



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 01:09 PM EDT

PDB ID : 5ODC / pdb_00005odc
Title : Heterodisulfide reductase / [NiFe]-hydrogenase complex from Methanothermococcus thermolithotrophicus at 2.3 Å resolution
Authors : Wagner, T.; Koch, J.; Ermler, U.; Shima, S.
Deposited on : 2017-07-05
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

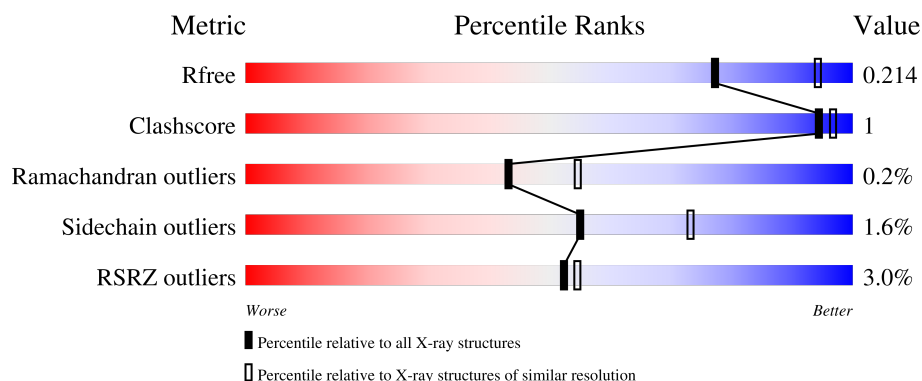
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	654	96%
1	G	654	94% 5%
2	B	291	97%
2	H	291	17% 96%
3	C	184	2% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	184	17% 90% 6%
4	D	140	91% 7%
4	J	140	90% 9%
5	E	299	% 96%
5	K	299	% 94% 5%
6	F	473	% 86% 8% 5%
6	L	473	3% 87% 7% 5%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 32275 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	653	Total	C	N	O	S	0	0	0
			4984	3145	846	944	49			
1	G	653	Total	C	N	O	S	0	0	0
			4984	3145	846	944	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2236	1420	379	413	24			
2	H	291	Total	C	N	O	S	0	0	0
			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
			1425	890	247	274	14			
3	I	173	Total	C	N	O	S	0	0	0
			1335	831	233	257	14			

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

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

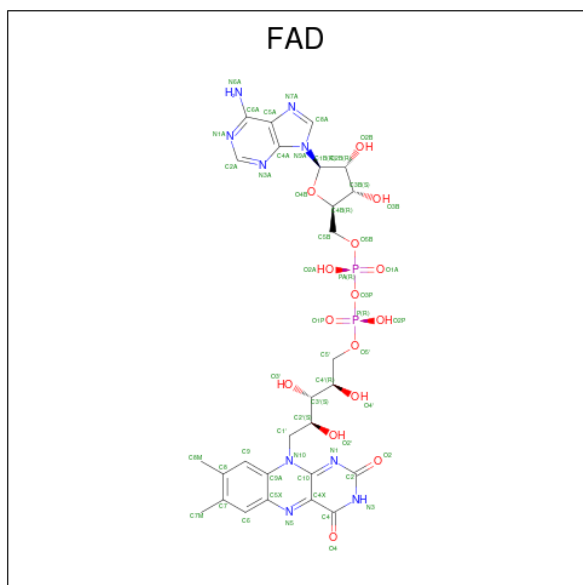
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase subunit G.

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

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

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

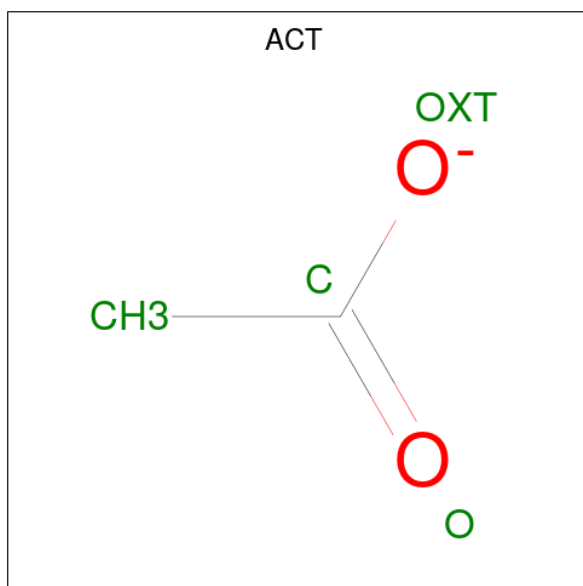
- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Continued from previous page...

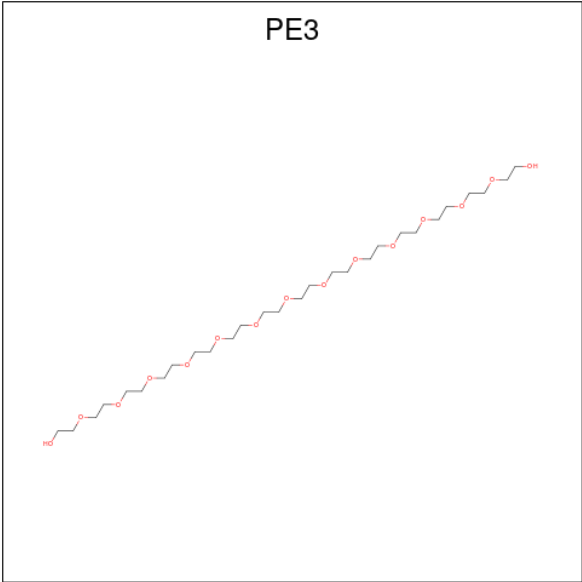
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Na	0	0
			1	1		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



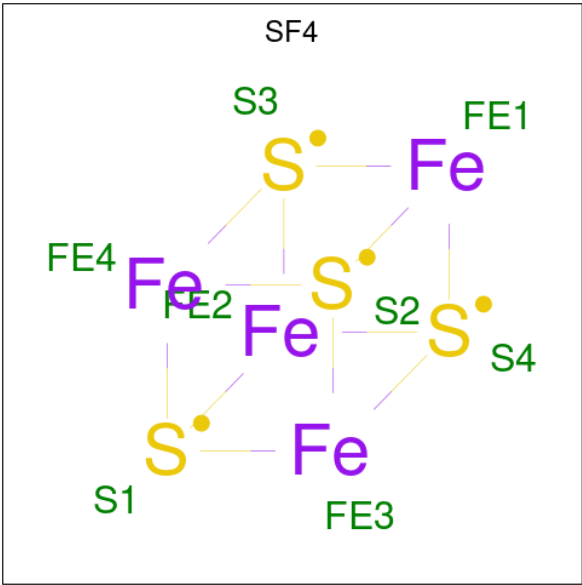
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (CCD ID: PE3) (formula: $C_{28}H_{58}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



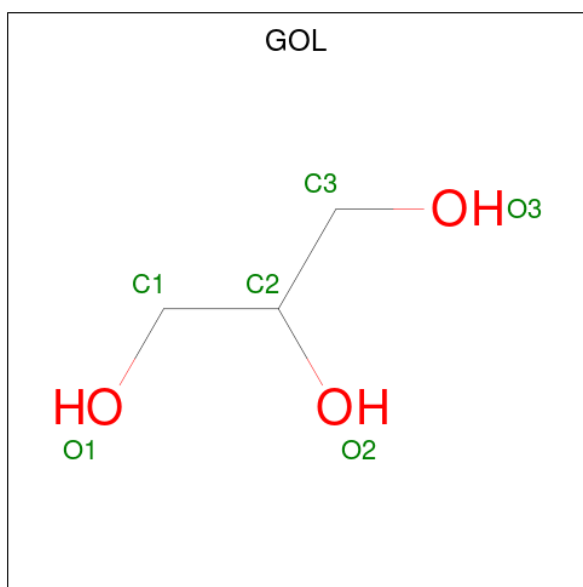
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	Fe	S	0	0
			8	4	4		
11	A	1	Total	Fe	S	0	0
			8	4	4		
11	A	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

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

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



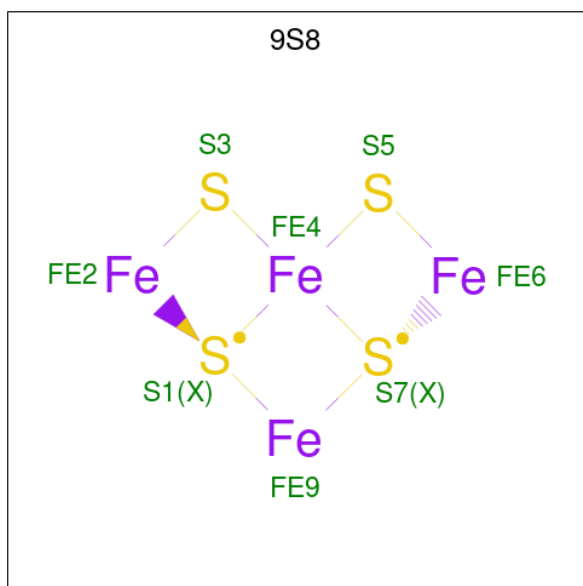
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	B	1	Total	C	O	0	0
			6	3	3		
12	C	1	Total	C	O	0	0
			6	3	3		
12	D	1	Total	C	O	0	0
			6	3	3		
12	E	1	Total	C	O	0	0
			6	3	3		
12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

Continued on next page...

Continued from previous page...

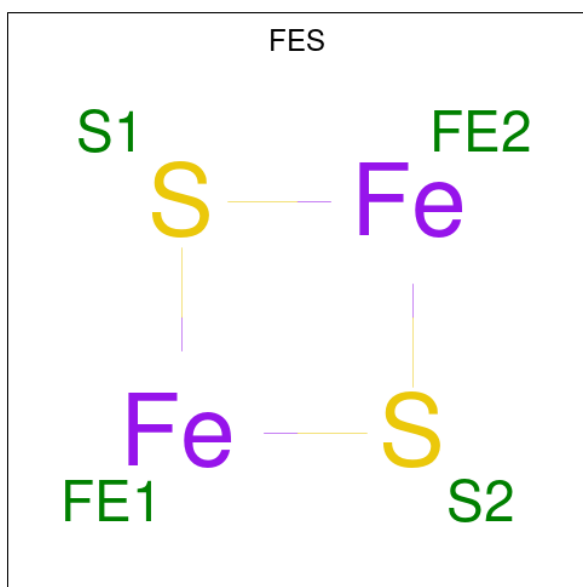
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe_4S_4).



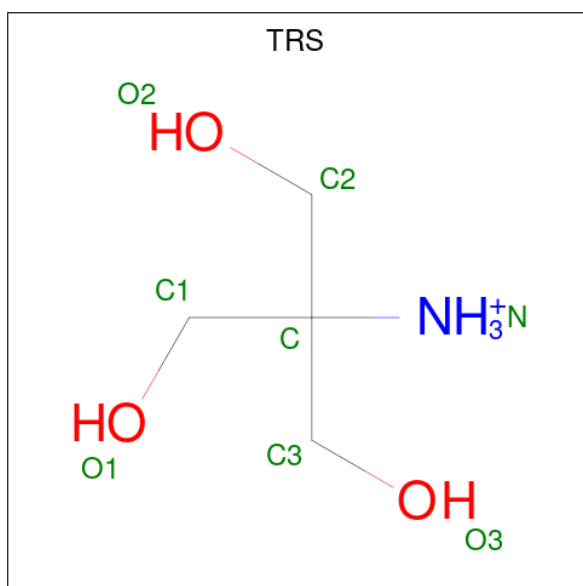
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	Fe	S	0	0
			8	4	4		
13	B	1	Total	Fe	S	0	0
			8	4	4		
13	H	1	Total	Fe	S	0	0
			8	4	4		
13	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 15 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

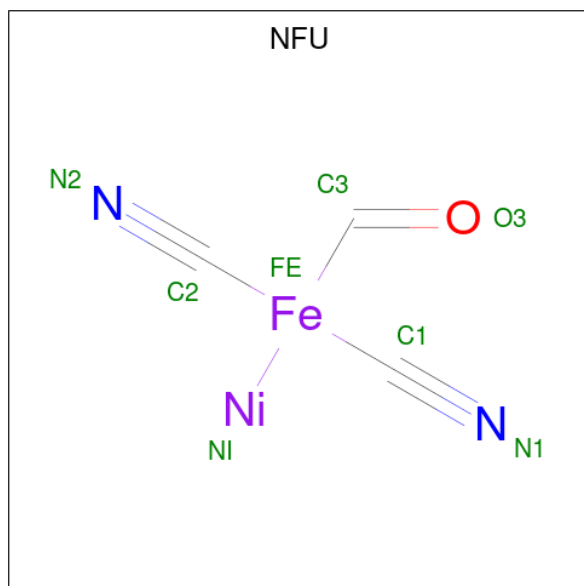
- Molecule 16 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	F	1	Total	Mg	0	0
			1	1		
17	I	1	Total	Mg	0	0
			1	1		

- Molecule 18 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C₃HFeN₂NiO).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	180	Total 180	O 180	0	0
19	B	52	Total 52	O 52	0	0
19	C	29	Total 29	O 29	0	0
19	D	52	Total 52	O 52	0	0
19	E	71	Total 71	O 71	0	0
19	F	78	Total 78	O 78	0	0
19	G	182	Total 182	O 182	0	0
19	H	10	Total 10	O 10	0	0
19	I	23	Total 23	O 23	0	0
19	J	48	Total 48	O 48	0	0
19	K	65	Total 65	O 65	0	0
19	L	42	Total 42	O 42	0	0

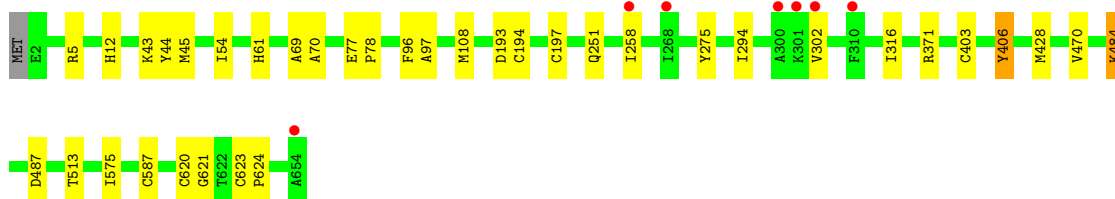
3 Residue-property plots [i](#)

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

- Molecule 1: Heterodisulfide reductase, subunit A



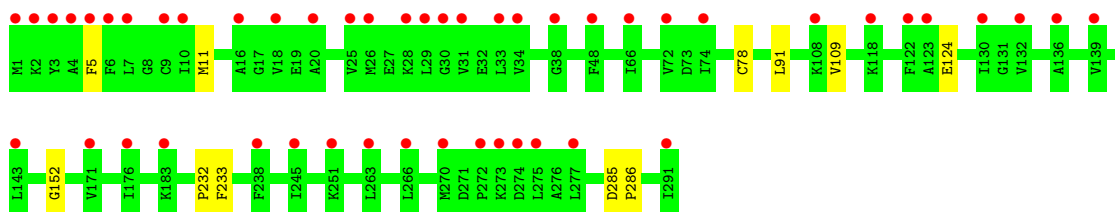
- Molecule 1: Heterodisulfide reductase, subunit A



- Molecule 2: Heterodisulfide reductase, subunit B



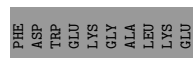
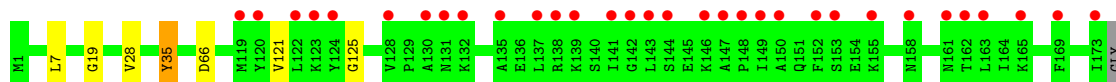
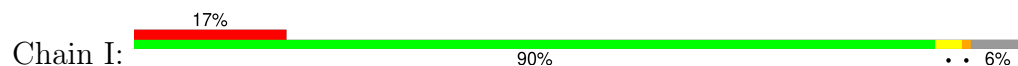
- Molecule 2: Heterodisulfide reductase, subunit B



- Molecule 3: Heterodisulfide reductase, subunit C



- Molecule 3: Heterodisulfide reductase, subunit C



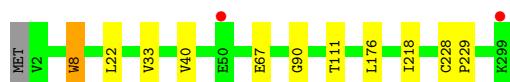
- Molecule 4: Methyl-viologen reducing hydrogenase subunit D



- Molecule 4: Methyl-viologen reducing hydrogenase subunit D



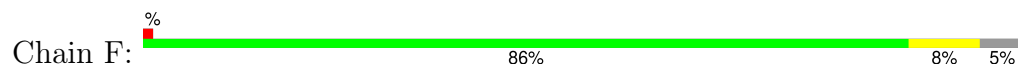
- Molecule 5: Methyl-viologen reducing hydrogenase subunit G

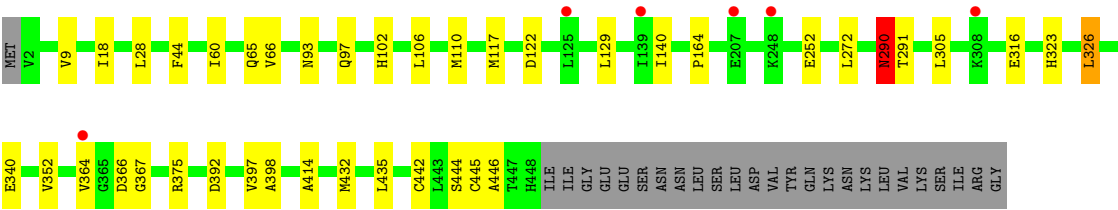


- Molecule 5: Methyl-viologen reducing hydrogenase subunit G

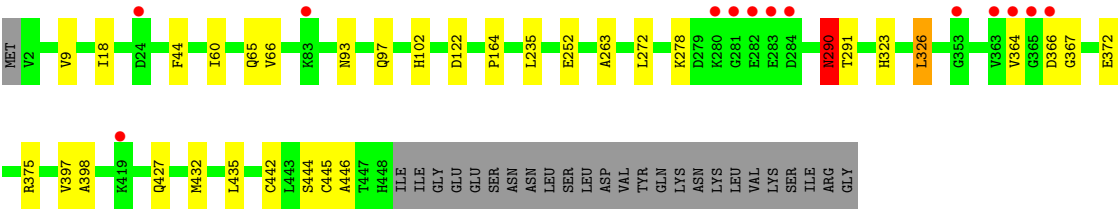
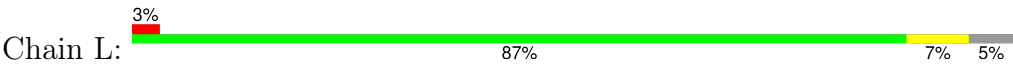


- Molecule 6: Methyl-viologen reducing hydrogenase subunit A





● 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	378.05Å 98.45Å 137.88Å 90.00° 110.70° 90.00°	Depositor
Resolution (Å)	49.22 – 2.30 49.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.22-2.30) 97.3 (49.22-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.178 , 0.200 0.193 , 0.214	Depositor DCC
R_{free} test set	10353 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32275	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: SF4, GOL, CA, PE3, ACT, FES, TRS, 9S8, NFU, MG, FAD, NA

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	0.53	0/5076	0.94	1/6860 (0.0%)
1	G	0.53	1/5076 (0.0%)	0.94	3/6860 (0.0%)
2	B	0.52	0/2277	0.95	2/3070 (0.1%)
2	H	0.52	0/2277	0.94	1/3070 (0.0%)
3	C	0.55	0/1446	0.97	2/1946 (0.1%)
3	I	0.52	0/1353	0.98	0/1822
4	D	0.51	0/1132	0.98	1/1520 (0.1%)
4	J	0.50	0/1132	0.98	1/1520 (0.1%)
5	E	0.53	0/2297	0.97	4/3113 (0.1%)
5	K	0.53	0/2297	0.96	5/3113 (0.2%)
6	F	0.53	0/3590	1.00	7/4853 (0.1%)
6	L	0.53	0/3590	1.00	7/4853 (0.1%)
All	All	0.53	1/31543 (0.0%)	0.97	34/42600 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	316	ILE	CG1-CD1	-5.10	1.31	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	22	LEU	N-CA-C	-7.88	103.12	112.89
5	K	22	LEU	N-CA-C	-7.85	103.16	112.89
6	L	290	ASN	CA-CB-CG	7.61	120.21	112.60
6	L	44	PHE	CA-CB-CG	6.49	120.29	113.80
6	F	44	PHE	CA-CB-CG	6.42	120.22	113.80
1	G	275	TYR	N-CA-C	6.37	117.90	108.60
1	A	275	TYR	N-CA-C	6.21	117.67	108.60
6	F	364	VAL	N-CA-C	-6.08	99.82	108.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	60	ILE	N-CA-C	-6.06	104.60	110.72
6	L	60	ILE	N-CA-C	-6.05	104.61	110.72
6	F	397	VAL	N-CA-C	6.02	116.48	107.51
3	C	26	ASP	CA-CB-CG	5.98	118.58	112.60
6	L	9	VAL	N-CA-C	-5.94	101.05	108.89
6	F	9	VAL	N-CA-C	-5.92	101.08	108.89
6	L	397	VAL	N-CA-C	5.90	116.30	107.51
6	L	444	SER	N-CA-C	-5.81	105.03	111.36
6	F	290	ASN	CA-CB-CG	5.77	118.37	112.60
5	E	176	LEU	N-CA-C	5.76	119.57	112.54
5	K	90	GLY	CA-C-N	5.71	123.84	120.24
5	K	90	GLY	C-N-CA	5.71	123.84	120.24
6	F	444	SER	N-CA-C	-5.70	105.14	111.36
5	K	130	VAL	N-CA-C	-5.64	103.90	110.05
6	L	364	VAL	N-CA-C	-5.47	101.67	108.89
2	H	152	GLY	N-CA-C	-5.47	105.79	112.68
2	B	152	GLY	N-CA-C	-5.45	105.81	112.68
1	G	193	ASP	N-CA-C	-5.41	103.25	110.55
5	E	90	GLY	CA-C-N	5.36	123.61	120.24
5	E	90	GLY	C-N-CA	5.36	123.61	120.24
1	G	428	MET	N-CA-C	-5.26	105.94	112.93
5	K	176	LEU	N-CA-C	5.26	118.95	112.54
4	D	32	PRO	N-CA-C	5.25	117.11	110.70
2	B	206	GLU	CB-CG-CD	5.17	121.39	112.60
4	J	32	PRO	N-CA-C	5.12	116.95	110.70
3	C	72	ASP	N-CA-C	-5.07	105.84	112.23

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	4984	0	4979	11	0
1	G	4984	0	4979	19	0
2	B	2236	0	2243	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2236	0	2243	3	0
3	C	1425	0	1441	3	0
3	I	1335	0	1358	5	0
4	D	1106	0	1074	5	0
4	J	1106	0	1074	6	0
5	E	2258	0	2265	3	0
5	K	2258	0	2265	3	0
6	F	3521	0	3503	16	0
6	L	3521	0	3503	15	0
7	A	53	0	31	0	0
7	G	53	0	31	0	0
8	A	1	0	0	0	0
8	G	1	0	0	0	0
9	A	4	0	3	0	0
9	B	4	0	3	0	0
9	F	4	0	3	0	0
9	G	8	0	6	0	0
10	A	11	0	12	0	0
11	A	48	0	0	0	0
11	C	16	0	0	0	0
11	E	24	0	0	0	0
11	G	48	0	0	0	0
11	I	16	0	0	0	0
11	K	24	0	0	0	0
12	A	24	0	32	0	0
12	B	6	0	8	0	0
12	C	6	0	8	0	0
12	D	6	0	8	0	0
12	E	6	0	8	0	0
12	G	24	0	32	1	0
12	K	18	0	24	0	0
13	B	16	0	0	0	0
13	H	16	0	0	0	0
14	D	4	0	0	0	0
14	J	4	0	0	0	0
15	D	8	0	12	0	0
16	F	1	0	0	0	0
16	L	1	0	0	0	0
17	F	1	0	0	0	0
17	I	1	0	0	0	0
18	F	8	0	0	0	0
18	L	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	180	0	0	0	0
19	B	52	0	0	0	0
19	C	29	0	0	0	0
19	D	52	0	0	0	0
19	E	71	0	0	0	0
19	F	78	0	0	0	0
19	G	182	0	0	0	0
19	H	10	0	0	0	0
19	I	23	0	0	0	0
19	J	48	0	0	0	0
19	K	65	0	0	0	0
19	L	42	0	0	0	0
All	All	32275	0	31148	80	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 (80) 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:L:323:HIS:HB2	6:L:326:LEU:HD23	1.64	0.78
1:A:194:CYS:HB2	1:A:197:CYS:SG	2.30	0.70
1:A:236:LYS:HD2	1:A:317:ILE:HD12	1.76	0.67
4:D:17:THR:HG21	4:D:65:GLY:HA3	1.79	0.65
2:H:5:PHE:CZ	2:H:11:MET:HE1	2.35	0.61
6:L:18:ILE:HG21	6:L:432:MET:HE2	1.83	0.61
6:L:323:HIS:CB	6:L:326:LEU:HD23	2.35	0.57
2:B:78:CYS:SG	2:B:232:PRO:HD2	2.46	0.56
12:G:711:GOL:H2	3:I:35:TYR:HA	1.88	0.56
2:H:78:CYS:SG	2:H:232:PRO:HD2	2.46	0.56
6:F:106:LEU:O	6:F:110:MET:HB2	2.09	0.52
1:A:587:CYS:HB2	5:E:218:ILE:HG22	1.91	0.51
1:G:623:CYS:SG	1:G:624:PRO:HD3	2.50	0.51
1:A:623:CYS:SG	1:A:624:PRO:HD3	2.51	0.51
5:E:8:TRP:CH2	5:E:40:VAL:HB	2.46	0.50
1:G:484:LYS:HD3	3:I:7:LEU:HD12	1.93	0.50
4:J:87:MET:HG3	5:K:257:CYS:SG	2.52	0.50
1:G:5:ARG:NH1	1:G:61:HIS:O	2.45	0.49
1:G:620:CYS:HB3	4:J:74:TYR:CG	2.48	0.49
6:F:352:VAL:O	6:F:352:VAL:HG12	2.13	0.49
4:J:17:THR:HG21	4:J:65:GLY:HA3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:VAL:O	3:C:125:GLY:HA2	2.13	0.48
6:F:272:LEU:HD11	6:F:446:ALA:HB1	1.96	0.48
6:L:290:ASN:HB3	6:L:375:ARG:C	2.39	0.48
1:G:45:MET:HE2	1:G:54:ILE:HD11	1.97	0.46
1:G:194:CYS:HB2	1:G:197:CYS:SG	2.55	0.46
1:G:621:GLY:C	1:G:624:PRO:HD2	2.41	0.46
1:A:483:GLU:HB2	3:C:1:MET:HE1	1.97	0.46
6:L:272:LEU:HD11	6:L:446:ALA:HB1	1.96	0.46
4:D:68:HIS:HA	4:D:106:TRP:HB3	1.97	0.46
1:G:406:TYR:CD1	1:G:406:TYR:C	2.94	0.46
3:I:121:VAL:O	3:I:125:GLY:HA2	2.16	0.46
1:A:620:CYS:HB3	4:D:74:TYR:CG	2.51	0.46
1:G:12:HIS:HB2	1:G:43:LYS:HA	1.97	0.45
2:B:285:ASP:N	2:B:286:PRO:HD2	2.31	0.45
6:L:263:ALA:HB2	6:L:278:LYS:HB3	1.96	0.45
1:A:621:GLY:C	1:A:624:PRO:HD2	2.41	0.45
2:H:285:ASP:N	2:H:286:PRO:HD2	2.32	0.45
6:F:129:LEU:HD12	6:F:140:ILE:HD12	1.98	0.45
4:D:16:CYS:SG	4:D:67:CYS:SG	3.15	0.45
1:G:251:GLN:HB3	1:G:302:VAL:CG1	2.46	0.44
6:F:117:MET:HE3	6:F:117:MET:HB2	1.90	0.44
5:K:228:CYS:HB2	5:K:229:PRO:HD3	1.99	0.44
1:A:77:GLU:N	1:A:78:PRO:CD	2.80	0.44
6:F:93:ASN:O	6:F:97:GLN:HG2	2.18	0.44
1:A:575:ILE:HD12	4:D:41:MET:HG3	1.99	0.44
1:G:77:GLU:N	1:G:78:PRO:CD	2.80	0.44
6:L:272:LEU:CD1	6:L:446:ALA:HB1	2.48	0.44
6:F:272:LEU:CD1	6:F:446:ALA:HB1	2.48	0.44
5:E:228:CYS:HB2	5:E:229:PRO:HD3	1.99	0.44
6:F:305:LEU:HB2	6:F:340:GLU:CD	2.43	0.43
1:A:196:ILE:HG21	1:G:44:TYR:CG	2.54	0.43
6:F:375:ARG:CD	6:F:442:CYS:HB2	2.49	0.43
1:G:258:ILE:HD11	1:G:294:ILE:HG23	2.00	0.43
6:L:375:ARG:CD	6:L:442:CYS:HB2	2.49	0.43
1:G:587:CYS:HB2	5:K:218:ILE:HG22	1.99	0.43
6:L:93:ASN:O	6:L:97:GLN:HG2	2.18	0.43
1:G:484:LYS:HD3	3:I:7:LEU:CD1	2.48	0.42
6:F:290:ASN:HB3	6:F:375:ARG:C	2.44	0.42
1:G:371:ARG:HD2	1:G:487:ASP:O	2.19	0.42
6:L:326:LEU:HD13	6:L:326:LEU:HA	1.94	0.42
6:F:28:LEU:HD21	6:F:414:ALA:HB1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:122:ASP:OD1	6:L:427:GLN:HG2	2.20	0.42
6:L:366:ASP:OD1	6:L:367:GLY:N	2.53	0.42
6:F:323:HIS:HB2	6:F:326:LEU:HD23	2.01	0.41
1:A:406:TYR:C	1:A:406:TYR:CD1	2.98	0.41
1:G:406:TYR:C	1:G:406:TYR:HD1	2.28	0.41
4:J:16:CYS:SG	4:J:67:CYS:SG	3.18	0.41
6:F:18:ILE:HG21	6:F:432:MET:HE2	2.03	0.41
1:G:108:MET:HE3	4:J:28:ARG:HG3	2.02	0.41
3:I:19:GLY:HA3	3:I:28:VAL:HG21	2.03	0.41
6:L:66:VAL:HG22	6:L:164:PRO:HG3	2.03	0.41
3:C:19:GLY:HA3	3:C:28:VAL:HG21	2.03	0.41
6:L:235:LEU:HA	6:L:372:GLU:HB2	2.03	0.41
4:J:68:HIS:HA	4:J:106:TRP:HB3	2.03	0.41
1:G:69:ALA:HA	1:G:97:ALA:HB3	2.03	0.41
6:F:66:VAL:HG22	6:F:164:PRO:HG3	2.02	0.40
6:F:435:LEU:C	6:F:435:LEU:HD13	2.46	0.40
6:L:435:LEU:C	6:L:435:LEU:HD13	2.46	0.40
6:F:366:ASP:OD1	6:F:367:GLY:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	651/654 (100%)	629 (97%)	21 (3%)	1 (0%)	43	55
1	G	651/654 (100%)	627 (96%)	22 (3%)	2 (0%)	36	46
2	B	289/291 (99%)	277 (96%)	12 (4%)	0	100	100
2	H	289/291 (99%)	275 (95%)	14 (5%)	0	100	100
3	C	182/184 (99%)	181 (100%)	1 (0%)	0	100	100
3	I	171/184 (93%)	170 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
4	J	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
5	E	296/299 (99%)	287 (97%)	9 (3%)	0	100	100
5	K	296/299 (99%)	287 (97%)	9 (3%)	0	100	100
6	F	445/473 (94%)	436 (98%)	7 (2%)	2 (0%)	30	38
6	L	445/473 (94%)	433 (97%)	10 (2%)	2 (0%)	30	38
All	All	3987/4082 (98%)	3866 (97%)	114 (3%)	7 (0%)	43	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	291	THR
6	F	398	ALA
6	L	291	THR
6	L	398	ALA
1	A	70	ALA
1	G	70	ALA
1	G	575	ILE

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%)	534 (99%)	6 (1%)	65	81
1	G	540/541 (100%)	534 (99%)	6 (1%)	65	81
2	B	242/242 (100%)	238 (98%)	4 (2%)	53	72
2	H	242/242 (100%)	238 (98%)	4 (2%)	53	72
3	C	157/157 (100%)	156 (99%)	1 (1%)	78	89
3	I	149/157 (95%)	147 (99%)	2 (1%)	61	77
4	D	117/119 (98%)	116 (99%)	1 (1%)	70	84
4	J	117/119 (98%)	115 (98%)	2 (2%)	53	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	255/256 (100%)	251 (98%)	4 (2%)	55	73
5	K	255/256 (100%)	247 (97%)	8 (3%)	35	52
6	F	386/410 (94%)	377 (98%)	9 (2%)	44	63
6	L	386/410 (94%)	380 (98%)	6 (2%)	55	73
All	All	3386/3450 (98%)	3333 (98%)	53 (2%)	55	73

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	96	PHE
1	A	403	CYS
1	A	406	TYR
1	A	470	VAL
1	A	513	THR
2	B	109	VAL
2	B	124	GLU
2	B	233	PHE
2	B	270	MET
3	C	35	TYR
4	D	47	GLU
5	E	8	TRP
5	E	33	VAL
5	E	67	GLU
5	E	111	THR
6	F	65	GLN
6	F	102	HIS
6	F	122	ASP
6	F	252	GLU
6	F	290	ASN
6	F	316	GLU
6	F	326	LEU
6	F	392	ASP
6	F	445	CYS
1	G	96	PHE
1	G	403	CYS
1	G	406	TYR
1	G	470	VAL
1	G	484	LYS
1	G	513	THR
2	H	91	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	109	VAL
2	H	124	GLU
2	H	233	PHE
3	I	35	TYR
3	I	66	ASP
4	J	47	GLU
4	J	133	LYS
5	K	8	TRP
5	K	25	GLU
5	K	33	VAL
5	K	61	ARG
5	K	111	THR
5	K	187	GLU
5	K	216	LEU
5	K	299	LYS
6	L	65	GLN
6	L	102	HIS
6	L	252	GLU
6	L	290	ASN
6	L	326	LEU
6	L	445	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	109	HIS
1	A	229	ASN
1	A	262	ASN
1	A	280	GLN
1	A	306	ASN
1	A	385	GLN
1	A	401	ASN
1	A	410	ASN
1	A	459	GLN
1	A	516	GLN
2	B	53	GLN
6	F	93	ASN
6	F	97	GLN
6	F	136	HIS
1	G	109	HIS
1	G	385	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	593	GLN
1	G	636	HIS
6	L	93	ASN
6	L	96	HIS
6	L	97	GLN
6	L	136	HIS
6	L	260	ASN
6	L	401	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 6 are monoatomic - leaving 54 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	$\# Z > 2$
12	GOL	G	713	-	5,5,5	0.33	0	5,5,5	0.26	0
12	GOL	K	306	-	5,5,5	0.27	0	5,5,5	0.14	0
11	SF4	E	302	5	0,12,12	-	-	-		
11	SF4	A	710	1	0,12,12	-	-	-		
11	SF4	K	302	5	0,12,12	-	-	-		
15	TRS	D	202	-	7,7,7	0.33	0	9,9,9	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	I	202	3	0,12,12	-	-	-		
10	PE3	A	704	-	10,10,42	0.53	0	9,9,41	0.14	0
11	SF4	K	301	5	0,12,12	-	-	-		
13	9S8	H	301	2	4,10,10	6.68	2 (50%)	-		
12	GOL	K	305	-	5,5,5	0.27	0	5,5,5	0.15	0
9	ACT	A	703	-	3,3,3	1.02	0	3,3,3	1.07	0
18	NFU	L	502	6	2,7,7	0.89	0	-		
13	9S8	H	302	2	4,10,10	6.62	2 (50%)	-		
12	GOL	E	304	-	5,5,5	0.28	0	5,5,5	0.19	0
7	FAD	G	701	-	58,58,58	1.52	9 (15%)	85,89,89	1.64	19 (22%)
12	GOL	B	304	-	5,5,5	0.33	0	5,5,5	0.41	0
12	GOL	C	203	-	5,5,5	0.27	0	5,5,5	0.33	0
12	GOL	G	714	-	5,5,5	0.32	0	5,5,5	0.24	0
11	SF4	A	705	1	0,12,12	-	-	-		
11	SF4	G	706	1	0,12,12	-	-	-		
11	SF4	G	707	1	0,12,12	-	-	-		
11	SF4	G	710	1	0,12,12	-	-	-		
11	SF4	C	202	3	0,12,12	-	-	-		
9	ACT	B	303	-	3,3,3	1.10	0	3,3,3	0.97	0
11	SF4	C	201	3	0,12,12	-	-	-		
12	GOL	A	712	-	5,5,5	0.28	0	5,5,5	0.11	0
14	FES	J	201	4	0,4,4	-	-	-		
12	GOL	G	712	-	5,5,5	0.29	0	5,5,5	0.10	0
11	SF4	A	707	1	0,12,12	-	-	-		
9	ACT	F	503	-	3,3,3	1.09	0	3,3,3	1.00	0
11	SF4	A	708	1	0,12,12	-	-	-		
11	SF4	I	203	3	0,12,12	-	-	-		
9	ACT	G	703	-	3,3,3	1.21	0	3,3,3	0.88	0
9	ACT	G	704	-	3,3,3	1.09	0	3,3,3	1.02	0
11	SF4	A	709	1	0,12,12	-	-	-		
11	SF4	K	303	5	0,12,12	-	-	-		
12	GOL	A	711	-	5,5,5	0.27	0	5,5,5	0.41	0
18	NFU	F	504	6	2,7,7	1.00	0	-		
12	GOL	G	711	-	5,5,5	0.21	0	5,5,5	0.28	0
12	GOL	A	714	-	5,5,5	0.27	0	5,5,5	0.24	0
12	GOL	K	304	-	5,5,5	0.31	0	5,5,5	0.65	0
11	SF4	A	706	1	0,12,12	-	-	-		
13	9S8	B	301	2	4,10,10	6.43	2 (50%)	-		
13	9S8	B	302	2	4,10,10	6.49	2 (50%)	-		
11	SF4	E	301	5	0,12,12	-	-	-		
11	SF4	G	708	1	0,12,12	-	-	-		
7	FAD	A	701	-	58,58,58	1.44	9 (15%)	85,89,89	1.68	20 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	GOL	A	713	-	5,5,5	0.30	0	5,5,5	0.46	0
12	GOL	D	203	-	5,5,5	0.27	0	5,5,5	0.31	0
11	SF4	G	709	1	0,12,12	-	-	-		
11	SF4	G	705	1	0,12,12	-	-	-		
11	SF4	E	303	5	0,12,12	-	-	-		
14	FES	D	201	4	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	GOL	G	713	-	-	2/4/4/4	-
12	GOL	K	306	-	-	2/4/4/4	-
11	SF4	E	302	5	-	-	0/6/5/5
11	SF4	A	710	1	-	-	0/6/5/5
11	SF4	K	302	5	-	-	0/6/5/5
15	TRS	D	202	-	-	6/9/9/9	-
11	SF4	I	202	3	-	-	0/6/5/5
10	PE3	A	704	-	-	4/8/8/40	-
11	SF4	K	301	5	-	-	0/6/5/5
13	9S8	H	301	2	-	-	0/3/3/3
12	GOL	K	305	-	-	2/4/4/4	-
13	9S8	H	302	2	-	-	0/3/3/3
7	FAD	G	701	-	-	1/34/50/50	0/6/6/6
12	GOL	B	304	-	-	4/4/4/4	-
12	GOL	C	203	-	-	4/4/4/4	-
12	GOL	G	714	-	-	0/4/4/4	-
12	GOL	D	203	-	-	0/4/4/4	-
11	SF4	A	705	1	-	-	0/6/5/5
11	SF4	G	706	1	-	-	0/6/5/5
11	SF4	G	707	1	-	-	0/6/5/5
11	SF4	G	710	1	-	-	0/6/5/5
11	SF4	C	202	3	-	-	0/6/5/5
11	SF4	C	201	3	-	-	0/6/5/5
12	GOL	A	712	-	-	4/4/4/4	-
14	FES	J	201	4	-	-	0/1/1/1
12	GOL	G	712	-	-	4/4/4/4	-
11	SF4	A	707	1	-	-	0/6/5/5
11	SF4	A	708	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	I	203	3	-	-	0/6/5/5
11	SF4	A	709	1	-	-	0/6/5/5
11	SF4	K	303	5	-	-	0/6/5/5
12	GOL	A	711	-	-	3/4/4/4	-
12	GOL	G	711	-	-	2/4/4/4	-
12	GOL	A	714	-	-	0/4/4/4	-
12	GOL	K	304	-	-	2/4/4/4	-
11	SF4	A	706	1	-	-	0/6/5/5
13	9S8	B	301	2	-	-	0/3/3/3
13	9S8	B	302	2	-	-	0/3/3/3
11	SF4	E	301	5	-	-	0/6/5/5
11	SF4	G	708	1	-	-	0/6/5/5
7	FAD	A	701	-	-	0/34/50/50	0/6/6/6
12	GOL	A	713	-	-	4/4/4/4	-
12	GOL	E	304	-	-	0/4/4/4	-
11	SF4	G	709	1	-	-	0/6/5/5
11	SF4	G	705	1	-	-	0/6/5/5
11	SF4	E	303	5	-	-	0/6/5/5
14	FES	D	201	4	-	-	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	301	9S8	S1-FE4	-10.04	2.12	2.28
13	H	302	9S8	S1-FE4	-9.94	2.12	2.28
13	B	302	9S8	S1-FE4	-9.76	2.12	2.28
13	B	301	9S8	S1-FE4	-9.39	2.13	2.28
13	B	301	9S8	S7-FE4	-8.69	2.14	2.28
13	H	301	9S8	S7-FE4	-8.69	2.14	2.28
13	H	302	9S8	S7-FE4	-8.62	2.14	2.28
13	B	302	9S8	S7-FE4	-8.33	2.15	2.28
7	G	701	FAD	C9A-C5X	5.62	1.50	1.41
7	A	701	FAD	C9A-C5X	5.55	1.50	1.41
7	G	701	FAD	C5A-C4A	4.75	1.47	1.39
7	A	701	FAD	C5A-C4A	4.40	1.46	1.39
7	A	701	FAD	C8-C7	3.44	1.49	1.40
7	G	701	FAD	C8-C7	3.36	1.49	1.40
7	G	701	FAD	C5A-C6A	2.63	1.48	1.41
7	A	701	FAD	C5A-C6A	2.59	1.48	1.41
7	G	701	FAD	C8A-N7A	2.51	1.36	1.31
7	G	701	FAD	PA-O3P	2.31	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	701	FAD	C5A-N7A	-2.26	1.34	1.39
7	A	701	FAD	C5A-N7A	-2.21	1.35	1.39
7	G	701	FAD	C4X-N5	2.21	1.35	1.30
7	A	701	FAD	C4-N3	-2.20	1.34	1.38
7	A	701	FAD	C8A-N7A	2.19	1.35	1.31
7	G	701	FAD	C4-N3	-2.13	1.34	1.38
7	A	701	FAD	C5X-N5	-2.12	1.35	1.39
7	A	701	FAD	C4X-N5	2.09	1.35	1.30

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	701	FAD	C5A-C4A-N3A	-5.77	118.78	126.72
7	A	701	FAD	C5A-C4A-N3A	-5.39	119.29	126.72
7	G	701	FAD	N3A-C4A-N9A	4.64	135.05	127.17
7	A	701	FAD	N3A-C4A-N9A	4.56	134.91	127.17
7	A	701	FAD	N3A-C2A-N1A	-3.99	122.55	128.58
7	G	701	FAD	C2A-N3A-C4A	3.95	121.47	111.83
7	G	701	FAD	N3A-C2A-N1A	-3.92	122.64	128.58
7	A	701	FAD	C2A-N3A-C4A	3.81	121.14	111.83
7	G	701	FAD	C4A-C5A-N7A	-3.50	106.58	110.58
7	A	701	FAD	C4A-N9A-C8A	3.30	109.20	105.74
7	A	701	FAD	C4-C4X-N5	3.14	122.55	118.21
7	A	701	FAD	C4A-C5A-N7A	-3.13	107.01	110.58
7	G	701	FAD	C4-C4X-N5	3.08	122.46	118.21
7	G	701	FAD	C4A-N9A-C8A	3.02	108.91	105.74
7	G	701	FAD	C5A-N7A-C8A	2.83	107.89	103.45
7	A	701	FAD	O4-C4-C4X	-2.76	119.24	126.53
7	A	701	FAD	O2-C2-N1	-2.72	117.28	121.80
7	A	701	FAD	C5A-N7A-C8A	2.66	107.63	103.45
7	G	701	FAD	O4-C4-C4X	-2.56	119.77	126.53
7	A	701	FAD	C4X-C10-N10	2.53	120.11	116.48
7	A	701	FAD	N9A-C8A-N7A	-2.51	110.37	113.94
7	A	701	FAD	C4X-C10-N1	-2.49	118.48	124.59
7	G	701	FAD	C4X-C10-N1	-2.47	118.55	124.59
7	G	701	FAD	N9A-C8A-N7A	-2.46	110.45	113.94
7	G	701	FAD	O2-C2-N1	-2.45	117.72	121.80
7	A	701	FAD	C10-N1-C2	2.45	122.14	116.85
7	G	701	FAD	C6A-C5A-N7A	2.40	136.71	132.09
7	A	701	FAD	C4X-C4-N3	2.34	119.21	113.25
7	A	701	FAD	C2A-N1A-C6A	2.33	122.55	118.73
7	A	701	FAD	C4-N3-C2	-2.32	121.53	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	701	FAD	C6A-C5A-N7A	2.30	136.53	132.09
7	G	701	FAD	C4-N3-C2	-2.29	121.57	125.64
7	G	701	FAD	C4X-C4-N3	2.26	119.02	113.25
7	G	701	FAD	C4X-C10-N10	2.19	119.61	116.48
7	A	701	FAD	O4'-C4'-C3'	2.19	114.36	109.25
7	A	701	FAD	O4B-C1B-N9A	2.16	112.25	108.09
7	G	701	FAD	C10-N1-C2	2.15	121.51	116.85
7	G	701	FAD	C9A-C5X-N5	-2.02	120.31	122.45
7	G	701	FAD	C2A-N1A-C6A	2.01	122.03	118.73

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	711	GOL	C1-C2-C3-O3
12	A	712	GOL	O1-C1-C2-C3
12	A	712	GOL	C1-C2-C3-O3
12	A	713	GOL	C1-C2-C3-O3
12	B	304	GOL	O1-C1-C2-C3
12	C	203	GOL	C1-C2-C3-O3
12	G	711	GOL	O1-C1-C2-C3
12	G	712	GOL	O1-C1-C2-C3
12	G	712	GOL	C1-C2-C3-O3
12	G	713	GOL	C1-C2-C3-O3
12	K	304	GOL	O1-C1-C2-C3
12	K	305	GOL	C1-C2-C3-O3
15	D	202	TRS	C1-C-C3-O3
15	D	202	TRS	N-C-C3-O3
12	A	712	GOL	O2-C2-C3-O3
12	A	713	GOL	O2-C2-C3-O3
10	A	704	PE3	O7-C8-C9-O10
12	A	713	GOL	O1-C1-C2-C3
12	B	304	GOL	C1-C2-C3-O3
12	C	203	GOL	O1-C1-C2-C3
12	K	306	GOL	C1-C2-C3-O3
12	A	711	GOL	O2-C2-C3-O3
12	A	712	GOL	O1-C1-C2-O2
12	B	304	GOL	O1-C1-C2-O2
12	G	711	GOL	O1-C1-C2-O2
12	G	712	GOL	O2-C2-C3-O3
12	G	713	GOL	O2-C2-C3-O3
12	G	712	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

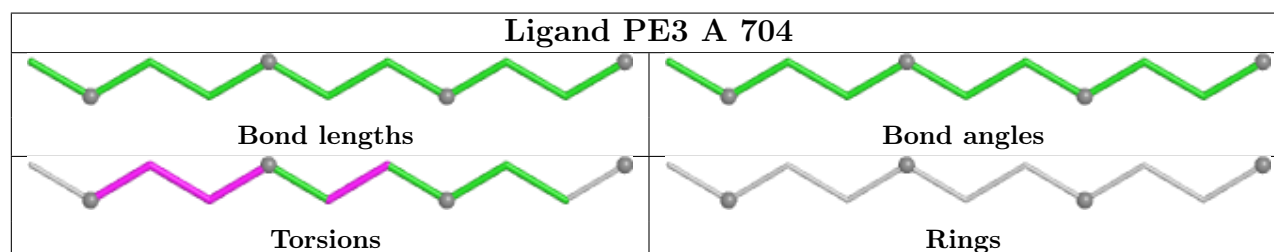
Mol	Chain	Res	Type	Atoms
12	K	304	GOL	O1-C1-C2-O2
12	K	305	GOL	O2-C2-C3-O3
10	A	704	PE3	O4-C5-C6-O7
12	A	711	GOL	O1-C1-C2-C3
12	B	304	GOL	O2-C2-C3-O3
15	D	202	TRS	C2-C-C3-O3
12	C	203	GOL	O2-C2-C3-O3
12	K	306	GOL	O2-C2-C3-O3
10	A	704	PE3	C6-C5-O4-C3
15	D	202	TRS	C2-C-C1-O1
15	D	202	TRS	C3-C-C2-O2
10	A	704	PE3	C5-C6-O7-C8
12	A	713	GOL	O1-C1-C2-O2
12	C	203	GOL	O1-C1-C2-O2
7	G	701	FAD	O4B-C4B-C5B-O5B
15	D	202	TRS	N-C-C2-O2

There are no ring outliers.

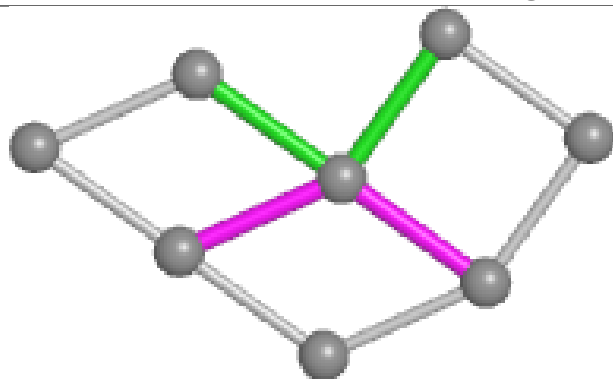
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	711	GOL	1	0

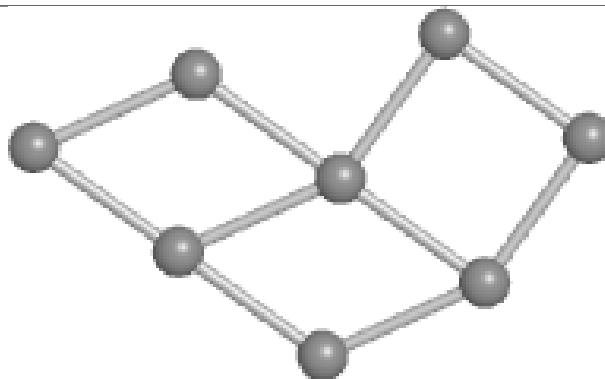
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



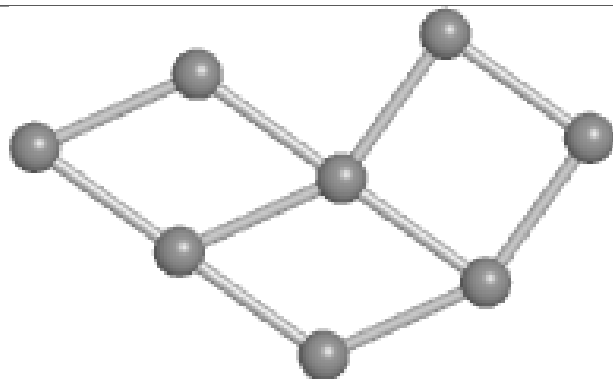
Ligand 9S8 H 301



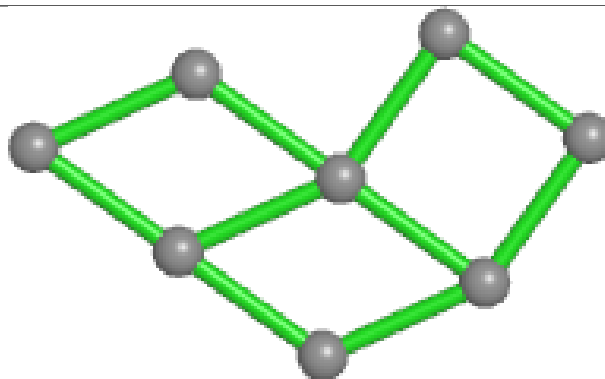
Bond lengths



Bond angles

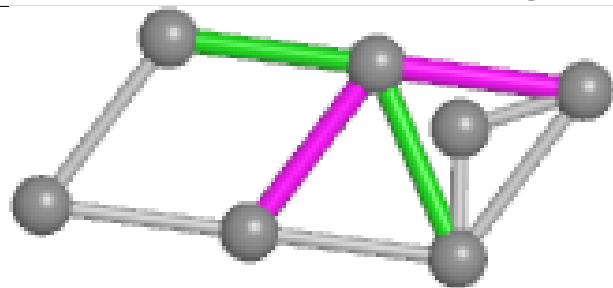


Torsions

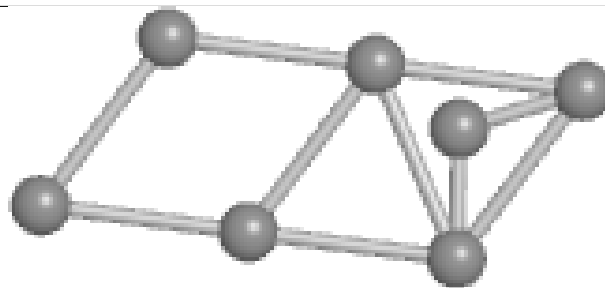


Rings

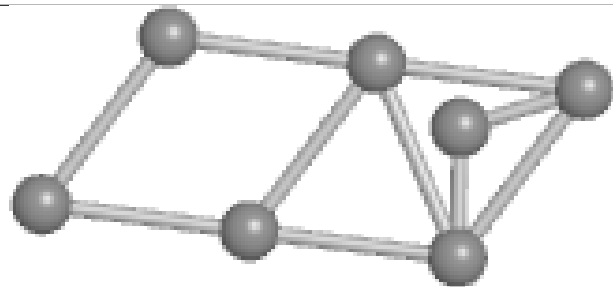
Ligand 9S8 H 302



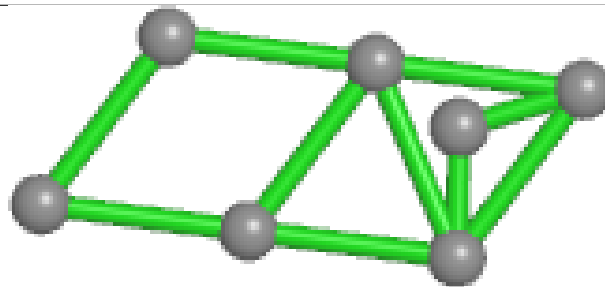
Bond lengths



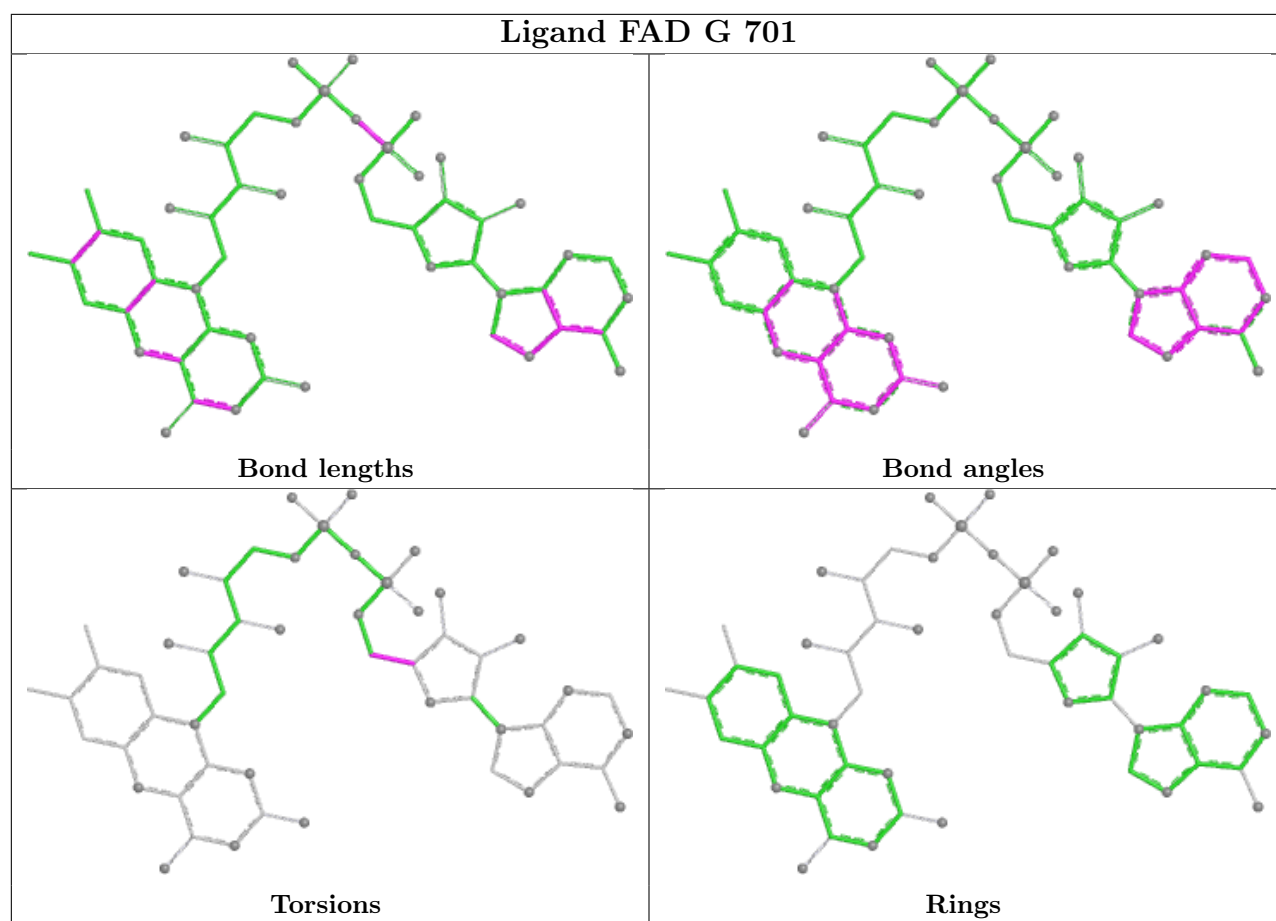
Bond angles



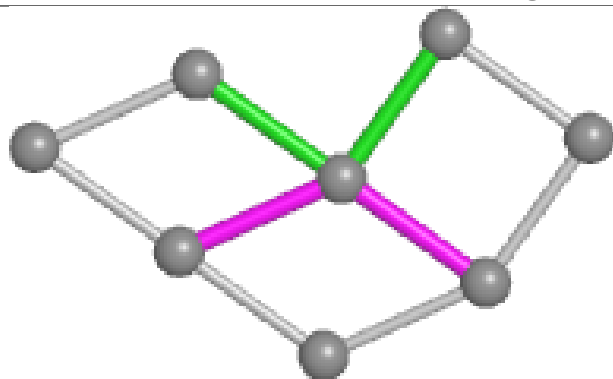
Torsions



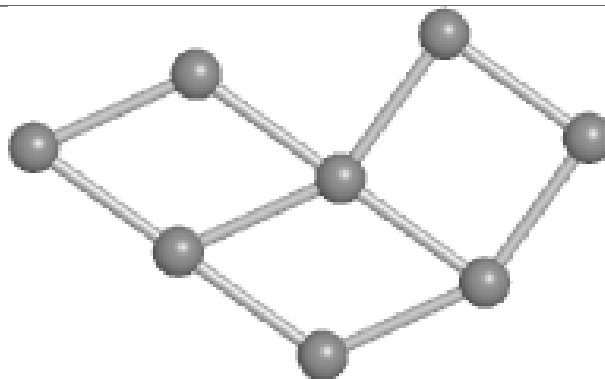
Rings



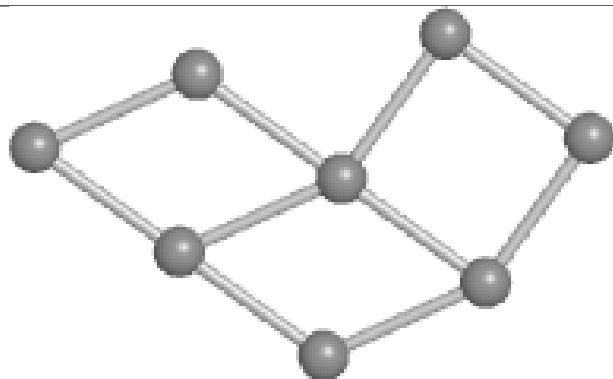
Ligand 9S8 B 301



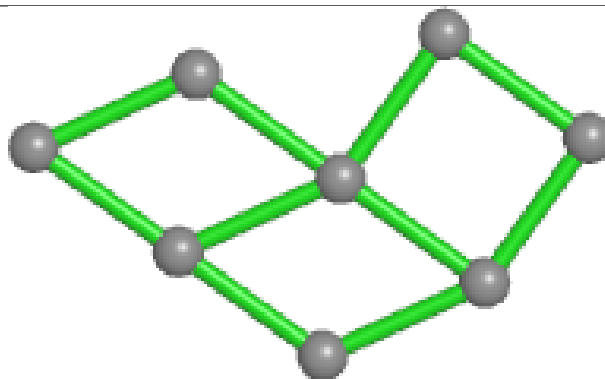
Bond lengths



Bond angles

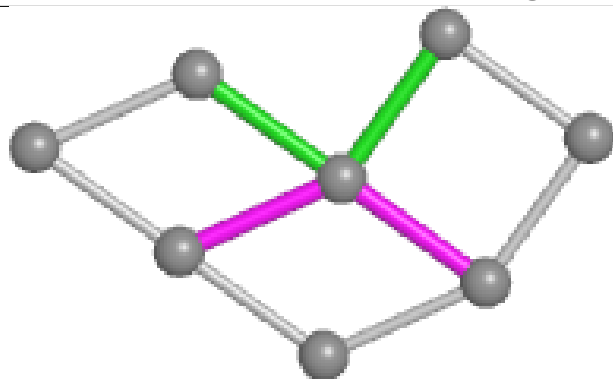


Torsions

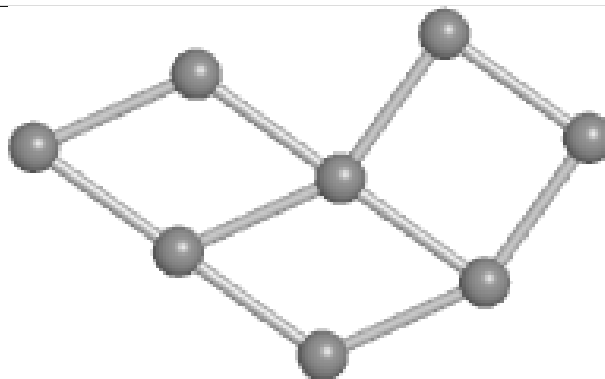


Rings

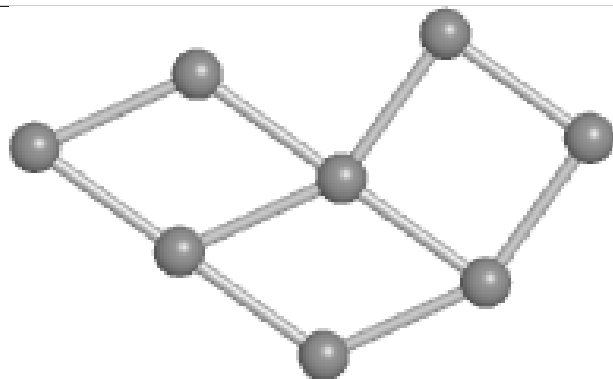
Ligand 9S8 B 302



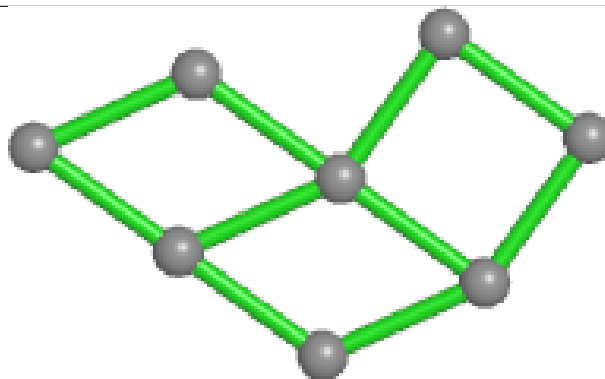
Bond lengths



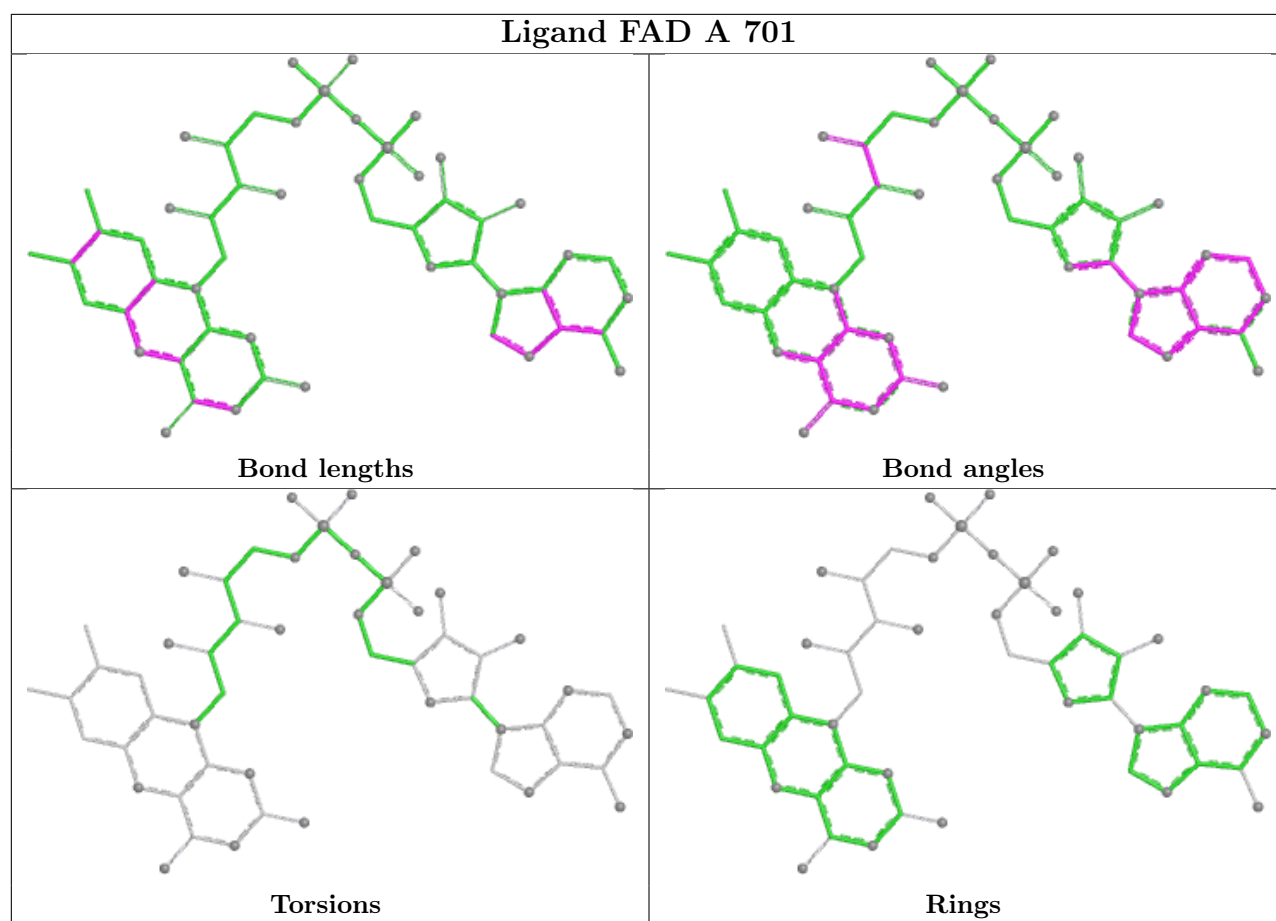
Bond angles



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	653/654 (99%)	-0.23	4 (0%) 85 86	24, 38, 65, 86	0
1	G	653/654 (99%)	-0.16	7 (1%) 78 79	25, 40, 78, 106	0
2	B	291/291 (100%)	0.25	2 (0%) 84 85	36, 50, 74, 90	0
2	H	291/291 (100%)	1.15	49 (16%) 4 5	42, 74, 109, 125	0
3	C	184/184 (100%)	0.14	3 (1%) 70 72	29, 49, 87, 126	0
3	I	173/184 (94%)	0.74	32 (18%) 3 4	27, 55, 113, 132	0
4	D	138/140 (98%)	-0.41	0 100 100	23, 34, 53, 80	0
4	J	138/140 (98%)	-0.31	0 100 100	29, 36, 62, 89	0
5	E	298/299 (99%)	-0.21	2 (0%) 84 85	23, 38, 66, 84	0
5	K	298/299 (99%)	0.09	3 (1%) 79 80	28, 45, 78, 98	0
6	F	447/473 (94%)	-0.01	6 (1%) 75 76	26, 45, 73, 91	0
6	L	447/473 (94%)	0.33	13 (2%) 53 56	32, 52, 85, 110	0
All	All	4011/4082 (98%)	0.08	121 (3%) 52 54	23, 44, 85, 132	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	654	ALA	5.1
1	A	654	ALA	5.1
3	I	122	LEU	4.4
2	H	291	ILE	4.4
6	L	282	GLU	4.3
2	H	132	VAL	4.0
3	I	143	LEU	4.0
3	I	147	ALA	3.8
3	I	173	ILE	3.6
3	I	148	PRO	3.6
3	I	141	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	33	LEU	3.4
2	H	34	VAL	3.3
2	H	122	PHE	3.3
2	H	31	VAL	3.2
3	I	123	LYS	3.2
2	H	136	ALA	3.2
2	H	275	LEU	3.2
2	H	28	LYS	3.1
6	L	83	LYS	3.1
2	B	291	ILE	3.1
2	H	18	VAL	3.0
3	I	132	LYS	2.9
3	I	130	ALA	2.9
2	H	274	ASP	2.9
2	H	139	VAL	2.9
2	H	1	MET	2.9
2	H	66	ILE	2.9
6	L	284	ASP	2.9
5	E	299	LYS	2.8
2	H	273	LYS	2.8
5	K	206	LYS	2.8
2	H	30	GLY	2.7
2	H	266	LEU	2.7
2	H	72	VAL	2.7
6	L	281	GLY	2.7
6	L	364	VAL	2.7
3	C	184	GLU	2.7
3	I	120	TYR	2.6
1	A	420	ASP	2.6
6	L	283	GLU	2.6
3	I	142	GLY	2.6
3	I	146	LYS	2.6
3	I	165	LYS	2.6
3	I	162	THR	2.6
2	H	25	VAL	2.6
6	L	363	VAL	2.6
5	K	112	ILE	2.6
6	L	365	GLY	2.5
3	I	119	MET	2.5
3	I	139	LYS	2.5
6	L	419	LYS	2.5
1	G	268	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	3	TYR	2.5
2	H	143	LEU	2.5
2	H	270	MET	2.5
2	H	238	PHE	2.4
2	H	251	LYS	2.4
2	H	245	ILE	2.4
3	C	131	ASN	2.3
6	L	24	ASP	2.3
3	I	144	SER	2.3
2	H	5	PHE	2.3
2	H	171	VAL	2.3
3	I	128	VAL	2.3
2	H	118	LYS	2.3
3	I	124	TYR	2.3
3	I	155	LYS	2.3
1	G	258	ILE	2.3
3	I	152	PHE	2.3
3	I	163	LEU	2.3
2	H	48	PHE	2.3
2	H	7	LEU	2.3
2	H	2	LYS	2.3
2	H	10	ILE	2.3
2	H	130	ILE	2.3
6	F	308	LYS	2.3
2	H	29	LEU	2.2
6	F	364	VAL	2.3
2	H	272	PRO	2.2
3	I	150	ALA	2.2
1	A	417	LYS	2.2
3	I	161	ASN	2.2
2	H	108	LYS	2.2
1	G	310	PHE	2.2
6	F	207	GLU	2.2
6	F	248	LYS	2.2
2	H	277	LEU	2.2
1	G	302	VAL	2.2
2	B	109	VAL	2.2
2	H	6	PHE	2.2
2	H	9	CYS	2.2
2	H	20	ALA	2.2
3	I	153	SER	2.2
6	L	366	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	4	ALA	2.1
3	I	135	ALA	2.1
1	A	268	ILE	2.1
2	H	26	MET	2.1
2	H	263	LEU	2.1
6	L	280	LYS	2.1
3	I	158	ASN	2.1
5	E	50	GLU	2.1
6	L	353	GLY	2.1
3	I	138	ARG	2.1
1	G	300	ALA	2.1
3	C	120	TYR	2.1
2	H	38	GLY	2.1
2	H	16	ALA	2.1
5	K	299	LYS	2.1
2	H	74	ILE	2.1
3	I	149	ILE	2.1
3	I	169	PHE	2.1
2	H	123	ALA	2.0
3	I	137	LEU	2.0
6	F	125	LEU	2.0
2	H	176	ILE	2.0
6	F	139	ILE	2.0
1	G	301	LYS	2.0
3	I	131	ASN	2.0
2	H	183	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
12	GOL	G	714	6/6	0.65	0.22	74,74,76,77	0
12	GOL	G	713	6/6	0.67	0.28	64,71,72,73	0
12	GOL	K	305	6/6	0.73	0.30	85,86,87,89	0
12	GOL	K	304	6/6	0.76	0.27	78,82,83,84	0
12	GOL	D	203	6/6	0.76	0.30	127,131,132,134	0
12	GOL	B	304	6/6	0.78	0.39	121,123,126,126	0
9	ACT	F	503	4/4	0.78	0.17	66,68,69,69	0
9	ACT	G	703	4/4	0.80	0.17	50,52,52,52	0
12	GOL	A	714	6/6	0.81	0.17	76,78,84,84	0
12	GOL	E	304	6/6	0.81	0.27	83,84,84,89	0
12	GOL	K	306	6/6	0.81	0.28	110,113,116,117	0
9	ACT	B	303	4/4	0.83	0.15	62,65,66,66	0
12	GOL	G	712	6/6	0.84	0.20	69,72,73,76	0
10	PE3	A	704	11/43	0.84	0.14	50,54,58,59	0
12	GOL	A	713	6/6	0.84	0.15	67,71,74,77	0
12	GOL	A	712	6/6	0.85	0.28	95,98,99,102	0
9	ACT	G	704	4/4	0.85	0.24	69,71,71,72	0
15	TRS	D	202	8/8	0.86	0.17	69,72,74,75	0
13	9S8	B	302	8/8	0.87	0.12	53,59,67,68	0
12	GOL	A	711	6/6	0.87	0.14	44,46,47,48	0
13	9S8	H	301	8/8	0.89	0.12	88,89,91,91	0
13	9S8	H	302	8/8	0.90	0.10	72,77,80,81	0
9	ACT	A	703	4/4	0.91	0.15	51,54,55,56	0
12	GOL	G	711	6/6	0.91	0.21	62,65,67,67	0
12	GOL	C	203	6/6	0.91	0.19	87,88,94,95	0
8	NA	A	702	1/1	0.91	0.26	49,49,49,49	0
13	9S8	B	301	8/8	0.93	0.07	51,57,59,60	0
11	SF4	G	707	8/8	0.94	0.07	98,100,100,103	0
11	SF4	G	709	8/8	0.95	0.07	88,90,91,92	0
17	MG	I	201	1/1	0.96	0.07	44,44,44,44	0
11	SF4	A	707	8/8	0.97	0.05	59,62,65,66	0
7	FAD	G	701	53/53	0.97	0.06	21,28,34,39	0
8	NA	G	702	1/1	0.97	0.18	43,43,43,43	0
11	SF4	A	706	8/8	0.97	0.04	52,56,58,62	0
11	SF4	I	202	8/8	0.98	0.04	44,46,52,53	0
11	SF4	I	203	8/8	0.98	0.05	41,44,47,48	0
11	SF4	K	301	8/8	0.98	0.07	43,44,50,51	0
11	SF4	K	302	8/8	0.98	0.05	40,49,54,55	0
11	SF4	K	303	8/8	0.98	0.04	50,54,57,59	0
11	SF4	A	709	8/8	0.98	0.05	31,40,42,45	0
11	SF4	C	202	8/8	0.98	0.05	44,48,52,53	0
11	SF4	E	302	8/8	0.98	0.06	39,45,49,49	0
11	SF4	G	705	8/8	0.98	0.05	42,49,50,52	0

Continued on next page...

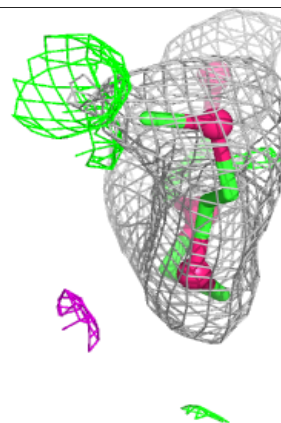
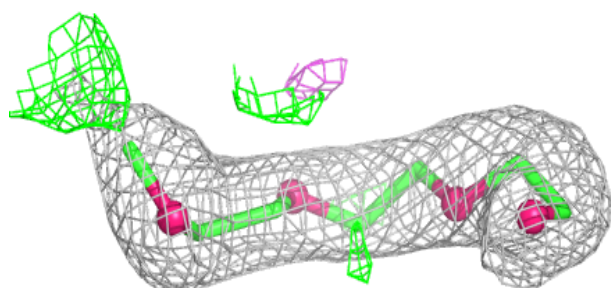
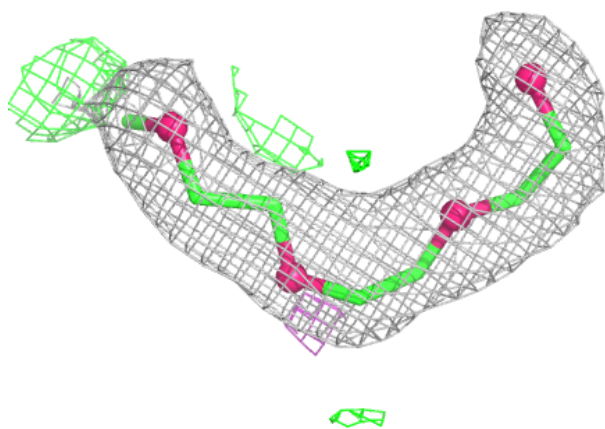
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	SF4	G	706	8/8	0.98	0.04	36,43,45,47	0
7	FAD	A	701	53/53	0.98	0.05	15,26,32,32	0
14	FES	D	201	4/4	0.98	0.05	32,34,36,39	0
14	FES	J	201	4/4	0.98	0.04	28,29,36,38	0
11	SF4	A	705	8/8	0.98	0.04	39,42,45,46	0
17	MG	F	502	1/1	0.98	0.08	39,39,39,39	0
11	SF4	G	710	8/8	0.98	0.05	42,45,49,51	0
11	SF4	E	303	8/8	0.99	0.04	36,40,47,47	0
11	SF4	C	201	8/8	0.99	0.04	34,39,44,46	0
11	SF4	A	708	8/8	0.99	0.04	26,32,35,36	0
11	SF4	E	301	8/8	0.99	0.05	32,36,40,45	0
16	CA	L	501	1/1	0.99	0.05	38,38,38,38	0
11	SF4	G	708	8/8	0.99	0.04	32,38,39,42	0
11	SF4	A	710	8/8	0.99	0.04	34,37,43,44	0
18	NFU	F	504	8/8	0.99	0.07	30,36,40,42	0
18	NFU	L	502	8/8	0.99	0.07	32,41,43,44	0
16	CA	F	501	1/1	1.00	0.02	31,31,31,31	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.

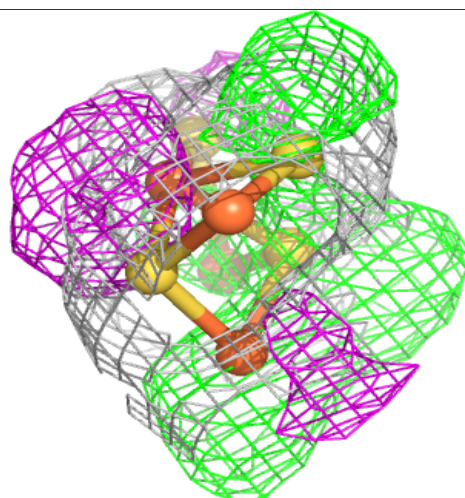
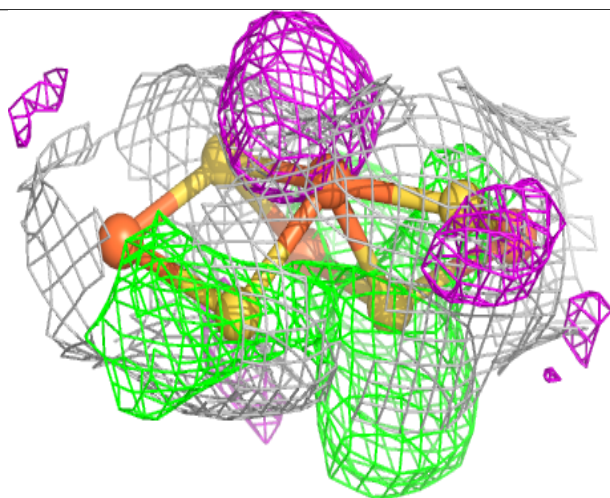
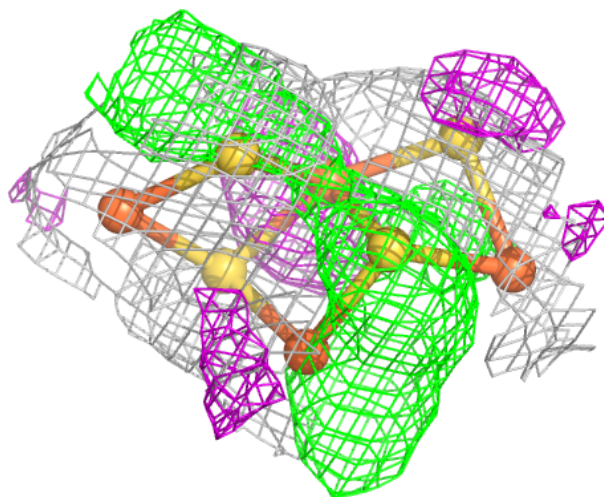
Electron density around PE3 A 704:

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



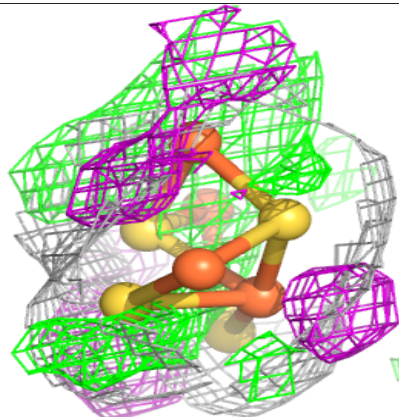
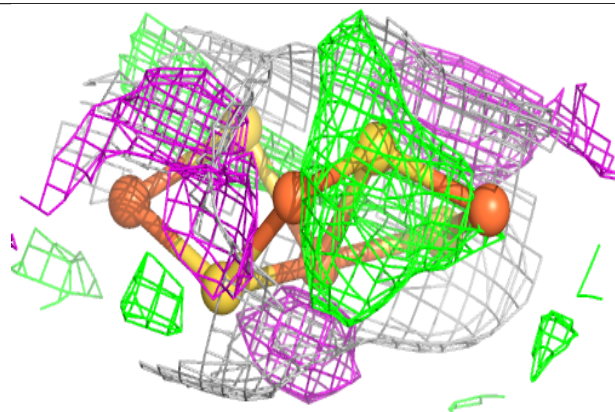
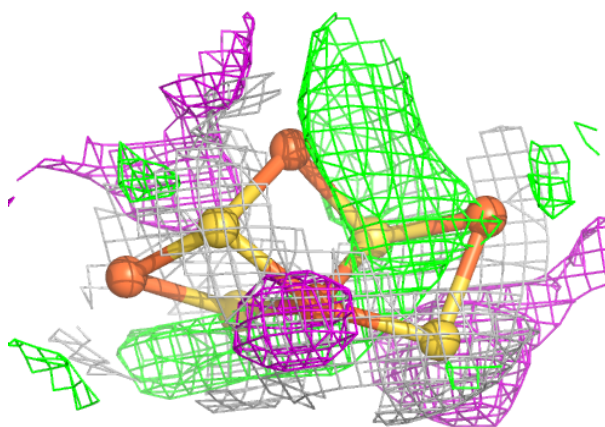
Electron density around 9S8 B 302:

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



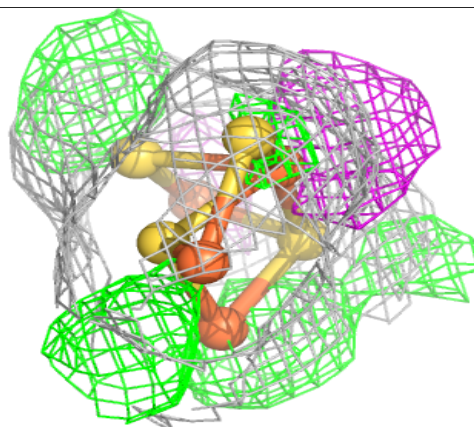
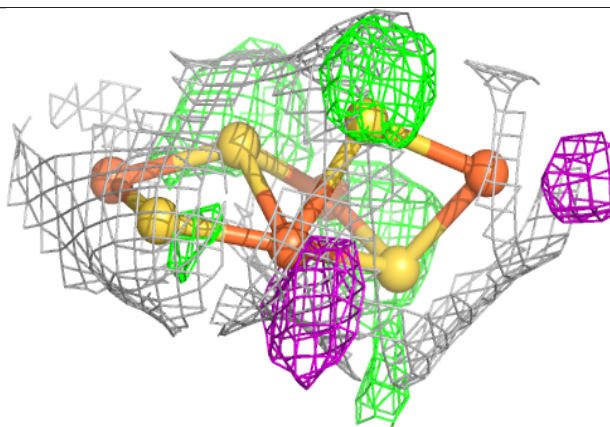
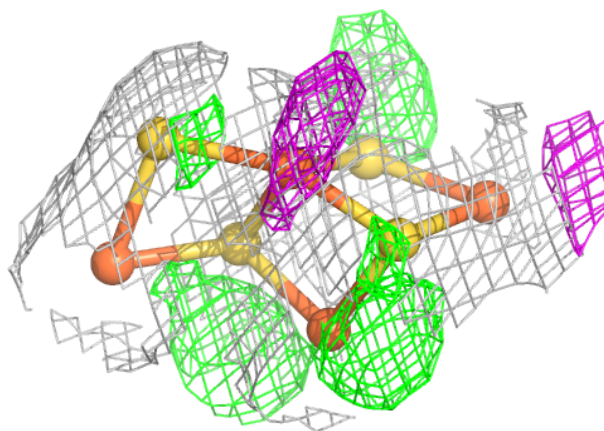
Electron density around 9S8 H 301:

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

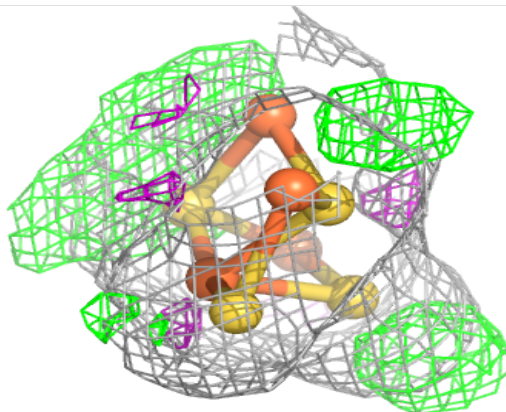
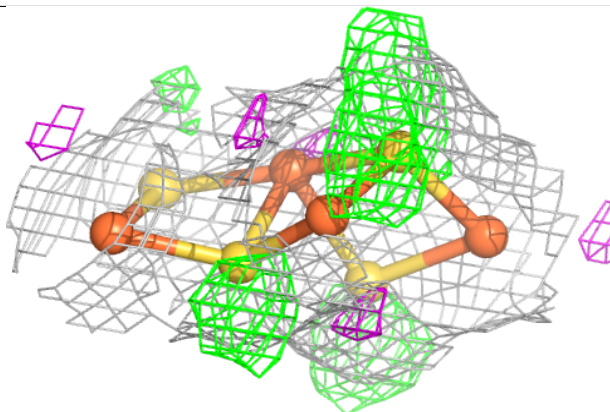
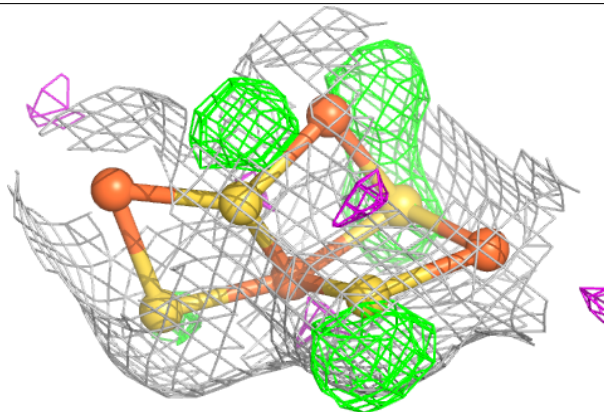


Electron density around 9S8 H 302:

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

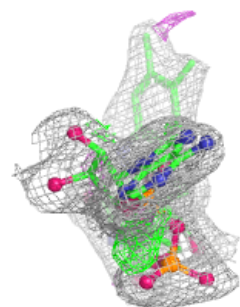
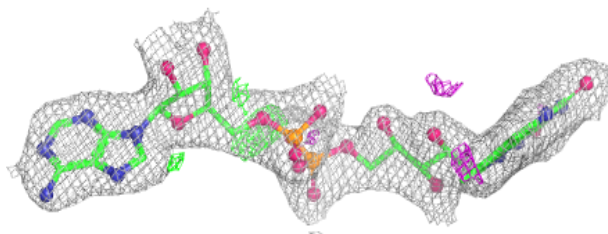
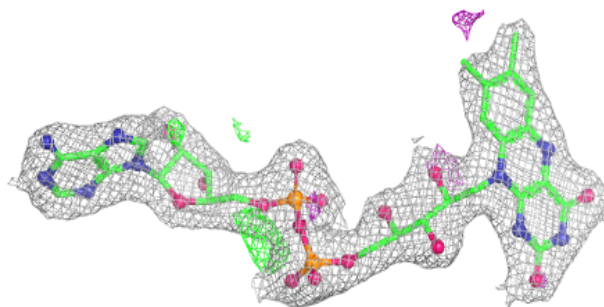
**Electron density around 9S8 B 301:**

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

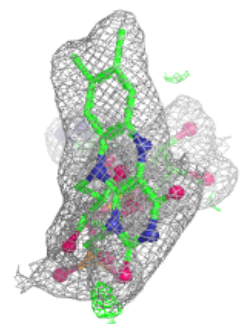
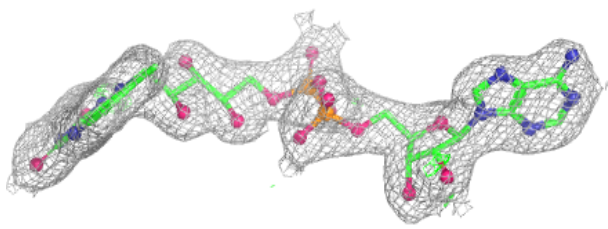
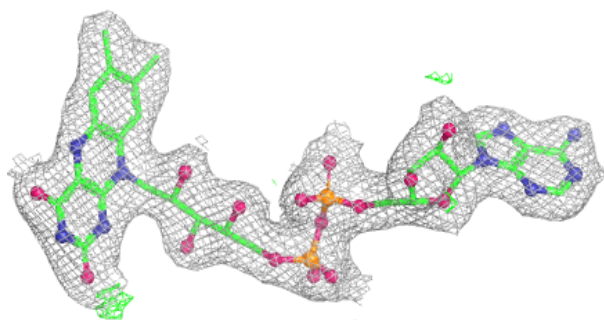


Electron density around FAD G 701:

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

**Electron density around 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.