



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:59 AM UTC

PDB ID : 5T61 / pdb_00005t61
Title : TUNGSTEN-CONTAINING FORMYLMETHANOFURAN DEHYDROGENASE FROM METHANOTHERMOBACTER WOLFEII, TRICLINIC FORM AT 2.55 Å
Authors : Wagner, T.; Ermler, U.; Shima, S.
Deposited on : 2016-09-01
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

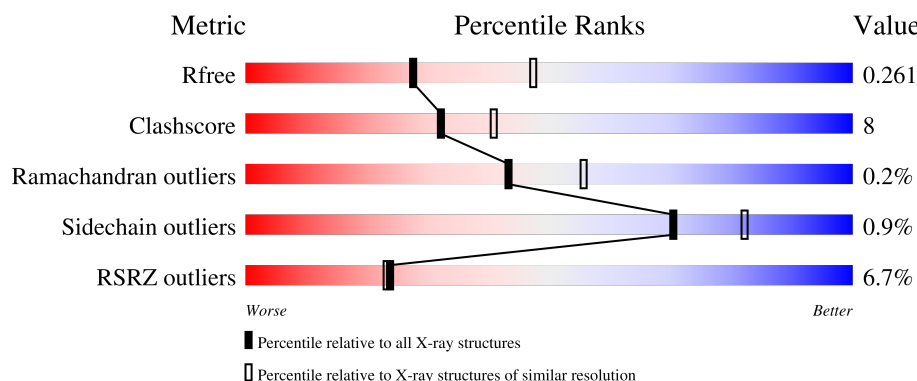
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	569	3% 86% 14%
1	G	569	8% 85% 14% .
1	M	569	13% 82% 17%
1	S	569	2% 86% 13% .

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Mol	Chain	Length	Quality of chain
1	Y	569	
1	e	569	
1	k	569	
1	q	569	
2	B	432	
2	H	432	
2	N	432	
2	T	432	
2	Z	432	
2	f	432	
2	l	432	
2	r	432	
3	C	270	
3	I	270	
3	O	270	
3	U	270	
3	a	270	
3	g	270	
3	m	270	
3	s	270	
4	D	130	
4	J	130	
4	P	130	
4	V	130	
4	b	130	

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Mol	Chain	Length	Quality of chain
4	h	130	
4	n	130	
4	t	130	
5	E	82	
5	K	82	
5	Q	82	
5	W	82	
5	c	82	
5	i	82	
5	o	82	
5	u	82	
6	F	349	
6	L	349	
6	R	349	
6	X	349	
6	d	349	
6	j	349	
6	p	349	
6	v	349	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	H2S	l	505	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 114321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	G	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	M	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	S	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	Y	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	e	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	k	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	q	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			

- Molecule 2 is a protein called Tungsten formylmethanofuran dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3364	2115	590	629	30			
2	H	427	Total	C	N	O	S	0	0	0
			3352	2109	587	626	30			
2	N	430	Total	C	N	O	S	0	0	0
			3369	2118	591	630	30			
2	T	429	Total	C	N	O	S	0	0	0
			3364	2115	590	629	30			
2	Z	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			
2	f	427	Total	C	N	O	S	0	0	0
			3352	2109	587	626	30			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	l	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			
2	r	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			

- Molecule 3 is a protein called Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			1982	1246	334	389	13			
3	I	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			
3	O	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	U	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	a	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	g	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	m	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	s	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			

- Molecule 4 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	J	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	P	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	V	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	b	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	h	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	n	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			

- Molecule 5 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	K	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	Q	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	W	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	c	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	i	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	o	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	u	81	Total	C	N	O	S	0	0	0
			581	359	97	116	9			

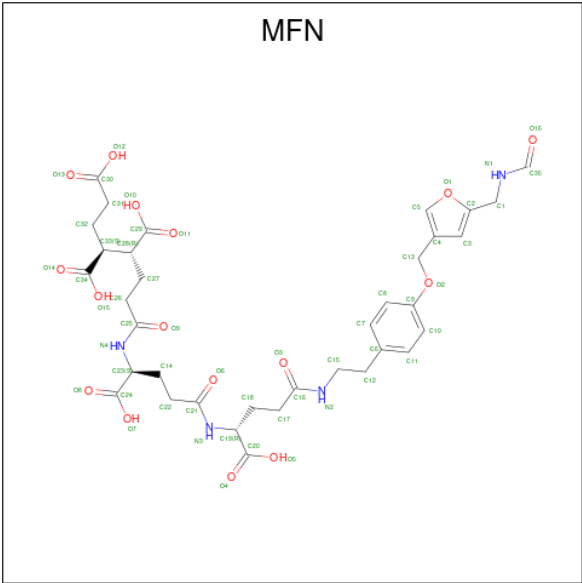
- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	345	Total	C	N	O	S	0	0	0
			2629	1626	438	523	42			
6	L	348	Total	C	N	O	S	0	0	0
			2656	1641	441	532	42			
6	R	341	Total	C	N	O	S	0	0	0
			2602	1611	434	515	42			
6	X	344	Total	C	N	O	S	0	0	0
			2627	1625	437	523	42			
6	d	340	Total	C	N	O	S	0	0	0
			2595	1606	433	514	42			
6	j	344	Total	C	N	O	S	0	0	0
			2625	1624	437	522	42			
6	p	348	Total	C	N	O	S	0	0	0
			2656	1641	441	532	42			
6	v	346	Total	C	N	O	S	0	0	0
			2643	1634	439	528	42			

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	G	2	Total	Zn	0	0
			2	2		
7	M	2	Total	Zn	0	0
			2	2		
7	S	2	Total	Zn	0	0
			2	2		
7	Y	2	Total	Zn	0	0
			2	2		
7	e	2	Total	Zn	0	0
			2	2		
7	k	2	Total	Zn	0	0
			2	2		
7	q	2	Total	Zn	0	0
			2	2		

- Molecule 8 is N-[4,5,7-TRICARBOXYHEPTANOYL]-L-GAMMA-GLUTAMYL-N-{2-[4-({5-[(FORMYLAMINO)METHYL]-3-FURYL}METHOXY)PHENYL]ETHYL}-D-GLUTAMINE (CCD ID: MFN) (formula: C₃₅H₄₄N₄O₁₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			53	34	4	15		
8	G	1	Total	C	N	O	0	0
			53	34	4	15		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			53	34	4	15		
8	S	1	Total	C	N	O	0	0
			53	34	4	15		
8	Y	1	Total	C	N	O	0	0
			53	34	4	15		
8	e	1	Total	C	N	O	0	0
			53	34	4	15		
8	k	1	Total	C	N	O	0	0
			53	34	4	15		
8	q	1	Total	C	N	O	0	0
			53	34	4	15		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		
9	G	1	Total	Na	0	0
			1	1		
9	M	1	Total	Na	0	0
			1	1		
9	S	1	Total	Na	0	0
			1	1		
9	e	1	Total	Na	0	0
			1	1		
9	k	1	Total	Na	0	0
			1	1		
9	q	1	Total	Na	0	0
			1	1		

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	K	0	0
			1	1		
10	B	1	Total	K	0	0
			1	1		
10	E	1	Total	K	0	0
			1	1		
10	F	4	Total	K	0	0
			4	4		

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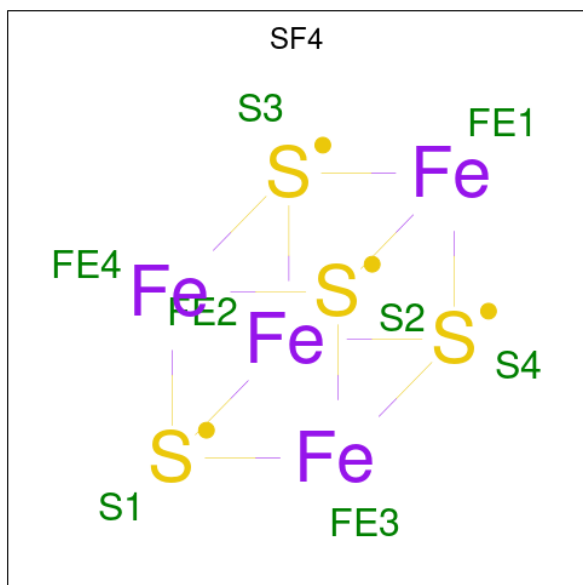
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	1	Total K 1 1	0	0
10	K	1	Total K 1 1	0	0
10	L	3	Total K 3 3	0	0
10	M	2	Total K 2 2	0	0
10	N	1	Total K 1 1	0	0
10	Q	1	Total K 1 1	0	0
10	R	3	Total K 3 3	0	0
10	S	2	Total K 2 2	0	0
10	T	1	Total K 1 1	0	0
10	X	3	Total K 3 3	0	0
10	Y	1	Total K 1 1	0	0
10	Z	1	Total K 1 1	0	0
10	c	1	Total K 1 1	0	0
10	d	2	Total K 2 2	0	0
10	e	4	Total K 4 4	0	0
10	i	1	Total K 1 1	0	0
10	j	6	Total K 6 6	0	0
10	k	1	Total K 1 1	0	0
10	o	1	Total K 1 1	0	0
10	p	3	Total K 3 3	0	0
10	q	2	Total K 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	r	1	Total	K	0	0
			1	1		
10	u	1	Total	K	0	0
			1	1		
10	v	7	Total	K	0	0
			7	7		

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	E	1	Total	Fe	S	0	0
			8	4	4		
11	E	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	H	1	Total 8	Fe 4	S 4	0	0
11	K	1	Total 8	Fe 4	S 4	0	0
11	K	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	N	1	Total 8	Fe 4	S 4	0	0
11	Q	1	Total 8	Fe 4	S 4	0	0
11	Q	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	T	1	Total 8	Fe 4	S 4	0	0
11	W	1	Total 8	Fe 4	S 4	0	0
11	W	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	Z	1	Total 8	Fe 4	S 4	0	0
11	c	1	Total 8	Fe 4	S 4	0	0
11	c	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	f	1	Total 8	Fe 4	S 4	0	0
11	i	1	Total 8	Fe 4	S 4	0	0
11	i	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	l	1	Total 8	Fe 4	S 4	0	0
11	o	1	Total 8	Fe 4	S 4	0	0

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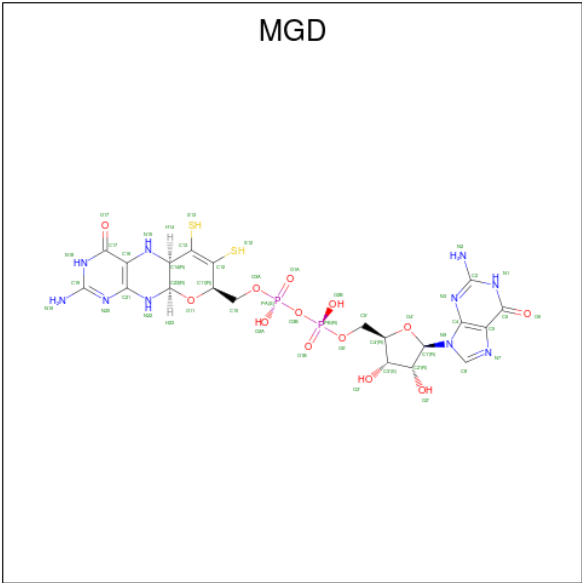
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	o	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	r	1	Total 8	Fe 4	S 4	0	0
11	u	1	Total 8	Fe 4	S 4	0	0
11	u	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0

- Molecule 12 is TUNGSTEN ION (CCD ID: W) (formula: W).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	W	0	0
			1	1		
12	H	1	Total	W	0	0
			1	1		
12	N	1	Total	W	0	0
			1	1		
12	T	1	Total	W	0	0
			1	1		
12	Z	1	Total	W	0	0
			1	1		
12	f	1	Total	W	0	0
			1	1		
12	l	1	Total	W	0	0
			1	1		
12	r	1	Total	W	0	0
			1	1		

- Molecule 13 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



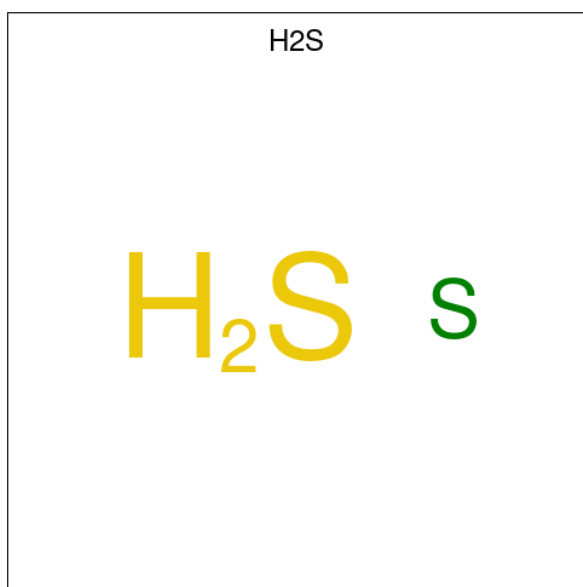
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	Z	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	Z	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	f	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	f	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	l	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	l	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	r	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	r	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 14 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total S 1 1	0	0
14	H	1	Total S 1 1	0	0
14	N	1	Total S 1 1	0	0
14	T	1	Total S 1 1	0	0
14	Z	1	Total S 1 1	0	0
14	f	1	Total S 1 1	0	0
14	l	1	Total S 1 1	0	0
14	r	1	Total S 1 1	0	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total Mg 1 1	0	0
15	H	1	Total Mg 1 1	0	0
15	O	1	Total Mg 1 1	0	0
15	T	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	Z	1	Total 1	Mg 1	0	0
15	f	1	Total 1	Mg 1	0	0
15	l	1	Total 1	Mg 1	0	0
15	r	1	Total 1	Mg 1	0	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	N	1	Total 1	Cl 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	22	Total 22	O 22	0	0
17	B	12	Total 12	O 12	0	0
17	C	7	Total 7	O 7	0	0
17	D	2	Total 2	O 2	0	0
17	E	1	Total 1	O 1	0	0
17	F	25	Total 25	O 25	0	0
17	G	14	Total 14	O 14	0	0
17	H	20	Total 20	O 20	0	0
17	I	17	Total 17	O 17	0	0
17	J	4	Total 4	O 4	0	0
17	K	8	Total 8	O 8	0	0
17	L	26	Total 26	O 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	5	Total O 5 5	0	0
17	N	24	Total O 24 24	0	0
17	O	9	Total O 9 9	0	0
17	P	4	Total O 4 4	0	0
17	Q	2	Total O 2 2	0	0
17	R	6	Total O 6 6	0	0
17	S	59	Total O 59 59	0	0
17	T	29	Total O 29 29	0	0
17	U	10	Total O 10 10	0	0
17	V	9	Total O 9 9	0	0
17	W	3	Total O 3 3	0	0
17	X	19	Total O 19 19	0	0
17	Y	17	Total O 17 17	0	0
17	Z	19	Total O 19 19	0	0
17	a	12	Total O 12 12	0	0
17	b	4	Total O 4 4	0	0
17	c	3	Total O 3 3	0	0
17	d	3	Total O 3 3	0	0
17	e	40	Total O 40 40	0	0
17	f	21	Total O 21 21	0	0
17	g	3	Total O 3 3	0	0

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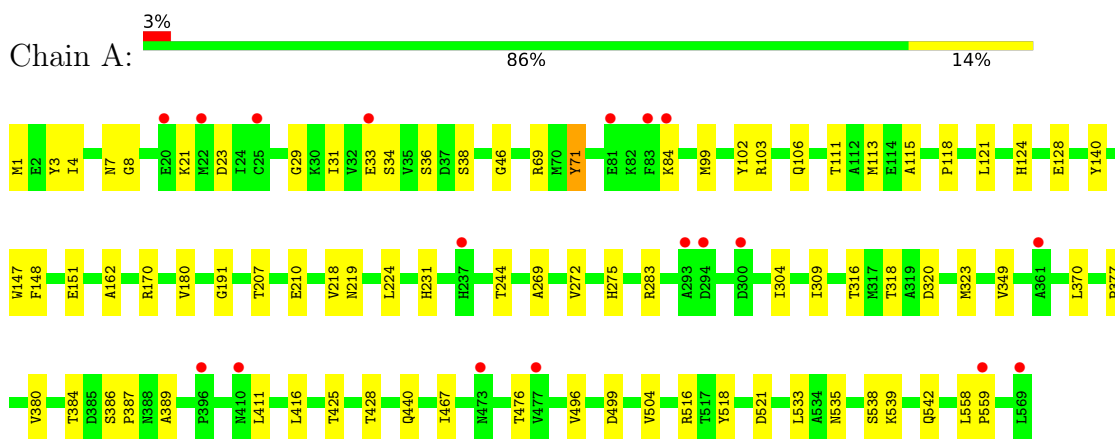
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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17	i	8	Total O 8 8	0	0
17	j	20	Total O 20 20	0	0
17	k	9	Total O 9 9	0	0
17	l	20	Total O 20 20	0	0
17	m	7	Total O 7 7	0	0
17	n	4	Total O 4 4	0	0
17	o	2	Total O 2 2	0	0
17	p	18	Total O 18 18	0	0
17	q	27	Total O 27 27	0	0
17	r	16	Total O 16 16	0	0
17	s	3	Total O 3 3	0	0
17	t	3	Total O 3 3	0	0
17	u	1	Total O 1 1	0	0
17	v	13	Total O 13 13	0	0

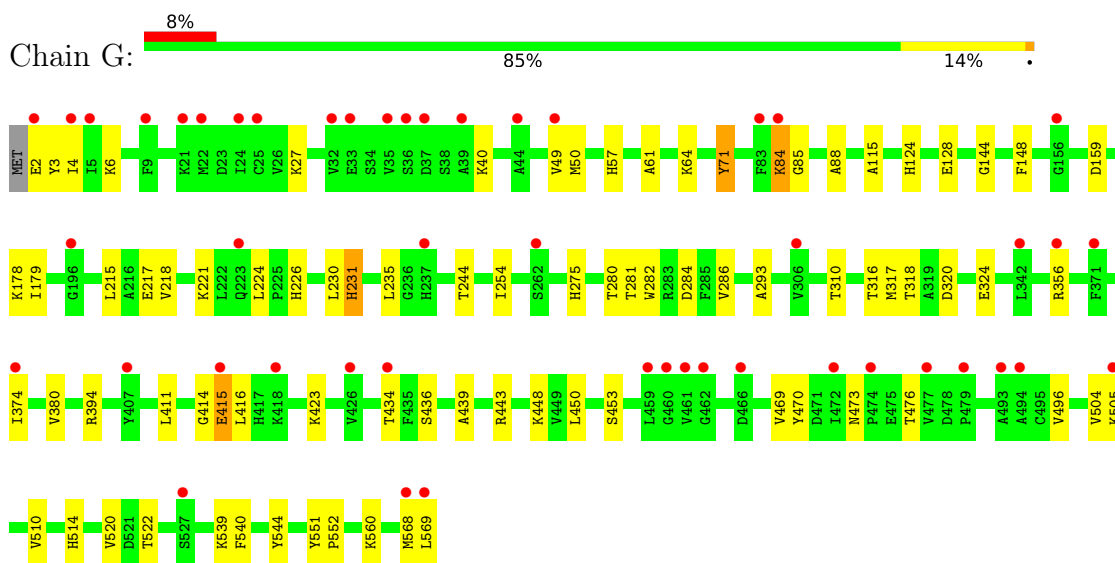
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

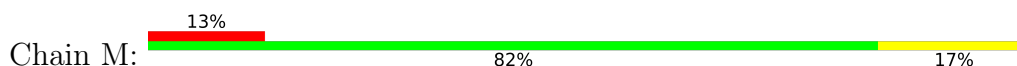
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

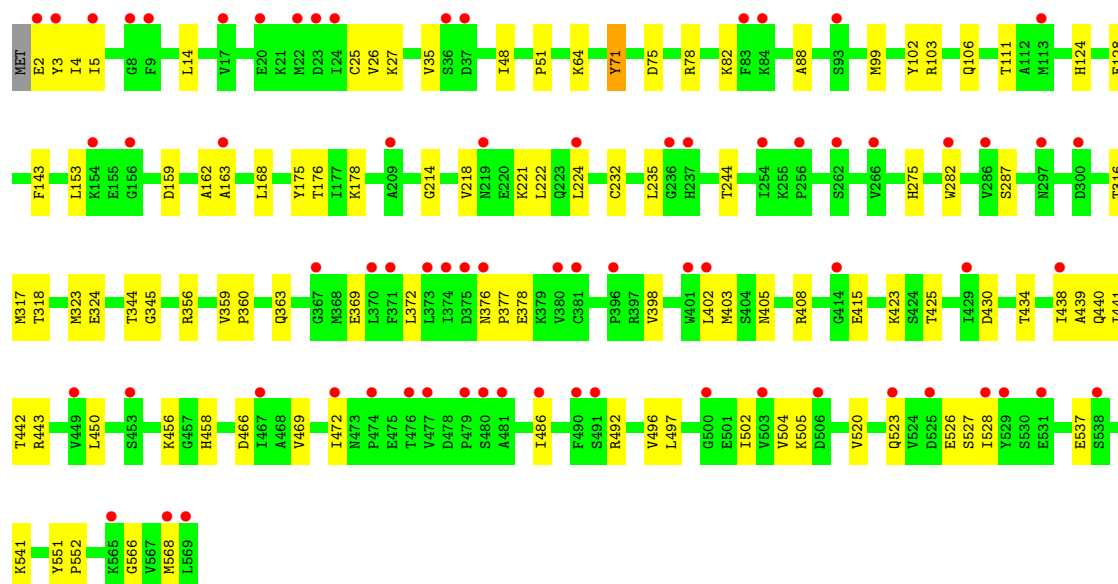


- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

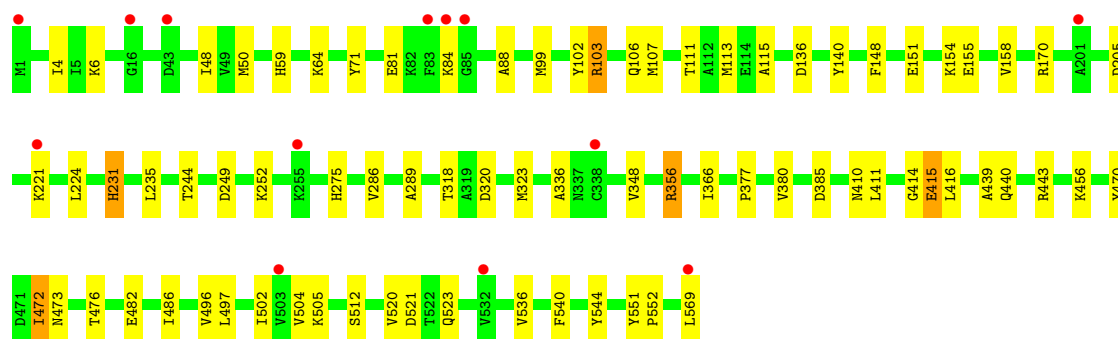
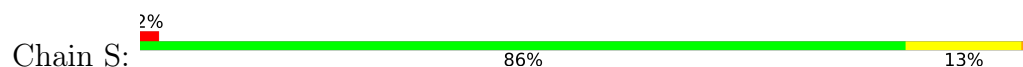


- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

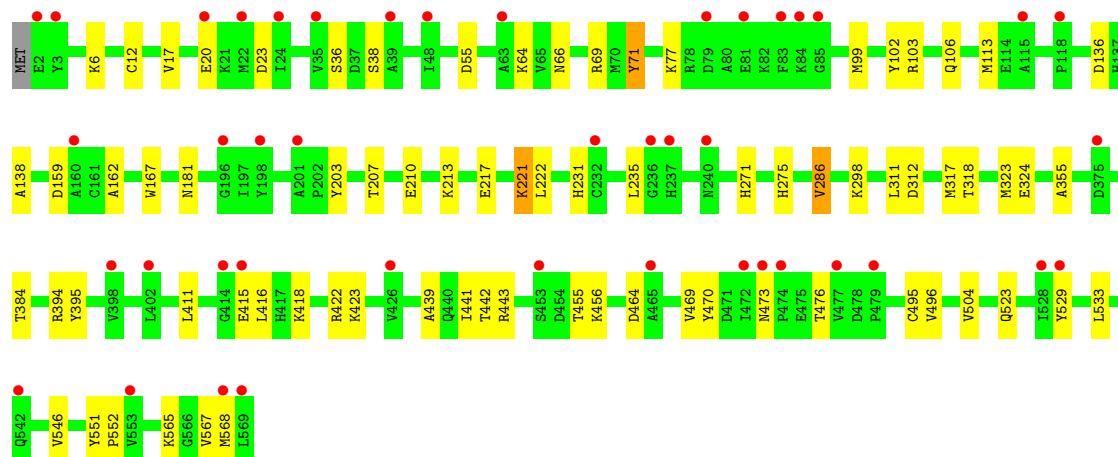
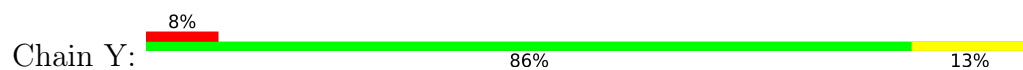




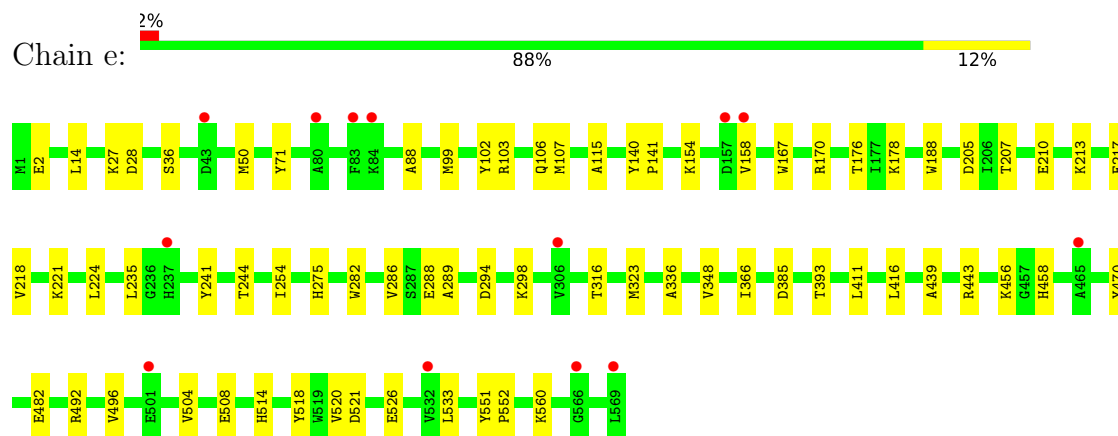
• Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



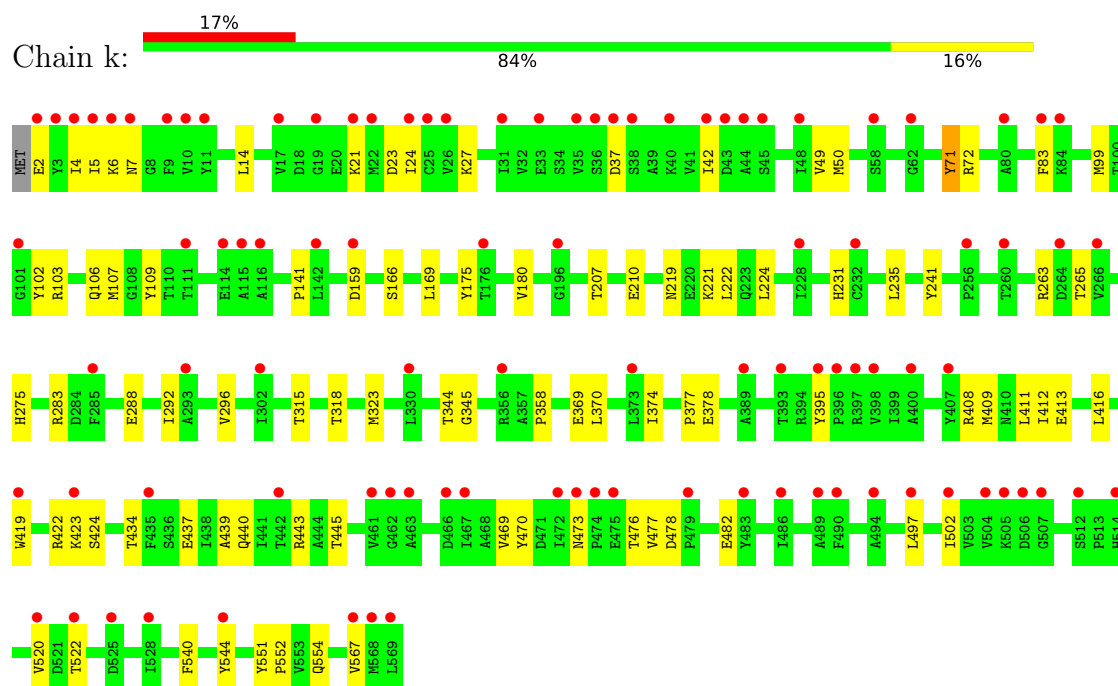
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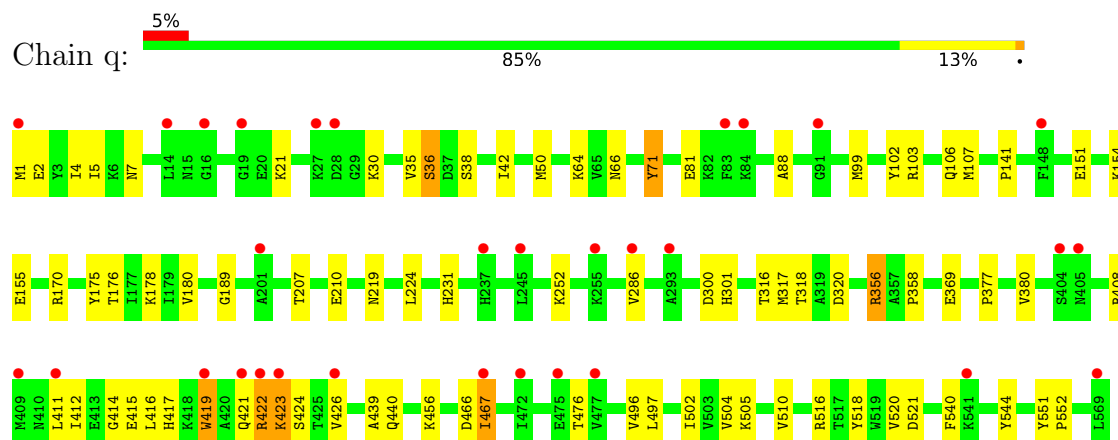
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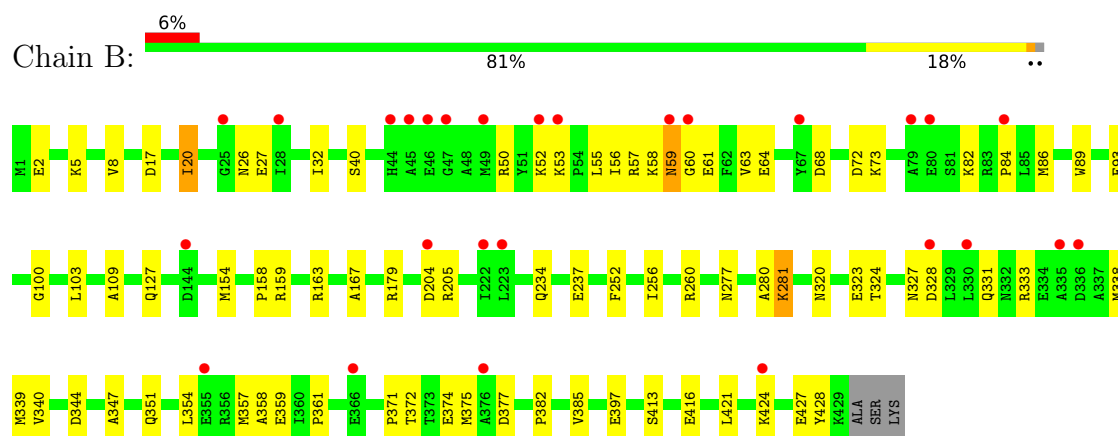
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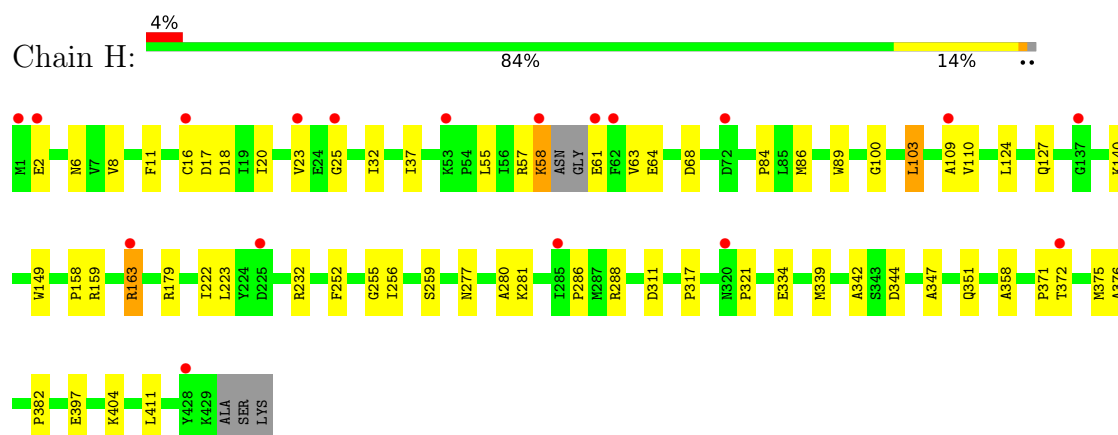
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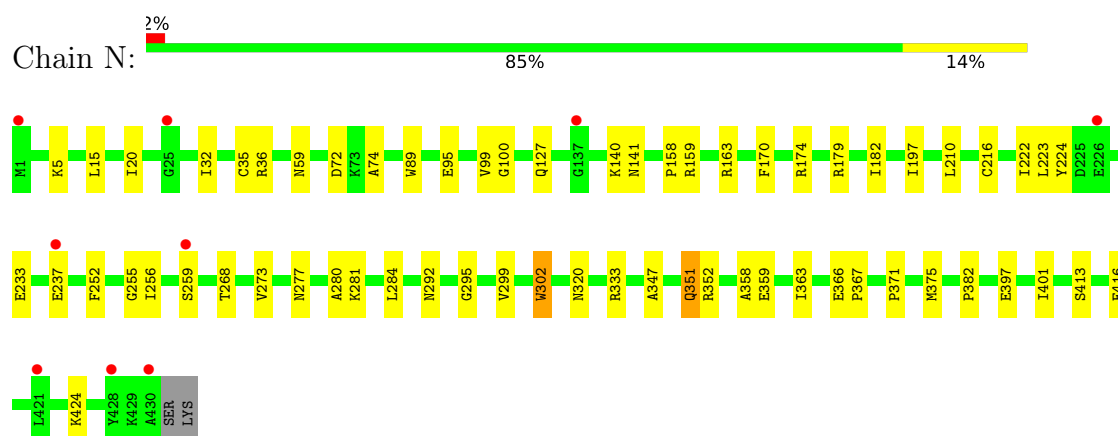
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



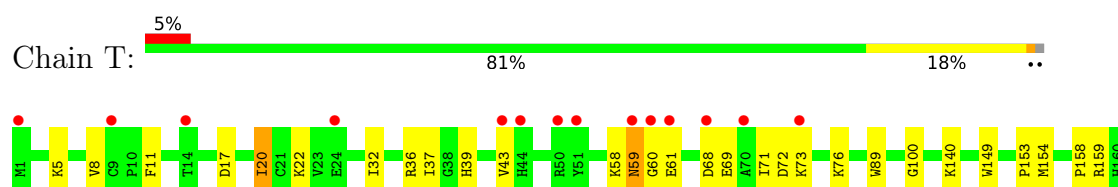
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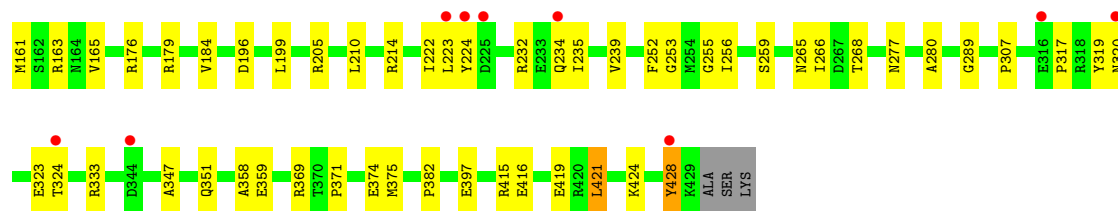


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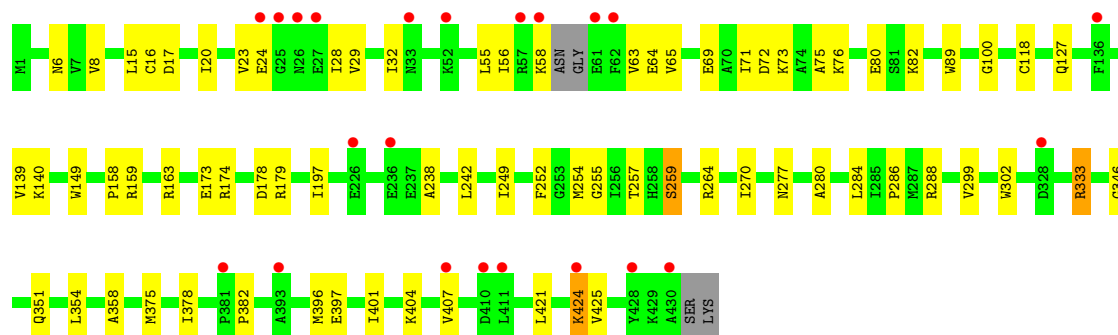
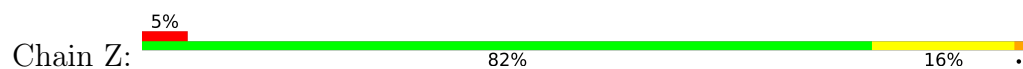


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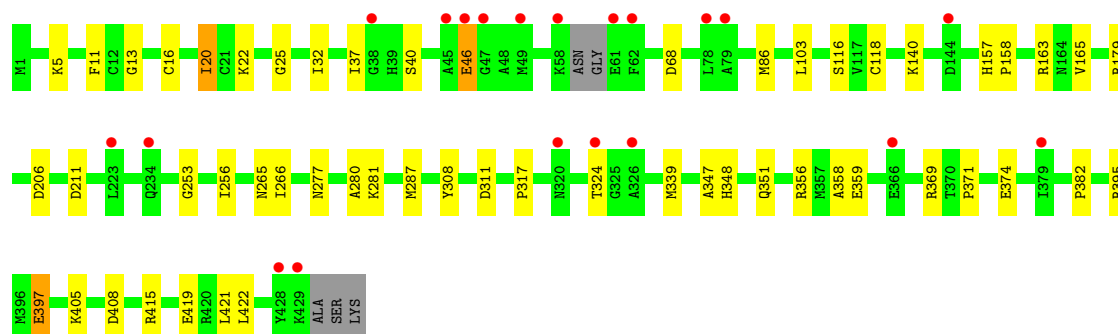
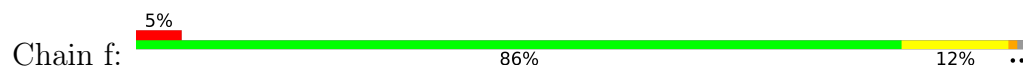




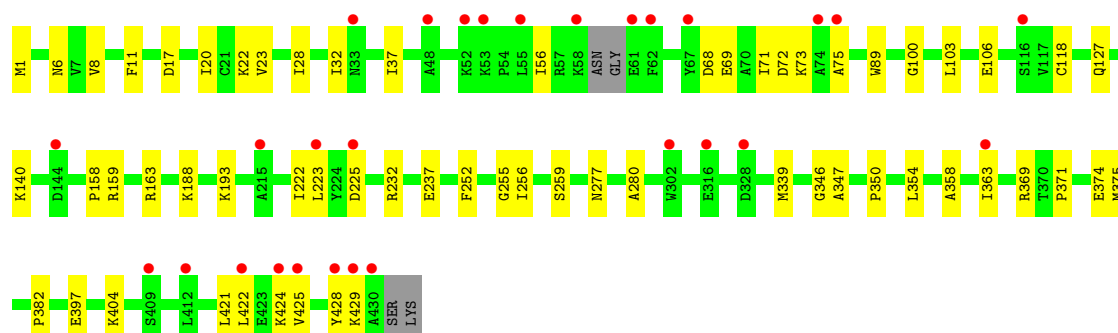
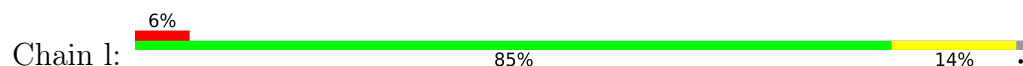
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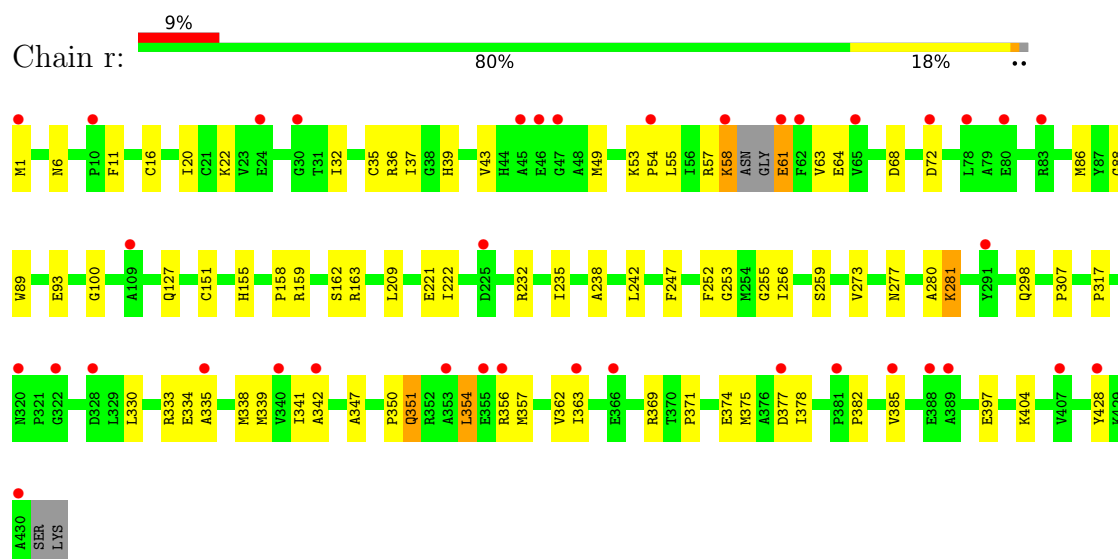
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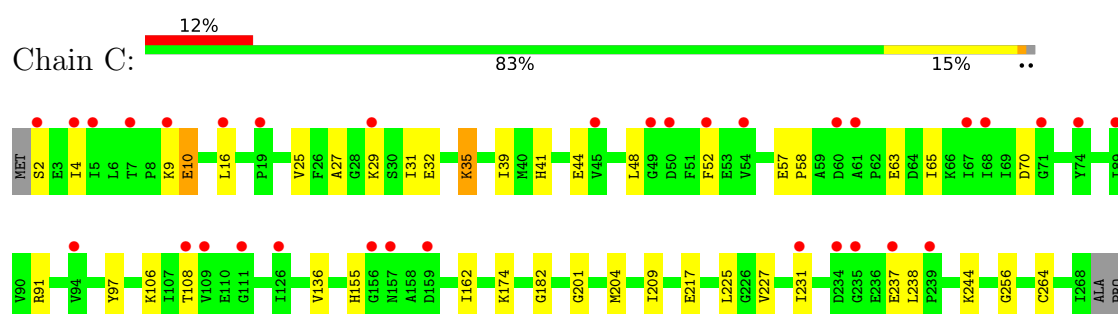
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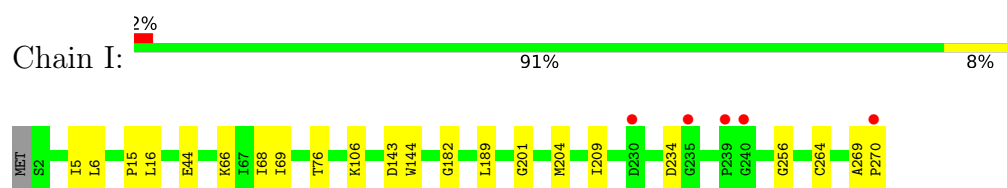
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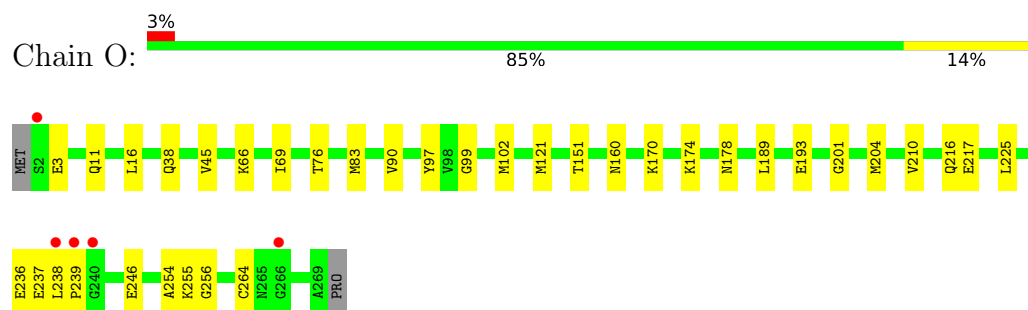
• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



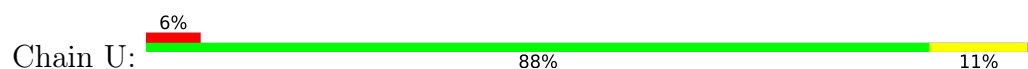
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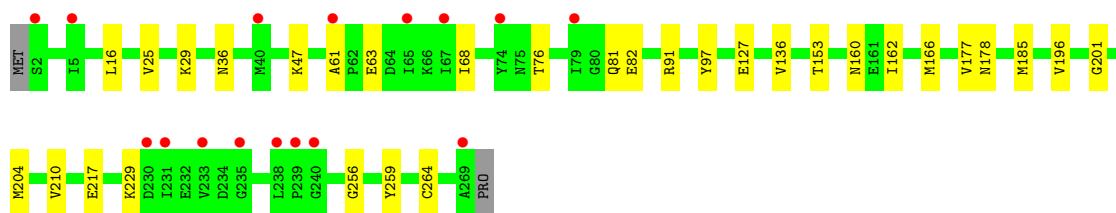


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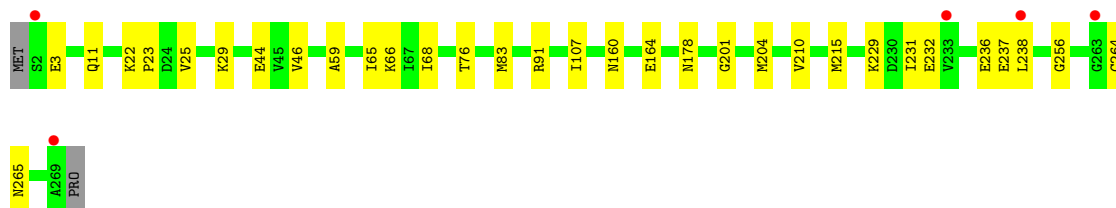
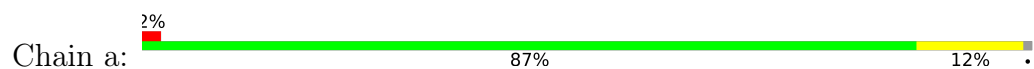


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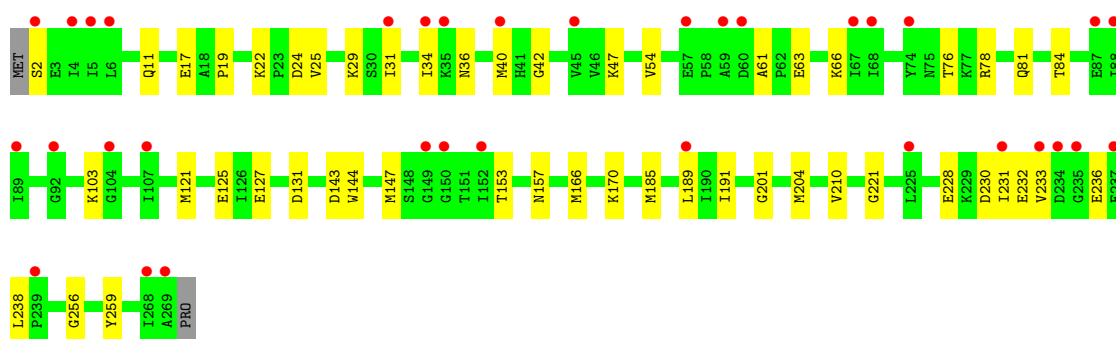
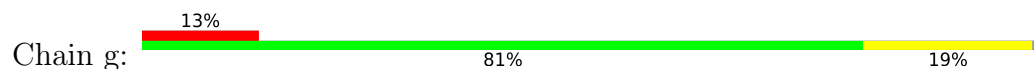




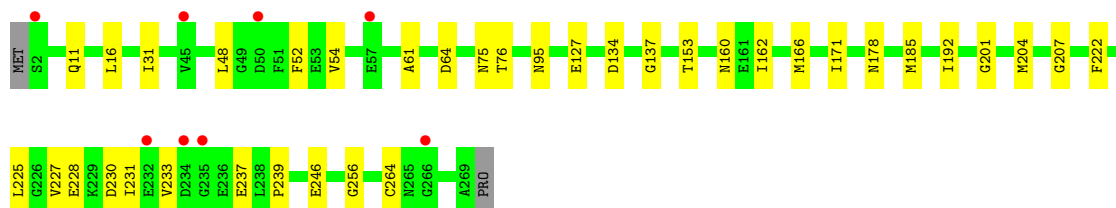
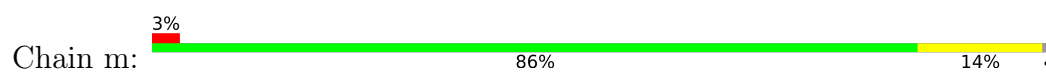
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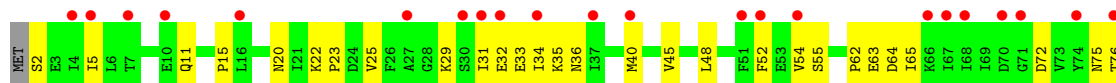
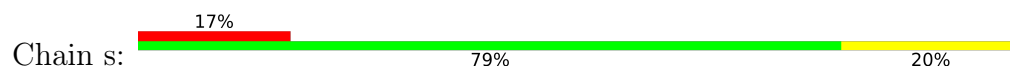
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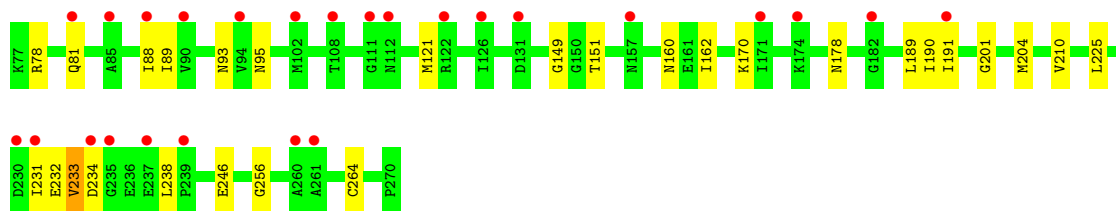


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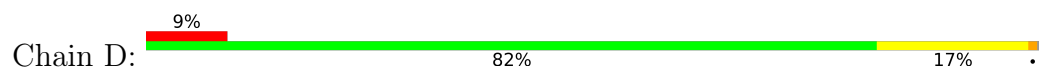


- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

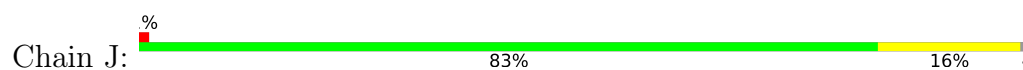




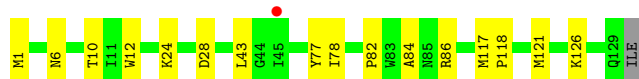
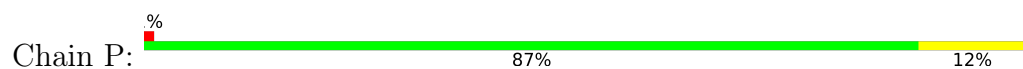
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



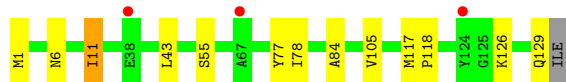
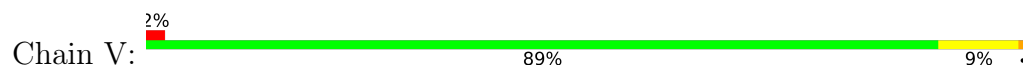
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



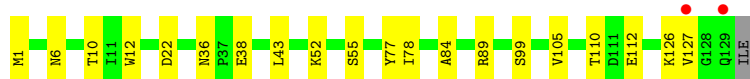
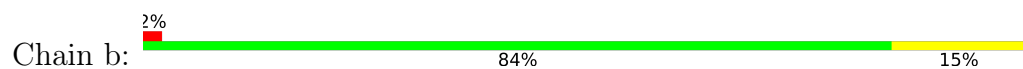
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



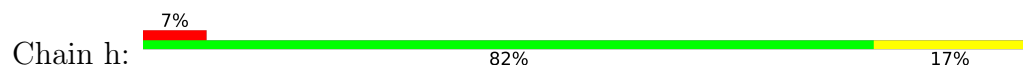
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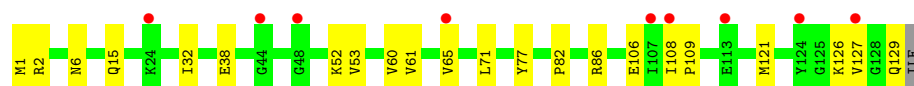


- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

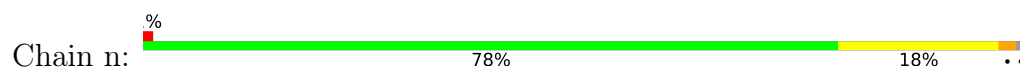


- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

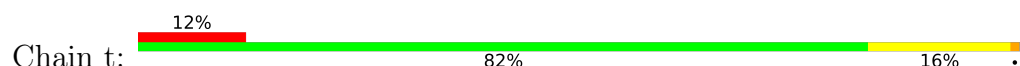




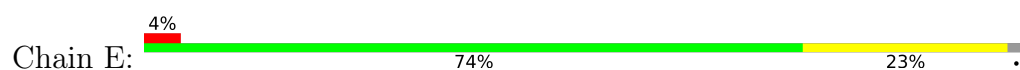
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



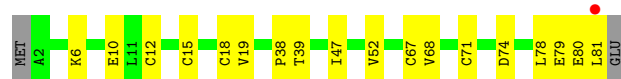
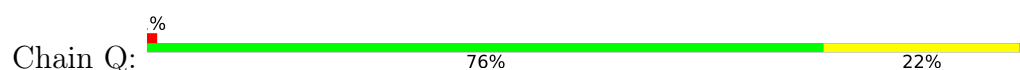
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



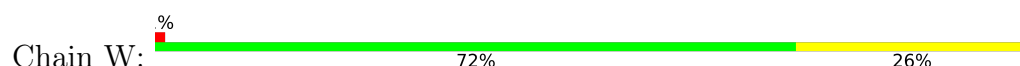
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



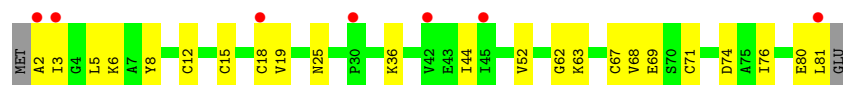
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



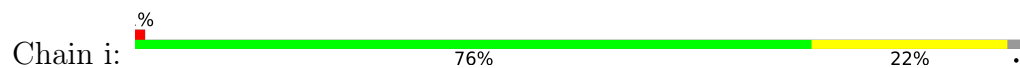
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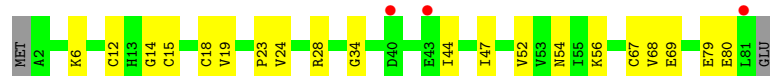
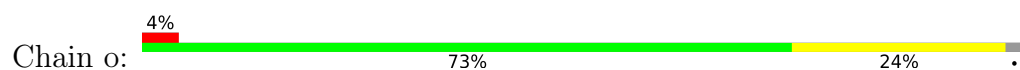
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



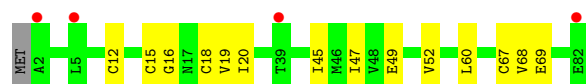
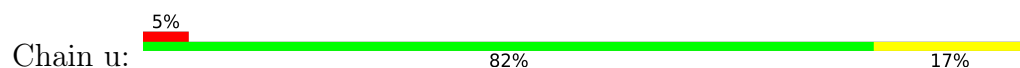
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



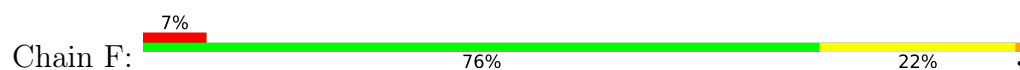
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



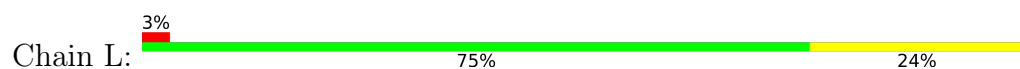
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

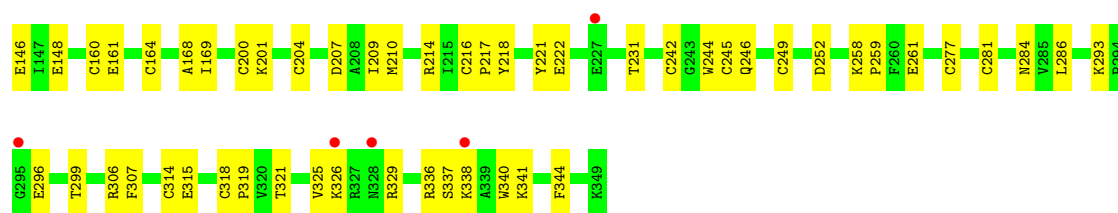


- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

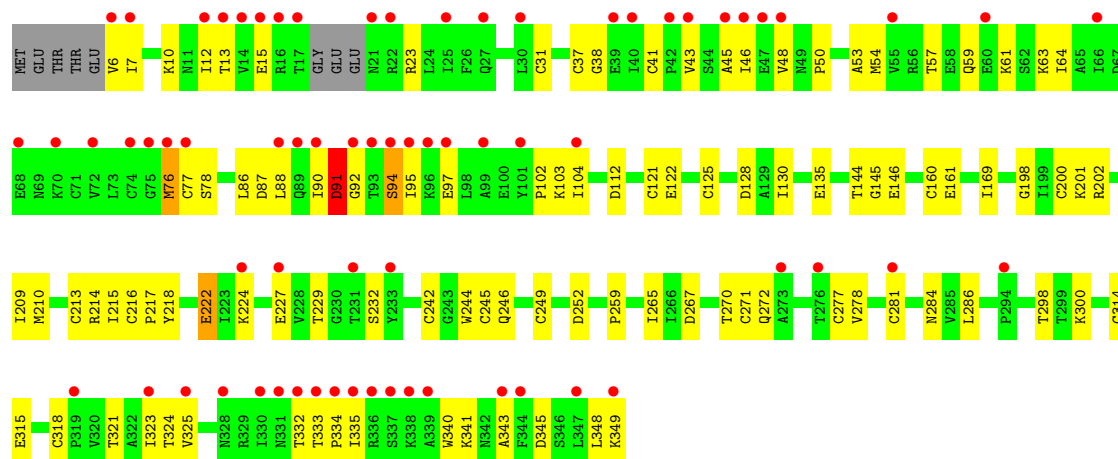


- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

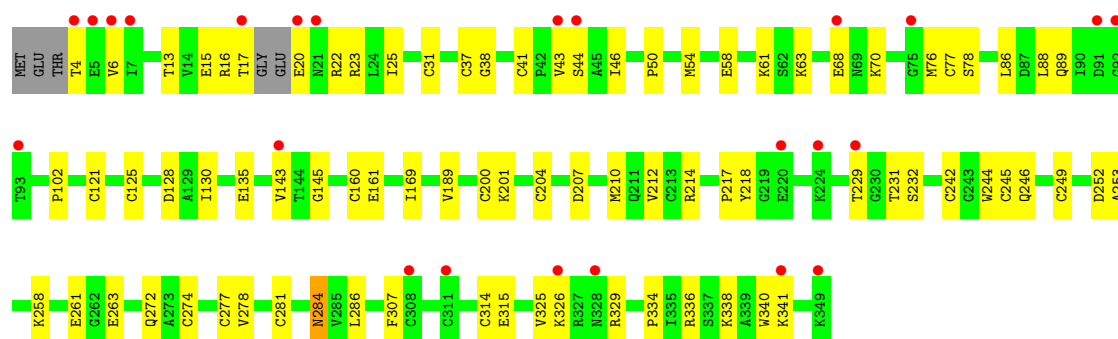
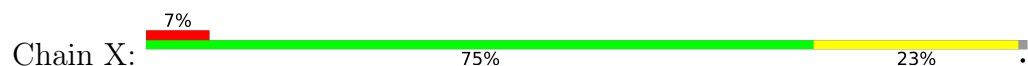




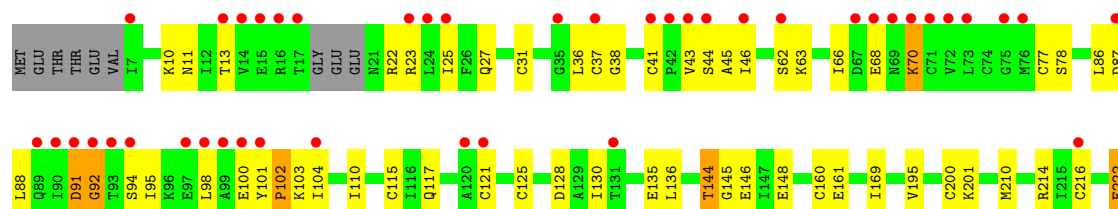
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

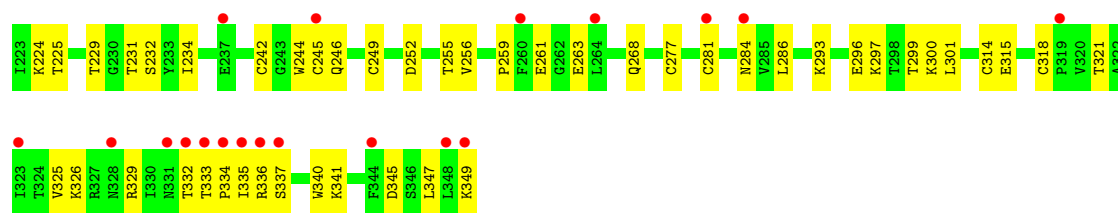


• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

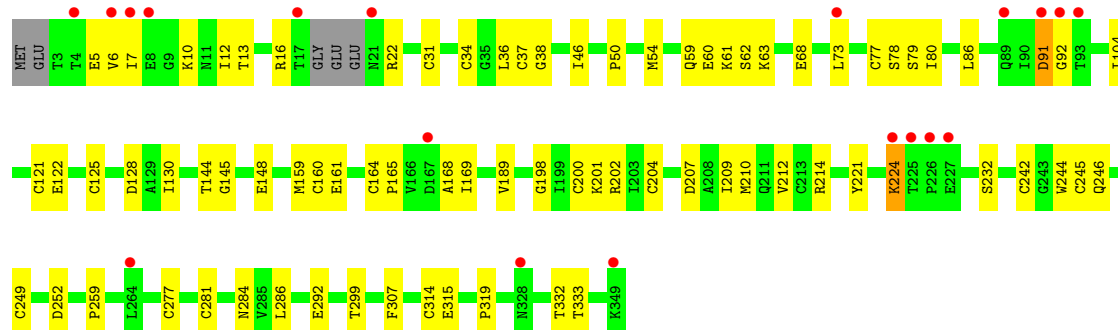
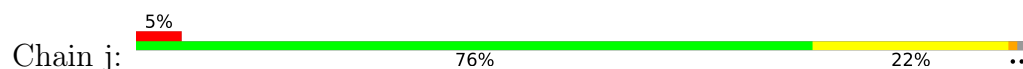


• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

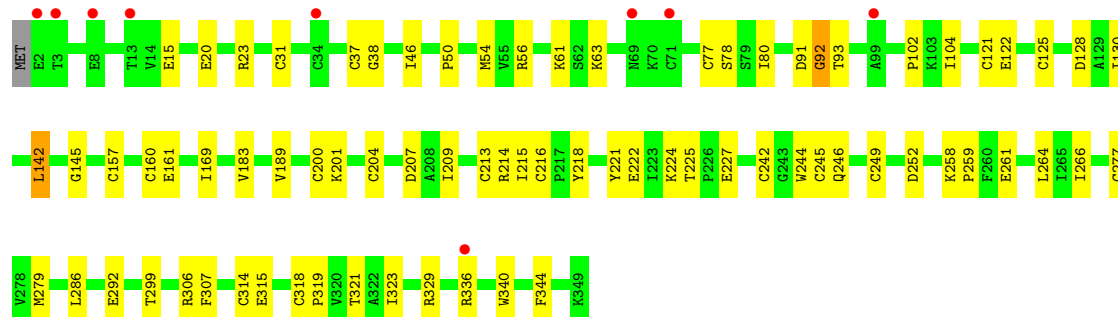
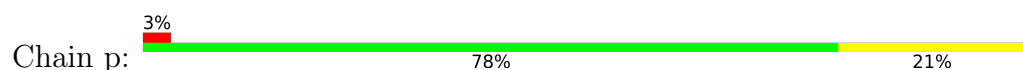




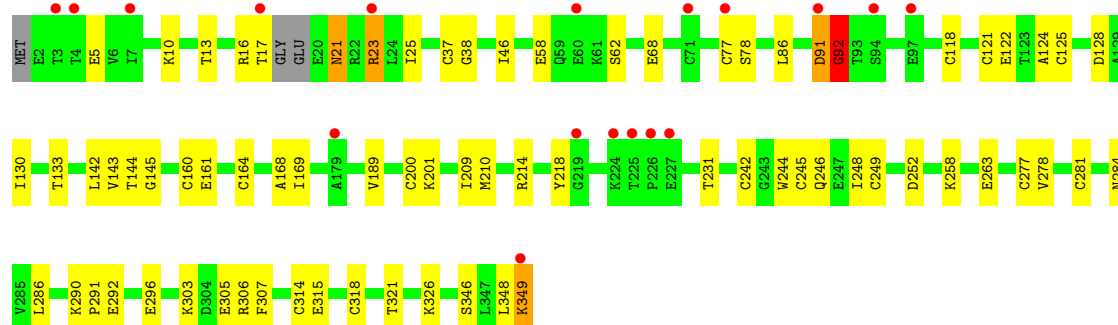
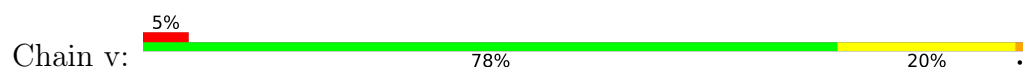
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	174.18Å 173.68Å 183.16Å 89.98° 95.42° 92.14°	Depositor
Resolution (Å)	48.97 – 2.55 48.97 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.97-2.55) 96.7 (48.97-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.229 , 0.259 0.231 , 0.261	Depositor DCC
R_{free} test set	34086 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.118 for -h,k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	114321	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MFN, SF4, NA, ZN, K, MG, H2S, MGD, KCX, CL, W

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	4/4523 (0.1%)	0.49	0/6161
1	G	0.24	0/4515	0.50	0/6151
1	M	0.30	0/4515	0.57	0/6151
1	S	0.28	1/4523 (0.0%)	0.51	1/6161 (0.0%)
1	Y	0.27	1/4515 (0.0%)	0.56	2/6151 (0.0%)
1	e	0.23	0/4523	0.49	0/6161
1	k	0.27	0/4515	0.55	0/6151
1	q	0.41	4/4523 (0.1%)	0.62	10/6161 (0.2%)
2	B	0.24	0/3434	0.55	3/4647 (0.1%)
2	H	0.28	1/3421 (0.0%)	0.54	4/4628 (0.1%)
2	N	0.21	0/3439	0.53	0/4654
2	T	0.26	0/3434	0.54	1/4647 (0.0%)
2	Z	0.36	5/3426 (0.1%)	0.57	0/4635
2	f	0.24	1/3421 (0.0%)	0.50	0/4628
2	l	0.24	0/3426	0.53	1/4635 (0.0%)
2	r	0.39	5/3426 (0.1%)	0.61	6/4635 (0.1%)
3	C	0.29	0/2014	0.61	3/2710 (0.1%)
3	I	0.29	0/2027	0.50	0/2729
3	O	0.19	0/2019	0.48	0/2717
3	U	0.20	0/2019	0.51	0/2717
3	a	0.21	0/2019	0.53	0/2717
3	g	0.27	0/2019	0.59	2/2717 (0.1%)
3	m	0.21	0/2019	0.50	0/2717
3	s	0.29	0/2027	0.57	0/2729
4	D	0.21	0/1016	0.50	0/1379
4	J	0.19	0/1016	0.46	0/1379
4	P	0.18	0/1016	0.48	0/1379
4	V	0.18	0/1016	0.50	0/1379
4	b	0.19	0/1016	0.49	0/1379
4	h	0.21	0/1016	0.53	0/1379
4	n	0.26	0/1016	0.56	1/1379 (0.1%)
4	t	0.31	0/1016	0.62	1/1379 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	E	0.23	0/579	0.46	0/787
5	K	0.32	0/579	0.55	0/787
5	Q	0.23	0/579	0.51	0/787
5	W	0.19	0/579	0.49	0/787
5	c	0.18	0/579	0.50	0/787
5	i	0.21	0/579	0.53	0/787
5	o	0.22	0/579	0.45	0/787
5	u	0.21	0/588	0.53	0/799
6	F	0.25	0/2667	0.54	1/3616 (0.0%)
6	L	0.27	0/2695	0.56	1/3655 (0.0%)
6	R	0.32	0/2640	0.67	5/3579 (0.1%)
6	X	0.32	0/2665	0.64	4/3613 (0.1%)
6	d	0.36	0/2633	0.65	2/3569 (0.1%)
6	j	0.23	0/2663	0.56	1/3611 (0.0%)
6	p	0.27	0/2695	0.54	1/3655 (0.0%)
6	v	0.40	4/2681 (0.1%)	0.62	1/3635 (0.0%)
All	All	0.28	26/113850 (0.0%)	0.55	51/154383 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	k	0	1
2	T	0	1
2	Z	0	1
6	F	0	1
6	L	0	1
6	R	0	1
6	d	0	1
6	p	0	1
6	v	0	1
All	All	0	9

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	558	LEU	CA-CB	10.60	1.68	1.53
1	q	423	LYS	CB-CG	-9.75	1.23	1.52
6	v	23	ARG	NE-CZ	-9.13	1.23	1.33
2	Z	333	ARG	NE-CZ	-8.82	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	58	LYS	CD-CE	-8.57	1.26	1.52
1	A	559	PRO	C-O	8.28	1.34	1.24
2	r	61	GLU	CD-OE1	7.74	1.40	1.25
1	S	356	ARG	C-N	-7.43	1.18	1.33
2	H	61	GLU	CD-OE2	7.11	1.38	1.25
1	A	559	PRO	N-CA	-7.10	1.38	1.47
2	r	61	GLU	CD-OE2	6.79	1.38	1.25
1	q	423	LYS	CD-CE	-6.73	1.32	1.52
2	Z	424	LYS	CE-NZ	-6.36	1.30	1.49
2	Z	333	ARG	CZ-NH1	-6.31	1.24	1.32
6	v	23	ARG	CZ-NH2	-6.31	1.25	1.33
1	q	419	TRP	CD1-NE1	5.88	1.50	1.37
2	Z	333	ARG	CD-NE	-5.75	1.38	1.46
1	A	558	LEU	N-CA	5.75	1.52	1.46
6	v	23	ARG	CD-NE	-5.69	1.38	1.46
2	Z	333	ARG	CZ-NH2	-5.66	1.26	1.33
6	v	349	LYS	CD-CE	-5.57	1.35	1.52
1	q	419	TRP	CE3-CZ3	-5.46	1.22	1.38
2	r	61	GLU	CA-CB	5.31	1.64	1.53
1	Y	181	ASN	C-O	5.26	1.26	1.23
2	f	46	GLU	CD-OE1	-5.26	1.15	1.25
2	r	354	LEU	CG-CD1	-5.08	1.35	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	58	LYS	CD-CE-NZ	-14.10	66.79	111.90
6	v	92	GLY	N-CA-C	11.99	141.59	113.18
1	q	423	LYS	CB-CA-C	-9.25	95.67	110.85
6	X	58	GLU	CB-CA-C	8.71	124.58	110.29
4	t	1	MET	CA-CB-CG	8.01	130.11	114.10
6	p	92	GLY	N-CA-C	7.95	132.03	113.18
3	g	125	GLU	CB-CA-C	7.73	122.94	109.80
2	B	27	GLU	CB-CG-CD	7.61	125.53	112.60
6	L	92	GLY	N-CA-C	7.48	130.92	113.18
6	d	92	GLY	N-CA-C	7.43	130.80	113.18
1	Y	221	LYS	CD-CE-NZ	-7.25	88.71	111.90
6	j	91	ASP	N-CA-C	7.06	120.98	111.24
6	R	91	ASP	N-CA-C	7.04	120.96	111.24
1	q	356	ARG	NE-CZ-NH1	-6.99	114.51	121.50
6	R	61	LYS	CG-CD-CE	6.97	127.34	111.30
2	r	333	ARG	CG-CD-NE	-6.97	96.67	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	92	GLY	N-CA-C	6.80	129.31	113.18
3	C	10	GLU	CA-C-N	6.78	130.12	120.49
3	C	10	GLU	C-N-CA	6.78	130.12	120.49
2	r	354	LEU	CB-CG-CD1	-6.77	90.38	110.70
2	r	1	MET	CG-SD-CE	-6.70	86.16	100.90
1	q	414	GLY	N-CA-C	-6.68	104.13	110.21
2	r	58	LYS	CB-CG-CD	-6.62	96.08	111.30
4	n	103	ILE	CA-CB-CG1	-6.50	99.35	110.40
2	H	61	GLU	OE1-CD-OE2	6.40	138.26	122.90
6	R	76	MET	CG-SD-CE	-6.29	87.06	100.90
1	q	422	ARG	CB-CG-CD	-6.26	96.89	111.30
2	B	26	ASN	CA-C-N	-6.26	111.96	122.29
2	B	26	ASN	C-N-CA	-6.26	111.96	122.29
3	C	35	LYS	CG-CD-CE	6.21	125.57	111.30
2	T	428	TYR	CA-CB-CG	-6.14	102.84	113.90
6	X	58	GLU	N-CA-CB	-6.12	99.90	109.87
1	q	467	ILE	CG1-CB-CG2	-6.12	92.35	110.70
6	d	70	LYS	CB-CG-CD	-6.01	97.47	111.30
6	R	97	GLU	CA-CB-CG	5.93	125.96	114.10
1	q	422	ARG	CB-CA-C	5.92	120.56	110.56
2	H	163	ARG	NE-CZ-NH1	-5.90	115.60	121.50
2	r	61	GLU	CA-CB-CG	5.76	125.62	114.10
2	H	163	ARG	NE-CZ-NH2	5.68	124.31	119.20
6	X	325	VAL	CA-C-N	5.64	131.05	122.65
6	X	325	VAL	C-N-CA	5.64	131.05	122.65
1	Y	221	LYS	CB-CA-C	-5.44	100.22	110.67
1	S	103	ARG	CA-CB-CG	-5.32	103.45	114.10
2	H	58	LYS	CD-CE-NZ	-5.25	95.10	111.90
3	g	125	GLU	N-CA-CB	-5.24	102.02	110.71
6	R	61	LYS	CD-CE-NZ	-5.23	95.16	111.90
1	q	356	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	l	237	GLU	CG-CD-OE1	-5.15	106.56	118.40
1	q	421	GLN	CA-C-N	-5.03	114.59	122.65
1	q	421	GLN	C-N-CA	-5.03	114.59	122.65
1	q	419	TRP	CH2-CZ2-CE2	-5.02	110.98	117.50

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	91	ASP	Peptide
6	L	91	ASP	Peptide

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Mol	Chain	Res	Type	Group
6	R	91	ASP	Peptide
2	T	58	LYS	Peptide
2	Z	173	GLU	Sidechain
6	d	91	ASP	Peptide
1	k	83	PHE	Peptide
6	p	91	ASP	Peptide
6	v	91	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4419	0	4273	48	0
1	G	4411	0	4261	56	0
1	M	4411	0	4260	85	0
1	S	4419	0	4272	50	0
1	Y	4411	0	4260	79	0
1	e	4419	0	4272	39	1
1	k	4411	0	4260	70	0
1	q	4419	0	4272	75	0
2	B	3364	0	3307	62	0
2	H	3352	0	3297	41	0
2	N	3369	0	3312	41	0
2	T	3364	0	3307	59	0
2	Z	3357	0	3302	56	0
2	f	3352	0	3297	37	0
2	l	3357	0	3302	50	0
2	r	3357	0	3300	67	0
3	C	1982	0	1950	35	0
3	I	1994	0	1962	15	0
3	O	1987	0	1955	31	0
3	U	1987	0	1955	20	0
3	a	1987	0	1955	21	0
3	g	1987	0	1955	54	0
3	m	1987	0	1955	25	0
3	s	1994	0	1962	43	0
4	D	997	0	1021	18	0
4	J	997	0	1022	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	997	0	1022	11	0
4	V	997	0	1022	8	0
4	b	997	0	1022	16	0
4	h	997	0	1022	14	0
4	n	997	0	1022	22	0
4	t	997	0	1022	24	0
5	E	572	0	567	15	0
5	K	572	0	567	14	0
5	Q	572	0	567	13	0
5	W	572	0	567	16	0
5	c	572	0	567	14	0
5	i	572	0	567	13	0
5	o	572	0	567	22	0
5	u	581	0	573	11	0
6	F	2629	0	2588	50	1
6	L	2656	0	2607	56	0
6	R	2602	0	2565	73	0
6	X	2627	0	2584	65	0
6	d	2595	0	2556	75	0
6	j	2625	0	2585	59	0
6	p	2656	0	2607	67	0
6	v	2643	0	2597	57	0
7	A	2	0	0	0	0
7	G	2	0	0	0	0
7	M	2	0	0	0	0
7	S	2	0	0	0	0
7	Y	2	0	0	0	0
7	e	2	0	0	0	0
7	k	2	0	0	0	0
7	q	2	0	0	0	0
8	A	53	0	37	0	0
8	G	53	0	37	2	0
8	M	53	0	37	3	0
8	S	53	0	37	3	0
8	Y	53	0	37	4	0
8	e	53	0	37	3	0
8	k	53	0	37	5	0
8	q	53	0	37	2	0
9	A	1	0	0	0	0
9	G	1	0	0	0	0
9	M	1	0	0	0	0
9	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	e	1	0	0	0	0
9	k	1	0	0	0	0
9	q	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
10	F	4	0	0	0	0
10	G	1	0	0	0	0
10	K	1	0	0	0	0
10	L	3	0	0	0	0
10	M	2	0	0	0	0
10	N	1	0	0	0	0
10	Q	1	0	0	0	0
10	R	3	0	0	0	0
10	S	2	0	0	0	0
10	T	1	0	0	0	0
10	X	3	0	0	0	0
10	Y	1	0	0	0	0
10	Z	1	0	0	0	0
10	c	1	0	0	0	0
10	d	2	0	0	0	0
10	e	4	0	0	0	0
10	i	1	0	0	0	0
10	j	6	0	0	0	0
10	k	1	0	0	0	0
10	o	1	0	0	0	0
10	p	3	0	0	0	0
10	q	2	0	0	0	0
10	r	1	0	0	0	0
10	u	1	0	0	0	0
10	v	7	0	0	0	0
11	B	8	0	0	0	0
11	E	16	0	0	1	0
11	F	72	0	0	0	0
11	H	8	0	0	0	0
11	K	16	0	0	0	0
11	L	64	0	0	0	0
11	N	8	0	0	0	0
11	Q	16	0	0	0	0
11	R	72	0	0	0	0
11	T	8	0	0	0	0
11	W	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	X	64	0	0	0	0
11	Z	8	0	0	0	0
11	c	16	0	0	0	0
11	d	72	0	0	0	0
11	f	8	0	0	0	0
11	i	16	0	0	1	0
11	j	64	0	0	0	0
11	l	8	0	0	0	0
11	o	16	0	0	0	0
11	p	72	0	0	0	0
11	r	8	0	0	0	0
11	u	16	0	0	0	0
11	v	64	0	0	0	0
12	B	1	0	0	0	0
12	H	1	0	0	0	0
12	N	1	0	0	0	0
12	T	1	0	0	0	0
12	Z	1	0	0	0	0
12	f	1	0	0	0	0
12	l	1	0	0	1	0
12	r	1	0	0	0	0
13	B	94	0	44	1	0
13	H	94	0	44	2	0
13	N	94	0	44	0	0
13	T	94	0	44	1	0
13	Z	94	0	44	1	0
13	f	94	0	44	0	0
13	l	94	0	44	3	0
13	r	94	0	44	1	0
14	B	1	0	0	0	0
14	H	1	0	0	0	0
14	N	1	0	0	0	0
14	T	1	0	0	0	0
14	Z	1	0	0	1	0
14	f	1	0	0	1	0
14	l	1	0	0	4	0
14	r	1	0	0	0	0
15	B	1	0	0	0	0
15	H	1	0	0	0	0
15	O	1	0	0	0	0
15	T	1	0	0	0	0
15	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	f	1	0	0	0	0
15	l	1	0	0	0	0
15	r	1	0	0	0	0
16	N	1	0	0	1	0
17	A	22	0	0	1	0
17	B	12	0	0	0	0
17	C	7	0	0	0	0
17	D	2	0	0	1	0
17	E	1	0	0	0	0
17	F	25	0	0	0	0
17	G	14	0	0	0	0
17	H	20	0	0	0	0
17	I	17	0	0	1	0
17	J	4	0	0	0	0
17	K	8	0	0	1	0
17	L	26	0	0	0	0
17	M	5	0	0	0	0
17	N	24	0	0	0	0
17	O	9	0	0	0	0
17	P	4	0	0	0	0
17	Q	2	0	0	0	0
17	R	6	0	0	0	0
17	S	59	0	0	0	0
17	T	29	0	0	1	0
17	U	10	0	0	0	0
17	V	9	0	0	0	0
17	W	3	0	0	0	0
17	X	19	0	0	0	0
17	Y	17	0	0	2	0
17	Z	19	0	0	0	0
17	a	12	0	0	0	0
17	b	4	0	0	0	0
17	c	3	0	0	0	0
17	d	3	0	0	1	0
17	e	40	0	0	0	0
17	f	21	0	0	1	0
17	g	3	0	0	0	0
17	h	3	0	0	0	0
17	i	8	0	0	0	0
17	j	20	0	0	1	0
17	k	9	0	0	0	0
17	l	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	m	7	0	0	0	0
17	n	4	0	0	0	0
17	o	2	0	0	0	0
17	p	18	0	0	1	0
17	q	27	0	0	1	0
17	r	16	0	0	0	0
17	s	3	0	0	0	0
17	t	3	0	0	0	0
17	u	1	0	0	0	0
17	v	13	0	0	0	0
All	All	114321	0	110257	1783	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1783) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:170:LYS:NZ	3:g:189:LEU:CD2	1.87	1.37
1:Y:418:LYS:NZ	1:Y:422:ARG:NH1	1.72	1.34
1:Y:418:LYS:NZ	1:Y:422:ARG:HH11	0.89	1.33
1:Y:17:VAL:HG23	1:Y:20:GLU:OE1	1.15	1.27
2:l:106:GLU:O	2:l:429:LYS:NZ	1.68	1.26
3:g:170:LYS:NZ	3:g:189:LEU:HD23	1.45	1.23
2:l:72:ASP:HA	2:l:424:LYS:CE	1.75	1.15
2:l:72:ASP:HA	2:l:424:LYS:HE2	1.14	1.13
3:g:170:LYS:HZ2	3:g:189:LEU:CD2	1.55	1.10
3:g:170:LYS:HZ3	3:g:189:LEU:CD2	1.55	1.10
6:p:213:CYS:SG	6:p:215:ILE:HD12	1.92	1.10
1:M:2:GLU:OE2	1:M:27:LYS:HB2	1.53	1.07
1:G:318:THR:HG22	1:G:320:ASP:H	1.17	1.07
1:Y:17:VAL:CG2	1:Y:20:GLU:OE1	2.02	1.06
2:r:374:GLU:HG3	4:t:117:MET:HE1	1.33	1.04
5:o:69:GLU:OE1	6:p:56:ARG:NH1	1.93	1.02
1:q:422:ARG:NH2	1:q:423:LYS:HE3	1.75	1.01
1:q:417:HIS:CE1	1:q:419:TRP:CD1	2.48	1.01
1:S:81:GLU:OE1	1:S:103:ARG:NH2	1.94	1.00
3:g:189:LEU:HD12	3:g:233:VAL:HG12	1.43	1.00
2:Z:75:ALA:HB3	2:Z:424:LYS:HE3	1.42	0.99
1:q:422:ARG:CZ	1:q:423:LYS:HE3	1.92	0.99
1:Y:418:LYS:NZ	1:Y:422:ARG:HD3	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:158:VAL:HG12	1:S:221:LYS:NZ	1.79	0.98
1:k:4:ILE:HG12	1:k:6:LYS:HD3	1.44	0.97
1:Y:418:LYS:HZ3	1:Y:422:ARG:HH11	1.02	0.96
1:Y:418:LYS:HZ2	1:Y:422:ARG:HH11	1.10	0.96
2:r:335:ALA:O	2:r:356:ARG:NH1	1.99	0.96
2:l:72:ASP:CA	2:l:424:LYS:HE2	1.95	0.95
4:t:11:ILE:HD12	4:t:12:TRP:N	1.82	0.95
3:C:231:ILE:HD11	3:C:238:LEU:HD12	1.49	0.94
2:N:36:ARG:NH2	16:N:506:CL:CL	2.38	0.94
3:g:189:LEU:CD1	3:g:233:VAL:HG12	1.97	0.94
1:Y:418:LYS:HZ1	1:Y:422:ARG:HH11	0.96	0.93
1:Y:418:LYS:HZ2	1:Y:422:ARG:HD3	1.29	0.93
3:g:189:LEU:HD12	3:g:233:VAL:CG1	1.97	0.93
2:T:76:LYS:NZ	2:T:428:TYR:OH	2.01	0.92
5:o:69:GLU:OE1	6:p:56:ARG:NE	2.03	0.91
2:r:363:ILE:HD13	2:r:378:ILE:HB	1.51	0.90
2:l:374:GLU:HG3	4:n:117:MET:HE1	1.54	0.90
1:M:403:MET:HE2	1:M:486:ILE:HG21	1.55	0.89
3:g:170:LYS:HZ2	3:g:189:LEU:HD23	0.75	0.89
1:k:283:ARG:NH1	8:k:603:MFN:O8	2.06	0.88
1:q:516:ARG:NH1	1:q:518:TYR:OH	2.07	0.88
2:Z:71:ILE:HG22	2:Z:424:LYS:NZ	1.88	0.88
1:M:51:PRO:O	1:M:443:ARG:NH1	2.07	0.87
5:o:69:GLU:OE1	6:p:56:ARG:CZ	2.23	0.86
1:M:2:GLU:OE2	1:M:27:LYS:CB	2.23	0.86
6:d:98:LEU:O	6:d:103:LYS:NZ	2.07	0.86
13:l:503:MGD:S12	14:l:505:H2S:S	2.75	0.85
1:q:467:ILE:HD11	1:q:497:LEU:HD13	1.59	0.84
2:l:424:LYS:NZ	2:l:428:TYR:HE2	1.75	0.84
2:Z:80:GLU:O	2:Z:82:LYS:NZ	2.10	0.84
6:d:224:LYS:NZ	6:d:225:THR:O	2.09	0.84
6:L:216:CYS:HB3	6:R:216:CYS:HB3	1.58	0.83
6:v:21:ASN:HD22	6:v:23:ARG:NH2	1.77	0.83
3:g:189:LEU:CD1	3:g:233:VAL:CG1	2.56	0.83
6:R:224:LYS:NZ	6:R:227:GLU:OE1	2.11	0.82
2:r:222:ILE:O	2:r:232:ARG:NH2	2.12	0.82
3:C:31:ILE:HG22	3:C:35:LYS:HE2	1.62	0.82
4:h:2:ARG:NH2	4:h:106:GLU:OE1	2.13	0.82
1:S:158:VAL:HG12	1:S:221:LYS:HZ1	1.44	0.81
6:d:333:THR:OG1	6:d:334:PRO:HD2	1.80	0.81
3:g:170:LYS:HZ3	3:g:189:LEU:HD21	1.41	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:78:ARG:HE	3:s:81:GLN:HE22	1.25	0.81
1:Y:418:LYS:HZ3	1:Y:422:ARG:NH1	1.54	0.81
5:W:23:PRO:HG3	6:X:274:CYS:HB3	1.64	0.80
2:H:6:ASN:O	2:H:404:LYS:NZ	2.15	0.80
6:F:338:LYS:NZ	6:F:342:ASN:HD21	1.79	0.80
1:e:492:ARG:NH2	1:e:508:GLU:OE1	2.11	0.80
1:G:473:ASN:HB3	1:G:476:THR:HG22	1.64	0.80
2:Z:76:LYS:NZ	2:Z:80:GLU:OE2	2.15	0.79
2:r:155:HIS:HA	4:t:11:ILE:HG23	1.65	0.79
1:e:514:HIS:O	1:e:560:LYS:NZ	2.15	0.79
6:p:264:LEU:HD22	6:p:323:ILE:HD11	1.62	0.79
3:s:189:LEU:HD11	3:s:233:VAL:HB	1.65	0.79
2:Z:75:ALA:CB	2:Z:424:LYS:HE3	2.12	0.79
6:R:10:LYS:NZ	6:R:59:GLN:O	2.16	0.79
6:d:216:CYS:HB3	6:p:216:CYS:HB3	1.64	0.79
6:v:346:SER:O	6:v:349:LYS:NZ	2.17	0.79
2:Z:24:GLU:OE2	2:Z:29:VAL:HG21	1.82	0.78
1:A:148:PHE:HE1	1:A:539:LYS:HG3	1.48	0.78
1:q:422:ARG:HD2	1:q:422:ARG:C	2.07	0.77
3:s:29:LYS:HB3	3:s:33:GLU:HG3	1.65	0.77
4:n:1:MET:HE2	4:n:43:LEU:HD13	1.66	0.77
2:N:140:LYS:O	2:N:179:ARG:NH2	2.18	0.77
1:k:159:ASP:OD1	1:k:221:LYS:NZ	2.17	0.77
1:Y:418:LYS:NZ	1:Y:422:ARG:CD	2.47	0.77
3:g:170:LYS:NZ	3:g:189:LEU:HD22	1.97	0.77
4:t:86:ARG:HD2	4:t:124:TYR:OH	1.85	0.77
2:B:374:GLU:HG3	4:D:117:MET:HE1	1.65	0.77
5:i:80:GLU:HG2	6:j:61:LYS:HE2	1.66	0.77
6:R:145:GLY:HA2	6:R:214:ARG:HG3	1.66	0.77
2:Z:71:ILE:HG22	2:Z:424:LYS:HZ1	1.48	0.77
6:d:103:LYS:H	6:d:333:THR:CG2	1.98	0.77
6:F:144:THR:HG21	6:F:222:GLU:HB3	1.66	0.76
6:L:314:CYS:SG	6:L:315:GLU:N	2.58	0.76
2:l:72:ASP:O	2:l:424:LYS:NZ	2.19	0.76
2:r:72:ASP:OD1	2:r:428:TYR:OH	2.02	0.76
1:Y:17:VAL:HG23	1:Y:20:GLU:CD	2.11	0.76
6:p:145:GLY:HA2	6:p:214:ARG:HG3	1.68	0.75
1:q:300:ASP:OD2	17:q:701:HOH:O	2.03	0.75
1:Y:418:LYS:HZ1	1:Y:422:ARG:NH1	1.55	0.75
1:M:497:LEU:HD21	1:M:502:ILE:HG12	1.68	0.75
4:t:11:ILE:HD11	4:t:12:TRP:CE2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:p:266:ILE:HG12	6:p:323:ILE:HD13	1.67	0.75
3:C:2:SER:N	3:C:57:GLU:OE1	2.20	0.74
6:d:95:ILE:O	6:d:103:LYS:NZ	2.20	0.74
6:j:292:GLU:OE1	17:j:601:HOH:O	2.04	0.74
1:M:2:GLU:CD	1:M:27:LYS:HB2	2.13	0.74
1:k:411:LEU:CD2	1:k:416:LEU:HG	2.18	0.74
6:L:242:CYS:SG	6:L:244:TRP:HD1	2.11	0.74
2:l:350:PRO:O	2:l:354:LEU:HD12	1.87	0.74
2:B:204:ASP:OD2	2:B:260:ARG:N	2.15	0.74
6:d:145:GLY:HA2	6:d:214:ARG:HG3	1.69	0.73
2:l:75:ALA:HB1	2:l:425:VAL:HG23	1.70	0.73
6:p:80:ILE:HD12	6:p:104:ILE:HD11	1.69	0.73
6:R:15:GLU:CD	6:R:23:ARG:HH12	1.96	0.73
2:Z:255:GLY:O	2:Z:259:SER:OG	2.05	0.73
6:v:292:GLU:HB2	6:v:296:GLU:OE1	1.89	0.73
2:r:338:MET:HE1	2:r:357:MET:HE3	1.71	0.73
3:s:225:LEU:HD11	3:s:246:GLU:HB2	1.70	0.73
2:H:57:ARG:NH2	2:H:376:ALA:O	2.20	0.73
1:k:50:MET:HE2	1:k:439:ALA:HB2	1.70	0.73
1:q:417:HIS:CE1	1:q:419:TRP:HD1	2.00	0.73
4:V:1:MET:HE2	4:V:43:LEU:HD13	1.70	0.72
6:X:16:ARG:HH21	6:X:22:ARG:HG3	1.52	0.72
6:X:145:GLY:HA2	6:X:214:ARG:HG3	1.71	0.72
1:G:215:LEU:HA	1:G:218:VAL:HG22	1.71	0.72
2:N:141:ASN:HD22	2:N:170:PHE:H	1.36	0.72
1:M:2:GLU:OE2	1:M:27:LYS:HG3	1.88	0.72
1:G:286:VAL:HG12	1:G:423:LYS:HD2	1.71	0.72
6:R:6:VAL:HG22	6:R:13:THR:OG1	1.90	0.72
3:C:32:GLU:HG2	3:C:35:LYS:HE3	1.72	0.71
3:a:11:GLN:NE2	3:a:76:THR:OG1	2.22	0.71
2:T:68:ASP:O	2:T:72:ASP:HB2	1.90	0.71
3:g:24:ASP:OD2	3:g:84:THR:OG1	2.08	0.71
1:q:417:HIS:HE1	1:q:419:TRP:CD1	2.08	0.71
1:q:419:TRP:CE3	1:q:423:LYS:NZ	2.59	0.71
2:r:354:LEU:HD11	4:t:124:TYR:CZ	2.25	0.71
1:S:356:ARG:HH11	1:S:415:GLU:CD	1.98	0.71
6:j:80:ILE:HD12	6:j:104:ILE:HD11	1.72	0.71
2:r:58:LYS:HE2	2:r:61:GLU:HG3	1.72	0.71
3:C:4:ILE:HD13	3:C:65:ILE:HG23	1.72	0.71
1:k:411:LEU:HD23	1:k:416:LEU:HG	1.71	0.71
6:L:144:THR:HG21	6:L:222:GLU:OE1	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:170:LYS:HZ3	3:g:189:LEU:HD22	1.53	0.71
6:X:334:PRO:HB2	6:X:336:ARG:HH12	1.55	0.71
5:o:69:GLU:CD	6:p:56:ARG:HH11	1.98	0.70
1:q:318:THR:HG22	1:q:320:ASP:H	1.56	0.70
2:B:103:LEU:HD21	2:B:421:LEU:HD23	1.71	0.70
6:X:314:CYS:SG	6:X:315:GLU:N	2.64	0.70
6:j:221:TYR:O	6:j:224:LYS:NZ	2.24	0.70
2:Z:140:LYS:O	2:Z:179:ARG:NH2	2.24	0.70
6:F:145:GLY:HA2	6:F:214:ARG:HG3	1.74	0.70
6:L:148:GLU:HG2	6:L:210:MET:HE3	1.73	0.70
2:B:323:GLU:OE2	3:C:97:TYR:OH	2.03	0.70
1:G:235:LEU:HD11	8:G:603:MFN:H11A	1.74	0.70
1:G:318:THR:HG22	1:G:320:ASP:N	2.00	0.70
2:B:59:ASN:HA	4:D:128:GLY:HA3	1.75	0.69
6:R:76:MET:HE1	6:R:343:ALA:HB3	1.74	0.69
2:T:319:TYR:O	2:T:320:ASN:ND2	2.23	0.69
1:S:356:ARG:NH1	1:S:415:GLU:OE2	2.25	0.69
1:e:294:ASP:OD2	1:e:298:LYS:NZ	2.21	0.69
4:t:11:ILE:HD12	4:t:11:ILE:C	2.16	0.69
2:T:59:ASN:O	2:T:61:GLU:N	2.23	0.69
2:B:72:ASP:OD1	2:B:428:TYR:OH	2.07	0.69
1:G:179:ILE:HB	1:G:230:LEU:HD12	1.74	0.69
5:W:18:CYS:HB2	5:W:67:CYS:HB2	1.74	0.69
2:l:75:ALA:HB1	2:l:425:VAL:CG2	2.23	0.69
3:g:63:GLU:CD	3:g:63:GLU:H	2.00	0.69
1:q:456:LYS:NZ	1:q:466:ASP:OD2	2.25	0.69
3:g:170:LYS:NZ	3:g:191:ILE:HG13	2.07	0.69
2:l:140:LYS:NZ	5:o:34:GLY:O	2.26	0.69
2:B:53:LYS:HE3	2:B:64:GLU:CD	2.18	0.68
1:G:49:VAL:HG22	1:G:469:VAL:HG22	1.74	0.68
2:r:58:LYS:CE	2:r:61:GLU:HG3	2.23	0.68
2:T:153:PRO:HG2	2:T:161:MET:HE2	1.74	0.68
5:i:18:CYS:HB2	5:i:67:CYS:HB2	1.74	0.68
2:l:118:CYS:SG	14:l:505:H2S:S	2.91	0.68
6:X:4:THR:N	6:X:68:GLU:OE2	2.27	0.68
2:H:358:ALA:HA	4:J:126:LYS:HD3	1.75	0.68
2:l:424:LYS:HZ2	2:l:428:TYR:HE2	1.41	0.68
2:Z:6:ASN:O	2:Z:404:LYS:NZ	2.26	0.68
6:d:37:CYS:SG	6:d:46:ILE:HG21	2.33	0.68
6:L:338:LYS:HD3	6:L:341:LYS:HE2	1.76	0.68
5:u:18:CYS:HB2	5:u:67:CYS:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:63:GLU:OE1	3:s:63:GLU:N	2.24	0.68
2:B:86:MET:HG2	2:B:339:MET:HE2	1.75	0.68
2:B:58:LYS:HD3	2:B:63:VAL:HG22	1.75	0.67
1:S:158:VAL:HG12	1:S:221:LYS:HZ2	1.59	0.67
6:d:46:ILE:HG12	6:d:66:ILE:HG12	1.75	0.67
3:a:25:VAL:O	3:a:29:LYS:HE2	1.94	0.67
1:S:497:LEU:HD22	1:S:502:ILE:HG12	1.76	0.67
2:f:158:PRO:O	5:i:15:CYS:HB2	1.95	0.67
3:s:2:SER:N	3:s:64:ASP:O	2.27	0.67
2:T:358:ALA:HA	4:V:126:LYS:HD3	1.77	0.67
1:q:1:MET:HG2	1:q:2:GLU:H	1.59	0.67
6:L:145:GLY:HA2	6:L:214:ARG:HG3	1.77	0.67
2:l:222:ILE:O	2:l:232:ARG:NH1	2.28	0.67
1:q:417:HIS:ND1	1:q:419:TRP:CD1	2.62	0.67
2:r:363:ILE:CD1	2:r:378:ILE:HB	2.25	0.67
3:C:70:ASP:OD2	3:C:91:ARG:NH1	2.27	0.67
4:D:73:GLU:OE1	17:D:201:HOH:O	2.13	0.67
2:T:154:MET:HA	2:T:154:MET:HE2	1.76	0.67
6:d:336:ARG:HD3	6:d:336:ARG:H	1.58	0.67
1:M:2:GLU:OE1	1:M:35:VAL:HB	1.96	0.66
3:O:232:GLU:CD	3:O:237:GLU:HG3	2.20	0.66
6:v:314:CYS:SG	6:v:315:GLU:N	2.68	0.66
3:C:9:LYS:HZ3	3:C:10:GLU:H	1.43	0.66
6:p:214:ARG:NH1	6:p:222:GLU:OE2	2.28	0.66
2:B:323:GLU:HG2	2:B:324:THR:HG23	1.76	0.66
2:f:5:LYS:HG2	2:f:20:ILE:HD13	1.77	0.66
6:p:249:CYS:SG	6:p:252:ASP:N	2.68	0.66
6:F:338:LYS:HZ2	6:F:342:ASN:HD21	1.42	0.66
1:S:170:ARG:NH2	1:S:521:ASP:OD1	2.25	0.66
2:l:72:ASP:HA	2:l:424:LYS:CD	2.25	0.66
2:B:61:GLU:N	2:B:61:GLU:OE2	2.29	0.66
2:T:76:LYS:HD2	2:T:428:TYR:CE2	2.30	0.66
6:d:103:LYS:H	6:d:333:THR:HG22	1.60	0.66
1:k:99:MET:O	1:k:103:ARG:HG3	1.96	0.66
3:s:78:ARG:HE	3:s:81:GLN:NE2	1.94	0.66
6:L:37:CYS:SG	6:L:46:ILE:HG21	2.35	0.66
13:l:504:MGD:S13	14:l:505:H2S:S	2.94	0.66
1:A:36:SER:HG	1:A:38:SER:HG	1.40	0.65
3:O:170:LYS:NZ	3:O:236:GLU:OE2	2.25	0.65
1:k:478:ASP:N	1:k:482:GLU:OE2	2.25	0.65
5:E:44:ILE:HD11	5:E:47:ILE:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:80:GLU:OE1	6:L:61:LYS:NZ	2.30	0.65
3:g:170:LYS:CD	3:g:189:LEU:HD22	2.27	0.65
3:C:32:GLU:CG	3:C:35:LYS:HE3	2.26	0.65
2:H:351:GLN:HG3	4:J:85:ASN:O	1.95	0.65
1:M:2:GLU:OE2	1:M:27:LYS:CG	2.43	0.65
6:X:16:ARG:NH2	6:X:20:GLU:O	2.28	0.65
6:j:16:ARG:HH11	6:j:22:ARG:HG3	1.60	0.65
5:E:18:CYS:HB2	5:E:67:CYS:HB2	1.79	0.65
6:X:6:VAL:CG1	6:X:13:THR:HB	2.26	0.65
3:g:17:GLU:HB2	3:g:40:MET:HG2	1.77	0.65
2:r:222:ILE:HB	2:r:232:ARG:HD3	1.79	0.65
2:r:252:PHE:HB2	2:r:256:ILE:HD11	1.78	0.65
3:m:230:ASP:OD1	3:m:239:PRO:HA	1.97	0.65
6:p:213:CYS:SG	6:p:215:ILE:CD1	2.78	0.65
3:I:66:LYS:HE3	3:I:68:ILE:HD11	1.78	0.65
2:T:140:LYS:O	2:T:179:ARG:NH2	2.28	0.65
6:d:326:LYS:HD3	6:d:349:LYS:O	1.97	0.65
6:R:315:GLU:OE2	6:R:325:VAL:N	2.24	0.65
5:o:80:GLU:HG2	6:p:61:LYS:NZ	2.12	0.65
2:l:23:VAL:HG22	2:l:28:ILE:HD13	1.79	0.65
6:R:135:GLU:OE2	6:R:229:THR:OG1	2.14	0.64
1:A:411:LEU:HD23	1:A:416:LEU:HG	1.79	0.64
6:R:267:ASP:OD1	6:R:270:THR:OG1	2.10	0.64
6:X:263:GLU:OE2	6:X:326:LYS:NZ	2.30	0.64
2:l:424:LYS:NZ	2:l:428:TYR:CE2	2.62	0.64
2:r:58:LYS:HD3	2:r:58:LYS:H	1.62	0.64
2:N:358:ALA:HA	4:P:126:LYS:HD3	1.78	0.64
4:b:38:GLU:H	4:b:38:GLU:CD	2.05	0.64
3:s:23:PRO:HB3	3:s:65:ILE:CG2	2.28	0.64
2:H:140:LYS:O	2:H:179:ARG:NH2	2.30	0.64
6:d:117:GLN:NE2	17:d:501:HOH:O	2.28	0.64
2:l:140:LYS:CE	5:o:34:GLY:O	2.44	0.64
6:p:292:GLU:OE1	6:p:292:GLU:N	2.28	0.64
1:q:286:VAL:HG23	1:q:423:LYS:HG2	1.80	0.64
1:q:419:TRP:HE1	8:q:603:MFN:H261	1.62	0.64
2:r:58:LYS:HD3	2:r:58:LYS:N	2.12	0.64
4:D:52:LYS:NZ	4:D:59:ASP:OD1	2.31	0.64
1:Y:418:LYS:HZ3	1:Y:422:ARG:CD	2.09	0.64
6:v:124:ALA:HB2	6:v:248:ILE:HD13	1.80	0.64
6:d:246:GLN:HE21	6:d:255:THR:HA	1.62	0.64
6:F:23:ARG:HD3	6:F:25:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:CD2	1:A:416:LEU:HG	2.27	0.64
6:F:314:CYS:SG	6:F:315:GLU:N	2.71	0.64
1:M:403:MET:HE2	1:M:486:ILE:CG2	2.28	0.64
3:U:36:ASN:OD1	3:U:47:LYS:NZ	2.29	0.64
2:N:36:ARG:NH1	5:Q:12:CYS:O	2.31	0.64
6:R:77:CYS:SG	6:R:86:LEU:HD13	2.38	0.64
1:k:369:GLU:OE2	1:k:424:SER:HB2	1.98	0.64
6:d:22:ARG:HB3	6:d:88:LEU:HD11	1.79	0.64
6:v:348:LEU:C	6:v:349:LYS:HD3	2.22	0.64
1:k:476:THR:HG23	1:k:477:VAL:HG23	1.79	0.63
6:X:160:CYS:SG	6:X:169:ILE:HG21	2.38	0.63
2:T:69:GLU:O	2:T:73:LYS:HG2	1.99	0.63
3:O:102:MET:HE2	3:O:121:MET:HE3	1.80	0.63
1:k:71:TYR:HA	2:l:127:GLN:HG2	1.79	0.63
6:p:37:CYS:SG	6:p:46:ILE:HG21	2.38	0.63
6:R:7:ILE:HD11	6:R:12:ILE:HG23	1.81	0.63
2:T:222:ILE:O	2:T:232:ARG:NH1	2.23	0.63
6:X:4:THR:HG23	6:X:15:GLU:HB3	1.81	0.63
2:f:348:HIS:NE2	17:f:601:HOH:O	2.30	0.63
3:s:32:GLU:OE1	3:s:36:ASN:ND2	2.31	0.63
6:X:242:CYS:O	6:X:258:LYS:NZ	2.30	0.63
3:m:201:GLY:HA3	3:m:204:MET:HE2	1.81	0.63
2:Z:75:ALA:HB2	2:Z:421:LEU:HD12	1.80	0.63
1:k:409:MET:HE1	1:k:413:GLU:CD	2.24	0.63
2:T:71:ILE:HG23	2:T:421:LEU:HG	1.81	0.62
2:B:333:ARG:NH2	2:B:359:GLU:OE1	2.32	0.62
2:r:351:GLN:HA	2:r:354:LEU:HD21	1.80	0.62
1:M:159:ASP:OD1	1:M:221:LYS:NZ	2.28	0.62
2:T:158:PRO:O	5:W:15:CYS:HB2	1.99	0.62
6:d:246:GLN:NE2	6:d:256:VAL:H	1.97	0.62
3:g:127:GLU:HG3	3:g:153:THR:HB	1.80	0.62
1:A:377:PRO:HB2	1:A:440:GLN:HG2	1.82	0.62
2:f:16:CYS:SG	2:f:163:ARG:NE	2.72	0.62
1:Y:162:ALA:CB	1:Y:221:LYS:HE2	2.29	0.62
6:R:77:CYS:SG	6:R:78:SER:N	2.72	0.62
6:F:37:CYS:SG	6:F:46:ILE:HG21	2.39	0.62
4:J:10:THR:HG22	4:J:12:TRP:H	1.64	0.62
5:K:67:CYS:SG	5:K:68:VAL:N	2.72	0.62
6:R:160:CYS:SG	6:R:169:ILE:HG21	2.40	0.62
6:d:314:CYS:SG	6:d:315:GLU:N	2.73	0.62
1:M:405:ASN:HD21	1:M:430:ASP:CA	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:24:LYS:NZ	4:P:28:ASP:OD2	2.33	0.62
3:O:210:VAL:HG11	3:O:238:LEU:HD21	1.82	0.61
1:Y:286:VAL:HG23	1:Y:423:LYS:HD2	1.81	0.61
6:j:314:CYS:SG	6:j:315:GLU:N	2.73	0.61
5:K:6:LYS:HG2	5:K:79:GLU:OE1	1.98	0.61
4:P:10:THR:HG22	4:P:12:TRP:H	1.65	0.61
6:d:160:CYS:SG	6:d:169:ILE:HG21	2.40	0.61
3:g:170:LYS:HD3	3:g:189:LEU:HD22	1.81	0.61
6:p:227:GLU:OE1	6:p:227:GLU:N	2.33	0.61
3:s:162:ILE:HD12	3:s:190:ILE:HD13	1.81	0.61
6:F:125:CYS:SG	6:F:128:ASP:N	2.73	0.61
2:T:424:LYS:O	2:T:428:TYR:HD1	1.84	0.61
1:Y:355:ALA:HB1	1:Y:416:LEU:HD23	1.81	0.61
2:Z:69:GLU:O	2:Z:73:LYS:HG2	2.00	0.61
2:f:140:LYS:O	2:f:179:ARG:NH2	2.33	0.61
6:v:23:ARG:HH22	6:v:91:ASP:H	1.48	0.61
1:S:443:ARG:NH2	1:S:470:TYR:OH	2.32	0.61
3:g:170:LYS:NZ	3:g:189:LEU:HD21	1.98	0.61
3:C:25:VAL:O	3:C:29:LYS:NZ	2.23	0.61
1:M:405:ASN:ND2	1:M:430:ASP:O	2.33	0.61
1:Y:565:LYS:HD2	1:Y:568:MET:HE2	1.82	0.61
12:l:502:W:W	14:l:505:H2S:S	1.84	0.61
3:s:23:PRO:HB3	3:s:65:ILE:HG21	1.82	0.61
6:v:37:CYS:SG	6:v:46:ILE:HG21	2.40	0.61
2:T:210:LEU:O	2:T:214:ARG:HG3	1.99	0.61
1:Y:565:LYS:HD2	1:Y:568:MET:CE	2.31	0.61
1:A:316:THR:OG1	1:A:349:VAL:O	2.18	0.61
1:A:516:ARG:NH1	1:A:518:TYR:OH	2.33	0.61
1:Y:66:ASN:OD1	1:Y:69:ARG:NH1	2.32	0.61
1:Y:77:LYS:NZ	17:Y:703:HOH:O	2.32	0.61
1:e:188:TRP:O	2:f:281:LYS:NZ	2.30	0.61
3:g:189:LEU:HD12	3:g:233:VAL:HG11	1.82	0.61
2:l:255:GLY:O	2:l:259:SER:OG	2.12	0.61
3:s:189:LEU:HD12	3:s:234:ASP:HB2	1.82	0.61
5:Q:6:LYS:HD3	5:Q:79:GLU:OE1	2.00	0.61
2:f:369:ARG:NH2	2:f:374:GLU:OE2	2.33	0.61
1:A:148:PHE:CE1	1:A:539:LYS:HG3	2.34	0.61
6:R:37:CYS:SG	6:R:46:ILE:HG21	2.40	0.61
6:d:100:GLU:HB2	6:d:101:TYR:CD1	2.35	0.61
5:K:39:THR:OG1	17:K:201:HOH:O	2.15	0.61
6:R:121:CYS:SG	6:R:130:ILE:HG21	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:415:ARG:NH1	2:T:419:GLU:OE1	2.34	0.61
2:r:347:ALA:HB2	2:r:371:PRO:HG2	1.83	0.61
6:v:145:GLY:HA2	6:v:214:ARG:HG3	1.83	0.61
2:f:356:ARG:NH1	2:f:359:GLU:OE1	2.33	0.60
3:C:227:VAL:HG23	6:L:231:THR:CG2	2.31	0.60
2:T:428:TYR:CD1	2:T:428:TYR:N	2.63	0.60
6:p:314:CYS:SG	6:p:315:GLU:N	2.74	0.60
1:M:5:ILE:HD11	1:M:469:VAL:HG21	1.82	0.60
6:d:98:LEU:HB3	6:d:100:GLU:HG2	1.82	0.60
1:G:434:THR:HG22	1:G:436:SER:H	1.66	0.60
1:G:84:LYS:HG3	1:G:85:GLY:N	2.17	0.60
1:S:224:LEU:HD22	1:S:520:VAL:HG11	1.84	0.60
6:v:77:CYS:SG	6:v:86:LEU:HD13	2.41	0.60
3:C:63:GLU:OE1	3:C:63:GLU:N	2.29	0.60
6:d:102:PRO:HG2	6:d:340:TRP:CE3	2.35	0.60
2:f:405:LYS:NZ	2:f:408:ASP:OD1	2.28	0.60
1:q:316:THR:HB	8:q:603:MFN:H5	1.84	0.60
5:Q:10:GLU:H	5:Q:10:GLU:CD	2.09	0.60
6:j:121:CYS:SG	6:j:130:ILE:HG21	2.41	0.60
3:s:191:ILE:HG12	3:s:210:VAL:HB	1.83	0.60
5:W:80:GLU:HG2	6:X:61:LYS:HE2	1.83	0.59
6:X:43:VAL:HG11	6:X:70:LYS:O	2.02	0.59
6:d:337:SER:HG	6:d:340:TRP:CD1	2.20	0.59
1:k:554:GLN:OE1	1:k:554:GLN:N	2.30	0.59
6:L:77:CYS:SG	6:L:86:LEU:HD13	2.41	0.59
6:R:249:CYS:SG	6:R:252:ASP:N	2.74	0.59
2:T:163:ARG:NH1	17:T:601:HOH:O	2.09	0.59
5:c:5:LEU:HD21	5:c:76:ILE:HD11	1.83	0.59
6:d:144:THR:HG21	6:d:222:GLU:HG2	1.84	0.59
2:N:158:PRO:O	5:Q:15:CYS:HB2	2.03	0.59
2:f:22:LYS:NZ	5:i:49:GLU:OE2	2.20	0.59
2:N:72:ASP:HB2	2:N:424:LYS:HZ1	1.67	0.59
6:X:16:ARG:NH1	6:X:17:THR:O	2.35	0.59
1:q:99:MET:O	1:q:103:ARG:HG3	2.02	0.59
1:M:492:ARG:HD2	1:M:492:ARG:O	2.02	0.59
1:e:443:ARG:NH2	1:e:470:TYR:OH	2.33	0.59
1:k:7:ASN:HD22	1:k:21:LYS:HE3	1.66	0.59
4:t:11:ILE:CD1	4:t:12:TRP:CD2	2.86	0.59
1:G:224:LEU:HD22	1:G:520:VAL:HG11	1.84	0.59
3:g:147:MET:HE3	3:g:166:MET:HE2	1.85	0.59
2:l:158:PRO:O	5:o:15:CYS:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:99:MET:O	1:S:103:ARG:HG3	2.03	0.59
4:n:2:ARG:HH12	4:n:4:ILE:CD1	2.16	0.59
6:v:169:ILE:HG12	6:v:189:VAL:HG22	1.85	0.59
1:A:147:TRP:O	1:A:151:GLU:HG3	2.03	0.59
2:B:154:MET:HE1	5:E:15:CYS:SG	2.43	0.59
2:B:158:PRO:O	5:E:15:CYS:HB2	2.03	0.59
4:J:36:ASN:HB3	4:J:38:GLU:OE1	2.02	0.59
6:X:37:CYS:SG	6:X:46:ILE:HG21	2.42	0.59
1:Y:312:ASP:OD1	1:Y:394:ARG:NH2	2.33	0.59
6:j:37:CYS:SG	6:j:46:ILE:HG21	2.43	0.59
3:a:83:MET:HE1	3:a:107:ILE:HG13	1.85	0.59
1:e:99:MET:O	1:e:103:ARG:HG3	2.02	0.59
1:e:154:LYS:HE2	1:e:205:ASP:O	2.02	0.59
6:j:281:CYS:SG	6:j:284:ASN:N	2.76	0.59
3:C:201:GLY:HA3	3:C:204:MET:HE2	1.85	0.58
1:M:360:PRO:HA	1:M:363:GLN:HE21	1.68	0.58
6:R:345:ASP:HA	6:R:348:LEU:CD1	2.32	0.58
6:d:115:CYS:SG	6:d:117:GLN:NE2	2.75	0.58
5:o:44:ILE:HD11	5:o:47:ILE:HG22	1.85	0.58
1:q:180:VAL:HA	1:q:231:HIS:HB3	1.85	0.58
6:X:77:CYS:SG	6:X:78:SER:N	2.76	0.58
6:X:135:GLU:HB2	6:X:229:THR:HG23	1.85	0.58
4:n:10:THR:HG22	4:n:12:TRP:H	1.69	0.58
2:B:53:LYS:HE2	2:B:55:LEU:HD21	1.84	0.58
6:L:160:CYS:SG	6:L:169:ILE:HG21	2.43	0.58
2:T:39:HIS:O	2:T:43:VAL:HG22	2.04	0.58
6:v:348:LEU:O	6:v:349:LYS:HD3	2.03	0.58
5:E:2:ALA:N	5:E:80:GLU:OE1	2.36	0.58
6:F:77:CYS:SG	6:F:78:SER:N	2.76	0.58
6:X:16:ARG:NH2	6:X:22:ARG:HG3	2.18	0.58
1:k:473:ASN:HB3	1:k:476:THR:CG2	2.32	0.58
3:U:136:VAL:HB	3:U:162:ILE:HD12	1.86	0.58
1:e:224:LEU:HD22	1:e:520:VAL:HG11	1.85	0.58
3:m:162:ILE:HD11	3:m:192:ILE:HD11	1.85	0.58
3:C:32:GLU:HA	3:C:35:LYS:HD2	1.85	0.58
6:L:249:CYS:SG	6:L:252:ASP:N	2.77	0.58
1:M:359:VAL:O	1:M:363:GLN:HG3	2.03	0.58
1:Y:418:LYS:HZ3	1:Y:422:ARG:CZ	2.14	0.58
1:G:568:MET:O	1:G:569:LEU:HG	2.03	0.58
6:d:87:ASP:OD1	6:d:94:SER:OG	2.15	0.58
2:l:20:ILE:HB	2:l:32:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:PRO:O	5:K:15:CYS:HB2	2.03	0.58
1:k:102:TYR:O	1:k:106:GLN:HG3	2.03	0.58
6:j:5:GLU:HB3	6:j:68:GLU:HG2	1.84	0.58
1:q:358:PRO:HB3	1:q:419:TRP:CG	2.39	0.58
3:s:201:GLY:HA3	3:s:204:MET:HE2	1.86	0.58
3:s:231:ILE:HD12	3:s:238:LEU:HD23	1.84	0.58
4:t:11:ILE:HD11	4:t:12:TRP:CD2	2.39	0.58
2:Z:375:MET:O	4:b:126:LYS:HE3	2.03	0.58
1:k:207:THR:OG1	1:k:210:GLU:HG3	2.03	0.58
6:v:5:GLU:HB3	6:v:68:GLU:HG2	1.86	0.58
1:G:514:HIS:HB2	1:G:560:LYS:NZ	2.18	0.57
6:L:160:CYS:SG	6:L:161:GLU:N	2.77	0.57
1:M:372:LEU:HD11	1:M:408:ARG:NH1	2.19	0.57
6:R:200:CYS:SG	6:R:201:LYS:N	2.77	0.57
6:p:160:CYS:SG	6:p:169:ILE:HG21	2.44	0.57
3:s:160:ASN:OD1	3:s:178:ASN:HB3	2.04	0.57
3:s:233:VAL:HG22	3:s:238:LEU:HD21	1.85	0.57
6:F:160:CYS:SG	6:F:169:ILE:HG21	2.44	0.57
1:M:224:LEU:HD22	1:M:520:VAL:HG11	1.84	0.57
3:g:170:LYS:CE	3:g:189:LEU:CD2	2.78	0.57
6:j:198:GLY:O	6:j:202:ARG:HG3	2.04	0.57
6:v:160:CYS:SG	6:v:169:ILE:HG21	2.44	0.57
6:v:245:CYS:SG	6:v:246:GLN:N	2.77	0.57
6:L:146:GLU:OE2	6:X:218:TYR:OH	2.19	0.57
1:M:2:GLU:OE1	1:M:35:VAL:HG12	2.04	0.57
2:N:233:GLU:O	2:N:237:GLU:HG3	2.02	0.57
1:e:235:LEU:HD22	1:e:323:MET:HE2	1.85	0.57
3:g:131:ASP:OD1	3:g:157:ASN:N	2.19	0.57
1:k:419:TRP:CD1	1:k:423:LYS:HZ2	2.21	0.57
1:k:422:ARG:CZ	1:k:423:LYS:HZ1	2.17	0.57
2:r:158:PRO:O	5:u:15:CYS:HB2	2.04	0.57
1:A:538:SER:O	1:A:542:GLN:HG3	2.05	0.57
1:M:502:ILE:HG21	1:M:505:LYS:CE	2.35	0.57
1:Y:12:CYS:HB3	1:Y:17:VAL:CG1	2.34	0.57
2:l:424:LYS:HZ3	2:l:428:TYR:HE2	1.51	0.57
1:A:69:ARG:NH2	1:A:128:GLU:OE1	2.34	0.57
5:E:53:VAL:HG21	11:E:101:SF4:S2	2.44	0.57
2:N:159:ARG:O	2:N:163:ARG:HG3	2.04	0.57
6:R:333:THR:HG23	6:R:334:PRO:HD2	1.85	0.57
1:G:414:GLY:O	1:G:415:GLU:HB2	2.03	0.57
2:N:333:ARG:NH1	2:N:359:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:77:CYS:SG	6:X:86:LEU:HD13	2.45	0.57
1:k:5:ILE:CG2	1:k:24:ILE:HB	2.35	0.57
6:R:314:CYS:SG	6:R:315:GLU:N	2.77	0.57
1:S:59:HIS:HD1	1:S:64:LYS:HZ1	1.52	0.57
1:S:414:GLY:O	1:S:415:GLU:HB2	2.04	0.57
3:g:170:LYS:HZ1	3:g:191:ILE:HG13	1.69	0.57
5:o:24:VAL:O	5:o:28:ARG:HG3	2.05	0.57
6:F:210:MET:HE2	6:F:212:VAL:HG23	1.85	0.57
2:H:16:CYS:SG	2:H:163:ARG:NH2	2.78	0.57
1:S:102:TYR:O	1:S:106:GLN:HG3	2.04	0.57
2:f:358:ALA:HA	4:h:126:LYS:HD3	1.87	0.57
2:B:53:LYS:HE3	2:B:64:GLU:OE2	2.04	0.57
2:B:347:ALA:HB2	2:B:371:PRO:HG2	1.87	0.57
5:Q:18:CYS:HB2	5:Q:67:CYS:HB2	1.87	0.57
1:Y:113:MET:HE3	1:Y:138:ALA:HB3	1.87	0.57
6:j:160:CYS:SG	6:j:169:ILE:HG21	2.45	0.57
3:s:31:ILE:O	3:s:35:LYS:HG3	2.04	0.57
3:s:31:ILE:O	3:s:34:ILE:HG12	2.04	0.57
2:B:424:LYS:NZ	2:B:427:GLU:OE1	2.29	0.56
2:H:58:LYS:NZ	2:H:63:VAL:HG11	2.20	0.56
2:H:223:LEU:HD11	3:I:270:PRO:HG3	1.87	0.56
6:R:213:CYS:SG	6:R:215:ILE:HD12	2.45	0.56
2:H:18:ASP:OD1	2:H:163:ARG:NH2	2.37	0.56
6:L:76:MET:HE2	6:L:340:TRP:HA	1.87	0.56
2:T:5:LYS:HG2	2:T:20:ILE:HD13	1.87	0.56
3:g:61:ALA:HB1	3:g:63:GLU:OE1	2.04	0.56
4:h:127:VAL:O	4:h:129:GLN:NE2	2.38	0.56
6:j:144:THR:HG23	6:j:214:ARG:HB2	1.86	0.56
1:k:292:ILE:O	1:k:296:VAL:HG23	2.05	0.56
1:G:159:ASP:OD1	1:G:221:LYS:NZ	2.37	0.56
6:R:160:CYS:SG	6:R:161:GLU:N	2.77	0.56
2:T:159:ARG:O	2:T:163:ARG:HG3	2.06	0.56
3:U:63:GLU:H	3:U:63:GLU:CD	2.14	0.56
5:W:23:PRO:HG3	6:X:274:CYS:CB	2.34	0.56
1:Y:311:LEU:HD22	1:Y:355:ALA:HB2	1.85	0.56
6:j:10:LYS:NZ	6:j:60:GLU:HA	2.20	0.56
1:k:222:LEU:C	1:k:567:VAL:HG23	2.30	0.56
2:r:159:ARG:O	2:r:163:ARG:HG3	2.05	0.56
2:N:72:ASP:HB2	2:N:424:LYS:NZ	2.21	0.56
2:T:428:TYR:HD1	2:T:428:TYR:H	1.54	0.56
2:r:53:LYS:HG3	2:r:54:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:LYS:HE2	2:B:52:LYS:HA	1.87	0.56
6:L:104:ILE:HD11	6:L:344:PHE:CE1	2.41	0.56
1:S:496:VAL:HB	1:S:504:VAL:HB	1.87	0.56
6:X:169:ILE:HG12	6:X:189:VAL:HG22	1.86	0.56
2:Z:158:PRO:O	5:c:15:CYS:HB2	2.05	0.56
1:k:473:ASN:HB3	1:k:476:THR:HG22	1.86	0.56
2:l:358:ALA:HA	4:n:126:LYS:HD3	1.88	0.56
2:r:354:LEU:HD23	2:r:354:LEU:H	1.71	0.56
6:v:77:CYS:SG	6:v:78:SER:N	2.77	0.56
3:C:32:GLU:CD	3:C:35:LYS:HE3	2.31	0.56
1:M:2:GLU:OE1	1:M:35:VAL:CB	2.54	0.56
5:W:18:CYS:SG	5:W:19:VAL:N	2.78	0.56
1:Y:103:ARG:NH2	1:Y:106:GLN:OE1	2.38	0.56
4:b:1:MET:HE2	4:b:43:LEU:HD13	1.87	0.56
2:N:273:VAL:HG21	2:N:284:LEU:HD23	1.87	0.56
2:T:256:ILE:HG13	2:T:265:ASN:HB3	1.88	0.56
6:d:332:THR:HG21	6:d:335:ILE:HD11	1.88	0.56
4:t:127:VAL:HG13	4:t:129:GLN:NE2	2.21	0.56
6:L:77:CYS:SG	6:L:78:SER:N	2.79	0.56
2:N:20:ILE:HB	2:N:32:ILE:HB	1.88	0.56
3:a:204:MET:SD	3:a:256:GLY:HA3	2.45	0.56
6:d:249:CYS:SG	6:d:252:ASP:N	2.78	0.56
1:q:419:TRP:CG	1:q:422:ARG:HH21	2.24	0.56
5:W:44:ILE:HD11	5:W:47:ILE:HG22	1.87	0.56
1:Y:6:LYS:HE2	1:Y:23:ASP:OD2	2.06	0.56
1:Y:231:HIS:NE2	1:Y:235:LEU:HD13	2.21	0.56
1:e:102:TYR:O	1:e:106:GLN:HG3	2.05	0.56
6:j:332:THR:HG22	6:j:333:THR:O	2.05	0.56
2:T:184:VAL:HG22	2:T:199:LEU:HD12	1.88	0.56
2:f:256:ILE:HG13	2:f:265:ASN:HB3	1.88	0.56
2:f:256:ILE:HG23	2:f:266:ILE:CD1	2.36	0.56
1:q:358:PRO:HB2	1:q:419:TRP:CD2	2.41	0.56
5:E:12:CYS:SG	5:E:53:VAL:HG23	2.46	0.55
6:j:77:CYS:SG	6:j:78:SER:N	2.79	0.55
1:k:231:HIS:CE1	1:k:235:LEU:HD13	2.40	0.55
2:l:346:GLY:HA2	2:l:354:LEU:HD21	1.87	0.55
3:m:227:VAL:HG23	6:v:231:THR:CG2	2.35	0.55
1:q:551:TYR:HB3	1:q:552:PRO:HD3	1.88	0.55
3:s:48:LEU:HD23	3:s:52:PHE:HB2	1.88	0.55
1:G:473:ASN:HB3	1:G:476:THR:CG2	2.34	0.55
4:J:38:GLU:H	4:J:38:GLU:CD	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:216:GLN:NE2	3:O:217:GLU:OE2	2.39	0.55
1:Y:411:LEU:CD2	1:Y:416:LEU:HG	2.36	0.55
6:d:77:CYS:SG	6:d:86:LEU:HD13	2.46	0.55
6:p:121:CYS:SG	6:p:130:ILE:HG21	2.46	0.55
1:M:442:THR:C	1:M:443:ARG:HD2	2.31	0.55
6:d:160:CYS:SG	6:d:161:GLU:N	2.79	0.55
2:f:415:ARG:HG2	2:f:419:GLU:OE1	2.06	0.55
8:k:603:MFN:C34	8:k:603:MFN:H262	2.35	0.55
1:q:358:PRO:CB	1:q:419:TRP:CD2	2.89	0.55
2:B:5:LYS:HG2	2:B:20:ILE:HD13	1.88	0.55
5:K:69:GLU:OE1	6:L:56:ARG:NE	2.37	0.55
1:M:377:PRO:HB2	1:M:440:GLN:HG2	1.88	0.55
6:R:103:LYS:H	6:R:333:THR:HB	1.70	0.55
3:a:68:ILE:HG21	3:a:91:ARG:HH21	1.72	0.55
1:k:235:LEU:HD12	1:k:275:HIS:CE1	2.42	0.55
5:Q:67:CYS:SG	5:Q:68:VAL:N	2.79	0.55
1:S:249:ASP:O	1:S:252:LYS:HG2	2.06	0.55
6:d:268:GLN:HE22	6:d:301:LEU:H	1.54	0.55
3:m:11:GLN:NE2	3:m:75:ASN:H	2.04	0.55
1:M:497:LEU:CD2	1:M:502:ILE:HG12	2.36	0.55
1:M:523:GLN:HG3	1:M:568:MET:HG3	1.89	0.55
3:a:210:VAL:HG11	3:a:238:LEU:HD22	1.89	0.55
2:r:350:PRO:O	2:r:354:LEU:HD23	2.07	0.55
3:C:9:LYS:NZ	3:C:10:GLU:HB3	2.22	0.55
1:M:3:TYR:HB2	1:M:26:VAL:CG2	2.37	0.55
1:M:456:LYS:HE3	1:M:466:ASP:OD2	2.07	0.55
3:C:227:VAL:HG22	6:L:133:THR:HG21	1.88	0.55
6:F:200:CYS:SG	6:F:201:LYS:N	2.80	0.55
5:c:2:ALA:N	5:c:80:GLU:OE2	2.40	0.55
1:S:551:TYR:HB3	1:S:552:PRO:HD3	1.88	0.55
1:Y:99:MET:O	1:Y:103:ARG:HG2	2.07	0.55
5:o:80:GLU:HG2	6:p:61:LYS:HZ3	1.72	0.55
1:M:405:ASN:HD21	1:M:430:ASP:HA	1.72	0.54
2:Z:55:LEU:HD21	2:Z:64:GLU:HG2	1.88	0.54
6:j:7:ILE:HD13	6:j:12:ILE:HG12	1.88	0.54
6:j:200:CYS:SG	6:j:201:LYS:N	2.80	0.54
1:k:5:ILE:HG22	1:k:24:ILE:HB	1.87	0.54
1:q:224:LEU:HD22	1:q:520:VAL:HG11	1.89	0.54
2:r:55:LEU:CD2	2:r:64:GLU:HG2	2.36	0.54
3:O:216:GLN:HG2	3:O:217:GLU:HG3	1.89	0.54
1:Y:203:TYR:CE1	6:d:297:LYS:HD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:10:LYS:O	6:d:62:SER:OG	2.20	0.54
5:o:67:CYS:SG	5:o:68:VAL:N	2.79	0.54
6:R:48:VAL:HG22	6:R:64:ILE:HD12	1.87	0.54
2:f:103:LEU:HD13	2:f:422:LEU:HA	1.89	0.54
3:m:227:VAL:HG23	6:v:231:THR:HG23	1.90	0.54
2:B:53:LYS:HD3	2:B:53:LYS:N	2.21	0.54
6:R:265:ILE:HB	6:R:324:THR:HG23	1.89	0.54
1:Y:355:ALA:HB3	1:Y:415:GLU:OE1	2.07	0.54
1:q:36:SER:OG	1:q:38:SER:N	2.38	0.54
6:d:36:LEU:HD22	6:d:347:LEU:HD13	1.89	0.54
6:d:43:VAL:HG21	6:d:70:LYS:O	2.07	0.54
6:d:121:CYS:SG	6:d:130:ILE:HG21	2.48	0.54
3:m:160:ASN:OD1	3:m:178:ASN:HB3	2.08	0.54
3:s:238:LEU:HD22	3:s:238:LEU:N	2.22	0.54
6:X:121:CYS:SG	6:X:130:ILE:HG21	2.46	0.54
3:a:22:LYS:HB2	3:a:83:MET:HG3	1.90	0.54
6:d:77:CYS:SG	6:d:78:SER:N	2.80	0.54
6:d:318:CYS:SG	6:d:321:THR:N	2.81	0.54
2:r:338:MET:HE2	2:r:362:VAL:HG22	1.89	0.54
2:r:363:ILE:HD11	2:r:378:ILE:HD12	1.90	0.54
2:B:56:ILE:HD13	2:B:73:LYS:HD2	1.89	0.54
3:C:136:VAL:HB	3:C:162:ILE:HG22	1.89	0.54
6:R:37:CYS:HB2	6:R:77:CYS:HB2	1.89	0.54
1:Y:55:ASP:O	1:Y:113:MET:HG2	2.08	0.54
5:o:18:CYS:HB2	5:o:67:CYS:HB2	1.90	0.54
6:p:37:CYS:SG	6:p:38:GLY:N	2.80	0.54
1:q:103:ARG:O	1:q:107:MET:HG2	2.07	0.54
1:Y:235:LEU:HD11	8:Y:603:MFN:H11A	1.89	0.54
1:q:170:ARG:NH2	1:q:521:ASP:OD1	2.30	0.54
1:M:566:GLY:N	1:M:568:MET:HE1	2.23	0.54
6:X:43:VAL:CG1	6:X:70:LYS:HB3	2.37	0.54
1:q:36:SER:OG	1:q:38:SER:OG	2.24	0.54
2:r:354:LEU:HD11	4:t:124:TYR:CE2	2.42	0.54
1:M:2:GLU:OE1	1:M:35:VAL:CG1	2.56	0.54
3:O:83:MET:HG2	3:O:102:MET:HG3	1.90	0.54
3:O:232:GLU:OE1	3:O:237:GLU:HA	2.08	0.54
2:T:277:ASN:HA	2:T:280:ALA:O	2.08	0.54
1:q:175:TYR:HA	1:q:520:VAL:HG23	1.91	0.54
2:r:86:MET:HG2	2:r:339:MET:HE2	1.89	0.54
2:r:155:HIS:HA	4:t:11:ILE:CG2	2.38	0.54
6:F:338:LYS:HZ3	6:F:342:ASN:HD21	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:496:VAL:HB	1:G:504:VAL:HB	1.90	0.53
1:M:356:ARG:NE	1:M:415:GLU:OE1	2.41	0.53
6:X:261:GLU:HB2	6:X:329:ARG:HB3	1.90	0.53
1:Y:213:LYS:O	1:Y:217:GLU:HG3	2.08	0.53
6:p:336:ARG:HG2	6:p:336:ARG:HH11	1.73	0.53
5:u:16:GLY:O	5:u:20:ILE:HG12	2.08	0.53
2:N:413:SER:OG	2:N:416:GLU:HG3	2.08	0.53
2:T:424:LYS:O	2:T:428:TYR:CD1	2.61	0.53
3:g:36:ASN:HA	3:g:47:LYS:HD2	1.90	0.53
4:h:32:ILE:HB	4:h:65:VAL:HG21	1.89	0.53
2:l:103:LEU:HA	2:l:422:LEU:HD13	1.89	0.53
6:p:125:CYS:SG	6:p:128:ASP:N	2.81	0.53
6:p:160:CYS:SG	6:p:161:GLU:N	2.81	0.53
6:p:336:ARG:HH11	6:p:336:ARG:CG	2.21	0.53
1:A:124:HIS:NE2	1:A:128:GLU:OE2	2.41	0.53
6:R:318:CYS:SG	6:R:321:THR:N	2.82	0.53
6:X:6:VAL:HG12	6:X:13:THR:HB	1.90	0.53
1:Y:411:LEU:HD23	1:Y:416:LEU:HG	1.90	0.53
5:o:6:LYS:HD3	5:o:79:GLU:OE1	2.09	0.53
3:O:216:GLN:HE21	3:O:217:GLU:HG3	1.73	0.53
6:R:345:ASP:HA	6:R:348:LEU:HD12	1.90	0.53
6:j:148:GLU:HG2	6:j:210:MET:HE3	1.90	0.53
1:k:5:ILE:HG13	1:k:42:ILE:HG22	1.91	0.53
3:s:189:LEU:CD1	3:s:234:ASP:HB2	2.38	0.53
6:R:146:GLU:HB2	6:R:210:MET:HE1	1.90	0.53
5:W:6:LYS:HD3	5:W:79:GLU:OE1	2.07	0.53
3:a:201:GLY:HA3	3:a:204:MET:HE2	1.89	0.53
6:d:136:LEU:HD21	6:j:159:MET:HG2	1.90	0.53
6:d:286:LEU:HB3	6:d:301:LEU:HD11	1.90	0.53
5:i:18:CYS:SG	5:i:19:VAL:N	2.82	0.53
2:B:234:GLN:NE2	2:B:237:GLU:OE1	2.42	0.53
4:D:86:ARG:HD2	4:D:124:TYR:OH	2.08	0.53
6:X:338:LYS:HZ2	6:X:341:LYS:HE2	1.73	0.53
1:k:318:THR:HG21	8:k:603:MFN:O1	2.07	0.53
3:m:166:MET:HB3	3:m:185:MET:HG3	1.91	0.53
6:p:15:GLU:HB2	6:p:23:ARG:HG3	1.90	0.53
6:F:148:GLU:HG3	6:F:210:MET:HB3	1.91	0.53
6:L:200:CYS:SG	6:L:201:LYS:N	2.82	0.53
2:Z:358:ALA:HA	4:b:126:LYS:HD3	1.90	0.53
3:g:19:PRO:O	3:g:22:LYS:NZ	2.42	0.53
6:j:169:ILE:HG12	6:j:189:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:HB3	1:A:21:LYS:HE3	1.90	0.53
3:I:201:GLY:HA3	3:I:204:MET:HE2	1.90	0.53
6:L:242:CYS:SG	6:L:244:TRP:CD1	2.98	0.53
2:Z:252:PHE:HE1	2:Z:284:LEU:HD13	1.74	0.53
6:d:261:GLU:HB2	6:d:329:ARG:HB3	1.90	0.53
6:j:245:CYS:SG	6:j:246:GLN:N	2.82	0.53
2:B:252:PHE:HB2	2:B:256:ILE:HD11	1.91	0.53
6:L:277:CYS:SG	6:L:286:LEU:HD13	2.48	0.53
2:N:347:ALA:HB2	2:N:371:PRO:HG2	1.91	0.53
6:X:231:THR:HG22	6:X:232:SER:H	1.74	0.53
6:d:41:CYS:SG	6:d:45:ALA:N	2.71	0.53
6:d:41:CYS:SG	6:d:44:SER:N	2.82	0.53
6:L:214:ARG:NH1	6:L:222:GLU:OE2	2.42	0.53
1:Y:17:VAL:CB	1:Y:20:GLU:OE1	2.56	0.53
2:r:20:ILE:HB	2:r:32:ILE:HB	1.91	0.53
6:F:6:VAL:HG22	6:F:13:THR:HB	1.91	0.52
1:M:153:LEU:HD13	1:M:214:GLY:HA3	1.91	0.52
3:O:231:ILE:HG13	3:O:238:LEU:HB2	1.92	0.52
6:R:242:CYS:SG	6:R:244:TRP:HD1	2.32	0.52
4:b:36:ASN:HB3	4:b:38:GLU:OE1	2.09	0.52
3:g:201:GLY:HA3	3:g:204:MET:HE2	1.91	0.52
2:l:369:ARG:NH2	2:l:374:GLU:OE2	2.41	0.52
3:s:233:VAL:HG22	3:s:238:LEU:CD2	2.39	0.52
2:B:159:ARG:O	2:B:163:ARG:HG3	2.09	0.52
6:F:245:CYS:SG	6:F:246:GLN:N	2.81	0.52
6:F:318:CYS:SG	6:F:321:THR:N	2.82	0.52
5:K:12:CYS:SG	5:K:52:VAL:HA	2.49	0.52
1:M:287:SER:OG	1:M:423:LYS:O	2.20	0.52
5:i:78:LEU:O	6:j:59:GLN:NE2	2.30	0.52
2:l:69:GLU:HG3	2:l:73:LYS:HE2	1.92	0.52
1:q:356:ARG:HG3	1:q:356:ARG:HH21	1.73	0.52
1:q:419:TRP:CD2	1:q:422:ARG:NH2	2.77	0.52
1:A:99:MET:O	1:A:103:ARG:HG3	2.10	0.52
6:L:104:ILE:HG23	6:L:259:PRO:HB3	1.89	0.52
6:L:218:TYR:OH	6:X:214:ARG:NH2	2.41	0.52
1:M:102:TYR:O	1:M:106:GLN:HG3	2.10	0.52
3:U:204:MET:SD	3:U:256:GLY:HA3	2.50	0.52
1:Y:455:THR:HB	1:Y:464:ASP:OD1	2.09	0.52
6:v:144:THR:HG23	6:v:214:ARG:HB2	1.92	0.52
6:F:249:CYS:SG	6:F:252:ASP:N	2.82	0.52
1:G:148:PHE:CE1	1:G:539:LYS:HE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:252:PHE:HB2	2:N:256:ILE:HD11	1.92	0.52
1:Y:418:LYS:NZ	1:Y:422:ARG:CZ	2.65	0.52
4:n:7:THR:HG22	4:n:101:LYS:HG2	1.91	0.52
6:L:119:LYS:HD2	6:L:134:ARG:CZ	2.39	0.52
2:N:277:ASN:HA	2:N:280:ALA:O	2.09	0.52
6:R:341:LYS:NZ	6:R:345:ASP:OD2	2.39	0.52
4:t:110:THR:OG1	4:t:112:GLU:HG3	2.10	0.52
1:A:102:TYR:O	1:A:106:GLN:HG3	2.09	0.52
1:G:71:TYR:HA	2:H:127:GLN:HG2	1.92	0.52
2:H:252:PHE:HB2	2:H:256:ILE:HD11	1.90	0.52
2:H:255:GLY:O	2:H:259:SER:OG	2.24	0.52
1:S:318:THR:HG23	1:S:320:ASP:H	1.75	0.52
1:Y:162:ALA:HB1	1:Y:222:LEU:HD21	1.91	0.52
1:Y:221:LYS:O	1:Y:567:VAL:HG21	2.09	0.52
3:s:189:LEU:CD2	3:s:191:ILE:HG13	2.40	0.52
2:T:347:ALA:HB2	2:T:371:PRO:HG2	1.92	0.52
6:X:160:CYS:HB2	6:X:200:CYS:HB2	1.92	0.52
1:Y:235:LEU:HD12	1:Y:275:HIS:CE1	2.45	0.52
1:e:27:LYS:HE3	1:e:28:ASP:OD2	2.10	0.52
2:l:71:ILE:O	2:l:424:LYS:HE2	2.10	0.52
6:p:183:VAL:HG13	6:v:248:ILE:HD11	1.90	0.52
6:p:200:CYS:SG	6:p:201:LYS:N	2.82	0.52
6:p:277:CYS:SG	6:p:286:LEU:HD13	2.49	0.52
2:Z:75:ALA:HB2	2:Z:421:LEU:CD1	2.40	0.52
6:p:292:GLU:H	6:p:292:GLU:CD	2.15	0.52
4:D:34:GLN:HA	4:D:65:VAL:HG23	1.92	0.52
6:L:258:LYS:NZ	6:L:306:ARG:O	2.35	0.52
6:R:104:ILE:CG2	6:R:259:PRO:HB3	2.39	0.52
5:c:18:CYS:SG	5:c:19:VAL:N	2.82	0.52
6:d:148:GLU:HG2	6:d:210:MET:HE3	1.92	0.52
2:B:413:SER:OG	2:B:416:GLU:HG3	2.11	0.51
6:F:77:CYS:SG	6:F:86:LEU:HD13	2.50	0.51
2:N:351:GLN:HG2	2:N:352:ARG:N	2.24	0.51
6:R:348:LEU:C	6:R:349:LYS:HG3	2.34	0.51
5:W:67:CYS:SG	5:W:68:VAL:N	2.83	0.51
6:d:341:LYS:HD2	6:d:345:ASP:OD2	2.10	0.51
6:p:242:CYS:SG	6:p:244:TRP:HD1	2.33	0.51
2:B:20:ILE:HB	2:B:32:ILE:HB	1.93	0.51
5:K:24:VAL:O	5:K:28:ARG:HG3	2.10	0.51
6:L:261:GLU:HB2	6:L:329:ARG:HB3	1.93	0.51
3:O:201:GLY:HA3	3:O:204:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:16:LEU:HD12	3:m:76:THR:HG22	1.92	0.51
6:p:56:ARG:CZ	6:p:279:MET:HE1	2.41	0.51
2:r:339:MET:HG3	2:r:363:ILE:CG2	2.41	0.51
6:L:121:CYS:SG	6:L:122:GLU:N	2.84	0.51
6:d:231:THR:HG22	6:d:232:SER:H	1.74	0.51
3:g:121:MET:HB3	3:g:147:MET:SD	2.50	0.51
1:k:5:ILE:HG13	1:k:42:ILE:CG2	2.39	0.51
2:r:16:CYS:SG	2:r:163:ARG:HD2	2.50	0.51
3:s:204:MET:SD	3:s:256:GLY:HA3	2.50	0.51
6:F:41:CYS:SG	6:F:44:SER:N	2.84	0.51
6:R:76:MET:HE1	6:R:343:ALA:CB	2.40	0.51
6:R:104:ILE:HG22	6:R:259:PRO:HB3	1.93	0.51
2:T:154:MET:HG2	2:T:161:MET:HE3	1.93	0.51
6:X:281:CYS:SG	6:X:284:ASN:N	2.83	0.51
3:a:210:VAL:HG11	3:a:238:LEU:CD2	2.40	0.51
1:q:102:TYR:O	1:q:106:GLN:HG3	2.11	0.51
4:J:10:THR:HG22	4:J:12:TRP:N	2.25	0.51
2:N:95:GLU:O	2:N:99:VAL:HG23	2.11	0.51
3:O:254:ALA:O	3:O:255:LYS:HE2	2.11	0.51
6:R:332:THR:HG21	6:R:335:ILE:HD11	1.93	0.51
1:S:235:LEU:HD11	8:S:603:MFN:H11A	1.92	0.51
2:f:277:ASN:HA	2:f:280:ALA:O	2.10	0.51
6:v:200:CYS:SG	6:v:201:LYS:N	2.83	0.51
1:Y:64:LYS:HD3	1:Y:317:MET:HB2	1.91	0.51
2:Z:20:ILE:HB	2:Z:32:ILE:HB	1.93	0.51
6:v:16:ARG:O	6:v:17:THR:HB	2.10	0.51
5:E:18:CYS:SG	5:E:19:VAL:N	2.83	0.51
6:L:160:CYS:SG	6:L:169:ILE:HD13	2.51	0.51
6:R:91:ASP:N	6:R:92:GLY:HA2	2.25	0.51
1:Y:318:THR:HG21	8:Y:603:MFN:O1	2.11	0.51
1:k:49:VAL:HG22	1:k:469:VAL:HG22	1.93	0.51
6:R:232:SER:O	3:U:229:LYS:HD3	2.10	0.51
1:S:377:PRO:HB2	1:S:440:GLN:HG2	1.92	0.51
5:c:80:GLU:HG3	5:c:81:LEU:HG	1.92	0.51
6:j:249:CYS:SG	6:j:252:ASP:N	2.84	0.51
3:m:185:MET:SD	3:m:207:GLY:HA3	2.51	0.51
1:Y:473:ASN:HB3	1:Y:476:THR:OG1	2.10	0.51
3:g:204:MET:SD	3:g:256:GLY:HA3	2.51	0.51
6:p:77:CYS:SG	6:p:78:SER:N	2.83	0.51
1:A:535:ASN:O	1:A:539:LYS:HG2	2.11	0.50
6:L:125:CYS:SG	6:L:128:ASP:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:200:CYS:SG	6:X:201:LYS:N	2.84	0.50
1:k:411:LEU:HD21	1:k:416:LEU:HG	1.92	0.50
1:q:66:ASN:ND2	2:r:298:GLN:OE1	2.34	0.50
2:B:2:GLU:HA	2:B:2:GLU:OE1	2.11	0.50
6:L:37:CYS:SG	6:L:38:GLY:N	2.85	0.50
2:N:320:ASN:ND2	3:O:97:TYR:OH	2.30	0.50
6:R:7:ILE:HG13	6:R:12:ILE:HG12	1.93	0.50
6:R:125:CYS:SG	6:R:128:ASP:N	2.85	0.50
3:U:210:VAL:HG22	3:U:259:TYR:HB2	1.93	0.50
5:c:67:CYS:SG	5:c:68:VAL:N	2.84	0.50
1:e:217:GLU:HG2	1:e:254:ILE:HD13	1.92	0.50
3:g:31:ILE:HG23	3:g:54:VAL:HG12	1.92	0.50
3:g:170:LYS:CE	3:g:189:LEU:HD22	2.42	0.50
1:k:377:PRO:HB2	1:k:440:GLN:HG2	1.93	0.50
1:q:151:GLU:O	1:q:155:GLU:HG3	2.11	0.50
6:v:242:CYS:SG	6:v:244:TRP:HD1	2.34	0.50
2:B:58:LYS:HD3	2:B:63:VAL:CG2	2.42	0.50
4:D:10:THR:HG22	4:D:12:TRP:H	1.76	0.50
2:H:20:ILE:HB	2:H:32:ILE:HB	1.93	0.50
3:I:6:LEU:HB2	3:I:69:ILE:HG12	1.92	0.50
6:L:37:CYS:HB2	6:L:77:CYS:HB2	1.93	0.50
1:M:175:TYR:HD2	1:M:176:THR:HG22	1.76	0.50
4:h:38:GLU:H	4:h:38:GLU:CD	2.19	0.50
1:k:37:ASP:OD1	1:k:37:ASP:N	2.43	0.50
2:T:253:GLY:O	2:T:256:ILE:HG22	2.12	0.50
3:g:228:GLU:HB3	3:g:231:ILE:HD11	1.93	0.50
1:k:2:GLU:HG3	1:k:27:LYS:HD2	1.93	0.50
2:l:252:PHE:HB2	2:l:256:ILE:HD11	1.94	0.50
6:p:160:CYS:SG	6:p:169:ILE:HD13	2.51	0.50
1:q:81:GLU:OE2	1:q:103:ARG:NH2	2.44	0.50
1:G:280:THR:HG23	1:G:281:THR:HG23	1.92	0.50
4:b:10:THR:HG22	4:b:12:TRP:H	1.77	0.50
1:k:4:ILE:HG12	1:k:6:LYS:CD	2.30	0.50
1:k:409:MET:HE1	1:k:413:GLU:OE2	2.11	0.50
6:p:160:CYS:HB2	6:p:200:CYS:HB2	1.93	0.50
6:R:245:CYS:SG	6:R:246:GLN:N	2.84	0.50
1:S:385:ASP:OD2	8:S:603:MFN:H12A	2.11	0.50
2:T:165:VAL:O	2:T:179:ARG:NH1	2.41	0.50
6:X:245:CYS:SG	6:X:246:GLN:N	2.84	0.50
2:B:338:MET:HE1	2:B:357:MET:HE3	1.94	0.50
3:C:27:ALA:O	3:C:29:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:MET:SD	3:C:256:GLY:HA3	2.52	0.50
2:H:347:ALA:HB2	2:H:371:PRO:HG2	1.94	0.50
1:M:497:LEU:HD23	1:M:502:ILE:HA	1.92	0.50
1:Y:102:TYR:O	1:Y:106:GLN:HG3	2.11	0.50
3:C:155:HIS:ND1	3:C:174:LYS:HE2	2.27	0.50
6:j:22:ARG:NH1	6:j:73:LEU:O	2.43	0.50
6:p:200:CYS:SG	6:p:209:ILE:HG21	2.51	0.50
2:r:162:SER:HB2	5:u:20:ILE:HG13	1.94	0.50
6:v:145:GLY:HA2	6:v:214:ARG:CG	2.42	0.50
1:Y:546:VAL:O	5:c:36:LYS:NZ	2.44	0.49
2:Z:174:ARG:NH2	6:d:299:THR:O	2.45	0.49
1:k:497:LEU:CD1	1:k:502:ILE:HG12	2.42	0.49
6:F:200:CYS:SG	6:F:209:ILE:HG21	2.53	0.49
2:H:351:GLN:HE21	4:J:86:ARG:C	2.21	0.49
2:T:256:ILE:HG23	2:T:266:ILE:CD1	2.42	0.49
2:f:116:SER:HA	2:f:308:TYR:HE2	1.76	0.49
5:o:18:CYS:SG	5:o:19:VAL:N	2.85	0.49
6:R:90:ILE:HD12	6:R:95:ILE:HG22	1.94	0.49
6:R:332:THR:HG23	6:R:333:THR:O	2.12	0.49
6:X:249:CYS:SG	6:X:252:ASP:N	2.85	0.49
6:j:10:LYS:O	6:j:62:SER:OG	2.26	0.49
6:v:121:CYS:SG	6:v:130:ILE:HG21	2.52	0.49
6:v:125:CYS:SG	6:v:128:ASP:N	2.86	0.49
6:v:277:CYS:SG	6:v:286:LEU:HD13	2.52	0.49
6:F:160:CYS:SG	6:F:169:ILE:HD13	2.53	0.49
6:F:277:CYS:SG	6:F:286:LEU:HD13	2.53	0.49
3:O:204:MET:SD	3:O:256:GLY:HA3	2.52	0.49
5:Q:38:PRO:HG2	5:Q:47:ILE:HD11	1.93	0.49
2:Z:56:ILE:HD12	2:Z:65:VAL:HG21	1.95	0.49
2:Z:118:CYS:SG	13:Z:504:MGD:S12	3.11	0.49
1:e:213:LYS:NZ	1:e:217:GLU:OE1	2.37	0.49
3:g:189:LEU:HD11	3:g:233:VAL:HB	1.94	0.49
2:B:205:ARG:NH2	3:C:217:GLU:OE2	2.45	0.49
6:F:104:ILE:HG23	6:F:259:PRO:HB3	1.94	0.49
6:F:146:GLU:HB2	6:F:210:MET:HE1	1.95	0.49
2:T:320:ASN:OD1	3:U:97:TYR:OH	2.21	0.49
6:j:200:CYS:SG	6:j:209:ILE:HG21	2.52	0.49
2:l:375:MET:O	4:n:126:LYS:HE3	2.12	0.49
3:m:137:GLY:HA3	3:m:171:ILE:HD11	1.94	0.49
2:N:216:CYS:HB2	2:N:222:ILE:HD11	1.94	0.49
1:S:497:LEU:CD2	1:S:502:ILE:HG12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:189:LEU:HD11	3:g:233:VAL:CG1	2.41	0.49
6:p:50:PRO:O	6:p:54:MET:HG2	2.11	0.49
6:F:169:ILE:HG12	6:F:189:VAL:HG22	1.94	0.49
1:M:3:TYR:HB2	1:M:26:VAL:HG22	1.93	0.49
3:O:232:GLU:OE1	3:O:237:GLU:HG3	2.12	0.49
5:Q:71:CYS:SG	5:Q:74:ASP:N	2.85	0.49
2:T:324:THR:O	2:T:324:THR:HG22	2.13	0.49
1:Y:318:THR:OG1	1:Y:324:GLU:OE2	2.20	0.49
6:j:34:CYS:SG	6:j:36:LEU:HG	2.53	0.49
2:r:247:PHE:CD2	2:r:281:LYS:HG2	2.47	0.49
1:A:162:ALA:HA	1:A:218:VAL:HG13	1.95	0.49
2:H:277:ASN:HA	2:H:280:ALA:O	2.12	0.49
6:L:31:CYS:SG	6:L:63:LYS:HD3	2.52	0.49
6:L:100:GLU:HG3	6:L:336:ARG:HH22	1.78	0.49
1:S:336:ALA:HB3	1:S:348:VAL:HB	1.95	0.49
6:d:125:CYS:SG	6:d:128:ASP:N	2.85	0.49
2:r:58:LYS:O	2:r:58:LYS:HG2	2.12	0.49
6:v:13:THR:HG23	6:v:25:ILE:HG13	1.93	0.49
1:A:36:SER:OG	1:A:38:SER:OG	2.20	0.49
3:C:106:LYS:NZ	3:C:108:THR:OG1	2.44	0.49
3:O:231:ILE:HG13	3:O:231:ILE:O	2.13	0.49
3:O:231:ILE:O	3:O:232:GLU:OE1	2.31	0.49
3:O:232:GLU:HG3	3:O:237:GLU:HA	1.95	0.49
1:S:158:VAL:CG1	1:S:221:LYS:HZ1	2.21	0.49
4:h:32:ILE:HB	4:h:65:VAL:CG2	2.43	0.49
6:j:125:CYS:SG	6:j:128:ASP:N	2.86	0.49
6:v:37:CYS:SG	6:v:38:GLY:N	2.86	0.49
2:H:222:ILE:O	2:H:232:ARG:NH2	2.45	0.49
1:M:175:TYR:HD2	1:M:176:THR:CG2	2.26	0.49
6:j:77:CYS:SG	6:j:86:LEU:HD13	2.52	0.49
6:p:31:CYS:SG	6:p:63:LYS:HD3	2.53	0.49
6:F:121:CYS:SG	6:F:130:ILE:HG21	2.52	0.48
6:L:318:CYS:SG	6:L:321:THR:N	2.86	0.48
1:M:175:TYR:OH	1:M:450:LEU:O	2.28	0.48
3:U:201:GLY:HA3	3:U:204:MET:HE2	1.95	0.48
2:Z:71:ILE:C	2:Z:424:LYS:HZ2	2.21	0.48
2:Z:277:ASN:HA	2:Z:280:ALA:O	2.13	0.48
5:c:18:CYS:HB2	5:c:67:CYS:HB2	1.94	0.48
3:m:201:GLY:CA	3:m:204:MET:HE2	2.43	0.48
1:M:356:ARG:NH1	1:M:415:GLU:OE2	2.45	0.48
3:O:174:LYS:HA	3:O:193:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:117:MET:HB3	4:P:118:PRO:HD3	1.94	0.48
2:T:22:LYS:NZ	5:W:49:GLU:OE1	2.37	0.48
2:T:154:MET:HG2	2:T:161:MET:CE	2.43	0.48
2:T:369:ARG:NH2	2:T:374:GLU:OE2	2.47	0.48
6:p:277:CYS:HB2	6:p:314:CYS:HB2	1.95	0.48
1:G:4:ILE:HG23	1:G:6:LYS:HE3	1.95	0.48
6:L:293:LYS:HE3	6:L:296:GLU:OE1	2.12	0.48
6:d:200:CYS:SG	6:d:201:LYS:N	2.87	0.48
1:e:551:TYR:HB3	1:e:552:PRO:HD3	1.95	0.48
13:l:504:MGD:O1B	4:n:101:LYS:NZ	2.41	0.48
3:m:204:MET:SD	3:m:256:GLY:HA3	2.52	0.48
6:L:281:CYS:SG	6:L:284:ASN:N	2.87	0.48
1:Y:443:ARG:NH2	1:Y:470:TYR:OH	2.41	0.48
2:B:57:ARG:C	2:B:58:LYS:HD2	2.39	0.48
4:D:110:THR:OG1	4:D:112:GLU:OE2	2.30	0.48
1:M:318:THR:HG22	1:M:324:GLU:OE1	2.13	0.48
6:R:15:GLU:HB2	6:R:23:ARG:NH2	2.28	0.48
6:X:41:CYS:SG	6:X:44:SER:N	2.87	0.48
6:X:135:GLU:HB2	6:X:229:THR:CG2	2.42	0.48
1:k:443:ARG:NH2	1:k:470:TYR:OH	2.44	0.48
2:l:159:ARG:O	2:l:163:ARG:HG3	2.14	0.48
6:p:261:GLU:HB2	6:p:329:ARG:HB3	1.95	0.48
1:q:4:ILE:HG12	1:q:35:VAL:HG21	1.95	0.48
1:q:356:ARG:HG3	1:q:356:ARG:NH2	2.28	0.48
1:q:417:HIS:C	1:q:419:TRP:N	2.71	0.48
6:F:264:LEU:N	6:F:305:GLU:OE1	2.47	0.48
3:O:225:LEU:HD11	3:O:246:GLU:HB2	1.96	0.48
3:U:160:ASN:OD1	3:U:178:ASN:HB3	2.13	0.48
6:X:37:CYS:SG	6:X:38:GLY:N	2.87	0.48
1:S:231:HIS:CE1	1:S:235:LEU:HD13	2.48	0.48
6:d:242:CYS:SG	6:d:244:TRP:HD1	2.37	0.48
5:o:12:CYS:SG	5:o:52:VAL:HA	2.53	0.48
1:q:5:ILE:HG13	1:q:42:ILE:HB	1.95	0.48
1:A:425:THR:O	1:A:428:THR:OG1	2.31	0.48
1:G:293:ALA:HA	1:G:374:ILE:HD11	1.96	0.48
13:H:503:MGD:S13	4:J:9:ARG:NH1	2.82	0.48
3:I:106:LYS:HG2	17:I:401:HOH:O	2.14	0.48
1:S:473:ASN:HB3	1:S:476:THR:OG1	2.14	0.48
3:U:127:GLU:HG3	3:U:153:THR:HB	1.96	0.48
6:p:336:ARG:CG	6:p:336:ARG:NH1	2.75	0.48
5:E:80:GLU:OE1	5:E:81:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:334:PRO:HB2	6:F:336:ARG:NH2	2.29	0.48
4:V:117:MET:HB3	4:V:118:PRO:HD3	1.95	0.48
6:X:204:CYS:SG	6:X:207:ASP:N	2.87	0.48
6:X:242:CYS:SG	6:X:244:TRP:HD1	2.37	0.48
6:j:210:MET:HG2	6:p:221:TYR:CE1	2.49	0.48
1:k:180:VAL:HA	1:k:231:HIS:HB3	1.95	0.48
4:t:1:MET:HG2	4:t:43:LEU:HD11	1.96	0.48
6:v:21:ASN:O	6:v:23:ARG:NH2	2.47	0.48
6:L:121:CYS:SG	6:L:130:ILE:HG21	2.54	0.48
1:Y:222:LEU:C	1:Y:567:VAL:HG23	2.39	0.48
3:g:40:MET:HE3	3:g:42:GLY:O	2.14	0.48
1:k:235:LEU:HD22	1:k:323:MET:HE2	1.95	0.48
6:v:21:ASN:ND2	6:v:23:ARG:CZ	2.77	0.48
1:A:318:THR:HG23	1:A:320:ASP:H	1.78	0.47
3:U:68:ILE:HD12	3:U:91:ARG:NH2	2.29	0.47
6:d:263:GLU:HG3	6:d:326:LYS:HB2	1.96	0.47
6:j:242:CYS:O	6:j:307:PHE:HA	2.14	0.47
6:j:242:CYS:SG	6:j:244:TRP:HD1	2.36	0.47
2:r:255:GLY:O	2:r:259:SER:OG	2.26	0.47
6:v:10:LYS:O	6:v:62:SER:OG	2.32	0.47
6:F:204:CYS:SG	6:F:207:ASP:N	2.87	0.47
2:H:344:ASP:OD1	2:H:372:THR:OG1	2.23	0.47
1:Y:439:ALA:O	1:Y:443:ARG:HB2	2.14	0.47
6:j:50:PRO:O	6:j:54:MET:HG2	2.13	0.47
1:q:419:TRP:CZ3	1:q:423:LYS:NZ	2.81	0.47
1:q:496:VAL:HB	1:q:504:VAL:HB	1.94	0.47
2:r:338:MET:HE1	2:r:357:MET:HG2	1.95	0.47
6:v:164:CYS:SG	6:v:168:ALA:N	2.77	0.47
1:A:170:ARG:NH2	1:A:521:ASP:OD1	2.32	0.47
3:C:225:LEU:HD12	3:C:244:LYS:HE2	1.96	0.47
6:F:49:ASN:OD1	6:F:61:LYS:HD2	2.14	0.47
3:I:189:LEU:HD22	3:I:234:ASP:HB2	1.96	0.47
1:M:526:GLU:HG3	1:M:527:SER:N	2.28	0.47
1:S:472:ILE:HD13	1:S:486:ILE:HD13	1.95	0.47
6:X:37:CYS:HB2	6:X:77:CYS:HB2	1.95	0.47
1:Y:551:TYR:HB3	1:Y:552:PRO:HD3	1.96	0.47
3:a:83:MET:HE1	3:a:107:ILE:CG1	2.44	0.47
6:j:31:CYS:SG	6:j:63:LYS:HD3	2.55	0.47
2:l:223:LEU:HD12	3:m:222:PHE:O	2.15	0.47
2:r:55:LEU:HD22	2:r:64:GLU:HG2	1.96	0.47
3:s:40:MET:SD	3:s:45:VAL:HG22	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:u:18:CYS:SG	5:u:19:VAL:N	2.87	0.47
6:L:200:CYS:SG	6:L:209:ILE:HG21	2.54	0.47
1:M:434:THR:O	1:M:438:ILE:HG23	2.14	0.47
5:o:69:GLU:CD	6:p:56:ARG:HE	2.21	0.47
1:M:111:THR:OG1	1:M:456:LYS:HE2	2.15	0.47
1:S:148:PHE:CE2	1:S:536:VAL:HG22	2.49	0.47
1:Y:64:LYS:HE2	1:Y:318:THR:C	2.39	0.47
2:Z:288:ARG:HG2	2:Z:396:MET:HB2	1.97	0.47
1:e:235:LEU:HD12	1:e:275:HIS:CE1	2.49	0.47
6:j:16:ARG:NH1	6:j:22:ARG:HG3	2.29	0.47
6:j:277:CYS:SG	6:j:286:LEU:HD13	2.54	0.47
1:k:141:PRO:HG2	1:k:169:LEU:HD23	1.95	0.47
6:v:160:CYS:SG	6:v:161:GLU:N	2.87	0.47
6:v:249:CYS:SG	6:v:252:ASP:N	2.88	0.47
1:A:1:MET:HG2	1:A:3:TYR:CE2	2.50	0.47
4:D:32:ILE:HD12	4:D:65:VAL:HG21	1.96	0.47
5:E:12:CYS:SG	5:E:52:VAL:HA	2.55	0.47
6:F:212:VAL:HG11	6:R:218:TYR:CE1	2.49	0.47
4:V:11:ILE:HG12	5:W:13:HIS:CE1	2.50	0.47
3:a:229:LYS:HD2	6:j:232:SER:O	2.15	0.47
1:e:167:TRP:CD1	1:e:533:LEU:HD21	2.49	0.47
2:l:1:MET:SD	2:l:22:LYS:HB3	2.55	0.47
2:l:56:ILE:HD13	2:l:73:LYS:HD2	1.97	0.47
2:l:75:ALA:HB2	2:l:421:LEU:CD2	2.44	0.47
4:n:10:THR:HG22	4:n:12:TRP:N	2.28	0.47
6:p:121:CYS:SG	6:p:122:GLU:N	2.87	0.47
5:u:47:ILE:HD13	5:u:49:GLU:HB2	1.95	0.47
2:B:385:VAL:HG23	13:B:503:MGD:O6	2.15	0.47
1:G:231:HIS:CE1	1:G:235:LEU:HD13	2.50	0.47
2:N:141:ASN:HD22	2:N:170:PHE:N	2.09	0.47
6:R:38:GLY:HA2	6:R:46:ILE:HB	1.96	0.47
6:X:50:PRO:O	6:X:54:MET:HG2	2.15	0.47
6:d:13:THR:HG23	6:d:25:ILE:HG13	1.97	0.47
6:d:31:CYS:SG	6:d:63:LYS:HD3	2.55	0.47
6:d:37:CYS:SG	6:d:38:GLY:N	2.87	0.47
2:f:165:VAL:O	2:f:179:ARG:NH1	2.48	0.47
2:f:347:ALA:HB2	2:f:371:PRO:HG2	1.97	0.47
1:k:175:TYR:HA	1:k:520:VAL:HG13	1.95	0.47
6:p:242:CYS:O	6:p:307:PHE:HA	2.14	0.47
6:v:281:CYS:SG	6:v:284:ASN:N	2.88	0.47
6:F:37:CYS:HB2	6:F:77:CYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:82:PRO:O	4:J:86:ARG:HG2	2.15	0.47
6:L:5:GLU:HB2	6:L:68:GLU:HG3	1.97	0.47
1:M:103:ARG:HA	1:M:106:GLN:HG3	1.97	0.47
6:X:125:CYS:SG	6:X:128:ASP:N	2.87	0.47
1:Y:162:ALA:HB3	1:Y:221:LYS:HE2	1.96	0.47
1:Y:415:GLU:C	1:Y:415:GLU:CD	2.83	0.47
6:j:212:VAL:HG21	6:p:218:TYR:CE1	2.49	0.47
2:B:375:MET:O	4:D:126:LYS:HE3	2.14	0.47
6:R:277:CYS:SG	6:R:286:LEU:HD13	2.55	0.47
1:S:540:PHE:HA	1:S:544:TYR:HB2	1.95	0.47
4:n:42:GLN:HA	4:t:41:LYS:HD3	1.97	0.47
6:p:37:CYS:HB2	6:p:77:CYS:HB2	1.96	0.47
6:p:169:ILE:HG12	6:p:189:VAL:HG22	1.97	0.47
3:s:62:PRO:O	3:s:65:ILE:HG22	2.15	0.47
4:t:11:ILE:C	4:t:11:ILE:CD1	2.87	0.47
5:E:67:CYS:SG	5:E:68:VAL:N	2.87	0.47
2:N:371:PRO:HB3	4:P:121:MET:SD	2.55	0.47
6:R:37:CYS:SG	6:R:38:GLY:N	2.88	0.47
1:S:410:ASN:OD1	6:p:20:GLU:HB2	2.15	0.47
5:W:12:CYS:SG	5:W:52:VAL:HA	2.54	0.47
5:W:76:ILE:C	5:W:77:ARG:HG2	2.40	0.47
1:Y:207:THR:OG1	1:Y:210:GLU:HG3	2.14	0.47
2:Z:358:ALA:O	4:b:127:VAL:HG22	2.15	0.47
5:i:71:CYS:SG	5:i:74:ASP:N	2.88	0.47
1:k:2:GLU:HG3	1:k:27:LYS:CD	2.45	0.47
1:k:551:TYR:HB3	1:k:552:PRO:HD3	1.96	0.47
2:B:344:ASP:OD1	2:B:372:THR:OG1	2.20	0.46
2:Z:159:ARG:O	2:Z:163:ARG:HG3	2.14	0.46
3:a:59:ALA:HB3	3:a:65:ILE:HG13	1.97	0.46
1:e:411:LEU:O	1:e:416:LEU:HB2	2.15	0.46
1:q:422:ARG:HD2	1:q:422:ARG:O	2.14	0.46
3:s:233:VAL:CG2	3:s:238:LEU:HD21	2.46	0.46
1:G:3:TYR:CE1	1:G:40:LYS:HD2	2.51	0.46
2:H:68:ASP:OD1	2:H:68:ASP:N	2.48	0.46
3:I:204:MET:SD	3:I:256:GLY:HA3	2.55	0.46
1:M:502:ILE:HG21	1:M:505:LYS:HE2	1.98	0.46
1:M:551:TYR:HB3	1:M:552:PRO:HD3	1.97	0.46
1:S:115:ALA:HA	1:S:140:TYR:CD2	2.50	0.46
1:Y:159:ASP:HA	1:Y:221:LYS:NZ	2.30	0.46
6:d:160:CYS:SG	6:d:169:ILE:HD13	2.56	0.46
4:h:53:VAL:HB	4:h:60:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:52:LYS:HD2	4:J:61:VAL:HG22	1.97	0.46
5:K:44:ILE:HD11	5:K:47:ILE:HG22	1.96	0.46
1:M:505:LYS:HE3	1:M:505:LYS:HB2	1.69	0.46
2:N:182:ILE:HG12	2:N:197:ILE:HB	1.97	0.46
2:N:375:MET:O	4:P:126:LYS:HE3	2.15	0.46
3:O:160:ASN:OD1	3:O:178:ASN:HB3	2.15	0.46
1:Y:523:GLN:HE22	1:Y:568:MET:CE	2.28	0.46
3:a:232:GLU:HG2	3:a:232:GLU:O	2.14	0.46
4:b:52:LYS:HE3	4:b:112:GLU:OE2	2.15	0.46
2:f:395:ARG:NH2	2:f:397:GLU:OE2	2.46	0.46
3:g:63:GLU:CD	3:g:63:GLU:N	2.69	0.46
2:r:39:HIS:O	2:r:43:VAL:HG22	2.15	0.46
5:u:12:CYS:SG	5:u:52:VAL:HA	2.56	0.46
2:H:11:PHE:CE2	2:H:37:ILE:HG21	2.50	0.46
3:I:182:GLY:HA3	3:I:209:ILE:HD11	1.97	0.46
4:J:117:MET:HB3	4:J:118:PRO:HD3	1.97	0.46
6:L:164:CYS:SG	6:L:168:ALA:N	2.78	0.46
1:M:2:GLU:HG2	1:M:27:LYS:CB	2.44	0.46
6:R:23:ARG:O	6:R:88:LEU:HA	2.14	0.46
6:R:315:GLU:HA	6:R:323:ILE:HG23	1.96	0.46
1:q:81:GLU:OE2	1:q:103:ARG:NH1	2.48	0.46
1:M:99:MET:O	1:M:103:ARG:HG3	2.14	0.46
1:S:235:LEU:HD22	1:S:323:MET:HE2	1.97	0.46
2:f:118:CYS:SG	14:f:505:H2S:S	3.13	0.46
6:j:10:LYS:HZ2	6:j:60:GLU:HA	1.80	0.46
2:l:347:ALA:HB2	2:l:371:PRO:HG2	1.96	0.46
6:v:200:CYS:SG	6:v:209:ILE:HG21	2.56	0.46
1:A:272:VAL:HG23	1:A:370:LEU:HD13	1.96	0.46
1:G:2:GLU:CG	1:G:27:LYS:HD2	2.45	0.46
1:M:398:VAL:O	1:M:402:LEU:HG	2.15	0.46
4:P:1:MET:HE2	4:P:43:LEU:HD13	1.96	0.46
5:Q:18:CYS:SG	5:Q:19:VAL:N	2.88	0.46
4:b:10:THR:HG22	4:b:12:TRP:N	2.31	0.46
6:d:277:CYS:HB2	6:d:314:CYS:HB2	1.97	0.46
2:B:327:ASN:O	2:B:331:GLN:HG3	2.15	0.46
5:Q:78:LEU:HD12	6:R:57:THR:HG21	1.98	0.46
6:R:43:VAL:HG13	6:R:45:ALA:HB2	1.97	0.46
5:c:3:ILE:O	5:c:63:LYS:NZ	2.36	0.46
6:d:293:LYS:HB2	6:d:296:GLU:HG3	1.98	0.46
6:j:160:CYS:SG	6:j:169:ILE:HD13	2.56	0.46
3:s:231:ILE:CD1	3:s:238:LEU:HD23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLY:O	17:A:701:HOH:O	2.20	0.46
1:A:111:THR:HG22	1:A:113:MET:HE3	1.98	0.46
1:G:217:GLU:HG3	1:G:254:ILE:HD13	1.97	0.46
2:H:86:MET:HE3	2:H:339:MET:HE1	1.98	0.46
1:M:502:ILE:HG21	1:M:505:LYS:HE3	1.97	0.46
3:O:210:VAL:HG11	3:O:238:LEU:CD2	2.46	0.46
6:R:50:PRO:O	6:R:54:MET:HG2	2.16	0.46
6:R:271:CYS:SG	6:R:300:LYS:HD2	2.56	0.46
6:d:103:LYS:H	6:d:333:THR:HG21	1.75	0.46
6:j:6:VAL:HG13	6:j:13:THR:HB	1.98	0.46
6:j:104:ILE:HG23	6:j:259:PRO:HB3	1.98	0.46
6:j:214:ARG:HD2	6:p:218:TYR:OH	2.16	0.46
6:p:56:ARG:NE	6:p:279:MET:HE1	2.31	0.46
2:r:54:PRO:O	2:r:55:LEU:HD23	2.15	0.46
1:A:115:ALA:HA	1:A:140:TYR:CD2	2.51	0.46
2:T:11:PHE:CE2	2:T:37:ILE:HG21	2.51	0.46
2:T:36:ARG:NH1	5:W:12:CYS:O	2.49	0.46
4:b:38:GLU:CD	4:b:38:GLU:N	2.73	0.46
6:d:144:THR:HG21	6:d:222:GLU:CG	2.44	0.46
1:q:189:GLY:O	2:r:281:LYS:HD3	2.16	0.46
3:s:162:ILE:CD1	3:s:190:ILE:HD13	2.44	0.46
6:v:242:CYS:O	6:v:307:PHE:HA	2.16	0.46
1:A:33:GLU:HG2	1:A:34:SER:N	2.31	0.46
2:B:50:ARG:O	2:B:52:LYS:HD2	2.15	0.46
2:B:68:ASP:OD1	2:B:68:ASP:N	2.49	0.46
3:C:32:GLU:HA	3:C:35:LYS:CD	2.46	0.46
4:D:34:GLN:HB2	4:D:77:TYR:HB3	1.96	0.46
1:M:71:TYR:HA	2:N:127:GLN:HG2	1.97	0.46
4:V:55:SER:HB3	4:V:105:VAL:HG12	1.97	0.46
2:Z:270:ILE:HG12	2:Z:284:LEU:HD21	1.98	0.46
2:f:253:GLY:O	2:f:256:ILE:HG22	2.16	0.46
4:h:82:PRO:O	4:h:86:ARG:HG2	2.16	0.46
1:k:6:LYS:HZ1	1:k:23:ASP:CG	2.23	0.46
5:o:54:ASN:OD1	5:o:56:LYS:HE2	2.16	0.46
3:C:57:GLU:HG2	3:C:58:PRO:O	2.15	0.45
1:G:310:THR:HB	1:G:394:ARG:HD2	1.98	0.45
1:G:505:LYS:HB2	1:G:510:VAL:HG11	1.97	0.45
3:I:143:ASP:OD1	3:I:144:TRP:N	2.49	0.45
6:L:217:PRO:HG3	6:X:217:PRO:HG3	1.97	0.45
6:L:315:GLU:OE2	6:L:325:VAL:N	2.48	0.45
1:S:411:LEU:O	1:S:416:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:159:ASP:OD1	1:Y:221:LYS:NZ	2.49	0.45
3:g:29:LYS:HB2	3:g:34:ILE:HD11	1.98	0.45
1:k:14:LEU:HD22	1:k:14:LEU:H	1.81	0.45
1:q:356:ARG:HE	1:q:415:GLU:CG	2.29	0.45
2:r:58:LYS:NZ	2:r:61:GLU:O	2.49	0.45
6:v:23:ARG:NH1	6:v:92:GLY:HA2	2.31	0.45
2:B:53:LYS:N	2:B:53:LYS:CD	2.79	0.45
6:L:204:CYS:SG	6:L:207:ASP:N	2.90	0.45
1:Y:231:HIS:ND1	1:Y:271:HIS:CE1	2.84	0.45
1:e:50:MET:HE2	1:e:439:ALA:HB2	1.98	0.45
6:j:91:ASP:N	6:j:92:GLY:HA2	2.31	0.45
4:n:117:MET:HB3	4:n:118:PRO:HD3	1.99	0.45
2:B:277:ASN:HA	2:B:280:ALA:O	2.15	0.45
6:F:242:CYS:SG	6:F:244:TRP:HD1	2.39	0.45
4:P:10:THR:HG22	4:P:12:TRP:N	2.30	0.45
6:R:87:ASP:OD2	6:R:94:SER:OG	2.34	0.45
1:Y:17:VAL:HA	1:Y:20:GLU:OE1	2.16	0.45
2:Z:238:ALA:O	2:Z:242:LEU:HG	2.16	0.45
3:g:170:LYS:HZ1	3:g:191:ILE:CG1	2.28	0.45
3:m:225:LEU:HD11	3:m:246:GLU:HB2	1.98	0.45
1:q:358:PRO:HB3	1:q:419:TRP:CD2	2.51	0.45
2:r:93:GLU:HB3	2:r:385:VAL:HG11	1.98	0.45
3:s:34:ILE:HD11	3:s:54:VAL:HG21	1.97	0.45
2:B:84:PRO:HG2	2:B:109:ALA:HB2	1.97	0.45
6:F:160:CYS:SG	6:F:161:GLU:N	2.89	0.45
6:L:102:PRO:HG2	6:L:340:TRP:CE3	2.52	0.45
1:M:235:LEU:HD11	8:M:603:MFN:H11A	1.98	0.45
3:O:3:GLU:HG2	3:O:66:LYS:HD3	1.98	0.45
2:T:73:LYS:HG2	2:T:73:LYS:H	1.56	0.45
2:Z:23:VAL:HG22	2:Z:28:ILE:CD1	2.47	0.45
6:d:68:GLU:H	6:d:68:GLU:CD	2.24	0.45
1:e:115:ALA:HA	1:e:140:TYR:CD2	2.52	0.45
6:p:204:CYS:SG	6:p:207:ASP:N	2.90	0.45
1:q:422:ARG:NH2	1:q:423:LYS:CE	2.64	0.45
6:v:21:ASN:HD22	6:v:23:ARG:CZ	2.27	0.45
1:A:309:ILE:HD13	1:A:309:ILE:HA	1.80	0.45
2:B:320:ASN:HB2	2:B:323:GLU:HB3	1.99	0.45
1:G:411:LEU:O	1:G:416:LEU:HB2	2.15	0.45
1:G:514:HIS:HB2	1:G:560:LYS:HZ2	1.79	0.45
1:S:48:ILE:HD12	1:S:472:ILE:HG23	1.97	0.45
2:Z:71:ILE:HG22	2:Z:424:LYS:HZ3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:67:CYS:SG	5:i:68:VAL:N	2.89	0.45
6:j:145:GLY:HA2	6:j:214:ARG:CG	2.47	0.45
6:j:164:CYS:SG	6:j:168:ALA:N	2.80	0.45
2:l:346:GLY:HA2	2:l:354:LEU:CD2	2.47	0.45
2:r:22:LYS:NZ	5:u:49:GLU:OE1	2.45	0.45
6:v:258:LYS:NZ	6:v:306:ARG:O	2.39	0.45
6:v:290:LYS:HG3	6:v:291:PRO:HD2	1.99	0.45
2:H:58:LYS:HZ2	2:H:63:VAL:HG11	1.80	0.45
4:J:1:MET:HE3	4:J:42:GLN:HG2	1.98	0.45
1:M:369:GLU:OE2	1:M:425:THR:HG22	2.16	0.45
3:O:189:LEU:HD13	3:O:233:VAL:HG11	1.98	0.45
1:S:148:PHE:HE2	1:S:536:VAL:HA	1.81	0.45
3:U:25:VAL:O	3:U:29:LYS:NZ	2.36	0.45
6:X:31:CYS:SG	6:X:63:LYS:HD3	2.56	0.45
3:a:160:ASN:OD1	3:a:178:ASN:HB3	2.16	0.45
1:e:289:ALA:HB2	1:e:366:ILE:HG23	1.99	0.45
5:o:80:GLU:HG2	6:p:61:LYS:HZ1	1.82	0.45
6:p:157:CYS:HB2	6:v:118:CYS:HA	1.99	0.45
6:p:224:LYS:HD3	6:p:225:THR:N	2.32	0.45
2:H:89:TRP:CH2	2:H:100:GLY:HA3	2.51	0.45
1:M:502:ILE:HD13	1:M:505:LYS:HE2	1.99	0.45
6:R:41:CYS:SG	6:R:43:VAL:HG12	2.56	0.45
6:R:200:CYS:SG	6:R:209:ILE:HG21	2.56	0.45
2:f:371:PRO:HB3	4:h:121:MET:SD	2.56	0.45
1:A:7:ASN:CB	1:A:21:LYS:HE3	2.46	0.45
1:M:82:LYS:HD3	1:M:88:ALA:HB2	1.98	0.45
3:O:238:LEU:HA	3:O:239:PRO:HD3	1.88	0.45
2:T:154:MET:HE3	2:T:161:MET:HE3	1.98	0.45
3:a:44:GLU:HG2	3:a:46:VAL:HG13	1.98	0.45
1:e:241:TYR:CD1	1:e:288:GLU:HG3	2.51	0.45
5:i:80:GLU:O	5:i:81:LEU:HG	2.17	0.45
1:q:505:LYS:HD2	1:q:510:VAL:HG11	1.98	0.45
3:s:20:ASN:O	3:s:25:VAL:HG11	2.17	0.45
4:t:61:VAL:HG12	4:t:114:VAL:HG12	1.99	0.45
1:A:191:GLY:N	2:B:281:LYS:HG3	2.32	0.45
2:B:361:PRO:HA	2:B:377:ASP:OD2	2.17	0.45
1:G:124:HIS:HE1	1:G:128:GLU:OE2	2.00	0.45
1:M:14:LEU:HD13	1:M:458:HIS:HB3	1.99	0.45
6:X:16:ARG:HH21	6:X:22:ARG:CG	2.25	0.45
2:Z:149:TRP:O	2:Z:252:PHE:HA	2.17	0.45
3:m:48:LEU:HD23	3:m:52:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:TYR:CZ	1:G:40:LYS:HD2	2.52	0.45
3:I:66:LYS:HG2	3:I:68:ILE:HD11	1.98	0.45
4:J:78:ILE:HG22	4:J:84:ALA:HB2	1.99	0.45
1:S:505:LYS:C	1:S:505:LYS:HD3	2.42	0.45
2:Z:75:ALA:HB1	2:Z:425:VAL:CG2	2.47	0.45
6:j:121:CYS:SG	6:j:122:GLU:N	2.90	0.45
1:q:207:THR:OG1	1:q:210:GLU:HG3	2.17	0.45
2:r:88:GLY:HA3	2:r:341:ILE:O	2.17	0.45
2:B:358:ALA:HA	4:D:126:LYS:HD3	1.98	0.44
1:G:282:TRP:HB3	8:G:603:MFN:O6	2.17	0.44
1:S:4:ILE:HG13	1:S:6:LYS:HG2	1.98	0.44
5:c:12:CYS:SG	5:c:52:VAL:HA	2.56	0.44
1:e:158:VAL:CG1	1:e:221:LYS:NZ	2.80	0.44
6:j:148:GLU:O	6:j:148:GLU:HG3	2.16	0.44
1:q:411:LEU:HG	1:q:416:LEU:HG	1.98	0.44
2:r:68:ASP:OD1	2:r:68:ASP:N	2.50	0.44
2:r:232:ARG:HA	2:r:235:ILE:HG12	1.98	0.44
1:G:316:THR:OG1	1:G:324:GLU:OE1	2.27	0.44
1:M:64:LYS:HG2	1:M:317:MET:HB2	2.00	0.44
2:Z:55:LEU:CD2	2:Z:64:GLU:HG2	2.47	0.44
2:f:324:THR:HG22	2:f:324:THR:O	2.16	0.44
6:v:23:ARG:NH1	6:v:92:GLY:CA	2.80	0.44
1:G:4:ILE:HG22	1:G:40:LYS:O	2.17	0.44
1:G:448:LYS:HA	1:G:453:SER:OG	2.17	0.44
2:H:2:GLU:HB2	2:H:23:VAL:HG13	1.98	0.44
2:H:55:LEU:HD23	2:H:64:GLU:HA	2.00	0.44
2:Z:16:CYS:SG	2:Z:163:ARG:NH1	2.91	0.44
1:e:107:MET:HE1	1:e:393:THR:HA	2.00	0.44
2:f:20:ILE:HB	2:f:32:ILE:HB	1.99	0.44
2:f:68:ASP:N	2:f:68:ASP:OD1	2.50	0.44
1:k:2:GLU:HG3	1:k:27:LYS:HE2	1.98	0.44
6:v:263:GLU:HB2	6:v:326:LYS:HB2	1.98	0.44
6:X:277:CYS:HB2	6:X:314:CYS:HB2	1.98	0.44
6:X:334:PRO:CB	6:X:336:ARG:HH12	2.28	0.44
2:Z:28:ILE:HD11	2:Z:407:VAL:HG13	1.98	0.44
6:d:110:ILE:HG13	6:d:234:ILE:HD11	2.00	0.44
1:e:456:LYS:HE2	1:e:518:TYR:OH	2.17	0.44
1:k:107:MET:HE3	1:k:109:TYR:CD1	2.53	0.44
1:k:434:THR:CG2	1:k:437:GLU:HG3	2.48	0.44
4:D:117:MET:HB3	4:D:118:PRO:HD3	1.99	0.44
6:F:71:CYS:SG	6:F:73:LEU:HG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:344:THR:OG1	1:M:345:GLY:N	2.50	0.44
6:R:277:CYS:SG	6:R:278:VAL:N	2.90	0.44
1:e:496:VAL:HB	1:e:504:VAL:HB	1.99	0.44
2:f:11:PHE:CE2	2:f:37:ILE:HG21	2.53	0.44
5:i:46:MET:HE1	11:i:102:SF4:S1	2.58	0.44
1:k:219:ASN:OD1	1:k:224:LEU:HD12	2.18	0.44
1:q:71:TYR:HA	2:r:127:GLN:HG2	1.99	0.44
1:q:417:HIS:C	1:q:419:TRP:H	2.25	0.44
6:v:160:CYS:SG	6:v:169:ILE:HD13	2.58	0.44
6:v:160:CYS:HB2	6:v:200:CYS:HB2	1.99	0.44
2:B:58:LYS:C	2:B:60:GLY:H	2.25	0.44
1:G:64:LYS:HG2	1:G:317:MET:HB2	1.98	0.44
1:M:75:ASP:O	1:M:78:ARG:HG2	2.18	0.44
2:N:292:ASN:OD1	2:N:295:GLY:HA3	2.18	0.44
6:R:277:CYS:HB2	6:R:314:CYS:HB2	1.98	0.44
3:U:81:GLN:HG2	3:U:82:GLU:HG3	1.99	0.44
6:X:277:CYS:SG	6:X:278:VAL:N	2.91	0.44
2:l:277:ASN:HA	2:l:280:ALA:O	2.17	0.44
1:q:64:LYS:HG2	1:q:317:MET:HB2	1.99	0.44
6:v:318:CYS:SG	6:v:321:THR:N	2.91	0.44
4:D:78:ILE:HG22	4:D:84:ALA:HB2	1.99	0.44
2:H:110:VAL:HG22	2:H:311:ASP:HA	2.00	0.44
4:J:22:ASP:OD1	4:J:22:ASP:N	2.48	0.44
6:L:245:CYS:SG	6:L:246:GLN:N	2.90	0.44
1:M:2:GLU:HG2	1:M:27:LYS:HA	1.98	0.44
2:N:15:LEU:HD23	2:N:401:ILE:HD12	1.99	0.44
2:T:210:LEU:HD13	2:T:268:THR:HG23	2.00	0.44
2:Z:174:ARG:HH21	6:d:300:LYS:C	2.26	0.44
1:e:336:ALA:HB3	1:e:348:VAL:HB	1.98	0.44
1:k:103:ARG:O	1:k:107:MET:HG2	2.16	0.44
1:k:221:LYS:O	1:k:567:VAL:HG21	2.17	0.44
4:n:9:ARG:NE	4:n:80:MET:SD	2.91	0.44
1:A:71:TYR:HA	2:B:127:GLN:HG2	2.00	0.44
1:A:386:SER:HA	1:A:387:PRO:HA	1.83	0.44
1:G:443:ARG:NH2	1:G:470:TYR:OH	2.49	0.44
1:M:537:GLU:HG2	1:M:541:LYS:HE3	1.99	0.44
2:N:5:LYS:HG2	2:N:20:ILE:HD12	1.99	0.44
1:Y:355:ALA:HB3	1:Y:415:GLU:CD	2.43	0.44
6:d:245:CYS:SG	6:d:246:GLN:N	2.91	0.44
2:f:157:HIS:CD2	2:f:287:MET:HE3	2.53	0.44
2:r:375:MET:O	4:t:126:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:v:121:CYS:SG	6:v:122:GLU:N	2.90	0.44
2:B:167:ALA:O	2:B:179:ARG:NH2	2.47	0.44
1:G:57:HIS:CE1	1:G:115:ALA:HB1	2.53	0.44
1:G:231:HIS:C	1:G:231:HIS:CD2	2.96	0.44
1:M:124:HIS:NE2	1:M:128:GLU:OE2	2.51	0.44
1:M:496:VAL:HB	1:M:504:VAL:HB	1.99	0.44
2:T:176:ARG:HH22	2:T:196:ASP:CG	2.26	0.44
6:X:160:CYS:SG	6:X:161:GLU:N	2.91	0.44
2:Z:82:LYS:HD2	3:a:44:GLU:OE1	2.17	0.44
5:i:12:CYS:SG	5:i:52:VAL:HA	2.57	0.44
5:o:12:CYS:SG	5:o:14:GLY:N	2.87	0.44
1:q:154:LYS:HA	1:q:154:LYS:HD2	1.91	0.44
3:s:88:ILE:C	3:s:89:ILE:HD12	2.43	0.44
5:E:25:ASN:HB3	5:E:32:VAL:HG11	1.99	0.43
6:F:95:ILE:HG13	6:F:96:LYS:HD3	1.99	0.43
1:G:244:THR:OG1	1:G:275:HIS:HB3	2.16	0.43
1:G:280:THR:HG22	1:G:284:ASP:OD2	2.18	0.43
5:K:18:CYS:HB2	5:K:67:CYS:HB2	2.00	0.43
1:Y:496:VAL:HB	1:Y:504:VAL:HB	2.00	0.43
1:k:14:LEU:HD22	1:k:14:LEU:N	2.32	0.43
1:q:377:PRO:HB2	1:q:440:GLN:HG2	1.99	0.43
3:C:16:LEU:HD23	3:C:41:HIS:HB2	2.00	0.43
1:G:3:TYR:CD1	1:G:40:LYS:HB2	2.51	0.43
5:K:5:LEU:HD21	5:K:76:ILE:HD11	2.00	0.43
2:T:333:ARG:NH1	2:T:359:GLU:OE1	2.49	0.43
6:X:277:CYS:SG	6:X:286:LEU:HD13	2.58	0.43
1:k:166:SER:HA	1:k:522:THR:HG21	2.00	0.43
2:l:6:ASN:O	2:l:404:LYS:NZ	2.50	0.43
6:F:164:CYS:SG	6:F:168:ALA:N	2.83	0.43
2:H:342:ALA:HA	13:H:503:MGD:N3	2.33	0.43
1:M:376:ASN:ND2	1:M:378:GLU:H	2.16	0.43
4:b:55:SER:HB3	4:b:105:VAL:HG12	2.00	0.43
1:q:408:ARG:O	1:q:412:ILE:HG13	2.17	0.43
1:q:424:SER:OG	1:q:426:VAL:HG22	2.19	0.43
3:s:72:ASP:OD1	3:s:93:ASN:N	2.47	0.43
2:B:58:LYS:HD2	2:B:58:LYS:N	2.33	0.43
6:F:242:CYS:O	6:F:307:PHE:HA	2.18	0.43
5:K:23:PRO:HG2	6:L:319:PRO:HG2	2.01	0.43
6:L:242:CYS:O	6:L:307:PHE:HA	2.19	0.43
4:P:6:ASN:O	4:P:77:TYR:HA	2.18	0.43
6:R:31:CYS:SG	6:R:63:LYS:HD3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:102:PRO:HG2	6:R:340:TRP:CE3	2.53	0.43
1:S:88:ALA:HB1	2:T:317:PRO:HD3	2.00	0.43
4:V:6:ASN:O	4:V:77:TYR:HA	2.18	0.43
6:X:43:VAL:HG12	6:X:70:LYS:HB3	2.00	0.43
1:Y:286:VAL:HG22	1:Y:423:LYS:HB3	2.01	0.43
1:e:316:THR:HB	8:e:603:MFN:H5	2.00	0.43
2:f:13:GLY:O	2:f:395:ARG:HG3	2.18	0.43
3:g:230:ASP:HA	3:g:238:LEU:O	2.19	0.43
6:j:37:CYS:HB2	6:j:77:CYS:HB2	1.99	0.43
1:k:358:PRO:HG2	8:k:603:MFN:H141	2.00	0.43
1:q:502:ILE:HG21	1:q:505:LYS:HE3	2.01	0.43
3:O:11:GLN:HE22	3:O:76:THR:CG2	2.32	0.43
1:Y:71:TYR:HA	2:Z:127:GLN:HG2	2.01	0.43
4:h:108:ILE:HG22	4:h:109:PRO:O	2.19	0.43
6:p:258:LYS:NZ	6:p:306:ARG:O	2.39	0.43
2:r:49:MET:HG2	2:r:369:ARG:HB2	2.00	0.43
6:v:303:LYS:NZ	6:v:305:GLU:OE2	2.33	0.43
6:F:217:PRO:HG3	6:R:217:PRO:HG3	2.00	0.43
1:G:293:ALA:HB1	1:G:374:ILE:HG13	1.99	0.43
3:I:269:ALA:HA	3:I:270:PRO:HD3	1.69	0.43
2:N:74:ALA:HB1	2:N:363:ILE:HD13	2.01	0.43
2:N:174:ARG:NH2	6:R:298:THR:OG1	2.51	0.43
1:S:103:ARG:O	1:S:107:MET:HG2	2.18	0.43
2:T:68:ASP:N	2:T:68:ASP:OD1	2.52	0.43
2:T:149:TRP:O	2:T:252:PHE:HA	2.18	0.43
1:Y:469:VAL:HG22	1:Y:495:CYS:HB3	1.99	0.43
6:d:160:CYS:HB2	6:d:200:CYS:HB2	2.00	0.43
1:e:88:ALA:HB1	2:f:317:PRO:HD3	2.01	0.43
2:l:75:ALA:HB2	2:l:421:LEU:HD23	1.99	0.43
2:l:188:LYS:HD2	2:l:193:LYS:HG3	1.99	0.43
3:m:231:ILE:HG22	3:m:233:VAL:HG23	1.99	0.43
5:o:23:PRO:HG2	6:p:319:PRO:HG2	2.00	0.43
2:r:428:TYR:N	2:r:428:TYR:CD2	2.86	0.43
1:M:323:MET:HE3	1:M:323:MET:HB3	1.96	0.43
1:S:231:HIS:CD2	1:S:231:HIS:C	2.96	0.43
5:W:25:ASN:HB3	5:W:32:VAL:HG11	2.00	0.43
6:X:88:LEU:HD23	6:X:89:GLN:N	2.33	0.43
6:j:37:CYS:SG	6:j:38:GLY:N	2.91	0.43
3:m:228:GLU:HB3	3:m:231:ILE:HD11	2.00	0.43
6:p:104:ILE:CG2	6:p:259:PRO:HB3	2.49	0.43
2:r:6:ASN:O	2:r:404:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:411:LEU:HG	1:G:416:LEU:HG	2.01	0.43
1:G:551:TYR:HB3	1:G:552:PRO:HD3	2.01	0.43
1:M:244:THR:OG1	1:M:275:HIS:HB3	2.19	0.43
1:S:84:LYS:HB2	1:S:84:LYS:HE2	1.92	0.43
1:S:151:GLU:O	1:S:155:GLU:HG2	2.19	0.43
2:Z:346:GLY:O	2:Z:354:LEU:HD21	2.19	0.43
2:f:211:ASP:OD1	3:g:221:GLY:N	2.52	0.43
1:k:231:HIS:NE2	1:k:235:LEU:HD13	2.34	0.43
4:n:54:ILE:HD13	4:n:59:ASP:HB2	2.00	0.43
1:q:219:ASN:OD1	1:q:224:LEU:HD12	2.18	0.43
4:t:22:ASP:OD1	4:t:22:ASP:N	2.50	0.43
1:A:180:VAL:HA	1:A:231:HIS:HB3	2.00	0.43
4:D:48:GLY:HA2	4:D:63:LYS:HD2	2.00	0.43
6:F:37:CYS:SG	6:F:38:GLY:N	2.91	0.43
5:K:18:CYS:SG	5:K:19:VAL:N	2.92	0.43
6:L:221:TYR:CE1	6:X:210:MET:HG2	2.54	0.43
1:M:4:ILE:HD13	1:M:35:VAL:CG2	2.48	0.43
4:P:78:ILE:HG22	4:P:84:ALA:HB2	1.99	0.43
4:V:78:ILE:HG22	4:V:84:ALA:HB2	2.01	0.43
1:Y:231:HIS:CE1	1:Y:235:LEU:HD13	2.54	0.43
2:Z:264:ARG:NH2	3:a:164:GLU:OE2	2.50	0.43
3:g:210:VAL:HG11	3:g:238:LEU:CD2	2.48	0.43
1:k:378:GLU:HA	1:k:445:THR:OG1	2.19	0.43
2:l:68:ASP:N	2:l:68:ASP:OD1	2.52	0.43
6:p:318:CYS:SG	6:p:321:THR:N	2.91	0.43
4:t:6:ASN:O	4:t:77:TYR:HA	2.19	0.43
2:B:89:TRP:CH2	2:B:100:GLY:HA3	2.54	0.43
3:C:48:LEU:HD23	3:C:52:PHE:HB2	2.01	0.43
2:H:149:TRP:O	2:H:252:PHE:HA	2.18	0.43
6:L:337:SER:O	6:L:341:LYS:HG3	2.19	0.43
3:U:16:LEU:HB2	3:U:76:THR:HG23	2.01	0.43
6:X:20:GLU:OE1	6:X:22:ARG:NE	2.50	0.43
3:a:201:GLY:CA	3:a:204:MET:HE2	2.49	0.43
2:f:206:ASP:CB	2:f:256:ILE:HD11	2.49	0.43
1:k:344:THR:OG1	1:k:345:GLY:N	2.52	0.43
5:u:67:CYS:SG	5:u:68:VAL:N	2.92	0.43
2:B:82:LYS:HE3	3:C:44:GLU:CD	2.44	0.42
6:F:213:CYS:SG	6:F:215:ILE:HD13	2.59	0.42
1:G:88:ALA:HB1	2:H:317:PRO:HD3	2.00	0.42
2:T:89:TRP:CH2	2:T:100:GLY:HA3	2.54	0.42
2:T:234:GLN:O	2:T:235:ILE:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:336:ARG:HD3	6:d:336:ARG:N	2.30	0.42
1:e:141:PRO:HD2	1:e:176:THR:O	2.19	0.42
3:m:61:ALA:HB3	3:m:64:ASP:OD1	2.18	0.42
3:s:121:MET:HG2	3:s:149:GLY:O	2.19	0.42
2:B:8:VAL:HA	2:B:17:ASP:HA	2.00	0.42
2:B:428:TYR:CD2	2:B:428:TYR:N	2.87	0.42
6:F:94:SER:OG	6:F:96:LYS:HG2	2.19	0.42
2:H:86:MET:SD	2:H:103:LEU:HD22	2.58	0.42
1:S:136:ASP:OD2	1:S:456:LYS:NZ	2.52	0.42
2:T:289:GLY:HA3	13:T:504:MGD:C13	2.49	0.42
1:Y:23:ASP:OD2	17:Y:701:HOH:O	2.20	0.42
2:Z:15:LEU:HD23	2:Z:401:ILE:HD12	2.02	0.42
3:a:23:PRO:HD2	3:a:83:MET:CG	2.48	0.42
5:c:71:CYS:SG	5:c:74:ASP:N	2.92	0.42
4:h:6:ASN:O	4:h:77:TYR:HA	2.19	0.42
4:h:71:LEU:HD21	4:h:77:TYR:HB2	2.01	0.42
2:l:188:LYS:HG3	4:n:70:PRO:HD2	2.00	0.42
3:m:11:GLN:HE22	3:m:75:ASN:H	1.65	0.42
2:r:35:CYS:SG	2:r:36:ARG:N	2.91	0.42
2:r:89:TRP:CH2	2:r:100:GLY:HA3	2.54	0.42
4:t:128:GLY:O	4:t:129:GLN:HG3	2.20	0.42
6:v:21:ASN:ND2	6:v:23:ARG:NH2	2.55	0.42
1:A:31:ILE:HD11	1:A:467:ILE:HD11	2.01	0.42
2:B:354:LEU:CD2	4:D:121:MET:HE1	2.50	0.42
3:C:182:GLY:HA3	3:C:209:ILE:HD11	2.01	0.42
5:E:71:CYS:SG	5:E:74:ASP:N	2.93	0.42
1:G:226:HIS:ND1	1:G:450:LEU:HD23	2.35	0.42
2:H:84:PRO:HG2	2:H:109:ALA:HB2	2.01	0.42
2:N:366:GLU:OE1	2:N:367:PRO:HD2	2.19	0.42
6:d:11:ASN:OD1	6:d:27:GLN:HA	2.19	0.42
1:e:207:THR:OG1	1:e:210:GLU:HG3	2.18	0.42
3:g:103:LYS:HB3	3:g:103:LYS:HE2	1.83	0.42
1:k:370:LEU:O	1:k:374:ILE:HD12	2.19	0.42
2:l:89:TRP:CH2	2:l:100:GLY:HA3	2.54	0.42
1:A:384:THR:O	1:A:389:ALA:HB3	2.20	0.42
6:R:198:GLY:O	6:R:202:ARG:HG3	2.19	0.42
6:X:54:MET:HE2	6:X:63:LYS:HA	2.01	0.42
2:Z:56:ILE:HG12	2:Z:378:ILE:HG12	2.01	0.42
5:c:25:ASN:OD1	5:c:44:ILE:HB	2.19	0.42
3:g:2:SER:O	3:g:66:LYS:N	2.46	0.42
6:j:54:MET:HE2	6:j:63:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:34:GLN:HB2	4:n:77:TYR:HB3	2.01	0.42
3:C:201:GLY:CA	3:C:204:MET:HE2	2.48	0.42
3:I:16:LEU:HD12	3:I:76:THR:HG22	2.01	0.42
1:M:163:ALA:HB2	1:M:528:ILE:HG22	2.01	0.42
1:M:438:ILE:HA	1:M:441:ILE:HG12	2.01	0.42
1:S:244:THR:OG1	1:S:275:HIS:HB3	2.18	0.42
6:X:88:LEU:HD23	6:X:88:LEU:C	2.44	0.42
3:g:166:MET:HB3	3:g:185:MET:HG3	2.01	0.42
1:k:72:ARG:NH1	1:k:315:THR:OG1	2.43	0.42
3:m:227:VAL:HG22	6:v:133:THR:HG21	2.01	0.42
6:v:23:ARG:HH12	6:v:92:GLY:N	2.18	0.42
2:B:424:LYS:HD2	2:B:428:TYR:CE2	2.55	0.42
1:G:540:PHE:HA	1:G:544:TYR:HB2	2.01	0.42
2:H:334:GLU:CD	3:I:15:PRO:HG2	2.44	0.42
1:M:232:CYS:HB2	1:M:275:HIS:CD2	2.54	0.42
6:R:281:CYS:SG	6:R:284:ASN:N	2.92	0.42
6:X:23:ARG:CZ	6:X:25:ILE:HD11	2.49	0.42
1:Y:231:HIS:HE1	8:Y:603:MFN:N1	2.18	0.42
2:Z:58:LYS:HA	2:Z:58:LYS:HD2	1.73	0.42
4:n:117:MET:HE2	4:n:117:MET:C	2.44	0.42
6:p:80:ILE:HD13	6:p:344:PHE:CE1	2.55	0.42
2:r:209:LEU:CD1	2:r:235:ILE:HD12	2.49	0.42
4:D:117:MET:HE2	4:D:117:MET:O	2.19	0.42
5:E:74:ASP:HB3	5:E:77:ARG:HE	1.85	0.42
1:G:61:ALA:HA	1:G:128:GLU:OE1	2.20	0.42
6:L:104:ILE:HD11	6:L:344:PHE:HE1	1.83	0.42
1:M:4:ILE:HD12	1:M:25:CYS:HA	2.02	0.42
2:N:299:VAL:HG22	2:N:302:TRP:CH2	2.54	0.42
6:R:46:ILE:HG23	6:R:64:ILE:HG23	2.02	0.42
1:Y:298:LYS:O	1:Y:298:LYS:NZ	2.49	0.42
3:g:22:LYS:HD2	3:g:24:ASP:HB2	2.01	0.42
1:k:408:ARG:O	1:k:412:ILE:HG13	2.18	0.42
1:q:467:ILE:O	1:q:467:ILE:HG13	2.19	0.42
1:A:219:ASN:OD1	1:A:224:LEU:HD12	2.20	0.42
2:B:328:ASP:OD1	2:B:328:ASP:N	2.51	0.42
2:B:338:MET:HE3	2:B:340:VAL:HG23	2.00	0.42
1:M:162:ALA:HA	1:M:218:VAL:HG13	2.02	0.42
1:M:282:TRP:CZ2	8:M:603:MFN:H152	2.55	0.42
1:M:438:ILE:HG13	1:M:439:ALA:N	2.34	0.42
3:O:99:GLY:O	3:O:102:MET:HB2	2.20	0.42
3:U:61:ALA:HB1	3:U:63:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:136:ASP:OD2	1:Y:456:LYS:NZ	2.51	0.42
2:Z:333:ARG:HH11	2:Z:333:ARG:HD2	1.53	0.42
6:d:146:GLU:OE2	6:v:218:TYR:OH	2.29	0.42
3:g:11:GLN:HE22	3:g:76:THR:CG2	2.32	0.42
4:h:52:LYS:HZ3	4:h:61:VAL:HG23	1.85	0.42
6:j:160:CYS:HB2	6:j:200:CYS:HB2	2.01	0.42
1:k:107:MET:HE1	1:k:395:TYR:CD2	2.55	0.42
2:r:55:LEU:HA	2:r:63:VAL:O	2.20	0.42
6:v:38:GLY:HA2	6:v:46:ILE:HB	2.01	0.42
3:l:201:GLY:CA	3:l:204:MET:HE2	2.49	0.42
2:T:8:VAL:HA	2:T:17:ASP:HA	2.01	0.42
4:b:6:ASN:O	4:b:77:TYR:HA	2.19	0.42
5:c:62:GLY:C	5:c:63:LYS:HG2	2.44	0.42
3:g:143:ASP:OD1	3:g:144:TRP:N	2.52	0.42
1:q:369:GLU:HG3	1:q:426:VAL:HG13	2.02	0.42
3:s:5:ILE:N	3:s:5:ILE:HD12	2.35	0.42
1:A:244:THR:OG1	1:A:275:HIS:HB3	2.20	0.42
2:H:159:ARG:O	2:H:163:ARG:HG3	2.19	0.42
2:N:223:LEU:HD23	2:N:224:TYR:CZ	2.54	0.42
2:N:333:ARG:HH12	2:N:359:GLU:CD	2.27	0.42
4:P:82:PRO:O	4:P:86:ARG:HG2	2.20	0.42
6:R:270:THR:O	6:R:272:GLN:NE2	2.48	0.42
2:T:375:MET:O	4:V:126:LYS:HE3	2.20	0.42
1:Y:235:LEU:CD1	8:Y:603:MFN:H11A	2.50	0.42
4:b:89:ARG:HB3	4:b:99:SER:HB2	2.00	0.42
1:e:282:TRP:CZ2	8:e:603:MFN:H152	2.55	0.42
2:l:8:VAL:HA	2:l:17:ASP:HA	2.02	0.42
2:r:330:LEU:O	2:r:356:ARG:HD2	2.20	0.42
3:s:151:THR:HA	3:s:170:LYS:O	2.19	0.42
4:t:23:LEU:HD23	4:t:23:LEU:HA	1.91	0.42
6:v:277:CYS:SG	6:v:278:VAL:N	2.92	0.42
6:F:23:ARG:O	6:F:88:LEU:HD12	2.20	0.41
6:F:277:CYS:SG	6:F:278:VAL:N	2.93	0.41
1:G:356:ARG:HD3	1:G:415:GLU:HG3	2.02	0.41
1:M:143:PHE:CE2	1:M:168:LEU:HD23	2.55	0.41
6:R:112:ASP:CG	3:U:229:LYS:HZ1	2.27	0.41
1:S:289:ALA:HB2	1:S:366:ILE:HG23	2.01	0.41
3:g:78:ARG:NH2	3:g:81:GLN:OE1	2.50	0.41
2:r:57:ARG:HG2	2:r:377:ASP:HA	2.02	0.41
2:r:238:ALA:O	2:r:242:LEU:HG	2.19	0.41
6:v:349:LYS:HD3	6:v:349:LYS:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLY:O	1:A:21:LYS:HA	2.20	0.41
2:B:93:GLU:HB3	2:B:385:VAL:HG11	2.03	0.41
3:C:70:ASP:OD2	3:C:91:ARG:HD2	2.20	0.41
6:X:4:THR:CG2	6:X:15:GLU:HB3	2.49	0.41
2:Z:118:CYS:SG	14:Z:505:H2S:S	3.18	0.41
4:b:110:THR:OG1	4:b:112:GLU:HG3	2.19	0.41
1:e:14:LEU:HD12	1:e:458:HIS:HB3	2.02	0.41
1:e:158:VAL:HG13	1:e:218:VAL:CG2	2.50	0.41
3:g:22:LYS:HE2	3:g:25:VAL:HG23	2.02	0.41
1:k:497:LEU:HD11	1:k:502:ILE:HG12	2.02	0.41
3:m:75:ASN:HA	3:m:95:ASN:HD22	1.85	0.41
1:q:7:ASN:HB3	1:q:21:LYS:HE2	2.01	0.41
1:q:30:LYS:HE3	1:q:30:LYS:HB3	1.88	0.41
2:r:151:CYS:HB3	2:r:253:GLY:HA3	2.02	0.41
3:O:201:GLY:CA	3:O:204:MET:HE2	2.50	0.41
6:R:315:GLU:OE2	6:R:324:THR:HA	2.20	0.41
6:X:160:CYS:SG	6:X:169:ILE:HD13	2.59	0.41
2:Z:71:ILE:C	2:Z:424:LYS:NZ	2.77	0.41
3:a:215:MET:H	3:a:265:ASN:HD21	1.68	0.41
6:d:23:ARG:CD	6:d:25:ILE:HD11	2.49	0.41
1:e:385:ASP:OD2	8:e:603:MFN:N1	2.53	0.41
1:k:4:ILE:CG1	1:k:6:LYS:HD3	2.31	0.41
6:p:102:PRO:HG2	6:p:340:TRP:CE3	2.55	0.41
1:q:50:MET:HE2	1:q:439:ALA:HB2	2.00	0.41
1:q:412:ILE:HA	1:q:416:LEU:HB2	2.01	0.41
2:r:11:PHE:CE2	2:r:37:ILE:HG21	2.55	0.41
2:B:86:MET:HE3	2:B:339:MET:HE1	2.02	0.41
1:M:316:THR:HB	8:M:603:MFN:H5	2.02	0.41
2:T:235:ILE:O	2:T:239:VAL:HG23	2.20	0.41
1:Y:323:MET:HE3	1:Y:323:MET:HB3	1.89	0.41
4:b:78:ILE:HG22	4:b:84:ALA:HB2	2.02	0.41
1:e:170:ARG:NH2	1:e:521:ASP:OD1	2.40	0.41
5:i:23:PRO:HG2	6:j:319:PRO:HG2	2.02	0.41
5:i:45:ILE:HG12	5:i:60:LEU:HB2	2.01	0.41
4:n:103:ILE:HA	4:n:104:PRO:HD3	1.95	0.41
1:q:540:PHE:HA	1:q:544:TYR:HB2	2.01	0.41
5:u:45:ILE:HG12	5:u:60:LEU:HB2	2.01	0.41
1:A:323:MET:HE3	1:A:323:MET:HB3	1.89	0.41
2:B:40:SER:OG	4:D:15:GLN:HG3	2.20	0.41
6:R:121:CYS:SG	6:R:122:GLU:N	2.94	0.41
8:S:603:MFN:H261	8:S:603:MFN:C34	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:299:VAL:HG22	2:Z:302:TRP:CZ2	2.55	0.41
6:d:104:ILE:HD11	6:d:259:PRO:HB2	2.02	0.41
2:f:40:SER:OG	4:h:15:GLN:HG3	2.20	0.41
1:k:263:ARG:HD2	1:k:265:THR:O	2.20	0.41
2:l:225:ASP:OD1	2:l:232:ARG:NH2	2.53	0.41
1:q:358:PRO:HB2	1:q:419:TRP:CE3	2.56	0.41
3:s:11:GLN:HE22	3:s:76:THR:CG2	2.33	0.41
1:A:207:THR:OG1	1:A:210:GLU:HG3	2.21	0.41
1:A:283:ARG:HE	1:A:283:ARG:HB3	1.73	0.41
5:E:23:PRO:HG2	6:F:319:PRO:HG2	2.02	0.41
6:F:96:LYS:HD3	6:F:96:LYS:N	2.36	0.41
2:N:210:LEU:HD13	2:N:268:THR:HG23	2.02	0.41
1:S:50:MET:HE2	1:S:439:ALA:HB2	2.02	0.41
1:S:154:LYS:HE2	1:S:205:ASP:O	2.21	0.41
1:S:496:VAL:C	1:S:497:LEU:HD23	2.45	0.41
2:T:255:GLY:O	2:T:259:SER:OG	2.34	0.41
6:X:242:CYS:O	6:X:307:PHE:HA	2.21	0.41
2:Z:8:VAL:HA	2:Z:17:ASP:HA	2.01	0.41
6:d:95:ILE:HG23	6:d:101:TYR:HB2	2.03	0.41
2:f:86:MET:HG2	2:f:339:MET:CE	2.51	0.41
3:m:127:GLU:HG3	3:m:153:THR:HB	2.03	0.41
4:n:89:ARG:H	4:n:103:ILE:HD12	1.84	0.41
4:n:117:MET:HE2	4:n:117:MET:O	2.20	0.41
1:q:175:TYR:HD1	1:q:176:THR:CG2	2.34	0.41
1:A:29:GLY:HA2	1:A:499:ASP:C	2.46	0.41
2:B:428:TYR:N	2:B:428:TYR:HD2	2.18	0.41
6:F:54:MET:HE2	6:F:63:LYS:HA	2.02	0.41
1:G:356:ARG:H	1:G:356:ARG:HG2	1.63	0.41
6:L:22:ARG:HG2	6:L:90:ILE:CD1	2.50	0.41
2:N:141:ASN:ND2	2:N:170:PHE:H	2.09	0.41
3:O:16:LEU:HD12	3:O:76:THR:HG22	2.02	0.41
5:Q:12:CYS:SG	5:Q:52:VAL:HA	2.61	0.41
5:Q:80:GLU:HG3	5:Q:81:LEU:HG	2.01	0.41
2:T:20:ILE:HB	2:T:32:ILE:HB	2.03	0.41
2:T:323:GLU:OE1	3:U:97:TYR:OH	2.38	0.41
2:Z:55:LEU:HD23	2:Z:63:VAL:C	2.45	0.41
2:Z:72:ASP:HA	2:Z:424:LYS:CD	2.51	0.41
2:Z:174:ARG:HB2	2:Z:178:ASP:CG	2.46	0.41
2:Z:254:MET:HA	2:Z:257:THR:OG1	2.21	0.41
6:d:277:CYS:SG	6:d:286:LEU:HD13	2.61	0.41
1:e:323:MET:HE3	1:e:323:MET:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:89:TRP:CD2	2:r:341:ILE:HG21	2.56	0.41
1:A:4:ILE:HD11	1:A:23:ASP:HB3	2.03	0.41
1:M:162:ALA:HB1	1:M:222:LEU:HD11	2.03	0.41
2:N:35:CYS:SG	2:N:36:ARG:N	2.93	0.41
6:R:214:ARG:NH1	6:R:222:GLU:OE2	2.53	0.41
1:S:111:THR:HG22	1:S:113:MET:HE3	2.03	0.41
3:U:166:MET:HB3	3:U:185:MET:HG3	2.03	0.41
6:X:102:PRO:HG2	6:X:340:TRP:CE3	2.55	0.41
1:Y:529:TYR:CE2	1:Y:533:LEU:HD11	2.56	0.41
6:d:281:CYS:SG	6:d:284:ASN:N	2.93	0.41
1:e:2:GLU:OE1	1:e:36:SER:OG	2.36	0.41
6:j:7:ILE:CD1	6:j:12:ILE:HG12	2.50	0.41
6:j:204:CYS:SG	6:j:207:ASP:N	2.93	0.41
3:s:75:ASN:HA	3:s:95:ASN:HD22	1.86	0.41
1:A:269:ALA:O	1:A:304:ILE:HA	2.21	0.41
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.83	0.41
2:H:18:ASP:CG	2:H:163:ARG:HH22	2.28	0.41
2:H:159:ARG:NH1	2:H:163:ARG:HH21	2.17	0.41
5:K:71:CYS:SG	5:K:74:ASP:N	2.94	0.41
1:M:2:GLU:CD	1:M:35:VAL:HG12	2.45	0.41
1:M:48:ILE:HD12	1:M:472:ILE:HB	2.02	0.41
2:N:89:TRP:CH2	2:N:100:GLY:HA3	2.56	0.41
3:O:69:ILE:HD12	3:O:90:VAL:HG22	2.03	0.41
6:R:53:ALA:O	6:R:57:THR:OG1	2.33	0.41
2:T:205:ARG:NH2	3:U:217:GLU:OE2	2.53	0.41
2:T:415:ARG:NH1	2:T:416:GLU:HG2	2.36	0.41
3:U:177:VAL:HG22	3:U:196:VAL:HG22	2.03	0.41
1:Y:36:SER:OG	1:Y:38:SER:OG	2.31	0.41
5:c:6:LYS:HG2	5:c:8:TYR:CE1	2.56	0.41
6:d:195:VAL:HG11	6:j:165:PRO:HG3	2.02	0.41
3:g:201:GLY:CA	3:g:204:MET:HE2	2.50	0.41
6:j:5:GLU:HA	6:j:13:THR:O	2.21	0.41
1:k:235:LEU:HD11	8:k:603:MFN:H11A	2.02	0.41
1:k:409:MET:HE3	1:k:409:MET:HB3	1.44	0.41
2:l:11:PHE:CE2	2:l:37:ILE:HG21	2.55	0.41
2:l:339:MET:HA	2:l:363:ILE:HB	2.03	0.41
6:p:80:ILE:HD13	6:p:344:PHE:HE1	1.86	0.41
6:p:225:THR:O	6:p:227:GLU:OE1	2.38	0.41
3:s:22:LYS:HG3	3:s:25:VAL:HG12	2.03	0.41
3:s:34:ILE:CD1	3:s:54:VAL:HG21	2.51	0.41
4:t:31:ALA:HB2	4:t:83:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LYS:HD3	2:B:53:LYS:H	1.85	0.41
3:C:231:ILE:HG13	3:C:238:LEU:HB2	2.03	0.41
1:G:84:LYS:HG3	1:G:85:GLY:H	1.84	0.41
1:S:523:GLN:NE2	1:S:569:LEU:H	2.19	0.41
5:W:23:PRO:HB3	6:X:272:GLN:HB2	2.02	0.41
1:Y:384:THR:HG23	1:Y:395:TYR:CE1	2.56	0.41
1:Y:441:ILE:HG13	1:Y:442:THR:HG23	2.01	0.41
2:Z:139:VAL:HG13	2:Z:249:ILE:HG21	2.02	0.41
6:j:160:CYS:SG	6:j:161:GLU:N	2.94	0.41
6:p:142:LEU:HD12	6:p:142:LEU:HA	1.94	0.41
6:p:245:CYS:SG	6:p:246:GLN:N	2.94	0.41
1:q:358:PRO:CB	1:q:419:TRP:CG	3.03	0.41
2:r:273:VAL:O	2:r:277:ASN:ND2	2.54	0.41
3:s:231:ILE:H	3:s:231:ILE:HG13	1.69	0.41
3:C:16:LEU:HD22	3:C:39:ILE:HD12	2.03	0.40
6:F:227:GLU:O	6:F:227:GLU:HG3	2.21	0.40
2:H:8:VAL:HA	2:H:17:ASP:HA	2.03	0.40
3:O:38:GLN:HG3	3:O:45:VAL:HG13	2.03	0.40
3:a:3:GLU:HG2	3:a:66:LYS:HD3	2.03	0.40
6:d:104:ILE:HG21	6:d:104:ILE:HD13	1.87	0.40
2:f:281:LYS:HA	2:f:281:LYS:HD2	1.94	0.40
4:n:1:MET:HG2	4:n:3:VAL:HG13	2.02	0.40
6:p:321:THR:HA	17:p:510:HOH:O	2.21	0.40
1:q:141:PRO:HD2	1:q:176:THR:O	2.20	0.40
1:A:118:PRO:HG2	1:A:121:LEU:HD12	2.03	0.40
1:G:144:GLY:HA3	1:G:179:ILE:HG23	2.03	0.40
1:G:520:VAL:HG12	1:G:522:THR:HG23	2.02	0.40
2:H:375:MET:O	4:J:126:LYS:HE3	2.21	0.40
6:L:326:LYS:HB3	6:L:326:LYS:NZ	2.36	0.40
1:M:439:ALA:O	1:M:443:ARG:HB2	2.20	0.40
2:N:255:GLY:O	2:N:259:SER:OG	2.20	0.40
4:b:22:ASP:OD1	4:b:22:ASP:N	2.48	0.40
1:e:213:LYS:O	1:e:217:GLU:HG3	2.22	0.40
1:e:244:THR:OG1	1:e:275:HIS:HB3	2.21	0.40
3:g:231:ILE:HD13	3:g:259:TYR:CE1	2.55	0.40
1:k:241:TYR:CD1	1:k:288:GLU:HG3	2.56	0.40
1:k:473:ASN:CB	1:k:476:THR:HG22	2.52	0.40
1:q:154:LYS:O	1:q:154:LYS:NZ	2.31	0.40
2:r:334:GLU:CD	3:s:15:PRO:HG2	2.46	0.40
2:r:342:ALA:HA	13:r:503:MGD:N3	2.36	0.40
4:t:43:LEU:HA	4:t:43:LEU:HD23	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:CYS:SG	6:F:63:LYS:HD3	2.61	0.40
6:X:76:MET:HE3	6:X:340:TRP:HA	2.04	0.40
1:Y:167:TRP:CD1	1:Y:533:LEU:HD21	2.57	0.40
6:d:135:GLU:OE2	6:d:229:THR:OG1	2.39	0.40
3:g:232:GLU:N	3:g:232:GLU:OE1	2.54	0.40
2:l:75:ALA:HB1	2:l:425:VAL:HG22	2.00	0.40
3:m:31:ILE:HG23	3:m:54:VAL:HG12	2.04	0.40
4:n:52:LYS:HB3	4:n:108:ILE:HG22	2.04	0.40
1:A:69:ARG:NH2	1:A:128:GLU:CD	2.79	0.40
3:C:32:GLU:HA	3:C:35:LYS:CE	2.51	0.40
2:H:351:GLN:HG2	4:J:86:ARG:O	2.22	0.40
4:J:34:GLN:HB2	4:J:77:TYR:HB3	2.03	0.40
1:M:443:ARG:HD2	1:M:443:ARG:N	2.35	0.40
1:M:526:GLU:CG	1:M:527:SER:N	2.84	0.40
2:N:5:LYS:HD3	5:Q:39:THR:HG22	2.03	0.40
6:X:249:CYS:SG	6:X:253:ALA:N	2.82	0.40
2:Z:89:TRP:CH2	2:Z:100:GLY:HA3	2.57	0.40
6:d:315:GLU:OE1	6:d:325:VAL:N	2.36	0.40
2:f:369:ARG:NE	2:f:374:GLU:OE2	2.52	0.40
4:n:78:ILE:HG22	4:n:84:ALA:HB2	2.04	0.40
1:q:81:GLU:OE2	1:q:103:ARG:CZ	2.70	0.40
2:r:277:ASN:HA	2:r:280:ALA:O	2.22	0.40
5:u:47:ILE:CD1	5:u:49:GLU:HB2	2.51	0.40
1:A:496:VAL:HB	1:A:504:VAL:HB	2.03	0.40
1:G:50:MET:HE2	1:G:439:ALA:HB2	2.03	0.40
2:H:124:LEU:HD21	2:H:321:PRO:HG2	2.04	0.40
2:H:286:PRO:HG2	2:H:288:ARG:HD3	2.02	0.40
3:I:5:ILE:N	3:I:5:ILE:HD12	2.36	0.40
6:L:41:CYS:SG	6:L:44:SER:N	2.95	0.40
2:T:76:LYS:HD2	2:T:428:TYR:CZ	2.56	0.40
2:T:223:LEU:HD23	2:T:224:TYR:CZ	2.56	0.40
2:Z:286:PRO:HG2	2:Z:288:ARG:HD3	2.02	0.40
2:f:311:ASP:HB2	2:f:324:THR:CG2	2.52	0.40
1:k:540:PHE:HA	1:k:544:TYR:HB2	2.04	0.40
3:m:134:ASP:OD1	3:m:160:ASN:HB2	2.21	0.40
5:o:44:ILE:HD11	5:o:47:ILE:CG2	2.50	0.40
1:q:88:ALA:HB1	2:r:317:PRO:HD3	2.02	0.40
1:q:252:LYS:HG3	1:q:301:HIS:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:336:ARG:NH1	1:e:526:GLU:OE1[1_544]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/569 (100%)	540 (95%)	25 (4%)	1 (0%)	43	56
1	G	565/569 (99%)	538 (95%)	25 (4%)	2 (0%)	30	39
1	M	565/569 (99%)	542 (96%)	23 (4%)	0	100	100
1	S	566/569 (100%)	540 (95%)	25 (4%)	1 (0%)	43	56
1	Y	565/569 (99%)	539 (95%)	26 (5%)	0	100	100
1	e	566/569 (100%)	542 (96%)	24 (4%)	0	100	100
1	k	565/569 (99%)	540 (96%)	25 (4%)	0	100	100
1	q	566/569 (100%)	542 (96%)	24 (4%)	0	100	100
2	B	427/432 (99%)	407 (95%)	18 (4%)	2 (0%)	24	34
2	H	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	24	34
2	N	428/432 (99%)	413 (96%)	13 (3%)	2 (0%)	24	34
2	T	427/432 (99%)	409 (96%)	14 (3%)	4 (1%)	14	20
2	Z	424/432 (98%)	409 (96%)	14 (3%)	1 (0%)	43	56
2	f	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	24	34
2	l	424/432 (98%)	408 (96%)	15 (4%)	1 (0%)	43	56
2	r	424/432 (98%)	409 (96%)	13 (3%)	2 (0%)	24	34
3	C	265/270 (98%)	256 (97%)	9 (3%)	0	100	100
3	I	267/270 (99%)	258 (97%)	9 (3%)	0	100	100
3	O	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	U	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	a	266/270 (98%)	257 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	m	266/270 (98%)	256 (96%)	10 (4%)	0	100	100
3	s	267/270 (99%)	258 (97%)	9 (3%)	0	100	100
4	D	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	J	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	P	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	V	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	b	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	h	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	n	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	t	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
5	E	78/82 (95%)	78 (100%)	0	0	100	100
5	K	78/82 (95%)	78 (100%)	0	0	100	100
5	Q	78/82 (95%)	78 (100%)	0	0	100	100
5	W	78/82 (95%)	78 (100%)	0	0	100	100
5	c	78/82 (95%)	78 (100%)	0	0	100	100
5	i	78/82 (95%)	78 (100%)	0	0	100	100
5	o	78/82 (95%)	78 (100%)	0	0	100	100
5	u	79/82 (96%)	79 (100%)	0	0	100	100
6	F	341/349 (98%)	337 (99%)	3 (1%)	1 (0%)	36	45
6	L	346/349 (99%)	340 (98%)	5 (1%)	1 (0%)	36	45
6	R	337/349 (97%)	330 (98%)	7 (2%)	0	100	100
6	X	340/349 (97%)	336 (99%)	4 (1%)	0	100	100
6	d	336/349 (96%)	331 (98%)	3 (1%)	2 (1%)	21	29
6	j	340/349 (97%)	336 (99%)	4 (1%)	0	100	100
6	p	346/349 (99%)	342 (99%)	3 (1%)	1 (0%)	36	45
6	v	342/349 (98%)	337 (98%)	4 (1%)	1 (0%)	36	45
All	All	14422/14656 (98%)	13934 (97%)	462 (3%)	26 (0%)	43	56

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS

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Mol	Chain	Res	Type
6	F	92	GLY
1	G	415	GLU
6	L	92	GLY
1	S	415	GLU
2	T	60	GLY
6	d	92	GLY
6	p	92	GLY
6	v	92	GLY
2	B	59	ASN
2	T	59	ASN
2	N	59	ASN
2	T	382	PRO
2	Z	382	PRO
2	r	382	PRO
2	B	382	PRO
2	H	382	PRO
2	N	382	PRO
2	f	382	PRO
2	l	382	PRO
1	G	84	LYS
6	d	102	PRO
2	H	25	GLY
2	f	25	GLY
2	r	307	PRO
2	T	307	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/470 (100%)	467 (99%)	3 (1%)	78	87
1	G	469/470 (100%)	466 (99%)	3 (1%)	78	87
1	M	469/470 (100%)	468 (100%)	1 (0%)	87	93
1	S	470/470 (100%)	463 (98%)	7 (2%)	57	74
1	Y	469/470 (100%)	467 (100%)	2 (0%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	470/470 (100%)	467 (99%)	3 (1%)	78	87
1	k	469/470 (100%)	468 (100%)	1 (0%)	87	93
1	q	470/470 (100%)	466 (99%)	4 (1%)	70	82
2	B	359/361 (99%)	355 (99%)	4 (1%)	65	79
2	H	358/361 (99%)	354 (99%)	4 (1%)	65	79
2	N	359/361 (99%)	355 (99%)	4 (1%)	65	79
2	T	359/361 (99%)	355 (99%)	4 (1%)	65	79
2	Z	358/361 (99%)	354 (99%)	4 (1%)	65	79
2	f	358/361 (99%)	353 (99%)	5 (1%)	59	75
2	l	358/361 (99%)	357 (100%)	1 (0%)	86	92
2	r	358/361 (99%)	354 (99%)	4 (1%)	65	79
3	C	202/204 (99%)	200 (99%)	2 (1%)	68	80
3	I	203/204 (100%)	201 (99%)	2 (1%)	68	80
3	O	202/204 (99%)	200 (99%)	2 (1%)	68	80
3	U	202/204 (99%)	201 (100%)	1 (0%)	81	88
3	a	202/204 (99%)	198 (98%)	4 (2%)	48	67
3	g	202/204 (99%)	201 (100%)	1 (0%)	81	88
3	m	202/204 (99%)	200 (99%)	2 (1%)	68	80
3	s	203/204 (100%)	199 (98%)	4 (2%)	48	67
4	D	110/111 (99%)	109 (99%)	1 (1%)	70	82
4	J	110/111 (99%)	109 (99%)	1 (1%)	70	82
4	P	110/111 (99%)	110 (100%)	0	100	100
4	V	110/111 (99%)	108 (98%)	2 (2%)	51	70
4	b	110/111 (99%)	110 (100%)	0	100	100
4	h	110/111 (99%)	109 (99%)	1 (1%)	70	82
4	n	110/111 (99%)	108 (98%)	2 (2%)	51	70
4	t	110/111 (99%)	110 (100%)	0	100	100
5	E	65/67 (97%)	65 (100%)	0	100	100
5	K	65/67 (97%)	64 (98%)	1 (2%)	57	74
5	Q	65/67 (97%)	65 (100%)	0	100	100
5	W	65/67 (97%)	63 (97%)	2 (3%)	35	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	c	65/67 (97%)	64 (98%)	1 (2%)	57	74
5	i	65/67 (97%)	64 (98%)	1 (2%)	57	74
5	o	65/67 (97%)	65 (100%)	0	100	100
5	u	66/67 (98%)	65 (98%)	1 (2%)	57	74
6	F	308/312 (99%)	302 (98%)	6 (2%)	50	69
6	L	311/312 (100%)	309 (99%)	2 (1%)	78	87
6	R	305/312 (98%)	302 (99%)	3 (1%)	68	80
6	X	308/312 (99%)	305 (99%)	3 (1%)	68	80
6	d	304/312 (97%)	301 (99%)	3 (1%)	68	80
6	j	308/312 (99%)	305 (99%)	3 (1%)	68	80
6	p	311/312 (100%)	308 (99%)	3 (1%)	68	80
6	v	310/312 (99%)	305 (98%)	5 (2%)	55	73
All	All	12107/12200 (99%)	11994 (99%)	113 (1%)	70	82

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	380	VAL
1	A	476	THR
2	B	20	ILE
2	B	281	LYS
2	B	351	GLN
2	B	397	GLU
3	C	237	GLU
3	C	264	CYS
4	D	117	MET
6	F	17	THR
6	F	143	VAL
6	F	222	GLU
6	F	240	VAL
6	F	299	THR
6	F	328	ASN
1	G	71	TYR
1	G	231	HIS
1	G	380	VAL
2	H	103	LEU
2	H	281	LYS

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Mol	Chain	Res	Type
2	H	397	GLU
2	H	411	LEU
3	I	44	GLU
3	I	264	CYS
4	J	129	GLN
5	K	69	GLU
6	L	2	GLU
6	L	299	THR
1	M	71	TYR
2	N	281	LYS
2	N	302	TRP
2	N	351	GLN
2	N	397	GLU
3	O	151	THR
3	O	264	CYS
6	R	94	SER
6	R	144	THR
6	R	222	GLU
1	S	71	TYR
1	S	231	HIS
1	S	286	VAL
1	S	380	VAL
1	S	472	ILE
1	S	482	GLU
1	S	512	SER
2	T	20	ILE
2	T	351	GLN
2	T	397	GLU
2	T	421	LEU
3	U	264	CYS
4	V	11	ILE
4	V	129	GLN
5	W	5	LEU
5	W	69	GLU
6	X	143	VAL
6	X	212	VAL
6	X	284	ASN
1	Y	71	TYR
1	Y	286	VAL
2	Z	197	ILE
2	Z	259	SER
2	Z	351	GLN

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Mol	Chain	Res	Type
2	Z	397	GLU
3	a	231	ILE
3	a	236	GLU
3	a	237	GLU
3	a	264	CYS
5	c	69	GLU
6	d	91	ASP
6	d	144	THR
6	d	222	GLU
1	e	71	TYR
1	e	286	VAL
1	e	482	GLU
2	f	20	ILE
2	f	46	GLU
2	f	351	GLN
2	f	397	GLU
2	f	421	LEU
3	g	236	GLU
4	h	1	MET
5	i	42	VAL
6	j	79	SER
6	j	224	LYS
6	j	299	THR
1	k	71	TYR
2	l	397	GLU
3	m	237	GLU
3	m	264	CYS
4	n	10	THR
4	n	117	MET
6	p	93	THR
6	p	142	LEU
6	p	299	THR
1	q	36	SER
1	q	71	TYR
1	q	380	VAL
1	q	476	THR
2	r	221	GLU
2	r	281	LYS
2	r	351	GLN
2	r	397	GLU
3	s	55	SER
3	s	232	GLU

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Mol	Chain	Res	Type
3	s	233	VAL
3	s	264	CYS
5	u	69	GLU
6	v	21	ASN
6	v	58	GLU
6	v	142	LEU
6	v	143	VAL
6	v	210	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	299	ASN
2	B	44	HIS
2	B	220	HIS
2	B	234	GLN
2	B	263	HIS
2	B	290	HIS
6	F	342	ASN
1	G	106	GLN
1	G	299	ASN
1	G	535	ASN
1	G	542	GLN
2	H	160	HIS
2	H	164	ASN
2	H	234	GLN
1	M	363	GLN
1	M	376	ASN
1	M	405	ASN
1	M	535	ASN
2	N	141	ASN
2	N	263	HIS
3	O	216	GLN
6	R	21	ASN
1	S	15	ASN
1	S	299	ASN
1	S	421	GLN
1	S	523	GLN
1	S	542	GLN
2	T	44	HIS
6	X	21	ASN

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Mol	Chain	Res	Type
6	X	174	GLN
6	X	331	ASN
1	Y	410	ASN
1	Y	523	GLN
1	Y	547	ASN
2	Z	6	ASN
2	Z	157	HIS
2	Z	160	HIS
2	Z	164	ASN
3	a	265	ASN
6	d	174	GLN
6	d	246	GLN
6	d	268	GLN
1	e	15	ASN
1	e	542	GLN
2	f	44	HIS
2	f	157	HIS
2	f	220	HIS
2	f	263	HIS
6	j	21	ASN
6	j	27	GLN
6	j	117	GLN
1	k	7	ASN
1	k	106	GLN
1	k	126	HIS
1	k	547	ASN
2	l	6	ASN
3	m	38	GLN
6	p	21	ASN
6	p	331	ASN
1	q	7	ASN
1	q	15	ASN
1	q	124	HIS
1	q	130	HIS
1	q	253	ASN
1	q	299	ASN
1	q	542	GLN
2	r	157	HIS
2	r	290	HIS
2	r	332	ASN
3	s	81	GLN
3	s	155	HIS

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Mol	Chain	Res	Type
6	v	21	ASN
6	v	27	GLN
6	v	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	G	178	7,1	10,11,12	2.13	1 (10%)	6,12,14	1.70	1 (16%)
1	KCX	k	178	7,1	10,11,12	0.60	0	6,12,14	0.79	0
1	KCX	A	178	7,1	10,11,12	0.58	0	6,12,14	0.69	0
1	KCX	Y	178	7,1	10,11,12	0.60	0	6,12,14	0.72	0
1	KCX	q	178	7,1	10,11,12	2.16	1 (10%)	6,12,14	1.38	1 (16%)
1	KCX	e	178	7,1	10,11,12	2.15	1 (10%)	6,12,14	1.73	1 (16%)
1	KCX	M	178	7,1	10,11,12	2.17	1 (10%)	6,12,14	1.51	1 (16%)
1	KCX	S	178	7,1	10,11,12	0.66	0	6,12,14	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	G	178	7,1	-	0/9/10/12	-
1	KCX	k	178	7,1	-	0/9/10/12	-
1	KCX	A	178	7,1	-	1/9/10/12	-
1	KCX	Y	178	7,1	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	q	178	7,1	-	0/9/10/12	-
1	KCX	e	178	7,1	-	0/9/10/12	-
1	KCX	M	178	7,1	-	0/9/10/12	-
1	KCX	S	178	7,1	-	0/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	178	KCX	OQ1-CX	6.47	1.33	1.21
1	q	178	KCX	OQ1-CX	6.44	1.33	1.21
1	e	178	KCX	OQ1-CX	6.35	1.33	1.21
1	G	178	KCX	OQ1-CX	6.33	1.33	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	178	KCX	OQ1-CX-NZ	-4.15	118.61	124.92
1	G	178	KCX	OQ1-CX-NZ	-4.04	118.78	124.92
1	M	178	KCX	OQ1-CX-NZ	-3.59	119.47	124.92
1	q	178	KCX	OQ1-CX-NZ	-3.16	120.11	124.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	178	KCX	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 221 ligands modelled in this entry, 97 are monoatomic and 8 are modelled with single atom - leaving 116 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	F	406	6	0,12,12	-	-	-		
11	SF4	d	408	6	0,12,12	-	-	-		
13	MGD	H	503	12	47,52,52	1.40	7 (14%)	58,81,81	1.88	13 (22%)
11	SF4	j	504	6	0,12,12	-	-	-		
11	SF4	X	501	6	0,12,12	-	-	-		
11	SF4	o	102	5	0,12,12	-	-	-		
8	MFN	Y	603	7	54,54,56	1.86	8 (14%)	63,71,73	2.39	16 (25%)
11	SF4	R	405	6	0,12,12	-	-	-		
11	SF4	p	407	6	0,12,12	-	-	-		
11	SF4	d	401	6	0,12,12	-	-	-		
13	MGD	r	504	12	47,52,52	1.48	7 (14%)	58,81,81	2.06	13 (22%)
11	SF4	j	507	6	0,12,12	-	-	-		
11	SF4	F	401	6	0,12,12	-	-	-		
13	MGD	T	504	12	47,52,52	1.47	7 (14%)	58,81,81	2.14	13 (22%)
13	MGD	Z	504	12	47,52,52	1.48	7 (14%)	58,81,81	2.10	15 (25%)
11	SF4	X	508	6	0,12,12	-	-	-		
11	SF4	j	505	6	0,12,12	-	-	-		
11	SF4	F	402	6	0,12,12	-	-	-		
11	SF4	u	101	5	0,12,12	-	-	-		
11	SF4	j	503	6	0,12,12	-	-	-		
11	SF4	E	102	5	0,12,12	-	-	-		
11	SF4	p	401	6	0,12,12	-	-	-		
11	SF4	v	508	6	0,12,12	-	-	-		
11	SF4	L	504	6	0,12,12	-	-	-		
11	SF4	F	408	6	0,12,12	-	-	-		
11	SF4	d	409	6	0,12,12	-	-	-		
11	SF4	v	505	6	0,12,12	-	-	-		
13	MGD	f	503	12	47,52,52	1.43	7 (14%)	58,81,81	1.86	11 (18%)
11	SF4	K	102	5	0,12,12	-	-	-		
11	SF4	H	501	2	0,12,12	-	-	-		
11	SF4	p	402	6	0,12,12	-	-	-		
11	SF4	d	407	6	0,12,12	-	-	-		
11	SF4	X	507	6	0,12,12	-	-	-		
11	SF4	R	401	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MFN	M	603	7	54,54,56	1.88	8 (14%)	63,71,73	2.44	20 (31%)
11	SF4	L	502	6	0,12,12	-	-	-		
11	SF4	L	508	6	0,12,12	-	-	-		
13	MGD	l	503	12	47,52,52	1.41	7 (14%)	58,81,81	1.98	13 (22%)
11	SF4	X	504	6	0,12,12	-	-	-		
11	SF4	Z	501	2	0,12,12	-	-	-		
11	SF4	f	501	2	0,12,12	-	-	-		
13	MGD	r	503	12	47,52,52	1.41	6 (12%)	58,81,81	1.93	13 (22%)
11	SF4	i	101	5	0,12,12	-	-	-		
11	SF4	L	507	6	0,12,12	-	-	-		
11	SF4	v	503	6	0,12,12	-	-	-		
11	SF4	F	404	6	0,12,12	-	-	-		
11	SF4	d	404	6	0,12,12	-	-	-		
11	SF4	R	408	6	0,12,12	-	-	-		
11	SF4	F	409	6	0,12,12	-	-	-		
11	SF4	R	406	6	0,12,12	-	-	-		
11	SF4	v	504	6	0,12,12	-	-	-		
11	SF4	R	407	6	0,12,12	-	-	-		
11	SF4	v	506	6	0,12,12	-	-	-		
11	SF4	F	405	6	0,12,12	-	-	-		
11	SF4	R	402	6	0,12,12	-	-	-		
11	SF4	i	102	5	0,12,12	-	-	-		
13	MGD	N	503	12	47,52,52	1.37	4 (8%)	58,81,81	1.92	12 (20%)
8	MFN	k	603	7	54,54,56	1.87	9 (16%)	63,71,73	2.90	22 (34%)
11	SF4	R	404	6	0,12,12	-	-	-		
8	MFN	A	603	7	54,54,56	1.98	12 (22%)	63,71,73	2.17	15 (23%)
11	SF4	c	102	5	0,12,12	-	-	-		
8	MFN	G	603	7	54,54,56	1.86	8 (14%)	63,71,73	2.26	14 (22%)
11	SF4	N	501	2	0,12,12	-	-	-		
11	SF4	l	501	2	0,12,12	-	-	-		
11	SF4	j	502	6	0,12,12	-	-	-		
13	MGD	l	504	12	47,52,52	1.48	7 (14%)	58,81,81	2.07	14 (24%)
11	SF4	X	505	6	0,12,12	-	-	-		
11	SF4	Q	102	5	0,12,12	-	-	-		
11	SF4	p	408	6	0,12,12	-	-	-		
11	SF4	p	409	6	0,12,12	-	-	-		
11	SF4	Q	101	5	0,12,12	-	-	-		
11	SF4	E	101	5	0,12,12	-	-	-		
11	SF4	T	501	2	0,12,12	-	-	-		
11	SF4	p	406	6	0,12,12	-	-	-		
11	SF4	u	102	5	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	R	409	6	0,12,12	-	-	-		
11	SF4	v	501	6	0,12,12	-	-	-		
11	SF4	K	101	5	0,12,12	-	-	-		
11	SF4	L	503	6	0,12,12	-	-	-		
11	SF4	c	101	5	0,12,12	-	-	-		
11	SF4	X	506	6	0,12,12	-	-	-		
11	SF4	d	405	6	0,12,12	-	-	-		
11	SF4	p	403	6	0,12,12	-	-	-		
11	SF4	W	201	5	0,12,12	-	-	-		
11	SF4	L	506	6	0,12,12	-	-	-		
11	SF4	d	402	6	0,12,12	-	-	-		
11	SF4	v	502	6	0,12,12	-	-	-		
11	SF4	B	501	2	0,12,12	-	-	-		
11	SF4	F	403	6	0,12,12	-	-	-		
13	MGD	Z	503	12	47,52,52	1.40	6 (12%)	58,81,81	1.97	13 (22%)
8	MFN	q	603	-	54,54,56	1.91	11 (20%)	63,71,73	2.18	14 (22%)
11	SF4	X	502	6	0,12,12	-	-	-		
11	SF4	d	406	6	0,12,12	-	-	-		
13	MGD	B	503	12	47,52,52	1.40	6 (12%)	58,81,81	1.96	13 (22%)
13	MGD	H	504	12	47,52,52	1.46	7 (14%)	58,81,81	2.10	11 (18%)
11	SF4	L	501	6	0,12,12	-	-	-		
11	SF4	o	101	5	0,12,12	-	-	-		
11	SF4	L	505	6	0,12,12	-	-	-		
11	SF4	v	507	6	0,12,12	-	-	-		
11	SF4	r	501	2	0,12,12	-	-	-		
13	MGD	f	504	12	47,52,52	1.46	8 (17%)	58,81,81	2.11	13 (22%)
11	SF4	j	506	6	0,12,12	-	-	-		
13	MGD	N	504	12	47,52,52	1.46	7 (14%)	58,81,81	2.06	14 (24%)
11	SF4	X	503	6	0,12,12	-	-	-		
11	SF4	F	407	6	0,12,12	-	-	-		
8	MFN	S	603	-	54,54,56	1.94	9 (16%)	63,71,73	2.23	16 (25%)
11	SF4	p	404	6	0,12,12	-	-	-		
11	SF4	d	403	6	0,12,12	-	-	-		
13	MGD	T	503	12	47,52,52	1.41	7 (14%)	58,81,81	1.90	13 (22%)
11	SF4	W	200	5	0,12,12	-	-	-		
13	MGD	B	504	12	47,52,52	1.47	8 (17%)	58,81,81	2.06	14 (24%)
11	SF4	p	405	6	0,12,12	-	-	-		
11	SF4	j	501	6	0,12,12	-	-	-		
11	SF4	R	403	6	0,12,12	-	-	-		
8	MFN	e	603	-	54,54,56	1.89	9 (16%)	63,71,73	2.42	13 (20%)
11	SF4	j	508	6	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	F	406	6	-	-	0/6/5/5
13	MGD	H	503	12	-	8/22/66/66	0/6/6/6
11	SF4	d	408	6	-	-	0/6/5/5
11	SF4	j	504	6	-	-	0/6/5/5
11	SF4	X	501	6	-	-	0/6/5/5
11	SF4	o	102	5	-	-	0/6/5/5
8	MFN	Y	603	7	-	28/61/61/63	0/2/2/2
11	SF4	R	405	6	-	-	0/6/5/5
13	MGD	r	504	12	-	1/22/66/66	0/6/6/6
11	SF4	d	401	6	-	-	0/6/5/5
11	SF4	p	407	6	-	-	0/6/5/5
11	SF4	j	507	6	-	-	0/6/5/5
13	MGD	T	504	12	-	1/22/66/66	0/6/6/6
11	SF4	F	401	6	-	-	0/6/5/5
13	MGD	Z	504	12	-	1/22/66/66	0/6/6/6
11	SF4	X	508	6	-	-	0/6/5/5
11	SF4	j	505	6	-	-	0/6/5/5
11	SF4	F	402	6	-	-	0/6/5/5
11	SF4	u	101	5	-	-	0/6/5/5
11	SF4	j	503	6	-	-	0/6/5/5
11	SF4	E	102	5	-	-	0/6/5/5
11	SF4	p	401	6	-	-	0/6/5/5
11	SF4	v	508	6	-	-	0/6/5/5
11	SF4	L	504	6	-	-	0/6/5/5
11	SF4	d	409	6	-	-	0/6/5/5
11	SF4	v	505	6	-	-	0/6/5/5
13	MGD	f	503	12	-	8/22/66/66	0/6/6/6
11	SF4	K	102	5	-	-	0/6/5/5
11	SF4	H	501	2	-	-	0/6/5/5
11	SF4	p	402	6	-	-	0/6/5/5
11	SF4	d	407	6	-	-	0/6/5/5
11	SF4	X	507	6	-	-	0/6/5/5
11	SF4	R	401	6	-	-	0/6/5/5
11	SF4	L	502	6	-	-	0/6/5/5
11	SF4	L	508	6	-	-	0/6/5/5
13	MGD	l	503	12	-	6/22/66/66	0/6/6/6
11	SF4	X	504	6	-	-	0/6/5/5
11	SF4	Z	501	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	f	501	2	-	-	0/6/5/5
13	MGD	r	503	12	-	9/22/66/66	0/6/6/6
11	SF4	i	101	5	-	-	0/6/5/5
11	SF4	L	507	6	-	-	0/6/5/5
11	SF4	v	503	6	-	-	0/6/5/5
11	SF4	F	404	6	-	-	0/6/5/5
11	SF4	d	404	6	-	-	0/6/5/5
11	SF4	R	408	6	-	-	0/6/5/5
11	SF4	F	409	6	-	-	0/6/5/5
11	SF4	R	406	6	-	-	0/6/5/5
11	SF4	v	504	6	-	-	0/6/5/5
11	SF4	R	407	6	-	-	0/6/5/5
11	SF4	v	506	6	-	-	0/6/5/5
11	SF4	F	405	6	-	-	0/6/5/5
11	SF4	R	402	6	-	-	0/6/5/5
11	SF4	i	102	5	-	-	0/6/5/5
13	MGD	N	503	12	-	7/22/66/66	0/6/6/6
8	MFN	k	603	7	-	19/61/61/63	0/2/2/2
11	SF4	R	404	6	-	-	0/6/5/5
8	MFN	A	603	7	-	12/61/61/63	0/2/2/2
11	SF4	c	102	5	-	-	0/6/5/5
8	MFN	G	603	7	-	17/61/61/63	0/2/2/2
11	SF4	N	501	2	-	-	0/6/5/5
11	SF4	l	501	2	-	-	0/6/5/5
11	SF4	j	502	6	-	-	0/6/5/5
13	MGD	l	504	12	-	1/22/66/66	0/6/6/6
11	SF4	X	505	6	-	-	0/6/5/5
11	SF4	Q	102	5	-	-	0/6/5/5
11	SF4	p	408	6	-	-	0/6/5/5
11	SF4	p	409	6	-	-	0/6/5/5
11	SF4	Q	101	5	-	-	0/6/5/5
11	SF4	E	101	5	-	-	0/6/5/5
11	SF4	T	501	2	-	-	0/6/5/5
11	SF4	p	406	6	-	-	0/6/5/5
11	SF4	u	102	5	-	-	0/6/5/5
11	SF4	R	409	6	-	-	0/6/5/5
11	SF4	v	501	6	-	-	0/6/5/5
11	SF4	K	101	5	-	-	0/6/5/5
11	SF4	L	503	6	-	-	0/6/5/5
11	SF4	c	101	5	-	-	0/6/5/5
11	SF4	X	506	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	d	405	6	-	-	0/6/5/5
11	SF4	p	403	6	-	-	0/6/5/5
11	SF4	W	201	5	-	-	0/6/5/5
11	SF4	L	506	6	-	-	0/6/5/5
11	SF4	d	402	6	-	-	0/6/5/5
11	SF4	v	502	6	-	-	0/6/5/5
11	SF4	B	501	2	-	-	0/6/5/5
11	SF4	F	403	6	-	-	0/6/5/5
13	MGD	Z	503	12	-	9/22/66/66	0/6/6/6
8	MFN	q	603	-	-	19/61/61/63	0/2/2/2
11	SF4	X	502	6	-	-	0/6/5/5
11	SF4	d	406	6	-	-	0/6/5/5
13	MGD	B	503	12	-	8/22/66/66	0/6/6/6
13	MGD	H	504	12	-	1/22/66/66	0/6/6/6
11	SF4	L	501	6	-	-	0/6/5/5
11	SF4	o	101	5	-	-	0/6/5/5
11	SF4	L	505	6	-	-	0/6/5/5
11	SF4	v	507	6	-	-	0/6/5/5
11	SF4	r	501	2	-	-	0/6/5/5
13	MGD	f	504	12	-	1/22/66/66	0/6/6/6
11	SF4	j	501	6	-	-	0/6/5/5
13	MGD	N	504	12	-	0/22/66/66	0/6/6/6
11	SF4	j	506	6	-	-	0/6/5/5
11	SF4	X	503	6	-	-	0/6/5/5
11	SF4	F	407	6	-	-	0/6/5/5
8	MFN	S	603	-	-	20/61/61/63	0/2/2/2
8	MFN	e	603	-	-	21/61/61/63	0/2/2/2
11	SF4	p	404	6	-	-	0/6/5/5
11	SF4	d	403	6	-	-	0/6/5/5
13	MGD	T	503	12	-	3/22/66/66	0/6/6/6
13	MGD	B	504	12	-	1/22/66/66	0/6/6/6
11	SF4	W	200	5	-	-	0/6/5/5
11	SF4	p	405	6	-	-	0/6/5/5
8	MFN	M	603	7	-	19/61/61/63	0/2/2/2
11	SF4	R	403	6	-	-	0/6/5/5
11	SF4	F	408	6	-	-	0/6/5/5
11	SF4	j	508	6	-	-	0/6/5/5

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	603	MFN	C21-N3	6.66	1.48	1.34
8	S	603	MFN	C21-N3	6.66	1.48	1.34
8	k	603	MFN	C21-N3	6.11	1.47	1.34
8	Y	603	MFN	C21-N3	6.05	1.46	1.34
8	A	603	MFN	C21-N3	5.97	1.46	1.34
13	r	504	MGD	C16-C21	5.90	1.48	1.38
8	q	603	MFN	C21-N3	5.85	1.46	1.34
13	Z	504	MGD	C16-C21	5.81	1.48	1.38
13	N	504	MGD	C16-C21	5.77	1.48	1.38
13	B	504	MGD	C16-C21	5.73	1.48	1.38
13	T	503	MGD	C16-C21	5.72	1.48	1.38
13	l	504	MGD	C16-C21	5.66	1.48	1.38
13	f	504	MGD	C16-C21	5.65	1.48	1.38
8	G	603	MFN	C21-N3	5.63	1.46	1.34
13	r	503	MGD	C16-C21	5.62	1.48	1.38
13	T	504	MGD	C16-C21	5.60	1.48	1.38
13	B	503	MGD	C16-C21	5.56	1.48	1.38
8	M	603	MFN	C21-N3	5.56	1.45	1.34
13	H	503	MGD	C16-C21	5.53	1.48	1.38
13	f	503	MGD	C16-C21	5.52	1.48	1.38
13	N	503	MGD	C16-C21	5.51	1.48	1.38
8	A	603	MFN	C16-N2	5.47	1.46	1.33
13	H	504	MGD	C16-C21	5.46	1.48	1.38
13	Z	503	MGD	C16-C21	5.41	1.47	1.38
13	l	503	MGD	C16-C21	5.39	1.47	1.38
8	M	603	MFN	C16-N2	5.30	1.46	1.33
8	Y	603	MFN	C16-N2	5.25	1.45	1.33
8	k	603	MFN	C16-N2	5.23	1.45	1.33
8	G	603	MFN	C16-N2	5.12	1.45	1.33
8	q	603	MFN	C16-N2	5.12	1.45	1.33
8	S	603	MFN	C16-N2	5.10	1.45	1.33
8	e	603	MFN	C16-N2	5.05	1.45	1.33
8	A	603	MFN	C25-N4	4.90	1.44	1.34
8	A	603	MFN	C3-C2	4.77	1.42	1.34
8	S	603	MFN	C25-N4	4.72	1.44	1.34
8	e	603	MFN	C25-N4	4.70	1.44	1.34
8	q	603	MFN	C25-N4	4.64	1.43	1.34
8	q	603	MFN	C3-C2	4.55	1.41	1.34
8	G	603	MFN	C25-N4	4.45	1.43	1.34
8	M	603	MFN	C3-C2	4.43	1.41	1.34
8	G	603	MFN	C3-C2	4.41	1.41	1.34
8	S	603	MFN	C3-C2	4.37	1.41	1.34
8	M	603	MFN	C25-N4	4.33	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	k	603	MFN	C3-C2	4.30	1.41	1.34
8	Y	603	MFN	C3-C2	4.27	1.41	1.34
8	Y	603	MFN	C25-N4	4.18	1.42	1.34
8	e	603	MFN	C3-C2	4.13	1.41	1.34
8	k	603	MFN	C25-N4	4.11	1.42	1.34
8	q	603	MFN	C8-C9	3.27	1.44	1.38
13	l	504	MGD	PB-O3B	3.27	1.63	1.59
8	k	603	MFN	C23-N4	-3.25	1.39	1.45
8	S	603	MFN	C8-C9	3.23	1.44	1.38
8	A	603	MFN	C8-C9	3.19	1.44	1.38
8	e	603	MFN	C8-C9	3.15	1.44	1.38
13	H	504	MGD	C5-C4	3.15	1.47	1.38
8	G	603	MFN	C8-C9	3.10	1.44	1.38
8	M	603	MFN	C8-C9	3.10	1.44	1.38
13	f	503	MGD	C5-C4	3.08	1.47	1.38
13	l	503	MGD	C5-C4	3.06	1.47	1.38
8	Y	603	MFN	C8-C9	3.06	1.44	1.38
13	T	504	MGD	PB-O3B	3.06	1.62	1.59
13	T	504	MGD	C5-C4	3.06	1.47	1.38
8	A	603	MFN	C10-C9	3.05	1.44	1.38
13	Z	504	MGD	C5-C4	3.05	1.47	1.38
13	N	504	MGD	C5-C4	3.04	1.47	1.38
13	N	503	MGD	C5-C4	3.03	1.47	1.38
8	k	603	MFN	C8-C9	3.02	1.44	1.38
13	H	503	MGD	C5-C4	3.02	1.47	1.38
13	r	504	MGD	C5-C4	3.02	1.47	1.38
13	Z	503	MGD	C5-C4	3.01	1.47	1.38
13	l	504	MGD	C5-C4	3.01	1.47	1.38
13	f	504	MGD	C5-C4	3.00	1.47	1.38
13	H	504	MGD	PB-O3B	2.99	1.62	1.59
13	r	503	MGD	C5-C4	2.97	1.46	1.38
13	T	503	MGD	C5-C4	2.95	1.46	1.38
13	B	504	MGD	C5-C4	2.95	1.46	1.38
13	l	504	MGD	PA-O3B	2.95	1.62	1.59
13	H	504	MGD	PA-O3B	2.93	1.62	1.59
8	M	603	MFN	C10-C9	2.91	1.44	1.38
13	r	504	MGD	PB-O3B	2.86	1.62	1.59
13	B	503	MGD	C5-C4	2.85	1.46	1.38
13	B	504	MGD	PB-O3B	2.79	1.62	1.59
13	Z	504	MGD	PA-O3B	2.79	1.62	1.59
8	q	603	MFN	C10-C9	2.78	1.43	1.38
13	Z	504	MGD	PB-O3B	2.77	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	504	MGD	PA-O3B	2.75	1.62	1.59
13	r	504	MGD	PA-O3B	2.75	1.62	1.59
8	Y	603	MFN	C10-C9	2.74	1.43	1.38
8	S	603	MFN	C10-C9	2.71	1.43	1.38
8	G	603	MFN	C10-C9	2.71	1.43	1.38
13	f	504	MGD	PB-O3B	2.70	1.62	1.59
13	N	504	MGD	PA-O3B	2.70	1.62	1.59
8	M	603	MFN	C17-C16	2.69	1.56	1.51
8	S	603	MFN	C17-C16	2.69	1.56	1.51
13	N	504	MGD	PB-O3B	2.69	1.62	1.59
8	k	603	MFN	C10-C9	2.67	1.43	1.38
13	f	503	MGD	PA-O3B	2.66	1.62	1.59
13	B	503	MGD	C17-N18	-2.62	1.33	1.38
13	f	504	MGD	PA-O3B	2.62	1.62	1.59
13	T	503	MGD	C17-N18	-2.60	1.34	1.38
8	e	603	MFN	C10-C9	2.59	1.43	1.38
13	Z	504	MGD	C17-N18	-2.58	1.34	1.38
13	T	504	MGD	PA-O3B	2.58	1.62	1.59
8	k	603	MFN	C17-C16	2.57	1.56	1.51
13	l	503	MGD	PA-O3B	2.53	1.62	1.59
13	Z	503	MGD	C17-N18	-2.53	1.34	1.38
8	M	603	MFN	C23-N4	-2.52	1.40	1.45
8	A	603	MFN	C17-C16	2.51	1.56	1.51
8	q	603	MFN	C17-C16	2.51	1.56	1.51
13	B	504	MGD	C17-N18	-2.49	1.34	1.38
13	N	503	MGD	C17-N18	-2.48	1.34	1.38
8	Y	603	MFN	C17-C16	2.48	1.56	1.51
13	N	504	MGD	C16-C17	2.47	1.49	1.41
13	r	503	MGD	C17-N18	-2.47	1.34	1.38
13	H	503	MGD	C17-N18	-2.46	1.34	1.38
13	r	504	MGD	C16-C17	2.46	1.49	1.41
8	G	603	MFN	C17-C16	2.45	1.56	1.51
13	T	504	MGD	C17-N18	-2.44	1.34	1.38
13	N	504	MGD	C17-N18	-2.43	1.34	1.38
8	Y	603	MFN	C23-N4	-2.42	1.40	1.45
13	f	504	MGD	C17-N18	-2.41	1.34	1.38
13	l	503	MGD	PB-O3B	2.40	1.62	1.59
13	H	504	MGD	C17-N18	-2.40	1.34	1.38
13	Z	503	MGD	PA-O3B	2.40	1.62	1.59
8	A	603	MFN	C26-C25	2.39	1.56	1.51
13	f	503	MGD	PB-O3B	2.38	1.62	1.59
8	A	603	MFN	O2-C9	2.37	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l	504	MGD	C17-N18	-2.36	1.34	1.38
13	B	504	MGD	C16-C17	2.36	1.48	1.41
13	Z	504	MGD	C16-C17	2.35	1.48	1.41
13	r	503	MGD	C16-C17	2.35	1.48	1.41
13	r	503	MGD	PA-O3B	2.34	1.62	1.59
13	f	503	MGD	C17-N18	-2.33	1.34	1.38
13	l	503	MGD	C17-N18	-2.32	1.34	1.38
13	f	503	MGD	C16-C17	2.32	1.48	1.41
13	H	503	MGD	PA-O3B	2.31	1.62	1.59
13	r	504	MGD	C17-N18	-2.30	1.34	1.38
13	Z	503	MGD	PB-O3B	2.30	1.62	1.59
13	f	504	MGD	C16-C17	2.26	1.48	1.41
13	T	504	MGD	C16-C17	2.25	1.48	1.41
13	l	503	MGD	C16-C17	2.25	1.48	1.41
13	r	504	MGD	C6-N1	-2.23	1.34	1.38
13	Z	503	MGD	C16-C17	2.20	1.48	1.41
13	N	503	MGD	C16-C17	2.19	1.48	1.41
13	H	503	MGD	C16-C17	2.19	1.48	1.41
13	T	504	MGD	C6-N1	-2.19	1.34	1.38
13	T	503	MGD	C16-C17	2.18	1.48	1.41
13	B	503	MGD	C16-C17	2.17	1.48	1.41
8	S	603	MFN	C26-C25	2.16	1.55	1.51
13	B	503	MGD	PA-O3B	2.16	1.61	1.59
8	A	603	MFN	C27-C26	2.16	1.59	1.52
8	e	603	MFN	C17-C16	2.15	1.55	1.51
8	k	603	MFN	C1-C2	2.15	1.53	1.48
8	G	603	MFN	C26-C25	2.14	1.55	1.51
13	l	503	MGD	C6-N1	-2.13	1.34	1.38
13	Z	504	MGD	C6-N1	-2.13	1.34	1.38
13	N	504	MGD	C6-N1	-2.13	1.34	1.38
13	B	504	MGD	C4-N9	-2.12	1.32	1.38
13	r	503	MGD	C6-N1	-2.11	1.34	1.38
8	A	603	MFN	C1-C2	2.11	1.53	1.48
13	B	504	MGD	C6-N1	-2.09	1.34	1.38
13	l	504	MGD	C16-C17	2.09	1.48	1.41
13	B	503	MGD	C6-N1	-2.09	1.34	1.38
8	e	603	MFN	C26-C25	2.09	1.55	1.51
13	T	503	MGD	C4-N9	-2.08	1.32	1.38
13	f	504	MGD	C6-N1	-2.08	1.35	1.38
13	T	503	MGD	C6-N1	-2.07	1.35	1.38
13	l	504	MGD	C6-N1	-2.07	1.35	1.38
13	H	504	MGD	C6-N1	-2.05	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	603	MFN	C13-C4	2.05	1.56	1.50
13	H	503	MGD	PB-O3B	2.04	1.61	1.59
13	H	504	MGD	C16-C17	2.04	1.48	1.41
13	f	503	MGD	C6-N1	-2.04	1.35	1.38
13	T	503	MGD	PA-O3B	2.04	1.61	1.59
8	q	603	MFN	C27-C26	2.04	1.59	1.52
8	q	603	MFN	O2-C9	2.04	1.42	1.37
8	e	603	MFN	C27-C26	2.02	1.58	1.52
8	S	603	MFN	C27-C26	2.02	1.58	1.52
8	q	603	MFN	C11-C6	-2.01	1.35	1.38
13	H	503	MGD	C6-N1	-2.01	1.35	1.38
8	q	603	MFN	C1-C2	2.01	1.52	1.48
13	f	504	MGD	C4-N9	-2.00	1.33	1.38

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	603	MFN	C1-C2-C3	-12.75	122.05	134.23
8	k	603	MFN	C1-C2-C3	-11.64	123.11	134.23
8	Y	603	MFN	C1-C2-C3	-11.60	123.15	134.23
8	G	603	MFN	C1-C2-C3	-11.26	123.48	134.23
8	M	603	MFN	C1-C2-C3	-11.16	123.57	134.23
8	S	603	MFN	C1-C2-C3	-10.68	124.03	134.23
8	q	603	MFN	C1-C2-C3	-10.68	124.03	134.23
8	A	603	MFN	C1-C2-C3	-10.32	124.38	134.23
8	k	603	MFN	C24-C23-N4	-8.02	91.97	110.57
13	T	504	MGD	C23-C14-N15	7.85	115.57	107.87
13	H	504	MGD	C23-C14-N15	7.26	115.00	107.87
13	f	504	MGD	C23-C14-N15	7.14	114.88	107.87
13	Z	504	MGD	C23-C14-N15	6.99	114.74	107.87
13	l	504	MGD	C23-C14-N15	6.88	114.62	107.87
13	B	504	MGD	C23-C14-N15	6.83	114.58	107.87
8	k	603	MFN	C22-C14-C23	-6.74	100.73	113.16
8	A	603	MFN	C8-C9-C10	-6.51	110.67	120.16
13	N	504	MGD	C23-C14-N15	6.33	114.08	107.87
13	l	503	MGD	C5-C4-N3	-6.31	118.34	128.39
13	r	504	MGD	C23-C14-N15	6.23	113.98	107.87
8	M	603	MFN	C8-C9-C10	-6.14	111.20	120.16
13	Z	504	MGD	C5-C4-N3	-6.06	118.74	128.39
8	q	603	MFN	C8-C9-C10	-6.04	111.34	120.16
13	T	504	MGD	C5-C4-N3	-6.01	118.82	128.39
13	B	503	MGD	C5-C4-N3	-5.99	118.85	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	503	MGD	C5-C4-N3	-5.98	118.88	128.39
13	H	503	MGD	C5-C4-N3	-5.97	118.89	128.39
13	Z	503	MGD	C5-C4-N3	-5.96	118.90	128.39
8	G	603	MFN	C8-C9-C10	-5.94	111.49	120.16
13	r	504	MGD	C5-C4-N3	-5.92	118.96	128.39
13	r	503	MGD	C5-C4-N3	-5.89	119.02	128.39
13	l	504	MGD	C5-C4-N3	-5.75	119.24	128.39
8	Y	603	MFN	C8-C9-C10	-5.73	111.80	120.16
13	l	503	MGD	C2-N3-C4	5.73	122.17	112.30
8	k	603	MFN	C8-C9-C10	-5.72	111.81	120.16
13	H	504	MGD	C5-C4-N3	-5.71	119.30	128.39
8	S	603	MFN	C8-C9-C10	-5.69	111.86	120.16
13	B	503	MGD	C2-N3-C4	5.64	122.01	112.30
13	N	504	MGD	C5-C4-N3	-5.61	119.46	128.39
13	Z	503	MGD	C2-N3-C4	5.60	121.94	112.30
13	r	503	MGD	C2-N3-C4	5.57	121.89	112.30
13	N	503	MGD	C2-N3-C4	5.53	121.83	112.30
13	H	503	MGD	C2-N3-C4	5.51	121.79	112.30
13	Z	504	MGD	C2-N3-C4	5.50	121.77	112.30
13	r	504	MGD	C2-N3-C4	5.49	121.76	112.30
13	f	504	MGD	C5-C4-N3	-5.49	119.66	128.39
13	f	503	MGD	C5-C4-N3	-5.49	119.66	128.39
13	T	503	MGD	C5-C4-N3	-5.41	119.78	128.39
8	e	603	MFN	C8-C9-C10	-5.39	112.30	120.16
13	T	504	MGD	C2-N3-C4	5.35	121.52	112.30
8	k	603	MFN	O1-C5-C4	-5.31	107.71	111.43
13	B	504	MGD	C5-C4-N3	-5.28	119.99	128.39
13	l	504	MGD	C2-N3-C4	5.28	121.39	112.30
13	f	504	MGD	C2-N3-C4	5.26	121.36	112.30
13	f	503	MGD	C2-N3-C4	5.25	121.34	112.30
13	T	503	MGD	C2-N3-C4	5.23	121.31	112.30
13	N	504	MGD	C2-N3-C4	5.22	121.30	112.30
13	H	504	MGD	C2-N3-C4	5.16	121.19	112.30
8	Y	603	MFN	O1-C5-C4	-5.09	107.86	111.43
13	B	504	MGD	C2-N3-C4	5.08	121.04	112.30
8	k	603	MFN	C26-C27-C28	-4.96	99.02	113.79
8	e	603	MFN	O1-C5-C4	-4.91	107.99	111.43
13	f	504	MGD	C19-N20-C21	4.75	121.75	113.36
13	Z	504	MGD	C19-N20-C21	4.75	121.73	113.36
13	Z	503	MGD	C19-N20-C21	4.74	121.72	113.36
13	H	504	MGD	C19-N20-C21	4.73	121.71	113.36
13	l	503	MGD	C19-N20-C21	4.70	121.66	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	f	503	MGD	C19-N20-C21	4.67	121.60	113.36
13	H	503	MGD	C19-N20-C21	4.66	121.59	113.36
13	B	503	MGD	C19-N20-C21	4.63	121.53	113.36
8	Y	603	MFN	C22-C14-C23	-4.60	104.69	113.16
13	r	504	MGD	C19-N20-C21	4.60	121.47	113.36
13	N	504	MGD	C19-N20-C21	4.58	121.45	113.36
8	M	603	MFN	C22-C14-C23	-4.58	104.71	113.16
13	r	503	MGD	C19-N20-C21	4.58	121.44	113.36
8	k	603	MFN	C26-C25-N4	-4.57	107.81	115.86
13	T	503	MGD	C19-N20-C21	4.57	121.42	113.36
8	Y	603	MFN	C27-C28-C29	-4.56	102.96	108.81
13	B	504	MGD	C19-N20-C21	4.56	121.40	113.36
13	T	504	MGD	C19-N20-C21	4.52	121.34	113.36
13	N	503	MGD	C19-N20-C21	4.52	121.33	113.36
8	G	603	MFN	C22-C14-C23	-4.52	104.83	113.16
8	q	603	MFN	C22-C14-C23	-4.51	104.84	113.16
13	B	503	MGD	C23-C14-N15	4.50	112.29	107.87
13	l	504	MGD	C19-N20-C21	4.48	121.27	113.36
8	k	603	MFN	C27-C26-C25	4.48	123.05	113.06
13	l	503	MGD	N9-C4-N3	4.37	134.69	125.95
13	r	503	MGD	C23-C14-N15	4.36	112.15	107.87
13	T	503	MGD	C6-C5-N7	4.35	138.20	130.29
13	B	504	MGD	C6-C5-N7	4.34	138.19	130.29
13	B	503	MGD	N9-C4-N3	4.34	134.63	125.95
13	f	504	MGD	C6-C5-N7	4.33	138.18	130.29
13	f	503	MGD	C6-C5-N7	4.32	138.14	130.29
13	Z	503	MGD	C23-C14-N15	4.25	112.05	107.87
13	Z	504	MGD	N9-C4-N3	4.24	134.43	125.95
13	r	503	MGD	C6-C5-N7	4.23	138.00	130.29
13	l	503	MGD	C23-C14-N15	4.20	111.99	107.87
13	N	503	MGD	C23-C14-N15	4.19	111.98	107.87
13	r	504	MGD	C6-C5-N7	4.17	137.89	130.29
13	Z	503	MGD	N9-C4-N3	4.17	134.30	125.95
13	Z	503	MGD	C6-C5-N7	4.15	137.85	130.29
13	H	503	MGD	N9-C4-N3	4.13	134.22	125.95
8	e	603	MFN	O2-C13-C4	-4.13	99.03	109.06
13	l	504	MGD	C6-C5-N7	4.11	137.77	130.29
13	N	503	MGD	N9-C4-N3	4.10	134.16	125.95
13	T	503	MGD	C23-C14-N15	4.09	111.89	107.87
13	f	503	MGD	C23-C14-N15	4.09	111.88	107.87
13	N	503	MGD	C6-C5-N7	4.08	137.71	130.29
13	T	504	MGD	N9-C4-N3	4.05	134.06	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	504	MGD	C6-C5-N7	4.05	137.66	130.29
13	T	504	MGD	C6-C5-N7	4.00	137.58	130.29
8	S	603	MFN	O1-C5-C4	-4.00	108.62	111.43
8	e	603	MFN	C24-C23-N4	-4.00	101.30	110.57
13	B	503	MGD	C6-C5-N7	3.98	137.54	130.29
13	l	503	MGD	C6-C5-N7	3.97	137.52	130.29
13	H	503	MGD	C6-C5-N7	3.96	137.50	130.29
8	S	603	MFN	C19-N3-C21	3.96	131.61	121.68
13	H	504	MGD	N9-C4-N3	3.95	133.85	125.95
13	r	504	MGD	N9-C4-N3	3.95	133.85	125.95
13	r	503	MGD	N9-C4-N3	3.92	133.80	125.95
13	N	504	MGD	N9-C4-N3	3.91	133.77	125.95
8	S	603	MFN	C24-C23-N4	-3.90	101.52	110.57
8	M	603	MFN	C20-C19-N3	-3.89	101.55	110.57
13	l	504	MGD	N9-C4-N3	3.88	133.70	125.95
13	Z	504	MGD	C6-C5-N7	3.85	137.30	130.29
13	H	504	MGD	C6-C5-N7	3.83	137.27	130.29
8	k	603	MFN	O2-C13-C4	-3.78	99.89	109.06
8	M	603	MFN	C26-C27-C28	-3.65	102.92	113.79
8	S	603	MFN	O2-C13-C4	-3.64	100.21	109.06
8	Y	603	MFN	O2-C13-C4	-3.61	100.29	109.06
8	G	603	MFN	O1-C5-C4	-3.58	108.92	111.43
13	f	503	MGD	N9-C4-N3	3.58	133.11	125.95
13	f	504	MGD	N9-C4-N3	3.56	133.07	125.95
13	H	504	MGD	O4'-C1'-N9	3.55	116.41	108.36
8	q	603	MFN	C20-C19-N3	-3.54	102.35	110.57
13	T	503	MGD	N9-C4-N3	3.53	133.02	125.95
13	N	504	MGD	O4'-C1'-N9	3.44	116.16	108.36
13	B	504	MGD	N9-C4-N3	3.44	132.82	125.95
8	q	603	MFN	O1-C5-C4	-3.42	109.03	111.43
8	G	603	MFN	O2-C13-C4	-3.39	100.82	109.06
8	M	603	MFN	O1-C5-C4	-3.39	109.05	111.43
8	A	603	MFN	C11-C10-C9	3.38	123.59	119.73
8	M	603	MFN	C24-C23-N4	-3.26	103.00	110.57
13	Z	504	MGD	O4'-C1'-N9	3.20	115.60	108.36
13	B	504	MGD	O11-C23-N22	-3.17	105.72	108.61
8	M	603	MFN	C11-C10-C9	3.16	123.34	119.73
8	M	603	MFN	O2-C13-C4	-3.15	101.42	109.06
13	f	503	MGD	C4-C5-N7	-3.10	105.76	110.67
13	r	503	MGD	C4-C5-N7	-3.09	105.78	110.67
13	f	504	MGD	C4-C5-N7	-3.09	105.78	110.67
13	T	504	MGD	C4-C5-N7	-3.06	105.82	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	r	504	MGD	C4-C5-N7	-3.05	105.84	110.67
13	T	503	MGD	C4-C5-N7	-3.04	105.85	110.67
8	q	603	MFN	C11-C10-C9	3.04	123.20	119.73
8	A	603	MFN	C20-C19-N3	-3.04	103.52	110.57
13	l	504	MGD	C4-C5-N7	-3.03	105.87	110.67
13	N	503	MGD	C4-C5-N7	-3.00	105.92	110.67
13	B	504	MGD	C4-C5-N7	-3.00	105.92	110.67
13	l	503	MGD	C4-C5-N7	-3.00	105.92	110.67
13	Z	503	MGD	C4-C5-N7	-2.97	105.96	110.67
8	e	603	MFN	C19-N3-C21	2.95	129.07	121.68
13	H	503	MGD	C4-C5-N7	-2.90	106.07	110.67
8	G	603	MFN	C20-C19-N3	-2.89	103.86	110.57
8	A	603	MFN	C26-C25-N4	2.87	120.92	115.86
8	e	603	MFN	O15-C34-C33	2.87	121.38	113.93
13	Z	504	MGD	C4-C5-N7	-2.86	106.13	110.67
8	e	603	MFN	O1-C2-C1	2.86	127.82	118.00
8	k	603	MFN	C27-C28-C29	-2.86	105.14	108.81
8	A	603	MFN	O1-C5-C4	-2.85	109.43	111.43
8	k	603	MFN	C14-C22-C21	2.85	119.41	113.06
13	N	504	MGD	C4-C5-N7	-2.82	106.19	110.67
13	H	504	MGD	C4-C5-N7	-2.79	106.24	110.67
13	f	504	MGD	O11-C23-N22	-2.79	106.07	108.61
8	G	603	MFN	C11-C10-C9	2.79	122.92	119.73
8	A	603	MFN	O7-C24-O8	-2.79	117.76	124.08
8	k	603	MFN	C20-C19-N3	-2.79	104.11	110.57
8	S	603	MFN	C11-C10-C9	2.78	122.91	119.73
13	B	503	MGD	C4-C5-N7	-2.77	106.28	110.67
8	k	603	MFN	O1-C2-C1	2.77	127.50	118.00
8	G	603	MFN	C32-C33-C34	2.74	112.33	108.81
13	N	504	MGD	C17-C16-N15	2.72	123.68	116.27
13	l	503	MGD	C17-C16-N15	2.72	123.68	116.27
8	e	603	MFN	O7-C24-O8	-2.71	117.93	124.08
8	G	603	MFN	O15-C34-C33	2.71	120.96	113.93
13	B	503	MGD	O6-C6-C5	-2.68	119.44	126.53
13	H	504	MGD	O17-C17-C16	-2.68	120.79	127.26
8	k	603	MFN	O15-C34-C33	2.68	120.89	113.93
8	Y	603	MFN	O1-C2-C1	2.68	127.19	118.00
8	M	603	MFN	O10-C29-C28	2.67	120.87	113.93
8	k	603	MFN	C11-C10-C9	2.67	122.78	119.73
8	M	603	MFN	O7-C24-O8	-2.67	118.03	124.08
8	Y	603	MFN	C11-C10-C9	2.66	122.77	119.73
13	l	504	MGD	O4'-C1'-N9	2.66	114.39	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	603	MFN	C19-N3-C21	2.65	128.33	121.68
8	S	603	MFN	O3-C16-N2	-2.65	117.84	123.03
8	k	603	MFN	O10-C29-C28	2.61	120.72	113.93
13	r	504	MGD	C17-C16-N15	2.60	123.35	116.27
8	q	603	MFN	O10-C29-C28	2.58	120.64	113.93
13	r	503	MGD	C17-C16-N15	2.58	123.30	116.27
13	H	503	MGD	C17-C16-N15	2.55	123.23	116.27
13	l	503	MGD	O17-C17-C16	-2.55	121.12	127.26
13	f	504	MGD	O17-C17-C16	-2.54	121.13	127.26
13	f	503	MGD	C17-C16-N15	2.51	123.12	116.27
13	Z	503	MGD	O17-C17-C16	-2.50	121.23	127.26
13	N	504	MGD	C4'-O4'-C1'	-2.50	103.94	109.47
13	l	504	MGD	O17-C17-C16	-2.50	121.23	127.26
8	M	603	MFN	C27-C26-C25	2.50	118.63	113.06
8	M	603	MFN	O15-C34-C33	2.46	120.33	113.93
13	Z	503	MGD	C17-C16-N15	2.46	122.99	116.27
8	Y	603	MFN	O15-C34-C33	2.44	120.26	113.93
8	e	603	MFN	O7-C24-C23	2.43	121.74	113.51
13	H	503	MGD	C23-C14-N15	2.43	110.25	107.87
8	q	603	MFN	O5-C20-C19	2.43	121.72	113.51
13	H	503	MGD	O17-C17-C16	-2.41	121.46	127.26
13	T	503	MGD	O17-C17-C16	-2.41	121.46	127.26
13	T	504	MGD	O17-C17-C16	-2.41	121.46	127.26
13	N	503	MGD	O17-C17-C16	-2.40	121.47	127.26
13	B	503	MGD	C5-C6-N1	2.39	119.34	113.25
13	f	503	MGD	O17-C17-C16	-2.38	121.51	127.26
13	B	503	MGD	C17-C16-N15	2.38	122.77	116.27
13	f	504	MGD	O4'-C1'-N9	2.38	113.74	108.36
8	e	603	MFN	C11-C10-C9	2.38	122.44	119.73
13	H	503	MGD	O6-C6-C5	-2.37	120.27	126.53
8	A	603	MFN	O10-C29-C28	2.37	120.07	113.93
13	Z	503	MGD	O6-C6-C5	-2.36	120.29	126.53
8	k	603	MFN	O3-C16-N2	-2.36	118.41	123.03
13	B	503	MGD	O17-C17-C16	-2.35	121.59	127.26
13	N	503	MGD	O6-C6-C5	-2.34	120.34	126.53
8	M	603	MFN	C7-C8-C9	2.34	122.40	119.73
13	N	503	MGD	C17-C16-N15	2.33	122.63	116.27
8	A	603	MFN	C22-C14-C23	-2.32	108.88	113.16
13	Z	504	MGD	C17-C16-N15	2.32	122.60	116.27
8	M	603	MFN	C22-C21-N3	-2.32	111.78	115.86
8	Y	603	MFN	C20-C19-N3	-2.31	105.20	110.57
8	M	603	MFN	O3-C16-N2	-2.31	118.49	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	q	603	MFN	O15-C34-C33	2.31	119.93	113.93
13	l	503	MGD	O6-C6-C5	-2.31	120.44	126.53
13	H	504	MGD	O6-C6-C5	-2.31	120.44	126.53
8	S	603	MFN	O7-C24-O8	-2.30	118.85	124.08
8	S	603	MFN	O10-C29-C28	2.30	119.90	113.93
8	A	603	MFN	O5-C20-C19	2.30	121.28	113.51
13	B	504	MGD	C17-C16-N15	2.29	122.52	116.27
8	e	603	MFN	O10-C29-C28	2.29	119.88	113.93
13	N	504	MGD	O6-C6-C5	-2.29	120.49	126.53
8	M	603	MFN	C19-N3-C21	2.29	127.42	121.68
13	Z	504	MGD	O6-C6-C5	-2.28	120.51	126.53
13	T	503	MGD	C17-C16-N15	2.28	122.49	116.27
8	k	603	MFN	C17-C16-N2	2.28	120.50	116.34
13	Z	504	MGD	C4'-O4'-C1'	-2.27	104.45	109.47
13	Z	503	MGD	C5-C6-N1	2.27	119.03	113.25
8	M	603	MFN	C26-C25-N4	-2.27	111.87	115.86
8	A	603	MFN	O15-C34-C33	2.26	119.81	113.93
8	A	603	MFN	C27-C26-C25	-2.26	108.02	113.06
8	G	603	MFN	O1-C2-C1	2.26	125.75	118.00
13	l	503	MGD	C5-C6-N1	2.25	118.98	113.25
8	k	603	MFN	O9-C25-C26	2.24	126.07	122.02
13	B	504	MGD	O17-C17-C16	-2.23	121.88	127.26
8	G	603	MFN	C26-C27-C28	-2.23	107.16	113.79
13	r	504	MGD	O6-C6-C5	-2.23	120.65	126.53
8	k	603	MFN	O15-C34-O14	-2.23	119.03	124.08
8	q	603	MFN	O2-C13-C4	-2.22	103.66	109.06
8	q	603	MFN	O3-C16-N2	-2.22	118.67	123.03
13	N	503	MGD	C5-C6-N1	2.22	118.90	113.25
13	T	504	MGD	O4'-C1'-N9	2.20	113.36	108.36
13	T	504	MGD	O6-C6-C5	-2.20	120.72	126.53
8	M	603	MFN	O1-C2-C1	2.20	125.55	118.00
8	k	603	MFN	O7-C24-O8	-2.20	119.10	124.08
13	r	503	MGD	O6-C6-C5	-2.20	120.74	126.53
8	e	603	MFN	O10-C29-O11	-2.19	119.10	124.08
13	B	504	MGD	O6-C6-C5	-2.19	120.76	126.53
8	Y	603	MFN	O10-C29-O11	-2.18	119.13	124.08
13	l	504	MGD	O6-C6-C5	-2.18	120.78	126.53
13	r	504	MGD	C5-C6-N1	2.17	118.77	113.25
13	T	503	MGD	O6-C6-C5	-2.17	120.81	126.53
13	r	504	MGD	O17-C17-C16	-2.16	122.04	127.26
8	A	603	MFN	O1-C2-C1	2.16	125.42	118.00
8	S	603	MFN	C7-C8-C9	2.16	122.19	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	603	MFN	C24-C23-N4	-2.16	105.57	110.57
8	q	603	MFN	O1-C2-C1	2.15	125.40	118.00
13	T	504	MGD	C17-C16-N15	2.15	122.14	116.27
13	l	504	MGD	O11-C23-N22	-2.15	106.66	108.61
13	r	503	MGD	O17-C17-C16	-2.15	122.08	127.26
13	Z	503	MGD	C8-N7-C5	2.14	108.08	104.26
13	r	503	MGD	O11-C23-C14	-2.14	107.54	108.96
13	l	503	MGD	C16-C17-N18	2.13	117.98	112.13
8	G	603	MFN	O5-C20-C19	2.13	120.72	113.51
8	Y	603	MFN	O5-C20-C19	2.13	120.71	113.51
8	S	603	MFN	O15-C34-C33	2.13	119.45	113.93
8	S	603	MFN	O1-C2-C1	2.13	125.30	118.00
13	H	503	MGD	C5-C6-N1	2.12	118.66	113.25
13	r	503	MGD	C5-C6-N1	2.12	118.66	113.25
13	l	504	MGD	C17-C16-N15	2.12	122.05	116.27
13	l	503	MGD	C8-N7-C5	2.12	108.03	104.26
13	N	504	MGD	O17-C17-C16	-2.12	122.15	127.26
8	S	603	MFN	O5-C20-C19	2.11	120.65	113.51
8	M	603	MFN	C14-C23-N4	-2.11	106.73	110.91
13	r	503	MGD	C8-N7-C5	2.11	108.02	104.26
13	Z	503	MGD	C16-C17-N18	2.11	117.92	112.13
8	G	603	MFN	O10-C29-O11	-2.10	119.31	124.08
13	N	503	MGD	C8-N7-C5	2.10	108.00	104.26
13	T	504	MGD	C8-N7-C5	2.10	108.00	104.26
13	r	504	MGD	C8-N7-C5	2.10	107.99	104.26
13	H	503	MGD	O11-C23-C14	-2.09	107.57	108.96
13	H	503	MGD	C16-C17-N18	2.09	117.87	112.13
13	Z	504	MGD	C5-C6-N1	2.09	118.57	113.25
13	Z	504	MGD	O17-C17-C16	-2.09	122.23	127.26
13	T	504	MGD	C5-C6-N1	2.09	118.56	113.25
8	S	603	MFN	C18-C19-N3	2.08	115.03	110.91
13	f	504	MGD	O6-C6-C5	-2.07	121.06	126.53
13	B	503	MGD	C8-N7-C5	2.07	107.95	104.26
13	B	504	MGD	C1'-N9-C4	-2.07	120.37	126.49
13	l	504	MGD	C8-N7-C5	2.07	107.94	104.26
8	S	603	MFN	C14-C23-C24	2.07	115.26	110.35
8	q	603	MFN	O5-C20-O4	-2.07	119.39	124.08
8	A	603	MFN	C7-C8-C9	2.06	122.09	119.73
8	Y	603	MFN	C26-C27-C28	-2.06	107.65	113.79
13	N	504	MGD	C5-C6-N1	2.06	118.49	113.25
13	T	503	MGD	C8-N7-C5	2.06	107.92	104.26
13	N	504	MGD	C16-C17-N18	2.05	117.77	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	603	MFN	O10-C29-C28	2.05	119.26	113.93
13	f	504	MGD	C17-C16-N15	2.05	121.86	116.27
13	T	503	MGD	O11-C23-C14	-2.05	107.60	108.96
8	A	603	MFN	C17-C16-N2	2.04	120.06	116.34
13	H	504	MGD	C17-C16-N15	2.04	121.82	116.27
13	l	504	MGD	C5-C6-N1	2.04	118.44	113.25
13	r	504	MGD	C16-C17-N18	2.03	117.71	112.13
13	f	503	MGD	C8-N7-C5	2.03	107.88	104.26
13	f	503	MGD	C16-C17-N18	2.03	117.71	112.13
13	f	504	MGD	C8-N7-C5	2.03	107.88	104.26
8	q	603	MFN	C26-C27-C28	-2.02	107.77	113.79
13	B	504	MGD	C8-N7-C5	2.02	107.86	104.26
13	B	504	MGD	C5-C6-N1	2.02	118.40	113.25
13	T	503	MGD	C5-C6-N1	2.02	118.39	113.25
13	B	503	MGD	C16-C17-N18	2.01	117.66	112.13
13	Z	504	MGD	C16-C17-N18	2.01	117.64	112.13
8	G	603	MFN	O15-C34-O14	-2.01	119.53	124.08
13	Z	504	MGD	O3B-PB-O1B	-2.00	104.67	110.70
8	k	603	MFN	O5-C20-O4	-2.00	119.54	124.08

There are no chirality outliers.

All (220) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	603	MFN	N1-C1-C2-O1
8	A	603	MFN	N1-C1-C2-C3
8	A	603	MFN	C6-C12-C15-N2
8	A	603	MFN	C31-C32-C33-C28
8	A	603	MFN	C31-C32-C33-C34
8	G	603	MFN	N1-C1-C2-O1
8	G	603	MFN	N1-C1-C2-C3
8	G	603	MFN	C26-C27-C28-C29
8	G	603	MFN	C6-C12-C15-N2
8	G	603	MFN	C31-C32-C33-C28
8	G	603	MFN	C31-C32-C33-C34
8	M	603	MFN	N1-C1-C2-O1
8	M	603	MFN	N1-C1-C2-C3
8	M	603	MFN	C26-C27-C28-C29
8	M	603	MFN	C26-C27-C28-C33
8	M	603	MFN	C27-C28-C33-C34
8	M	603	MFN	C29-C28-C33-C32
8	M	603	MFN	C29-C28-C33-C34

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Mol	Chain	Res	Type	Atoms
8	M	603	MFN	C6-C12-C15-N2
8	M	603	MFN	C31-C32-C33-C28
8	M	603	MFN	C31-C32-C33-C34
8	S	603	MFN	N1-C1-C2-O1
8	S	603	MFN	N1-C1-C2-C3
8	S	603	MFN	C18-C19-N3-C21
8	S	603	MFN	C26-C27-C28-C29
8	S	603	MFN	C29-C28-C33-C34
8	S	603	MFN	C17-C18-C19-N3
8	S	603	MFN	C6-C12-C15-N2
8	Y	603	MFN	N1-C1-C2-O1
8	Y	603	MFN	N1-C1-C2-C3
8	Y	603	MFN	C26-C27-C28-C29
8	Y	603	MFN	C26-C27-C28-C33
8	Y	603	MFN	C6-C12-C15-N2
8	Y	603	MFN	C31-C32-C33-C28
8	Y	603	MFN	C31-C32-C33-C34
8	e	603	MFN	C27-C28-C33-C32
8	e	603	MFN	C29-C28-C33-C32
8	e	603	MFN	C29-C28-C33-C34
8	e	603	MFN	C6-C12-C15-N2
8	k	603	MFN	N1-C1-C2-O1
8	k	603	MFN	N1-C1-C2-C3
8	k	603	MFN	C26-C27-C28-C29
8	k	603	MFN	C26-C27-C28-C33
8	k	603	MFN	C27-C28-C33-C34
8	k	603	MFN	C29-C28-C33-C32
8	k	603	MFN	C29-C28-C33-C34
8	k	603	MFN	C6-C12-C15-N2
8	k	603	MFN	C31-C32-C33-C28
8	k	603	MFN	C31-C32-C33-C34
8	q	603	MFN	N1-C1-C2-O1
8	q	603	MFN	N1-C1-C2-C3
8	q	603	MFN	C26-C27-C28-C29
8	q	603	MFN	C26-C27-C28-C33
8	q	603	MFN	C6-C12-C15-N2
8	q	603	MFN	C31-C32-C33-C28
8	q	603	MFN	C31-C32-C33-C34
13	B	503	MGD	C5'-O5'-PB-O2B
13	B	503	MGD	C5'-O5'-PB-O3B
13	B	503	MGD	O3A-C10-C11-C12
13	H	503	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
13	H	503	MGD	C5'-O5'-PB-O2B
13	H	503	MGD	C5'-O5'-PB-O3B
13	H	503	MGD	O3A-C10-C11-C12
13	N	503	MGD	C5'-O5'-PB-O2B
13	N	503	MGD	C5'-O5'-PB-O3B
13	N	503	MGD	O3A-C10-C11-C12
13	T	503	MGD	PA-O3B-PB-O5'
13	T	503	MGD	O3A-C10-C11-C12
13	Z	503	MGD	PA-O3B-PB-O5'
13	Z	503	MGD	C5'-O5'-PB-O1B
13	Z	503	MGD	C5'-O5'-PB-O2B
13	Z	503	MGD	C5'-O5'-PB-O3B
13	Z	503	MGD	O3A-C10-C11-C12
13	f	503	MGD	C5'-O5'-PB-O1B
13	f	503	MGD	C5'-O5'-PB-O2B
13	f	503	MGD	C5'-O5'-PB-O3B
13	f	503	MGD	O3A-C10-C11-C12
13	l	503	MGD	C5'-O5'-PB-O2B
13	l	503	MGD	O3A-C10-C11-C12
13	r	503	MGD	C5'-O5'-PB-O1B
13	r	503	MGD	C5'-O5'-PB-O2B
13	r	503	MGD	C5'-O5'-PB-O3B
13	r	503	MGD	O3A-C10-C11-C12
8	e	603	MFN	C18-C19-N3-C21
8	e	603	MFN	C17-C18-C19-N3
8	Y	603	MFN	C18-C19-N3-C21
8	k	603	MFN	C30-C31-C32-C33
8	q	603	MFN	C30-C31-C32-C33
8	Y	603	MFN	C23-C14-C22-C21
8	G	603	MFN	N3-C19-C20-O4
8	G	603	MFN	N3-C19-C20-O5
8	e	603	MFN	N3-C19-C20-O4
8	S	603	MFN	C17-C18-C19-C20
8	S	603	MFN	C18-C19-C20-O5
8	G	603	MFN	C30-C31-C32-C33
8	M	603	MFN	C8-C9-O2-C13
8	e	603	MFN	N3-C19-C20-O5
8	q	603	MFN	C23-C14-C22-C21
8	e	603	MFN	N4-C23-C24-O8
13	B	503	MGD	O4'-C4'-C5'-O5'
13	H	503	MGD	O4'-C4'-C5'-O5'
13	H	503	MGD	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	M	603	MFN	C27-C28-C33-C32
8	k	603	MFN	C27-C28-C33-C32
8	A	603	MFN	N3-C19-C20-O4
8	Y	603	MFN	N4-C23-C24-O7
8	q	603	MFN	N4-C23-C24-O7
8	q	603	MFN	N3-C19-C20-O4
8	q	603	MFN	N3-C19-C20-O5
8	S	603	MFN	C18-C19-C20-O4
8	S	603	MFN	C25-C26-C27-C28
8	G	603	MFN	C27-C28-C33-C34
8	e	603	MFN	C27-C28-C33-C34
8	A	603	MFN	N3-C19-C20-O5
8	Y	603	MFN	N4-C23-C24-O8
8	Y	603	MFN	N3-C19-C20-O4
8	Y	603	MFN	N3-C19-C20-O5
8	q	603	MFN	N4-C23-C24-O8
8	k	603	MFN	C32-C33-C34-O14
8	G	603	MFN	C33-C28-C29-O10
8	G	603	MFN	C33-C28-C29-O11
8	Y	603	MFN	C33-C28-C29-O10
8	Y	603	MFN	C33-C28-C29-O11
8	k	603	MFN	C28-C33-C34-O15
8	Y	603	MFN	C29-C28-C33-C34
13	B	503	MGD	O3A-C10-C11-O11
13	H	503	MGD	O3A-C10-C11-O11
13	N	503	MGD	O3A-C10-C11-O11
13	T	503	MGD	O3A-C10-C11-O11
13	Z	503	MGD	O3A-C10-C11-O11
13	f	503	MGD	O3A-C10-C11-O11
13	l	503	MGD	O3A-C10-C11-O11
8	A	603	MFN	C18-C19-C20-O4
8	q	603	MFN	C18-C19-C20-O4
13	B	503	MGD	PA-O3B-PB-O5'
13	H	503	MGD	PA-O3B-PB-O5'
13	N	503	MGD	PA-O3B-PB-O5'
13	Z	504	MGD	PA-O3B-PB-O5'
13	f	503	MGD	PA-O3B-PB-O5'
13	l	503	MGD	PA-O3B-PB-O5'
13	l	504	MGD	PA-O3B-PB-O5'
13	r	503	MGD	PA-O3B-PB-O5'
8	e	603	MFN	N4-C23-C24-O7
8	A	603	MFN	C15-C12-C6-C7

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Mol	Chain	Res	Type	Atoms
8	e	603	MFN	C17-C18-C19-C20
13	B	503	MGD	C3'-C4'-C5'-O5'
8	A	603	MFN	C18-C19-C20-O5
8	Y	603	MFN	C18-C19-C20-O4
8	Y	603	MFN	C18-C19-C20-O5
8	q	603	MFN	C18-C19-C20-O5
8	M	603	MFN	N3-C19-C20-O4
8	S	603	MFN	N3-C19-C20-O5
13	B	504	MGD	PB-O3B-PA-O1A
8	e	603	MFN	C31-C32-C33-C34
13	B	503	MGD	C5'-O5'-PB-O1B
13	N	503	MGD	C5'-O5'-PB-O1B
13	T	504	MGD	C10-O3A-PA-O3B
13	l	503	MGD	C5'-O5'-PB-O1B
13	l	503	MGD	C5'-O5'-PB-O3B
8	q	603	MFN	C14-C23-C24-O8
8	S	603	MFN	C27-C28-C33-C32
8	Y	603	MFN	C27-C28-C33-C32
13	f	503	MGD	O4'-C4'-C5'-O5'
8	M	603	MFN	N3-C19-C20-O5
8	S	603	MFN	N3-C19-C20-O4
8	S	603	MFN	C27-C28-C33-C34
8	S	603	MFN	C29-C28-C33-C32
8	Y	603	MFN	C27-C28-C33-C34
8	Y	603	MFN	C29-C28-C33-C32
8	q	603	MFN	C14-C23-C24-O7
8	k	603	MFN	N3-C19-C20-O4
8	S	603	MFN	C32-C33-C34-O15
8	Y	603	MFN	C27-C28-C29-O10
8	Y	603	MFN	C27-C28-C29-O11
8	Y	603	MFN	C32-C33-C34-O15
8	e	603	MFN	C27-C28-C29-O11
8	k	603	MFN	C32-C33-C34-O15
8	G	603	MFN	C29-C28-C33-C34
8	k	603	MFN	N3-C19-C20-O5
13	r	503	MGD	O3A-C10-C11-O11
8	M	603	MFN	O12-C30-C31-C32
8	A	603	MFN	O13-C30-C31-C32
8	A	603	MFN	O12-C30-C31-C32
8	Y	603	MFN	O13-C30-C31-C32
8	e	603	MFN	O12-C30-C31-C32
8	e	603	MFN	O13-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
8	M	603	MFN	O13-C30-C31-C32
8	S	603	MFN	O12-C30-C31-C32
8	Y	603	MFN	O12-C30-C31-C32
13	r	503	MGD	O4'-C4'-C5'-O5'
8	G	603	MFN	C18-C19-C20-O4
8	M	603	MFN	C14-C23-C24-O8
8	M	603	MFN	N4-C23-C24-O8
8	G	603	MFN	C18-C19-C20-O5
8	S	603	MFN	O13-C30-C31-C32
8	q	603	MFN	O13-C30-C31-C32
8	G	603	MFN	C15-C12-C6-C7
8	e	603	MFN	N1-C1-C2-C3
13	N	503	MGD	O4'-C4'-C5'-O5'
13	Z	503	MGD	PA-O3B-PB-O1B
8	M	603	MFN	C14-C23-C24-O7
8	e	603	MFN	N1-C1-C2-O1
8	G	603	MFN	C27-C28-C29-O10
8	S	603	MFN	C32-C33-C34-O14
8	Y	603	MFN	C32-C33-C34-O14
8	e	603	MFN	C27-C28-C29-O10
13	f	503	MGD	C3'-C4'-C5'-O5'
8	q	603	MFN	O12-C30-C31-C32
8	k	603	MFN	O12-C30-C31-C32
8	e	603	MFN	C14-C23-C24-O7
8	e	603	MFN	C14-C23-C24-O8
8	Y	603	MFN	C15-C12-C6-C7
8	k	603	MFN	O13-C30-C31-C32
13	H	504	MGD	PB-O3B-PA-O2A
13	Z	503	MGD	PA-O3B-PB-O2B
13	f	504	MGD	PB-O3B-PA-O2A
13	r	503	MGD	PA-O3B-PB-O1B
13	r	503	MGD	PA-O3B-PB-O2B
13	r	504	MGD	PB-O3B-PA-O2A
13	Z	503	MGD	O4'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 33 short contacts:

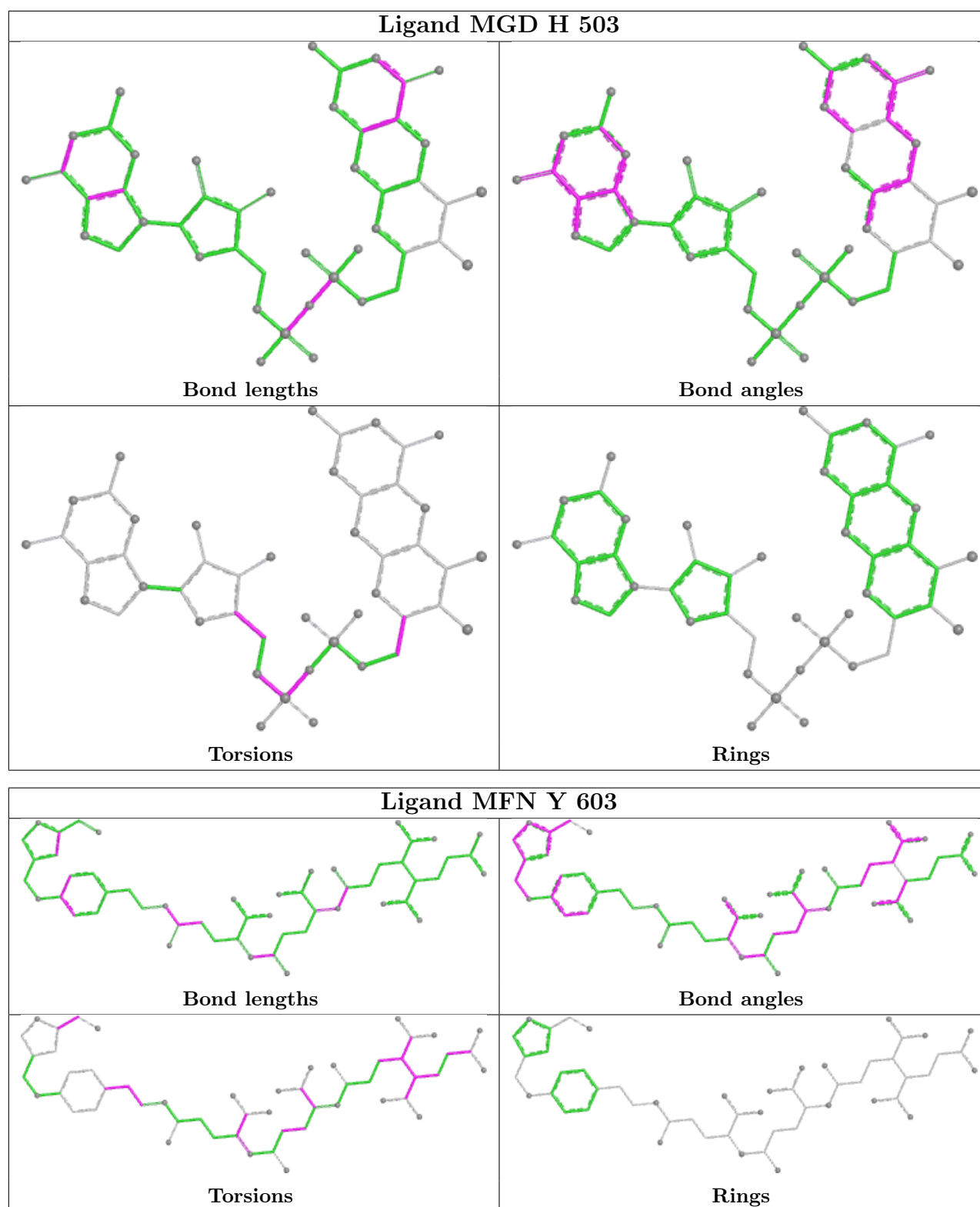
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	503	MGD	2	0
8	Y	603	MFN	4	0
13	T	504	MGD	1	0

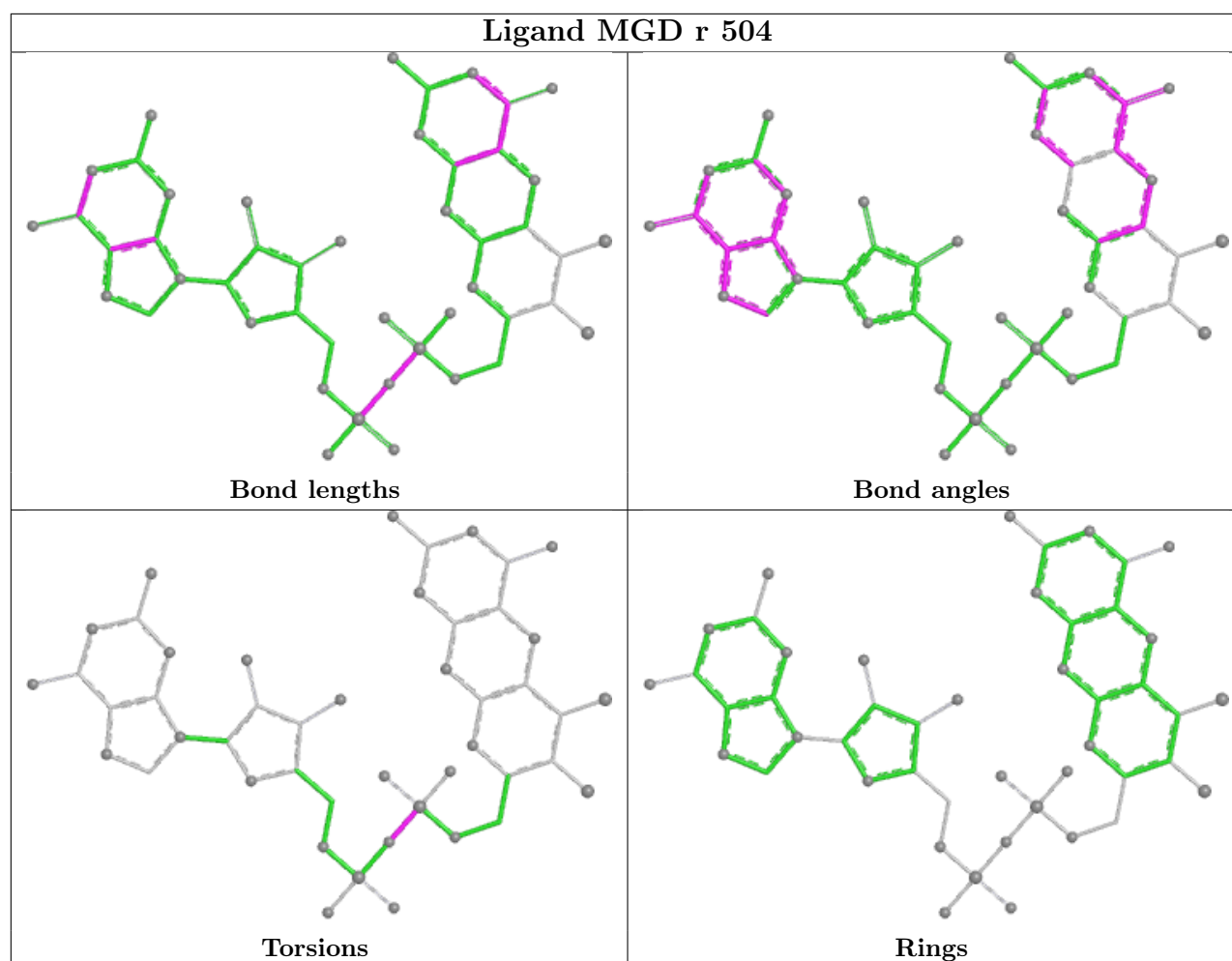
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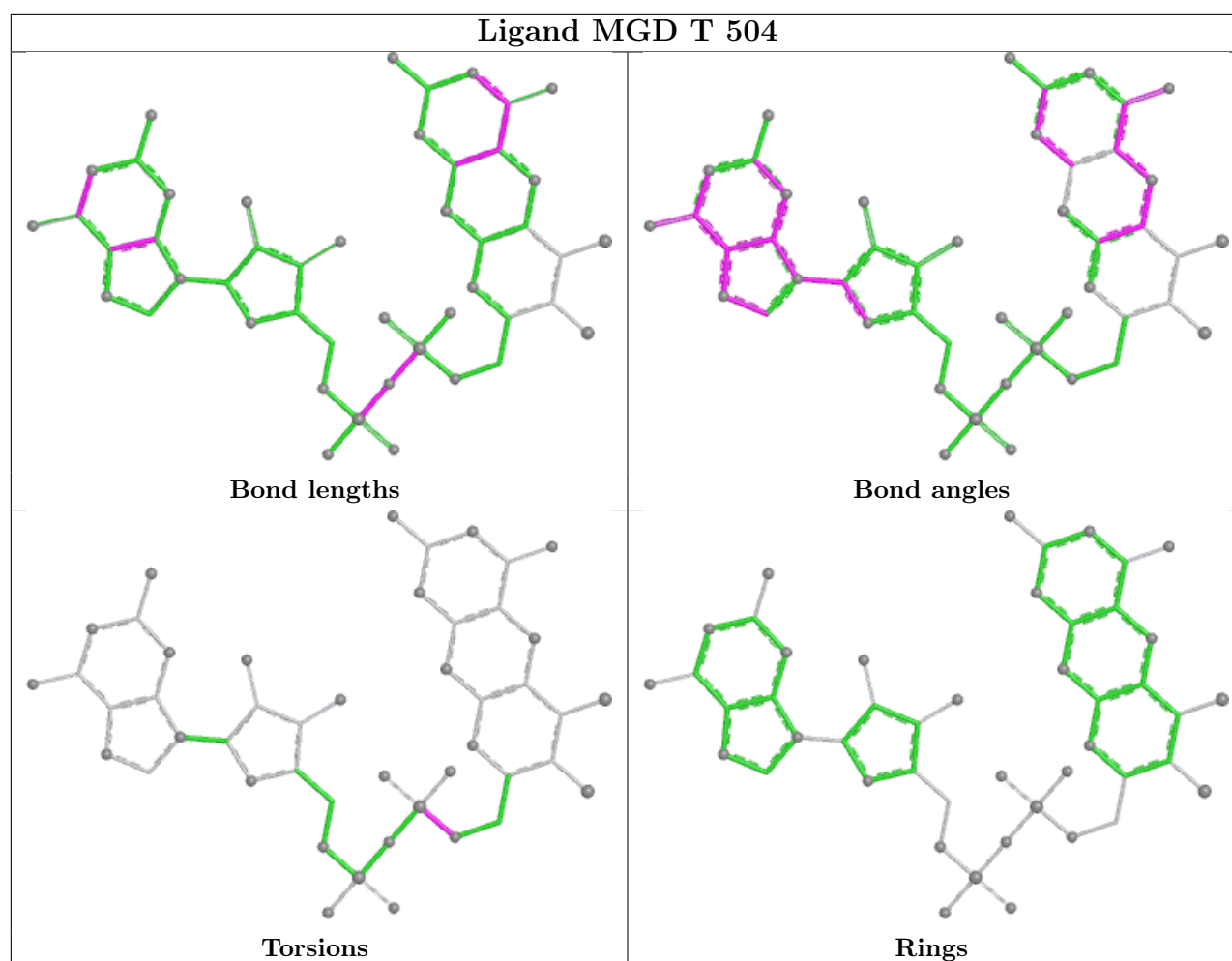
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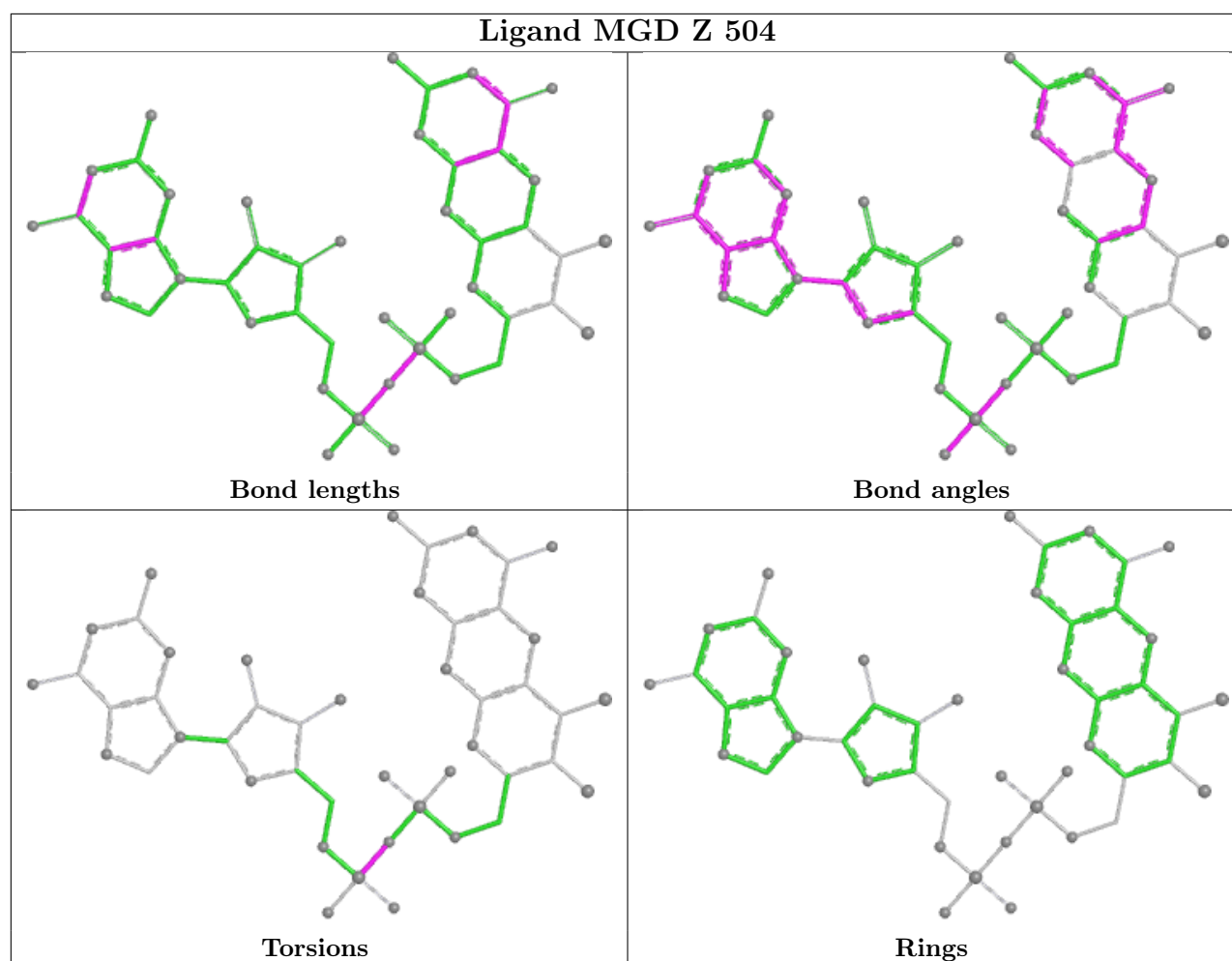
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Z	504	MGD	1	0
8	M	603	MFN	3	0
13	l	503	MGD	1	0
13	r	503	MGD	1	0
11	i	102	SF4	1	0
8	k	603	MFN	5	0
8	G	603	MFN	2	0
13	l	504	MGD	2	0
11	E	101	SF4	1	0
8	q	603	MFN	2	0
13	B	503	MGD	1	0
8	S	603	MFN	3	0
8	e	603	MFN	3	0

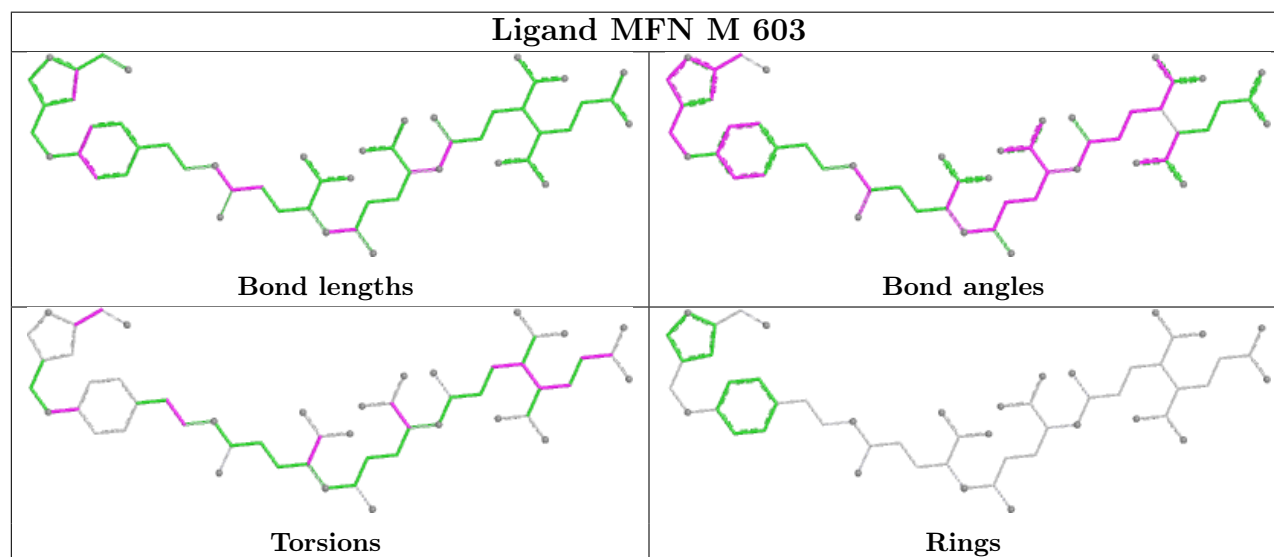
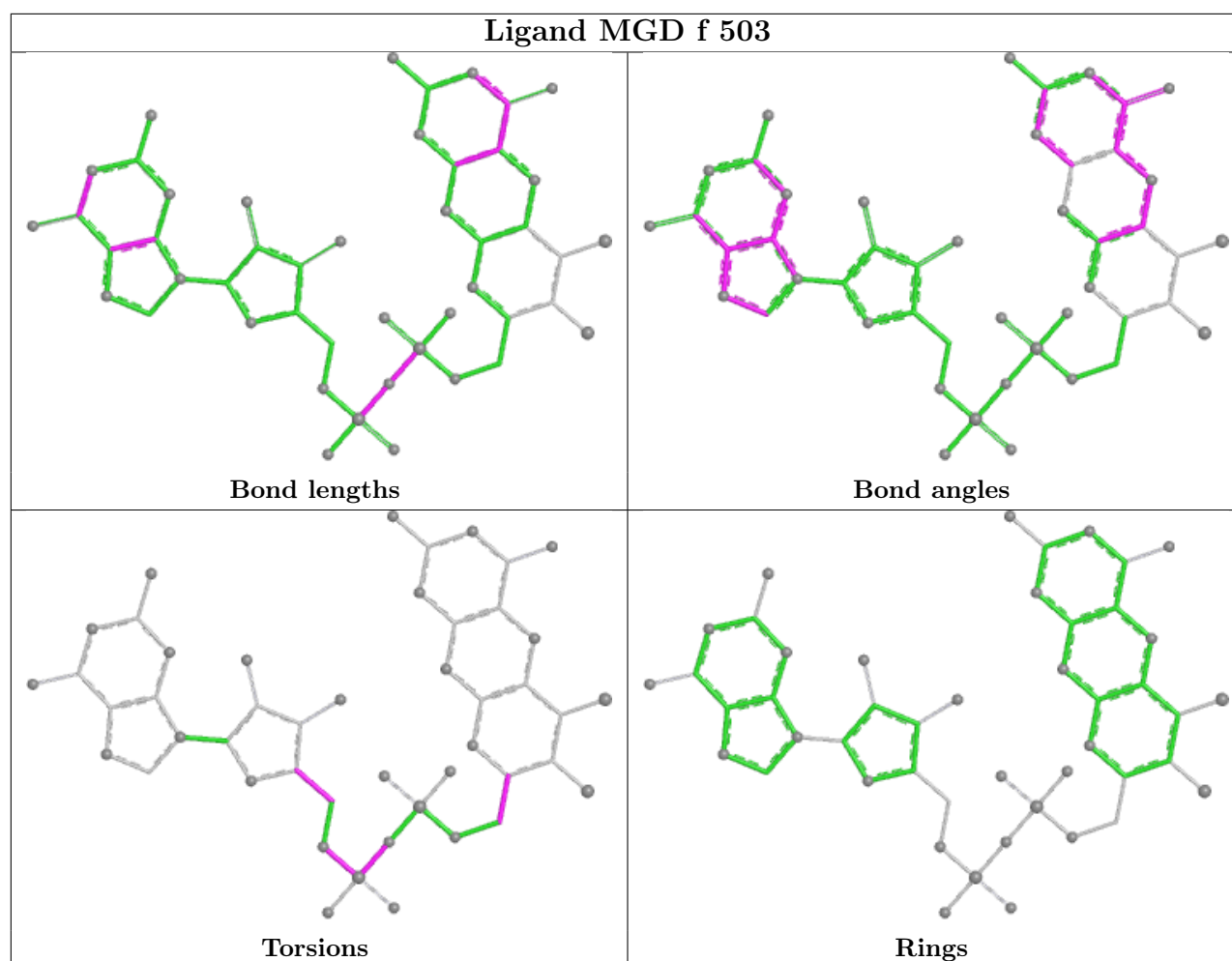
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

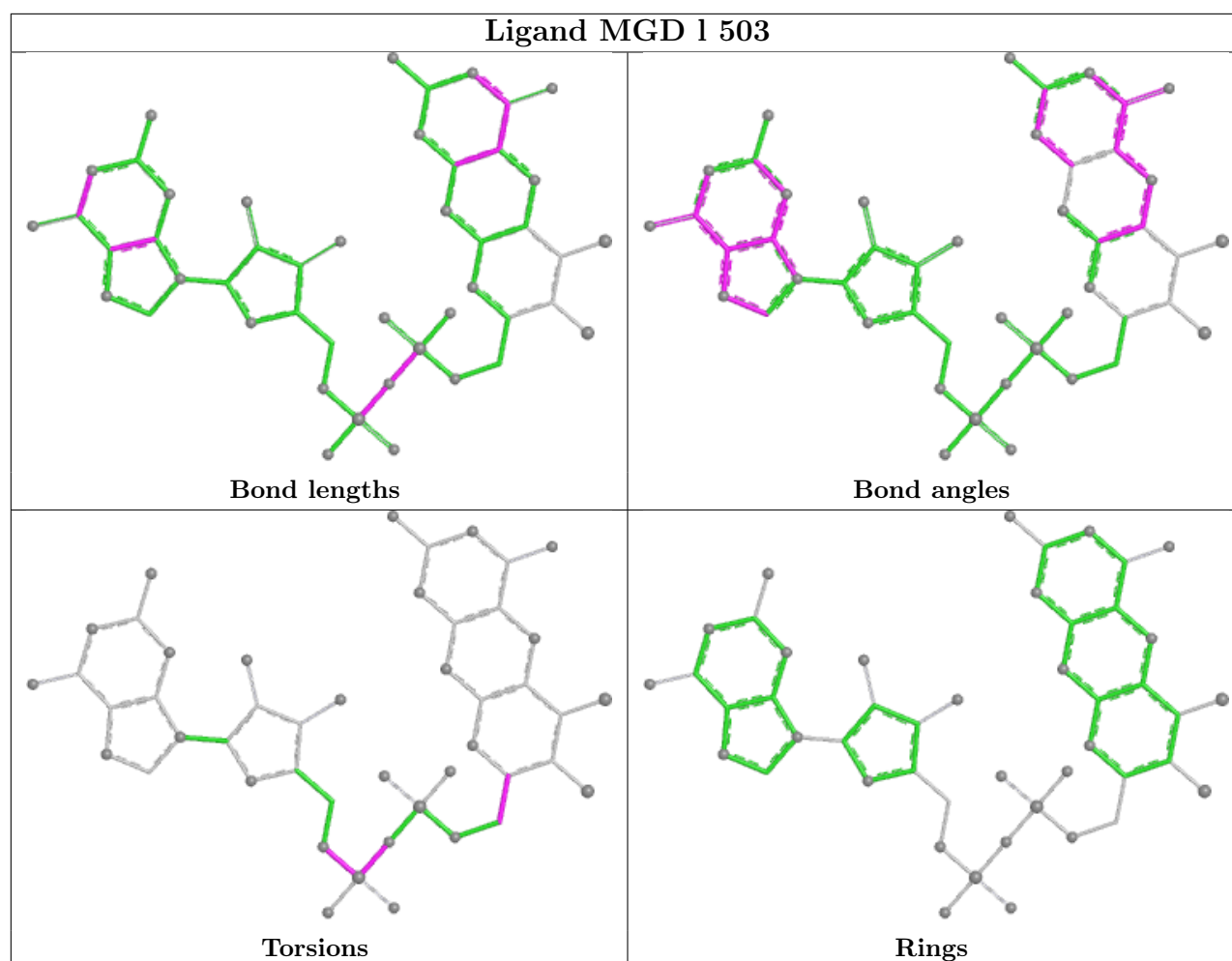


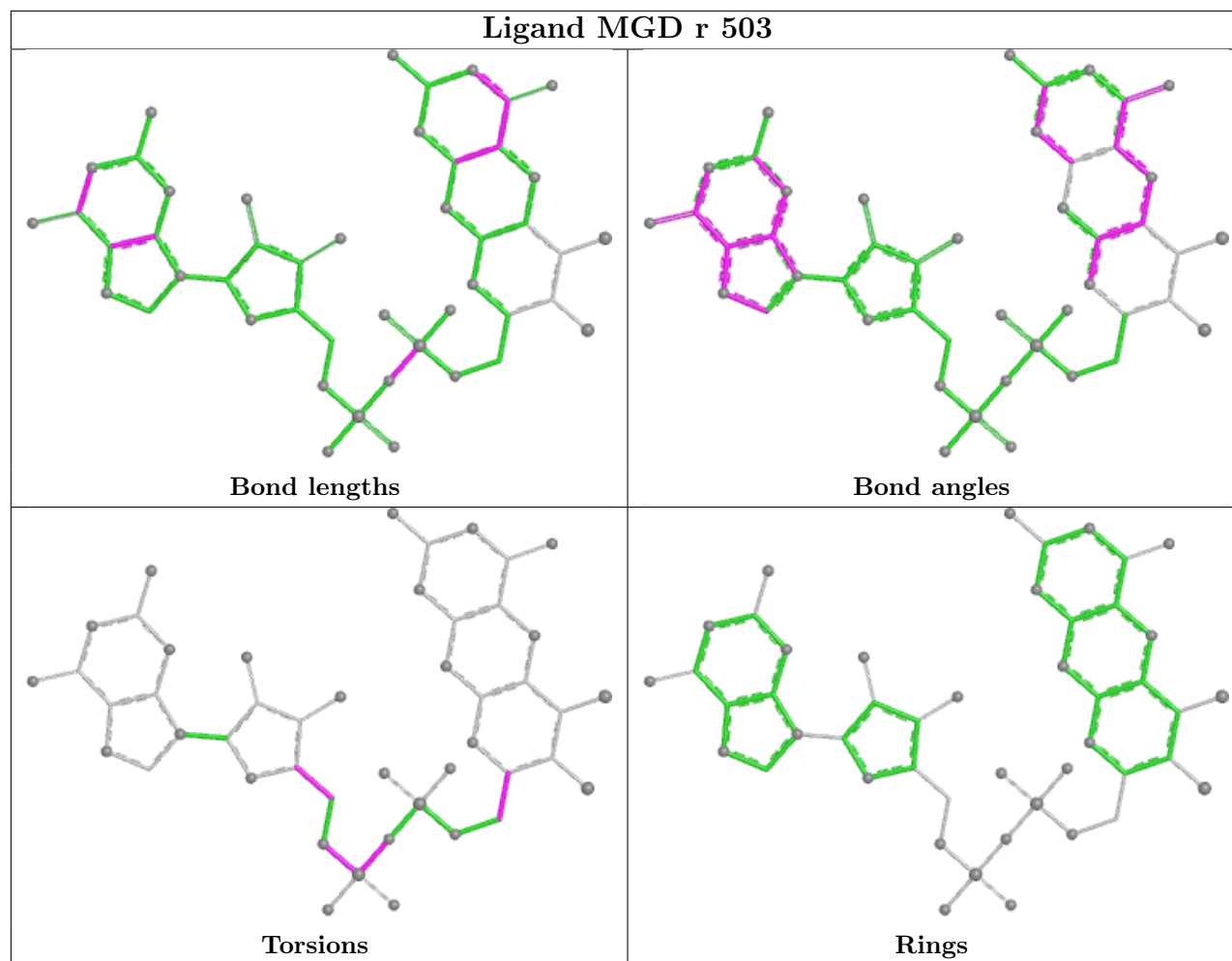


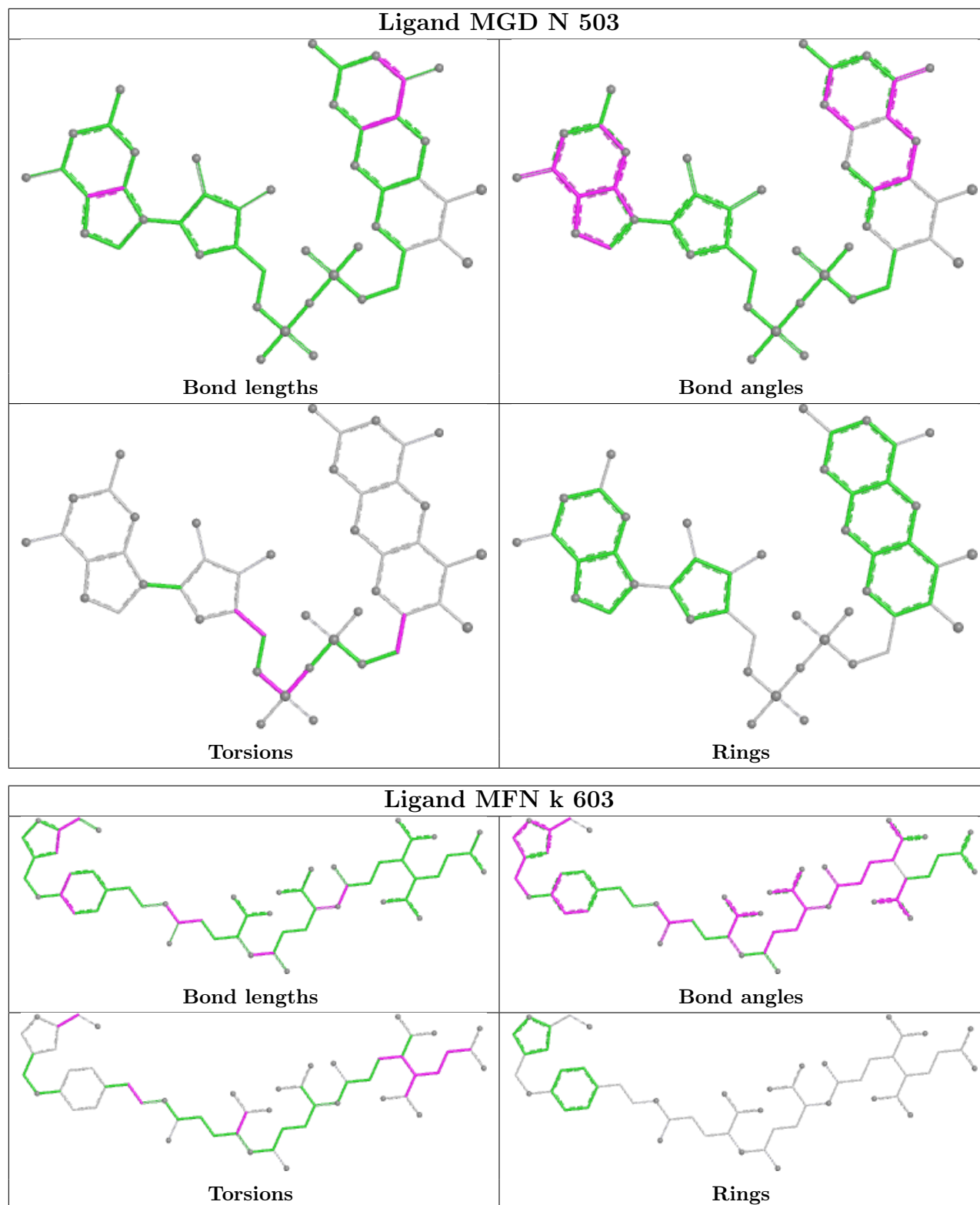


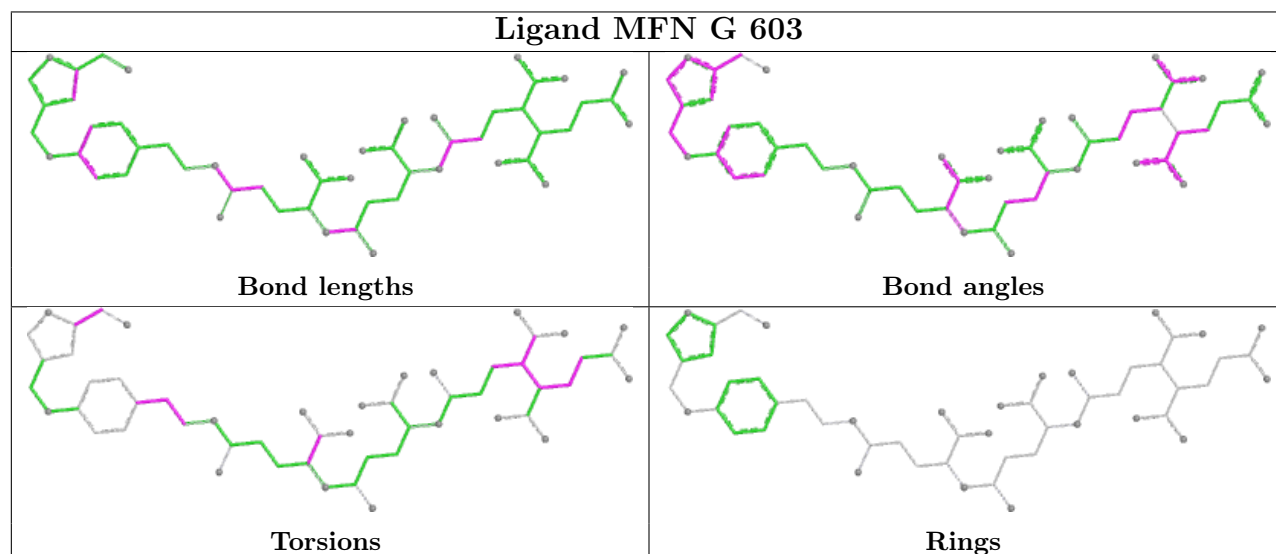
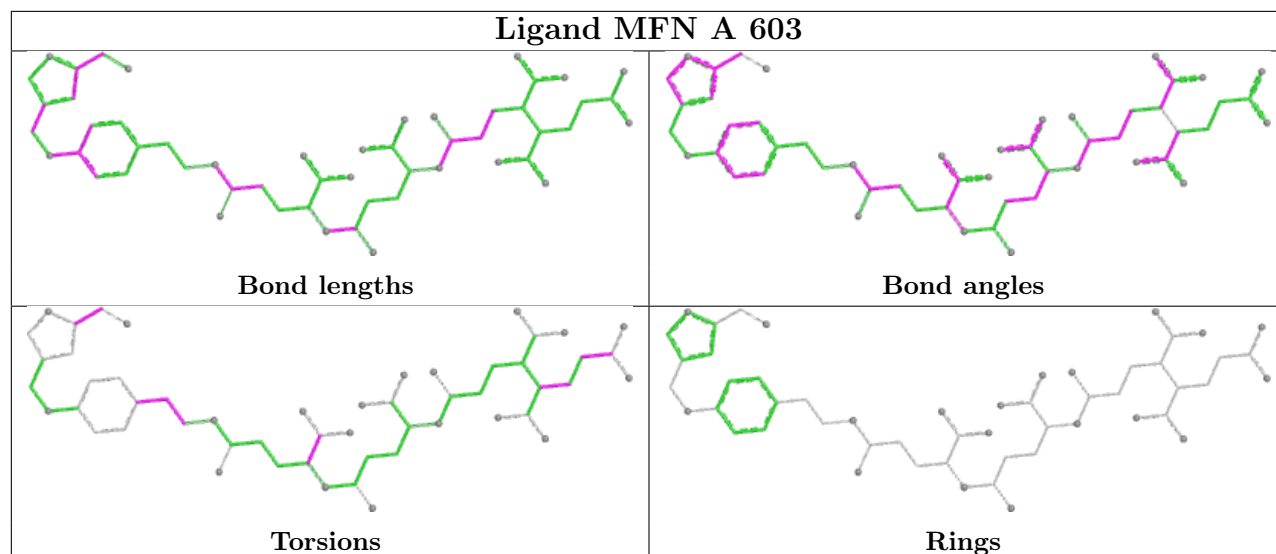


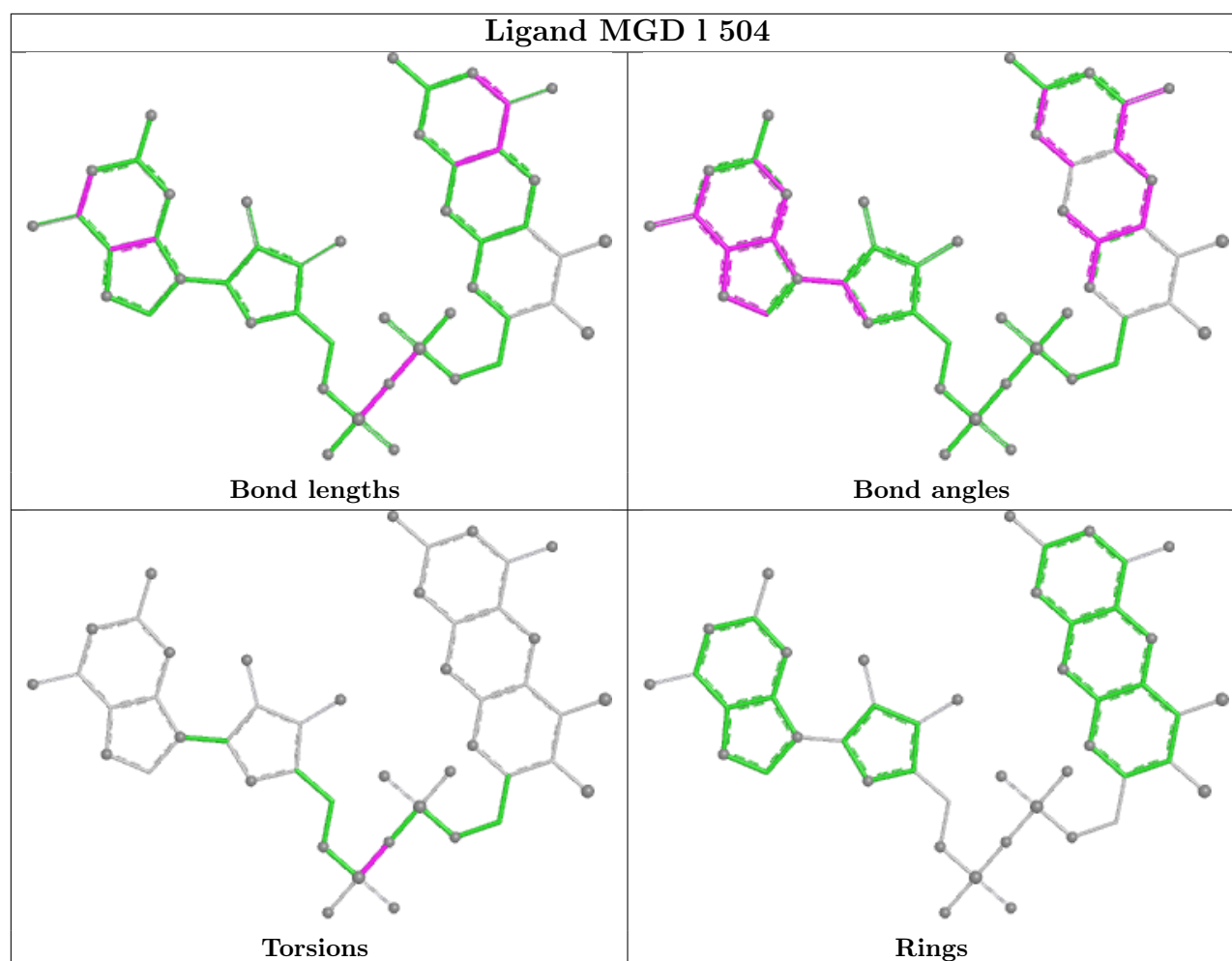


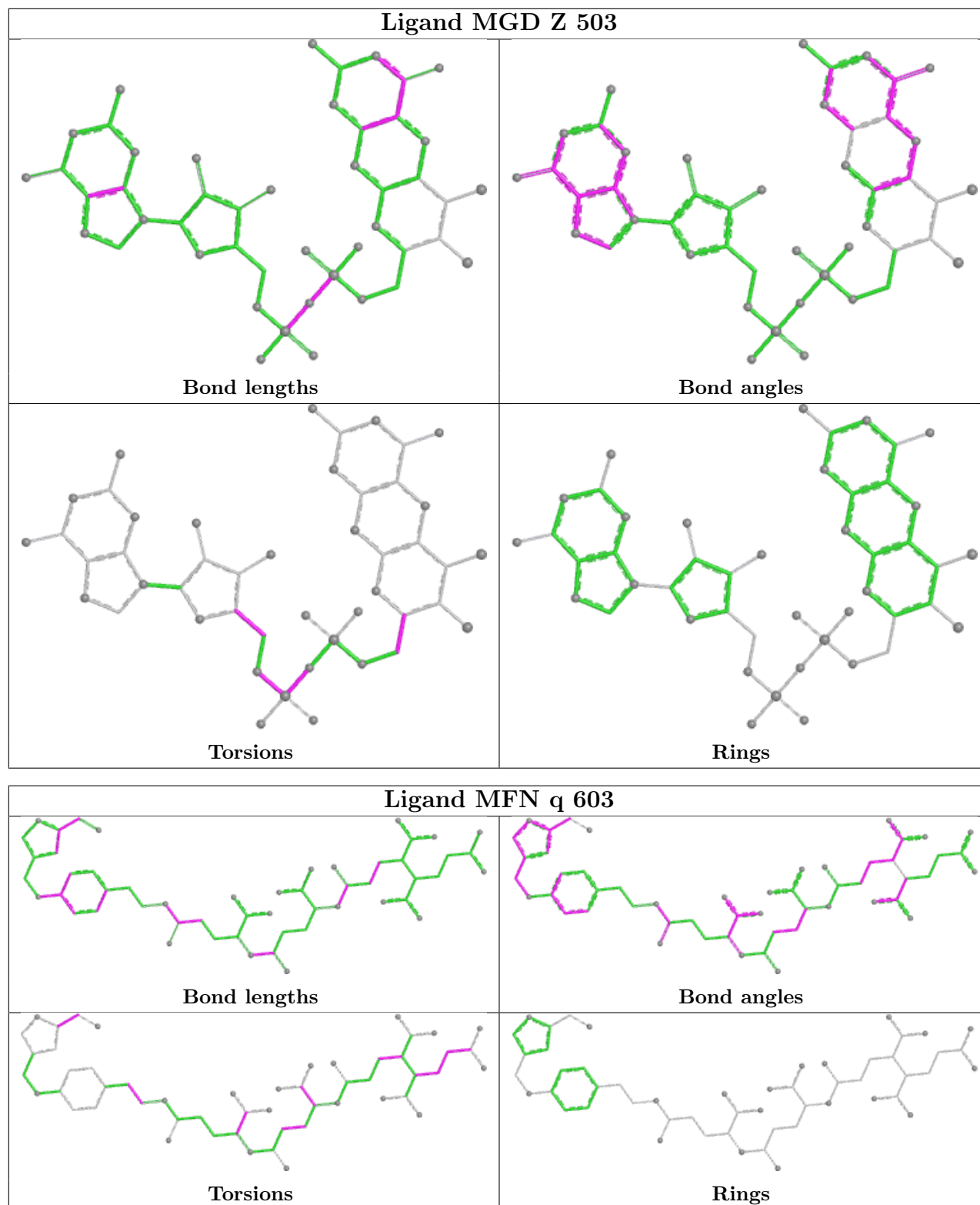


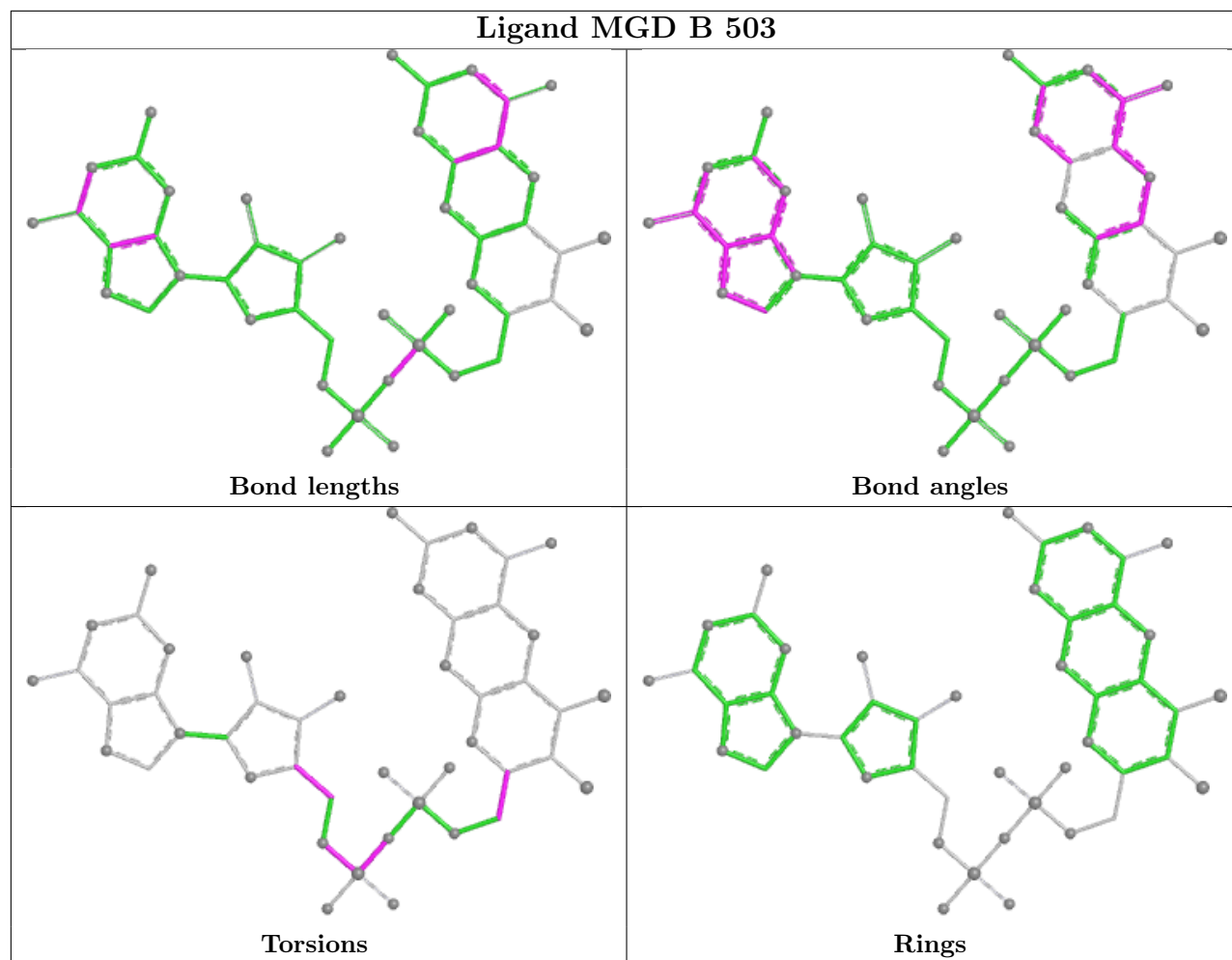


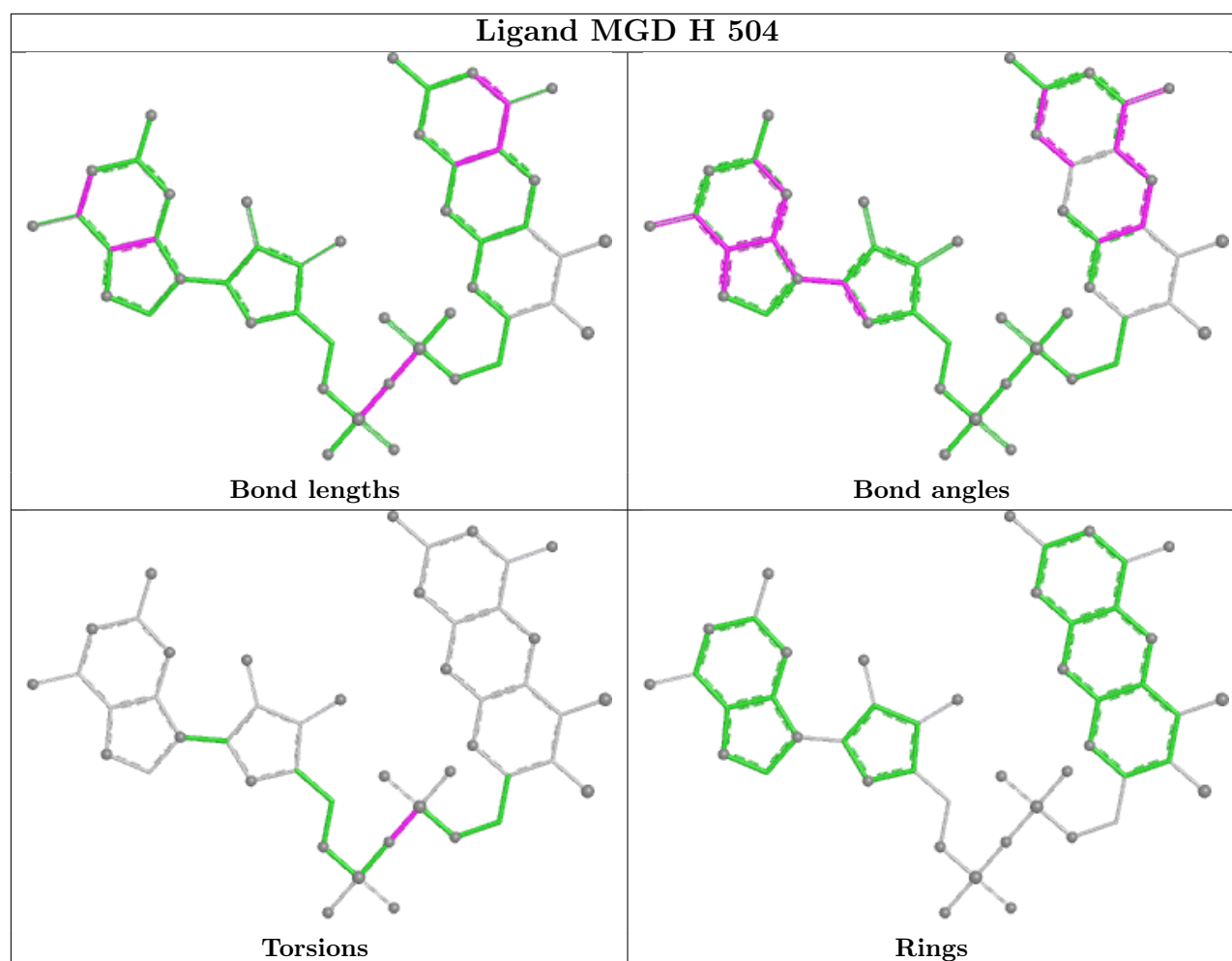


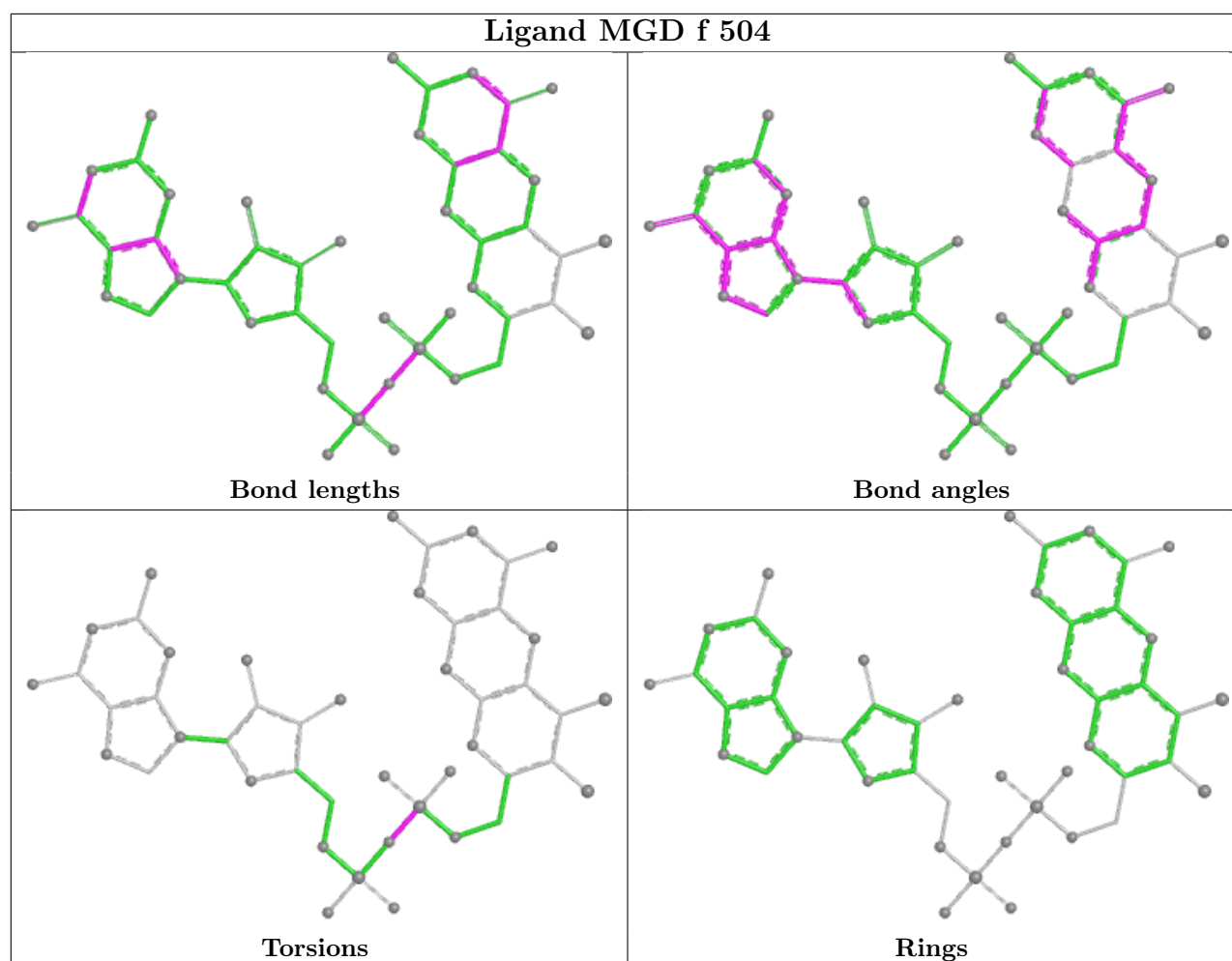


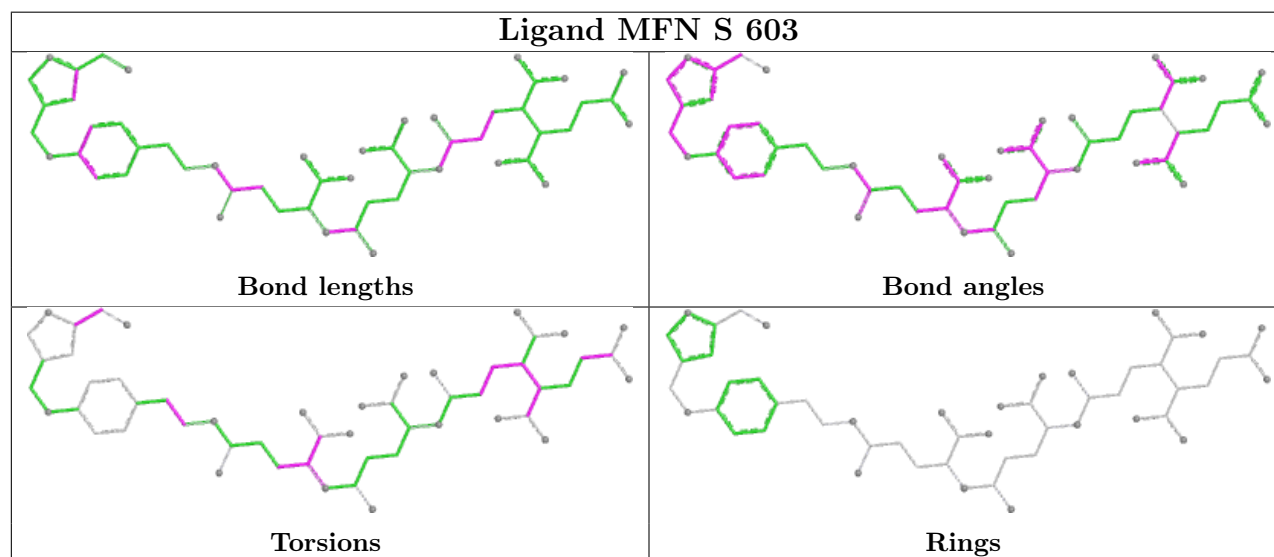
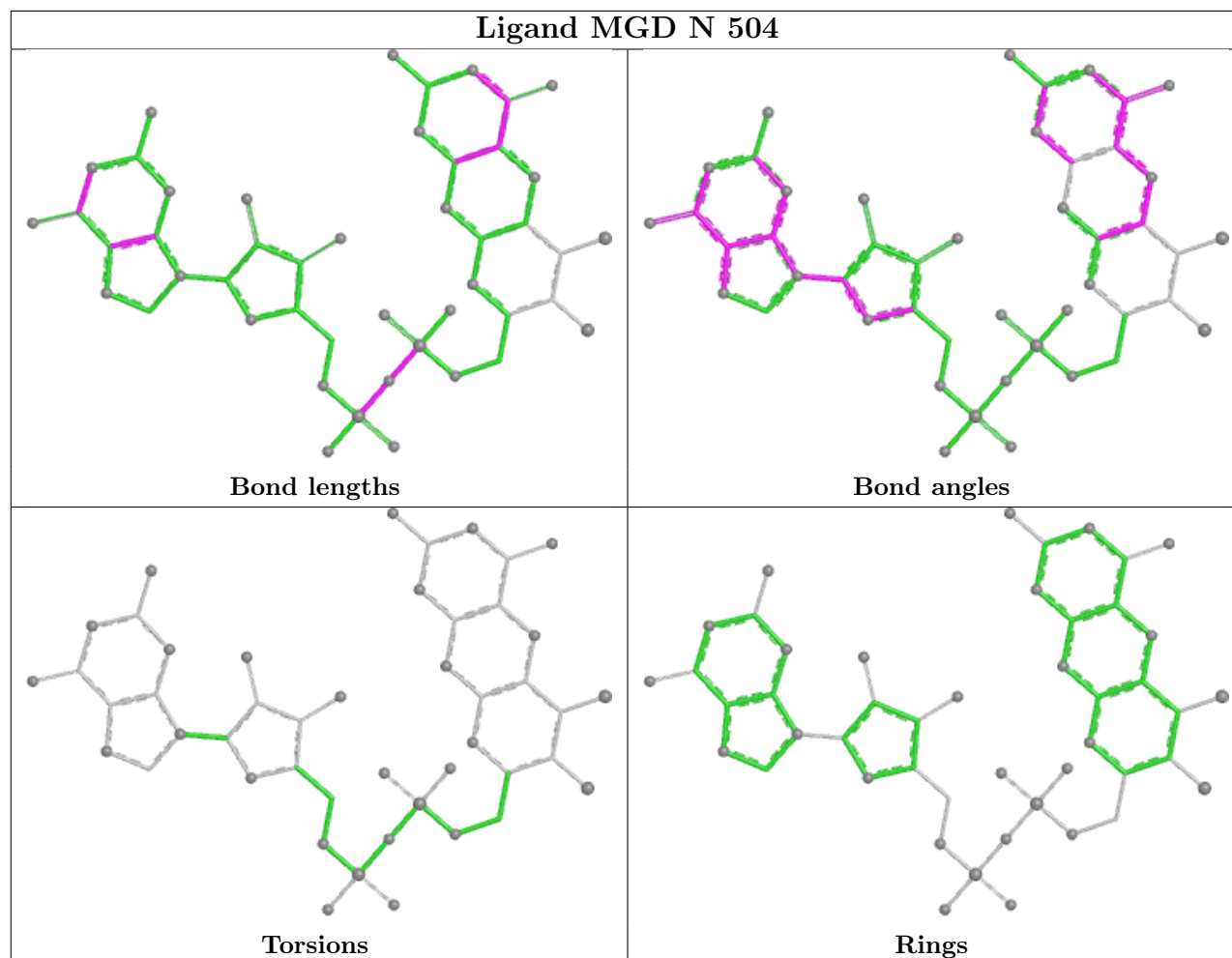


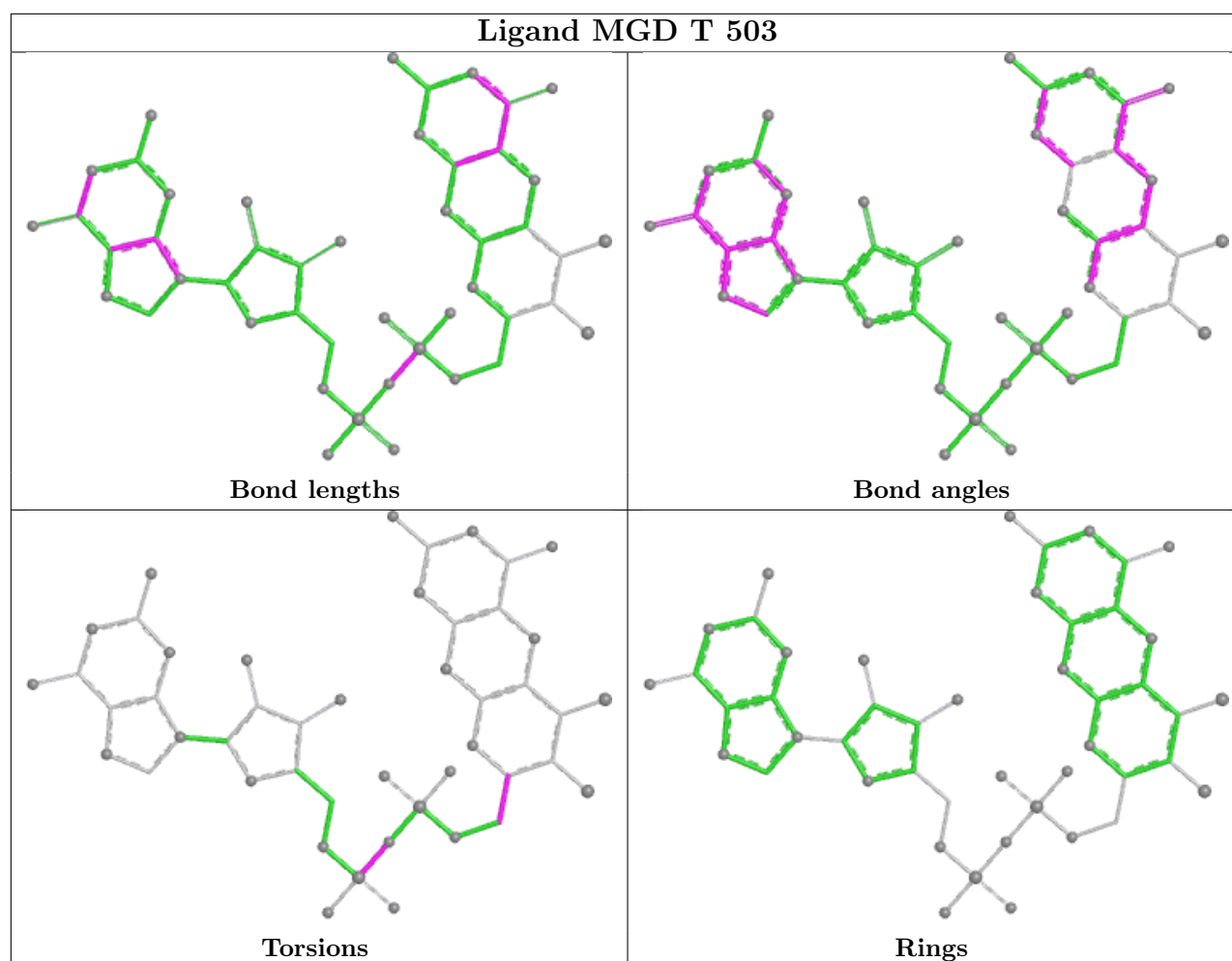


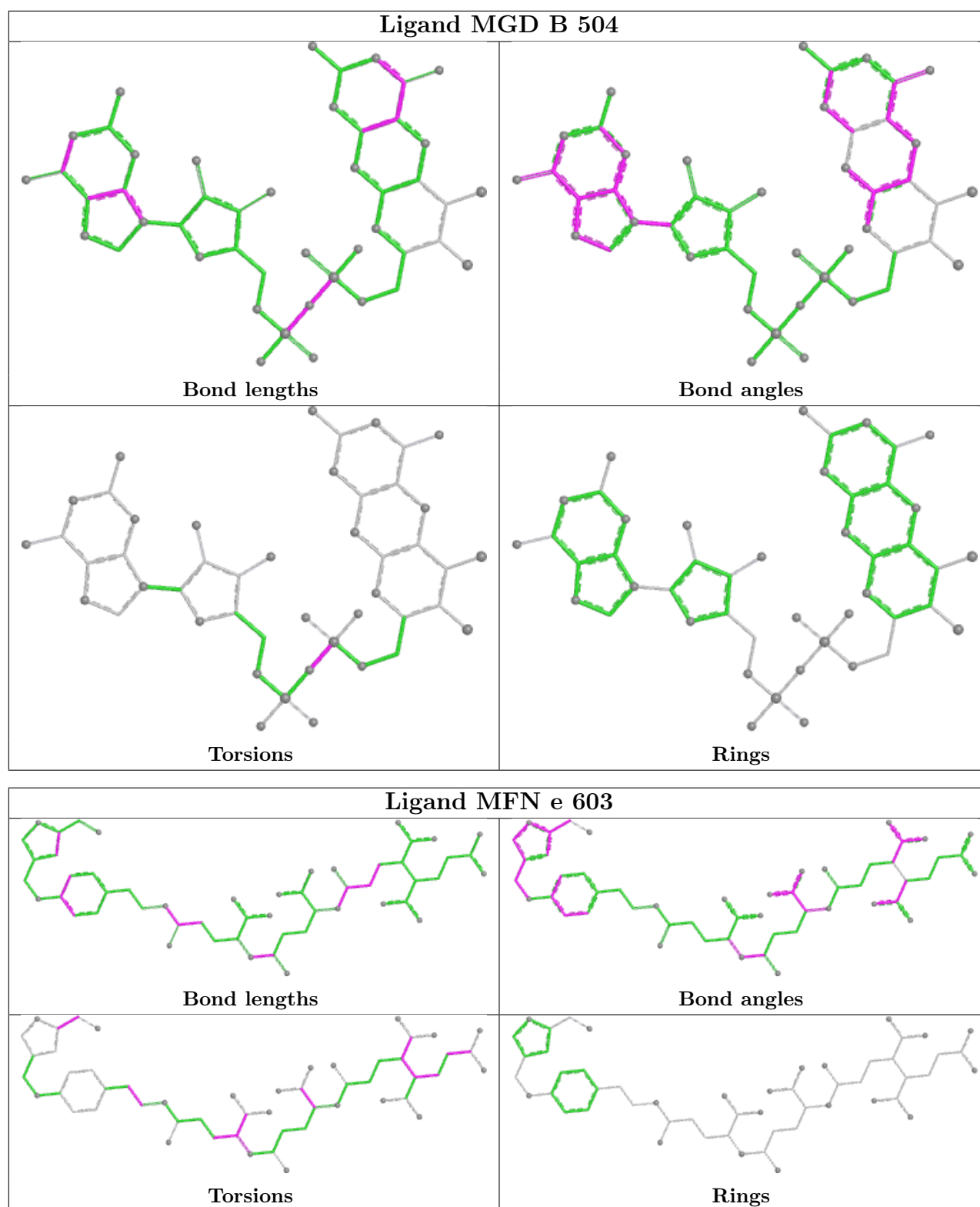












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	q	1
1	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	356:ARG	C	357:ALA	N	1.20
1	S	356:ARG	C	357:ALA	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	568/569 (99%)	0.59	18 (3%)	50	51	29, 43, 63, 91	0
1	G	567/569 (99%)	0.85	48 (8%)	16	16	31, 48, 73, 117	0
1	M	567/569 (99%)	1.16	72 (12%)	8	7	34, 55, 81, 113	0
1	S	568/569 (99%)	0.33	13 (2%)	61	62	25, 36, 54, 94	0
1	Y	567/569 (99%)	0.92	43 (7%)	20	19	31, 51, 75, 109	0
1	e	568/569 (99%)	0.33	13 (2%)	61	62	27, 37, 53, 88	0
1	k	567/569 (99%)	1.27	97 (17%)	4	3	33, 56, 80, 102	0
1	q	568/569 (99%)	0.70	31 (5%)	30	30	31, 46, 66, 105	0
2	B	429/432 (99%)	0.69	27 (6%)	26	25	29, 42, 69, 124	0
2	H	427/432 (98%)	0.49	18 (4%)	40	41	26, 38, 61, 87	0
2	N	430/432 (99%)	0.44	9 (2%)	63	64	30, 39, 57, 71	0
2	T	429/432 (99%)	0.62	23 (5%)	31	31	26, 39, 65, 104	0
2	Z	428/432 (99%)	0.63	22 (5%)	33	33	28, 40, 64, 122	0
2	f	427/432 (98%)	0.57	20 (4%)	36	36	25, 39, 61, 109	0
2	l	428/432 (99%)	0.73	28 (6%)	25	24	29, 43, 68, 98	0
2	r	428/432 (99%)	0.84	38 (8%)	15	14	29, 44, 69, 106	0
3	C	267/270 (98%)	1.10	33 (12%)	8	7	35, 53, 78, 108	0
3	I	269/270 (99%)	0.35	5 (1%)	66	66	26, 38, 56, 90	0
3	O	268/270 (99%)	0.46	7 (2%)	57	58	30, 41, 61, 86	0
3	U	268/270 (99%)	0.73	16 (5%)	27	27	28, 46, 70, 110	0
3	a	268/270 (99%)	0.42	5 (1%)	66	66	30, 39, 55, 83	0
3	g	268/270 (99%)	0.97	34 (12%)	8	7	31, 50, 78, 101	0
3	m	268/270 (99%)	0.54	8 (2%)	52	54	28, 41, 62, 93	0
3	s	269/270 (99%)	1.23	47 (17%)	4	3	36, 56, 80, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	D	129/130 (99%)	1.07	12 (9%) 14 13	36, 52, 70, 91	0
4	J	129/130 (99%)	0.34	1 (0%) 82 84	31, 41, 56, 66	0
4	P	129/130 (99%)	0.20	1 (0%) 82 84	29, 38, 54, 65	0
4	V	129/130 (99%)	0.63	3 (2%) 61 62	33, 43, 58, 68	0
4	b	129/130 (99%)	0.47	2 (1%) 70 71	33, 41, 56, 83	0
4	h	129/130 (99%)	0.85	9 (6%) 22 21	34, 48, 65, 84	0
4	n	129/130 (99%)	0.46	1 (0%) 82 84	34, 42, 61, 78	0
4	t	129/130 (99%)	0.99	15 (11%) 9 8	37, 51, 70, 83	0
5	E	80/82 (97%)	0.83	3 (3%) 44 45	33, 42, 57, 67	0
5	K	80/82 (97%)	0.60	1 (1%) 75 75	32, 40, 55, 72	0
5	Q	80/82 (97%)	0.75	1 (1%) 75 75	34, 44, 60, 69	0
5	W	80/82 (97%)	0.64	1 (1%) 75 75	31, 39, 52, 68	0
5	c	80/82 (97%)	0.91	7 (8%) 15 15	37, 46, 63, 72	0
5	i	80/82 (97%)	0.57	1 (1%) 75 75	28, 37, 50, 70	0
5	o	80/82 (97%)	0.86	3 (3%) 44 45	34, 43, 57, 71	0
5	u	81/82 (98%)	0.77	4 (4%) 35 34	32, 40, 61, 84	0
6	F	345/349 (98%)	0.74	26 (7%) 20 19	29, 40, 67, 116	0
6	L	348/349 (99%)	0.51	9 (2%) 57 58	28, 38, 60, 83	0
6	R	341/349 (97%)	1.19	69 (20%) 3 2	29, 48, 87, 147	0
6	X	344/349 (98%)	0.72	24 (6%) 22 21	29, 41, 71, 107	0
6	d	340/349 (97%)	1.15	62 (18%) 3 3	28, 49, 96, 130	0
6	j	344/349 (98%)	0.66	19 (5%) 30 30	26, 39, 69, 99	0
6	p	348/349 (99%)	0.53	9 (2%) 57 58	29, 37, 58, 85	0
6	v	346/349 (99%)	0.54	18 (5%) 33 32	27, 38, 63, 87	0
All	All	14540/14656 (99%)	0.71	976 (6%) 24 23	25, 43, 71, 147	0

All (976) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	83	PHE	8.3
2	l	430	ALA	6.7
1	q	467	ILE	5.9
1	A	83	PHE	5.9
6	R	17	THR	5.9

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Mol	Chain	Res	Type	RSRZ
6	X	6	VAL	5.7
1	Y	83	PHE	5.7
1	q	83	PHE	5.6
3	U	235	GLY	5.6
6	d	17	THR	5.4
1	M	569	LEU	5.4
2	l	75	ALA	5.4
6	j	92	GLY	5.3
1	k	4	ILE	5.2
1	S	569	LEU	5.1
1	M	8	GLY	5.1
1	q	419	TRP	5.0
6	R	6	VAL	5.0
5	o	81	LEU	5.0
6	p	2	GLU	4.9
1	k	569	LEU	4.9
6	j	6	VAL	4.8
6	X	7	ILE	4.7
3	g	234	ASP	4.7
6	F	3	THR	4.7
1	k	159	ASP	4.6
1	S	83	PHE	4.6
2	B	45	ALA	4.5
3	C	234	ASP	4.5
2	f	58	LYS	4.4
2	Z	430	ALA	4.4
4	b	129	GLN	4.4
2	r	1	MET	4.4
1	G	569	LEU	4.3
1	k	84	LYS	4.3
2	B	336	ASP	4.3
1	S	16	GLY	4.3
6	d	99	ALA	4.3
6	j	7	ILE	4.3
1	q	477	VAL	4.3
3	s	10	GLU	4.3
3	m	234	ASP	4.3
1	k	25	CYS	4.3
1	Y	415	GLU	4.2
2	Z	428	TYR	4.2
6	d	14	VAL	4.2
1	M	83	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
6	R	334	PRO	4.2
1	k	83	PHE	4.2
1	k	19	GLY	4.1
4	h	108	ILE	4.1
4	D	127	VAL	4.1
6	d	70	LYS	4.1
3	O	239	PRO	4.1
1	q	422	ARG	4.1
6	j	17	THR	4.1
1	M	237	HIS	4.1
1	M	479	PRO	4.0
2	r	430	ALA	4.0
1	M	396	PRO	4.0
6	d	334	PRO	4.0
3	s	235	GLY	4.0
1	k	393	THR	4.0
6	p	71	CYS	3.9
1	Y	84	LYS	3.9
1	M	481	ALA	3.9
1	G	22	MET	3.9
1	Y	237	HIS	3.9
6	d	245	CYS	3.9
3	C	235	GLY	3.9
4	t	123	VAL	3.9
2	r	61	GLU	3.8
3	s	52	PHE	3.8
6	d	75	GLY	3.8
5	E	12	CYS	3.8
6	d	120	ALA	3.8
2	B	59	ASN	3.8
6	v	17	THR	3.8
1	G	84	LYS	3.8
6	d	328	ASN	3.8
6	d	42	PRO	3.8
1	G	25	CYS	3.7
2	f	46	GLU	3.7
3	s	231	ILE	3.7
6	d	73	LEU	3.7
1	k	11	TYR	3.7
6	R	349	LYS	3.7
6	d	16	ARG	3.7
4	b	127	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
6	R	97	GLU	3.7
1	G	24	ILE	3.7
3	g	239	PRO	3.7
5	E	75	ALA	3.7
2	r	355	GLU	3.6
6	R	339	ALA	3.6
6	R	43	VAL	3.6
1	A	559	PRO	3.6
6	R	14	VAL	3.6
4	V	67	ALA	3.6
2	r	62	PHE	3.6
6	j	91	ASP	3.6
2	Z	61	GLU	3.5
3	I	270	PRO	3.5
3	g	5	ILE	3.5
1	q	84	LYS	3.5
4	h	65	VAL	3.5
1	M	156	GLY	3.5
3	s	71	GLY	3.5
1	A	237	HIS	3.5
6	F	16	ARG	3.5
6	F	17	THR	3.5
6	R	40	ILE	3.5
3	U	231	ILE	3.5
1	k	9	PHE	3.5
1	e	237	HIS	3.5
1	k	36	SER	3.4
2	Z	424	LYS	3.4
1	k	462	GLY	3.4
1	Y	63	ALA	3.4
1	Y	160	ALA	3.4
3	U	2	SER	3.4
6	v	7	ILE	3.4
2	T	44	HIS	3.4
2	Z	410	ASP	3.4
2	T	320	ASN	3.4
1	k	6	LYS	3.4
3	U	269	ALA	3.4
3	s	68	ILE	3.4
2	H	58	LYS	3.4
1	G	461	VAL	3.4
3	U	239	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
6	d	92	GLY	3.4
6	d	335	ILE	3.4
2	H	61	GLU	3.4
4	t	129	GLN	3.3
6	X	93	THR	3.3
1	Y	414	GLY	3.3
1	q	237	HIS	3.3
4	t	124	TYR	3.3
3	s	112	ASN	3.3
3	C	2	SER	3.3
1	e	569	LEU	3.3
2	B	44	HIS	3.3
1	k	176	THR	3.3
3	O	235	GLY	3.3
6	R	46	ILE	3.3
6	d	46	ILE	3.3
6	v	224	LYS	3.3
6	L	328	ASN	3.2
5	E	81	LEU	3.2
1	k	461	VAL	3.2
1	G	156	GLY	3.2
1	k	101	GLY	3.2
1	M	84	LYS	3.2
2	r	363	ILE	3.2
6	d	7	ILE	3.2
2	f	62	PHE	3.2
3	O	2	SER	3.2
6	j	167	ASP	3.2
2	l	55	LEU	3.2
3	g	235	GLY	3.2
6	p	3	THR	3.2
1	k	486	ILE	3.2
1	Y	465	ALA	3.2
1	G	462	GLY	3.2
4	h	48	GLY	3.2
4	t	81	GLY	3.2
3	U	238	LEU	3.2
4	h	127	VAL	3.2
1	M	374	ILE	3.2
3	g	152	ILE	3.2
1	M	36	SER	3.1
1	k	435	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	375	ASP	3.1
1	k	43	ASP	3.1
1	k	423	LYS	3.1
3	m	50	ASP	3.1
1	G	460	GLY	3.1
3	s	191	ILE	3.1
3	s	230	ASP	3.1
3	g	2	SER	3.1
1	q	405	ASN	3.1
6	R	328	ASN	3.1
4	D	108	ILE	3.1
1	M	2	GLU	3.1
2	B	46	GLU	3.1
6	R	16	ARG	3.1
6	X	349	LYS	3.0
1	k	115	ALA	3.0
6	R	45	ALA	3.0
2	r	366	GLU	3.0
3	O	238	LEU	3.0
1	q	423	LYS	3.0
2	B	25	GLY	3.0
6	X	326	LYS	3.0
1	k	35	VAL	3.0
6	R	333	THR	3.0
1	Y	3	TYR	3.0
2	T	428	TYR	3.0
5	c	81	LEU	3.0
1	k	37	ASP	3.0
1	k	490	PHE	3.0
6	d	94	SER	3.0
1	G	505	LYS	3.0
1	M	297	ASN	3.0
2	Z	58	LYS	3.0
6	R	25	ILE	3.0
6	R	72	VAL	3.0
3	s	76	THR	3.0
1	G	568	MET	3.0
1	Y	81	GLU	3.0
6	R	42	PRO	3.0
6	R	344	PHE	3.0
2	l	429	LYS	3.0
2	r	58	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	m	2	SER	3.0
3	s	157	ASN	3.0
1	Y	24	ILE	3.0
3	g	67	ILE	3.0
4	t	11	ILE	3.0
6	d	23	ARG	3.0
1	M	371	PHE	3.0
6	F	77	CYS	3.0
2	B	222	ILE	2.9
3	s	4	ILE	2.9
3	s	37	ILE	2.9
1	k	396	PRO	2.9
1	k	3	TYR	2.9
2	B	53	LYS	2.9
4	t	23	LEU	2.9
1	e	83	PHE	2.9
6	d	37	CYS	2.9
6	F	7	ILE	2.9
1	k	10	VAL	2.9
6	F	6	VAL	2.9
6	d	336	ARG	2.9
5	Q	81	LEU	2.9
3	g	34	ILE	2.9
3	s	5	ILE	2.9
1	k	80	ALA	2.9
2	l	422	LEU	2.9
1	Y	375	ASP	2.9
2	B	144	ASP	2.9
3	s	74	TYR	2.9
2	H	25	GLY	2.9
2	Z	226	GLU	2.9
3	m	232	GLU	2.9
6	F	49	ASN	2.9
6	X	20	GLU	2.9
6	d	284	ASN	2.9
3	g	68	ILE	2.9
1	Y	426	VAL	2.9
1	k	21	LYS	2.9
1	G	37	ASP	2.9
1	S	1	MET	2.9
2	f	61	GLU	2.9
4	V	38	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
6	p	8	GLU	2.9
1	M	438	ILE	2.8
1	k	472	ILE	2.8
3	C	5	ILE	2.8
6	p	336	ARG	2.8
6	j	224	LYS	2.8
3	s	239	PRO	2.8
1	A	293	ALA	2.8
1	G	493	ALA	2.8
3	s	131	ASP	2.8
6	F	68	GLU	2.8
1	G	36	SER	2.8
6	R	66	ILE	2.8
6	R	335	ILE	2.8
3	C	16	LEU	2.8
3	s	70	ASP	2.8
2	Z	62	PHE	2.8
6	F	9	GLY	2.8
6	R	101	TYR	2.8
6	d	101	TYR	2.8
3	C	126	ILE	2.8
6	F	223	ILE	2.8
6	R	90	ILE	2.8
1	G	474	PRO	2.8
3	U	233	VAL	2.8
6	v	225	THR	2.8
6	p	34	CYS	2.8
2	Z	24	GLU	2.8
6	X	341	LYS	2.8
6	X	92	GLY	2.8
1	M	429	ILE	2.8
2	l	428	TYR	2.8
6	d	104	ILE	2.8
3	C	157	ASN	2.8
1	M	256	PRO	2.8
1	k	479	PRO	2.8
3	s	94	VAL	2.8
2	l	215	ALA	2.8
2	r	78	LEU	2.8
6	R	273	ALA	2.8
1	A	81	GLU	2.8
1	k	2	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	r	356	ARG	2.8
6	R	60	GLU	2.8
2	H	225	ASP	2.8
1	M	5	ILE	2.7
3	C	231	ILE	2.7
6	R	95	ILE	2.7
1	k	407	TYR	2.7
1	M	93	SER	2.7
3	C	45	VAL	2.7
1	A	569	LEU	2.7
2	H	109	ALA	2.7
3	s	108	THR	2.7
6	F	224	LYS	2.7
6	R	47	GLU	2.7
6	j	89	GLN	2.7
1	M	486	ILE	2.7
6	p	69	ASN	2.7
6	R	233	TYR	2.7
6	R	337	SER	2.7
2	f	326	ALA	2.7
5	c	2	ALA	2.7
6	v	3	THR	2.7
2	r	83	ARG	2.7
2	r	46	GLU	2.7
6	v	60	GLU	2.7
2	r	328	ASP	2.7
6	R	74	CYS	2.7
2	r	322	GLY	2.7
6	L	295	GLY	2.7
3	C	239	PRO	2.7
1	G	426	VAL	2.7
3	a	2	SER	2.7
6	d	43	VAL	2.7
1	M	113	MET	2.7
2	l	412	LEU	2.7
1	k	400	ALA	2.7
2	N	430	ALA	2.7
1	k	506	ASP	2.7
2	B	204	ASP	2.7
1	Y	236	GLY	2.7
1	G	4	ILE	2.7
3	U	65	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
6	R	319	PRO	2.7
1	M	286	VAL	2.7
1	k	22	MET	2.7
1	k	520	VAL	2.7
2	Z	411	LEU	2.7
2	B	355	GLU	2.7
2	l	74	ALA	2.7
3	C	60	ASP	2.6
6	d	91	ASP	2.6
1	q	91	GLY	2.6
6	R	92	GLY	2.6
6	X	75	GLY	2.6
6	d	216	CYS	2.6
6	X	328	ASN	2.6
1	G	49	VAL	2.6
1	k	497	LEU	2.6
3	C	237	GLU	2.6
6	L	227	GLU	2.6
6	d	68	GLU	2.6
4	D	129	GLN	2.6
2	l	302	TRP	2.6
2	r	377	ASP	2.6
6	X	91	ASP	2.6
1	G	9	PHE	2.6
1	M	490	PHE	2.6
1	k	467	ILE	2.6
3	s	34	ILE	2.6
4	h	107	ILE	2.6
6	R	104	ILE	2.6
6	F	23	ARG	2.6
1	A	25	CYS	2.6
1	q	245	LEU	2.6
6	R	88	LEU	2.6
6	X	21	ASN	2.6
2	T	43	VAL	2.6
3	s	54	VAL	2.6
4	t	114	VAL	2.6
6	d	15	GLU	2.6
1	Y	201	ALA	2.6
6	R	93	THR	2.6
6	R	332	THR	2.6
2	B	328	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
6	R	336	ARG	2.6
6	d	319	PRO	2.6
1	k	568	MET	2.6
2	B	223	LEU	2.6
2	T	316	GLU	2.6
2	l	61	GLU	2.6
6	F	71	CYS	2.6
6	R	39	GLU	2.6
1	Y	35	VAL	2.6
3	g	233	VAL	2.6
6	R	331	ASN	2.6
6	j	328	ASN	2.6
1	Y	453	SER	2.6
1	M	209	ALA	2.6
1	e	465	ALA	2.6
1	k	44	ALA	2.6
2	B	376	ALA	2.6
6	R	13	THR	2.6
6	R	343	ALA	2.6
3	s	66	LYS	2.6
6	L	338	LYS	2.6
1	A	300	ASP	2.6
1	M	23	ASP	2.6
1	M	525	ASP	2.6
1	Y	474	PRO	2.6
2	N	137	GLY	2.6
2	B	49	MET	2.6
2	r	381	PRO	2.6
3	U	240	GLY	2.6
6	d	76	MET	2.6
3	U	5	ILE	2.6
3	C	52	PHE	2.6
1	q	411	LEU	2.6
2	Z	27	GLU	2.6
6	R	15	GLU	2.6
2	Z	407	VAL	2.6
4	D	65	VAL	2.6
6	j	21	ASN	2.6
1	G	527	SER	2.6
2	r	353	ALA	2.6
3	g	59	ALA	2.6
6	j	225	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	q	255	LYS	2.6
2	N	428	TYR	2.6
2	l	67	TYR	2.6
1	q	1	MET	2.5
2	B	60	GLY	2.5
3	g	92	GLY	2.5
4	D	25	MET	2.5
1	G	374	ILE	2.5
2	H	2	GLU	2.5
2	r	24	GLU	2.5
6	d	260	PHE	2.5
6	v	97	GLU	2.5
6	R	347	LEU	2.5
1	A	477	VAL	2.5
6	R	325	VAL	2.5
1	G	39	ALA	2.5
1	k	232	CYS	2.5
2	H	16	CYS	2.5
6	F	349	LYS	2.5
6	R	224	LYS	2.5
6	d	13	THR	2.5
6	d	93	THR	2.5
1	Y	198	TYR	2.5
3	C	68	ILE	2.5
1	S	221	LYS	2.5
1	Y	553	VAL	2.5
2	f	429	LYS	2.5
6	R	55	VAL	2.5
6	d	349	LYS	2.5
6	j	349	LYS	2.5
6	v	349	LYS	2.5
1	q	293	ALA	2.5
2	r	45	ALA	2.5
6	R	99	ALA	2.5
1	k	522	THR	2.5
6	R	77	CYS	2.5
6	X	308	CYS	2.5
3	s	40	MET	2.5
1	k	474	PRO	2.5
4	D	128	GLY	2.5
1	Y	528	ILE	2.5
1	k	31	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
6	F	25	ILE	2.5
6	R	12	ILE	2.5
6	R	227	GLU	2.5
6	R	330	ILE	2.5
6	j	227	GLU	2.5
1	M	282	TRP	2.5
2	Z	136	PHE	2.5
1	S	84	LYS	2.5
1	Y	542	GLN	2.5
2	B	424	LYS	2.5
2	l	424	LYS	2.5
3	s	81	GLN	2.5
1	G	477	VAL	2.5
3	C	94	VAL	2.5
1	k	463	ALA	2.5
1	M	480	SER	2.5
2	f	324	THR	2.5
1	M	22	MET	2.5
1	M	568	MET	2.5
2	N	1	MET	2.5
2	f	47	GLY	2.5
6	v	219	GLY	2.5
1	M	506	ASP	2.5
1	k	5	ILE	2.5
2	T	344	ASP	2.5
5	c	3	ILE	2.5
1	G	21	LYS	2.5
1	S	255	LYS	2.5
1	k	142	LEU	2.5
2	H	62	PHE	2.5
6	d	89	GLN	2.5
1	M	449	VAL	2.5
2	l	425	VAL	2.5
6	X	17	THR	2.5
6	R	281	CYS	2.4
1	Y	196	GLY	2.4
2	B	47	GLY	2.4
3	I	235	GLY	2.4
1	M	24	ILE	2.4
1	k	505	LYS	2.4
2	l	52	LYS	2.4
3	g	4	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	s	234	ASP	2.4
4	P	45	ILE	2.4
6	d	25	ILE	2.4
1	M	224	LEU	2.4
1	M	402	LEU	2.4
5	i	81	LEU	2.4
1	M	523	GLN	2.4
1	M	9	PHE	2.4
3	s	122	ARG	2.4
4	D	64	ALA	2.4
6	L	3	THR	2.4
1	M	262	SER	2.4
6	d	62	SER	2.4
3	I	239	PRO	2.4
2	Z	236	GLU	2.4
3	g	87	GLU	2.4
2	T	73	LYS	2.4
3	g	104	GLY	2.4
4	t	24	LYS	2.4
1	k	48	ILE	2.4
2	f	379	ILE	2.4
4	D	42	GLN	2.4
1	G	237	HIS	2.4
1	M	219	ASN	2.4
1	q	286	VAL	2.4
6	R	21	ASN	2.4
1	k	494	ALA	2.4
2	B	79	ALA	2.4
5	c	30	PRO	2.4
1	q	27	LYS	2.4
1	e	157	ASP	2.4
1	k	502	ILE	2.4
4	D	78	ILE	2.4
6	d	71	CYS	2.4
2	f	223	LEU	2.4
6	R	30	LEU	2.4
1	k	483	TYR	2.4
1	G	306	VAL	2.4
6	R	76	MET	2.4
6	X	43	VAL	2.4
1	k	7	ASN	2.4
1	k	389	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	r	342	ALA	2.4
2	N	237	GLU	2.4
2	l	316	GLU	2.4
3	C	108	THR	2.4
6	v	4	THR	2.4
2	r	54	PRO	2.4
3	g	150	GLY	2.4
3	g	268	ILE	2.4
4	t	78	ILE	2.4
1	k	466	ASP	2.4
2	B	330	LEU	2.4
5	W	81	LEU	2.4
6	L	91	ASP	2.4
6	d	264	LEU	2.4
6	v	23	ARG	2.4
2	H	428	TYR	2.4
3	s	90	VAL	2.4
2	r	335	ALA	2.4
6	R	96	LYS	2.4
1	q	475	GLU	2.4
6	F	97	GLU	2.4
1	M	476	THR	2.3
1	k	260	THR	2.3
6	F	4	THR	2.3
6	R	94	SER	2.3
3	C	71	GLY	2.3
1	G	472	ILE	2.3
2	H	163	ARG	2.3
1	k	514	HIS	2.3
1	q	14	LEU	2.3
2	T	234	GLN	2.3
2	T	68	ASP	2.3
1	G	371	PHE	2.3
1	k	395	TYR	2.3
2	B	67	TYR	2.3
2	l	62	PHE	2.3
3	g	74	TYR	2.3
6	d	344	PHE	2.3
3	g	35	LYS	2.3
4	t	127	VAL	2.3
1	M	376	ASN	2.3
1	A	361	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	33	GLU	2.3
1	G	415	GLU	2.3
1	k	293	ALA	2.3
6	d	97	GLU	2.3
2	l	409	SER	2.3
6	d	337	SER	2.3
1	M	414	GLY	2.3
1	k	62	GLY	2.3
2	T	60	GLY	2.3
3	a	263	GLY	2.3
4	t	128	GLY	2.3
6	d	35	GLY	2.3
3	C	67	ILE	2.3
3	U	79	ILE	2.3
3	g	31	ILE	2.3
4	t	103	ILE	2.3
2	H	72	ASP	2.3
2	l	144	ASP	2.3
3	I	230	ASP	2.3
1	Y	568	MET	2.3
2	H	1	MET	2.3
2	f	49	MET	2.3
2	Z	52	LYS	2.3
1	M	380	VAL	2.3
1	M	529	TYR	2.3
4	V	124	TYR	2.3
2	r	80	GLU	2.3
3	g	237	GLU	2.3
1	Y	115	ALA	2.3
1	Y	118	PRO	2.3
1	q	201	ALA	2.3
3	s	85	ALA	2.3
6	j	93	THR	2.3
1	k	45	SER	2.3
1	k	419	TRP	2.3
1	k	512	SER	2.3
6	R	89	GLN	2.3
1	k	373	LEU	2.3
1	q	472	ILE	2.3
2	T	223	LEU	2.3
3	g	225	LEU	2.3
3	g	231	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
5	c	45	ILE	2.3
1	Y	79	ASP	2.3
1	k	264	ASP	2.3
5	K	50	ASP	2.3
4	h	24	LYS	2.3
1	Y	2	GLU	2.3
1	e	501	GLU	2.3
6	d	41	CYS	2.3
6	d	281	CYS	2.3
6	v	227	GLU	2.3
1	M	163	ALA	2.3
1	S	201	ALA	2.3
2	l	33	ASN	2.3
3	U	61	ALA	2.3
1	G	434	THR	2.3
5	u	39	THR	2.3
1	k	507	GLY	2.3
2	Z	25	GLY	2.3
3	I	240	GLY	2.3
3	m	235	GLY	2.3
6	R	27	GLN	2.3
1	G	5	ILE	2.3
1	k	330	LEU	2.3
2	l	223	LEU	2.3
3	s	16	LEU	2.3
5	u	5	LEU	2.3
6	R	7	ILE	2.3
6	d	90	ILE	2.3
1	k	40	LYS	2.3
2	H	53	LYS	2.3
2	f	144	ASP	2.3
2	r	225	ASP	2.3
3	C	159	ASP	2.3
3	U	230	ASP	2.3
6	v	91	ASP	2.3
4	D	123	VAL	2.3
6	R	294	PRO	2.3
1	A	473	ASN	2.2
2	Z	33	ASN	2.2
2	f	79	ALA	2.2
6	F	21	ASN	2.2
6	v	71	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	a	269	ALA	2.2
3	m	266	GLY	2.2
1	M	254	ILE	2.2
1	Y	569	LEU	2.2
1	e	84	LYS	2.2
2	N	259	SER	2.2
3	s	30	SER	2.2
3	s	102	MET	2.2
3	s	126	ILE	2.2
3	s	174	LYS	2.2
4	t	117	MET	2.2
6	X	224	LYS	2.2
6	v	94	SER	2.2
1	A	294	ASP	2.2
1	A	33	GLU	2.2
2	T	24	GLU	2.2
1	M	266	VAL	2.2
1	M	477	VAL	2.2
1	e	532	VAL	2.2
2	T	50	ARG	2.2
3	a	233	VAL	2.2
6	R	48	VAL	2.2
1	Y	39	ALA	2.2
2	T	70	ALA	2.2
2	f	320	ASN	2.2
1	Y	232	CYS	2.2
2	T	51	TYR	2.2
3	C	74	TYR	2.2
6	X	311	CYS	2.2
4	J	129	GLN	2.2
4	h	44	GLY	2.2
1	Y	402	LEU	2.2
2	T	1	MET	2.2
2	r	30	GLY	2.2
1	M	472	ILE	2.2
1	k	302	ILE	2.2
6	F	215	ILE	2.2
2	T	225	ASP	2.2
2	f	366	GLU	2.2
6	R	22	ARG	2.2
1	G	35	VAL	2.2
1	e	306	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	k	26	VAL	2.2
1	k	256	PRO	2.2
1	k	266	VAL	2.2
1	k	398	VAL	2.2
1	G	494	ALA	2.2
1	Y	473	ASN	2.2
1	k	473	ASN	2.2
1	k	489	ALA	2.2
3	C	61	ALA	2.2
3	s	260	ALA	2.2
1	k	442	THR	2.2
2	T	14	THR	2.2
3	U	40	MET	2.2
3	g	40	MET	2.2
6	F	225	THR	2.2
6	X	4	THR	2.2
6	d	121	CYS	2.2
6	d	332	THR	2.2
6	j	4	THR	2.2
4	D	43	LEU	2.2
6	d	348	LEU	2.2
1	S	43	ASP	2.2
1	G	2	GLU	2.2
3	m	57	GLU	2.2
1	M	401	TRP	2.2
2	Z	381	PRO	2.2
3	s	51	PHE	2.2
1	k	567	VAL	2.2
1	q	426	VAL	2.2
2	r	385	VAL	2.2
2	r	407	VAL	2.2
3	C	54	VAL	2.2
1	M	154	LYS	2.2
2	T	59	ASN	2.2
2	Z	26	ASN	2.2
2	r	320	ASN	2.2
1	Y	22	MET	2.2
1	k	544	TYR	2.2
3	C	7	THR	2.2
6	d	131	THR	2.2
1	S	338	CYS	2.2
1	q	569	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	49	GLY	2.2
3	a	238	LEU	2.2
6	v	77	CYS	2.2
1	k	228	ILE	2.2
3	g	57	GLU	2.2
6	R	68	GLU	2.2
6	d	87	ASP	2.2
6	d	100	GLU	2.2
1	Y	479	PRO	2.2
2	B	84	PRO	2.2
1	A	84	LYS	2.2
1	G	418	LYS	2.2
2	l	53	LYS	2.2
2	l	58	LYS	2.2
4	t	68	LYS	2.2
6	L	326	LYS	2.2
1	M	503	VAL	2.1
1	e	158	VAL	2.1
1	G	44	ALA	2.1
1	Y	240	ASN	2.1
1	q	421	GLN	2.1
2	B	335	ALA	2.1
2	f	45	ALA	2.1
2	r	389	ALA	2.1
3	s	27	ALA	2.1
2	N	421	LEU	2.1
1	M	3	TYR	2.1
1	Y	529	TYR	2.1
2	r	428	TYR	2.1
3	C	4	ILE	2.1
1	G	356	ARG	2.1
1	M	20	GLU	2.1
2	r	388	GLU	2.1
6	X	220	GLU	2.1
1	k	38	SER	2.1
2	Z	57	ARG	2.1
2	r	72	ASP	2.1
3	g	60	ASP	2.1
4	t	59	ASP	2.1
1	q	541	LYS	2.1
3	C	19	PRO	2.1
6	R	70	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	532	VAL	2.1
1	Y	398	VAL	2.1
1	k	504	VAL	2.1
2	r	65	VAL	2.1
3	m	45	VAL	2.1
4	n	127	VAL	2.1
2	f	234	GLN	2.1
2	Z	393	ALA	2.1
2	l	48	ALA	2.1
3	s	261	ALA	2.1
6	v	179	ALA	2.1
1	A	410	ASN	2.1
2	H	320	ASN	2.1
6	d	331	ASN	2.1
1	k	196	GLY	2.1
2	r	47	GLY	2.1
3	g	6	LEU	2.1
6	R	75	GLY	2.1
6	j	73	LEU	2.1
1	M	467	ILE	2.1
1	k	24	ILE	2.1
3	U	67	ILE	2.1
3	g	107	ILE	2.1
1	k	356	ARG	2.1
2	T	61	GLU	2.1
2	f	428	TYR	2.1
2	r	291	TYR	2.1
3	s	32	GLU	2.1
4	h	124	TYR	2.1
6	X	68	GLU	2.1
6	d	237	GLU	2.1
5	c	18	CYS	2.1
1	q	404	SER	2.1
2	l	116	SER	2.1
2	l	328	ASP	2.1
6	d	67	ASP	2.1
6	F	226	PRO	2.1
1	k	285	PHE	2.1
3	g	45	VAL	2.1
5	c	42	VAL	2.1
2	r	109	ALA	2.1
6	p	99	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	196	GLY	2.1
1	k	111	THR	2.1
1	q	16	GLY	2.1
2	T	324	THR	2.1
3	O	240	GLY	2.1
6	R	231	THR	2.1
6	X	229	THR	2.1
1	k	397	ARG	2.1
1	A	20	GLU	2.1
1	Y	20	GLU	2.1
1	k	42	ILE	2.1
3	s	67	ILE	2.1
3	s	237	GLU	2.1
4	h	113	GLU	2.1
6	X	5	GLU	2.1
1	e	43	ASP	2.1
6	R	338	LYS	2.1
6	d	44	SER	2.1
1	G	479	PRO	2.1
1	M	474	PRO	2.1
1	M	17	VAL	2.1
1	k	17	VAL	2.1
1	q	148	PHE	2.1
2	H	23	VAL	2.1
6	X	143	VAL	2.1
3	g	269	ALA	2.1
5	u	2	ALA	2.1
1	G	459	LEU	2.1
1	M	370	LEU	2.1
1	M	373	LEU	2.1
6	d	69	ASN	2.1
6	j	264	LEU	2.1
1	Y	85	GLY	2.1
1	q	19	GLY	2.1
2	f	38	GLY	2.1
3	C	111	GLY	2.1
3	C	156	GLY	2.1
3	O	266	GLY	2.1
1	k	33	GLU	2.1
3	s	7	THR	2.1
5	o	43	GLU	2.1
6	F	15	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
6	R	276	THR	2.1
1	M	528	ILE	2.1
1	Y	472	ILE	2.1
3	s	31	ILE	2.1
3	s	171	ILE	2.1
6	R	323	ILE	2.1
1	M	565	LYS	2.1
1	q	28	ASP	2.1
2	Z	328	ASP	2.1
2	l	225	ASP	2.1
3	C	50	ASP	2.1
3	U	74	TYR	2.1
5	o	40	ASP	2.1
1	M	538	SER	2.1
1	k	58	SER	2.1
1	M	381	CYS	2.1
1	G	32	VAL	2.0
1	Y	477	VAL	2.0
2	r	340	VAL	2.0
3	C	109	VAL	2.0
4	D	114	VAL	2.0
6	d	72	VAL	2.0
1	G	342	LEU	2.0
2	f	78	LEU	2.0
3	g	189	LEU	2.0
1	M	367	GLY	2.0
1	k	475	GLU	2.0
2	B	366	GLU	2.0
2	H	137	GLY	2.0
3	O	232	GLU	2.0
3	s	111	GLY	2.0
3	s	182	GLY	2.0
5	u	82	GLU	2.0
6	L	100	GLU	2.0
1	k	528	ILE	2.0
2	B	28	ILE	2.0
2	l	363	ILE	2.0
3	C	29	LYS	2.0
3	g	88	ILE	2.0
3	g	89	ILE	2.0
3	s	88	ILE	2.0
6	d	323	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
6	d	333	THR	2.0
6	p	13	THR	2.0
1	M	37	ASP	2.0
6	F	28	ASP	2.0
1	A	396	PRO	2.0
2	r	10	PRO	2.0
6	j	226	PRO	2.0
1	A	22	MET	2.0
1	M	453	SER	2.0
1	M	491	SER	2.0
1	q	409	MET	2.0
1	G	223	GLN	2.0
2	T	9	CYS	2.0
1	S	503	VAL	2.0
1	e	80	ALA	2.0
1	k	116	ALA	2.0
6	L	99	ALA	2.0
1	M	531	GLU	2.0
1	k	114	GLU	2.0
6	F	148	GLU	2.0
6	d	24	LEU	2.0
6	d	98	LEU	2.0
1	M	236	GLY	2.0
1	M	500	GLY	2.0
1	S	85	GLY	2.0
1	e	566	GLY	2.0
2	B	52	LYS	2.0
2	B	80	GLU	2.0
2	N	226	GLU	2.0
2	N	25	GLY	2.0
3	C	9	LYS	2.0
6	j	8	GLU	2.0
3	g	149	GLY	2.0
1	Y	48	ILE	2.0
2	H	285	ILE	2.0
2	H	372	THR	2.0
3	C	89	ILE	2.0
6	F	335	ILE	2.0
1	G	466	ASP	2.0
1	M	300	ASP	2.0
1	k	525	ASP	2.0
6	v	226	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	262	SER	2.0
1	G	407	TYR	2.0
2	T	224	TYR	2.0
6	F	221	TYR	2.0
6	X	44	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	k	178	12/13	0.92	0.15	39,45,52,53	0
1	KCX	M	178	12/13	0.94	0.12	41,47,48,50	0
1	KCX	e	178	12/13	0.94	0.09	21,27,33,35	0
1	KCX	G	178	12/13	0.94	0.11	33,38,40,44	0
1	KCX	A	178	12/13	0.95	0.08	28,35,40,43	0
1	KCX	Y	178	12/13	0.95	0.12	36,43,50,51	0
1	KCX	q	178	12/13	0.95	0.08	31,35,42,44	0
1	KCX	S	178	12/13	0.97	0.07	25,29,38,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MFN	M	603	53/55	0.79	0.21	46,85,111,116	0
8	MFN	k	603	53/55	0.80	0.20	51,77,108,110	0
10	K	v	515	1/1	0.82	0.15	78,78,78,78	0
8	MFN	q	603	53/55	0.84	0.17	40,85,115,121	0
8	MFN	A	603	53/55	0.84	0.17	40,72,97,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MFN	Y	603	53/55	0.85	0.17	44,75,101,103	0
9	NA	q	604	1/1	0.85	0.18	47,47,47,47	0
8	MFN	G	603	53/55	0.85	0.17	43,68,86,90	0
9	NA	G	604	1/1	0.86	0.23	54,54,54,54	0
8	MFN	e	603	53/55	0.87	0.15	35,59,92,101	0
10	K	L	511	1/1	0.88	0.12	80,80,80,80	0
8	MFN	S	603	53/55	0.88	0.13	30,56,87,89	0
10	K	Z	506	1/1	0.89	0.13	63,63,63,63	0
16	CL	N	506	1/1	0.89	0.10	62,62,62,62	0
9	NA	A	604	1/1	0.90	0.14	41,41,41,41	0
10	K	v	511	1/1	0.90	0.10	53,53,53,53	0
10	K	e	608	1/1	0.91	0.09	68,68,68,68	0
9	NA	M	604	1/1	0.91	0.18	56,56,56,56	0
10	K	d	411	1/1	0.93	0.11	60,60,60,60	0
10	K	X	511	1/1	0.94	0.10	59,59,59,59	0
10	K	T	506	1/1	0.94	0.09	59,59,59,59	0
13	MGD	Z	503	47/47	0.94	0.10	29,37,45,56	0
14	H2S	l	505	1/1	0.94	0.24	66,66,66,66	0
14	H2S	r	505	1/1	0.94	0.13	52,52,52,52	0
10	K	v	510	1/1	0.94	0.07	57,57,57,57	0
11	SF4	R	403	8/8	0.95	0.06	67,74,83,94	0
11	SF4	c	102	8/8	0.95	0.08	42,53,64,69	0
11	SF4	d	403	8/8	0.95	0.06	60,74,85,92	0
11	SF4	l	501	8/8	0.95	0.07	30,37,53,53	0
13	MGD	T	504	47/47	0.95	0.10	25,37,43,55	0
10	K	R	411	1/1	0.95	0.07	59,59,59,59	0
13	MGD	Z	504	47/47	0.95	0.09	23,37,43,65	0
13	MGD	f	503	47/47	0.95	0.09	26,37,43,46	0
13	MGD	r	503	47/47	0.95	0.09	37,46,53,55	0
13	MGD	r	504	47/47	0.95	0.09	27,36,45,47	0
9	NA	e	604	1/1	0.95	0.09	30,30,30,30	0
10	K	v	514	1/1	0.95	0.09	42,42,42,42	0
10	K	M	606	1/1	0.95	0.10	55,55,55,55	0
10	K	v	509	1/1	0.96	0.08	58,58,58,58	0
11	SF4	d	404	8/8	0.96	0.06	44,57,65,69	0
11	SF4	d	405	8/8	0.96	0.05	38,43,61,62	0
11	SF4	d	406	8/8	0.96	0.06	34,42,54,61	0
11	SF4	f	501	8/8	0.96	0.08	38,41,64,66	0
11	SF4	i	101	8/8	0.96	0.05	26,34,41,47	0
11	SF4	j	505	8/8	0.96	0.05	33,47,54,55	0
10	K	X	510	1/1	0.96	0.06	52,52,52,52	0
11	SF4	p	402	8/8	0.96	0.06	28,37,44,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	MGD	B	503	47/47	0.96	0.09	34,40,48,51	0
13	MGD	H	503	47/47	0.96	0.08	29,35,41,47	0
13	MGD	T	503	47/47	0.96	0.09	28,38,46,47	0
10	K	N	507	1/1	0.96	0.06	55,55,55,55	0
10	K	F	412	1/1	0.96	0.06	53,53,53,53	0
10	K	R	412	1/1	0.96	0.06	61,61,61,61	0
11	SF4	F	407	8/8	0.96	0.05	29,31,44,53	0
13	MGD	l	504	47/47	0.96	0.09	25,36,47,50	0
10	K	L	509	1/1	0.96	0.06	43,43,43,43	0
11	SF4	R	404	8/8	0.96	0.06	48,54,65,78	0
11	SF4	R	407	8/8	0.96	0.06	23,35,43,46	0
11	SF4	X	504	8/8	0.96	0.06	25,30,48,57	0
15	MG	B	507	1/1	0.96	0.13	36,36,36,36	0
15	MG	r	507	1/1	0.96	0.14	34,34,34,34	0
10	K	p	411	1/1	0.96	0.07	57,57,57,57	0
11	SF4	R	402	8/8	0.97	0.06	28,41,51,59	0
10	K	j	512	1/1	0.97	0.08	58,58,58,58	0
10	K	j	514	1/1	0.97	0.16	48,48,48,48	0
11	SF4	R	405	8/8	0.97	0.05	32,44,55,65	0
10	K	p	410	1/1	0.97	0.10	63,63,63,63	0
11	SF4	R	409	8/8	0.97	0.04	31,35,47,50	0
11	SF4	T	501	8/8	0.97	0.06	28,39,53,60	0
11	SF4	W	200	8/8	0.97	0.05	32,40,47,54	0
11	SF4	W	201	8/8	0.97	0.04	21,33,41,47	0
10	K	F	410	1/1	0.97	0.07	53,53,53,53	0
11	SF4	X	505	8/8	0.97	0.05	33,46,57,60	0
11	SF4	X	506	8/8	0.97	0.04	22,31,42,42	0
11	SF4	X	507	8/8	0.97	0.05	30,31,40,48	0
11	SF4	Z	501	8/8	0.97	0.05	26,36,44,53	0
11	SF4	c	101	8/8	0.97	0.06	39,45,51,66	0
10	K	p	412	1/1	0.97	0.07	53,53,53,53	0
11	SF4	d	401	8/8	0.97	0.04	34,50,53,59	0
11	SF4	d	402	8/8	0.97	0.06	37,48,56,66	0
10	K	q	605	1/1	0.97	0.06	47,47,47,47	0
10	K	r	506	1/1	0.97	0.08	57,57,57,57	0
10	K	L	510	1/1	0.97	0.05	52,52,52,52	0
10	K	F	411	1/1	0.97	0.06	38,38,38,38	0
11	SF4	d	407	8/8	0.97	0.04	34,42,53,55	0
9	NA	k	604	1/1	0.97	0.08	52,52,52,52	0
10	K	v	512	1/1	0.97	0.09	56,56,56,56	0
11	SF4	i	102	8/8	0.97	0.05	20,31,41,52	0
11	SF4	j	501	8/8	0.97	0.05	27,38,44,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	SF4	j	502	8/8	0.97	0.05	18,31,50,53	0
11	SF4	j	503	8/8	0.97	0.04	33,38,44,49	0
11	SF4	j	504	8/8	0.97	0.05	25,37,42,51	0
10	K	v	513	1/1	0.97	0.07	59,59,59,59	0
11	SF4	j	507	8/8	0.97	0.04	16,26,43,45	0
10	K	F	413	1/1	0.97	0.05	40,40,40,40	0
11	SF4	o	102	8/8	0.97	0.05	31,38,49,51	0
10	K	R	410	1/1	0.97	0.04	40,40,40,40	0
11	SF4	p	403	8/8	0.97	0.07	20,35,47,51	0
11	SF4	p	404	8/8	0.97	0.05	20,30,41,42	0
11	SF4	p	406	8/8	0.97	0.05	24,37,43,44	0
11	SF4	p	409	8/8	0.97	0.04	28,41,43,45	0
11	SF4	u	101	8/8	0.97	0.05	25,39,46,61	0
11	SF4	v	503	8/8	0.97	0.04	27,31,39,44	0
11	SF4	v	505	8/8	0.97	0.05	33,39,51,51	0
11	SF4	v	507	8/8	0.97	0.04	21,33,45,47	0
11	SF4	v	508	8/8	0.97	0.05	27,41,48,52	0
11	SF4	B	501	8/8	0.97	0.05	29,38,55,56	0
13	MGD	B	504	47/47	0.97	0.08	27,36,42,44	0
11	SF4	E	102	8/8	0.97	0.06	33,37,52,61	0
13	MGD	H	504	47/47	0.97	0.08	21,32,38,41	0
13	MGD	N	503	47/47	0.97	0.08	26,34,43,48	0
13	MGD	N	504	47/47	0.97	0.08	24,32,40,44	0
11	SF4	F	401	8/8	0.97	0.05	26,38,46,46	0
11	SF4	F	403	8/8	0.97	0.05	41,48,60,66	0
11	SF4	F	405	8/8	0.97	0.05	29,37,49,56	0
10	K	K	103	1/1	0.97	0.05	48,48,48,48	0
11	SF4	F	408	8/8	0.97	0.05	26,33,40,49	0
13	MGD	f	504	47/47	0.97	0.08	23,33,38,43	0
13	MGD	l	503	47/47	0.97	0.08	30,37,44,51	0
11	SF4	F	409	8/8	0.97	0.04	18,29,38,39	0
11	SF4	H	501	8/8	0.97	0.05	28,33,40,45	0
11	SF4	K	102	8/8	0.97	0.04	27,41,47,60	0
11	SF4	L	504	8/8	0.97	0.05	25,31,39,41	0
11	SF4	L	508	8/8	0.97	0.06	27,34,46,52	0
11	SF4	N	501	8/8	0.97	0.07	30,38,48,55	0
15	MG	Z	507	1/1	0.97	0.12	30,30,30,30	0
15	MG	l	506	1/1	0.97	0.05	32,32,32,32	0
11	SF4	Q	102	8/8	0.97	0.06	32,45,54,63	0
11	SF4	R	401	8/8	0.97	0.05	31,47,53,59	0
10	K	j	510	1/1	0.98	0.07	49,49,49,49	0
11	SF4	j	506	8/8	0.98	0.04	25,30,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	K	j	511	1/1	0.98	0.04	35,35,35,35	0
11	SF4	j	508	8/8	0.98	0.04	22,36,40,59	0
10	K	Q	103	1/1	0.98	0.07	53,53,53,53	0
11	SF4	o	101	8/8	0.98	0.04	27,35,45,55	0
11	SF4	R	406	8/8	0.98	0.04	33,36,50,59	0
11	SF4	p	401	8/8	0.98	0.04	24,34,47,52	0
11	SF4	E	101	8/8	0.98	0.06	36,43,51,58	0
11	SF4	R	408	8/8	0.98	0.03	21,28,40,41	0
10	K	j	513	1/1	0.98	0.04	53,53,53,53	0
11	SF4	p	405	8/8	0.98	0.04	17,21,36,39	0
10	K	X	509	1/1	0.98	0.05	42,42,42,42	0
11	SF4	p	407	8/8	0.98	0.04	25,32,44,51	0
11	SF4	F	402	8/8	0.98	0.04	18,36,46,49	0
11	SF4	r	501	8/8	0.98	0.05	31,43,47,51	0
10	K	o	103	1/1	0.98	0.04	42,42,42,42	0
11	SF4	u	102	8/8	0.98	0.06	26,34,43,46	0
11	SF4	v	501	8/8	0.98	0.04	20,33,44,46	0
11	SF4	v	502	8/8	0.98	0.04	15,26,36,42	0
11	SF4	X	501	8/8	0.98	0.05	34,41,58,62	0
11	SF4	v	504	8/8	0.98	0.05	18,36,41,42	0
11	SF4	X	502	8/8	0.98	0.04	22,36,39,53	0
11	SF4	v	506	8/8	0.98	0.04	19,27,43,47	0
11	SF4	X	503	8/8	0.98	0.04	28,33,40,61	0
11	SF4	F	404	8/8	0.98	0.04	22,35,44,57	0
7	ZN	q	602	1/1	0.98	0.03	39,39,39,39	0
11	SF4	F	406	8/8	0.98	0.04	20,35,46,49	0
10	K	B	506	1/1	0.98	0.10	54,54,54,54	0
11	SF4	X	508	8/8	0.98	0.04	26,29,41,46	0
9	NA	S	604	1/1	0.98	0.05	32,32,32,32	0
10	K	c	103	1/1	0.98	0.04	57,57,57,57	0
10	K	q	606	1/1	0.98	0.07	47,47,47,47	0
11	SF4	K	101	8/8	0.98	0.04	25,34,43,52	0
10	K	d	410	1/1	0.98	0.04	47,47,47,47	0
11	SF4	L	501	8/8	0.98	0.04	21,34,47,49	0
11	SF4	L	502	8/8	0.98	0.05	27,40,50,52	0
11	SF4	L	503	8/8	0.98	0.04	24,34,46,47	0
10	K	u	103	1/1	0.98	0.11	53,53,53,53	0
11	SF4	L	506	8/8	0.98	0.03	15,26,33,44	0
11	SF4	d	408	8/8	0.98	0.05	20,34,50,59	0
11	SF4	d	409	8/8	0.98	0.04	24,29,38,60	0
14	H2S	Z	505	1/1	0.98	0.11	63,63,63,63	0
11	SF4	L	507	8/8	0.98	0.04	21,27,40,43	0

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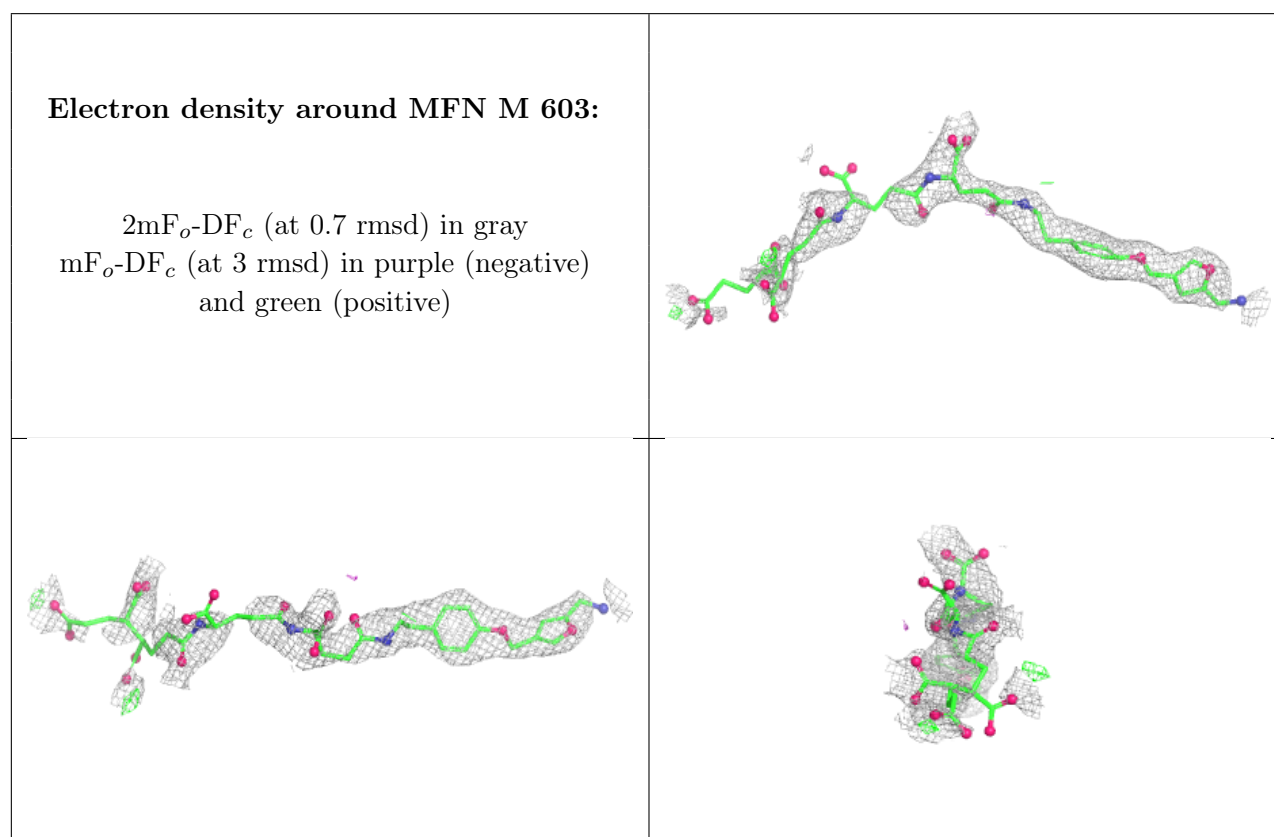
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	K	S	605	1/1	0.98	0.04	32,32,32,32	0
10	K	e	605	1/1	0.98	0.06	34,34,34,34	0
15	MG	T	507	1/1	0.98	0.10	27,27,27,27	0
11	SF4	Q	101	8/8	0.98	0.04	23,36,48,49	0
10	K	e	606	1/1	0.98	0.04	37,37,37,37	0
10	K	S	606	1/1	0.98	0.08	46,46,46,46	0
10	K	i	103	1/1	0.98	0.03	36,36,36,36	0
11	SF4	L	505	8/8	0.99	0.03	22,32,41,49	0
7	ZN	M	601	1/1	0.99	0.02	51,51,51,51	0
10	K	k	605	1/1	0.99	0.03	36,36,36,36	0
11	SF4	p	408	8/8	0.99	0.03	21,34,40,44	0
7	ZN	M	602	1/1	0.99	0.06	46,46,46,46	0
10	K	Y	604	1/1	0.99	0.10	38,38,38,38	0
7	ZN	S	601	1/1	0.99	0.04	40,40,40,40	0
10	K	M	605	1/1	0.99	0.03	37,37,37,37	0
7	ZN	S	602	1/1	0.99	0.02	32,32,32,32	0
10	K	A	605	1/1	0.99	0.04	49,49,49,49	0
7	ZN	Y	602	1/1	0.99	0.04	47,47,47,47	0
10	K	E	103	1/1	0.99	0.04	43,43,43,43	0
14	H2S	B	505	1/1	0.99	0.08	44,44,44,44	0
14	H2S	H	505	1/1	0.99	0.11	41,41,41,41	0
14	H2S	N	505	1/1	0.99	0.10	50,50,50,50	0
14	H2S	T	505	1/1	0.99	0.10	50,50,50,50	0
10	K	e	607	1/1	0.99	0.04	51,51,51,51	0
14	H2S	f	505	1/1	0.99	0.06	38,38,38,38	0
7	ZN	e	602	1/1	0.99	0.03	34,34,34,34	0
7	ZN	k	601	1/1	0.99	0.03	46,46,46,46	0
10	K	j	509	1/1	0.99	0.08	37,37,37,37	0
15	MG	H	506	1/1	0.99	0.06	24,24,24,24	0
15	MG	O	301	1/1	0.99	0.10	31,31,31,31	0
12	W	Z	502	1/1	0.99	0.11	63,63,63,63	0
7	ZN	q	601	1/1	0.99	0.03	39,39,39,39	0
15	MG	f	506	1/1	0.99	0.10	28,28,28,28	0
7	ZN	A	601	1/1	0.99	0.03	40,40,40,40	0
10	K	G	605	1/1	0.99	0.05	62,62,62,62	0
7	ZN	G	602	1/1	0.99	0.02	40,40,40,40	0
12	W	f	502	1/1	1.00	0.10	52,52,52,52	0
12	W	l	502	1/1	1.00	0.08	48,48,48,48	0
12	W	r	502	1/1	1.00	0.05	48,48,48,48	0
7	ZN	A	602	1/1	1.00	0.02	41,41,41,41	0
7	ZN	Y	601	1/1	1.00	0.04	45,45,45,45	0
7	ZN	k	602	1/1	1.00	0.02	44,44,44,44	0

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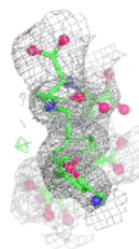
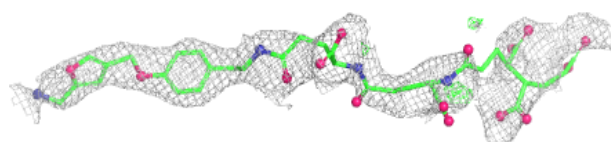
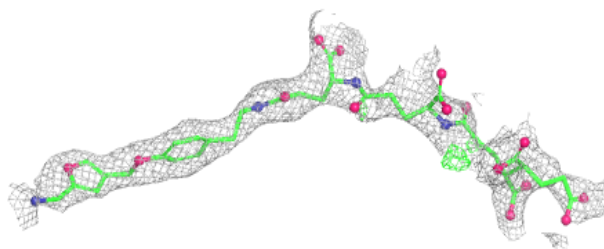
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ZN	G	601	1/1	1.00	0.02	41,41,41,41	0
12	W	B	502	1/1	1.00	0.04	43,43,43,43	0
12	W	H	502	1/1	1.00	0.04	37,37,37,37	0
12	W	N	502	1/1	1.00	0.02	34,34,34,34	0
12	W	T	502	1/1	1.00	0.08	49,49,49,49	0
7	ZN	e	601	1/1	1.00	0.02	38,38,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

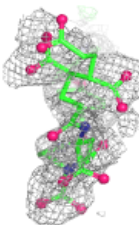
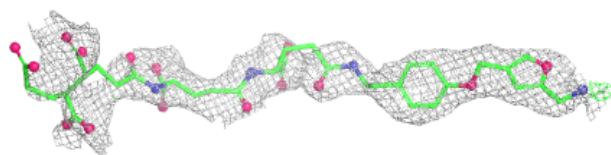
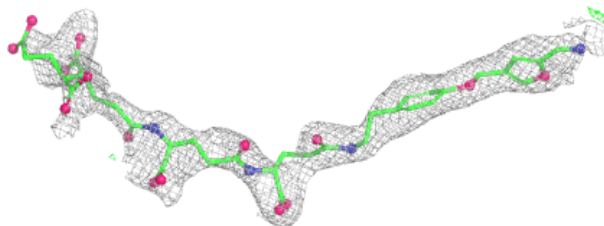


Electron density around MFN k 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

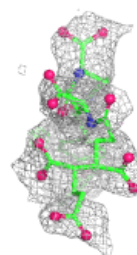
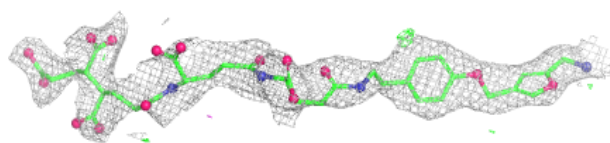
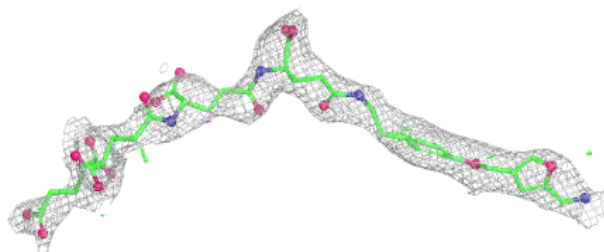
**Electron density around MFN q 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

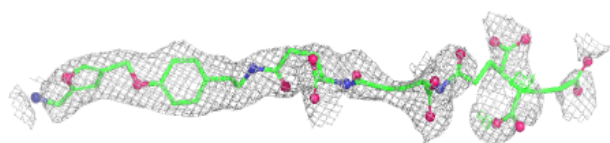
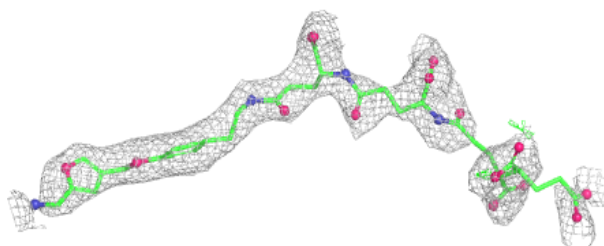


Electron density around MFN A 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

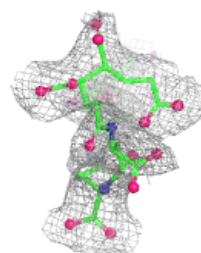
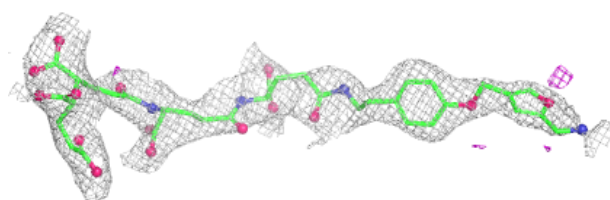
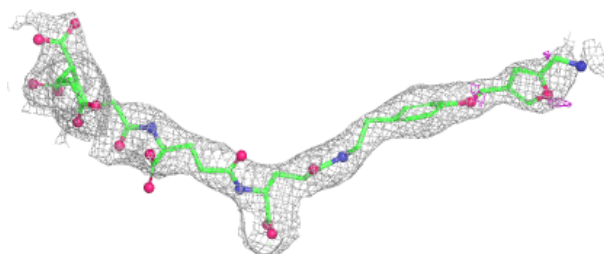
**Electron density around MFN Y 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

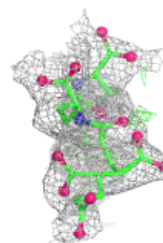
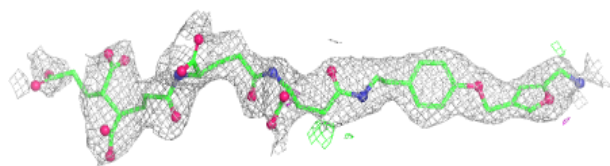
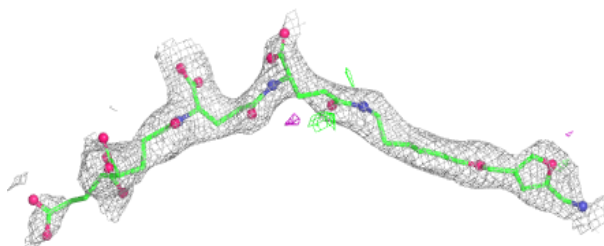


Electron density around MFN G 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

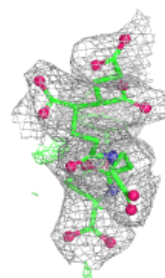
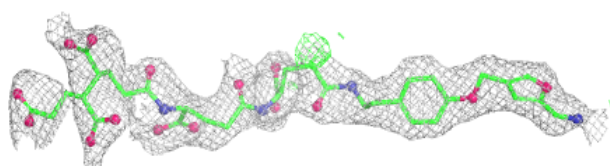
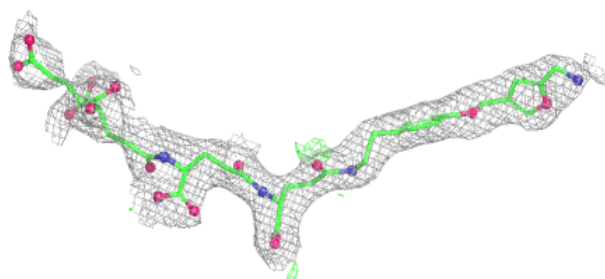
**Electron density around MFN e 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

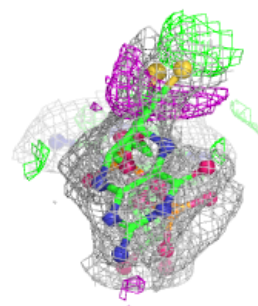
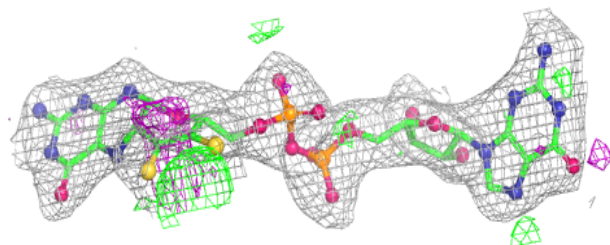
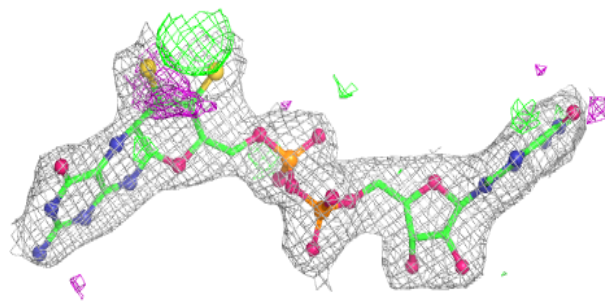


Electron density around MFN S 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

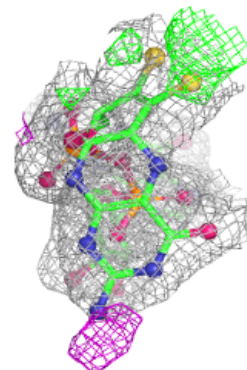
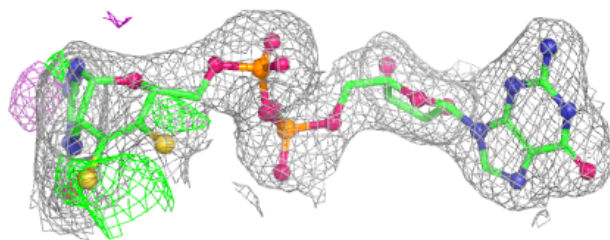
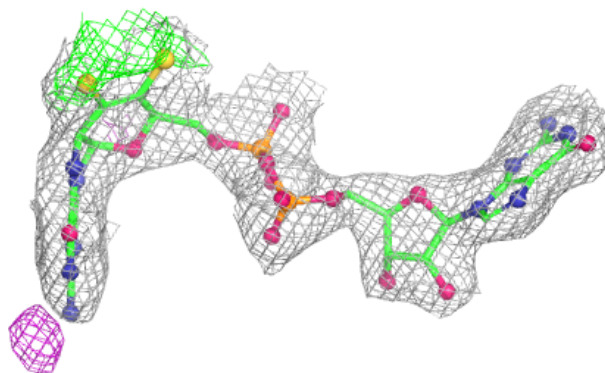
**Electron density around MGD Z 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

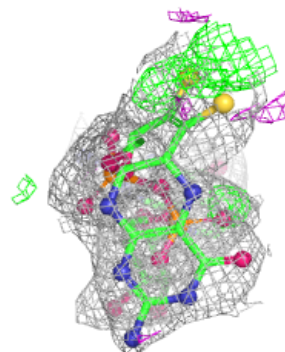
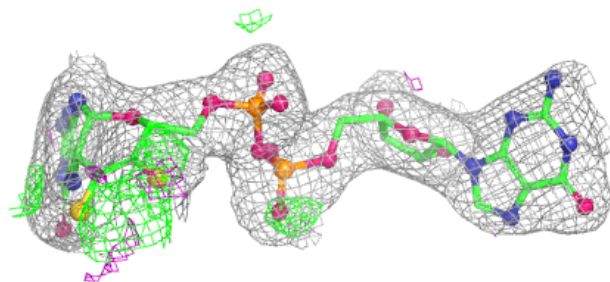
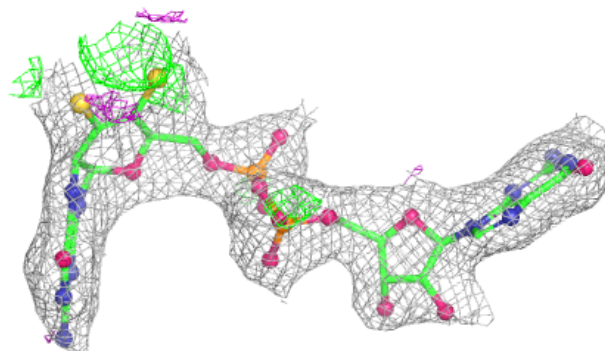


Electron density around MGD T 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

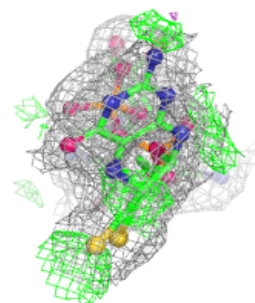
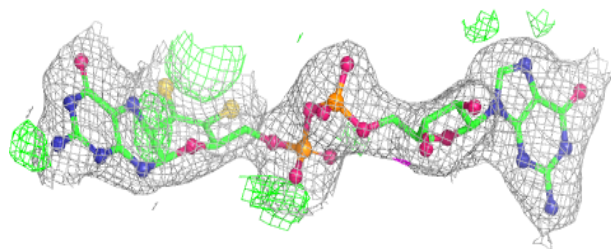
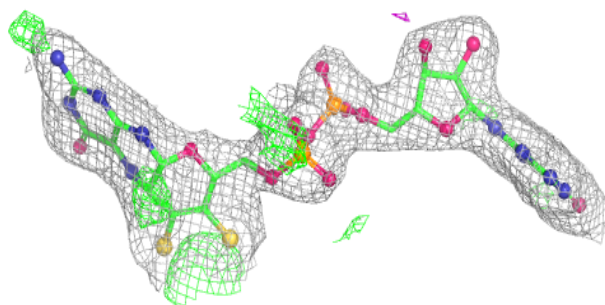
**Electron density around MGD Z 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

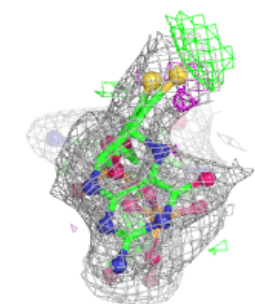
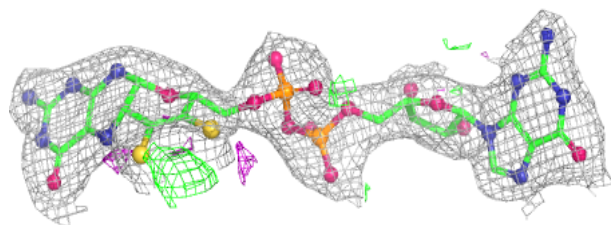
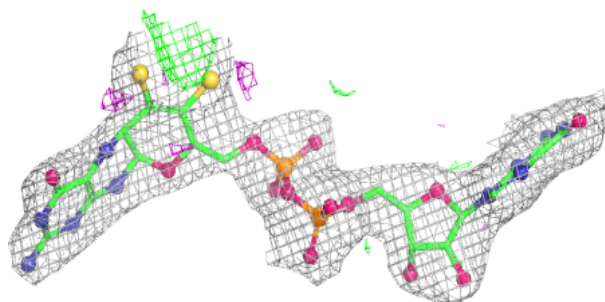


Electron density around MGD f 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

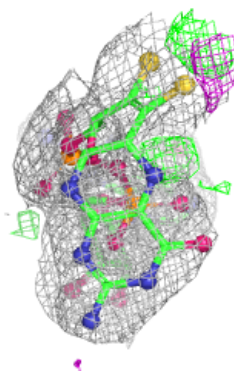
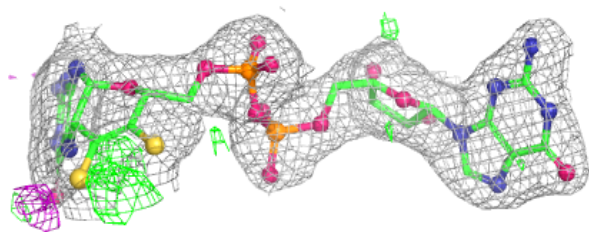
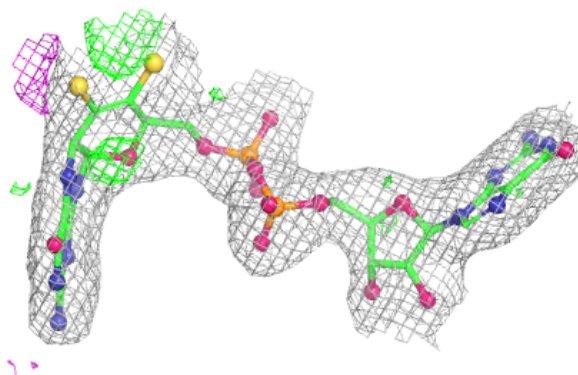
**Electron density around MGD r 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

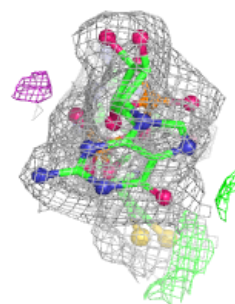
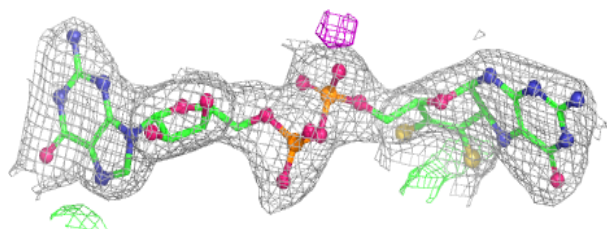
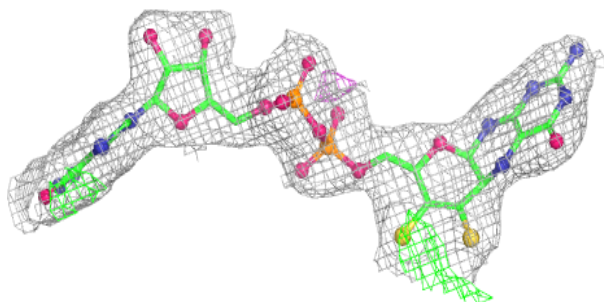


Electron density around MGD r 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

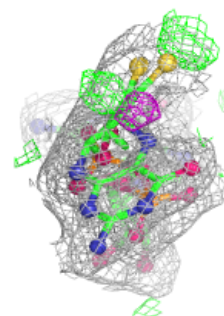
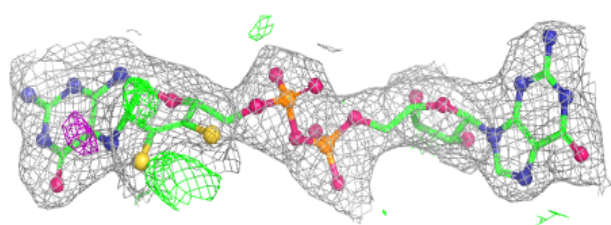
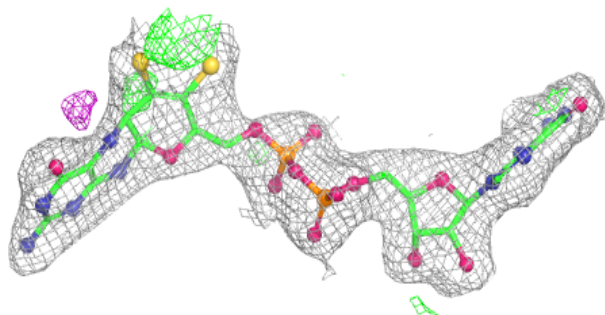
**Electron density around MGD B 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

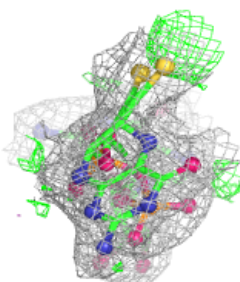
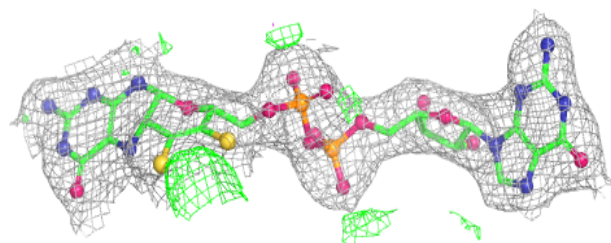
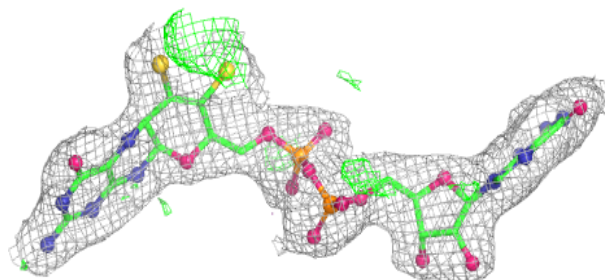


Electron density around MGD H 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

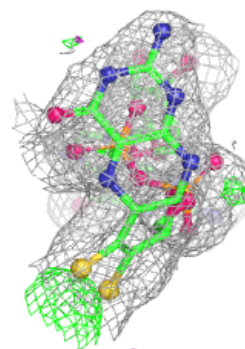
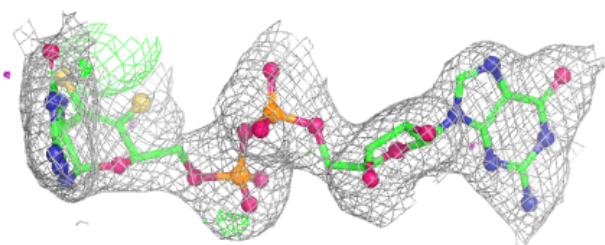
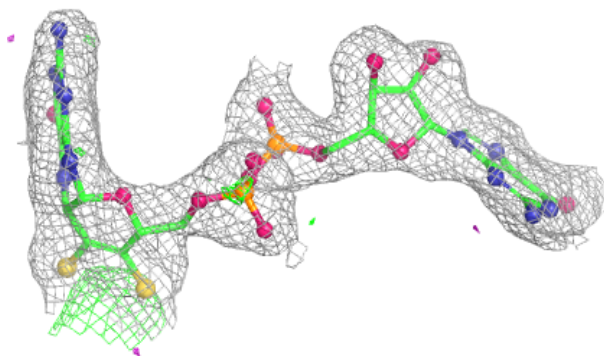
**Electron density around MGD T 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

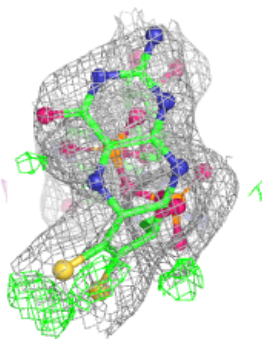
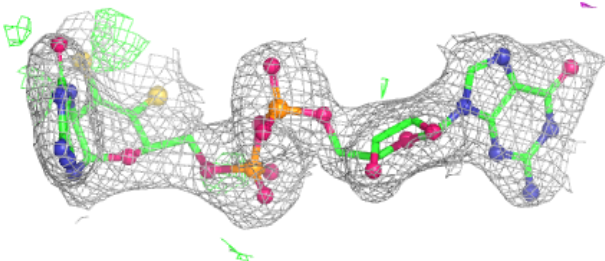
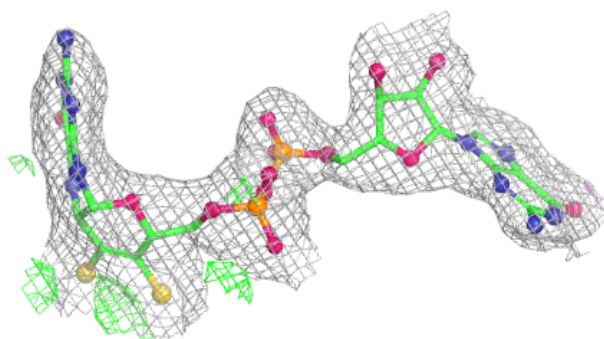


Electron density around MGD 1 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

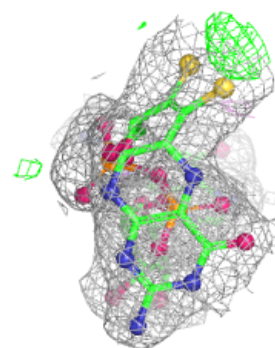
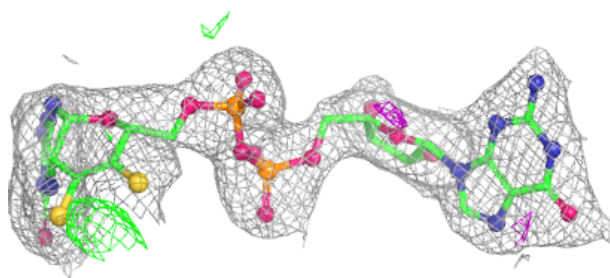
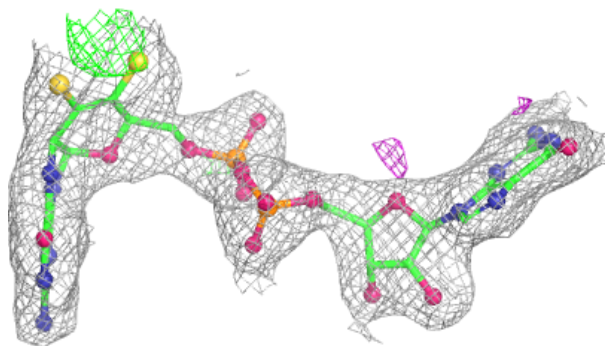
**Electron density around MGD B 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

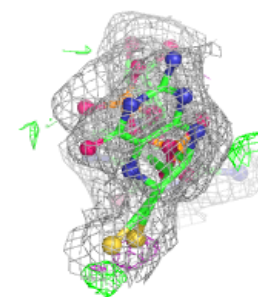
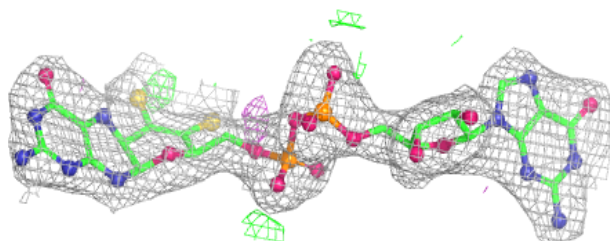
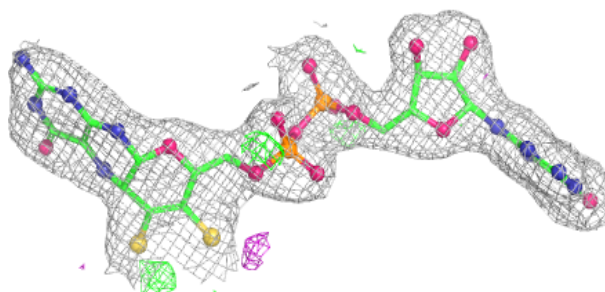


Electron density around MGD H 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

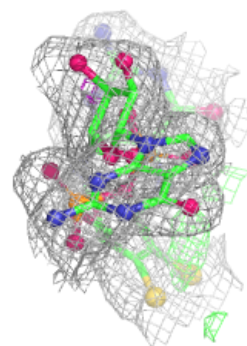
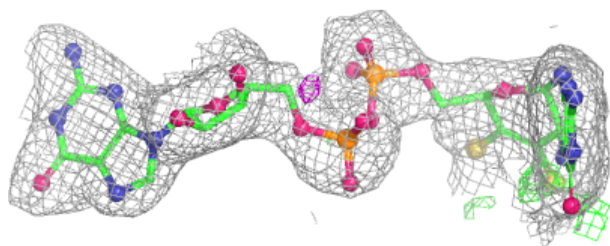
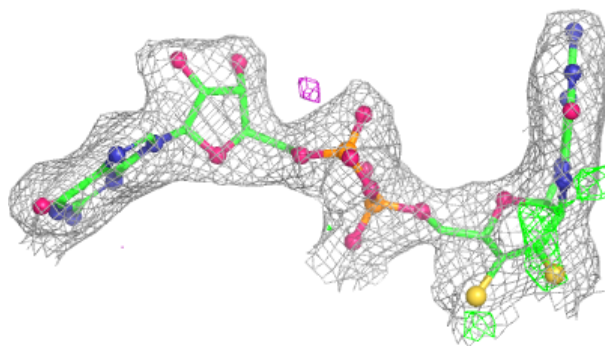
**Electron density around MGD N 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

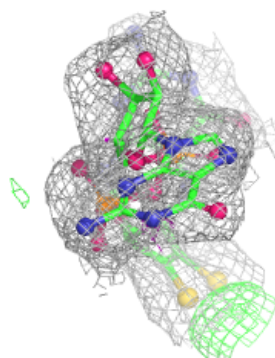
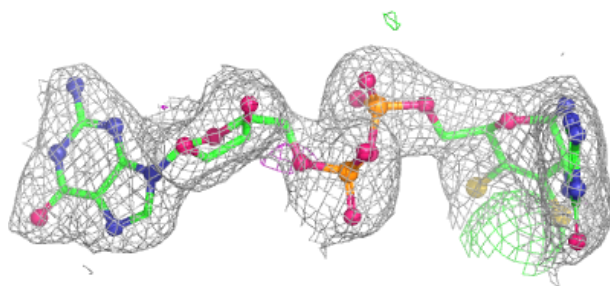
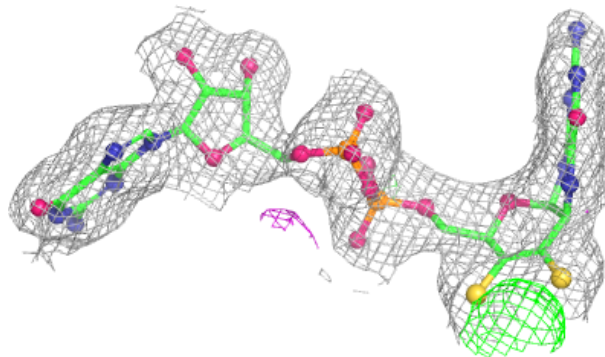


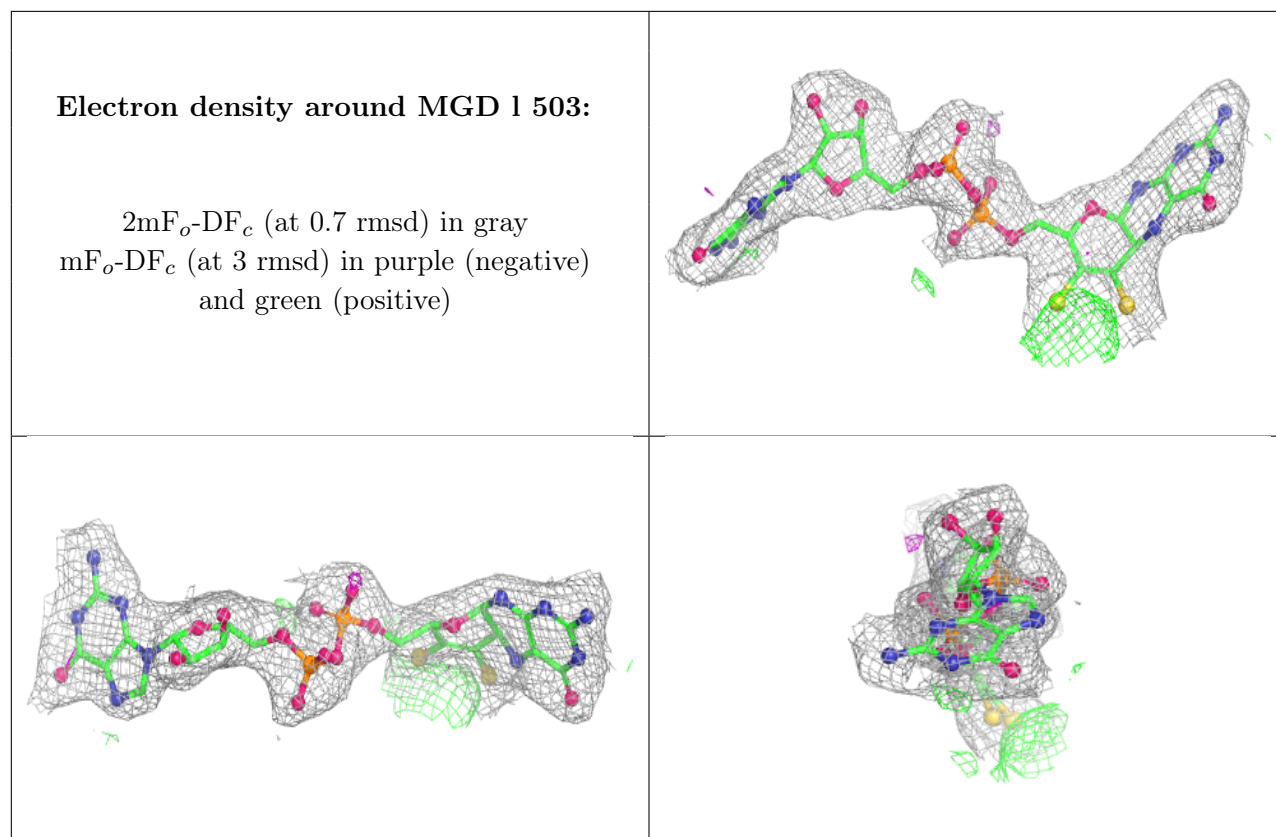
Electron density around MGD N 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MGD f 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.