



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:20 AM UTC

PDB ID : 7YRS / pdb_00007yrs
Title : Crystal structure of Lactobacillus rhamnosus 4-deoxy-L-threo-5-hexosulose-urionate ketol-isomerase KduI complexed with MOPS
Authors : Yamamoto, Y.; Oiki, S.; Takase, R.; Mikami, B.; Hashimoto, W.
Deposited on : 2022-08-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

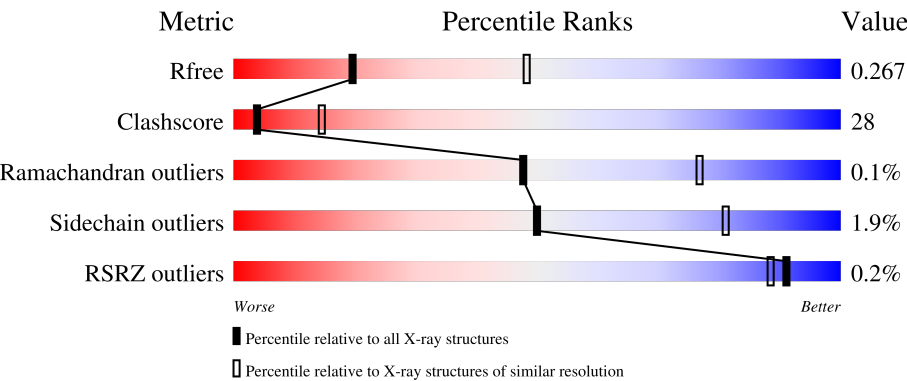
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	289	53% 40% ••
1	B	289	47% 46% ••
1	C	289	52% 42% ••
1	D	289	46% 41% • 10%
1	E	289	54% 39% ••

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Mol	Chain	Length	Quality of chain
1	F	289	46% 46% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			
1	B	276	Total	C	N	O	S	0	0	0
			2219	1408	374	420	17			
1	C	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			
1	D	261	Total	C	N	O	S	0	0	0
			2100	1337	355	392	16			
1	E	276	Total	C	N	O	S	0	0	0
			2222	1409	375	421	17			
1	F	276	Total	C	N	O	S	0	0	0
			2219	1411	374	416	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	LEU	-	expression tag	UNP C2JUP1
A	283	GLU	-	expression tag	UNP C2JUP1
A	284	HIS	-	expression tag	UNP C2JUP1
A	285	HIS	-	expression tag	UNP C2JUP1
A	286	HIS	-	expression tag	UNP C2JUP1
A	287	HIS	-	expression tag	UNP C2JUP1
A	288	HIS	-	expression tag	UNP C2JUP1
A	289	HIS	-	expression tag	UNP C2JUP1
B	282	LEU	-	expression tag	UNP C2JUP1
B	283	GLU	-	expression tag	UNP C2JUP1
B	284	HIS	-	expression tag	UNP C2JUP1
B	285	HIS	-	expression tag	UNP C2JUP1
B	286	HIS	-	expression tag	UNP C2JUP1
B	287	HIS	-	expression tag	UNP C2JUP1
B	288	HIS	-	expression tag	UNP C2JUP1
B	289	HIS	-	expression tag	UNP C2JUP1
C	282	LEU	-	expression tag	UNP C2JUP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	283	GLU	-	expression tag	UNP C2JUP1
C	284	HIS	-	expression tag	UNP C2JUP1
C	285	HIS	-	expression tag	UNP C2JUP1
C	286	HIS	-	expression tag	UNP C2JUP1
C	287	HIS	-	expression tag	UNP C2JUP1
C	288	HIS	-	expression tag	UNP C2JUP1
C	289	HIS	-	expression tag	UNP C2JUP1
D	282	LEU	-	expression tag	UNP C2JUP1
D	283	GLU	-	expression tag	UNP C2JUP1
D	284	HIS	-	expression tag	UNP C2JUP1
D	285	HIS	-	expression tag	UNP C2JUP1
D	286	HIS	-	expression tag	UNP C2JUP1
D	287	HIS	-	expression tag	UNP C2JUP1
D	288	HIS	-	expression tag	UNP C2JUP1
D	289	HIS	-	expression tag	UNP C2JUP1
E	282	LEU	-	expression tag	UNP C2JUP1
E	283	GLU	-	expression tag	UNP C2JUP1
E	284	HIS	-	expression tag	UNP C2JUP1
E	285	HIS	-	expression tag	UNP C2JUP1
E	286	HIS	-	expression tag	UNP C2JUP1
E	287	HIS	-	expression tag	UNP C2JUP1
E	288	HIS	-	expression tag	UNP C2JUP1
E	289	HIS	-	expression tag	UNP C2JUP1
F	282	LEU	-	expression tag	UNP C2JUP1
F	283	GLU	-	expression tag	UNP C2JUP1
F	284	HIS	-	expression tag	UNP C2JUP1
F	285	HIS	-	expression tag	UNP C2JUP1
F	286	HIS	-	expression tag	UNP C2JUP1
F	287	HIS	-	expression tag	UNP C2JUP1
F	288	HIS	-	expression tag	UNP C2JUP1
F	289	HIS	-	expression tag	UNP C2JUP1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

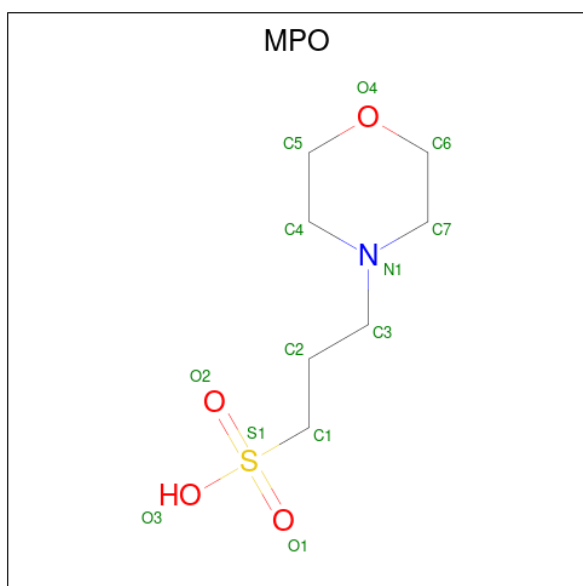
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: C₇H₁₅NO₄S) (labeled as "Ligand of Interest" by depositor).

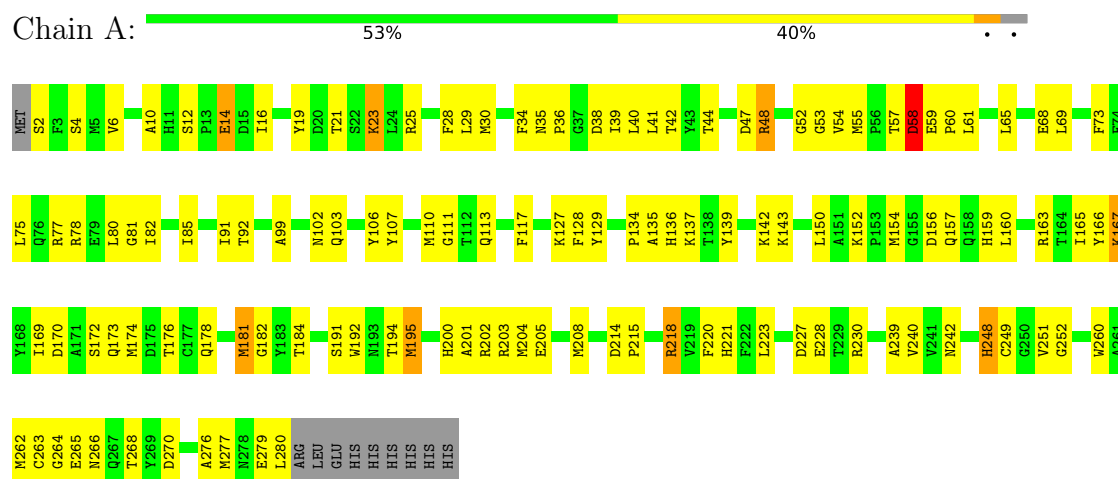


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

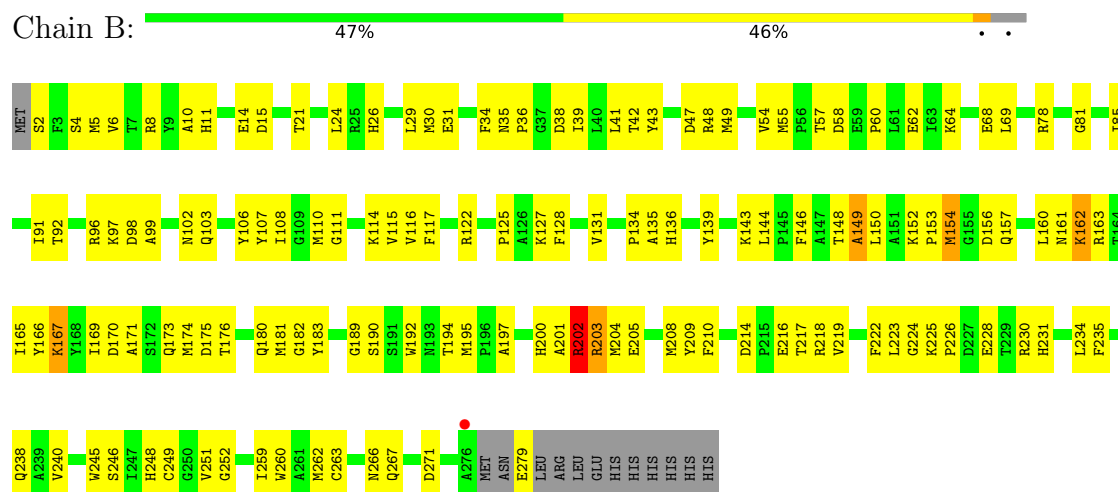
3 Residue-property plots

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

- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



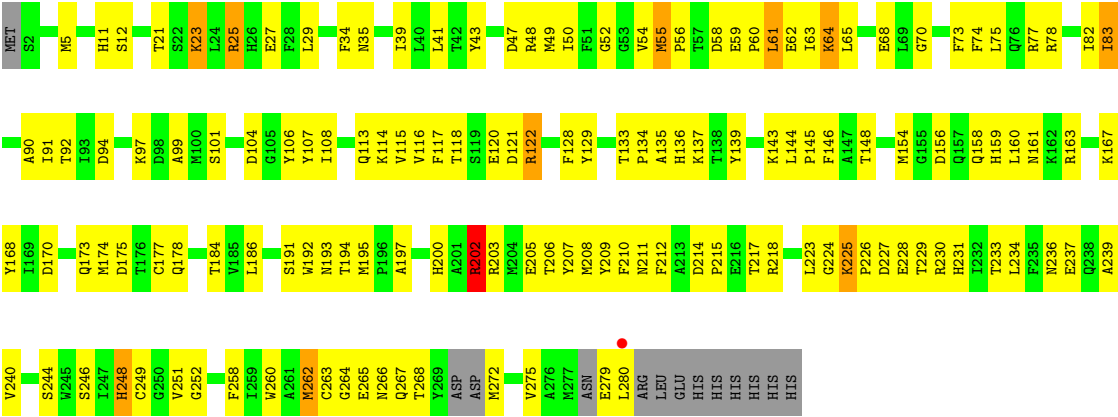
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.40Å 187.40Å 108.93Å 90.00° 112.49° 90.00°	Depositor
Resolution (Å)	49.55 – 2.80 49.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.55-2.80) 99.1 (49.55-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.189 , 0.265 0.194 , 0.267	Depositor DCC
R_{free} test set	2034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13304	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MPO

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	0.55	1/2303 (0.0%)	0.96	11/3121 (0.4%)
1	B	0.71	7/2278 (0.3%)	1.02	11/3086 (0.4%)
1	C	0.59	2/2303 (0.1%)	0.99	11/3121 (0.4%)
1	D	0.61	4/2156 (0.2%)	1.00	9/2918 (0.3%)
1	E	0.49	0/2281	0.94	8/3090 (0.3%)
1	F	0.69	6/2277 (0.3%)	1.03	14/3082 (0.5%)
All	All	0.61	20/13598 (0.1%)	0.99	64/18418 (0.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	ARG	NE-CZ	-9.58	1.22	1.33
1	F	202	ARG	NE-CZ	-9.29	1.22	1.33
1	F	202	ARG	CG-CD	-8.59	1.26	1.52
1	D	202	ARG	CZ-NH1	-7.98	1.21	1.32
1	A	58	ASP	C-N	7.63	1.49	1.33
1	B	202	ARG	NE-CZ	-7.52	1.24	1.33
1	B	202	ARG	CZ-NH1	-7.30	1.22	1.32
1	B	203	ARG	NE-CZ	-6.34	1.26	1.33
1	F	202	ARG	CZ-NH2	-5.97	1.25	1.33
1	D	202	ARG	CZ-NH2	-5.97	1.25	1.33
1	F	23	LYS	CD-CE	-5.90	1.34	1.52
1	B	203	ARG	CZ-NH2	-5.87	1.25	1.33
1	B	203	ARG	CZ-NH1	-5.50	1.25	1.32
1	F	202	ARG	CZ-NH1	-5.49	1.25	1.32
1	F	202	ARG	CD-NE	-5.41	1.38	1.46
1	C	154	MET	SD-CE	5.30	1.92	1.79
1	B	153	PRO	N-CA	5.30	1.53	1.47
1	D	202	ARG	CD-NE	-5.14	1.39	1.46
1	B	248	HIS	CE1-NE2	-5.02	1.27	1.32
1	C	25	ARG	NE-CZ	-5.01	1.27	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	ARG	CB-CG-CD	-15.08	76.62	111.30
1	C	77	ARG	CG-CD-NE	-13.83	81.57	112.00
1	A	194	THR	CA-C-N	-8.91	109.94	119.83
1	A	194	THR	C-N-CA	-8.91	109.94	119.83
1	E	122	ARG	CA-CB-CG	8.62	131.35	114.10
1	D	114	LYS	CB-CG-CD	-8.49	91.77	111.30
1	F	202	ARG	NE-CZ-NH1	-8.15	113.35	121.50
1	D	114	LYS	CA-CB-CG	8.07	130.25	114.10
1	B	64	LYS	CA-CB-CG	7.82	129.73	114.10
1	F	225	LYS	CB-CG-CD	-7.41	94.26	111.30
1	C	167	LYS	CA-CB-CG	7.23	128.56	114.10
1	D	201	ALA	CA-C-N	-7.23	110.62	122.54
1	D	201	ALA	C-N-CA	-7.23	110.62	122.54
1	D	31	GLU	CA-C-N	-7.19	111.08	122.73
1	D	31	GLU	C-N-CA	-7.19	111.08	122.73
1	B	202	ARG	CG-CD-NE	6.64	126.61	112.00
1	B	154	MET	N-CA-CB	-6.61	99.40	110.57
1	F	202	ARG	CG-CD-NE	-6.58	97.52	112.00
1	E	59	GLU	CB-CA-C	6.40	117.58	108.68
1	A	167	LYS	CB-CG-CD	-6.39	96.60	111.30
1	A	218	ARG	CG-CD-NE	-6.36	98.01	112.00
1	F	202	ARG	CB-CA-C	-6.30	99.57	110.09
1	F	120	GLU	CA-CB-CG	6.27	126.64	114.10
1	C	61	LEU	CB-CA-C	6.21	121.65	109.35
1	F	25	ARG	CB-CG-CD	6.05	125.23	111.30
1	E	59	GLU	N-CA-CB	-6.00	100.21	110.11
1	E	196	PRO	N-CA-C	-5.99	100.12	112.47
1	B	154	MET	CB-CA-C	5.99	120.01	109.89
1	A	23	LYS	CG-CD-CE	-5.90	97.73	111.30
1	D	203	ARG	CA-CB-CG	5.89	125.87	114.10
1	F	144	LEU	CA-CB-CG	5.84	136.75	116.30
1	D	232	ILE	CG1-CB-CG2	-5.83	93.21	110.70
1	F	64	LYS	CA-C-N	-5.79	112.59	122.33
1	F	64	LYS	C-N-CA	-5.79	112.59	122.33
1	C	25	ARG	CG-CD-NE	5.69	124.52	112.00
1	A	48	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	F	202	ARG	CA-C-N	-5.61	112.21	121.80
1	F	202	ARG	C-N-CA	-5.61	112.21	121.80
1	C	69	LEU	CA-CB-CG	5.49	135.53	116.30
1	F	64	LYS	CA-CB-CG	5.45	124.99	114.10
1	A	167	LYS	CD-CE-NZ	-5.44	94.48	111.90
1	E	119	SER	CA-C-N	5.42	129.02	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	SER	C-N-CA	5.42	129.02	120.89
1	C	166	TYR	CA-C-N	-5.42	114.55	122.19
1	C	166	TYR	C-N-CA	-5.42	114.55	122.19
1	B	201	ALA	CA-C-N	5.39	130.58	121.14
1	B	201	ALA	C-N-CA	5.39	130.58	121.14
1	A	14	GLU	N-CA-CB	-5.34	101.52	110.39
1	B	152	LYS	N-CA-CB	5.34	119.60	110.05
1	B	14	GLU	CB-CA-C	-5.32	100.46	110.67
1	B	162	LYS	CA-CB-CG	5.31	124.72	114.10
1	A	276	ALA	CA-C-N	-5.25	113.08	122.32
1	A	276	ALA	C-N-CA	-5.25	113.08	122.32
1	E	162	LYS	CB-CA-C	-5.25	101.97	109.84
1	A	195	MET	N-CA-CB	5.23	115.36	110.39
1	C	61	LEU	N-CA-CB	-5.20	101.59	111.00
1	D	55	MET	CA-CB-CG	5.14	124.38	114.10
1	B	167	LYS	CB-CG-CD	-5.12	99.52	111.30
1	F	262	MET	CB-CG-SD	-5.12	97.33	112.70
1	C	77	ARG	CA-CB-CG	-5.09	103.92	114.10
1	B	202	ARG	N-CA-CB	-5.08	102.12	110.40
1	F	122	ARG	CG-CD-NE	-5.06	100.86	112.00
1	C	76	GLN	CA-C-N	-5.05	114.64	122.67
1	C	76	GLN	C-N-CA	-5.05	114.64	122.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2243	0	2144	121	0
1	B	2219	0	2117	167	0
1	C	2243	0	2144	135	0
1	D	2100	0	2018	128	0
1	E	2222	0	2118	120	0
1	F	2219	0	2128	154	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	13	0	14	1	0
3	B	13	0	14	1	0
3	E	13	0	15	0	0
3	F	13	0	15	4	0
All	All	13304	0	12727	742	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 28.

All (742) 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)
1:B:154:MET:HE1	1:B:163:ARG:CZ	1.50	1.40
1:B:154:MET:HE1	1:B:163:ARG:NH1	1.46	1.31
1:A:19:TYR:CG	1:A:23:LYS:NZ	2.00	1.28
1:B:154:MET:HE1	1:B:163:ARG:NE	1.68	1.09
1:D:75:LEU:HD12	1:D:78:ARG:HB2	1.31	1.08
1:A:19:TYR:CD2	1:A:23:LYS:NZ	2.21	1.07
1:F:92:THR:HG22	1:F:97:LYS:HG3	1.38	1.06
1:B:154:MET:CE	1:B:163:ARG:CZ	2.34	1.05
1:E:48:ARG:NH1	1:F:47:ASP:OD1	1.91	1.03
1:A:279:GLU:H	1:E:218:ARG:HH12	1.07	0.99
1:B:154:MET:CE	1:B:163:ARG:NH1	2.27	0.98
1:A:142:LYS:NZ	1:A:174:MET:HB3	1.77	0.98
1:F:228:GLU:HG3	1:F:230:ARG:HH12	1.29	0.97
1:B:216:GLU:HB3	1:C:277:MET:HG3	1.44	0.97
1:C:78:ARG:NH1	1:D:265:GLU:OE2	2.01	0.94
1:D:75:LEU:CD1	1:D:78:ARG:HB2	1.98	0.93
1:B:131:VAL:HB	1:B:181:MET:HE2	1.50	0.93
1:B:39:ILE:HD13	1:B:54:VAL:HG12	1.52	0.90
1:F:99:ALA:O	1:F:143:LYS:NZ	2.04	0.90
1:B:85:ILE:HD11	1:B:210:PHE:CG	2.07	0.89
1:D:203:ARG:HB2	1:D:263:CYS:O	1.71	0.88
1:F:65:LEU:HD22	1:F:68:GLU:OE1	1.72	0.88
1:A:48:ARG:NH1	1:B:47:ASP:OD1	2.07	0.87
1:A:69:LEU:HA	1:B:202:ARG:NE	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:MET:CE	1:B:163:ARG:NE	2.37	0.86
1:A:142:LYS:HZ3	1:A:174:MET:HB3	1.41	0.84
1:F:225:LYS:NZ	1:F:225:LYS:HB3	1.91	0.84
1:B:154:MET:HE1	1:B:163:ARG:HH11	1.42	0.82
1:A:48:ARG:HH12	1:B:47:ASP:CG	1.86	0.82
1:D:16:ILE:O	1:D:230:ARG:NH2	2.13	0.82
1:C:92:THR:OG1	1:C:116:VAL:HG12	1.81	0.81
1:B:99:ALA:O	1:B:143:LYS:NZ	2.14	0.80
1:F:58:ASP:HB2	1:F:122:ARG:NH1	1.96	0.80
1:F:163:ARG:NH1	3:F:302:MPO:O3	2.15	0.79
1:C:226:PRO:HB3	1:C:275:VAL:HG21	1.64	0.79
1:A:279:GLU:H	1:E:218:ARG:NH1	1.80	0.78
1:A:279:GLU:N	1:E:218:ARG:HH12	1.81	0.78
1:E:85:ILE:HD11	1:E:259:ILE:HD11	1.65	0.78
1:C:136:HIS:H	1:D:136:HIS:HD2	1.32	0.77
1:C:221:HIS:HE1	1:C:242:ASN:HD21	1.32	0.77
1:A:200:HIS:NE2	1:A:205:GLU:OE2	2.14	0.77
1:A:160:LEU:HD23	1:E:160:LEU:HD23	1.67	0.77
1:D:32:LYS:HD3	1:D:33:ILE:H	1.47	0.77
1:E:48:ARG:O	1:E:78:ARG:NH2	2.18	0.77
1:F:167:LYS:HD2	1:F:173:GLN:HB2	1.65	0.77
1:E:267:GLN:HE21	1:F:77:ARG:HH22	1.30	0.77
1:D:203:ARG:HH11	1:D:263:CYS:HA	1.50	0.77
1:E:203:ARG:NH2	1:E:268:THR:O	2.18	0.77
1:C:266:ASN:ND2	1:C:268:THR:H	1.83	0.76
1:C:78:ARG:HD2	1:C:132:SER:OG	1.85	0.76
1:A:169:ILE:HD12	1:A:181:MET:HG3	1.68	0.76
1:F:92:THR:HG22	1:F:97:LYS:CG	2.16	0.76
1:A:19:TYR:CB	1:A:23:LYS:NZ	2.48	0.76
1:E:69:LEU:C	1:F:202:ARG:HH12	1.94	0.76
1:D:191:SER:OG	1:D:252:GLY:N	2.18	0.76
1:D:233:THR:HG23	1:F:280:LEU:HD22	1.68	0.75
1:C:266:ASN:HD21	1:C:268:THR:HG23	1.51	0.75
1:A:19:TYR:HB3	1:A:23:LYS:HZ1	1.52	0.75
1:A:142:LYS:HZ1	1:A:174:MET:HB3	1.50	0.75
1:B:214:ASP:HB3	1:B:217:THR:OG1	1.87	0.75
1:B:114:LYS:HE2	1:B:116:VAL:HB	1.68	0.75
1:D:75:LEU:HD12	1:D:78:ARG:CB	2.13	0.74
1:E:8:ARG:NH1	1:E:26:HIS:O	2.19	0.74
1:E:200:HIS:HB2	1:E:202:ARG:NH2	2.02	0.74
1:B:225:LYS:H	1:B:225:LYS:HD3	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HA	1:B:174:MET:HE1	1.70	0.73
1:E:32:LYS:HE3	1:E:35:ASN:HB2	1.69	0.73
1:C:136:HIS:H	1:D:136:HIS:CD2	2.06	0.73
1:B:160:LEU:HD23	1:C:160:LEU:HD23	1.71	0.72
1:D:32:LYS:HD3	1:D:33:ILE:N	2.04	0.72
1:D:174:MET:HG2	1:D:175:ASP:H	1.55	0.72
1:D:160:LEU:HD23	1:F:160:LEU:HD23	1.71	0.72
1:E:78:ARG:NH1	1:F:265:GLU:OE1	2.22	0.72
1:D:39:ILE:HG12	1:D:54:VAL:HG13	1.72	0.71
1:D:59:GLU:HG3	1:D:60:PRO:HD2	1.73	0.71
1:F:210:PHE:HD2	1:F:211:ASN:HD22	1.38	0.71
1:E:202:ARG:HH21	1:E:203:ARG:NH1	1.87	0.71
1:F:228:GLU:CG	1:F:230:ARG:HH12	2.03	0.71
1:E:266:ASN:ND2	1:F:70:GLY:O	2.24	0.71
1:B:225:LYS:HE2	1:B:228:GLU:HB3	1.72	0.70
1:E:195:MET:HB3	1:E:196:PRO:HD3	1.73	0.70
1:B:5:MET:HE3	1:B:43:TYR:HB2	1.74	0.70
1:B:54:VAL:HG22	1:B:128:PHE:HB2	1.74	0.70
1:E:129:TYR:CE1	1:E:208:MET:HG3	2.27	0.69
1:F:167:LYS:HG3	1:F:170:ASP:HB3	1.74	0.69
1:F:203:ARG:HB2	1:F:263:CYS:O	1.92	0.69
1:D:19:TYR:O	1:D:230:ARG:NH1	2.19	0.69
1:D:19:TYR:CD1	1:D:23:LYS:HG2	2.27	0.69
1:E:34:PHE:HZ	1:E:129:TYR:HB2	1.57	0.69
1:B:21:THR:HG23	1:C:230:ARG:HH12	1.57	0.69
1:D:16:ILE:HA	1:D:19:TYR:CD2	2.26	0.69
1:F:114:LYS:HD2	1:F:114:LYS:C	2.16	0.69
1:A:195:MET:HE2	1:A:277:MET:HE1	1.74	0.69
1:F:56:PRO:HG2	1:F:128:PHE:HE2	1.56	0.69
1:F:225:LYS:HB3	1:F:225:LYS:HZ2	1.54	0.69
1:F:200:HIS:ND1	1:F:203:ARG:O	2.23	0.69
1:D:203:ARG:NH2	1:D:266:ASN:O	2.20	0.68
1:A:191:SER:OG	1:A:252:GLY:N	2.26	0.68
1:A:200:HIS:ND1	1:A:203:ARG:O	2.26	0.68
1:F:191:SER:HB2	1:F:252:GLY:H	1.58	0.68
1:B:161:ASN:HB2	1:B:163:ARG:NH2	2.08	0.68
1:C:219:VAL:HA	1:C:252:GLY:HA2	1.74	0.68
1:C:91:ILE:HD11	1:C:106:TYR:CE2	2.29	0.68
1:B:176:THR:OG1	1:B:267:GLN:NE2	2.27	0.68
1:E:57:THR:OG1	1:E:58:ASP:N	2.27	0.68
1:C:203:ARG:NH2	1:C:271:ASP:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:HIS:CE1	1:C:242:ASN:HD21	2.12	0.67
1:D:41:LEU:HD23	1:D:52:GLY:HA3	1.75	0.67
1:C:225:LYS:CD	1:C:225:LYS:H	2.07	0.67
1:D:49:MET:HE3	1:D:263:CYS:SG	2.35	0.67
1:E:155:GLY:HA3	1:E:162:LYS:HA	1.76	0.67
1:B:154:MET:HE1	1:B:163:ARG:HE	1.60	0.67
1:C:165:ILE:C	1:C:166:TYR:HD2	2.02	0.67
1:C:195:MET:O	1:C:197:ALA:N	2.27	0.67
1:F:202:ARG:HG2	1:F:265:GLU:HB3	1.77	0.67
1:B:167:LYS:HG2	1:B:170:ASP:HB2	1.77	0.66
1:E:133:THR:HG21	1:E:179:LEU:HB2	1.75	0.66
1:B:150:LEU:O	1:B:166:TYR:HA	1.95	0.66
1:C:177:CYS:O	1:D:77:ARG:NH2	2.29	0.66
1:D:223:LEU:HD21	1:D:232:ILE:HD11	1.78	0.66
1:C:78:ARG:HG3	1:C:134:PRO:HA	1.77	0.66
1:F:228:GLU:HG3	1:F:230:ARG:NH1	2.06	0.66
1:E:167:LYS:HD2	1:E:170:ASP:OD2	1.95	0.66
1:B:30:MET:HE3	1:B:42:THR:HG23	1.78	0.65
1:E:6:VAL:HG21	1:E:8:ARG:HH21	1.62	0.65
1:B:85:ILE:HD11	1:B:210:PHE:CD2	2.32	0.65
1:B:39:ILE:HD13	1:B:54:VAL:CG1	2.24	0.65
1:A:203:ARG:HH11	1:A:266:ASN:HD21	1.45	0.65
1:A:69:LEU:HA	1:B:202:ARG:HE	1.61	0.64
1:A:59:GLU:HG3	1:A:60:PRO:HD2	1.79	0.64
1:F:193:ASN:OD1	1:F:194:THR:HG22	1.97	0.64
1:B:230:ARG:HH12	1:C:230:ARG:CZ	2.10	0.64
1:C:54:VAL:HG22	1:C:128:PHE:HB2	1.77	0.64
1:A:68:GLU:O	1:B:202:ARG:NH2	2.30	0.64
1:E:69:LEU:HA	1:F:202:ARG:NH1	2.14	0.63
1:D:75:LEU:CD1	1:D:78:ARG:CB	2.74	0.63
1:C:43:TYR:OH	1:C:48:ARG:HG2	1.98	0.63
1:F:203:ARG:HB3	1:F:264:GLY:HA3	1.79	0.63
1:B:49:MET:HE3	1:B:204:MET:HE1	1.81	0.63
1:F:21:THR:O	1:F:25:ARG:HG3	1.99	0.62
1:A:21:THR:O	1:A:25:ARG:HG3	1.99	0.62
1:B:107:TYR:HD1	1:B:108:ILE:N	1.97	0.62
1:E:202:ARG:CZ	1:E:271:ASP:HB2	2.29	0.62
1:E:266:ASN:OD1	1:E:267:GLN:N	2.32	0.62
1:C:92:THR:HG22	1:C:97:LYS:HB2	1.80	0.62
1:B:102:ASN:OD1	1:B:103:GLN:HG2	2.00	0.62
1:E:91:ILE:HD12	1:E:100:MET:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ILE:HD13	1:F:168:TYR:CD2	2.34	0.62
1:C:11:HIS:HD2	1:D:15:ASP:OD1	1.82	0.61
1:F:48:ARG:O	1:F:78:ARG:NH1	2.31	0.61
1:E:38:ASP:OD2	1:E:39:ILE:N	2.33	0.61
1:F:41:LEU:HD23	1:F:52:GLY:HA3	1.83	0.61
1:B:85:ILE:HG22	1:B:127:LYS:O	2.00	0.61
1:B:225:LYS:H	1:B:225:LYS:CD	2.13	0.61
1:F:91:ILE:HG22	1:F:117:PHE:HA	1.81	0.61
1:F:200:HIS:HB3	1:F:272:MET:HG3	1.82	0.61
1:B:218:ARG:O	1:B:252:GLY:HA2	2.01	0.61
1:F:63:ILE:HD11	1:F:74:PHE:CE2	2.36	0.61
1:A:182:GLY:HA3	1:A:260:TRP:CE2	2.36	0.61
1:F:5:MET:HE3	1:F:43:TYR:HB2	1.82	0.61
1:A:57:THR:OG1	1:A:58:ASP:N	2.33	0.61
1:A:150:LEU:O	1:A:166:TYR:HA	2.01	0.61
1:B:54:VAL:CG2	1:B:128:PHE:HB2	2.31	0.61
1:F:163:ARG:NH1	3:F:302:MPO:S1	2.74	0.61
1:B:24:LEU:HD12	1:B:230:ARG:HH21	1.66	0.60
1:B:110:MET:HE1	1:B:136:HIS:C	2.26	0.60
1:C:214:ASP:OD1	1:C:217:THR:OG1	2.19	0.60
1:F:203:ARG:HE	1:F:262:MET:CE	2.13	0.60
1:B:146:PHE:HE1	1:B:166:TYR:CD1	2.20	0.60
1:E:136:HIS:H	1:F:136:HIS:CD2	2.19	0.60
1:E:170:ASP:OD2	1:E:172:SER:OG	2.13	0.60
1:C:62:GLU:OE1	1:C:115:VAL:N	2.34	0.60
1:F:62:GLU:HB2	1:F:115:VAL:O	2.01	0.60
1:E:58:ASP:HA	1:E:122:ARG:CZ	2.31	0.60
1:A:41:LEU:HD23	1:A:52:GLY:HA3	1.84	0.60
1:F:203:ARG:NH1	1:F:266:ASN:OD1	2.35	0.60
1:B:103:GLN:OE1	1:B:103:GLN:HA	2.02	0.60
1:C:135:ALA:HA	1:D:136:HIS:HD2	1.67	0.60
1:B:139:TYR:CE1	1:B:175:ASP:HB3	2.37	0.59
1:E:203:ARG:HB2	1:E:263:CYS:O	2.02	0.59
1:A:110:MET:HE1	1:A:136:HIS:C	2.26	0.59
1:A:34:PHE:CE1	1:A:127:LYS:HB3	2.37	0.59
1:B:156:ASP:HA	1:B:162:LYS:HD2	1.83	0.59
1:C:92:THR:HG22	1:C:97:LYS:CB	2.32	0.59
1:F:43:TYR:OH	1:F:48:ARG:NH1	2.36	0.59
1:B:235:PHE:H	1:B:238:GLN:NE2	2.01	0.59
1:D:21:THR:O	1:D:25:ARG:HG3	2.02	0.59
1:E:34:PHE:HB3	1:E:55:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD13	1:B:173:GLN:HE22	1.66	0.59
1:A:65:LEU:HD13	1:A:69:LEU:HD11	1.85	0.59
1:E:198:HIS:HB3	1:E:272:MET:HE2	1.85	0.58
1:C:103:GLN:HB2	1:C:146:PHE:CD2	2.37	0.58
1:F:23:LYS:O	1:F:23:LYS:HG3	2.03	0.58
1:F:203:ARG:CB	1:F:264:GLY:HA3	2.33	0.58
1:C:58:ASP:OD1	1:C:59:GLU:N	2.36	0.58
1:E:191:SER:OG	1:E:252:GLY:N	2.37	0.58
1:D:55:MET:HE2	1:D:125:PRO:HG2	1.85	0.58
1:C:135:ALA:HA	1:D:136:HIS:CD2	2.39	0.58
1:D:35:ASN:OD1	1:D:36:PRO:HD2	2.02	0.58
1:F:223:LEU:HD12	1:F:224:GLY:H	1.69	0.58
1:D:110:MET:HE1	1:D:136:HIS:C	2.29	0.58
1:B:107:TYR:CE2	1:B:176:THR:HG22	2.39	0.58
1:F:192:TRP:CD2	1:F:251:VAL:HG22	2.39	0.58
1:A:48:ARG:O	1:A:78:ARG:NH1	2.29	0.58
1:D:182:GLY:HA3	1:D:260:TRP:CZ2	2.39	0.58
1:C:70:GLY:HA3	1:D:202:ARG:NH1	2.19	0.57
1:D:55:MET:HE3	1:D:127:LYS:HG2	1.85	0.57
1:F:174:MET:HG2	1:F:175:ASP:H	1.70	0.57
1:D:85:ILE:HG13	1:D:127:LYS:HB2	1.86	0.57
1:F:50:ILE:HG13	1:F:78:ARG:NH1	2.19	0.57
1:A:35:ASN:OD1	1:A:36:PRO:HD2	2.05	0.57
1:D:174:MET:HG2	1:D:175:ASP:N	2.19	0.57
1:E:39:ILE:HD11	1:E:61:LEU:HB3	1.84	0.57
1:C:34:PHE:HB3	1:C:55:MET:CE	2.34	0.57
1:B:131:VAL:HB	1:B:181:MET:CE	2.31	0.57
1:B:157:GLN:O	1:C:189:GLY:HA2	2.04	0.57
1:B:203:ARG:HH11	1:B:262:MET:HE2	1.69	0.57
1:D:102:ASN:OD1	1:D:103:GLN:HG2	2.05	0.57
1:B:81:GLY:HA3	1:B:181:MET:HE3	1.87	0.57
1:C:75:LEU:HD21	1:C:80:LEU:HB2	1.85	0.57
1:E:45:TYR:HE2	1:F:244:SER:HB2	1.70	0.57
1:E:272:MET:HA	1:E:272:MET:HE3	1.86	0.57
1:B:182:GLY:HA3	1:B:260:TRP:CZ2	2.40	0.57
1:C:205:GLU:OE1	1:C:248:HIS:NE2	2.38	0.56
1:E:43:TYR:OH	1:E:48:ARG:HD3	2.05	0.56
1:F:59:GLU:CD	1:F:59:GLU:H	2.12	0.56
1:A:165:ILE:HD11	1:A:260:TRP:HE1	1.70	0.56
1:A:136:HIS:HB2	1:B:136:HIS:HB2	1.86	0.56
1:B:34:PHE:CD1	1:B:127:LYS:HB3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HD21	1:B:240:VAL:HG23	1.87	0.56
1:B:165:ILE:C	1:B:166:TYR:HD2	2.14	0.56
1:D:100:MET:HE1	1:D:106:TYR:HB2	1.86	0.56
1:A:68:GLU:O	1:B:202:ARG:NE	2.36	0.56
1:C:91:ILE:O	1:C:91:ILE:HD12	2.05	0.56
1:F:163:ARG:NH1	3:F:302:MPO:O2	2.39	0.56
1:B:30:MET:CE	1:B:42:THR:HG23	2.36	0.56
1:E:64:LYS:O	1:E:65:LEU:HD23	2.05	0.56
1:F:205:GLU:OE2	1:F:248:HIS:NE2	2.38	0.56
1:C:154:MET:HG3	1:C:165:ILE:CD1	2.35	0.56
1:D:107:TYR:CE1	1:D:176:THR:HG22	2.41	0.56
1:B:150:LEU:CD1	1:B:173:GLN:HE22	2.19	0.56
1:D:203:ARG:HH11	1:D:263:CYS:CA	2.19	0.56
1:E:133:THR:CG2	1:E:179:LEU:HB2	2.35	0.56
1:E:148:THR:O	1:E:150:LEU:HD12	2.06	0.56
1:A:260:TRP:CD2	3:A:302:MPO:H72	2.41	0.55
1:B:34:PHE:HB3	1:B:55:MET:CE	2.37	0.55
1:B:57:THR:OG1	1:B:58:ASP:N	2.35	0.55
1:D:182:GLY:O	1:D:259:ILE:HG23	2.06	0.55
1:E:268:THR:HG22	1:E:270:ASP:H	1.71	0.55
1:D:8:ARG:HH12	1:D:26:HIS:CD2	2.23	0.55
1:A:203:ARG:HB2	1:A:263:CYS:O	2.06	0.55
1:C:134:PRO:O	1:C:178:GLN:NE2	2.33	0.55
1:D:218:ARG:O	1:D:252:GLY:HA2	2.06	0.55
1:C:146:PHE:HD1	1:C:146:PHE:O	1.89	0.55
1:A:69:LEU:HA	1:B:202:ARG:CZ	2.35	0.55
1:B:92:THR:O	1:B:114:LYS:NZ	2.39	0.55
1:D:33:ILE:HD13	1:D:238:GLN:HA	1.87	0.55
1:D:203:ARG:NH1	1:D:263:CYS:HA	2.19	0.55
1:F:62:GLU:OE1	1:F:116:VAL:HG12	2.06	0.55
1:C:200:HIS:ND1	1:C:203:ARG:O	2.39	0.55
1:A:242:ASN:ND2	1:A:248:HIS:HB3	2.22	0.55
1:B:203:ARG:HH11	1:B:262:MET:CE	2.19	0.55
1:D:93:ILE:HD11	1:D:141:ASN:ND2	2.22	0.55
1:E:266:ASN:OD1	1:E:268:THR:N	2.28	0.55
1:F:25:ARG:HH12	1:F:233:THR:H	1.55	0.55
1:F:121:ASP:OD1	1:F:122:ARG:N	2.39	0.55
1:A:30:MET:SD	1:A:42:THR:HG23	2.47	0.54
1:C:218:ARG:HH21	1:C:234:LEU:C	2.14	0.54
1:D:156:ASP:OD1	1:D:159:HIS:N	2.39	0.54
1:E:123:ASP:O	1:E:124:HIS:ND1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ARG:HE	1:F:262:MET:HE2	1.71	0.54
1:D:14:GLU:O	1:D:14:GLU:HG2	2.05	0.54
1:D:223:LEU:HD21	1:D:232:ILE:CD1	2.37	0.54
1:E:220:PHE:CD1	1:E:233:THR:HG22	2.42	0.54
1:F:137:LYS:HE2	1:F:139:TYR:CE1	2.43	0.54
1:B:171:ALA:H	1:B:180:GLN:HE22	1.55	0.54
1:C:12:SER:HB3	1:C:15:ASP:CG	2.32	0.54
1:C:92:THR:HA	1:C:97:LYS:HA	1.90	0.54
1:B:210:PHE:HE1	1:B:259:ILE:HG13	1.71	0.54
1:C:47:ASP:OD1	1:D:48:ARG:NH1	2.41	0.54
1:E:34:PHE:HB3	1:E:55:MET:CE	2.38	0.54
1:E:267:GLN:HE21	1:F:77:ARG:NH2	2.01	0.54
1:C:57:THR:OG1	1:C:58:ASP:N	2.39	0.54
1:E:139:TYR:CD1	1:E:175:ASP:HB3	2.42	0.54
1:A:279:GLU:O	1:E:233:THR:OG1	2.12	0.54
1:D:57:THR:OG1	1:D:58:ASP:N	2.37	0.54
1:D:210:PHE:HA	1:D:236:ASN:ND2	2.23	0.54
1:C:108:ILE:CD1	1:C:115:VAL:HG21	2.38	0.54
1:C:103:GLN:HB2	1:C:146:PHE:HD2	1.73	0.53
1:B:195:MET:O	1:B:197:ALA:N	2.41	0.53
1:D:219:VAL:HA	1:D:251:VAL:O	2.08	0.53
1:F:83:ILE:HD13	1:F:168:TYR:CE2	2.44	0.53
1:B:43:TYR:OH	1:B:48:ARG:NE	2.36	0.53
1:D:106:TYR:CD1	1:D:142:LYS:O	2.62	0.53
1:F:207:TYR:OH	1:F:248:HIS:HD2	1.91	0.53
1:A:4:SER:HB3	1:A:40:LEU:HD23	1.91	0.53
1:A:107:TYR:CE2	1:A:176:THR:HG22	2.44	0.53
1:A:265:GLU:OE1	1:B:69:LEU:HD23	2.09	0.53
1:B:183:TYR:CE1	1:B:210:PHE:HZ	2.27	0.53
1:E:17:GLN:O	1:E:230:ARG:NH2	2.33	0.53
1:E:34:PHE:CD1	1:E:127:LYS:HB3	2.43	0.53
1:F:234:LEU:HD21	1:F:240:VAL:HG23	1.91	0.53
1:C:47:ASP:OD2	1:D:48:ARG:NH1	2.42	0.53
1:C:170:ASP:OD1	1:C:171:ALA:N	2.42	0.53
1:E:223:LEU:HD12	1:E:246:SER:OG	2.09	0.53
1:C:136:HIS:N	1:D:136:HIS:HD2	2.02	0.52
1:D:58:ASP:HA	1:D:122:ARG:HD3	1.90	0.52
1:E:88:ALA:CB	1:E:120:GLU:HG3	2.40	0.52
1:D:203:ARG:HH21	1:D:266:ASN:C	2.14	0.52
1:E:67:THR:C	1:E:70:GLY:H	2.18	0.52
1:E:200:HIS:CB	1:E:202:ARG:HH22	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:ASP:OD1	1:F:146:PHE:N	2.38	0.52
1:A:10:ALA:HB3	1:B:10:ALA:HB3	1.91	0.52
1:A:110:MET:HE2	1:A:135:ALA:O	2.10	0.52
1:A:47:ASP:OD2	1:B:48:ARG:HD2	2.10	0.51
1:A:205:GLU:HG2	1:A:262:MET:HB2	1.91	0.51
1:B:78:ARG:HB3	1:B:134:PRO:HA	1.92	0.51
1:B:154:MET:CE	1:B:163:ARG:HE	2.21	0.51
1:C:179:LEU:HD12	1:C:180:GLN:N	2.25	0.51
1:D:155:GLY:HA3	1:D:162:LYS:HA	1.93	0.51
1:B:223:LEU:HD12	1:B:246:SER:OG	2.11	0.51
1:C:56:PRO:HA	1:C:61:LEU:HD12	1.91	0.51
1:F:227:ASP:O	1:F:280:LEU:HA	2.11	0.51
1:B:57:THR:HG22	1:B:125:PRO:HG3	1.91	0.51
1:D:78:ARG:HD3	1:D:134:PRO:HA	1.91	0.51
1:E:77:ARG:HH11	1:E:77:ARG:HB3	1.75	0.51
1:F:161:ASN:O	1:F:163:ARG:HD3	2.10	0.51
1:A:218:ARG:O	1:A:252:GLY:HA2	2.09	0.51
1:B:167:LYS:HD3	1:B:170:ASP:OD1	2.11	0.51
1:A:137:LYS:HE2	1:A:139:TYR:CE1	2.46	0.51
1:F:62:GLU:HB3	1:F:116:VAL:HA	1.91	0.51
1:A:107:TYR:CZ	1:A:176:THR:HG22	2.46	0.51
1:B:139:TYR:CD1	1:B:175:ASP:HB3	2.46	0.51
1:B:230:ARG:HH12	1:C:230:ARG:NE	2.09	0.51
1:C:76:GLN:O	1:C:110:MET:HG3	2.11	0.51
1:C:79:GLU:HG2	1:C:133:THR:O	2.11	0.51
1:F:163:ARG:HB3	1:F:186:LEU:HD13	1.92	0.51
1:A:54:VAL:HG12	1:A:61:LEU:HD12	1.93	0.51
1:C:225:LYS:HE2	1:C:228:GLU:HB3	1.92	0.51
1:E:11:HIS:CE1	1:F:12:SER:HB3	2.46	0.51
1:E:136:HIS:HB2	1:F:136:HIS:HB2	1.93	0.51
1:B:34:PHE:CE1	1:B:127:LYS:HB3	2.46	0.50
1:C:10:ALA:HB3	1:D:10:ALA:HB3	1.93	0.50
1:C:165:ILE:C	1:C:166:TYR:CD2	2.86	0.50
1:E:88:ALA:HB3	1:E:120:GLU:HG3	1.93	0.50
1:B:154:MET:SD	1:B:163:ARG:NH1	2.84	0.50
1:E:58:ASP:HA	1:E:122:ARG:NH1	2.26	0.50
1:E:66:SER:O	1:E:70:GLY:N	2.45	0.50
1:C:37:GLY:O	1:C:61:LEU:HD11	2.11	0.50
1:C:240:VAL:HG12	1:C:242:ASN:OD1	2.11	0.50
1:C:182:GLY:O	1:C:259:ILE:HG23	2.12	0.50
1:D:31:GLU:O	1:D:238:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ASP:OD1	1:E:171:ALA:N	2.44	0.50
1:F:59:GLU:O	1:F:60:PRO:C	2.55	0.50
1:F:91:ILE:HD11	1:F:106:TYR:CD2	2.46	0.50
1:A:2:SER:HB3	1:A:38:ASP:OD1	2.11	0.50
1:C:225:LYS:H	1:C:225:LYS:HD2	1.75	0.50
1:D:59:GLU:HG3	1:D:60:PRO:CD	2.42	0.50
1:F:90:ALA:O	1:F:118:THR:HG22	2.11	0.50
1:A:110:MET:HE1	1:A:137:LYS:N	2.26	0.49
1:B:30:MET:HE3	1:B:42:THR:CG2	2.41	0.49
1:B:210:PHE:CE1	1:B:259:ILE:HG13	2.46	0.49
1:F:133:THR:HG21	1:F:178:GLN:HG3	1.93	0.49
1:A:36:PRO:N	1:A:55:MET:HE3	2.26	0.49
1:A:170:ASP:OD2	1:A:172:SER:OG	2.29	0.49
1:B:202:ARG:C	1:B:203:ARG:HG2	2.36	0.49
1:F:210:PHE:HA	1:F:236:ASN:OD1	2.13	0.49
1:D:203:ARG:NE	1:D:262:MET:HG2	2.27	0.49
1:F:203:ARG:NH2	1:F:268:THR:O	2.44	0.49
1:A:16:ILE:HG22	1:A:19:TYR:CE2	2.47	0.49
1:D:82:ILE:HD13	1:D:117:PHE:HE2	1.77	0.49
1:E:200:HIS:HB2	1:E:202:ARG:HH22	1.78	0.49
1:F:63:ILE:O	1:F:63:ILE:HG13	2.11	0.49
1:F:75:LEU:HD12	1:F:78:ARG:HB2	1.94	0.49
1:A:277:MET:HE2	1:E:216:GLU:O	2.12	0.49
1:B:218:ARG:NH2	1:B:235:PHE:CD2	2.79	0.49
1:C:225:LYS:HD3	1:C:228:GLU:O	2.13	0.49
1:D:166:TYR:HB2	1:D:183:TYR:HB3	1.95	0.49
1:F:39:ILE:HG23	1:F:54:VAL:HG12	1.94	0.49
1:B:183:TYR:HE1	1:B:210:PHE:CZ	2.30	0.49
1:A:19:TYR:CD1	1:A:23:LYS:NZ	2.54	0.49
1:C:39:ILE:HG23	1:C:54:VAL:HG12	1.94	0.49
1:B:161:ASN:HB2	1:B:163:ARG:HH22	1.77	0.49
1:D:62:GLU:HG3	1:D:115:VAL:O	2.13	0.48
1:E:200:HIS:CB	1:E:202:ARG:NH2	2.74	0.48
1:E:203:ARG:CB	1:E:264:GLY:HA3	2.43	0.48
1:F:223:LEU:HD12	1:F:246:SER:OG	2.13	0.48
1:A:157:GLN:O	1:E:189:GLY:HA2	2.13	0.48
1:A:205:GLU:OE2	1:A:248:HIS:CE1	2.66	0.48
1:B:21:THR:HG21	1:C:228:GLU:HA	1.94	0.48
1:F:11:HIS:NE2	1:F:27:GLU:OE2	2.46	0.48
1:F:137:LYS:HD3	1:F:139:TYR:CZ	2.48	0.48
1:F:167:LYS:HG3	1:F:170:ASP:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:OD1	1:A:159:HIS:N	2.42	0.48
1:C:99:ALA:O	1:C:143:LYS:NZ	2.45	0.48
1:F:64:LYS:O	1:F:65:LEU:HD23	2.13	0.48
1:C:225:LYS:H	1:C:225:LYS:HD3	1.76	0.48
1:F:56:PRO:HG2	1:F:128:PHE:CE2	2.44	0.48
1:B:117:PHE:HB3	1:B:128:PHE:CE2	2.48	0.48
1:E:69:LEU:CA	1:F:202:ARG:HH12	2.26	0.48
1:C:115:VAL:HG13	1:C:115:VAL:O	2.12	0.48
1:F:91:ILE:HD12	1:F:91:ILE:O	2.13	0.48
1:C:41:LEU:HD23	1:C:52:GLY:HA3	1.96	0.48
1:E:200:HIS:CD2	1:E:272:MET:HE1	2.49	0.48
1:A:53:GLY:HA2	1:A:128:PHE:O	2.13	0.47
1:A:68:GLU:C	1:B:202:ARG:HH21	2.22	0.47
1:C:266:ASN:ND2	1:C:268:THR:HG23	2.24	0.47
1:D:253:THR:HG21	1:F:195:MET:HE2	1.96	0.47
1:E:29:LEU:CD2	1:E:31:GLU:HG2	2.44	0.47
1:F:39:ILE:HD13	1:F:63:ILE:HG22	1.96	0.47
1:F:82:ILE:HD13	1:F:106:TYR:HB3	1.96	0.47
1:B:144:LEU:HD21	1:B:174:MET:SD	2.54	0.47
1:C:82:ILE:HD13	1:C:117:PHE:HE2	1.78	0.47
1:F:63:ILE:HD11	1:F:74:PHE:CZ	2.49	0.47
1:F:94:ASP:HA	1:F:114:LYS:HE3	1.96	0.47
1:B:55:MET:HE2	1:B:127:LYS:HG2	1.96	0.47
1:C:203:ARG:HB2	1:C:263:CYS:O	2.15	0.47
1:C:214:ASP:OD1	1:C:214:ASP:N	2.46	0.47
1:D:204:MET:HE3	1:D:263:CYS:SG	2.54	0.47
1:E:107:TYR:O	1:E:108:ILE:HD13	2.14	0.47
1:E:200:HIS:ND1	1:E:203:ARG:O	2.48	0.47
1:C:91:ILE:HA	1:C:116:VAL:O	2.14	0.47
1:F:91:ILE:HA	1:F:116:VAL:O	2.14	0.47
1:F:205:GLU:HG2	1:F:262:MET:HB2	1.96	0.47
1:B:110:MET:HG2	1:B:111:GLY:N	2.28	0.47
1:B:171:ALA:N	1:B:180:GLN:HE22	2.11	0.47
1:C:144:LEU:HD22	1:C:168:TYR:O	2.14	0.47
1:A:34:PHE:CD1	1:A:127:LYS:HB3	2.50	0.47
1:A:137:LYS:HE2	1:A:139:TYR:CZ	2.49	0.47
1:A:163:ARG:HD3	1:A:184:THR:CG2	2.44	0.47
1:A:182:GLY:HA3	1:A:260:TRP:CZ2	2.50	0.47
1:B:29:LEU:HD23	1:B:31:GLU:HG2	1.96	0.47
1:B:170:ASP:H	1:B:174:MET:CE	2.28	0.47
1:C:150:LEU:HG	1:C:151:ALA:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:TYR:CD2	1:C:166:TYR:N	2.83	0.47
1:D:115:VAL:HG12	1:D:117:PHE:CE1	2.50	0.47
1:E:29:LEU:CD1	1:E:234:LEU:HD22	2.44	0.47
1:E:179:LEU:HD11	1:E:181:MET:HG3	1.97	0.47
1:F:34:PHE:HE2	1:F:208:MET:HE3	1.79	0.47
1:A:142:LYS:HZ1	1:A:174:MET:CB	2.22	0.47
1:C:29:LEU:CD2	1:C:31:GLU:HG2	2.45	0.47
1:D:19:TYR:HE1	1:D:27:GLU:HG3	1.79	0.47
1:C:29:LEU:HD23	1:C:31:GLU:HG2	1.97	0.47
1:A:202:ARG:HB2	1:A:266:ASN:ND2	2.29	0.47
1:B:29:LEU:CD2	1:B:31:GLU:HG2	2.45	0.47
1:B:226:PRO:O	1:B:279:GLU:HA	2.15	0.47
1:F:73:PHE:CD2	1:F:113:GLN:HA	2.50	0.47
1:F:210:PHE:HD2	1:F:211:ASN:ND2	2.10	0.47
1:F:212:PHE:HB3	1:F:217:THR:HB	1.96	0.47
1:A:228:GLU:HG3	1:A:230:ARG:HH12	1.80	0.46
1:B:146:PHE:HE1	1:B:166:TYR:HD1	1.61	0.46
1:C:92:THR:OG1	1:C:116:VAL:CG1	2.60	0.46
1:C:220:PHE:N	1:C:251:VAL:O	2.30	0.46
1:E:40:LEU:O	1:E:52:GLY:HA3	2.15	0.46
1:E:136:HIS:H	1:F:136:HIS:HD2	1.60	0.46
1:F:25:ARG:NH1	1:F:233:THR:H	2.13	0.46
1:D:207:TYR:HH	1:D:248:HIS:HD1	1.59	0.46
1:E:179:LEU:HD12	1:E:180:GLN:N	2.30	0.46
1:E:195:MET:HB3	1:E:196:PRO:CD	2.44	0.46
1:F:226:PRO:O	1:F:279:GLU:HA	2.16	0.46
1:B:107:TYR:CD1	1:B:107:TYR:C	2.93	0.46
1:C:217:THR:C	1:C:218:ARG:HG2	2.41	0.46
1:B:35:ASN:OD1	1:B:36:PRO:HD2	2.15	0.46
1:C:34:PHE:HB3	1:C:55:MET:HE2	1.97	0.46
1:A:110:MET:HG2	1:A:111:GLY:N	2.27	0.46
1:A:277:MET:HG3	1:E:216:GLU:HB3	1.98	0.46
1:B:6:VAL:HG22	1:B:42:THR:HG22	1.98	0.46
1:F:200:HIS:NE2	1:F:205:GLU:OE2	2.48	0.46
1:D:205:GLU:HG2	1:D:262:MET:HB2	1.98	0.46
1:C:82:ILE:HD13	1:C:117:PHE:CE2	2.51	0.46
1:A:279:GLU:N	1:E:218:ARG:NH1	2.52	0.46
1:B:5:MET:HA	1:B:41:LEU:O	2.15	0.46
1:B:114:LYS:HZ2	1:B:114:LYS:HG3	1.67	0.46
1:D:35:ASN:O	1:D:55:MET:HG2	2.16	0.46
1:E:77:ARG:HH21	1:F:267:GLN:HE21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:PRO:HA	1:F:61:LEU:HD12	1.98	0.46
1:F:195:MET:O	1:F:197:ALA:N	2.49	0.46
1:C:165:ILE:O	1:C:166:TYR:HD2	1.99	0.46
1:C:78:ARG:HG3	1:C:133:THR:C	2.41	0.46
1:C:198:HIS:HB2	1:C:272:MET:HB2	1.98	0.46
1:D:231:HIS:NE2	1:F:229:THR:OG1	2.41	0.46
1:D:21:THR:HG23	1:F:230:ARG:NH1	2.31	0.45
1:E:200:HIS:HB3	1:E:272:MET:CE	2.45	0.45
1:F:260:TRP:CE2	3:F:302:MPO:H72	2.51	0.45
1:B:21:THR:N	1:C:228:GLU:OE2	2.45	0.45
1:B:96:ARG:NH1	1:B:96:ARG:HA	2.29	0.45
1:B:107:TYR:CD1	1:B:108:ILE:N	2.80	0.45
1:B:189:GLY:HA2	1:C:157:GLN:O	2.15	0.45
1:C:210:PHE:HE1	1:C:259:ILE:HG13	1.81	0.45
1:D:32:LYS:HD2	1:D:34:PHE:O	2.16	0.45
1:B:2:SER:HB2	1:B:38:ASP:OD1	2.16	0.45
1:C:179:LEU:HD12	1:C:180:GLN:H	1.81	0.45
1:C:187:GLU:O	1:C:190:SER:HB2	2.16	0.45
1:F:61:LEU:O	1:F:117:PHE:N	2.37	0.45
1:F:158:GLN:O	1:F:158:GLN:HG3	2.15	0.45
1:B:11:HIS:HB3	1:B:15:ASP:HB2	1.98	0.45
1:C:19:TYR:HE2	1:C:27:GLU:HG3	1.81	0.45
1:C:216:GLU:N	1:C:216:GLU:OE1	2.49	0.45
1:D:3:PHE:HD1	1:D:39:ILE:HB	1.80	0.45
1:A:19:TYR:CB	1:A:23:LYS:HZ1	2.15	0.45
1:B:170:ASP:H	1:B:174:MET:HE3	1.82	0.45
1:C:224:GLY:O	1:C:247:ILE:HG12	2.16	0.45
1:D:218:ARG:NH2	1:F:279:GLU:O	2.48	0.45
1:F:62:GLU:CB	1:F:116:VAL:HA	2.46	0.45
1:A:91:ILE:HD11	1:A:106:TYR:CD2	2.52	0.45
1:C:30:MET:SD	1:C:42:THR:HG23	2.57	0.45
1:C:71:VAL:HB	1:C:76:GLN:OE1	2.16	0.45
1:C:100:MET:HE2	1:C:100:MET:HB3	1.84	0.45
1:D:194:THR:HG22	1:D:194:THR:O	2.15	0.45
1:E:152:LYS:O	1:E:165:ILE:HG22	2.17	0.45
1:E:203:ARG:HH21	1:E:262:MET:CE	2.29	0.45
1:B:200:HIS:ND1	1:B:203:ARG:O	2.50	0.45
1:D:30:MET:HE2	1:D:42:THR:OG1	2.16	0.45
1:D:192:TRP:CD2	1:D:251:VAL:HG12	2.51	0.45
1:F:214:ASP:OD1	1:F:215:PRO:HD3	2.17	0.45
1:A:154:MET:HE2	1:A:165:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:HB	1:C:280:LEU:CD1	2.47	0.45
1:B:98:ASP:OD1	1:B:143:LYS:NZ	2.49	0.45
1:B:174:MET:HE3	1:B:174:MET:HB3	1.63	0.45
1:D:42:THR:HB	1:D:51:PHE:CE1	2.51	0.45
1:D:179:LEU:HD12	1:D:180:GLN:N	2.32	0.45
1:D:227:ASP:OD1	1:D:228:GLU:N	2.50	0.45
1:E:3:PHE:CZ	1:E:65:LEU:HD21	2.51	0.45
1:E:5:MET:HE3	1:E:43:TYR:CD2	2.51	0.45
1:A:85:ILE:HA	1:A:103:GLN:NE2	2.32	0.45
1:A:221:HIS:CD2	1:A:240:VAL:HG11	2.52	0.45
3:B:302:MPO:H42	3:B:302:MPO:H11	1.98	0.45
1:D:92:THR:HG22	1:D:97:LYS:HB2	1.98	0.45
1:F:49:MET:HE1	1:F:206:THR:HB	1.98	0.45
1:B:48:ARG:O	1:B:78:ARG:NH2	2.49	0.44
1:C:269:TYR:O	1:C:272:MET:HE3	2.16	0.44
1:F:129:TYR:CE1	1:F:208:MET:HG3	2.53	0.44
1:C:34:PHE:CD1	1:C:127:LYS:HB3	2.52	0.44
1:D:129:TYR:CE2	1:D:208:MET:HG3	2.52	0.44
1:A:6:VAL:HG22	1:A:42:THR:HG22	1.98	0.44
1:B:114:LYS:HE2	1:B:116:VAL:CB	2.41	0.44
1:C:47:ASP:CG	1:D:48:ARG:NH1	2.75	0.44
1:C:92:THR:HG22	1:C:97:LYS:CG	2.47	0.44
1:D:73:PHE:CD2	1:D:113:GLN:HA	2.53	0.44
1:D:145:PRO:HD2	1:D:148:THR:OG1	2.17	0.44
1:A:23:LYS:HB3	1:A:23:LYS:HE3	1.20	0.44
1:A:102:ASN:OD1	1:A:103:GLN:HG2	2.17	0.44
1:B:231:HIS:NE2	1:C:229:THR:HG23	2.33	0.44
1:C:210:PHE:CE1	1:C:259:ILE:HG13	2.52	0.44
1:E:6:VAL:HG21	1:E:8:ARG:NH2	2.31	0.44
1:E:214:ASP:OD1	1:E:215:PRO:HD2	2.17	0.44
1:F:92:THR:HG22	1:F:97:LYS:CD	2.48	0.44
1:A:19:TYR:HB3	1:A:23:LYS:NZ	2.15	0.44
1:B:69:LEU:N	1:B:69:LEU:HD12	2.33	0.44
1:C:179:LEU:O	1:C:180:GLN:HG2	2.18	0.44
1:E:102:ASN:OD1	1:E:103:GLN:HG2	2.18	0.44
1:E:208:MET:HG2	1:E:239:ALA:HB2	1.99	0.44
1:A:68:GLU:O	1:B:202:ARG:CZ	2.65	0.44
1:A:81:GLY:HA3	1:A:181:MET:HE2	2.00	0.44
1:A:129:TYR:CE1	1:A:208:MET:HG3	2.52	0.44
1:F:174:MET:HG2	1:F:175:ASP:N	2.32	0.44
1:A:75:LEU:HD21	1:A:80:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ARG:NH2	1:B:271:ASP:O	2.51	0.44
1:B:224:GLY:HA2	1:B:245:TRP:HZ3	1.82	0.44
1:C:54:VAL:HG21	1:C:117:PHE:CG	2.53	0.44
1:F:107:TYR:O	1:F:108:ILE:HD13	2.17	0.44
1:A:12:SER:OG	1:A:14:GLU:HB2	2.18	0.44
1:A:39:ILE:HG12	1:A:54:VAL:HG13	1.98	0.44
1:B:91:ILE:HD11	1:B:106:TYR:CD1	2.53	0.44
1:C:75:LEU:CD2	1:C:80:LEU:HB2	2.46	0.44
1:C:203:ARG:HE	1:C:262:MET:HE2	1.82	0.44
1:D:82:ILE:HD13	1:D:117:PHE:CE2	2.52	0.44
1:A:73:PHE:CD2	1:A:113:GLN:HA	2.53	0.43
1:D:51:PHE:CD2	1:D:206:THR:HG21	2.53	0.43
1:D:93:ILE:HD11	1:D:141:ASN:HD22	1.81	0.43
1:D:134:PRO:HD2	1:D:178:GLN:NE2	2.33	0.43
1:D:234:LEU:HD21	1:D:240:VAL:HG23	1.99	0.43
1:A:178:GLN:HE21	1:A:264:GLY:N	2.17	0.43
1:B:30:MET:SD	1:B:42:THR:HG23	2.58	0.43
1:F:209:TYR:HB3	1:F:212:PHE:HE1	1.83	0.43
1:B:204:MET:HE3	1:B:204:MET:HB3	1.48	0.43
1:C:221:HIS:HE1	1:C:242:ASN:ND2	2.08	0.43
1:D:34:PHE:CE2	1:D:85:ILE:HD11	2.53	0.43
1:E:2:SER:OG	1:E:3:PHE:N	2.51	0.43
1:E:174:MET:HE3	1:E:174:MET:HB2	1.83	0.43
1:F:225:LYS:HB3	1:F:225:LYS:HZ3	1.80	0.43
1:A:156:ASP:CG	1:A:159:HIS:HD1	2.26	0.43
1:B:85:ILE:HD12	1:B:208:MET:HE1	2.00	0.43
1:B:154:MET:CE	1:B:163:ARG:HH11	2.15	0.43
1:C:78:ARG:HG3	1:C:134:PRO:CA	2.45	0.43
1:E:48:ARG:HD2	1:F:265:GLU:HB2	1.99	0.43
1:F:226:PRO:HG3	1:F:275:VAL:HG11	2.01	0.43
1:A:16:ILE:O	1:A:19:TYR:HB2	2.19	0.43
1:A:77:ARG:NE	1:B:266:ASN:HA	2.34	0.43
1:A:270:ASP:OD2	1:A:270:ASP:N	2.42	0.43
1:B:85:ILE:CG2	1:B:127:LYS:HB2	2.49	0.43
1:B:218:ARG:NH2	1:B:235:PHE:CE2	2.83	0.43
1:C:7:THR:O	1:C:8:ARG:NH1	2.52	0.43
1:E:70:GLY:HA3	1:F:202:ARG:HH22	1.84	0.43
1:F:139:TYR:HD1	1:F:139:TYR:HA	1.73	0.43
1:F:156:ASP:OD1	1:F:159:HIS:N	2.47	0.43
1:A:167:LYS:HZ2	1:A:173:GLN:HG2	1.83	0.43
1:A:200:HIS:CE1	1:A:203:ARG:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HD2	1:B:68:GLU:O	2.17	0.43
1:B:92:THR:HA	1:B:97:LYS:HA	1.99	0.43
1:C:15:ASP:OD1	1:D:11:HIS:HD2	2.02	0.43
1:C:266:ASN:HD21	1:C:268:THR:CG2	2.26	0.43
1:E:162:LYS:N	1:E:190:SER:OG	2.51	0.43
1:F:11:HIS:CE1	1:F:27:GLU:OE2	2.72	0.43
1:B:68:GLU:HB2	1:B:69:LEU:HD12	2.01	0.43
1:B:228:GLU:OE1	1:C:20:ASP:HB2	2.18	0.43
1:B:222:PHE:HB2	1:B:249:CYS:HB2	2.01	0.43
1:E:77:ARG:NH2	1:F:267:GLN:HE21	2.17	0.43
1:E:198:HIS:HB3	1:E:272:MET:CE	2.48	0.43
1:E:203:ARG:HB2	1:E:264:GLY:HA3	2.00	0.43
1:F:202:ARG:HE	1:F:202:ARG:HB2	1.22	0.43
1:A:82:ILE:HD13	1:A:117:PHE:HE1	1.84	0.43
1:C:69:LEU:HD13	1:D:265:GLU:OE1	2.18	0.43
1:E:40:LEU:O	1:E:41:LEU:HD23	2.19	0.43
1:E:78:ARG:HG2	1:E:134:PRO:HA	1.99	0.43
1:E:200:HIS:HB3	1:E:272:MET:HE1	2.00	0.43
1:E:221:HIS:CG	1:E:240:VAL:HG11	2.53	0.43
1:F:145:PRO:O	1:F:148:THR:HG22	2.19	0.43
1:B:21:THR:HG23	1:C:228:GLU:HG3	2.01	0.42
1:B:62:GLU:HG3	1:B:115:VAL:O	2.19	0.42
1:B:146:PHE:HE1	1:B:166:TYR:CE1	2.36	0.42
1:C:37:GLY:C	1:C:61:LEU:HD11	2.44	0.42
1:E:165:ILE:HD12	1:E:183:TYR:O	2.19	0.42
1:A:266:ASN:OD1	1:A:268:THR:N	2.52	0.42
1:B:202:ARG:HD3	1:B:202:ARG:HA	1.57	0.42
1:E:23:LYS:O	1:E:27:GLU:HB2	2.19	0.42
1:F:184:THR:HB	1:F:258:PHE:CE1	2.54	0.42
1:C:31:GLU:O	1:C:238:GLN:HG2	2.20	0.42
1:A:28:PHE:CD2	1:A:223:LEU:HD21	2.53	0.42
1:B:166:TYR:N	1:B:166:TYR:CD2	2.88	0.42
1:D:3:PHE:CD1	1:D:39:ILE:HB	2.54	0.42
1:D:24:LEU:HD23	1:D:24:LEU:HA	1.81	0.42
1:D:25:ARG:HG2	1:D:232:ILE:HG23	2.00	0.42
1:F:25:ARG:O	1:F:29:LEU:HB3	2.19	0.42
1:F:35:ASN:C	1:F:55:MET:HE3	2.44	0.42
1:F:202:ARG:NH2	1:F:266:ASN:ND2	2.67	0.42
1:A:152:LYS:HB3	1:A:165:ILE:CG2	2.49	0.42
1:A:227:ASP:OD2	1:A:280:LEU:HD13	2.19	0.42
1:C:136:HIS:CG	1:D:177:CYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HA	1:D:19:TYR:CE2	2.54	0.42
1:D:25:ARG:O	1:D:29:LEU:HB3	2.18	0.42
1:D:39:ILE:HG23	1:D:54:VAL:HG22	2.01	0.42
1:D:83:ILE:HG13	1:D:181:MET:HE1	2.02	0.42
1:B:209:TYR:CE2	1:B:219:VAL:HG11	2.55	0.42
1:D:36:PRO:HA	1:D:55:MET:HG3	2.01	0.42
1:A:152:LYS:HB3	1:A:165:ILE:HG23	2.02	0.42
1:A:204:MET:HE2	1:A:204:MET:HB2	1.93	0.42
1:A:44:THR:O	1:A:48:ARG:HA	2.19	0.42
1:C:133:THR:CG2	1:C:178:GLN:HG3	2.50	0.42
1:D:135:ALA:HB1	1:D:177:CYS:SG	2.60	0.42
1:E:16:ILE:HG22	1:E:19:TYR:CE2	2.54	0.42
1:F:202:ARG:CG	1:F:265:GLU:HB3	2.48	0.42
1:A:99:ALA:O	1:A:143:LYS:NZ	2.42	0.42
1:B:106:TYR:CE1	1:B:143:LYS:HB2	2.55	0.42
1:B:154:MET:HE3	1:B:163:ARG:NE	2.29	0.42
1:E:184:THR:HB	1:E:258:PHE:CE1	2.54	0.42
1:F:202:ARG:HH11	1:F:202:ARG:HD2	1.31	0.42
1:A:12:SER:HB2	1:B:11:HIS:HE1	1.85	0.42
1:A:40:LEU:O	1:A:52:GLY:HA3	2.20	0.42
1:A:91:ILE:HG22	1:A:117:PHE:HA	2.02	0.42
1:A:201:ALA:O	1:B:48:ARG:NH2	2.53	0.42
1:D:11:HIS:CE1	1:D:27:GLU:OE1	2.73	0.42
1:D:228:GLU:CD	1:F:21:THR:HG23	2.45	0.42
1:D:139:TYR:CE1	1:D:175:ASP:HB3	2.55	0.41
1:D:200:HIS:CE1	1:D:203:ARG:O	2.73	0.41
1:D:229:THR:HG23	1:F:231:HIS:NE2	2.35	0.41
1:E:107:TYR:CZ	1:E:176:THR:HG22	2.54	0.41
1:B:92:THR:HG22	1:B:116:VAL:HG12	2.02	0.41
1:B:234:LEU:HD21	1:B:240:VAL:CG2	2.50	0.41
1:C:92:THR:CG2	1:C:97:LYS:HB2	2.48	0.41
1:D:8:ARG:NH1	1:D:26:HIS:O	2.53	0.41
1:A:29:LEU:HD12	1:A:239:ALA:O	2.19	0.41
1:A:178:GLN:HG2	1:A:264:GLY:O	2.20	0.41
1:B:69:LEU:CD2	1:B:78:ARG:HH11	2.33	0.41
1:B:110:MET:HE2	1:B:135:ALA:O	2.21	0.41
1:C:198:HIS:CD2	1:C:248:HIS:NE2	2.88	0.41
1:D:162:LYS:HE3	1:D:187:GLU:CD	2.44	0.41
1:E:273:ASP:OD1	1:E:273:ASP:N	2.54	0.41
1:F:94:ASP:CA	1:F:114:LYS:HE3	2.49	0.41
1:F:203:ARG:NH1	1:F:272:MET:HE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:THR:O	1:B:149:ALA:C	2.64	0.41
1:D:65:LEU:HD13	1:D:69:LEU:HD11	2.02	0.41
1:D:200:HIS:ND1	1:D:203:ARG:O	2.53	0.41
1:D:207:TYR:O	1:D:239:ALA:HA	2.19	0.41
1:F:101:SER:O	1:F:104:ASP:HB2	2.20	0.41
1:B:85:ILE:HG21	1:B:85:ILE:HD13	1.77	0.41
1:B:192:TRP:CD2	1:B:251:VAL:HG12	2.54	0.41
1:C:34:PHE:HE2	1:C:208:MET:HE3	1.85	0.41
1:E:198:HIS:CB	1:E:272:MET:HE2	2.50	0.41
1:A:35:ASN:C	1:A:55:MET:HE3	2.46	0.41
1:A:150:LEU:HD13	1:A:167:LYS:HG3	2.02	0.41
1:B:57:THR:HB	1:B:122:ARG:HG3	2.03	0.41
1:C:107:TYR:CZ	1:C:176:THR:HG22	2.56	0.41
1:D:55:MET:CE	1:D:127:LYS:HG2	2.48	0.41
1:E:78:ARG:NH1	1:F:265:GLU:CD	2.79	0.41
1:F:29:LEU:HD12	1:F:239:ALA:O	2.20	0.41
1:F:208:MET:HE2	1:F:237:GLU:HA	2.03	0.41
1:F:218:ARG:O	1:F:252:GLY:HA2	2.20	0.41
1:F:39:ILE:HG12	1:F:54:VAL:HG12	2.03	0.41
1:C:78:ARG:HH21	1:C:78:ARG:HD3	1.67	0.41
1:E:136:HIS:N	1:F:136:HIS:HD2	2.17	0.41
1:A:220:PHE:HB2	1:A:251:VAL:CG2	2.51	0.41
1:B:34:PHE:HB3	1:B:55:MET:HE2	2.02	0.41
1:B:202:ARG:HD3	1:B:202:ARG:HH11	1.61	0.41
1:C:90:ALA:HB3	1:C:97:LYS:NZ	2.36	0.41
1:D:191:SER:OG	1:D:252:GLY:O	2.28	0.41
1:D:211:ASN:N	1:D:236:ASN:HD21	2.19	0.41
1:E:87:GLY:N	1:E:126:ALA:HA	2.36	0.41
1:F:91:ILE:HG21	1:F:117:PHE:CD2	2.56	0.41
1:B:8:ARG:NH1	1:B:26:HIS:O	2.50	0.41
1:C:43:TYR:CZ	1:C:48:ARG:HG2	2.56	0.41
1:E:107:TYR:CE1	1:E:176:THR:HG22	2.56	0.41
1:E:195:MET:O	1:E:196:PRO:C	2.61	0.41
1:F:78:ARG:HG2	1:F:134:PRO:HA	2.01	0.41
1:F:143:LYS:O	1:F:145:PRO:HD3	2.21	0.41
1:B:60:PRO:HB2	1:B:116:VAL:HG21	2.02	0.40
1:B:156:ASP:CA	1:B:162:LYS:HD2	2.48	0.40
1:C:51:PHE:CD1	1:C:51:PHE:C	2.98	0.40
1:C:228:GLU:CD	1:C:230:ARG:HH22	2.25	0.40
1:F:135:ALA:HB1	1:F:177:CYS:SG	2.61	0.40
1:B:169:ILE:CG2	1:B:176:THR:HG21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:NH1	1:D:47:ASP:OD2	2.45	0.40
1:D:41:LEU:HD23	1:D:52:GLY:CA	2.49	0.40
1:E:156:ASP:OD2	1:E:159:HIS:N	2.50	0.40
1:A:192:TRP:CD2	1:A:251:VAL:HG12	2.56	0.40
1:B:24:LEU:HD23	1:B:24:LEU:HA	1.75	0.40
1:B:169:ILE:HA	1:B:174:MET:CE	2.46	0.40
1:B:235:PHE:N	1:B:238:GLN:NE2	2.69	0.40
1:C:34:PHE:CE2	1:C:85:ILE:HD11	2.56	0.40
1:D:203:ARG:NH2	1:D:266:ASN:C	2.76	0.40
1:E:29:LEU:HD12	1:E:234:LEU:HD22	2.04	0.40
1:E:69:LEU:C	1:F:202:ARG:NH1	2.71	0.40
1:F:154:MET:HE3	1:F:154:MET:HB3	1.89	0.40
1:D:8:ARG:NH1	1:D:26:HIS:CE1	2.89	0.40
1:D:36:PRO:HA	1:D:55:MET:CG	2.51	0.40
1:F:65:LEU:HD23	1:F:65:LEU:HA	1.96	0.40
1:F:115:VAL:O	1:F:115:VAL:HG13	2.21	0.40
1:A:78:ARG:HG2	1:A:134:PRO:HA	2.04	0.40
1:A:178:GLN:HE21	1:A:264:GLY:H	1.68	0.40
1:A:214:ASP:OD1	1:A:215:PRO:N	2.54	0.40
1:B:114:LYS:HD2	1:B:115:VAL:N	2.36	0.40
1:E:91:ILE:HG22	1:E:93:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/289 (96%)	270 (98%)	7 (2%)	0	100	100
1	B	273/289 (94%)	261 (96%)	11 (4%)	1 (0%)	30	60
1	C	277/289 (96%)	268 (97%)	8 (3%)	1 (0%)	30	60
1	D	257/289 (89%)	250 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	272/289 (94%)	264 (97%)	8 (3%)	0	100	100
1	F	270/289 (93%)	262 (97%)	8 (3%)	0	100	100
All	All	1626/1734 (94%)	1575 (97%)	49 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ALA
1	C	196	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/253 (96%)	238 (98%)	5 (2%)	47	79
1	B	240/253 (95%)	234 (98%)	6 (2%)	42	76
1	C	243/253 (96%)	240 (99%)	3 (1%)	63	87
1	D	227/253 (90%)	224 (99%)	3 (1%)	61	86
1	E	241/253 (95%)	237 (98%)	4 (2%)	53	83
1	F	240/253 (95%)	234 (98%)	6 (2%)	42	76
All	All	1434/1518 (94%)	1407 (98%)	27 (2%)	50	81

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	92	THR
1	A	181	MET
1	A	248	HIS
1	A	249	CYS
1	B	4	SER
1	B	190	SER
1	B	194	THR

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Mol	Chain	Res	Type
1	B	202	ARG
1	B	205	GLU
1	B	263	CYS
1	C	133	THR
1	C	181	MET
1	C	248	HIS
1	D	75	LEU
1	D	233	THR
1	D	248	HIS
1	E	133	THR
1	E	164	THR
1	E	248	HIS
1	E	263	CYS
1	F	55	MET
1	F	61	LEU
1	F	83	ILE
1	F	202	ARG
1	F	248	HIS
1	F	249	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	173	GLN
1	A	178	GLN
1	A	193	ASN
1	A	242	ASN
1	B	46	ASN
1	B	76	GLN
1	B	124	HIS
1	B	173	GLN
1	B	180	GLN
1	B	238	GLN
1	B	248	HIS
1	C	11	HIS
1	C	180	GLN
1	C	198	HIS
1	C	221	HIS
1	C	266	ASN
1	D	11	HIS
1	D	18	HIS

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Mol	Chain	Res	Type
1	D	46	ASN
1	D	84	ASN
1	D	136	HIS
1	D	193	ASN
1	D	236	ASN
1	E	46	ASN
1	E	84	ASN
1	E	103	GLN
1	E	157	GLN
1	E	267	GLN
1	F	26	HIS
1	F	46	ASN
1	F	76	GLN
1	F	136	HIS
1	F	267	GLN
1	F	274	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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
3	MPO	A	302	-	13,13,13	1.10	1 (7%)	17,17,17	1.35	2 (11%)
3	MPO	E	302	-	13,13,13	0.67	1 (7%)	17,17,17	0.56	0
3	MPO	B	302	-	13,13,13	1.08	1 (7%)	17,17,17	1.06	1 (5%)
3	MPO	F	302	-	13,13,13	0.62	1 (7%)	17,17,17	0.91	2 (11%)

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
3	MPO	A	302	-	-	2/7/15/15	0/1/1/1
3	MPO	E	302	-	-	0/7/15/15	0/1/1/1
3	MPO	B	302	-	-	1/7/15/15	0/1/1/1
3	MPO	F	302	-	-	2/7/15/15	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	MPO	O1-S1	3.84	1.55	1.45
3	B	302	MPO	O2-S1	3.77	1.55	1.45
3	E	302	MPO	O3-S1	2.32	1.55	1.47
3	F	302	MPO	O3-S1	2.14	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	MPO	O3-S1-O2	3.71	120.69	111.40
3	A	302	MPO	O1-S1-C1	-3.53	101.40	106.73
3	B	302	MPO	O3-S1-O1	3.37	119.82	111.40
3	F	302	MPO	O2-S1-O1	2.35	121.47	113.82
3	F	302	MPO	O3-S1-C1	-2.07	101.95	106.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	302	MPO	C2-C3-N1-C4
3	F	302	MPO	C2-C3-N1-C7
3	A	302	MPO	C2-C1-S1-O1

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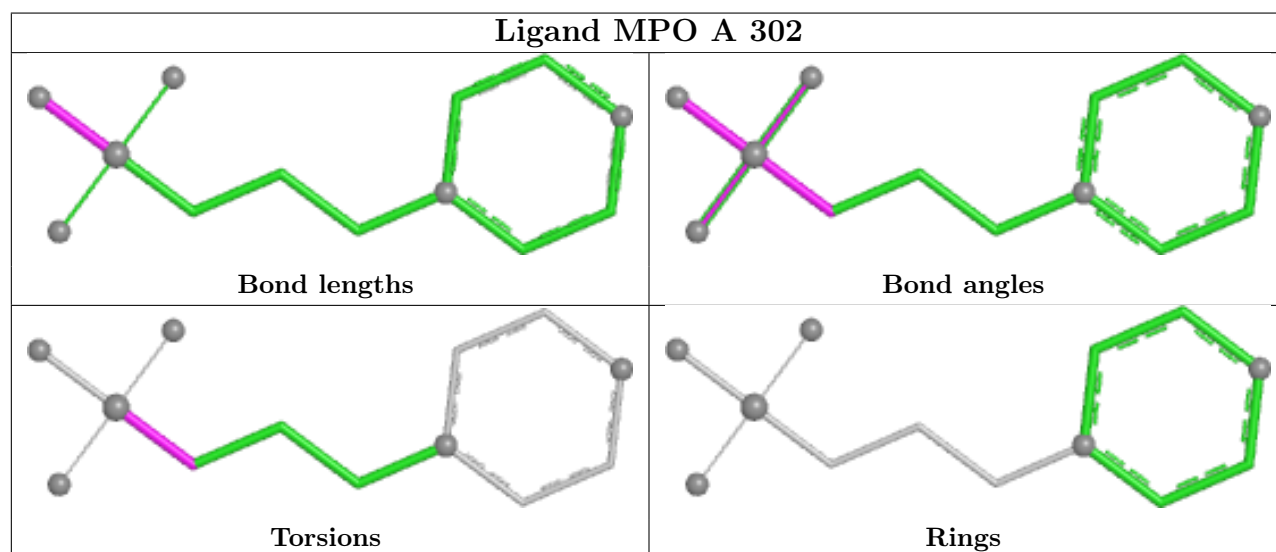
Mol	Chain	Res	Type	Atoms
3	A	302	MPO	C2-C1-S1-O2
3	B	302	MPO	C1-C2-C3-N1

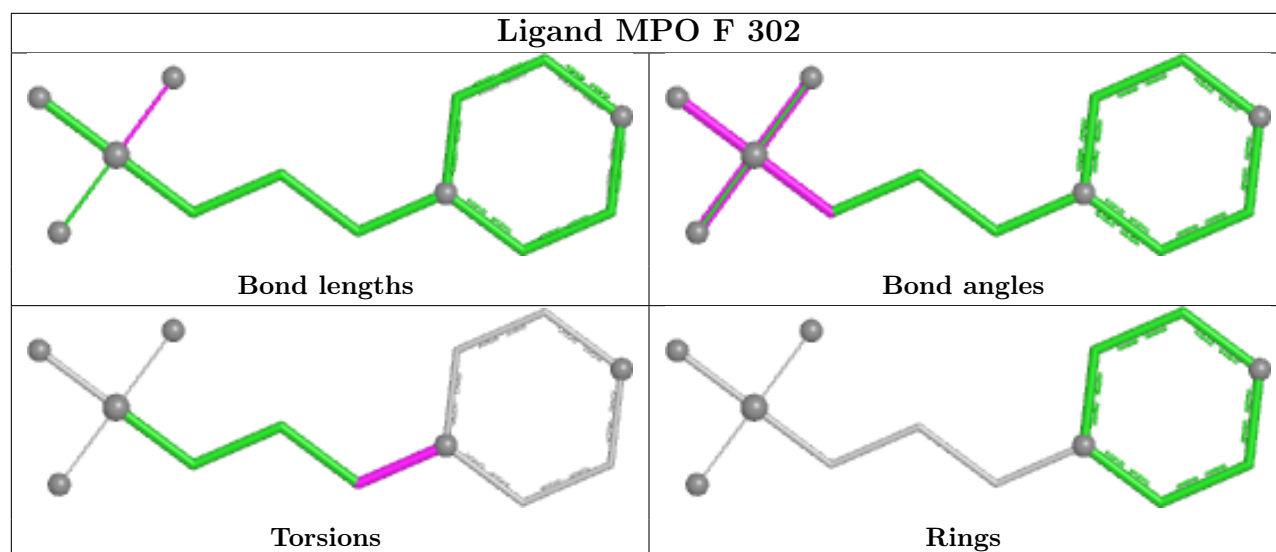
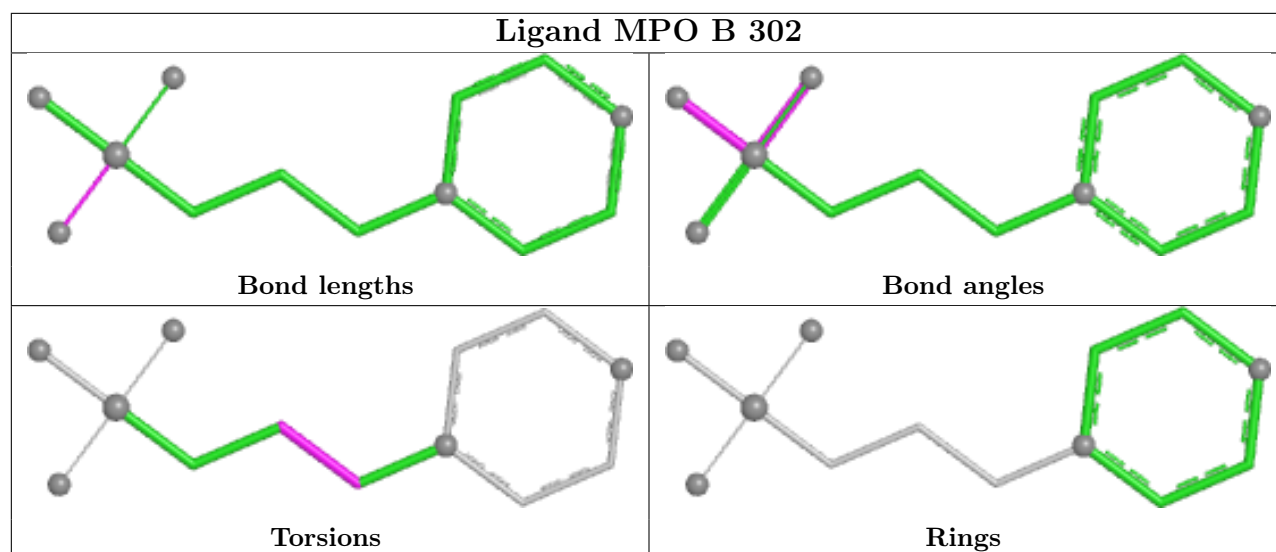
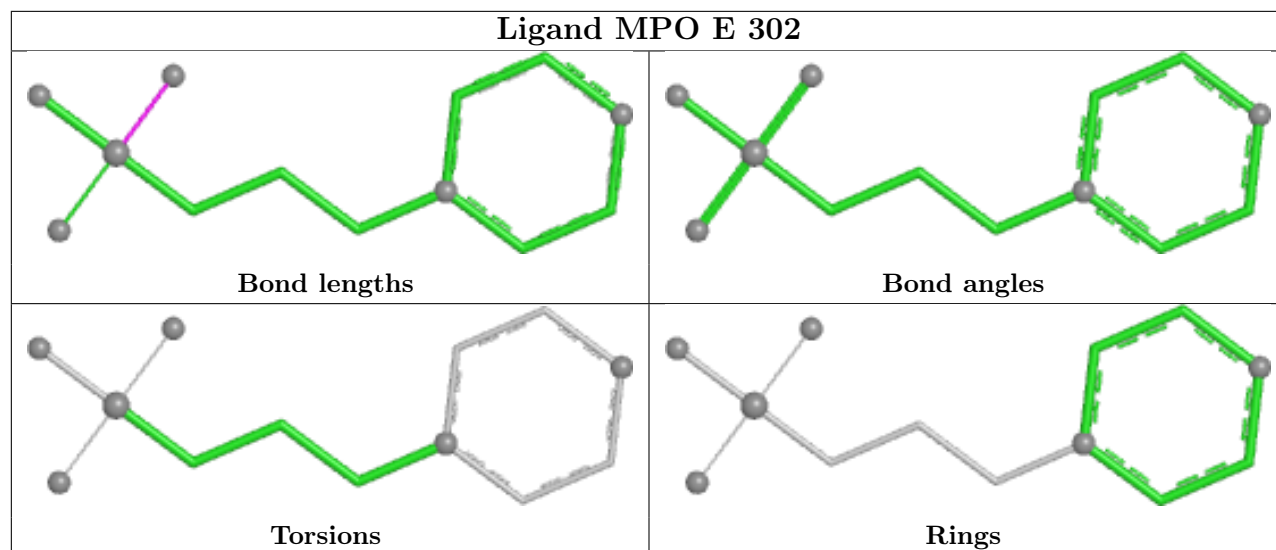
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	MPO	1	0
3	B	302	MPO	1	0
3	F	302	MPO	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	279/289 (96%)	-0.56	0	100 100	46, 68, 113, 171	0
1	B	276/289 (95%)	-0.42	1 (0%)	88 84	30, 81, 129, 175	0
1	C	279/289 (96%)	-0.38	1 (0%)	88 84	49, 88, 132, 160	0
1	D	261/289 (90%)	-0.50	0	100 100	41, 73, 110, 164	0
1	E	276/289 (95%)	-0.42	0	100 100	42, 78, 137, 226	0
1	F	276/289 (95%)	-0.32	1 (0%)	88 84	44, 80, 131, 200	0
All	All	1647/1734 (94%)	-0.43	3 (0%)	91 88	30, 77, 130, 226	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	ALA	3.7
1	F	280	LEU	2.8
1	C	280	LEU	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

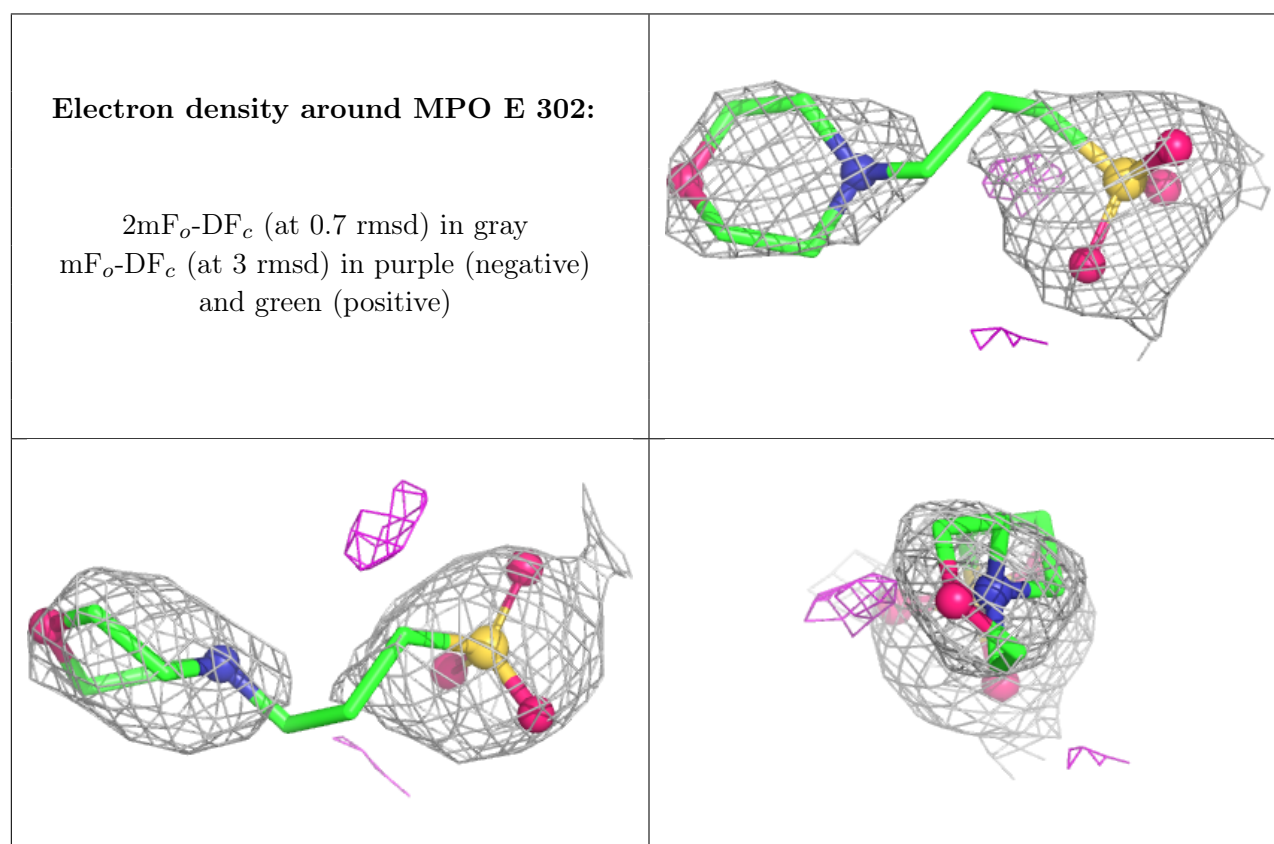
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

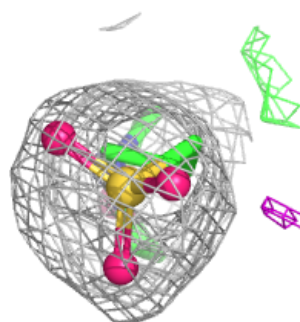
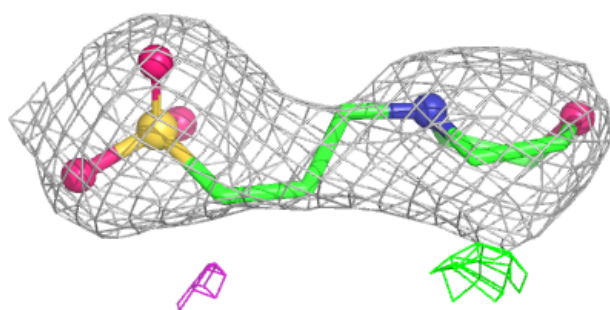
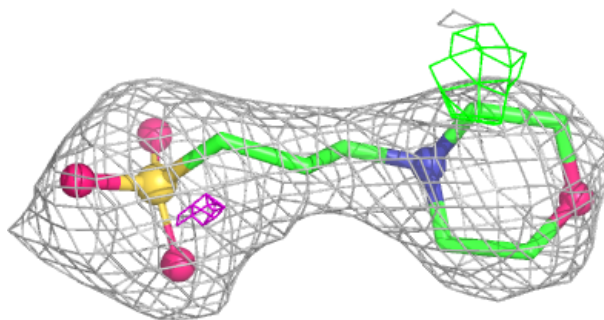
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPO	E	302	13/13	0.85	0.13	102,114,124,128	0
3	MPO	A	302	13/13	0.91	0.10	86,96,102,102	0
3	MPO	B	302	13/13	0.93	0.10	80,92,114,116	0
3	MPO	F	302	13/13	0.93	0.09	93,102,108,117	0
2	ZN	E	301	1/1	0.94	0.06	134,134,134,134	0
2	ZN	D	301	1/1	0.97	0.05	163,163,163,163	0
2	ZN	C	301	1/1	0.97	0.07	122,122,122,122	0
2	ZN	B	301	1/1	0.98	0.04	108,108,108,108	0
2	ZN	F	301	1/1	0.98	0.04	110,110,110,110	0
2	ZN	A	301	1/1	0.99	0.03	87,87,87,87	0

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

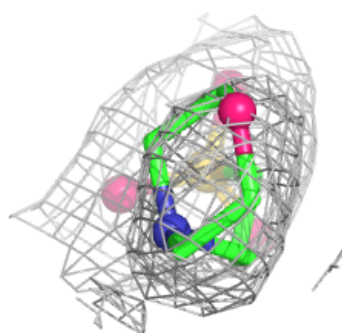
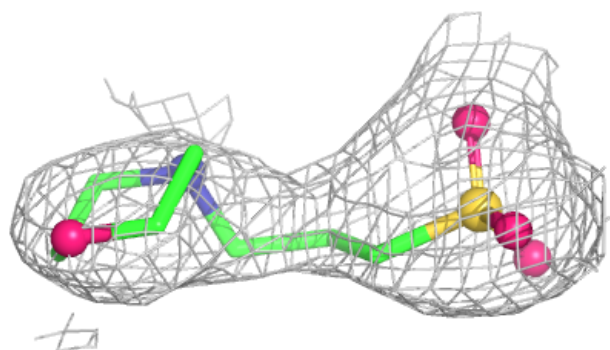
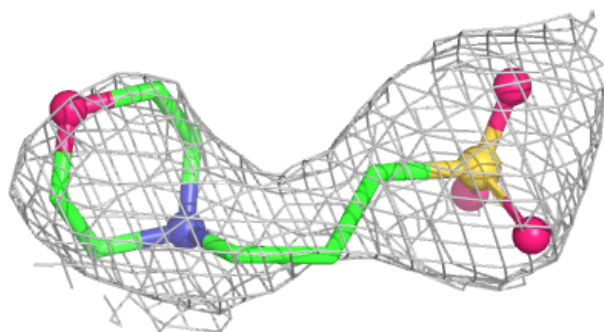


Electron density around MPO A 302:

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

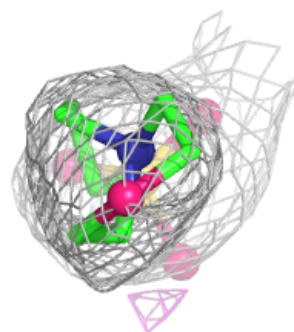
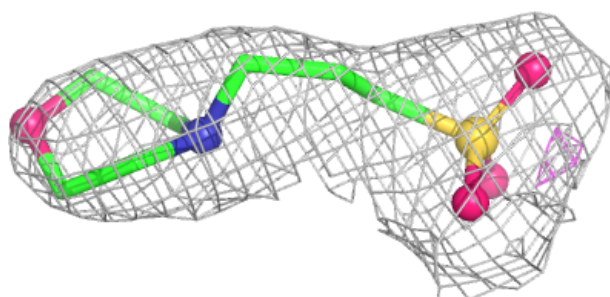
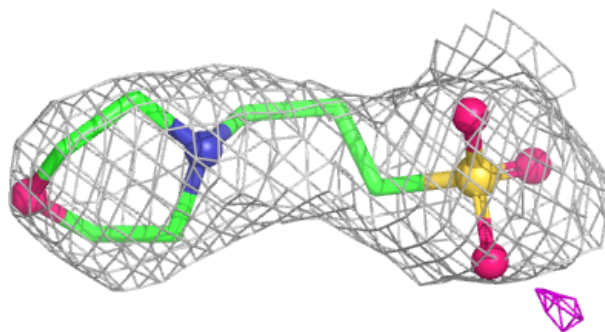
**Electron density around MPO B 302:**

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



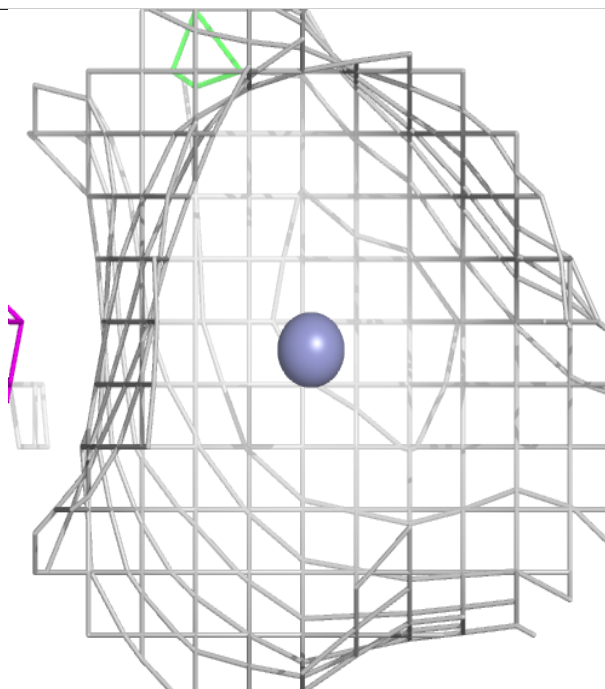
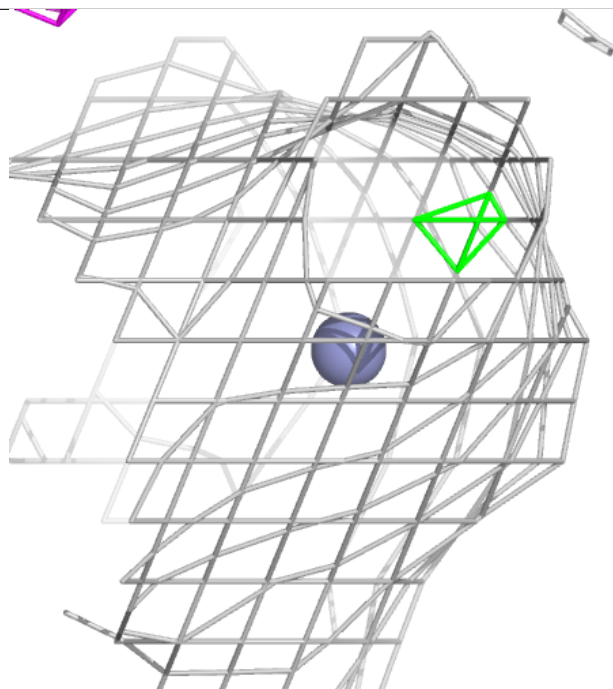
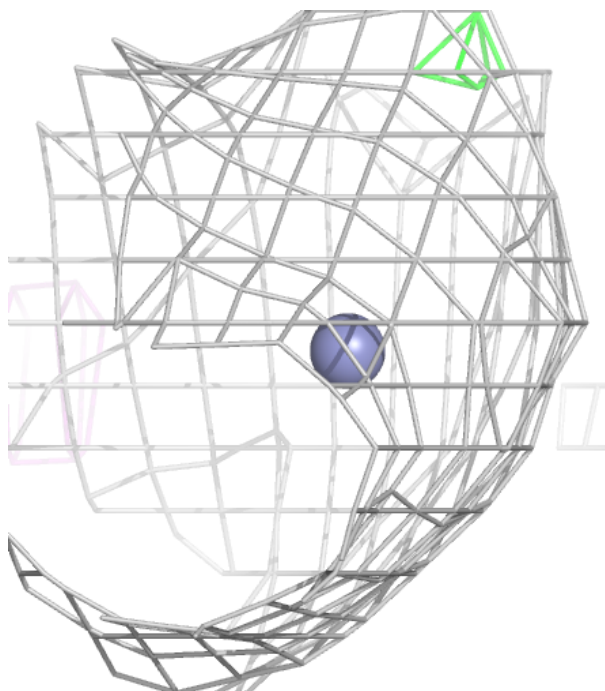
Electron density around MPO F 302:

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



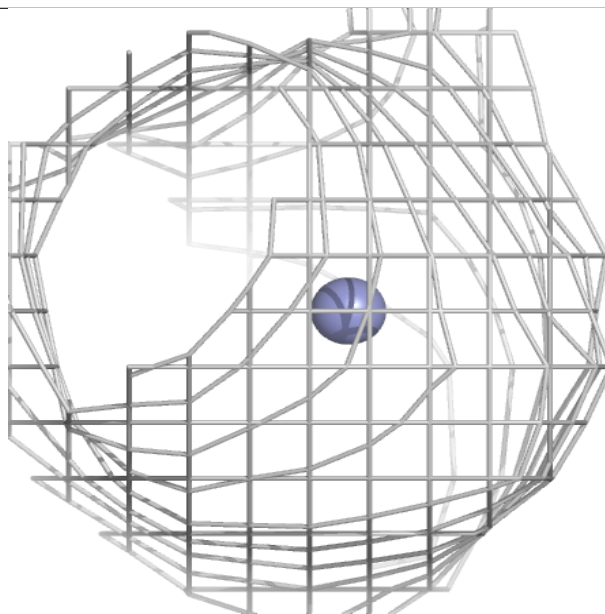
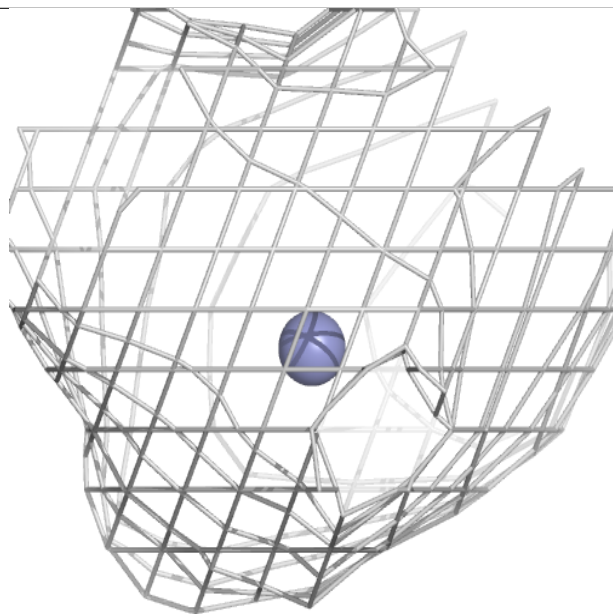
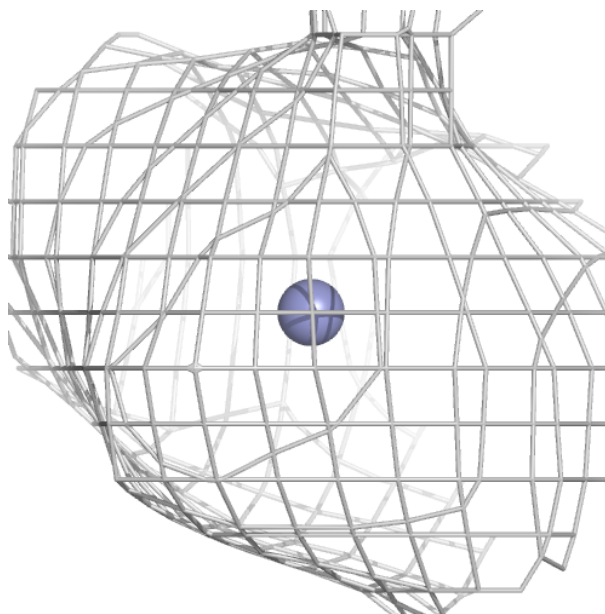
Electron density around ZN E 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



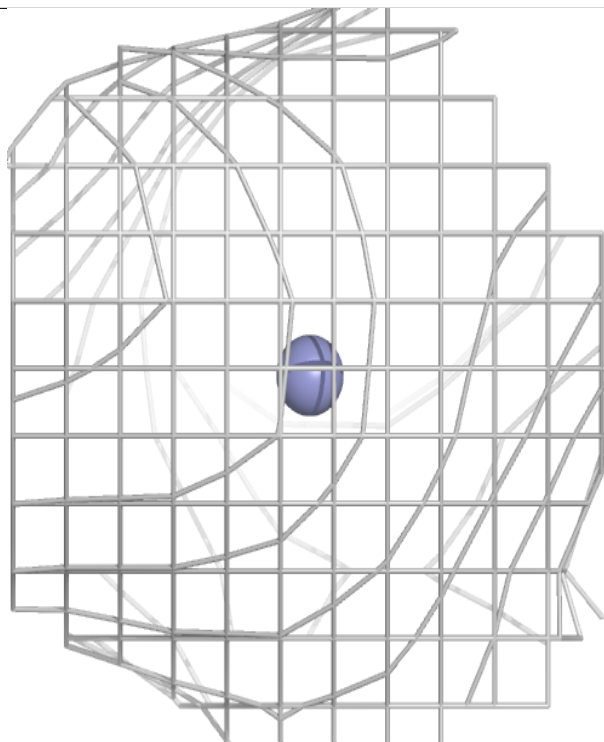
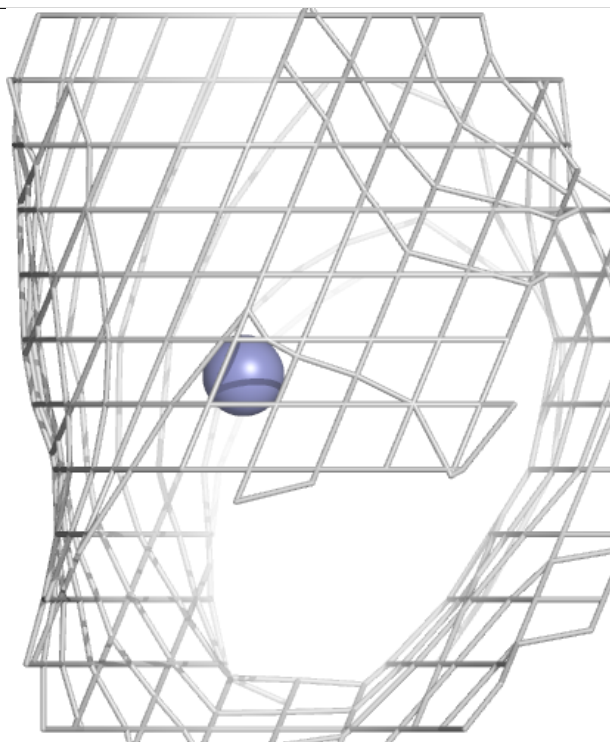
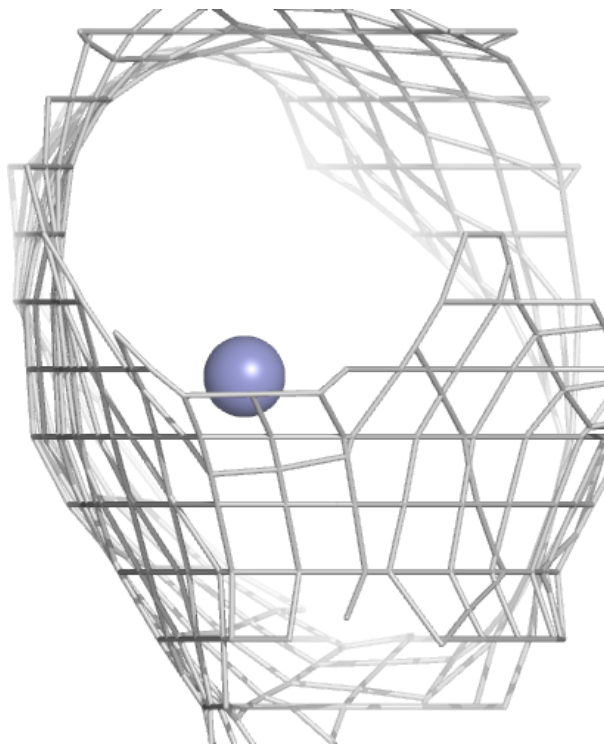
Electron density around ZN D 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



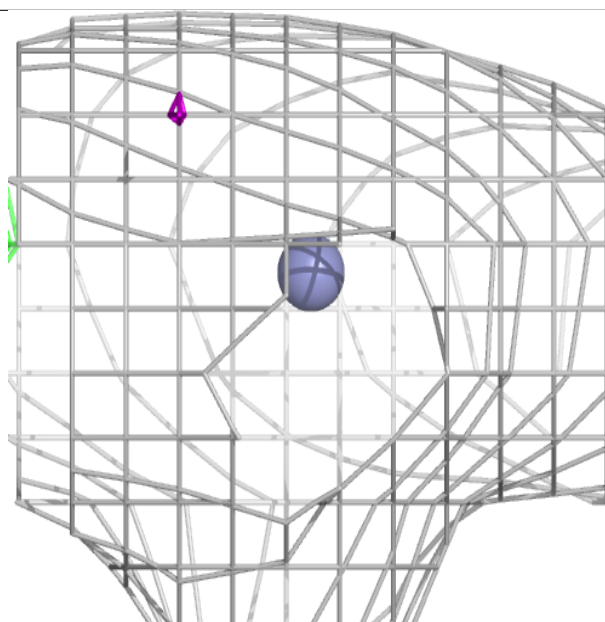
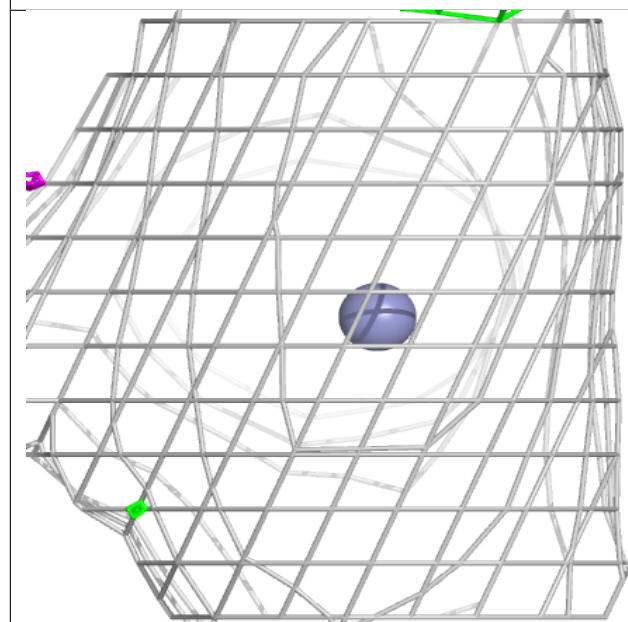
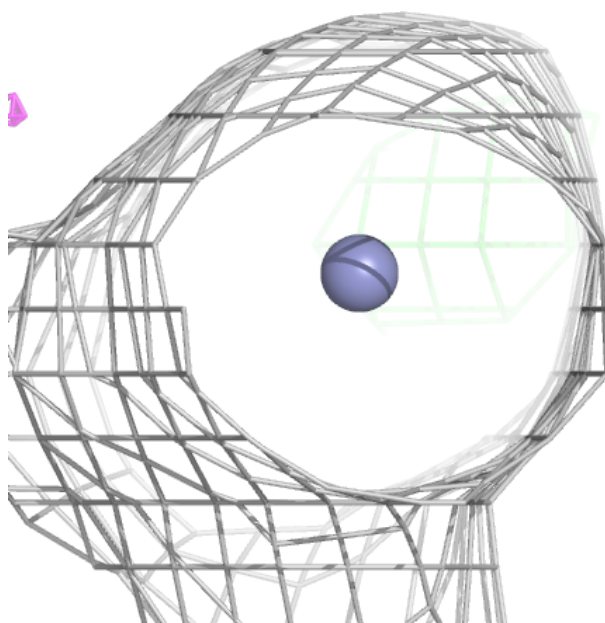
Electron density around ZN C 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



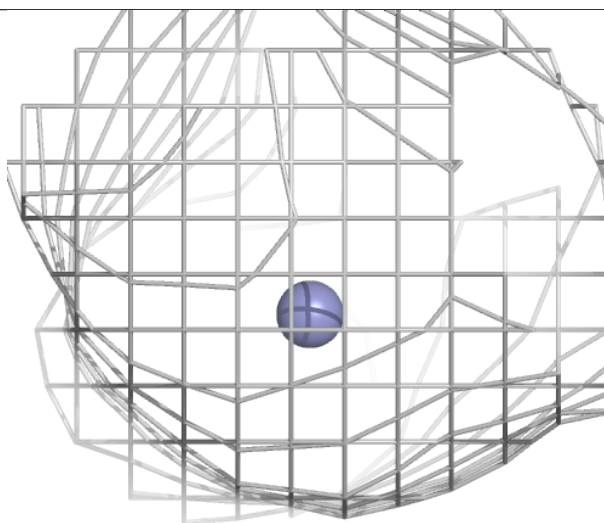
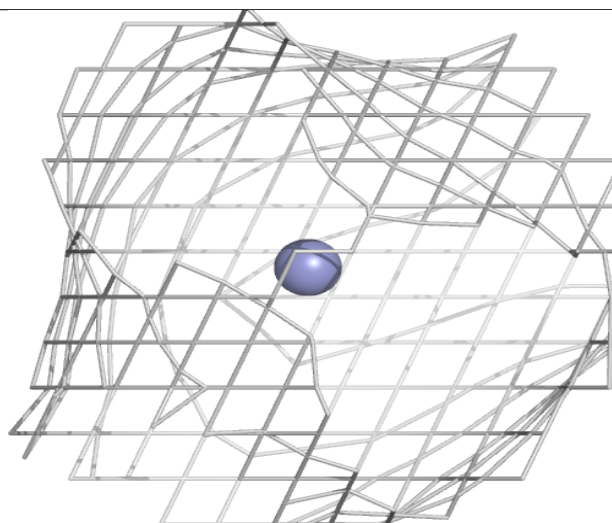
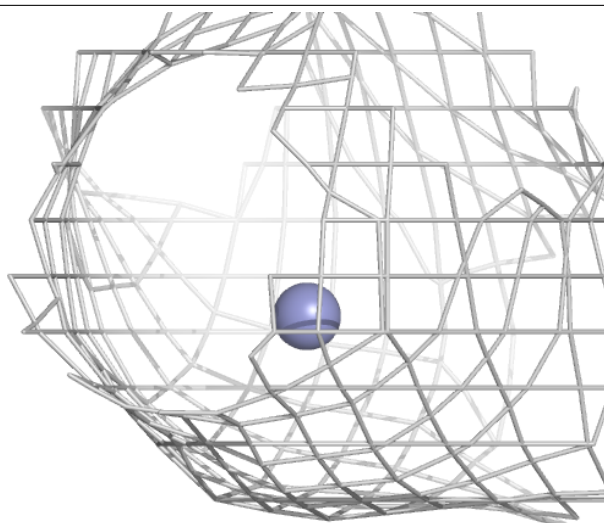
Electron density around ZN B 301:

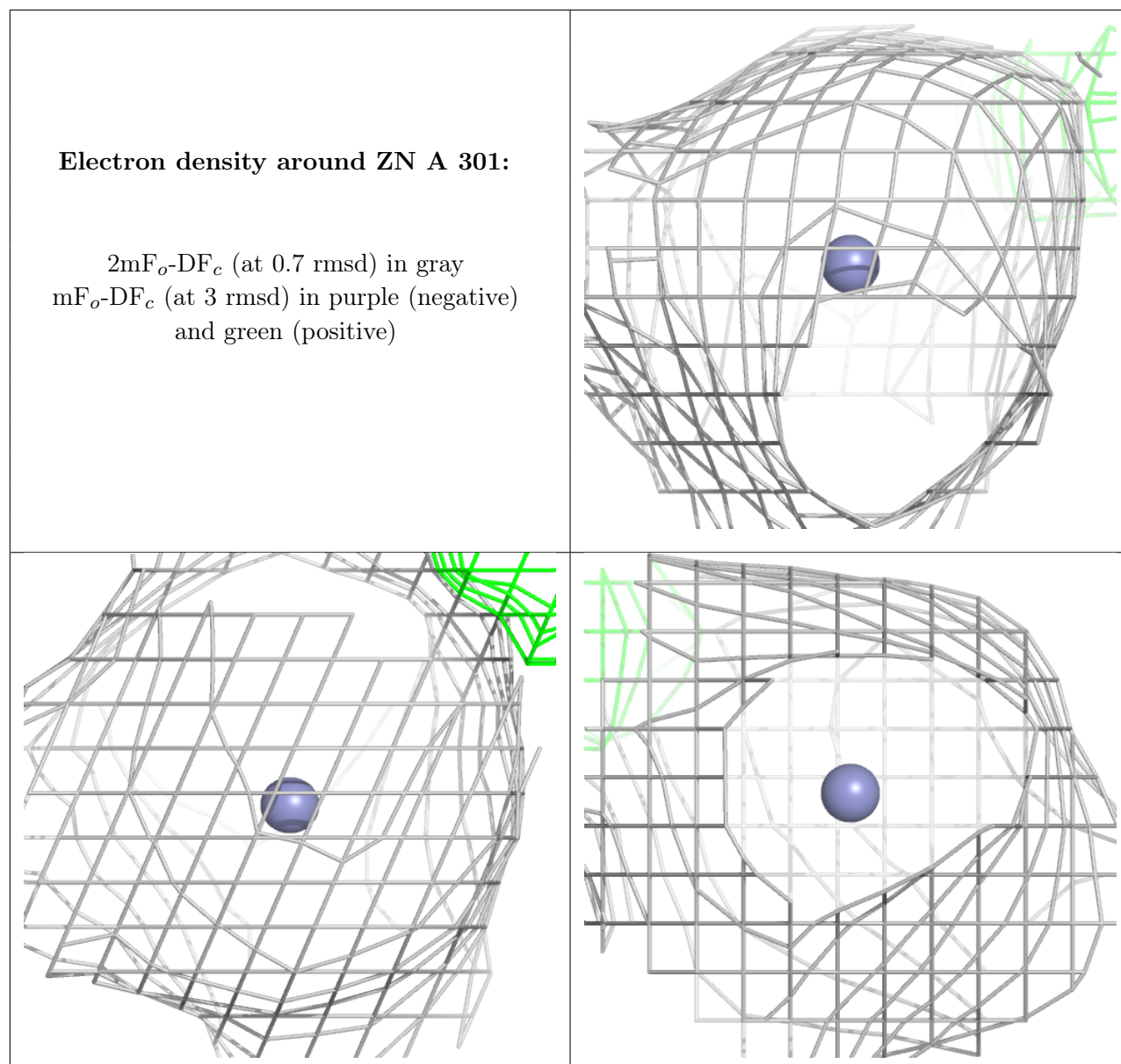
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN F 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.