Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2026 – 05:11 pm BST

PDB ID	:	5ODH / pdb_00005odh
Title	:	Heterodisulfide reductase / [NiFe]-hydrogenase complex from Methanothermococcus thermolithotrophicus soaked with heterodisulfide for 3.5 minutes
Authors	:	Wagner, T.; Koch, J.; Ermler, U.; Shima, S.
Deposited on	:	2017-07-05
Resolution	:	2.20 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

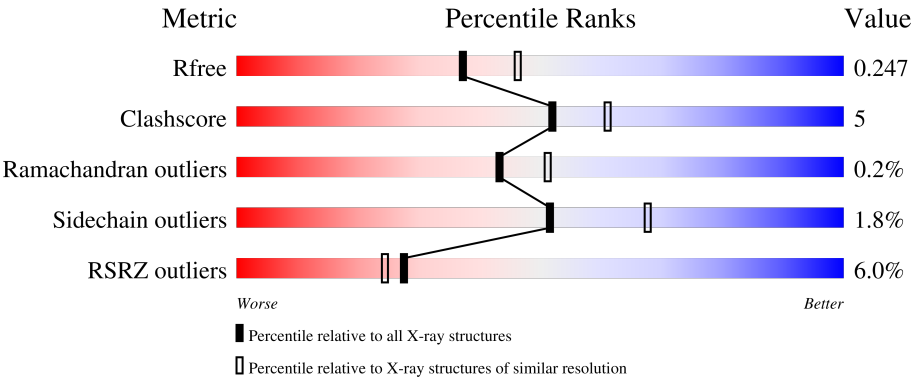
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	654	10% 88% 11%
1	G	654	5% 88% 11%
2	B	291	2% 87% 13%
2	H	291	27% 73% 27%
3	C	184	3% 84% 15%

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Mol	Chain	Length	Quality of chain
3	I	184	8% 79% 20%
4	D	140	84% 14%
4	J	140	2% 89% 9%
5	E	299	5% 88% 10%
5	K	299	2% 89% 10%
6	F	473	% 85% 9% 5%
6	L	473	2% 87% 7% 5%

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
12	COM	B	303	-	X	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 32106 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 Heterodisulfide reductase, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	0	0	0
			4977	3140	845	943	49			
1	G	653	Total	C	N	O	S	0	0	0
			4984	3145	846	944	49			

- Molecule 2 is a protein called Heterodisulfide reductase, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2236	1420	379	413	24			
2	H	291	Total	C	N	O	S	0	0	0
			2232	1417	378	413	24			

- Molecule 3 is a protein called Heterodisulfide reductase, subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	184	Total	C	N	O	S	0	0	0
			1421	887	246	274	14			
3	I	183	Total	C	N	O	S	0	0	0
			1416	885	246	271	14			

- Molecule 4 is a protein called Methyl-viologen reducing hydrogenase, subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	137	Total	C	N	O	S	0	0	0
			1097	698	187	200	12			
4	J	138	Total	C	N	O	S	0	0	0
			1106	703	188	203	12			

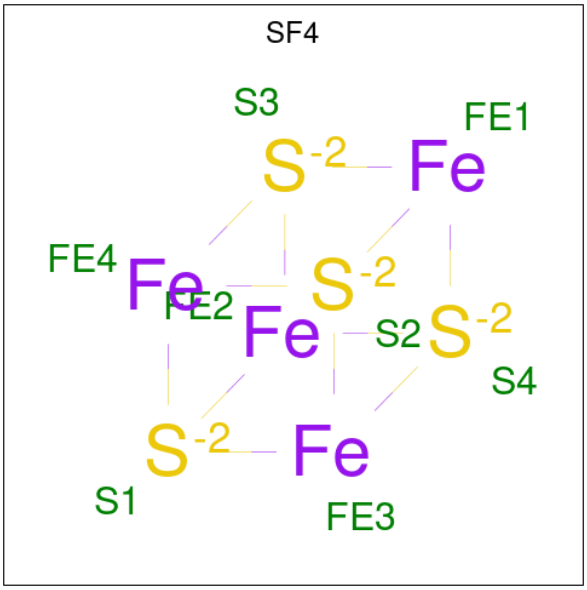
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	298	Total	C	N	O	S	0	0	0
			2258	1425	369	445	19			
5	K	298	Total	C	N	O	S	0	0	0
			2258	1425	369	445	19			

- Molecule 6 is a protein called Methyl-viologen reducing hydrogenase, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	447	Total	C	N	O	S	0	0	0
			3521	2230	600	672	19			
6	L	447	Total	C	N	O	S	0	0	0
			3521	2230	600	672	19			

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



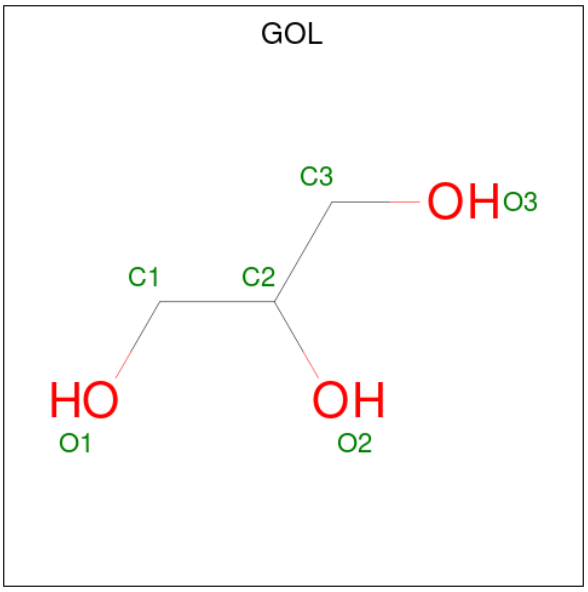
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Fe	S		0	0
			8	4	4			
7	A	1	Total	Fe	S		0	0
			8	4	4			
7	A	1	Total	Fe	S		0	0
			8	4	4			
7	A	1	Total	Fe	S		0	0
			8	4	4			
7	A	1	Total	Fe	S		0	0
			8	4	4			
7	A	1	Total	Fe	S		0	0
			8	4	4			

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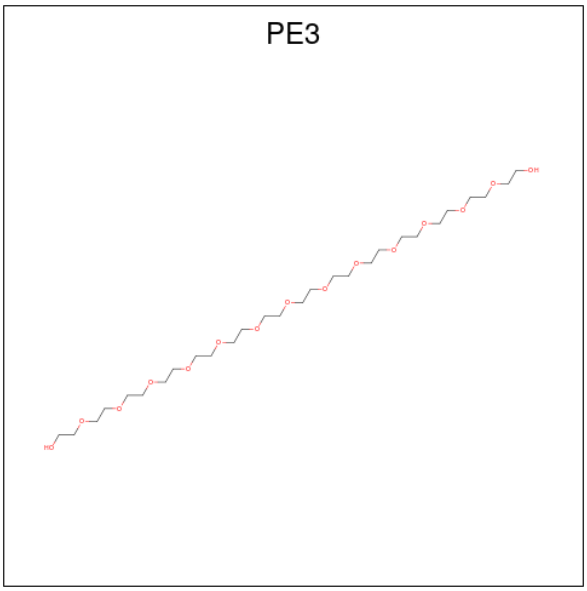
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Fe S 8 4 4	0	0
7	C	1	Total Fe S 8 4 4	0	0
7	E	1	Total Fe S 8 4 4	0	0
7	E	1	Total Fe S 8 4 4	0	0
7	E	1	Total Fe S 8 4 4	0	0
7	G	1	Total Fe S 8 4 4	0	0
7	G	1	Total Fe S 8 4 4	0	0
7	G	1	Total Fe S 8 4 4	0	0
7	G	1	Total Fe S 8 4 4	0	0
7	G	1	Total Fe S 8 4 4	0	0
7	G	1	Total Fe S 8 4 4	0	0
7	I	1	Total Fe S 8 4 4	0	0
7	I	1	Total Fe S 8 4 4	0	0
7	K	1	Total Fe S 8 4 4	0	0
7	K	1	Total Fe S 8 4 4	0	0
7	K	1	Total Fe S 8 4 4	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



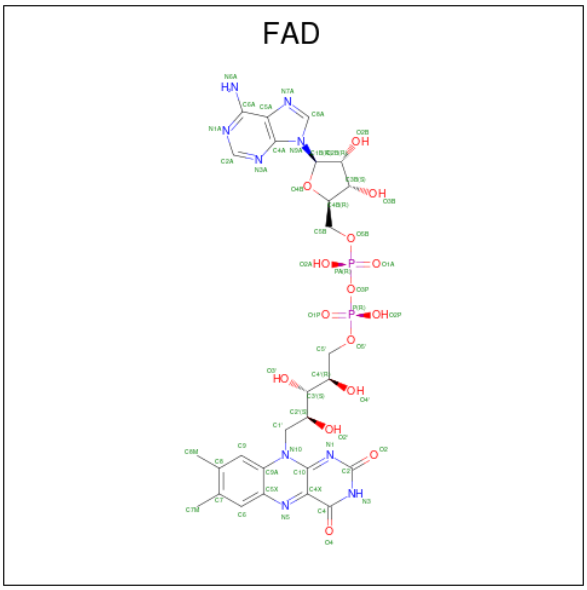
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	E	1	Total C O 6 3 3	0	0
8	G	1	Total C O 6 3 3	0	0
8	K	1	Total C O 6 3 3	0	0

- Molecule 9 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1 ,41-DIOL (CCD ID: PE3) (formula: $C_{28}H_{58}O_{15}$).



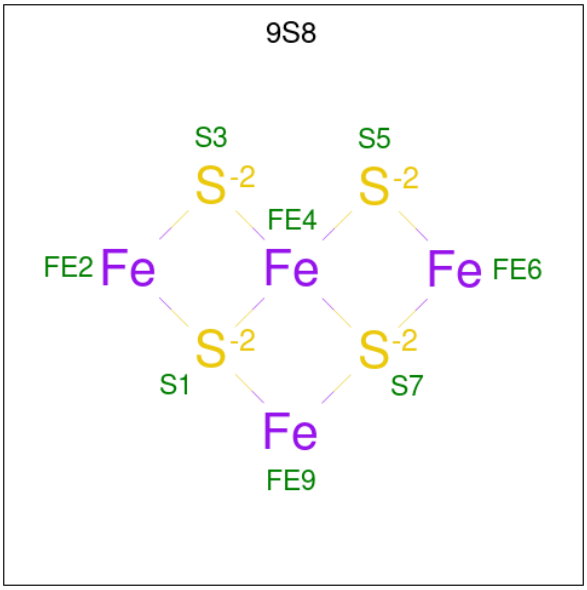
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 14 9 5	0	0
9	F	1	Total C O 9 6 3	0	0
9	F	1	Total C O 9 6 3	0	0
9	L	1	Total C O 9 6 3	0	0

- Molecule 10 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



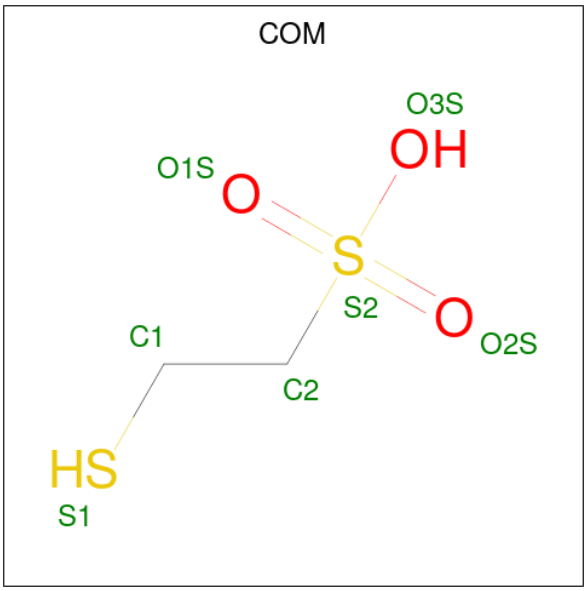
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
10	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 11 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe_4S_4).



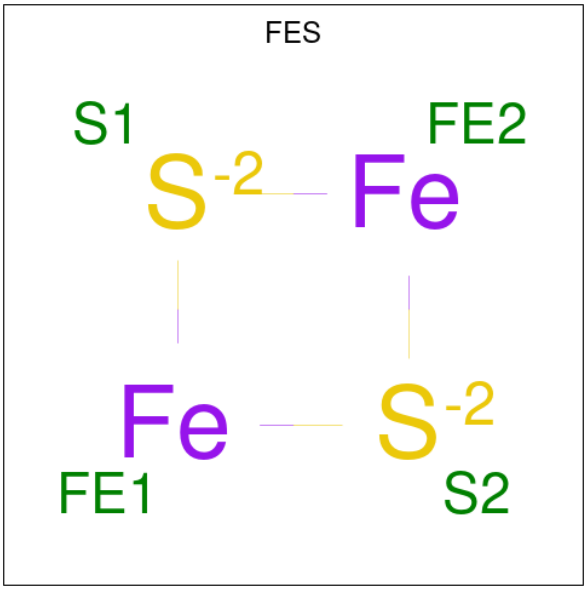
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	H	1	Total	Fe	S	0	0
			8	4	4		
11	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



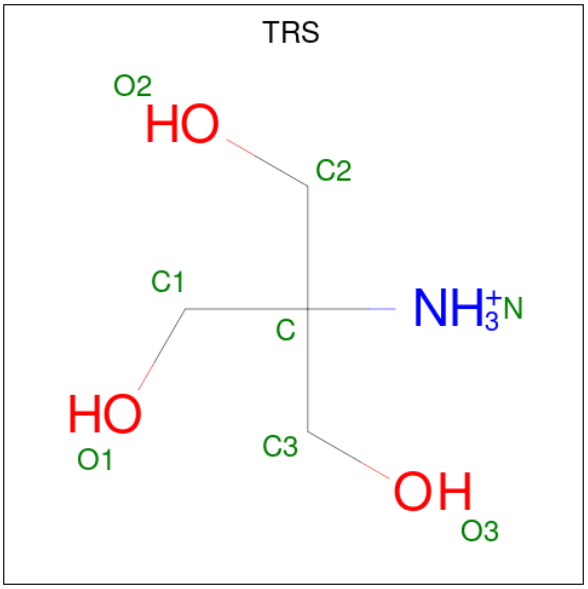
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O S 7 2 3 2	0	0
12	H	1	Total C O S 7 2 3 2	0	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total Fe S 4 2 2	0	0
13	J	1	Total Fe S 4 2 2	0	0

- Molecule 14 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).

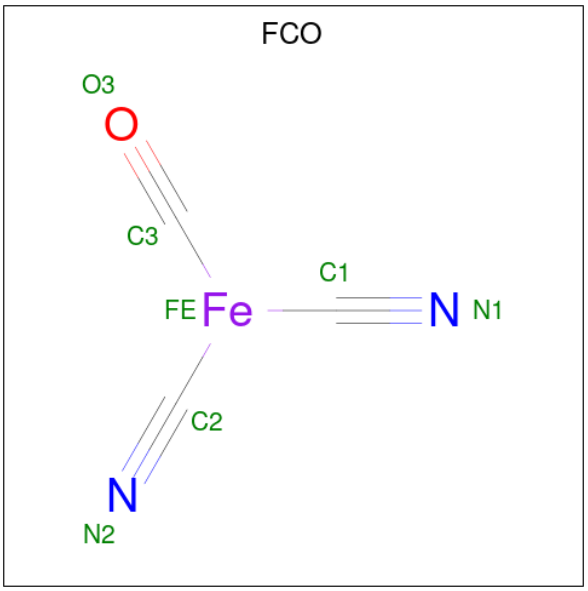


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	1	Total C N O 8 4 1 3	0	0

- Molecule 15 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	F	1	Total Fe 1 1	0	0
15	G	1	Total Fe 1 1	0	0
15	L	1	Total Fe 1 1	0	0

- Molecule 16 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O).

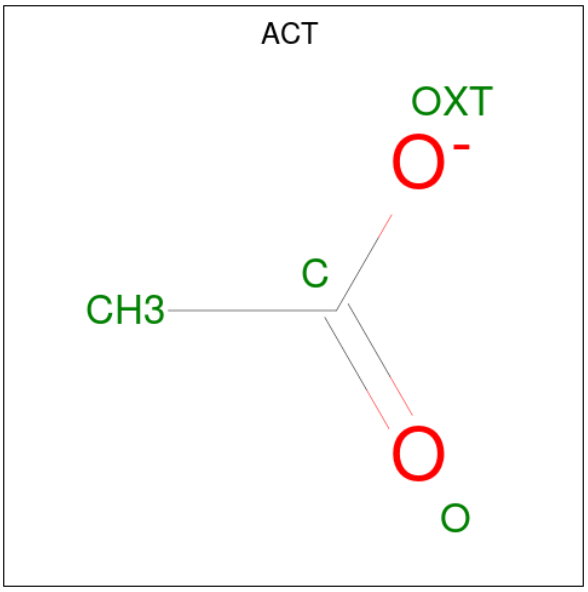


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	F	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
16	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 17 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

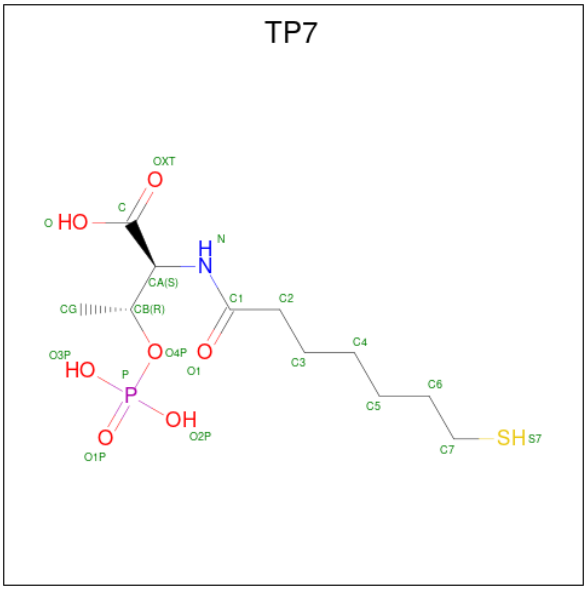
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	F	1	Total	Ni	0	0
			1	1		
17	L	1	Total	Ni	0	0
			1	1		

- Molecule 18 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	1	Total C O 4 2 2	0	0
18	G	1	Total C O 4 2 2	0	0

- Molecule 19 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	H	1	Total C N O P S 21 11 1 7 1 1	0	0

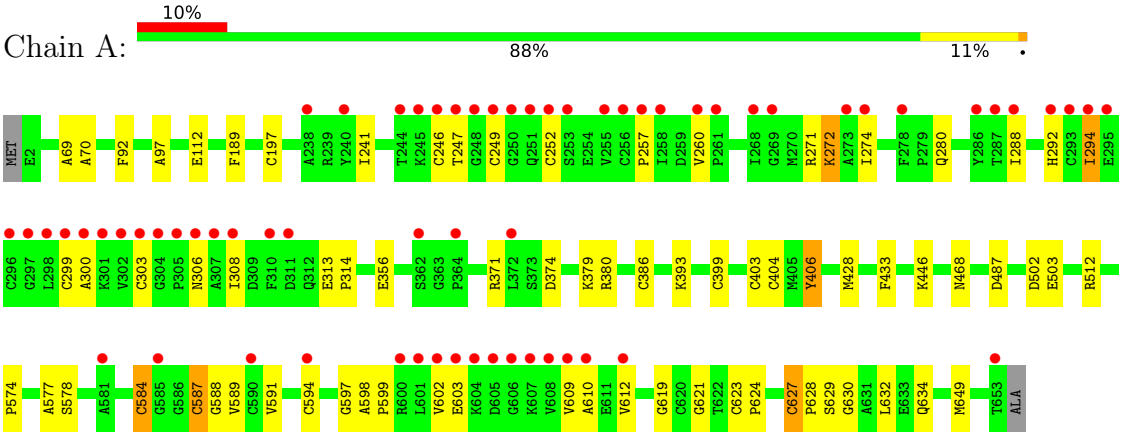
- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	111	Total O 111 111	0	0
20	B	27	Total O 27 27	0	0
20	C	25	Total O 25 25	0	0
20	D	29	Total O 29 29	0	0
20	E	37	Total O 37 37	0	0
20	F	67	Total O 67 67	0	0
20	G	134	Total O 134 134	0	0
20	H	5	Total O 5 5	0	0
20	I	14	Total O 14 14	0	0
20	J	31	Total O 31 31	0	0
20	K	51	Total O 51 51	0	0
20	L	79	Total O 79 79	0	0

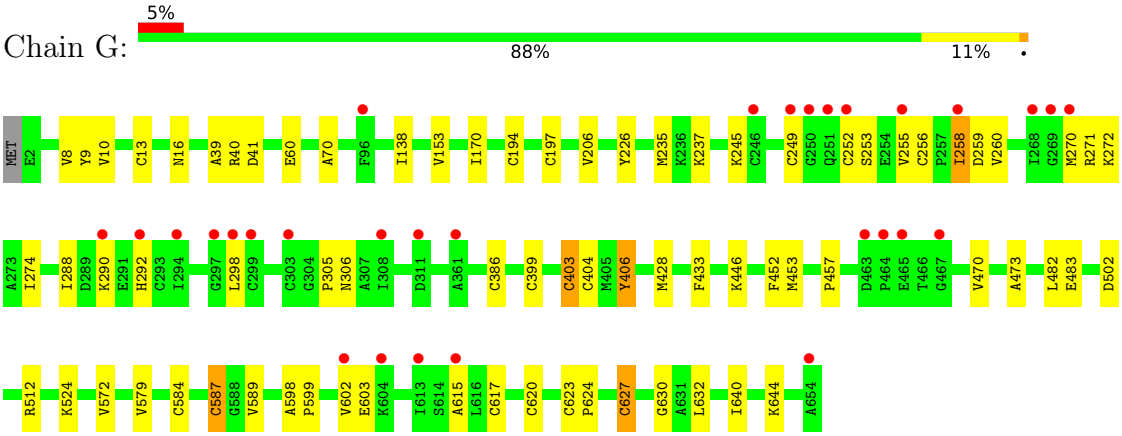
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

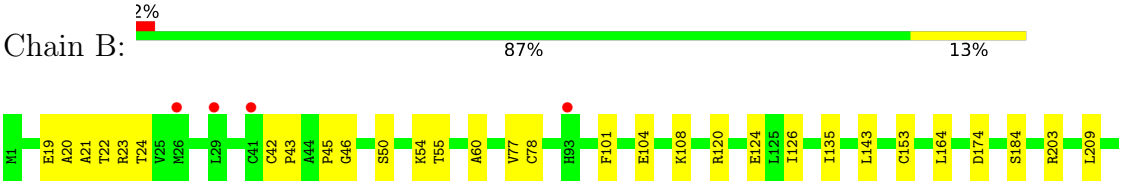
• Molecule 1: Heterodisulfide reductase, subunit A

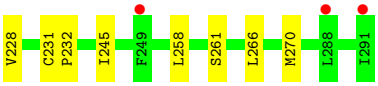


• Molecule 1: Heterodisulfide reductase, subunit A



• Molecule 2: Heterodisulfide reductase, subunit B

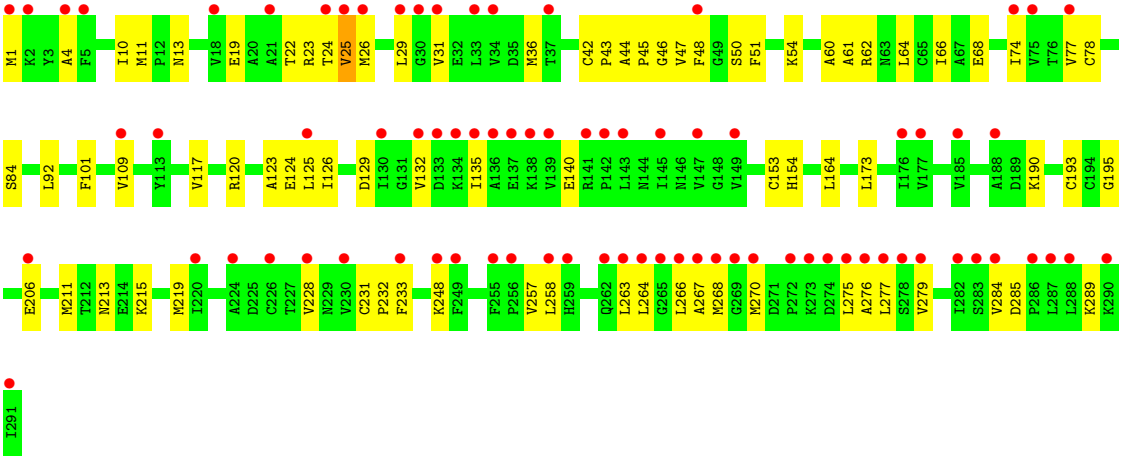




• Molecule 2: Heterodisulfide reductase, subunit B

Chain H:





• Molecule 3: Heterodisulfide reductase, subunit C

Chain C:

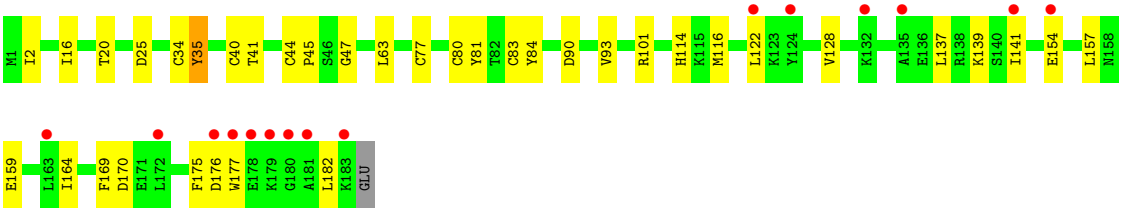




• Molecule 3: Heterodisulfide reductase, subunit C

Chain I:

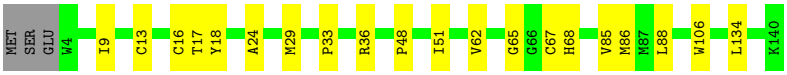




• Molecule 4: Methyl-viologen reducing hydrogenase, subunit D

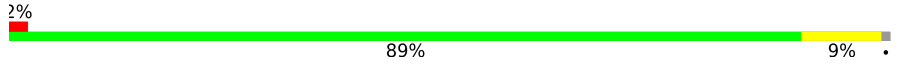
Chain D:

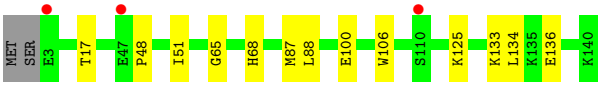




• Molecule 4: Methyl-viologen reducing hydrogenase, subunit D

Chain J:

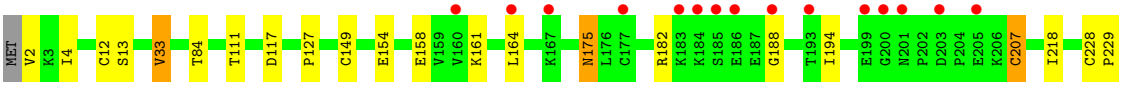


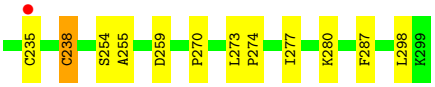


• Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

Chain E:



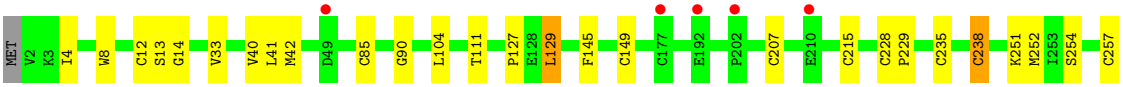


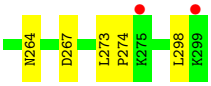


• Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

Chain K:



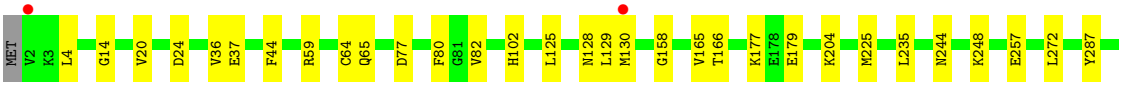


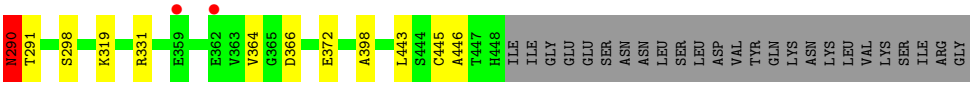


• Molecule 6: Methyl-viologen reducing hydrogenase, subunit A

Chain F:



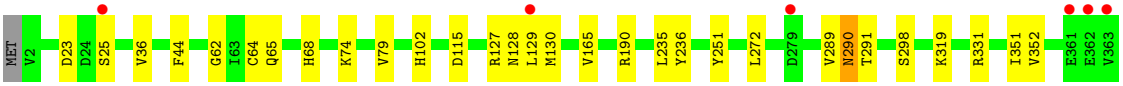


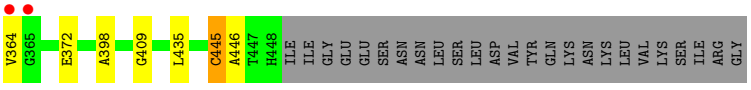


• Molecule 6: Methyl-viologen reducing hydrogenase, subunit A

Chain L:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	366.38Å 97.10Å 133.97Å 90.00° 108.43° 90.00°	Depositor
Resolution (Å)	48.55 – 2.20 48.55 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.55-2.20) 99.8 (48.55-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.214 , 0.245 0.218 , 0.247	Depositor DCC
R_{free} test set	11273 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32106	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FES, FCO, SF4, FE, 9S8, FAD, NI, TRS, TP7, ACT, COM, GOL, PE3

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	0.19	0/5069	0.36	0/6850
1	G	0.18	0/5076	0.36	0/6860
2	B	0.20	0/2277	0.43	0/3070
2	H	0.20	0/2273	0.47	0/3066
3	C	0.21	0/1442	0.42	0/1942
3	I	0.21	0/1437	0.46	0/1934
4	D	0.20	0/1123	0.39	0/1508
4	J	0.18	0/1132	0.36	0/1520
5	E	0.20	0/2297	0.41	0/3113
5	K	0.19	0/2297	0.40	0/3113
6	F	0.18	0/3590	0.39	0/4853
6	L	0.19	0/3590	0.39	0/4853
All	All	0.19	0/31603	0.40	0/42682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4977	0	4968	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4984	0	4979	45	0
2	B	2236	0	2243	28	0
2	H	2232	0	2234	64	0
3	C	1421	0	1431	18	0
3	I	1416	0	1435	28	0
4	D	1097	0	1068	14	0
4	J	1106	0	1074	9	0
5	E	2258	0	2265	26	0
5	K	2258	0	2265	21	0
6	F	3521	0	3506	26	1
6	L	3521	0	3505	22	1
7	A	48	0	0	1	0
7	C	16	0	0	0	0
7	E	24	0	0	0	0
7	G	48	0	0	1	0
7	I	16	0	0	0	0
7	K	24	0	0	0	0
8	A	6	0	8	0	0
8	B	12	0	16	0	0
8	E	6	0	8	0	0
8	G	6	0	8	2	0
8	K	6	0	8	1	0
9	A	14	0	16	0	0
9	F	18	0	18	1	0
9	L	9	0	10	0	0
10	A	53	0	31	0	0
10	G	53	0	31	0	0
11	B	16	0	0	1	0
11	H	16	0	0	1	0
12	B	7	0	6	1	0
12	H	7	0	6	2	0
13	D	4	0	0	0	0
13	J	4	0	0	0	0
14	D	8	0	12	0	0
15	F	1	0	0	0	0
15	G	1	0	0	0	0
15	L	1	0	0	0	0
16	F	7	0	0	1	0
16	L	7	0	0	1	0
17	F	1	0	0	0	0
17	L	1	0	0	0	0
18	G	8	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	H	21	0	19	3	0
20	A	111	0	0	2	0
20	B	27	0	0	1	0
20	C	25	0	0	0	0
20	D	29	0	0	0	0
20	E	37	0	0	0	0
20	F	67	0	0	1	0
20	G	134	0	0	0	0
20	H	5	0	0	0	0
20	I	14	0	0	0	0
20	J	31	0	0	0	0
20	K	51	0	0	0	0
20	L	79	0	0	0	0
All	All	32106	0	31176	318	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (318) 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)
6:F:290:ASN:OD1	6:F:291:THR:N	2.09	0.85
1:G:587:CYS:SG	1:G:589:VAL:HG23	2.24	0.77
1:A:197:CYS:SG	20:A:910:HOH:O	2.49	0.71
2:B:104:GLU:OE2	20:B:401:HOH:O	2.10	0.67
6:L:289:VAL:O	6:L:290:ASN:HB2	1.95	0.67
1:A:619:GLY:O	1:A:634:GLN:NE2	2.30	0.64
2:B:120:ARG:NH2	2:B:124:GLU:OE1	2.30	0.63
1:G:170:ILE:HD11	18:G:710:ACT:H2	1.79	0.63
1:A:257:PRO:HG2	1:A:294:ILE:HD11	1.80	0.63
5:E:149:CYS:SG	6:F:59:ARG:NE	2.72	0.62
2:B:153:CYS:SG	3:C:80:CYS:HB2	2.39	0.62
2:H:13:ASN:ND2	3:I:128:VAL:O	2.31	0.62
3:I:154:GLU:HG3	3:I:157:LEU:HD12	1.82	0.62
1:G:259:ASP:HB3	1:G:270:MET:HG2	1.83	0.61
6:F:125:LEU:O	6:F:128:ASN:ND2	2.34	0.60
5:K:149:CYS:HB3	5:K:238:CYS:SG	2.42	0.60
1:A:271:ARG:NH2	1:A:272:LYS:O	2.34	0.59
1:A:241:ILE:HD11	1:A:288:ILE:HD11	1.83	0.59
1:G:252:CYS:SG	1:G:253:SER:N	2.77	0.58
2:H:140:GLU:N	2:H:267:ALA:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2:VAL:HG11	5:E:164:LEU:HD22	1.87	0.57
6:L:272:LEU:HD11	6:L:446:ALA:HB1	1.87	0.57
6:F:129:LEU:HD12	6:F:130:MET:N	2.21	0.56
3:I:154:GLU:HA	3:I:157:LEU:HB2	1.86	0.56
6:L:289:VAL:O	6:L:290:ASN:CB	2.52	0.56
3:I:164:ILE:HG23	3:I:169:PHE:HB3	1.88	0.56
19:H:304:TP7:HG1C	19:H:304:TP7:C1	2.36	0.55
2:B:54:LYS:HD3	2:B:101:PHE:CZ	2.41	0.55
2:B:124:GLU:HG3	2:B:164:LEU:CD2	2.37	0.55
2:H:78:CYS:SG	2:H:231:CYS:SG	3.05	0.55
4:D:16:CYS:HB2	4:D:67:CYS:SG	2.47	0.55
6:F:257:GLU:OE2	20:F:601:HOH:O	2.18	0.54
3:C:63:LEU:HD23	3:C:65:MET:HE2	1.88	0.54
1:G:482:LEU:HD23	3:I:2:ILE:HB	1.89	0.54
3:C:60:LYS:HG2	3:C:65:MET:HE3	1.89	0.54
5:E:175:ASN:OD1	5:E:175:ASN:N	2.41	0.54
11:H:301:9S8:S5	19:H:304:TP7:H71C	2.48	0.54
6:F:298:SER:O	6:F:319:LYS:NZ	2.40	0.53
1:G:274:ILE:HD13	1:G:288:ILE:HG12	1.90	0.53
2:H:11:MET:SD	2:H:77:VAL:HG21	2.48	0.53
1:A:303:CYS:SG	1:A:306:ASN:N	2.83	0.52
2:H:45:PRO:HD3	2:H:84:SER:HB2	1.92	0.52
2:H:132:VAL:HA	2:H:135:ILE:HG12	1.93	0.51
2:B:78:CYS:SG	2:B:232:PRO:HD2	2.50	0.51
5:E:182:ARG:HG2	5:E:207:CYS:HA	1.92	0.51
2:H:190:LYS:O	2:H:215:LYS:NZ	2.42	0.51
3:C:83:CYS:SG	3:C:93:VAL:HB	2.51	0.51
2:H:215:LYS:O	2:H:219:MET:HG3	2.10	0.51
3:I:83:CYS:SG	3:I:84:TYR:N	2.83	0.51
1:A:628:PRO:HG3	5:E:255:ALA:HB2	1.93	0.50
1:A:649:MET:HE1	4:D:9:ILE:HB	1.93	0.50
5:E:127:PRO:HD3	6:F:36:VAL:HB	1.93	0.50
2:H:50:SER:HB3	3:I:101:ARG:HD3	1.93	0.50
1:A:589:VAL:HG11	1:A:628:PRO:HD3	1.93	0.50
1:A:627:CYS:SG	1:A:630:GLY:N	2.84	0.50
2:B:126:ILE:HG21	2:B:135:ILE:HD11	1.94	0.50
1:A:584:CYS:SG	1:A:610:ALA:N	2.77	0.50
1:A:623:CYS:SG	1:A:624:PRO:HD3	2.52	0.50
3:I:44:CYS:SG	3:I:47:GLY:N	2.83	0.50
2:H:42:CYS:SG	2:H:43:PRO:C	2.95	0.50
1:A:502:ASP:OD1	1:A:512:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:SER:OG	7:A:706:SF4:S3	2.69	0.49
4:D:134:LEU:HA	5:E:298:LEU:HD21	1.94	0.49
3:C:83:CYS:SG	3:C:84:TYR:N	2.85	0.49
6:F:204:LYS:HD2	9:F:502:PE3:H332	1.94	0.49
6:F:4:LEU:HB2	6:F:20:VAL:CG2	2.41	0.49
2:H:285:ASP:O	2:H:289:LYS:HG2	2.12	0.49
5:E:277:ILE:O	5:E:280:LYS:NZ	2.45	0.49
6:L:23:ASP:OD1	6:L:25:SER:OG	2.31	0.49
1:A:374:ASP:OD1	1:A:374:ASP:N	2.44	0.49
6:L:298:SER:O	6:L:319:LYS:NZ	2.46	0.49
1:G:194:CYS:HB2	1:G:197:CYS:SG	2.52	0.48
19:H:304:TP7:O	19:H:304:TP7:HG3C	2.12	0.48
3:I:122:LEU:C	3:I:122:LEU:HD23	2.38	0.48
1:G:623:CYS:SG	1:G:632:LEU:HD21	2.53	0.48
2:H:43:PRO:HB2	2:H:48:PHE:CD2	2.48	0.48
1:G:258:ILE:CG2	1:G:259:ASP:N	2.77	0.48
1:G:579:VAL:HG22	1:G:632:LEU:HD13	1.96	0.48
1:A:628:PRO:HB2	5:E:218:ILE:O	2.13	0.48
5:E:228:CYS:SG	6:F:165:VAL:HG11	2.54	0.48
1:A:628:PRO:HG3	5:E:255:ALA:CB	2.43	0.48
2:H:62:ARG:HH22	2:H:66:ILE:HD11	1.78	0.48
1:A:589:VAL:HG23	5:E:259:ASP:OD2	2.14	0.48
1:A:300:ALA:HA	1:A:308:ILE:HD12	1.96	0.47
8:G:707:GOL:H2	3:I:35:TYR:HA	1.96	0.47
5:K:104:LEU:HD21	5:K:129:LEU:HD21	1.96	0.47
1:A:623:CYS:SG	1:A:632:LEU:HD13	2.54	0.47
1:G:10:VAL:O	1:G:41:ASP:HA	2.14	0.47
2:H:270:MET:SD	2:H:275:LEU:HD21	2.54	0.47
5:K:228:CYS:SG	6:L:165:VAL:HG11	2.53	0.47
1:G:623:CYS:SG	1:G:624:PRO:HD3	2.55	0.47
1:A:406:TYR:CD1	1:A:406:TYR:C	2.93	0.47
2:H:124:GLU:HG3	2:H:164:LEU:HD21	1.97	0.47
1:G:502:ASP:OD1	1:G:512:ARG:NH1	2.48	0.47
2:H:42:CYS:N	2:H:43:PRO:HA	2.29	0.47
2:H:228:VAL:HG21	2:H:263:LEU:HD13	1.97	0.47
6:L:291:THR:HG21	6:L:331:ARG:HG3	1.97	0.47
2:B:42:CYS:N	2:B:43:PRO:HA	2.29	0.47
2:B:124:GLU:HG3	2:B:164:LEU:HD22	1.95	0.47
5:E:273:LEU:HB3	5:E:274:PRO:HD3	1.97	0.47
1:G:138:ILE:HB	1:G:572:VAL:CG2	2.45	0.47
1:G:627:CYS:SG	1:G:630:GLY:N	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:HIS:CE1	12:H:303:COM:H11	2.50	0.47
2:H:211:MET:HE3	3:I:45:PRO:HB2	1.97	0.47
3:C:132:LYS:O	3:C:132:LYS:HD3	2.14	0.47
5:E:194:ILE:HG13	5:E:273:LEU:CD1	2.45	0.47
2:B:203:ARG:HD3	3:C:75:TRP:HB3	1.96	0.47
2:B:46:GLY:O	2:B:50:SER:OG	2.33	0.46
6:F:272:LEU:HD11	6:F:446:ALA:HB1	1.96	0.46
2:H:54:LYS:HD2	2:H:101:PHE:CZ	2.50	0.46
2:H:78:CYS:SG	2:H:232:PRO:HD2	2.55	0.46
1:A:274:ILE:HD12	1:A:288:ILE:HG12	1.97	0.46
1:A:399:CYS:SG	1:G:433:PHE:HA	2.55	0.46
1:A:433:PHE:HA	1:G:399:CYS:SG	2.55	0.46
4:D:51:ILE:HD13	4:D:62:VAL:HG11	1.97	0.46
6:F:128:ASN:OD1	6:F:130:MET:HB2	2.15	0.46
2:H:25:VAL:O	2:H:29:LEU:HG	2.15	0.46
1:G:598:ALA:HB3	1:G:599:PRO:HD3	1.96	0.46
2:H:26:MET:HB3	2:H:31:VAL:CG2	2.44	0.46
2:H:51:PHE:CZ	3:I:114:HIS:HB3	2.51	0.46
4:J:134:LEU:HA	5:K:298:LEU:HD21	1.97	0.46
6:L:74:LYS:NZ	6:L:236:TYR:O	2.49	0.46
5:E:12:CYS:O	5:E:13:SER:OG	2.32	0.46
2:H:24:THR:OG1	2:H:270:MET:HE1	2.16	0.46
1:A:584:CYS:SG	1:A:609:VAL:HA	2.56	0.46
1:A:594:CYS:SG	1:A:597:GLY:N	2.89	0.46
3:C:31:LEU:HD12	3:C:58:ILE:HG23	1.98	0.46
3:C:80:CYS:HG	3:C:82:THR:HG1	1.59	0.46
3:I:40:CYS:SG	3:I:41:THR:N	2.89	0.46
3:I:175:PHE:HD1	3:I:182:LEU:HD23	1.80	0.46
1:A:386:CYS:SG	1:A:428:MET:HE2	2.55	0.46
1:A:299:CYS:SG	1:A:308:ILE:HD13	2.56	0.46
1:A:379:LYS:HG3	1:A:380:ARG:HG3	1.97	0.46
1:A:621:GLY:C	1:A:624:PRO:HD2	2.40	0.46
2:B:24:THR:OG1	2:B:270:MET:CE	2.63	0.46
1:G:138:ILE:HB	1:G:572:VAL:HG23	1.97	0.46
2:H:264:LEU:O	2:H:268:MET:HG2	2.15	0.46
4:J:17:THR:HG21	4:J:65:GLY:HA3	1.97	0.46
1:A:252:CYS:SG	1:A:274:ILE:HG21	2.56	0.46
4:J:68:HIS:HA	4:J:106:TRP:HB3	1.98	0.45
1:A:189:PHE:O	1:G:524:LYS:NZ	2.35	0.45
1:G:470:VAL:CG1	1:G:483:GLU:HG3	2.47	0.45
6:F:4:LEU:HB2	6:F:20:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:TYR:HE1	1:G:40:ARG:HD3	1.81	0.45
2:H:46:GLY:N	12:H:303:COM:O3S	2.48	0.45
3:C:80:CYS:O	3:C:81:TYR:HB2	2.15	0.45
5:E:182:ARG:NH2	5:E:229:PRO:O	2.45	0.45
1:G:255:VAL:HG12	1:G:298:LEU:HB3	1.99	0.45
1:G:245:LYS:HE2	1:G:305:PRO:O	2.17	0.45
1:A:446:LYS:HD3	3:C:33:ALA:HB2	1.99	0.45
2:H:266:LEU:HD12	2:H:275:LEU:HD11	1.99	0.45
4:J:51:ILE:HB	4:J:88:LEU:HD21	1.99	0.45
1:A:92:PHE:CZ	1:A:574:PRO:HD2	2.52	0.45
2:H:44:ALA:HB3	2:H:47:VAL:HG22	1.97	0.45
1:A:247:THR:OG1	1:A:249:CYS:N	2.50	0.45
2:B:21:ALA:HB1	2:B:261:SER:O	2.17	0.44
1:A:393:LYS:NZ	3:I:90:ASP:OD1	2.48	0.44
2:B:45:PRO:HD2	12:B:303:COM:O2S	2.18	0.44
1:A:371:ARG:NH1	1:A:468:ASN:OD1	2.48	0.44
1:G:226:TYR:CZ	1:G:615:ALA:HB1	2.52	0.44
4:D:13:CYS:O	4:D:18:TYR:HB2	2.16	0.44
1:G:386:CYS:SG	1:G:428:MET:HE2	2.58	0.44
1:G:457:PRO:HA	1:G:473:ALA:HB2	1.99	0.44
1:A:299:CYS:SG	1:A:300:ALA:N	2.90	0.44
1:G:453:MET:HE1	3:I:63:LEU:HD13	1.99	0.44
1:A:577:ALA:O	1:A:612:VAL:HG21	2.17	0.44
2:H:109:VAL:HB	3:I:159:GLU:HG2	1.98	0.44
6:L:409:GLY:HA3	6:L:435:LEU:HD11	1.99	0.44
2:B:20:ALA:HB2	3:C:143:LEU:HD21	1.99	0.44
3:C:137:LEU:O	3:C:141:ILE:HG12	2.18	0.44
6:F:177:LYS:HE2	6:F:179:GLU:HB3	1.99	0.44
2:H:22:THR:HG21	2:H:77:VAL:HG11	1.98	0.44
6:F:14:GLY:HA3	6:F:443:LEU:HB2	2.00	0.44
2:H:1:MET:HE3	2:H:31:VAL:HG12	2.00	0.44
1:A:589:VAL:HG11	1:A:628:PRO:CD	2.48	0.43
2:B:153:CYS:HB2	11:B:302:9S8:S3	2.58	0.43
4:D:86:MET:HG3	5:E:270:PRO:HB2	1.99	0.43
5:K:145:PHE:CD1	8:K:304:GOL:H11	2.53	0.43
4:D:85:VAL:HG13	4:D:86:MET:HE2	2.00	0.43
5:E:154:GLU:O	5:E:158:GLU:HG3	2.18	0.43
4:J:133:LYS:HA	4:J:136:GLU:OE1	2.18	0.43
6:L:129:LEU:HD12	6:L:130:MET:N	2.33	0.43
5:E:2:VAL:HG13	5:E:2:VAL:O	2.17	0.43
2:H:124:GLU:HG3	2:H:164:LEU:CD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:100:GLU:HB3	4:J:125:LYS:HE3	1.99	0.43
2:B:124:GLU:HG3	2:B:164:LEU:HD21	1.99	0.43
6:F:290:ASN:CG	6:F:291:THR:H	2.25	0.43
1:G:255:VAL:CG1	1:G:298:LEU:HB3	2.48	0.43
1:G:305:PRO:O	1:G:306:ASN:HB2	2.18	0.43
5:K:4:ILE:HG12	5:K:33:VAL:CG1	2.48	0.43
5:K:14:GLY:HA2	6:L:62:GLY:HA3	2.00	0.43
2:B:22:THR:HG21	2:B:77:VAL:HG11	2.01	0.43
2:B:78:CYS:SG	2:B:231:CYS:SG	3.16	0.43
5:K:273:LEU:HB3	5:K:274:PRO:HD3	2.01	0.43
6:L:351:ILE:HG23	6:L:352:VAL:HG13	2.01	0.43
1:A:112:GLU:CD	1:A:112:GLU:H	2.26	0.43
1:A:371:ARG:HD2	1:A:487:ASP:O	2.18	0.43
2:H:42:CYS:O	2:H:60:ALA:HA	2.17	0.43
1:A:578:SER:HA	1:A:612:VAL:HG21	2.01	0.43
2:B:19:GLU:O	2:B:23:ARG:HG3	2.19	0.43
1:G:406:TYR:CD1	1:G:406:TYR:C	2.96	0.43
1:A:356:GLU:OE1	20:A:801:HOH:O	2.21	0.43
5:E:149:CYS:HB3	5:E:238:CYS:HB2	2.00	0.43
4:D:51:ILE:HG13	4:D:88:LEU:HD21	1.99	0.43
1:G:403:CYS:HB2	7:G:702:SF4:S3	2.59	0.43
1:A:587:CYS:SG	1:A:589:VAL:N	2.77	0.42
3:C:65:MET:O	3:C:68:VAL:HG22	2.19	0.42
4:D:68:HIS:HA	4:D:106:TRP:HB3	2.01	0.42
6:F:20:VAL:O	6:F:20:VAL:HG23	2.19	0.42
1:G:602:VAL:HG12	1:G:603:GLU:N	2.34	0.42
2:H:19:GLU:OE2	2:H:23:ARG:NH1	2.48	0.42
2:H:193:CYS:SG	2:H:195:GLY:N	2.88	0.42
4:J:48:PRO:HD2	5:K:254:SER:HB2	2.01	0.42
4:J:134:LEU:HB2	5:K:298:LEU:HD11	2.01	0.42
6:L:64:CYS:SG	16:L:504:FCO:C3	3.07	0.42
2:H:68:GLU:HB2	2:H:117:VAL:CG2	2.49	0.42
2:H:206:GLU:OE2	2:H:248:LYS:HD3	2.19	0.42
6:F:225:MET:HE2	6:F:287:TYR:CE2	2.55	0.42
4:J:87:MET:HG3	5:K:257:CYS:SG	2.58	0.42
5:K:12:CYS:O	5:K:13:SER:OG	2.34	0.42
6:F:235:LEU:HA	6:F:372:GLU:HB2	2.00	0.42
2:H:62:ARG:HG2	2:H:62:ARG:HH21	1.83	0.42
2:H:153:CYS:SG	3:I:80:CYS:HB2	2.59	0.42
2:H:284:VAL:O	2:H:284:VAL:HG22	2.19	0.42
4:D:134:LEU:HB2	5:E:298:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:ALA:HB2	2:H:92:LEU:HD11	2.01	0.42
3:I:16:ILE:O	3:I:20:THR:HG23	2.19	0.42
3:I:20:THR:HG22	3:I:25:ASP:HA	2.01	0.42
1:A:403:CYS:HA	1:A:406:TYR:CE2	2.55	0.42
1:A:587:CYS:SG	1:A:589:VAL:HB	2.59	0.42
4:D:33:PRO:O	4:D:36:ARG:NH1	2.52	0.42
6:F:77:ASP:O	6:F:80:PHE:O	2.36	0.42
6:F:364:VAL:HG12	6:F:366:ASP:H	1.84	0.42
2:H:279:VAL:HG21	3:I:137:LEU:CD1	2.50	0.42
3:I:170:ASP:OD1	3:I:170:ASP:N	2.53	0.42
6:L:115:ASP:OD1	6:L:127:ARG:HD3	2.19	0.42
6:L:68:HIS:NE2	6:L:445:CYS:SG	2.73	0.42
2:B:42:CYS:O	2:B:60:ALA:HA	2.20	0.42
4:D:24:ALA:HA	4:D:29:MET:HE3	2.02	0.42
4:D:48:PRO:HD2	5:E:254:SER:HB2	2.02	0.42
5:K:12:CYS:SG	6:L:62:GLY:N	2.93	0.42
5:K:85:CYS:SG	5:K:90:GLY:HA3	2.60	0.42
1:A:406:TYR:C	1:A:406:TYR:HD1	2.27	0.42
1:A:69:ALA:HA	1:A:97:ALA:HB3	2.02	0.42
1:A:252:CYS:SG	1:A:274:ILE:HD13	2.60	0.42
2:B:55:THR:HA	3:C:167:LEU:HD13	2.02	0.42
3:I:80:CYS:O	3:I:81:TYR:HB2	2.19	0.42
1:G:305:PRO:O	1:G:306:ASN:CB	2.68	0.41
2:H:64:LEU:HD23	2:H:74:ILE:HD12	2.02	0.41
2:H:266:LEU:CD1	2:H:275:LEU:CD1	2.98	0.41
5:E:84:THR:HG21	5:E:287:PHE:HB3	2.02	0.41
6:F:44:PHE:CD1	6:F:44:PHE:C	2.98	0.41
2:H:61:ALA:HA	2:H:64:LEU:HD12	2.01	0.41
2:H:120:ARG:NH2	2:H:124:GLU:OE2	2.53	0.41
2:H:123:ALA:HB1	2:H:173:LEU:HD21	2.02	0.41
2:H:276:ALA:HB2	3:I:141:ILE:HD11	2.02	0.41
6:F:158:GLY:HA2	6:F:166:THR:OG1	2.21	0.41
1:A:587:CYS:SG	1:A:588:GLY:N	2.93	0.41
2:B:228:VAL:HA	2:B:258:LEU:O	2.20	0.41
1:G:235:MET:HE3	1:G:237:LYS:HG2	2.02	0.41
3:I:116:MET:HE1	3:I:182:LEU:HD12	2.02	0.41
2:H:47:VAL:HG23	2:H:48:PHE:N	2.34	0.41
1:A:260:VAL:HG13	1:A:292:HIS:CD2	2.55	0.41
1:A:313:GLU:HG3	1:A:314:PRO:HD2	2.03	0.41
2:B:42:CYS:SG	2:B:43:PRO:C	3.04	0.41
6:F:244:ASN:HD21	6:F:248:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:CYS:SG	1:G:16:ASN:HB2	2.60	0.41
5:K:40:VAL:HG13	5:K:41:LEU:HG	2.02	0.41
3:C:40:CYS:SG	3:C:41:THR:N	2.94	0.41
1:G:290:LYS:O	1:G:292:HIS:N	2.53	0.41
5:K:251:LYS:HD3	5:K:251:LYS:HA	1.95	0.41
6:L:235:LEU:HA	6:L:372:GLU:HB2	2.02	0.41
1:A:598:ALA:HB3	1:A:599:PRO:HD3	2.03	0.41
1:G:256:CYS:SG	1:G:272:LYS:HB3	2.61	0.41
1:G:403:CYS:HA	1:G:406:TYR:CE2	2.56	0.41
1:G:452:PHE:HB2	8:G:707:GOL:H12	2.03	0.41
1:G:587:CYS:SG	1:G:589:VAL:CG2	3.01	0.41
2:H:4:ALA:HB1	2:H:36:MET:CG	2.50	0.41
2:H:10:ILE:HD11	3:I:128:VAL:HG21	2.03	0.41
2:H:126:ILE:HG23	2:H:135:ILE:HD11	2.03	0.41
1:A:591:VAL:CG2	5:E:188:GLY:HA3	2.51	0.41
2:B:108:LYS:HD3	3:C:166:GLU:HG3	2.02	0.41
2:B:143:LEU:HD11	2:B:266:LEU:HB2	2.03	0.41
6:F:64:CYS:SG	16:F:505:FCO:C3	3.09	0.41
1:G:8:VAL:O	1:G:39:ALA:HA	2.21	0.41
1:G:260:VAL:N	1:G:271:ARG:O	2.53	0.41
1:G:640:ILE:O	1:G:644:LYS:HG2	2.21	0.41
2:H:1:MET:HB2	2:H:31:VAL:HG12	2.02	0.41
2:H:31:VAL:O	2:H:31:VAL:HG23	2.21	0.41
2:H:47:VAL:HG23	2:H:48:PHE:CD2	2.56	0.41
2:H:270:MET:SD	2:H:275:LEU:CD2	3.09	0.41
2:H:277:LEU:HD13	2:H:284:VAL:HG11	2.02	0.41
5:K:127:PRO:HD3	6:L:36:VAL:HB	2.03	0.41
6:L:79:VAL:O	6:L:364:VAL:N	2.49	0.41
4:D:17:THR:HG21	4:D:65:GLY:HA3	2.03	0.41
5:E:4:ILE:CD1	5:E:33:VAL:HG21	2.51	0.41
5:E:4:ILE:HD11	5:E:33:VAL:HG21	2.02	0.41
5:K:228:CYS:HB2	5:K:229:PRO:HD3	2.03	0.41
2:H:4:ALA:HB1	2:H:36:MET:HG2	2.03	0.40
2:H:228:VAL:HA	2:H:258:LEU:O	2.21	0.40
5:K:42:MET:HE3	6:L:130:MET:HE1	2.02	0.40
6:L:435:LEU:HD13	6:L:435:LEU:C	2.46	0.40
1:A:280:GLN:OE1	1:A:280:GLN:N	2.52	0.40
6:F:291:THR:HG21	6:F:331:ARG:HG3	2.03	0.40
1:G:290:LYS:C	1:G:292:HIS:N	2.76	0.40
2:H:213:ASN:HD22	2:H:213:ASN:C	2.28	0.40
2:H:257:VAL:O	2:H:258:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:215:CYS:O	5:K:252:MET:HE1	2.22	0.40
2:B:174:ASP:OD1	2:B:184:SER:OG	2.35	0.40
2:H:22:THR:HG21	2:H:77:VAL:CG1	2.51	0.40
2:H:125:LEU:HD12	2:H:129:ASP:HB2	2.02	0.40
5:K:264:ASN:OD1	5:K:267:ASP:HB2	2.22	0.40
6:L:44:PHE:CD1	6:L:44:PHE:C	3.00	0.40
1:A:602:VAL:CG1	1:A:603:GLU:N	2.85	0.40
2:B:209:LEU:HD22	2:B:245:ILE:HG13	2.03	0.40
3:C:116:MET:HE2	3:C:182:LEU:HD12	2.02	0.40
3:I:122:LEU:HD21	3:I:177:TRP:CZ3	2.56	0.40
3:I:176:ASP:OD1	3:I:177:TRP:N	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:ASP:OD2	6:L:190:ARG:NH1[3_546]	1.99	0.21

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	650/654 (99%)	624 (96%)	25 (4%)	1 (0%)	43	51
1	G	651/654 (100%)	615 (94%)	35 (5%)	1 (0%)	43	51
2	B	289/291 (99%)	281 (97%)	8 (3%)	0	100	100
2	H	289/291 (99%)	278 (96%)	11 (4%)	0	100	100
3	C	182/184 (99%)	177 (97%)	5 (3%)	0	100	100
3	I	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
4	D	135/140 (96%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	J	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
5	E	296/299 (99%)	286 (97%)	10 (3%)	0	100	100
5	K	296/299 (99%)	287 (97%)	9 (3%)	0	100	100
6	F	445/473 (94%)	437 (98%)	6 (1%)	2 (0%)	30	34
6	L	445/473 (94%)	439 (99%)	4 (1%)	2 (0%)	30	34
All	All	3995/4082 (98%)	3866 (97%)	123 (3%)	6 (0%)	43	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	290	ASN
6	F	290	ASN
6	L	398	ALA
1	A	70	ALA
6	F	398	ALA
1	G	70	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	539/541 (100%)	530 (98%)	9 (2%)	53	69
1	G	540/541 (100%)	526 (97%)	14 (3%)	40	55
2	B	242/242 (100%)	242 (100%)	0	100	100
2	H	241/242 (100%)	239 (99%)	2 (1%)	73	85
3	C	156/157 (99%)	150 (96%)	6 (4%)	29	40
3	I	156/157 (99%)	151 (97%)	5 (3%)	34	47
4	D	116/119 (98%)	116 (100%)	0	100	100
4	J	117/119 (98%)	117 (100%)	0	100	100
5	E	255/256 (100%)	247 (97%)	8 (3%)	35	48
5	K	255/256 (100%)	249 (98%)	6 (2%)	43	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	386/410 (94%)	380 (98%)	6 (2%)	55 71
6	L	386/410 (94%)	381 (99%)	5 (1%)	61 76
All	All	3389/3450 (98%)	3328 (98%)	61 (2%)	51 68

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	CYS
1	A	272	LYS
1	A	294	ILE
1	A	404	CYS
1	A	406	TYR
1	A	503	GLU
1	A	584	CYS
1	A	587	CYS
1	A	627	CYS
3	C	34	CYS
3	C	35	TYR
3	C	60	LYS
3	C	77	CYS
3	C	115	LYS
3	C	184	GLU
5	E	33	VAL
5	E	111	THR
5	E	117	ASP
5	E	161	LYS
5	E	175	ASN
5	E	207	CYS
5	E	235	CYS
5	E	238	CYS
6	F	37	GLU
6	F	65	GLN
6	F	82	VAL
6	F	102	HIS
6	F	290	ASN
6	F	445	CYS
1	G	60	GLU
1	G	153	VAL
1	G	206	VAL
1	G	249	CYS
1	G	258	ILE

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Mol	Chain	Res	Type
1	G	403	CYS
1	G	404	CYS
1	G	406	TYR
1	G	446	LYS
1	G	584	CYS
1	G	587	CYS
1	G	617	CYS
1	G	620	CYS
1	G	627	CYS
2	H	25	VAL
2	H	233	PHE
3	I	34	CYS
3	I	35	TYR
3	I	77	CYS
3	I	93	VAL
3	I	139	LYS
5	K	8	TRP
5	K	111	THR
5	K	129	LEU
5	K	207	CYS
5	K	235	CYS
5	K	238	CYS
6	L	65	GLN
6	L	102	HIS
6	L	128	ASN
6	L	251	TYR
6	L	445	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	224	GLN
1	A	229	ASN
1	A	251	GLN
1	A	593	GLN
4	D	124	ASN
1	G	61	HIS
1	G	62	ASN
1	G	102	HIS
1	G	109	HIS
1	G	192	ASN

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Mol	Chain	Res	Type
1	G	385	GLN
2	H	229	ASN
2	H	235	HIS
2	H	262	GLN
2	H	280	HIS
3	I	109	ASN
4	J	124	ASN
6	L	97	GLN
6	L	394	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 5 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SF4	G	703	1	0,12,12	-	-	-		
10	FAD	A	709	-	56,58,58	1.43	9 (16%)	81,89,89	1.64	17 (20%)
18	ACT	G	710	-	3,3,3	0.76	0	3,3,3	1.44	0
7	SF4	I	201	3	0,12,12	-	-	-		
7	SF4	A	702	-	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SF4	G	704	1	0,12,12	-	-	-		
11	9S8	H	302	2	2,10,10	1.14	0	-		
7	SF4	E	303	5	0,12,12	-	-	-		
12	COM	B	303	-	6,6,6	1.33	1 (16%)	7,8,8	2.99	4 (57%)
11	9S8	B	301	2	2,10,10	1.55	1 (50%)	-		
7	SF4	K	303	5	0,12,12	-	-	-		
19	TP7	H	304	-	19,20,20	0.64	0	24,26,26	1.05	0
7	SF4	C	202	3	0,12,12	-	-	-		
11	9S8	H	301	2	2,10,10	1.13	0	-		
9	PE3	F	501	-	8,8,42	0.45	0	7,7,41	0.31	0
8	GOL	B	304	-	5,5,5	0.38	0	5,5,5	0.19	0
8	GOL	G	707	-	5,5,5	0.35	0	5,5,5	0.13	0
18	ACT	G	709	-	3,3,3	0.80	0	3,3,3	1.35	0
9	PE3	F	502	-	8,8,42	0.46	0	7,7,41	0.22	0
7	SF4	G	702	1	0,12,12	-	-	-		
8	GOL	E	304	-	5,5,5	0.34	0	5,5,5	0.22	0
9	PE3	A	708	-	13,13,42	0.49	0	12,12,41	0.19	0
7	SF4	A	701	1	0,12,12	-	-	-		
7	SF4	E	302	5	0,12,12	-	-	-		
7	SF4	E	301	5	0,12,12	-	-	-		
9	PE3	L	501	-	8,8,42	0.50	0	7,7,41	0.21	0
7	SF4	G	705	1	0,12,12	-	-	-		
16	FCO	F	505	6	1,6,6	3.98	1 (100%)	-		
7	SF4	A	705	1	0,12,12	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
7	SF4	A	706	1	0,12,12	-	-	-		
7	SF4	K	301	5	0,12,12	-	-	-		
14	TRS	D	202	-	7,7,7	0.27	0	9,9,9	0.39	0
8	GOL	B	305	-	5,5,5	0.30	0	5,5,5	0.25	0
7	SF4	C	201	3	0,12,12	-	-	-		
7	SF4	I	202	3	0,12,12	-	-	-		
7	SF4	G	701	1,15	0,12,12	-	-	-		
7	SF4	G	706	1	0,12,12	-	-	-		
7	SF4	A	703	1	0,12,12	-	-	-		
8	GOL	A	707	-	5,5,5	0.31	0	5,5,5	0.35	0
10	FAD	G	711	-	56,58,58	1.45	9 (16%)	81,89,89	1.61	12 (14%)
13	FES	D	201	4	0,4,4	-	-	-		
12	COM	H	303	-	6,6,6	1.42	2 (33%)	7,8,8	2.67	4 (57%)
11	9S8	B	302	2	2,10,10	1.40	0	-		
7	SF4	K	302	5	0,12,12	-	-	-		
8	GOL	K	304	-	5,5,5	0.35	0	5,5,5	0.22	0
16	FCO	L	504	6	1,6,6	4.21	1 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	FES	J	201	4	0,4,4	-	-	-		

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
7	SF4	G	703	1	-	-	0/6/5/5
10	FAD	A	709	-	-	2/34/50/50	0/6/6/6
7	SF4	I	201	3	-	-	0/6/5/5
7	SF4	A	702	-	-	-	0/6/5/5
7	SF4	G	704	1	-	-	0/6/5/5
11	9S8	H	302	2	-	-	0/3/3/3
7	SF4	E	303	5	-	-	0/6/5/5
12	COM	B	303	-	-	4/4/4/4	-
11	9S8	B	301	2	-	-	0/3/3/3
7	SF4	K	303	5	-	-	0/6/5/5
19	TP7	H	304	-	-	10/24/24/24	-
7	SF4	C	202	3	-	-	0/6/5/5
11	9S8	H	301	2	-	-	0/3/3/3
9	PE3	F	501	-	-	3/6/6/40	-
8	GOL	B	304	-	-	4/4/4/4	-
8	GOL	G	707	-	-	2/4/4/4	-
9	PE3	F	502	-	-	5/6/6/40	-
7	SF4	G	702	1	-	-	0/6/5/5
8	GOL	E	304	-	-	1/4/4/4	-
9	PE3	A	708	-	-	5/11/11/40	-
7	SF4	A	701	1	-	-	0/6/5/5
9	PE3	L	501	-	-	2/6/6/40	-
7	SF4	E	301	5	-	-	0/6/5/5
7	SF4	E	302	5	-	-	0/6/5/5
7	SF4	G	705	1	-	-	0/6/5/5
7	SF4	A	704	1	-	-	0/6/5/5
7	SF4	A	705	1	-	-	0/6/5/5
7	SF4	A	706	1	-	-	0/6/5/5
7	SF4	K	301	5	-	-	0/6/5/5
14	TRS	D	202	-	-	8/9/9/9	-
8	GOL	B	305	-	-	0/4/4/4	-
7	SF4	C	201	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	I	202	3	-	-	0/6/5/5
7	SF4	G	701	1,15	-	-	0/6/5/5
7	SF4	G	706	1	-	-	0/6/5/5
8	GOL	A	707	-	-	2/4/4/4	-
7	SF4	A	703	1	-	-	0/6/5/5
10	FAD	G	711	-	-	1/34/50/50	0/6/6/6
13	FES	D	201	4	-	-	0/1/1/1
12	COM	H	303	-	-	1/4/4/4	-
11	9S8	B	302	2	-	-	0/3/3/3
7	SF4	K	302	5	-	-	0/6/5/5
8	GOL	K	304	-	-	2/4/4/4	-
13	FES	J	201	4	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	711	FAD	C9A-C5X	5.35	1.50	1.41
10	A	709	FAD	C9A-C5X	5.01	1.49	1.41
10	A	709	FAD	C5A-C4A	4.51	1.47	1.39
10	G	711	FAD	C5A-C4A	4.33	1.47	1.39
16	L	504	FCO	O3-C3	4.21	1.21	1.16
16	F	505	FCO	O3-C3	3.98	1.21	1.16
10	G	711	FAD	C8-C7	3.57	1.49	1.40
10	A	709	FAD	C8-C7	3.23	1.49	1.40
10	A	709	FAD	C5A-C6A	2.79	1.48	1.41
10	G	711	FAD	C5X-N5	-2.65	1.34	1.39
10	G	711	FAD	C5A-C6A	2.65	1.48	1.41
10	A	709	FAD	C8A-N7A	2.52	1.36	1.31
10	G	711	FAD	C4-N3	-2.50	1.34	1.38
10	A	709	FAD	C4-N3	-2.49	1.34	1.38
10	G	711	FAD	C8A-N7A	2.29	1.35	1.31
12	H	303	COM	O1S-S2	2.28	1.51	1.45
12	H	303	COM	O2S-S2	2.17	1.51	1.45
12	B	303	COM	O1S-S2	2.17	1.51	1.45
10	G	711	FAD	C5A-N7A	-2.15	1.35	1.39
10	G	711	FAD	C4X-N5	2.13	1.34	1.30
10	A	709	FAD	C5X-N5	-2.12	1.35	1.39
10	A	709	FAD	C4X-N5	2.10	1.34	1.30
10	A	709	FAD	C5A-N7A	-2.05	1.35	1.39
11	B	301	9S8	S3-FE4	-2.05	2.20	2.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	711	FAD	C5A-C4A-N3A	-6.08	118.82	126.75
10	A	709	FAD	C5A-C4A-N3A	-5.86	119.11	126.75
10	G	711	FAD	N3A-C4A-N9A	4.84	135.06	127.08
12	B	303	COM	O3S-S2-O2S	-4.42	100.48	111.27
10	A	709	FAD	N3A-C4A-N9A	4.34	134.24	127.08
12	H	303	COM	O3S-S2-C2	4.14	112.46	105.77
12	H	303	COM	O3S-S2-O2S	-4.06	101.36	111.27
12	B	303	COM	O1S-S2-C2	3.96	111.68	106.92
10	A	709	FAD	C2A-N3A-C4A	3.82	120.78	111.75
10	A	709	FAD	P-O3P-PA	-3.82	119.72	132.83
10	G	711	FAD	C2A-N3A-C4A	3.81	120.74	111.75
10	A	709	FAD	C4A-C5A-N7A	-3.62	106.21	110.62
12	B	303	COM	O3S-S2-C2	3.53	111.48	105.77
12	B	303	COM	O2S-S2-C2	3.43	111.05	106.92
10	A	709	FAD	N3A-C2A-N1A	-3.31	123.43	128.60
10	G	711	FAD	P-O3P-PA	-3.30	121.50	132.83
10	G	711	FAD	C4A-C5A-N7A	-3.26	106.64	110.62
10	G	711	FAD	N3A-C2A-N1A	-3.06	123.82	128.60
10	A	709	FAD	C5A-N7A-C8A	3.04	107.83	103.51
12	H	303	COM	O2S-S2-C2	2.99	110.52	106.92
10	G	711	FAD	C5A-N7A-C8A	2.92	107.66	103.51
10	A	709	FAD	C4X-C10-N1	-2.83	118.17	124.73
10	G	711	FAD	C4A-N9A-C8A	2.81	108.78	105.73
10	A	709	FAD	O4-C4-C4X	-2.73	119.35	126.60
10	G	711	FAD	C4X-C10-N1	-2.68	118.50	124.73
10	A	709	FAD	C4A-N9A-C8A	2.64	108.59	105.73
10	A	709	FAD	C6A-C5A-N7A	2.57	136.82	132.02
10	G	711	FAD	O4-C4-C4X	-2.46	120.06	126.60
10	A	709	FAD	N9A-C8A-N7A	-2.34	110.71	113.91
12	H	303	COM	O1S-S2-C2	2.29	109.67	106.92
10	G	711	FAD	N9A-C8A-N7A	-2.28	110.80	113.91
10	A	709	FAD	C10-N1-C2	2.26	121.43	116.90
10	G	711	FAD	C6A-C5A-N7A	2.19	136.10	132.02
10	A	709	FAD	O2-C2-N1	-2.17	118.23	121.83
10	A	709	FAD	C4X-C4-N3	2.09	118.49	113.19
10	A	709	FAD	C2A-N1A-C6A	2.02	122.23	118.77
10	A	709	FAD	C4X-C10-N10	2.00	119.41	116.48

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	304	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	B	304	GOL	C1-C2-C3-O3
12	B	303	COM	S1-C1-C2-S2
12	B	303	COM	C1-C2-S2-O1S
12	B	303	COM	C1-C2-S2-O2S
12	B	303	COM	C1-C2-S2-O3S
14	D	202	TRS	C3-C-C2-O2
14	D	202	TRS	N-C-C3-O3
19	H	304	TP7	O1-C1-N-CA
19	H	304	TP7	C2-C1-N-CA
19	H	304	TP7	CB-O4P-P-O2P
19	H	304	TP7	OXT-C-CA-N
19	H	304	TP7	C5-C6-C7-S7
9	L	501	PE3	O34-C35-C36-O37
19	H	304	TP7	C4-C5-C6-C7
8	A	707	GOL	C1-C2-C3-O3
8	G	707	GOL	O1-C1-C2-C3
8	K	304	GOL	O1-C1-C2-C3
9	F	502	PE3	C32-C33-O34-C35
8	B	304	GOL	O1-C1-C2-O2
8	B	304	GOL	O2-C2-C3-O3
19	H	304	TP7	O-C-CA-N
14	D	202	TRS	C1-C-C3-O3
12	H	303	COM	S1-C1-C2-S2
8	A	707	GOL	O2-C2-C3-O3
8	K	304	GOL	O1-C1-C2-O2
9	A	708	PE3	O37-C38-C39-O40
8	G	707	GOL	O1-C1-C2-O2
9	F	502	PE3	C33-C32-O31-C30
19	H	304	TP7	C1-C2-C3-C4
9	L	501	PE3	C38-C39-O40-C41
9	F	502	PE3	C36-C35-O34-C33
9	A	708	PE3	C33-C32-O31-C30
14	D	202	TRS	N-C-C1-O1
14	D	202	TRS	C1-C-C2-O2
14	D	202	TRS	C2-C-C1-O1
9	A	708	PE3	C32-C33-O34-C35
19	H	304	TP7	CB-CA-N-C1
19	H	304	TP7	CB-O4P-P-O1P
9	F	502	PE3	O31-C32-C33-O34
9	F	501	PE3	C36-C35-O34-C33
9	F	501	PE3	O31-C32-C33-O34
9	F	502	PE3	O34-C35-C36-O37

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Mol	Chain	Res	Type	Atoms
10	A	709	FAD	O4B-C4B-C5B-O5B
14	D	202	TRS	N-C-C2-O2
14	D	202	TRS	C2-C-C3-O3
8	E	304	GOL	C1-C2-C3-O3
9	A	708	PE3	O34-C35-C36-O37
9	A	708	PE3	O31-C32-C33-O34
10	G	711	FAD	O4B-C4B-C5B-O5B
10	A	709	FAD	C2B-C1B-N9A-C8A
9	F	501	PE3	C32-C33-O34-C35

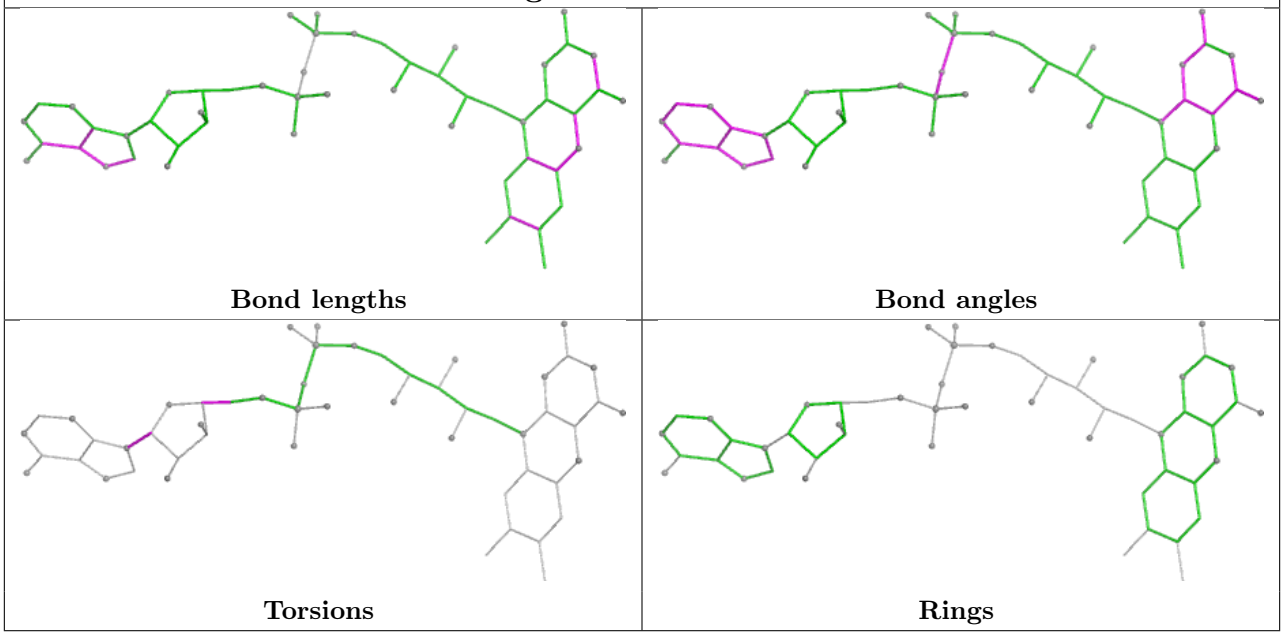
There are no ring outliers.

13 monomers are involved in 16 short contacts:

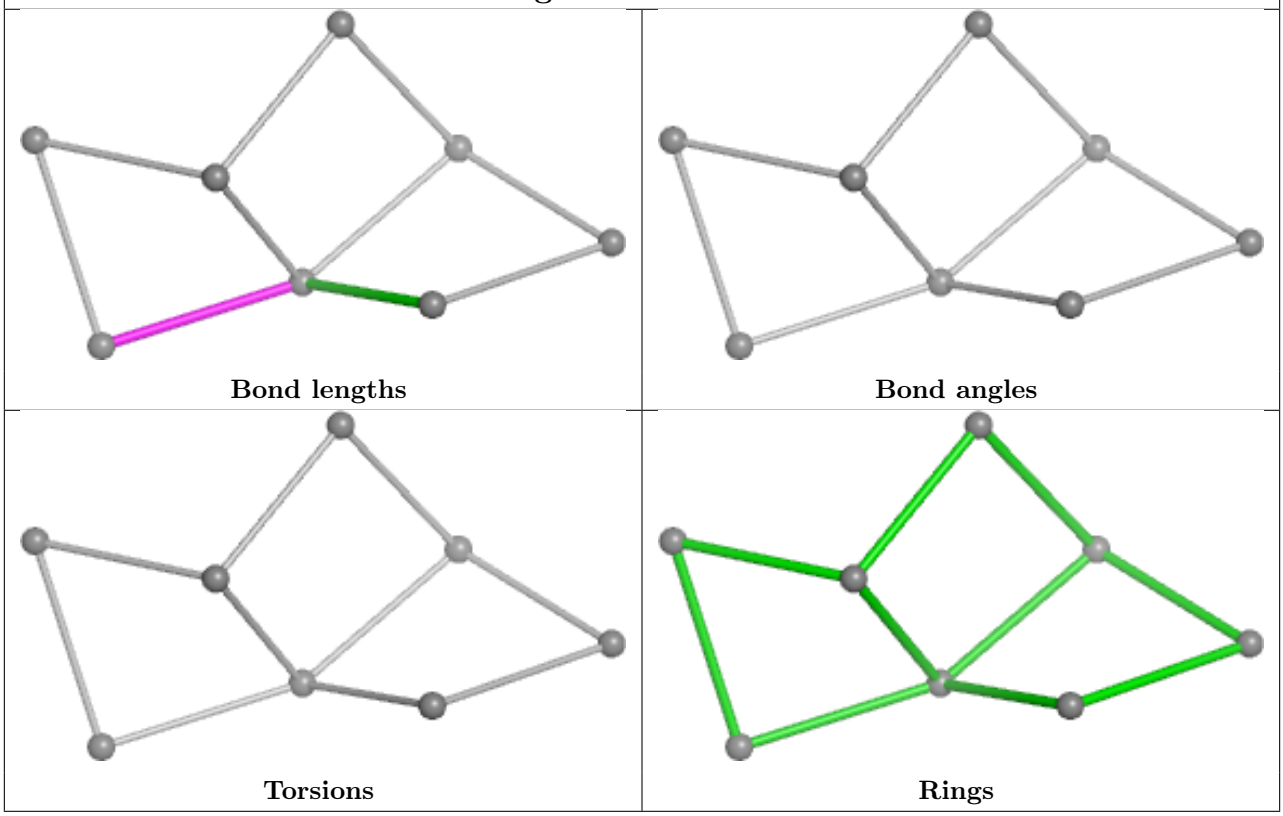
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	710	ACT	1	0
12	B	303	COM	1	0
19	H	304	TP7	3	0
11	H	301	9S8	1	0
8	G	707	GOL	2	0
9	F	502	PE3	1	0
7	G	702	SF4	1	0
16	F	505	FCO	1	0
7	A	706	SF4	1	0
12	H	303	COM	2	0
11	B	302	9S8	1	0
8	K	304	GOL	1	0
16	L	504	FCO	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

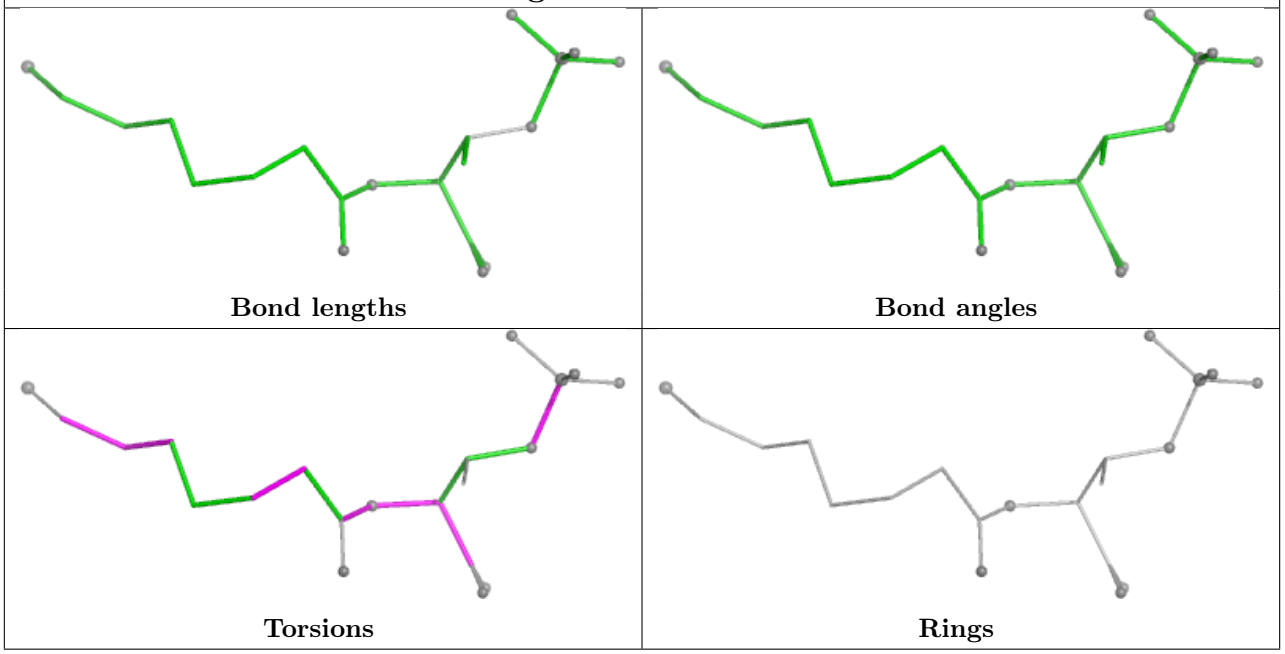
Ligand FAD A 709



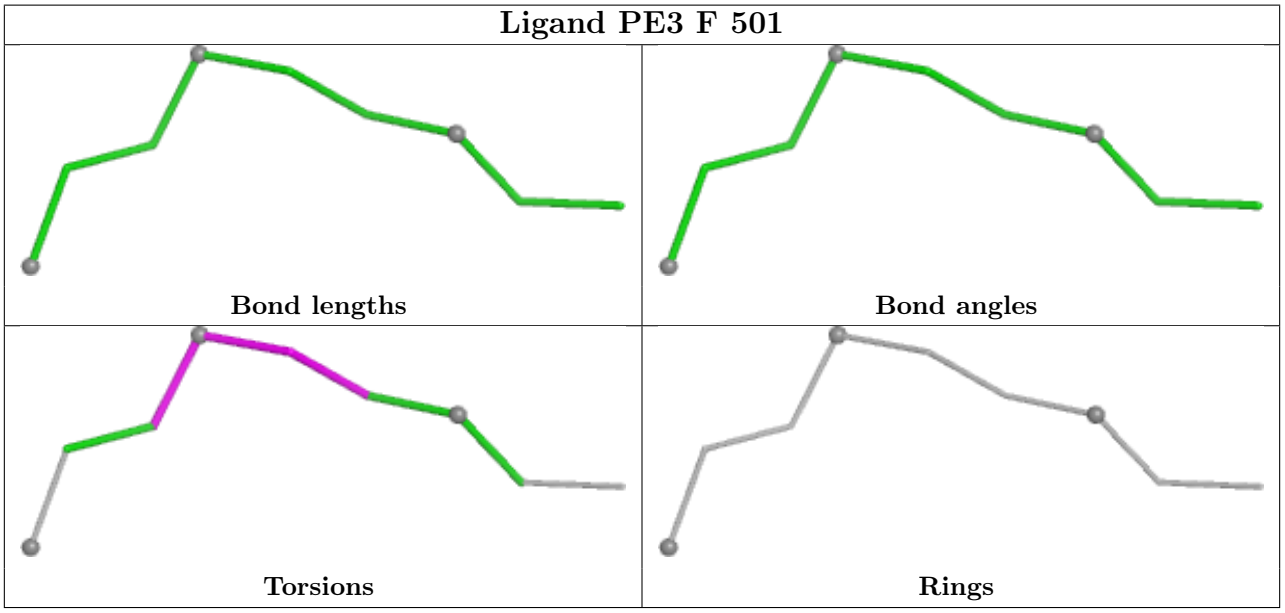
Ligand 9S8 B 301



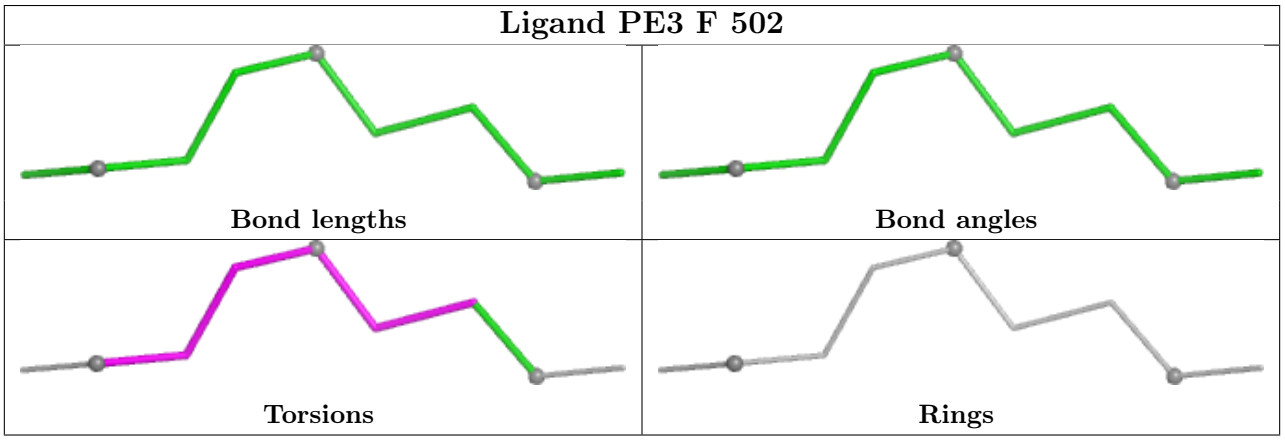
Ligand TP7 H 304



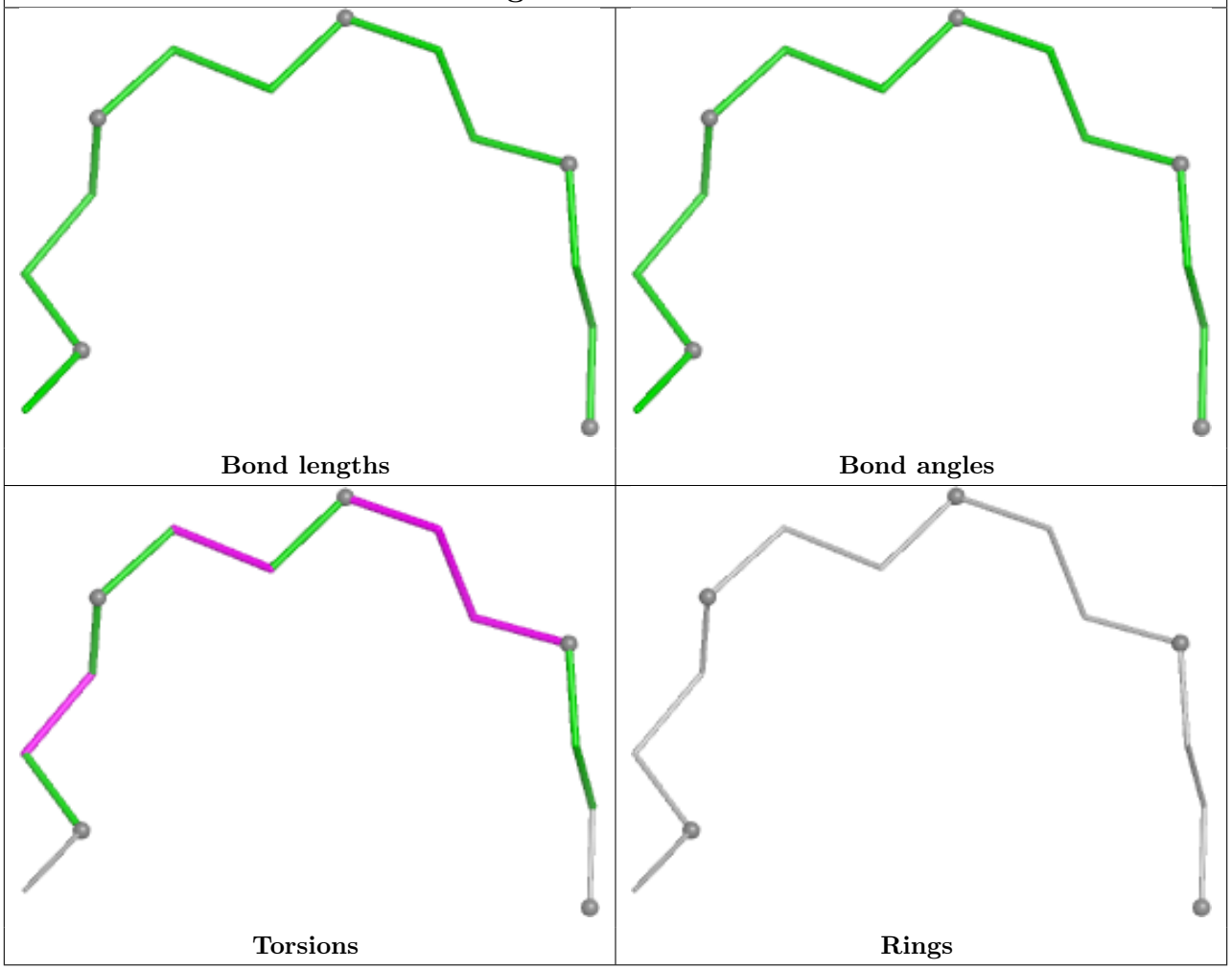
Ligand PE3 F 501



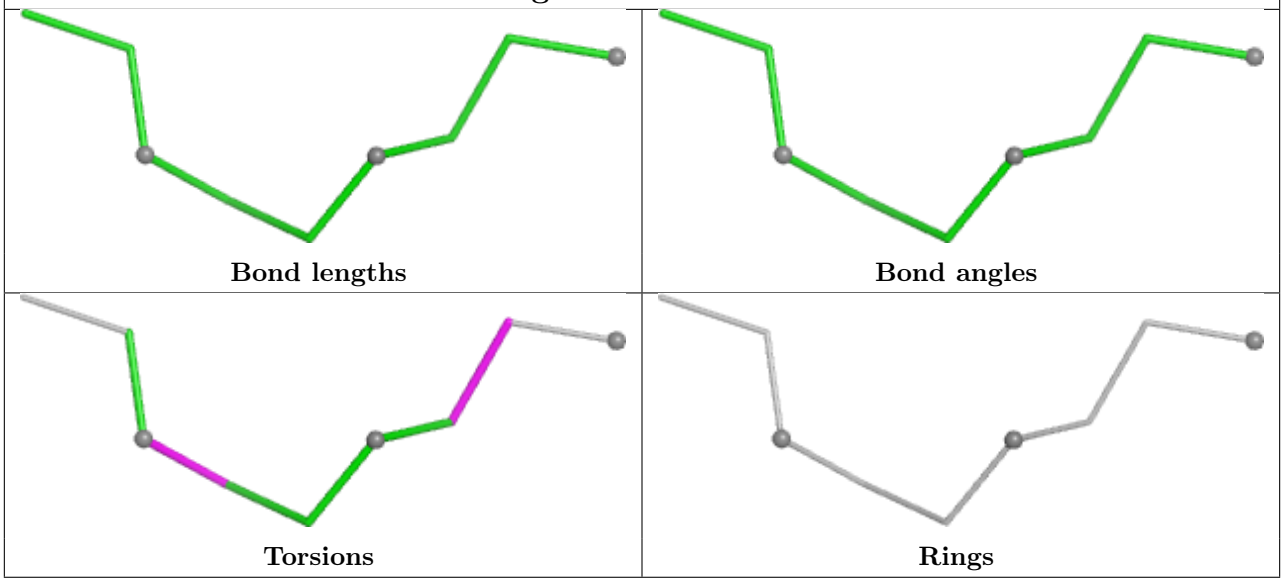
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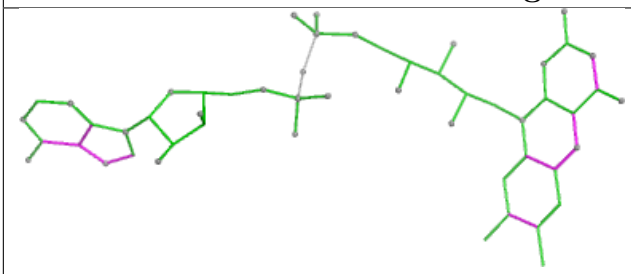
Ligand PE3 A 708



Ligand PE3 L 501



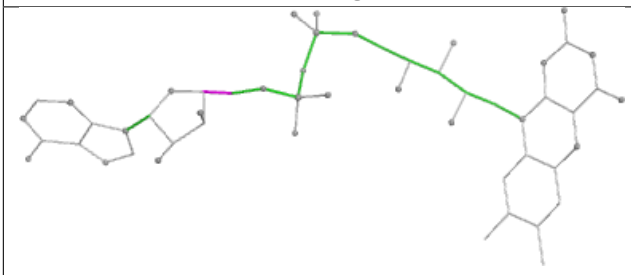
Ligand FAD G 711



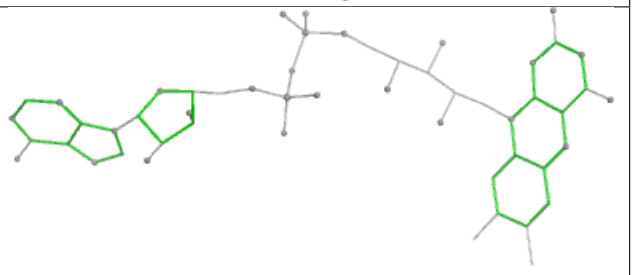
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	652/654 (99%)	0.46	65 (9%) 12 10	13, 31, 81, 112	0
1	G	653/654 (99%)	0.34	30 (4%) 37 34	16, 31, 71, 90	0
2	B	291/291 (100%)	0.54	7 (2%) 59 56	21, 40, 55, 70	0
2	H	291/291 (100%)	1.42	79 (27%) 1 1	31, 54, 98, 116	0
3	C	184/184 (100%)	0.41	6 (3%) 49 46	21, 35, 53, 74	0
3	I	183/184 (99%)	0.80	15 (8%) 17 15	19, 43, 71, 98	0
4	D	137/140 (97%)	0.04	0 100 100	19, 28, 40, 54	0
4	J	138/140 (98%)	0.25	3 (2%) 62 59	21, 30, 43, 76	0
5	E	298/299 (99%)	0.72	16 (5%) 31 28	18, 34, 62, 81	0
5	K	298/299 (99%)	0.26	7 (2%) 61 58	16, 29, 50, 66	0
6	F	447/473 (94%)	0.24	4 (0%) 81 79	15, 30, 52, 75	0
6	L	447/473 (94%)	0.11	8 (1%) 67 64	15, 28, 49, 106	0
All	All	4019/4082 (98%)	0.45	240 (5%) 27 24	13, 33, 67, 116	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	ALA	5.4
1	A	602	VAL	5.4
2	H	25	VAL	5.2
1	G	258	ILE	4.7
3	I	179	LYS	4.6
2	H	263	LEU	4.6
1	A	653	THR	4.5
1	A	248	GLY	4.4
1	A	274	ILE	4.1
1	A	608	VAL	4.1
1	A	247	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	654	ALA	4.0
1	A	310	PHE	4.0
1	A	245	LYS	3.9
2	H	143	LEU	3.9
1	A	288	ILE	3.9
1	A	305	PRO	3.9
1	A	606	GLY	3.8
2	H	33	LEU	3.8
2	H	279	VAL	3.7
1	A	252	CYS	3.7
1	A	249	CYS	3.7
1	A	301	LYS	3.7
1	A	308	ILE	3.6
3	I	180	GLY	3.6
2	H	26	MET	3.6
1	A	605	ASP	3.6
1	A	302	VAL	3.6
2	H	145	ILE	3.6
1	A	306	ASN	3.6
2	H	288	LEU	3.6
1	A	256	CYS	3.6
3	I	177	TRP	3.6
1	A	604	LYS	3.5
2	H	270	MET	3.5
1	A	269	GLY	3.5
2	H	272	PRO	3.5
2	H	18	VAL	3.5
6	L	363	VAL	3.5
2	H	4	ALA	3.5
1	A	298	LEU	3.5
1	G	294	ILE	3.4
2	H	277	LEU	3.4
1	A	590	CYS	3.4
1	A	600	ARG	3.3
2	H	248	LYS	3.3
2	H	224	ALA	3.3
2	H	269	GLY	3.3
2	H	266	LEU	3.3
2	H	132	VAL	3.3
2	H	276	ALA	3.2
1	A	603	GLU	3.2
1	G	252	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	361	ALA	3.2
1	A	294	ILE	3.2
6	F	130	MET	3.2
2	H	278	SER	3.2
2	H	176	ILE	3.2
1	A	303	CYS	3.1
1	G	249	CYS	3.1
2	H	177	VAL	3.1
5	E	200	GLY	3.1
5	E	193	THR	3.1
1	A	307	ALA	3.1
1	A	240	TYR	3.0
1	A	258	ILE	3.0
2	H	31	VAL	3.0
2	H	149	VAL	3.0
3	I	122	LEU	3.0
1	A	607	LYS	3.0
3	I	181	ALA	3.0
1	G	465	GLU	3.0
5	E	164	LEU	2.9
3	I	141	ILE	2.9
2	B	249	PHE	2.9
1	G	602	VAL	2.9
1	A	299	CYS	2.9
6	L	25	SER	2.9
1	G	290	LYS	2.9
2	H	147	VAL	2.9
2	H	291	ILE	2.9
1	A	253	SER	2.9
1	A	255	VAL	2.9
1	G	255	VAL	2.9
1	A	246	CYS	2.9
1	A	286	TYR	2.8
2	H	142	PRO	2.8
6	L	364	VAL	2.8
5	E	205	GLU	2.8
2	B	26	MET	2.8
1	A	244	THR	2.8
5	E	184	LYS	2.8
1	A	609	VAL	2.8
1	A	296	CYS	2.8
4	J	110	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	181	ALA	2.8
2	H	5	PHE	2.8
5	E	235	CYS	2.8
1	A	251	GLN	2.8
6	F	362	GLU	2.8
2	H	135	ILE	2.7
1	A	250	GLY	2.7
1	A	304	GLY	2.7
2	H	30	GLY	2.7
1	G	604	LYS	2.7
1	A	601	LEU	2.7
2	H	230	VAL	2.7
3	I	178	GLU	2.7
5	E	186	GLU	2.7
1	A	297	GLY	2.7
6	L	365	GLY	2.7
2	H	226	CYS	2.6
2	H	287	LEU	2.6
1	A	581	ALA	2.6
1	A	594	CYS	2.6
2	H	220	ILE	2.6
3	I	154	GLU	2.5
6	L	362	GLU	2.5
5	E	177	CYS	2.5
2	H	264	LEU	2.5
3	C	66	ASP	2.5
3	I	176	ASP	2.5
2	H	48	PHE	2.5
2	H	255	PHE	2.5
2	H	139	VAL	2.5
1	A	268	ILE	2.5
2	H	141	ARG	2.5
1	A	273	ALA	2.5
3	I	183	LYS	2.5
1	G	308	ILE	2.5
3	I	172	LEU	2.4
2	H	268	MET	2.4
5	E	203	ASP	2.4
2	H	113	TYR	2.4
2	H	286	PRO	2.4
2	B	291	ILE	2.4
3	I	132	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	275	LEU	2.4
5	K	202	PRO	2.4
1	G	467	GLY	2.4
2	H	75	VAL	2.4
5	K	210	GLU	2.4
2	H	134	LYS	2.3
2	H	130	ILE	2.3
1	G	303	CYS	2.3
5	K	177	CYS	2.3
2	H	259	HIS	2.3
2	B	288	LEU	2.3
2	H	274	ASP	2.3
5	K	49	ASP	2.3
2	H	273	LYS	2.3
1	A	300	ALA	2.3
1	A	612	VAL	2.3
2	H	109	VAL	2.3
2	H	137	GLU	2.3
2	H	262	GLN	2.3
2	H	1	MET	2.3
2	H	136	ALA	2.3
5	E	185	SER	2.3
2	B	93	HIS	2.3
6	L	361	GLU	2.3
1	G	268	ILE	2.3
6	F	2	VAL	2.3
3	C	8	ASN	2.3
2	H	37	THR	2.3
3	C	5	SER	2.3
6	F	359	GLU	2.3
2	H	125	LEU	2.2
2	H	249	PHE	2.2
6	L	129	LEU	2.2
1	G	311	ASP	2.2
2	B	41	CYS	2.2
1	G	615	ALA	2.2
4	J	3	GLU	2.2
5	E	167	LYS	2.2
3	I	163	LEU	2.2
2	H	233	PHE	2.2
5	E	160	VAL	2.2
1	A	311	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	464	PRO	2.2
5	E	199	GLU	2.2
5	K	192	GLU	2.2
1	A	287	THR	2.2
2	H	29	LEU	2.2
2	H	77	VAL	2.2
1	A	278	PHE	2.2
1	G	463	ASP	2.2
2	H	133	ASP	2.2
1	G	270	MET	2.2
3	C	180	GLY	2.2
1	G	292	HIS	2.2
4	J	47	GLU	2.2
2	H	21	ALA	2.2
3	I	135	ALA	2.2
2	H	283	SER	2.2
1	G	298	LEU	2.2
2	H	258	LEU	2.2
2	H	228	VAL	2.2
1	A	261	PRO	2.2
1	A	364	PRO	2.2
1	G	250	GLY	2.2
1	G	246	CYS	2.2
1	A	362	SER	2.2
3	C	84	TYR	2.1
2	B	29	LEU	2.1
1	A	260	VAL	2.1
2	H	34	VAL	2.1
2	H	138	LYS	2.1
5	E	188	GLY	2.1
1	A	293	CYS	2.1
2	H	188	ALA	2.1
2	H	282	ILE	2.1
1	A	295	GLU	2.1
6	L	279	ASP	2.1
1	A	257	PRO	2.1
2	H	256	PRO	2.1
1	A	238	ALA	2.1
2	H	290	LYS	2.1
1	A	292	HIS	2.1
1	A	372	LEU	2.1
1	G	251	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	201	ASN	2.1
2	H	185	VAL	2.1
2	H	284	VAL	2.1
1	A	585	GLY	2.1
2	H	265	GLY	2.1
5	K	299	LYS	2.0
1	G	299	CYS	2.0
1	G	613	ILE	2.0
3	I	124	TYR	2.0
1	G	269	GLY	2.0
1	G	297	GLY	2.0
1	G	96	PHE	2.0
5	K	275	LYS	2.0
2	H	24	THR	2.0
2	H	206	GLU	2.0
2	H	267	ALA	2.0
2	H	74	ILE	2.0
2	H	2	LYS	2.0
5	E	183	LYS	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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	ACT	G	709	4/4	0.74	0.14	38,38,38,47	0
19	TP7	H	304	21/21	0.75	0.16	39,61,74,80	0
18	ACT	G	710	4/4	0.77	0.17	31,39,39,47	0
9	PE3	A	708	14/43	0.82	0.14	30,41,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	B	304	6/6	0.82	0.16	31,38,41,48	0
8	GOL	E	304	6/6	0.82	0.14	38,42,50,53	0
8	GOL	K	304	6/6	0.82	0.16	29,36,41,49	0
9	PE3	L	501	9/43	0.83	0.13	28,39,44,50	0
12	COM	B	303	7/7	0.86	0.12	34,50,61,71	0
9	PE3	F	501	9/43	0.87	0.13	31,33,43,46	0
7	SF4	A	702	8/8	0.87	0.10	101,125,137,146	0
8	GOL	A	707	6/6	0.88	0.12	33,38,40,47	0
8	GOL	B	305	6/6	0.89	0.10	28,39,41,49	0
8	GOL	G	707	6/6	0.90	0.15	26,36,45,46	0
11	9S8	H	301	8/8	0.90	0.10	38,54,72,77	0
9	PE3	F	502	9/43	0.91	0.11	32,41,47,47	0
14	TRS	D	202	8/8	0.92	0.09	25,31,38,40	0
7	SF4	A	703	8/8	0.92	0.08	72,84,107,111	0
11	9S8	H	302	8/8	0.92	0.07	30,44,52,57	0
11	9S8	B	302	8/8	0.92	0.08	21,31,36,37	0
11	9S8	B	301	8/8	0.93	0.10	30,40,47,58	0
7	SF4	G	703	8/8	0.93	0.07	66,69,73,95	0
7	SF4	G	704	8/8	0.93	0.08	73,87,106,125	0
7	SF4	A	706	8/8	0.94	0.05	19,34,42,43	0
12	COM	H	303	7/7	0.94	0.09	34,36,45,53	0
7	SF4	A	704	8/8	0.95	0.06	27,30,37,37	0
7	SF4	C	202	8/8	0.95	0.05	21,29,31,32	0
17	NI	F	506	1/1	0.95	0.10	23,23,23,23	0
7	SF4	G	705	8/8	0.95	0.06	27,30,38,41	0
7	SF4	I	201	8/8	0.95	0.06	19,24,25,28	0
7	SF4	K	303	8/8	0.95	0.06	27,29,36,37	0
7	SF4	E	302	8/8	0.96	0.05	17,31,38,39	0
7	SF4	K	301	8/8	0.96	0.05	15,21,23,23	0
7	SF4	K	302	8/8	0.96	0.06	23,34,36,37	0
7	SF4	E	303	8/8	0.96	0.06	28,39,49,63	0
7	SF4	C	201	8/8	0.96	0.06	20,25,27,32	0
7	SF4	A	705	8/8	0.96	0.05	27,31,42,43	0
10	FAD	A	709	53/53	0.96	0.07	10,19,34,37	0
7	SF4	E	301	8/8	0.96	0.05	20,27,29,34	0
7	SF4	G	706	8/8	0.96	0.05	21,30,36,40	0
7	SF4	I	202	8/8	0.97	0.04	21,23,31,33	0
16	FCO	L	504	7/7	0.97	0.10	20,22,25,29	0
7	SF4	G	702	8/8	0.97	0.05	19,21,24,26	0
7	SF4	A	701	8/8	0.97	0.04	14,20,22,25	0
10	FAD	G	711	53/53	0.97	0.06	10,20,27,28	0
7	SF4	G	701	8/8	0.97	0.05	18,28,37,40	0

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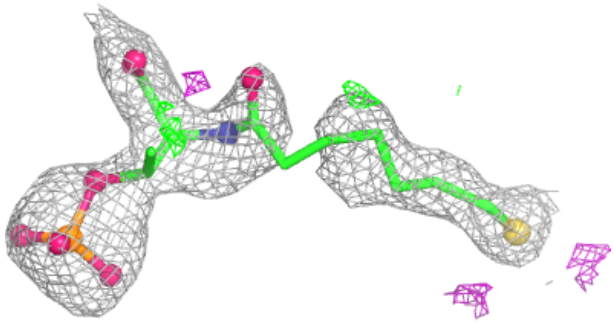
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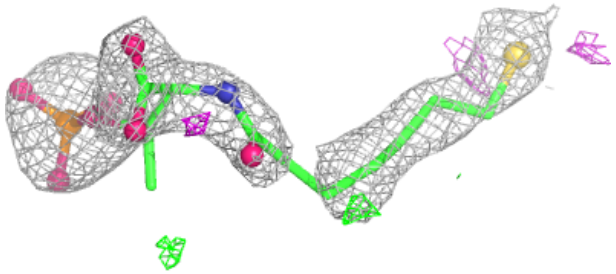
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	NI	L	505	1/1	0.98	0.09	25,25,25,25	0
16	FCO	F	505	7/7	0.98	0.08	14,21,23,24	0
13	FES	D	201	4/4	0.98	0.04	24,24,25,27	0
15	FE	F	504	1/1	0.98	0.03	23,23,23,23	0
15	FE	G	708	1/1	0.99	0.03	32,32,32,32	1
15	FE	L	503	1/1	0.99	0.03	20,20,20,20	0
13	FES	J	201	4/4	0.99	0.04	20,21,26,29	0

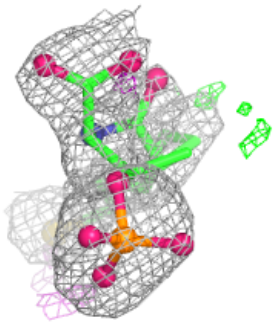
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TP7 H 304:

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

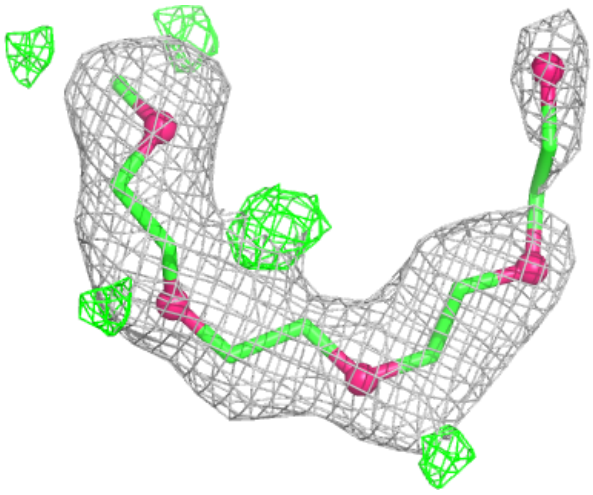


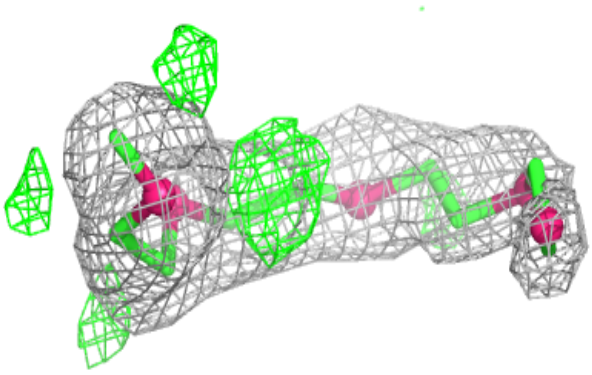


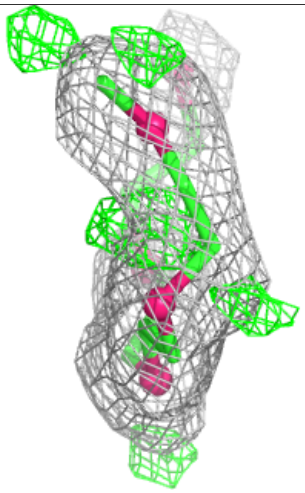


Electron density around PE3 A 708:

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

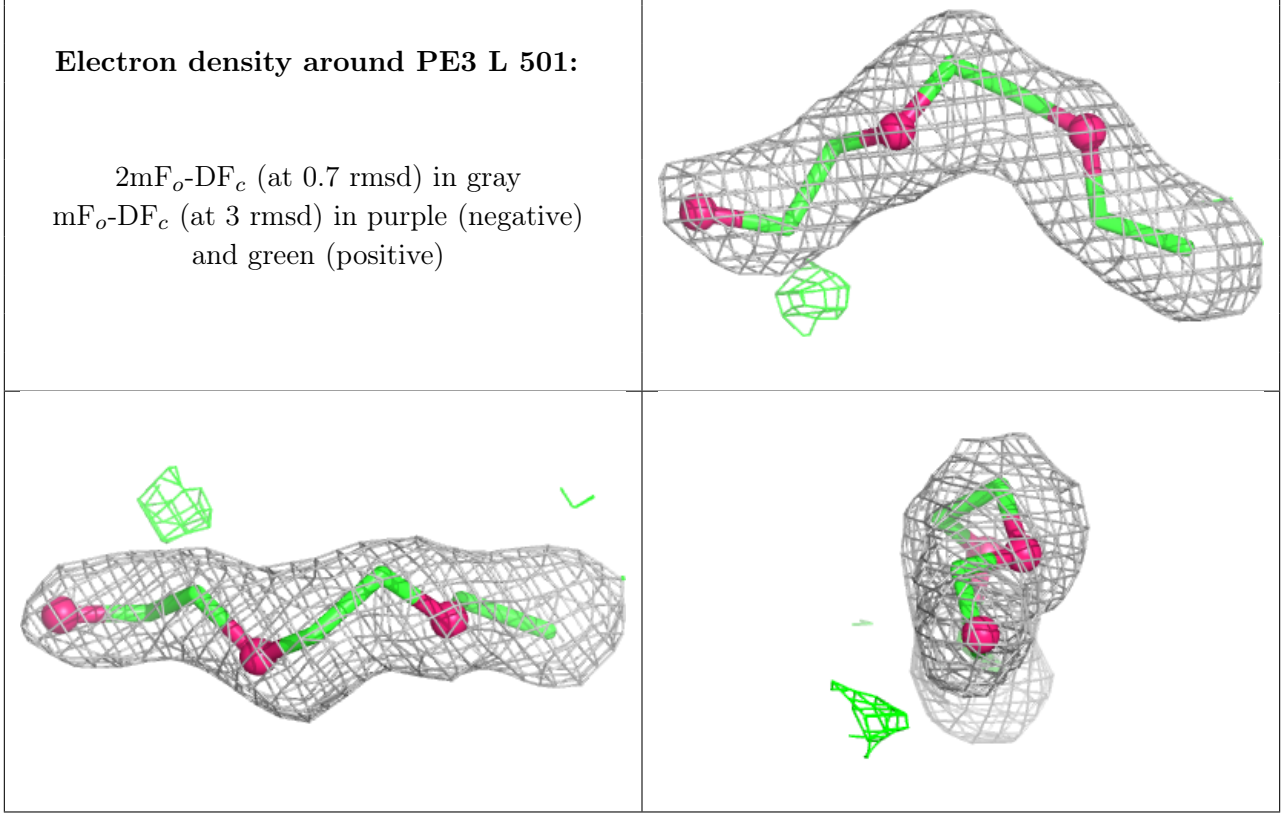






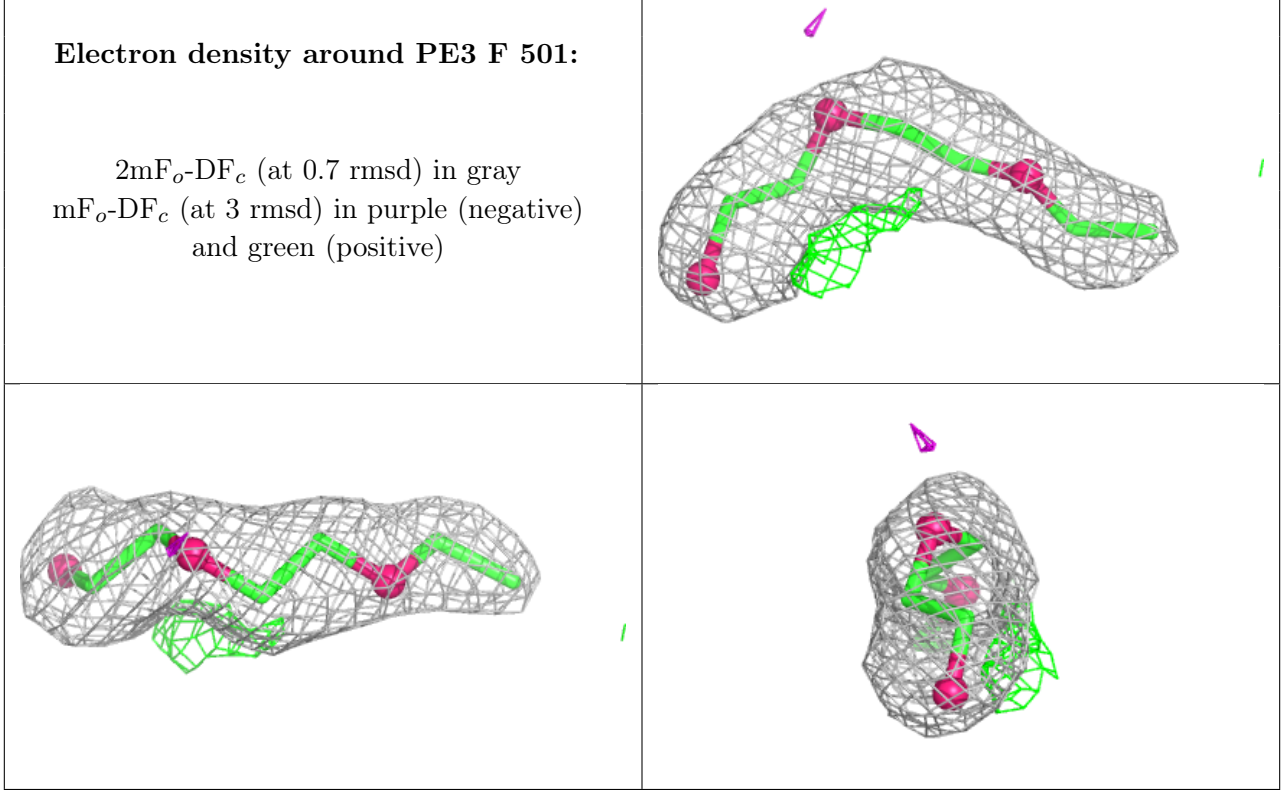
Electron density around PE3 L 501:

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



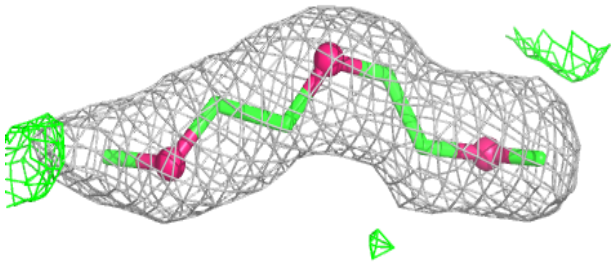
Electron density around PE3 F 501:

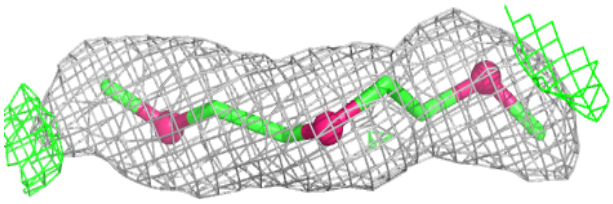
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

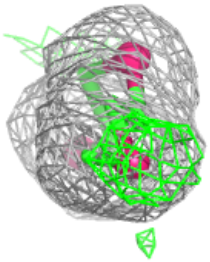


Electron density around PE3 F 502:

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

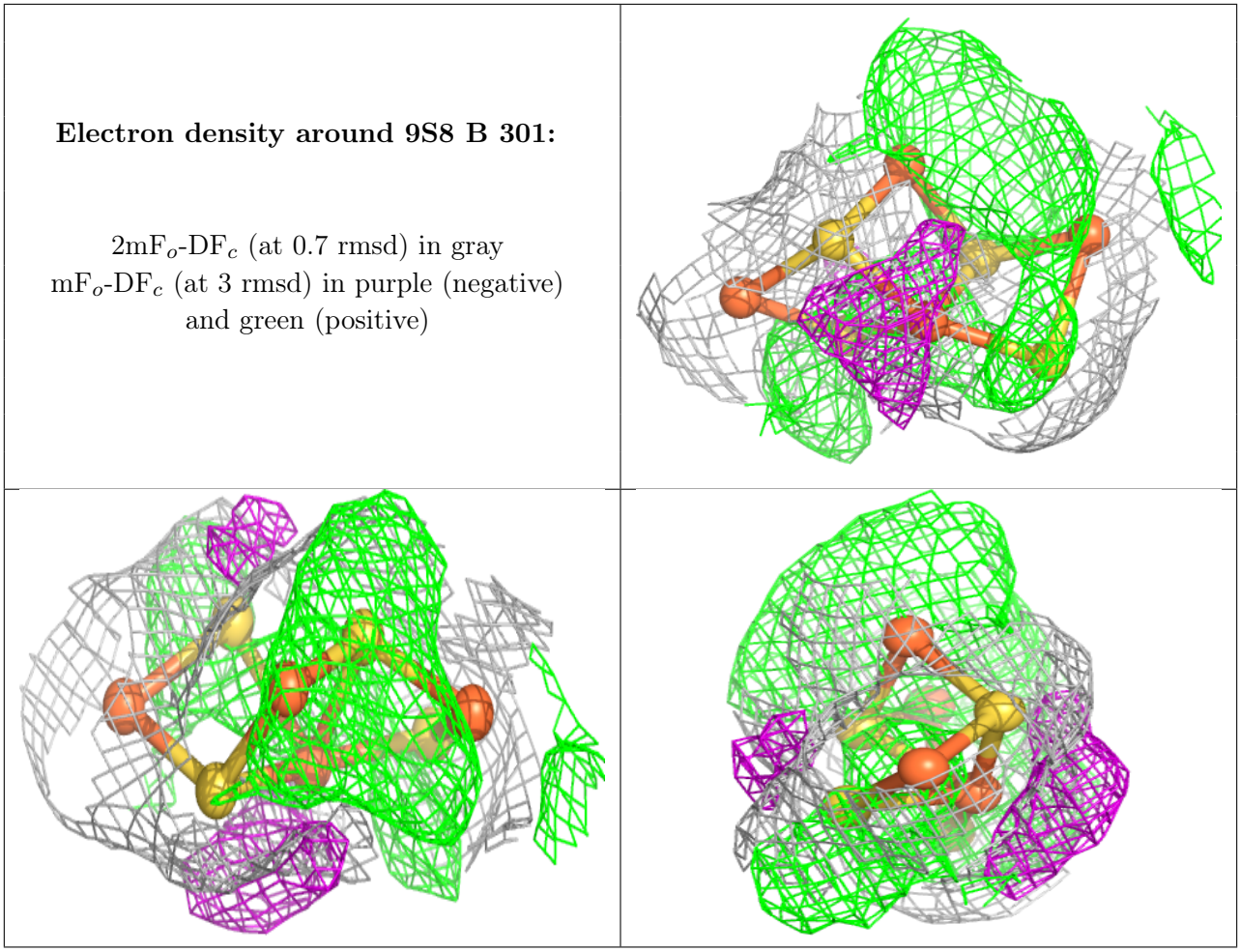






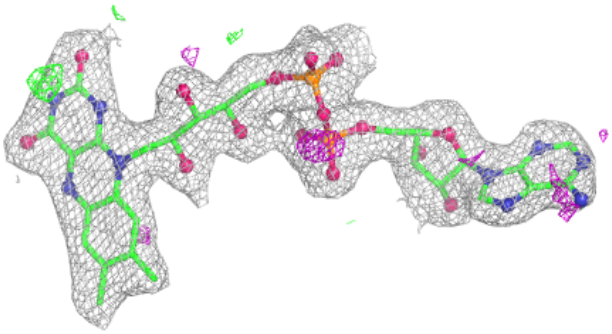
Electron density around 9S8 B 301:

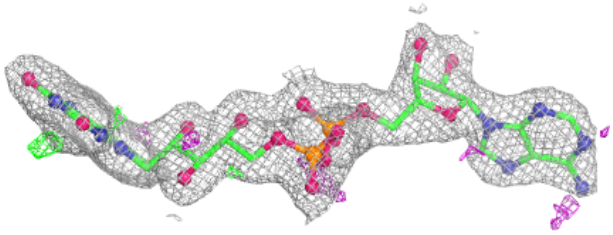
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

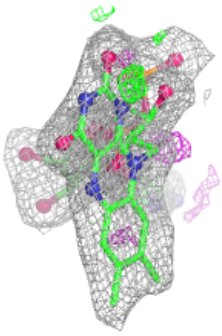


Electron density around FAD A 709:

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

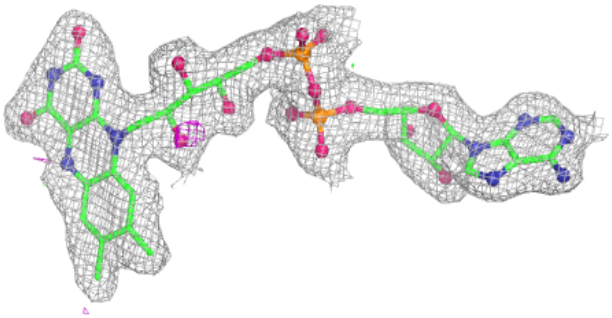


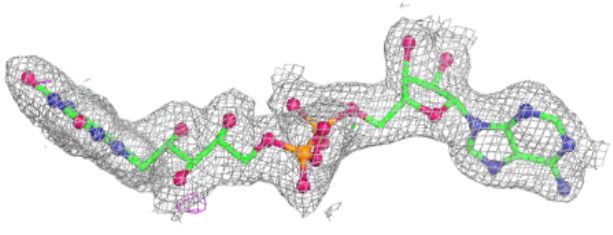


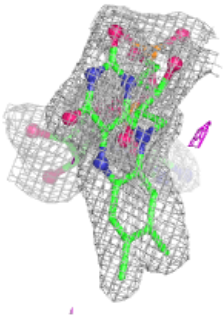


Electron density around FAD G 711:

$2mF_o$-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.