



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:50 pm BST

PDB ID : 5ODR
Title : Heterodisulfide reductase / [NiFe]-hydrogenase complex from Methanothermococcus thermolithotrophicus soaked with heterodisulfide for 2 minutes.
Authors : Wagner, T.; Koch, J.; Ermler, U.; Shima, S.
Deposited on : 2017-07-06
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 ⓘ 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

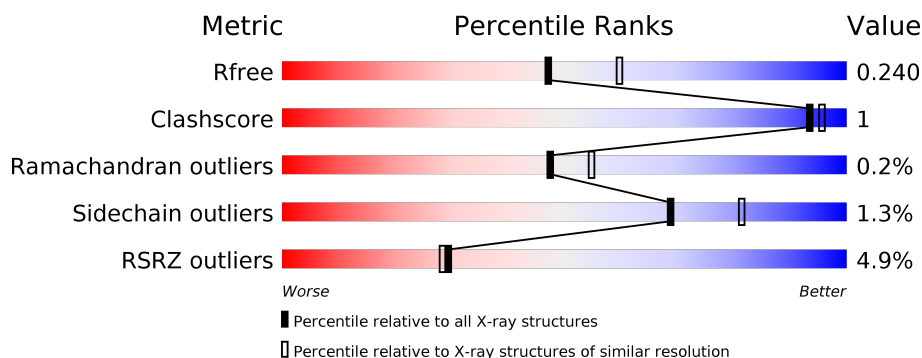
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	654	<div> <div>6%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	G	654	<div> <div>6%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
2	B	291	<div> <div>4%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>
2	H	291	<div> <div>20%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
3	C	184	<div> <div>3%</div> <div> <div></div> <div>99%</div> <div>..</div> </div> </div>
3	I	184	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>6% ..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	140	
4	J	140	
5	E	299	
5	K	299	
6	F	473	
6	L	473	

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
10	9S8	B	302	-	-	X	-
11	COM	B	303	-	X	-	-
8	SF4	G	706	-	-	X	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 32577 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
			4979	3142	845	943	49			
1	G	652	Total	C	N	O	S	0	0	0
			4979	3142	845	943	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
			2236	1420	379	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
			1426	890	247	275	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			

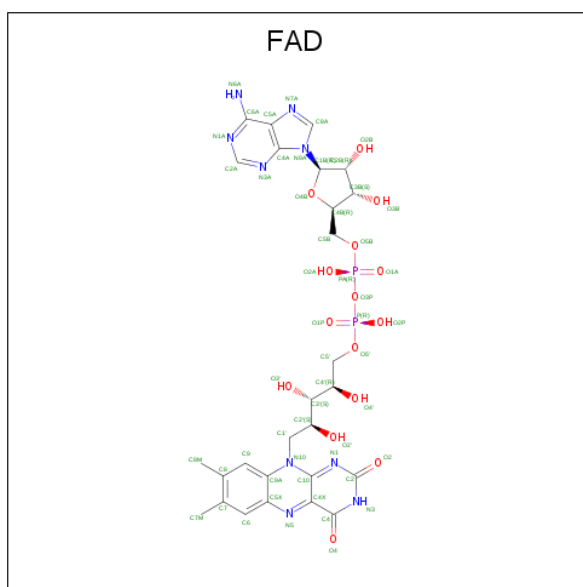
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	297	Total	C	N	O	S	0	0	0
			2249	1419	367	444	19			
5	K	297	Total	C	N	O	S	0	1	0
			2257	1424	370	444	19			

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

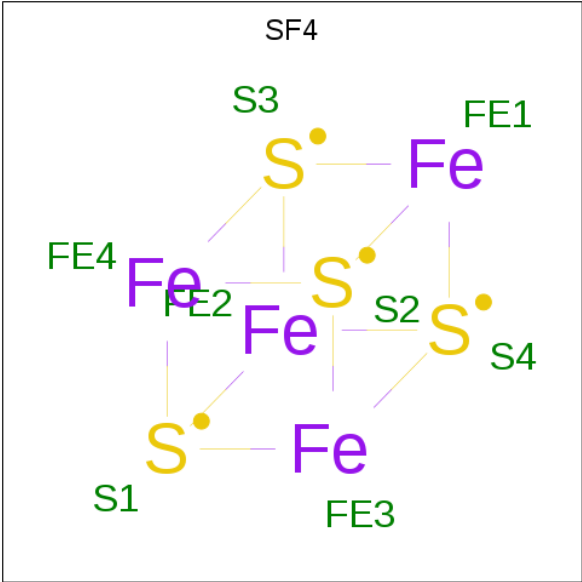
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	447	Total	C	N	O	S	0	0	0
			3521	2230	600	672	19			
6	L	447	Total	C	N	O	S	0	0	0
			3521	2230	600	672	19			

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



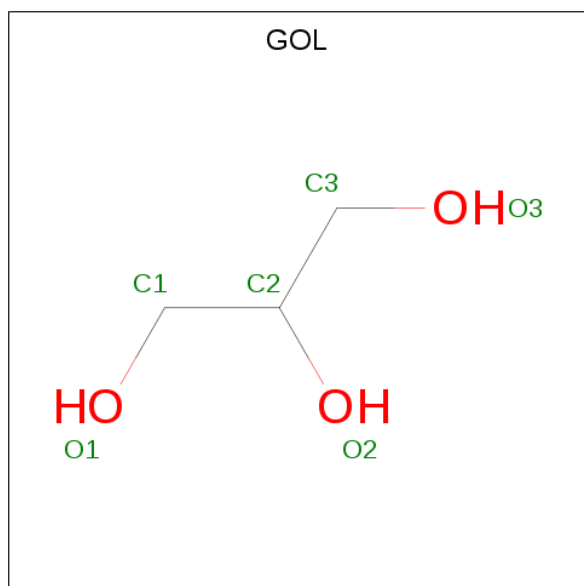
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Fe	S	0	0
			8	4	4		
8	A	1	Total	Fe	S	0	0
			8	4	4		
8	A	1	Total	Fe	S	0	0
			8	4	4		
8	A	1	Total	Fe	S	0	0
			8	4	4		
8	A	1	Total	Fe	S	0	0
			8	4	4		
8	C	1	Total	Fe	S	0	0
			8	4	4		
8	C	1	Total	Fe	S	0	0
			8	4	4		
8	E	1	Total	Fe	S	0	0
			8	4	4		
8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

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



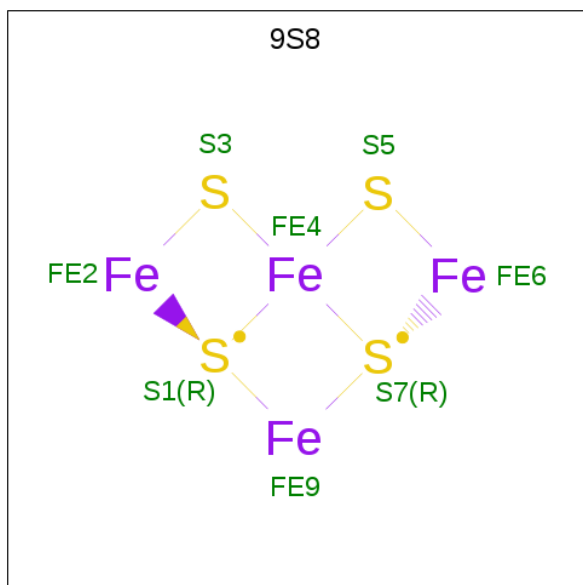
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		

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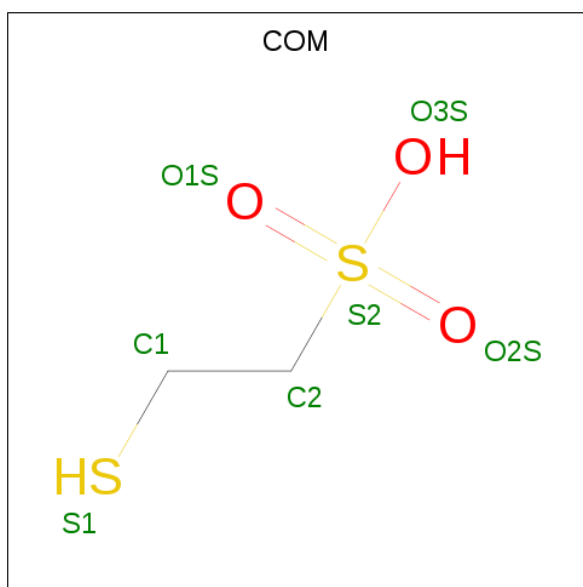
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			6	3	3		
9	I	1	Total	C	O	0	0
			6	3	3		
9	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is Non-cubane [4Fe-4S]-cluster (three-letter code: 9S8) (formula: Fe₄S₄).



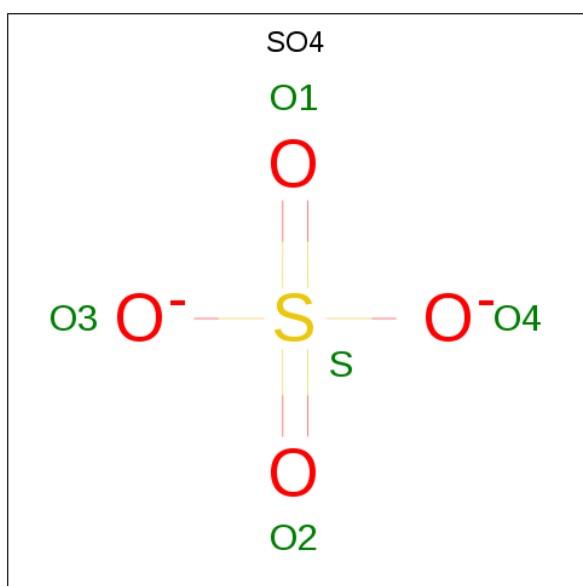
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			8	4	4		
10	B	1	Total	Fe	S	0	0
			8	4	4		
10	H	1	Total	Fe	S	0	0
			8	4	4		
10	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 11 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: C₂H₆O₃S₂).



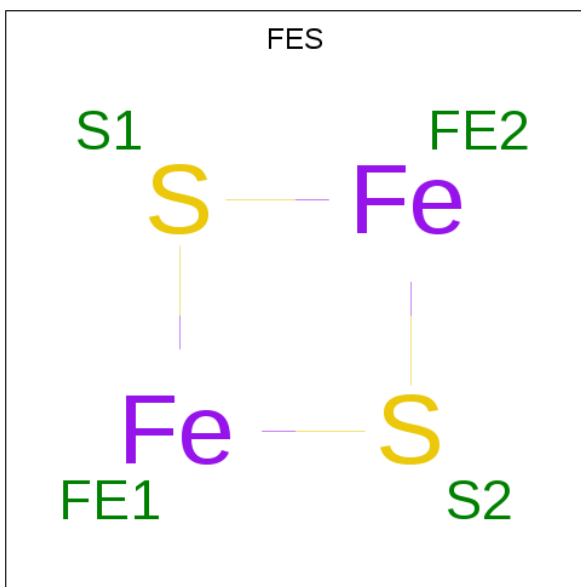
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	O	S	0	0
			7	2	3	2		
11	H	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



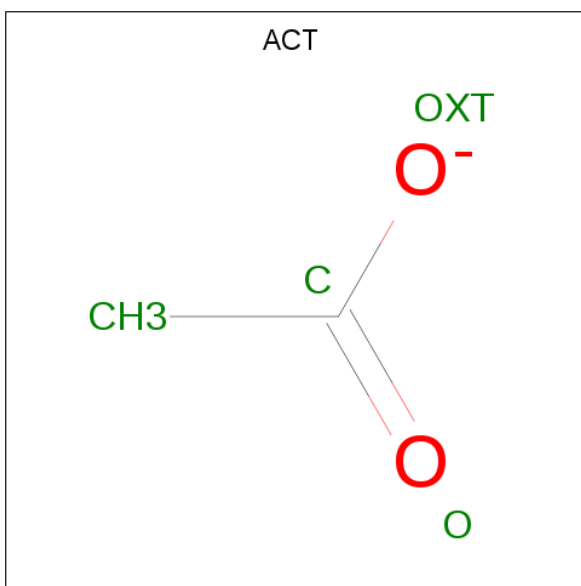
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 14 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



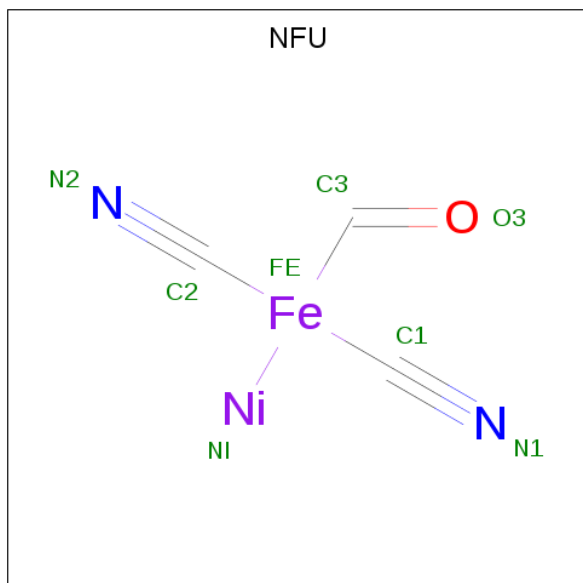
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			4	2	2		
14	E	1	Total	C	O	0	0
			4	2	2		

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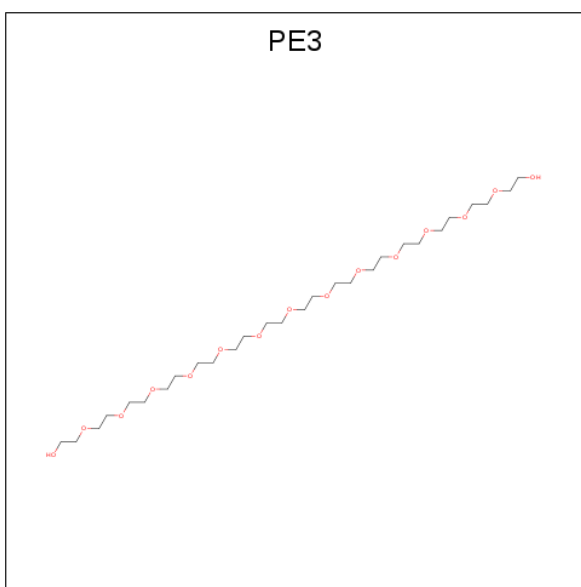
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	F	1	Total	C	O	0	0
			4	2	2		
14	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 15 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (three-letter code: NFU) (formula: C_3HFeN_2NiO).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
15	F	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
15	L	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

- Molecule 16 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).

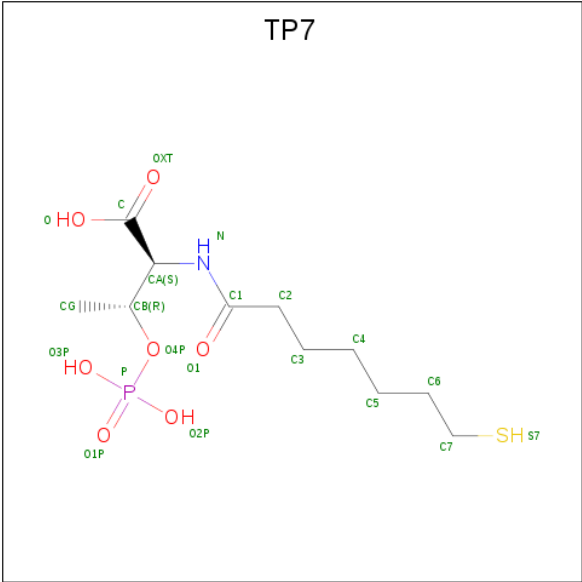


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	F	1	Total	C	O	0	0
			9	6	3		
16	F	1	Total	C	O	0	0
			13	8	5		
16	G	1	Total	C	O	0	0
			10	7	3		
16	L	1	Total	C	O	0	0
			9	6	3		

- Molecule 17 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 18 is Coenzyme B (three-letter code: TP7) (formula: C₁₁H₂₂NO₇PS).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	198	Total	O	0	0
			198	198		
19	B	52	Total	O	0	0
			52	52		
19	C	48	Total	O	0	0
			48	48		
19	D	46	Total	O	0	0
			46	46		
19	E	86	Total	O	0	0
			86	86		
19	F	137	Total	O	0	0
			137	137		
19	G	181	Total	O	0	0
			181	181		
19	H	24	Total	O	0	0
			24	24		
19	I	35	Total	O	0	0
			35	35		
19	J	54	Total	O	0	0
			54	54		
19	K	87	Total	O	0	0
			87	87		

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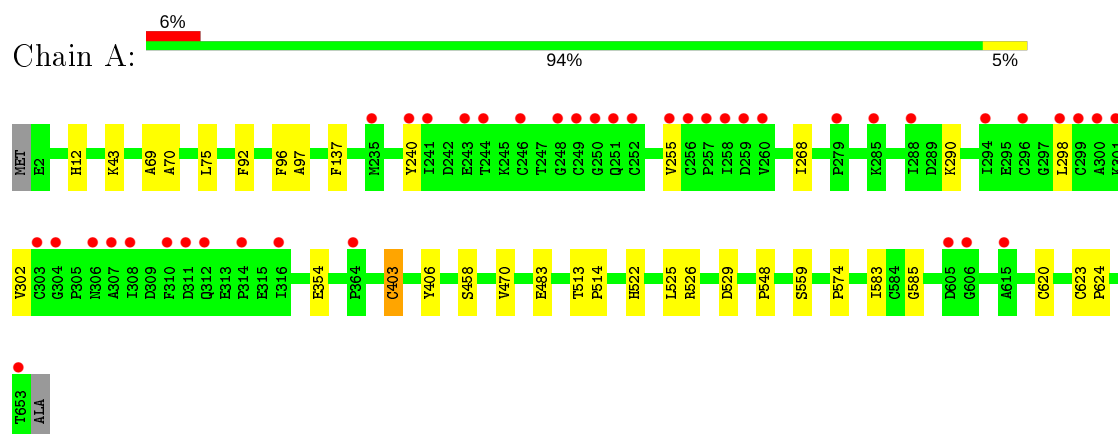
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	132	Total 132	O 132	0	0

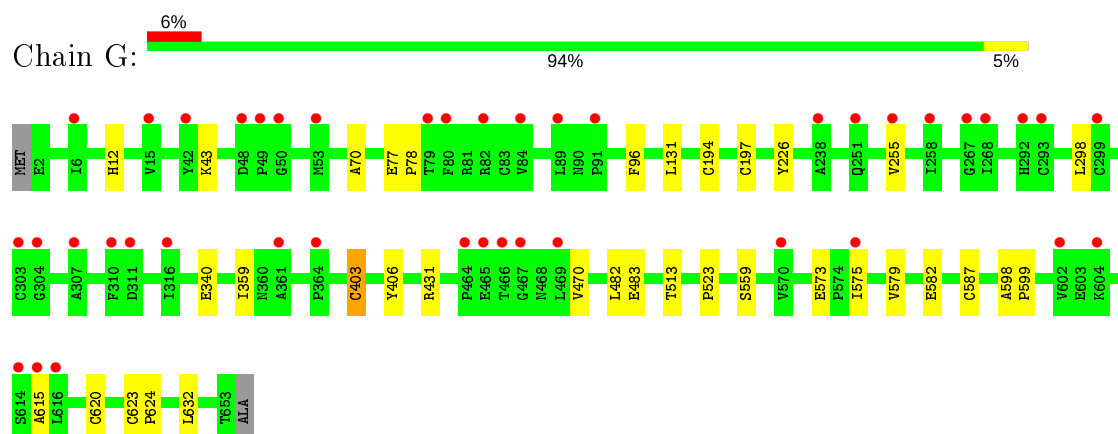
3 Residue-property plots [i](#)

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.

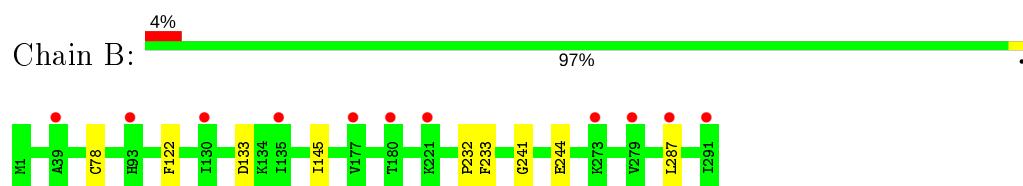
- Molecule 1: Heterodisulfide reductase, subunit A



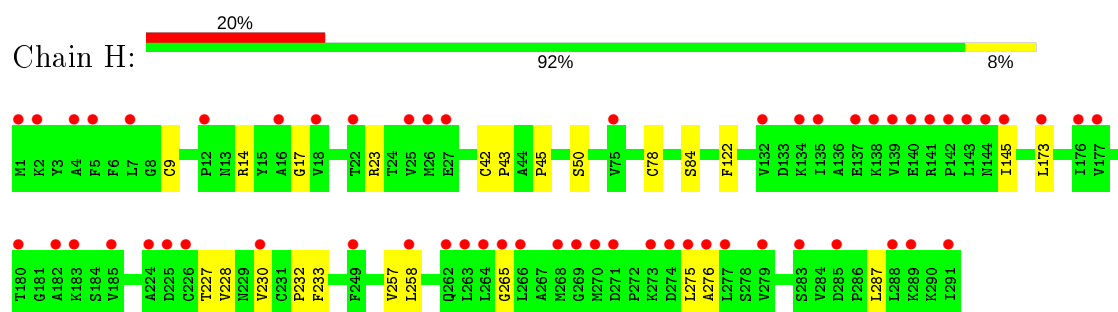
- Molecule 1: Heterodisulfide reductase, subunit A



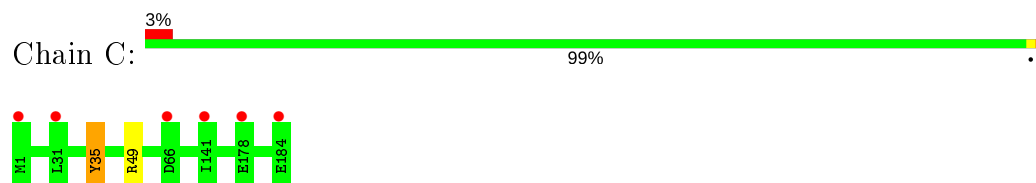
- Molecule 2: Heterodisulfide reductase, subunit B



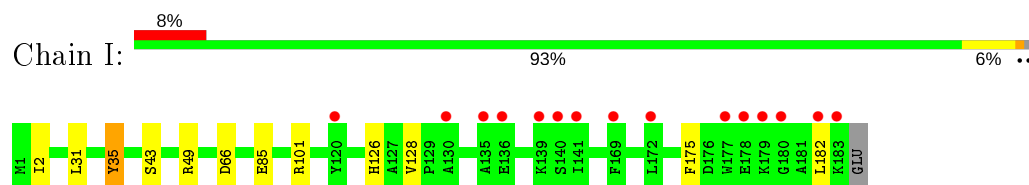
- Molecule 2: Heterodisulfide reductase, subunit B



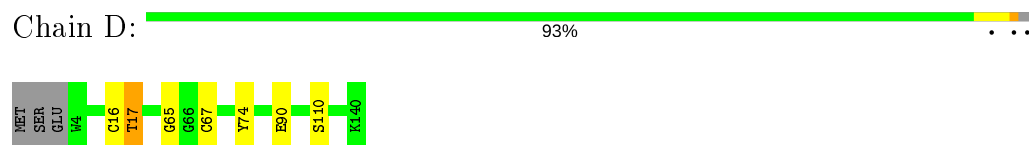
- Molecule 3: Heterodisulfide reductase, subunit C



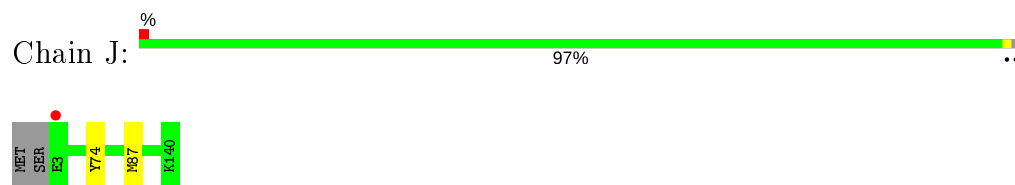
- Molecule 3: Heterodisulfide reductase, subunit C



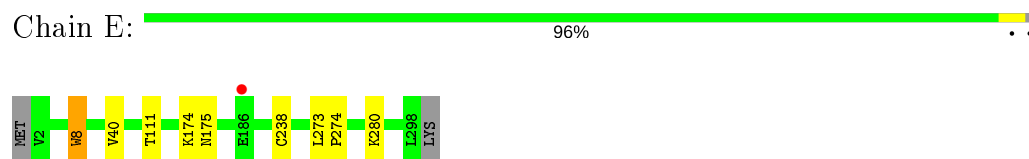
- Molecule 4: Methyl-viologen reducing hydrogenase, subunit D



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

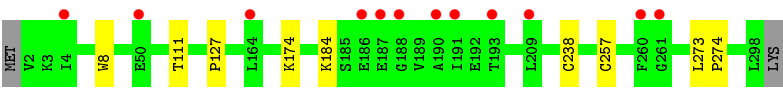


- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

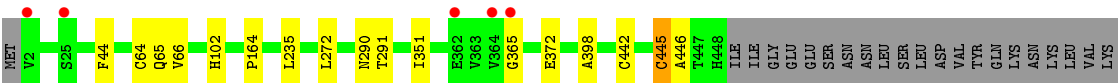
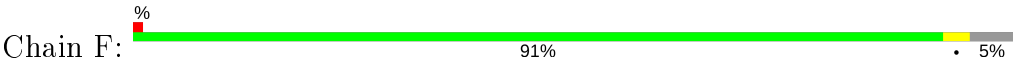


- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G





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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	366.22Å 96.92Å 134.45Å 90.00° 108.30° 90.00°	Depositor
Resolution (Å)	90.26 – 2.20 90.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (90.26-2.20) 99.2 (90.26-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.204 , 0.225 0.218 , 0.240	Depositor DCC
R_{free} test set	11228 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32577	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, SO4, SF4, PE3, TP7, NFU, 9S8, FE, ACT, COM, FAD, FES

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	0.31	0/5071	0.54	0/6853
1	G	0.31	0/5071	0.55	0/6853
2	B	0.30	0/2277	0.48	0/3070
2	H	0.30	0/2277	0.47	0/3070
3	C	0.31	0/1447	0.47	0/1946
3	I	0.31	0/1437	0.46	0/1934
4	D	0.29	0/1123	0.53	0/1508
4	J	0.30	0/1132	0.52	0/1520
5	E	0.28	0/2288	0.55	0/3102
5	K	0.29	0/2299	0.55	0/3116
6	F	0.30	0/3590	0.55	0/4853
6	L	0.29	0/3590	0.54	0/4853
All	All	0.30	0/31602	0.53	0/42678

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	4979	0	4975	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4979	0	4974	19	0
2	B	2236	0	2243	3	0
2	H	2236	0	2243	14	0
3	C	1426	0	1441	1	0
3	I	1416	0	1435	10	0
4	D	1097	0	1068	5	0
4	J	1106	0	1074	2	0
5	E	2249	0	2252	5	0
5	K	2257	0	2265	5	0
6	F	3521	0	3503	5	0
6	L	3521	0	3503	7	0
7	A	53	0	31	0	0
7	G	53	0	31	0	0
8	A	48	0	0	1	0
8	C	16	0	0	0	0
8	E	24	0	0	0	0
8	G	48	0	0	2	0
8	I	16	0	0	0	0
8	K	24	0	0	0	0
9	A	12	0	16	2	0
9	D	6	0	8	0	0
9	I	12	0	16	1	0
9	K	6	0	8	0	0
10	B	16	0	0	3	0
10	H	16	0	0	0	0
11	B	7	0	6	0	0
11	H	7	0	5	0	0
12	B	5	0	0	0	0
13	D	4	0	0	0	0
13	J	4	0	0	0	0
14	D	4	0	3	0	0
14	E	4	0	3	0	0
14	F	4	0	3	0	0
14	G	4	0	3	0	0
15	F	8	0	0	1	0
15	L	8	0	0	1	0
16	F	22	0	27	0	0
16	G	10	0	10	0	0
16	L	9	0	10	0	0
17	F	1	0	0	0	0
17	G	1	0	0	0	0
17	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	21	0	19	0	0
19	A	198	0	0	0	0
19	B	52	0	0	1	0
19	C	48	0	0	0	0
19	D	46	0	0	0	0
19	E	86	0	0	0	0
19	F	137	0	0	0	0
19	G	181	0	0	0	0
19	H	24	0	0	0	0
19	I	35	0	0	1	0
19	J	54	0	0	0	0
19	K	87	0	0	0	0
19	L	132	0	0	0	0
All	All	32577	0	31175	86	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 1.

All (86) 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:A:255:VAL:HG21	1:A:302:VAL:HG21	1.47	0.96
10:B:302:9S8:S1	10:B:302:9S8:S5	2.73	0.86
10:B:302:9S8:S1	19:B:402:HOH:O	2.42	0.77
3:I:35:TYR:HA	9:I:203:GOL:H2	1.65	0.76
2:B:145:ILE:HD12	2:B:287:LEU:HD11	1.68	0.74
1:G:226:TYR:CZ	1:G:615:ALA:HB1	2.28	0.68
1:A:403:CYS:HB2	8:A:702:SF4:S1	2.36	0.66
10:B:302:9S8:FE4	10:B:302:9S8:S1	1.90	0.63
1:G:598:ALA:HB3	1:G:599:PRO:HD3	1.87	0.55
4:D:17:THR:HG21	4:D:65:GLY:HA3	1.88	0.55
4:D:16:CYS:HB2	4:D:67:CYS:SG	2.48	0.54
6:F:272:LEU:HD11	6:F:446:ALA:HB1	1.90	0.54
1:A:255:VAL:CG2	1:A:302:VAL:HG21	2.30	0.53
1:G:470:VAL:CG1	1:G:483:GLU:HG2	2.39	0.53
1:A:12:HIS:HB2	1:A:43:LYS:HA	1.90	0.52
1:G:403:CYS:HB2	8:G:706:SF4:S3	2.50	0.52
1:A:470:VAL:CG1	1:A:483:GLU:HG2	2.39	0.51
2:H:42:CYS:SG	2:H:43:PRO:C	2.89	0.51
2:H:257:VAL:C	2:H:258:LEU:HD12	2.31	0.51
2:H:50:SER:HB3	3:I:101:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:C	1:A:526:ARG:HG3	2.31	0.50
2:H:228:VAL:HA	2:H:258:LEU:O	2.10	0.50
1:A:623:CYS:SG	1:A:624:PRO:HD3	2.52	0.50
6:F:442:CYS:SG	6:F:445:CYS:HB2	2.52	0.49
1:A:458:SER:HB2	3:I:43:SER:OG	2.12	0.49
4:J:87:MET:HG3	5:K:257:CYS:SG	2.53	0.49
1:A:470:VAL:HG11	1:A:483:GLU:HG2	1.95	0.49
2:B:78:CYS:SG	2:B:232:PRO:HD2	2.53	0.48
1:G:623:CYS:SG	1:G:624:PRO:HD3	2.53	0.48
2:H:173:LEU:HD21	2:H:230:VAL:HG11	1.95	0.48
2:H:265:GLY:HA3	2:H:275:LEU:HD21	1.96	0.48
1:A:255:VAL:HG21	1:A:302:VAL:CG2	2.32	0.47
1:A:525:LEU:O	1:A:526:ARG:HG3	2.14	0.47
1:A:514:PRO:HA	4:D:110:SER:HB2	1.96	0.47
1:G:482:LEU:HD23	3:I:2:ILE:HB	1.96	0.47
1:A:75:LEU:HD13	1:A:522:HIS:CD2	2.49	0.47
1:G:470:VAL:HG11	1:G:483:GLU:HG2	1.97	0.47
6:L:442:CYS:SG	6:L:445:CYS:HB2	2.55	0.47
5:K:273:LEU:HB3	5:K:274:PRO:HD3	1.97	0.47
3:I:175:PHE:HD1	3:I:182:LEU:HD12	1.80	0.46
5:K:127:PRO:HD3	6:L:36:VAL:HB	1.98	0.46
2:H:227:THR:CG2	2:H:257:VAL:HG13	2.47	0.45
4:D:90:GLU:HB3	5:E:280:LYS:HE3	1.99	0.45
2:H:145:ILE:CD1	2:H:287:LEU:HD11	2.47	0.45
3:I:66:ASP:HB3	19:I:302:HOH:O	2.17	0.45
1:A:526:ARG:HB3	1:A:529:ASP:HB2	2.00	0.44
1:A:548:PRO:HB3	1:G:523:PRO:O	2.18	0.44
2:H:17:GLY:HA3	2:H:276:ALA:HB3	2.00	0.44
1:A:255:VAL:HG12	1:A:298:LEU:HB3	1.99	0.44
1:A:92:PHE:CZ	1:A:574:PRO:HD2	2.52	0.44
6:F:66:VAL:HG22	6:F:164:PRO:HG3	2.00	0.43
3:I:31:LEU:C	3:I:31:LEU:HD12	2.38	0.43
1:A:268:ILE:HD11	1:A:354:GLU:HB3	2.01	0.43
1:G:582:GLU:O	5:K:174:LYS:HG3	2.19	0.43
9:A:708:GOL:H31	3:I:85:GLU:O	2.18	0.43
1:G:255:VAL:HG12	1:G:298:LEU:HB3	2.01	0.43
1:G:579:VAL:HG22	1:G:632:LEU:HD13	2.01	0.43
6:L:235:LEU:HA	6:L:372:GLU:HB2	2.01	0.43
2:B:241:GLY:HA2	2:B:244:GLU:OE1	2.19	0.43
1:G:194:CYS:HB2	1:G:197:CYS:SG	2.59	0.43
1:A:583:ILE:O	5:E:174:LYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:620:CYS:HB3	4:J:74:TYR:CG	2.54	0.42
1:A:69:ALA:HA	1:A:97:ALA:HB3	2.01	0.42
6:F:235:LEU:HA	6:F:372:GLU:HB2	2.01	0.42
2:H:14:ARG:HD3	3:I:128:VAL:HG11	2.01	0.42
9:A:709:GOL:H2	3:C:35:TYR:HA	2.01	0.42
1:A:240:TYR:CE2	1:A:290:LYS:HG3	2.54	0.42
5:E:273:LEU:HB3	5:E:274:PRO:HD3	2.00	0.42
1:G:131:LEU:HD22	1:G:131:LEU:N	2.34	0.42
6:L:272:LEU:HD11	6:L:446:ALA:HB1	2.01	0.42
1:A:620:CYS:HB3	4:D:74:TYR:CG	2.55	0.42
2:H:9:CYS:SG	3:I:126:HIS:HB3	2.60	0.42
1:A:559:SER:HB2	1:G:559:SER:HB2	2.02	0.41
5:E:8:TRP:CH2	5:E:40:VAL:HB	2.55	0.41
1:G:12:HIS:HB2	1:G:43:LYS:HA	2.02	0.41
6:L:66:VAL:HG22	6:L:164:PRO:HG3	2.02	0.41
2:H:145:ILE:HD12	2:H:287:LEU:HD11	2.02	0.41
1:A:585:GLY:HA3	5:E:175:ASN:OD1	2.21	0.41
1:G:77:GLU:N	1:G:78:PRO:CD	2.83	0.41
2:H:45:PRO:HD3	2:H:84:SER:HB2	2.02	0.41
1:G:587:CYS:HA	5:K:184:LYS:HE3	2.02	0.41
6:F:64:CYS:CB	15:F:501:NFU:C1	2.99	0.40
6:L:272:LEU:HD11	6:L:400:VAL:HA	2.03	0.40
6:L:442:CYS:HB3	15:L:501:NFU:N2	2.37	0.40
2:H:78:CYS:SG	2:H:232:PRO:HD2	2.62	0.40
1:G:431:ARG:HD2	8:G:706:SF4:S1	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	629 (97%)	20 (3%)	1 (0%)	47 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	650/654 (99%)	629 (97%)	19 (3%)	2 (0%)	41	46
2	B	289/291 (99%)	274 (95%)	15 (5%)	0	100	100
2	H	289/291 (99%)	278 (96%)	11 (4%)	0	100	100
3	C	182/184 (99%)	182 (100%)	0	0	100	100
3	I	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
4	D	135/140 (96%)	130 (96%)	5 (4%)	0	100	100
4	J	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
5	E	295/299 (99%)	285 (97%)	10 (3%)	0	100	100
5	K	296/299 (99%)	285 (96%)	11 (4%)	0	100	100
6	F	445/473 (94%)	431 (97%)	11 (2%)	3 (1%)	22	22
6	L	445/473 (94%)	431 (97%)	12 (3%)	2 (0%)	34	37
All	All	3993/4082 (98%)	3865 (97%)	120 (3%)	8 (0%)	47	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	398	ALA
6	L	398	ALA
6	F	291	THR
6	L	291	THR
1	A	70	ALA
1	G	70	ALA
1	G	575	ILE
6	F	365	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	540/541 (100%)	535 (99%)	5 (1%)	78	88
1	G	540/541 (100%)	533 (99%)	7 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	242/242 (100%)	239 (99%)	3 (1%)	71	83
2	H	242/242 (100%)	239 (99%)	3 (1%)	71	83
3	C	157/157 (100%)	155 (99%)	2 (1%)	69	81
3	I	156/157 (99%)	154 (99%)	2 (1%)	69	81
4	D	116/119 (98%)	115 (99%)	1 (1%)	78	88
4	J	117/119 (98%)	117 (100%)	0	100	100
5	E	254/256 (99%)	251 (99%)	3 (1%)	71	83
5	K	255/256 (100%)	252 (99%)	3 (1%)	71	83
6	F	386/410 (94%)	380 (98%)	6 (2%)	62	76
6	L	386/410 (94%)	378 (98%)	8 (2%)	53	67
All	All	3391/3450 (98%)	3348 (99%)	43 (1%)	69	81

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	137	PHE
1	A	403	CYS
1	A	406	TYR
1	A	513	THR
2	B	122	PHE
2	B	133	ASP
2	B	233	PHE
3	C	35	TYR
3	C	49	ARG
4	D	17	THR
5	E	8	TRP
5	E	111	THR
5	E	238	CYS
6	F	44	PHE
6	F	65	GLN
6	F	102	HIS
6	F	290	ASN
6	F	351	ILE
6	F	445	CYS
1	G	96	PHE
1	G	340	GLU
1	G	359	ILE

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Mol	Chain	Res	Type
1	G	403	CYS
1	G	406	TYR
1	G	513	THR
1	G	573	GLU
2	H	23	ARG
2	H	122	PHE
2	H	233	PHE
3	I	35	TYR
3	I	49	ARG
5	K	8	TRP
5	K	111	THR
5	K	238	CYS
6	L	65	GLN
6	L	72	SER
6	L	102	HIS
6	L	251	TYR
6	L	290	ASN
6	L	311	ASP
6	L	422	GLU
6	L	445	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 53 ligands modelled in this entry, 3 are monoatomic - leaving 50 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	$\# Z > 2$
8	SF4	I	202	3	0,12,12	0.00	-	-		
8	SF4	I	201	3	0,12,12	0.00	-	-		
8	SF4	E	304	5	0,12,12	0.00	-	-		
15	NFU	L	501	6	2,7,7	1.01	0	-		
8	SF4	A	705	1	0,12,12	0.00	-	-		
13	FES	D	201	4	0,4,4	0.00	-	-		
9	GOL	I	204	-	5,5,5	0.36	0	5,5,5	0.19	0
8	SF4	A	706	1	0,12,12	0.00	-	-		
16	PE3	L	502	-	8,8,42	0.50	0	7,7,41	0.18	0
11	COM	H	303	-	6,6,6	1.38	2 (33%)	7,8,8	2.63	4 (57%)
8	SF4	A	702	1	0,12,12	0.00	-	-		
9	GOL	K	304	-	5,5,5	0.35	0	5,5,5	0.41	0
14	ACT	F	504	-	1,3,3	5.23	1 (100%)	0,3,3	0.00	-
14	ACT	G	702	-	1,3,3	4.97	1 (100%)	0,3,3	0.00	-
8	SF4	A	704	1	0,12,12	0.00	-	-		
18	TP7	H	304	-	16,20,20	0.55	0	18,26,26	0.94	0
14	ACT	E	301	-	1,3,3	4.97	1 (100%)	0,3,3	0.00	-
10	9S8	B	301	2	2,10,10	3.98	1 (50%)	-		
11	COM	B	303	-	6,6,6	1.30	1 (16%)	7,8,8	2.71	4 (57%)
7	FAD	G	704	-	51,58,58	1.81	6 (11%)	60,89,89	1.96	11 (18%)
8	SF4	K	303	5	0,12,12	0.00	-	-		
9	GOL	I	203	-	5,5,5	0.23	0	5,5,5	0.52	0
8	SF4	A	707	1	0,12,12	0.00	-	-		
8	SF4	G	707	1	0,12,12	0.00	-	-		
16	PE3	F	502	-	8,8,42	0.47	0	7,7,41	0.28	0
8	SF4	E	303	5	0,12,12	0.00	-	-		
9	GOL	A	708	-	5,5,5	0.31	0	5,5,5	0.35	0
8	SF4	K	301	5	0,12,12	0.00	-	-		
14	ACT	D	202	-	1,3,3	4.50	1 (100%)	0,3,3	0.00	-
15	NFU	F	501	6	2,7,7	1.09	0	-		
8	SF4	K	302	5	0,12,12	0.00	-	-		
8	SF4	G	705	1,17	0,12,12	0.00	-	-		
10	9S8	H	301	2	2,10,10	3.44	2 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SF4	G	708	1	0,12,12	0.00	-	-		
10	9S8	H	302	2	2,10,10	3.26	2 (100%)	-		
16	PE3	G	701	-	9,9,42	0.50	0	8,8,41	0.20	0
8	SF4	A	703	1	0,12,12	0.00	-	-		
8	SF4	G	709	1	0,12,12	0.00	-	-		
16	PE3	F	503	-	12,12,42	0.47	0	11,11,41	0.28	0
12	SO4	B	304	-	4,4,4	0.17	0	6,6,6	0.08	0
8	SF4	G	706	1	0,12,12	0.00	-	-		
9	GOL	D	203	-	5,5,5	0.33	0	5,5,5	0.37	0
13	FES	J	200	4	0,4,4	0.00	-	-		
10	9S8	B	302	2	2,10,10	3.16	1 (50%)	-		
8	SF4	C	202	3	0,12,12	0.00	-	-		
8	SF4	E	302	5	0,12,12	0.00	-	-		
7	FAD	A	701	-	51,58,58	1.85	6 (11%)	60,89,89	1.95	12 (20%)
9	GOL	A	709	-	5,5,5	0.36	0	5,5,5	0.70	0
8	SF4	C	201	3	0,12,12	0.00	-	-		
8	SF4	G	710	1	0,12,12	0.00	-	-		

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
8	SF4	I	202	3	-	-	0/6/5/5
8	SF4	I	201	3	-	-	0/6/5/5
8	SF4	E	304	5	-	-	0/6/5/5
8	SF4	A	705	1	-	-	0/6/5/5
13	FES	D	201	4	-	-	0/1/1/1
9	GOL	I	204	-	-	2/4/4/4	-
8	SF4	A	706	1	-	-	0/6/5/5
16	PE3	L	502	-	-	2/6/6/40	-
11	COM	H	303	-	-	0/4/4/4	-
8	SF4	A	702	1	-	-	0/6/5/5
9	GOL	K	304	-	-	0/4/4/4	-
9	GOL	I	203	-	-	2/4/4/4	-
8	SF4	A	704	1	-	-	0/6/5/5
18	TP7	H	304	-	-	1/20/24/24	-
10	9S8	B	301	2	-	-	0/3/3/3
8	SF4	G	708	1	-	-	0/6/5/5
7	FAD	G	704	-	-	1/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SF4	K	303	5	-	-	0/6/5/5
8	SF4	A	707	1	-	-	0/6/5/5
8	SF4	G	707	1	-	-	0/6/5/5
16	PE3	F	502	-	-	4/6/6/40	-
8	SF4	E	303	5	-	-	0/6/5/5
9	GOL	A	708	-	-	0/4/4/4	-
8	SF4	K	301	5	-	-	0/6/5/5
16	PE3	G	701	-	-	3/7/7/40	-
8	SF4	K	302	5	-	-	0/6/5/5
8	SF4	G	705	1,17	-	-	0/6/5/5
10	9S8	H	301	2	-	-	0/3/3/3
11	COM	B	303	-	-	3/4/4/4	-
10	9S8	H	302	2	-	-	0/3/3/3
8	SF4	A	703	1	-	-	0/6/5/5
8	SF4	G	709	1	-	-	0/6/5/5
16	PE3	F	503	-	-	7/10/10/40	-
8	SF4	G	706	1	-	-	0/6/5/5
9	GOL	D	203	-	-	2/4/4/4	-
13	FES	J	200	4	-	-	0/1/1/1
10	9S8	B	302	2	-	-	0/3/3/3
8	SF4	C	202	3	-	-	0/6/5/5
8	SF4	E	302	5	-	-	0/6/5/5
8	SF4	G	710	1	-	-	0/6/5/5
9	GOL	A	709	-	-	2/4/4/4	-
8	SF4	C	201	3	-	-	0/6/5/5
7	FAD	A	701	-	-	2/30/50/50	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	701	FAD	C4X-C10	9.36	1.48	1.38
7	G	704	FAD	C4X-C10	9.17	1.48	1.38
10	B	301	9S8	S3-FE4	-5.40	2.12	2.24
14	F	504	ACT	CH3-C	5.23	1.55	1.48
14	E	301	ACT	CH3-C	4.97	1.55	1.48
14	G	702	ACT	CH3-C	4.97	1.55	1.48
14	D	202	ACT	CH3-C	4.50	1.54	1.48
10	B	302	9S8	S3-FE4	-4.32	2.14	2.24
10	H	302	9S8	S3-FE4	-4.08	2.15	2.24
10	H	301	9S8	S3-FE4	-4.06	2.15	2.24
7	A	701	FAD	C4-C4X	3.84	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	701	FAD	C9A-C5X	3.81	1.50	1.42
7	G	704	FAD	C4-C4X	3.72	1.47	1.41
7	G	704	FAD	C9A-C5X	3.52	1.49	1.42
7	G	704	FAD	C8-C7	3.49	1.49	1.40
7	A	701	FAD	C8-C7	3.28	1.49	1.40
7	A	701	FAD	C9A-N10	3.19	1.42	1.38
7	G	704	FAD	C9A-N10	3.03	1.42	1.38
10	H	301	9S8	S5-FE4	-2.69	2.18	2.24
7	A	701	FAD	C5A-C4A	2.26	1.46	1.40
7	G	704	FAD	C5A-C4A	2.25	1.46	1.40
11	H	303	COM	O2S-S2	2.20	1.51	1.45
10	H	302	9S8	S5-FE4	-2.14	2.19	2.24
11	H	303	COM	O1S-S2	2.11	1.51	1.45
11	B	303	COM	O1S-S2	2.00	1.50	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	704	FAD	C4-N3-C2	7.65	121.60	115.14
7	A	701	FAD	C4-N3-C2	7.19	121.21	115.14
7	A	701	FAD	C1'-N10-C9A	6.70	123.56	118.29
7	G	704	FAD	C1'-N10-C9A	6.18	123.16	118.29
7	G	704	FAD	C4-C4X-C10	-4.97	116.66	119.95
7	A	701	FAD	C4-C4X-C10	-4.80	116.77	119.95
7	G	704	FAD	C4X-N5-C5X	4.11	120.87	116.77
11	B	303	COM	O3S-S2-C2	4.03	112.28	105.77
7	A	701	FAD	N3A-C2A-N1A	-4.01	122.40	128.68
11	H	303	COM	O3S-S2-O1S	-3.99	101.52	111.27
7	G	704	FAD	N3A-C2A-N1A	-3.98	122.45	128.68
11	H	303	COM	O3S-S2-C2	3.98	112.20	105.77
11	B	303	COM	O3S-S2-O2S	-3.89	101.76	111.27
7	A	701	FAD	C4X-N5-C5X	3.63	120.40	116.77
7	G	704	FAD	C4X-C4-N3	-3.30	118.92	123.43
7	A	701	FAD	C4X-C4-N3	-3.27	118.96	123.43
7	A	701	FAD	C9A-N10-C10	-3.09	117.86	121.91
11	B	303	COM	O1S-S2-C2	2.98	110.50	106.92
7	A	701	FAD	P-O3P-PA	-2.97	122.64	132.83
7	G	704	FAD	P-O3P-PA	-2.89	122.91	132.83
7	G	704	FAD	C4-C4X-N5	2.75	121.74	118.60
11	H	303	COM	O2S-S2-C2	2.66	110.12	106.92
7	A	701	FAD	C4A-C5A-N7A	-2.66	106.63	109.40
11	B	303	COM	O2S-S2-C2	2.56	110.00	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	701	FAD	C4-C4X-N5	2.53	121.49	118.60
11	H	303	COM	O1S-S2-C2	2.51	109.94	106.92
7	G	704	FAD	C9A-N10-C10	-2.47	118.68	121.91
7	G	704	FAD	C4A-C5A-N7A	-2.38	106.92	109.40
7	A	701	FAD	C5X-C9A-N10	2.19	119.30	117.72
7	G	704	FAD	C2A-N1A-C6A	2.11	122.37	118.75
7	A	701	FAD	C2A-N1A-C6A	2.07	122.29	118.75

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	204	GOL	O1-C1-C2-C3
11	B	303	COM	S1-C1-C2-S2
9	D	203	GOL	O1-C1-C2-C3
9	A	709	GOL	C1-C2-C3-O3
16	F	502	PE3	O31-C32-C33-O34
16	F	503	PE3	O4-C5-C6-O7
9	A	709	GOL	O2-C2-C3-O3
16	G	701	PE3	O34-C35-C36-O37
16	F	502	PE3	O34-C35-C36-O37
16	F	503	PE3	O7-C8-C9-O10
9	I	203	GOL	C1-C2-C3-O3
9	I	204	GOL	O1-C1-C2-O2
9	I	203	GOL	O2-C2-C3-O3
9	D	203	GOL	O1-C1-C2-O2
16	G	701	PE3	C32-C33-O34-C35
7	A	701	FAD	PA-O3P-P-O5'
16	L	502	PE3	C39-C38-O37-C36
16	F	503	PE3	C9-C8-O7-C6
16	F	502	PE3	C32-C33-O34-C35
16	G	701	PE3	C35-C36-O37-C38
16	F	502	PE3	C33-C32-O31-C30
11	B	303	COM	C1-C2-S2-O2S
18	H	304	TP7	O1-C1-N-CA
16	F	503	PE3	C12-C11-O10-C9
16	F	503	PE3	C8-C9-O10-C11
16	L	502	PE3	C42-C41-O40-C39
16	F	503	PE3	O10-C11-C12-O13
16	F	503	PE3	C5-C6-O7-C8
7	G	704	FAD	O4B-C4B-C5B-O5B
11	B	303	COM	C1-C2-S2-O1S

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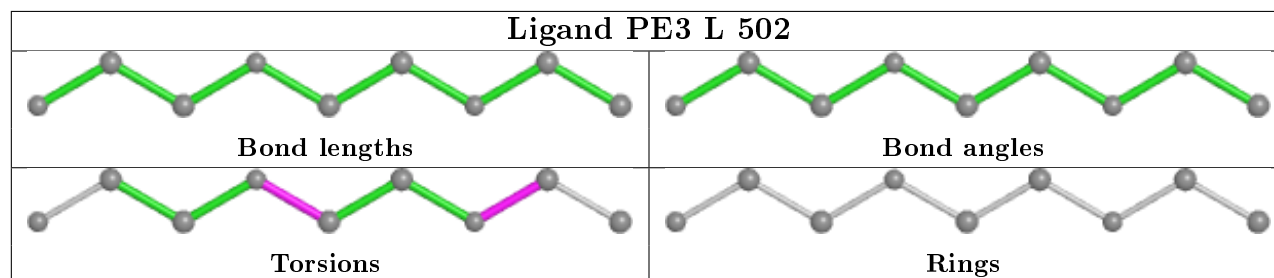
Mol	Chain	Res	Type	Atoms
7	A	701	FAD	O4B-C4B-C5B-O5B

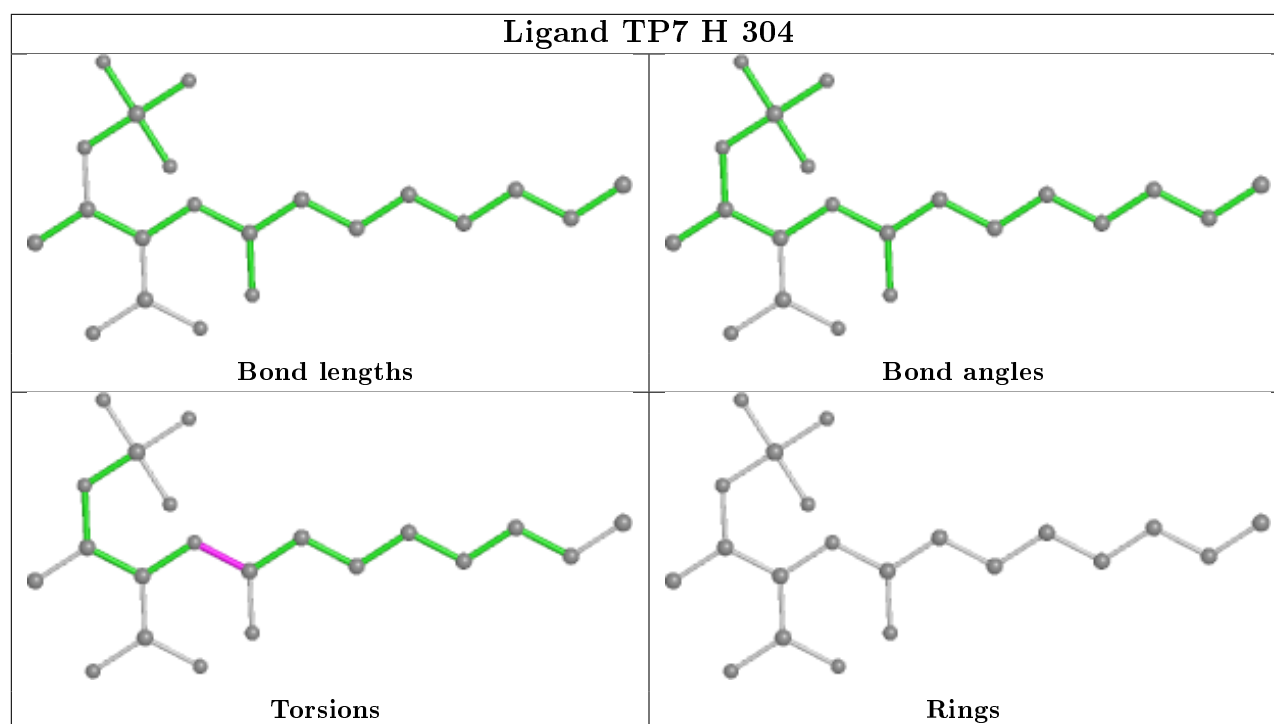
There are no ring outliers.

8 monomers are involved in 11 short contacts:

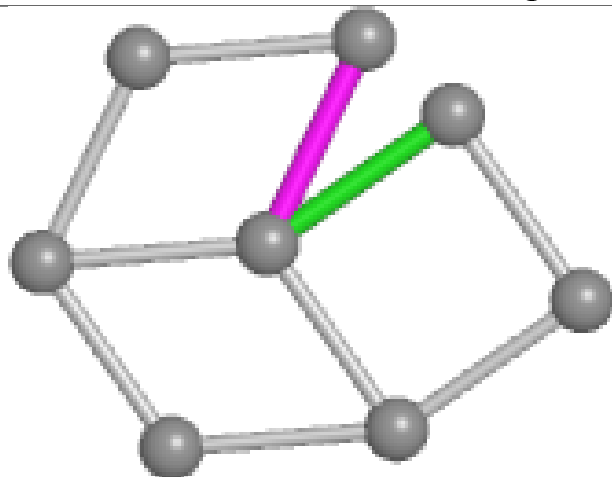
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L	501	NFU	1	0
8	A	702	SF4	1	0
9	I	203	GOL	1	0
9	A	708	GOL	1	0
15	F	501	NFU	1	0
8	G	706	SF4	2	0
10	B	302	9S8	3	0
9	A	709	GOL	1	0

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

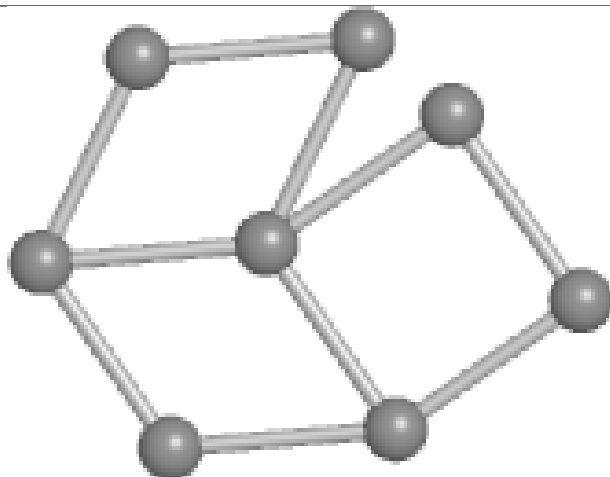




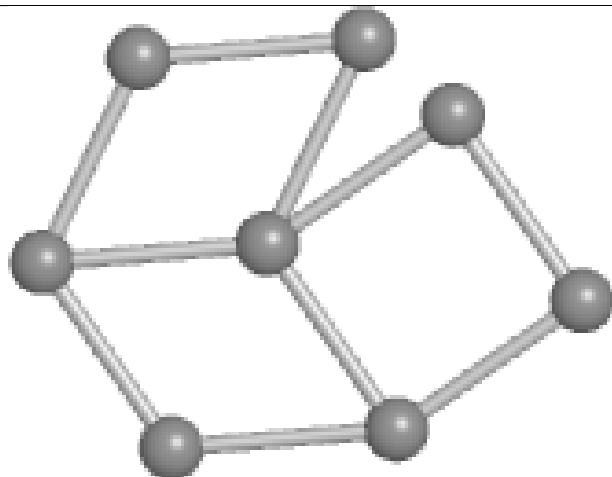
Ligand 9S8 B 301



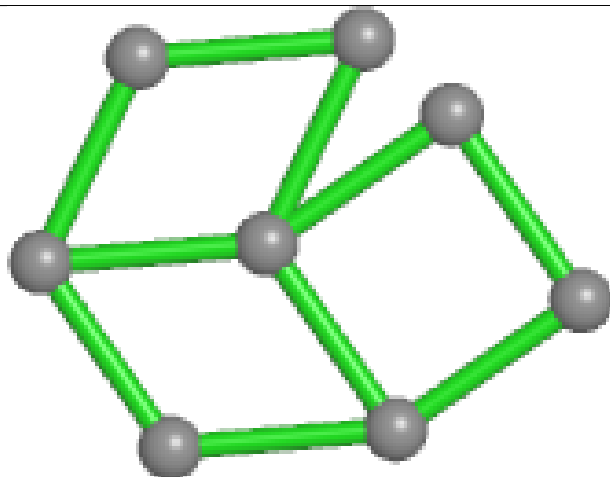
Bond lengths



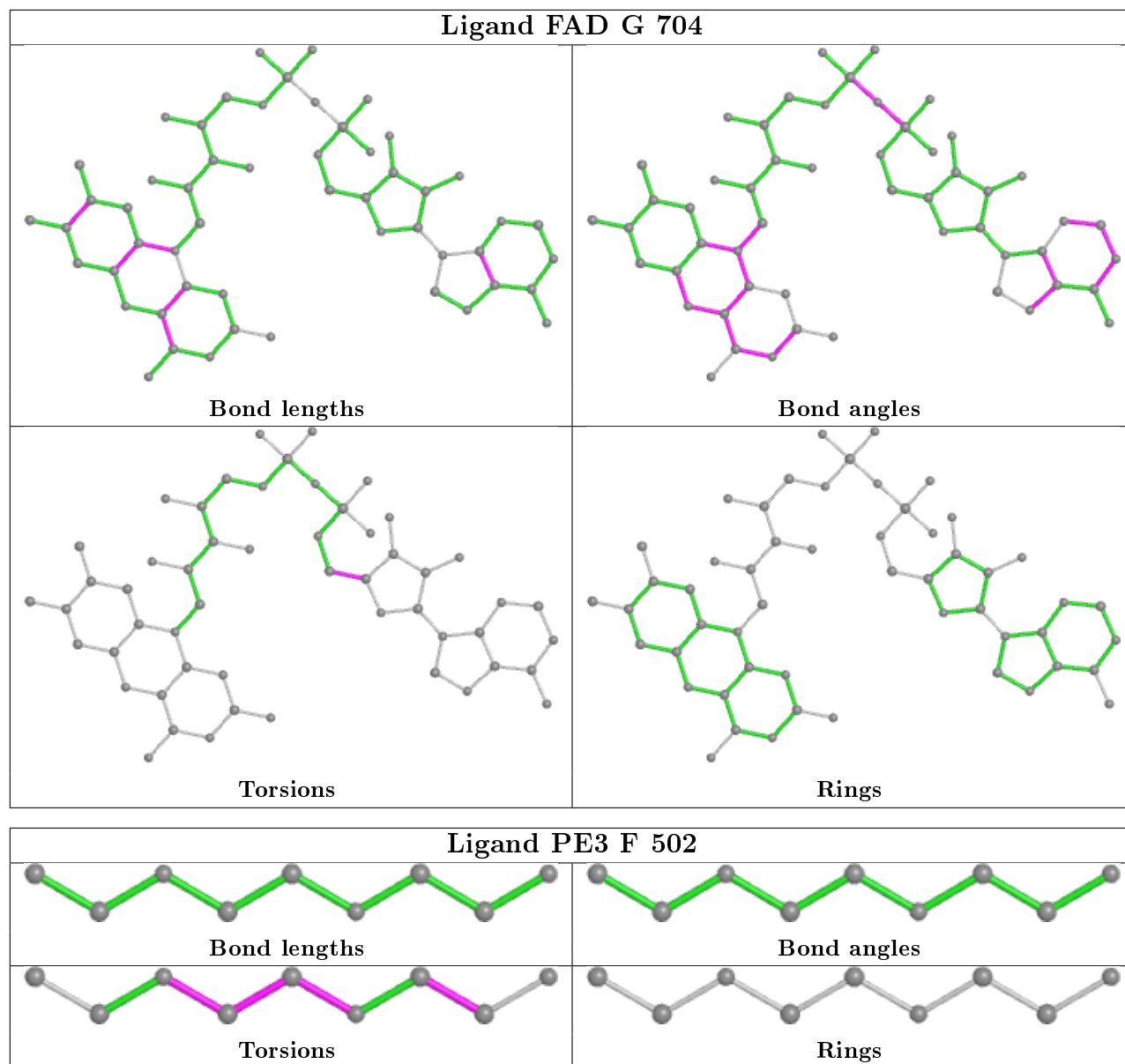
Bond angles

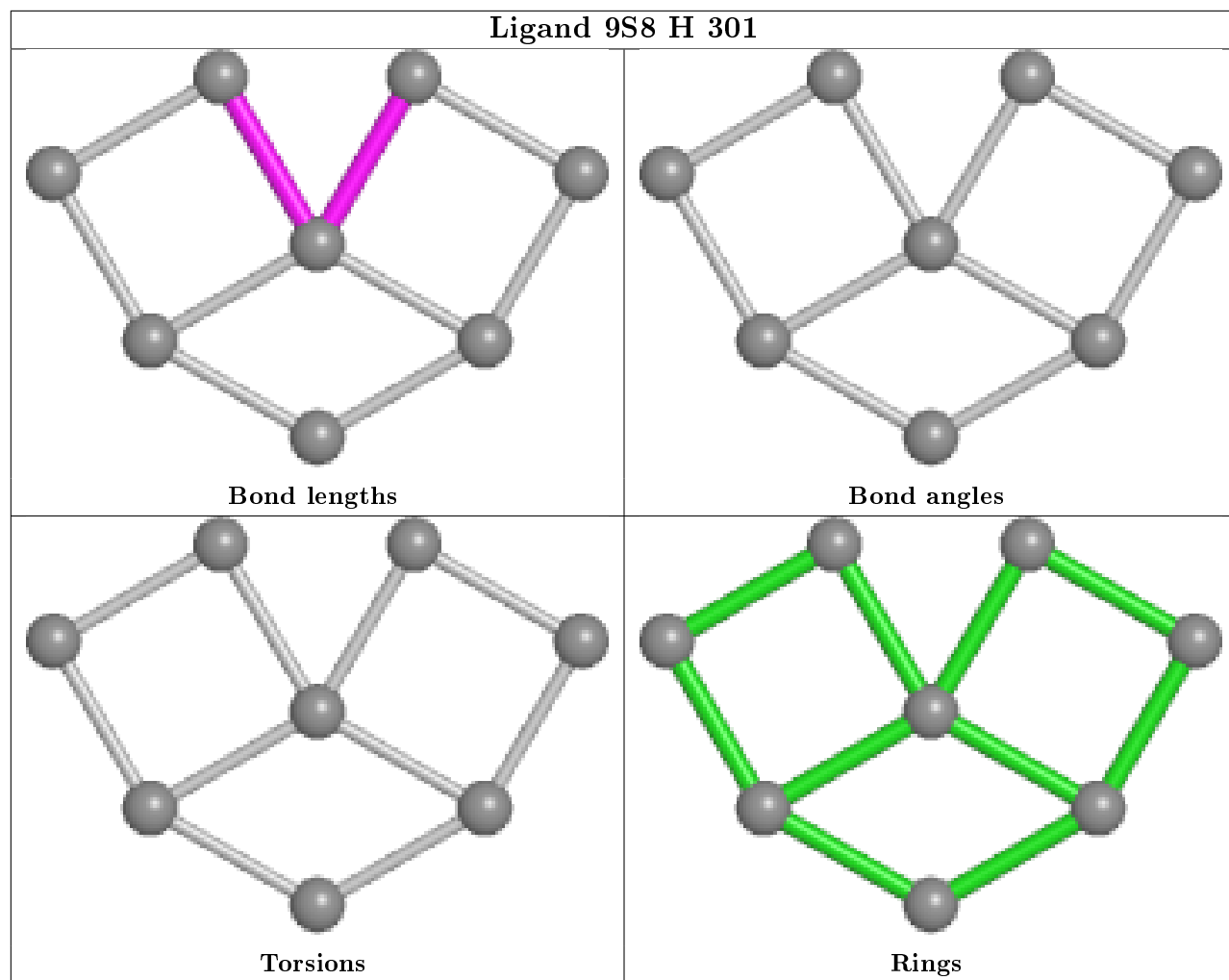


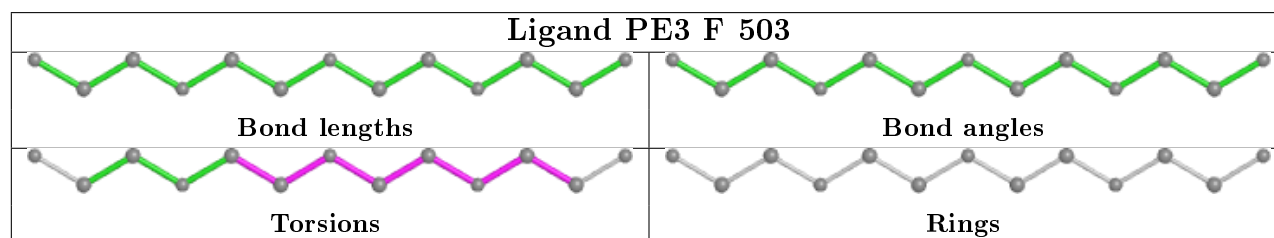
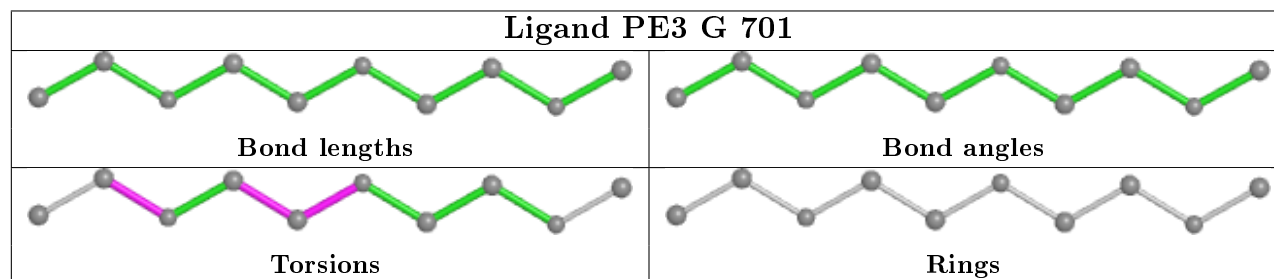
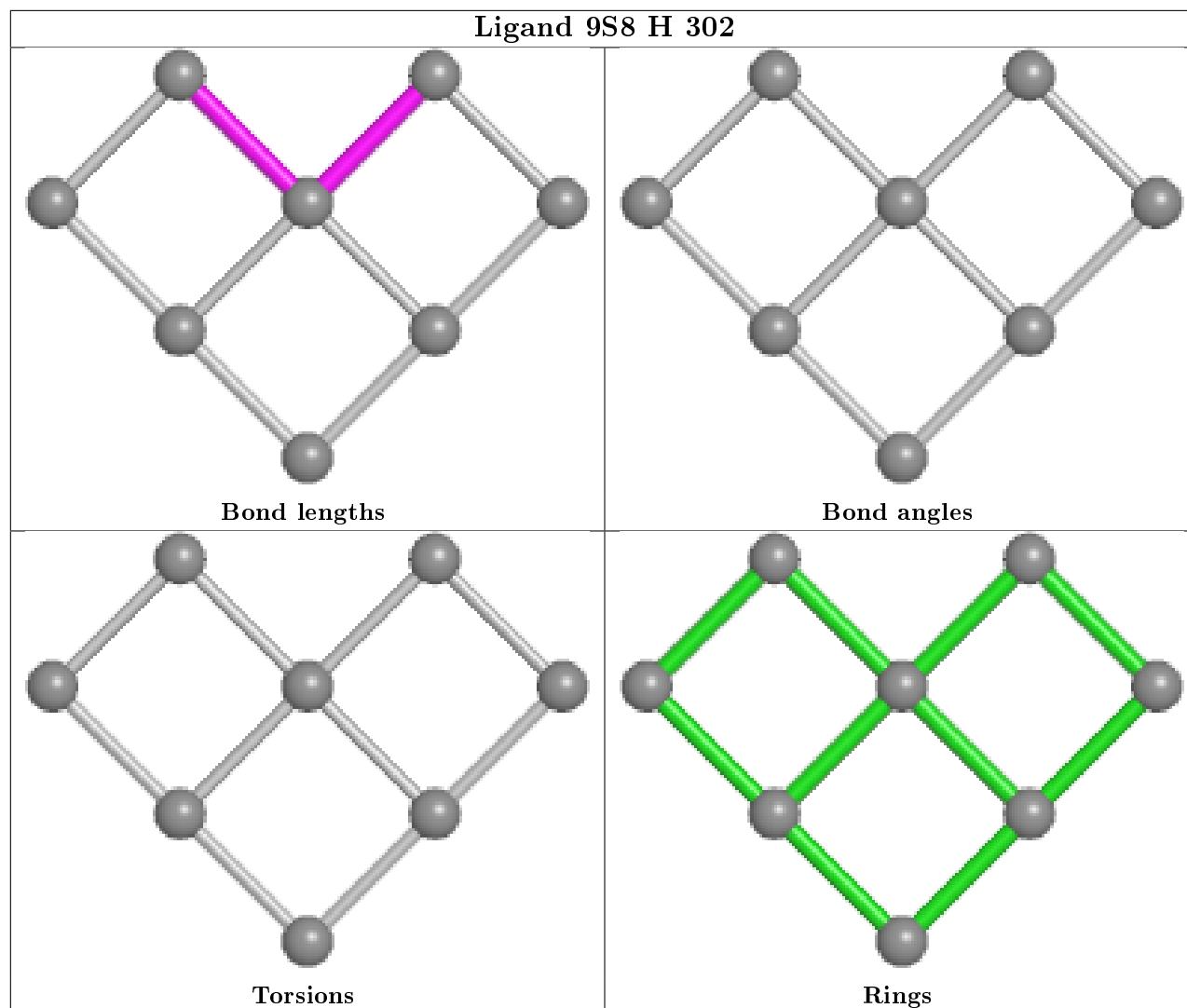
Torsions

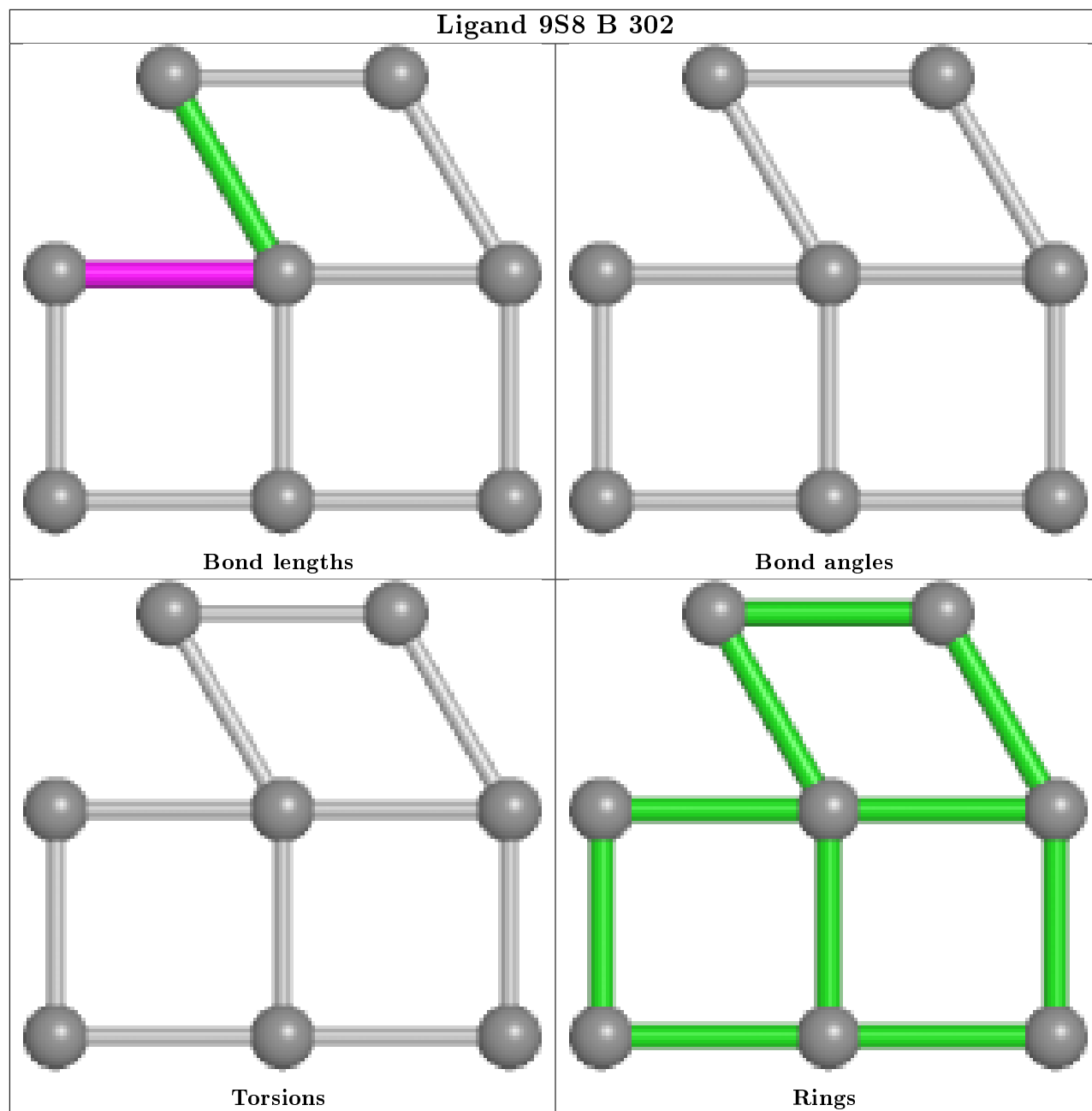


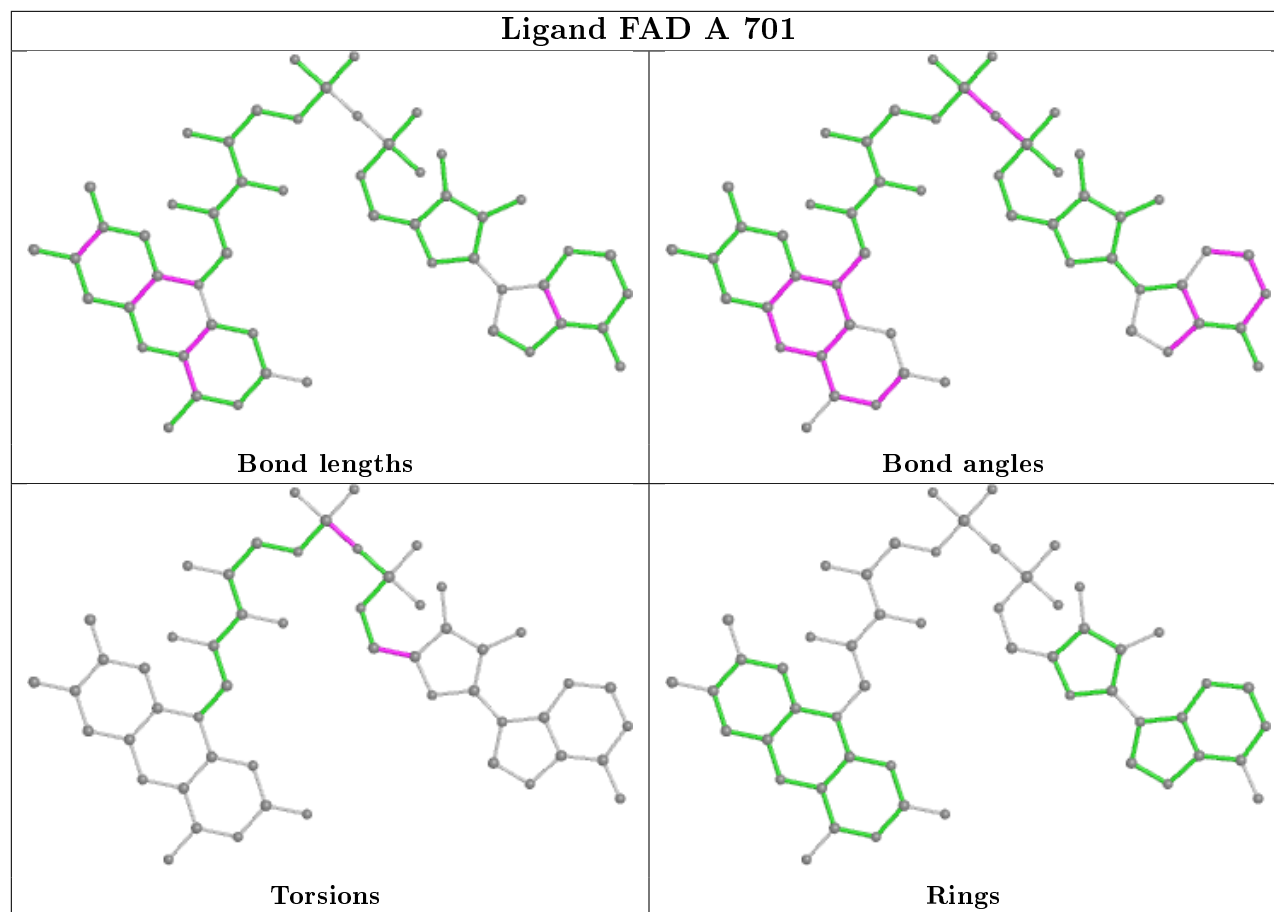
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9
1	A	652/654 (99%)	0.18	41 (6%) <div>2019</div>	25, 44, 135, 185	0
1	G	652/654 (99%)	0.26	42 (6%) <div>1918</div>	24, 44, 108, 142	0
2	B	291/291 (100%)	0.33	11 (3%) <div>4038</div>	33, 53, 76, 88	0
2	H	291/291 (100%)	1.27	58 (19%) <div>11</div>	44, 75, 123, 151	0
3	C	184/184 (100%)	0.16	6 (3%) <div>4644</div>	29, 49, 73, 88	0
3	I	183/184 (99%)	0.44	15 (8%) <div>1110</div>	28, 57, 105, 124	0
4	D	137/140 (97%)	-0.25	0 <div>100100</div>	29, 38, 58, 88	0
4	J	138/140 (98%)	0.21	1 (0%) <div>8786</div>	33, 43, 63, 100	0
5	E	297/299 (99%)	-0.05	1 (0%) <div>9493</div>	29, 43, 78, 101	0
5	K	297/299 (99%)	0.11	12 (4%) <div>3836</div>	27, 42, 79, 103	0
6	F	447/473 (94%)	-0.25	5 (1%) <div>8079</div>	27, 41, 69, 87	0
6	L	447/473 (94%)	-0.06	4 (0%) <div>8483</div>	24, 42, 69, 109	0
All	All	4016/4082 (98%)	0.19	196 (4%) <div>2928</div>	24, 46, 96, 185	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	143	LEU	13.8
1	A	246	CYS	8.5
2	H	291	ILE	8.1
2	H	268	MET	8.0
2	H	141	ARG	7.9
2	H	266	LEU	7.8
2	H	269	GLY	6.8
2	H	263	LEU	6.4
1	G	465	GLU	6.1
2	H	265	GLY	5.9
2	H	277	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
2	H	145	ILE	5.4
1	A	240	TYR	5.3
2	H	288	LEU	5.3
6	L	361	GLU	5.2
2	H	180	THR	5.1
2	H	140	GLU	5.1
6	L	362	GLU	5.1
1	A	251	GLN	5.0
1	A	605	ASP	4.9
1	A	294	ILE	4.9
1	A	255	VAL	4.9
1	A	306	ASN	4.8
1	A	311	ASP	4.8
2	H	279	VAL	4.6
2	H	274	ASP	4.6
2	H	270	MET	4.5
5	K	188	GLY	4.5
1	A	303	CYS	4.5
1	A	248	GLY	4.4
1	G	615	ALA	4.4
3	I	177	TRP	4.4
2	H	142	PRO	4.3
1	A	249	CYS	4.3
2	H	75	VAL	4.3
1	A	250	GLY	4.3
5	K	191	ILE	4.2
2	H	258	LEU	4.2
1	A	308	ILE	4.2
3	I	136	GLU	4.2
1	G	464	PRO	4.2
1	G	258	ILE	4.1
2	H	275	LEU	4.1
2	H	7	LEU	4.0
2	H	25	VAL	4.0
2	H	276	ALA	3.9
2	H	285	ASP	3.9
3	C	178	GLU	3.9
1	A	310	PHE	3.9
5	K	190	ALA	3.9
6	F	362	GLU	3.8
6	L	364	VAL	3.7
1	G	466	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	289	LYS	3.7
1	A	301	LYS	3.7
1	A	258	ILE	3.7
1	A	243	GLU	3.6
2	H	224	ALA	3.6
1	G	80	PHE	3.6
1	A	244	THR	3.6
3	I	141	ILE	3.6
1	G	6	ILE	3.5
1	A	257	PRO	3.5
1	A	252	CYS	3.4
2	H	249	PHE	3.4
1	G	570	VAL	3.4
1	A	653	THR	3.3
4	J	3	GLU	3.3
1	G	361	ALA	3.2
1	G	267	GLY	3.2
3	I	130	ALA	3.2
1	G	79	THR	3.2
2	H	5	PHE	3.2
1	A	288	ILE	3.1
2	H	177	VAL	3.1
3	I	183	LYS	3.0
2	H	12	PRO	3.0
1	G	311	ASP	3.0
2	H	225	ASP	3.0
2	H	27	GLU	2.9
6	L	363	VAL	2.9
2	H	138	LYS	2.9
1	G	604	LYS	2.9
5	K	193	THR	2.9
2	H	18	VAL	2.9
1	A	364	PRO	2.9
1	A	259	ASP	2.9
2	H	185	VAL	2.9
5	E	186	GLU	2.9
5	K	187	GLU	2.9
1	G	292	HIS	2.9
2	B	93	HIS	2.8
1	G	53	MET	2.8
2	B	287	LEU	2.8
1	G	303	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	299	CYS	2.8
3	I	140	SER	2.7
2	H	264	LEU	2.7
2	H	135	ILE	2.7
2	H	22	THR	2.7
3	I	178	GLU	2.7
1	A	241	ILE	2.7
5	K	50	GLU	2.7
1	G	50	GLY	2.7
1	G	614	SER	2.7
1	G	293	CYS	2.6
3	C	184	GLU	2.6
1	G	602	VAL	2.6
1	G	91	PRO	2.6
2	H	262	GLN	2.6
2	B	39	ALA	2.6
2	H	139	VAL	2.6
2	B	221	LYS	2.6
1	G	42	TYR	2.6
3	C	66	ASP	2.6
1	A	296	CYS	2.5
2	H	271	ASP	2.5
1	G	84	VAL	2.5
2	H	2	LYS	2.5
2	H	134	LYS	2.5
6	F	365	GLY	2.5
1	G	15	VAL	2.5
3	I	139	LYS	2.5
1	G	316	ILE	2.5
2	H	173	LEU	2.5
2	H	26	MET	2.4
1	G	49	PRO	2.4
1	A	316	ILE	2.4
1	A	299	CYS	2.4
2	H	182	ALA	2.4
2	H	137	GLU	2.4
5	K	186	GLU	2.4
1	G	89	LEU	2.4
1	A	300	ALA	2.4
1	G	48	ASP	2.3
1	G	575	ILE	2.3
2	B	135	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	LEU	2.3
1	G	255	VAL	2.3
2	H	144	ASN	2.3
2	H	1	MET	2.3
2	B	273	LYS	2.3
2	H	230	VAL	2.3
5	K	261	GLY	2.3
2	H	4	ALA	2.3
1	G	307	ALA	2.3
5	K	164	LEU	2.3
3	I	180	GLY	2.3
6	F	25	SER	2.3
2	H	226	CYS	2.2
1	A	285	LYS	2.2
2	H	183	LYS	2.2
2	H	132	VAL	2.2
5	K	260	PHE	2.2
2	B	130	ILE	2.2
1	G	469	LEU	2.2
3	I	120	TYR	2.2
1	G	310	PHE	2.2
1	A	235	MET	2.2
2	H	273	LYS	2.2
2	H	283	SER	2.2
2	B	279	VAL	2.2
6	F	2	VAL	2.2
1	A	256	CYS	2.2
1	A	314	PRO	2.2
2	B	177	VAL	2.2
3	I	179	LYS	2.1
1	G	82	ARG	2.1
1	A	615	ALA	2.1
1	G	238	ALA	2.1
3	I	172	LEU	2.1
1	G	304	GLY	2.1
1	G	364	PRO	2.1
1	A	307	ALA	2.1
3	C	141	ILE	2.1
1	G	616	LEU	2.1
2	H	16	ALA	2.1
2	B	180	THR	2.1
1	A	260	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
6	F	364	VAL	2.1
1	A	279	PRO	2.1
2	B	291	ILE	2.0
2	H	176	ILE	2.0
1	A	606	GLY	2.0
3	I	135	ALA	2.0
3	C	31	LEU	2.0
5	K	4	ILE	2.0
5	K	209	LEU	2.0
3	I	169	PHE	2.0
1	G	268	ILE	2.0
3	I	182	LEU	2.0
1	A	304	GLY	2.0
1	A	312	GLN	2.0
1	G	251	GLN	2.0
1	G	467	GLY	2.0
3	C	1	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GOL	A	709	6/6	0.59	0.30	61,63,64,65	0
9	GOL	I	204	6/6	0.71	0.20	52,52,54,54	0
9	GOL	I	203	6/6	0.74	0.27	54,55,58,58	0
9	GOL	A	708	6/6	0.77	0.19	58,59,59,60	0
16	PE3	G	701	10/43	0.77	0.19	63,69,76,78	0
9	GOL	K	304	6/6	0.77	0.23	67,69,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SF4	A	703	8/8	0.78	0.13	176,177,177,177	0
16	PE3	L	502	9/43	0.79	0.18	61,66,69,70	0
14	ACT	G	702	4/4	0.79	0.24	88,90,90,91	0
16	PE3	F	503	13/43	0.80	0.18	63,64,72,73	0
16	PE3	F	502	9/43	0.81	0.18	74,74,76,77	0
14	ACT	D	202	4/4	0.81	0.19	75,75,76,76	0
14	ACT	E	301	4/4	0.82	0.15	56,59,60,60	0
18	TP7	H	304	21/21	0.85	0.19	72,78,84,85	0
9	GOL	D	203	6/6	0.88	0.18	58,63,64,65	0
10	9S8	H	301	8/8	0.88	0.13	65,71,77,78	0
8	SF4	A	704	8/8	0.89	0.09	132,134,134,134	0
17	FE	G	703	1/1	0.91	0.15	28,28,28,28	1
8	SF4	G	708	8/8	0.93	0.08	102,102,104,104	0
8	SF4	K	303	8/8	0.94	0.10	47,48,49,52	0
8	SF4	G	709	8/8	0.94	0.08	39,41,45,46	0
8	SF4	G	710	8/8	0.94	0.10	35,41,43,43	0
10	9S8	B	301	8/8	0.95	0.09	39,43,47,47	0
10	9S8	H	302	8/8	0.95	0.09	56,58,61,61	0
10	9S8	B	302	8/8	0.95	0.08	41,43,47,47	0
14	ACT	F	504	4/4	0.95	0.14	40,42,44,46	0
12	SO4	B	304	5/5	0.95	0.18	74,76,76,77	0
11	COM	H	303	7/7	0.96	0.11	53,56,61,64	0
8	SF4	G	707	8/8	0.96	0.06	72,73,75,75	0
8	SF4	G	705	8/8	0.96	0.07	38,42,45,47	0
11	COM	B	303	7/7	0.96	0.11	65,66,67,69	0
7	FAD	A	701	53/53	0.97	0.13	25,31,45,49	0
13	FES	J	200	4/4	0.97	0.09	36,38,39,41	0
7	FAD	G	704	53/53	0.97	0.11	25,31,46,52	0
8	SF4	E	304	8/8	0.98	0.12	45,46,50,51	0
8	SF4	A	707	8/8	0.98	0.12	42,44,46,48	0
13	FES	D	201	4/4	0.98	0.12	34,35,36,39	0
8	SF4	I	201	8/8	0.98	0.12	32,33,35,35	0
8	SF4	A	706	8/8	0.98	0.10	38,40,42,43	0
8	SF4	K	301	8/8	0.98	0.13	29,30,31,33	0
8	SF4	I	202	8/8	0.98	0.13	38,42,42,43	0
8	SF4	C	201	8/8	0.98	0.14	33,34,36,36	0
8	SF4	K	302	8/8	0.98	0.13	38,40,40,41	0
15	NFU	F	501	8/8	0.99	0.12	28,29,32,32	0
8	SF4	A	705	8/8	0.99	0.09	29,33,33,33	0
8	SF4	E	303	8/8	0.99	0.12	42,44,47,49	0
8	SF4	C	202	8/8	0.99	0.12	38,38,41,41	0
8	SF4	E	302	8/8	0.99	0.14	38,40,41,42	0

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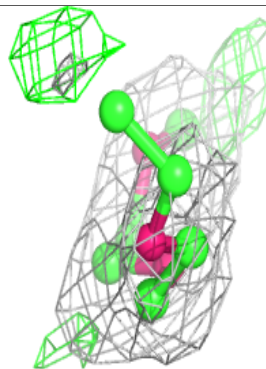
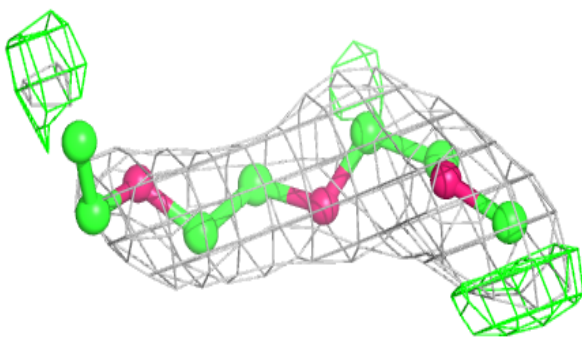
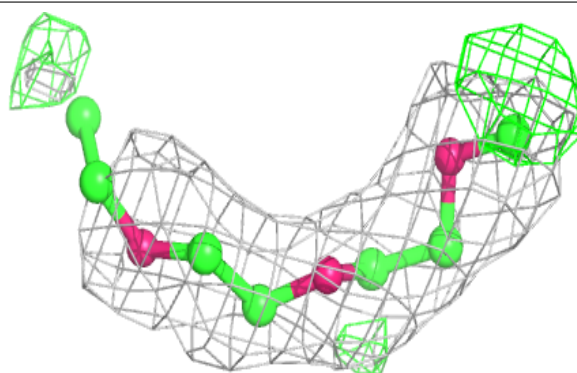
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	NFU	L	501	8/8	0.99	0.15	26,29,31,31	0
17	FE	F	505	1/1	0.99	0.10	29,29,29,29	0
8	SF4	G	706	8/8	0.99	0.12	26,27,28,29	0
8	SF4	A	702	8/8	0.99	0.12	27,28,29,29	0
17	FE	L	503	1/1	1.00	0.13	29,29,29,29	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.

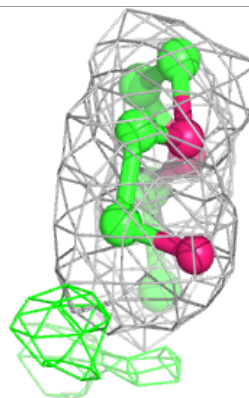
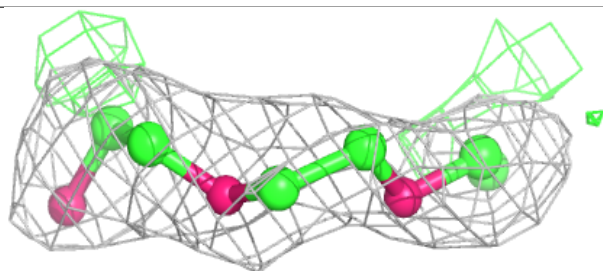
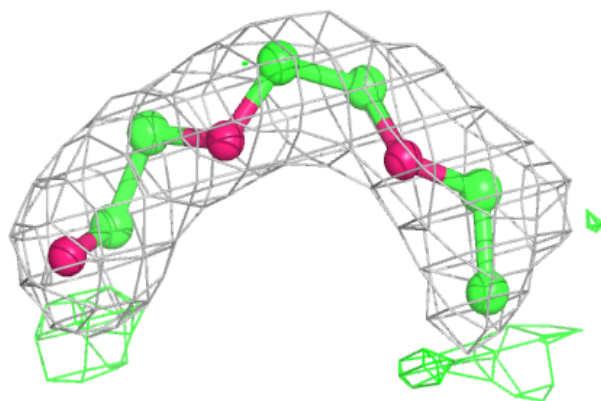
Electron density around PE3 G 701:

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

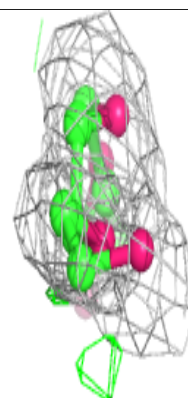
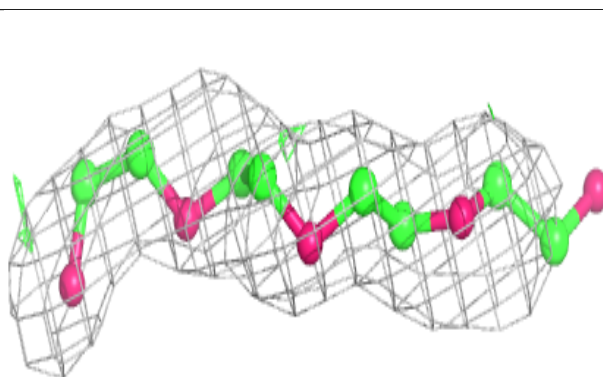
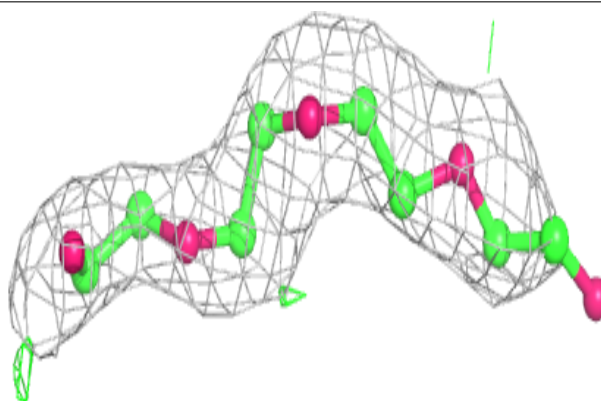


Electron density around PE3 L 502:

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

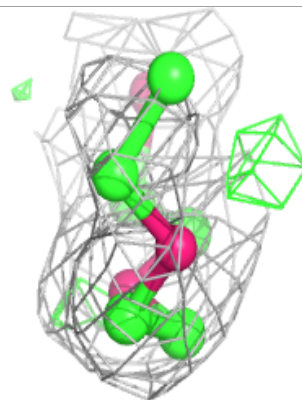
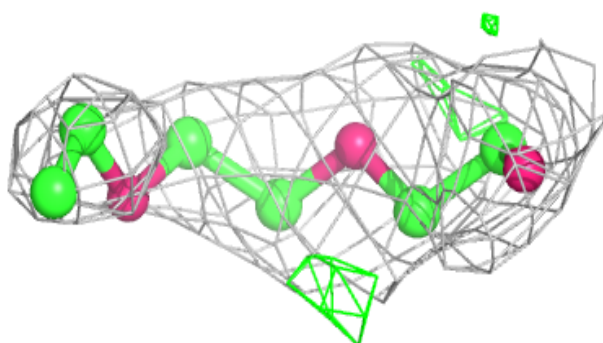
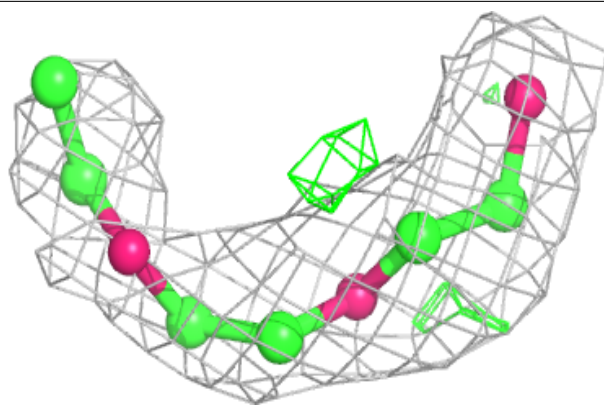
**Electron density around PE3 F 503:**

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

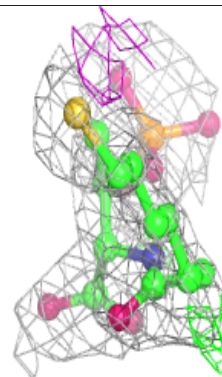
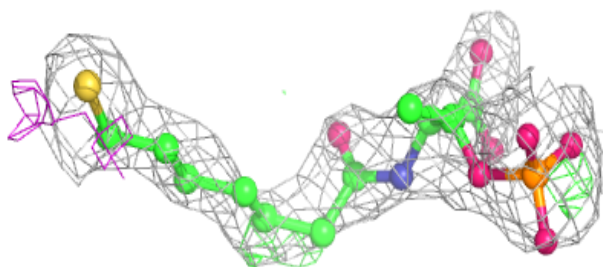
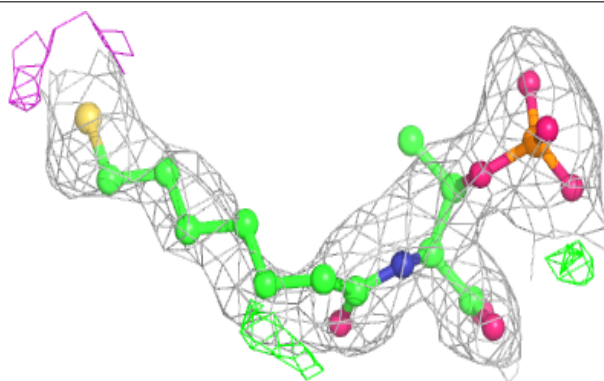


Electron density around PE3 F 502:

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

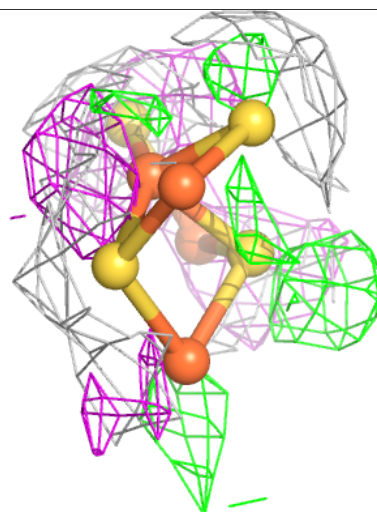
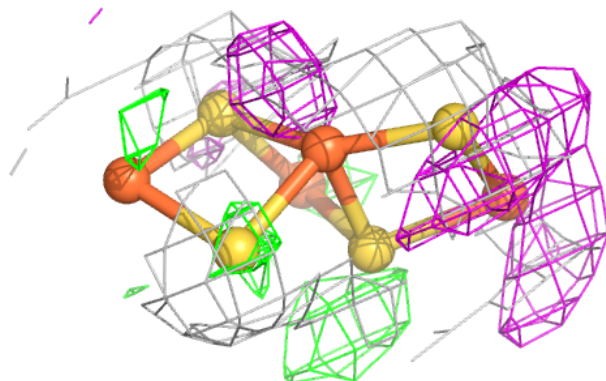
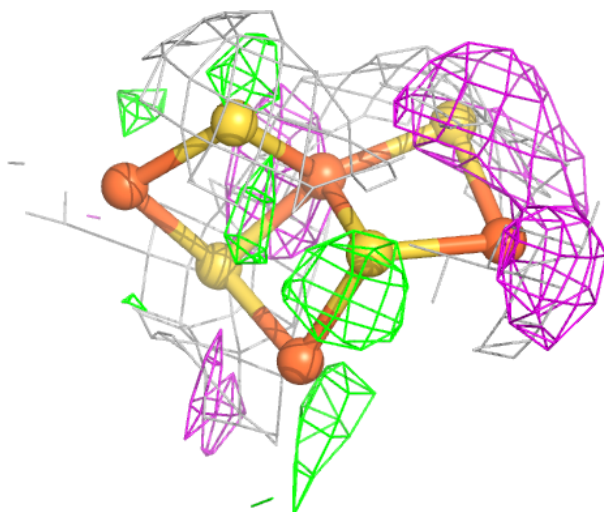
**Electron density around TP7 H 304:**

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



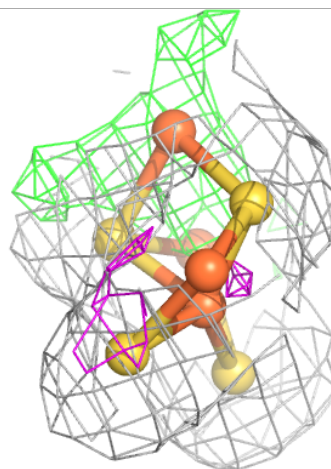
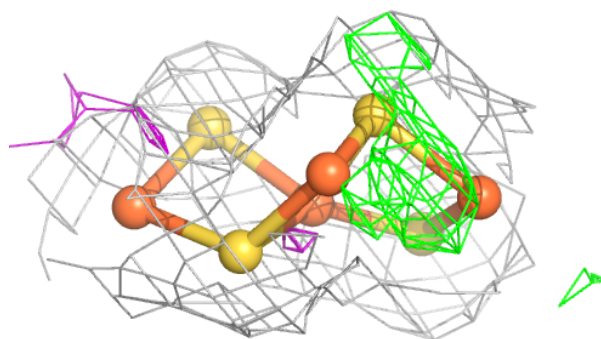
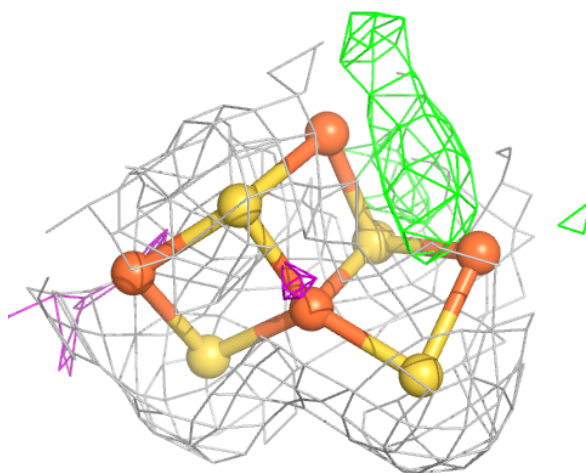
Electron density around 9S8 H 301:

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



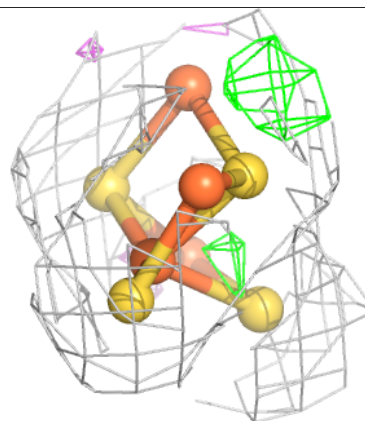
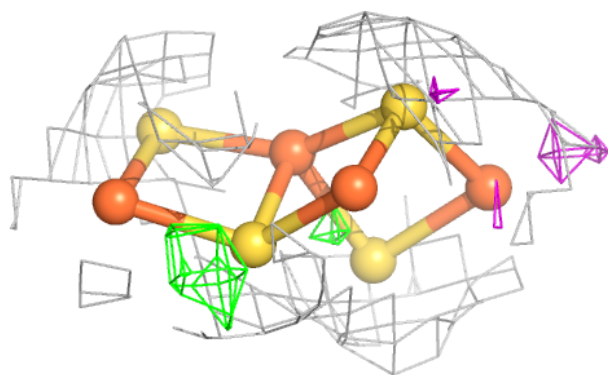
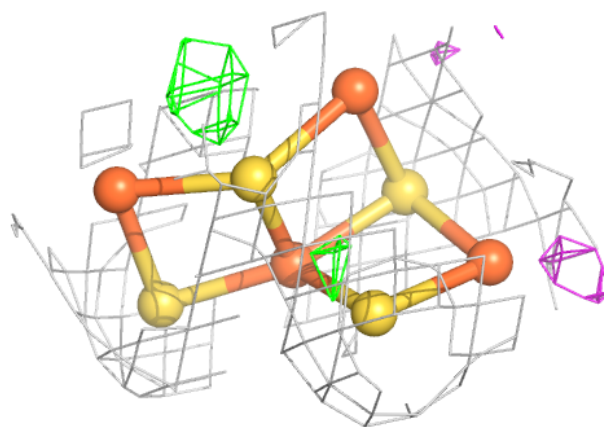
Electron density around 9S8 B 301:

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



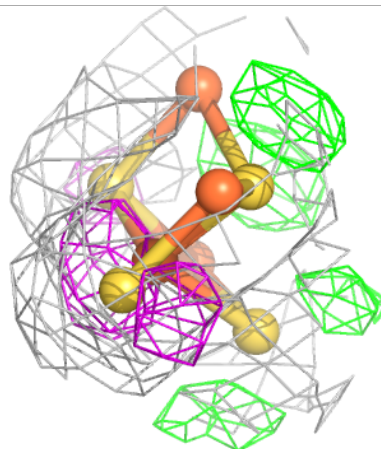
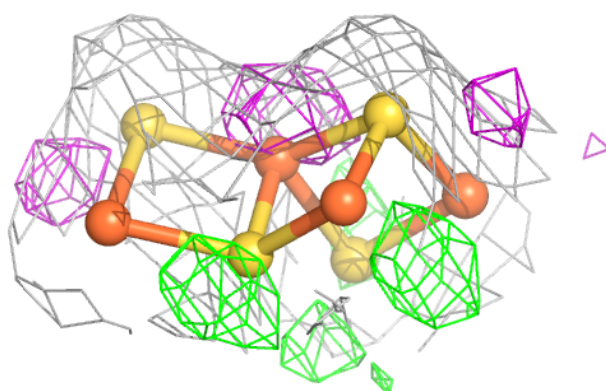
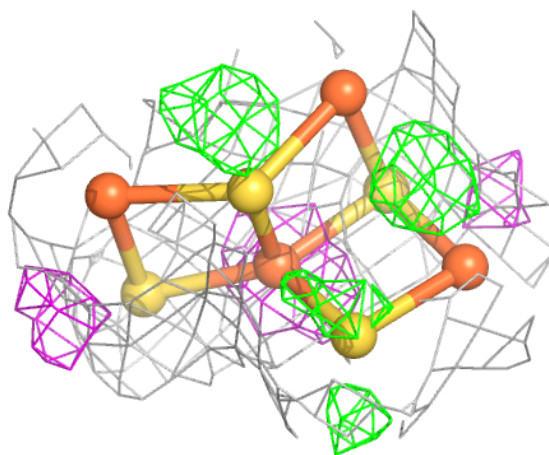
Electron density around 9S8 H 302:

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

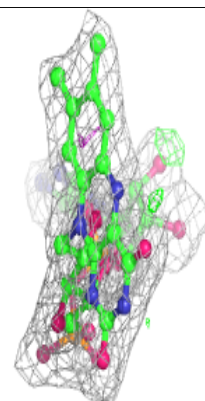
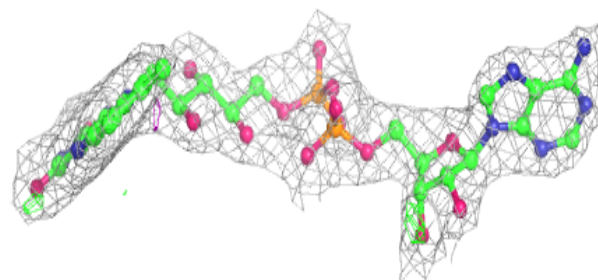
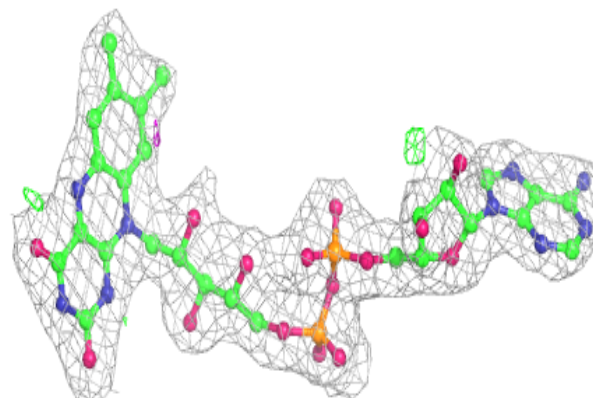


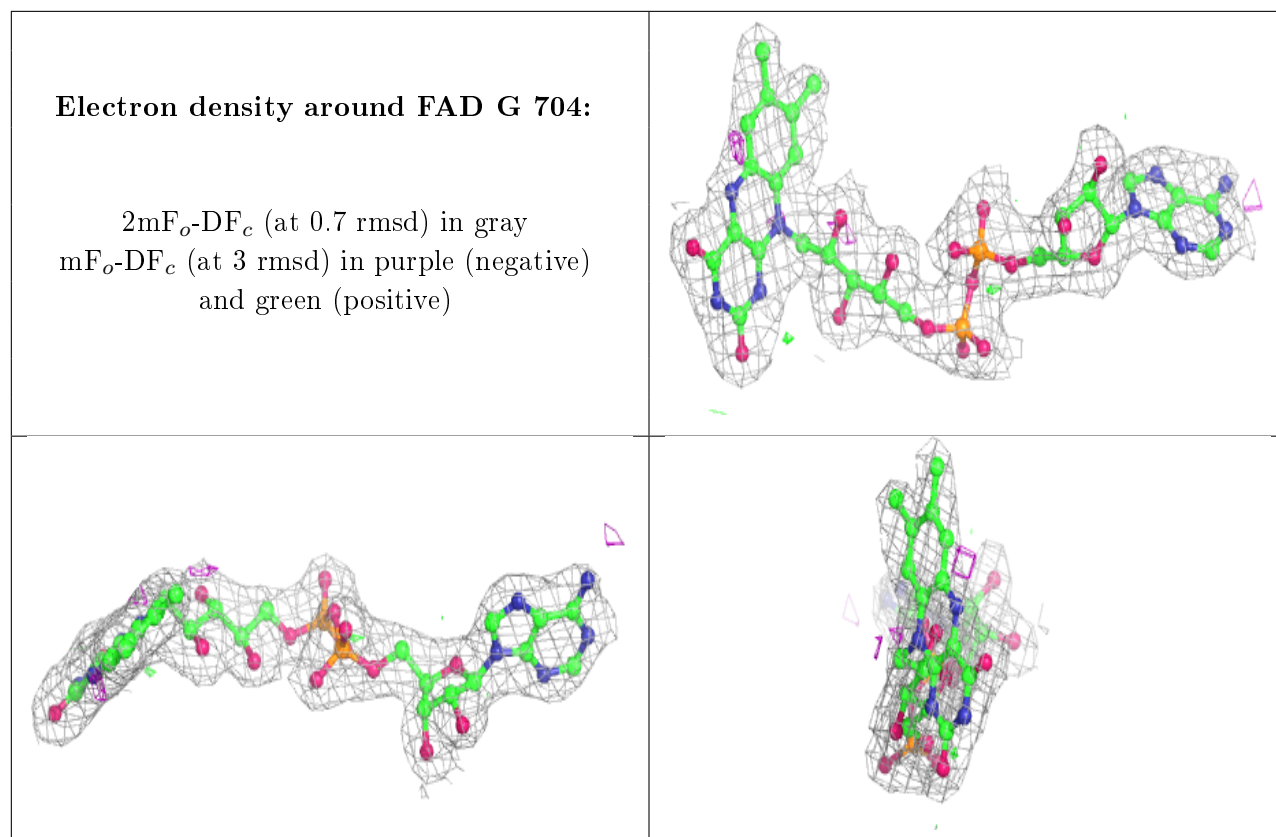
Electron density around 9S8 B 302:

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

**Electron density around FAD A 701:**

$2mF_o-DF_c$ (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.