



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:41 AM UTC

PDB ID : 7ARD / pdb_00007ard
EMDB ID : EMD-11880
Title : Cryo-EM structure of Polytomella Complex-I (complete composition)
Authors : Klusch, N.; Kuehlbrandt, W.; Yildiz, O.
Deposited on : 2020-10-23
Resolution : 3.11 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

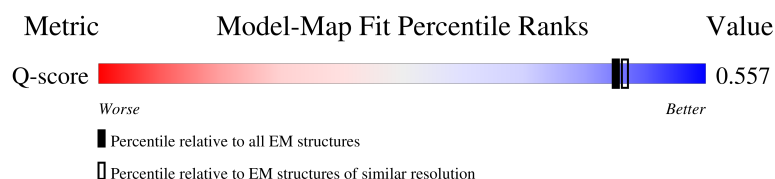
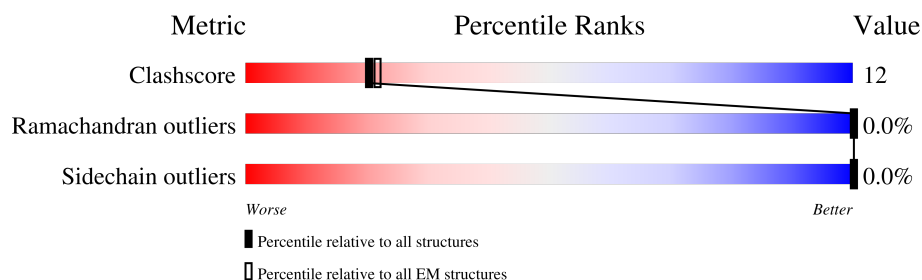
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.61 - 3.61)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	154	12% 52% 27% 21%
2	B	164	18% 63% 31% 6%
3	C	217	6% 70% 30%
4	D	395	8% 65% 35%

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Mol	Chain	Length	Quality of chain
5	E	276	
6	F	469	
7	G	720	
8	H	293	
9	I	229	
10	J	145	
11	K	127	
12	L	536	
13	M	438	
14	N	375	
15	O	200	
16	P	370	
17	Q	185	
18	R	132	
19	S	98	
20	T	123	
21	U	122	
22	V	159	
23	W	137	
24	X	100	
25	Y	206	
26	Z	142	
27	a	71	
28	b	54	
29	c	110	

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Mol	Chain	Length	Quality of chain
30	d	83	
31	e	75	
32	f	121	
33	g	172	
34	h	81	
35	i	128	
36	j	87	
37	k	55	
38	l	151	
39	m	138	
40	n	121	
41	o	85	
42	p	156	
43	q	155	
44	r	121	
45	s	118	
46	t	134	
47	u	50	
48	w	41	
49	x	280	
50	y	310	
51	z	227	

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
53	SF4	F	501	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 70559 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ND3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			999	673	148	172	6		

- Molecule 2 is a protein called PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	154	Total	C	N	O	S	0	0
			1206	774	208	211	13		

- Molecule 3 is a protein called ND9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	216	Total	C	N	O	S	0	0
			1808	1169	302	332	5		

- Molecule 4 is a protein called ND7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	395	Total	C	N	O	S	0	0
			3178	2029	557	569	23		

- Molecule 5 is a protein called 24 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	235	Total	C	N	O	S	0	0
			1806	1135	306	350	15		

- Molecule 6 is a protein called 51 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3322	2088	594	617	23		

- Molecule 7 is a protein called 75 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	682	Total	C	N	O	S	0	0
			5166	3243	919	980	24		

- Molecule 8 is a protein called ND1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	293	Total	C	N	O	S	0	0
			2237	1487	346	387	17		

- Molecule 9 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	199	Total	C	N	O	S	0	0
			1602	1000	274	317	11		

- Molecule 10 is a protein called ND6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	145	Total	C	N	O	S	0	0
			1120	755	159	197	9		

- Molecule 11 is a protein called ND4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	104	Total	C	N	O	S	0	0
			798	518	128	145	7		

- Molecule 12 is a protein called ND5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	536	Total	C	N	O	S	0	0
			4111	2697	654	735	25		

- Molecule 13 is a protein called ND4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	438	Total	C	N	O	S	0	0
			3425	2314	520	572	19		

- Molecule 14 is a protein called ND2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	375	Total	C	N	O	S	0	0
			2967	1998	450	505	14		

- Molecule 15 is a protein called C1-FDX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	161	Total	C	N	O	S	0	0
			1336	871	213	247	5		

- Molecule 16 is a protein called 39 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	347	Total	C	N	O	S	0	0
			2701	1713	464	514	10		

- Molecule 17 is a protein called 18 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	162	Total	C	N	O	S	0	0
			1276	812	227	233	4		

- Molecule 18 is a protein called 13 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	108	Total	C	N	O	S	0	0
			812	510	138	159	5		

- Molecule 19 is a protein called B8.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	95	Total	C	N	O	0	0
			716	450	124	142		

- Molecule 20 is a protein called SDAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			645	406	103	134	2		

- Molecule 21 is a protein called SDAP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	84	Total	C	N	O	0	0
			655	414	103	138		

- Molecule 22 is a protein called B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	134	Total	C	N	O	S	0	0
			1052	671	170	209	2		

- Molecule 23 is a protein called B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	127	Total	C	N	O	S	0	0
			1074	695	185	188	6		

- Molecule 24 is a protein called PGIV.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	99	Total	C	N	O	S	0	0
			816	522	139	149	6		

- Molecule 25 is a protein called B14.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	205	Total	C	N	O	S	0	0
			1583	1027	259	293	4		

- Molecule 26 is a protein called B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	124	Total	C	N	O	S	0	0
			1003	639	184	178	2		

- Molecule 27 is a protein called MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	60	Total	C	N	O	S	0	0
			515	335	89	90	1		

- Molecule 28 is a protein called B9.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	54	Total	C	N	O	0	0
			270	162	54	54		

- Molecule 29 is a protein called KFYI.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	97	Total	C	N	O	S	0	0
			785	512	134	136	3		

- Molecule 30 is a protein called B14.5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	80	Total	C	N	O	S	0	0
			650	420	112	116	2		

- Molecule 31 is a protein called 15 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	71	Total	C	N	O	S	0	0
			592	370	103	112	7		

- Molecule 32 is a protein called MNLL.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	111	Total	C	N	O	S	0	0
			877	566	146	163	2		

- Molecule 33 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	147	Total	C	N	O	S	0	0
			1176	763	194	213	6		

- Molecule 34 is a protein called NUOP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	77	Total	C	N	O	S	0	0
			625	411	94	118	2		

- Molecule 35 is a protein called NUOP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	i	111	Total	C	N	O	0	0
			922	576	170	176		

- Molecule 36 is a protein called AGGG.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	j	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 37 is a protein called B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	44	Total	C	N	O	S	0	0
			367	247	60	59	1		

- Molecule 38 is a protein called ASHL.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	127	Total	C	N	O	S	0	0
			1018	666	161	184	7		

- Molecule 39 is a protein called B15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	111	Total	C	N	O	S	0	0
			934	601	158	172	3		

- Molecule 40 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	120	Total	C	N	O	S	0	0
			1008	648	183	173	4		

- Molecule 41 is a protein called B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	83	Total	C	N	O	S	0	0
			704	448	129	120	7		

- Molecule 42 is a protein called PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	155	Total	C	N	O	S	0	0
			1287	803	242	238	4		

- Molecule 43 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	28	Total	C	N	O	S	0	0
			243	160	43	39	1		

- Molecule 44 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	60	Total	C	N	O	S	0	0
			493	317	88	87	1		

- Molecule 45 is a protein called NUOP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	115	Total	C	N	O	S	0	0
			933	613	155	164	1		

- Molecule 46 is a protein called NUOP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	82	Total	C	N	O	S	0	0
			706	476	112	116	2		

- Molecule 47 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	u	50	Total	C	N	O	0	0
			250	150	50	50		

- Molecule 48 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	w	41	Total	C	N	O	0	0
			204	122	41	41		

- Molecule 49 is a protein called CAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	250	Total	C	N	O	S	0	0
			1967	1240	346	375	6		

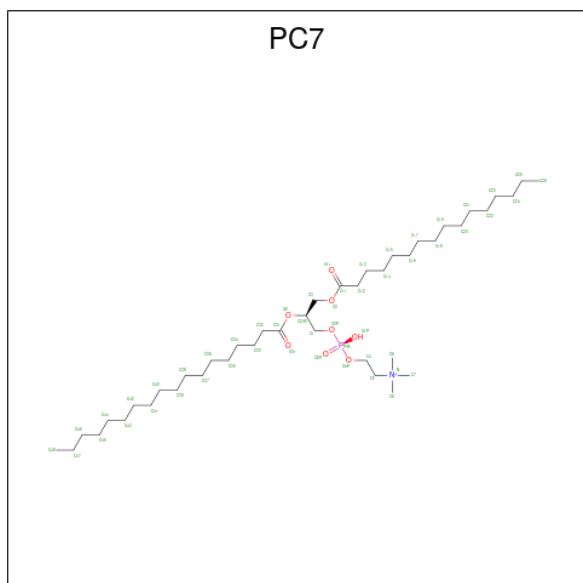
- Molecule 50 is a protein called CA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	308	Total	C	N	O	S	0	0
			2316	1470	401	438	7		

- Molecule 51 is a protein called CA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	226	Total	C	N	O	S	0	0
			1687	1069	279	334	5		

- Molecule 52 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: $C_{42}H_{85}NO_8P$).



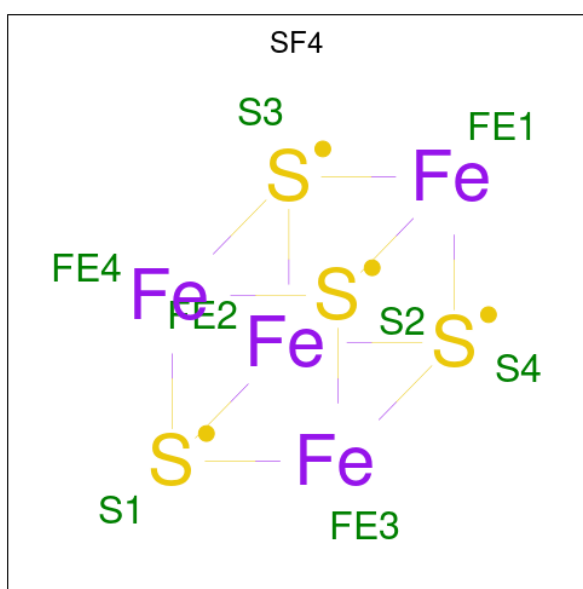
Mol	Chain	Residues	Atoms					AltConf
52	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	L	1	Total	C	N	O	P	0
			48	38	1	8	1	
52	M	1	Total	C	N	O	P	0
			52	42	1	8	1	

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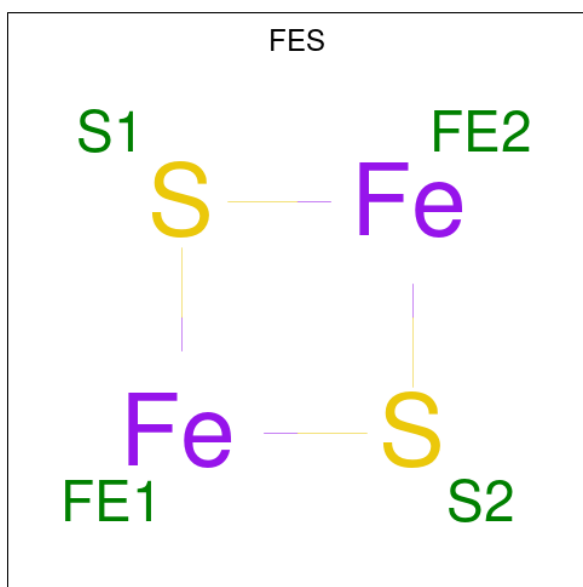
Mol	Chain	Residues	Atoms					AltConf
52	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	N	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	N	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	z	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 53 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



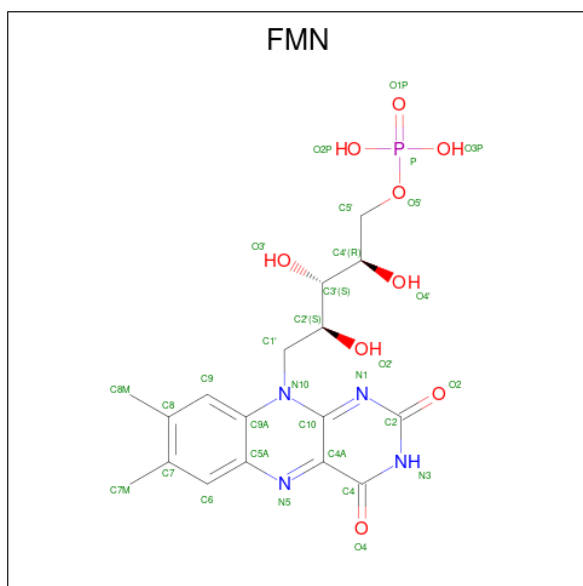
Mol	Chain	Residues	Atoms			AltConf
53	B	1	Total	Fe	S	0
			8	4	4	
53	F	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	
53	I	1	Total	Fe	S	0
			8	4	4	
53	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



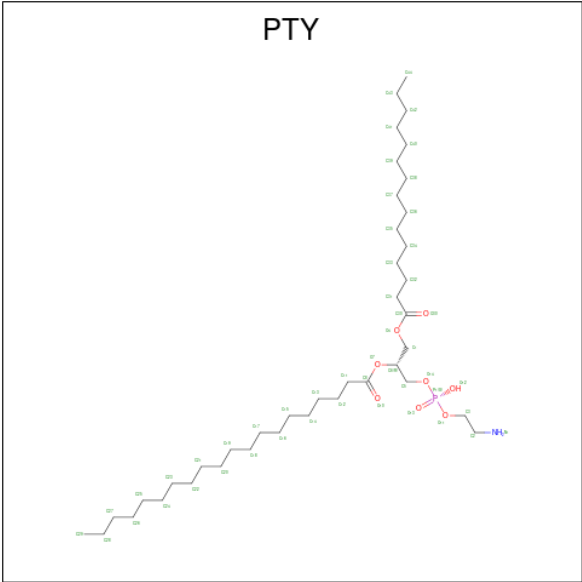
Mol	Chain	Residues	Atoms			AltConf
54	E	1	Total	Fe	S	0
			4	2	2	
54	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



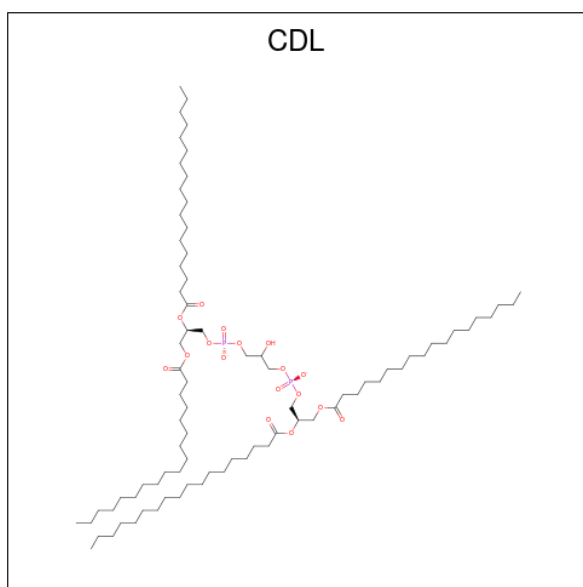
Mol	Chain	Residues	Atoms					AltConf
55	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 56 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
56	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	L	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	M	1	Total	C	N	O	P	0
			47	37	1	8	1	
56	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	m	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	m	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 57 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
57	L	1	Total	C	O	P	0
			89	70	17	2	
57	M	1	Total	C	O	P	0
			100	81	17	2	
57	N	1	Total	C	O	P	0
			100	81	17	2	
57	d	1	Total	C	O	P	0
			100	81	17	2	
57	t	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 58 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
58	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	R	1	Total Zn 1 1	0

- Molecule 60 is S-[2-($\{N-[(2R)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alanyl}\}$ amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
60	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
60	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	A	6	Total	O	0
			6	6	
61	B	15	Total	O	0
			15	15	
61	C	37	Total	O	0
			37	37	
61	D	43	Total	O	0
			43	43	
61	E	15	Total	O	0
			15	15	
61	F	16	Total	O	0
			16	16	
61	G	114	Total	O	0
			114	114	
61	H	11	Total	O	0
			11	11	
61	I	33	Total	O	0
			33	33	
61	J	3	Total	O	0
			3	3	
61	K	5	Total	O	0
			5	5	
61	L	38	Total	O	0
			38	38	
61	M	39	Total	O	0
			39	39	
61	N	22	Total	O	0
			22	22	
61	O	15	Total	O	0
			15	15	
61	P	54	Total	O	0
			54	54	
61	Q	36	Total	O	0
			36	36	
61	R	9	Total	O	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
61	S	7	Total 7	O 7	0
61	T	3	Total 3	O 3	0
61	V	8	Total 8	O 8	0
61	W	12	Total 12	O 12	0
61	X	2	Total 2	O 2	0
61	Y	13	Total 13	O 13	0
61	Z	10	Total 10	O 10	0
61	a	6	Total 6	O 6	0
61	c	7	Total 7	O 7	0
61	d	5	Total 5	O 5	0
61	e	6	Total 6	O 6	0
61	f	1	Total 1	O 1	0
61	g	9	Total 9	O 9	0
61	h	2	Total 2	O 2	0
61	i	9	Total 9	O 9	0
61	k	1	Total 1	O 1	0
61	l	21	Total 21	O 21	0
61	m	22	Total 22	O 22	0
61	n	5	Total 5	O 5	0
61	o	1	Total 1	O 1	0
61	p	14	Total 14	O 14	0

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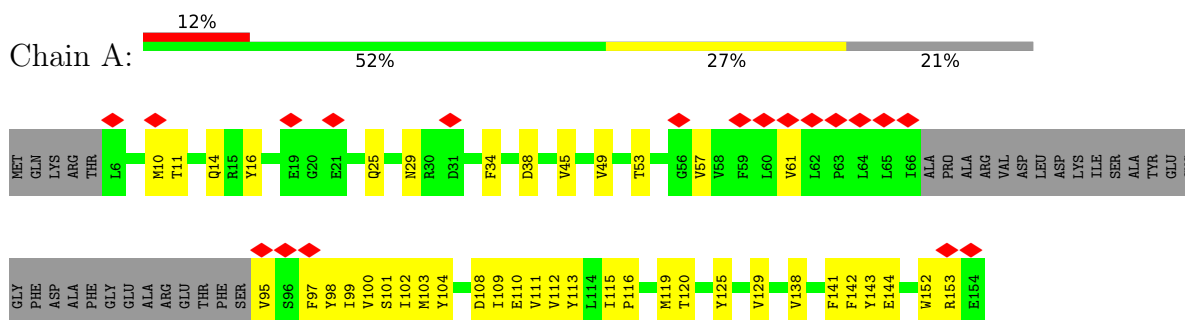
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Mol	Chain	Residues	Atoms		AltConf
61	q	8	Total 8	O 8	0
61	r	7	Total 7	O 7	0
61	s	8	Total 8	O 8	0
61	t	7	Total 7	O 7	0
61	x	25	Total 25	O 25	0
61	y	28	Total 28	O 28	0
61	z	24	Total 24	O 24	0

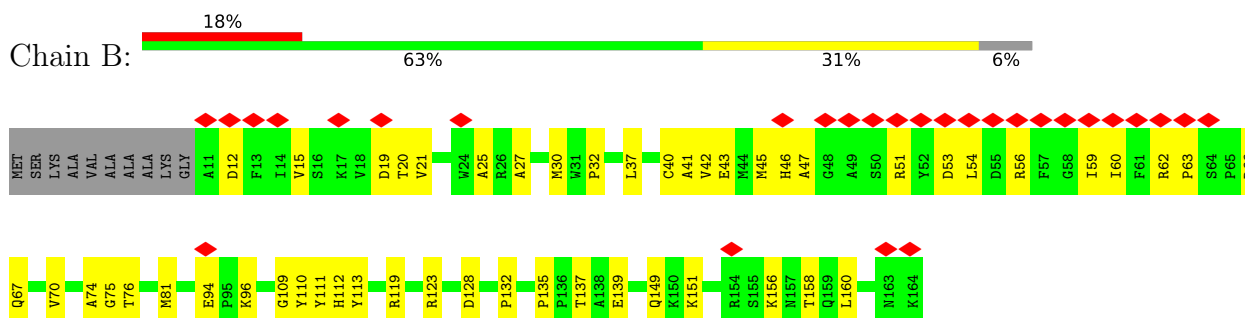
3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

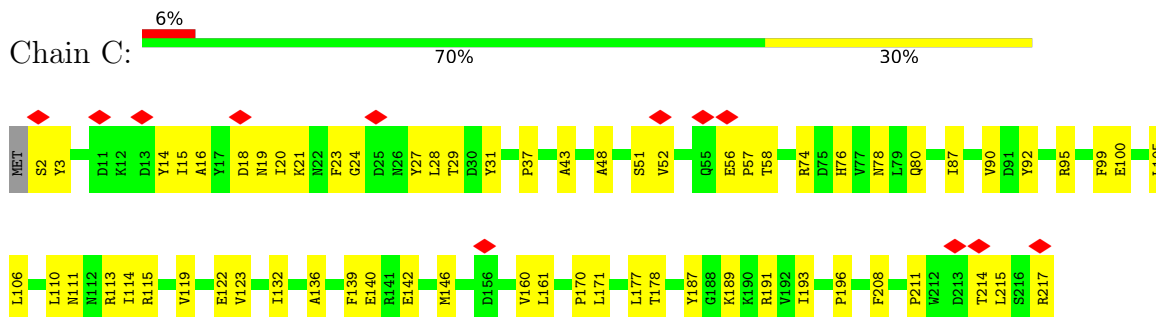
• Molecule 1: ND3



• Molecule 2: PSST

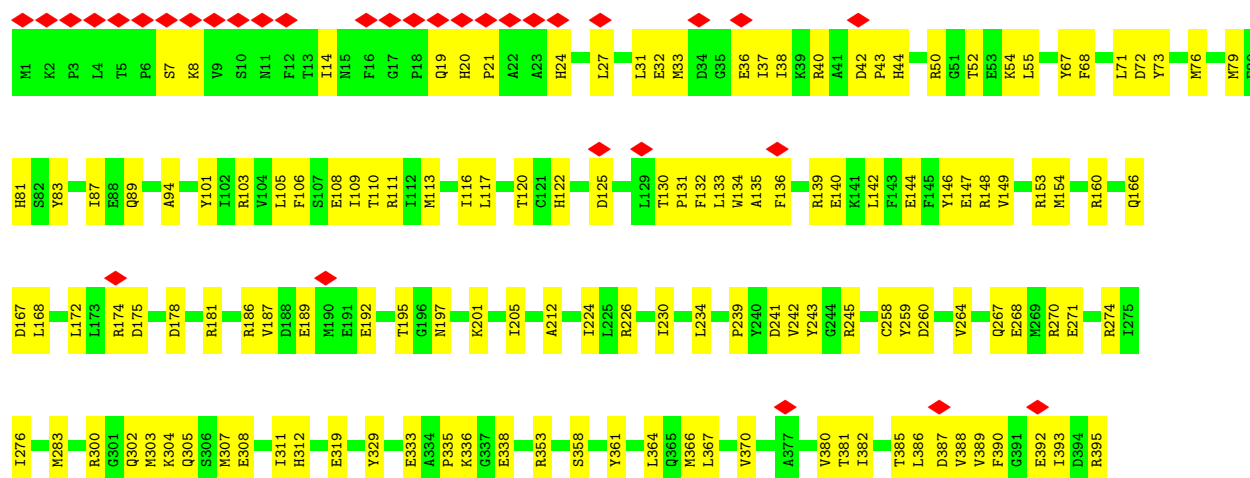


• Molecule 3: ND9

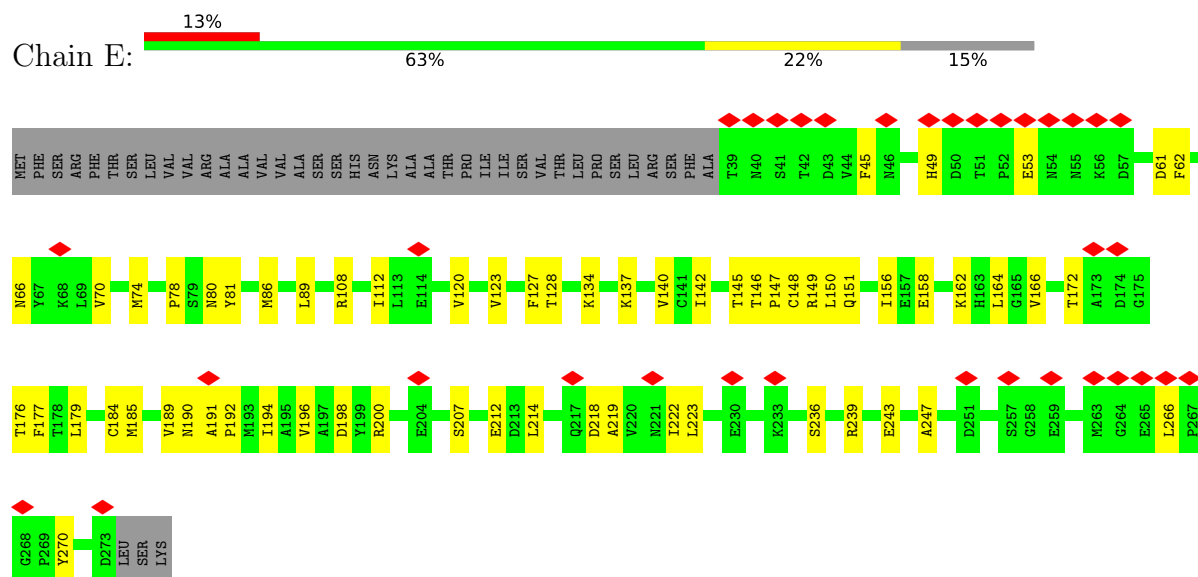


• Molecule 4: ND7

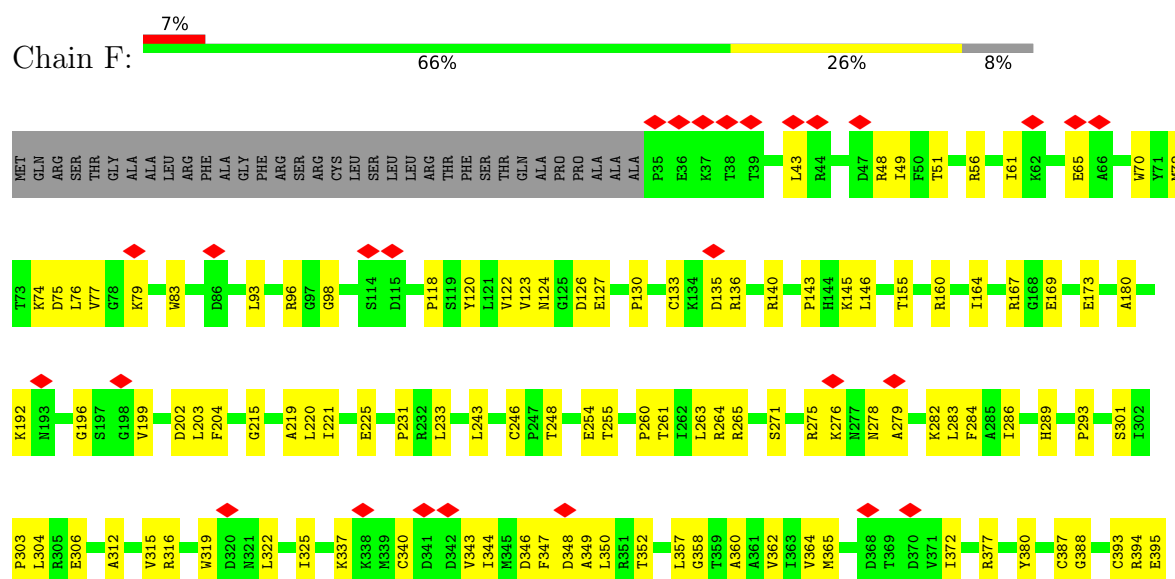




• Molecule 5: 24 kDa

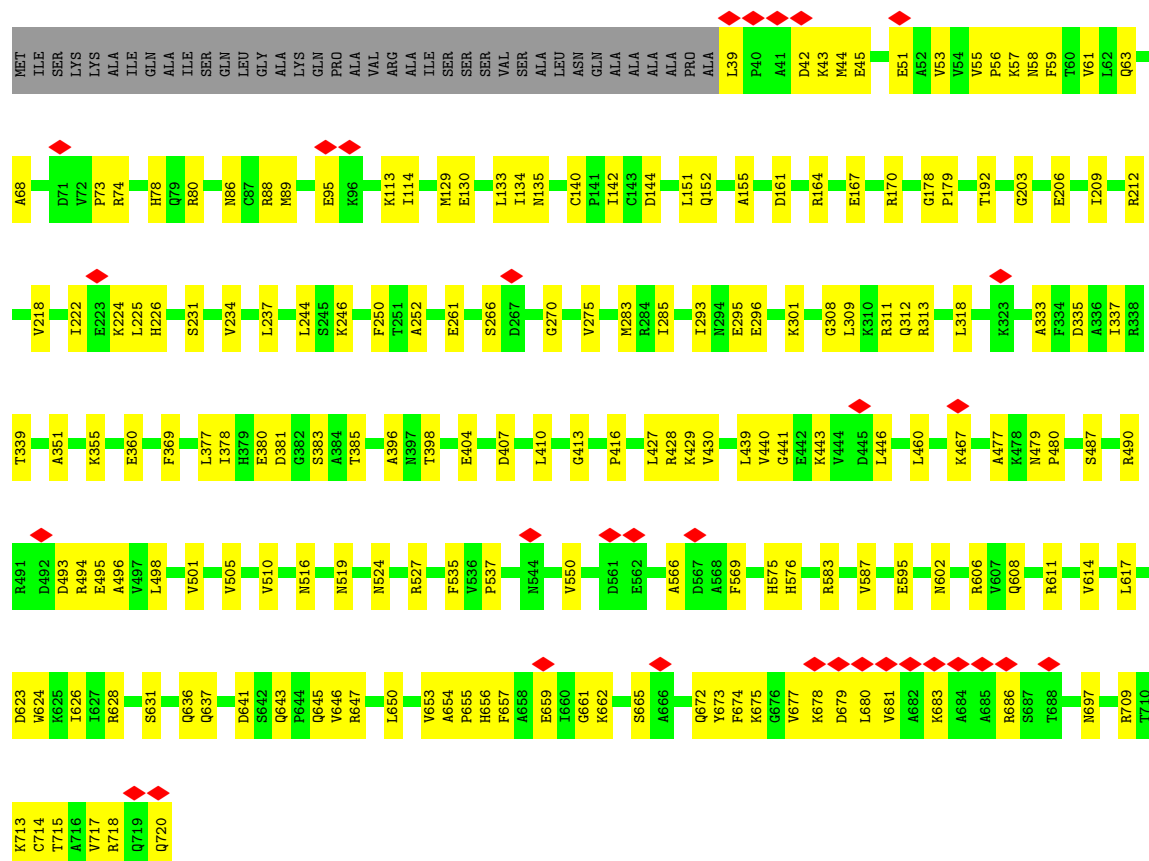


• Molecule 6: 51 kDa

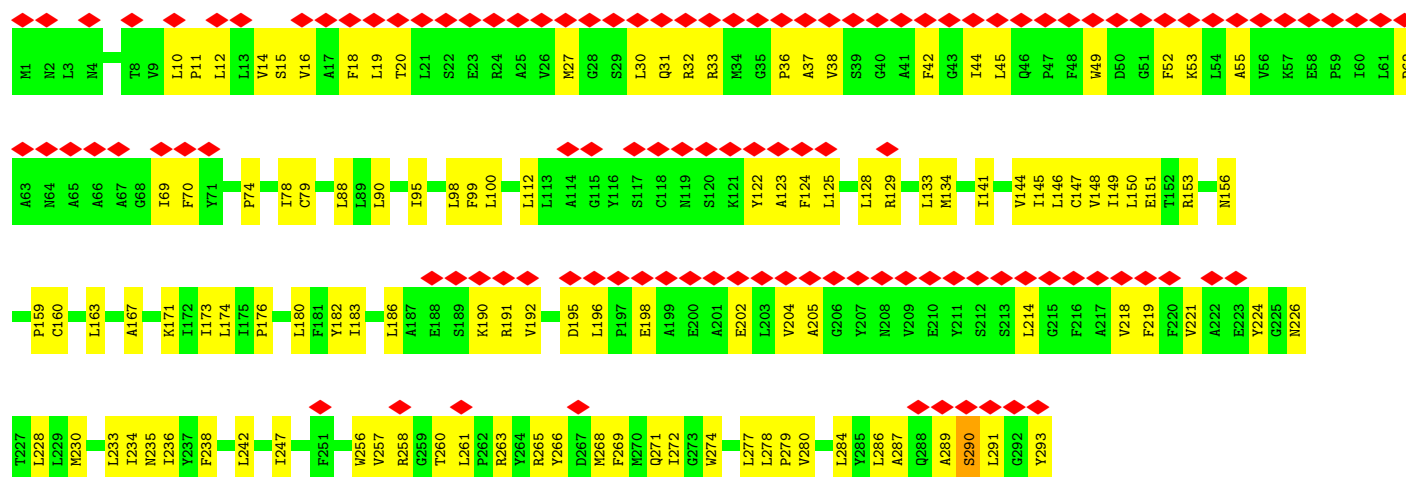
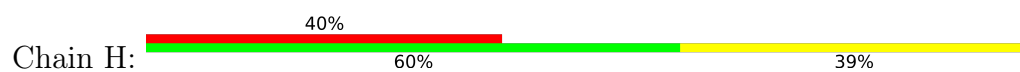




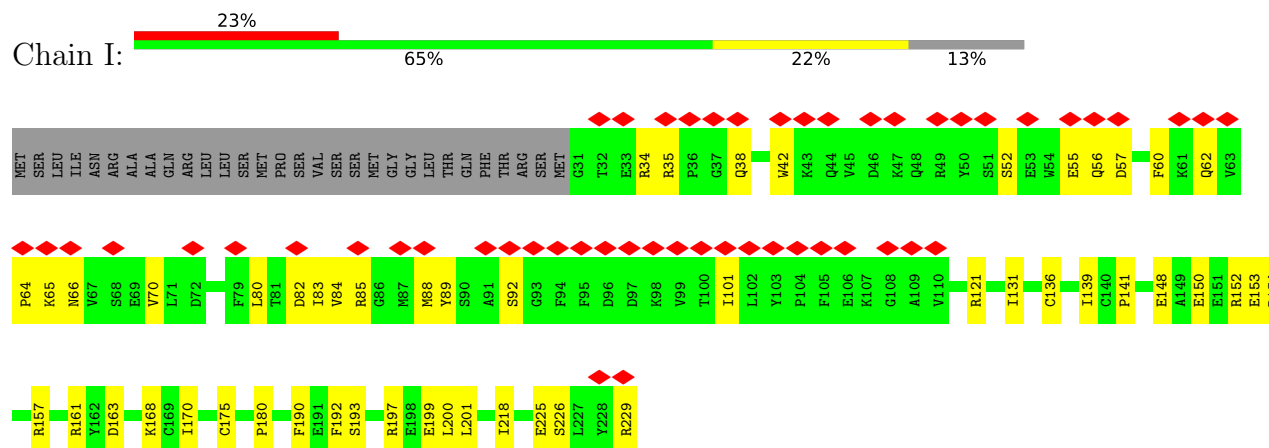
• Molecule 7: 75 kDa



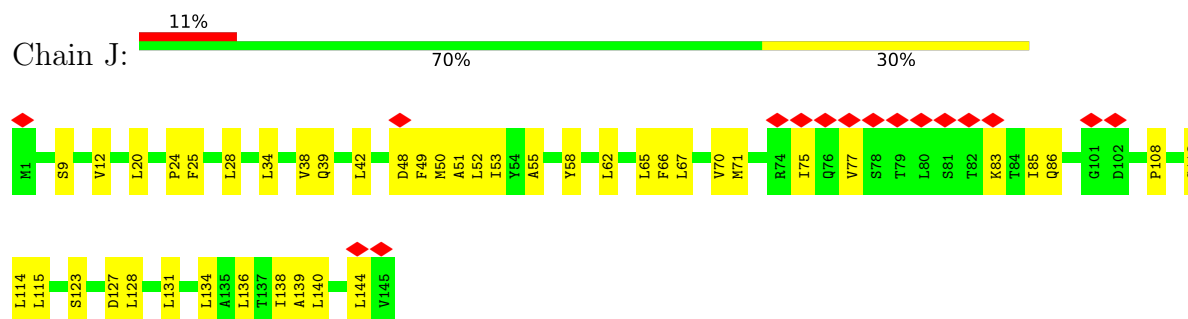
• Molecule 8: ND1



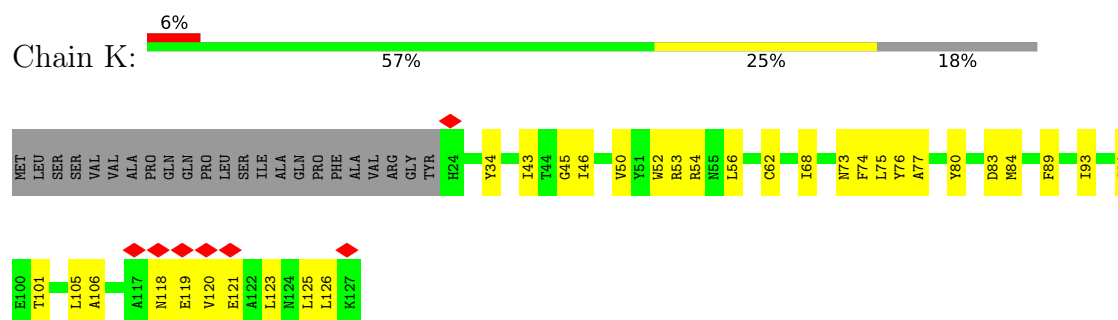
- Molecule 9: TYKY



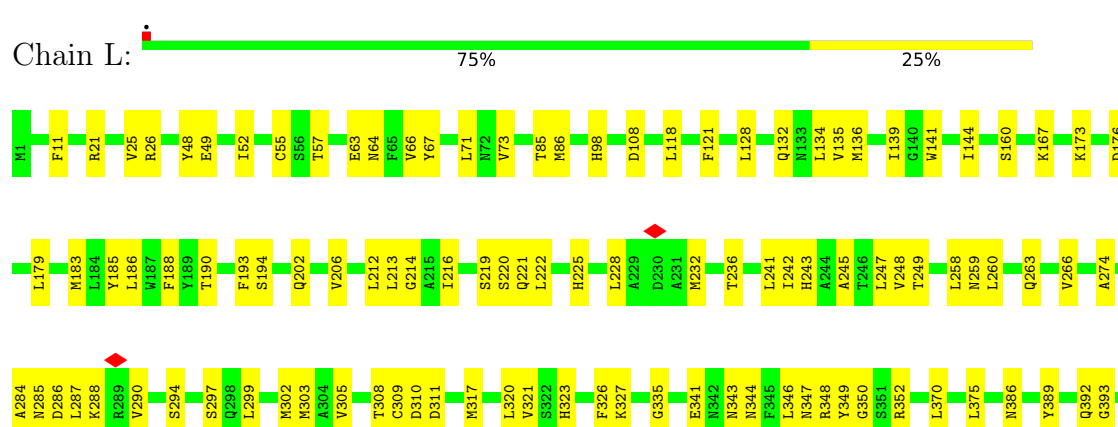
- Molecule 10: ND6



- Molecule 11: ND4L

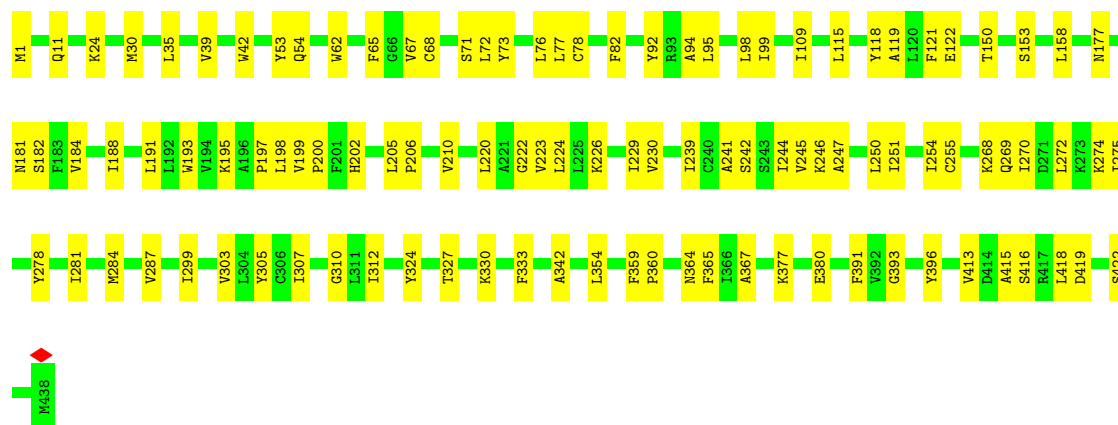
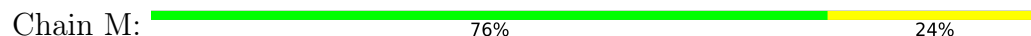


- Molecule 12: ND5





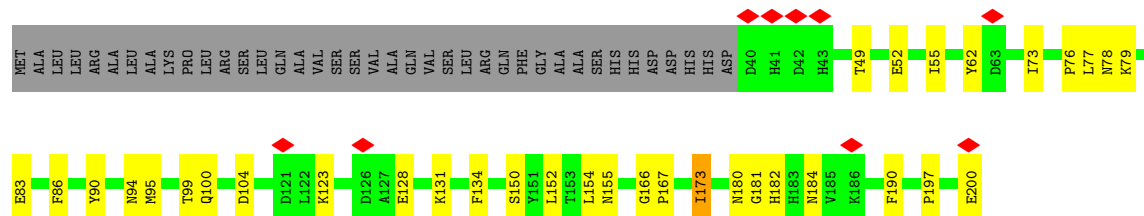
• Molecule 13: ND4



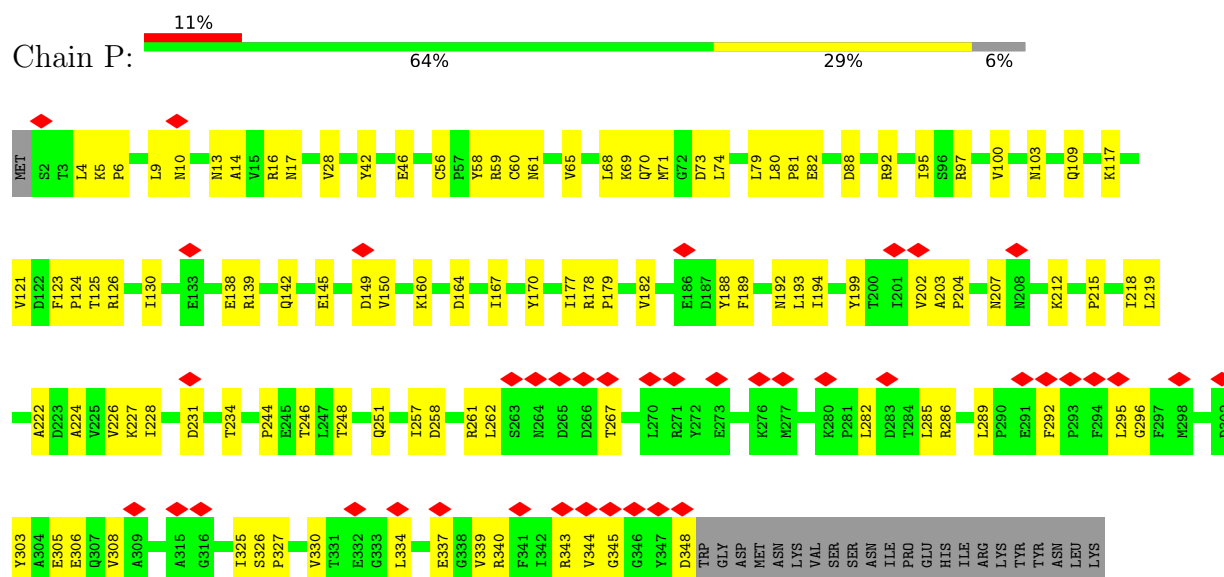
• Molecule 14: ND2



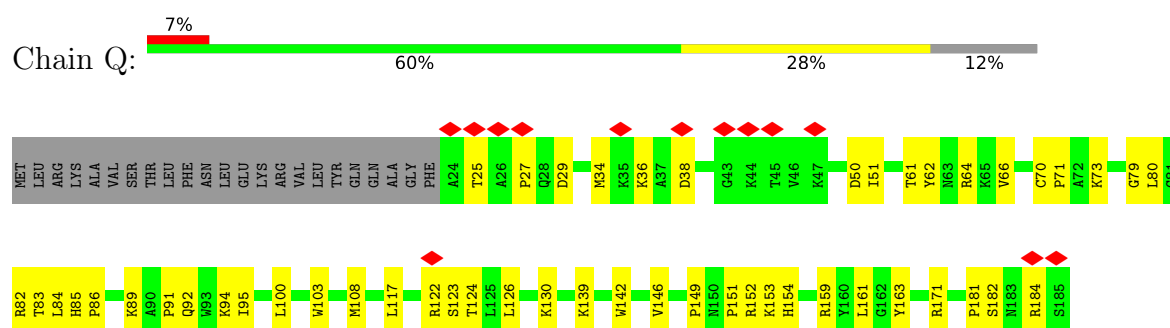
• Molecule 15: C1-FDX



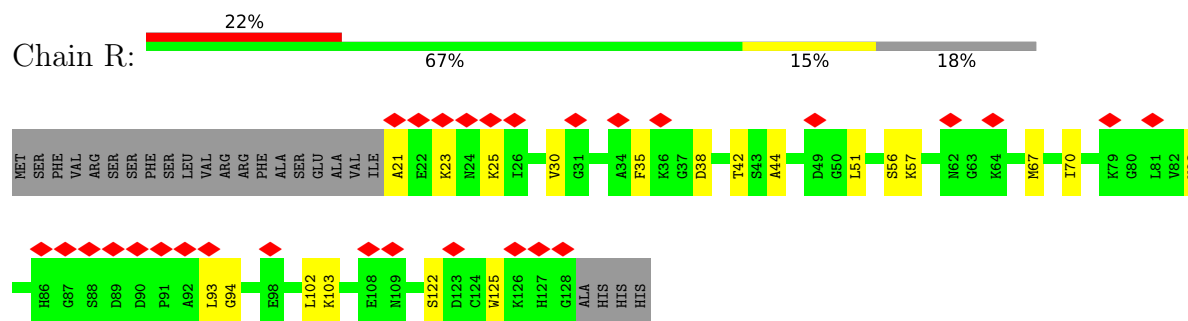
- Molecule 16: 39 kDa



- Molecule 17: 18 kDa



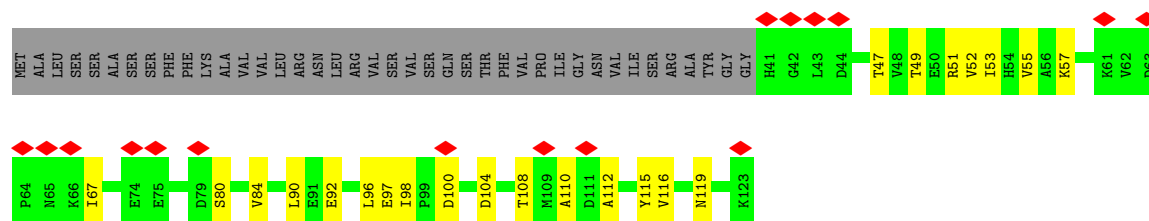
- Molecule 18: 13 kDa



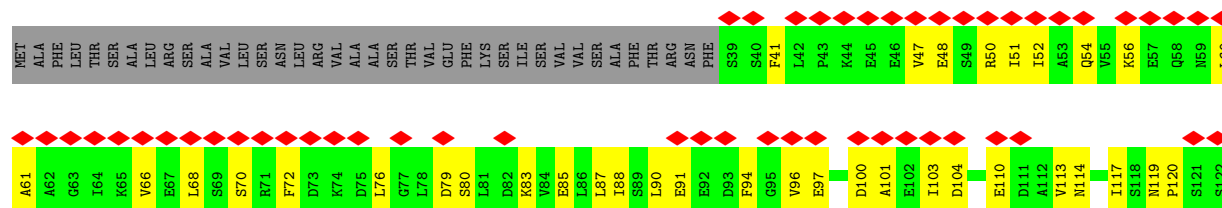
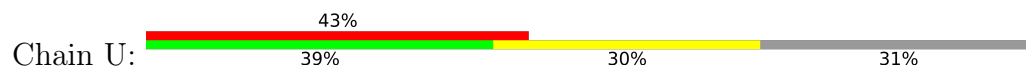
- Molecule 19: B8



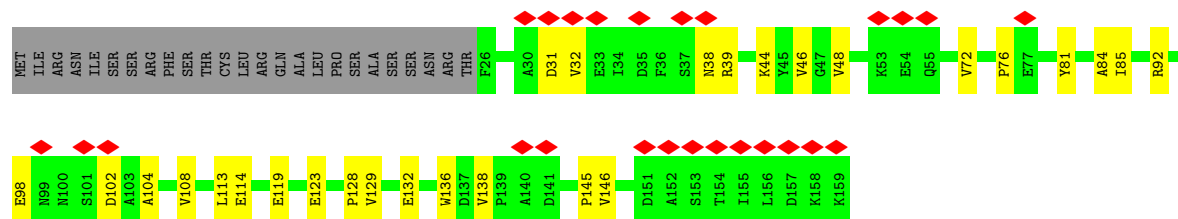
- Molecule 20: SDAP1



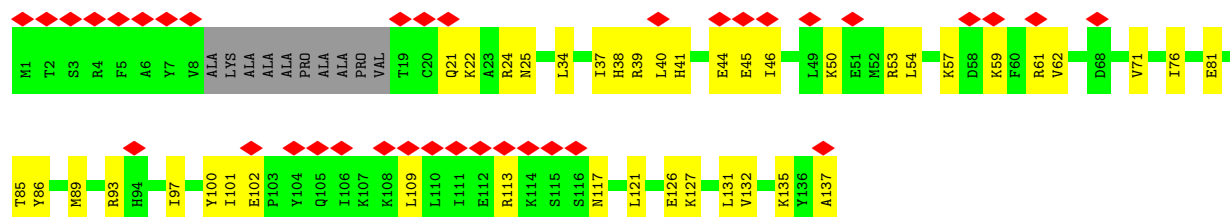
- Molecule 21: SDAP2



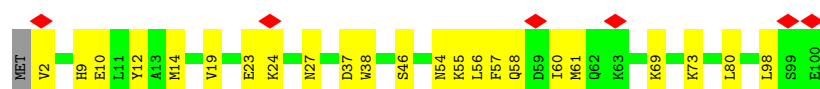
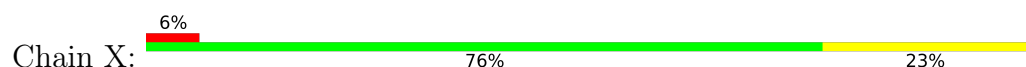
- Molecule 22: B13



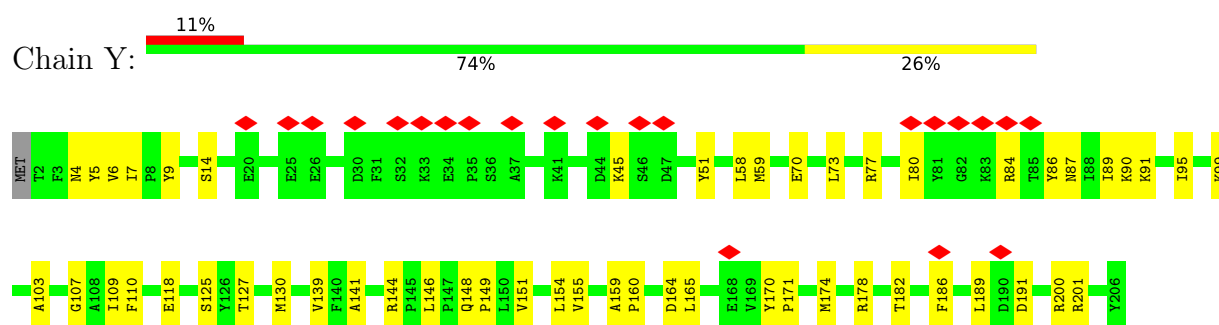
- Molecule 23: B14



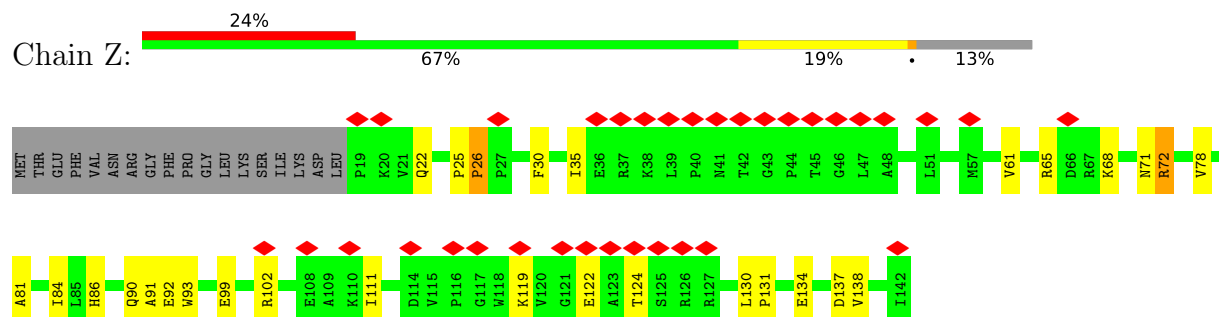
- Molecule 24: PGIV



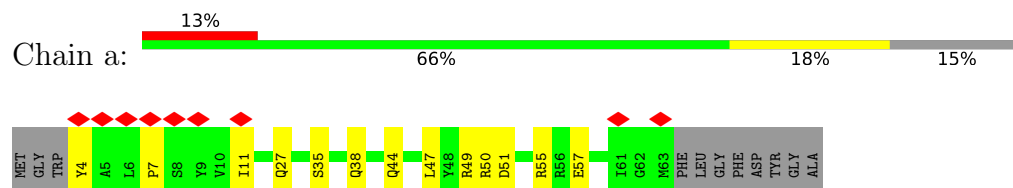
- Molecule 25: B14.7



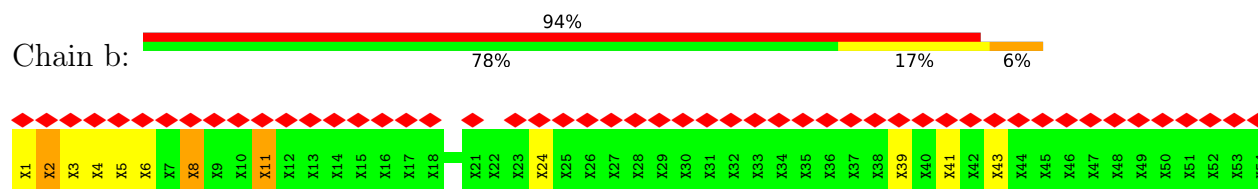
- Molecule 26: B16.6



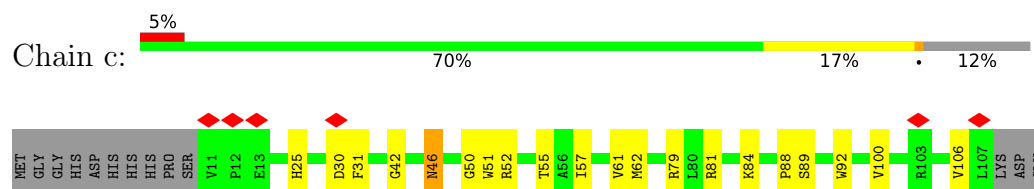
- Molecule 27: MWFE



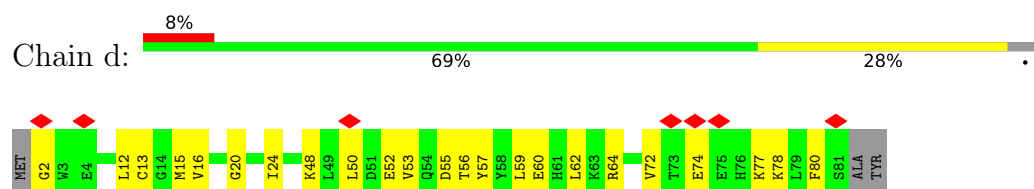
- Molecule 28: B9



- Molecule 29: KFYI

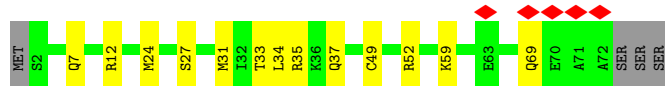


- Molecule 30: B14.5b



- Molecule 31: 15 kDa

Chain e: 



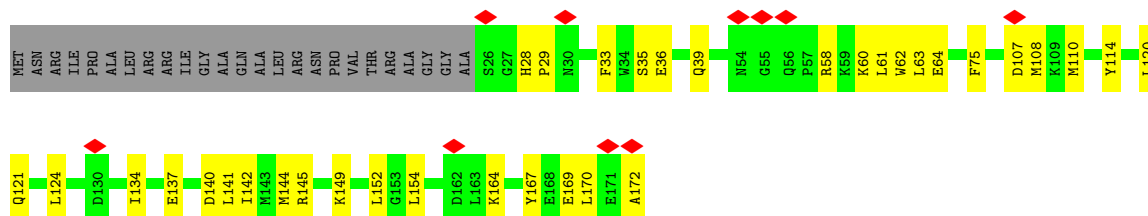
- Molecule 32: MNLL

Chain f: 



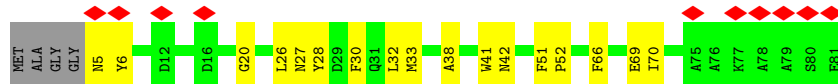
- Molecule 33: ESSS

Chain g: 



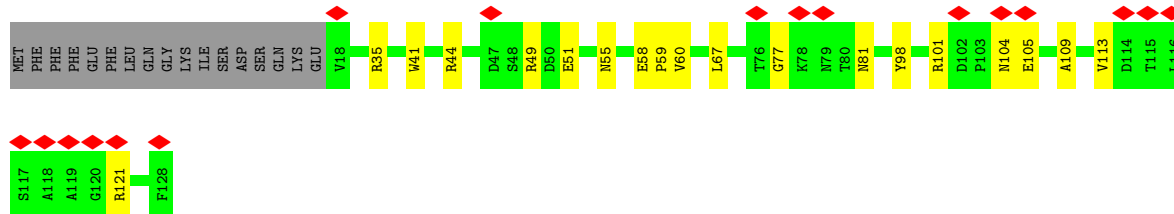
- Molecule 34: NUOP4

Chain h: 

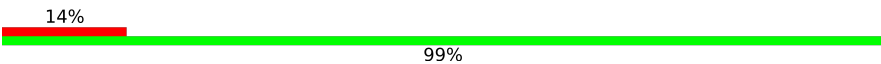


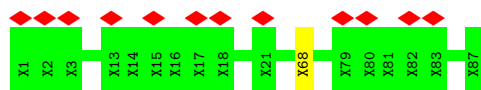
- Molecule 35: NUOP5

Chain i: 

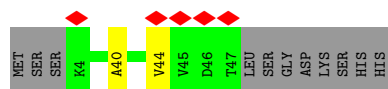
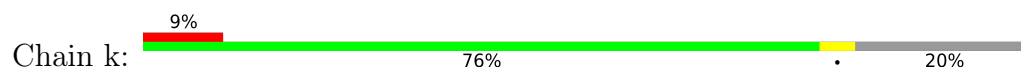


- Molecule 36: AGGG

Chain j: 



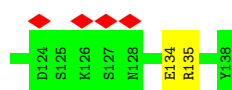
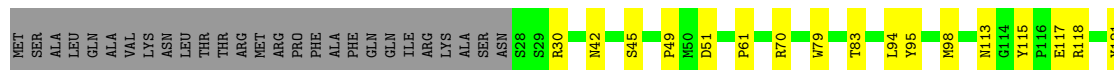
• Molecule 37: B12



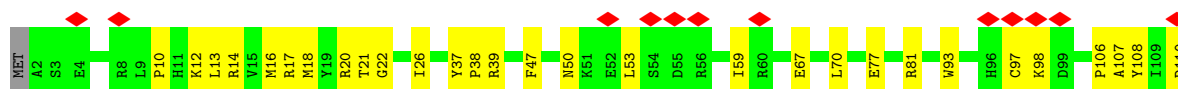
• Molecule 38: ASHI



• Molecule 39: B15



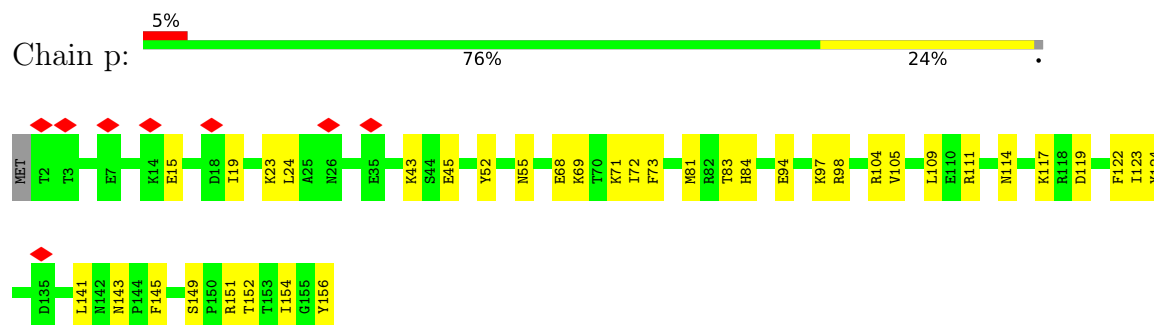
• Molecule 40: Complex I-B22



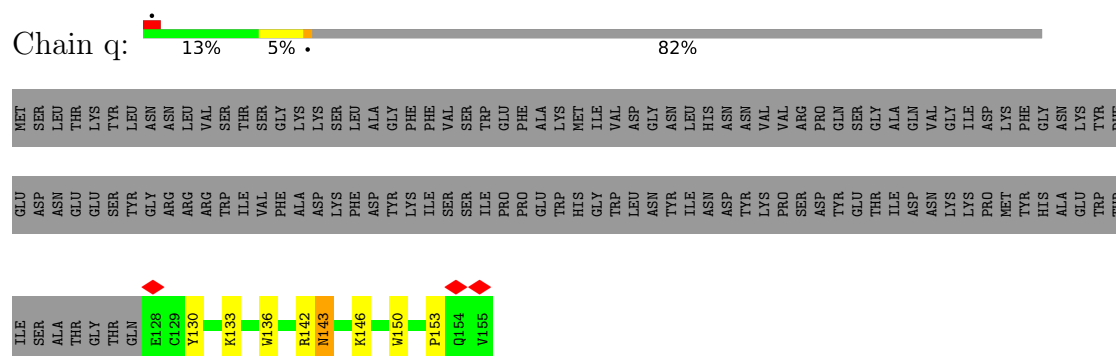
• Molecule 41: B18



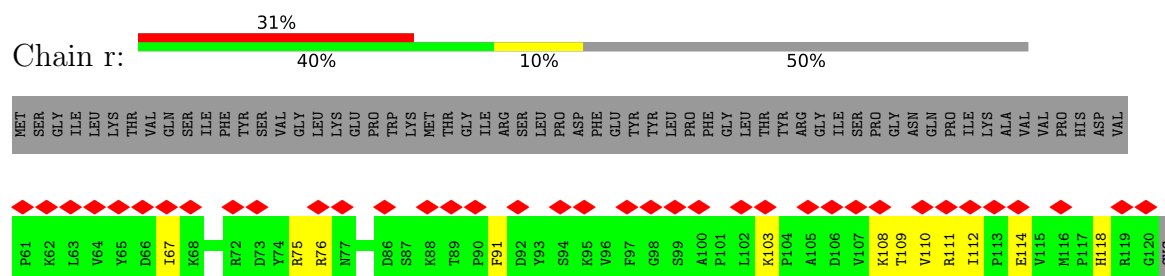
- Molecule 42: PDSW



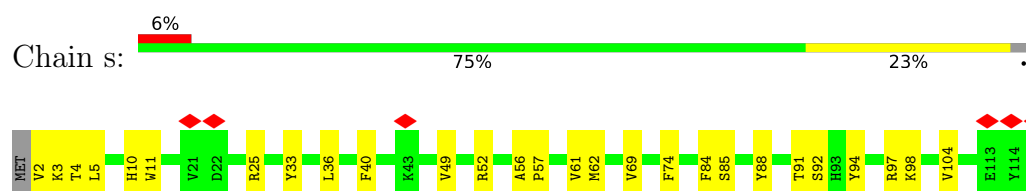
- Molecule 43: B17.2



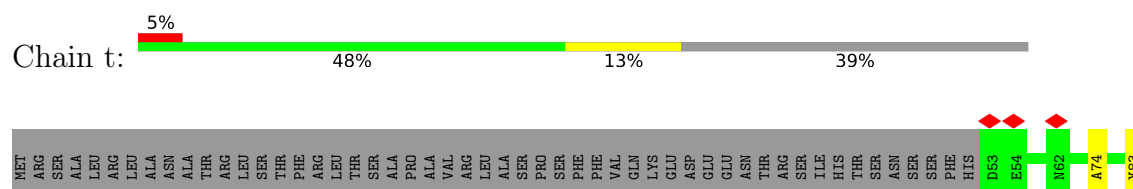
- Molecule 44: B14.5a

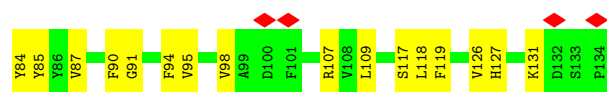


- Molecule 45: NUOP7

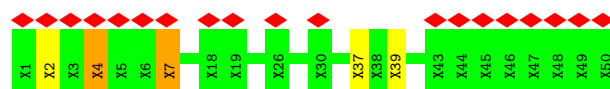
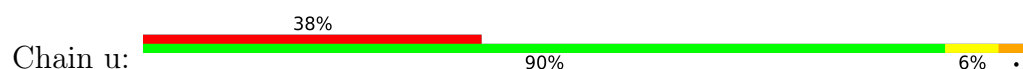


- Molecule 46: NUOP8

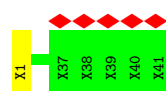




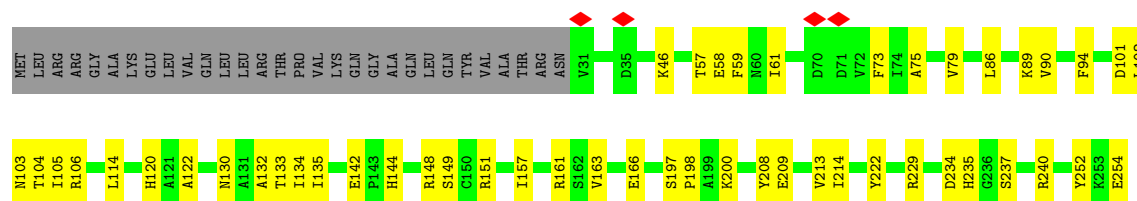
- Molecule 47: unknown



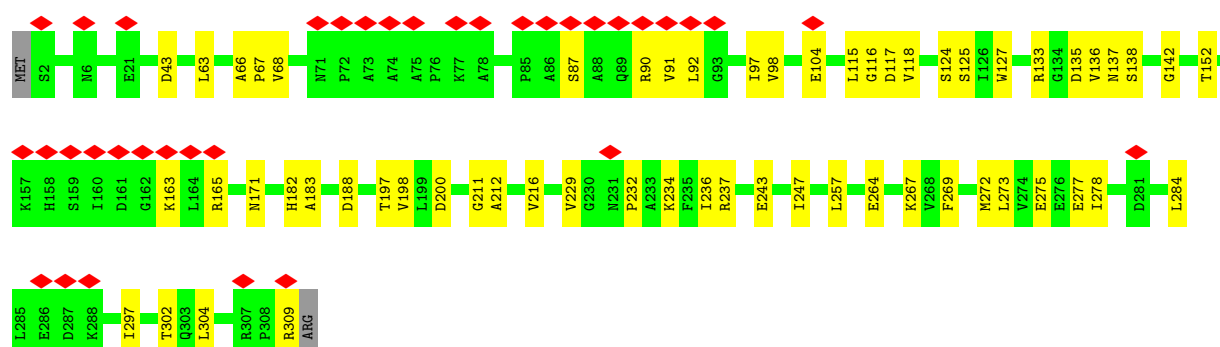
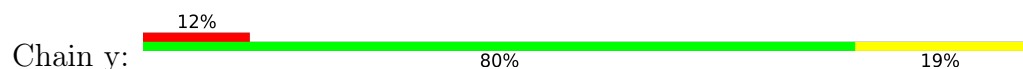
- Molecule 48: unknown



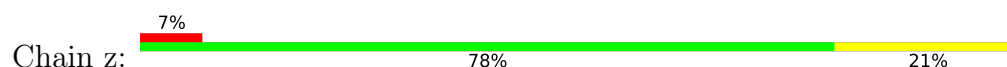
- Molecule 49: CAL

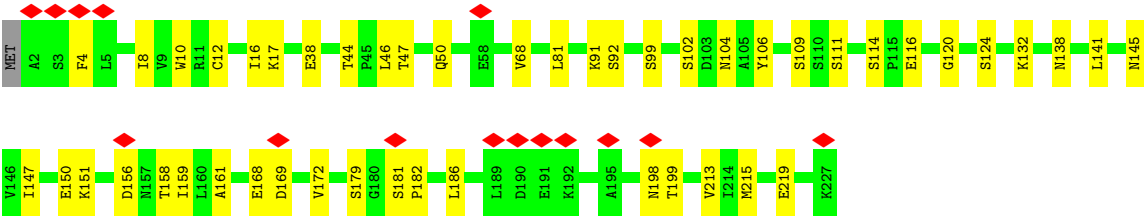


- Molecule 50: CA2



- Molecule 51: CA3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FMN, PTY, ZN, 8Q1, SF4, NDP, PC7, CDL

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	0.20	0/1028	0.42	0/1405
2	B	0.21	0/1240	0.46	0/1685
3	C	0.14	0/1862	0.36	0/2537
4	D	0.21	0/3257	0.47	0/4406
5	E	0.17	0/1843	0.42	0/2497
6	F	0.17	0/3394	0.42	0/4577
7	G	0.15	0/5254	0.36	0/7114
8	H	0.29	0/2287	0.59	1/3116 (0.0%)
9	I	0.17	0/1634	0.41	0/2204
10	J	0.17	0/1142	0.41	0/1558
11	K	0.17	0/812	0.38	0/1102
12	L	0.18	0/4210	0.41	0/5713
13	M	0.18	0/3529	0.41	0/4813
14	N	0.18	0/3050	0.43	0/4154
15	O	0.15	0/1380	0.41	1/1875 (0.1%)
16	P	0.17	0/2750	0.40	0/3726
17	Q	0.14	0/1311	0.35	0/1774
18	R	0.14	0/832	0.35	0/1125
19	S	0.15	0/725	0.36	0/979
20	T	0.17	0/655	0.42	0/891
21	U	0.22	0/663	0.51	0/895
22	V	0.15	0/1069	0.34	0/1448
23	W	0.19	0/1097	0.43	0/1472
24	X	0.18	0/838	0.42	0/1128
25	Y	0.19	0/1630	0.41	0/2227
26	Z	0.23	0/1029	0.50	1/1395 (0.1%)
27	a	0.19	0/532	0.42	0/722
29	c	0.13	0/816	0.39	1/1117 (0.1%)
30	d	0.17	0/667	0.38	0/902
31	e	0.14	0/602	0.41	0/803
32	f	0.17	0/906	0.32	0/1236
33	g	0.17	0/1210	0.38	0/1638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	h	0.13	0/643	0.35	0/870
35	i	0.15	0/943	0.39	0/1275
37	k	0.14	0/381	0.31	0/517
38	l	0.15	0/1053	0.34	0/1435
39	m	0.15	0/967	0.36	0/1314
40	n	0.19	0/1036	0.39	0/1399
41	o	0.15	0/724	0.37	0/974
42	p	0.17	0/1314	0.38	0/1766
43	q	0.13	0/254	0.40	0/346
44	r	0.13	0/507	0.35	0/685
45	s	0.16	0/963	0.42	0/1317
46	t	0.17	0/736	0.36	0/1003
49	x	0.15	0/2010	0.37	0/2733
50	y	0.15	0/2363	0.37	0/3215
51	z	0.16	0/1713	0.34	0/2320
All	All	0.17	0/68861	0.41	4/93403 (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
8	H	0	1
26	Z	0	1
28	b	0	3
47	u	0	2
All	All	0	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	46	ASN	CB-CA-C	-6.17	109.45	116.54
15	O	173	ILE	N-CA-C	-5.99	106.89	111.62
26	Z	26	PRO	CA-N-CD	-5.35	104.51	112.00
8	H	30	LEU	CA-CB-CG	5.15	134.33	116.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	290	SER	Peptide
26	Z	72	ARG	Sidechain
28	b	11	UNK	Peptide
28	b	2	UNK	Peptide
28	b	8	UNK	Peptide
47	u	4	UNK	Peptide
47	u	7	UNK	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	999	0	989	40	0
2	B	1206	0	1193	59	0
3	C	1808	0	1750	61	0
4	D	3178	0	3148	118	0
5	E	1806	0	1769	52	0
6	F	3322	0	3278	87	0
7	G	5166	0	5193	141	0
8	H	2237	0	2336	113	0
9	I	1602	0	1534	49	0
10	J	1120	0	1189	42	0
11	K	798	0	801	31	0
12	L	4111	0	4124	120	0
13	M	3425	0	3509	86	0
14	N	2967	0	3053	99	0
15	O	1336	0	1273	25	0
16	P	2701	0	2719	84	0
17	Q	1276	0	1264	43	0
18	R	812	0	781	17	0
19	S	716	0	730	26	0
20	T	645	0	633	20	0
21	U	655	0	647	30	0
22	V	1052	0	1059	22	0
23	W	1074	0	1101	34	0
24	X	816	0	788	21	0
25	Y	1583	0	1559	50	0
26	Z	1003	0	1015	38	0
27	a	515	0	488	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	270	0	58	13	0
29	c	785	0	750	19	0
30	d	650	0	641	17	0
31	e	592	0	580	14	0
32	f	877	0	843	15	0
33	g	1176	0	1154	38	0
34	h	625	0	590	16	0
35	i	922	0	893	21	0
36	j	435	0	91	1	0
37	k	367	0	353	1	0
38	l	1018	0	982	31	0
39	m	934	0	861	20	0
40	n	1008	0	997	33	0
41	o	704	0	689	17	0
42	p	1287	0	1275	32	0
43	q	243	0	233	8	0
44	r	493	0	498	18	0
45	s	933	0	942	25	0
46	t	706	0	673	21	0
47	u	250	0	53	5	0
48	w	204	0	42	1	0
49	x	1967	0	1918	41	0
50	y	2316	0	2334	44	0
51	z	1687	0	1709	36	0
52	A	49	0	72	5	0
52	L	48	0	73	11	0
52	M	104	0	168	7	0
52	N	104	0	168	13	0
52	z	52	0	84	6	0
53	B	8	0	0	0	0
53	F	8	0	0	2	0
53	G	16	0	0	1	0
53	I	16	0	0	1	0
54	E	4	0	0	1	0
54	G	4	0	0	0	0
55	F	31	0	19	1	0
56	H	50	0	79	7	0
56	L	50	0	79	2	0
56	M	47	0	67	8	0
56	N	50	0	79	1	0
56	Y	50	0	79	4	0
56	m	100	0	158	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	L	89	0	128	9	0
57	M	100	0	156	7	0
57	N	100	0	156	10	0
57	d	100	0	156	3	0
57	t	100	0	156	9	0
58	P	48	0	26	1	0
59	R	1	0	0	0	0
60	W	35	0	0	1	0
60	n	35	0	0	0	0
61	A	6	0	0	0	0
61	B	15	0	0	2	0
61	C	37	0	0	0	0
61	D	43	0	0	3	0
61	E	15	0	0	0	0
61	F	16	0	0	0	0
61	G	114	0	0	3	0
61	H	11	0	0	0	0
61	I	33	0	0	1	0
61	J	3	0	0	0	0
61	K	5	0	0	0	0
61	L	38	0	0	1	0
61	M	39	0	0	0	0
61	N	22	0	0	0	0
61	O	15	0	0	1	0
61	P	54	0	0	2	0
61	Q	36	0	0	2	0
61	R	9	0	0	0	0
61	S	7	0	0	0	0
61	T	3	0	0	1	0
61	V	8	0	0	1	0
61	W	12	0	0	0	0
61	X	2	0	0	0	0
61	Y	13	0	0	0	0
61	Z	10	0	0	0	0
61	a	6	0	0	0	0
61	c	7	0	0	0	0
61	d	5	0	0	0	0
61	e	6	0	0	0	0
61	f	1	0	0	0	0
61	g	9	0	0	0	0
61	h	2	0	0	0	0
61	i	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	k	1	0	0	0	0
61	l	21	0	0	0	0
61	m	22	0	0	1	0
61	n	5	0	0	0	0
61	o	1	0	0	0	0
61	p	14	0	0	0	0
61	q	8	0	0	0	0
61	r	7	0	0	0	0
61	s	8	0	0	0	0
61	t	7	0	0	0	0
61	x	25	0	0	0	0
61	y	28	0	0	0	0
61	z	24	0	0	0	0
All	All	70559	0	68985	1689	0

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 12.

All (1689) 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)
8:H:286:LEU:O	8:H:290:SER:OG	1.85	0.92
47:u:37:UNK:O	47:u:39:UNK:N	2.03	0.92
2:B:62:ARG:HE	2:B:63:PRO:HD2	1.32	0.91
28:b:41:UNK:O	28:b:43:UNK:N	2.03	0.91
12:L:26:ARG:HH21	33:g:29:PRO:HD2	1.37	0.89
47:u:4:UNK:HA	47:u:7:UNK:N	1.87	0.89
28:b:8:UNK:HA	28:b:11:UNK:N	1.87	0.88
24:X:80:LEU:HD12	27:a:44:GLN:HE22	1.35	0.88
3:C:95:ARG:NH2	17:Q:34:MET:SD	2.46	0.87
33:g:108:MET:HE1	42:p:98:ARG:HD3	1.54	0.87
7:G:709:ARG:NH2	18:R:23:LYS:O	2.06	0.87
35:i:55:ASN:O	35:i:81:ASN:ND2	2.06	0.86
7:G:311:ARG:HE	7:G:709:ARG:HH21	1.23	0.86
50:y:197:THR:OG1	51:z:145:ASN:ND2	2.08	0.86
27:a:47:LEU:HD23	27:a:50:ARG:HD3	1.56	0.86
6:F:120:TYR:HB2	6:F:248:THR:HG22	1.58	0.86
4:D:101:TYR:OH	4:D:245:ARG:NH1	2.07	0.85
7:G:44:MET:HE3	7:G:57:LYS:HA	1.58	0.85
42:p:81:MET:HE1	42:p:154:ILE:HG12	1.59	0.85
25:Y:77:ARG:HH12	46:t:127:HIS:HA	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:294:SER:OG	12:L:327:LYS:NZ	2.10	0.84
4:D:201:LYS:HE2	4:D:205:ILE:HD11	1.58	0.84
49:x:132:ALA:O	49:x:151:ARG:NH1	2.10	0.84
7:G:665:SER:O	19:S:20:GLN:NE2	2.11	0.83
6:F:271:SER:HA	6:F:279:ALA:HB1	1.60	0.83
15:O:190:PHE:O	49:x:106:ARG:NH2	2.12	0.82
3:C:106:LEU:HD13	3:C:113:ARG:HE	1.45	0.82
15:O:55:ILE:HG23	15:O:73:ILE:HD11	1.62	0.82
7:G:80:ARG:NH1	7:G:295:GLU:OE2	2.14	0.81
7:G:129:MET:HE2	7:G:155:ALA:HB2	1.62	0.81
4:D:388:VAL:HB	4:D:393:ILE:HD11	1.63	0.80
1:A:112:VAL:HG13	10:J:53:ILE:HD12	1.61	0.80
16:P:194:ILE:HD11	16:P:339:VAL:HG12	1.61	0.80
25:Y:148:GLN:HA	25:Y:151:VAL:HG22	1.62	0.80
28:b:4:UNK:HA	28:b:8:UNK:CB	2.12	0.80
33:g:152:LEU:HD22	39:m:135:ARG:HD2	1.64	0.80
16:P:177:ILE:HG22	16:P:179:PRO:HD3	1.62	0.80
26:Z:131:PRO:O	31:e:52:ARG:NH2	2.16	0.79
6:F:315:VAL:HG21	6:F:322:LEU:HD21	1.65	0.79
14:N:248:LEU:HD11	14:N:310:LEU:HD11	1.64	0.79
33:g:149:LYS:NZ	39:m:134:GLU:O	2.15	0.79
12:L:248:VAL:HB	12:L:299:LEU:HD11	1.64	0.78
16:P:257:ILE:HG12	16:P:262:LEU:HD12	1.65	0.78
31:e:24:MET:O	31:e:35:ARG:NH2	2.16	0.78
2:B:46:HIS:ND1	4:D:140:GLU:OE2	2.17	0.78
5:E:266:LEU:HD12	6:F:51:THR:HB	1.65	0.78
7:G:164:ARG:HH21	44:r:67:ILE:HG12	1.47	0.78
14:N:208:ASN:ND2	35:i:51:GLU:OE2	2.17	0.77
13:M:181:ASN:ND2	25:Y:174:MET:SD	2.57	0.77
3:C:74:ARG:NH1	3:C:132:ILE:O	2.17	0.77
6:F:140:ARG:HB3	6:F:173:GLU:HG3	1.66	0.77
1:A:99:ILE:HG22	1:A:103:MET:HE2	1.67	0.77
12:L:202:GLN:NE2	38:l:121:LEU:O	2.17	0.76
8:H:242:LEU:HD11	8:H:247:ILE:HD11	1.67	0.76
12:L:259:ASN:O	38:l:124:ASN:ND2	2.18	0.76
16:P:244:PRO:HD3	16:P:327:PRO:HB2	1.66	0.76
7:G:398:THR:OG1	7:G:516:ASN:O	2.04	0.76
17:Q:61:THR:HG23	17:Q:117:LEU:HD11	1.66	0.76
8:H:45:LEU:HD12	8:H:49:TRP:HE1	1.50	0.76
12:L:511:ARG:HH12	38:l:67:MET:HE2	1.51	0.76
50:y:211:GLY:HA3	50:y:229:VAL:HG12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:161:ARG:NH2	17:Q:108:MET:O	2.20	0.75
49:x:161:ARG:HH22	51:z:145:ASN:ND2	1.84	0.75
52:M:503:PC7:H411	52:M:503:PC7:H171	1.68	0.75
4:D:178:ASP:O	4:D:181:ARG:HG2	1.86	0.75
6:F:395:GLU:HB3	7:G:134:ILE:HD11	1.69	0.75
14:N:171:ALA:HB3	14:N:172:PRO:HD3	1.67	0.75
2:B:27:ALA:HB1	2:B:149:GLN:HG3	1.68	0.75
3:C:177:LEU:HD11	4:D:55:LEU:HD23	1.66	0.75
12:L:26:ARG:NH1	33:g:35:SER:O	2.20	0.75
2:B:15:VAL:HG23	2:B:158:THR:HG22	1.69	0.75
16:P:227:LYS:HG3	16:P:325:ILE:HD11	1.68	0.75
21:U:60:LEU:HG	21:U:61:ALA:H	1.51	0.74
39:m:42:ASN:HB3	39:m:45:SER:HB3	1.69	0.74
7:G:222:ILE:HD11	7:G:224:LYS:HE2	1.67	0.74
15:O:73:ILE:HG23	15:O:155:ASN:HA	1.69	0.74
12:L:245:ALA:O	12:L:249:THR:OG1	2.05	0.74
7:G:309:LEU:O	7:G:313:ARG:NH2	2.20	0.74
21:U:51:ILE:HD13	21:U:113:VAL:HB	1.69	0.74
7:G:709:ARG:NH1	18:R:25:LYS:O	2.20	0.74
7:G:381:ASP:OD2	7:G:524:ASN:ND2	2.20	0.73
16:P:262:LEU:HD23	16:P:343:ARG:HH22	1.53	0.73
7:G:480:PRO:HG2	7:G:510:VAL:HA	1.70	0.73
49:x:148:ARG:NH1	49:x:166:GLU:OE2	2.21	0.73
49:x:161:ARG:HB2	51:z:147:ILE:HD11	1.69	0.73
20:T:108:THR:HG22	20:T:110:ALA:H	1.53	0.73
49:x:86:LEU:HD22	49:x:90:VAL:HG11	1.71	0.73
6:F:49:ILE:O	6:F:145:LYS:NZ	2.22	0.72
8:H:261:LEU:HD21	9:I:83:ILE:HG23	1.72	0.72
13:M:11:GLN:HG2	13:M:30:MET:HB3	1.71	0.72
20:T:84:VAL:HG13	40:n:20:ARG:HG2	1.71	0.72
14:N:70:PHE:HE2	14:N:111:ILE:HG21	1.54	0.72
6:F:350:LEU:HD12	6:F:357:LEU:HB2	1.70	0.72
13:M:197:PRO:HG2	13:M:205:LEU:HD22	1.71	0.72
4:D:239:PRO:HG3	44:r:112:ILE:HG23	1.72	0.72
4:D:226:ARG:NH2	4:D:268:GLU:OE1	2.23	0.71
1:A:10:MET:HG3	1:A:11:THR:HG23	1.72	0.71
5:E:166:VAL:HG11	5:E:172:THR:HA	1.71	0.71
12:L:167:LYS:HG3	52:L:602:PC7:H322	1.70	0.71
6:F:319:TRP:O	6:F:337:LYS:NZ	2.24	0.71
25:Y:182:THR:HG22	25:Y:191:ASP:HB2	1.72	0.71
2:B:56:ARG:HA	8:H:36:PRO:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:164:ASP:OD2	61:P:601:HOH:O	2.09	0.71
3:C:100:GLU:HG3	3:C:119:VAL:HG22	1.72	0.71
60:W:200:8Q1:O40	60:W:200:8Q1:N36	2.22	0.71
38:l:53:ILE:HG22	38:l:55:PRO:HD2	1.71	0.71
17:Q:82:ARG:O	17:Q:92:GLN:NE2	2.23	0.70
1:A:111:VAL:HG13	8:H:146:LEU:HD11	1.71	0.70
10:J:67:LEU:HD21	10:J:71:MET:HE3	1.72	0.70
13:M:393:GLY:HA2	13:M:396:TYR:CE2	2.26	0.70
17:Q:130:LYS:HE3	17:Q:146:VAL:HG11	1.72	0.70
12:L:242:ILE:HG13	12:L:243:HIS:HD2	1.55	0.70
22:V:102:ASP:HB2	22:V:113:LEU:HD11	1.72	0.70
8:H:27:MET:SD	8:H:258:ARG:NH2	2.62	0.70
4:D:19:GLN:NE2	4:D:21:PRO:HD2	2.07	0.70
5:E:150:LEU:HD21	6:F:365:MET:HG2	1.74	0.70
9:I:197:ARG:HD3	16:P:74:LEU:HD21	1.74	0.70
2:B:62:ARG:NE	2:B:63:PRO:HD2	2.06	0.70
16:P:258:ASP:O	16:P:261:ARG:HD3	1.92	0.70
8:H:150:LEU:HD13	8:H:289:ALA:N	2.07	0.69
25:Y:110:PHE:HZ	46:t:107:ARG:HG2	1.56	0.69
27:a:50:ARG:HD2	32:f:3:TRP:HH2	1.57	0.69
50:y:297:ILE:HD11	50:y:309:ARG:HD2	1.75	0.69
20:T:96:LEU:HD22	20:T:119:ASN:HD22	1.57	0.69
19:S:15:ARG:NH2	19:S:69:GLU:OE1	2.26	0.69
6:F:412:ALA:HB1	6:F:416:GLU:HG3	1.74	0.69
7:G:566:ALA:HA	7:G:583:ARG:HH21	1.57	0.69
40:n:17:ARG:HD3	40:n:20:ARG:HH21	1.57	0.69
6:F:346:ASP:OD1	6:F:347:PHE:N	2.25	0.69
13:M:220:LEU:HD23	13:M:224:LEU:HD22	1.75	0.69
16:P:257:ILE:HG23	16:P:262:LEU:HB2	1.73	0.69
50:y:115:LEU:HD12	50:y:133:ARG:HG2	1.74	0.69
13:M:153:SER:HB2	13:M:191:LEU:HA	1.74	0.69
15:O:104:ASP:OD1	15:O:150:SER:OG	2.11	0.69
33:g:145:ARG:NH1	33:g:172:ALA:O	2.25	0.69
5:E:214:LEU:HD13	5:E:219:ALA:HB2	1.75	0.69
10:J:49:PHE:O	10:J:53:ILE:HG12	1.93	0.69
15:O:86:PHE:HB3	15:O:90:TYR:HD2	1.59	0.69
3:C:24:GLY:HA2	3:C:28:LEU:HB2	1.74	0.68
26:Z:68:LYS:O	26:Z:72:ARG:NH1	2.26	0.68
57:L:601:CDL:H211	57:L:601:CDL:H361	1.74	0.68
33:g:110:MET:HE1	33:g:145:ARG:HD3	1.74	0.68
12:L:405:THR:HA	12:L:408:TYR:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:q:143:ASN:O	43:q:143:ASN:ND2	2.26	0.68
27:a:50:ARG:HD2	32:f:3:TRP:CH2	2.27	0.68
7:G:378:ILE:HG22	7:G:537:PRO:HG3	1.76	0.68
7:G:495:GLU:HB3	7:G:681:VAL:HG12	1.75	0.68
12:L:134:LEU:HB3	12:L:183:MET:HE3	1.74	0.68
7:G:550:VAL:HG22	7:G:569:PHE:HB3	1.76	0.68
8:H:78:ILE:HD11	8:H:218:VAL:HB	1.74	0.68
26:Z:93:TRP:HB2	32:f:3:TRP:HE1	1.59	0.68
33:g:124:LEU:HD11	33:g:141:LEU:HD23	1.77	0.68
56:H:301:PTY:H331	9:I:80:LEU:HD21	1.76	0.67
14:N:84:PHE:HE2	52:N:403:PC7:H483	1.58	0.67
7:G:398:THR:HB	7:G:519:ASN:HD21	1.59	0.67
20:T:92:GLU:OE2	61:T:201:HOH:O	2.11	0.67
57:L:601:CDL:H592	25:Y:155:VAL:HG13	1.77	0.67
14:N:12:ILE:O	14:N:16:ILE:HG12	1.94	0.67
7:G:63:GLN:HG2	17:Q:154:HIS:CD2	2.30	0.67
13:M:42:TRP:CE2	56:M:501:PTY:H312	2.30	0.67
2:B:110:TYR:HE1	9:I:141:PRO:HB2	1.59	0.67
7:G:718:ARG:NH2	61:G:903:HOH:O	2.27	0.67
7:G:381:ASP:HB3	7:G:490:ARG:HD3	1.76	0.67
49:x:46:LYS:NZ	50:y:104:GLU:OE1	2.26	0.67
38:l:94:GLU:O	38:l:103:ARG:NH1	2.27	0.66
12:L:67:TYR:HE2	42:p:71:LYS:HD3	1.60	0.66
5:E:137:LYS:HD2	5:E:200:ARG:HG2	1.78	0.66
24:X:56:LEU:O	24:X:60:ILE:HG13	1.95	0.66
14:N:88:SER:O	35:i:49:ARG:NH2	2.28	0.66
20:T:100:ASP:HB3	40:n:17:ARG:NH1	2.10	0.66
23:W:34:LEU:HD23	23:W:37:ILE:HD11	1.77	0.66
16:P:286:ARG:HH12	16:P:296:GLY:HA2	1.61	0.66
16:P:100:VAL:HG12	16:P:139:ARG:HB2	1.78	0.66
5:E:236:SER:OG	5:E:239:ARG:O	2.14	0.66
12:L:242:ILE:HG13	12:L:243:HIS:CD2	2.31	0.66
2:B:51:ARG:NH2	4:D:140:GLU:OE1	2.29	0.65
9:I:35:ARG:HB2	9:I:38:GLN:HG2	1.78	0.65
33:g:108:MET:HA	33:g:108:MET:HE2	1.79	0.65
3:C:122:GLU:OE2	17:Q:139:LYS:NZ	2.29	0.65
5:E:247:ALA:HB1	6:F:316:ARG:HH21	1.61	0.65
12:L:26:ARG:NH2	33:g:29:PRO:HD2	2.10	0.65
4:D:271:GLU:OE1	4:D:274:ARG:NH1	2.29	0.65
30:d:2:GLY:N	30:d:55:ASP:OD1	2.30	0.65
16:P:182:VAL:HG23	58:P:500:NDP:H42N	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:94:LEU:HG	39:m:98:MET:HE2	1.78	0.65
8:H:192:VAL:HA	8:H:195:ASP:HB2	1.78	0.65
23:W:97:ILE:HD13	23:W:101:ILE:HD12	1.78	0.65
22:V:72:VAL:HG11	22:V:85:ILE:HG21	1.79	0.65
50:y:92:LEU:HD12	51:z:213:VAL:HG13	1.79	0.65
12:L:511:ARG:HH22	38:l:67:MET:HE2	1.62	0.65
6:F:155:THR:HG22	6:F:199:VAL:HG21	1.78	0.64
7:G:628:ARG:HH12	7:G:637:GLN:HG3	1.62	0.64
34:h:20:GLY:O	38:l:32:LYS:NZ	2.27	0.64
8:H:88:LEU:HD12	8:H:163:LEU:HD13	1.79	0.64
8:H:266:TYR:HA	8:H:269:PHE:CE1	2.32	0.64
6:F:402:ASP:HB3	7:G:167:GLU:HG2	1.79	0.64
7:G:383:SER:O	7:G:527:ARG:NH2	2.30	0.64
20:T:49:THR:O	20:T:53:ILE:HG13	1.97	0.64
51:z:138:ASN:N	51:z:156:ASP:OD1	2.31	0.64
14:N:31:LYS:HE2	50:y:284:LEU:HD21	1.79	0.64
13:M:76:LEU:HG	56:M:501:PTY:H332	1.79	0.64
25:Y:144:ARG:HB3	25:Y:148:GLN:OE1	1.98	0.64
1:A:16:TYR:OH	26:Z:92:GLU:OE2	2.16	0.64
4:D:147:GLU:OE1	61:D:401:HOH:O	2.14	0.64
23:W:34:LEU:O	23:W:38:HIS:ND1	2.31	0.64
2:B:43:GLU:OE2	4:D:153:ARG:NH2	2.30	0.63
8:H:192:VAL:HB	8:H:258:ARG:HG2	1.80	0.63
12:L:494:ASN:OD1	12:L:495:PHE:N	2.30	0.63
25:Y:148:GLN:HE21	45:s:11:TRP:NE1	1.96	0.63
21:U:91:GLU:OE1	21:U:97:GLU:HA	1.98	0.63
47:u:37:UNK:C	47:u:39:UNK:N	2.60	0.63
14:N:252:VAL:HG21	14:N:306:ILE:HG23	1.79	0.63
25:Y:77:ARG:NH1	46:t:127:HIS:HA	2.12	0.63
7:G:275:VAL:HG22	7:G:285:ILE:HG12	1.80	0.63
49:x:114:LEU:HD12	49:x:142:GLU:HA	1.80	0.63
4:D:109:ILE:HG23	4:D:142:LEU:HD22	1.80	0.63
6:F:77:VAL:HG11	6:F:199:VAL:HG11	1.81	0.63
28:b:41:UNK:C	28:b:43:UNK:N	2.60	0.63
25:Y:141:ALA:HA	25:Y:144:ARG:HG3	1.81	0.63
6:F:74:LYS:HE2	6:F:196:GLY:HA3	1.80	0.63
2:B:132:PRO:HG3	9:I:200:LEU:HD11	1.81	0.63
8:H:192:VAL:HA	8:H:195:ASP:CB	2.29	0.63
16:P:215:PRO:HB2	16:P:330:VAL:HG21	1.81	0.62
2:B:110:TYR:HB2	9:I:170:ILE:HG21	1.79	0.62
6:F:275:ARG:NH2	6:F:346:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PRO:HG3	2:B:59:ILE:HG23	1.81	0.62
15:O:134:PHE:HB3	46:t:74:ALA:HB2	1.81	0.62
4:D:389:VAL:O	4:D:393:ILE:HG13	2.00	0.62
21:U:104:ASP:OD1	23:W:24:ARG:NH2	2.33	0.62
3:C:18:ASP:OD1	3:C:19:ASN:N	2.32	0.62
4:D:134:TRP:HA	8:H:32:ARG:HH21	1.65	0.62
10:J:48:ASP:OD1	10:J:49:PHE:N	2.32	0.62
5:E:164:LEU:HD12	5:E:179:LEU:HD21	1.82	0.62
10:J:138:ILE:HG23	14:N:74:PHE:HE1	1.64	0.62
12:L:212:LEU:HD11	12:L:303:MET:HE3	1.80	0.62
3:C:28:LEU:HD23	3:C:57:PRO:HG2	1.82	0.62
49:x:261:ARG:HE	50:y:304:LEU:HD21	1.65	0.62
2:B:119:ARG:HH22	3:C:178:THR:HG23	1.64	0.61
4:D:68:PHE:HA	4:D:71:LEU:HD12	1.81	0.61
1:A:138:VAL:HG13	52:A:201:PC7:H412	1.82	0.61
4:D:358:SER:HB3	4:D:361:TYR:HB2	1.80	0.61
12:L:236:THR:HG21	12:L:335:GLY:HA3	1.80	0.61
3:C:16:ALA:HB3	3:C:21:LYS:HE3	1.80	0.61
10:J:131:LEU:HD23	10:J:134:LEU:HD12	1.81	0.61
15:O:78:ASN:OD1	15:O:79:LYS:N	2.32	0.61
21:U:85:GLU:HG3	23:W:53:ARG:HD2	1.81	0.61
2:B:128:ASP:OD1	16:P:69:LYS:NZ	2.34	0.61
3:C:177:LEU:HA	4:D:54:LYS:HE3	1.82	0.61
16:P:109:GLN:OE1	16:P:286:ARG:NH1	2.33	0.61
33:g:110:MET:HE3	33:g:170:LEU:HB2	1.81	0.61
2:B:25:ALA:HB1	8:H:53:LYS:HB2	1.83	0.61
4:D:111:ARG:NH2	4:D:333:GLU:O	2.33	0.61
6:F:387:CYS:HA	7:G:212:ARG:HG3	1.82	0.61
12:L:511:ARG:NE	38:l:62:GLY:O	2.25	0.61
11:K:43:ILE:HD12	11:K:46:ILE:HD11	1.83	0.61
16:P:6:PRO:HB3	16:P:16:ARG:NH1	2.15	0.61
5:E:149:ARG:HE	6:F:377:ARG:HG2	1.65	0.61
4:D:111:ARG:NH1	61:D:403:HOH:O	2.33	0.60
8:H:167:ALA:HB2	8:H:236:ILE:HG13	1.83	0.60
12:L:343:ASN:ND2	12:L:348:ARG:HB2	2.16	0.60
15:O:123:LYS:HE3	45:s:10:HIS:HB3	1.83	0.60
46:t:94:PHE:O	46:t:98:VAL:HG23	2.00	0.60
3:C:214:THR:O	3:C:217:ARG:NH1	2.34	0.60
4:D:304:LYS:NZ	18:R:94:GLY:O	2.29	0.60
6:F:127:GLU:O	6:F:127:GLU:HG2	2.01	0.60
7:G:42:ASP:O	7:G:57:LYS:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:222:LEU:HD21	56:L:603:PTY:H261	1.83	0.60
14:N:349:LYS:HE2	14:N:349:LYS:HA	1.83	0.60
12:L:323:HIS:HA	12:L:326:PHE:CE1	2.37	0.60
39:m:30:ARG:CZ	39:m:42:ASN:HB2	2.31	0.60
40:n:67:GLU:HG2	45:s:33:TYR:CE1	2.36	0.60
42:p:119:ASP:OD2	42:p:122:PHE:HA	2.00	0.60
12:L:274:ALA:HA	12:L:297:SER:HA	1.83	0.60
14:N:354:SER:HB2	14:N:357:ILE:HB	1.81	0.60
20:T:51:ARG:O	20:T:55:VAL:HG23	2.01	0.60
25:Y:164:ASP:CG	46:t:107:ARG:HH21	2.09	0.60
12:L:202:GLN:HE21	38:l:142:ARG:HD2	1.67	0.60
40:n:16:MET:HE2	40:n:20:ARG:HH12	1.67	0.60
8:H:180:LEU:HD23	8:H:277:LEU:HD22	1.84	0.60
17:Q:100:LEU:HD13	23:W:132:VAL:HG22	1.83	0.60
2:B:110:TYR:HB2	9:I:170:ILE:CG2	2.32	0.60
8:H:144:VAL:O	8:H:148:VAL:HG23	2.02	0.60
12:L:506:ASP:OD1	38:l:60:TYR:OH	2.19	0.60
21:U:88:ILE:O	21:U:91:GLU:HB2	2.02	0.60
49:x:130:ASN:HB3	49:x:151:ARG:NH2	2.17	0.60
4:D:304:LYS:NZ	9:I:180:PRO:O	2.34	0.60
7:G:313:ARG:HD3	7:G:575:HIS:O	2.01	0.60
13:M:122:GLU:HB3	14:N:295:PRO:HG2	1.81	0.60
1:A:119:MET:HE1	8:H:160:CYS:HA	1.83	0.60
15:O:79:LYS:O	15:O:83:GLU:HG3	2.02	0.60
20:T:53:ILE:HG23	20:T:67:ILE:HD12	1.82	0.60
3:C:189:LYS:HD2	3:C:193:ILE:HG21	1.82	0.59
7:G:164:ARG:NH2	44:r:67:ILE:HG12	2.16	0.59
14:N:66:PHE:HZ	14:N:191:VAL:HG21	1.66	0.59
7:G:39:LEU:HD11	7:G:45:GLU:HB2	1.84	0.59
15:O:128:GLU:HA	15:O:131:LYS:HG2	1.85	0.59
52:L:602:PC7:H2	38:l:60:TYR:HD1	1.67	0.59
13:M:119:ALA:HA	14:N:295:PRO:HB3	1.84	0.59
39:m:115:TYR:OH	42:p:111:ARG:NH2	2.35	0.59
3:C:29:THR:HG22	3:C:57:PRO:HB3	1.84	0.59
31:e:33:THR:O	31:e:37:GLN:HG3	2.03	0.59
40:n:16:MET:HB3	40:n:20:ARG:HH12	1.67	0.59
6:F:192:LYS:HG3	17:Q:182:SER:HB3	1.84	0.59
12:L:341:GLU:HA	12:L:428:LYS:HD3	1.83	0.59
21:U:85:GLU:OE1	23:W:57:LYS:NZ	2.23	0.59
12:L:467:ALA:HB2	36:j:68:UNK:HA	1.84	0.59
20:T:98:ILE:HG12	20:T:115:TYR:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:130:THR:HG23	4:D:131:PRO:HD3	1.84	0.59
12:L:433:ASP:OD1	12:L:434:ALA:N	2.34	0.59
16:P:188:TYR:O	16:P:192:ASN:ND2	2.35	0.59
49:x:252:TYR:HB2	49:x:254:GLU:OE1	2.02	0.59
8:H:42:PHE:HD1	8:H:44:ILE:HB	1.68	0.59
3:C:146:MET:HB3	3:C:171:LEU:HD12	1.85	0.59
7:G:496:ALA:HB3	7:G:686:ARG:NH2	2.17	0.59
7:G:714:CYS:O	7:G:718:ARG:HG2	2.03	0.59
8:H:45:LEU:HD12	8:H:49:TRP:NE1	2.17	0.59
8:H:98:LEU:HB3	10:J:52:LEU:HD21	1.84	0.59
9:I:55:GLU:OE2	9:I:56:GLN:NE2	2.36	0.59
50:y:269:PHE:CE1	51:z:38:GLU:HA	2.38	0.59
2:B:37:LEU:HB2	2:B:75:GLY:HA3	1.85	0.58
7:G:61:VAL:HG13	7:G:114:ILE:HD13	1.85	0.58
8:H:16:VAL:O	8:H:20:THR:HG23	2.03	0.58
7:G:74:ARG:HH22	17:Q:80:LEU:HD23	1.68	0.58
12:L:392:GLN:HE21	45:s:97:ARG:CZ	2.16	0.58
20:T:100:ASP:C	40:n:17:ARG:HH12	2.11	0.58
16:P:60:CYS:SG	16:P:82:GLU:HG3	2.43	0.58
28:b:2:UNK:O	28:b:3:UNK:C	2.50	0.58
7:G:355:LYS:HG3	7:G:380:GLU:OE2	2.03	0.58
12:L:21:ARG:HG2	29:c:42:GLY:HA2	1.84	0.58
17:Q:152:ARG:NH1	17:Q:154:HIS:HB2	2.18	0.58
2:B:19:ASP:OD2	2:B:20:THR:N	2.37	0.58
32:f:29:ILE:HD12	32:f:29:ILE:H	1.69	0.58
6:F:83:TRP:CZ3	6:F:263:LEU:HD12	2.39	0.58
5:E:189:VAL:HG12	5:E:239:ARG:HH22	1.69	0.58
16:P:145:GLU:HG2	16:P:160:LYS:HE2	1.85	0.58
49:x:57:THR:OG1	49:x:58:GLU:OE1	2.20	0.58
11:K:118:ASN:ND2	11:K:119:GLU:OE1	2.36	0.58
3:C:217:ARG:NE	17:Q:29:ASP:OD2	2.30	0.58
5:E:239:ARG:NH1	5:E:243:GLU:O	2.37	0.58
7:G:266:SER:HB3	7:G:301:LYS:HE3	1.86	0.58
9:I:201:LEU:HB3	17:Q:108:MET:HE2	1.84	0.58
28:b:1:UNK:O	28:b:4:UNK:N	2.37	0.58
5:E:74:MET:HE1	5:E:112:ILE:HG22	1.85	0.57
29:c:52:ARG:NH2	33:g:36:GLU:OE1	2.37	0.57
30:d:12:LEU:O	30:d:16:VAL:HG23	2.05	0.57
4:D:264:VAL:O	4:D:268:GLU:HG3	2.05	0.57
9:I:201:LEU:HD11	16:P:74:LEU:HD13	1.86	0.57
9:I:55:GLU:HA	9:I:62:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:333:TYR:O	14:N:337:ILE:HD12	2.04	0.57
4:D:42:ASP:OD2	4:D:44:HIS:HE1	1.87	0.57
26:Z:130:LEU:HB3	31:e:52:ARG:HH12	1.68	0.57
50:y:275:GLU:HA	50:y:278:ILE:HD12	1.86	0.57
7:G:209:ILE:HG12	7:G:218:VAL:HG22	1.87	0.57
7:G:396:ALA:HB1	7:G:519:ASN:HD22	1.70	0.57
14:N:11:LEU:HD21	52:N:403:PC7:H462	1.86	0.57
14:N:105:LEU:HD13	14:N:192:PHE:CG	2.40	0.57
17:Q:152:ARG:NH2	61:Q:201:HOH:O	2.38	0.57
19:S:13:GLU:OE1	19:S:15:ARG:HG3	2.05	0.57
19:S:90:VAL:O	19:S:94:GLN:HG2	2.04	0.57
2:B:137:THR:HA	4:D:153:ARG:HH21	1.70	0.57
12:L:263:GLN:NE2	38:l:124:ASN:O	2.38	0.57
17:Q:66:VAL:HG13	17:Q:95:ILE:HG23	1.85	0.57
11:K:52:TRP:O	11:K:54:ARG:HG2	2.03	0.57
21:U:79:ASP:OD1	21:U:80:SER:N	2.35	0.57
27:a:4:TYR:O	27:a:7:PRO:HD2	2.05	0.57
16:P:42:TYR:O	16:P:46:GLU:HG2	2.05	0.57
16:P:262:LEU:HD23	16:P:343:ARG:NH2	2.19	0.57
49:x:161:ARG:HH12	51:z:145:ASN:CG	2.11	0.57
7:G:410:LEU:HD11	7:G:440:VAL:HG23	1.87	0.57
12:L:350:GLY:HA3	12:L:421:TYR:HA	1.86	0.57
35:i:59:PRO:HB3	35:i:77:GLY:HA2	1.85	0.57
13:M:78:CYS:HB3	13:M:223:VAL:HG11	1.86	0.56
13:M:150:THR:OG1	13:M:195:LYS:NZ	2.37	0.56
16:P:46:GLU:HG3	16:P:222:ALA:HB1	1.86	0.56
23:W:54:LEU:HA	23:W:57:LYS:NZ	2.20	0.56
41:o:31:ALA:HA	41:o:34:ILE:HG22	1.86	0.56
42:p:45:GLU:OE2	42:p:55:ASN:HB2	2.04	0.56
3:C:21:LYS:NZ	3:C:111:ASN:HB3	2.20	0.56
5:E:190:ASN:HB3	5:E:212:GLU:HB3	1.87	0.56
7:G:250:PHE:HB3	9:I:157:ARG:HG3	1.87	0.56
9:I:153:GLU:HB3	18:R:30:VAL:HG23	1.87	0.56
12:L:11:PHE:CE2	29:c:62:MET:HB2	2.41	0.56
12:L:511:ARG:NH1	38:l:67:MET:HE2	2.20	0.56
14:N:154:ILE:HG22	14:N:156:ASP:H	1.69	0.56
14:N:181:PHE:HA	14:N:184:VAL:HG22	1.87	0.56
17:Q:84:LEU:HD12	17:Q:149:PRO:HG3	1.87	0.56
40:n:16:MET:HB3	40:n:20:ARG:NH1	2.20	0.56
45:s:88:TYR:HA	45:s:91:THR:HG22	1.86	0.56
49:x:234:ASP:OD1	49:x:235:HIS:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:PHE:HE2	3:C:78:ASN:HB3	1.71	0.56
3:C:191:ARG:NH2	23:W:102:GLU:OE1	2.37	0.56
25:Y:165:LEU:HD21	56:m:201:PTY:H342	1.88	0.56
26:Z:90:GLN:HA	32:f:3:TRP:CD1	2.41	0.56
28:b:2:UNK:C	28:b:4:UNK:N	2.67	0.56
44:r:111:ARG:HH22	44:r:114:GLU:CD	2.13	0.56
6:F:286:ILE:HG21	6:F:312:ALA:HB2	1.88	0.56
7:G:680:LEU:HD11	19:S:44:PRO:HB3	1.88	0.56
8:H:16:VAL:HG11	8:H:221:VAL:HG13	1.88	0.56
24:X:37:ASP:HB3	35:i:98:TYR:CD2	2.40	0.56
24:X:80:LEU:HD12	27:a:44:GLN:NE2	2.15	0.56
26:Z:137:ASP:OD1	26:Z:138:VAL:N	2.38	0.56
8:H:268:MET:O	8:H:272:ILE:HG12	2.06	0.56
17:Q:181:PRO:HG3	17:Q:184:ARG:HH21	1.71	0.56
18:R:51:LEU:HD12	43:q:142:ARG:HH12	1.70	0.56
3:C:106:LEU:HD13	3:C:113:ARG:NE	2.18	0.56
4:D:307:MET:HE2	4:D:311:ILE:HG13	1.86	0.56
5:E:247:ALA:HB2	6:F:293:PRO:HD3	1.88	0.56
25:Y:77:ARG:HH22	46:t:127:HIS:HB2	1.71	0.56
49:x:163:VAL:HG11	50:y:212:ALA:HB1	1.88	0.56
6:F:419:MET:HG3	7:G:164:ARG:HD3	1.87	0.56
12:L:49:GLU:HG2	29:c:88:PRO:HD2	1.88	0.56
12:L:386:ASN:HB3	12:L:463:THR:HG21	1.87	0.56
14:N:271:SER:HA	14:N:364:LEU:HD11	1.88	0.56
4:D:106:PHE:CZ	4:D:149:VAL:HG11	2.41	0.56
14:N:108:LEU:HD23	14:N:111:ILE:HD11	1.88	0.56
14:N:118:ARG:NH1	14:N:122:TYR:OH	2.38	0.56
16:P:286:ARG:NH1	16:P:296:GLY:HA2	2.20	0.56
16:P:289:LEU:HD23	16:P:292:PHE:HE2	1.70	0.56
3:C:21:LYS:HZ1	3:C:111:ASN:HB3	1.71	0.55
12:L:220:SER:HB2	12:L:225:HIS:HA	1.88	0.55
42:p:105:VAL:O	42:p:109:LEU:HD23	2.05	0.55
12:L:132:GLN:HE22	12:L:194:SER:HB3	1.70	0.55
12:L:527:LEU:HD22	39:m:83:THR:HG23	1.87	0.55
14:N:92:LEU:HD23	35:i:67:LEU:HD21	1.89	0.55
6:F:164:ILE:HD11	6:F:203:LEU:HD21	1.87	0.55
7:G:583:ARG:O	7:G:583:ARG:HG3	2.07	0.55
11:K:56:LEU:HD13	14:N:126:LEU:HD13	1.88	0.55
12:L:258:LEU:HD13	12:L:260:LEU:HD12	1.86	0.55
1:A:108:ASP:O	1:A:112:VAL:HG23	2.06	0.55
8:H:69:ILE:HG21	10:J:25:PHE:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:ILE:HG23	10:J:77:VAL:HG13	1.88	0.55
11:K:89:PHE:HD1	14:N:92:LEU:HD13	1.71	0.55
13:M:184:VAL:O	13:M:188:ILE:HG13	2.07	0.55
15:O:182:HIS:HB3	15:O:184:ASN:ND2	2.22	0.55
4:D:120:THR:HG21	4:D:135:ALA:HB2	1.88	0.55
8:H:173:ILE:HD11	8:H:291:LEU:HD13	1.87	0.55
8:H:191:ARG:O	8:H:195:ASP:N	2.39	0.55
16:P:68:LEU:HA	16:P:71:MET:HG2	1.87	0.55
38:l:99:ASP:O	38:l:103:ARG:HG3	2.07	0.55
5:E:185:MET:HE1	6:F:169:GLU:HG2	1.89	0.55
5:E:191:ALA:HB3	5:E:192:PRO:HD3	1.87	0.55
12:L:512:LYS:HD2	34:h:41:TRP:CE2	2.41	0.55
23:W:54:LEU:HA	23:W:57:LYS:HZ3	1.71	0.55
9:I:229:ARG:NH2	61:I:602:HOH:O	2.39	0.55
10:J:20:LEU:HD22	10:J:83:LYS:HE3	1.89	0.55
33:g:61:LEU:HB2	33:g:64:GLU:HG3	1.86	0.55
42:p:151:ARG:NH2	42:p:154:ILE:O	2.39	0.55
1:A:45:VAL:HG11	8:H:99:PHE:HE2	1.71	0.55
12:L:186:LEU:O	12:L:190:THR:OG1	2.17	0.55
14:N:63:ILE:HB	14:N:75:LEU:HD23	1.88	0.55
33:g:140:ASP:O	33:g:144:MET:HG2	2.07	0.55
4:D:108:GLU:OE2	4:D:243:TYR:OH	2.22	0.55
8:H:233:LEU:HA	8:H:236:ILE:HG22	1.89	0.55
19:S:81:GLY:O	19:S:85:LYS:HG2	2.07	0.55
24:X:12:TYR:CE2	24:X:80:LEU:HD13	2.42	0.55
26:Z:99:GLU:O	26:Z:102:ARG:HG3	2.07	0.55
26:Z:137:ASP:O	27:a:49:ARG:NH1	2.39	0.55
33:g:110:MET:HG2	33:g:170:LEU:O	2.06	0.55
35:i:104:ASN:OD1	35:i:105:GLU:N	2.40	0.55
4:D:42:ASP:OD2	4:D:44:HIS:CE1	2.60	0.54
5:E:148:CYS:HA	5:E:191:ALA:HB1	1.89	0.54
8:H:12:LEU:O	8:H:16:VAL:HG23	2.07	0.54
8:H:171:LYS:HB3	8:H:173:ILE:HG22	1.87	0.54
16:P:73:ASP:OD1	16:P:74:LEU:N	2.37	0.54
45:s:49:VAL:HG22	45:s:52:ARG:HH21	1.72	0.54
4:D:197:ASN:O	4:D:201:LYS:HG2	2.07	0.54
5:E:145:THR:HG22	5:E:146:THR:H	1.71	0.54
17:Q:71:PRO:HG3	17:Q:94:LYS:HE2	1.88	0.54
10:J:24:PRO:HD3	10:J:77:VAL:HG21	1.89	0.54
40:n:13:LEU:O	40:n:17:ARG:HG2	2.08	0.54
4:D:14:ILE:HG22	8:H:122:TYR:CE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:180:LEU:HD11	8:H:280:VAL:HG12	1.89	0.54
27:a:4:TYR:HD2	27:a:7:PRO:HD3	1.72	0.54
29:c:84:LYS:NZ	41:o:21:ASP:OD2	2.28	0.54
42:p:69:LYS:HA	42:p:72:ILE:HD12	1.90	0.54
6:F:123:VAL:HG11	6:F:146:LEU:HD11	1.88	0.54
7:G:261:GLU:O	7:G:611:ARG:HD3	2.06	0.54
9:I:148:GLU:HG2	9:I:161:ARG:HB3	1.88	0.54
24:X:54:ASN:O	24:X:58:GLN:HG3	2.07	0.54
28:b:4:UNK:O	28:b:5:UNK:C	2.55	0.54
8:H:123:ALA:HA	8:H:205:ALA:O	2.08	0.54
9:I:161:ARG:NH2	9:I:163:ASP:OD2	2.38	0.54
13:M:77:LEU:HD21	13:M:310:GLY:HA3	1.89	0.54
13:M:210:VAL:HG21	13:M:274:LYS:HG3	1.89	0.54
14:N:34:ASP:OD1	14:N:35:LEU:N	2.41	0.54
16:P:95:ILE:HD11	16:P:130:ILE:HG22	1.90	0.54
29:c:46:ASN:O	33:g:39:GLN:NE2	2.41	0.54
8:H:133:LEU:HD13	8:H:269:PHE:CD2	2.43	0.54
4:D:241:ASP:C	4:D:243:TYR:H	2.16	0.54
33:g:154:LEU:HD22	33:g:164:LYS:HE3	1.89	0.54
2:B:43:GLU:HG3	2:B:135:PRO:HB2	1.90	0.54
5:E:218:ASP:O	5:E:222:ILE:HG12	2.07	0.54
9:I:225:GLU:HB3	9:I:229:ARG:NH1	2.22	0.54
28:b:6:UNK:C	28:b:8:UNK:N	2.68	0.54
35:i:41:TRP:NE1	35:i:44:ARG:HH21	2.06	0.54
51:z:141:LEU:HB3	51:z:159:ILE:HG12	1.89	0.54
1:A:49:VAL:HG13	8:H:79:CYS:SG	2.48	0.53
6:F:75:ASP:O	6:F:79:LYS:HG3	2.07	0.53
6:F:122:VAL:HG11	6:F:220:LEU:HD21	1.90	0.53
7:G:360:GLU:HB3	7:G:646:VAL:HG11	1.89	0.53
19:S:7:LEU:HB2	19:S:43:ASN:ND2	2.23	0.53
3:C:136:ALA:O	3:C:140:GLU:HG3	2.08	0.53
14:N:64:LEU:HD22	52:N:402:PC7:H32	1.91	0.53
14:N:72:SER:O	14:N:76:VAL:HG23	2.09	0.53
22:V:81:TYR:OH	22:V:123:GLU:OE2	2.15	0.53
5:E:128:THR:HG23	7:G:212:ARG:HH12	1.73	0.53
6:F:160:ARG:HH22	17:Q:182:SER:HB2	1.74	0.53
7:G:206:GLU:OE1	7:G:226:HIS:HA	2.09	0.53
14:N:186:ARG:N	15:O:200:GLU:OE2	2.42	0.53
14:N:255:GLU:O	25:Y:200:ARG:HD2	2.08	0.53
15:O:78:ASN:ND2	15:O:150:SER:OG	2.41	0.53
16:P:189:PHE:O	16:P:193:LEU:HG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:35:SER:HB2	27:a:38:GLN:HG2	1.91	0.53
3:C:160:VAL:HG23	3:C:161:LEU:HG	1.91	0.53
12:L:346:LEU:HA	12:L:349:TYR:HD2	1.74	0.53
56:Y:301:PTY:H382	56:m:201:PTY:H262	1.91	0.53
41:o:77:GLU:HB3	41:o:81:ARG:HH12	1.73	0.53
47:u:2:UNK:C	47:u:4:UNK:N	2.68	0.53
49:x:101:ASP:OD1	49:x:102:LEU:N	2.40	0.53
50:y:152:THR:HG1	51:z:104:ASN:HD22	1.54	0.53
1:A:142:PHE:HD1	52:A:201:PC7:H382	1.73	0.53
8:H:62:PRO:HD2	16:P:199:TYR:OH	2.09	0.53
8:H:129:ARG:HH21	8:H:266:TYR:HB2	1.74	0.53
13:M:95:LEU:O	13:M:99:ILE:HG12	2.09	0.53
14:N:134:ILE:HD11	46:t:85:TYR:CE1	2.43	0.53
25:Y:186:PHE:HB3	25:Y:189:LEU:HD12	1.89	0.53
3:C:43:ALA:HB3	22:V:146:VAL:HG22	1.89	0.53
3:C:211:PRO:HB2	17:Q:79:GLY:HA3	1.91	0.53
57:N:401:CDL:O1	30:d:64:ARG:NH2	2.41	0.53
26:Z:124:THR:HG23	26:Z:130:LEU:HD12	1.89	0.53
45:s:5:LEU:HD12	46:t:118:LEU:HD23	1.90	0.53
11:K:120:VAL:HG23	11:K:121:GLU:H	1.74	0.53
13:M:327:THR:HG22	13:M:413:VAL:HG11	1.91	0.53
11:K:89:PHE:CE2	11:K:93:ILE:HD11	2.43	0.53
12:L:160:SER:HA	52:L:602:PC7:H62	1.91	0.53
35:i:58:GLU:HB2	35:i:81:ASN:HD21	1.74	0.53
41:o:71:VAL:HB	45:s:104:VAL:HG21	1.89	0.53
4:D:168:LEU:HD22	4:D:172:LEU:HD23	1.90	0.53
23:W:50:LYS:O	23:W:54:LEU:HG	2.09	0.53
1:A:34:PHE:HA	1:A:38:ASP:O	2.09	0.53
5:E:66:ASN:O	5:E:70:VAL:HG23	2.08	0.53
8:H:198:GLU:HB3	8:H:263:ARG:NH2	2.25	0.53
10:J:39:GLN:OE1	10:J:55:ALA:HB2	2.09	0.53
12:L:492:SER:OG	12:L:494:ASN:OD1	2.27	0.53
14:N:74:PHE:CZ	14:N:107:VAL:HG11	2.44	0.53
14:N:201:LEU:HD22	14:N:253:LEU:HD22	1.91	0.53
15:O:123:LYS:NZ	61:O:302:HOH:O	2.34	0.53
16:P:203:ALA:HB3	16:P:267:THR:HA	1.92	0.53
50:y:135:ASP:OD1	50:y:136:VAL:N	2.41	0.53
1:A:45:VAL:HG11	8:H:99:PHE:CE2	2.43	0.52
7:G:140:CYS:SG	7:G:152:GLN:NE2	2.82	0.52
33:g:134:ILE:HG12	33:g:137:GLU:HG3	1.91	0.52
50:y:137:ASN:OD1	50:y:138:SER:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:z:99:SER:OG	51:z:120:GLY:O	2.26	0.52
8:H:125:LEU:O	8:H:129:ARG:HG3	2.10	0.52
8:H:183:ILE:HA	8:H:186:LEU:HD12	1.90	0.52
40:n:37:TYR:HB2	40:n:38:PRO:HD3	1.90	0.52
50:y:152:THR:OG1	51:z:104:ASN:ND2	2.34	0.52
16:P:224:ALA:O	16:P:228:ILE:HG12	2.09	0.52
50:y:273:LEU:O	50:y:277:GLU:HG2	2.10	0.52
4:D:14:ILE:CG1	4:D:31:LEU:HB2	2.39	0.52
6:F:372:ILE:HD11	6:F:454:MET:HG2	1.91	0.52
12:L:352:ARG:HH12	12:L:428:LYS:HG3	1.75	0.52
25:Y:109:ILE:HD13	25:Y:139:VAL:HG21	1.90	0.52
50:y:87:SER:O	50:y:91:VAL:HG23	2.10	0.52
1:A:152:TRP:HD1	8:H:271:GLN:HG3	1.74	0.52
8:H:15:SER:O	8:H:19:LEU:HG	2.08	0.52
17:Q:91:PRO:HB2	17:Q:126:LEU:HB3	1.92	0.52
20:T:98:ILE:HG12	20:T:115:TYR:CE2	2.44	0.52
22:V:104:ALA:O	22:V:108:VAL:HG23	2.09	0.52
25:Y:170:TYR:HB3	25:Y:171:PRO:HD3	1.91	0.52
4:D:186:ARG:HH21	4:D:189:GLU:CD	2.17	0.52
7:G:231:SER:O	7:G:234:VAL:HG22	2.10	0.52
10:J:66:PHE:O	10:J:70:VAL:HG23	2.09	0.52
34:h:51:PHE:CD2	34:h:52:PRO:HD3	2.45	0.52
40:n:67:GLU:HG2	45:s:33:TYR:HE1	1.74	0.52
51:z:158:THR:HG21	51:z:172:VAL:HG12	1.91	0.52
4:D:105:LEU:HD11	4:D:276:ILE:HG23	1.90	0.52
4:D:144:GLU:OE2	4:D:148:ARG:HD2	2.08	0.52
5:E:198:ASP:OD2	5:E:207:SER:OG	2.28	0.52
14:N:171:ALA:CB	14:N:172:PRO:HD3	2.38	0.52
23:W:81:GLU:O	23:W:85:THR:HG23	2.10	0.52
25:Y:14:SER:O	42:p:43:LYS:NZ	2.37	0.52
41:o:3:ASP:OD1	41:o:4:ARG:N	2.43	0.52
4:D:245:ARG:HG2	44:r:114:GLU:HB3	1.92	0.52
21:U:68:LEU:HD23	21:U:110:GLU:HG2	1.91	0.52
25:Y:87:ASN:HD22	25:Y:90:LYS:H	1.56	0.52
34:h:38:ALA:O	34:h:42:ASN:ND2	2.42	0.52
2:B:32:PRO:HA	2:B:70:VAL:O	2.09	0.52
3:C:80:GLN:HE22	22:V:119:GLU:CD	2.17	0.52
5:E:53:GLU:OE2	5:E:134:LYS:HB2	2.09	0.52
7:G:78:HIS:CE1	7:G:237:LEU:HD21	2.45	0.52
13:M:342:ALA:HB2	13:M:413:VAL:O	2.10	0.52
22:V:92:ARG:NH1	61:V:201:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:40:LEU:HG	23:W:89:MET:HE2	1.92	0.52
25:Y:103:ALA:HB2	46:t:119:PHE:CE2	2.45	0.52
42:p:97:LYS:HG2	42:p:156:TYR:CD1	2.45	0.52
3:C:187:TYR:CG	16:P:71:MET:HE1	2.45	0.52
4:D:117:LEU:HD22	4:D:139:ARG:NH1	2.25	0.52
8:H:100:LEU:HD13	8:H:233:LEU:HD21	1.91	0.52
8:H:226:ASN:O	8:H:230:MET:HG2	2.10	0.52
51:z:150:GLU:O	51:z:168:GLU:HG2	2.10	0.52
5:E:270:TYR:CD2	6:F:265:ARG:HD3	2.45	0.51
6:F:304:LEU:HD11	6:F:362:VAL:HG21	1.92	0.51
7:G:711:MET:O	7:G:715:THR:HG23	2.10	0.51
19:S:74:ILE:HB	19:S:82:ILE:HD12	1.91	0.51
29:c:100:VAL:HG12	29:c:106:VAL:HG12	1.93	0.51
44:r:111:ARG:NH2	44:r:114:GLU:OE2	2.36	0.51
50:y:171:ASN:N	50:y:188:ASP:OD1	2.41	0.51
3:C:48:ALA:HB1	3:C:56:GLU:HG2	1.92	0.51
3:C:123:VAL:HG13	17:Q:51:ILE:HD11	1.92	0.51
4:D:148:ARG:NH1	4:D:175:ASP:OD1	2.39	0.51
14:N:255:GLU:HA	25:Y:201:ARG:HD3	1.92	0.51
41:o:23:PRO:HD2	41:o:26:TYR:HD2	1.75	0.51
49:x:101:ASP:OD2	50:y:257:LEU:HD13	2.10	0.51
4:D:258:CYS:SG	4:D:385:THR:HG21	2.50	0.51
6:F:93:LEU:HD21	6:F:255:THR:HG23	1.91	0.51
7:G:439:LEU:HG	7:G:441:GLY:H	1.75	0.51
12:L:222:LEU:HD11	12:L:505:PHE:CZ	2.44	0.51
12:L:310:ASP:OD1	12:L:311:ASP:N	2.43	0.51
15:O:100:GLN:HB3	15:O:197:PRO:HD2	1.92	0.51
35:i:55:ASN:C	35:i:81:ASN:HD22	2.11	0.51
6:F:348:ASP:O	6:F:352:THR:HG23	2.11	0.51
7:G:493:ASP:HB2	7:G:686:ARG:NH2	2.25	0.51
8:H:272:ILE:HG21	56:H:301:PTY:H312	1.93	0.51
12:L:118:LEU:HD22	12:L:241:LEU:HD12	1.92	0.51
12:L:266:VAL:HA	12:L:303:MET:HE2	1.91	0.51
21:U:51:ILE:CD1	21:U:113:VAL:HB	2.39	0.51
21:U:72:PHE:HD2	21:U:83:LYS:HE3	1.75	0.51
24:X:19:VAL:HG11	26:Z:84:ILE:HG12	1.93	0.51
51:z:141:LEU:HD23	51:z:159:ILE:HG23	1.93	0.51
7:G:56:PRO:HD2	7:G:59:PHE:CE2	2.45	0.51
7:G:311:ARG:HG2	7:G:312:GLN:HG2	1.93	0.51
8:H:272:ILE:HD12	56:H:301:PTY:HC51	1.91	0.51
14:N:175:MET:HG2	46:t:84:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:61:ASN:O	16:P:65:VAL:HG22	2.11	0.51
24:X:57:PHE:O	24:X:61:MET:HG2	2.10	0.51
4:D:144:GLU:HA	4:D:147:GLU:HG2	1.92	0.51
6:F:348:ASP:OD1	6:F:349:ALA:N	2.43	0.51
7:G:252:ALA:HB2	7:G:283:MET:HE2	1.93	0.51
19:S:74:ILE:HB	19:S:82:ILE:CD1	2.41	0.51
24:X:46:SER:HB3	26:Z:91:ALA:HB1	1.93	0.51
51:z:198:ASN:OD1	51:z:199:THR:N	2.43	0.51
1:A:144:GLU:OE2	10:J:144:LEU:HG	2.10	0.51
7:G:717:VAL:O	7:G:720:GLN:HG2	2.10	0.51
14:N:84:PHE:HZ	52:N:403:PC7:H472	1.75	0.51
14:N:366:VAL:HG13	30:d:13:CYS:SG	2.51	0.51
16:P:202:VAL:O	16:P:204:PRO:HD3	2.11	0.51
17:Q:70:CYS:SG	17:Q:84:LEU:HG	2.51	0.51
23:W:41:HIS:O	23:W:93:ARG:HD2	2.11	0.51
49:x:122:ALA:H	49:x:149:SER:HG	1.58	0.51
4:D:366:MET:HG2	4:D:370:VAL:HG23	1.93	0.51
7:G:606:ARG:NH1	7:G:661:GLY:O	2.41	0.51
12:L:515:ASN:HB3	34:h:33:MET:HE3	1.92	0.51
14:N:164:LEU:HD11	14:N:203:LEU:HD23	1.93	0.51
15:O:77:LEU:HD22	15:O:152:LEU:HD23	1.93	0.51
39:m:118:ARG:NH2	61:m:301:HOH:O	2.38	0.51
51:z:215:MET:O	51:z:219:GLU:HG3	2.11	0.51
6:F:243:LEU:H	6:F:248:THR:HG21	1.76	0.51
25:Y:91:LYS:NZ	46:t:131:LYS:O	2.44	0.51
42:p:94:GLU:HG3	42:p:98:ARG:HE	1.76	0.51
7:G:203:GLY:HA3	7:G:428:ARG:HH12	1.76	0.50
16:P:334:LEU:HA	16:P:337:GLU:HG3	1.92	0.50
26:Z:130:LEU:HB3	31:e:52:ARG:NH1	2.26	0.50
39:m:30:ARG:NH2	39:m:42:ASN:HB2	2.26	0.50
49:x:120:HIS:O	49:x:148:ARG:HA	2.11	0.50
50:y:66:ALA:HB3	50:y:115:LEU:HD23	1.93	0.50
2:B:109:GLY:HA2	9:I:168:LYS:HA	1.93	0.50
8:H:133:LEU:HD13	8:H:269:PHE:CE2	2.46	0.50
9:I:56:GLN:HB3	22:V:44:LYS:NZ	2.27	0.50
9:I:175:CYS:HB3	53:I:500:SF4:S2	2.51	0.50
12:L:67:TYR:CE2	42:p:71:LYS:HD3	2.43	0.50
12:L:343:ASN:OD1	12:L:344:ASN:N	2.44	0.50
14:N:7:TYR:HB2	52:N:403:PC7:H421	1.92	0.50
24:X:37:ASP:OD1	24:X:38:TRP:N	2.44	0.50
34:h:26:LEU:HG	34:h:28:TYR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:o:46:LEU:HD12	41:o:47:THR:HG23	1.94	0.50
4:D:94:ALA:HB1	44:r:118:HIS:HA	1.93	0.50
5:E:243:GLU:HG2	6:F:56:ARG:HH21	1.76	0.50
6:F:77:VAL:HG13	6:F:155:THR:HG21	1.94	0.50
7:G:130:GLU:O	7:G:134:ILE:HG23	2.12	0.50
20:T:104:ASP:OD2	40:n:17:ARG:NH2	2.44	0.50
40:n:18:MET:HG2	40:n:47:PHE:HZ	1.77	0.50
41:o:31:ALA:O	41:o:35:ILE:HG13	2.12	0.50
8:H:74:PRO:HB3	8:H:218:VAL:HG21	1.93	0.50
17:Q:27:PRO:HB3	17:Q:89:LYS:HD2	1.94	0.50
49:x:198:PRO:O	49:x:200:LYS:HG2	2.11	0.50
3:C:208:PHE:HB3	4:D:319:GLU:HG3	1.92	0.50
9:I:84:VAL:HG12	9:I:88:MET:HE1	1.92	0.50
12:L:511:ARG:NH2	38:l:67:MET:HE2	2.27	0.50
13:M:73:TYR:HB3	13:M:307:ILE:HD11	1.94	0.50
19:S:70:LYS:HD3	19:S:89:LEU:HD23	1.94	0.50
27:a:7:PRO:O	27:a:11:ILE:HG12	2.10	0.50
49:x:197:SER:HB2	49:x:198:PRO:HD3	1.92	0.50
51:z:44:THR:HB	51:z:47:THR:HG22	1.93	0.50
57:L:601:CDL:H252	39:m:95:TYR:HE2	1.76	0.50
17:Q:159:ARG:HH22	17:Q:171:ARG:HG2	1.77	0.50
33:g:120:LEU:HD21	33:g:169:GLU:OE1	2.12	0.50
40:n:39:ARG:NH2	48:w:1:UNK:O	2.45	0.50
4:D:212:ALA:HB1	4:D:230:ILE:HD11	1.94	0.50
6:F:301:SER:O	6:F:344:ILE:HD11	2.12	0.50
8:H:293:TYR:C	26:Z:68:LYS:HD2	2.37	0.50
12:L:512:LYS:HD2	34:h:41:TRP:NE1	2.27	0.50
23:W:45:GLU:HG2	23:W:46:ILE:N	2.27	0.50
23:W:57:LYS:O	23:W:61:ARG:HG2	2.11	0.50
2:B:32:PRO:HG3	2:B:59:ILE:CG2	2.42	0.50
5:E:80:ASN:OD1	5:E:81:TYR:N	2.45	0.50
7:G:501:VAL:O	7:G:505:VAL:HG23	2.12	0.50
7:G:679:ASP:O	7:G:683:LYS:HG2	2.10	0.50
13:M:206:PRO:CG	13:M:278:TYR:HE1	2.24	0.50
16:P:58:TYR:HE2	16:P:61:ASN:H	1.60	0.50
21:U:50:ARG:O	21:U:54:GLN:HG2	2.12	0.50
33:g:63:LEU:HD23	33:g:63:LEU:H	1.77	0.50
6:F:61:ILE:O	6:F:65:GLU:HG2	2.12	0.50
7:G:51:GLU:HG3	17:Q:25:THR:HG22	1.94	0.50
7:G:659:GLU:HB3	7:G:662:LYS:HE2	1.93	0.50
12:L:57:THR:HG22	29:c:79:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:50:ASP:HB3	23:W:71:VAL:HG21	1.93	0.50
23:W:86:TYR:CE2	23:W:100:TYR:HE2	2.30	0.50
29:c:89:SER:HA	29:c:92:TRP:CE2	2.47	0.50
46:t:91:GLY:O	46:t:95:VAL:HG23	2.11	0.50
2:B:119:ARG:HH22	3:C:178:THR:CG2	2.25	0.49
4:D:27:LEU:HD13	4:D:390:PHE:CE2	2.47	0.49
5:E:140:VAL:HG22	5:E:196:VAL:HG22	1.94	0.49
6:F:127:GLU:CD	6:F:135:ASP:HB2	2.37	0.49
7:G:440:VAL:HG11	7:G:460:LEU:HB2	1.94	0.49
13:M:324:TYR:CD1	13:M:330:LYS:HG3	2.47	0.49
17:Q:151:PRO:HB2	17:Q:153:LYS:HE3	1.94	0.49
7:G:78:HIS:CE1	7:G:296:GLU:OE2	2.65	0.49
7:G:653:VAL:HA	19:S:15:ARG:HH11	1.76	0.49
15:O:55:ILE:HD11	15:O:154:LEU:HB3	1.93	0.49
16:P:46:GLU:CG	16:P:222:ALA:HB1	2.42	0.49
2:B:139:GLU:HB2	9:I:190:PHE:CE2	2.47	0.49
5:E:190:ASN:OD1	5:E:239:ARG:NH2	2.36	0.49
6:F:143:PRO:HB2	6:F:180:ALA:HB2	1.95	0.49
4:D:234:LEU:HD21	4:D:338:GLU:HG3	1.94	0.49
7:G:58:ASN:HB2	17:Q:161:LEU:HD21	1.94	0.49
12:L:86:MET:HG2	12:L:317:MET:HE1	1.94	0.49
12:L:167:LYS:HA	52:L:602:PC7:O31	2.12	0.49
25:Y:58:LEU:HD21	46:t:109:LEU:HD23	1.94	0.49
50:y:43:ASP:OD1	51:z:17:LYS:NZ	2.40	0.49
50:y:43:ASP:OD1	51:z:17:LYS:HG3	2.12	0.49
5:E:149:ARG:NH2	6:F:377:ARG:HE	2.10	0.49
12:L:206:VAL:HG21	38:l:148:THR:HG22	1.94	0.49
13:M:1:MET:HB2	13:M:54:GLN:OE1	2.13	0.49
17:Q:123:SER:OG	17:Q:124:THR:HG23	2.12	0.49
22:V:129:VAL:HG22	49:x:280:LEU:HD22	1.94	0.49
25:Y:6:VAL:HG12	25:Y:7:ILE:HG23	1.93	0.49
25:Y:146:LEU:O	25:Y:149:PRO:HD2	2.13	0.49
21:U:119:ASN:OD1	21:U:120:PRO:HD2	2.13	0.49
44:r:75:ARG:HD2	44:r:76:ARG:HD3	1.93	0.49
51:z:46:LEU:HD23	51:z:68:VAL:HB	1.94	0.49
3:C:113:ARG:HH12	4:D:329:TYR:HE2	1.59	0.49
4:D:120:THR:HB	4:D:132:PHE:HA	1.94	0.49
5:E:147:PRO:HG2	6:F:130:PRO:O	2.11	0.49
10:J:9:SER:O	10:J:12:VAL:HG22	2.13	0.49
11:K:53:ARG:HD2	25:Y:80:ILE:HG21	1.93	0.49
12:L:25:VAL:HG13	29:c:46:ASN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:210:VAL:CG2	13:M:274:LYS:HG3	2.43	0.49
13:M:223:VAL:HG23	13:M:224:LEU:HD12	1.94	0.49
15:O:76:PRO:HD2	15:O:79:LYS:HD2	1.95	0.49
27:a:4:TYR:CD2	27:a:7:PRO:HD3	2.48	0.49
50:y:98:VAL:HG11	50:y:117:ASP:OD1	2.12	0.49
50:y:124:SER:OG	50:y:142:GLY:O	2.28	0.49
51:z:106:TYR:HE2	51:z:132:LYS:HG2	1.78	0.49
2:B:32:PRO:HD2	2:B:60:ILE:O	2.13	0.49
4:D:36:GLU:OE1	4:D:36:GLU:N	2.45	0.49
6:F:303:PRO:HD2	6:F:306:GLU:OE1	2.13	0.49
9:I:52:SER:O	9:I:55:GLU:HG3	2.13	0.49
12:L:346:LEU:HA	12:L:349:TYR:CD2	2.48	0.49
25:Y:178:ARG:HD2	25:Y:182:THR:O	2.11	0.49
7:G:129:MET:HE1	7:G:151:LEU:HD12	1.94	0.49
7:G:641:ASP:OD1	7:G:645:GLN:NE2	2.46	0.49
7:G:650:LEU:HA	7:G:653:VAL:HG22	1.95	0.49
16:P:88:ASP:HB3	16:P:92:ARG:NH1	2.28	0.49
21:U:87:LEU:O	21:U:91:GLU:HG2	2.13	0.49
22:V:92:ARG:NH2	22:V:119:GLU:OE2	2.39	0.49
4:D:167:ASP:OD2	26:Z:22:GLN:NE2	2.45	0.48
7:G:178:GLY:HA2	7:G:225:LEU:HD23	1.95	0.48
13:M:118:TYR:CD1	13:M:158:LEU:HD13	2.48	0.48
14:N:115:GLU:OE1	14:N:118:ARG:NE	2.46	0.48
16:P:178:ARG:NH1	61:P:601:HOH:O	2.20	0.48
8:H:173:ILE:O	8:H:176:PRO:HD2	2.13	0.48
12:L:285:ASN:HD21	12:L:347:ASN:ND2	2.11	0.48
23:W:39:ARG:HA	23:W:44:GLU:OE2	2.13	0.48
7:G:653:VAL:HA	19:S:15:ARG:NH1	2.29	0.48
10:J:128:LEU:HD12	14:N:96:LEU:HD22	1.95	0.48
14:N:108:LEU:HD12	14:N:192:PHE:HE2	1.79	0.48
16:P:17:ASN:ND2	17:Q:103:TRP:HB3	2.29	0.48
33:g:142:ILE:O	33:g:145:ARG:HG3	2.13	0.48
46:t:83:TYR:O	46:t:87:VAL:HG23	2.12	0.48
50:y:269:PHE:HE1	51:z:38:GLU:HA	1.78	0.48
7:G:505:VAL:HG13	7:G:510:VAL:HG22	1.95	0.48
8:H:293:TYR:C	26:Z:72:ARG:HH22	2.21	0.48
9:I:57:ASP:HB3	9:I:60:PHE:CD2	2.48	0.48
10:J:85:ILE:H	10:J:85:ILE:HD12	1.77	0.48
12:L:302:MET:O	12:L:305:VAL:HG12	2.13	0.48
26:Z:137:ASP:OD1	26:Z:138:VAL:HG23	2.14	0.48
34:h:26:LEU:HD12	34:h:27:ASN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:117:GLU:N	39:m:117:GLU:OE2	2.44	0.48
7:G:440:VAL:HG12	7:G:440:VAL:O	2.14	0.48
14:N:60:SER:HA	14:N:63:ILE:HG22	1.94	0.48
14:N:268:TYR:CE2	14:N:272:LEU:HD11	2.48	0.48
4:D:27:LEU:HD22	4:D:390:PHE:HZ	1.78	0.48
4:D:122:HIS:NE2	4:D:381:THR:HG23	2.28	0.48
6:F:43:LEU:HD23	6:F:48:ARG:HG2	1.95	0.48
7:G:86:ASN:O	7:G:88:ARG:HG2	2.14	0.48
8:H:291:LEU:HD11	26:Z:61:VAL:HG22	1.94	0.48
4:D:245:ARG:CG	44:r:114:GLU:HB3	2.44	0.48
6:F:49:ILE:HG23	6:F:261:THR:HG21	1.96	0.48
12:L:202:GLN:OE1	42:p:152:THR:HA	2.13	0.48
52:L:602:PC7:H211	52:L:602:PC7:H241	1.45	0.48
13:M:68:CYS:H	13:M:71:SER:HB2	1.79	0.48
13:M:222:GLY:O	13:M:226:LYS:HD3	2.14	0.48
13:M:242:SER:O	13:M:246:LYS:HG3	2.14	0.48
13:M:312:ILE:HG13	13:M:364:ASN:OD1	2.13	0.48
45:s:61:VAL:HG12	45:s:62:MET:HG3	1.96	0.48
50:y:117:ASP:HB3	50:y:138:SER:HA	1.95	0.48
1:A:110:GLU:HG2	10:J:136:LEU:HD13	1.96	0.48
4:D:24:HIS:HB2	4:D:73:TYR:OH	2.14	0.48
4:D:37:ILE:HD11	9:I:42:TRP:CZ3	2.49	0.48
8:H:19:LEU:HD21	8:H:228:LEU:HD13	1.96	0.48
8:H:265:ARG:HE	8:H:268:MET:HE3	1.78	0.48
10:J:127:ASP:OD1	10:J:128:LEU:N	2.47	0.48
13:M:109:ILE:HG23	13:M:230:VAL:HG21	1.95	0.48
13:M:419:ASP:O	13:M:422:SER:OG	2.15	0.48
16:P:81:PRO:HB2	16:P:82:GLU:OE1	2.14	0.48
16:P:261:ARG:HG3	16:P:344:VAL:C	2.39	0.48
30:d:20:GLY:O	30:d:24:ILE:HG12	2.14	0.48
49:x:75:ALA:HB1	49:x:94:PHE:CD1	2.48	0.48
2:B:42:VAL:HG21	4:D:73:TYR:CE2	2.49	0.48
3:C:87:ILE:HB	3:C:139:PHE:HB3	1.96	0.48
8:H:277:LEU:HD23	56:H:301:PTY:H132	1.96	0.48
10:J:50:MET:HE2	11:K:75:LEU:HD21	1.96	0.48
12:L:232:MET:SD	12:L:288:LYS:HB3	2.54	0.48
52:L:602:PC7:C2	38:l:60:TYR:HD1	2.26	0.48
13:M:241:ALA:O	13:M:244:ILE:HG22	2.13	0.48
57:M:502:CDL:H652	30:d:20:GLY:HA3	1.96	0.48
52:M:504:PC7:H62	52:M:504:PC7:H41	1.60	0.48
14:N:277:HIS:ND1	14:N:357:ILE:HD11	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:27:SER:O	31:e:35:ARG:NH1	2.44	0.48
32:f:59:VAL:HG13	52:z:301:PC7:H361	1.95	0.48
1:A:11:THR:OG1	26:Z:134:GLU:HG3	2.14	0.48
5:E:150:LEU:HD23	6:F:289:HIS:CE1	2.49	0.48
10:J:131:LEU:HB2	14:N:96:LEU:HD21	1.96	0.48
12:L:48:TYR:HD1	12:L:52:ILE:HD12	1.79	0.48
13:M:195:LYS:HE2	13:M:195:LYS:HA	1.96	0.48
14:N:63:ILE:HD11	14:N:72:SER:HB3	1.96	0.48
14:N:221:LEU:HD21	14:N:322:SER:HA	1.96	0.48
19:S:13:GLU:HG3	19:S:63:ARG:HB3	1.95	0.48
25:Y:4:ASN:O	25:Y:9:TYR:HE1	1.97	0.48
33:g:114:TYR:CZ	33:g:121:GLN:HG2	2.49	0.48
51:z:161:ALA:HB3	51:z:179:SER:HB2	1.96	0.48
9:I:150:GLU:HG2	18:R:42:THR:HA	1.95	0.47
10:J:65:LEU:HG	11:K:105:LEU:HD12	1.96	0.47
13:M:92:TYR:OH	57:M:502:CDL:OA7	2.30	0.47
13:M:229:ILE:HD11	13:M:287:VAL:HG12	1.95	0.47
57:M:502:CDL:H411	57:M:502:CDL:H381	1.45	0.47
16:P:88:ASP:OD1	16:P:126:ARG:HD3	2.14	0.47
28:b:4:UNK:O	28:b:8:UNK:C	2.62	0.47
29:c:81:ARG:NH1	42:p:84:HIS:O	2.46	0.47
4:D:33:MET:HG2	4:D:38:ILE:HG12	1.96	0.47
7:G:270:GLY:HA3	7:G:602:ASN:HD21	1.78	0.47
7:G:427:LEU:HA	7:G:430:VAL:HG22	1.96	0.47
8:H:147:CYS:O	8:H:150:LEU:HB2	2.14	0.47
8:H:156:ASN:OD1	26:Z:78:VAL:HG11	2.14	0.47
12:L:213:LEU:HD23	12:L:216:ILE:HD11	1.96	0.47
13:M:193:TRP:CD1	13:M:198:LEU:HD23	2.49	0.47
14:N:105:LEU:HD23	14:N:128:TYR:CZ	2.49	0.47
19:S:13:GLU:HG2	19:S:63:ARG:NH1	2.30	0.47
5:E:189:VAL:HG12	5:E:239:ARG:NH2	2.29	0.47
7:G:53:VAL:HG21	7:G:68:ALA:HB2	1.95	0.47
7:G:407:ASP:OD2	7:G:479:ASN:N	2.47	0.47
8:H:173:ILE:CD1	8:H:291:LEU:HD13	2.43	0.47
12:L:510:ALA:HB2	38:l:60:TYR:CE2	2.49	0.47
16:P:4:LEU:HD13	23:W:137:ALA:HA	1.97	0.47
16:P:125:THR:HG23	16:P:170:TYR:CE2	2.50	0.47
21:U:52:ILE:O	21:U:56:LYS:HG3	2.15	0.47
24:X:55:LYS:NZ	35:i:121:ARG:O	2.29	0.47
29:c:81:ARG:HD3	42:p:83:THR:O	2.14	0.47
40:n:50:ASN:HA	40:n:53:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:o:10:MET:HE3	41:o:12:ALA:HB3	1.96	0.47
4:D:267:GLN:O	4:D:271:GLU:HG2	2.14	0.47
8:H:90:LEU:HD22	27:a:27:GLN:HE21	1.78	0.47
13:M:35:LEU:O	13:M:39:VAL:HG23	2.14	0.47
17:Q:66:VAL:CG1	17:Q:95:ILE:HG23	2.44	0.47
50:y:198:VAL:HA	50:y:216:VAL:HG12	1.97	0.47
1:A:97:PHE:O	1:A:100:VAL:HG12	2.14	0.47
5:E:108:ARG:O	5:E:112:ILE:HG13	2.15	0.47
7:G:53:VAL:HG12	7:G:55:VAL:HG13	1.95	0.47
8:H:14:VAL:O	8:H:18:PHE:HD1	1.97	0.47
12:L:173:LYS:HA	12:L:176:ASP:OD2	2.15	0.47
14:N:158:LEU:O	14:N:162:VAL:HG23	2.14	0.47
21:U:51:ILE:HG22	21:U:90:LEU:HD11	1.96	0.47
22:V:98:GLU:HG2	44:r:103:LYS:NZ	2.30	0.47
28:b:6:UNK:O	28:b:8:UNK:N	2.48	0.47
42:p:104:ARG:HH12	42:p:156:TYR:HD2	1.58	0.47
47:u:2:UNK:O	47:u:4:UNK:N	2.48	0.47
49:x:142:GLU:OE1	51:z:132:LYS:NZ	2.47	0.47
3:C:142:GLU:OE2	4:D:395:ARG:NH2	2.47	0.47
13:M:287:VAL:CG2	13:M:305:TYR:HD2	2.27	0.47
18:R:21:ALA:O	18:R:25:LYS:HG3	2.14	0.47
20:T:97:GLU:OE2	40:n:81:ARG:NH1	2.47	0.47
23:W:34:LEU:C	23:W:38:HIS:HD1	2.21	0.47
3:C:14:TYR:HB3	44:r:109:THR:HB	1.96	0.47
4:D:81:HIS:NE2	4:D:103:ARG:HD3	2.30	0.47
5:E:176:THR:HG23	5:E:177:PHE:CD2	2.50	0.47
6:F:447:ILE:HG12	6:F:454:MET:HE1	1.96	0.47
8:H:287:ALA:O	8:H:291:LEU:HB2	2.15	0.47
8:H:290:SER:O	28:b:24:UNK:O	2.33	0.47
10:J:86:GLN:NE2	25:Y:89:ILE:HD12	2.28	0.47
11:K:77:ALA:HA	14:N:148:LEU:HD13	1.97	0.47
12:L:64:ASN:HB3	12:L:67:TYR:HB2	1.95	0.47
52:L:602:PC7:H191	52:L:602:PC7:H222	1.33	0.47
13:M:418:LEU:HD23	33:g:61:LEU:HD13	1.96	0.47
14:N:197:LYS:O	14:N:201:LEU:HG	2.14	0.47
16:P:5:LYS:HE2	23:W:113:ARG:HH21	1.79	0.47
16:P:177:ILE:HD11	16:P:228:ILE:HG13	1.97	0.47
21:U:100:ASP:OD1	21:U:101:ALA:N	2.47	0.47
25:Y:59:MET:HG3	25:Y:107:GLY:HA3	1.96	0.47
26:Z:26:PRO:HD2	26:Z:26:PRO:O	2.14	0.47
27:a:47:LEU:HD23	27:a:50:ARG:CD	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:30:ASP:OD1	29:c:31:PHE:N	2.48	0.47
32:f:27:PRO:O	32:f:104:ASN:ND2	2.48	0.47
45:s:84:PHE:O	45:s:88:TYR:HB2	2.15	0.47
50:y:267:LYS:O	50:y:272:MET:HE3	2.13	0.47
51:z:111:SER:OG	51:z:114:SER:HB2	2.14	0.47
2:B:94:GLU:O	2:B:96:LYS:HG2	2.15	0.47
5:E:149:ARG:HH21	6:F:377:ARG:HE	1.62	0.47
16:P:303:TYR:HA	16:P:306:GLU:HG2	1.95	0.47
25:Y:189:LEU:HD13	35:i:35:ARG:HH12	1.80	0.47
6:F:118:PRO:O	6:F:246:CYS:HB3	2.15	0.47
9:I:89:TYR:O	9:I:92:SER:OG	2.21	0.47
17:Q:64:ARG:HD2	23:W:131:LEU:HD13	1.97	0.47
19:S:15:ARG:HH21	19:S:61:THR:HG21	1.79	0.47
56:Y:301:PTY:H422	56:Y:301:PTY:H392	1.65	0.47
45:s:5:LEU:HD21	57:t:201:CDL:H121	1.97	0.47
49:x:61:ILE:HD13	50:y:264:GLU:HG3	1.97	0.47
6:F:419:MET:CG	7:G:164:ARG:HD3	2.43	0.47
52:L:602:PC7:H171	52:L:602:PC7:H142	1.45	0.47
13:M:193:TRP:HD1	13:M:198:LEU:HB3	1.80	0.47
18:R:35:PHE:HB2	18:R:38:ASP:OD2	2.14	0.47
22:V:76:PRO:HG2	22:V:136:TRP:NE1	2.30	0.47
35:i:101:ARG:HH22	35:i:109:ALA:HB2	1.79	0.47
2:B:160:LEU:HD13	16:P:60:CYS:O	2.15	0.46
8:H:265:ARG:NE	8:H:268:MET:HE3	2.29	0.46
9:I:152:ARG:HB3	9:I:154:ASP:OD1	2.15	0.46
10:J:140:LEU:O	10:J:144:LEU:HD23	2.14	0.46
13:M:24:LYS:HG2	33:g:62:TRP:CH2	2.50	0.46
13:M:199:VAL:HG22	13:M:202:HIS:CE1	2.50	0.46
21:U:47:VAL:HG21	21:U:117:ILE:CG2	2.45	0.46
49:x:157:ILE:HG13	49:x:214:ILE:HG23	1.96	0.46
52:z:301:PC7:H201	52:z:301:PC7:H171	1.70	0.46
4:D:106:PHE:HZ	4:D:149:VAL:HG11	1.81	0.46
12:L:66:VAL:HB	12:L:73:VAL:HG12	1.98	0.46
12:L:326:PHE:HA	12:L:447:MET:HE2	1.98	0.46
12:L:370:LEU:HD11	12:L:481:ALA:HB2	1.97	0.46
16:P:212:LYS:HE3	16:P:246:THR:HG22	1.96	0.46
56:m:202:PTY:H382	56:m:202:PTY:H352	1.52	0.46
42:p:19:ILE:HG22	42:p:23:LYS:HE2	1.96	0.46
43:q:150:TRP:CZ2	43:q:153:PRO:HD3	2.50	0.46
52:A:201:PC7:H362	52:A:201:PC7:H332	1.59	0.46
9:I:56:GLN:HB3	22:V:44:LYS:HZ1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:284:ALA:HB3	12:L:290:VAL:HG22	1.98	0.46
56:M:501:PTY:H202	56:M:501:PTY:H172	1.74	0.46
24:X:10:GLU:O	24:X:14:MET:HG2	2.16	0.46
50:y:67:PRO:CB	50:y:97:ILE:HD12	2.45	0.46
3:C:92:TYR:CB	3:C:95:ARG:HD2	2.45	0.46
7:G:654:ALA:HB1	7:G:656:HIS:NE2	2.30	0.46
8:H:284:LEU:HA	8:H:287:ALA:HB3	1.97	0.46
12:L:434:ALA:O	12:L:438:ILE:HG12	2.15	0.46
19:S:58:ALA:HB1	19:S:74:ILE:HG13	1.98	0.46
5:E:74:MET:HE1	5:E:112:ILE:CG2	2.44	0.46
7:G:42:ASP:OD1	7:G:43:LYS:N	2.48	0.46
16:P:13:ASN:OD1	16:P:14:ALA:N	2.48	0.46
16:P:125:THR:HG23	16:P:170:TYR:HE2	1.81	0.46
24:X:69:LYS:O	24:X:73:LYS:HG2	2.16	0.46
50:y:302:THR:O	50:y:304:LEU:N	2.46	0.46
1:A:25:GLN:NE2	1:A:29:ASN:HD22	2.14	0.46
2:B:123:ARG:O	16:P:70:GLN:NE2	2.43	0.46
8:H:145:ILE:O	8:H:149:ILE:HG13	2.15	0.46
10:J:62:LEU:HD11	11:K:101:THR:HG21	1.98	0.46
13:M:82:PHE:CZ	13:M:99:ILE:HD13	2.50	0.46
26:Z:71:ASN:HD22	26:Z:71:ASN:C	2.21	0.46
26:Z:86:HIS:CE1	32:f:5:LYS:HD2	2.51	0.46
35:i:55:ASN:HB3	35:i:58:GLU:HG2	1.97	0.46
4:D:260:ASP:O	4:D:264:VAL:HG23	2.16	0.46
7:G:95:GLU:OE1	7:G:113:LYS:HB2	2.16	0.46
8:H:10:LEU:HB3	8:H:11:PRO:HD3	1.97	0.46
14:N:268:TYR:HE1	14:N:291:ILE:HG23	1.81	0.46
49:x:263:GLN:O	49:x:267:MET:HG3	2.16	0.46
2:B:76:THR:HG21	4:D:50:ARG:HG2	1.96	0.46
6:F:98:GLY:HA2	6:F:358:GLY:HA2	1.96	0.46
55:F:500:FMN:N1	55:F:500:FMN:H3'	2.31	0.46
12:L:346:LEU:HB3	12:L:415:GLN:OE1	2.15	0.46
13:M:62:TRP:CH2	13:M:115:LEU:HB3	2.51	0.46
16:P:248:THR:HG22	16:P:251:GLN:OE1	2.15	0.46
34:h:69:GLU:HG2	42:p:141:LEU:HD21	1.98	0.46
35:i:60:VAL:HG11	35:i:81:ASN:OD1	2.16	0.46
56:m:201:PTY:H142	56:m:201:PTY:H172	1.46	0.46
40:n:22:GLY:HA2	40:n:70:LEU:HD21	1.97	0.46
50:y:163:LYS:HD2	50:y:165:ARG:NH2	2.31	0.46
1:A:98:TYR:CZ	1:A:102:ILE:HD11	2.50	0.46
6:F:282:LYS:HE3	6:F:360:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:393:CYS:HB2	53:F:501:SF4:S3	2.55	0.46
13:M:82:PHE:HZ	13:M:99:ILE:HD13	1.79	0.46
16:P:6:PRO:HB3	16:P:16:ARG:HH11	1.81	0.46
26:Z:72:ARG:HG3	32:f:10:TYR:CD2	2.51	0.46
1:A:111:VAL:O	1:A:115:ILE:HG13	2.16	0.46
1:A:113:TYR:O	1:A:116:PRO:HD2	2.16	0.46
1:A:152:TRP:HZ2	8:H:274:TRP:CD1	2.34	0.46
3:C:16:ALA:CB	3:C:21:LYS:HE3	2.45	0.46
3:C:74:ARG:HH22	49:x:279:LEU:HD21	1.81	0.46
4:D:72:ASP:OD2	4:D:392:GLU:HG3	2.15	0.46
57:L:601:CDL:H371	57:L:601:CDL:H532	1.97	0.46
16:P:207:ASN:ND2	16:P:308:VAL:HG23	2.31	0.46
23:W:22:LYS:HB3	23:W:76:ILE:HD13	1.98	0.46
6:F:403:ILE:HG12	6:F:406:ARG:HH21	1.81	0.45
7:G:144:ASP:HB2	7:G:244:LEU:HD13	1.97	0.45
8:H:16:VAL:HG13	8:H:224:TYR:HB2	1.98	0.45
8:H:18:PHE:HE2	8:H:44:ILE:HG13	1.81	0.45
12:L:141:TRP:O	12:L:144:ILE:HG12	2.17	0.45
52:L:602:PC7:H263	13:M:391:PHE:HZ	1.81	0.45
57:M:502:CDL:H722	57:M:502:CDL:H751	1.51	0.45
14:N:41:ILE:HD11	32:f:60:MET:HE1	1.98	0.45
52:N:402:PC7:H122	52:N:402:PC7:H152	1.48	0.45
19:S:57:GLN:HB3	19:S:75:GLU:OE2	2.16	0.45
23:W:59:LYS:O	23:W:62:VAL:HG12	2.16	0.45
26:Z:130:LEU:HD21	31:e:49:CYS:HA	1.97	0.45
35:i:109:ALA:O	35:i:113:VAL:HG23	2.16	0.45
57:t:201:CDL:H812	57:t:201:CDL:H841	1.63	0.45
49:x:237:SER:HB2	49:x:240:ARG:NE	2.31	0.45
3:C:215:LEU:O	3:C:217:ARG:HD2	2.16	0.45
4:D:270:ARG:HD2	26:Z:35:ILE:O	2.16	0.45
7:G:494:ARG:NH1	7:G:495:GLU:OE2	2.48	0.45
8:H:74:PRO:HG3	8:H:219:PHE:CE2	2.51	0.45
12:L:85:THR:HG22	12:L:321:VAL:HG11	1.98	0.45
57:L:601:CDL:H362	57:L:601:CDL:H392	1.82	0.45
13:M:270:ILE:HG22	13:M:333:PHE:HE1	1.81	0.45
52:N:403:PC7:H471	52:N:403:PC7:H442	1.65	0.45
38:l:130:ASP:OD1	38:l:132:SER:OG	2.30	0.45
41:o:67:PHE:O	41:o:71:VAL:HG23	2.16	0.45
57:t:201:CDL:H532	57:t:201:CDL:H821	1.98	0.45
52:A:201:PC7:H121	52:A:201:PC7:H31	1.79	0.45
4:D:186:ARG:NH2	4:D:189:GLU:OE2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:80:ARG:CZ	7:G:295:GLU:HB3	2.45	0.45
7:G:673:TYR:O	7:G:677:VAL:HG22	2.17	0.45
57:L:601:CDL:H572	25:Y:155:VAL:HG22	1.97	0.45
14:N:171:ALA:N	14:N:220:SER:OG	2.48	0.45
19:S:63:ARG:HG3	19:S:69:GLU:HG2	1.99	0.45
27:a:47:LEU:O	27:a:50:ARG:HG2	2.16	0.45
34:h:66:PHE:CE2	34:h:70:ILE:HD11	2.52	0.45
42:p:149:SER:OG	42:p:152:THR:OG1	2.33	0.45
1:A:95:VAL:O	1:A:99:ILE:HG12	2.16	0.45
5:E:194:ILE:HG12	5:E:214:LEU:HD21	1.99	0.45
7:G:628:ARG:NH1	7:G:637:GLN:HG3	2.30	0.45
8:H:153:ARG:HD3	8:H:159:PRO:HA	1.99	0.45
9:I:150:GLU:OE2	18:R:57:LYS:NZ	2.50	0.45
12:L:249:THR:HG22	12:L:320:LEU:HD11	1.97	0.45
18:R:125:TRP:CD1	18:R:125:TRP:H	2.34	0.45
23:W:89:MET:HG3	23:W:89:MET:O	2.16	0.45
24:X:98:LEU:H	24:X:98:LEU:HD23	1.81	0.45
1:A:112:VAL:CG1	10:J:53:ILE:HD12	2.40	0.45
1:A:125:TYR:HE2	10:J:123:SER:HA	1.82	0.45
3:C:18:ASP:OD2	44:r:108:LYS:HB2	2.15	0.45
3:C:27:TYR:HB3	44:r:91:PHE:HZ	1.81	0.45
7:G:152:GLN:NE2	53:G:802:SF4:S2	2.89	0.45
7:G:643:GLN:HE21	7:G:647:ARG:NE	2.15	0.45
8:H:55:ALA:HA	8:H:214:LEU:HD21	1.99	0.45
12:L:228:LEU:HG	12:L:243:HIS:CE1	2.51	0.45
52:N:403:PC7:H73	52:N:403:PC7:H42	1.58	0.45
37:k:40:ALA:O	37:k:44:VAL:HG23	2.16	0.45
41:o:21:ASP:O	41:o:38:LYS:NZ	2.50	0.45
50:y:116:GLY:O	50:y:118:VAL:N	2.50	0.45
51:z:181:SER:HB3	51:z:182:PRO:HD3	1.98	0.45
52:z:301:PC7:H321	52:z:301:PC7:H352	1.55	0.45
1:A:57:VAL:O	1:A:61:VAL:HG22	2.17	0.45
4:D:134:TRP:HA	8:H:32:ARG:NH2	2.30	0.45
5:E:158:GLU:O	5:E:162:LYS:HG2	2.16	0.45
6:F:65:GLU:OE2	6:F:70:TRP:HB2	2.17	0.45
20:T:52:VAL:HG13	20:T:90:LEU:HD21	1.99	0.45
24:X:80:LEU:HD23	24:X:80:LEU:HA	1.78	0.45
3:C:76:HIS:HA	22:V:123:GLU:OE1	2.16	0.45
3:C:146:MET:HA	3:C:170:PRO:HD2	1.98	0.45
4:D:195:THR:HG23	4:D:259:TYR:OH	2.15	0.45
16:P:340:ARG:HG3	16:P:344:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:54:LEU:HD23	23:W:57:LYS:HZ1	1.82	0.45
41:o:8:PRO:HG2	41:o:66:GLU:OE2	2.16	0.45
3:C:52:VAL:HA	4:D:89:GLN:NE2	2.32	0.45
3:C:99:PHE:CE2	3:C:122:GLU:HG3	2.52	0.45
5:E:61:ASP:OD1	5:E:62:PHE:N	2.50	0.45
7:G:192:THR:HG22	7:G:209:ILE:HD11	1.99	0.45
11:K:106:ALA:HB1	14:N:110:LYS:NZ	2.32	0.45
18:R:51:LEU:HD22	18:R:56:SER:HB2	1.99	0.45
21:U:85:GLU:HG3	23:W:53:ARG:CD	2.46	0.45
22:V:38:ASN:O	22:V:39:ARG:HG2	2.16	0.45
30:d:59:LEU:HD23	30:d:80:PHE:HB3	1.98	0.45
4:D:7:SER:C	4:D:8:LYS:HD3	2.42	0.45
4:D:76:MET:N	4:D:76:MET:SD	2.89	0.45
11:K:53:ARG:HB3	11:K:126:LEU:O	2.17	0.45
57:N:401:CDL:H252	57:N:401:CDL:H221	1.70	0.45
15:O:62:TYR:HE1	15:O:167:PRO:HA	1.82	0.45
16:P:97:ARG:HD2	43:q:136:TRP:CD1	2.52	0.45
29:c:57:ILE:O	29:c:61:VAL:HG23	2.17	0.45
39:m:30:ARG:CZ	39:m:49:PRO:HB3	2.46	0.45
49:x:89:LYS:HG2	49:x:222:TYR:CZ	2.52	0.45
2:B:62:ARG:HG2	2:B:67:GLN:HB2	1.99	0.45
5:E:78:PRO:HG2	5:E:81:TYR:HB2	1.99	0.45
6:F:372:ILE:HD13	6:F:446:LEU:HD21	1.98	0.45
8:H:112:LEU:HD11	10:J:67:LEU:HD22	1.99	0.45
8:H:124:PHE:O	8:H:128:LEU:HG	2.17	0.45
12:L:185:TYR:CE1	13:M:380:GLU:HG2	2.52	0.45
12:L:516:VAL:HG21	34:h:41:TRP:HB3	1.99	0.45
13:M:268:LYS:C	39:m:70:ARG:HH21	2.23	0.45
56:M:501:PTY:H241	33:g:75:PHE:HB3	1.98	0.45
33:g:58:ARG:NH1	33:g:60:LYS:HA	2.32	0.45
33:g:120:LEU:HD23	33:g:120:LEU:HA	1.58	0.45
41:o:77:GLU:HB3	41:o:81:ARG:NH1	2.32	0.45
6:F:219:ALA:HB2	6:F:231:PRO:HG3	1.99	0.44
7:G:653:VAL:HG12	19:S:15:ARG:NH1	2.33	0.44
8:H:134:MET:SD	8:H:190:LYS:NZ	2.89	0.44
13:M:94:ALA:O	13:M:98:LEU:HD23	2.16	0.44
13:M:197:PRO:HB2	13:M:281:ILE:HG12	1.99	0.44
56:M:501:PTY:H122	56:M:501:PTY:H151	1.63	0.44
20:T:112:ALA:O	20:T:116:VAL:HG23	2.17	0.44
21:U:66:VAL:HG13	21:U:66:VAL:O	2.17	0.44
25:Y:146:LEU:HD23	39:m:79:TRP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:61:VAL:O	26:Z:65:ARG:HG2	2.17	0.44
29:c:25:HIS:CE1	33:g:29:PRO:HA	2.53	0.44
30:d:62:LEU:HD22	30:d:80:PHE:HB2	1.99	0.44
42:p:68:GLU:O	42:p:72:ILE:HG13	2.16	0.44
4:D:125:ASP:HB3	4:D:380:VAL:CG1	2.46	0.44
6:F:221:ILE:O	6:F:225:GLU:HG3	2.17	0.44
7:G:164:ARG:NH2	44:r:67:ILE:H	2.15	0.44
8:H:286:LEU:O	8:H:290:SER:CB	2.65	0.44
12:L:219:SER:OG	12:L:248:VAL:O	2.26	0.44
12:L:258:LEU:HD12	12:L:258:LEU:O	2.17	0.44
13:M:245:VAL:HG23	42:p:114:ASN:OD1	2.17	0.44
13:M:416:SER:HB2	40:n:107:ALA:HB2	2.00	0.44
57:N:401:CDL:H531	57:N:401:CDL:H562	1.65	0.44
16:P:305:GLU:O	16:P:308:VAL:HG12	2.16	0.44
21:U:114:ASN:HA	21:U:117:ILE:HG12	1.99	0.44
25:Y:148:GLN:NE2	45:s:11:TRP:NE1	2.64	0.44
3:C:58:THR:HG23	3:C:115:ARG:HG2	1.99	0.44
7:G:443:LYS:NZ	61:G:906:HOH:O	2.48	0.44
10:J:39:GLN:HG3	10:J:51:ALA:O	2.18	0.44
13:M:250:LEU:O	13:M:254:ILE:HG23	2.17	0.44
13:M:416:SER:HB3	40:n:106:PRO:HB2	2.00	0.44
14:N:136:GLY:O	14:N:140:ILE:HG12	2.18	0.44
21:U:48:GLU:HA	21:U:51:ILE:HG12	1.99	0.44
26:Z:130:LEU:HB3	31:e:52:ARG:HH22	1.81	0.44
29:c:50:GLY:N	33:g:36:GLU:OE2	2.45	0.44
33:g:108:MET:HE3	42:p:73:PHE:CE1	2.53	0.44
35:i:101:ARG:HH22	35:i:109:ALA:CB	2.30	0.44
56:m:202:PTY:H201	56:m:202:PTY:H171	1.85	0.44
2:B:81:MET:O	2:B:81:MET:HG3	2.17	0.44
3:C:31:TYR:OH	22:V:84:ALA:HB1	2.18	0.44
3:C:48:ALA:HB3	3:C:51:SER:O	2.18	0.44
3:C:92:TYR:HB2	3:C:95:ARG:HD2	1.99	0.44
4:D:174:ARG:HD2	26:Z:30:PHE:CE1	2.52	0.44
5:E:189:VAL:HG23	6:F:133:CYS:SG	2.58	0.44
7:G:496:ALA:HB3	7:G:686:ARG:HH22	1.83	0.44
8:H:278:LEU:HB3	8:H:279:PRO:HD3	2.00	0.44
12:L:139:ILE:HG12	13:M:360:PRO:HB3	1.99	0.44
12:L:285:ASN:HB3	40:n:77:GLU:CD	2.42	0.44
57:L:601:CDL:H201	57:L:601:CDL:H171	1.56	0.44
14:N:206:ASN:HB3	35:i:49:ARG:HG2	1.98	0.44
17:Q:62:TYR:HA	17:Q:142:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:26:ALA:HA	19:S:29:ARG:HE	1.83	0.44
25:Y:4:ASN:OD1	25:Y:5:TYR:N	2.47	0.44
57:t:201:CDL:H551	57:t:201:CDL:H661	2.00	0.44
50:y:182:HIS:CG	50:y:183:ALA:H	2.36	0.44
52:z:301:PC7:H132	52:z:301:PC7:H161	1.80	0.44
5:E:70:VAL:HG13	5:E:89:LEU:CD2	2.47	0.44
7:G:142:ILE:HG23	9:I:131:ILE:HD12	1.99	0.44
7:G:377:LEU:HB3	7:G:535:PHE:CE1	2.53	0.44
11:K:83:ASP:OD1	11:K:84:MET:N	2.51	0.44
52:M:503:PC7:H483	52:M:503:PC7:H452	1.84	0.44
14:N:105:LEU:HD13	14:N:192:PHE:CD1	2.53	0.44
16:P:343:ARG:HG2	16:P:348:ASP:OD1	2.17	0.44
33:g:28:HIS:CE1	33:g:33:PHE:HD1	2.36	0.44
42:p:15:GLU:O	42:p:19:ILE:HG13	2.18	0.44
45:s:88:TYR:O	45:s:92:SER:HB3	2.18	0.44
3:C:37:PRO:HB2	22:V:138:VAL:HG11	1.98	0.44
4:D:111:ARG:HA	4:D:335:PRO:HG3	1.99	0.44
4:D:311:ILE:HG12	7:G:152:GLN:HG2	2.00	0.44
4:D:364:LEU:HD22	4:D:393:ILE:HD13	2.00	0.44
9:I:199:GLU:HG2	43:q:130:TYR:O	2.18	0.44
10:J:108:PRO:HD2	11:K:76:TYR:CE2	2.52	0.44
12:L:141:TRP:CZ2	12:L:179:LEU:HD11	2.52	0.44
12:L:286:ASP:O	12:L:290:VAL:HG23	2.18	0.44
13:M:78:CYS:CB	13:M:223:VAL:HG11	2.47	0.44
14:N:36:LYS:NZ	14:N:66:PHE:O	2.44	0.44
14:N:49:ASP:HB3	14:N:51:PRO:HD2	1.98	0.44
20:T:53:ILE:O	20:T:57:LYS:HG3	2.18	0.44
7:G:73:PRO:HB2	7:G:89:MET:HG3	2.00	0.44
12:L:511:ARG:HH12	38:l:67:MET:CE	2.24	0.44
13:M:354:LEU:HD22	13:M:359:PHE:CE2	2.53	0.44
16:P:56:CYS:HB2	16:P:79:LEU:HD23	2.00	0.44
25:Y:159:ALA:HB3	25:Y:160:PRO:HD3	2.00	0.44
40:n:10:PRO:HG2	40:n:13:LEU:HD12	2.00	0.44
57:t:201:CDL:H151	57:t:201:CDL:H122	1.45	0.44
49:x:209:GLU:HA	49:x:213:VAL:HG22	2.00	0.44
49:x:209:GLU:O	49:x:213:VAL:HG22	2.18	0.44
1:A:129:VAL:HG22	52:N:403:PC7:H381	2.00	0.44
4:D:31:LEU:HD22	4:D:38:ILE:HD13	1.99	0.44
5:E:164:LEU:HD11	5:E:223:LEU:HD13	1.99	0.44
6:F:283:LEU:O	6:F:360:ALA:HB3	2.17	0.44
7:G:44:MET:HE2	7:G:57:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:64:PRO:O	9:I:65:LYS:HG2	2.18	0.44
13:M:303:VAL:O	13:M:307:ILE:HG12	2.18	0.44
21:U:41:PHE:CZ	21:U:120:PRO:HB3	2.52	0.44
21:U:51:ILE:HG13	21:U:52:ILE:N	2.33	0.44
21:U:70:SER:HB3	21:U:76:LEU:CD1	2.48	0.44
24:X:61:MET:HE1	24:X:69:LYS:NZ	2.32	0.44
43:q:143:ASN:HD22	43:q:143:ASN:C	2.18	0.44
49:x:103:ASN:OD1	49:x:104:THR:N	2.38	0.44
3:C:95:ARG:HG2	17:Q:38:ASP:OD1	2.17	0.44
4:D:21:PRO:HD3	8:H:202:GLU:HG3	1.99	0.44
5:E:142:ILE:HG13	5:E:194:ILE:HG22	1.99	0.44
57:L:601:CDL:H262	13:M:200:PRO:HG3	2.00	0.44
20:T:84:VAL:HG13	40:n:20:ARG:CG	2.45	0.44
23:W:21:GLN:HE22	23:W:25:ASN:HD21	1.66	0.44
25:Y:110:PHE:CZ	46:t:107:ARG:HG2	2.45	0.44
33:g:145:ARG:HG2	33:g:167:TYR:CE1	2.52	0.44
56:m:201:PTY:H172	56:m:201:PTY:H202	1.51	0.44
7:G:59:PHE:HA	7:G:63:GLN:OE1	2.17	0.43
8:H:235:ASN:C	8:H:235:ASN:HD22	2.25	0.43
52:L:602:PC7:H402	52:L:602:PC7:H372	1.63	0.43
13:M:360:PRO:HA	13:M:365:PHE:CG	2.53	0.43
57:N:401:CDL:H112	57:N:401:CDL:HA4	1.63	0.43
16:P:149:ASP:OD1	16:P:150:VAL:N	2.51	0.43
18:R:83:VAL:HG12	18:R:102:LEU:HD21	2.00	0.43
49:x:105:ILE:HG12	49:x:133:THR:HB	1.99	0.43
51:z:81:LEU:HD12	51:z:102:SER:HA	2.00	0.43
51:z:91:LYS:O	51:z:109:SER:OG	2.36	0.43
2:B:132:PRO:HD3	9:I:193:SER:HA	1.99	0.43
4:D:32:GLU:OE2	4:D:40:ARG:NH2	2.51	0.43
6:F:72:MET:HG3	6:F:76:LEU:CD1	2.48	0.43
6:F:124:ASN:ND2	6:F:215:GLY:O	2.51	0.43
6:F:304:LEU:HD21	6:F:325:ILE:HG21	1.99	0.43
7:G:270:GLY:HA3	7:G:602:ASN:ND2	2.33	0.43
7:G:335:ASP:O	7:G:339:THR:HG23	2.18	0.43
56:L:603:PTY:H171	56:L:603:PTY:H201	1.69	0.43
13:M:415:ALA:HB1	13:M:419:ASP:HB2	2.00	0.43
14:N:155:SER:O	14:N:160:THR:HG21	2.18	0.43
34:h:6:TYR:CD2	39:m:61:PRO:HG3	2.53	0.43
39:m:51:ASP:OD2	49:x:208:TYR:HB3	2.17	0.43
39:m:113:ASN:HA	42:p:117:LYS:HE2	1.99	0.43
49:x:144:HIS:HB3	49:x:161:ARG:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:y:236:ILE:HG13	50:y:237:ARG:N	2.33	0.43
1:A:153:ARG:HE	9:I:42:TRP:CG	2.36	0.43
4:D:336:LYS:HE2	4:D:387:ASP:HB3	2.01	0.43
6:F:260:PRO:HB2	6:F:264:ARG:HH12	1.83	0.43
6:F:388:GLY:HA2	6:F:394:ARG:HB2	1.99	0.43
7:G:313:ARG:HG2	7:G:617:LEU:HD23	2.01	0.43
7:G:318:LEU:HB2	7:G:587:VAL:HB	2.00	0.43
7:G:675:LYS:O	7:G:678:LYS:HG3	2.17	0.43
56:H:301:PTY:H443	56:H:301:PTY:H411	1.76	0.43
13:M:272:LEU:HA	13:M:275:ILE:HD12	2.00	0.43
14:N:13:ASN:O	14:N:17:ILE:HG13	2.18	0.43
14:N:60:SER:O	14:N:63:ILE:HG22	2.17	0.43
14:N:170:VAL:HG12	14:N:246:ILE:HG23	1.99	0.43
16:P:9:LEU:HD12	16:P:28:VAL:HG22	2.00	0.43
31:e:59:LYS:HD2	31:e:59:LYS:HA	1.81	0.43
51:z:10:TRP:CZ2	51:z:50:GLN:HA	2.54	0.43
1:A:120:THR:HG22	10:J:115:LEU:HA	2.00	0.43
3:C:20:ILE:HG23	3:C:110:LEU:HD23	1.99	0.43
5:E:86:MET:HE2	5:E:120:VAL:HG22	2.01	0.43
7:G:164:ARG:HH21	44:r:67:ILE:H	1.65	0.43
7:G:624:TRP:NE1	7:G:643:GLN:OE1	2.51	0.43
8:H:141:ILE:O	8:H:145:ILE:HG12	2.18	0.43
11:K:74:PHE:CE2	11:K:89:PHE:CE2	3.07	0.43
17:Q:122:ARG:NH2	61:Q:202:HOH:O	2.51	0.43
24:X:9:HIS:H	24:X:9:HIS:CD2	2.37	0.43
25:Y:45:LYS:HE2	25:Y:51:TYR:CZ	2.53	0.43
25:Y:127:THR:HA	25:Y:130:MET:HE3	1.99	0.43
33:g:58:ARG:HD3	40:n:108:TYR:OH	2.18	0.43
7:G:351:ALA:HB2	7:G:369:PHE:CE2	2.54	0.43
12:L:512:LYS:O	12:L:516:VAL:HG23	2.19	0.43
57:d:101:CDL:H251	57:d:101:CDL:H221	1.76	0.43
45:s:25:ARG:HD3	45:s:25:ARG:HA	1.76	0.43
4:D:300:ARG:O	4:D:303:MET:HG2	2.19	0.43
7:G:404:GLU:OE1	7:G:429:LYS:HD2	2.18	0.43
8:H:74:PRO:HB3	8:H:218:VAL:CG2	2.47	0.43
13:M:268:LYS:O	39:m:70:ARG:NH2	2.45	0.43
52:M:503:PC7:H352	52:M:503:PC7:H381	1.75	0.43
14:N:161:TYR:O	14:N:165:LEU:HG	2.18	0.43
23:W:34:LEU:HD22	23:W:38:HIS:CE1	2.54	0.43
25:Y:45:LYS:HD2	25:Y:118:GLU:OE1	2.19	0.43
2:B:66:ARG:HH22	8:H:204:VAL:HG11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:63:GLU:HG2	12:L:64:ASN:OD1	2.19	0.43
12:L:393:GLY:H	38:l:94:GLU:CD	2.26	0.43
13:M:270:ILE:HD13	39:m:70:ARG:HD3	2.00	0.43
56:M:501:PTY:H252	56:M:501:PTY:H222	1.58	0.43
14:N:70:PHE:CZ	14:N:74:PHE:HE2	2.37	0.43
20:T:80:SER:OG	40:n:12:LYS:NZ	2.29	0.43
21:U:87:LEU:HD13	21:U:103:ILE:HG12	2.01	0.43
2:B:112:HIS:CD2	2:B:119:ARG:HE	2.36	0.43
3:C:160:VAL:HG23	3:C:161:LEU:N	2.34	0.43
4:D:133:LEU:HG	8:H:31:GLN:NE2	2.33	0.43
7:G:203:GLY:HA3	7:G:428:ARG:NH1	2.34	0.43
12:L:118:LEU:HD22	12:L:241:LEU:CD1	2.47	0.43
12:L:510:ALA:HB2	38:l:60:TYR:CD2	2.53	0.43
57:M:502:CDL:H471	30:d:15:MET:HG3	2.00	0.43
14:N:39:PHE:CD1	14:N:76:VAL:HG21	2.54	0.43
57:N:401:CDL:H561	57:N:401:CDL:H591	1.77	0.43
16:P:286:ARG:HH22	16:P:296:GLY:N	2.17	0.43
25:Y:99:LYS:HD2	45:s:2:VAL:HG13	2.01	0.43
2:B:30:MET:O	2:B:32:PRO:HD3	2.19	0.43
4:D:20:HIS:HB2	4:D:21:PRO:HD3	2.01	0.43
4:D:52:THR:HG23	4:D:67:TYR:CD1	2.54	0.43
7:G:179:PRO:O	7:G:246:LYS:HD2	2.18	0.43
7:G:595:GLU:HG2	7:G:614:VAL:HG23	2.01	0.43
12:L:285:ASN:ND2	61:L:701:HOH:O	2.36	0.43
18:R:44:ALA:HB1	43:q:146:LYS:O	2.19	0.43
20:T:47:THR:O	20:T:51:ARG:HG3	2.18	0.43
24:X:24:LYS:HE3	24:X:24:LYS:HB3	1.66	0.43
40:n:21:THR:HB	40:n:70:LEU:HD13	2.00	0.43
42:p:24:LEU:HD23	42:p:24:LEU:HA	1.91	0.43
2:B:56:ARG:O	8:H:38:VAL:HG22	2.19	0.43
2:B:151:LYS:NZ	61:B:601:HOH:O	2.42	0.43
4:D:192:GLU:OE1	9:I:85:ARG:HG3	2.18	0.43
4:D:302:GLN:HA	4:D:305:GLN:HG2	2.01	0.43
6:F:406:ARG:NE	7:G:167:GLU:OE2	2.51	0.43
7:G:308:GLY:O	7:G:576:HIS:NE2	2.51	0.43
8:H:261:LEU:CD2	9:I:83:ILE:HD12	2.49	0.43
12:L:128:LEU:HD11	12:L:141:TRP:HE3	1.84	0.43
14:N:84:PHE:CZ	52:N:403:PC7:H472	2.54	0.43
14:N:262:PHE:HD2	57:N:401:CDL:H122	1.83	0.43
15:O:62:TYR:OH	15:O:166:GLY:O	2.29	0.43
16:P:117:LYS:O	16:P:121:VAL:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:100:ASP:HA	21:U:103:ILE:HD12	2.00	0.43
29:c:51:TRP:O	29:c:55:THR:HG23	2.18	0.43
40:n:17:ARG:HD3	40:n:20:ARG:NH2	2.30	0.43
57:t:201:CDL:H572	57:t:201:CDL:H602	1.62	0.43
2:B:81:MET:HE2	2:B:81:MET:HB2	1.83	0.42
4:D:110:THR:HB	4:D:146:TYR:OH	2.19	0.42
7:G:293:ILE:HD12	7:G:608:GLN:HE22	1.84	0.42
7:G:631:SER:HB2	7:G:636:GLN:O	2.19	0.42
9:I:136:CYS:HA	9:I:139:ILE:HG22	2.00	0.42
12:L:136:MET:HE1	52:M:504:PC7:H251	2.01	0.42
12:L:469:ILE:CD1	45:s:92:SER:HB2	2.49	0.42
14:N:139:PHE:CD1	14:N:159:VAL:HG12	2.54	0.42
15:O:128:GLU:O	15:O:131:LYS:HG2	2.18	0.42
16:P:218:ILE:HG23	16:P:219:LEU:HD22	2.00	0.42
34:h:32:LEU:HD21	38:l:47:PHE:CZ	2.54	0.42
50:y:232:PRO:O	50:y:234:LYS:HG3	2.19	0.42
1:A:53:THR:O	1:A:57:VAL:HG23	2.19	0.42
1:A:141:PHE:HD2	52:A:201:PC7:H411	1.84	0.42
6:F:126:ASP:HA	6:F:167:ARG:HG3	2.00	0.42
7:G:333:ALA:O	7:G:337:ILE:HG13	2.18	0.42
7:G:480:PRO:HB2	7:G:510:VAL:HG12	2.00	0.42
14:N:21:GLY:CA	14:N:35:LEU:HD21	2.49	0.42
14:N:96:LEU:O	14:N:100:MET:HG3	2.19	0.42
18:R:102:LEU:HB3	18:R:122:SER:HB3	2.01	0.42
31:e:31:MET:HE3	31:e:34:LEU:HD23	2.00	0.42
34:h:28:TYR:CE2	34:h:30:PHE:HA	2.55	0.42
38:l:109:ARG:HA	41:o:70:ARG:HD3	2.00	0.42
40:n:10:PRO:O	40:n:14:ARG:HG3	2.19	0.42
50:y:243:GLU:O	50:y:247:ILE:HG13	2.19	0.42
11:K:34:TYR:OH	11:K:73:ASN:HA	2.19	0.42
16:P:59:ARG:O	16:P:60:CYS:C	2.63	0.42
26:Z:71:ASN:C	26:Z:71:ASN:ND2	2.77	0.42
32:f:93:ASN:O	32:f:97:ARG:HG3	2.19	0.42
33:g:108:MET:HE3	42:p:73:PHE:HE1	1.84	0.42
41:o:76:GLU:O	41:o:80:ARG:HG3	2.18	0.42
50:y:67:PRO:HB3	50:y:97:ILE:HD12	1.99	0.42
51:z:4:PHE:O	51:z:8:ILE:HG12	2.19	0.42
5:E:184:CYS:HB2	6:F:130:PRO:HA	2.00	0.42
7:G:293:ILE:HD11	7:G:606:ARG:HD2	2.02	0.42
7:G:655:PRO:HB2	19:S:53:SER:HB3	2.02	0.42
8:H:256:TRP:O	8:H:260:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:89:PHE:CD1	14:N:92:LEU:HD13	2.52	0.42
12:L:98:HIS:CE1	12:L:118:LEU:HB3	2.54	0.42
57:L:601:CDL:H312	57:L:601:CDL:H341	1.69	0.42
13:M:177:ASN:O	13:M:239:ILE:HG22	2.19	0.42
13:M:299:ILE:HD13	25:Y:9:TYR:CE1	2.55	0.42
52:N:403:PC7:H142	52:N:403:PC7:H171	1.78	0.42
3:C:113:ARG:NH1	4:D:329:TYR:HE2	2.17	0.42
4:D:43:PRO:HG3	4:D:367:LEU:HD23	2.01	0.42
4:D:174:ARG:HD2	26:Z:30:PHE:HE1	1.84	0.42
7:G:672:GLN:HG3	61:G:1007:HOH:O	2.20	0.42
7:G:697:ASN:HD21	7:G:715:THR:CG2	2.32	0.42
11:K:45:GLY:O	11:K:62:CYS:HB3	2.19	0.42
11:K:89:PHE:HA	14:N:92:LEU:HD13	2.02	0.42
12:L:212:LEU:O	12:L:216:ILE:HG23	2.20	0.42
13:M:413:VAL:O	13:M:413:VAL:HG23	2.20	0.42
14:N:292:ALA:HB3	14:N:294:LEU:HG	2.00	0.42
15:O:49:THR:OG1	15:O:52:GLU:OE1	2.18	0.42
40:n:22:GLY:O	40:n:26:ILE:HG12	2.18	0.42
50:y:165:ARG:CZ	50:y:200:ASP:HB3	2.50	0.42
2:B:19:ASP:HB3	2:B:158:THR:HB	2.01	0.42
4:D:117:LEU:HD22	4:D:139:ARG:HH12	1.83	0.42
6:F:233:LEU:HB2	17:Q:163:TYR:CE2	2.55	0.42
7:G:237:LEU:HD23	7:G:237:LEU:HA	1.91	0.42
8:H:261:LEU:HD21	9:I:83:ILE:HD12	2.02	0.42
13:M:73:TYR:HE1	56:M:501:PTY:C30	2.33	0.42
13:M:121:PHE:CZ	13:M:195:LYS:HD2	2.54	0.42
56:N:404:PTY:H412	56:N:404:PTY:H381	1.84	0.42
45:s:2:VAL:HG12	45:s:4:THR:HG23	2.02	0.42
57:t:201:CDL:H741	57:t:201:CDL:H772	1.68	0.42
49:x:73:PHE:HB2	49:x:229:ARG:HD3	2.01	0.42
50:y:68:VAL:HG21	50:y:135:ASP:HA	2.00	0.42
5:E:123:VAL:HG13	5:E:127:PHE:HE2	1.85	0.42
6:F:380:TYR:HB2	6:F:401:TYR:CE1	2.55	0.42
7:G:643:GLN:HE21	7:G:647:ARG:HE	1.68	0.42
14:N:8:LEU:HD22	52:N:403:PC7:H341	2.00	0.42
14:N:141:PHE:O	14:N:144:SER:OG	2.31	0.42
16:P:231:ASP:HB3	16:P:234:THR:HG23	2.02	0.42
25:Y:73:LEU:HB3	46:t:126:VAL:HG11	2.02	0.42
25:Y:189:LEU:HD13	35:i:35:ARG:HH22	1.85	0.42
26:Z:119:LYS:O	26:Z:122:GLU:HG3	2.19	0.42
32:f:57:THR:HB	32:f:78:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:120:ALA:O	38:l:128:LEU:HD21	2.19	0.42
42:p:143:ASN:ND2	42:p:145:PHE:O	2.53	0.42
1:A:45:VAL:O	1:A:49:VAL:HG23	2.19	0.42
4:D:76:MET:HE3	4:D:154:MET:O	2.19	0.42
8:H:18:PHE:CE2	27:a:11:ILE:HG21	2.55	0.42
8:H:27:MET:HE3	8:H:27:MET:HB3	1.88	0.42
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.65	0.42
8:H:257:VAL:HG11	56:H:301:PTY:H372	2.02	0.42
13:M:1:MET:HE2	13:M:65:PHE:HB3	2.02	0.42
14:N:226:ILE:HD12	57:t:201:CDL:H311	2.01	0.42
57:N:401:CDL:H711	57:N:401:CDL:HB61	1.95	0.42
16:P:282:LEU:HD21	16:P:295:LEU:HD13	2.00	0.42
18:R:67:MET:HA	18:R:70:ILE:HG22	2.02	0.42
45:s:36:LEU:HD23	45:s:36:LEU:HA	1.80	0.42
49:x:59:PHE:HE1	49:x:79:VAL:HG13	1.85	0.42
52:z:301:PC7:H222	52:z:301:PC7:H192	1.96	0.42
2:B:47:ALA:O	2:B:54:LEU:HG	2.19	0.42
2:B:53:ASP:HA	8:H:33:ARG:HE	1.84	0.42
61:B:601:HOH:O	16:P:69:LYS:NZ	2.43	0.42
4:D:83:TYR:CZ	4:D:87:ILE:HD11	2.54	0.42
6:F:96:ARG:HG2	6:F:254:GLU:CD	2.45	0.42
6:F:136:ARG:O	6:F:140:ARG:HG2	2.19	0.42
6:F:204:PHE:CZ	17:Q:181:PRO:HD3	2.54	0.42
6:F:315:VAL:HG22	6:F:364:VAL:HG11	2.01	0.42
7:G:407:ASP:HB2	7:G:477:ALA:HB1	2.02	0.42
7:G:416:PRO:HD2	7:G:446:LEU:HD21	2.01	0.42
7:G:623:ASP:HA	7:G:626:ILE:HD12	2.01	0.42
10:J:49:PHE:CE1	10:J:53:ILE:HD11	2.54	0.42
12:L:26:ARG:HH12	33:g:35:SER:C	2.27	0.42
12:L:392:GLN:N	38:l:94:GLU:OE1	2.53	0.42
52:L:602:PC7:H262	52:L:602:PC7:H232	1.68	0.42
19:S:70:LYS:HD2	19:S:92:HIS:ND1	2.35	0.42
26:Z:111:ILE:O	31:e:69:GLN:NE2	2.50	0.42
57:d:101:CDL:H822	57:d:101:CDL:H852	1.81	0.42
34:h:32:LEU:HD21	38:l:47:PHE:HZ	1.85	0.42
43:q:133:LYS:HB3	43:q:142:ARG:HD3	2.02	0.42
46:t:90:PHE:O	46:t:94:PHE:HB2	2.19	0.42
2:B:21:VAL:HG12	8:H:52:PHE:HE2	1.84	0.42
2:B:132:PRO:HB2	9:I:192:PHE:CE2	2.55	0.42
11:K:80:TYR:O	31:e:12:ARG:NE	2.49	0.42
12:L:108:ASP:OD1	40:n:93:TRP:NE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:285:LEU:O	16:P:289:LEU:HD13	2.20	0.42
40:n:53:LEU:O	40:n:59:ILE:HD11	2.19	0.42
42:p:45:GLU:HG2	42:p:52:TYR:HA	2.02	0.42
1:A:104:TYR:O	1:A:108:ASP:HB2	2.20	0.41
2:B:41:ALA:O	2:B:45:MET:HG3	2.20	0.41
2:B:51:ARG:HD3	9:I:101:ILE:HD12	2.01	0.41
2:B:137:THR:HA	4:D:153:ARG:NH2	2.32	0.41
4:D:224:ILE:H	4:D:224:ILE:HD12	1.85	0.41
7:G:467:LYS:O	7:G:467:LYS:HD2	2.19	0.41
7:G:713:LYS:O	7:G:717:VAL:HG23	2.19	0.41
8:H:182:TYR:CE1	8:H:186:LEU:HD11	2.55	0.41
9:I:66:ASN:O	9:I:70:VAL:HG23	2.20	0.41
10:J:42:LEU:HB2	10:J:51:ALA:HB2	2.01	0.41
12:L:179:LEU:HG	12:L:214:GLY:HA3	2.02	0.41
13:M:73:TYR:HD2	13:M:303:VAL:HG12	1.84	0.41
13:M:269:GLN:NE2	13:M:278:TYR:HE2	2.18	0.41
14:N:50:ILE:HD11	30:d:57:TYR:OH	2.20	0.41
29:c:25:HIS:HB3	33:g:29:PRO:HG3	2.02	0.41
30:d:48:LYS:O	30:d:52:GLU:OE1	2.38	0.41
42:p:123:ILE:HG13	42:p:124:TYR:N	2.35	0.41
2:B:12:ASP:HA	2:B:15:VAL:HG12	2.01	0.41
3:C:2:SER:OG	3:C:3:TYR:N	2.50	0.41
3:C:15:ILE:HG22	44:r:110:VAL:O	2.20	0.41
5:E:145:THR:HB	54:E:500:FES:S1	2.60	0.41
10:J:113:SER:HB2	31:e:7:GLN:OE1	2.20	0.41
11:K:89:PHE:HZ	14:N:140:ILE:HG22	1.85	0.41
14:N:307:LEU:HD23	14:N:310:LEU:HD12	2.01	0.41
15:O:94:ASN:HB3	15:O:99:THR:O	2.19	0.41
16:P:326:SER:HB3	23:W:109:LEU:O	2.20	0.41
22:V:46:VAL:HG23	22:V:48:VAL:HG23	2.01	0.41
24:X:23:GLU:HG3	24:X:27:ASN:ND2	2.35	0.41
26:Z:93:TRP:HB2	32:f:3:TRP:NE1	2.31	0.41
26:Z:130:LEU:HB3	31:e:52:ARG:NH2	2.35	0.41
30:d:56:THR:O	30:d:60:GLU:HG2	2.21	0.41
51:z:92:SER:OG	51:z:116:GLU:OE2	2.37	0.41
1:A:119:MET:HG3	10:J:114:LEU:CD2	2.50	0.41
2:B:112:HIS:CE1	2:B:119:ARG:HD3	2.55	0.41
3:C:196:PRO:O	23:W:135:LYS:NZ	2.52	0.41
4:D:308:GLU:HG3	7:G:133:LEU:HD13	2.02	0.41
6:F:160:ARG:NH1	6:F:202:ASP:OD2	2.45	0.41
6:F:284:PHE:CD2	6:F:360:ALA:HB1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:121:ARG:HD3	9:I:218:ILE:HG21	2.02	0.41
12:L:121:PHE:HZ	12:L:242:ILE:HG22	1.85	0.41
12:L:242:ILE:HG22	12:L:247:LEU:HD23	2.01	0.41
13:M:121:PHE:HZ	13:M:195:LYS:HD2	1.85	0.41
57:M:502:CDL:H542	57:M:502:CDL:H512	1.54	0.41
21:U:47:VAL:HG12	21:U:94:PHE:CZ	2.55	0.41
22:V:128:PRO:O	22:V:132:GLU:HG2	2.20	0.41
30:d:50:LEU:HD22	57:d:101:CDL:H842	2.02	0.41
45:s:56:ALA:N	45:s:57:PRO:HD2	2.36	0.41
2:B:53:ASP:HA	8:H:33:ARG:HH21	1.85	0.41
2:B:111:TYR:CE2	4:D:50:ARG:HD2	2.56	0.41
3:C:105:LEU:HB2	3:C:114:ILE:HG22	2.02	0.41
4:D:72:ASP:HB2	4:D:79:MET:HE3	2.02	0.41
7:G:135:ASN:HB3	7:G:170:ARG:HG2	2.02	0.41
8:H:129:ARG:NH2	8:H:196:LEU:HD11	2.36	0.41
13:M:198:LEU:HD11	13:M:255:CYS:HA	2.03	0.41
13:M:251:ILE:O	13:M:254:ILE:HG12	2.20	0.41
13:M:305:TYR:HB2	13:M:367:ALA:HB1	2.02	0.41
14:N:338:ARG:O	14:N:343:VAL:HG23	2.21	0.41
52:N:403:PC7:H322	52:N:403:PC7:H351	1.83	0.41
19:S:78:SER:O	19:S:82:ILE:HG12	2.21	0.41
19:S:86:LEU:O	19:S:90:VAL:HG23	2.21	0.41
34:h:5:ASN:HB3	34:h:6:TYR:H	1.60	0.41
38:l:38:ASP:OD2	38:l:38:ASP:N	2.54	0.41
45:s:94:TYR:O	45:s:98:LYS:HG2	2.21	0.41
49:x:133:THR:HG22	49:x:135:ILE:HD11	2.02	0.41
4:D:283:MET:HB3	26:Z:25:PRO:HD3	2.02	0.41
8:H:174:LEU:HB3	8:H:238:PHE:CE1	2.56	0.41
11:K:56:LEU:HG	11:K:123:LEU:O	2.20	0.41
13:M:53:TYR:HB2	13:M:67:VAL:HG23	2.03	0.41
57:M:502:CDL:H382	30:d:16:VAL:HG22	2.02	0.41
14:N:50:ILE:O	14:N:54:ILE:HG13	2.21	0.41
14:N:51:PRO:HA	14:N:54:ILE:HD12	2.02	0.41
57:N:401:CDL:H752	57:N:401:CDL:H722	1.29	0.41
25:Y:84:ARG:HD2	25:Y:86:TYR:CE1	2.55	0.41
33:g:58:ARG:HH11	33:g:60:LYS:HA	1.85	0.41
38:l:75:TYR:CE2	45:s:40:PHE:HA	2.55	0.41
42:p:104:ARG:HH22	42:p:156:TYR:HE2	1.67	0.41
44:r:67:ILE:O	44:r:67:ILE:HG13	2.19	0.41
6:F:202:ASP:CG	17:Q:181:PRO:HD2	2.46	0.41
7:G:656:HIS:CD2	7:G:656:HIS:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:149:ILE:O	8:H:153:ARG:NH1	2.53	0.41
8:H:151:GLU:HG2	8:H:173:ILE:HG21	2.02	0.41
9:I:34:ARG:HD2	9:I:60:PHE:CZ	2.56	0.41
10:J:86:GLN:HE21	25:Y:89:ILE:HD12	1.85	0.41
11:K:120:VAL:HG23	11:K:121:GLU:OE1	2.20	0.41
12:L:308:THR:OG1	12:L:309:CYS:N	2.53	0.41
12:L:476:VAL:HG22	45:s:85:SER:HB2	2.02	0.41
13:M:193:TRP:CD1	13:M:198:LEU:HB3	2.56	0.41
57:N:401:CDL:H842	30:d:53:VAL:HG22	2.03	0.41
19:S:53:SER:HB3	19:S:56:ALA:HB2	2.03	0.41
21:U:96:VAL:HG21	21:U:119:ASN:ND2	2.36	0.41
23:W:117:ASN:HB3	23:W:121:LEU:HB3	2.02	0.41
25:Y:95:ILE:O	25:Y:99:LYS:HG2	2.19	0.41
30:d:74:GLU:O	30:d:78:LYS:HG3	2.20	0.41
38:l:78:LYS:O	38:l:82:VAL:HG23	2.20	0.41
49:x:106:ARG:HD2	49:x:134:ILE:HD12	2.01	0.41
2:B:40:CYS:HB2	2:B:74:ALA:HB1	2.02	0.41
4:D:21:PRO:CD	8:H:202:GLU:HG3	2.50	0.41
4:D:120:THR:HG21	4:D:135:ALA:CB	2.51	0.41
14:N:168:LEU:HD23	14:N:168:LEU:HA	1.95	0.41
16:P:261:ARG:HG3	16:P:345:GLY:N	2.36	0.41
17:Q:159:ARG:HD2	17:Q:159:ARG:O	2.20	0.41
24:X:61:MET:HE1	24:X:69:LYS:HZ3	1.86	0.41
35:i:58:GLU:HB2	35:i:81:ASN:ND2	2.35	0.41
1:A:11:THR:OG1	1:A:14:GLN:HG3	2.21	0.41
1:A:119:MET:SD	8:H:149:ILE:HG21	2.61	0.41
2:B:45:MET:SD	4:D:24:HIS:CE1	3.14	0.41
4:D:113:MET:HE1	4:D:146:TYR:CE2	2.55	0.41
4:D:187:VAL:HG11	4:D:270:ARG:HE	1.84	0.41
4:D:241:ASP:C	4:D:243:TYR:N	2.78	0.41
5:E:156:ILE:HD12	5:E:214:LEU:HD12	2.03	0.41
6:F:276:LYS:C	6:F:278:ASN:H	2.28	0.41
6:F:435:LEU:HD23	53:F:501:SF4:S1	2.61	0.41
8:H:230:MET:O	8:H:234:ILE:HG13	2.21	0.41
56:H:301:PTY:H141	56:H:301:PTY:H111	1.80	0.41
10:J:34:LEU:O	10:J:38:VAL:HG23	2.20	0.41
12:L:188:PHE:HE1	13:M:377:LYS:HG2	1.86	0.41
12:L:287:LEU:HD13	12:L:346:LEU:HD21	2.02	0.41
52:M:503:PC7:H321	52:M:503:PC7:H2	1.84	0.41
14:N:228:GLN:NE2	14:N:241:SER:OG	2.54	0.41
15:O:180:ASN:OD1	15:O:181:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:222:ALA:O	16:P:226:VAL:HG23	2.21	0.41
25:Y:154:LEU:HD22	56:Y:301:PTY:H191	2.01	0.41
50:y:63:LEU:HA	50:y:66:ALA:HB2	2.02	0.41
50:y:125:SER:OG	50:y:127:TRP:NE1	2.54	0.41
51:z:151:LYS:HE2	51:z:169:ASP:OD1	2.20	0.41
1:A:101:SER:OG	10:J:65:LEU:HD13	2.21	0.41
1:A:109:ILE:O	1:A:112:VAL:HB	2.21	0.41
1:A:143:TYR:HD1	14:N:22:LEU:HD21	1.86	0.41
3:C:90:VAL:HG22	4:D:353:ARG:HG2	2.02	0.41
4:D:103:ARG:NH2	4:D:160:ARG:O	2.54	0.41
4:D:111:ARG:HH22	4:D:333:GLU:HG3	1.86	0.41
4:D:382:ILE:O	4:D:386:LEU:HG	2.19	0.41
8:H:18:PHE:CE2	8:H:44:ILE:HG13	2.55	0.41
8:H:69:ILE:HG13	8:H:70:PHE:N	2.36	0.41
8:H:95:ILE:HD12	10:J:52:LEU:HD22	2.02	0.41
8:H:163:LEU:HB3	8:H:236:ILE:CD1	2.51	0.41
9:I:226:SER:HB3	18:R:93:LEU:HD21	2.01	0.41
12:L:216:ILE:HB	12:L:221:GLN:HB2	2.03	0.41
12:L:249:THR:HB	12:L:320:LEU:HD21	2.02	0.41
12:L:523:VAL:HA	12:L:527:LEU:HD12	2.02	0.41
13:M:247:ALA:HB2	39:m:121:TYR:CD2	2.55	0.41
14:N:66:PHE:CE2	14:N:75:LEU:HD22	2.56	0.41
57:N:401:CDL:H852	57:N:401:CDL:H822	1.30	0.41
16:P:88:ASP:HB3	16:P:92:ARG:HH12	1.85	0.41
20:T:96:LEU:O	40:n:81:ARG:NH1	2.54	0.41
22:V:31:ASP:OD1	22:V:32:VAL:N	2.54	0.41
22:V:114:GLU:OE1	22:V:114:GLU:N	2.54	0.41
25:Y:70:GLU:OE2	45:s:3:LYS:HD3	2.21	0.41
27:a:51:ASP:O	27:a:55:ARG:HG3	2.21	0.41
32:f:28:VAL:HG22	32:f:99:MET:O	2.20	0.41
41:o:44:HIS:O	41:o:48:TRP:HB3	2.20	0.41
51:z:12:CYS:O	51:z:16:ILE:HG13	2.21	0.41
2:B:156:LYS:O	2:B:156:LYS:HG3	2.21	0.41
8:H:192:VAL:HA	8:H:195:ASP:HB3	2.00	0.41
11:K:83:ASP:HB3	14:N:147:TYR:OH	2.20	0.41
14:N:313:ILE:HD12	14:N:315:LEU:HD12	2.03	0.41
15:O:95:MET:HE2	15:O:173:ILE:HD11	2.02	0.41
16:P:207:ASN:HD21	16:P:308:VAL:HG23	1.86	0.41
23:W:126:GLU:OE1	23:W:127:LYS:HE3	2.21	0.41
26:Z:72:ARG:HD3	28:b:39:UNK:CB	2.51	0.41
26:Z:81:ALA:HA	26:Z:84:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:95:ALA:O	32:f:99:MET:HG3	2.21	0.41
56:m:201:PTY:H151	56:m:201:PTY:H122	1.71	0.41
45:s:69:VAL:HA	45:s:74:PHE:CD2	2.56	0.41
50:y:197:THR:HG1	51:z:145:ASN:HD22	1.68	0.41
52:z:301:PC7:H381	52:z:301:PC7:H411	1.88	0.41
2:B:42:VAL:O	2:B:45:MET:HB2	2.20	0.40
2:B:113:TYR:HA	2:B:119:ARG:HH21	1.86	0.40
4:D:136:PHE:O	4:D:140:GLU:HG2	2.21	0.40
5:E:151:GLN:OE1	5:E:192:PRO:HD3	2.21	0.40
6:F:420:LEU:O	6:F:424:THR:HG23	2.21	0.40
10:J:139:ALA:HB2	11:K:99:CYS:HB3	2.04	0.40
11:K:50:VAL:HG21	46:t:85:TYR:CD2	2.56	0.40
13:M:182:SER:HB2	56:m:201:PTY:H152	2.02	0.40
16:P:124:PRO:HB3	16:P:167:ILE:HD11	2.02	0.40
17:Q:85:HIS:CG	17:Q:86:PRO:HD2	2.56	0.40
30:d:72:VAL:HG23	30:d:77:LYS:NZ	2.36	0.40
33:g:107:ASP:OD2	42:p:69:LYS:NZ	2.34	0.40
40:n:110:ASP:OD2	40:n:113:LYS:HB2	2.21	0.40
4:D:166:GLN:NE2	61:D:402:HOH:O	2.16	0.40
4:D:312:HIS:NE2	7:G:161:ASP:HA	2.36	0.40
5:E:45:PHE:CE1	18:R:103:LYS:HB3	2.56	0.40
7:G:385:THR:O	7:G:494:ARG:NH2	2.54	0.40
7:G:413:GLY:O	7:G:487:SER:OG	2.33	0.40
7:G:654:ALA:HB3	7:G:657:PHE:HD2	1.86	0.40
11:K:56:LEU:HD21	11:K:125:LEU:HD13	2.03	0.40
11:K:89:PHE:HD1	14:N:92:LEU:CD1	2.34	0.40
12:L:375:LEU:HD23	12:L:375:LEU:HA	1.94	0.40
13:M:72:LEU:O	13:M:76:LEU:HD23	2.21	0.40
13:M:72:LEU:HD23	56:M:501:PTY:O30	2.21	0.40
52:M:503:PC7:H401	52:M:503:PC7:H431	1.63	0.40
16:P:10:ASN:HB2	16:P:138:GLU:OE2	2.20	0.40
24:X:2:VAL:HG21	27:a:57:GLU:OE2	2.20	0.40
49:x:130:ASN:HB3	49:x:151:ARG:HH22	1.85	0.40
3:C:14:TYR:CB	44:r:109:THR:HB	2.51	0.40
9:I:82:ASP:OD2	9:I:83:ILE:N	2.54	0.40
10:J:28:LEU:CD2	10:J:67:LEU:HB2	2.51	0.40
10:J:58:TYR:CE1	11:K:68:ILE:HD11	2.56	0.40
12:L:55:CYS:SG	29:c:79:ARG:HD3	2.61	0.40
12:L:73:VAL:HG21	12:L:135:VAL:HB	2.03	0.40
12:L:389:TYR:CD2	12:L:465:LEU:HD21	2.57	0.40
13:M:118:TYR:CE1	13:M:158:LEU:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:80:LEU:HA	16:P:81:PRO:HD3	1.84	0.40
17:Q:36:LYS:NZ	22:V:145:PRO:HG2	2.36	0.40
17:Q:73:LYS:HB2	17:Q:83:THR:CG2	2.52	0.40
27:a:35:SER:O	27:a:38:GLN:HG3	2.21	0.40
50:y:87:SER:HA	50:y:90:ARG:HG2	2.03	0.40
51:z:124:SER:OG	51:z:141:LEU:HD12	2.21	0.40
51:z:179:SER:HB3	51:z:186:LEU:HD11	2.01	0.40
2:B:15:VAL:CG2	2:B:158:THR:HG22	2.44	0.40
2:B:56:ARG:HG3	8:H:37:ALA:H	1.87	0.40
5:E:247:ALA:HB1	6:F:316:ARG:NH2	2.32	0.40
7:G:498:LEU:HB3	7:G:674:PHE:HZ	1.86	0.40
12:L:71:LEU:HD11	12:L:193:PHE:HE2	1.86	0.40
12:L:228:LEU:HD12	12:L:228:LEU:HA	1.96	0.40
14:N:21:GLY:HA3	14:N:35:LEU:HD21	2.02	0.40
14:N:87:GLN:HA	35:i:49:ARG:HH12	1.86	0.40
14:N:165:LEU:HD22	14:N:170:VAL:HG21	2.02	0.40
21:U:70:SER:HB3	21:U:76:LEU:HD11	2.03	0.40
25:Y:125:SER:HB2	56:Y:301:PTY:O12	2.22	0.40
40:n:97:CYS:SG	40:n:98:LYS:N	2.95	0.40
4:D:116:ILE:CG2	4:D:135:ALA:HB1	2.52	0.40
6:F:340:CYS:HA	6:F:343:VAL:HG12	2.03	0.40
13:M:197:PRO:HD2	13:M:284:MET:HG3	2.02	0.40
14:N:134:ILE:HD11	46:t:85:TYR:CD1	2.56	0.40
16:P:103:ASN:ND2	16:P:142:GLN:OE1	2.45	0.40
16:P:123:PHE:HB3	16:P:124:PRO:HD3	2.04	0.40
16:P:194:ILE:CD1	16:P:339:VAL:HG12	2.42	0.40
19:S:15:ARG:NH2	19:S:61:THR:HG21	2.36	0.40
38:l:109:ARG:HH21	41:o:28:ASP:CG	2.30	0.40
46:t:117:SER:HB3	57:t:201:CDL:H142	2.04	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	117/154 (76%)	115 (98%)	2 (2%)	0	100	100
2	B	152/164 (93%)	146 (96%)	6 (4%)	0	100	100
3	C	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
4	D	393/395 (100%)	386 (98%)	6 (2%)	1 (0%)	36	65
5	E	233/276 (84%)	226 (97%)	7 (3%)	0	100	100
6	F	428/469 (91%)	415 (97%)	13 (3%)	0	100	100
7	G	680/720 (94%)	665 (98%)	15 (2%)	0	100	100
8	H	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
9	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
10	J	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
11	K	102/127 (80%)	101 (99%)	1 (1%)	0	100	100
12	L	534/536 (100%)	525 (98%)	9 (2%)	0	100	100
13	M	436/438 (100%)	425 (98%)	11 (2%)	0	100	100
14	N	373/375 (100%)	369 (99%)	3 (1%)	1 (0%)	36	65
15	O	159/200 (80%)	154 (97%)	5 (3%)	0	100	100
16	P	345/370 (93%)	332 (96%)	13 (4%)	0	100	100
17	Q	160/185 (86%)	156 (98%)	4 (2%)	0	100	100
18	R	106/132 (80%)	103 (97%)	3 (3%)	0	100	100
19	S	93/98 (95%)	92 (99%)	1 (1%)	0	100	100
20	T	81/123 (66%)	81 (100%)	0	0	100	100
21	U	82/122 (67%)	72 (88%)	10 (12%)	0	100	100
22	V	132/159 (83%)	129 (98%)	3 (2%)	0	100	100
23	W	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
24	X	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
25	Y	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
26	Z	122/142 (86%)	118 (97%)	4 (3%)	0	100	100
27	a	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
29	c	95/110 (86%)	94 (99%)	1 (1%)	0	100	100
30	d	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
31	e	69/75 (92%)	67 (97%)	2 (3%)	0	100	100
32	f	109/121 (90%)	109 (100%)	0	0	100	100
33	g	145/172 (84%)	143 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	h	75/81 (93%)	75 (100%)	0	0	100	100
35	i	109/128 (85%)	108 (99%)	1 (1%)	0	100	100
37	k	42/55 (76%)	41 (98%)	1 (2%)	0	100	100
38	l	125/151 (83%)	124 (99%)	1 (1%)	0	100	100
39	m	109/138 (79%)	107 (98%)	2 (2%)	0	100	100
40	n	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
41	o	81/85 (95%)	81 (100%)	0	0	100	100
42	p	153/156 (98%)	152 (99%)	1 (1%)	0	100	100
43	q	26/155 (17%)	26 (100%)	0	0	100	100
44	r	58/121 (48%)	58 (100%)	0	0	100	100
45	s	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
46	t	80/134 (60%)	80 (100%)	0	0	100	100
49	x	248/280 (89%)	245 (99%)	3 (1%)	0	100	100
50	y	306/310 (99%)	298 (97%)	8 (3%)	0	100	100
51	z	224/227 (99%)	219 (98%)	5 (2%)	0	100	100
All	All	8417/9404 (90%)	8239 (98%)	176 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	171	ALA
4	D	242	VAL

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 PDB entries followed by that with respect to all EM entries.

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	107/133 (80%)	107 (100%)	0	100	100
2	B	129/134 (96%)	129 (100%)	0	100	100
3	C	199/200 (100%)	199 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	339/339 (100%)	339 (100%)	0	100	100
5	E	197/232 (85%)	196 (100%)	1 (0%)	81	83
6	F	343/372 (92%)	343 (100%)	0	100	100
7	G	544/570 (95%)	544 (100%)	0	100	100
8	H	240/240 (100%)	240 (100%)	0	100	100
9	I	175/201 (87%)	175 (100%)	0	100	100
10	J	129/129 (100%)	129 (100%)	0	100	100
11	K	84/103 (82%)	84 (100%)	0	100	100
12	L	438/438 (100%)	438 (100%)	0	100	100
13	M	376/376 (100%)	376 (100%)	0	100	100
14	N	331/331 (100%)	330 (100%)	1 (0%)	86	86
15	O	146/177 (82%)	146 (100%)	0	100	100
16	P	296/318 (93%)	296 (100%)	0	100	100
17	Q	134/154 (87%)	134 (100%)	0	100	100
18	R	86/107 (80%)	86 (100%)	0	100	100
19	S	77/79 (98%)	77 (100%)	0	100	100
20	T	73/106 (69%)	73 (100%)	0	100	100
21	U	76/108 (70%)	76 (100%)	0	100	100
22	V	116/139 (84%)	116 (100%)	0	100	100
23	W	119/123 (97%)	119 (100%)	0	100	100
24	X	85/86 (99%)	85 (100%)	0	100	100
25	Y	165/166 (99%)	165 (100%)	0	100	100
26	Z	107/123 (87%)	107 (100%)	0	100	100
27	a	50/57 (88%)	50 (100%)	0	100	100
29	c	80/91 (88%)	80 (100%)	0	100	100
30	d	68/70 (97%)	68 (100%)	0	100	100
31	e	64/68 (94%)	64 (100%)	0	100	100
32	f	92/100 (92%)	92 (100%)	0	100	100
33	g	122/139 (88%)	122 (100%)	0	100	100
34	h	64/65 (98%)	64 (100%)	0	100	100
35	i	97/113 (86%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	k	35/45 (78%)	35 (100%)	0	100	100
38	l	110/128 (86%)	110 (100%)	0	100	100
39	m	100/123 (81%)	100 (100%)	0	100	100
40	n	106/107 (99%)	106 (100%)	0	100	100
41	o	74/76 (97%)	74 (100%)	0	100	100
42	p	140/141 (99%)	140 (100%)	0	100	100
43	q	26/138 (19%)	25 (96%)	1 (4%)	29	58
44	r	55/109 (50%)	55 (100%)	0	100	100
45	s	105/108 (97%)	105 (100%)	0	100	100
46	t	73/119 (61%)	73 (100%)	0	100	100
49	x	209/234 (89%)	209 (100%)	0	100	100
50	y	250/252 (99%)	250 (100%)	0	100	100
51	z	188/189 (100%)	188 (100%)	0	100	100
All	All	7219/7956 (91%)	7216 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	49	HIS
14	N	305	GLN
43	q	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	22	HIS
1	A	29	ASN
1	A	47	HIS
2	B	157	ASN
3	C	80	GLN
3	C	154	HIS
4	D	44	HIS
4	D	89	GLN
4	D	214	GLN
4	D	238	GLN

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Mol	Chain	Res	Type
4	D	293	GLN
5	E	66	ASN
6	F	172	ASN
6	F	228	GLN
6	F	289	HIS
6	F	291	ASN
7	G	78	HIS
7	G	135	ASN
7	G	186	ASN
7	G	415	ASN
7	G	519	ASN
7	G	608	GLN
7	G	643	GLN
7	G	656	HIS
7	G	697	ASN
9	I	56	GLN
11	K	124	ASN
12	L	58	ASN
12	L	132	GLN
12	L	243	HIS
12	L	285	ASN
12	L	298	GLN
12	L	319	HIS
12	L	392	GLN
12	L	468	HIS
12	L	471	ASN
12	L	519	HIS
12	L	520	ASN
13	M	145	ASN
13	M	202	HIS
13	M	300	GLN
13	M	411	GLN
14	N	65	ASN
14	N	142	HIS
14	N	206	ASN
14	N	208	ASN
14	N	228	GLN
15	O	58	ASN
15	O	160	ASN
16	P	61	ASN
16	P	76	GLN
16	P	103	ASN

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Mol	Chain	Res	Type
16	P	142	GLN
16	P	214	GLN
16	P	264	ASN
17	Q	140	HIS
17	Q	150	ASN
17	Q	154	HIS
18	R	86	HIS
18	R	127	HIS
19	S	54	ASN
20	T	41	HIS
21	U	107	HIS
22	V	50	HIS
23	W	21	GLN
23	W	25	ASN
23	W	92	GLN
23	W	94	HIS
25	Y	87	ASN
25	Y	204	HIS
25	Y	205	HIS
26	Z	41	ASN
26	Z	86	HIS
26	Z	101	GLN
27	a	27	GLN
27	a	42	GLN
27	a	44	GLN
32	f	111	ASN
33	g	132	ASN
34	h	17	HIS
39	m	72	ASN
39	m	82	GLN
39	m	108	GLN
40	n	34	HIS
41	o	44	HIS
42	p	54	HIS
42	p	93	GLN
43	q	143	ASN
46	t	62	ASN
49	x	44	GLN
49	x	55	GLN
49	x	77	ASN
49	x	144	HIS
49	x	155	ASN

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Mol	Chain	Res	Type
50	y	146	ASN
50	y	172	ASN
50	y	189	ASN
50	y	219	ASN
50	y	244	ASN
51	z	122	ASN
51	z	145	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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
57	CDL	L	601	-	88,88,99	0.94	8 (9%)	94,100,111	1.11	4 (4%)
53	SF4	I	500	9	0,12,12	-	-	-		
52	PC7	M	503	-	51,51,51	0.99	4 (7%)	57,59,59	1.10	2 (3%)
60	8Q1	n	200	-	32,34,34	1.67	6 (18%)	39,43,43	1.76	5 (12%)
53	SF4	F	501	6	0,12,12	-	-	-		
56	PTY	m	201	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	NDP	P	500	-	51,52,52	2.43	7 (13%)	71,80,80	1.56	17 (23%)
57	CDL	d	101	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	4 (3%)
52	PC7	N	403	-	51,51,51	1.00	4 (7%)	57,59,59	1.07	2 (3%)
52	PC7	z	301	-	51,51,51	0.96	4 (7%)	57,59,59	1.02	2 (3%)
53	SF4	G	802	7	0,12,12	-	-	-	-	-
55	FMN	F	500	-	33,33,33	1.03	2 (6%)	48,50,50	1.22	8 (16%)
53	SF4	G	803	7	0,12,12	-	-	-	-	-
56	PTY	Y	301	-	49,49,49	0.88	4 (8%)	52,54,54	1.11	2 (3%)
52	PC7	A	201	-	48,48,51	0.99	4 (8%)	54,56,59	1.08	2 (3%)
56	PTY	M	501	-	46,46,49	0.92	4 (8%)	49,51,54	1.14	2 (4%)
52	PC7	M	504	-	51,51,51	0.97	4 (7%)	57,59,59	1.09	2 (3%)
56	PTY	m	202	-	49,49,49	0.88	4 (8%)	52,54,54	1.06	2 (3%)
52	PC7	L	602	-	47,47,51	1.03	3 (6%)	53,55,59	1.04	2 (3%)
60	8Q1	W	200	-	32,34,34	1.60	6 (18%)	39,43,43	1.57	4 (10%)
56	PTY	N	404	-	49,49,49	0.89	4 (8%)	52,54,54	1.11	2 (3%)
57	CDL	t	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.09	4 (3%)
52	PC7	N	402	-	51,51,51	0.97	4 (7%)	57,59,59	1.05	2 (3%)
57	CDL	M	502	-	99,99,99	0.88	7 (7%)	105,111,111	1.06	4 (3%)
54	FES	E	500	5	0,4,4	-	-	-	-	-
53	SF4	I	501	9	0,12,12	-	-	-	-	-
56	PTY	H	301	-	49,49,49	0.88	4 (8%)	52,54,54	1.06	2 (3%)
56	PTY	L	603	-	49,49,49	0.89	4 (8%)	52,54,54	1.12	2 (3%)
57	CDL	N	401	-	99,99,99	0.90	8 (8%)	105,111,111	1.10	4 (3%)
54	FES	G	801	7	0,4,4	-	-	-	-	-
53	SF4	B	500	2	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
57	CDL	L	601	-	-	51/99/99/110	-
53	SF4	I	500	9	-	-	0/6/5/5
52	PC7	M	503	-	-	25/55/55/55	-
60	8Q1	n	200	-	-	17/41/41/41	-
53	SF4	F	501	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PTY	m	201	-	-	24/53/53/53	-
58	NDP	P	500	-	-	10/34/77/77	0/5/5/5
57	CDL	d	101	-	-	59/110/110/110	-
52	PC7	N	403	-	-	34/55/55/55	-
52	PC7	z	301	-	-	29/55/55/55	-
53	SF4	G	802	7	-	-	0/6/5/5
55	FMN	F	500	-	-	9/18/18/18	0/3/3/3
56	PTY	Y	301	-	-	33/53/53/53	-
53	SF4	G	803	7	-	-	0/6/5/5
52	PC7	A	201	-	-	36/52/52/55	-
56	PTY	M	501	-	-	22/50/50/53	-
52	PC7	M	504	-	-	33/55/55/55	-
56	PTY	m	202	-	-	25/53/53/53	-
52	PC7	L	602	-	-	33/51/51/55	-
60	8Q1	W	200	-	-	11/41/41/41	-
56	PTY	N	404	-	-	22/53/53/53	-
57	CDL	t	201	-	-	64/110/110/110	-
52	PC7	N	402	-	-	26/55/55/55	-
57	CDL	M	502	-	-	66/110/110/110	-
54	FES	E	500	5	-	-	0/1/1/1
56	PTY	H	301	-	-	32/53/53/53	-
56	PTY	L	603	-	-	26/53/53/53	-
57	CDL	N	401	-	-	63/110/110/110	-
53	SF4	I	501	9	-	-	0/6/5/5
54	FES	G	801	7	-	-	0/1/1/1
53	SF4	B	500	2	-	-	0/6/5/5

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	P	500	NDP	P2B-O2B	13.50	1.83	1.59
58	P	500	NDP	PA-O3	5.54	1.65	1.59
60	n	200	8Q1	C34-N36	5.33	1.46	1.33
60	n	200	8Q1	C39-N41	5.27	1.45	1.33
60	W	200	8Q1	C34-N36	5.06	1.45	1.33
60	W	200	8Q1	C39-N41	4.90	1.45	1.33
58	P	500	NDP	PN-O5D	4.05	1.75	1.59
55	F	500	FMN	C4A-N5	3.39	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	P	500	NDP	O2B-C2B	-3.39	1.32	1.44
52	N	403	PC7	O2-C2	-2.83	1.39	1.46
57	M	502	CDL	OA6-CA5	2.77	1.42	1.34
57	L	601	CDL	OB6-CB4	-2.77	1.40	1.46
57	d	101	CDL	OA6-CA4	-2.76	1.40	1.46
57	d	101	CDL	OB6-CB4	-2.75	1.40	1.46
52	L	602	PC7	O3-C11	2.75	1.41	1.33
57	M	502	CDL	OB6-CB4	-2.74	1.40	1.46
57	N	401	CDL	OA6-CA4	-2.71	1.40	1.46
56	M	501	PTY	O7-C6	-2.70	1.40	1.46
57	L	601	CDL	OA6-CA4	-2.70	1.40	1.46
57	t	201	CDL	OB6-CB4	-2.70	1.40	1.46
52	A	201	PC7	O2-C2	-2.70	1.40	1.46
57	t	201	CDL	OA6-CA4	-2.69	1.40	1.46
52	M	503	PC7	O2-C2	-2.66	1.40	1.46
56	N	404	PTY	O7-C6	-2.66	1.40	1.46
56	m	202	PTY	O7-C6	-2.65	1.40	1.46
52	N	402	PC7	O2-C2	-2.64	1.40	1.46
56	L	603	PTY	O7-C6	-2.64	1.40	1.46
57	N	401	CDL	OA8-CA7	2.61	1.41	1.33
57	N	401	CDL	OB6-CB4	-2.60	1.40	1.46
56	m	201	PTY	O7-C6	-2.59	1.40	1.46
52	M	504	PC7	O2-C2	-2.59	1.40	1.46
56	Y	301	PTY	O7-C6	-2.58	1.40	1.46
57	N	401	CDL	OB8-CB7	2.54	1.40	1.33
57	L	601	CDL	OA8-CA7	2.53	1.40	1.33
57	t	201	CDL	OA8-CA7	2.52	1.40	1.33
57	L	601	CDL	OB8-CB7	2.51	1.40	1.33
57	M	502	CDL	OA8-CA7	2.51	1.40	1.33
60	n	200	8Q1	C1-S44	2.49	1.82	1.76
57	t	201	CDL	OB8-CB7	2.49	1.40	1.33
57	d	101	CDL	OA8-CA7	2.48	1.40	1.33
60	n	200	8Q1	O40-C39	-2.47	1.18	1.23
52	N	403	PC7	O3-C11	2.47	1.40	1.33
57	d	101	CDL	OB8-CB7	2.47	1.40	1.33
60	W	200	8Q1	C1-S44	2.46	1.82	1.76
57	M	502	CDL	OB8-CB7	2.45	1.40	1.33
52	M	503	PC7	O3-C11	2.45	1.40	1.33
56	M	501	PTY	O4-C30	2.44	1.40	1.33
52	z	301	PC7	O3-C11	2.43	1.40	1.33
55	F	500	FMN	C10-N1	2.43	1.38	1.33
60	W	200	8Q1	O35-C34	-2.41	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	N	404	PTY	O4-C30	2.41	1.40	1.33
56	H	301	PTY	O4-C30	2.40	1.40	1.33
52	N	402	PC7	O3-C11	2.40	1.40	1.33
56	H	301	PTY	O7-C6	-2.40	1.41	1.46
56	m	202	PTY	O4-C30	2.40	1.40	1.33
56	m	201	PTY	O4-C30	2.38	1.40	1.33
56	Y	301	PTY	O4-C30	2.38	1.40	1.33
60	W	200	8Q1	O40-C39	-2.35	1.18	1.23
56	L	603	PTY	O4-C30	2.34	1.40	1.33
52	A	201	PC7	O3-C11	2.34	1.40	1.33
52	N	403	PC7	O3-C3	-2.33	1.40	1.45
56	H	301	PTY	O7-C8	2.33	1.40	1.34
52	M	504	PC7	O3-C11	2.33	1.40	1.33
52	M	504	PC7	O3-C3	-2.32	1.40	1.45
52	z	301	PC7	O2-C31	2.32	1.40	1.34
52	z	301	PC7	O2-C2	-2.31	1.41	1.46
60	n	200	8Q1	O35-C34	-2.31	1.19	1.23
60	W	200	8Q1	C6-C1	2.30	1.53	1.50
58	P	500	NDP	O5D-C5D	-2.29	1.35	1.44
58	P	500	NDP	C5A-C4A	2.28	1.43	1.39
57	t	201	CDL	OA6-CA5	2.28	1.40	1.34
52	M	503	PC7	O2-C31	2.27	1.40	1.34
56	H	301	PTY	O4-C1	-2.27	1.40	1.45
56	N	404	PTY	O4-C1	-2.26	1.40	1.45
56	M	501	PTY	O4-C1	-2.26	1.40	1.45
57	N	401	CDL	OA6-CA5	2.25	1.40	1.34
57	N	401	CDL	OB6-CB5	2.24	1.40	1.34
56	m	201	PTY	O4-C1	-2.23	1.40	1.45
52	L	602	PC7	O2-C31	2.23	1.40	1.34
56	Y	301	PTY	O4-C1	-2.23	1.40	1.45
52	M	503	PC7	O3-C3	-2.22	1.40	1.45
57	L	601	CDL	OA6-CA5	2.22	1.40	1.34
52	A	201	PC7	O3-C3	-2.21	1.40	1.45
56	m	202	PTY	O4-C1	-2.21	1.40	1.45
52	N	402	PC7	O3-C3	-2.21	1.40	1.45
60	n	200	8Q1	C6-C1	2.21	1.53	1.50
56	L	603	PTY	O4-C1	-2.20	1.40	1.45
57	d	101	CDL	OA6-CA5	2.19	1.40	1.34
52	N	403	PC7	O2-C31	2.19	1.40	1.34
56	m	201	PTY	O7-C8	2.19	1.40	1.34
52	M	504	PC7	O2-C31	2.18	1.40	1.34
56	L	603	PTY	O7-C8	2.18	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	N	404	PTY	O7-C8	2.17	1.40	1.34
57	t	201	CDL	OB6-CB5	2.16	1.40	1.34
52	N	402	PC7	O2-C31	2.15	1.40	1.34
56	Y	301	PTY	O7-C8	2.15	1.40	1.34
52	A	201	PC7	O2-C31	2.15	1.40	1.34
56	m	202	PTY	O7-C8	2.13	1.40	1.34
58	P	500	NDP	C2A-N1A	2.13	1.37	1.33
57	d	101	CDL	OB6-CB5	2.13	1.40	1.34
52	L	602	PC7	P-O3P	2.12	1.67	1.59
56	M	501	PTY	O7-C8	2.11	1.40	1.34
57	L	601	CDL	OB6-CB5	2.11	1.40	1.34
57	d	101	CDL	OB8-CB6	-2.10	1.40	1.45
57	M	502	CDL	OB6-CB5	2.09	1.40	1.34
57	d	101	CDL	OA8-CA6	-2.09	1.40	1.45
52	z	301	PC7	O3-C3	-2.09	1.40	1.45
57	L	601	CDL	OA8-CA6	-2.08	1.40	1.45
57	t	201	CDL	OA8-CA6	-2.07	1.40	1.45
57	M	502	CDL	OB8-CB6	-2.05	1.40	1.45
57	N	401	CDL	OB8-CB6	-2.05	1.40	1.45
57	M	502	CDL	OA8-CA6	-2.04	1.40	1.45
57	N	401	CDL	OA8-CA6	-2.04	1.40	1.45
57	L	601	CDL	OB8-CB6	-2.03	1.40	1.45
57	t	201	CDL	OB8-CB6	-2.03	1.40	1.45

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	n	200	8Q1	C6-C1-S44	6.88	121.61	113.40
60	W	200	8Q1	C6-C1-S44	5.93	120.47	113.40
52	M	503	PC7	O2-C31-C32	4.75	121.76	111.48
58	P	500	NDP	P2B-O2B-C2B	-4.60	111.16	123.43
57	N	401	CDL	OA6-CA5-C11	4.39	120.98	111.48
56	L	603	PTY	O7-C8-C11	4.39	120.98	111.48
57	L	601	CDL	OA6-CA5-C11	4.17	120.50	111.48
57	t	201	CDL	OA6-CA5-C11	4.07	120.28	111.48
56	m	201	PTY	O7-C8-C11	4.02	120.18	111.48
56	N	404	PTY	O7-C8-C11	4.00	120.13	111.48
57	N	401	CDL	OB6-CB5-C51	3.99	120.12	111.48
56	Y	301	PTY	O7-C8-C11	3.94	120.00	111.48
57	t	201	CDL	OB6-CB5-C51	3.88	119.87	111.48
52	A	201	PC7	O2-C31-C32	3.87	119.85	111.48
52	M	504	PC7	O2-C31-C32	3.87	119.85	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	n	200	8Q1	O4-C1-C6	-3.87	119.52	123.98
56	M	501	PTY	O7-C8-C11	3.85	119.81	111.48
56	H	301	PTY	O7-C8-C11	3.84	119.78	111.48
57	M	502	CDL	OB6-CB5-C51	3.77	119.65	111.48
52	z	301	PC7	O2-C31-C32	3.76	119.61	111.48
52	N	402	PC7	O2-C31-C32	3.75	119.60	111.48
57	d	101	CDL	OA6-CA5-C11	3.72	119.52	111.48
57	d	101	CDL	OB6-CB5-C51	3.66	119.39	111.48
52	N	403	PC7	O2-C31-C32	3.64	119.35	111.48
56	m	202	PTY	O7-C8-C11	3.62	119.31	111.48
58	P	500	NDP	O2B-P2B-O1X	-3.59	96.54	109.33
57	L	601	CDL	OB6-CB5-C51	3.58	119.22	111.48
58	P	500	NDP	O3-PA-O1A	-3.48	100.25	110.70
57	M	502	CDL	OA6-CA5-C11	3.34	118.70	111.48
60	W	200	8Q1	O4-C1-C6	-3.29	120.19	123.98
55	F	500	FMN	C4-N3-C2	-3.25	119.87	125.64
52	L	602	PC7	O2-C31-C32	3.18	118.35	111.48
52	N	403	PC7	O3-C11-C12	3.05	121.15	111.83
60	n	200	8Q1	O4-C1-S44	-3.00	118.87	122.68
58	P	500	NDP	PN-O5D-C5D	-2.99	104.20	121.35
58	P	500	NDP	PA-O5B-C5B	-2.99	104.21	121.35
52	L	602	PC7	O3-C11-C12	2.97	120.91	111.83
60	n	200	8Q1	C32-C34-N36	2.96	122.09	116.48
56	M	501	PTY	O4-C30-C31	2.92	120.74	111.83
57	d	101	CDL	OA8-CA7-C31	2.85	120.53	111.83
57	M	502	CDL	OB8-CB7-C71	2.82	120.43	111.83
52	A	201	PC7	O3-C11-C12	2.78	120.31	111.83
57	N	401	CDL	OB8-CB7-C71	2.77	120.28	111.83
58	P	500	NDP	O2N-PN-O3	2.77	114.75	107.27
57	t	201	CDL	OA8-CA7-C31	2.76	120.24	111.83
57	N	401	CDL	OA8-CA7-C31	2.75	120.22	111.83
56	H	301	PTY	O4-C30-C31	2.75	120.22	111.83
57	L	601	CDL	OB8-CB7-C71	2.74	120.20	111.83
52	M	503	PC7	O3-C11-C12	2.73	120.15	111.83
57	t	201	CDL	OB8-CB7-C71	2.72	120.12	111.83
56	L	603	PTY	O4-C30-C31	2.71	120.09	111.83
56	Y	301	PTY	O4-C30-C31	2.69	120.03	111.83
52	z	301	PC7	O3-C11-C12	2.67	119.96	111.83
56	m	202	PTY	O4-C30-C31	2.66	119.95	111.83
57	L	601	CDL	OA8-CA7-C31	2.66	119.94	111.83
57	d	101	CDL	OB8-CB7-C71	2.65	119.92	111.83
55	F	500	FMN	C4A-C4-N3	2.65	120.00	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	N	402	PC7	O3-C11-C12	2.63	119.85	111.83
60	W	200	8Q1	O4-C1-S44	-2.62	119.35	122.68
52	M	504	PC7	O3-C11-C12	2.60	119.76	111.83
58	P	500	NDP	O3X-P2B-O2X	2.60	117.55	107.80
60	W	200	8Q1	C38-C37-N36	-2.59	106.49	112.00
56	m	201	PTY	O4-C30-C31	2.56	119.63	111.83
58	P	500	NDP	C5B-C4B-C3B	-2.53	106.12	115.21
56	N	404	PTY	O4-C30-C31	2.51	119.50	111.83
55	F	500	FMN	C4A-C10-N10	2.51	120.08	116.48
55	F	500	FMN	O4-C4-C4A	-2.51	119.91	126.53
58	P	500	NDP	O2N-PN-O1N	2.51	124.11	112.44
58	P	500	NDP	O4B-C4B-C3B	2.47	110.06	105.15
58	P	500	NDP	O5D-PN-O1N	-2.45	99.21	108.94
60	n	200	8Q1	O35-C34-N36	-2.27	118.18	122.98
58	P	500	NDP	C2A-N1A-C6A	-2.26	115.01	118.73
55	F	500	FMN	C10-C4A-N5	-2.24	120.23	124.81
58	P	500	NDP	N3A-C4A-N9A	2.20	130.91	127.17
55	F	500	FMN	C5A-C9A-N10	2.19	119.95	117.97
58	P	500	NDP	O3X-P2B-O2B	-2.16	97.44	105.85
57	M	502	CDL	OA8-CA7-C31	2.15	118.40	111.83
58	P	500	NDP	C3N-C2N-N1N	-2.10	120.12	123.20
55	F	500	FMN	C4A-C10-N1	-2.08	119.50	124.59
58	P	500	NDP	C5A-C4A-N3A	-2.06	123.88	126.72
58	P	500	NDP	C5D-C4D-C3D	-2.06	107.81	115.21
55	F	500	FMN	C9A-C5A-N5	-2.06	120.27	122.45

There are no chirality outliers.

All (750) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	A	201	PC7	O31-C31-O2-C2
52	A	201	PC7	C1-O3P-P-O1P
52	A	201	PC7	C1-O3P-P-O2P
52	A	201	PC7	C1-O3P-P-O4P
52	A	201	PC7	C4-O4P-P-O3P
52	A	201	PC7	C4-O4P-P-O1P
52	A	201	PC7	C4-O4P-P-O2P
52	A	201	PC7	O11-C11-O3-C3
52	A	201	PC7	C12-C11-O3-C3
52	L	602	PC7	C1-O3P-P-O2P
52	L	602	PC7	C4-O4P-P-O3P
52	L	602	PC7	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
52	L	602	PC7	C4-O4P-P-O2P
52	M	503	PC7	C32-C31-O2-C2
52	M	503	PC7	O31-C31-O2-C2
52	M	504	PC7	C1-O3P-P-O1P
52	M	504	PC7	C4-O4P-P-O3P
52	M	504	PC7	C4-O4P-P-O1P
52	M	504	PC7	C4-O4P-P-O2P
52	N	402	PC7	C4-O4P-P-O2P
52	N	403	PC7	C32-C31-O2-C2
52	N	403	PC7	C1-O3P-P-O1P
52	N	403	PC7	C1-O3P-P-O2P
52	N	403	PC7	C1-O3P-P-O4P
52	N	403	PC7	C4-O4P-P-O3P
52	N	403	PC7	C4-O4P-P-O1P
52	N	403	PC7	C4-O4P-P-O2P
52	N	403	PC7	O4P-C4-C5-N
52	z	301	PC7	O2-C2-C3-O3
52	z	301	PC7	O4P-C4-C5-N
55	F	500	FMN	N10-C1'-C2'-O2'
55	F	500	FMN	N10-C1'-C2'-C3'
55	F	500	FMN	C1'-C2'-C3'-O3'
55	F	500	FMN	C1'-C2'-C3'-C4'
55	F	500	FMN	C5'-O5'-P-O2P
55	F	500	FMN	C5'-O5'-P-O3P
56	H	301	PTY	C11-C8-O7-C6
56	H	301	PTY	C3-O11-P1-O12
56	H	301	PTY	C3-O11-P1-O13
56	H	301	PTY	C3-O11-P1-O14
56	H	301	PTY	C5-O14-P1-O11
56	H	301	PTY	C5-O14-P1-O12
56	H	301	PTY	C5-O14-P1-O13
56	L	603	PTY	N1-C2-C3-O11
56	L	603	PTY	O10-C8-O7-C6
56	L	603	PTY	C11-C8-O7-C6
56	L	603	PTY	C3-O11-P1-O13
56	L	603	PTY	C5-O14-P1-O11
56	M	501	PTY	N1-C2-C3-O11
56	M	501	PTY	C31-C30-O4-C1
56	M	501	PTY	O30-C30-O4-C1
56	M	501	PTY	O10-C8-O7-C6
56	M	501	PTY	C11-C8-O7-C6
56	M	501	PTY	C3-O11-P1-O13

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Mol	Chain	Res	Type	Atoms
56	M	501	PTY	C5-O14-P1-O11
56	M	501	PTY	C5-O14-P1-O12
56	N	404	PTY	O4-C1-C6-O7
56	N	404	PTY	N1-C2-C3-O11
56	Y	301	PTY	N1-C2-C3-O11
56	Y	301	PTY	C11-C8-O7-C6
56	Y	301	PTY	C3-O11-P1-O12
56	Y	301	PTY	C3-O11-P1-O14
56	m	201	PTY	N1-C2-C3-O11
56	m	201	PTY	C5-O14-P1-O11
56	m	201	PTY	C5-O14-P1-O12
56	m	201	PTY	C5-O14-P1-O13
56	m	202	PTY	N1-C2-C3-O11
56	m	202	PTY	C5-O14-P1-O11
56	m	202	PTY	C5-O14-P1-O13
57	L	601	CDL	CA2-OA2-PA1-OA3
57	L	601	CDL	CA3-OA5-PA1-OA2
57	L	601	CDL	CA3-OA5-PA1-OA3
57	L	601	CDL	CA3-OA5-PA1-OA4
57	L	601	CDL	C11-CA5-OA6-CA4
57	L	601	CDL	CB2-OB2-PB2-OB3
57	L	601	CDL	CB2-OB2-PB2-OB4
57	L	601	CDL	CB2-OB2-PB2-OB5
57	L	601	CDL	CB3-OB5-PB2-OB2
57	L	601	CDL	CB3-OB5-PB2-OB3
57	M	502	CDL	CA2-OA2-PA1-OA4
57	M	502	CDL	CA2-OA2-PA1-OA5
57	M	502	CDL	CA3-OA5-PA1-OA2
57	M	502	CDL	CA3-OA5-PA1-OA3
57	M	502	CDL	C11-CA5-OA6-CA4
57	M	502	CDL	CA4-CA6-OA8-CA7
57	M	502	CDL	CB3-OB5-PB2-OB2
57	M	502	CDL	CB3-OB5-PB2-OB3
57	N	401	CDL	CA2-OA2-PA1-OA4
57	N	401	CDL	CA3-OA5-PA1-OA2
57	N	401	CDL	CA3-OA5-PA1-OA3
57	N	401	CDL	CA3-OA5-PA1-OA4
57	N	401	CDL	CA4-CA3-OA5-PA1
57	N	401	CDL	OA7-CA5-OA6-CA4
57	N	401	CDL	C11-CA5-OA6-CA4
57	N	401	CDL	CB3-OB5-PB2-OB3
57	d	101	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
57	d	101	CDL	O1-C1-CB2-OB2
57	d	101	CDL	CA2-OA2-PA1-OA3
57	d	101	CDL	CA2-OA2-PA1-OA4
57	d	101	CDL	CA2-OA2-PA1-OA5
57	d	101	CDL	CA3-OA5-PA1-OA2
57	d	101	CDL	CA3-OA5-PA1-OA3
57	d	101	CDL	CA3-OA5-PA1-OA4
57	d	101	CDL	C11-CA5-OA6-CA4
57	d	101	CDL	OB9-CB7-OB8-CB6
57	t	201	CDL	O1-C1-CA2-OA2
57	t	201	CDL	CB2-C1-CA2-OA2
57	t	201	CDL	CA3-OA5-PA1-OA2
57	t	201	CDL	CA3-OA5-PA1-OA3
57	t	201	CDL	CB2-OB2-PB2-OB3
57	t	201	CDL	CB2-OB2-PB2-OB5
58	P	500	NDP	C5B-O5B-PA-O1A
58	P	500	NDP	C2N-C3N-C7N-O7N
60	W	200	8Q1	O27-C28-C29-C30
60	W	200	8Q1	O27-C28-C29-C31
60	W	200	8Q1	O27-C28-C29-C32
60	W	200	8Q1	N36-C37-C38-C39
60	W	200	8Q1	C42-C43-S44-C1
60	W	200	8Q1	C28-O27-P24-O3
60	W	200	8Q1	C28-O27-P24-O2
60	W	200	8Q1	C28-O27-P24-O1
60	n	200	8Q1	C1-C6-C7-C8
60	n	200	8Q1	O27-C28-C29-C30
60	n	200	8Q1	O27-C28-C29-C31
60	n	200	8Q1	O27-C28-C29-C32
60	n	200	8Q1	O33-C32-C34-N36
60	n	200	8Q1	C42-C43-S44-C1
60	n	200	8Q1	C28-O27-P24-O2
60	n	200	8Q1	C28-O27-P24-O1
52	N	402	PC7	O11-C11-O3-C3
56	m	202	PTY	O30-C30-O4-C1
57	N	401	CDL	OB9-CB7-OB8-CB6
52	N	402	PC7	C12-C11-O3-C3
57	N	401	CDL	C71-CB7-OB8-CB6
52	N	403	PC7	O11-C11-O3-C3
52	N	403	PC7	O31-C31-O2-C2
56	H	301	PTY	O10-C8-O7-C6
56	Y	301	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
57	L	601	CDL	OA7-CA5-OA6-CA4
57	M	502	CDL	OA7-CA5-OA6-CA4
57	d	101	CDL	OA7-CA5-OA6-CA4
52	L	602	PC7	C12-C11-O3-C3
56	m	202	PTY	C31-C30-O4-C1
57	d	101	CDL	C71-CB7-OB8-CB6
52	A	201	PC7	C32-C31-O2-C2
60	W	200	8Q1	C38-C39-N41-C42
52	N	403	PC7	C12-C11-O3-C3
52	L	602	PC7	O11-C11-O3-C3
57	N	401	CDL	C53-C54-C55-C56
57	t	201	CDL	C77-C78-C79-C80
57	L	601	CDL	O1-C1-CB2-OB2
57	N	401	CDL	O1-C1-CB2-OB2
57	d	101	CDL	O1-C1-CA2-OA2
56	H	301	PTY	O30-C30-O4-C1
55	F	500	FMN	O2'-C2'-C3'-C4'
58	P	500	NDP	O4D-C4D-C5D-O5D
56	H	301	PTY	C31-C30-O4-C1
52	L	602	PC7	C21-C22-C23-C24
52	z	301	PC7	C32-C33-C34-C35
57	d	101	CDL	C22-C23-C24-C25
60	W	200	8Q1	O40-C39-N41-C42
57	N	401	CDL	C72-C73-C74-C75
57	L	601	CDL	C17-C18-C19-C20
57	d	101	CDL	C19-C20-C21-C22
57	t	201	CDL	C55-C56-C57-C58
56	Y	301	PTY	O30-C30-O4-C1
57	L	601	CDL	CA2-C1-CB2-OB2
57	d	101	CDL	CA2-C1-CB2-OB2
57	t	201	CDL	CA2-C1-CB2-OB2
56	Y	301	PTY	C31-C30-O4-C1
57	M	502	CDL	C31-CA7-OA8-CA6
52	L	602	PC7	C19-C20-C21-C22
52	M	503	PC7	C40-C41-C42-C43
56	m	201	PTY	C34-C35-C36-C37
57	N	401	CDL	C82-C83-C84-C85
52	M	503	PC7	C4-C5-N-C6
52	M	503	PC7	C13-C14-C15-C16
56	L	603	PTY	C38-C39-C40-C41
56	m	201	PTY	C12-C13-C14-C15
56	N	404	PTY	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
57	L	601	CDL	O1-C1-CA2-OA2
57	d	101	CDL	C82-C83-C84-C85
57	t	201	CDL	CB7-C71-C72-C73
56	H	301	PTY	C11-C12-C13-C14
57	M	502	CDL	OA9-CA7-OA8-CA6
52	M	503	PC7	O2-C2-C3-O3
57	d	101	CDL	OB6-CB4-CB6-OB8
57	t	201	CDL	C12-C13-C14-C15
56	m	201	PTY	C17-C18-C19-C20
52	M	503	PC7	C12-C11-O3-C3
57	M	502	CDL	C38-C39-C40-C41
56	m	201	PTY	C14-C15-C16-C17
56	m	201	PTY	C22-C23-C24-C25
52	M	503	PC7	C4-C5-N-C7
52	z	301	PC7	C4-C5-N-C6
56	L	603	PTY	C30-C31-C32-C33
56	N	404	PTY	C8-C11-C12-C13
56	Y	301	PTY	C8-C11-C12-C13
56	Y	301	PTY	C30-C31-C32-C33
57	L	601	CDL	CA5-C11-C12-C13
57	N	401	CDL	CB7-C71-C72-C73
57	t	201	CDL	CA7-C31-C32-C33
52	M	503	PC7	C11-C12-C13-C14
52	M	504	PC7	C31-C32-C33-C34
52	M	504	PC7	C11-C12-C13-C14
52	N	403	PC7	C31-C32-C33-C34
56	H	301	PTY	C8-C11-C12-C13
52	A	201	PC7	C33-C34-C35-C36
52	L	602	PC7	C14-C15-C16-C17
57	M	502	CDL	O1-C1-CA2-OA2
57	t	201	CDL	O1-C1-CB2-OB2
52	A	201	PC7	C31-C32-C33-C34
52	L	602	PC7	C31-C32-C33-C34
52	L	602	PC7	C11-C12-C13-C14
56	N	404	PTY	C30-C31-C32-C33
55	F	500	FMN	O2'-C2'-C3'-O3'
56	L	603	PTY	C8-C11-C12-C13
56	L	603	PTY	C31-C30-O4-C1
52	M	503	PC7	O11-C11-O3-C3
52	z	301	PC7	O31-C31-O2-C2
57	M	502	CDL	CB2-C1-CA2-OA2
57	N	401	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
52	A	201	PC7	C4-C5-N-C6
52	N	402	PC7	C4-C5-N-C7
52	N	402	PC7	C4-C5-N-C6
52	z	301	PC7	C4-C5-N-C8
52	z	301	PC7	C32-C31-O2-C2
52	L	602	PC7	C40-C41-C42-C43
52	M	504	PC7	C32-C31-O2-C2
52	A	201	PC7	C4-C5-N-C7
52	A	201	PC7	C4-C5-N-C8
52	N	402	PC7	C4-C5-N-C8
57	L	601	CDL	C22-C23-C24-C25
52	N	402	PC7	C32-C33-C34-C35
56	Y	301	PTY	C40-C41-C42-C43
52	L	602	PC7	C32-C33-C34-C35
52	M	504	PC7	C38-C39-C40-C41
56	H	301	PTY	C24-C25-C26-C27
56	Y	301	PTY	C13-C14-C15-C16
57	L	601	CDL	C11-C12-C13-C14
57	L	601	CDL	C21-C22-C23-C24
57	d	101	CDL	C34-C35-C36-C37
57	t	201	CDL	C17-C18-C19-C20
57	t	201	CDL	C20-C21-C22-C23
57	t	201	CDL	C52-C53-C54-C55
56	m	202	PTY	C8-C11-C12-C13
56	Y	301	PTY	C12-C13-C14-C15
57	N	401	CDL	C14-C15-C16-C17
52	A	201	PC7	C21-C22-C23-C24
56	N	404	PTY	C34-C35-C36-C37
56	Y	301	PTY	C19-C20-C21-C22
56	m	202	PTY	C32-C33-C34-C35
57	M	502	CDL	C15-C16-C17-C18
57	d	101	CDL	C80-C81-C82-C83
56	m	202	PTY	C21-C22-C23-C24
57	N	401	CDL	C37-C38-C39-C40
57	d	101	CDL	C41-C42-C43-C44
57	t	201	CDL	C11-CA5-OA6-CA4
56	L	603	PTY	C39-C40-C41-C42
52	N	403	PC7	C19-C20-C21-C22
52	N	402	PC7	C31-C32-C33-C34
52	N	402	PC7	C11-C12-C13-C14
57	N	401	CDL	CA5-C11-C12-C13
52	L	602	PC7	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
52	M	504	PC7	C32-C33-C34-C35
56	N	404	PTY	C17-C18-C19-C20
56	Y	301	PTY	C21-C22-C23-C24
56	m	202	PTY	C11-C12-C13-C14
57	N	401	CDL	C83-C84-C85-C86
56	L	603	PTY	O30-C30-O4-C1
57	d	101	CDL	C12-C13-C14-C15
52	L	602	PC7	C15-C16-C17-C18
57	N	401	CDL	C80-C81-C82-C83
52	L	602	PC7	C38-C39-C40-C41
57	M	502	CDL	C71-C72-C73-C74
57	M	502	CDL	C78-C79-C80-C81
57	t	201	CDL	C71-C72-C73-C74
52	M	504	PC7	O31-C31-O2-C2
52	z	301	PC7	C18-C19-C20-C21
52	M	503	PC7	C20-C21-C22-C23
57	M	502	CDL	C13-C14-C15-C16
57	M	502	CDL	C14-C15-C16-C17
57	d	101	CDL	CB7-C71-C72-C73
52	A	201	PC7	C32-C33-C34-C35
52	L	602	PC7	C13-C14-C15-C16
52	M	503	PC7	C17-C18-C19-C20
52	M	503	PC7	C19-C20-C21-C22
56	N	404	PTY	C33-C34-C35-C36
57	M	502	CDL	C82-C83-C84-C85
52	A	201	PC7	C40-C41-C42-C43
57	N	401	CDL	C39-C40-C41-C42
57	d	101	CDL	C56-C57-C58-C59
56	m	202	PTY	C34-C35-C36-C37
57	M	502	CDL	C17-C18-C19-C20
57	M	502	CDL	C83-C84-C85-C86
52	M	503	PC7	C4-C5-N-C8
52	A	201	PC7	C41-C42-C43-C44
52	A	201	PC7	C13-C14-C15-C16
57	L	601	CDL	C53-C54-C55-C56
52	z	301	PC7	C42-C43-C44-C45
57	d	101	CDL	C31-C32-C33-C34
57	t	201	CDL	C60-C61-C62-C63
56	N	404	PTY	C11-C8-O7-C6
57	M	502	CDL	C79-C80-C81-C82
57	t	201	CDL	C19-C20-C21-C22
56	H	301	PTY	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
56	Y	301	PTY	C11-C12-C13-C14
56	Y	301	PTY	C25-C26-C27-C28
57	d	101	CDL	C61-C62-C63-C64
52	M	503	PC7	C32-C33-C34-C35
57	L	601	CDL	C37-C38-C39-C40
52	N	403	PC7	C20-C21-C22-C23
52	z	301	PC7	C43-C44-C45-C46
52	z	301	PC7	C35-C36-C37-C38
57	t	201	CDL	C73-C74-C75-C76
57	t	201	CDL	OA7-CA5-OA6-CA4
56	m	202	PTY	C15-C16-C17-C18
52	L	602	PC7	C35-C36-C37-C38
52	M	504	PC7	C18-C19-C20-C21
56	N	404	PTY	C15-C16-C17-C18
57	N	401	CDL	C13-C14-C15-C16
57	N	401	CDL	C15-C16-C17-C18
57	t	201	CDL	C71-CB7-OB8-CB6
52	M	504	PC7	C16-C17-C18-C19
56	m	201	PTY	C16-C17-C18-C19
57	M	502	CDL	C52-C53-C54-C55
57	N	401	CDL	C54-C55-C56-C57
57	t	201	CDL	C61-C62-C63-C64
56	L	603	PTY	C20-C21-C22-C23
57	d	101	CDL	C77-C78-C79-C80
56	m	201	PTY	C18-C19-C20-C21
57	L	601	CDL	C33-C34-C35-C36
57	t	201	CDL	C36-C37-C38-C39
52	M	504	PC7	C17-C18-C19-C20
56	m	202	PTY	C37-C38-C39-C40
52	L	602	PC7	C32-C31-O2-C2
57	t	201	CDL	C51-CB5-OB6-CB4
57	M	502	CDL	CB5-C51-C52-C53
56	m	201	PTY	C32-C33-C34-C35
52	L	602	PC7	O31-C31-O2-C2
57	t	201	CDL	OB7-CB5-OB6-CB4
52	M	504	PC7	C33-C34-C35-C36
57	M	502	CDL	C59-C60-C61-C62
57	N	401	CDL	C31-C32-C33-C34
57	t	201	CDL	C58-C59-C60-C61
57	N	401	CDL	C75-C76-C77-C78
52	A	201	PC7	C11-C12-C13-C14
52	M	503	PC7	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
57	M	502	CDL	C18-C19-C20-C21
52	N	402	PC7	C22-C23-C24-C25
57	N	401	CDL	C73-C74-C75-C76
56	Y	301	PTY	C31-C32-C33-C34
52	z	301	PC7	C4-C5-N-C7
52	z	301	PC7	C34-C35-C36-C37
56	L	603	PTY	C15-C16-C17-C18
57	M	502	CDL	C39-C40-C41-C42
52	M	503	PC7	C18-C19-C20-C21
56	m	201	PTY	C15-C16-C17-C18
57	M	502	CDL	C55-C56-C57-C58
52	A	201	PC7	C37-C38-C39-C40
56	m	201	PTY	C24-C25-C26-C27
56	M	501	PTY	C21-C22-C23-C24
57	M	502	CDL	C54-C55-C56-C57
57	M	502	CDL	C33-C34-C35-C36
56	M	501	PTY	C14-C15-C16-C17
52	N	402	PC7	C21-C22-C23-C24
57	L	601	CDL	C56-C57-C58-C59
57	N	401	CDL	C41-C42-C43-C44
57	d	101	CDL	C51-C52-C53-C54
57	L	601	CDL	OB6-CB4-CB6-OB8
56	H	301	PTY	C13-C14-C15-C16
57	L	601	CDL	C59-C60-C61-C62
57	d	101	CDL	C43-C44-C45-C46
57	M	502	CDL	C19-C20-C21-C22
52	M	504	PC7	C35-C36-C37-C38
56	m	201	PTY	C33-C34-C35-C36
56	m	202	PTY	C25-C26-C27-C28
56	N	404	PTY	C11-C12-C13-C14
56	L	603	PTY	C11-C12-C13-C14
56	N	404	PTY	C13-C14-C15-C16
57	M	502	CDL	C71-CB7-OB8-CB6
57	M	502	CDL	C42-C43-C44-C45
56	m	202	PTY	C39-C40-C41-C42
52	N	402	PC7	C44-C45-C46-C47
52	N	402	PC7	C12-C13-C14-C15
56	M	501	PTY	C17-C18-C19-C20
57	M	502	CDL	C72-C73-C74-C75
57	M	502	CDL	C34-C35-C36-C37
60	n	200	8Q1	O33-C32-C34-O35
52	A	201	PC7	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
56	m	202	PTY	C35-C36-C37-C38
57	t	201	CDL	OB9-CB7-OB8-CB6
52	A	201	PC7	O3P-C1-C2-C3
56	H	301	PTY	O14-C5-C6-C1
57	N	401	CDL	OA5-CA3-CA4-CA6
56	N	404	PTY	O10-C8-O7-C6
57	M	502	CDL	C35-C36-C37-C38
57	N	401	CDL	C74-C75-C76-C77
56	N	404	PTY	C40-C41-C42-C43
57	L	601	CDL	C36-C37-C38-C39
52	z	301	PC7	C40-C41-C42-C43
56	M	501	PTY	C16-C17-C18-C19
56	Y	301	PTY	C32-C33-C34-C35
52	N	403	PC7	C21-C22-C23-C24
56	N	404	PTY	C31-C32-C33-C34
57	d	101	CDL	C42-C43-C44-C45
52	M	503	PC7	C1-C2-C3-O3
52	z	301	PC7	C1-C2-C3-O3
56	H	301	PTY	O4-C1-C6-C5
56	N	404	PTY	O4-C1-C6-C5
57	L	601	CDL	CB3-CB4-CB6-OB8
57	N	401	CDL	CA3-CA4-CA6-OA8
57	t	201	CDL	CB3-CB4-CB6-OB8
56	L	603	PTY	C35-C36-C37-C38
52	M	503	PC7	C21-C22-C23-C24
52	M	504	PC7	C19-C20-C21-C22
57	L	601	CDL	C19-C20-C21-C22
57	M	502	CDL	C31-C32-C33-C34
57	N	401	CDL	C36-C37-C38-C39
57	d	101	CDL	C11-C12-C13-C14
57	d	101	CDL	C71-C72-C73-C74
57	t	201	CDL	C74-C75-C76-C77
57	t	201	CDL	C14-C15-C16-C17
52	M	503	PC7	C36-C37-C38-C39
57	L	601	CDL	C76-C77-C78-C79
56	L	603	PTY	C34-C35-C36-C37
56	N	404	PTY	C32-C33-C34-C35
56	H	301	PTY	C15-C16-C17-C18
57	N	401	CDL	C71-C72-C73-C74
57	M	502	CDL	OB9-CB7-OB8-CB6
60	n	200	8Q1	C28-O27-P24-O3
60	n	200	8Q1	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
52	M	504	PC7	C39-C40-C41-C42
57	M	502	CDL	C41-C42-C43-C44
52	z	301	PC7	C1-C2-O2-C31
57	M	502	CDL	CA3-CA4-OA6-CA5
52	z	301	PC7	C33-C34-C35-C36
56	M	501	PTY	C39-C40-C41-C42
57	N	401	CDL	C81-C82-C83-C84
56	L	603	PTY	C18-C19-C20-C21
58	P	500	NDP	C3D-C4D-C5D-O5D
60	n	200	8Q1	C12-C13-C14-C15
57	t	201	CDL	C31-CA7-OA8-CA6
52	N	403	PC7	C23-C24-C25-C26
57	t	201	CDL	C33-C34-C35-C36
52	N	403	PC7	C44-C45-C46-C47
56	Y	301	PTY	C36-C37-C38-C39
57	t	201	CDL	C43-C44-C45-C46
57	M	502	CDL	C36-C37-C38-C39
57	M	502	CDL	C62-C63-C64-C65
57	N	401	CDL	C20-C21-C22-C23
57	d	101	CDL	C83-C84-C85-C86
56	Y	301	PTY	C20-C21-C22-C23
57	M	502	CDL	C58-C59-C60-C61
57	t	201	CDL	C59-C60-C61-C62
57	d	101	CDL	OA6-CA4-CA6-OA8
56	N	404	PTY	C35-C36-C37-C38
57	d	101	CDL	C84-C85-C86-C87
57	t	201	CDL	C84-C85-C86-C87
56	L	603	PTY	C31-C32-C33-C34
52	L	602	PC7	C4-C5-N-C7
52	L	602	PC7	C18-C19-C20-C21
52	N	402	PC7	C20-C21-C22-C23
52	z	301	PC7	C41-C42-C43-C44
57	M	502	CDL	C53-C54-C55-C56
56	m	201	PTY	C26-C27-C28-C29
57	t	201	CDL	C75-C76-C77-C78
57	N	401	CDL	C31-CA7-OA8-CA6
56	Y	301	PTY	C41-C42-C43-C44
60	n	200	8Q1	C29-C32-C34-O35
52	N	402	PC7	C43-C44-C45-C46
56	H	301	PTY	C18-C19-C20-C21
57	M	502	CDL	C37-C38-C39-C40
60	n	200	8Q1	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
52	N	402	PC7	O3P-C1-C2-C3
57	M	502	CDL	OB5-CB3-CB4-CB6
57	t	201	CDL	OA5-CA3-CA4-CA6
52	z	301	PC7	C22-C23-C24-C25
57	M	502	CDL	C16-C17-C18-C19
57	L	601	CDL	C64-C65-C66-C67
57	M	502	CDL	C40-C41-C42-C43
57	L	601	CDL	C55-C56-C57-C58
56	H	301	PTY	C25-C26-C27-C28
57	M	502	CDL	C44-C45-C46-C47
56	H	301	PTY	C26-C27-C28-C29
57	N	401	CDL	CB5-C51-C52-C53
60	W	200	8Q1	C6-C7-C8-C9
52	N	403	PC7	C1-C2-C3-O3
57	M	502	CDL	CB3-CB4-CB6-OB8
57	d	101	CDL	CB3-CB4-CB6-OB8
57	L	601	CDL	C51-C52-C53-C54
56	N	404	PTY	C37-C38-C39-C40
52	A	201	PC7	C15-C16-C17-C18
56	L	603	PTY	C32-C33-C34-C35
60	n	200	8Q1	C9-C10-C11-C12
56	m	201	PTY	C25-C26-C27-C28
57	t	201	CDL	OA9-CA7-OA8-CA6
57	N	401	CDL	C34-C35-C36-C37
52	A	201	PC7	O3P-C1-C2-O2
52	N	403	PC7	O3P-C1-C2-O2
57	M	502	CDL	OB5-CB3-CB4-OB6
52	M	503	PC7	C43-C44-C45-C46
56	L	603	PTY	C14-C15-C16-C17
56	Y	301	PTY	C18-C19-C20-C21
56	m	202	PTY	C20-C21-C22-C23
57	L	601	CDL	C72-C73-C74-C75
56	M	501	PTY	C13-C14-C15-C16
57	N	401	CDL	C19-C20-C21-C22
57	t	201	CDL	C63-C64-C65-C66
52	L	602	PC7	C20-C21-C22-C23
52	N	403	PC7	C32-C33-C34-C35
56	L	603	PTY	C13-C14-C15-C16
57	M	502	CDL	C22-C23-C24-C25
57	M	502	CDL	OB6-CB4-CB6-OB8
57	N	401	CDL	OA6-CA4-CA6-OA8
57	N	401	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
57	t	201	CDL	OA6-CA4-CA6-OA8
57	t	201	CDL	C57-C58-C59-C60
58	P	500	NDP	C2N-C3N-C7N-N7N
52	M	504	PC7	C41-C42-C43-C44
57	d	101	CDL	C37-C38-C39-C40
57	t	201	CDL	CB5-C51-C52-C53
57	M	502	CDL	C57-C58-C59-C60
57	t	201	CDL	C51-C52-C53-C54
57	d	101	CDL	C52-C53-C54-C55
52	N	402	PC7	C45-C46-C47-C48
52	N	403	PC7	C35-C36-C37-C38
56	Y	301	PTY	C14-C15-C16-C17
57	N	401	CDL	C78-C79-C80-C81
57	t	201	CDL	C42-C43-C44-C45
56	H	301	PTY	C37-C38-C39-C40
56	m	202	PTY	C11-C8-O7-C6
52	L	602	PC7	C12-C13-C14-C15
52	M	504	PC7	C37-C38-C39-C40
52	M	504	PC7	C14-C15-C16-C17
57	N	401	CDL	OA9-CA7-OA8-CA6
56	Y	301	PTY	O14-C5-C6-C1
57	d	101	CDL	OA5-CA3-CA4-CA6
57	M	502	CDL	C64-C65-C66-C67
52	N	402	PC7	C40-C41-C42-C43
57	N	401	CDL	C55-C56-C57-C58
57	L	601	CDL	C20-C21-C22-C23
52	M	504	PC7	C15-C16-C17-C18
52	N	402	PC7	C38-C39-C40-C41
56	M	501	PTY	C33-C34-C35-C36
57	d	101	CDL	CA5-C11-C12-C13
56	H	301	PTY	C23-C24-C25-C26
57	L	601	CDL	C61-C62-C63-C64
56	H	301	PTY	C1-C6-O7-C8
57	L	601	CDL	C40-C41-C42-C43
56	Y	301	PTY	O14-C5-C6-O7
57	d	101	CDL	OA5-CA3-CA4-OA6
57	t	201	CDL	OA5-CA3-CA4-OA6
52	L	602	PC7	C1-C2-C3-O3
52	M	504	PC7	C1-C2-C3-O3
57	N	401	CDL	CB3-CB4-CB6-OB8
57	t	201	CDL	CA3-CA4-CA6-OA8
57	t	201	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
52	A	201	PC7	C5-C4-O4P-P
57	M	502	CDL	C51-C52-C53-C54
56	Y	301	PTY	C37-C38-C39-C40
52	L	602	PC7	O2-C2-C3-O3
52	N	403	PC7	O2-C2-C3-O3
57	t	201	CDL	OB6-CB4-CB6-OB8
57	M	502	CDL	C43-C44-C45-C46
57	d	101	CDL	C36-C37-C38-C39
52	L	602	PC7	C4-C5-N-C8
52	N	403	PC7	C4-C5-N-C7
52	N	403	PC7	C4-C5-N-C8
52	L	602	PC7	C34-C35-C36-C37
57	L	601	CDL	C62-C63-C64-C65
52	A	201	PC7	O4P-C4-C5-N
52	N	402	PC7	O4P-C4-C5-N
56	M	501	PTY	C19-C20-C21-C22
52	M	503	PC7	C31-C32-C33-C34
56	m	202	PTY	O10-C8-O7-C6
57	N	401	CDL	C35-C36-C37-C38
56	m	202	PTY	C22-C23-C24-C25
57	M	502	CDL	C74-C75-C76-C77
56	Y	301	PTY	C17-C18-C19-C20
56	m	201	PTY	C21-C22-C23-C24
52	N	403	PC7	C40-C41-C42-C43
57	d	101	CDL	C75-C76-C77-C78
57	L	601	CDL	C18-C19-C20-C21
52	L	602	PC7	C4-C5-N-C6
57	M	502	CDL	C21-C22-C23-C24
57	M	502	CDL	C73-C74-C75-C76
57	N	401	CDL	OB5-CB3-CB4-CB6
56	Y	301	PTY	C26-C27-C28-C29
56	H	301	PTY	C17-C18-C19-C20
57	d	101	CDL	C59-C60-C61-C62
52	N	402	PC7	C18-C19-C20-C21
52	z	301	PC7	C39-C40-C41-C42
52	N	402	PC7	O3P-C1-C2-O2
56	H	301	PTY	O14-C5-C6-O7
57	L	601	CDL	OB5-CB3-CB4-OB6
57	N	401	CDL	OA5-CA3-CA4-OA6
57	N	401	CDL	OB5-CB3-CB4-OB6
52	N	403	PC7	C15-C16-C17-C18
57	d	101	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
56	L	603	PTY	C17-C18-C19-C20
57	N	401	CDL	C76-C77-C78-C79
57	t	201	CDL	C31-C32-C33-C34
52	A	201	PC7	C18-C19-C20-C21
56	L	603	PTY	C33-C34-C35-C36
52	M	504	PC7	C1-O3P-P-O2P
52	M	504	PC7	C1-O3P-P-O4P
52	N	402	PC7	C4-O4P-P-O3P
52	N	403	PC7	C4-C5-N-C6
52	z	301	PC7	C1-O3P-P-O2P
56	L	603	PTY	C5-O14-P1-O13
56	M	501	PTY	C5-O14-P1-O13
56	Y	301	PTY	C3-O11-P1-O13
57	L	601	CDL	CA2-OA2-PA1-OA5
57	L	601	CDL	CB3-OB5-PB2-OB4
57	M	502	CDL	CB3-OB5-PB2-OB4
57	N	401	CDL	CA2-OA2-PA1-OA3
57	N	401	CDL	CA2-OA2-PA1-OA5
57	N	401	CDL	CB3-OB5-PB2-OB2
57	N	401	CDL	CB3-OB5-PB2-OB4
57	t	201	CDL	CA3-OA5-PA1-OA4
57	t	201	CDL	CB2-OB2-PB2-OB4
58	P	500	NDP	C5D-O5D-PN-O1N
52	M	504	PC7	C22-C23-C24-C25
56	m	202	PTY	C6-C5-O14-P1
52	A	201	PC7	C12-C13-C14-C15
57	L	601	CDL	C38-C39-C40-C41
56	M	501	PTY	C38-C39-C40-C41
56	Y	301	PTY	C23-C24-C25-C26
52	N	403	PC7	O3P-C1-C2-C3
57	L	601	CDL	OB5-CB3-CB4-CB6
57	L	601	CDL	CB2-C1-CA2-OA2
57	L	601	CDL	C74-C75-C76-C77
57	M	502	CDL	C12-C13-C14-C15
57	L	601	CDL	C23-C24-C25-C26
56	H	301	PTY	C32-C33-C34-C35
52	M	504	PC7	O2-C2-C3-O3
56	H	301	PTY	O4-C1-C6-O7
56	L	603	PTY	C37-C38-C39-C40
57	d	101	CDL	C35-C36-C37-C38
52	z	301	PC7	C31-C32-C33-C34
57	N	401	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
57	t	201	CDL	C39-C40-C41-C42
57	d	101	CDL	CA3-CA4-CA6-OA8
57	t	201	CDL	C79-C80-C81-C82
57	L	601	CDL	C32-C31-CA7-OA8
52	N	403	PC7	C16-C17-C18-C19
56	Y	301	PTY	C39-C40-C41-C42
57	d	101	CDL	C38-C39-C40-C41
52	z	301	PC7	C19-C20-C21-C22
57	t	201	CDL	C41-C42-C43-C44
56	Y	301	PTY	C16-C17-C18-C19
60	n	200	8Q1	C29-C32-C34-N36
52	N	402	PC7	C15-C16-C17-C18
56	Y	301	PTY	C35-C36-C37-C38
57	N	401	CDL	C23-C24-C25-C26
52	A	201	PC7	C36-C37-C38-C39
60	n	200	8Q1	C13-C14-C15-C16
57	N	401	CDL	C1-CA2-OA2-PA1
57	d	101	CDL	C33-C34-C35-C36
57	d	101	CDL	C57-C58-C59-C60
57	L	601	CDL	C31-C32-C33-C34
57	t	201	CDL	C38-C39-C40-C41
52	L	602	PC7	C1-C2-O2-C31
52	L	602	PC7	C23-C24-C25-C26
52	N	402	PC7	C41-C42-C43-C44
56	m	201	PTY	O14-C5-C6-O7
57	d	101	CDL	C18-C19-C20-C21
56	m	201	PTY	C20-C21-C22-C23
52	L	602	PC7	C41-C42-C43-C44
52	N	403	PC7	C2-C1-O3P-P
56	M	501	PTY	C22-C23-C24-C25
57	N	401	CDL	C38-C39-C40-C41
57	t	201	CDL	C24-C25-C26-C27
52	z	301	PC7	C23-C24-C25-C26
52	M	504	PC7	C12-C13-C14-C15
58	P	500	NDP	O4D-C1D-N1N-C6N
57	M	502	CDL	C12-C11-CA5-OA6
56	m	202	PTY	C26-C27-C28-C29
57	d	101	CDL	C1-CB2-OB2-PB2
57	t	201	CDL	C1-CA2-OA2-PA1
52	A	201	PC7	C38-C39-C40-C41
56	m	201	PTY	C38-C39-C40-C41
56	N	404	PTY	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
58	P	500	NDP	C2D-C1D-N1N-C6N
57	d	101	CDL	OB5-CB3-CB4-OB6
52	N	402	PC7	C23-C24-C25-C26
56	M	501	PTY	C31-C32-C33-C34
56	m	201	PTY	C39-C40-C41-C42
52	N	403	PC7	C11-C12-C13-C14
52	A	201	PC7	O2-C2-C3-O3
57	N	401	CDL	CB4-CB3-OB5-PB2
55	F	500	FMN	C5'-O5'-P-O1P
52	A	201	PC7	C22-C23-C24-C25
52	N	403	PC7	C33-C34-C35-C36
52	A	201	PC7	C39-C40-C41-C42
52	M	503	PC7	C22-C23-C24-C25
52	M	504	PC7	C44-C45-C46-C47
56	H	301	PTY	C22-C23-C24-C25
52	A	201	PC7	C43-C44-C45-C46
57	d	101	CDL	C79-C80-C81-C82
52	M	503	PC7	C37-C38-C39-C40
57	L	601	CDL	OA5-CA3-CA4-CA6
57	M	502	CDL	CA5-C11-C12-C13
57	L	601	CDL	C12-C11-CA5-OA6
57	d	101	CDL	C58-C59-C60-C61
52	z	301	PC7	C20-C21-C22-C23
58	P	500	NDP	O4B-C4B-C5B-O5B
56	N	404	PTY	C19-C20-C21-C22
52	N	403	PC7	C41-C42-C43-C44
57	N	401	CDL	OB7-CB5-OB6-CB4
57	N	401	CDL	C51-CB5-OB6-CB4
57	t	201	CDL	C16-C17-C18-C19
56	L	603	PTY	C24-C25-C26-C27
52	M	504	PC7	C4-C5-N-C6
52	M	504	PC7	C42-C43-C44-C45
52	z	301	PC7	C14-C15-C16-C17
52	L	602	PC7	C22-C23-C24-C25
58	P	500	NDP	C2B-O2B-P2B-O3X
56	H	301	PTY	C6-C5-O14-P1
57	t	201	CDL	CA5-C11-C12-C13
56	m	201	PTY	C12-C11-C8-O7
52	z	301	PC7	O3-C11-C12-C13
56	m	202	PTY	C12-C11-C8-O7
57	d	101	CDL	C24-C25-C26-C27
57	N	401	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
57	t	201	CDL	CA3-CA4-OA6-CA5
56	H	301	PTY	C39-C40-C41-C42
52	z	301	PC7	C13-C14-C15-C16
56	m	202	PTY	C23-C24-C25-C26
57	d	101	CDL	C72-C71-CB7-OB8
57	d	101	CDL	C16-C17-C18-C19
56	H	301	PTY	C20-C21-C22-C23
52	M	504	PC7	C20-C21-C22-C23
56	m	202	PTY	C38-C39-C40-C41
52	M	504	PC7	C4-C5-N-C8
57	M	502	CDL	C75-C76-C77-C78
57	t	201	CDL	C32-C33-C34-C35
52	M	504	PC7	C45-C46-C47-C48
52	N	403	PC7	C36-C37-C38-C39
57	t	201	CDL	C82-C83-C84-C85
57	L	601	CDL	C12-C11-CA5-OA7
56	m	202	PTY	C12-C11-C8-O10
57	d	101	CDL	C72-C71-CB7-OB9
56	m	201	PTY	C12-C11-C8-O10
56	M	501	PTY	C35-C36-C37-C38
56	N	404	PTY	C36-C37-C38-C39
52	M	503	PC7	O3-C11-C12-C13
52	z	301	PC7	O2-C31-C32-C33
56	M	501	PTY	C34-C35-C36-C37

There are no ring outliers.

26 monomers are involved in 117 short contacts:

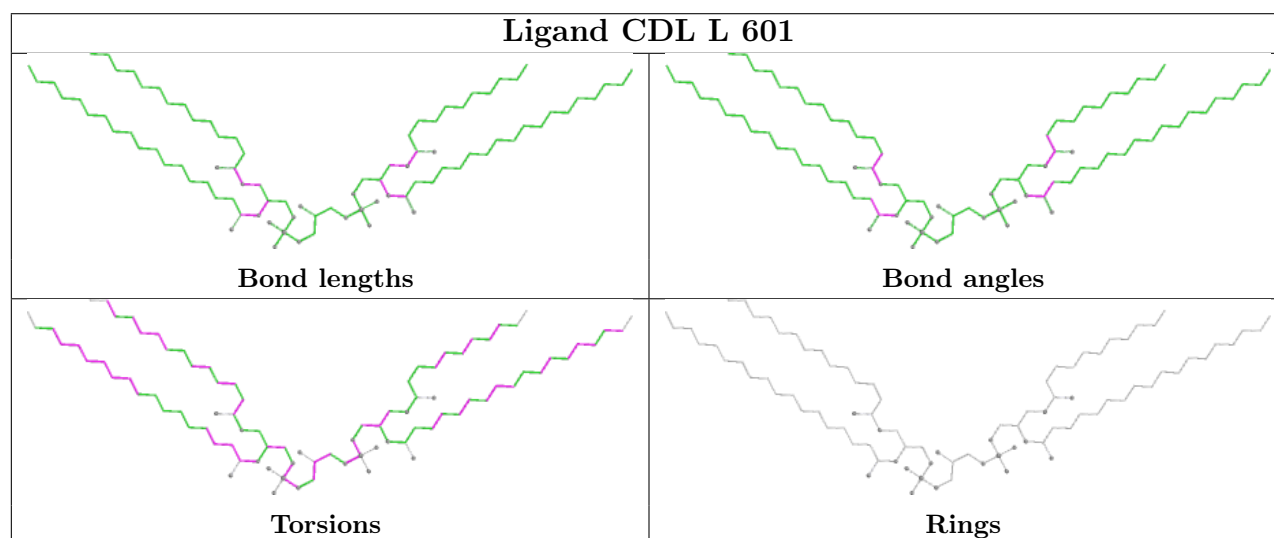
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	L	601	CDL	9	0
53	I	500	SF4	1	0
52	M	503	PC7	5	0
53	F	501	SF4	2	0
56	m	201	PTY	6	0
58	P	500	NDP	1	0
57	d	101	CDL	3	0
52	N	403	PC7	11	0
52	z	301	PC7	6	0
53	G	802	SF4	1	0
55	F	500	FMN	1	0
56	Y	301	PTY	4	0
52	A	201	PC7	5	0

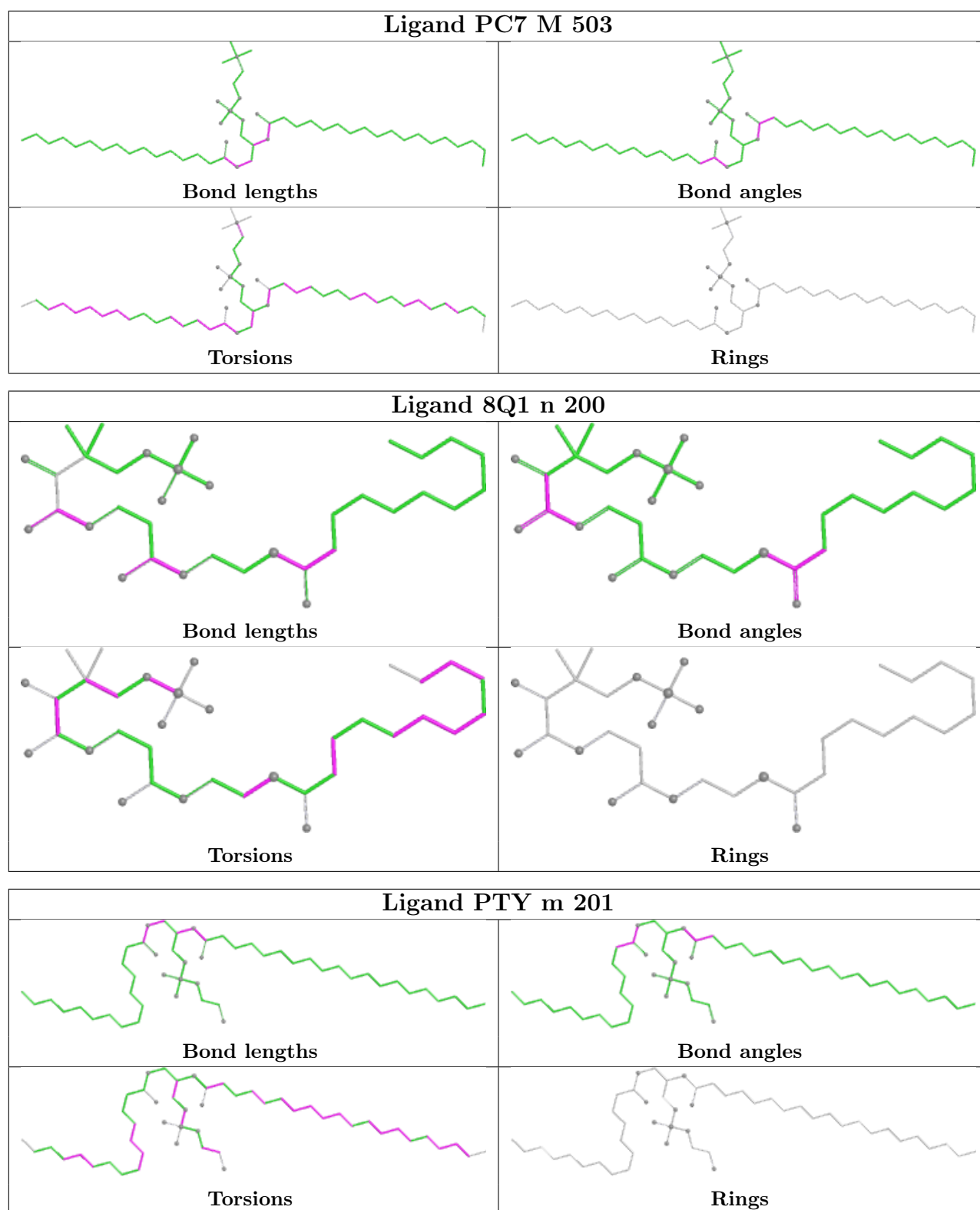
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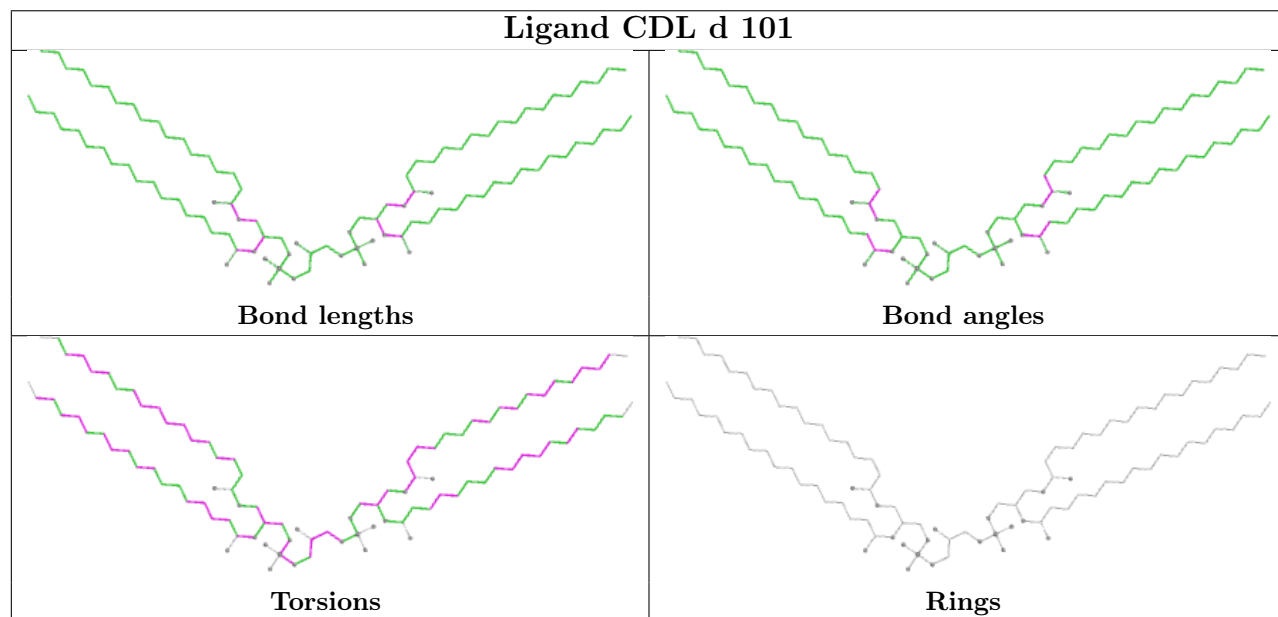
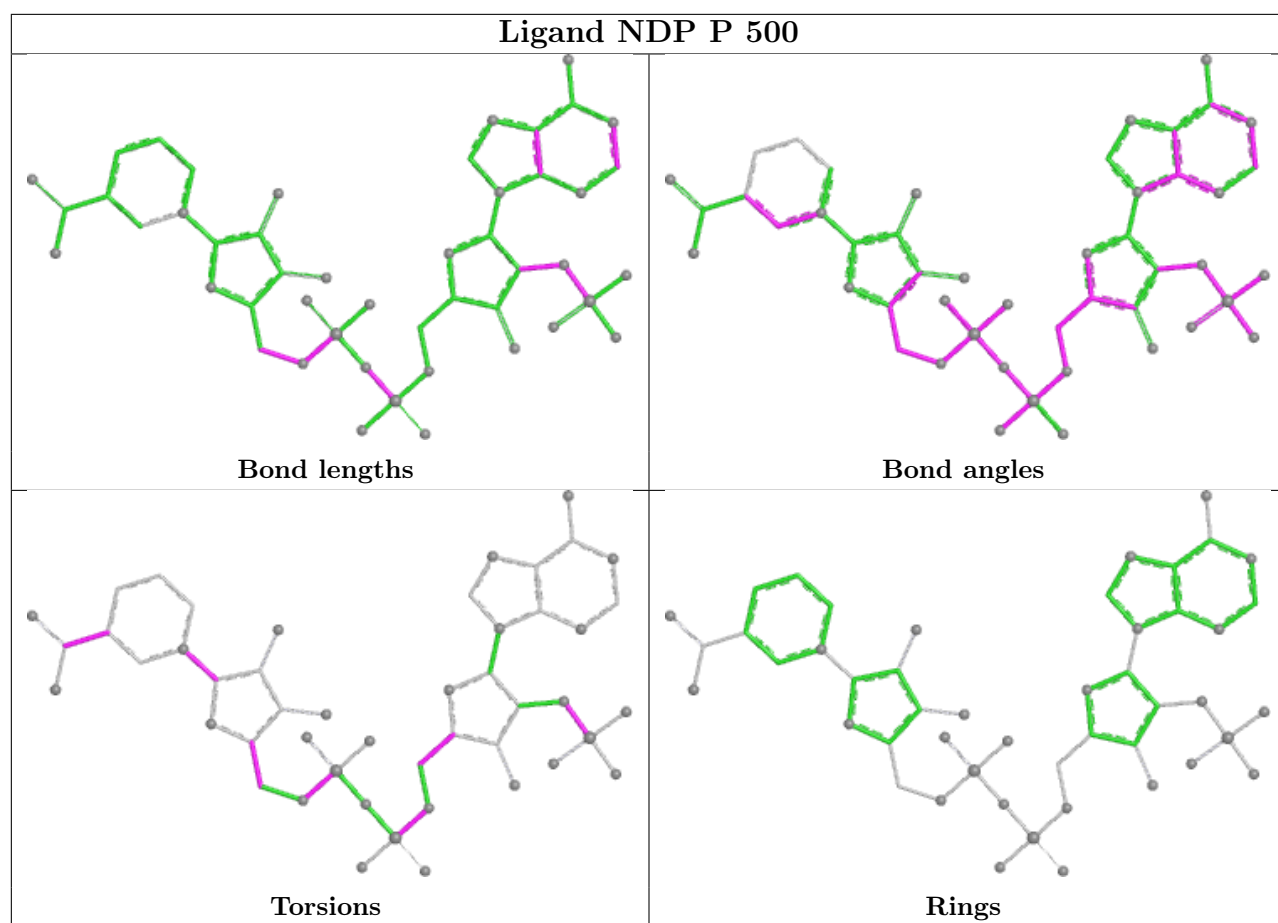
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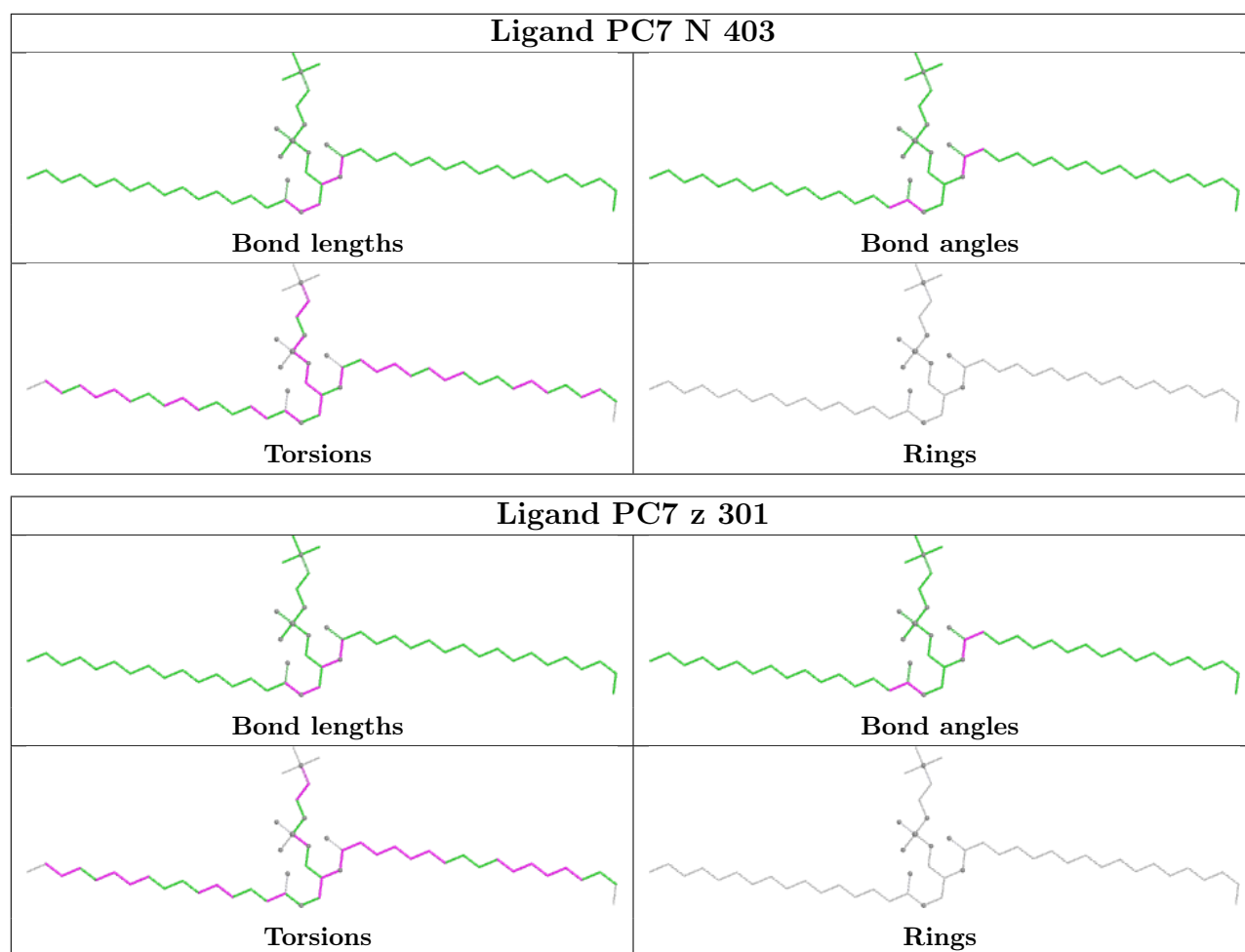
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	M	501	PTY	8	0
52	M	504	PC7	2	0
56	m	202	PTY	2	0
52	L	602	PC7	11	0
60	W	200	8Q1	1	0
56	N	404	PTY	1	0
57	t	201	CDL	9	0
52	N	402	PC7	2	0
57	M	502	CDL	7	0
54	E	500	FES	1	0
56	H	301	PTY	7	0
56	L	603	PTY	2	0
57	N	401	CDL	10	0

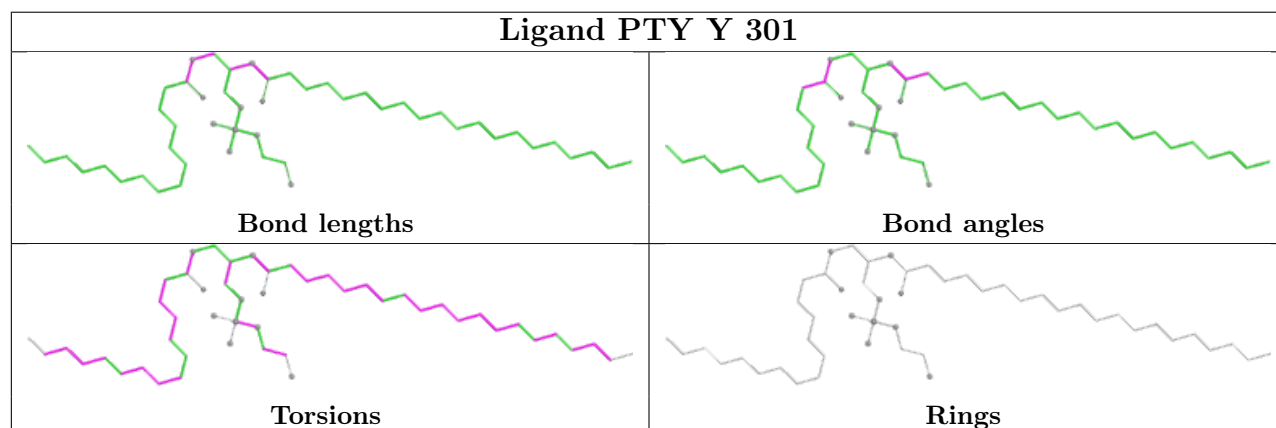
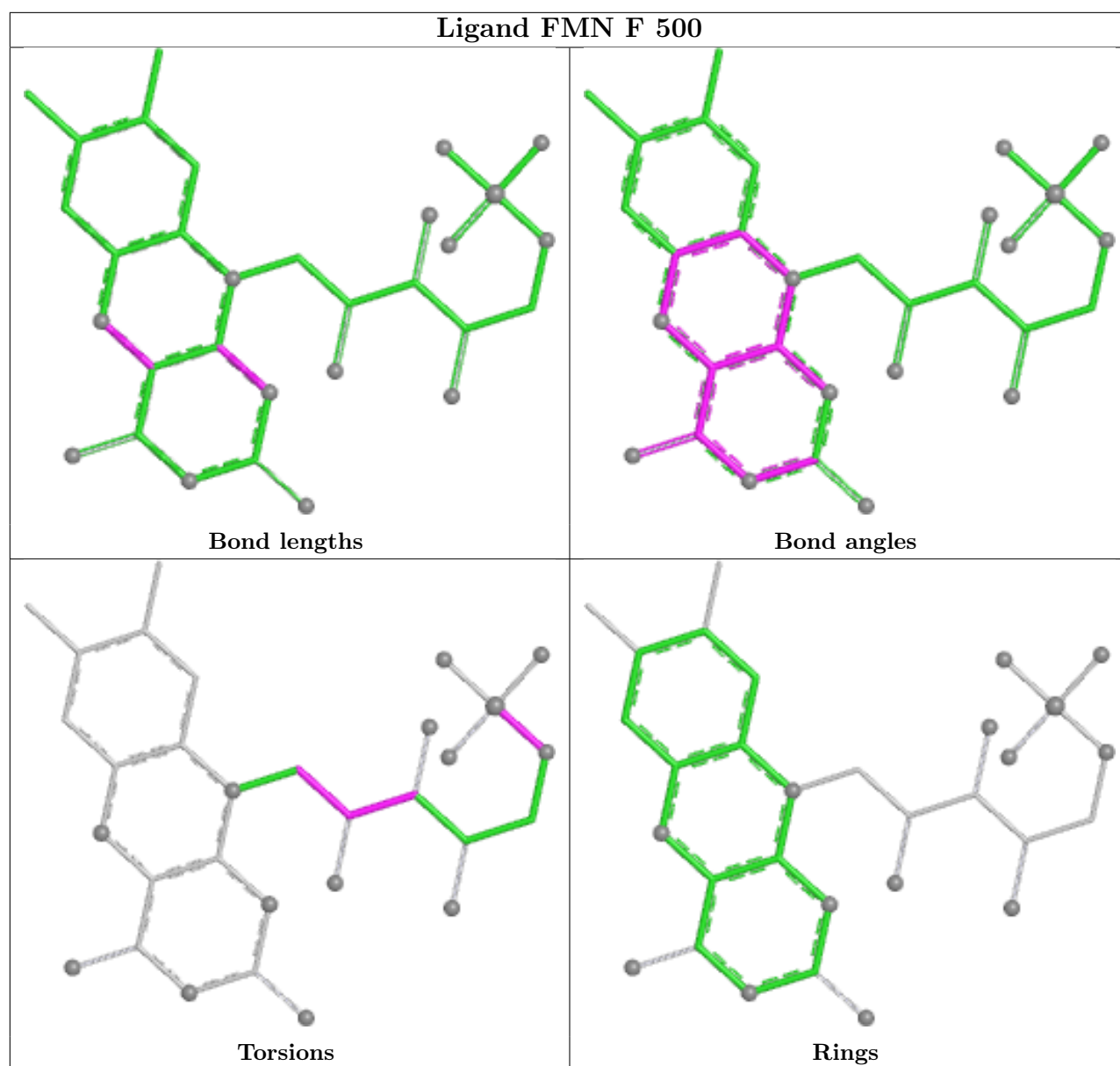
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

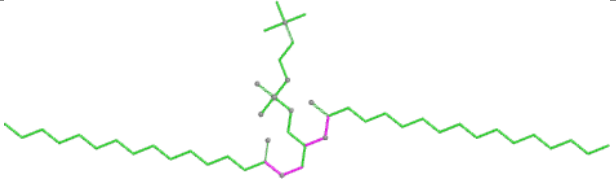
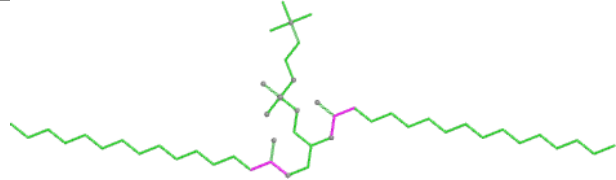
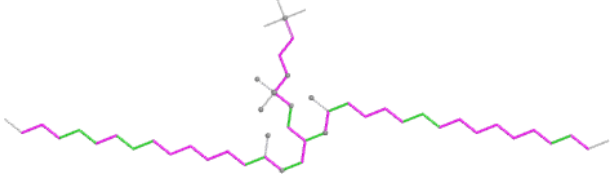
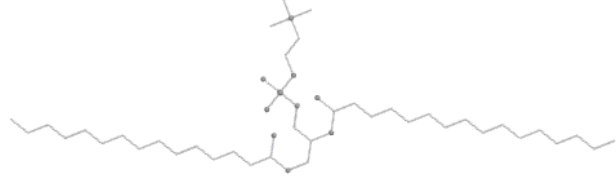


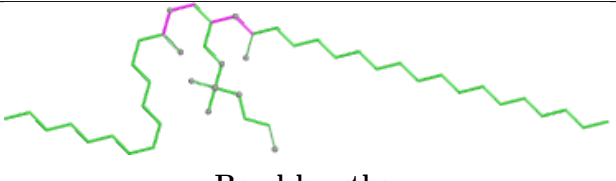
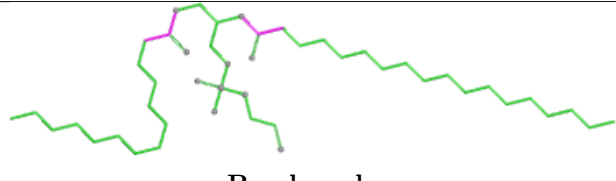
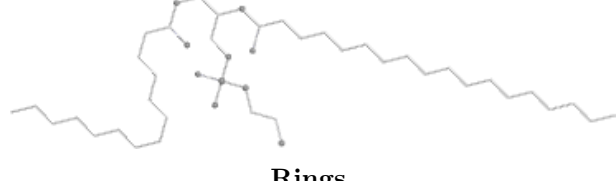


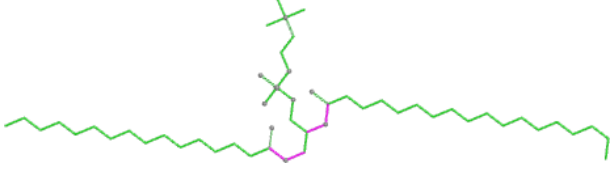
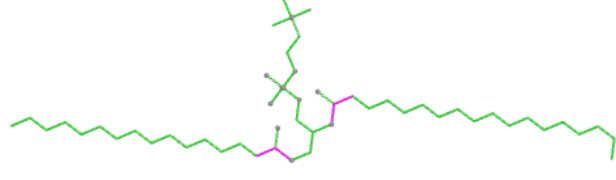
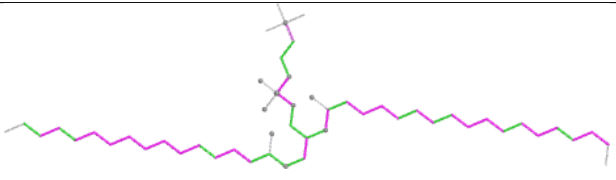
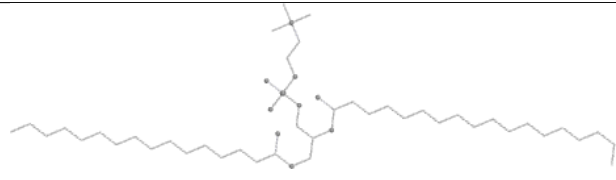


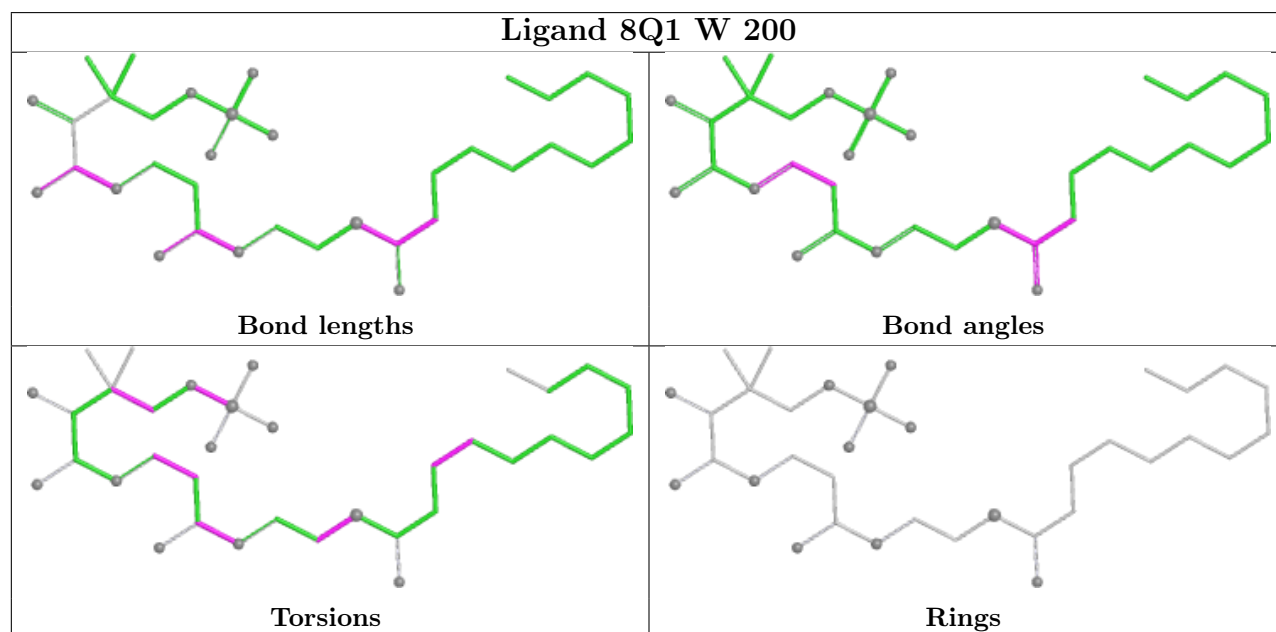
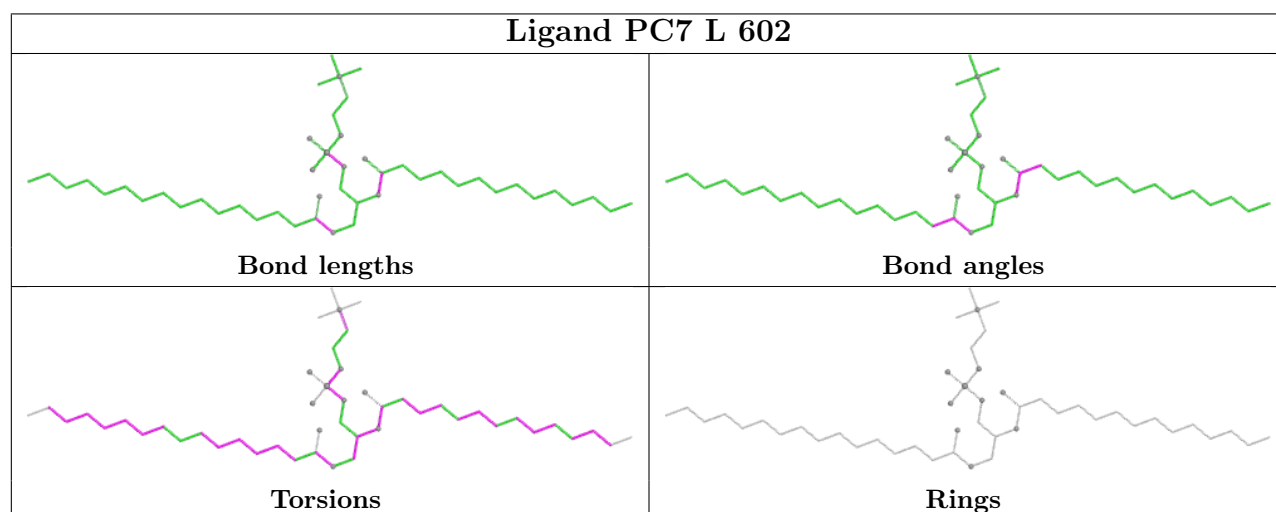
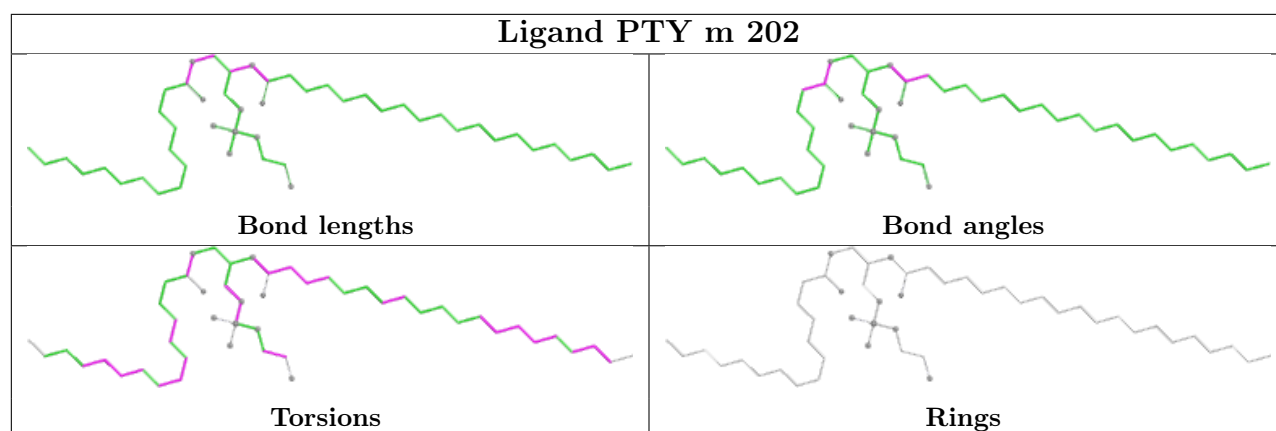


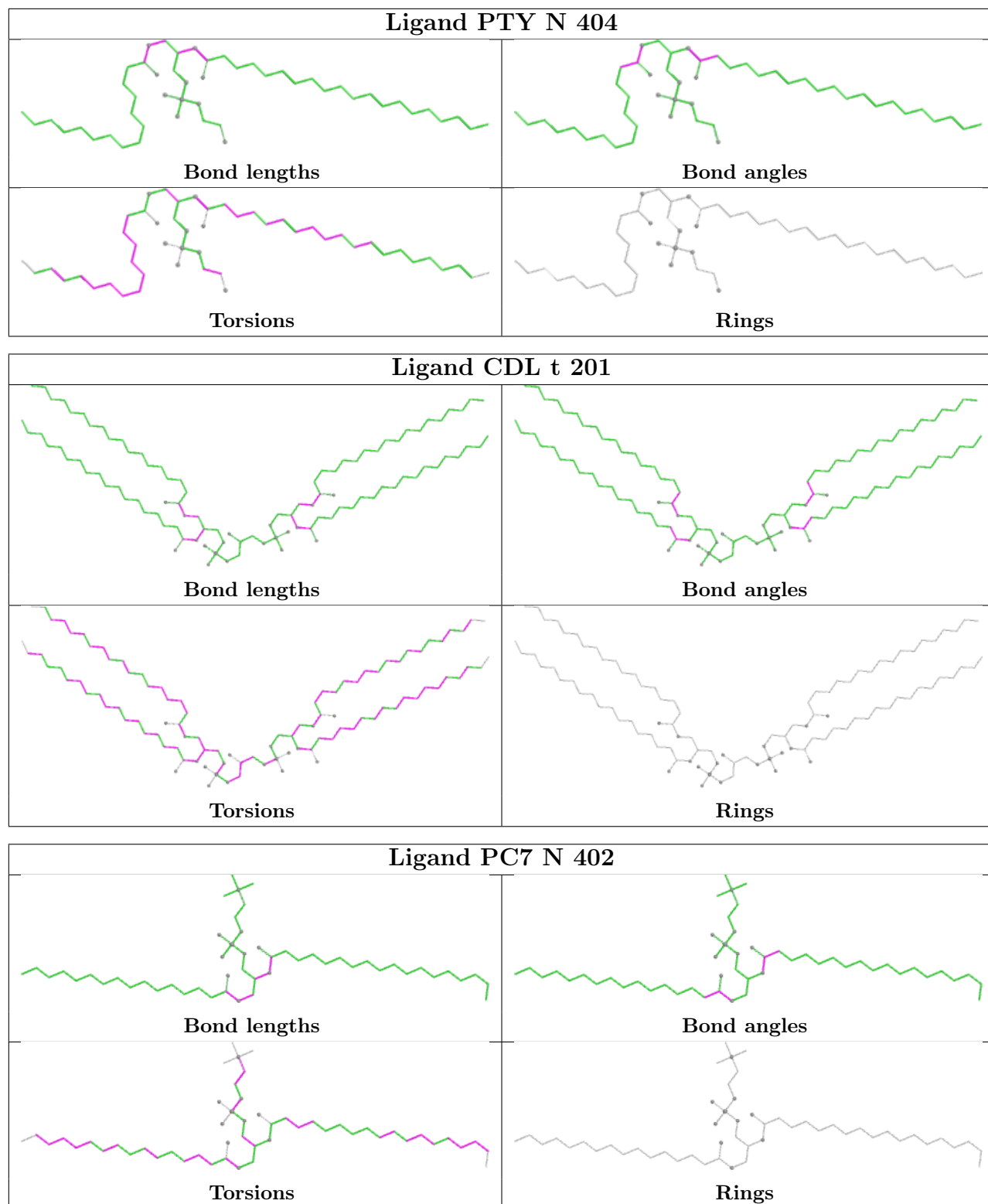


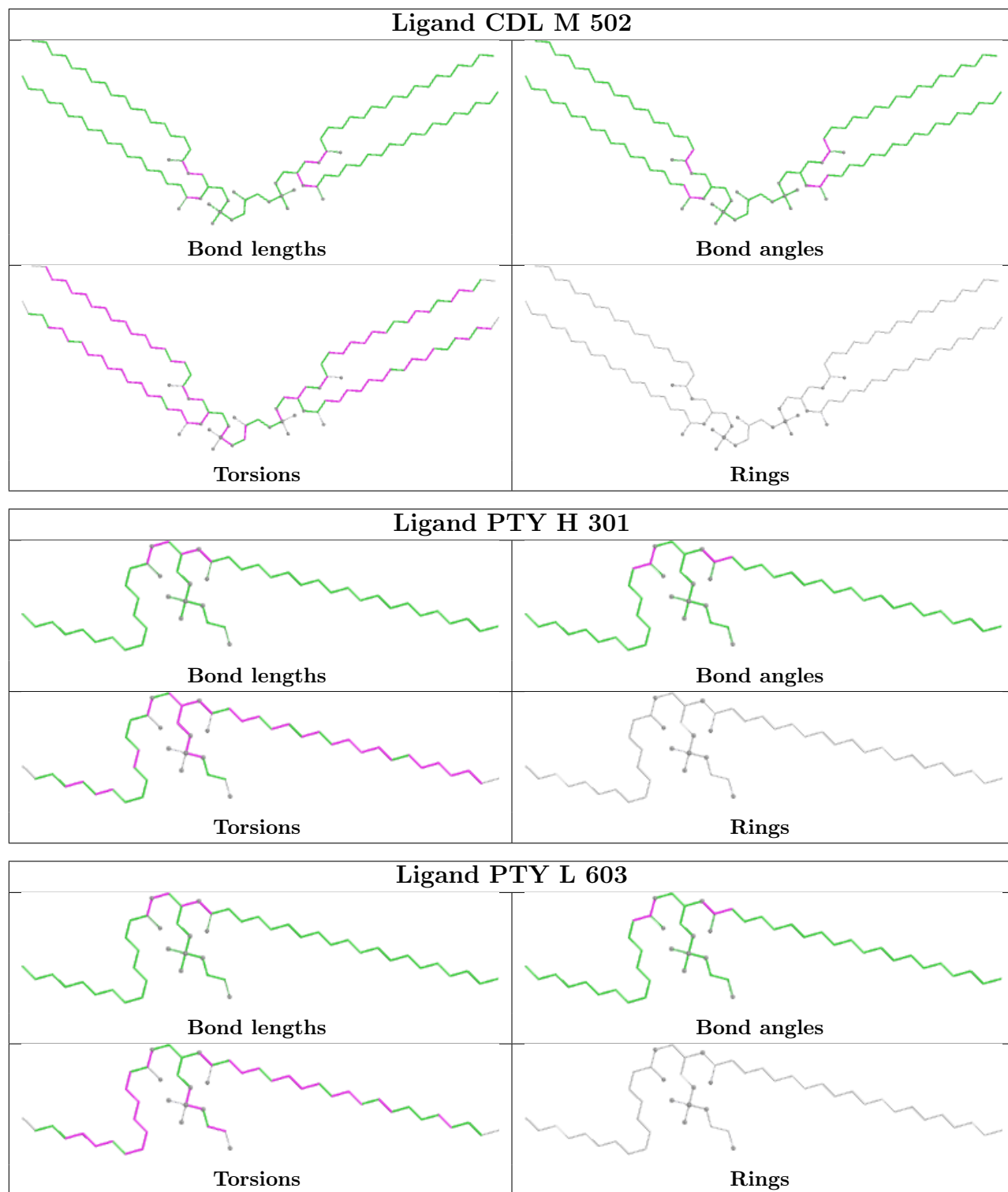
Ligand PC7 A 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

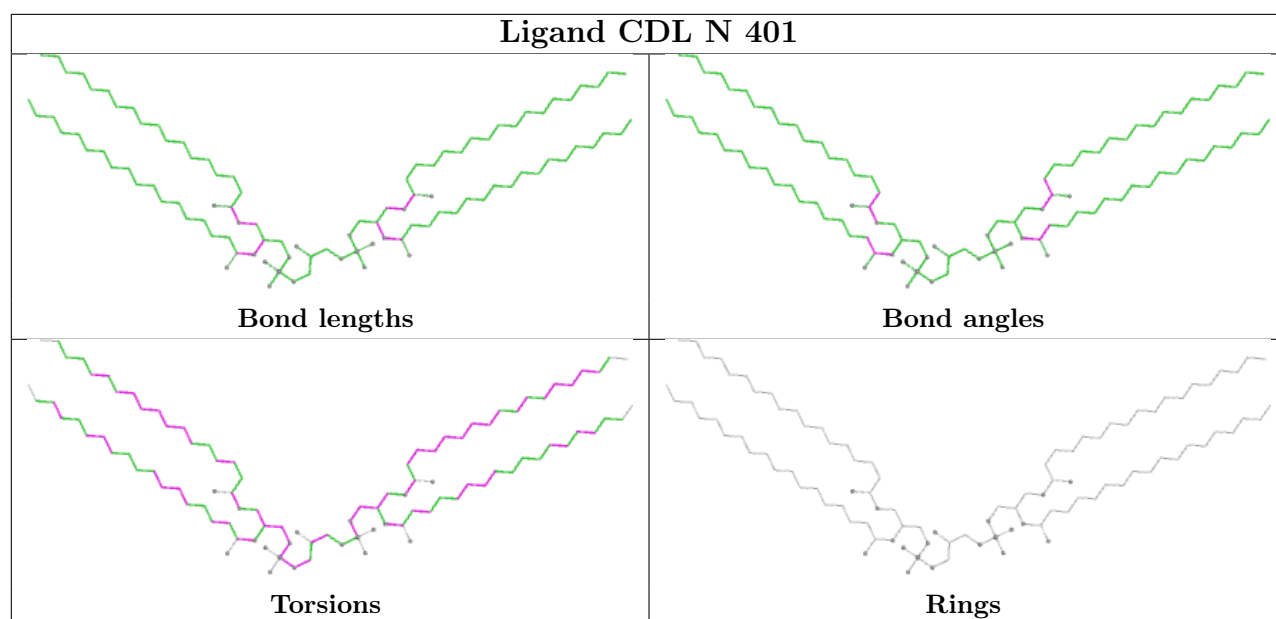
Ligand PTY M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC7 M 504	
 Bond lengths	 Bond angles
 Torsions	 Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

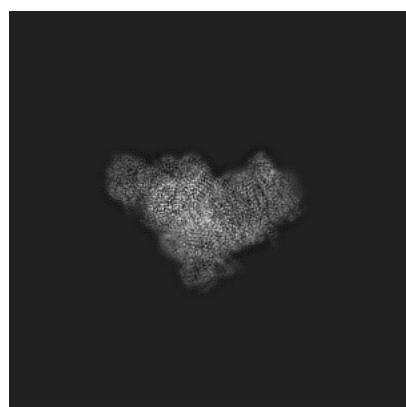
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11880. These allow visual inspection of the internal detail of the map and identification of artifacts.

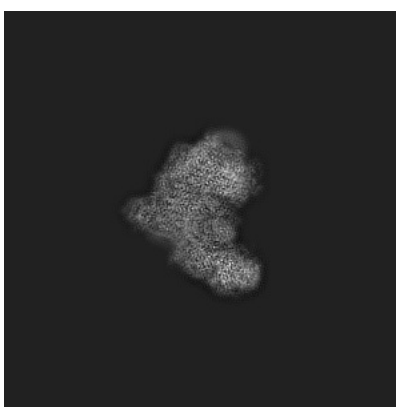
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

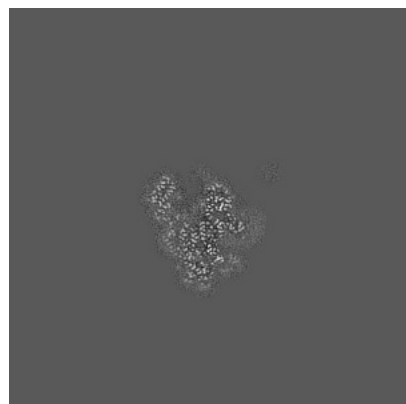


Z

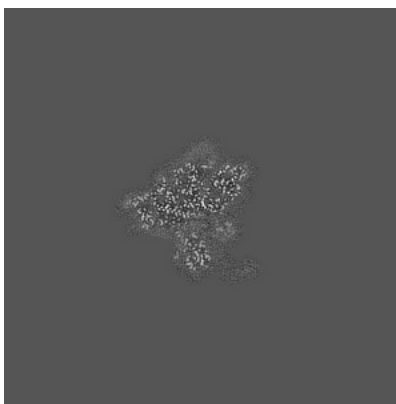
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

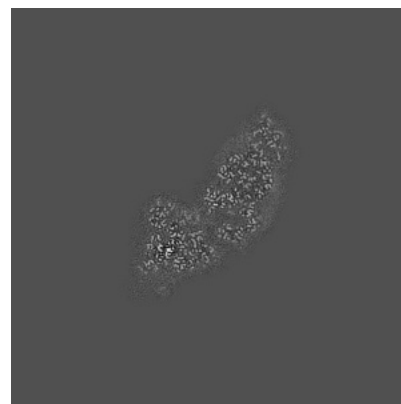
6.2.1 Primary map



X Index: 300



Y Index: 300

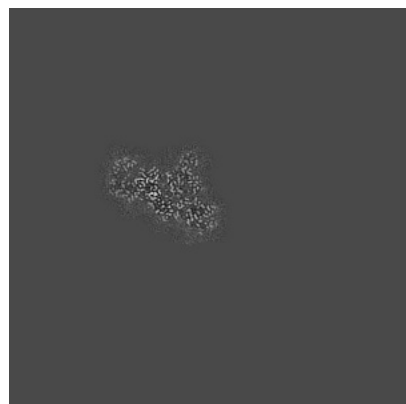


Z Index: 300

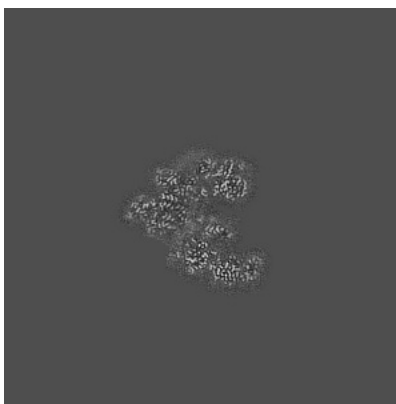
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

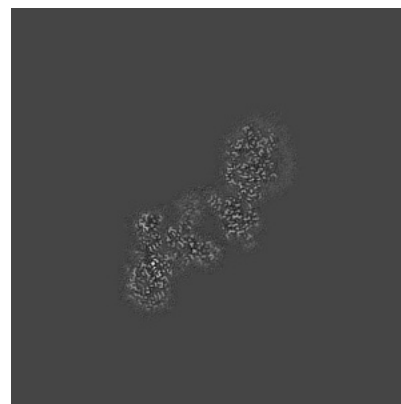
6.3.1 Primary map



X Index: 220



Y Index: 274

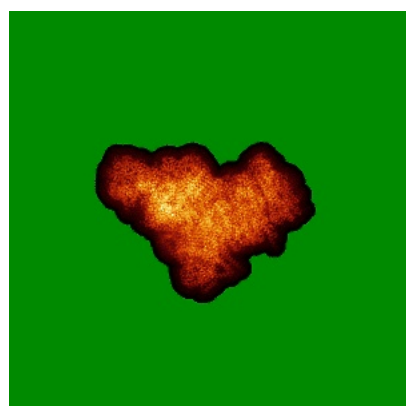


Z Index: 332

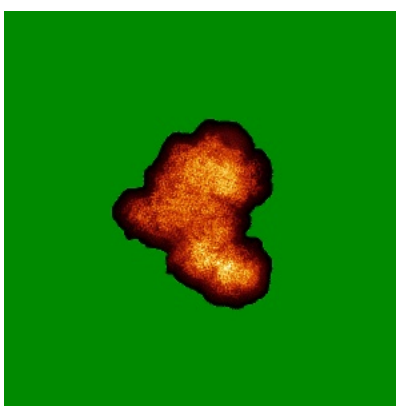
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

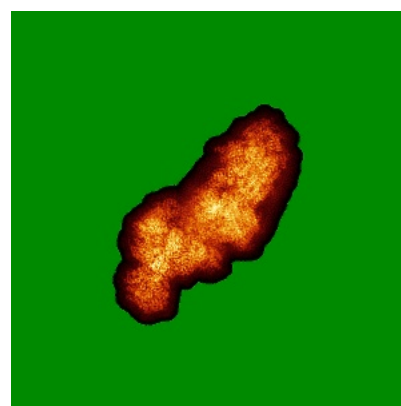
6.4.1 Primary map



X



Y

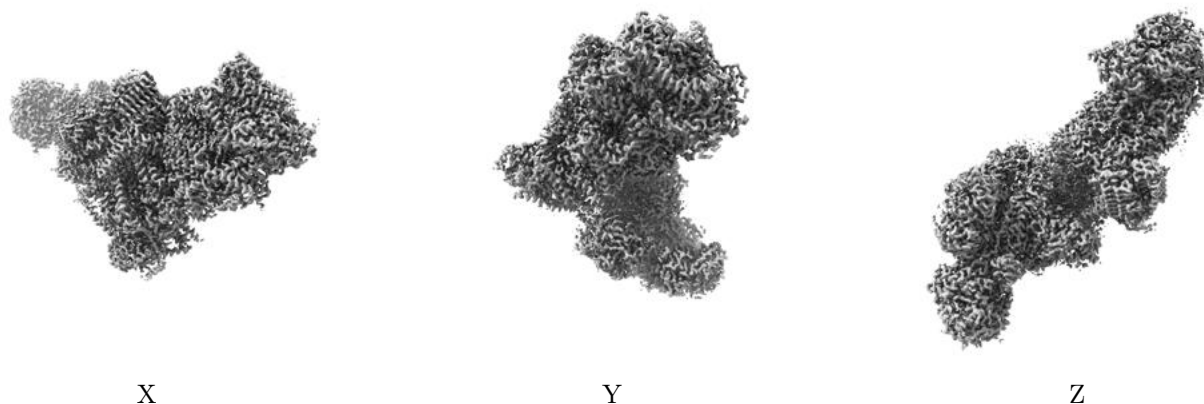


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

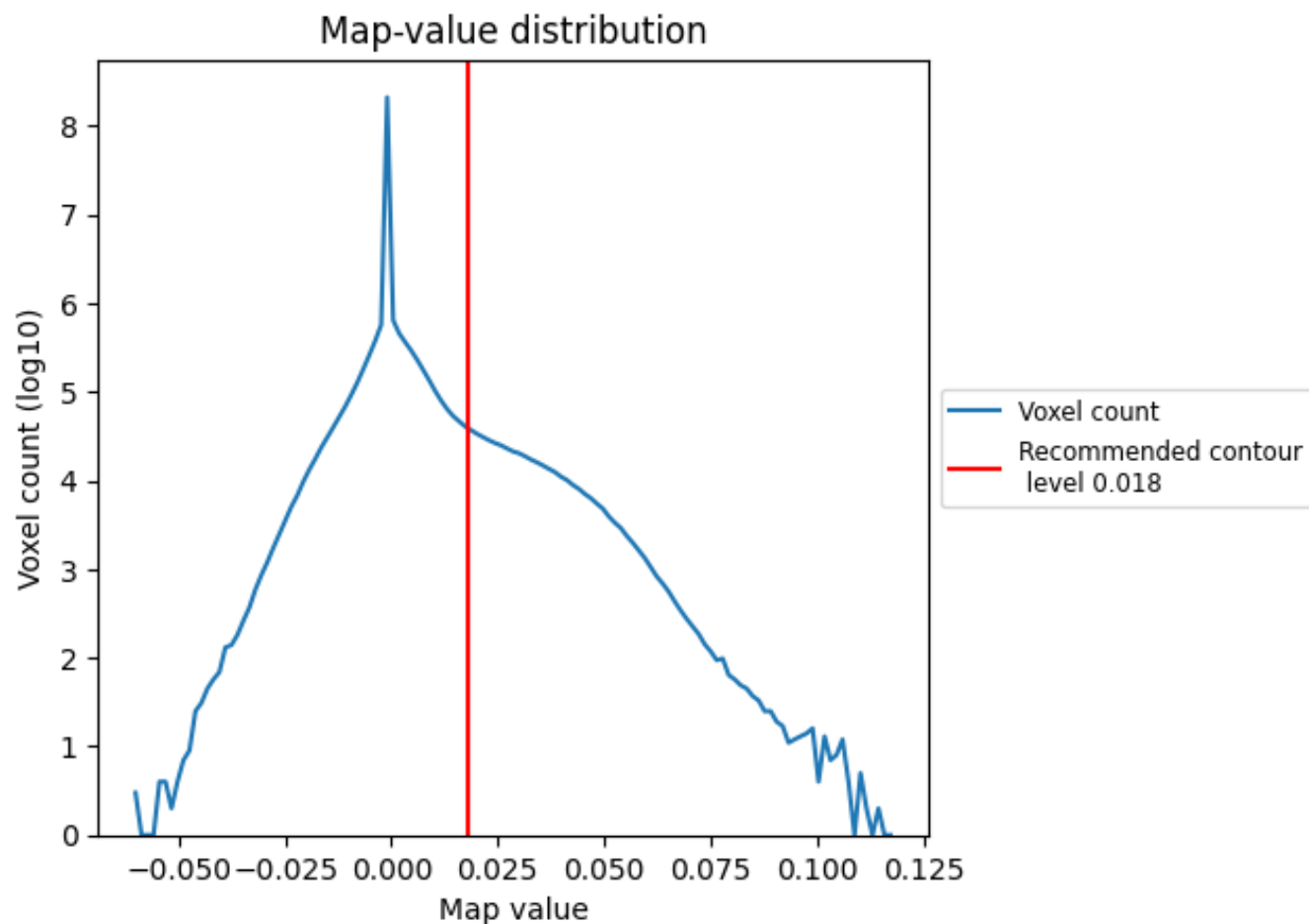
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

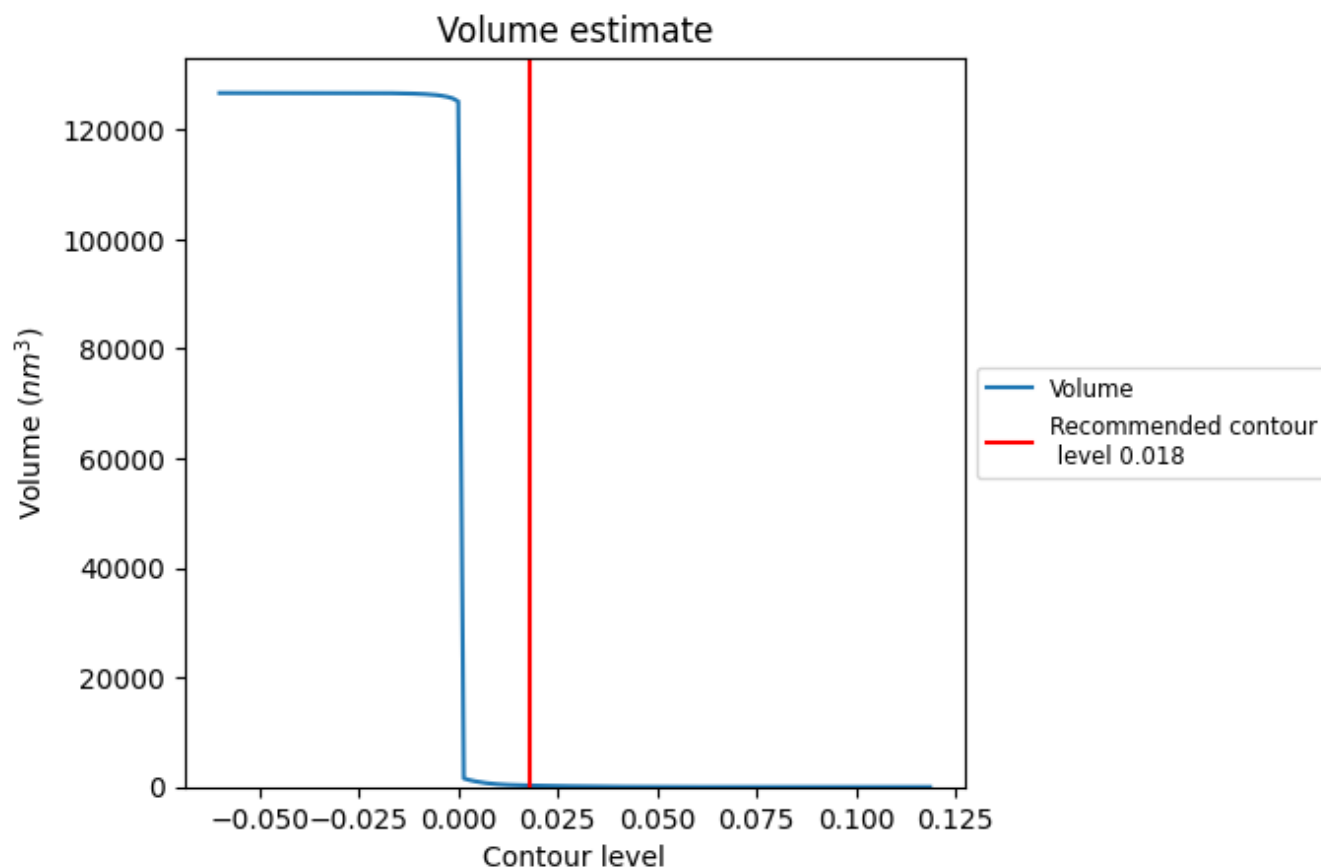
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

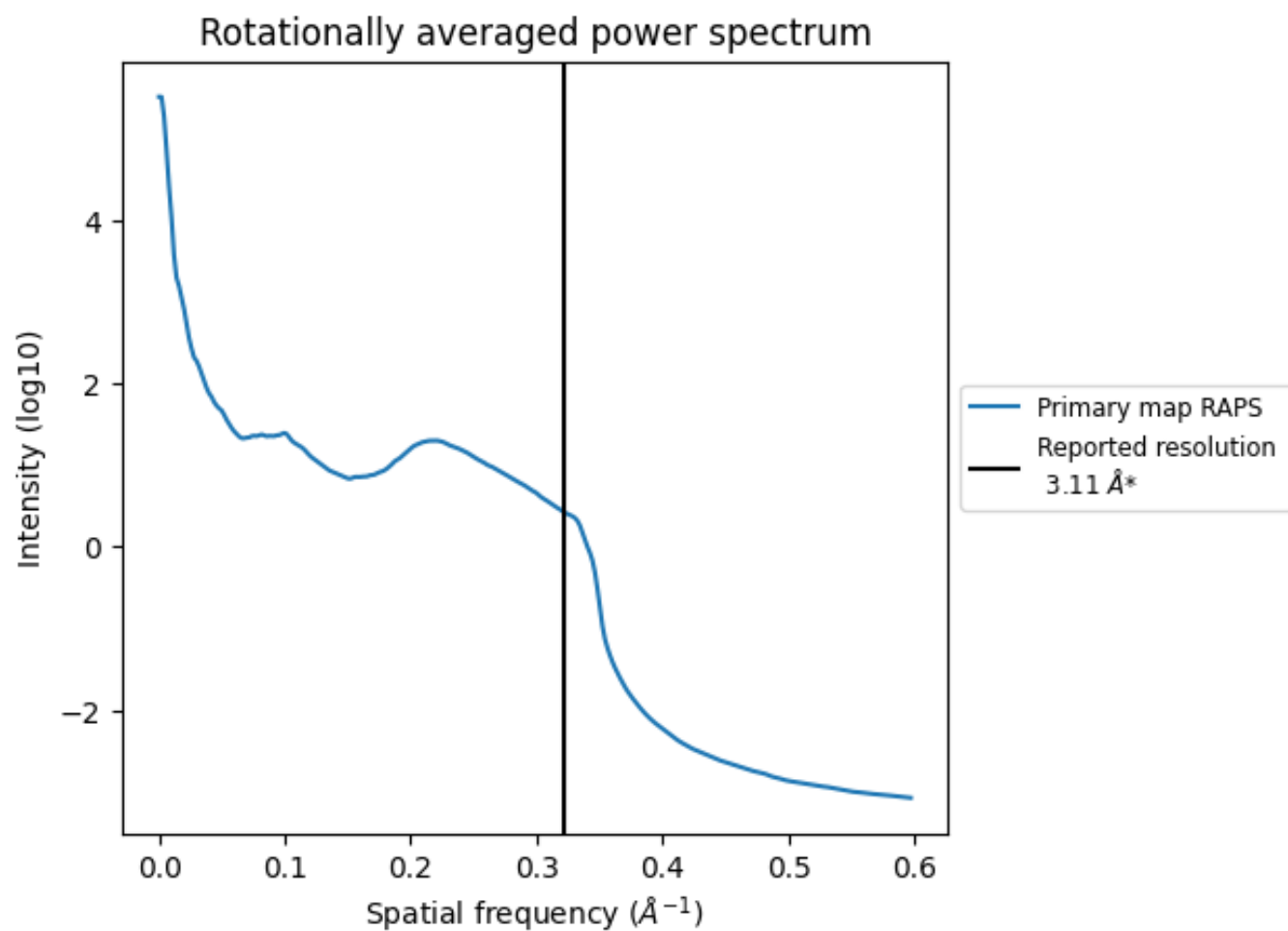
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm³; this corresponds to an approximate mass of 235 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

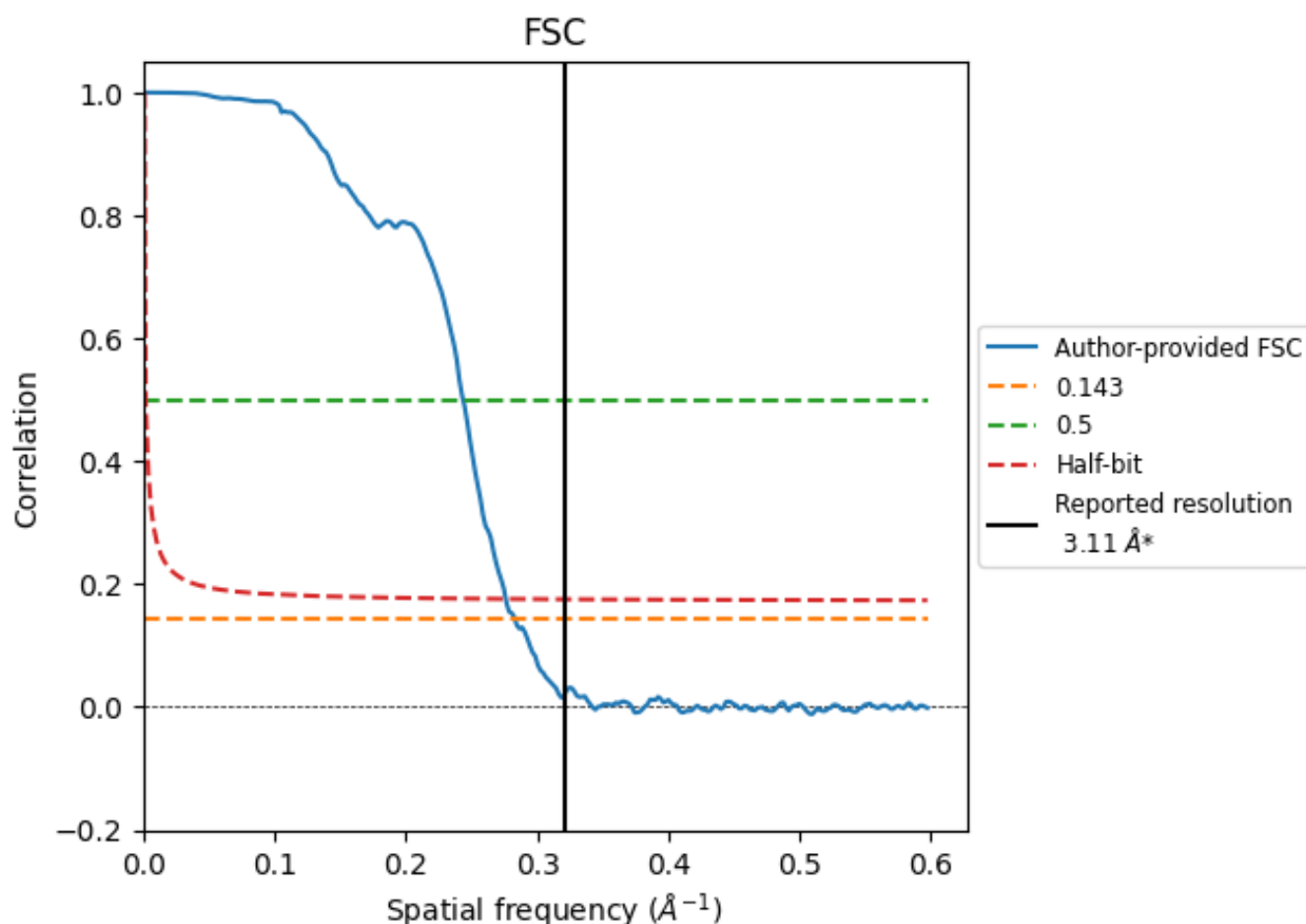


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8.2 Resolution estimates [i](#)

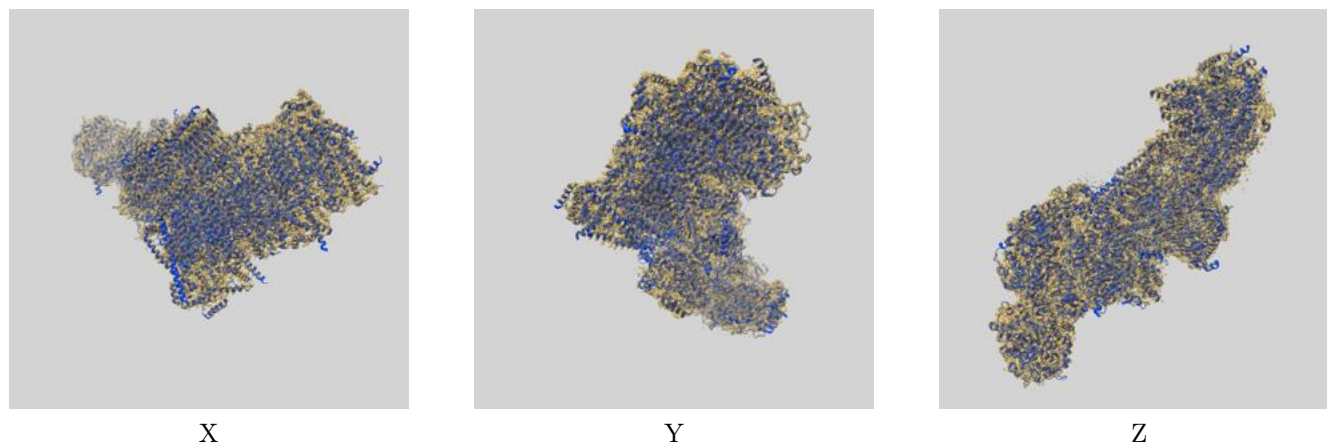
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.53	4.10	3.62
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

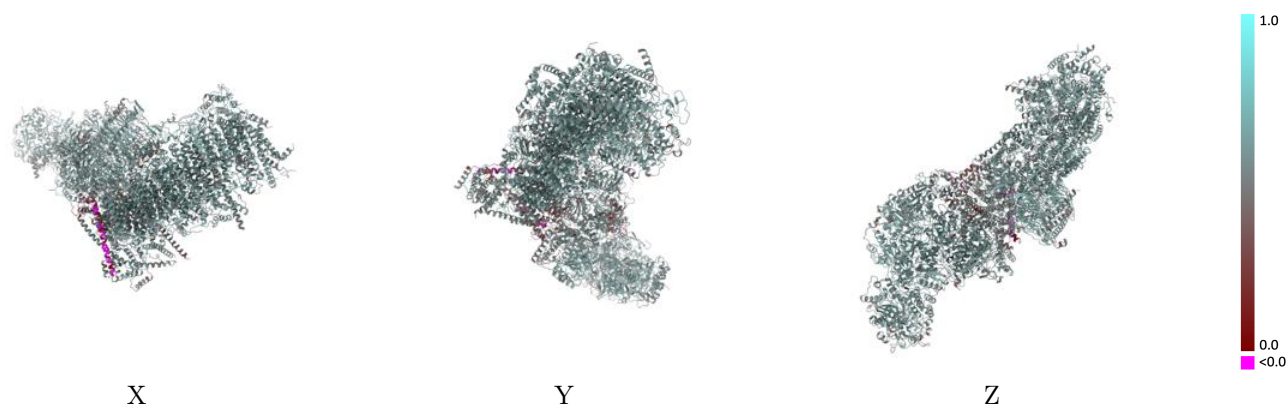
This section contains information regarding the fit between EMDB map EMD-11880 and PDB model 7ARD. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



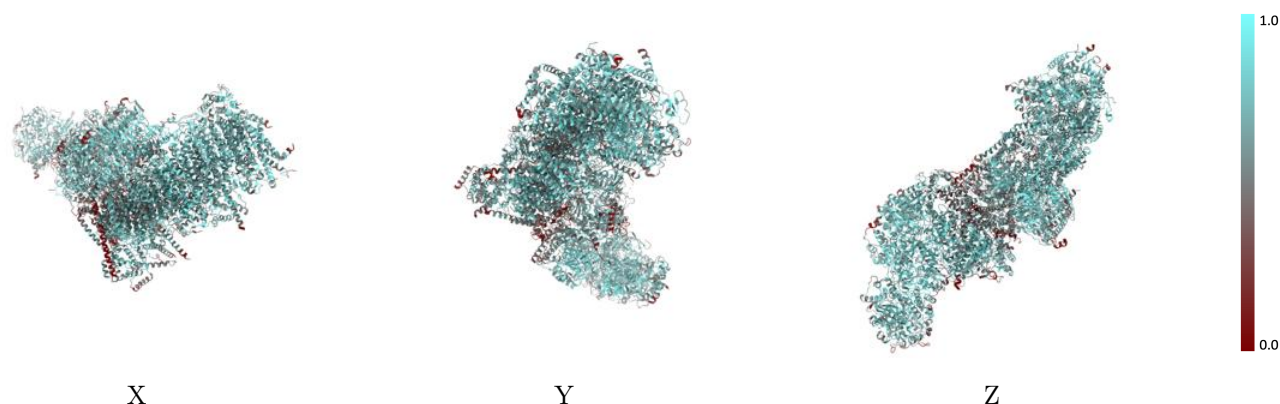
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



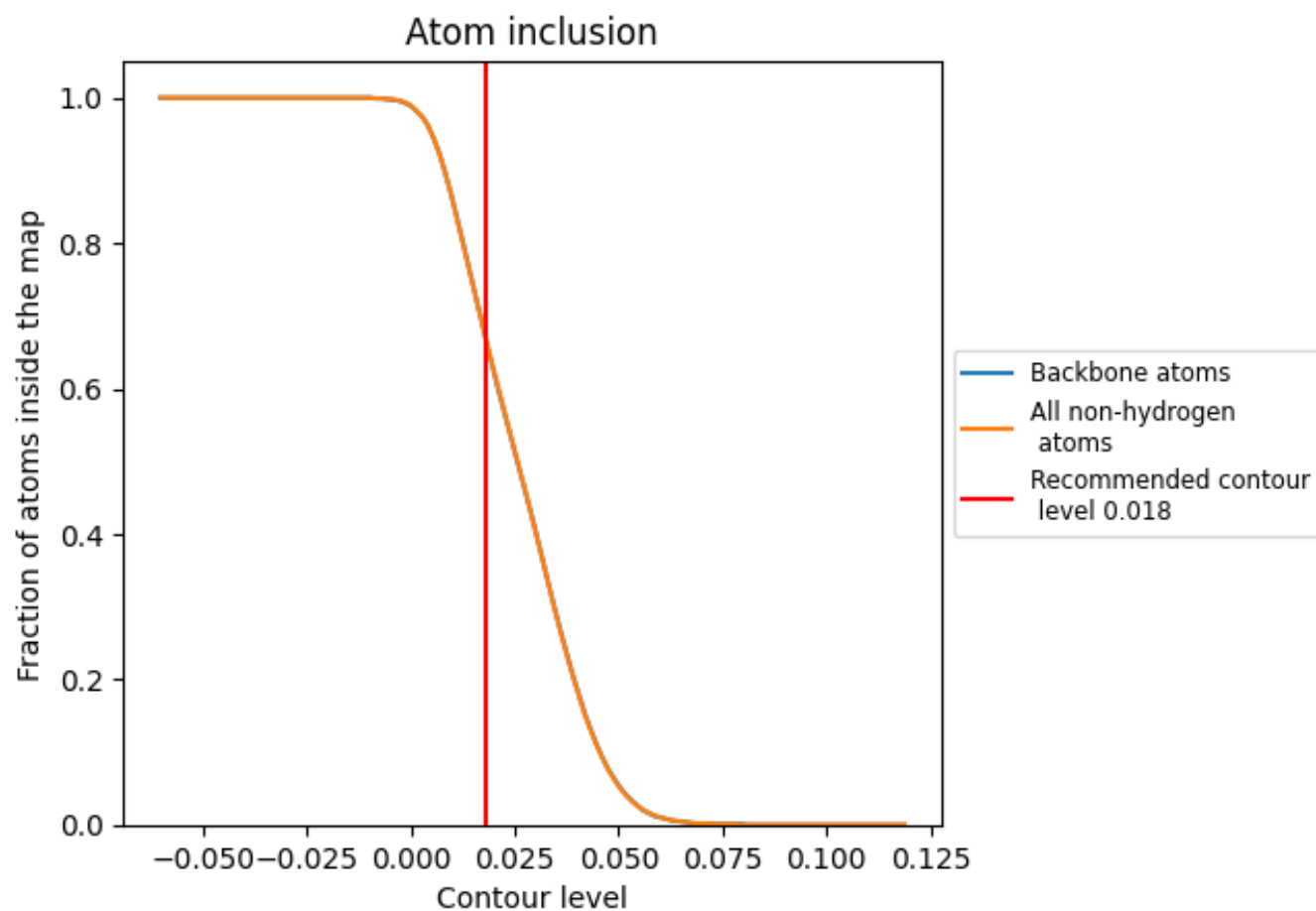
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6700	 0.5570
A	 0.6110	 0.5460
B	 0.6760	 0.5450
C	 0.7840	 0.5960
D	 0.7370	 0.5650
E	 0.6400	 0.5430
F	 0.6980	 0.5580
G	 0.7560	 0.5830
H	 0.4370	 0.4690
I	 0.6200	 0.5250
J	 0.6680	 0.5570
K	 0.7220	 0.5660
L	 0.7250	 0.5890
M	 0.7540	 0.5950
N	 0.7040	 0.5850
O	 0.7450	 0.5800
P	 0.6750	 0.5490
Q	 0.7110	 0.5810
R	 0.5850	 0.5360
S	 0.6580	 0.5420
T	 0.5840	 0.5220
U	 0.2990	 0.3850
V	 0.5760	 0.5250
W	 0.5510	 0.5010
X	 0.6420	 0.5480
Y	 0.6490	 0.5520
Z	 0.5640	 0.4950
a	 0.6240	 0.5280
b	 0.1000	 -0.0330
c	 0.7420	 0.5800
d	 0.6360	 0.5610
e	 0.6650	 0.5560
f	 0.6950	 0.5720
g	 0.7000	 0.5670
h	 0.6600	 0.5560



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Chain	Atom inclusion	Q-score
i	 0.6380	 0.5370
j	 0.6940	 0.5450
k	 0.6670	 0.5500
l	 0.7530	 0.5870
m	 0.7300	 0.5910
n	 0.6970	 0.5550
o	 0.7180	 0.5670
p	 0.7180	 0.5750
q	 0.7260	 0.5790
r	 0.3150	 0.5110
s	 0.6670	 0.5650
t	 0.6810	 0.5880
u	 0.5200	 0.3570
w	 0.6860	 0.5650
x	 0.7460	 0.5780
y	 0.6640	 0.5630
z	 0.6910	 0.5650