wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 06:19 am GMT

PDB ID	:	5ODH
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 wwPDB X-ray Structure Validation Summary 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:

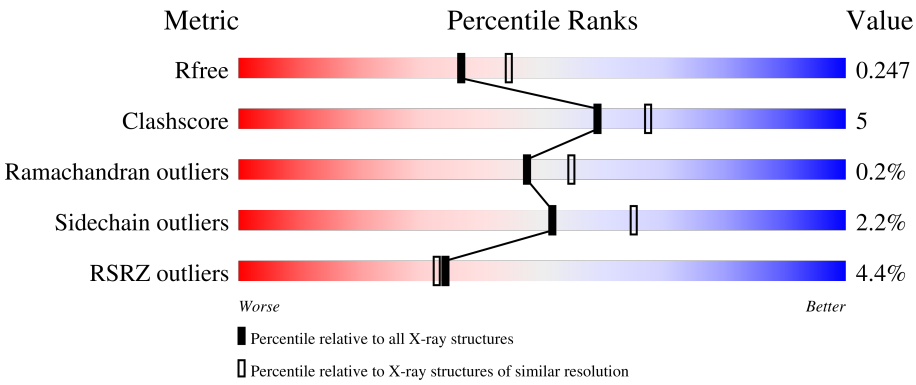
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	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 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	7%, 88%, 10%
1	G	654	5%, 89%, 11%
2	B	291	2%, 87%, 13%
2	H	291	13%, 72%, 28%
3	C	184	2%, 86%, 14%

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Mol	Chain	Length	Quality of chain
3	I	184	5% 79% 20%
4	D	140	84% 14%
4	J	140	2% 89% 9%
5	E	299	4% 89% 10%
5	K	299	3% 90% 9%
6	F	473	% 86% 8% 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 19 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
			Total	C	N	O	S			
1	A	652	4977	3140	845	943	49	0	0	0
1	G	653	4984	3145	846	944	49	0	0	0

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

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

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

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

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

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

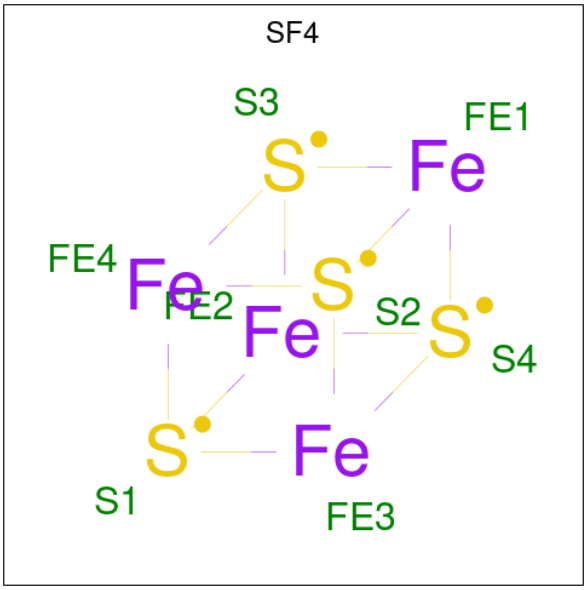
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

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

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

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

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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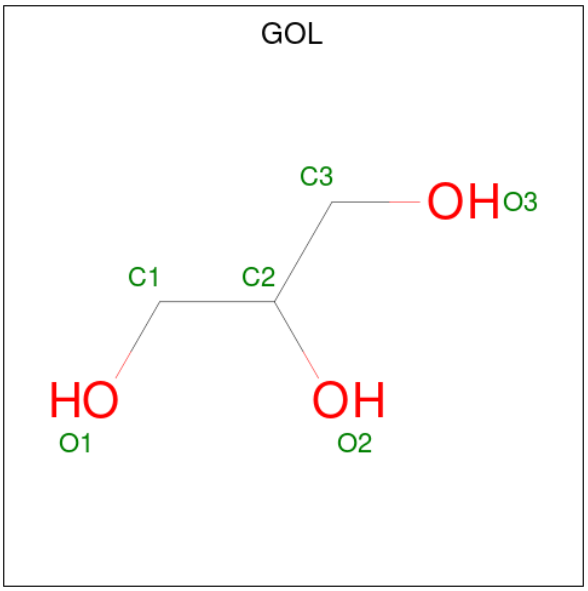
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	C	1	8	4	4	0	0
			Total	Fe	S		
7	C	1	8	4	4	0	0
			Total	Fe	S		
7	E	1	8	4	4	0	0
			Total	Fe	S		
7	E	1	8	4	4	0	0
			Total	Fe	S		
7	E	1	8	4	4	0	0
			Total	Fe	S		
7	G	1	8	4	4	0	0
			Total	Fe	S		
7	G	1	8	4	4	0	0
			Total	Fe	S		
7	G	1	8	4	4	0	0
	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

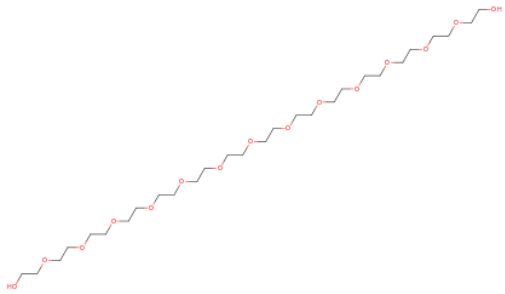
- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0
8	B	1	6	3	3	0	0
8	B	1	6	3	3	0	0
8	E	1	6	3	3	0	0
8	G	1	6	3	3	0	0
8	K	1	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 (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).

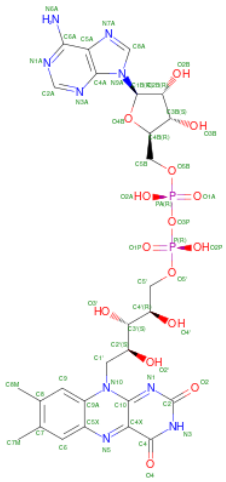
PE3



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

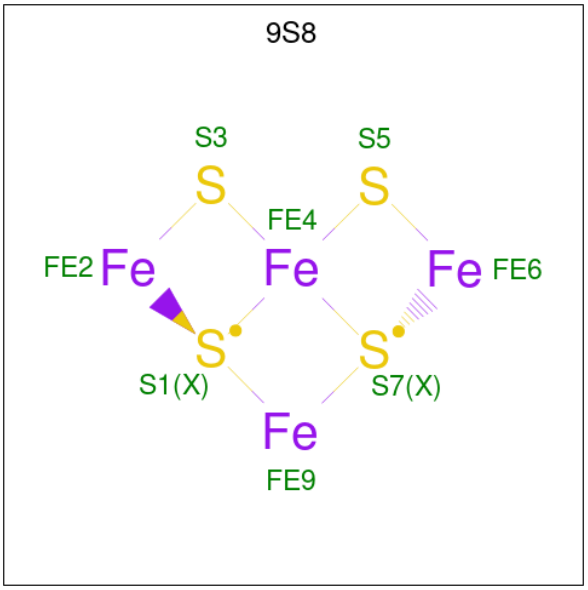
- Molecule 10 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD



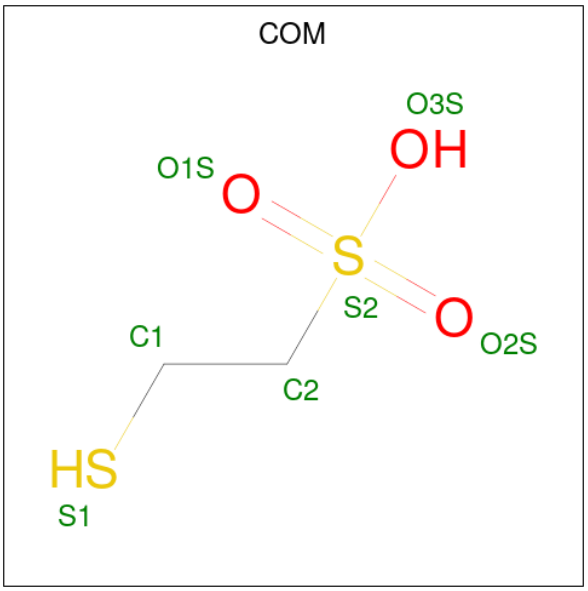
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
10	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
10	G	1	53	27	9	15	2	0	0

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



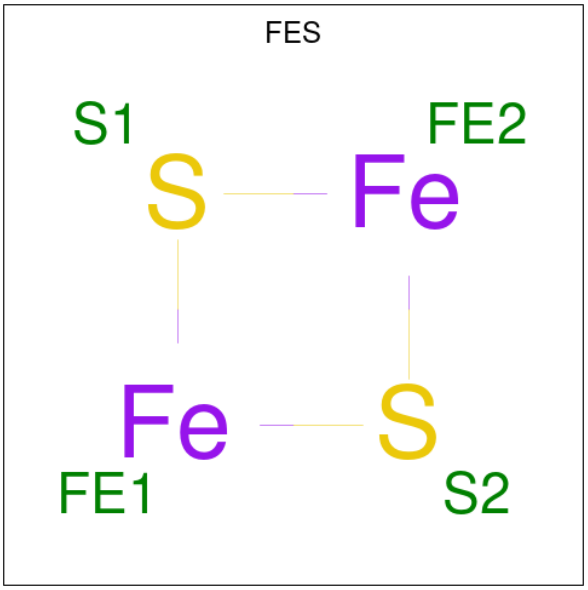
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	B	1	8	4	4	0	0
			Total	Fe	S		
11	B	1	8	4	4	0	0
			Total	Fe	S		
11	H	1	8	4	4	0	0
			Total	Fe	S		
11	H	1	8	4	4	0	0

- Molecule 12 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



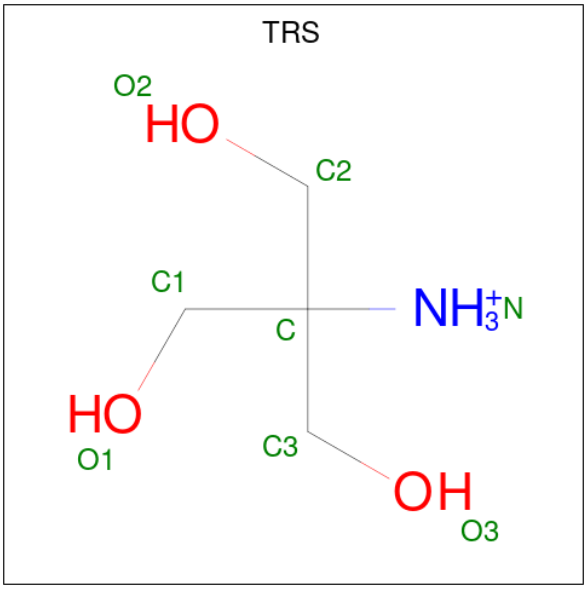
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
12	B	1	7	2	3	2	0	0
			Total	C	O	S		
12	H	1	7	2	3	2	0	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



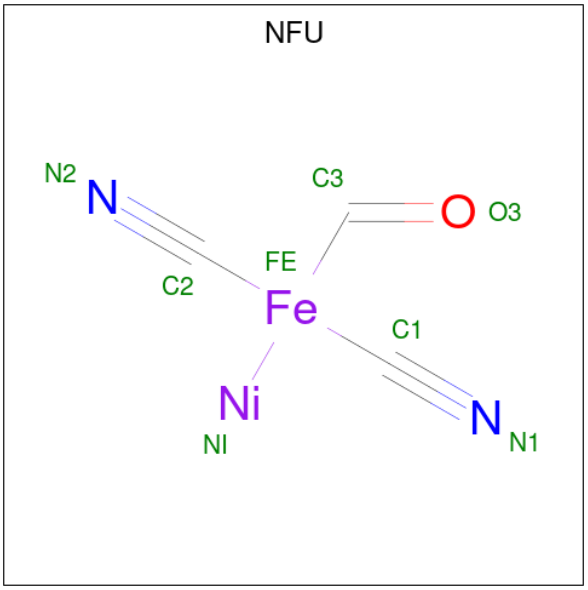
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
13	D	1	4	2	2	0	0
			Total	Fe	S		
13	J	1	4	2	2	0	0

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



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

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



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

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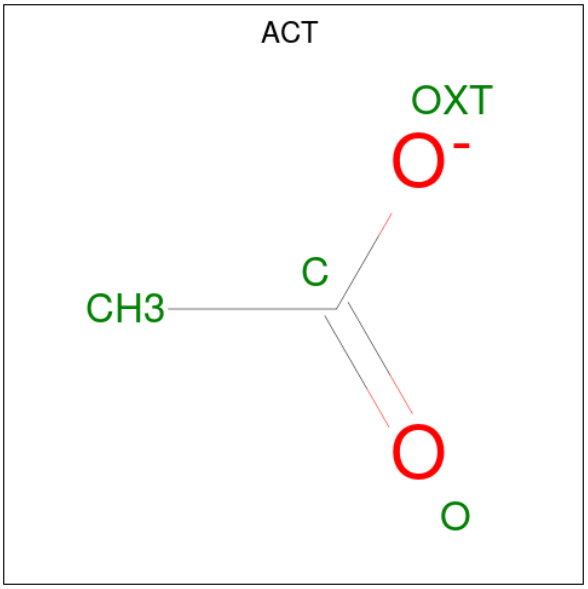
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	N	Ni	O		
15	L	1	8	3	1	2	1	1	0	0

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

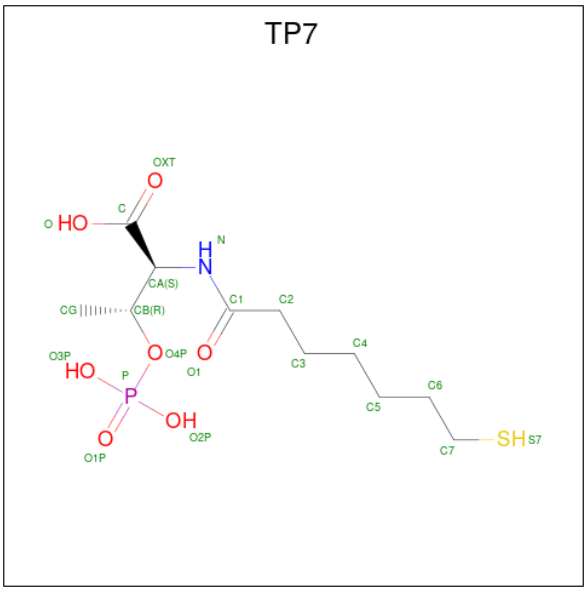
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
16	F	1	1	1	0	0
16	G	1	1	1	0	0
16	L	1	1	1	0	0

- Molecule 17 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 18 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



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

- Molecule 19 is water.

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

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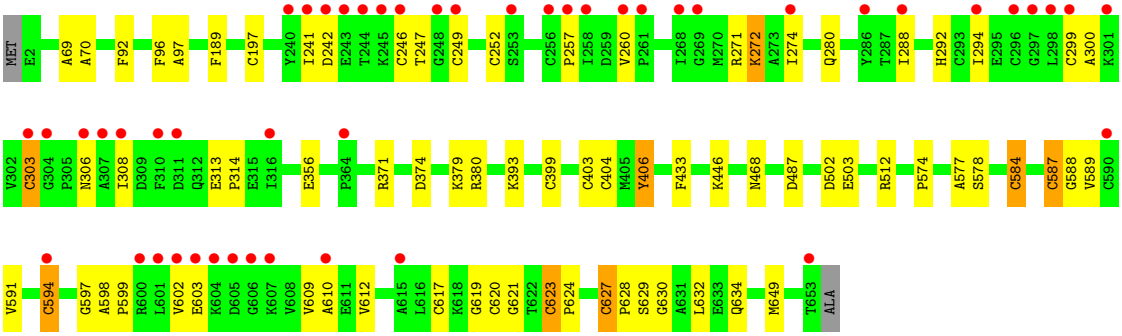
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	L	79	79	79	0	0

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.

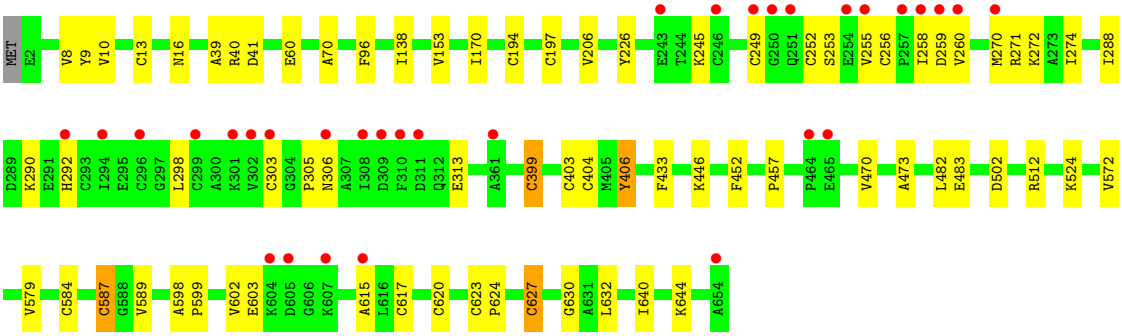
• Molecule 1: Heterodisulfide reductase, subunit A

Chain A:



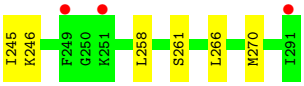
• Molecule 1: Heterodisulfide reductase, subunit A

Chain G:



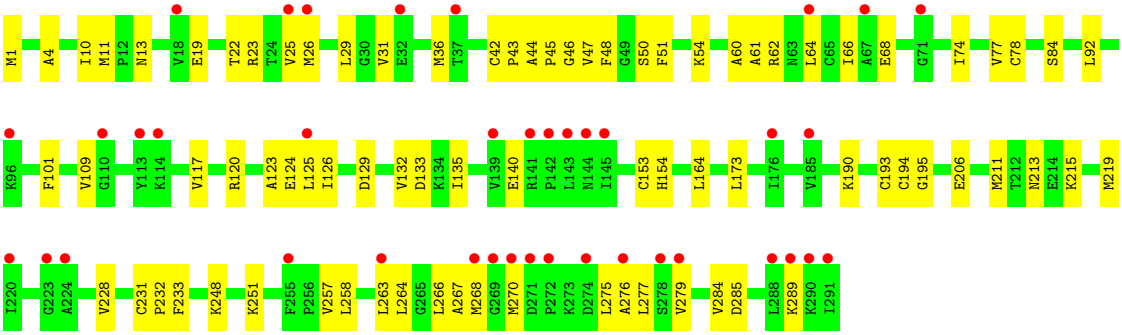
• Molecule 2: Heterodisulfide reductase, subunit B

Chain B:



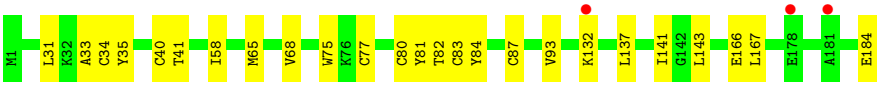
• Molecule 2: Heterodisulfide reductase, subunit B

Chain H:



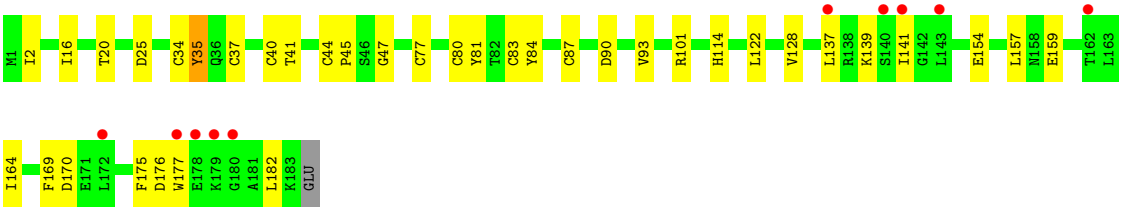
• Molecule 3: Heterodisulfide reductase, subunit C

Chain C:



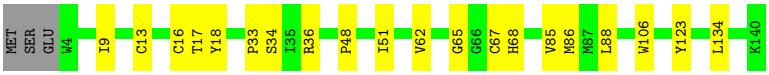
• Molecule 3: Heterodisulfide reductase, subunit C

Chain I:



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

Chain D:

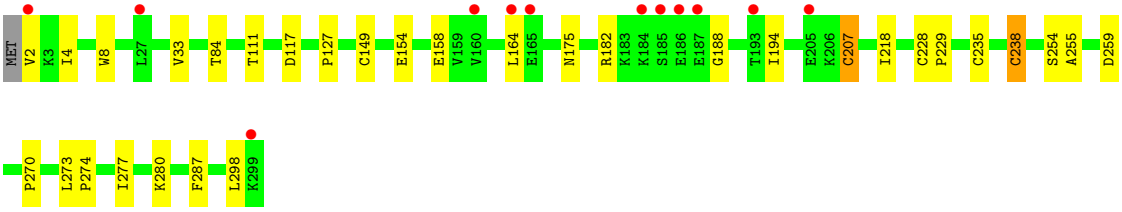


• Molecule 4: Methyl-viologen reducing hydrogenase, subunit D

Chain J:

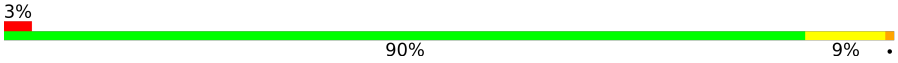
• Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

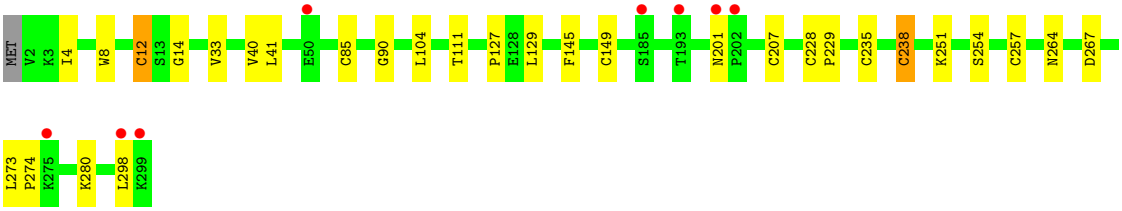
Chain E:



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

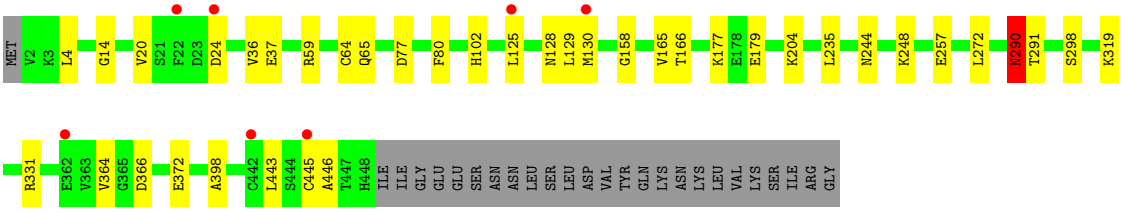
Chain K:





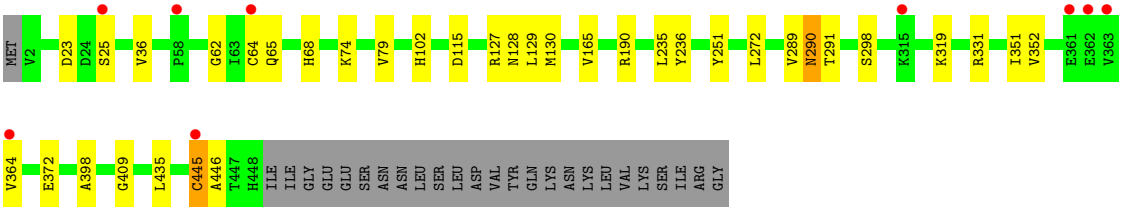
• Molecule 6: Methyl-viologen reducing hydrogenase, subunit A

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 (5.00%)	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 , 42.2	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	0.93	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PE3, FAD, SF4, FES, COM, GOL, NFU, ACT, TP7, 9S8, FE, TRS

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	0.30	0/5069	0.47	0/6850
1	G	0.30	0/5076	0.46	0/6860
2	B	0.29	0/2277	0.51	0/3070
2	H	0.31	0/2273	0.52	0/3066
3	C	0.32	0/1442	0.49	0/1942
3	I	0.30	0/1437	0.50	0/1934
4	D	0.30	0/1123	0.47	0/1508
4	J	0.29	0/1132	0.46	0/1520
5	E	0.31	0/2297	0.52	0/3113
5	K	0.30	0/2297	0.51	0/3113
6	F	0.29	0/3590	0.48	0/4853
6	L	0.29	0/3590	0.47	0/4853
All	All	0.30	0/31603	0.48	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4977	0	4968	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4984	0	4979	40	0
2	B	2236	0	2243	26	0
2	H	2232	0	2234	62	0
3	C	1421	0	1431	15	0
3	I	1416	0	1435	26	0
4	D	1097	0	1068	14	0
4	J	1106	0	1074	9	0
5	E	2258	0	2265	25	0
5	K	2258	0	2265	19	0
6	F	3521	0	3506	23	1
6	L	3521	0	3505	19	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	8	0	0	1	0
15	L	8	0	0	1	0
16	F	1	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
17	G	8	0	6	1	0
18	H	21	0	19	3	0
19	A	111	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	27	0	0	1	0
19	C	25	0	0	0	0
19	D	29	0	0	0	0
19	E	37	0	0	0	0
19	F	67	0	0	1	0
19	G	134	0	0	0	0
19	H	5	0	0	0	0
19	I	14	0	0	0	0
19	J	31	0	0	0	0
19	K	51	0	0	0	0
19	L	79	0	0	0	0
All	All	32106	0	31176	294	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.

The worst 5 of 294 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	19:A:910:HOH:O	2.49	0.71
2:B:104:GLU:OE2	19:B:401:HOH:O	2.10	0.67
6:L:289:VAL:O	6:L:290:ASN:HB2	1.95	0.67

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%)	47	55
1	G	651/654 (100%)	615 (94%)	35 (5%)	1 (0%)	47	55
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
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%)	34	37
6	L	445/473 (94%)	439 (99%)	4 (1%)	2 (0%)	34	37
All	All	3995/4082 (98%)	3866 (97%)	123 (3%)	6 (0%)	47	55

5 of 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

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%)	524 (97%)	15 (3%)	43	56
1	G	540/541 (100%)	524 (97%)	16 (3%)	41	53
2	B	242/242 (100%)	238 (98%)	4 (2%)	60	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	241/242 (100%)	236 (98%)	5 (2%)	53	67
3	C	156/157 (99%)	151 (97%)	5 (3%)	39	50
3	I	156/157 (99%)	149 (96%)	7 (4%)	27	34
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%)	249 (98%)	6 (2%)	49	62
5	K	255/256 (100%)	248 (97%)	7 (3%)	44	57
6	F	386/410 (94%)	381 (99%)	5 (1%)	69	81
6	L	386/410 (94%)	381 (99%)	5 (1%)	69	81
All	All	3389/3450 (98%)	3314 (98%)	75 (2%)	52	65

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	35	TYR
6	L	102	HIS
3	I	77	CYS
5	K	111	THR
5	E	8	TRP

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
11	9S8	B	302	2	2,10,10	1.40	0	-		
8	GOL	B	304	-	5,5,5	0.38	0	5,5,5	0.19	0
15	NFU	L	502	6	2,7,7	1.21	0	-		
17	ACT	G	709	-	3,3,3	0.80	0	3,3,3	1.35	0
13	FES	D	201	4	0,4,4	-	-	-		
13	FES	J	201	4	0,4,4	-	-	-		
7	SF4	G	706	1	0,12,12	-	-	-		
7	SF4	C	201	3	0,12,12	-	-	-		
7	SF4	A	701	1	0,12,12	-	-	-		
15	NFU	F	503	6	2,7,7	1.40	0	-		
7	SF4	I	201	3	0,12,12	-	-	-		
11	9S8	H	301	2	2,10,10	1.13	0	-		
10	FAD	A	709	-	53,58,58	1.27	6 (11%)	68,89,89	1.33	10 (14%)
18	TP7	H	304	-	19,20,20	0.64	0	24,26,26	1.05	0
7	SF4	K	301	5	0,12,12	-	-	-		
8	GOL	K	304	-	5,5,5	0.35	0	5,5,5	0.22	0
12	COM	H	303	-	6,6,6	1.42	2 (33%)	7,8,8	2.67	4 (57%)
7	SF4	A	704	1	0,12,12	-	-	-		
7	SF4	E	301	5	0,12,12	-	-	-		
8	GOL	B	305	-	5,5,5	0.30	0	5,5,5	0.25	0
7	SF4	K	303	5	0,12,12	-	-	-		
9	PE3	A	708	-	13,13,42	0.49	0	12,12,41	0.19	0
7	SF4	G	703	1	0,12,12	-	-	-		
9	PE3	F	502	-	8,8,42	0.46	0	7,7,41	0.22	0
11	9S8	H	302	2	2,10,10	1.14	0	-		
9	PE3	F	501	-	8,8,42	0.45	0	7,7,41	0.31	0
7	SF4	A	702	-	0,12,12	-	-	-		
7	SF4	E	303	5	0,12,12	-	-	-		
8	GOL	A	707	-	5,5,5	0.31	0	5,5,5	0.35	0
7	SF4	A	705	1	0,12,12	-	-	-		
11	9S8	B	301	2	2,10,10	1.55	1 (50%)	-		

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	-	-	-		
7	SF4	A	706	1	0,12,12	-	-	-		
7	SF4	G	702	1	0,12,12	-	-	-		
7	SF4	A	703	1	0,12,12	-	-	-		
7	SF4	I	202	3	0,12,12	-	-	-		
7	SF4	K	302	5	0,12,12	-	-	-		
14	TRS	D	202	-	7,7,7	0.27	0	9,9,9	0.39	0
10	FAD	G	711	-	53,58,58	1.31	6 (11%)	68,89,89	1.23	5 (7%)
8	GOL	G	707	-	5,5,5	0.35	0	5,5,5	0.13	0
7	SF4	G	705	1	0,12,12	-	-	-		
17	ACT	G	710	-	3,3,3	0.76	0	3,3,3	1.44	0
7	SF4	E	302	5	0,12,12	-	-	-		
9	PE3	L	501	-	8,8,42	0.50	0	7,7,41	0.21	0
12	COM	B	303	-	6,6,6	1.33	1 (16%)	7,8,8	2.99	4 (57%)
7	SF4	C	202	3	0,12,12	-	-	-		
8	GOL	E	304	-	5,5,5	0.34	0	5,5,5	0.22	0
7	SF4	G	701	16,1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	9S8	B	302	2	-	-	0/3/3/3
8	GOL	B	304	-	-	4/4/4/4	-
13	FES	D	201	4	-	-	0/1/1/1
13	FES	J	201	4	-	-	0/1/1/1
7	SF4	G	706	1	-	-	0/6/5/5
7	SF4	C	201	3	-	-	0/6/5/5
7	SF4	A	701	1	-	-	0/6/5/5
7	SF4	I	201	3	-	-	0/6/5/5
11	9S8	H	301	2	-	-	0/3/3/3
10	FAD	A	709	-	-	1/30/50/50	0/6/6/6
18	TP7	H	304	-	-	10/24/24/24	-
12	COM	H	303	-	-	1/4/4/4	-
8	GOL	K	304	-	-	2/4/4/4	-
7	SF4	K	301	5	-	-	0/6/5/5
7	SF4	A	704	1	-	-	0/6/5/5
7	SF4	E	301	5	-	-	0/6/5/5
8	GOL	B	305	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PE3	F	502	-	-	5/6/6/40	-
9	PE3	A	708	-	-	5/11/11/40	-
7	SF4	G	703	1	-	-	0/6/5/5
7	SF4	K	303	5	-	-	0/6/5/5
11	9S8	H	302	2	-	-	0/3/3/3
9	PE3	F	501	-	-	3/6/6/40	-
7	SF4	A	702	-	-	-	0/6/5/5
8	GOL	A	707	-	-	2/4/4/4	-
7	SF4	E	303	5	-	-	0/6/5/5
7	SF4	A	705	1	-	-	0/6/5/5
11	9S8	B	301	2	-	-	0/3/3/3
7	SF4	G	704	1	-	-	0/6/5/5
7	SF4	A	706	1	-	-	0/6/5/5
7	SF4	G	702	1	-	-	0/6/5/5
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	I	202	3	-	-	0/6/5/5
7	SF4	K	302	5	-	-	0/6/5/5
14	TRS	D	202	-	-	8/9/9/9	-
10	FAD	G	711	-	-	1/30/50/50	0/6/6/6
8	GOL	G	707	-	-	2/4/4/4	-
7	SF4	G	705	1	-	-	0/6/5/5
9	PE3	L	501	-	-	2/6/6/40	-
7	SF4	E	302	5	-	-	0/6/5/5
12	COM	B	303	-	-	4/4/4/4	-
7	SF4	C	202	3	-	-	0/6/5/5
8	GOL	E	304	-	-	1/4/4/4	-
7	SF4	G	701	16,1	-	-	0/6/5/5

The worst 5 of 16 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	G	711	FAD	C8-C7	3.57	1.49	1.40
10	A	709	FAD	C8-C7	3.23	1.49	1.40
10	G	711	FAD	C5X-N5	-2.65	1.34	1.39

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	303	COM	O3S-S2-O2S	-4.42	100.48	111.27
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	P-O3P-PA	-3.82	119.72	132.83

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

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

There are no ring outliers.

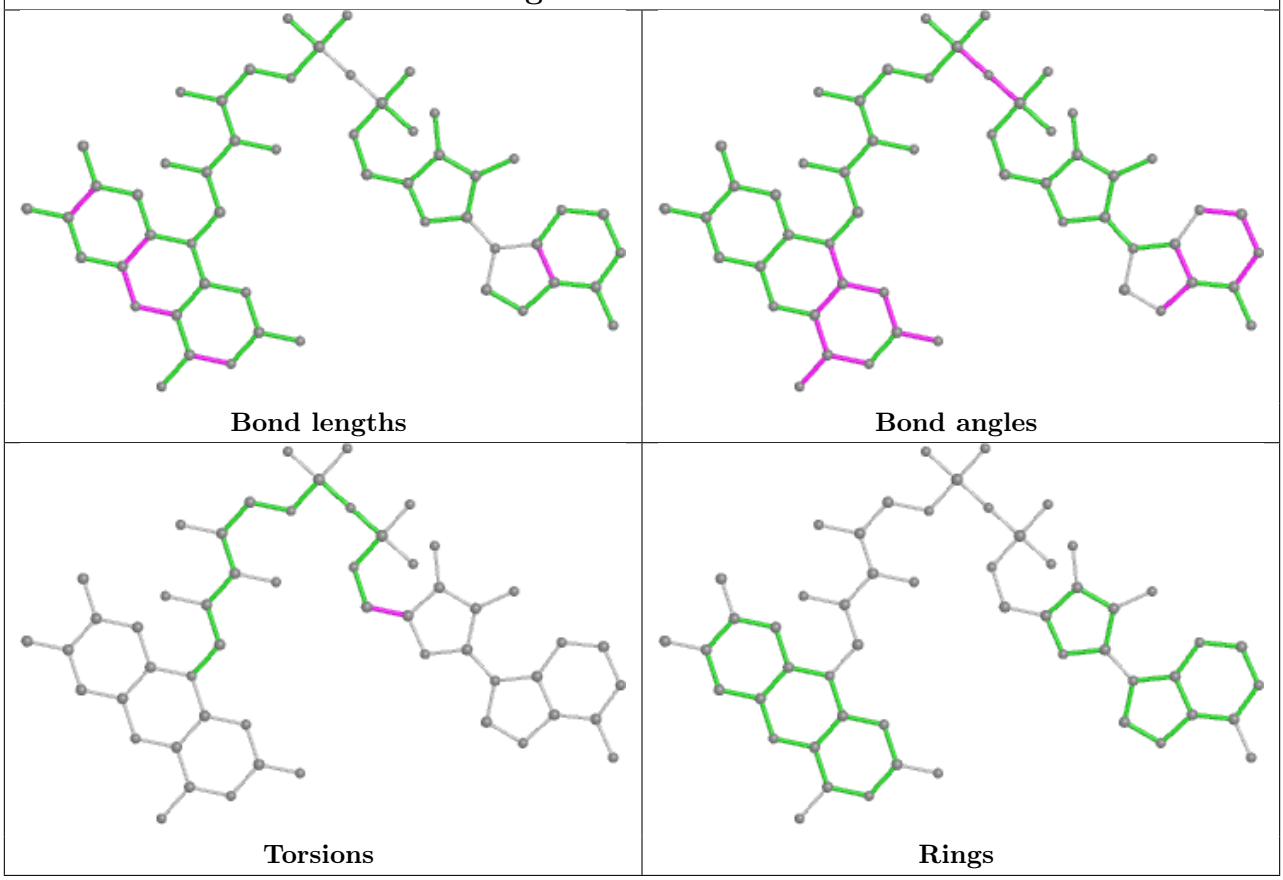
13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	302	9S8	1	0
15	L	502	NFU	1	0
15	F	503	NFU	1	0
11	H	301	9S8	1	0
18	H	304	TP7	3	0
8	K	304	GOL	1	0
12	H	303	COM	2	0
9	F	502	PE3	1	0
7	A	706	SF4	1	0
7	G	702	SF4	1	0
8	G	707	GOL	2	0
17	G	710	ACT	1	0
12	B	303	COM	1	0

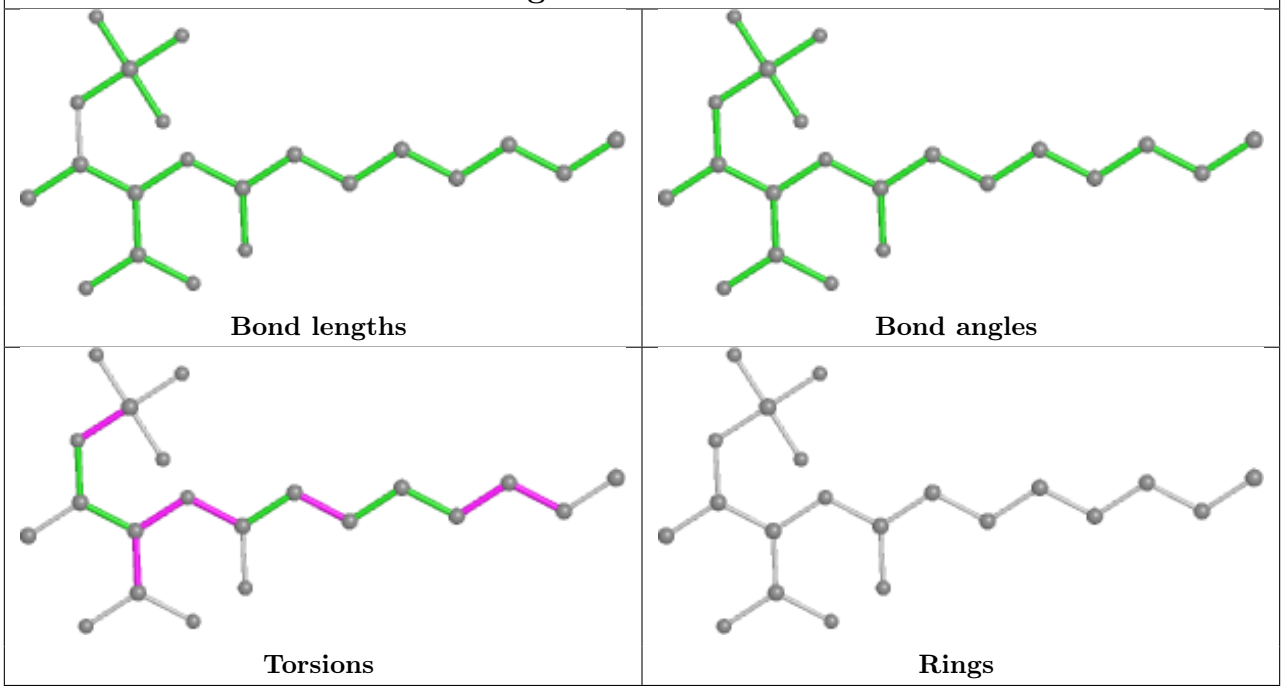
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



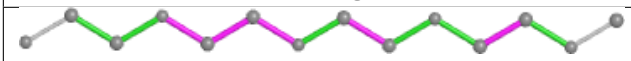
Ligand TP7 H 304



Ligand PE3 A 708

Bond lengths

Bond angles

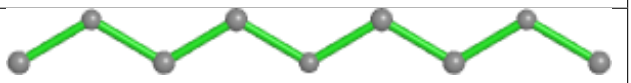


Torsions

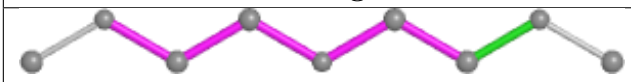
Rings

Ligand PE3 F 502

Bond lengths



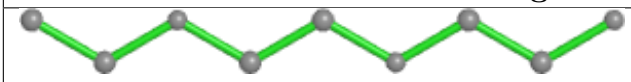
Bond angles



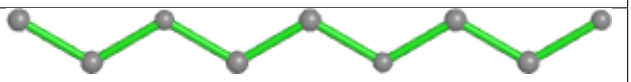
Torsions

Rings

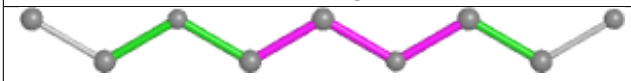
Ligand PE3 F 501



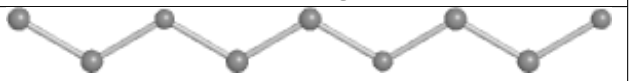
Bond lengths



Bond angles

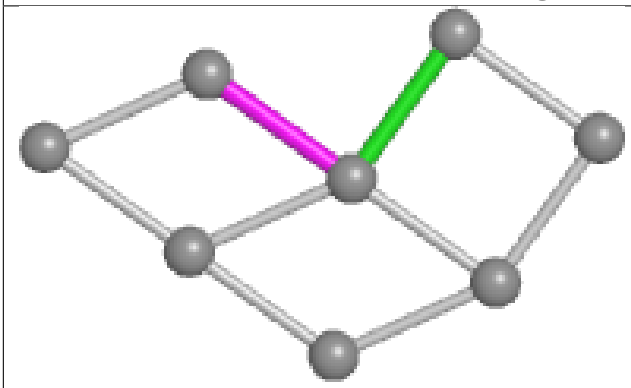


Torsions

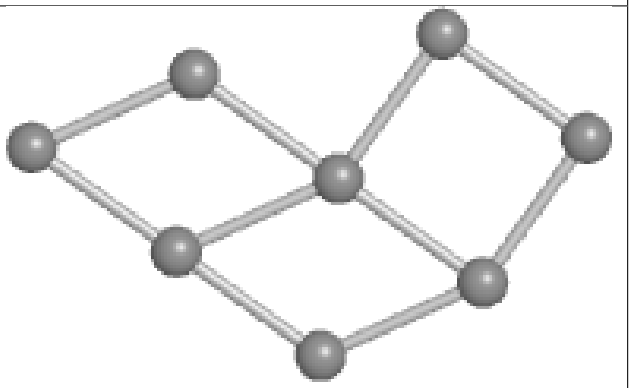


Rings

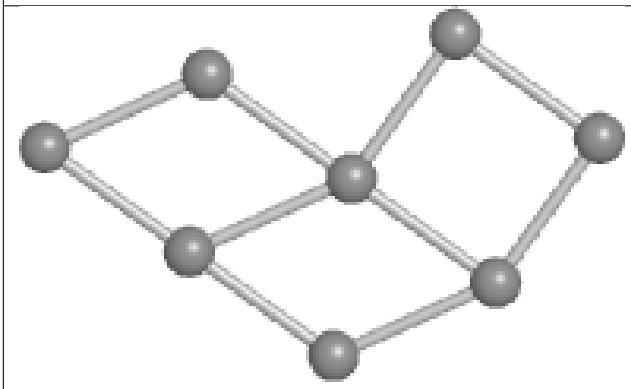
Ligand 9S8 B 301



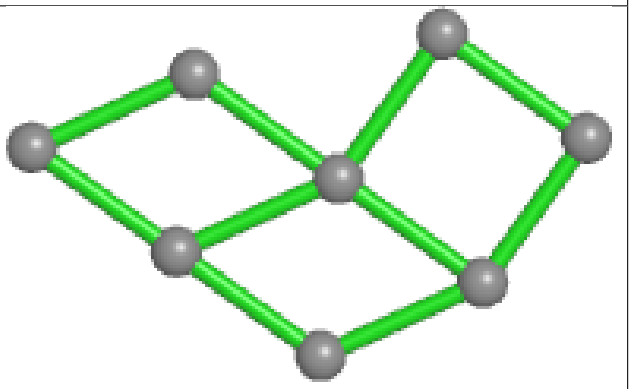
Bond lengths



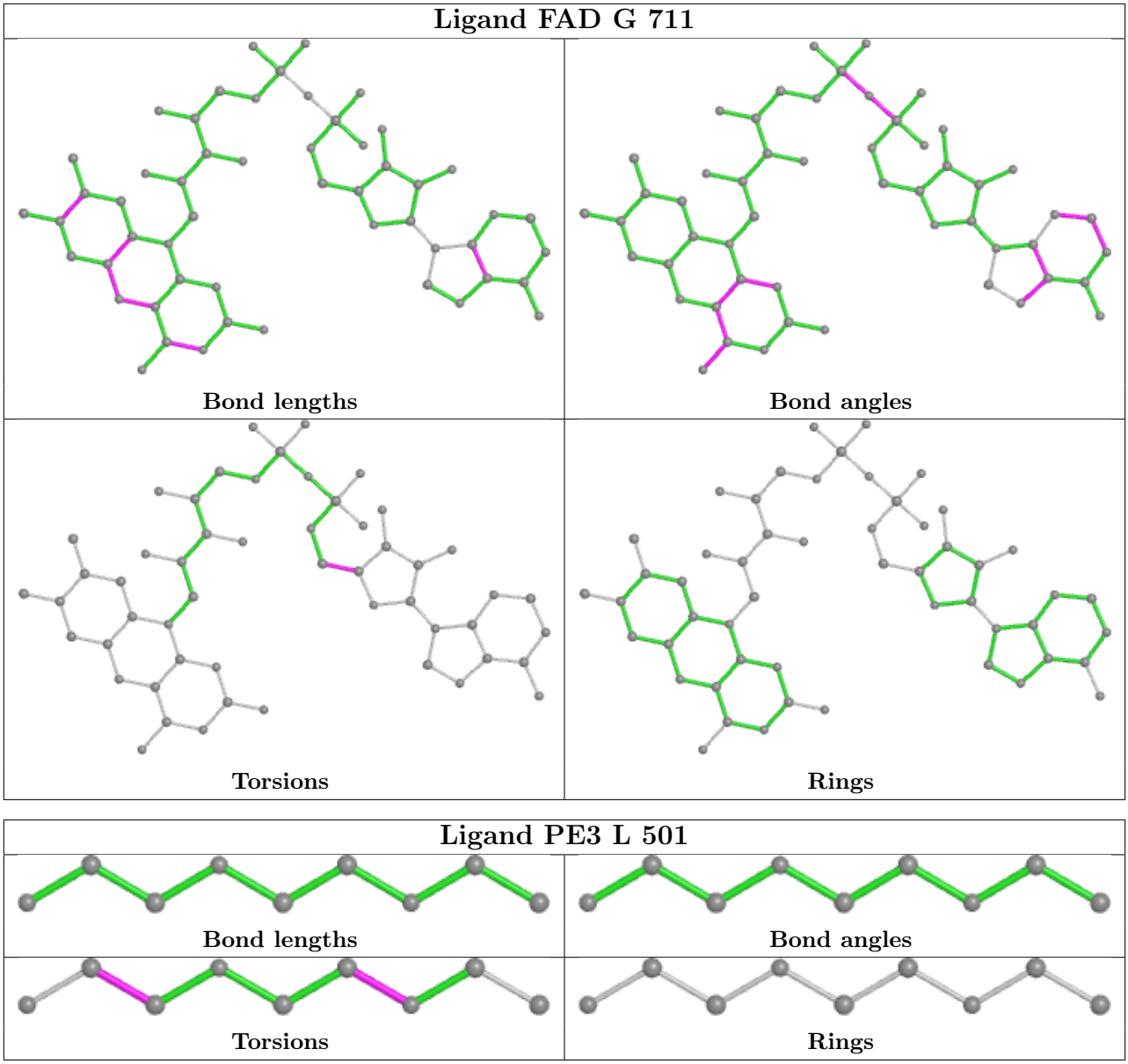
Bond angles



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(Å^2)	Q<0.9
1	A	652/654 (99%)	0.16	48 (7%)	14	13	13, 31, 81, 112	0
1	G	653/654 (99%)	0.14	32 (4%)	29	28	16, 31, 71, 90	0
2	B	291/291 (100%)	0.11	5 (1%)	70	68	21, 40, 55, 70	0
2	H	291/291 (100%)	0.95	39 (13%)	3	2	31, 54, 98, 116	0
3	C	184/184 (100%)	0.09	3 (1%)	72	70	21, 35, 53, 74	0
3	I	183/184 (99%)	0.34	10 (5%)	25	24	19, 43, 71, 98	0
4	D	137/140 (97%)	-0.18	0	100	100	19, 28, 40, 54	0
4	J	138/140 (98%)	0.01	3 (2%)	62	59	21, 30, 43, 76	0
5	E	298/299 (99%)	0.40	12 (4%)	38	36	18, 34, 62, 81	0
5	K	298/299 (99%)	0.17	8 (2%)	54	52	16, 29, 50, 66	0
6	F	447/473 (94%)	0.00	7 (1%)	72	70	15, 30, 52, 75	0
6	L	447/473 (94%)	0.02	9 (2%)	65	63	15, 28, 49, 106	0
All	All	4019/4082 (98%)	0.18	176 (4%)	34	32	13, 33, 67, 116	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	164	LEU	7.0
2	H	279	VAL	6.4
2	H	276	ALA	6.3
2	H	143	LEU	6.2
6	L	362	GLU	5.8

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	K	304	6/6	0.79	0.21	29,36,41,49	0
17	ACT	G	710	4/4	0.79	0.32	31,39,39,47	0
9	PE3	A	708	14/43	0.82	0.25	30,41,56,57	0
8	GOL	A	707	6/6	0.82	0.14	33,38,40,47	0
8	GOL	E	304	6/6	0.83	0.18	38,42,50,53	0
17	ACT	G	709	4/4	0.87	0.25	38,38,38,47	0
12	COM	B	303	7/7	0.87	0.20	34,50,61,71	0
7	SF4	A	702	8/8	0.88	0.10	101,125,137,146	0
18	TP7	H	304	21/21	0.88	0.23	39,61,74,80	0
9	PE3	L	501	9/43	0.89	0.26	28,39,44,50	0
9	PE3	F	501	9/43	0.90	0.17	31,33,43,46	0
8	GOL	B	304	6/6	0.90	0.28	31,38,41,48	0
11	9S8	H	301	8/8	0.90	0.16	38,54,72,77	0
11	9S8	H	302	8/8	0.90	0.13	30,44,52,57	0
14	TRS	D	202	8/8	0.91	0.21	25,31,38,40	0
7	SF4	G	705	8/8	0.92	0.12	27,30,38,41	0
7	SF4	A	703	8/8	0.92	0.07	72,84,107,111	0
7	SF4	A	706	8/8	0.92	0.10	19,34,42,43	0
7	SF4	G	703	8/8	0.92	0.10	66,69,73,95	0
11	9S8	B	302	8/8	0.92	0.12	21,31,36,37	0
8	GOL	G	707	6/6	0.92	0.20	26,36,45,46	0
7	SF4	G	704	8/8	0.93	0.07	73,87,106,125	0
7	SF4	K	303	8/8	0.93	0.12	27,29,36,37	0
7	SF4	G	706	8/8	0.94	0.11	21,30,36,40	0
7	SF4	I	201	8/8	0.94	0.14	19,24,25,28	0
7	SF4	C	202	8/8	0.94	0.13	21,29,31,32	0
7	SF4	E	301	8/8	0.94	0.15	20,27,29,34	0
7	SF4	E	303	8/8	0.94	0.11	28,39,49,63	0
9	PE3	F	502	9/43	0.94	0.09	32,41,47,47	0
8	GOL	B	305	6/6	0.94	0.17	28,39,41,49	0
11	9S8	B	301	8/8	0.94	0.15	30,40,47,58	0
7	SF4	K	302	8/8	0.95	0.16	23,34,36,37	0

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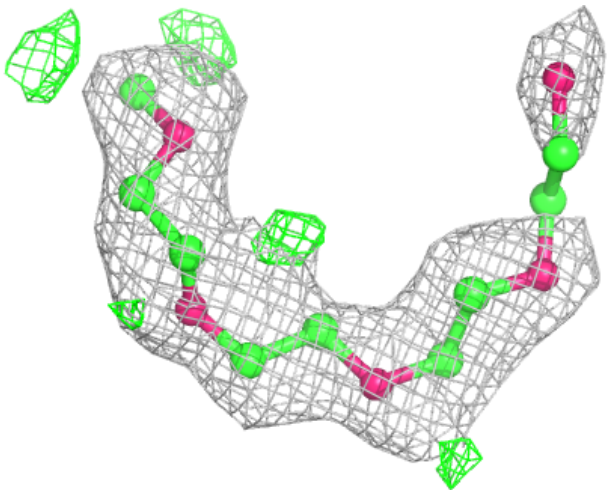
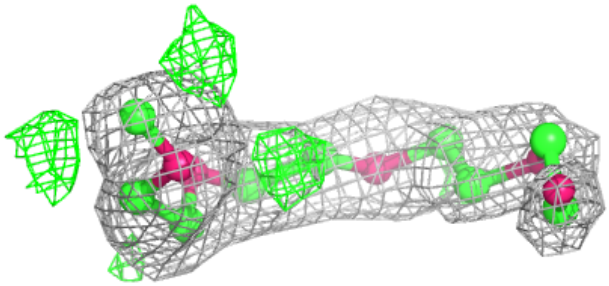
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SF4	A	704	8/8	0.95	0.13	27,30,37,37	0
7	SF4	E	302	8/8	0.95	0.13	17,31,38,39	0
10	FAD	A	709	53/53	0.96	0.14	10,19,34,37	0
12	COM	H	303	7/7	0.96	0.10	34,36,45,53	0
7	SF4	C	201	8/8	0.96	0.15	20,25,27,32	0
7	SF4	A	705	8/8	0.96	0.11	27,31,42,43	0
7	SF4	I	202	8/8	0.96	0.11	21,23,31,33	0
7	SF4	K	301	8/8	0.96	0.16	15,21,23,23	0
7	SF4	G	701	8/8	0.97	0.09	18,28,37,40	0
15	NFU	F	503	8/8	0.97	0.17	14,21,23,24	0
15	NFU	L	502	8/8	0.97	0.18	20,22,25,29	0
10	FAD	G	711	53/53	0.97	0.13	10,20,27,28	0
7	SF4	G	702	8/8	0.97	0.15	19,21,24,26	0
7	SF4	A	701	8/8	0.97	0.13	14,20,22,25	0
13	FES	D	201	4/4	0.98	0.12	24,24,25,27	0
13	FES	J	201	4/4	0.98	0.13	20,21,26,29	0
16	FE	F	504	1/1	0.99	0.10	23,23,23,23	0
16	FE	G	708	1/1	0.99	0.08	32,32,32,32	1
16	FE	L	503	1/1	0.99	0.13	20,20,20,20	0

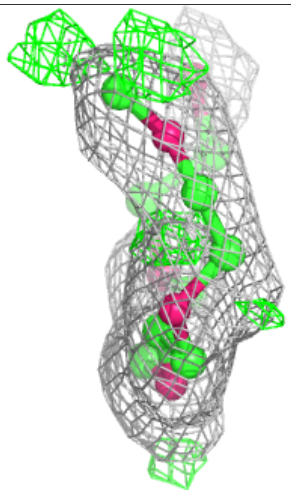
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE3 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)

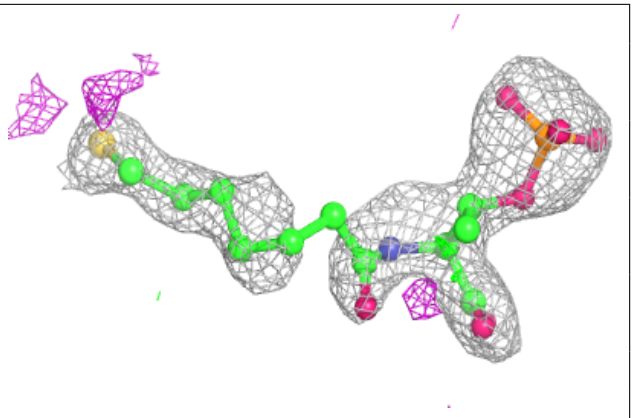


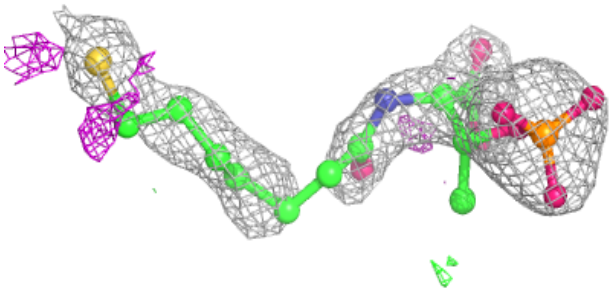


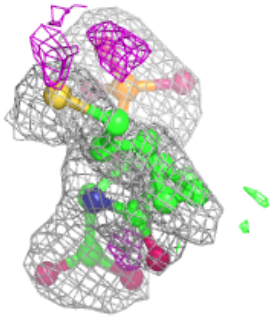


Electron density around TP7 H 304:

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

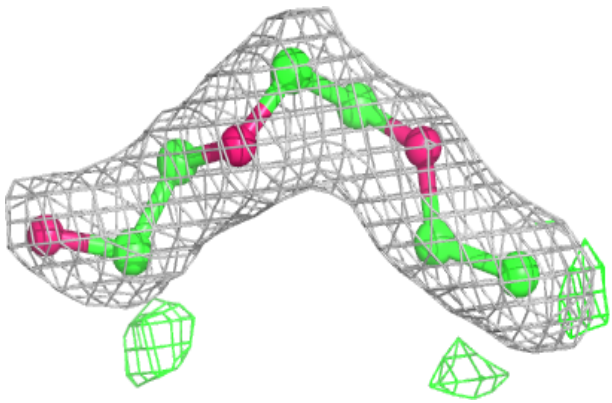


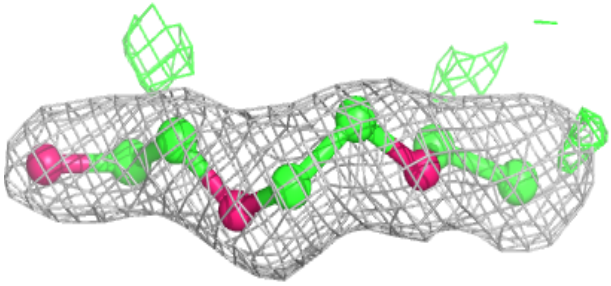


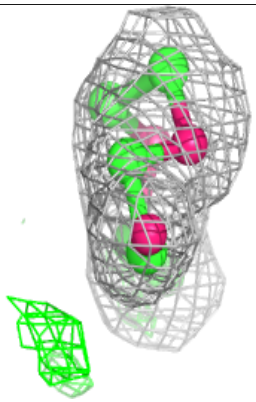


Electron density around PE3 L 501:

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

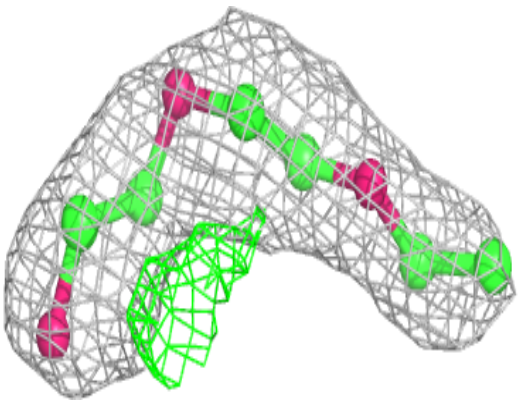


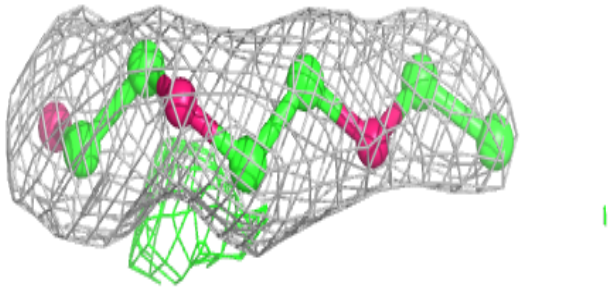


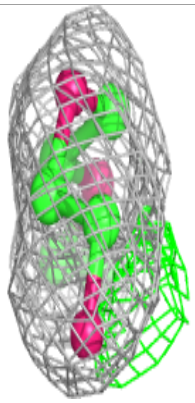


Electron density around PE3 F 501:

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

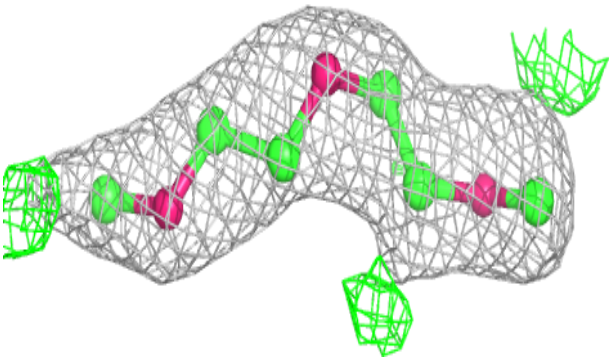


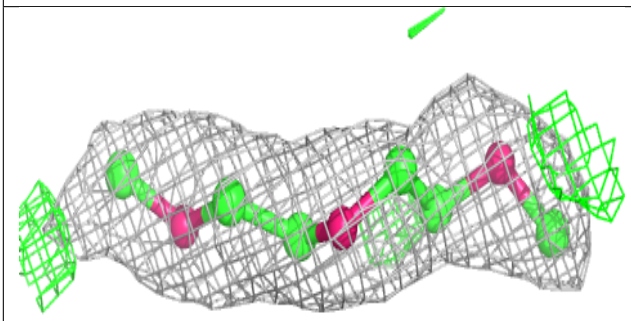


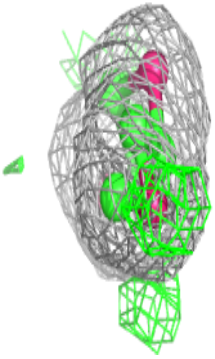


Electron density around PE3 F 502:

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

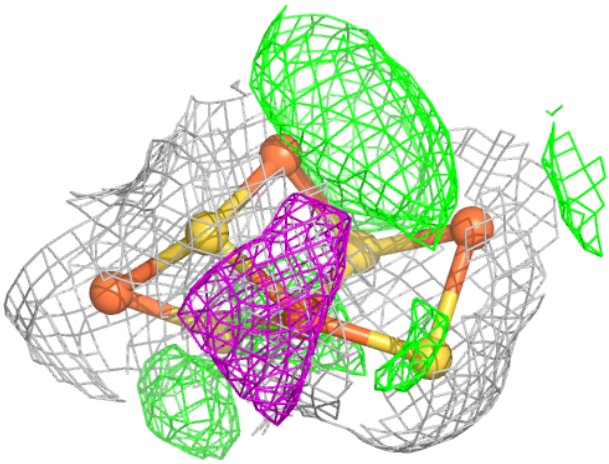


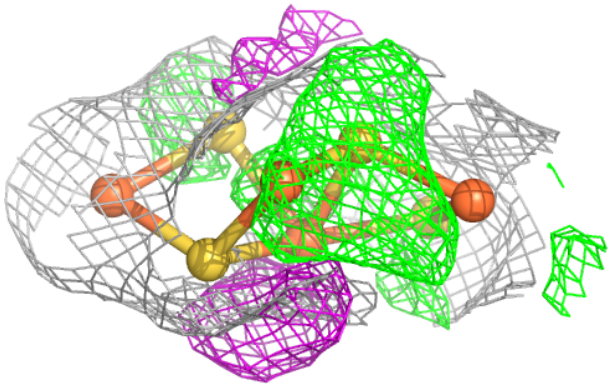


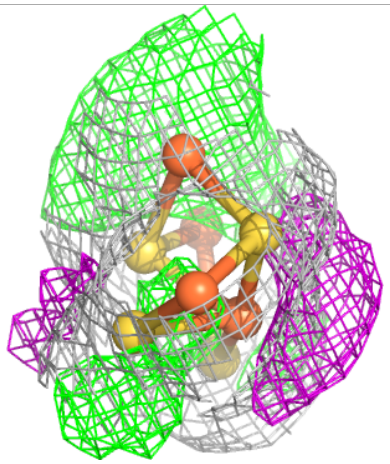


Electron density around 9S8 B 301:

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

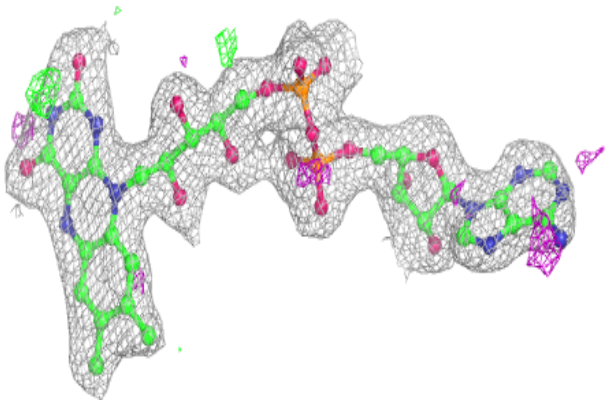


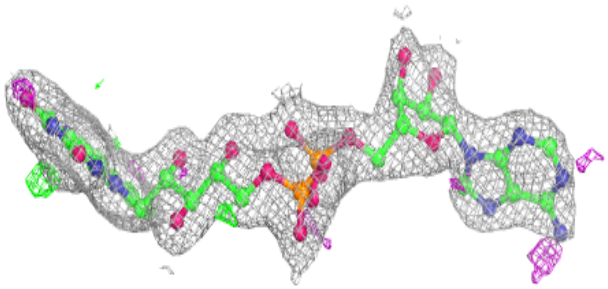


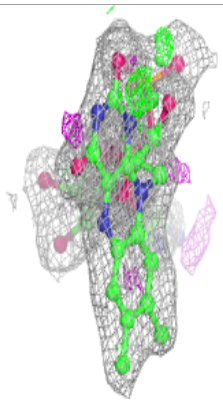


Electron density around FAD A 709:

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

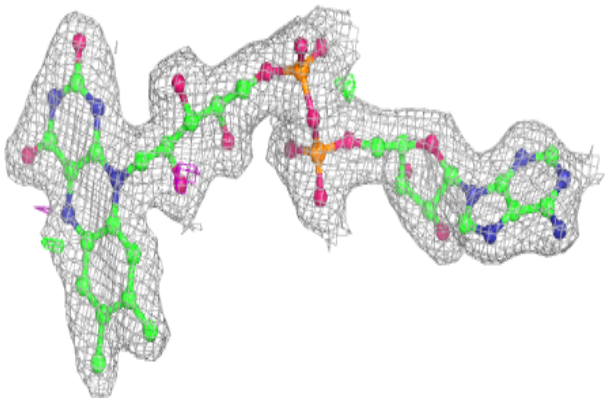


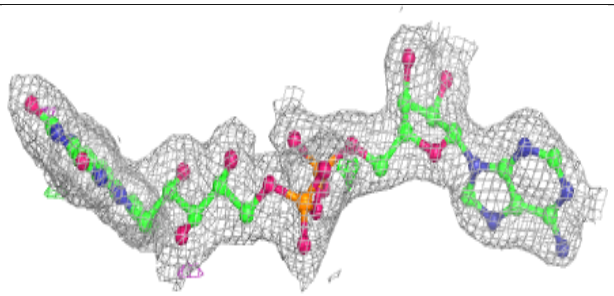


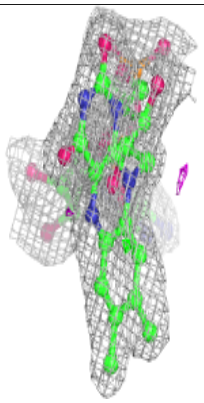


Electron density around FAD G 711:

$2mF_o$-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.