



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:44 pm BST

PDB ID : 1S4D
Title : Crystal Structure Analysis of the S-adenosyl-L-methionine dependent uroporphyrinogen-III C-methyltransferase SUMT
Authors : Vevodova, J.; Graham, R.M.; Raux, E.; Schubert, H.L.; Roper, D.I.; Brindley, A.A.; Scott, A.I.; Roessner, C.A.; Stamford, N.P.J.; Stroupe, M.E.; Getzoff, E.D.; Warren, M.J.; Wilson, K.S.
Deposited on : 2004-01-16
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

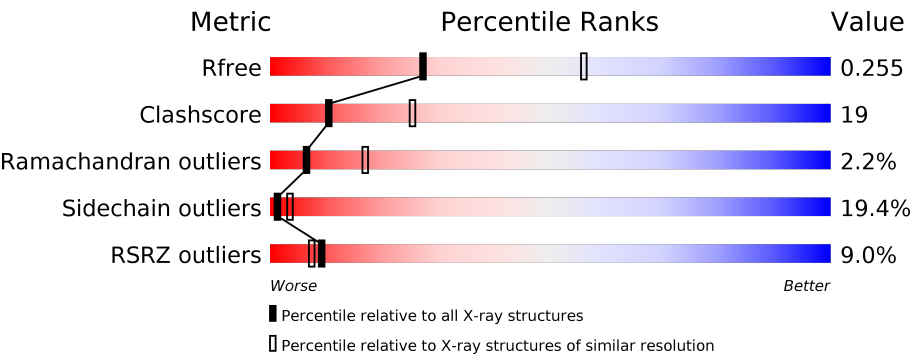
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	280	<div><div>5%</div><div><div>55%</div><div>27%</div><div>9%</div><div>•</div><div>9%</div></div></div>
1	B	280	<div><div>7%</div><div><div>60%</div><div>24%</div><div>9%</div><div>•</div><div>6%</div></div></div>
1	D	280	<div><div>3%</div><div><div>54%</div><div>25%</div><div>9%</div><div>•</div><div>11%</div></div></div>
1	E	280	<div><div>7%</div><div><div>60%</div><div>24%</div><div>9%</div><div>•</div><div>5%</div></div></div>
1	F	280	<div><div>5%</div><div><div>61%</div><div>21%</div><div>7%</div><div>•</div><div>9%</div></div></div>
1	G	280	<div><div>9%</div><div><div>63%</div><div>21%</div><div>8%</div><div>•</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	H	280	
1	I	280	
1	J	280	
1	K	280	
1	L	280	
1	M	280	

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
3	GOL	D	2011	-	-	X	-
3	GOL	E	2001	-	-	X	-
3	GOL	G	3003	-	-	X	-
3	GOL	H	4012	-	-	X	-
3	GOL	I	4002	-	-	X	-
3	GOL	K	5001	-	-	X	-
3	GOL	K	5012	-	-	X	-

2 Entry composition

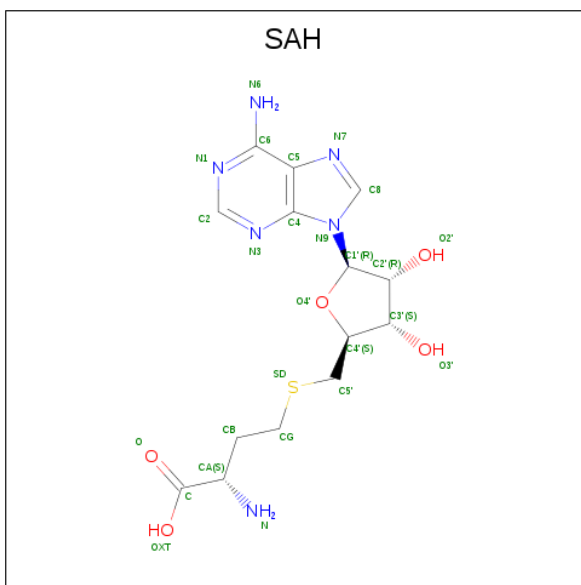
There are 4 unique types of molecules in this entry. The entry contains 23427 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uroporphyrin-III C-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	1	0
			1878	1195	341	337	5			
1	B	263	Total	C	N	O	S	0	1	0
			1915	1213	348	349	5			
1	D	248	Total	C	N	O	S	0	0	0
			1806	1146	326	329	5			
1	E	265	Total	C	N	O	S	0	0	0
			1922	1218	349	350	5			
1	F	254	Total	C	N	O	S	0	0	0
			1852	1176	336	335	5			
1	G	258	Total	C	N	O	S	0	0	0
			1877	1186	345	341	5			
1	H	259	Total	C	N	O	S	0	0	0
			1894	1205	344	340	5			
1	I	263	Total	C	N	O	S	0	1	0
			1932	1224	352	351	5			
1	J	252	Total	C	N	O	S	0	0	0
			1840	1171	333	331	5			
1	K	258	Total	C	N	O	S	0	1	0
			1883	1197	342	339	5			
1	L	247	Total	C	N	O	S	0	0	0
			1795	1141	325	324	5			
1	M	252	Total	C	N	O	S	0	0	0
			1842	1165	339	333	5			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	54	Total O 54 54	0	0
4	D	54	Total O 54 54	0	0
4	E	50	Total O 50 50	0	0
4	F	41	Total O 41 41	0	0
4	G	38	Total O 38 38	0	0
4	H	69	Total O 69 69	0	0

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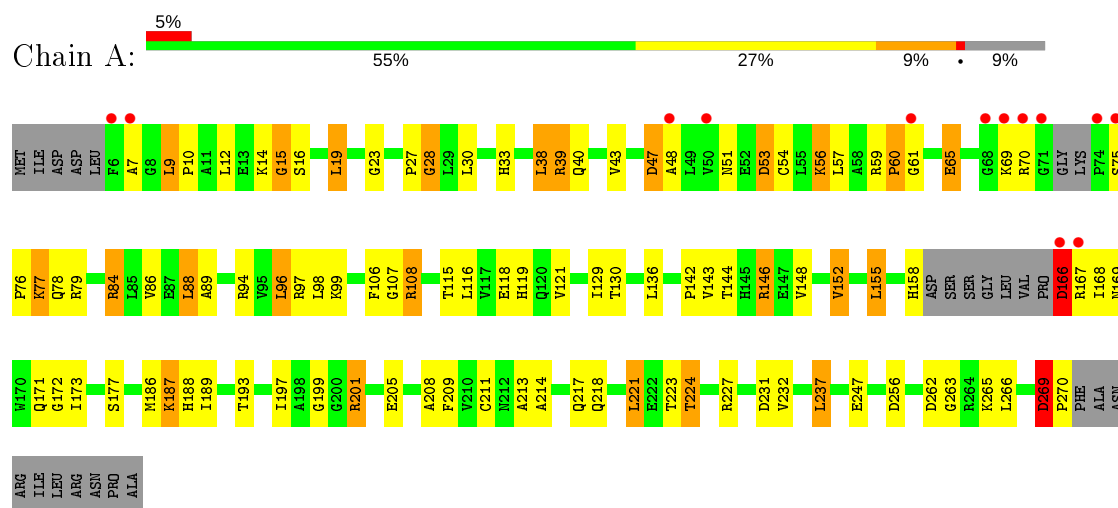
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	59	Total 59	O 59	0	0
4	J	30	Total 30	O 30	0	0
4	K	44	Total 44	O 44	0	0
4	L	24	Total 24	O 24	0	0
4	M	14	Total 14	O 14	0	0

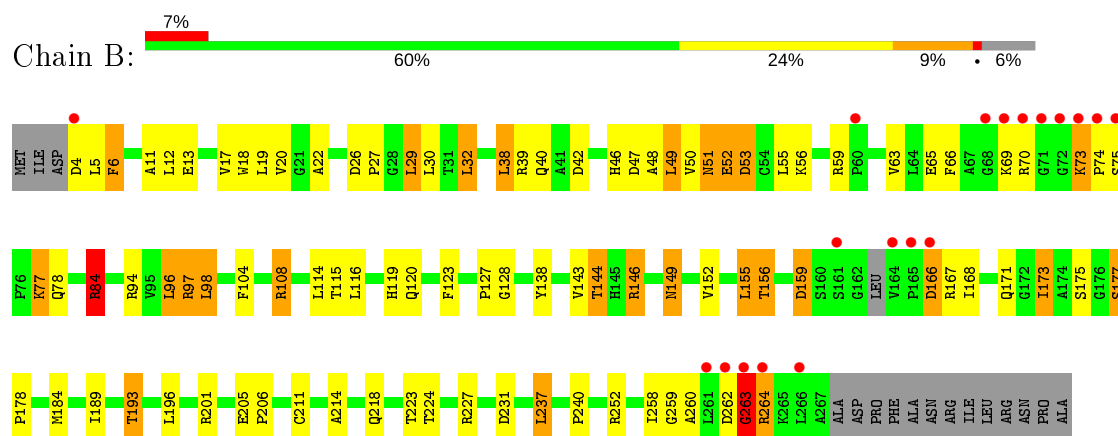
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

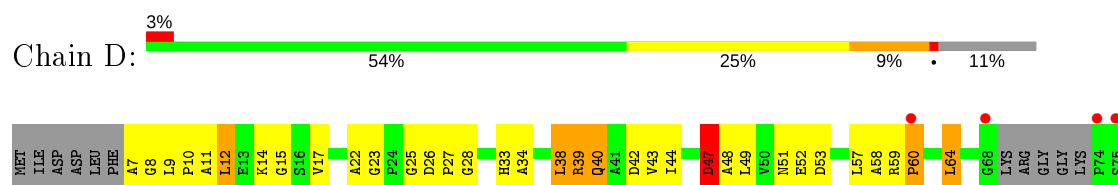
• Molecule 1: Uroporphyrin-III C-methyltransferase

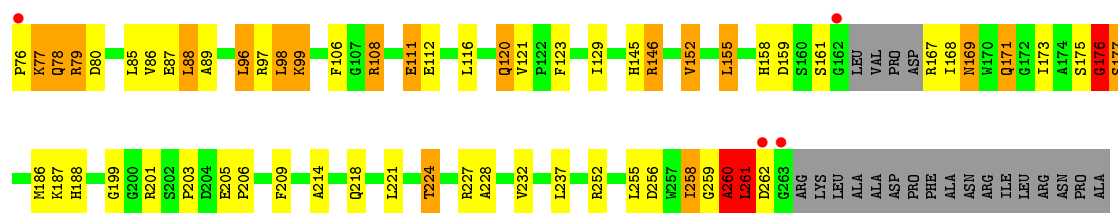


• Molecule 1: Uroporphyrin-III C-methyltransferase

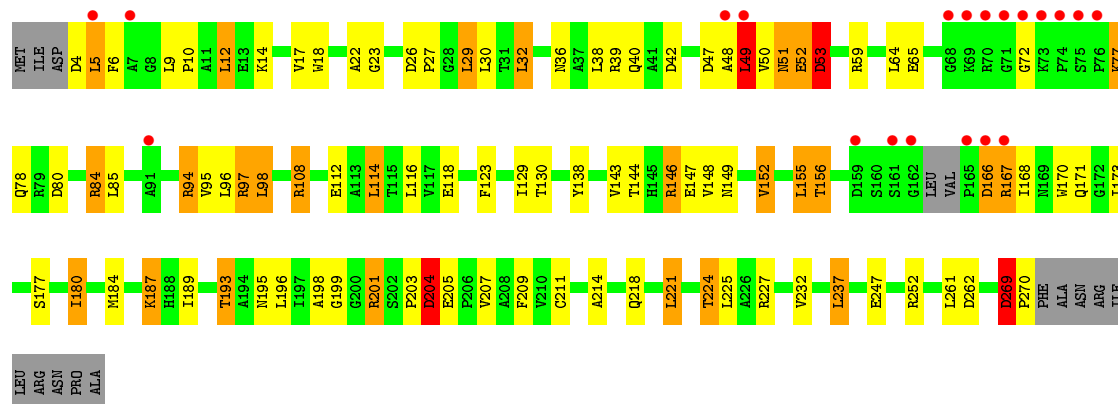


• Molecule 1: Uroporphyrin-III C-methyltransferase

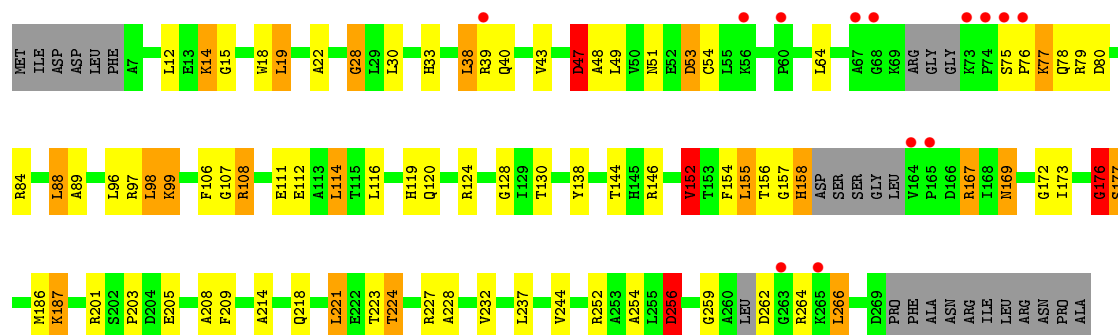




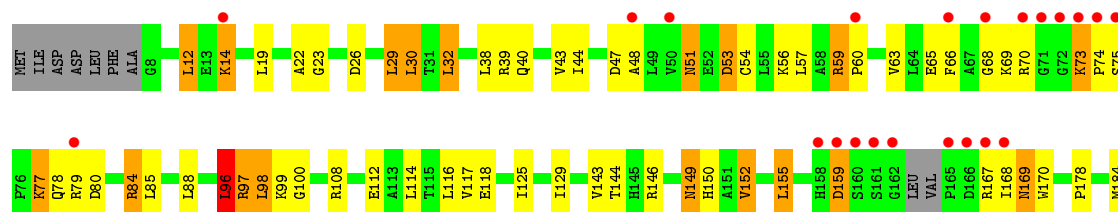
• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase

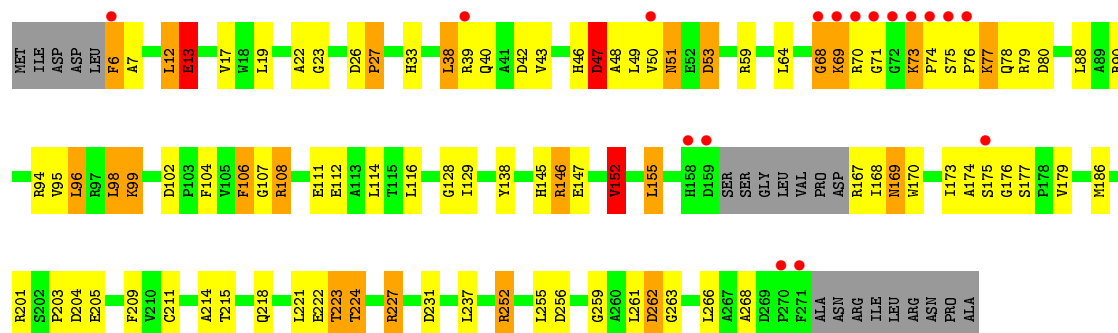


• Molecule 1: Uroporphyrin-III C-methyltransferase

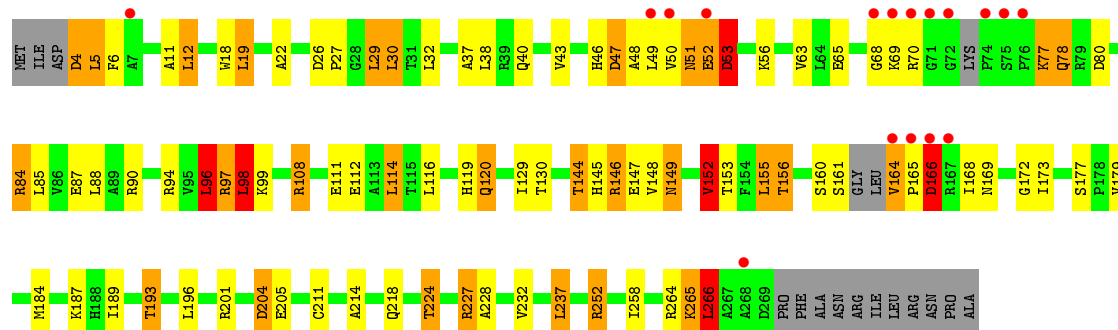




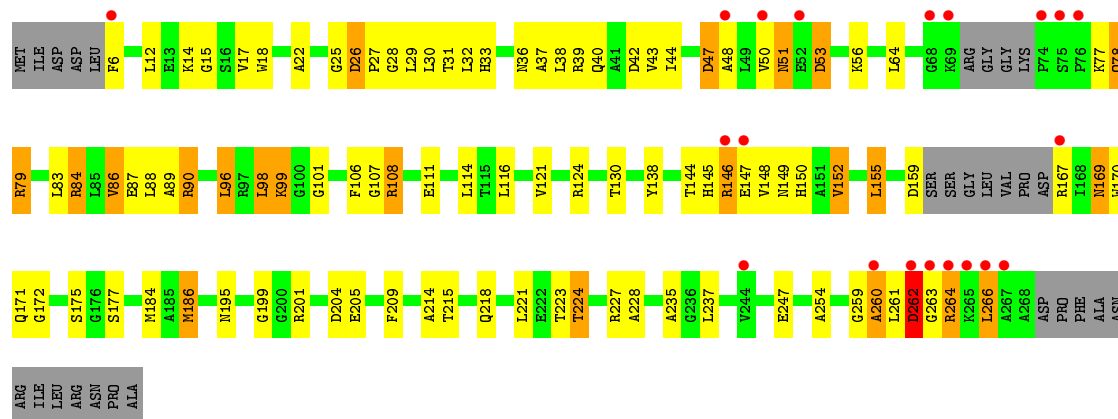
• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	218.10Å 218.10Å 190.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 2.70 19.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.84-2.70) 100.0 (19.84-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.213 , 0.260 0.211 , 0.255	Depositor DCC
R_{free} test set	6099 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23427	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.67	2/1918 (0.1%)	0.95	11/2609 (0.4%)
1	B	0.62	1/1956 (0.1%)	0.96	9/2666 (0.3%)
1	D	0.64	1/1840 (0.1%)	0.92	7/2506 (0.3%)
1	E	0.56	0/1960	0.96	12/2672 (0.4%)
1	F	0.63	1/1886 (0.1%)	0.91	10/2569 (0.4%)
1	G	0.53	0/1913	0.86	5/2605 (0.2%)
1	H	0.71	1/1932 (0.1%)	0.97	15/2632 (0.6%)
1	I	0.62	0/1972	0.98	12/2683 (0.4%)
1	J	0.60	1/1875 (0.1%)	0.88	8/2554 (0.3%)
1	K	0.58	1/1924 (0.1%)	0.88	8/2621 (0.3%)
1	L	0.59	1/1828 (0.1%)	0.81	4/2490 (0.2%)
1	M	0.51	0/1876	1.00	15/2552 (0.6%)
All	All	0.61	9/22880 (0.0%)	0.93	116/31159 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	D	0	5
1	E	0	4
1	F	0	5
1	H	0	2
1	I	0	1
1	J	0	4
1	K	0	4
1	L	0	2
1	M	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	39

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	79	ARG	NE-CZ	14.01	1.51	1.33
1	H	79	ARG	NE-CZ	13.53	1.50	1.33
1	F	79	ARG	NE-CZ	13.34	1.50	1.33
1	J	79	ARG	NE-CZ	13.03	1.50	1.33
1	A	79	ARG	NE-CZ	12.89	1.49	1.33
1	D	79	ARG	NE-CZ	12.80	1.49	1.33
1	B	263	GLY	C-O	5.34	1.32	1.23
1	K	7	ALA	C-N	5.22	1.42	1.33
1	A	70	ARG	C-N	5.11	1.42	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	266	LEU	O-C-N	-21.33	88.57	122.70
1	M	263	GLY	C-N-CA	9.86	146.35	121.70
1	H	79	ARG	CD-NE-CZ	-8.97	111.04	123.60
1	M	264	ARG	C-N-CA	8.77	143.62	121.70
1	A	79	ARG	CD-NE-CZ	-8.68	111.45	123.60
1	F	79	ARG	CD-NE-CZ	-8.64	111.50	123.60
1	D	155	LEU	CA-CB-CG	8.31	134.42	115.30
1	D	79	ARG	CD-NE-CZ	-8.21	112.10	123.60
1	M	264	ARG	O-C-N	-8.20	109.58	122.70
1	M	265	LYS	N-CA-C	7.95	132.47	111.00
1	G	155	LEU	CA-CB-CG	7.81	133.26	115.30
1	E	201	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	D	256	ASP	CB-CG-OD2	7.63	125.17	118.30
1	J	79	ARG	CD-NE-CZ	-7.62	112.93	123.60
1	E	152	VAL	CB-CA-C	-7.35	97.43	111.40
1	F	256	ASP	CB-CG-OD2	7.27	124.84	118.30
1	H	262	ASP	CB-CG-OD2	7.25	124.83	118.30
1	M	155	LEU	CA-CB-CG	7.13	131.70	115.30
1	B	155	LEU	CA-CB-CG	7.05	131.52	115.30
1	F	176	GLY	N-CA-C	7.02	130.65	113.10
1	I	155	LEU	CA-CB-CG	6.98	131.36	115.30
1	K	152	VAL	CB-CA-C	-6.96	98.18	111.40
1	L	155	LEU	CA-CB-CG	6.90	131.17	115.30
1	J	155	LEU	CA-CB-CG	6.86	131.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	27	PRO	C-N-CA	-6.86	107.90	122.30
1	B	159	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	201	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	K	80	ASP	CB-CG-OD2	6.61	124.25	118.30
1	H	102	ASP	CB-CG-OD2	6.61	124.25	118.30
1	K	155	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	262	ASP	CB-CG-OD2	6.55	124.19	118.30
1	I	98	LEU	CA-CB-CG	6.53	130.32	115.30
1	J	47	ASP	CB-CG-OD2	6.53	124.17	118.30
1	I	204	ASP	CB-CG-OD2	6.50	124.15	118.30
1	E	5	LEU	CA-CB-CG	6.47	130.19	115.30
1	E	262	ASP	CB-CG-OD2	6.46	124.12	118.30
1	E	49	LEU	CA-CB-CG	6.45	130.14	115.30
1	M	225	LEU	CA-CB-CG	6.44	130.10	115.30
1	M	261	LEU	CA-CB-CG	6.43	130.10	115.30
1	F	155	LEU	CA-CB-CG	6.41	130.03	115.30
1	H	155	LEU	CA-CB-CG	6.37	129.94	115.30
1	H	42	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	231	ASP	CB-CG-OD2	6.35	124.01	118.30
1	E	155	LEU	CA-CB-CG	6.35	129.90	115.30
1	F	114	LEU	CA-CB-CG	6.29	129.77	115.30
1	E	166	ASP	CB-CG-OD2	6.25	123.93	118.30
1	K	159	ASP	CB-CG-OD2	6.25	123.92	118.30
1	E	4	ASP	CB-CG-OD2	6.24	123.92	118.30
1	H	13	GLU	O-C-N	-6.22	112.75	122.70
1	J	152	VAL	CB-CA-C	-6.21	99.59	111.40
1	B	84	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	H	152	VAL	CB-CA-C	-6.19	99.64	111.40
1	G	96	LEU	CA-CB-CG	6.19	129.53	115.30
1	I	166	ASP	CB-CG-OD2	6.12	123.81	118.30
1	F	152	VAL	CB-CA-C	-6.12	99.77	111.40
1	A	155	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	152	VAL	CB-CA-C	-6.04	99.92	111.40
1	G	262	ASP	CB-CG-OD2	5.99	123.69	118.30
1	M	102	ASP	CB-CG-OD2	5.90	123.61	118.30
1	F	47	ASP	CB-CG-OD2	5.86	123.57	118.30
1	L	79	ARG	CD-NE-CZ	-5.86	115.40	123.60
1	K	102	ASP	CB-CG-OD2	5.82	123.54	118.30
1	E	80	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	80	ASP	CB-CG-OD2	5.78	123.50	118.30
1	M	269	ASP	CB-CG-OD2	5.77	123.49	118.30
1	I	152	VAL	CB-CA-C	-5.77	100.44	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	GLY	C-N-CA	-5.73	107.38	121.70
1	E	53	ASP	CB-CG-OD2	5.72	123.44	118.30
1	F	80	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	47	ASP	CB-CG-OD2	5.66	123.39	118.30
1	E	204	ASP	CB-CG-OD2	5.65	123.39	118.30
1	I	96	LEU	CA-CB-CG	5.62	128.22	115.30
1	H	27	PRO	N-CA-C	-5.59	97.57	112.10
1	M	80	ASP	CB-CG-OD2	5.59	123.33	118.30
1	F	221	LEU	CA-CB-CG	5.58	128.13	115.30
1	B	42	ASP	CB-CG-OD2	5.55	123.30	118.30
1	K	47	ASP	CB-CG-OD2	5.55	123.30	118.30
1	H	204	ASP	CB-CG-OD2	5.53	123.28	118.30
1	G	204	ASP	CB-CG-OD2	5.53	123.27	118.30
1	J	159	ASP	CB-CG-OD2	5.53	123.27	118.30
1	I	4	ASP	CB-CG-OD2	5.51	123.26	118.30
1	I	80	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	264	ARG	CA-C-N	-5.44	105.24	117.20
1	L	256	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	27	PRO	C-N-CA	-5.40	110.95	122.30
1	A	256	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	152	VAL	CB-CA-C	-5.38	101.18	111.40
1	K	231	ASP	CB-CA-C	5.37	121.15	110.40
1	H	256	ASP	CB-CG-OD2	5.36	123.13	118.30
1	L	47	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	42	ASP	CB-CG-OD2	5.36	123.12	118.30
1	M	47	ASP	CB-CG-OD2	5.34	123.11	118.30
1	H	68	GLY	N-CA-C	5.33	126.42	113.10
1	M	204	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	4	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	231	ASP	CB-CG-OD2	5.29	123.06	118.30
1	I	53	ASP	CB-CG-OD2	5.29	123.06	118.30
1	I	30	LEU	CA-CB-CG	5.26	127.40	115.30
1	J	204	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	263	GLY	N-CA-C	5.21	126.13	113.10
1	D	8	GLY	N-CA-C	-5.21	100.07	113.10
1	E	203	PRO	N-CA-C	-5.20	98.57	112.10
1	J	42	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	166	ASP	CB-CG-OD2	5.16	122.95	118.30
1	M	42	ASP	CB-CG-OD2	5.14	122.93	118.30
1	J	26	ASP	CB-CG-OD2	5.14	122.93	118.30
1	I	266	LEU	CA-CB-CG	5.14	127.11	115.30
1	I	252	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	ASP	CB-CG-OD2	5.11	122.90	118.30
1	K	119	HIS	N-CA-C	5.08	124.72	111.00
1	M	159	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	166	ASP	CB-CG-OD2	5.05	122.85	118.30
1	H	80	ASP	CB-CG-OD2	5.05	122.84	118.30
1	H	47	ASP	CB-CG-OD2	5.03	122.83	118.30
1	H	13	GLU	CA-C-N	5.01	128.23	117.20
1	F	262	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	ASP	Peptide
1	A	28	GLY	Peptide
1	A	47	ASP	Peptide
1	B	167	ARG	Peptide
1	B	263	GLY	Peptide
1	B	264	ARG	Peptide
1	D	176	GLY	Peptide
1	D	260	ALA	Peptide
1	D	261	LEU	Peptide
1	D	47	ASP	Peptide
1	D	7	ALA	Mainchain
1	E	10	PRO	Mainchain,Peptide
1	E	167	ARG	Peptide
1	E	269	ASP	Peptide
1	F	119	HIS	Peptide
1	F	176	GLY	Peptide
1	F	28	GLY	Peptide
1	F	47	ASP	Peptide
1	F	75	SER	Peptide
1	H	13	GLU	Mainchain
1	H	47	ASP	Peptide
1	I	164	VAL	Peptide
1	J	146	ARG	Peptide
1	J	147	GLU	Peptide
1	J	260	ALA	Peptide
1	J	47	ASP	Peptide
1	K	119	HIS	Peptide
1	K	164	VAL	Peptide
1	K	166	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	K	5	LEU	Peptide
1	L	165	PRO	Peptide
1	L	166	ASP	Peptide
1	M	232	VAL	Mainchain
1	M	264	ARG	Sidechain,Mainchain,Peptide
1	M	265	LYS	Peptide
1	M	266	LEU	Mainchain

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	1878	0	1911	86	0
1	B	1915	0	1933	79	0
1	D	1806	0	1836	75	0
1	E	1922	0	1942	78	0
1	F	1852	0	1881	70	0
1	G	1877	0	1903	65	0
1	H	1894	0	1922	80	0
1	I	1932	0	1968	94	0
1	J	1840	0	1870	84	0
1	K	1883	0	1920	71	0
1	L	1795	0	1822	55	0
1	M	1842	0	1870	75	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	D	26	0	19	0	0
2	E	26	0	19	1	0
2	F	26	0	19	0	0
2	G	26	0	19	2	0
2	H	26	0	19	0	0
2	I	26	0	19	0	0
2	J	26	0	19	2	0
2	K	26	0	19	1	0
2	L	26	0	19	0	0
2	M	26	0	19	2	0
3	A	18	0	24	5	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	0	16	7	0
3	E	18	0	24	9	0
3	F	12	0	16	2	0
3	G	18	0	24	7	0
3	H	12	0	16	6	0
3	I	12	0	16	4	0
3	J	18	0	24	5	0
3	K	12	0	16	9	0
3	L	12	0	16	1	0
3	M	6	0	8	0	0
4	A	46	0	0	2	0
4	B	54	0	0	7	0
4	D	54	0	0	3	0
4	E	50	0	0	4	0
4	F	41	0	0	2	0
4	G	38	0	0	2	0
4	H	69	0	0	7	0
4	I	59	0	0	3	0
4	J	30	0	0	3	0
4	K	44	0	0	8	0
4	L	24	0	0	2	0
4	M	14	0	0	0	0
All	All	23427	0	23214	856	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 19.

All (856) 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:I:160:SER:HA	1:I:166:ASP:OD2	1.41	1.20
1:J:186:MET:CE	1:J:209:PHE:HD1	1.55	1.20
1:J:186:MET:HE1	1:J:209:PHE:HD1	1.01	1.14
1:L:9:LEU:HB2	1:L:10:PRO:HD2	1.29	1.14
1:J:186:MET:CE	1:J:209:PHE:CD1	2.31	1.12
1:E:168:ILE:HG23	4:E:2542:HOH:O	1.46	1.12
1:J:186:MET:HE1	1:J:209:PHE:CD1	1.84	1.12
1:I:164:VAL:HG23	4:I:4561:HOH:O	1.51	1.09
1:G:51:ASN:HD22	1:G:53:ASP:HB2	1.15	1.08
1:I:146:ARG:H	1:I:146:ARG:HD2	1.17	1.08
1:A:39:ARG:HH21	1:A:39:ARG:HG2	1.17	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:186:MET:HE2	1:M:209:PHE:CD1	1.89	1.07
1:J:223:THR:HG22	1:J:224:THR:H	0.97	1.07
1:F:157:GLY:O	1:F:158:HIS:HB2	1.31	1.05
1:M:186:MET:CE	1:M:209:PHE:HD1	1.68	1.05
1:D:39:ARG:HH11	1:D:39:ARG:HG3	1.19	1.05
1:I:50:VAL:HG12	1:I:51:ASN:H	1.17	1.05
1:M:186:MET:HE2	1:M:209:PHE:HD1	1.17	1.05
1:D:158:HIS:HB3	4:D:2517:HOH:O	1.57	1.05
1:A:146:ARG:H	3:A:1012:GOL:H32	1.17	1.04
3:D:2011:GOL:C3	1:E:108:ARG:HA	1.88	1.04
3:D:2011:GOL:H31	1:E:108:ARG:CA	1.88	1.03
1:F:28:GLY:HA2	1:G:32:LEU:HB2	1.42	1.01
1:A:28:GLY:HA2	1:B:32:LEU:HB2	1.40	1.01
1:H:128:GLY:O	3:I:4002:GOL:H11	1.59	1.01
1:J:223:THR:HG22	1:J:224:THR:N	1.77	0.99
1:K:224:THR:HG21	4:K:5523:HOH:O	1.59	0.99
1:H:175:SER:HB3	4:H:4562:HOH:O	1.62	0.99
1:F:223:THR:HG22	1:F:224:THR:H	1.27	0.98
1:E:269:ASP:OD1	1:E:270:PRO:HD2	1.64	0.98
1:J:146:ARG:H	3:J:5011:GOL:H11	1.25	0.96
1:E:84:ARG:HG3	1:E:84:ARG:HH21	1.29	0.96
1:E:84:ARG:CG	1:E:84:ARG:HH21	1.78	0.96
1:J:186:MET:HE2	1:J:209:PHE:CE1	2.02	0.95
1:M:223:THR:HG22	1:M:224:THR:H	1.31	0.94
1:K:204:ASP:HB3	4:K:5523:HOH:O	1.65	0.94
3:H:4012:GOL:H31	1:I:111:GLU:OE1	1.70	0.92
1:J:223:THR:CG2	1:J:224:THR:H	1.80	0.92
1:J:6:PHE:CE2	1:J:32:LEU:HD13	2.04	0.92
1:B:6:PHE:HA	4:B:1562:HOH:O	1.68	0.92
1:D:228:ALA:O	1:D:232:VAL:HG23	1.70	0.91
1:G:224:THR:HG21	4:G:3514:HOH:O	1.68	0.91
1:B:50:VAL:CG1	1:B:51:ASN:H	1.82	0.91
1:D:28:GLY:HA2	1:E:32:LEU:HB2	1.53	0.90
1:L:106:PHE:H	1:M:144:THR:HG21	1.36	0.90
1:F:167:ARG:HH21	1:G:150:HIS:H	0.93	0.90
1:D:224:THR:HG21	4:D:2526:HOH:O	1.71	0.89
1:F:214:ALA:H	1:F:218:GLN:HE21	1.16	0.89
1:I:146:ARG:H	1:I:146:ARG:CD	1.79	0.89
1:I:50:VAL:HG12	1:I:51:ASN:N	1.84	0.89
1:I:50:VAL:CG1	1:I:51:ASN:H	1.85	0.88
1:I:160:SER:CA	1:I:166:ASP:OD2	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:THR:HG22	1:G:227:ARG:H	1.39	0.88
1:B:50:VAL:HG13	1:B:51:ASN:H	1.36	0.88
1:I:214:ALA:H	1:I:218:GLN:HE21	1.22	0.88
1:F:12:LEU:H	1:F:40:GLN:HE22	1.18	0.87
1:I:228:ALA:O	1:I:232:VAL:HG13	1.73	0.87
1:J:186:MET:HE2	1:J:209:PHE:CD1	2.05	0.87
1:A:146:ARG:HG3	4:B:1561:HOH:O	1.74	0.87
1:J:28:GLY:HA2	1:K:32:LEU:HB2	1.56	0.87
1:E:214:ALA:H	1:E:218:GLN:HE21	1.22	0.87
1:J:146:ARG:HH22	1:K:108:ARG:NE	1.72	0.86
3:H:4012:GOL:H11	1:I:108:ARG:H	1.40	0.86
1:I:214:ALA:H	1:I:218:GLN:NE2	1.73	0.86
1:I:204:ASP:HA	1:I:224:THR:HG23	1.57	0.86
1:L:9:LEU:HB2	1:L:10:PRO:CD	2.05	0.86
1:F:259:GLY:O	1:F:264:ARG:HB3	1.76	0.85
1:D:108:ARG:H	3:E:2003:GOL:H11	1.42	0.85
1:I:169:ASN:ND2	1:I:172:GLY:H	1.75	0.84
1:F:223:THR:HG22	1:F:224:THR:N	1.92	0.84
1:F:167:ARG:NH2	1:G:150:HIS:H	1.75	0.84
1:E:224:THR:HG22	1:E:227:ARG:H	1.41	0.84
1:D:186:MET:HE3	1:D:209:PHE:HD1	1.43	0.83
1:H:146:ARG:HG3	1:H:146:ARG:HH11	1.43	0.83
1:H:214:ALA:H	1:H:218:GLN:HE21	1.23	0.83
1:H:224:THR:HG22	1:H:227:ARG:H	1.44	0.83
1:F:157:GLY:O	1:F:158:HIS:CB	2.17	0.83
1:H:146:ARG:H	3:H:4012:GOL:H32	1.43	0.83
3:D:2011:GOL:H11	1:E:108:ARG:H	1.43	0.83
1:G:146:ARG:H	3:G:3003:GOL:H32	1.44	0.82
1:J:224:THR:HG22	1:J:227:ARG:H	1.42	0.82
1:B:260:ALA:HB3	4:B:1563:HOH:O	1.79	0.82
1:F:12:LEU:H	1:F:40:GLN:NE2	1.77	0.82
1:F:176:GLY:HA2	4:F:3536:HOH:O	1.78	0.82
1:G:204:ASP:HB3	4:G:3514:HOH:O	1.79	0.82
1:E:130:THR:HG22	3:E:2001:GOL:O2	1.79	0.82
1:B:12:LEU:H	1:B:40:GLN:NE2	1.77	0.82
1:D:39:ARG:HH11	1:D:39:ARG:CG	1.92	0.82
3:A:1001:GOL:H11	1:B:128:GLY:O	1.81	0.81
1:F:128:GLY:O	3:G:3002:GOL:H11	1.81	0.81
1:H:13:GLU:O	1:H:94:ARG:HG2	1.79	0.81
1:H:255:LEU:HD21	1:I:114:LEU:HD13	1.63	0.81
1:L:184:MET:HB3	3:L:6002:GOL:H12	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:204:ASP:HA	1:M:224:THR:HB	1.61	0.81
1:F:214:ALA:H	1:F:218:GLN:NE2	1.79	0.80
1:I:169:ASN:HD22	1:I:172:GLY:H	1.26	0.80
1:K:9:LEU:HB3	1:K:10:PRO:CD	2.12	0.80
1:A:169:ASN:HD22	1:A:172:GLY:H	1.29	0.80
1:F:51:ASN:HD22	1:F:53:ASP:HB2	1.45	0.80
1:F:167:ARG:HH21	1:G:150:HIS:N	1.76	0.80
1:J:12:LEU:H	1:J:40:GLN:NE2	1.78	0.80
1:E:84:ARG:NH2	1:E:84:ARG:HG3	1.94	0.80
1:F:108:ARG:H	3:G:3003:GOL:H11	1.46	0.79
1:I:224:THR:HG22	1:I:227:ARG:H	1.48	0.78
1:A:146:ARG:HB3	4:A:1547:HOH:O	1.82	0.78
1:E:214:ALA:H	1:E:218:GLN:NE2	1.80	0.78
1:J:28:GLY:HA2	1:K:32:LEU:CB	2.14	0.78
1:B:26:ASP:HB3	1:B:29:LEU:HD22	1.66	0.77
1:D:39:ARG:HG3	1:D:39:ARG:NH1	1.93	0.77
1:L:165:PRO:HB3	1:L:167:ARG:HG3	1.66	0.77
1:M:186:MET:CE	1:M:209:PHE:CD1	2.56	0.76
1:K:214:ALA:H	1:K:218:GLN:HE21	1.32	0.76
1:F:224:THR:HG22	1:F:227:ARG:H	1.50	0.76
1:K:12:LEU:H	1:K:40:GLN:HE22	1.31	0.76
3:J:5002:GOL:H32	1:K:133:ILE:HB	1.66	0.76
1:L:228:ALA:O	1:L:232:VAL:HG23	1.84	0.76
1:A:146:ARG:N	3:A:1012:GOL:H32	1.98	0.75
1:B:38:LEU:HD13	1:B:96:LEU:HD11	1.68	0.75
1:B:146:ARG:HB3	1:B:146:ARG:HH21	1.51	0.75
1:H:111:GLU:OE1	1:I:146:ARG:HG3	1.87	0.75
1:H:224:THR:HG21	4:H:4507:HOH:O	1.86	0.75
1:B:27:PRO:HG3	1:B:53:ASP:HB2	1.67	0.74
1:D:259:GLY:O	1:D:260:ALA:HB2	1.87	0.74
1:B:65:GLU:OE1	1:B:84:ARG:NH2	2.21	0.74
1:G:51:ASN:HD22	1:G:53:ASP:CB	1.97	0.74
1:B:73:LYS:N	1:B:74:PRO:HD3	2.02	0.74
1:H:214:ALA:H	1:H:218:GLN:NE2	1.85	0.74
1:B:214:ALA:H	1:B:218:GLN:HE21	1.36	0.74
1:B:214:ALA:H	1:B:218:GLN:NE2	1.84	0.74
1:I:204:ASP:HA	1:I:224:THR:CG2	2.17	0.74
1:I:119:HIS:O	1:I:120[A]:GLN:NE2	2.20	0.74
1:J:169:ASN:HD22	1:J:172:GLY:H	1.35	0.74
1:A:33:HIS:HE1	1:B:26:ASP:OD2	1.71	0.73
1:D:11:ALA:HA	1:D:40:GLN:HE22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:THR:HG22	1:D:227:ARG:H	1.54	0.73
1:E:156:THR:HG21	4:E:2540:HOH:O	1.86	0.73
1:G:214:ALA:H	1:G:218:GLN:HE21	1.35	0.73
1:A:186:MET:HE3	1:A:209:PHE:CD1	2.23	0.73
1:K:224:THR:HG22	1:K:227:ARG:H	1.53	0.73
1:A:77:LYS:HD3	1:A:78:GLN:H	1.52	0.73
1:A:269:ASP:CB	1:A:270:PRO:HD3	2.18	0.73
1:A:77:LYS:HD3	1:A:78:GLN:N	2.04	0.73
1:K:204:ASP:HA	1:K:224:THR:HG23	1.70	0.73
1:E:269:ASP:OD1	1:E:270:PRO:CD	2.36	0.73
1:F:28:GLY:HA2	1:G:32:LEU:CB	2.19	0.73
1:A:269:ASP:HB2	1:A:270:PRO:HD3	1.71	0.72
1:H:51:ASN:HD22	1:H:53:ASP:HB2	1.53	0.72
1:K:12:LEU:H	1:K:40:GLN:NE2	1.87	0.72
1:E:49:LEU:HD21	4:E:2544:HOH:O	1.88	0.72
1:B:149:ASN:CB	1:B:178:PRO:HG2	2.19	0.72
1:H:38:LEU:HD13	1:H:96:LEU:HD21	1.71	0.72
1:J:108:ARG:NH2	1:J:111:GLU:OE2	2.23	0.72
1:B:50:VAL:CG1	1:B:51:ASN:N	2.50	0.72
1:E:204:ASP:HA	1:E:224:THR:OG1	1.90	0.72
1:A:221:LEU:HD12	1:A:232:VAL:HG22	1.71	0.72
1:A:224:THR:HG22	1:A:227:ARG:H	1.55	0.72
1:B:48:ALA:C	1:B:50:VAL:H	1.94	0.72
1:I:26:ASP:HB3	1:I:29:LEU:HD22	1.72	0.72
1:F:186:MET:HE1	1:F:209:PHE:HE1	1.55	0.71
1:J:6:PHE:HE2	1:J:32:LEU:CD1	2.02	0.71
1:M:264:ARG:HG2	1:M:265:LYS:N	2.06	0.71
1:I:266:LEU:CD2	1:I:266:LEU:H	2.03	0.71
1:E:204:ASP:HA	1:E:224:THR:HG23	1.72	0.71
1:I:48:ALA:C	1:I:50:VAL:H	1.90	0.71
1:A:214:ALA:H	1:A:218:GLN:NE2	1.88	0.71
1:B:12:LEU:H	1:B:40:GLN:HE22	1.39	0.70
1:A:39:ARG:NH2	1:A:39:ARG:HG2	1.97	0.70
1:B:149:ASN:HB3	1:B:178:PRO:HG2	1.73	0.70
1:F:38:LEU:HD13	1:F:96:LEU:HD21	1.74	0.70
1:H:268:ALA:HA	4:H:4556:HOH:O	1.91	0.70
1:J:214:ALA:H	1:J:218:GLN:HE21	1.40	0.70
1:L:177:SER:O	1:L:201:ARG:NH2	2.24	0.70
1:A:217:GLN:HG3	4:A:1524:HOH:O	1.89	0.70
1:D:28:GLY:HA2	1:E:32:LEU:CB	2.21	0.70
1:I:146:ARG:HD2	1:I:146:ARG:N	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:PHE:CE2	1:J:32:LEU:CD1	2.74	0.70
1:K:163:LEU:HD23	1:K:164:VAL:H	1.57	0.69
1:L:201:ARG:HD3	1:L:205:GLU:OE1	1.92	0.69
1:E:193:THR:HG21	4:E:2513:HOH:O	1.91	0.69
1:I:48:ALA:O	1:I:50:VAL:N	2.26	0.69
1:I:265:LYS:HE3	1:I:265:LYS:H	1.57	0.69
1:L:9:LEU:CB	1:L:10:PRO:HD2	2.11	0.69
1:H:211:CYS:SG	1:H:237:LEU:HG	2.33	0.69
1:L:168:ILE:CG2	1:L:173:ILE:HD13	2.23	0.69
1:E:47:ASP:HB3	1:E:97:ARG:NH2	2.08	0.69
1:I:22:ALA:HB2	1:I:98:LEU:HD22	1.74	0.69
1:A:186:MET:HE2	1:A:186:MET:HA	1.73	0.69
1:B:177:SER:O	1:B:201:ARG:NH1	2.25	0.68
1:E:204:ASP:HA	1:E:224:THR:CG2	2.23	0.68
1:J:86:VAL:O	1:J:90:ARG:HG2	1.93	0.68
1:M:179:VAL:HA	1:M:245:VAL:O	1.93	0.68
1:I:130:THR:HG22	3:I:4002:GOL:O2	1.94	0.68
1:E:146:ARG:H	3:E:2003:GOL:H32	1.58	0.68
1:A:130:THR:HG22	3:A:1001:GOL:O2	1.93	0.68
1:D:186:MET:HE3	1:D:209:PHE:CD1	2.29	0.68
1:B:201:ARG:HD2	1:B:205:GLU:OE2	1.93	0.68
1:A:214:ALA:H	1:A:218:GLN:HE21	1.42	0.68
3:H:4012:GOL:C3	1:I:111:GLU:OE1	2.41	0.68
1:I:161:SER:C	1:I:164:VAL:HG22	2.14	0.68
1:F:176:GLY:HA3	1:G:169:ASN:HB3	1.76	0.67
1:J:186:MET:HE2	1:J:209:PHE:HE1	1.58	0.67
1:J:214:ALA:H	1:J:218:GLN:NE2	1.91	0.67
1:M:19:LEU:HD12	1:M:97:ARG:HB3	1.75	0.67
1:E:47:ASP:HB3	1:E:97:ARG:HH22	1.59	0.67
1:D:177:SER:O	1:D:201:ARG:NH2	2.28	0.67
3:J:5011:GOL:H2	1:K:108:ARG:H	1.59	0.67
1:M:37:ALA:HB1	1:M:96:LEU:HD21	1.76	0.67
1:G:214:ALA:H	1:G:218:GLN:NE2	1.92	0.67
1:G:14:LYS:HD3	1:G:14:LYS:O	1.95	0.67
1:D:108:ARG:NH2	1:D:111:GLU:OE2	2.28	0.66
1:H:168:ILE:CG2	1:H:173:ILE:HD12	2.24	0.66
1:A:186:MET:CE	1:A:209:PHE:CE1	2.78	0.66
4:H:4545:HOH:O	1:I:146:ARG:HD3	1.94	0.66
1:I:161:SER:C	1:I:164:VAL:CG2	2.63	0.66
1:H:201:ARG:HD2	1:H:205:GLU:OE1	1.95	0.66
1:J:6:PHE:CD2	1:J:32:LEU:HD13	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:ARG:HH22	1:K:227:ARG:NH1	1.94	0.66
1:E:177:SER:O	1:E:201:ARG:NH1	2.25	0.66
1:E:6:PHE:HB2	1:E:9:LEU:HG	1.78	0.66
1:K:214:ALA:H	1:K:218:GLN:NE2	1.94	0.66
1:J:50:VAL:HG23	4:J:5530:HOH:O	1.95	0.65
1:A:232:VAL:HG13	1:A:237:LEU:HB2	1.79	0.65
1:D:186:MET:HE1	1:D:209:PHE:CE1	2.31	0.65
1:B:6:PHE:O	1:B:6:PHE:CD1	2.49	0.65
1:J:223:THR:CG2	1:J:224:THR:N	2.50	0.65
1:K:193:THR:HG21	4:K:5512:HOH:O	1.97	0.65
1:E:51:ASN:O	1:E:53:ASP:N	2.30	0.65
1:E:211:CYS:SG	1:E:237:LEU:HG	2.37	0.65
1:A:38:LEU:HD13	1:A:96:LEU:HD21	1.79	0.65
1:K:204:ASP:HA	1:K:224:THR:CG2	2.27	0.65
1:H:186:MET:HE1	1:H:209:PHE:HE1	1.61	0.64
1:B:12:LEU:HG	1:B:94:ARG:HB3	1.79	0.64
1:B:38:LEU:HD13	1:B:96:LEU:CD1	2.28	0.64
1:J:260:ALA:HA	1:J:262:ASP:H	1.62	0.64
1:K:227:ARG:NH2	1:K:231:ASP:OD1	2.29	0.64
1:D:129:ILE:HA	3:E:2001:GOL:H31	1.79	0.64
1:D:171:GLN:HG2	4:D:2542:HOH:O	1.98	0.64
1:H:186:MET:HE1	1:H:209:PHE:CE1	2.33	0.64
1:A:30:LEU:HD11	1:A:54:CYS:HB2	1.80	0.64
1:B:51:ASN:O	1:B:52:GLU:C	2.37	0.64
1:J:235:ALA:HB1	1:J:237:LEU:HD13	1.80	0.64
1:J:148:VAL:CG1	1:J:247:GLU:HB2	2.28	0.63
1:D:146:ARG:N	3:D:2011:GOL:O2	2.27	0.63
1:H:177:SER:O	1:H:201:ARG:NH2	2.32	0.63
1:B:22:ALA:HB2	1:B:98:LEU:HD22	1.81	0.63
1:F:146:ARG:HB2	3:F:3011:GOL:H11	1.80	0.63
1:H:227:ARG:HD3	4:H:4507:HOH:O	1.98	0.63
1:E:198:ALA:O	1:H:252:ARG:NH1	2.32	0.63
1:H:77:LYS:HG3	1:H:78:GLN:N	2.14	0.63
1:M:149:ASN:N	1:M:149:ASN:HD22	1.94	0.63
1:F:22:ALA:HB2	1:F:98:LEU:HD22	1.80	0.63
1:A:169:ASN:ND2	1:A:172:GLY:H	1.96	0.62
1:G:51:ASN:ND2	1:G:53:ASP:HB2	2.00	0.62
1:I:204:ASP:CA	1:I:224:THR:HG23	2.29	0.62
1:D:260:ALA:H	1:D:261:LEU:HB2	1.63	0.62
1:G:204:ASP:HA	1:G:224:THR:HG23	1.81	0.62
1:J:201:ARG:HD2	1:J:205:GLU:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:MET:CE	1:D:209:PHE:CD1	2.83	0.61
1:F:14:LYS:HD3	1:F:14:LYS:O	2.00	0.61
1:I:50:VAL:CG1	1:I:51:ASN:N	2.52	0.61
1:K:17:VAL:HG22	1:K:95:VAL:HB	1.81	0.61
1:M:186:MET:HE1	1:M:209:PHE:HD1	1.62	0.61
1:A:186:MET:HE1	1:A:209:PHE:CE1	2.36	0.61
1:H:99:LYS:NZ	1:H:107:GLY:O	2.27	0.61
1:A:19:LEU:HD12	1:A:97:ARG:HB3	1.83	0.61
1:E:17:VAL:HG22	1:E:95:VAL:HB	1.82	0.61
1:D:22:ALA:HB2	1:D:98:LEU:HD22	1.83	0.61
1:G:65:GLU:OE1	1:G:84:ARG:NH2	2.32	0.61
1:I:12:LEU:HG	1:I:94:ARG:HB3	1.83	0.61
1:L:214:ALA:H	1:L:218:GLN:HE21	1.48	0.61
1:A:186:MET:CE	1:A:209:PHE:HE1	2.14	0.61
1:F:169:ASN:HD22	1:F:169:ASN:C	2.04	0.60
1:J:26:ASP:OD1	1:J:27:PRO:O	2.20	0.60
1:L:108:ARG:HG2	1:L:108:ARG:HH21	1.67	0.60
1:H:46:HIS:HD2	1:H:47:ASP:O	1.84	0.60
1:K:9:LEU:HB3	1:K:10:PRO:HD2	1.83	0.60
1:D:43:VAL:HG11	1:D:88:LEU:HG	1.83	0.60
1:E:26:ASP:HB3	1:E:29:LEU:HD22	1.81	0.60
1:A:186:MET:HE3	1:A:209:PHE:HD1	1.66	0.60
1:A:186:MET:HE1	1:A:209:PHE:HE1	1.67	0.60
1:A:201:ARG:HD2	1:A:205:GLU:OE1	2.01	0.60
1:D:9:LEU:HB3	1:D:10:PRO:HD2	1.83	0.60
1:D:186:MET:CE	1:D:209:PHE:HD1	2.14	0.60
1:M:156:THR:HG22	1:M:184:MET:CE	2.31	0.60
1:D:175:SER:O	1:D:176:GLY:C	2.40	0.59
1:K:189:ILE:O	1:K:193:THR:HB	2.01	0.59
1:M:225:LEU:HD21	1:M:245:VAL:HG11	1.83	0.59
1:M:266:LEU:O	1:M:267:ALA:HB2	2.02	0.59
1:A:186:MET:HE3	1:A:209:PHE:CE1	2.37	0.59
1:B:193:THR:HG21	4:B:1529:HOH:O	2.01	0.59
1:L:106:PHE:N	1:M:144:THR:HG21	2.13	0.59
1:M:223:THR:HG21	1:M:228:ALA:HA	1.85	0.59
1:H:186:MET:HE3	1:H:209:PHE:HD1	1.67	0.59
1:D:12:LEU:H	1:D:40:GLN:NE2	2.00	0.59
1:H:59:ARG:HH22	1:K:227:ARG:HH12	1.49	0.59
1:J:146:ARG:NH2	1:K:108:ARG:NE	2.47	0.59
1:L:214:ALA:H	1:L:218:GLN:NE2	2.00	0.59
1:M:148:VAL:HG13	1:M:247:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:ILE:HA	4:I:4562:HOH:O	2.02	0.59
1:A:99:LYS:NZ	1:A:107:GLY:O	2.27	0.59
1:G:129:ILE:HA	3:G:3002:GOL:O2	2.01	0.59
1:I:177:SER:O	1:I:201:ARG:NH1	2.32	0.59
1:I:265:LYS:H	1:I:265:LYS:CD	2.15	0.59
1:B:258:ILE:C	1:B:260:ALA:H	2.05	0.58
1:G:26:ASP:HB3	1:G:29:LEU:HD22	1.84	0.58
1:H:227:ARG:HG2	1:H:227:ARG:HH11	1.67	0.58
1:I:51:ASN:O	1:I:53:ASP:N	2.36	0.58
1:H:205:GLU:O	1:H:224:THR:HA	2.04	0.58
1:I:37:ALA:HB1	1:I:96:LEU:HD22	1.84	0.58
1:D:259:GLY:O	1:D:260:ALA:CB	2.51	0.58
1:E:77:LYS:HE3	1:E:108:ARG:HH12	1.68	0.58
1:M:201:ARG:NH2	1:M:205:GLU:OE2	2.35	0.58
1:M:149:ASN:H	1:M:149:ASN:HD22	1.51	0.58
1:M:156:THR:HG22	1:M:184:MET:HE3	1.86	0.58
1:J:146:ARG:HH22	1:K:108:ARG:CD	2.16	0.58
1:A:51:ASN:HD22	1:A:53:ASP:HB2	1.67	0.58
1:E:129:ILE:HD12	3:E:2001:GOL:H11	1.85	0.58
3:F:3011:GOL:H12	1:G:108:ARG:HD3	1.84	0.58
1:B:12:LEU:N	1:B:40:GLN:HE22	2.02	0.58
1:D:258:ILE:O	1:D:261:LEU:HB2	2.03	0.58
1:I:211:CYS:SG	1:I:237:LEU:HG	2.44	0.58
1:B:138:TYR:CD2	1:B:258:ILE:HD11	2.39	0.57
1:K:258:ILE:C	1:K:260:ALA:H	2.07	0.57
1:F:186:MET:HE1	1:F:209:PHE:CE1	2.37	0.57
1:I:265:LYS:CE	1:I:265:LYS:H	2.16	0.57
1:J:84:ARG:NH1	1:J:87:GLU:OE1	2.38	0.57
1:K:204:ASP:HA	1:K:224:THR:OG1	2.04	0.57
1:L:108:ARG:HG2	1:L:108:ARG:NH2	2.18	0.57
1:D:201:ARG:HD2	1:D:205:GLU:OE1	2.05	0.57
1:F:99:LYS:NZ	1:F:107:GLY:O	2.26	0.57
1:J:37:ALA:HB1	1:J:96:LEU:HD22	1.87	0.57
1:K:7:ALA:HB3	4:K:5549:HOH:O	2.04	0.57
1:M:266:LEU:O	1:M:267:ALA:CB	2.51	0.57
1:B:73:LYS:H	1:B:74:PRO:HD3	1.69	0.57
1:F:214:ALA:N	1:F:218:GLN:HE21	1.95	0.57
1:G:204:ASP:HA	1:G:224:THR:OG1	2.05	0.57
1:M:224:THR:OG1	1:M:227:ARG:HB2	2.05	0.57
1:G:73:LYS:N	1:G:74:PRO:CD	2.68	0.57
1:M:82:SER:HB3	1:M:115:THR:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:186:MET:HE2	1:M:209:PHE:CE1	2.38	0.57
1:H:6:PHE:HD1	1:H:7:ALA:N	2.03	0.56
1:L:18:TRP:CD1	1:L:124:ARG:HB3	2.39	0.56
1:G:204:ASP:HA	1:G:224:THR:CG2	2.35	0.56
1:J:99:LYS:NZ	1:J:107:GLY:O	2.32	0.56
1:J:148:VAL:HG13	1:J:247:GLU:HB2	1.88	0.56
1:H:68:GLY:HA3	1:H:76:PRO:HD2	1.88	0.56
1:A:12:LEU:H	1:A:40:GLN:NE2	2.02	0.56
1:F:108:ARG:HG2	1:F:108:ARG:HH21	1.69	0.56
1:H:146:ARG:N	3:H:4012:GOL:H32	2.18	0.56
1:I:266:LEU:HD23	1:I:266:LEU:H	1.69	0.56
1:M:191:ALA:O	1:M:195:ASN:HB2	2.05	0.56
1:M:223:THR:HG22	1:M:224:THR:N	2.11	0.56
1:A:15:GLY:O	1:A:121:VAL:HG13	2.06	0.56
1:J:33:HIS:HE1	1:K:26:ASP:OD2	1.88	0.56
1:L:17:VAL:HG22	1:L:95:VAL:HB	1.87	0.56
1:D:186:MET:HE1	1:D:209:PHE:HE1	1.71	0.56
1:I:201:ARG:HD2	1:I:205:GLU:OE2	2.06	0.56
1:A:39:ARG:CG	1:A:39:ARG:HH21	2.04	0.56
1:B:189:ILE:O	1:B:193:THR:HB	2.06	0.56
1:E:12:LEU:HD13	1:E:18:TRP:CD1	2.42	0.55
3:K:5012:GOL:H11	4:K:5552:HOH:O	2.07	0.55
1:D:203:PRO:O	1:D:224:THR:HG23	2.05	0.55
1:E:170:TRP:HB3	1:E:195:ASN:ND2	2.22	0.55
1:K:51:ASN:HD22	1:K:53:ASP:HB2	1.71	0.55
1:L:257:TRP:CZ3	1:M:124:ARG:HG3	2.42	0.55
1:F:108:ARG:HG2	1:F:108:ARG:NH2	2.21	0.55
1:F:78:GLN:NE2	1:F:112:GLU:HG2	2.22	0.55
1:D:214:ALA:H	1:D:218:GLN:NE2	2.04	0.55
1:D:59:ARG:HB2	1:D:60:PRO:HD2	1.88	0.55
1:H:146:ARG:HG3	1:H:146:ARG:NH1	2.15	0.55
1:I:193:THR:HG21	4:I:4526:HOH:O	2.06	0.55
1:M:156:THR:CG2	1:M:184:MET:HE1	2.37	0.55
1:D:77:LYS:HG3	1:D:78:GLN:N	2.22	0.55
1:G:149:ASN:HD22	1:G:149:ASN:N	2.05	0.55
1:I:149:ASN:HD22	1:I:149:ASN:N	2.05	0.55
1:F:201:ARG:HD2	1:F:205:GLU:OE1	2.07	0.54
1:D:11:ALA:HA	1:D:40:GLN:NE2	2.21	0.54
1:F:108:ARG:N	3:G:3003:GOL:H11	2.20	0.54
1:H:168:ILE:CG2	1:H:173:ILE:CD1	2.86	0.54
1:K:138:TYR:HB3	1:K:218:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LEU:O	1:E:118:GLU:HG2	2.07	0.54
1:J:177:SER:O	1:J:201:ARG:NH2	2.39	0.54
1:I:214:ALA:N	1:I:218:GLN:HE21	1.97	0.54
1:F:177:SER:O	1:F:201:ARG:NH2	2.41	0.54
1:F:223:THR:CG2	1:F:224:THR:H	1.97	0.54
1:H:168:ILE:HG23	1:H:173:ILE:HD12	1.89	0.54
1:A:269:ASP:CG	1:A:270:PRO:HD3	2.28	0.54
1:B:11:ALA:HA	1:B:40:GLN:HE22	1.71	0.54
1:B:227:ARG:NH2	4:B:1542:HOH:O	2.40	0.54
1:G:39:ARG:O	1:G:59:ARG:HG2	2.07	0.54
1:H:77:LYS:HE3	1:H:108:ARG:HH12	1.73	0.54
1:F:169:ASN:ND2	1:F:172:GLY:H	2.04	0.54
1:G:22:ALA:HB2	1:G:98:LEU:HD22	1.89	0.54
1:I:19:LEU:HD12	1:I:97:ARG:HG2	1.90	0.54
1:M:47:ASP:OD2	1:M:97:ARG:NH2	2.39	0.54
1:B:5:LEU:HD12	4:B:1562:HOH:O	2.07	0.54
1:G:19:LEU:HD12	1:G:125:ILE:CD1	2.38	0.54
1:H:169:ASN:HD22	1:H:169:ASN:C	2.12	0.54
1:J:108:ARG:H	3:K:5001:GOL:H11	1.72	0.54
1:K:19:LEU:HD12	1:K:125:ILE:CD1	2.37	0.54
3:D:2011:GOL:H31	1:E:108:ARG:HA	0.91	0.53
1:E:22:ALA:HB2	1:E:98:LEU:HD22	1.90	0.53
1:L:205:GLU:O	1:L:224:THR:HA	2.08	0.53
1:I:145:HIS:H	1:I:149:ASN:HD21	1.55	0.53
1:B:48:ALA:O	1:B:50:VAL:N	2.42	0.53
1:D:169:ASN:C	1:D:169:ASN:HD22	2.11	0.53
1:G:100:GLY:O	2:G:3511:SAH:N	2.39	0.53
1:L:31:THR:HG21	1:L:127:PRO:O	2.08	0.53
1:L:168:ILE:HG23	1:L:173:ILE:CD1	2.38	0.53
1:E:173:ILE:CG2	1:E:180:ILE:HD12	2.38	0.53
1:K:146[A]:ARG:HH21	3:K:5001:GOL:H12	1.73	0.53
1:M:253:ALA:HA	1:M:264:ARG:HH11	1.73	0.53
1:F:33:HIS:HD2	4:F:3537:HOH:O	1.90	0.53
1:K:177:SER:O	1:K:201:ARG:NH1	2.41	0.53
1:I:19:LEU:HD12	1:I:97:ARG:HB3	1.89	0.53
1:E:171:GLN:HE22	1:E:199:GLY:HA2	1.73	0.53
1:G:189:ILE:HG12	1:G:209:PHE:HZ	1.74	0.53
1:I:48:ALA:C	1:I:50:VAL:N	2.62	0.53
1:J:83:LEU:HA	1:J:86:VAL:HG13	1.90	0.53
1:L:19:LEU:HD12	1:L:97:ARG:HB3	1.91	0.53
1:G:77:LYS:HE3	1:G:78:GLN:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:ASP:HB3	1:M:29:LEU:HD22	1.91	0.53
1:A:186:MET:CE	1:A:209:PHE:CD1	2.92	0.52
1:B:73:LYS:N	1:B:74:PRO:CD	2.71	0.52
1:B:77:LYS:HG3	1:B:78:GLN:N	2.25	0.52
1:H:223:THR:HG23	1:H:231:ASP:OD2	2.08	0.52
1:K:156:THR:HG23	1:K:184:MET:CE	2.40	0.52
1:E:156:THR:CG2	1:E:184:MET:HE1	2.39	0.52
1:G:168:ILE:O	1:G:170:TRP:N	2.42	0.52
1:J:169:ASN:ND2	1:J:172:GLY:H	2.04	0.52
1:A:65:GLU:OE1	1:A:84:ARG:NH2	2.41	0.52
1:B:50:VAL:HG13	1:B:51:ASN:N	2.15	0.52
1:F:108:ARG:CG	1:F:108:ARG:HH21	2.22	0.52
1:H:186:MET:HE3	1:H:209:PHE:CD1	2.44	0.52
1:G:23:GLY:HA2	1:G:129:ILE:O	2.10	0.52
4:L:6525:HOH:O	1:M:134:GLY:HA2	2.09	0.52
1:A:209:PHE:CE1	1:A:232:VAL:HG21	2.45	0.52
1:B:168:ILE:HG23	1:B:173:ILE:CD1	2.39	0.52
1:H:50:VAL:HG12	1:H:215:THR:HG21	1.92	0.52
1:J:130:THR:H	3:J:5002:GOL:H11	1.75	0.52
1:K:149:ASN:N	1:K:149:ASN:HD22	2.08	0.52
1:J:266:LEU:HD23	1:K:117:VAL:HG22	1.92	0.52
1:L:186:MET:HE1	1:L:209:PHE:CE1	2.45	0.52
1:B:149:ASN:HD22	1:B:149:ASN:N	2.09	0.51
1:D:39:ARG:NH1	1:D:39:ARG:CG	2.62	0.51
1:H:168:ILE:HG23	1:H:173:ILE:CD1	2.40	0.51
1:I:144:THR:CG2	1:I:146:ARG:HH12	2.23	0.51
1:J:30:LEU:HB2	1:K:32:LEU:HD22	1.92	0.51
1:B:49:LEU:HD21	1:B:240:PRO:HG3	1.91	0.51
1:G:73:LYS:H	1:G:74:PRO:CD	2.22	0.51
1:K:143:VAL:HG22	1:K:152:VAL:HG11	1.93	0.51
1:A:193:THR:O	1:A:197:ILE:HG13	2.10	0.51
1:E:201:ARG:HD2	1:E:205:GLU:OE2	2.10	0.51
1:L:20:VAL:HB	1:L:96:LEU:HD11	1.92	0.51
1:A:7:ALA:HB1	1:A:9:LEU:HD21	1.92	0.51
1:I:27:PRO:HG3	1:I:53:ASP:HB2	1.93	0.51
1:M:197:ILE:HD11	1:M:225:LEU:O	2.10	0.51
1:A:213:ALA:HA	1:A:218:GLN:HE21	1.76	0.51
1:A:28:GLY:HA2	1:B:32:LEU:CB	2.28	0.51
1:D:17:VAL:O	1:D:123:PHE:HA	2.10	0.51
1:H:6:PHE:CD1	1:H:7:ALA:N	2.79	0.51
1:H:73:LYS:CB	1:H:74:PRO:HD3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ASP:CA	1:E:224:THR:HG23	2.41	0.51
1:M:143:VAL:HG22	1:M:152:VAL:HG11	1.91	0.51
1:B:50:VAL:HG12	1:B:51:ASN:H	1.73	0.51
1:D:171:GLN:HB3	1:H:263:GLY:HA3	1.93	0.51
1:D:258:ILE:HA	1:D:261:LEU:HD12	1.93	0.51
1:D:51:ASN:OD1	1:D:53:ASP:N	2.43	0.51
1:F:130:THR:HG22	3:G:3002:GOL:H31	1.92	0.51
1:H:69:LYS:HA	1:H:75:SER:HB3	1.91	0.51
1:A:108:ARG:HH21	1:A:108:ARG:CG	2.24	0.51
1:D:12:LEU:H	1:D:40:GLN:HE21	1.58	0.51
1:E:12:LEU:HG	1:E:94:ARG:HB2	1.93	0.51
1:I:189:ILE:O	1:I:193:THR:HB	2.11	0.51
1:K:26:ASP:HB3	1:K:29:LEU:HD22	1.91	0.51
1:M:138:TYR:CD2	1:M:214:ALA:HA	2.46	0.51
1:B:52:GLU:O	1:B:55:LEU:N	2.42	0.51
1:G:159:ASP:N	1:G:159:ASP:OD1	2.43	0.50
1:I:90:ARG:HE	1:I:120[A]:GLN:HE22	1.57	0.50
1:L:18:TRP:CE2	1:L:124:ARG:HD2	2.46	0.50
1:A:23:GLY:HA2	1:A:129:ILE:O	2.11	0.50
1:B:48:ALA:HB2	1:B:66:PHE:HE1	1.75	0.50
1:L:221:LEU:HB2	1:L:237:LEU:HD21	1.92	0.50
1:L:27:PRO:O	1:L:30:LEU:HB2	2.10	0.50
1:A:9:LEU:N	1:A:9:LEU:HD23	2.26	0.50
1:G:99:LYS:NZ	1:G:112:GLU:OE1	2.43	0.50
1:G:170:TRP:HB3	1:G:195:ASN:ND2	2.27	0.50
1:K:163:LEU:O	1:K:164:VAL:C	2.49	0.50
1:A:15:GLY:HA2	1:A:89:ALA:O	2.12	0.50
1:D:33:HIS:HE1	1:E:26:ASP:OD2	1.94	0.50
1:H:104:PHE:O	1:I:144:THR:HB	2.11	0.50
1:L:148:VAL:HG13	1:L:247:GLU:HB2	1.94	0.50
1:M:145:HIS:H	1:M:149:ASN:HD21	1.60	0.50
1:B:48:ALA:HB2	1:B:66:PHE:CE1	2.46	0.50
1:E:189:ILE:HG12	1:E:209:PHE:HZ	1.76	0.50
1:I:145:HIS:H	1:I:149:ASN:ND2	2.09	0.50
1:I:204:ASP:HA	1:I:224:THR:OG1	2.11	0.50
1:K:156:THR:HG22	1:K:158:HIS:H	1.75	0.50
1:L:168:ILE:CG2	1:L:173:ILE:CD1	2.90	0.50
1:M:169:ASN:ND2	1:M:172:GLY:H	2.10	0.50
1:A:223:THR:OG1	1:A:224:THR:N	2.44	0.50
1:B:48:ALA:C	1:B:50:VAL:N	2.63	0.50
1:J:31:THR:HG23	4:J:5510:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:GLY:CA	1:K:32:LEU:HB2	2.37	0.50
1:F:12:LEU:N	1:F:40:GLN:HE22	1.97	0.50
1:J:138:TYR:HB3	1:J:218:GLN:HE22	1.75	0.50
1:J:25:GLY:O	1:J:51:ASN:HB2	2.12	0.50
1:B:258:ILE:O	1:B:260:ALA:N	2.44	0.49
1:J:214:ALA:N	1:J:218:GLN:HE21	2.10	0.49
1:A:211:CYS:SG	1:A:237:LEU:HG	2.52	0.49
1:J:259:GLY:O	1:J:262:ASP:HB2	2.12	0.49
1:A:43:VAL:HG11	1:A:88:LEU:HG	1.95	0.49
1:G:73:LYS:H	1:G:74:PRO:HD3	1.77	0.49
1:A:189:ILE:HG12	1:A:209:PHE:HZ	1.78	0.49
1:D:44:ILE:HB	1:D:64:LEU:HD12	1.94	0.49
1:F:208:ALA:HB3	1:F:244:VAL:CG1	2.43	0.49
1:L:117:VAL:HG11	1:M:267:ALA:HB2	1.94	0.49
1:B:47:ASP:O	1:B:50:VAL:HB	2.13	0.49
1:J:108:ARG:N	3:K:5001:GOL:H11	2.28	0.49
1:L:51:ASN:O	1:L:53:ASP:N	2.46	0.49
1:M:85:LEU:HD21	1:M:97:ARG:HD2	1.94	0.49
1:A:167:ARG:O	1:A:168:ILE:HG13	2.13	0.49
1:D:78:GLN:NE2	1:D:112:GLU:OE2	2.46	0.49
1:D:161:SER:HB3	1:D:188:HIS:CE1	2.48	0.49
1:F:14:LYS:HD3	1:F:14:LYS:N	2.28	0.49
1:K:106:PHE:CE2	1:K:156:THR:OG1	2.66	0.49
1:I:228:ALA:O	1:I:232:VAL:CG1	2.54	0.49
1:K:204:ASP:CA	1:K:224:THR:HG23	2.42	0.49
1:L:186:MET:CE	1:L:209:PHE:CE1	2.96	0.49
1:L:75:SER:O	1:L:77:LYS:N	2.45	0.49
1:E:156:THR:CG2	1:E:184:MET:CE	2.91	0.48
1:G:12:LEU:H	1:G:40:GLN:NE2	2.10	0.48
1:I:47:ASP:OD2	1:I:97:ARG:NH2	2.41	0.48
1:L:108:ARG:HH21	1:L:108:ARG:CG	2.26	0.48
1:A:232:VAL:HG13	1:A:237:LEU:CB	2.43	0.48
1:B:115:THR:O	1:B:119:HIS:HD2	1.96	0.48
3:A:1001:GOL:C1	1:B:128:GLY:O	2.59	0.48
1:B:214:ALA:N	1:B:218:GLN:HE21	2.08	0.48
1:H:51:ASN:HD22	1:H:53:ASP:CB	2.25	0.48
1:L:38:LEU:HD22	1:L:96:LEU:HD21	1.95	0.48
4:L:6525:HOH:O	1:M:133:ILE:HG22	2.13	0.48
1:B:50:VAL:HG12	1:B:51:ASN:N	2.28	0.48
1:F:256:ASP:OD1	1:F:264:ARG:NH2	2.45	0.48
1:F:30:LEU:HD11	1:F:54:CYS:HB2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:LYS:HB3	1:G:75:SER:OG	2.13	0.48
1:M:19:LEU:HD12	1:M:97:ARG:CB	2.43	0.48
1:E:130:THR:HG22	3:E:2001:GOL:HO2	1.74	0.48
1:A:187:LYS:HA	1:A:187:LYS:HD2	1.47	0.48
1:J:170:TRP:CB	1:J:195:ASN:ND2	2.77	0.48
1:J:106:PHE:N	1:K:144:THR:HG21	2.29	0.48
1:D:108:ARG:N	3:E:2003:GOL:H11	2.21	0.48
1:K:203:PRO:O	1:K:204:ASP:C	2.51	0.48
1:D:171:GLN:NE2	1:D:199:GLY:HA2	2.29	0.48
1:K:23:GLY:HA2	1:K:129:ILE:O	2.13	0.48
1:L:203:PRO:O	1:L:224:THR:HG23	2.14	0.48
1:F:203:PRO:O	1:F:224:THR:HG23	2.14	0.47
1:J:101:GLY:HA3	2:J:5501:SAH:C	2.44	0.47
1:A:158[B]:HIS:HD2	1:A:188:HIS:CD2	2.31	0.47
1:G:43:VAL:HG11	1:G:88:LEU:HD22	1.95	0.47
1:I:97:ARG:HD3	1:I:112:GLU:OE2	2.14	0.47
1:I:129:ILE:CD1	3:I:4002:GOL:H12	2.44	0.47
1:I:77:LYS:HD2	1:I:78:GLN:H	1.79	0.47
1:E:97:ARG:NH1	1:E:112:GLU:OE2	2.47	0.47
1:H:138:TYR:HB3	1:H:218:GLN:HE22	1.79	0.47
1:L:20:VAL:HG22	1:L:126:VAL:HB	1.96	0.47
1:B:156:THR:CG2	1:B:184:MET:CE	2.92	0.47
4:H:4545:HOH:O	1:I:145:HIS:HD2	1.97	0.47
1:M:78:GLN:HE22	1:M:112:GLU:HG3	1.80	0.47
1:B:12:LEU:N	1:B:40:GLN:NE2	2.53	0.47
1:F:19:LEU:HD12	1:F:97:ARG:HB3	1.97	0.47
1:F:186:MET:CE	1:F:209:PHE:CE1	2.97	0.47
1:H:111:GLU:CD	1:I:146:ARG:HG3	2.35	0.47
1:B:20:VAL:HG21	1:B:96:LEU:HD21	1.96	0.47
1:D:38:LEU:HD13	1:D:96:LEU:HD21	1.97	0.47
1:F:47:ASP:O	1:F:49:LEU:HG	2.14	0.47
1:F:18:TRP:CD1	1:F:124:ARG:HB3	2.50	0.47
1:A:209:PHE:CZ	1:A:232:VAL:HG21	2.50	0.47
1:B:12:LEU:HD13	1:B:18:TRP:CD1	2.50	0.47
1:J:26:ASP:O	1:J:29:LEU:HB2	2.14	0.47
1:A:28:GLY:CA	1:B:32:LEU:HB2	2.29	0.47
1:F:187:LYS:HD3	1:F:187:LYS:HA	1.64	0.47
1:F:51:ASN:HD22	1:F:53:ASP:CB	2.21	0.47
1:H:203:PRO:O	1:H:224:THR:HG23	2.14	0.47
1:M:264:ARG:CG	1:M:265:LYS:N	2.77	0.47
1:D:108:ARG:CG	1:D:108:ARG:HH21	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ARG:HA	1:G:60:PRO:HD3	1.80	0.47
1:H:78:GLN:HB2	1:H:108:ARG:NH1	2.29	0.47
1:I:46:HIS:HB2	1:I:50:VAL:HG21	1.96	0.47
1:J:28:GLY:HA2	1:K:32:LEU:HB3	1.97	0.47
1:J:99:LYS:HB3	4:J:5529:HOH:O	2.13	0.47
1:J:146:ARG:NH2	1:K:108:ARG:HD2	2.30	0.47
1:E:214:ALA:N	1:E:218:GLN:HE21	2.01	0.47
1:H:12:LEU:H	1:H:40:GLN:NE2	2.12	0.47
1:I:65:GLU:OE2	1:I:84:ARG:HD3	2.15	0.47
1:J:148:VAL:HG11	1:J:247:GLU:HB2	1.96	0.47
1:J:15:GLY:HA2	1:J:89:ALA:O	2.15	0.47
1:M:169:ASN:HD22	1:M:172:GLY:H	1.62	0.47
1:I:12:LEU:HD13	1:I:18:TRP:CD1	2.50	0.46
1:J:145:HIS:O	1:J:148:VAL:N	2.49	0.46
1:H:78:GLN:NE2	1:H:112:GLU:HG2	2.30	0.46
1:I:156:THR:HG23	1:I:184:MET:CE	2.45	0.46
1:D:146:ARG:H	3:D:2011:GOL:HO2	1.59	0.46
1:D:255:LEU:HD21	1:E:114:LEU:HD13	1.97	0.46
1:D:57:LEU:HD11	1:E:6:PHE:CZ	2.51	0.46
1:F:223:THR:HG21	1:F:228:ALA:HA	1.97	0.46
1:H:78:GLN:NE2	1:H:112:GLU:CG	2.78	0.46
1:M:156:THR:HG21	1:M:184:MET:HE1	1.97	0.46
1:A:148:VAL:HG13	1:A:247:GLU:HB2	1.98	0.46
1:F:186:MET:HE3	1:F:209:PHE:CD1	2.50	0.46
1:J:223:THR:HG21	1:J:228:ALA:HA	1.98	0.46
1:M:186:MET:HE1	1:M:209:PHE:CD1	2.45	0.46
1:K:214:ALA:N	1:K:218:GLN:HE21	2.09	0.46
1:H:17:VAL:HG22	1:H:95:VAL:HB	1.98	0.46
1:I:169:ASN:ND2	1:I:172:GLY:N	2.54	0.46
1:A:269:ASP:HB2	1:A:270:PRO:CD	2.44	0.46
1:I:43:VAL:HG11	1:I:88:LEU:HD22	1.97	0.46
1:J:17:VAL:HG23	1:J:121:VAL:HG11	1.98	0.46
1:M:24:PRO:HB2	1:M:214:ALA:HB3	1.97	0.46
1:B:47:ASP:OD2	1:B:97:ARG:NH2	2.48	0.46
1:D:49:LEU:HB3	1:D:51:ASN:O	2.16	0.46
1:H:33:HIS:HE1	1:I:26:ASP:OD2	1.99	0.46
1:L:104:PHE:CZ	1:L:125:ILE:HG13	2.51	0.46
1:M:155:LEU:HD12	1:M:173:ILE:HD13	1.96	0.46
1:I:145:HIS:O	1:I:148:VAL:N	2.48	0.46
1:M:223:THR:HG23	1:M:231:ASP:OD2	2.15	0.46
1:E:22:ALA:HB2	1:E:98:LEU:CD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:184:MET:HA	3:K:5012:GOL:H32	1.97	0.45
1:M:26:ASP:HB2	1:M:214:ALA:O	2.16	0.45
1:A:177:SER:O	1:A:201:ARG:NH2	2.42	0.45
1:B:77:LYS:NZ	1:B:108:ARG:HH22	2.14	0.45
1:A:269:ASP:CB	1:A:270:PRO:CD	2.93	0.45
1:F:77:LYS:HE3	1:F:78:GLN:H	1.82	0.45
1:G:44:ILE:HG12	1:G:96:LEU:HG	1.98	0.45
1:I:264:ARG:HA	1:I:265:LYS:HE3	1.98	0.45
1:K:156:THR:HG23	1:K:184:MET:HE3	1.98	0.45
1:F:84:ARG:O	1:F:88:LEU:HB2	2.17	0.45
1:G:65:GLU:OE2	1:G:84:ARG:HD3	2.17	0.45
1:I:5:LEU:HG	1:I:5:LEU:H	1.47	0.45
1:J:22:ALA:HB2	1:J:98:LEU:HD22	1.98	0.45
1:A:14:LYS:C	1:A:16:SER:N	2.70	0.45
1:A:39:ARG:O	1:A:59:ARG:HB3	2.17	0.45
1:E:138:TYR:HB3	1:E:218:GLN:HE22	1.80	0.45
1:E:77:LYS:HD2	1:E:77:LYS:HA	1.77	0.45
1:H:106:PHE:HA	1:I:146:ARG:HH22	1.80	0.45
1:M:253:ALA:HA	1:M:264:ARG:NH1	2.32	0.45
1:M:184:MET:HE2	2:M:6511:SAH:SD	2.56	0.45
1:F:33:HIS:HE1	1:G:26:ASP:OD2	1.99	0.45
1:L:211:CYS:SG	1:L:241:ALA:HB2	2.56	0.45
1:A:59:ARG:O	1:A:60:PRO:C	2.55	0.45
1:G:189:ILE:HG12	1:G:209:PHE:CZ	2.52	0.45
1:I:129:ILE:HD12	3:I:4002:GOL:H12	1.98	0.45
1:B:258:ILE:C	1:B:260:ALA:N	2.69	0.45
1:D:85:LEU:HD11	1:D:97:ARG:HD3	1.99	0.45
1:K:97:ARG:NH1	1:K:112:GLU:OE2	2.45	0.45
1:J:254:ALA:O	1:K:117:VAL:HG21	2.17	0.45
1:I:266:LEU:H	1:I:266:LEU:HD22	1.80	0.45
1:I:85:LEU:HD11	1:I:97:ARG:HD2	1.99	0.45
1:D:38:LEU:O	1:D:58:ALA:HA	2.18	0.44
1:E:204:ASP:C	1:E:204:ASP:OD1	2.56	0.44
1:J:184:MET:HE2	2:J:5501:SAH:SD	2.56	0.44
1:F:144:THR:HG22	1:F:152:VAL:HG22	1.99	0.44
1:A:7:ALA:HA	1:A:9:LEU:CD2	2.48	0.44
1:F:138:TYR:HB3	1:F:218:GLN:HE22	1.82	0.44
1:H:169:ASN:ND2	1:H:169:ASN:C	2.71	0.44
1:D:214:ALA:H	1:D:218:GLN:HE21	1.65	0.44
1:K:17:VAL:O	1:K:123:PHE:HA	2.18	0.44
1:L:33:HIS:HE1	1:M:26:ASP:OD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:O	1:A:119:HIS:HD2	2.00	0.44
1:B:46:HIS:HE1	4:B:1523:HOH:O	2.00	0.44
1:H:186:MET:CE	1:H:209:PHE:CD1	3.00	0.44
1:A:9:LEU:HB2	1:A:10:PRO:CD	2.48	0.44
1:F:154:PHE:HB2	1:G:152:VAL:HG23	2.00	0.44
1:I:144:THR:HG23	1:I:146:ARG:HH12	1.82	0.44
1:J:108:ARG:HH21	1:J:108:ARG:CG	2.29	0.44
1:J:175:SER:HB3	1:K:169:ASN:ND2	2.32	0.44
1:J:260:ALA:HB2	1:J:264:ARG:O	2.17	0.44
1:L:133:ILE:HG12	1:L:143:VAL:HG21	1.99	0.44
1:I:156:THR:CG2	1:I:184:MET:CE	2.96	0.44
1:J:51:ASN:HD22	1:J:53:ASP:HB2	1.83	0.44
1:B:156:THR:HG23	1:B:184:MET:HE3	1.99	0.44
1:B:168:ILE:HG23	1:B:173:ILE:HD13	1.98	0.44
1:D:59:ARG:O	1:D:60:PRO:C	2.56	0.44
1:E:129:ILE:CD1	3:E:2001:GOL:H11	2.46	0.44
1:G:184:MET:HG2	2:G:3511:SAH:O3'	2.18	0.44
1:M:25:GLY:O	1:M:51:ASN:HB2	2.18	0.44
1:D:26:ASP:HA	1:D:27:PRO:HD2	1.92	0.44
1:E:204:ASP:HA	1:E:224:THR:CB	2.48	0.44
1:F:208:ALA:HB3	1:F:244:VAL:HG13	1.99	0.44
1:L:168:ILE:HG21	1:L:173:ILE:HD13	1.98	0.44
1:L:196:LEU:O	1:L:201:ARG:HB2	2.18	0.44
1:D:209:PHE:CZ	1:D:232:VAL:CG2	3.01	0.43
1:L:201:ARG:CD	1:L:205:GLU:OE1	2.65	0.43
1:B:19:LEU:HD12	1:B:19:LEU:N	2.33	0.43
1:D:120:GLN:HB2	1:D:120:GLN:HE21	1.66	0.43
1:I:266:LEU:N	1:I:266:LEU:CD2	2.76	0.43
1:J:262:ASP:HB3	1:J:263:GLY:H	1.63	0.43
1:J:146:ARG:N	3:J:5011:GOL:H11	2.09	0.43
1:M:138:TYR:HB3	1:M:218:GLN:HE22	1.83	0.43
1:A:173:ILE:O	1:A:177:SER:HB2	2.18	0.43
1:E:78:GLN:HB2	1:E:108:ARG:NH1	2.33	0.43
1:I:156:THR:CG2	1:I:184:MET:HE1	2.48	0.43
1:B:211:CYS:SG	1:B:237:LEU:HG	2.58	0.43
1:D:23:GLY:HA2	1:D:129:ILE:O	2.18	0.43
1:J:144:THR:HA	1:J:149:ASN:HD21	1.82	0.43
1:M:78:GLN:HG3	1:M:108:ARG:NE	2.33	0.43
1:B:156:THR:CG2	1:B:184:MET:HE3	2.48	0.43
1:E:85:LEU:HD21	1:E:97:ARG:HD2	2.00	0.43
1:H:186:MET:CE	1:H:209:PHE:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:VAL:HG13	1:I:179:VAL:HB	2.01	0.43
1:A:189:ILE:O	1:A:193:THR:HG23	2.19	0.43
1:D:86:VAL:HB	1:D:121:VAL:HG21	2.00	0.43
1:E:173:ILE:HG22	1:E:180:ILE:HD12	2.00	0.43
1:M:149:ASN:ND2	1:M:149:ASN:N	2.65	0.43
1:G:30:LEU:HD21	1:G:54:CYS:HB2	1.99	0.43
1:F:28:GLY:CA	1:G:32:LEU:HB2	2.29	0.43
1:E:42:ASP:OD2	1:E:94:ARG:HG2	2.19	0.43
1:G:12:LEU:H	1:G:40:GLN:HE22	1.67	0.43
1:I:11:ALA:HA	1:I:40:GLN:HE22	1.84	0.43
1:J:106:PHE:HA	1:K:144:THR:HG21	2.01	0.43
1:E:148:VAL:HG13	1:E:247:GLU:HB2	2.00	0.43
1:A:142:PRO:HB3	1:B:104:PHE:CG	2.54	0.43
1:B:159:ASP:O	1:B:166:ASP:OD2	2.36	0.43
1:E:193:THR:CG2	1:E:225:LEU:O	2.67	0.43
1:I:43:VAL:HG23	1:I:63:VAL:HG22	2.01	0.43
1:J:111:GLU:OE1	3:K:5001:GOL:H31	2.19	0.43
1:E:23:GLY:HA2	1:E:129:ILE:O	2.19	0.42
1:A:108:ARG:NH2	1:A:108:ARG:CG	2.82	0.42
1:M:156:THR:HG22	1:M:184:MET:HE1	1.99	0.42
1:D:15:GLY:HA2	1:D:89:ALA:O	2.19	0.42
1:F:51:ASN:C	1:F:53:ASP:H	2.21	0.42
1:H:152:VAL:HG13	1:H:179:VAL:HB	2.00	0.42
1:I:160:SER:CB	1:I:166:ASP:OD2	2.67	0.42
1:K:258:ILE:C	1:K:260:ALA:N	2.71	0.42
1:D:77:LYS:O	1:D:80:ASP:HB2	2.19	0.42
1:E:27:PRO:HG3	1:E:53:ASP:HB2	2.01	0.42
1:G:53:ASP:O	1:G:56:LYS:HB2	2.19	0.42
1:M:153:THR:HG21	1:M:173:ILE:HG12	2.02	0.42
1:A:56:LYS:HD2	1:A:56:LYS:HA	1.66	0.42
1:D:34:ALA:O	1:D:38:LEU:HD22	2.20	0.42
1:E:84:ARG:HH21	1:E:84:ARG:HG2	1.71	0.42
1:L:86:VAL:HG12	1:L:116:LEU:HD12	2.01	0.42
1:G:258:ILE:C	1:G:260:ALA:H	2.23	0.42
1:H:222:GLU:OE1	1:H:252:ARG:HD3	2.20	0.42
1:M:145:HIS:H	1:M:149:ASN:ND2	2.16	0.42
1:M:156:THR:CG2	1:M:184:MET:CE	2.96	0.42
1:A:269:ASP:OD1	1:A:269:ASP:N	2.47	0.42
1:H:59:ARG:NH2	1:K:227:ARG:NH1	2.66	0.42
1:L:85:LEU:HD21	1:L:97:ARG:HD3	2.02	0.42
1:M:97:ARG:HG3	1:M:99:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:O	1:B:123:PHE:HA	2.19	0.42
1:L:117:VAL:HG11	1:M:267:ALA:CB	2.49	0.42
1:L:78:GLN:HA	1:L:78:GLN:HE21	1.84	0.42
1:M:193:THR:HG21	1:M:228:ALA:HB3	2.02	0.42
1:D:168:ILE:HG23	1:D:173:ILE:HD13	2.02	0.42
1:E:184:MET:HE2	2:E:2511:SAH:SD	2.60	0.42
1:E:36:ASN:O	1:E:40:GLN:HG2	2.20	0.42
1:G:69:LYS:HB2	1:G:69:LYS:HE2	1.84	0.42
1:H:22:ALA:HB2	1:H:98:LEU:HD22	2.00	0.42
1:H:47:ASP:O	1:H:49:LEU:HG	2.20	0.42
1:K:102:ASP:HB2	1:K:128:GLY:O	2.19	0.42
1:M:177:SER:O	1:M:201:ARG:NH1	2.52	0.42
1:H:33:HIS:HD2	4:H:4552:HOH:O	2.03	0.42
1:B:223:THR:HG23	1:B:224:THR:N	2.34	0.41
1:D:186:MET:CE	1:D:209:PHE:CE1	3.03	0.41
1:I:204:ASP:N	1:I:224:THR:HG23	2.35	0.41
3:K:5012:GOL:H31	4:K:5541:HOH:O	2.19	0.41
1:E:207:VAL:HG21	1:E:225:LEU:HD23	2.02	0.41
1:F:15:GLY:HA2	1:F:89:ALA:O	2.20	0.41
1:D:209:PHE:CZ	1:D:232:VAL:HG22	2.55	0.41
1:E:17:VAL:O	1:E:123:PHE:HA	2.21	0.41
1:G:224:THR:HG22	1:G:227:ARG:N	2.20	0.41
1:H:145:HIS:HA	3:H:4012:GOL:H32	2.01	0.41
1:L:17:VAL:HA	1:L:95:VAL:O	2.20	0.41
1:A:59:ARG:HB2	1:A:60:PRO:HD2	2.03	0.41
1:E:166:ASP:OD2	1:E:167:ARG:N	2.52	0.41
1:E:156:THR:HG23	1:E:184:MET:CE	2.50	0.41
1:H:169:ASN:HD22	1:H:170:TRP:N	2.19	0.41
1:H:70:ARG:HB3	1:H:71:GLY:H	1.58	0.41
1:H:106:PHE:N	1:I:144:THR:HG21	2.36	0.41
1:I:153:THR:HG21	1:I:173:ILE:HD13	2.02	0.41
1:J:172:GLY:O	1:J:175:SER:O	2.38	0.41
1:K:12:LEU:HD13	1:K:18:TRP:CD1	2.56	0.41
1:K:163:LEU:HD23	1:K:164:VAL:N	2.30	0.41
3:K:5012:GOL:H12	4:K:5530:HOH:O	2.20	0.41
1:M:97:ARG:NH1	1:M:112:GLU:OE2	2.53	0.41
1:A:208:ALA:HA	1:A:221:LEU:O	2.21	0.41
1:H:259:GLY:O	1:H:262:ASP:O	2.39	0.41
1:H:77:LYS:HE3	1:H:108:ARG:NH1	2.35	0.41
1:H:176:GLY:HA2	1:I:169:ASN:HB3	2.02	0.41
1:M:207:VAL:HG22	1:M:245:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:GLY:HA2	1:H:129:ILE:O	2.20	0.41
1:H:214:ALA:N	1:H:218:GLN:HE21	2.03	0.41
1:J:150:HIS:CD2	4:K:5528:HOH:O	2.73	0.41
1:L:23:GLY:HA2	1:L:129:ILE:O	2.19	0.41
1:L:165:PRO:HB3	1:L:167:ARG:CG	2.45	0.41
1:A:143:VAL:HG23	1:A:144:THR:HG23	2.03	0.41
1:A:30:LEU:HD11	1:A:54:CYS:CB	2.50	0.41
1:F:108:ARG:NH2	1:F:111:GLU:OE1	2.52	0.41
1:F:167:ARG:NH2	1:G:178:PRO:HG2	2.36	0.41
1:G:47:ASP:HB3	1:G:97:ARG:NH2	2.34	0.41
1:H:108:ARG:HG2	1:H:108:ARG:NH2	2.36	0.41
1:K:42:ASP:OD1	1:K:59:ARG:NH1	2.51	0.41
1:M:225:LEU:HD21	1:M:245:VAL:CG1	2.47	0.41
1:G:204:ASP:H	1:G:224:THR:HG23	1.86	0.41
1:J:18:TRP:CE2	1:J:124:ARG:HD2	2.56	0.41
1:L:146:ARG:HG2	1:L:147:GLU:N	2.36	0.41
1:L:206:PRO:HA	1:L:223:THR:O	2.21	0.41
1:L:59:ARG:HA	1:L:60:PRO:HD3	1.85	0.41
1:M:154:PHE:CD2	1:M:154:PHE:N	2.88	0.41
1:M:210:VAL:O	2:M:6511:SAH:H2	2.20	0.41
1:A:12:LEU:HD22	1:A:94:ARG:HB3	2.02	0.41
1:D:171:GLN:HB3	1:H:263:GLY:CA	2.51	0.41
1:D:205:GLU:HA	1:D:206:PRO:HD3	1.97	0.41
1:D:99:LYS:HE3	1:D:99:LYS:HB3	1.80	0.41
1:J:146:ARG:NH2	1:K:108:ARG:CD	2.82	0.41
1:F:18:TRP:CE2	1:F:124:ARG:HD2	2.56	0.41
1:J:171:GLN:HE22	1:J:199:GLY:HA2	1.85	0.41
1:K:82:SER:O	1:K:85:LEU:HB2	2.21	0.41
1:A:169:ASN:HD22	1:A:172:GLY:N	2.08	0.41
1:A:171:GLN:HE22	1:A:199:GLY:HA2	1.86	0.41
1:F:30:LEU:HB2	1:G:32:LEU:HD22	2.03	0.41
1:A:106:PHE:N	1:B:144:THR:HG21	2.36	0.40
1:B:205:GLU:HA	1:B:206:PRO:HD3	1.97	0.40
1:E:51:ASN:O	1:E:52:GLU:C	2.59	0.40
1:F:254:ALA:O	1:G:117:VAL:HG21	2.21	0.40
1:G:146:ARG:HG3	3:G:3003:GOL:C3	2.52	0.40
1:J:50:VAL:HG12	1:J:215:THR:HG21	2.02	0.40
1:K:101:GLY:HA3	2:K:5511:SAH:C	2.50	0.40
1:L:186:MET:HE3	1:L:209:PHE:HE1	1.86	0.40
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.69	0.40
1:E:209:PHE:CZ	1:E:232:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:LEU:HD23	1:E:237:LEU:HD22	2.03	0.40
1:E:65:GLU:OE2	1:E:84:ARG:NH2	2.54	0.40
1:F:266:LEU:HD23	1:G:117:VAL:HG22	2.03	0.40
1:G:73:LYS:N	1:G:74:PRO:HD2	2.36	0.40
1:H:26:ASP:C	1:H:27:PRO:O	2.56	0.40
1:K:26:ASP:HA	1:K:27:PRO:HD2	1.98	0.40
1:B:11:ALA:CA	1:B:40:GLN:HE22	2.33	0.40
1:D:145:HIS:HA	3:D:2011:GOL:H2	2.03	0.40
1:G:78:GLN:NE2	1:G:112:GLU:OE2	2.54	0.40
1:J:44:ILE:HG23	1:J:96:LEU:HG	2.03	0.40
1:M:154:PHE:HD2	1:M:154:PHE:N	2.19	0.40
1:E:187:LYS:HB3	3:E:2012:GOL:H11	2.04	0.40
1:G:85:LEU:HD21	1:G:97:ARG:HD2	2.03	0.40
1:K:99:LYS:NZ	1:K:112:GLU:OE1	2.53	0.40
1:K:132:GLY:HA3	1:K:183:TYR:OH	2.21	0.40
1:K:29:LEU:HG	1:K:129:ILE:HG13	2.03	0.40
1:M:15:GLY:HA2	1:M:89:ALA:O	2.20	0.40
1:M:190:GLY:HA2	1:M:229:GLU:HG3	2.03	0.40
1:B:262:ASP:O	1:B:263:GLY:C	2.58	0.40
1:H:108:ARG:HH21	1:H:108:ARG:HG2	1.87	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	250/280 (89%)	225 (90%)	18 (7%)	7 (3%)	5 11
1	B	260/280 (93%)	236 (91%)	20 (8%)	4 (2%)	10 26
1	D	242/280 (86%)	222 (92%)	13 (5%)	7 (3%)	4 10
1	E	261/280 (93%)	239 (92%)	18 (7%)	4 (2%)	10 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	246/280 (88%)	229 (93%)	12 (5%)	5 (2%)	7	19
1	G	254/280 (91%)	232 (91%)	16 (6%)	6 (2%)	6	15
1	H	255/280 (91%)	234 (92%)	15 (6%)	6 (2%)	6	15
1	I	258/280 (92%)	239 (93%)	14 (5%)	5 (2%)	8	20
1	J	246/280 (88%)	231 (94%)	12 (5%)	3 (1%)	13	32
1	K	255/280 (91%)	229 (90%)	18 (7%)	8 (3%)	4	9
1	L	239/280 (85%)	222 (93%)	14 (6%)	3 (1%)	12	30
1	M	246/280 (88%)	225 (92%)	12 (5%)	9 (4%)	3	7
All	All	3012/3360 (90%)	2763 (92%)	182 (6%)	67 (2%)	6	17

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	A	269	ASP
1	B	52	GLU
1	D	48	ALA
1	D	260	ALA
1	E	48	ALA
1	E	52	GLU
1	F	176	GLY
1	G	169	ASN
1	I	49	LEU
1	I	52	GLU
1	I	165	PRO
1	K	48	ALA
1	K	261	LEU
1	M	120	GLN
1	M	264	ARG
1	M	265	LYS
1	M	267	ALA
1	A	61	GLY
1	B	49	LEU
1	B	259	GLY
1	D	106	PHE
1	D	176	GLY
1	F	48	ALA
1	H	48	ALA
1	H	69	LYS

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Mol	Chain	Res	Type
1	H	73	LYS
1	I	68	GLY
1	J	48	ALA
1	K	9	LEU
1	L	52	GLU
1	A	60	PRO
1	F	106	PHE
1	G	48	ALA
1	G	264	ARG
1	H	174	ALA
1	L	8	GLY
1	L	10	PRO
1	M	261	LEU
1	M	263	GLY
1	M	266	LEU
1	A	118	GLU
1	D	60	PRO
1	E	12	LEU
1	G	68	GLY
1	G	73	LYS
1	I	78	GLN
1	K	260	ALA
1	M	48	ALA
1	F	256	ASP
1	G	259	GLY
1	H	106	PHE
1	J	262	ASP
1	K	259	GLY
1	M	179	VAL
1	D	261	LEU
1	H	13	GLU
1	J	78	GLN
1	K	71	GLY
1	K	108	ARG
1	D	25	GLY
1	F	76	PRO
1	A	15	GLY
1	B	73	LYS
1	K	25	GLY
1	A	76	PRO
1	E	72	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/207 (90%)	158 (84%)	29 (16%)	2	7
1	B	190/207 (92%)	151 (80%)	39 (20%)	1	3
1	D	181/207 (87%)	145 (80%)	36 (20%)	1	3
1	E	190/207 (92%)	149 (78%)	41 (22%)	1	3
1	F	184/207 (89%)	154 (84%)	30 (16%)	2	6
1	G	186/207 (90%)	152 (82%)	34 (18%)	1	4
1	H	187/207 (90%)	155 (83%)	32 (17%)	2	5
1	I	194/207 (94%)	148 (76%)	46 (24%)	1	2
1	J	182/207 (88%)	149 (82%)	33 (18%)	1	4
1	K	188/207 (91%)	152 (81%)	36 (19%)	1	4
1	L	178/207 (86%)	140 (79%)	38 (21%)	1	3
1	M	182/207 (88%)	144 (79%)	38 (21%)	1	3
All	All	2229/2484 (90%)	1797 (81%)	432 (19%)	1	3

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	LEU
1	A	38	LEU
1	A	39	ARG
1	A	53	ASP
1	A	56	LYS
1	A	57	LEU
1	A	65	GLU
1	A	69	LYS
1	A	75	SER
1	A	77	LYS
1	A	84	ARG
1	A	86	VAL
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	96	LEU
1	A	98	LEU
1	A	108	ARG
1	A	116	LEU
1	A	146	ARG
1	A	152	VAL
1	A	155	LEU
1	A	166	ASP
1	A	187	LYS
1	A	221	LEU
1	A	224	THR
1	A	237	LEU
1	A	265	LYS
1	A	266	LEU
1	A	269	ASP
1	B	6	PHE
1	B	13	GLU
1	B	29	LEU
1	B	30	LEU
1	B	32	LEU
1	B	38	LEU
1	B	39	ARG
1	B	51	ASN
1	B	53	ASP
1	B	56	LYS
1	B	59	ARG
1	B	63	VAL
1	B	69	LYS
1	B	70	ARG
1	B	75	SER
1	B	77	LYS
1	B	84	ARG
1	B	96	LEU
1	B	97	ARG
1	B	98	LEU
1	B	108	ARG
1	B	114	LEU
1	B	116	LEU
1	B	127	PRO
1	B	143	VAL
1	B	144	THR
1	B	146	ARG

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Mol	Chain	Res	Type
1	B	149	ASN
1	B	152	VAL
1	B	155	LEU
1	B	156	THR
1	B	171	GLN
1	B	173	ILE
1	B	175	SER
1	B	177	SER
1	B	193	THR
1	B	196	LEU
1	B	237	LEU
1	B	252	ARG
1	D	12	LEU
1	D	14	LYS
1	D	38	LEU
1	D	39	ARG
1	D	40	GLN
1	D	47	ASP
1	D	52	GLU
1	D	64	LEU
1	D	76	PRO
1	D	77	LYS
1	D	78	GLN
1	D	79	ARG
1	D	87	GLU
1	D	88	LEU
1	D	96	LEU
1	D	98	LEU
1	D	99	LYS
1	D	108	ARG
1	D	111	GLU
1	D	116	LEU
1	D	120	GLN
1	D	146	ARG
1	D	152	VAL
1	D	155	LEU
1	D	159	ASP
1	D	167	ARG
1	D	169	ASN
1	D	171	GLN
1	D	177	SER
1	D	187	LYS

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Mol	Chain	Res	Type
1	D	221	LEU
1	D	224	THR
1	D	237	LEU
1	D	252	ARG
1	D	258	ILE
1	D	262	ASP
1	E	5	LEU
1	E	14	LYS
1	E	29	LEU
1	E	30	LEU
1	E	32	LEU
1	E	38	LEU
1	E	39	ARG
1	E	49	LEU
1	E	50	VAL
1	E	51	ASN
1	E	53	ASP
1	E	59	ARG
1	E	64	LEU
1	E	77	LYS
1	E	84	ARG
1	E	94	ARG
1	E	96	LEU
1	E	97	ARG
1	E	98	LEU
1	E	108	ARG
1	E	114	LEU
1	E	116	LEU
1	E	143	VAL
1	E	144	THR
1	E	146	ARG
1	E	147	GLU
1	E	149	ASN
1	E	152	VAL
1	E	155	LEU
1	E	156	THR
1	E	180	ILE
1	E	187	LYS
1	E	193	THR
1	E	196	LEU
1	E	204	ASP
1	E	221	LEU

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Mol	Chain	Res	Type
1	E	224	THR
1	E	237	LEU
1	E	252	ARG
1	E	261	LEU
1	E	269	ASP
1	F	14	LYS
1	F	19	LEU
1	F	38	LEU
1	F	39	ARG
1	F	43	VAL
1	F	53	ASP
1	F	64	LEU
1	F	77	LYS
1	F	88	LEU
1	F	98	LEU
1	F	99	LYS
1	F	108	ARG
1	F	114	LEU
1	F	116	LEU
1	F	120	GLN
1	F	152	VAL
1	F	155	LEU
1	F	156	THR
1	F	158	HIS
1	F	167	ARG
1	F	169	ASN
1	F	173	ILE
1	F	177	SER
1	F	187	LYS
1	F	221	LEU
1	F	224	THR
1	F	232	VAL
1	F	237	LEU
1	F	252	ARG
1	F	266	LEU
1	G	12	LEU
1	G	14	LYS
1	G	29	LEU
1	G	30	LEU
1	G	32	LEU
1	G	38	LEU
1	G	51	ASN

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Mol	Chain	Res	Type
1	G	53	ASP
1	G	57	LEU
1	G	59	ARG
1	G	63	VAL
1	G	66	PHE
1	G	70	ARG
1	G	77	LYS
1	G	79	ARG
1	G	84	ARG
1	G	96	LEU
1	G	97	ARG
1	G	98	LEU
1	G	114	LEU
1	G	116	LEU
1	G	118	GLU
1	G	143	VAL
1	G	144	THR
1	G	149	ASN
1	G	152	VAL
1	G	155	LEU
1	G	159	ASP
1	G	167	ARG
1	G	187	LYS
1	G	221	LEU
1	G	224	THR
1	G	262	ASP
1	G	264	ARG
1	H	6	PHE
1	H	12	LEU
1	H	13	GLU
1	H	19	LEU
1	H	38	LEU
1	H	39	ARG
1	H	43	VAL
1	H	51	ASN
1	H	53	ASP
1	H	64	LEU
1	H	77	LYS
1	H	88	LEU
1	H	90	ARG
1	H	96	LEU
1	H	98	LEU

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Mol	Chain	Res	Type
1	H	99	LYS
1	H	108	ARG
1	H	114	LEU
1	H	116	LEU
1	H	146	ARG
1	H	147	GLU
1	H	152	VAL
1	H	155	LEU
1	H	167	ARG
1	H	169	ASN
1	H	221	LEU
1	H	223	THR
1	H	224	THR
1	H	227	ARG
1	H	252	ARG
1	H	261	LEU
1	H	266	LEU
1	I	4	ASP
1	I	5	LEU
1	I	6	PHE
1	I	12	LEU
1	I	19	LEU
1	I	29	LEU
1	I	30	LEU
1	I	32	LEU
1	I	38	LEU
1	I	47	ASP
1	I	51	ASN
1	I	52	GLU
1	I	53	ASP
1	I	56	LYS
1	I	69	LYS
1	I	70	ARG
1	I	77	LYS
1	I	84	ARG
1	I	87	GLU
1	I	96	LEU
1	I	97	ARG
1	I	98	LEU
1	I	99	LYS
1	I	108	ARG
1	I	114	LEU

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Mol	Chain	Res	Type
1	I	116	LEU
1	I	120[A]	GLN
1	I	120[B]	GLN
1	I	144	THR
1	I	146	ARG
1	I	147	GLU
1	I	149	ASN
1	I	152	VAL
1	I	155	LEU
1	I	156	THR
1	I	166	ASP
1	I	187	LYS
1	I	193	THR
1	I	196	LEU
1	I	224	THR
1	I	227	ARG
1	I	237	LEU
1	I	252	ARG
1	I	258	ILE
1	I	265	LYS
1	I	266	LEU
1	J	14	LYS
1	J	36	ASN
1	J	38	LEU
1	J	39	ARG
1	J	43	VAL
1	J	51	ASN
1	J	53	ASP
1	J	56	LYS
1	J	64	LEU
1	J	77	LYS
1	J	78	GLN
1	J	79	ARG
1	J	84	ARG
1	J	86	VAL
1	J	88	LEU
1	J	90	ARG
1	J	96	LEU
1	J	98	LEU
1	J	99	LYS
1	J	108	ARG
1	J	114	LEU

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Mol	Chain	Res	Type
1	J	116	LEU
1	J	152	VAL
1	J	155	LEU
1	J	167	ARG
1	J	169	ASN
1	J	186	MET
1	J	221	LEU
1	J	224	THR
1	J	261	LEU
1	J	262	ASP
1	J	264	ARG
1	J	266	LEU
1	K	12	LEU
1	K	13	GLU
1	K	29	LEU
1	K	30	LEU
1	K	31	THR
1	K	32	LEU
1	K	38	LEU
1	K	51	ASN
1	K	53	ASP
1	K	59	ARG
1	K	66	PHE
1	K	75	SER
1	K	77	LYS
1	K	84	ARG
1	K	97	ARG
1	K	98	LEU
1	K	108	ARG
1	K	116	LEU
1	K	118	GLU
1	K	120	GLN
1	K	143	VAL
1	K	144	THR
1	K	147	GLU
1	K	149	ASN
1	K	152	VAL
1	K	155	LEU
1	K	163	LEU
1	K	173	ILE
1	K	177	SER
1	K	193	THR

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Mol	Chain	Res	Type
1	K	196	LEU
1	K	224	THR
1	K	231	ASP
1	K	232	VAL
1	K	237	LEU
1	K	258	ILE
1	L	9	LEU
1	L	12	LEU
1	L	14	LYS
1	L	19	LEU
1	L	31	THR
1	L	36	ASN
1	L	47	ASP
1	L	52	GLU
1	L	57	LEU
1	L	59	ARG
1	L	63	VAL
1	L	77	LYS
1	L	78	GLN
1	L	79	ARG
1	L	86	VAL
1	L	88	LEU
1	L	90	ARG
1	L	108	ARG
1	L	114	LEU
1	L	116	LEU
1	L	118	GLU
1	L	143	VAL
1	L	146	ARG
1	L	147	GLU
1	L	152	VAL
1	L	155	LEU
1	L	156	THR
1	L	167	ARG
1	L	169	ASN
1	L	173	ILE
1	L	186	MET
1	L	217	GLN
1	L	221	LEU
1	L	223	THR
1	L	224	THR
1	L	231	ASP

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Mol	Chain	Res	Type
1	L	237	LEU
1	L	252	ARG
1	M	10	PRO
1	M	14	LYS
1	M	19	LEU
1	M	29	LEU
1	M	32	LEU
1	M	50	VAL
1	M	51	ASN
1	M	56	LYS
1	M	63	VAL
1	M	66	PHE
1	M	69	LYS
1	M	78	GLN
1	M	81	ILE
1	M	87	GLU
1	M	95	VAL
1	M	96	LEU
1	M	97	ARG
1	M	98	LEU
1	M	108	ARG
1	M	114	LEU
1	M	115	THR
1	M	118	GLU
1	M	120	GLN
1	M	143	VAL
1	M	144	THR
1	M	146	ARG
1	M	149	ASN
1	M	152	VAL
1	M	155	LEU
1	M	156	THR
1	M	158	HIS
1	M	159	ASP
1	M	167	ARG
1	M	177	SER
1	M	195	ASN
1	M	225	LEU
1	M	252	ARG
1	M	262	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	36	ASN
1	A	40	GLN
1	A	51	ASN
1	A	119	HIS
1	A	120	GLN
1	A	169	ASN
1	A	171	GLN
1	A	188	HIS
1	A	195	ASN
1	A	212	ASN
1	A	218	GLN
1	B	40	GLN
1	B	46	HIS
1	B	78	GLN
1	B	119	HIS
1	B	149	ASN
1	B	195	ASN
1	B	218	GLN
1	D	33	HIS
1	D	40	GLN
1	D	46	HIS
1	D	93	ASN
1	D	119	HIS
1	D	120	GLN
1	D	169	ASN
1	D	171	GLN
1	D	188	HIS
1	D	195	ASN
1	D	212	ASN
1	D	218	GLN
1	E	149	ASN
1	E	171	GLN
1	E	188	HIS
1	E	195	ASN
1	E	218	GLN
1	F	33	HIS
1	F	40	GLN
1	F	46	HIS
1	F	51	ASN
1	F	93	ASN
1	F	169	ASN
1	F	171	GLN

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Mol	Chain	Res	Type
1	F	195	ASN
1	F	212	ASN
1	F	218	GLN
1	G	40	GLN
1	G	51	ASN
1	G	145	HIS
1	G	149	ASN
1	G	171	GLN
1	G	188	HIS
1	G	195	ASN
1	G	218	GLN
1	H	33	HIS
1	H	40	GLN
1	H	46	HIS
1	H	51	ASN
1	H	78	GLN
1	H	93	ASN
1	H	119	HIS
1	H	169	ASN
1	H	195	ASN
1	H	212	ASN
1	H	218	GLN
1	I	40	GLN
1	I	46	HIS
1	I	119	HIS
1	I	149	ASN
1	I	169	ASN
1	I	171	GLN
1	I	218	GLN
1	J	33	HIS
1	J	36	ASN
1	J	40	GLN
1	J	51	ASN
1	J	93	ASN
1	J	169	ASN
1	J	171	GLN
1	J	195	ASN
1	J	218	GLN
1	K	40	GLN
1	K	51	ASN
1	K	78	GLN
1	K	149	ASN

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Mol	Chain	Res	Type
1	K	218	GLN
1	L	40	GLN
1	L	145	HIS
1	L	158	HIS
1	L	171	GLN
1	L	212	ASN
1	L	218	GLN
1	M	51	ASN
1	M	78	GLN
1	M	119	HIS
1	M	149	ASN
1	M	169	ASN
1	M	195	ASN
1	M	218	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

38 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	K	5511	-	21,28,28	1.20	2 (9%)	20,40,40	1.51	2 (10%)
3	GOL	D	2011	-	5,5,5	0.58	0	5,5,5	0.64	0
3	GOL	A	1001	-	5,5,5	0.71	0	5,5,5	1.03	0
3	GOL	B	1011	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	F	3001	-	5,5,5	0.36	0	5,5,5	0.48	0
3	GOL	L	6002	-	5,5,5	0.46	0	5,5,5	0.15	0
3	GOL	I	4011	-	5,5,5	0.39	0	5,5,5	0.40	0
3	GOL	E	2003	-	5,5,5	0.48	0	5,5,5	0.45	0
3	GOL	L	6001	-	5,5,5	0.47	0	5,5,5	0.22	0
2	SAH	M	6511	-	21,28,28	1.31	2 (9%)	20,40,40	1.60	2 (10%)
2	SAH	D	2501	-	21,28,28	1.08	1 (4%)	20,40,40	1.62	2 (10%)
3	GOL	G	3012	-	5,5,5	0.39	0	5,5,5	0.26	0
3	GOL	J	5003	-	5,5,5	0.43	0	5,5,5	0.36	0
3	GOL	A	1002	-	5,5,5	0.39	0	5,5,5	0.34	0
2	SAH	B	1511	-	21,28,28	1.26	2 (9%)	20,40,40	1.65	2 (10%)
3	GOL	E	2001	-	5,5,5	0.66	0	5,5,5	0.62	0
3	GOL	G	3002	-	5,5,5	0.52	0	5,5,5	0.73	0
3	GOL	K	5012	-	5,5,5	0.46	0	5,5,5	0.50	0
2	SAH	E	2511	-	21,28,28	1.28	2 (9%)	20,40,40	1.55	2 (10%)
2	SAH	G	3511	-	21,28,28	1.20	2 (9%)	20,40,40	1.72	2 (10%)
2	SAH	A	1501	-	21,28,28	1.16	2 (9%)	20,40,40	1.56	2 (10%)
3	GOL	A	1012	-	5,5,5	0.41	0	5,5,5	0.68	0
3	GOL	D	2002	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	H	4003	-	5,5,5	0.52	0	5,5,5	0.50	0
3	GOL	F	3011	-	5,5,5	0.39	0	5,5,5	0.38	0
3	GOL	I	4002	-	5,5,5	0.75	0	5,5,5	1.19	0
2	SAH	I	4511	-	21,28,28	1.03	2 (9%)	20,40,40	1.67	2 (10%)
3	GOL	H	4012	-	5,5,5	0.41	0	5,5,5	0.63	0
3	GOL	J	5011	-	5,5,5	0.41	0	5,5,5	0.45	0
3	GOL	E	2012	-	5,5,5	0.44	0	5,5,5	0.38	0
2	SAH	J	5501	-	21,28,28	1.29	3 (14%)	20,40,40	1.74	3 (15%)
2	SAH	H	4501	-	21,28,28	1.22	2 (9%)	20,40,40	1.73	4 (20%)
3	GOL	M	6011	-	5,5,5	0.33	0	5,5,5	0.47	0
2	SAH	L	6501	-	21,28,28	1.20	2 (9%)	20,40,40	1.65	2 (10%)
2	SAH	F	3501	-	21,28,28	1.17	2 (9%)	20,40,40	1.68	4 (20%)
3	GOL	K	5001	-	5,5,5	0.52	0	5,5,5	0.71	0
3	GOL	G	3003	-	5,5,5	0.50	0	5,5,5	0.53	0
3	GOL	J	5002	-	5,5,5	0.56	0	5,5,5	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	K	5511	-	-	2/7/31/31	0/3/3/3
3	GOL	D	2011	-	-	2/4/4/4	-
3	GOL	A	1001	-	-	2/4/4/4	-
3	GOL	B	1011	-	-	4/4/4/4	-
3	GOL	F	3001	-	-	2/4/4/4	-
3	GOL	L	6002	-	-	2/4/4/4	-
3	GOL	I	4011	-	-	4/4/4/4	-
3	GOL	E	2003	-	-	4/4/4/4	-
3	GOL	L	6001	-	-	2/4/4/4	-
2	SAH	M	6511	-	-	0/7/31/31	0/3/3/3
2	SAH	D	2501	-	-	1/7/31/31	0/3/3/3
3	GOL	G	3012	-	-	1/4/4/4	-
3	GOL	J	5003	-	-	2/4/4/4	-
3	GOL	A	1002	-	-	3/4/4/4	-
2	SAH	B	1511	-	-	0/7/31/31	0/3/3/3
3	GOL	E	2001	-	-	2/4/4/4	-
3	GOL	G	3002	-	-	4/4/4/4	-
3	GOL	K	5012	-	-	2/4/4/4	-
2	SAH	E	2511	-	-	2/7/31/31	0/3/3/3
2	SAH	G	3511	-	-	2/7/31/31	0/3/3/3
2	SAH	A	1501	-	-	2/7/31/31	0/3/3/3
3	GOL	A	1012	-	-	4/4/4/4	-
3	GOL	D	2002	-	-	2/4/4/4	-
3	GOL	H	4003	-	-	3/4/4/4	-
3	GOL	F	3011	-	-	2/4/4/4	-
3	GOL	I	4002	-	-	2/4/4/4	-
2	SAH	I	4511	-	-	2/7/31/31	0/3/3/3
3	GOL	H	4012	-	-	4/4/4/4	-
3	GOL	J	5011	-	-	2/4/4/4	-
3	GOL	E	2012	-	-	2/4/4/4	-
2	SAH	J	5501	-	-	2/7/31/31	0/3/3/3
2	SAH	H	4501	-	-	2/7/31/31	0/3/3/3
3	GOL	M	6011	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	L	6501	-	-	0/7/31/31	0/3/3/3
2	SAH	F	3501	-	-	2/7/31/31	0/3/3/3
3	GOL	K	5001	-	-	2/4/4/4	-
3	GOL	G	3003	-	-	4/4/4/4	-
3	GOL	J	5002	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	6511	SAH	C2-N3	4.24	1.38	1.32
2	B	1511	SAH	C2-N3	4.24	1.38	1.32
2	L	6501	SAH	C2-N3	4.00	1.38	1.32
2	E	2511	SAH	C2-N3	3.94	1.38	1.32
2	H	4501	SAH	C2-N3	3.79	1.38	1.32
2	J	5501	SAH	C2-N3	3.67	1.38	1.32
2	K	5511	SAH	C2-N3	3.59	1.37	1.32
2	F	3501	SAH	C2-N3	3.45	1.37	1.32
2	G	3511	SAH	C2-N3	3.43	1.37	1.32
2	A	1501	SAH	C2-N3	3.37	1.37	1.32
2	D	2501	SAH	C2-N3	3.27	1.37	1.32
2	I	4511	SAH	C2-N3	3.12	1.37	1.32
2	M	6511	SAH	C2-N1	2.86	1.39	1.33
2	J	5501	SAH	C2-N1	2.54	1.38	1.33
2	B	1511	SAH	C2-N1	2.38	1.38	1.33
2	L	6501	SAH	C2-N1	2.33	1.38	1.33
2	A	1501	SAH	C2-N1	2.31	1.38	1.33
2	E	2511	SAH	C2-N1	2.30	1.38	1.33
2	H	4501	SAH	C2-N1	2.30	1.38	1.33
2	K	5511	SAH	C2-N1	2.22	1.38	1.33
2	G	3511	SAH	C2-N1	2.18	1.38	1.33
2	I	4511	SAH	C2-N1	2.17	1.38	1.33
2	J	5501	SAH	O4'-C4'	-2.01	1.40	1.45
2	F	3501	SAH	C2-N1	2.00	1.37	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	5501	SAH	N3-C2-N1	-6.19	119.01	128.68
2	G	3511	SAH	N3-C2-N1	-6.16	119.05	128.68
2	M	6511	SAH	N3-C2-N1	-5.88	119.49	128.68
2	L	6501	SAH	N3-C2-N1	-5.75	119.69	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4511	SAH	N3-C2-N1	-5.72	119.74	128.68
2	F	3501	SAH	N3-C2-N1	-5.54	120.02	128.68
2	K	5511	SAH	N3-C2-N1	-5.46	120.15	128.68
2	H	4501	SAH	N3-C2-N1	-5.38	120.27	128.68
2	D	2501	SAH	N3-C2-N1	-5.36	120.31	128.68
2	A	1501	SAH	N3-C2-N1	-5.26	120.46	128.68
2	E	2511	SAH	N3-C2-N1	-5.25	120.47	128.68
2	B	1511	SAH	N3-C2-N1	-4.87	121.07	128.68
2	B	1511	SAH	C5'-SD-CG	-3.89	90.59	102.27
2	G	3511	SAH	C5'-SD-CG	-3.59	91.50	102.27
2	L	6501	SAH	C5'-SD-CG	-3.48	91.83	102.27
2	H	4501	SAH	CB-CG-SD	3.35	120.82	113.31
2	D	2501	SAH	C5'-SD-CG	-3.24	92.54	102.27
2	F	3501	SAH	C5'-SD-CG	-2.76	93.97	102.27
2	M	6511	SAH	C5'-SD-CG	-2.69	94.21	102.27
2	A	1501	SAH	C5'-SD-CG	-2.67	94.27	102.27
2	J	5501	SAH	C5'-SD-CG	-2.42	95.01	102.27
2	K	5511	SAH	C5'-SD-CG	-2.41	95.04	102.27
2	H	4501	SAH	C4-C5-N7	-2.37	106.93	109.40
2	E	2511	SAH	CB-CG-SD	2.30	118.45	113.31
2	F	3501	SAH	CB-CG-SD	2.14	118.11	113.31
2	H	4501	SAH	C5'-SD-CG	-2.12	95.91	102.27
2	F	3501	SAH	C4-C5-N7	-2.12	107.19	109.40
2	I	4511	SAH	C4-C5-N7	-2.09	107.22	109.40
2	J	5501	SAH	CB-CG-SD	2.05	117.89	113.31

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	5511	SAH	O4'-C4'-C5'-SD
2	K	5511	SAH	C3'-C4'-C5'-SD
3	D	2011	GOL	C1-C2-C3-O3
3	D	2011	GOL	O2-C2-C3-O3
3	B	1011	GOL	O1-C1-C2-C3
3	B	1011	GOL	C1-C2-C3-O3
3	B	1011	GOL	O2-C2-C3-O3
3	F	3001	GOL	O1-C1-C2-O2
3	I	4011	GOL	O1-C1-C2-C3
3	I	4011	GOL	C1-C2-C3-O3
3	E	2003	GOL	O1-C1-C2-C3
3	E	2003	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	L	6001	GOL	O1-C1-C2-C3
3	J	5003	GOL	O1-C1-C2-C3
3	A	1002	GOL	O1-C1-C2-O2
3	A	1002	GOL	O1-C1-C2-C3
3	E	2001	GOL	O1-C1-C2-C3
3	G	3002	GOL	O1-C1-C2-O2
3	G	3002	GOL	O1-C1-C2-C3
3	G	3002	GOL	C1-C2-C3-O3
3	K	5012	GOL	C1-C2-C3-O3
2	E	2511	SAH	O4'-C4'-C5'-SD
2	E	2511	SAH	C3'-C4'-C5'-SD
2	G	3511	SAH	O4'-C4'-C5'-SD
2	G	3511	SAH	C3'-C4'-C5'-SD
3	A	1012	GOL	C1-C2-C3-O3
3	A	1012	GOL	O2-C2-C3-O3
3	D	2002	GOL	C1-C2-C3-O3
3	H	4003	GOL	C1-C2-C3-O3
3	F	3011	GOL	C1-C2-C3-O3
3	F	3011	GOL	O2-C2-C3-O3
3	I	4002	GOL	C1-C2-C3-O3
3	H	4012	GOL	O1-C1-C2-C3
3	H	4012	GOL	C1-C2-C3-O3
3	J	5002	GOL	C1-C2-C3-O3
3	J	5002	GOL	O2-C2-C3-O3
3	M	6011	GOL	O1-C1-C2-C3
3	K	5001	GOL	C1-C2-C3-O3
3	G	3003	GOL	O1-C1-C2-C3
3	G	3003	GOL	C1-C2-C3-O3
3	E	2003	GOL	O2-C2-C3-O3
3	A	1001	GOL	C1-C2-C3-O3
3	F	3001	GOL	O1-C1-C2-C3
3	L	6002	GOL	C1-C2-C3-O3
3	J	5011	GOL	C1-C2-C3-O3
3	L	6002	GOL	O2-C2-C3-O3
3	I	4011	GOL	O1-C1-C2-O2
3	I	4011	GOL	O2-C2-C3-O3
3	L	6001	GOL	O1-C1-C2-O2
3	E	2001	GOL	O1-C1-C2-O2
3	D	2002	GOL	O2-C2-C3-O3
3	H	4003	GOL	O2-C2-C3-O3
3	I	4002	GOL	O2-C2-C3-O3
3	H	4012	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	M	6011	GOL	O1-C1-C2-O2
3	K	5001	GOL	O2-C2-C3-O3
3	G	3003	GOL	O2-C2-C3-O3
3	G	3002	GOL	O2-C2-C3-O3
3	K	5012	GOL	O2-C2-C3-O3
3	H	4012	GOL	O1-C1-C2-O2
3	G	3003	GOL	O1-C1-C2-O2
3	B	1011	GOL	O1-C1-C2-O2
3	J	5011	GOL	O2-C2-C3-O3
3	E	2003	GOL	O1-C1-C2-O2
3	J	5003	GOL	O1-C1-C2-O2
3	A	1012	GOL	O1-C1-C2-O2
3	E	2012	GOL	O2-C2-C3-O3
2	D	2501	SAH	C3'-C4'-C5'-SD
2	A	1501	SAH	C3'-C4'-C5'-SD
2	I	4511	SAH	C3'-C4'-C5'-SD
2	J	5501	SAH	C3'-C4'-C5'-SD
2	H	4501	SAH	C3'-C4'-C5'-SD
2	F	3501	SAH	C3'-C4'-C5'-SD
2	A	1501	SAH	O4'-C4'-C5'-SD
2	I	4511	SAH	O4'-C4'-C5'-SD
2	J	5501	SAH	O4'-C4'-C5'-SD
2	H	4501	SAH	O4'-C4'-C5'-SD
2	F	3501	SAH	O4'-C4'-C5'-SD
3	A	1001	GOL	O1-C1-C2-O2
3	G	3012	GOL	C1-C2-C3-O3
3	A	1012	GOL	O1-C1-C2-C3
3	H	4003	GOL	O1-C1-C2-C3
3	E	2012	GOL	C1-C2-C3-O3
3	A	1002	GOL	O2-C2-C3-O3

There are no ring outliers.

21 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	5511	SAH	1	0
3	D	2011	GOL	7	0
3	A	1001	GOL	3	0
3	L	6002	GOL	1	0
3	E	2003	GOL	3	0
2	M	6511	SAH	2	0
3	E	2001	GOL	5	0

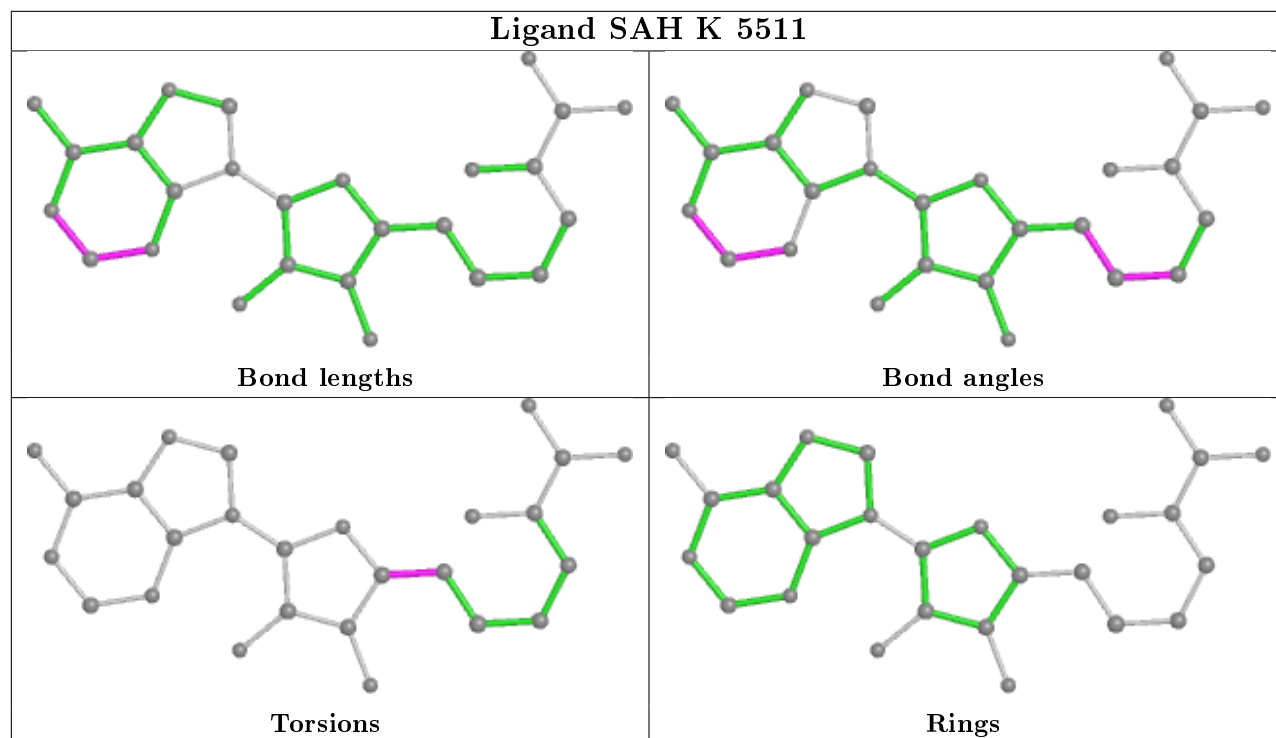
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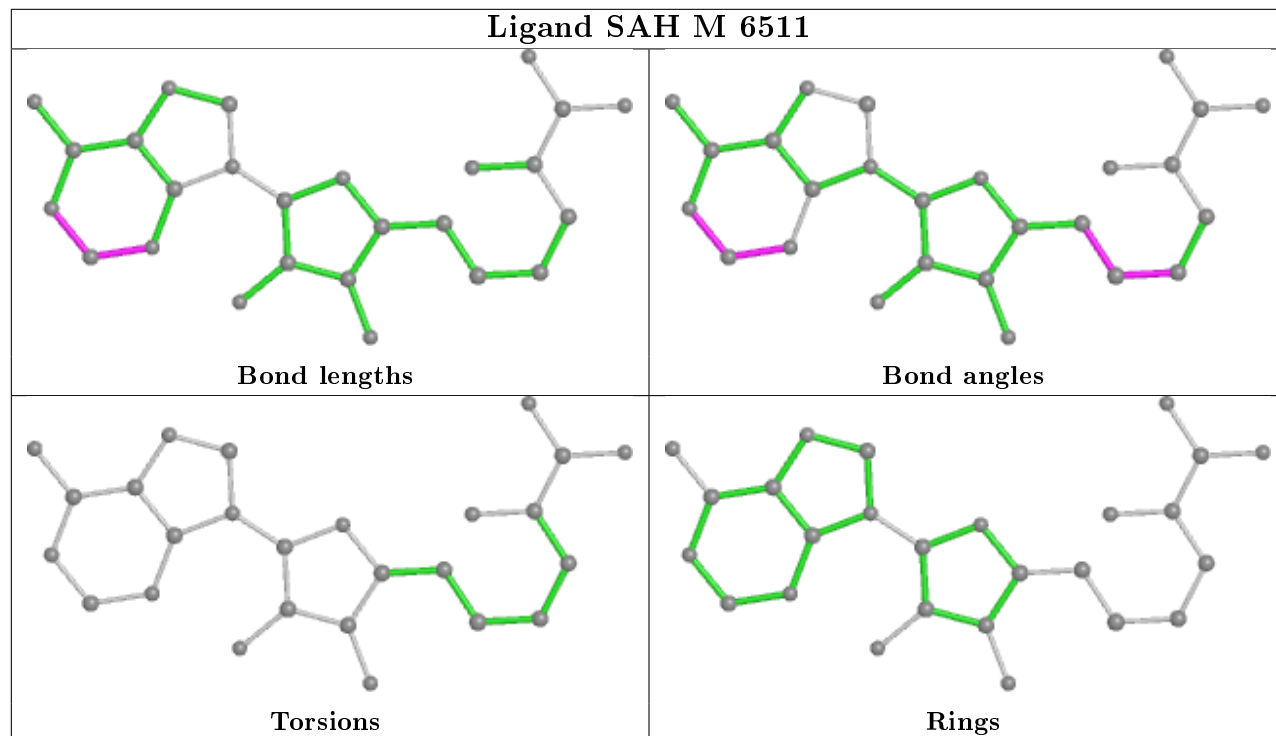
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3002	GOL	3	0
3	K	5012	GOL	4	0
2	E	2511	SAH	1	0
2	G	3511	SAH	2	0
3	A	1012	GOL	2	0
3	F	3011	GOL	2	0
3	I	4002	GOL	4	0
3	H	4012	GOL	6	0
3	J	5011	GOL	3	0
3	E	2012	GOL	1	0
2	J	5501	SAH	2	0
3	K	5001	GOL	5	0
3	G	3003	GOL	4	0
3	J	5002	GOL	2	0

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.

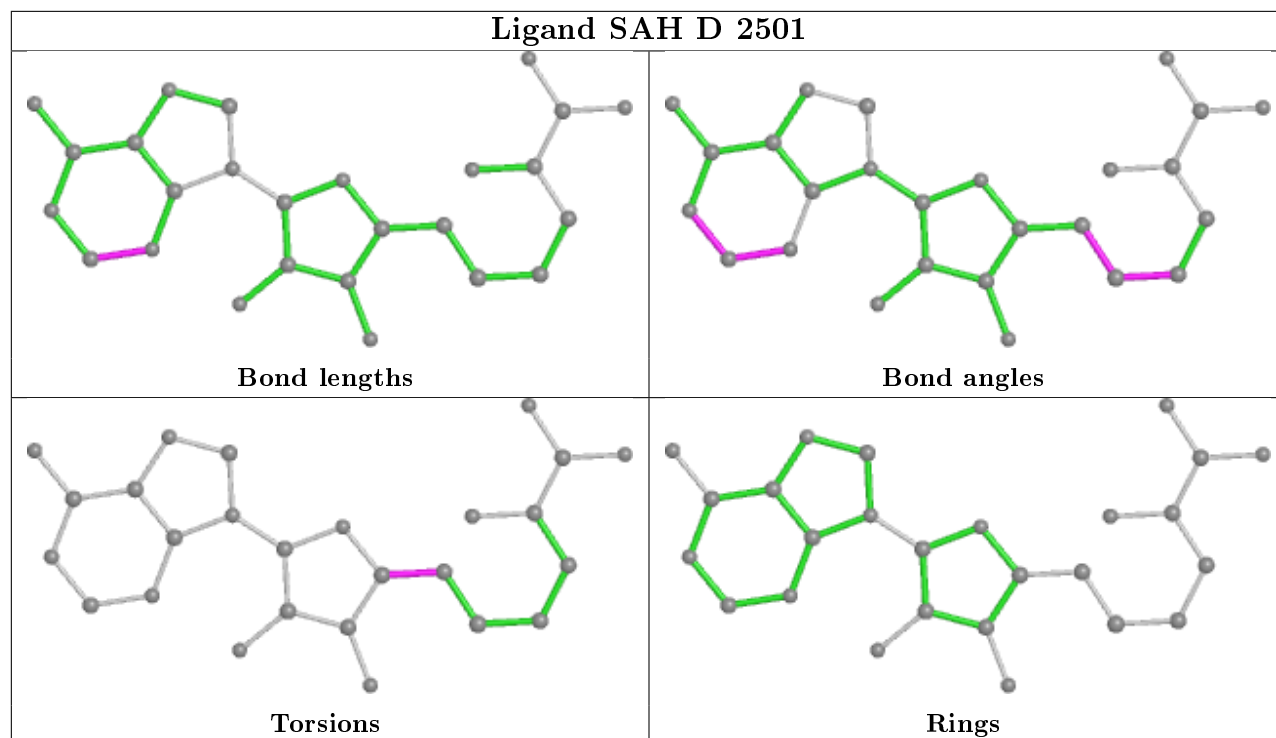
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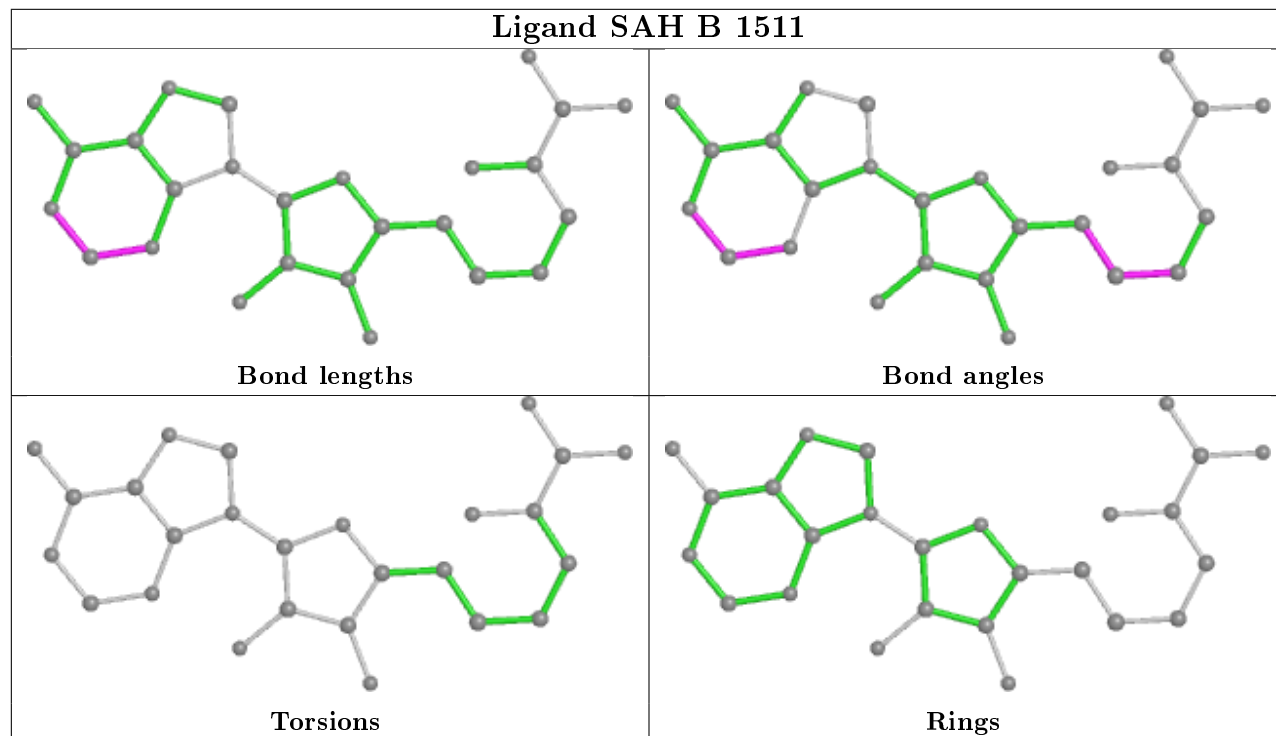
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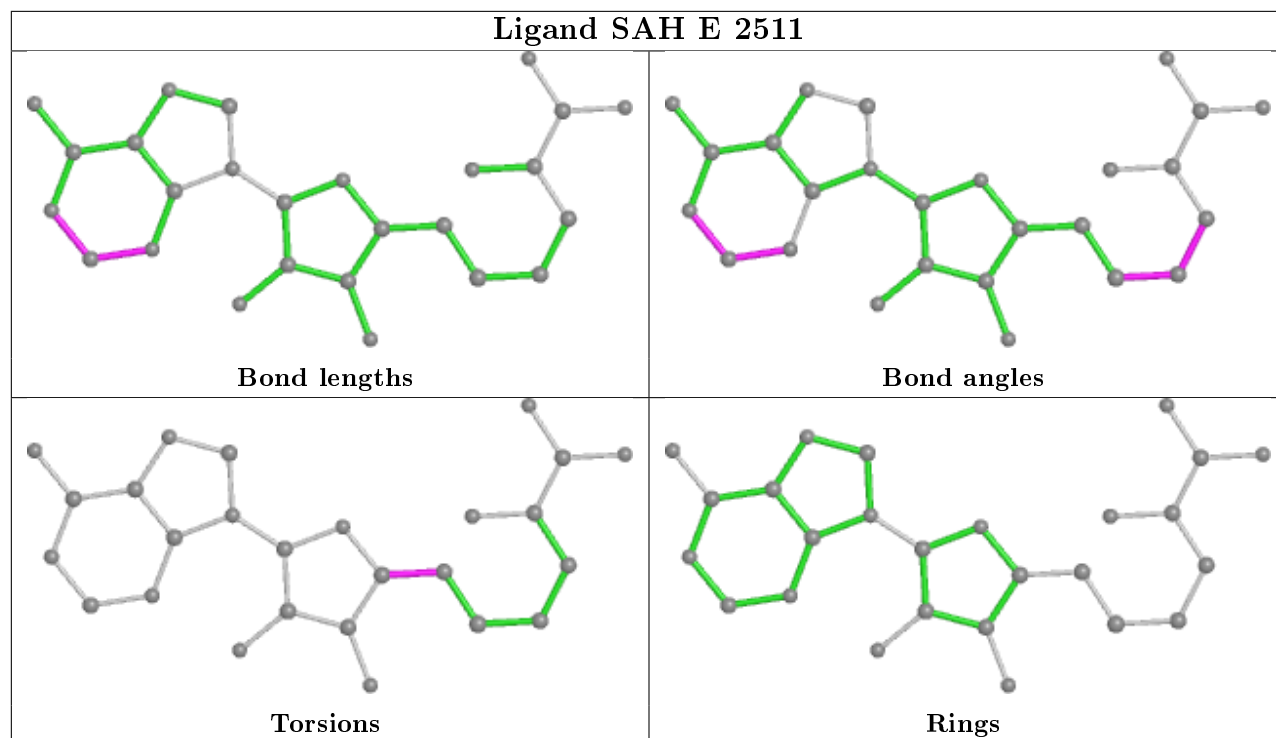
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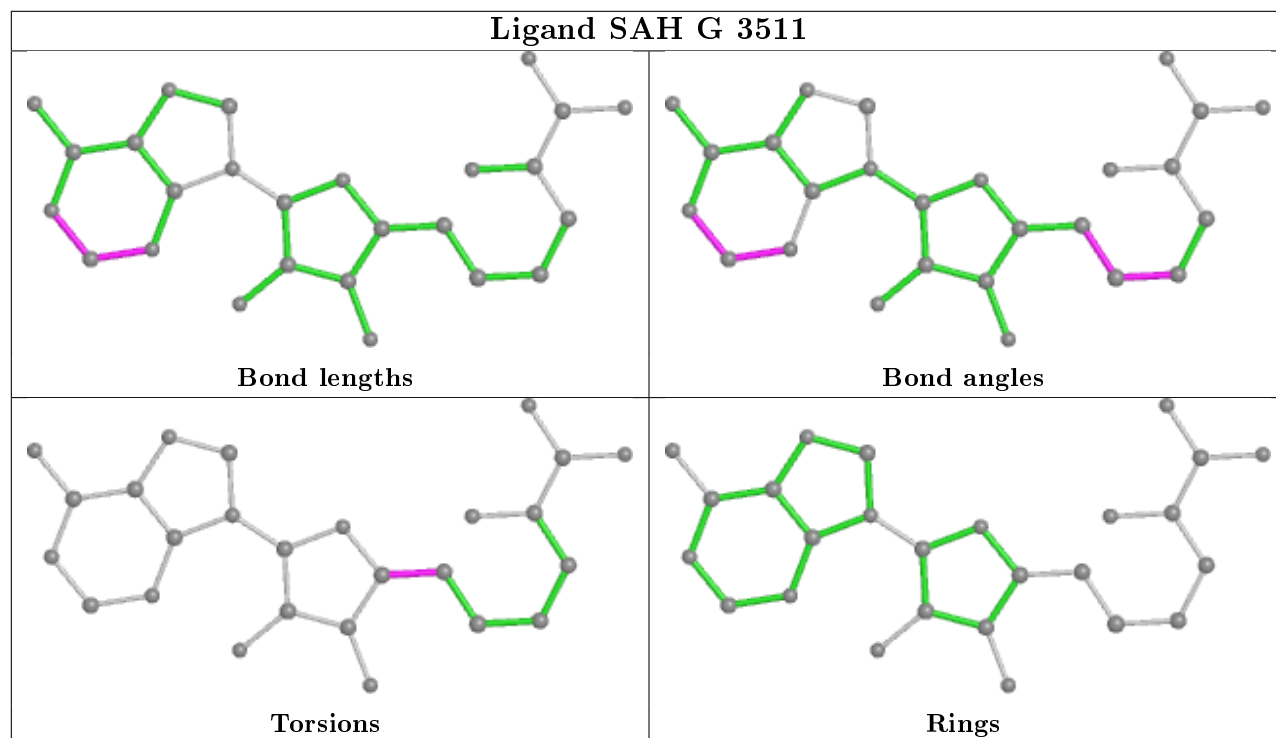
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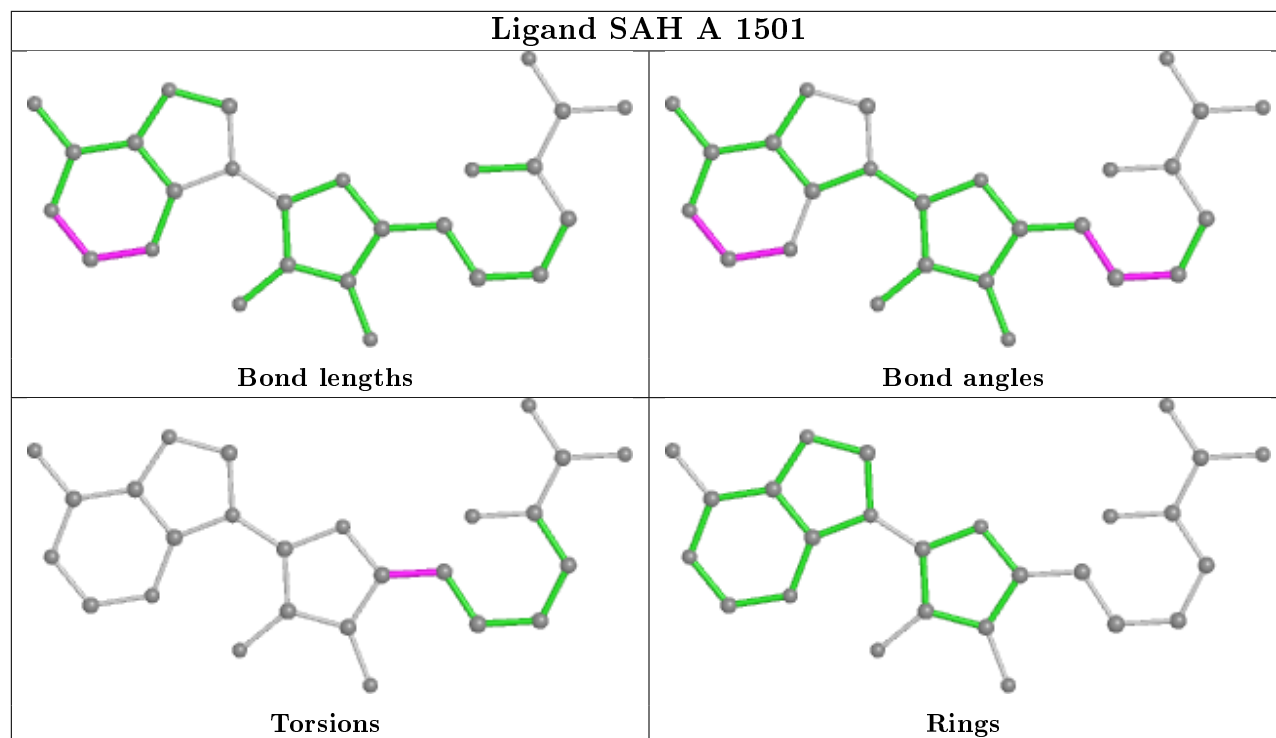
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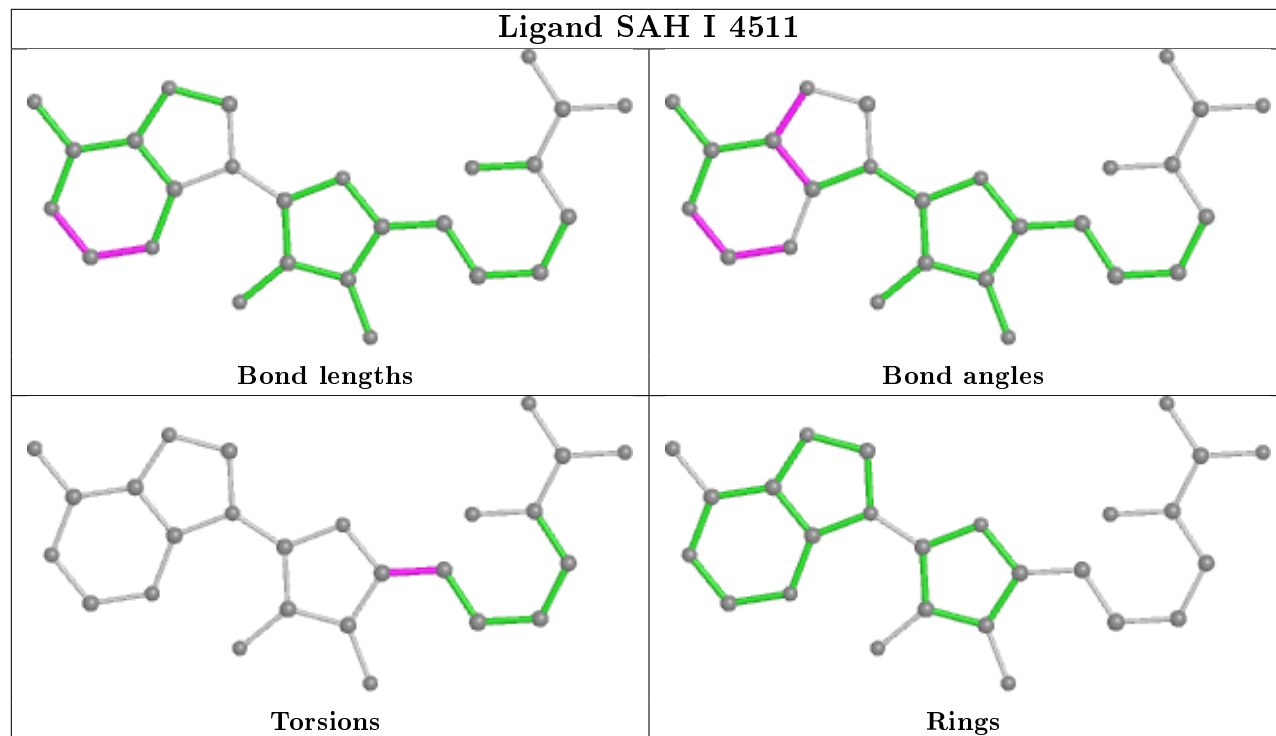
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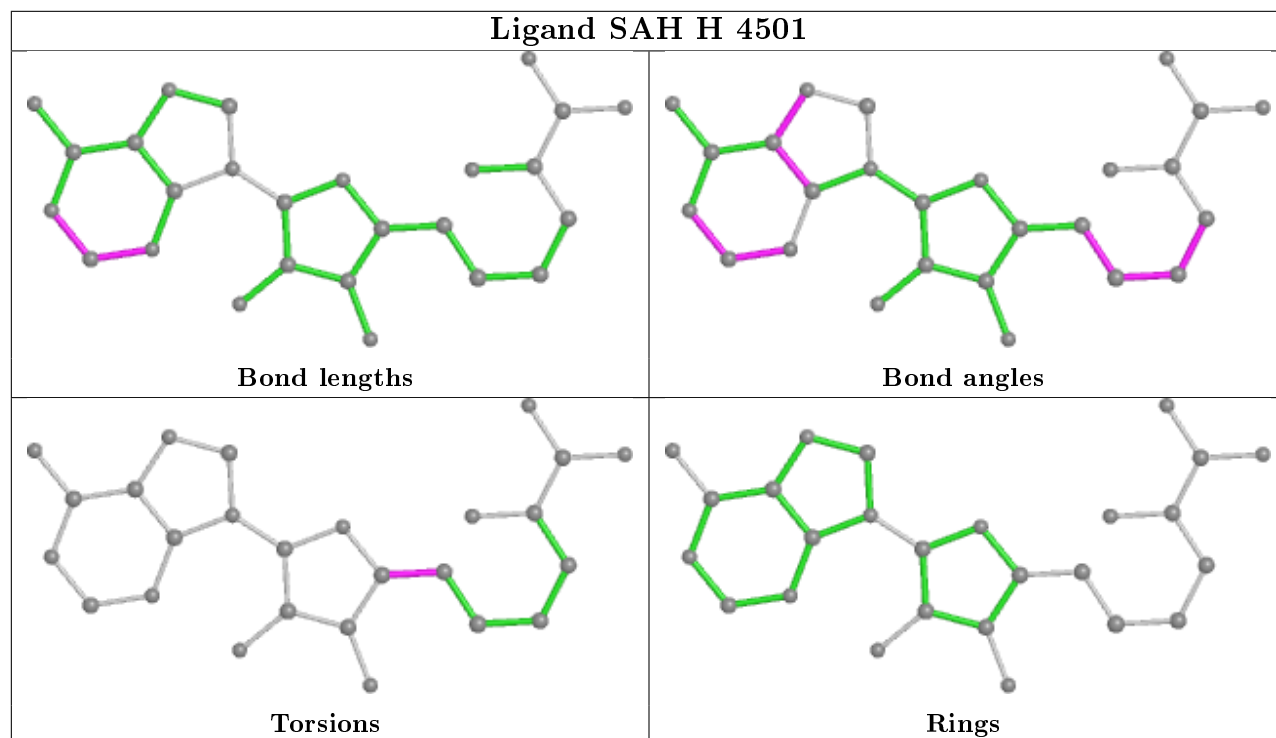
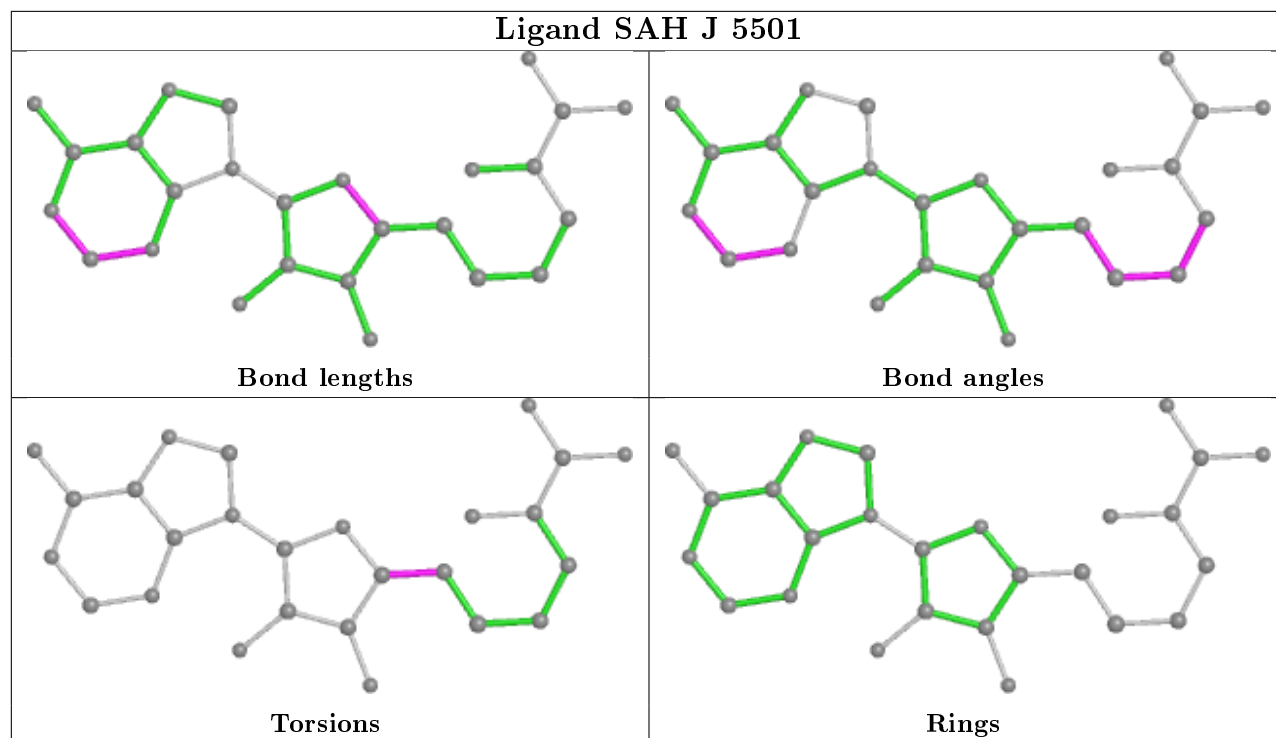


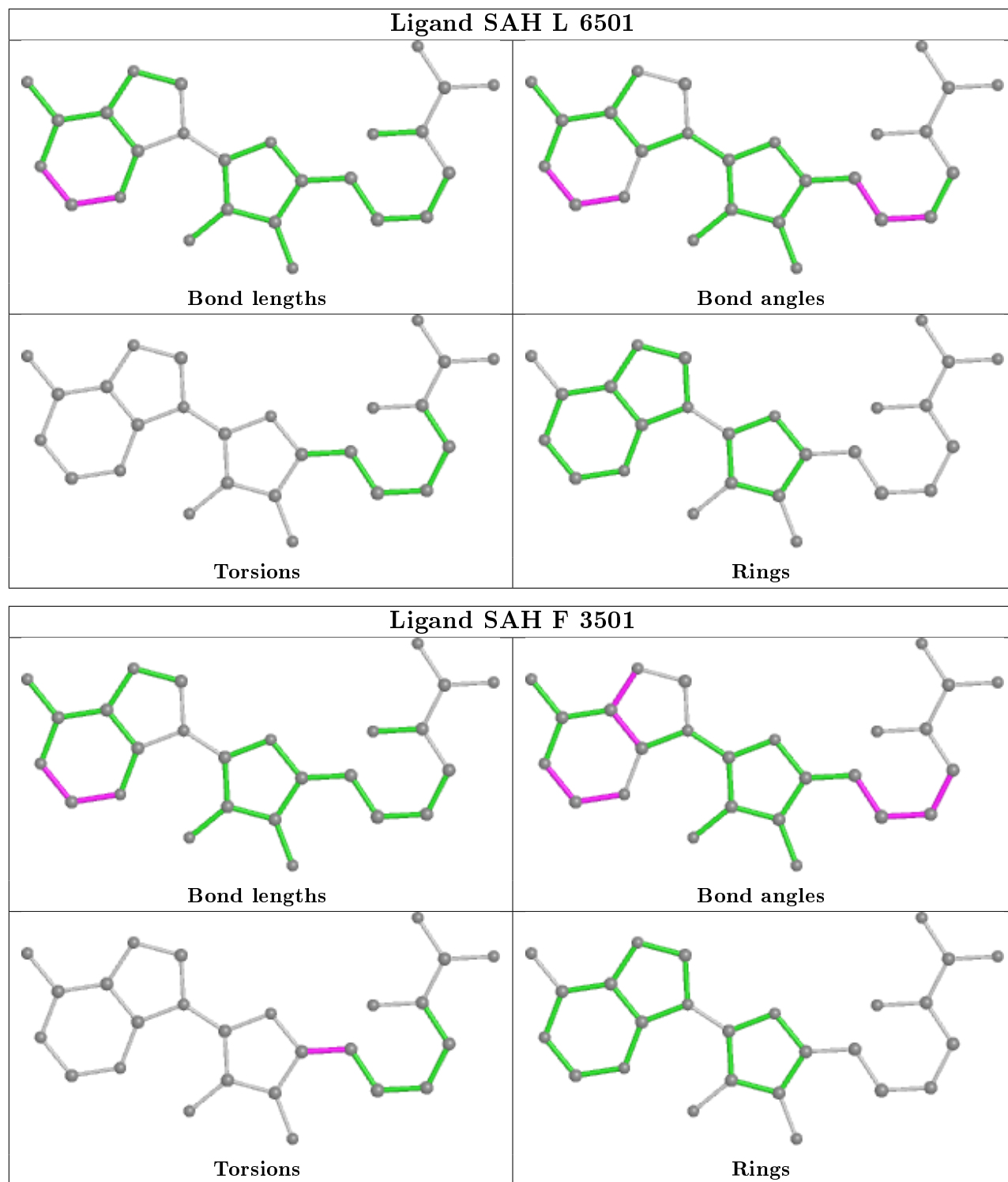
Ligand SAH A 1501



Ligand SAH I 4511







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/280 (91%)	-0.12	13 (5%) 28 26	16, 23, 53, 83	0
1	B	263/280 (93%)	-0.03	19 (7%) 15 13	14, 23, 56, 79	0
1	D	248/280 (88%)	-0.18	8 (3%) 47 48	15, 22, 45, 69	0
1	E	265/280 (94%)	0.00	20 (7%) 14 12	13, 23, 64, 80	0
1	F	254/280 (90%)	-0.01	13 (5%) 28 26	14, 23, 55, 63	0
1	G	258/280 (92%)	0.21	26 (10%) 7 5	14, 25, 62, 73	0
1	H	259/280 (92%)	-0.12	17 (6%) 18 16	16, 23, 53, 79	0
1	I	263/280 (93%)	-0.10	17 (6%) 18 17	12, 22, 55, 78	0
1	J	252/280 (90%)	0.07	20 (7%) 12 10	14, 24, 54, 79	0
1	K	258/280 (92%)	0.07	21 (8%) 12 10	10, 24, 69, 88	0
1	L	247/280 (88%)	0.73	47 (19%) 1 0	15, 25, 87, 92	0
1	M	252/280 (90%)	0.93	55 (21%) 0 0	16, 27, 85, 88	0
All	All	3075/3360 (91%)	0.12	276 (8%) 9 7	10, 24, 62, 92	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	71	GLY	9.3
1	M	72	GLY	7.9
1	L	49	LEU	7.7
1	L	74	PRO	7.6
1	M	50	VAL	7.5
1	B	73	LYS	7.4
1	H	74	PRO	7.2
1	J	263	GLY	7.1
1	B	72	GLY	7.0
1	G	71	GLY	7.0
1	G	161	SER	6.5

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Mol	Chain	Res	Type	RSRZ
1	I	75	SER	6.5
1	D	75	SER	6.1
1	B	264	ARG	6.1
1	H	72	GLY	6.0
1	I	71	GLY	6.0
1	L	60	PRO	6.0
1	J	267	ALA	6.0
1	M	71	GLY	5.9
1	K	164	VAL	5.9
1	J	74	PRO	5.9
1	K	74	PRO	5.9
1	I	72	GLY	5.8
1	L	72	GLY	5.8
1	H	68	GLY	5.7
1	M	233	ALA	5.7
1	E	165	PRO	5.7
1	B	71	GLY	5.5
1	F	74	PRO	5.4
1	K	69	LYS	5.3
1	E	74	PRO	5.3
1	M	266	LEU	5.3
1	G	262	ASP	5.3
1	M	66	PHE	5.2
1	I	74	PRO	5.2
1	J	265	LYS	5.2
1	B	74	PRO	5.1
1	K	75	SER	5.1
1	M	70	ARG	5.0
1	J	264	ARG	5.0
1	G	162	GLY	5.0
1	H	73	LYS	5.0
1	B	262	ASP	4.9
1	D	262	ASP	4.9
1	M	48	ALA	4.7
1	K	165	PRO	4.7
1	M	167	ARG	4.7
1	J	167	ARG	4.7
1	K	70	ARG	4.6
1	A	75	SER	4.6
1	B	69	LYS	4.6
1	L	164	VAL	4.5
1	G	68	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	70	ARG	4.5
1	A	166	ASP	4.4
1	A	68	GLY	4.4
1	H	71	GLY	4.4
1	I	50	VAL	4.4
1	G	166	ASP	4.3
1	K	262	ASP	4.3
1	A	74	PRO	4.3
1	M	60	PRO	4.3
1	I	49	LEU	4.3
1	M	91	ALA	4.3
1	L	166	ASP	4.3
1	I	164	VAL	4.2
1	L	73	LYS	4.2
1	E	75	SER	4.2
1	E	166	ASP	4.1
1	E	7	ALA	4.1
1	F	263	GLY	4.1
1	K	6	PHE	4.1
1	L	216	PRO	4.1
1	L	259	GLY	4.1
1	A	71	GLY	4.0
1	G	74	PRO	4.0
1	M	63	VAL	4.0
1	M	216	PRO	4.0
1	E	72	GLY	4.0
1	A	69	LYS	4.0
1	B	263	GLY	4.0
1	D	60	PRO	4.0
1	L	75	SER	4.0
1	E	71	GLY	3.9
1	M	268	ALA	3.9
1	L	165	PRO	3.9
1	D	263	GLY	3.9
1	E	73	LYS	3.9
1	F	68	GLY	3.9
1	I	68	GLY	3.9
1	A	70	ARG	3.9
1	B	75	SER	3.9
1	B	164	VAL	3.8
1	M	51	ASN	3.8
1	H	6	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	162	GLY	3.8
1	H	75	SER	3.8
1	F	164	VAL	3.8
1	H	70	ARG	3.8
1	M	267	ALA	3.8
1	L	167	ARG	3.7
1	G	165	PRO	3.7
1	B	165	PRO	3.7
1	F	165	PRO	3.7
1	G	264	ARG	3.7
1	B	166	ASP	3.7
1	L	67	ALA	3.7
1	J	146	ARG	3.7
1	L	14	LYS	3.7
1	G	73	LYS	3.6
1	M	11	ALA	3.6
1	M	69	LYS	3.6
1	L	52	GLU	3.6
1	H	271	PHE	3.6
1	I	165	PRO	3.6
1	K	71	GLY	3.6
1	M	79	ARG	3.6
1	F	76	PRO	3.6
1	L	55	LEU	3.6
1	D	74	PRO	3.5
1	E	70	ARG	3.5
1	G	261	LEU	3.5
1	B	68	GLY	3.4
1	A	48	ALA	3.4
1	K	76	PRO	3.4
1	G	75	SER	3.4
1	K	163	LEU	3.4
1	F	75	SER	3.4
1	H	69	LYS	3.4
1	L	69	LYS	3.4
1	G	48	ALA	3.3
1	J	266	LEU	3.3
1	E	69	LYS	3.3
1	L	66	PHE	3.3
1	I	268	ALA	3.3
1	M	10	PRO	3.3
1	L	39	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	72	GLY	3.3
1	I	70	ARG	3.3
1	M	269	ASP	3.2
1	M	14	LYS	3.2
1	E	49	LEU	3.2
1	J	68	GLY	3.2
1	B	266	LEU	3.2
1	G	66	PHE	3.2
1	J	75	SER	3.1
1	M	120	GLN	3.1
1	F	265	LYS	3.1
1	M	68	GLY	3.1
1	L	260	ALA	3.1
1	J	6	PHE	3.1
1	B	261	LEU	3.1
1	K	7	ALA	3.1
1	M	15	GLY	3.0
1	M	75	SER	3.0
1	B	70	ARG	3.0
1	K	166	ASP	3.0
1	G	60	PRO	3.0
1	E	159	ASP	3.0
1	M	59	ARG	3.0
1	L	63	VAL	2.9
1	M	76	PRO	2.9
1	J	147	GLU	2.9
1	E	91	ALA	2.9
1	L	77	LYS	2.8
1	M	191	ALA	2.8
1	I	69	LYS	2.8
1	G	167	ARG	2.8
1	L	236	GLY	2.8
1	M	262	ASP	2.8
1	B	60	PRO	2.8
1	L	234	ALA	2.8
1	M	74	PRO	2.8
1	A	50	VAL	2.7
1	I	76	PRO	2.7
1	M	52	GLU	2.7
1	M	217	GLN	2.7
1	J	50	VAL	2.7
1	K	263	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	52	GLU	2.7
1	A	61	GLY	2.7
1	G	168	ILE	2.7
1	J	69	LYS	2.7
1	F	60	PRO	2.7
1	L	7	ALA	2.7
1	G	50	VAL	2.7
1	E	161	SER	2.7
1	L	58	ALA	2.6
1	G	79	ARG	2.6
1	M	67	ALA	2.6
1	M	77	LYS	2.6
1	L	61	GLY	2.6
1	E	48	ALA	2.6
1	M	159	ASP	2.6
1	L	56	LYS	2.6
1	L	119	HIS	2.6
1	D	68	GLY	2.6
1	J	260	ALA	2.5
1	J	262	ASP	2.5
1	L	9	LEU	2.5
1	I	167	ARG	2.5
1	F	73	LYS	2.5
1	J	48	ALA	2.5
1	M	158	HIS	2.5
1	M	230	ALA	2.5
1	G	158	HIS	2.5
1	L	90	ARG	2.5
1	I	52	GLU	2.5
1	L	50	VAL	2.5
1	L	118	GLU	2.5
1	G	160	SER	2.5
1	M	58	ALA	2.5
1	G	159	ASP	2.5
1	L	147	GLU	2.4
1	F	67	ALA	2.4
1	J	52	GLU	2.4
1	M	265	LYS	2.4
1	H	175	SER	2.4
1	L	146	ARG	2.4
1	I	166	ASP	2.4
1	G	267	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	233	ALA	2.4
1	M	53	ASP	2.4
1	A	6	PHE	2.4
1	M	187	LYS	2.4
1	L	53	ASP	2.4
1	L	54	CYS	2.4
1	E	167	ARG	2.4
1	G	14	LYS	2.3
1	M	56	LYS	2.3
1	M	16	SER	2.3
1	K	50	VAL	2.3
1	M	90	ARG	2.3
1	H	270	PRO	2.3
1	K	68	GLY	2.3
1	I	7	ALA	2.3
1	K	90	ARG	2.3
1	M	234	ALA	2.3
1	J	244	VAL	2.3
1	K	162	GLY	2.3
1	H	159	ASP	2.3
1	K	5	LEU	2.2
1	M	92	GLY	2.2
1	E	76	PRO	2.2
1	L	13	GLU	2.2
1	M	168	ILE	2.2
1	D	76	PRO	2.2
1	M	96	LEU	2.2
1	M	118	GLU	2.2
1	A	167	ARG	2.2
1	H	76	PRO	2.2
1	B	4	ASP	2.2
1	E	68	GLY	2.1
1	M	238	GLU	2.1
1	K	72	GLY	2.1
1	L	42	ASP	2.1
1	M	202	SER	2.1
1	L	8	GLY	2.1
1	L	68	GLY	2.1
1	F	56	LYS	2.1
1	M	35	ALA	2.1
1	D	162	GLY	2.1
1	M	188	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	91	ALA	2.1
1	F	39	ARG	2.1
1	B	161	SER	2.1
1	E	5	LEU	2.0
1	M	88	LEU	2.0
1	L	79	ARG	2.0
1	H	50	VAL	2.0
1	H	158	HIS	2.0
1	A	7	ALA	2.0
1	L	120	GLN	2.0
1	H	39	ARG	2.0
1	J	76	PRO	2.0
1	L	253	ALA	2.0

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 carbohydrates 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(\AA^2)	Q<0.9
3	GOL	D	2002	6/6	0.68	0.27	77,86,87,88	0
3	GOL	A	1002	6/6	0.72	0.26	78,84,86,88	0
3	GOL	F	3001	6/6	0.72	0.26	83,90,92,93	0
3	GOL	D	2011	6/6	0.74	0.36	74,82,83,85	0
3	GOL	L	6001	6/6	0.79	0.33	105,106,106,106	0
3	GOL	I	4011	6/6	0.80	0.32	88,91,92,93	0
3	GOL	G	3012	6/6	0.80	0.28	91,93,94,96	0
3	GOL	M	6011	6/6	0.80	0.20	83,85,87,89	0
3	GOL	A	1012	6/6	0.83	0.39	71,75,76,78	0
3	GOL	H	4003	6/6	0.84	0.30	77,82,82,82	0

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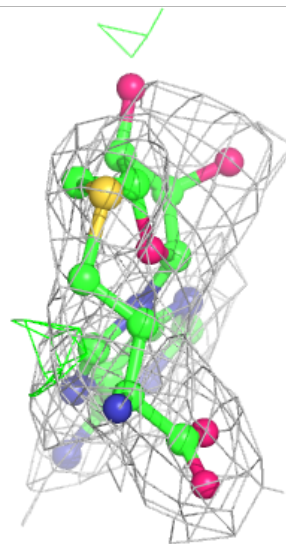
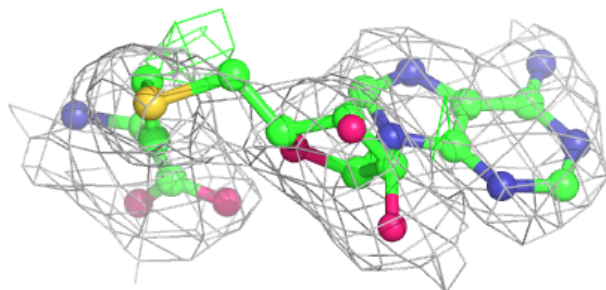
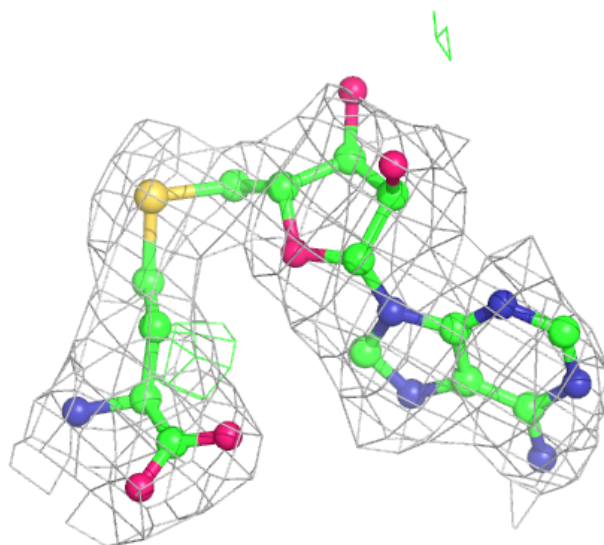
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	1001	6/6	0.84	0.31	51,57,60,61	0
3	GOL	J	5011	6/6	0.85	0.36	95,95,97,98	0
3	GOL	E	2003	6/6	0.85	0.28	73,76,77,79	0
3	GOL	F	3011	6/6	0.86	0.43	92,93,94,95	0
3	GOL	E	2012	6/6	0.87	0.29	89,95,96,97	0
3	GOL	B	1011	6/6	0.87	0.22	67,77,79,79	0
3	GOL	E	2001	6/6	0.88	0.29	57,63,65,67	0
3	GOL	H	4012	6/6	0.88	0.30	73,74,76,77	0
3	GOL	G	3002	6/6	0.88	0.34	78,80,81,81	0
2	SAH	M	6511	26/26	0.88	0.18	67,69,71,73	0
3	GOL	L	6002	6/6	0.89	0.18	91,95,96,97	0
3	GOL	J	5002	6/6	0.89	0.32	66,70,70,71	0
3	GOL	K	5001	6/6	0.89	0.34	74,77,77,77	0
3	GOL	I	4002	6/6	0.90	0.27	50,53,57,57	0
3	GOL	G	3003	6/6	0.90	0.37	73,76,77,77	0
3	GOL	K	5012	6/6	0.91	0.20	94,95,96,96	0
2	SAH	L	6501	26/26	0.92	0.24	88,96,102,102	0
3	GOL	J	5003	6/6	0.93	0.19	78,82,86,88	0
2	SAH	I	4511	26/26	0.95	0.21	52,60,64,65	0
2	SAH	J	5501	26/26	0.95	0.21	66,68,69,70	0
2	SAH	G	3511	26/26	0.95	0.23	60,69,78,78	0
2	SAH	K	5511	26/26	0.96	0.21	56,62,64,64	0
2	SAH	H	4501	26/26	0.96	0.20	50,56,60,62	0
2	SAH	B	1511	26/26	0.96	0.18	45,49,50,51	0
2	SAH	E	2511	26/26	0.96	0.19	51,58,59,59	0
2	SAH	F	3501	26/26	0.96	0.19	54,62,63,64	0
2	SAH	D	2501	26/26	0.96	0.22	55,60,64,64	0
2	SAH	A	1501	26/26	0.96	0.21	46,59,67,67	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.

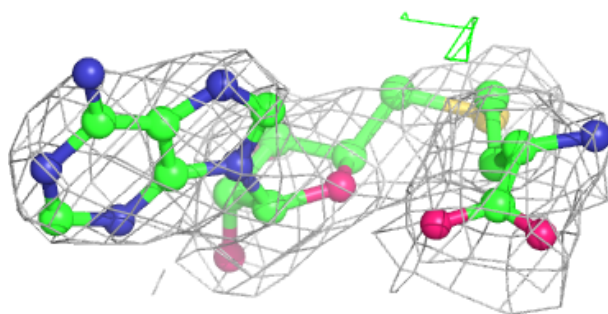
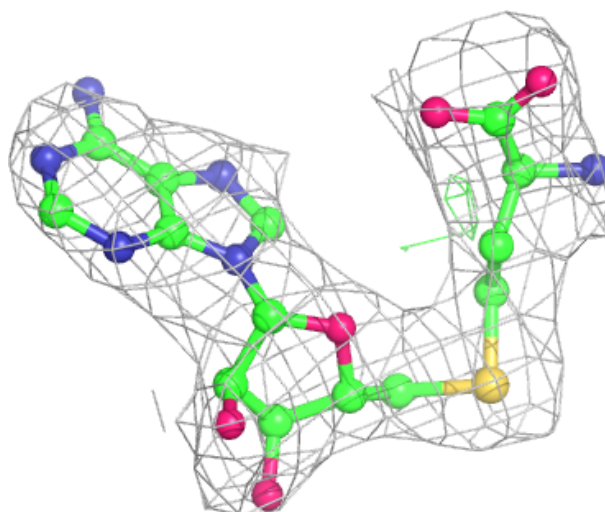
Electron density around SAH M 6511:

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



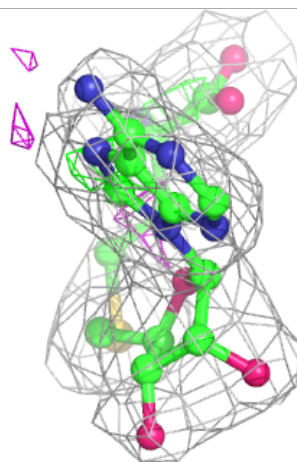
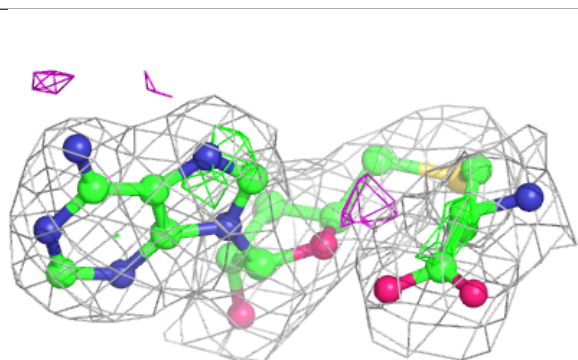
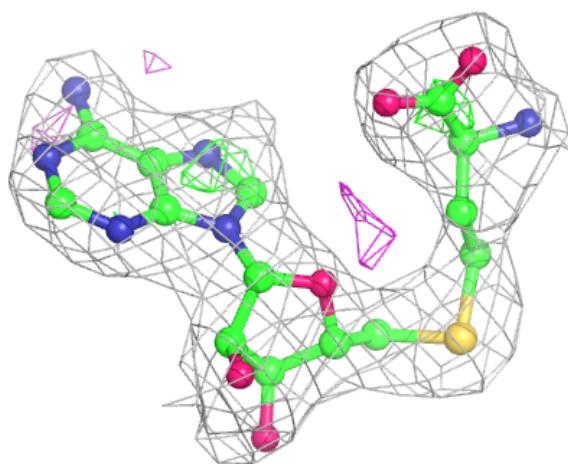
Electron density around SAH L 6501:

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



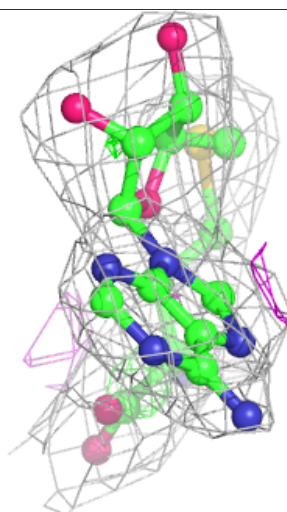
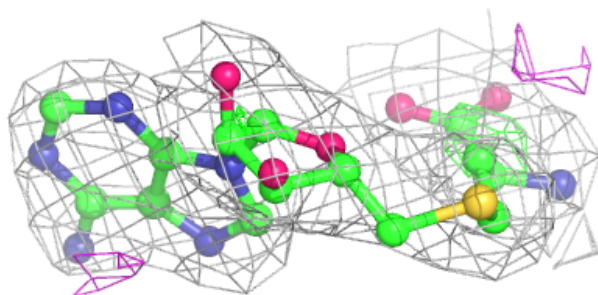
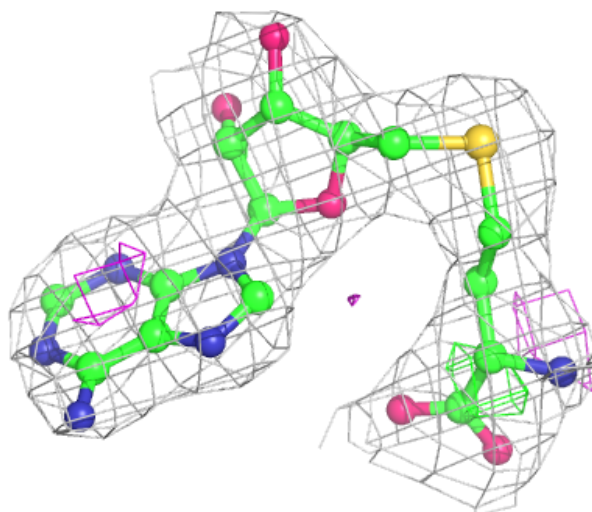
Electron density around SAH I 4511:

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



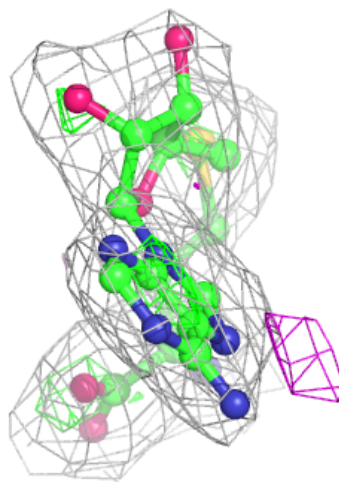
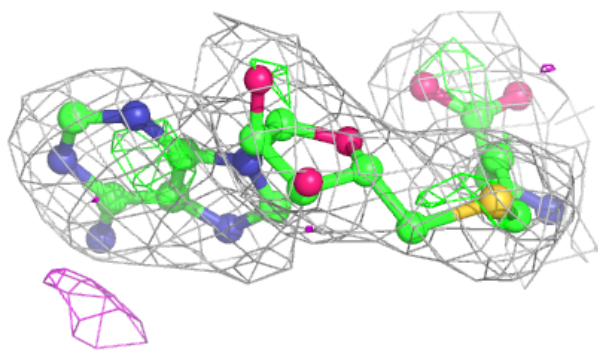
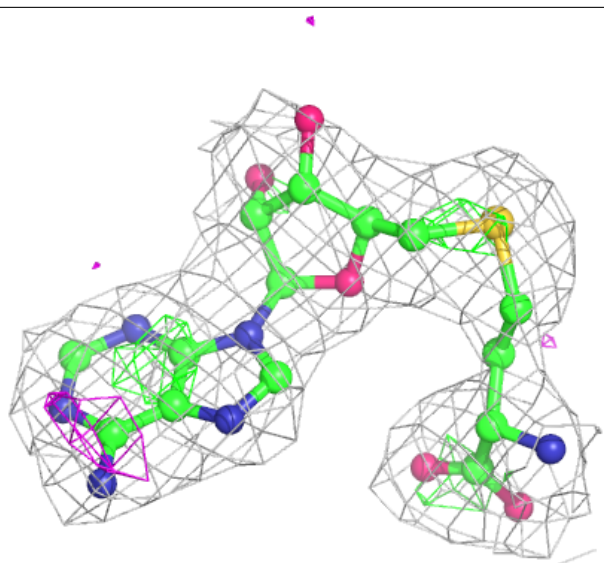
Electron density around SAH J 5501:

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



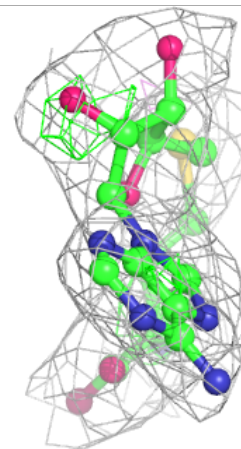
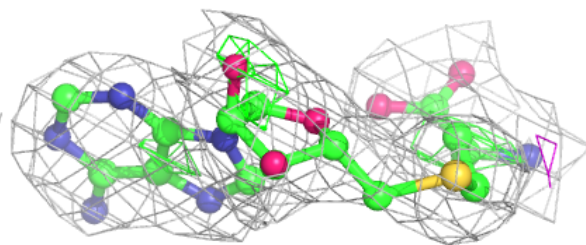
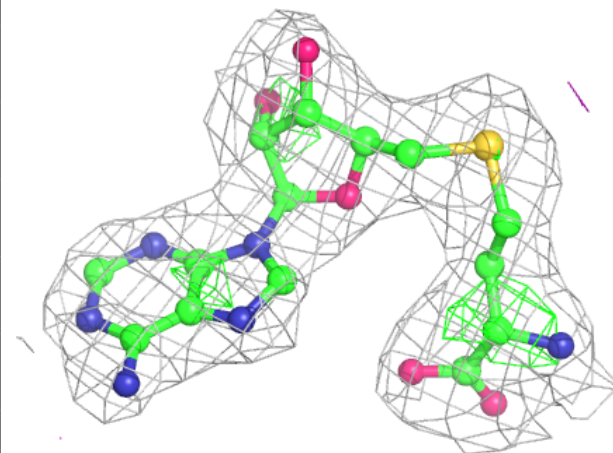
Electron density around SAH G 3511:

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



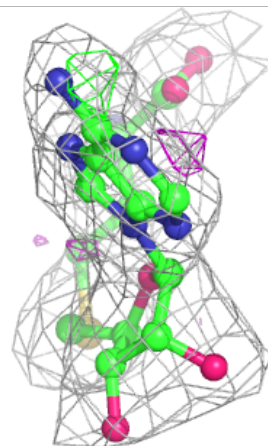
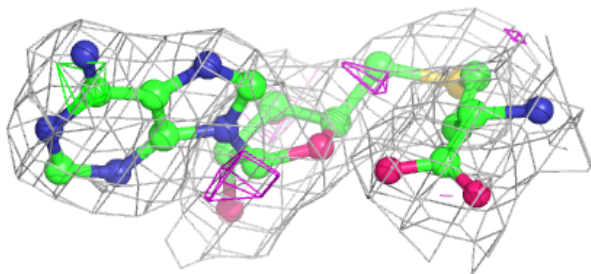
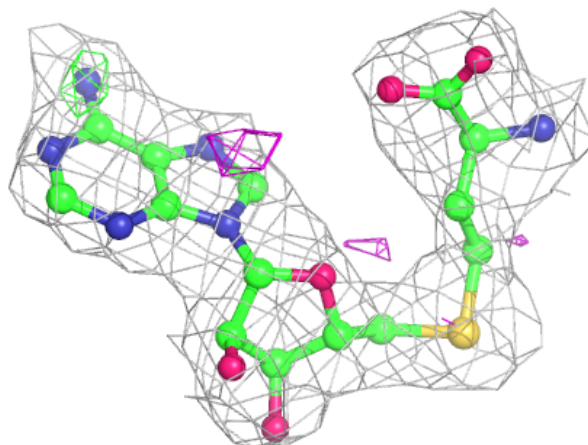
Electron density around SAH K 5511:

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



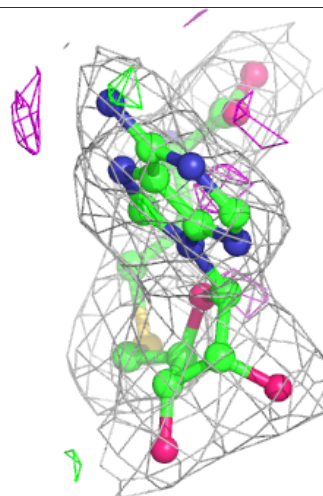
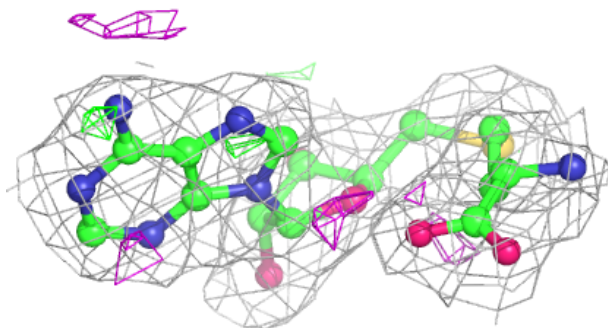
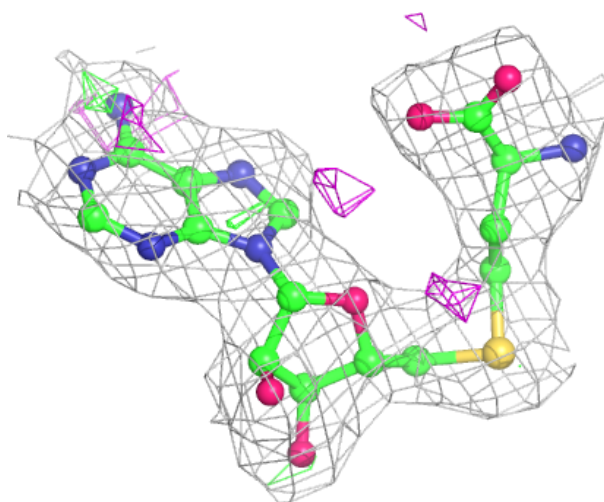
Electron density around SAH H 4501:

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



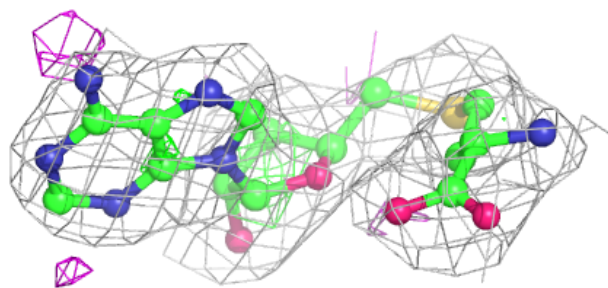
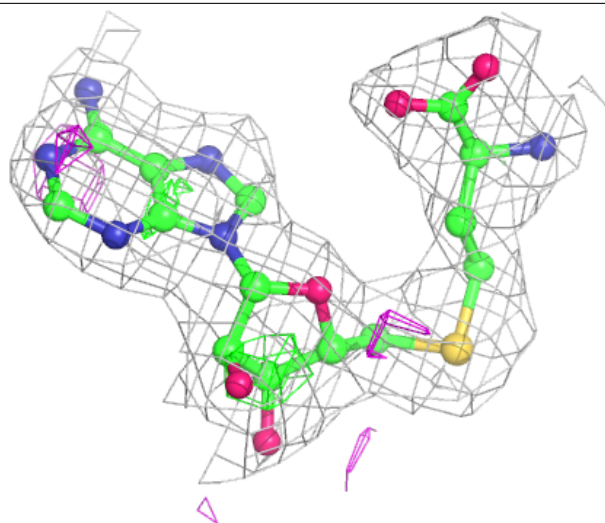
Electron density around SAH B 1511:

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



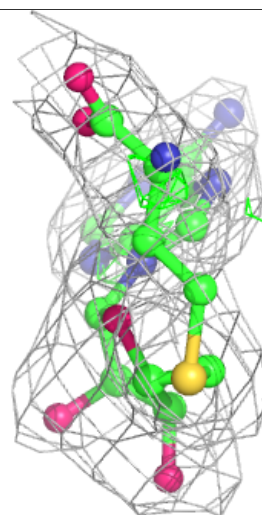
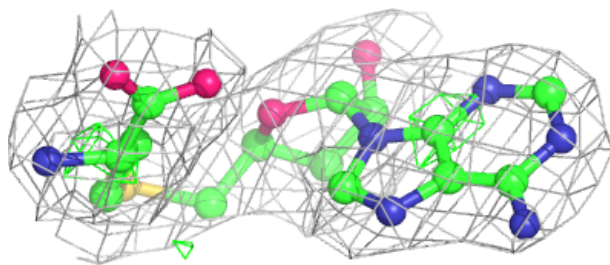
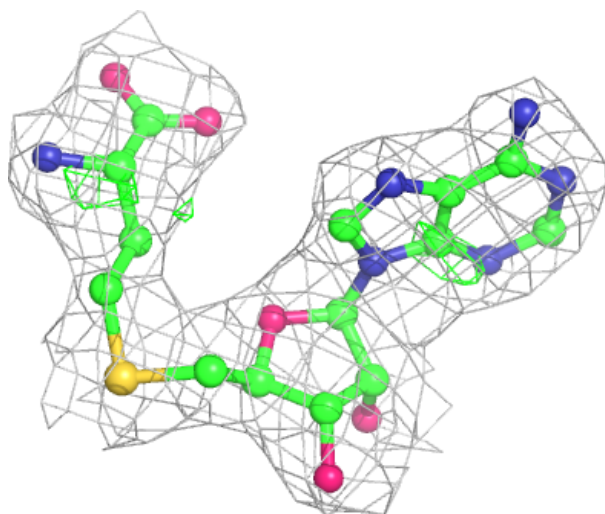
Electron density around SAH E 2511:

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



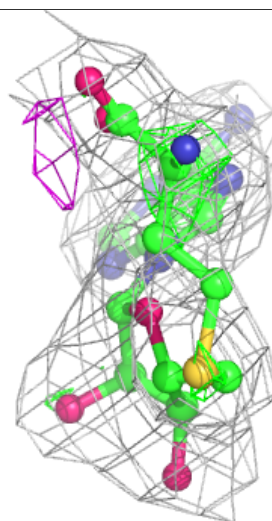
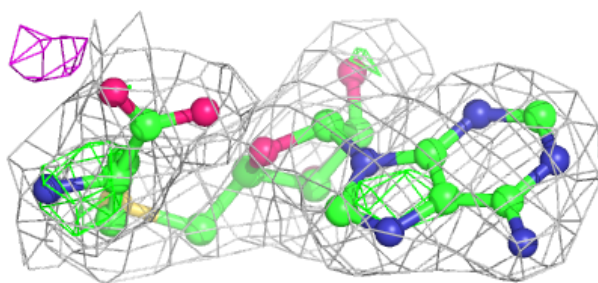
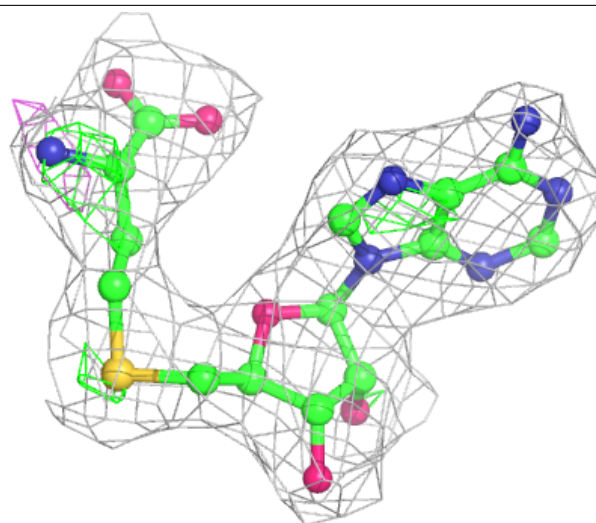
Electron density around SAH F 3501:

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



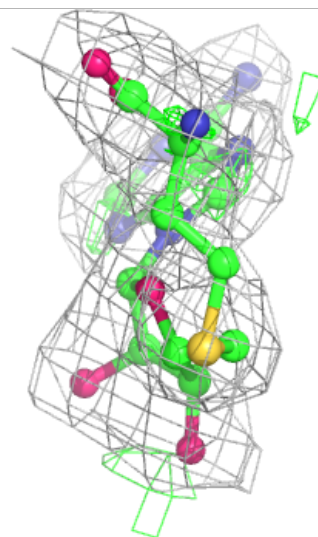
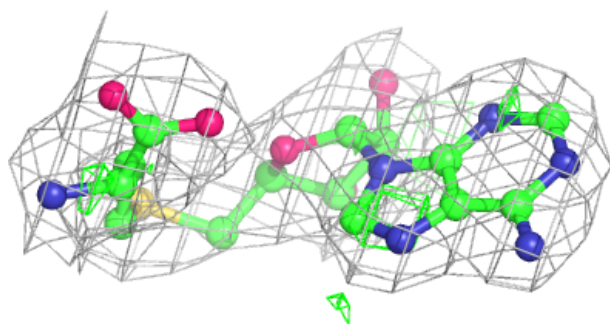
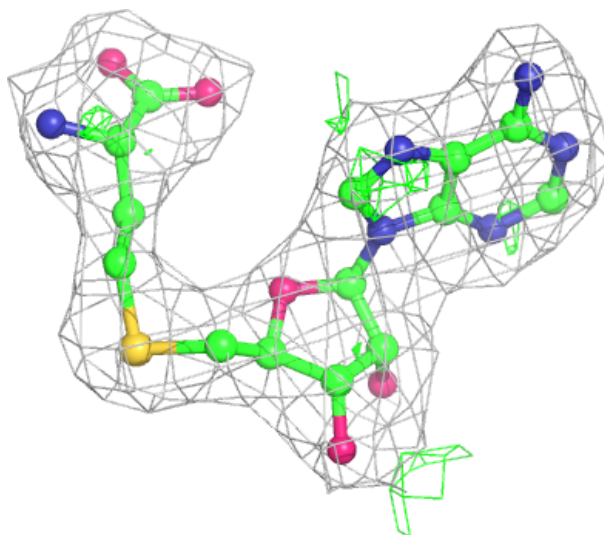
Electron density around SAH D 2501:

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



Electron density around SAH A 1501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.