



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:47 PM UTC

PDB ID : 5ODI / pdb_00005odi
Title : Heterodisulfide reductase / [NiFe]-hydrogenase complex from Methanothermococcus thermolithotrophicus cocrystallized with CoM-SH
Authors : Wagner, T.; Koch, J.; Ermler, U.; Shima, S.
Deposited on : 2017-07-05
Resolution : 2.40 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

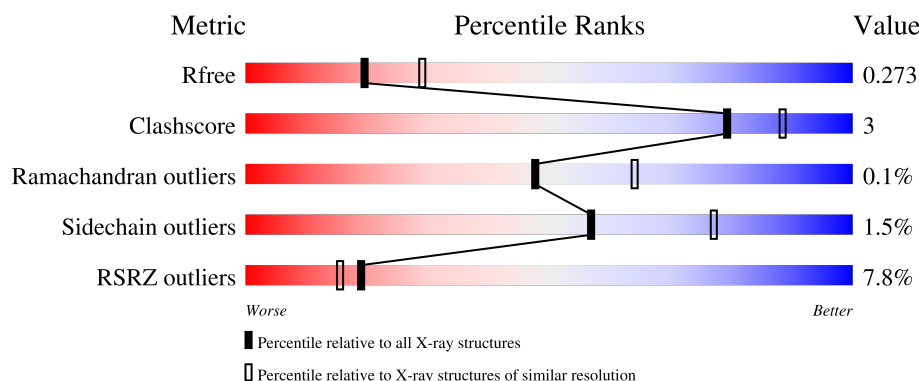
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	
1	G	654	
2	B	291	
2	H	291	
3	C	184	

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Mol	Chain	Length	Quality of chain
3	I	184	 91% 9%
4	D	140	 90% 8%
4	J	140	 91% 8% 11%
5	E	299	 92% 8%
5	K	299	 91% 9% 11%
6	F	473	 89% 5%
6	L	473	 87% 6% 8%

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	H	303	-	X	-	-
15	NFU	F	501	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31986 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	651	Total	C	N	O	S	0	0	0
			4970	3137	844	940	49			
1	G	652	Total	C	N	O	S	0	0	0
			4979	3142	845	943	49			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	184	Total	C	N	O	S	0	0	0
			1426	890	247	275	14			
3	I	183	Total	C	N	O	S	0	0	0
			1416	885	246	271	14			

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

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

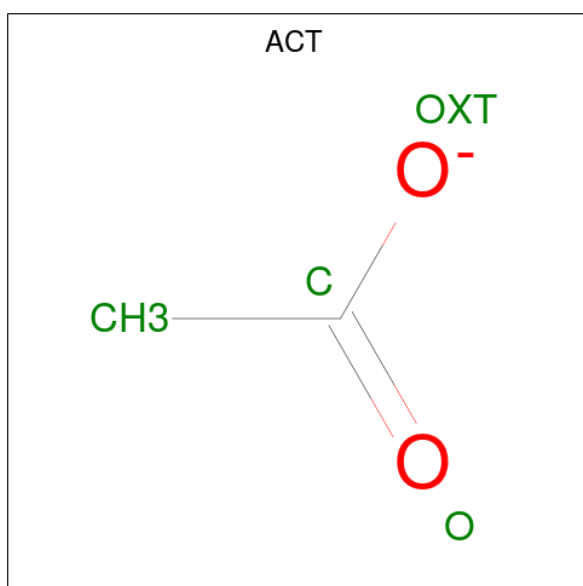
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

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

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

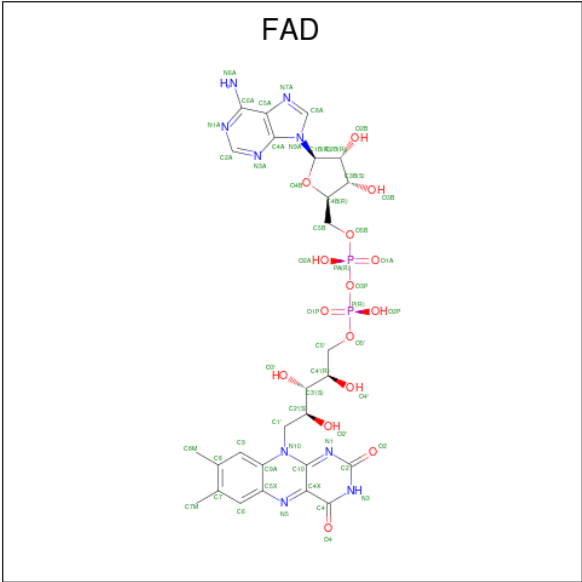
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	447	Total	C	N	O	S	0	0	0
			3521	2230	600	672	19			
6	L	447	Total	C	N	O	S	0	0	0
			3521	2230	600	672	19			

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



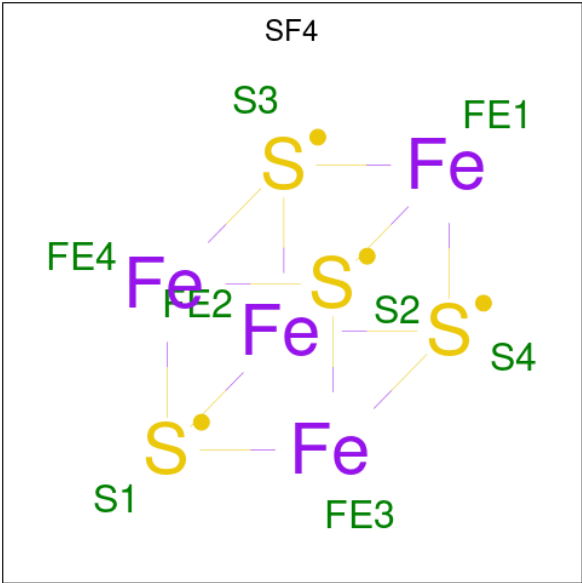
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



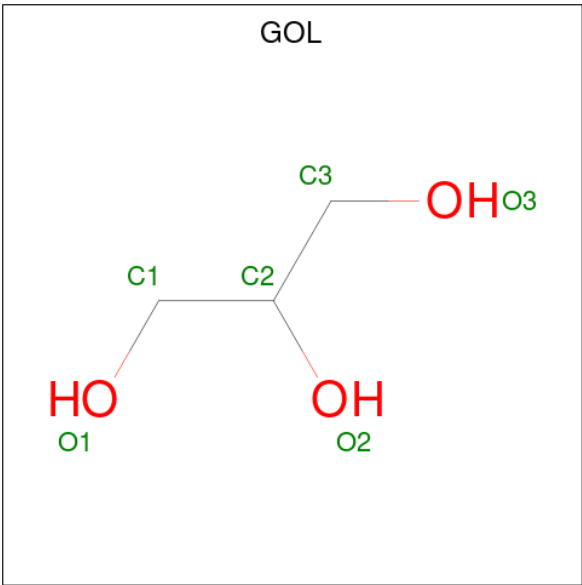
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Fe S	0	0
			8	4 4		
9	A	1	Total	Fe S	0	0
			8	4 4		

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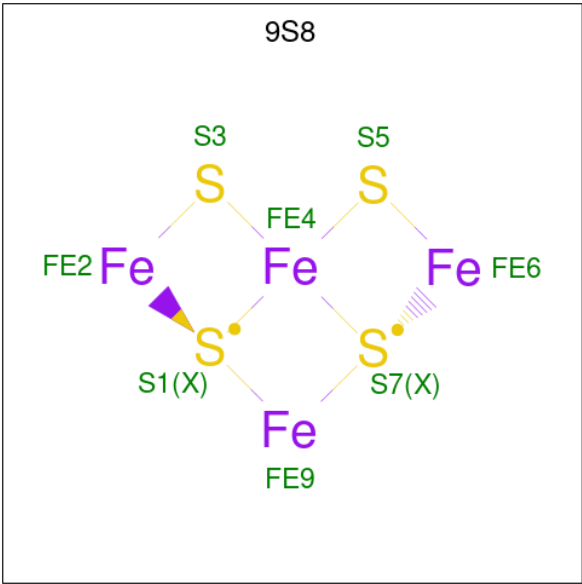
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	Fe	S	0	0
			8	4	4		
9	A	1	Total	Fe	S	0	0
			8	4	4		
9	A	1	Total	Fe	S	0	0
			8	4	4		
9	A	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



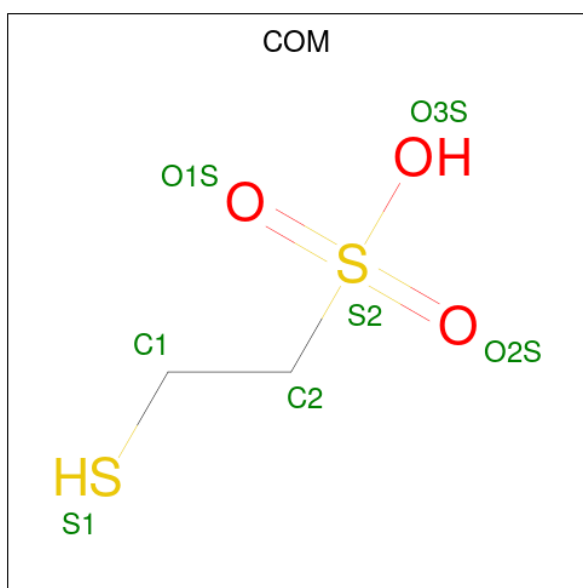
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	G	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe₄S₄).



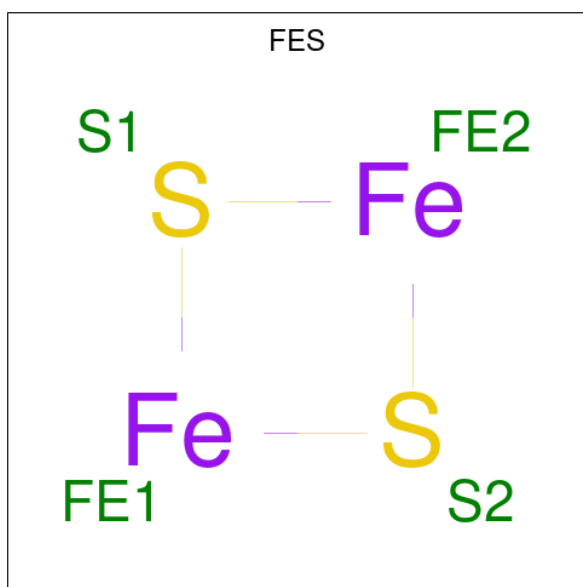
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	H	1	Total	Fe	S	0	0
			8	4	4		
11	H	1	Total	Fe	S	0	0
			8	4	4		

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



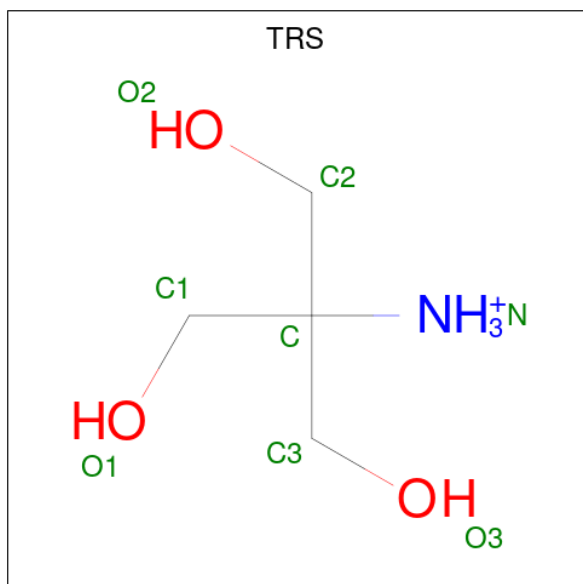
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	O	S	0	0
			7	2	3	2		
12	H	1	Total	C	O	S	0	0
			7	2	3	2		

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



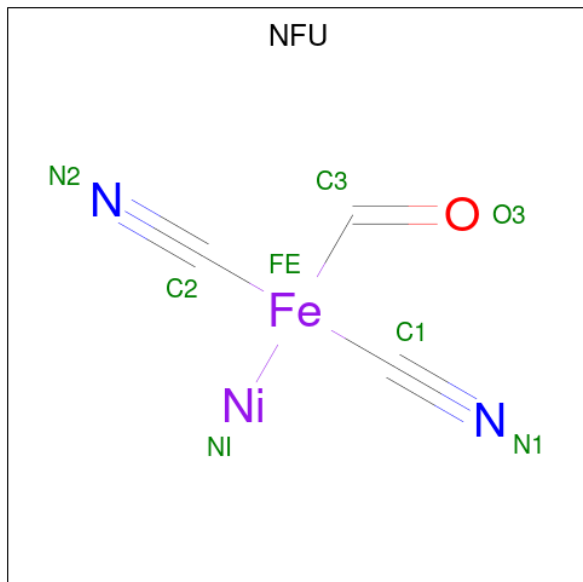
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	Fe	S	0	0
			4	2	2		
13	J	1	Total	Fe	S	0	0
			4	2	2		

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



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

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

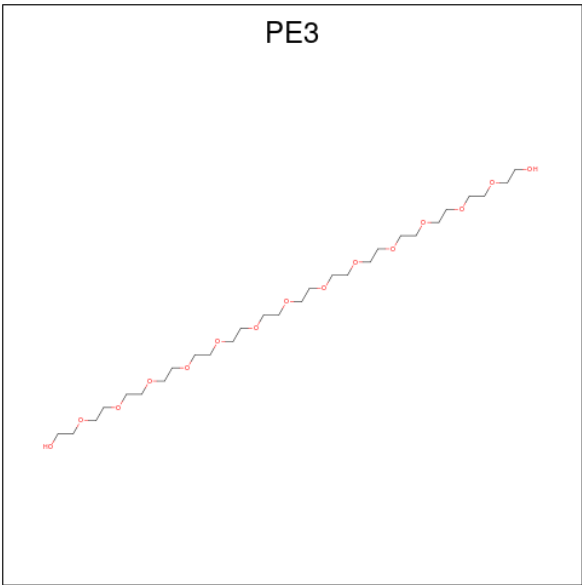


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
15	F	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
15	L	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

- Molecule 16 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 17 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
17	G	1	Total	C	O	0	0
			14	9	5		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	125	Total	O	0	0
			125	125		
18	B	14	Total	O	0	0
			14	14		
18	C	19	Total	O	0	0
			19	19		
18	D	36	Total	O	0	0
			36	36		
18	E	49	Total	O	0	0
			49	49		
18	F	65	Total	O	0	0
			65	65		
18	G	87	Total	O	0	0
			87	87		
18	H	23	Total	O	0	0
			23	23		
18	I	27	Total	O	0	0
			27	27		
18	J	5	Total	O	0	0
			5	5		
18	K	42	Total	O	0	0
			42	42		

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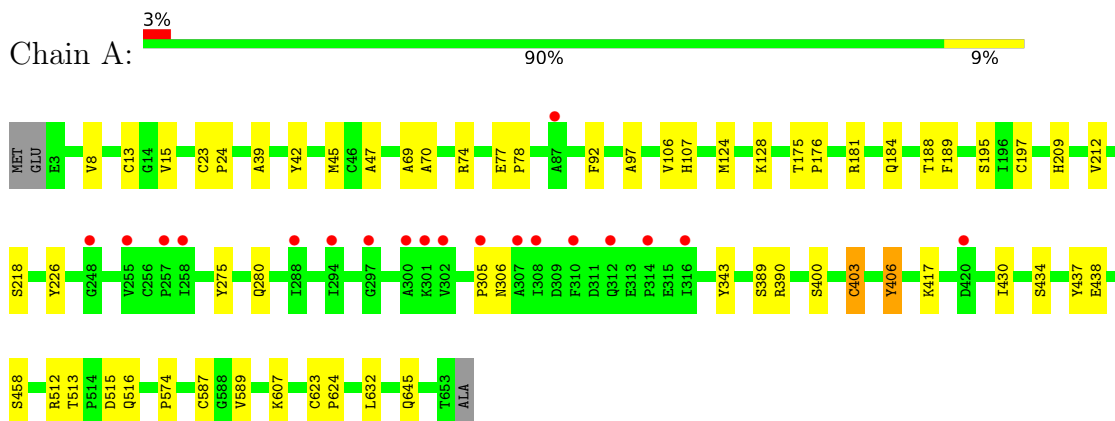
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	62	Total	O	0	0
			62	62		

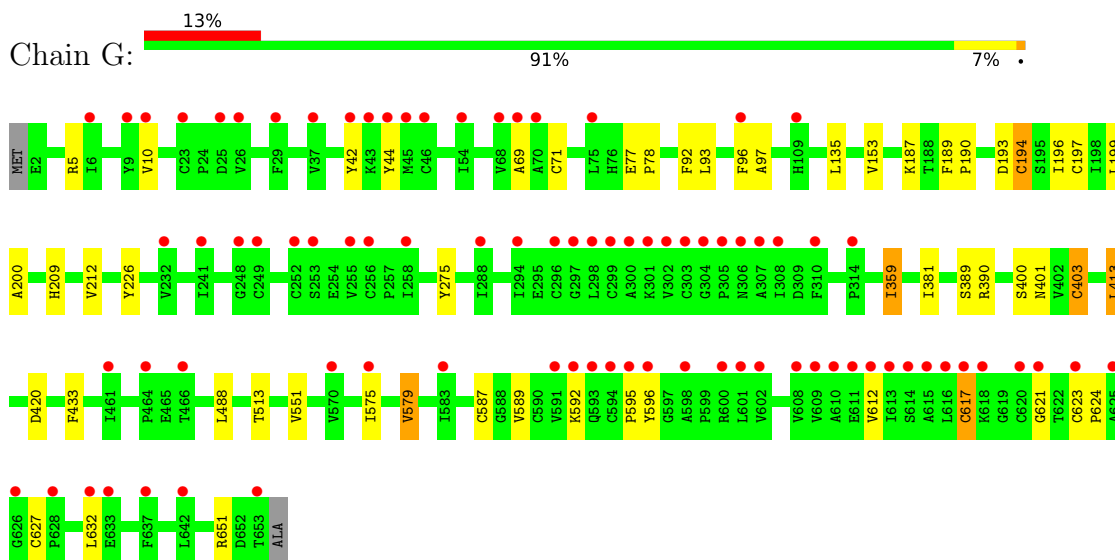
3 Residue-property plots

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.

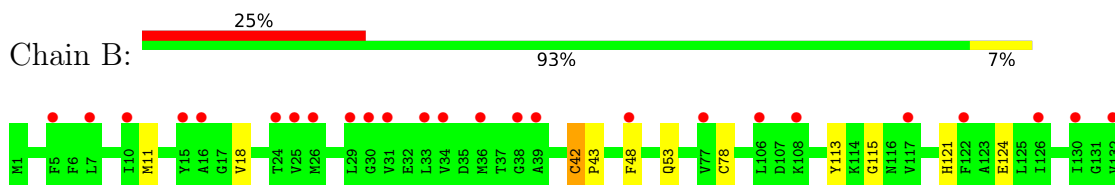
• Molecule 1: Heterodisulfide reductase, subunit A

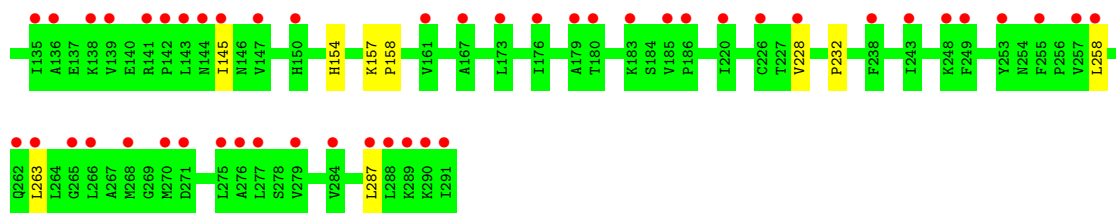


• Molecule 1: Heterodisulfide reductase, subunit A

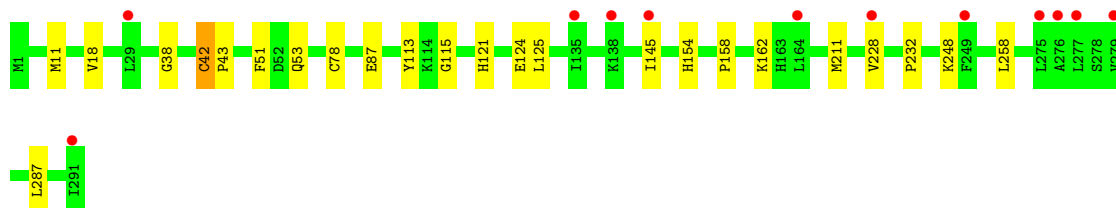
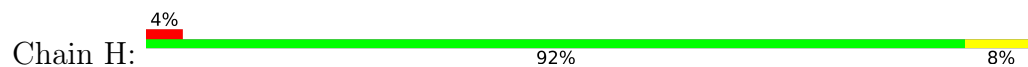


• Molecule 2: Heterodisulfide reductase, subunit B

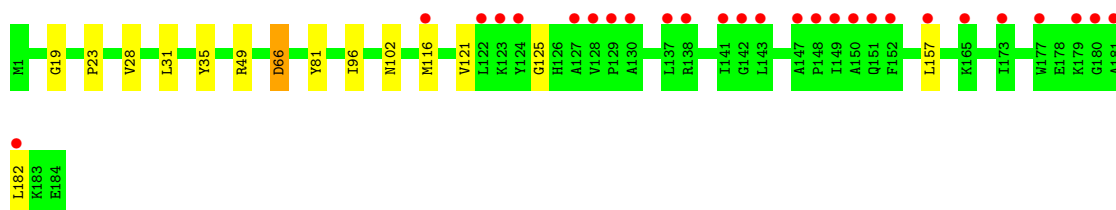
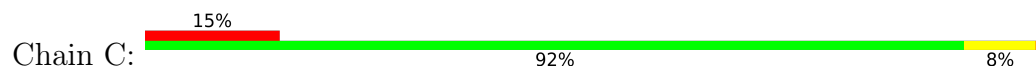




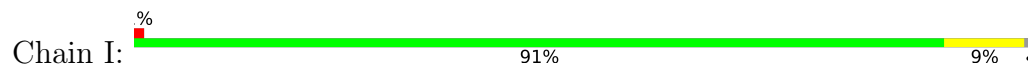
• Molecule 2: Heterodisulfide reductase, subunit B



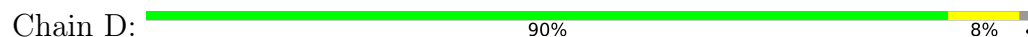
• Molecule 3: Heterodisulfide reductase, subunit C



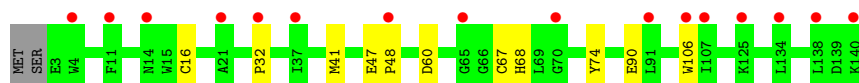
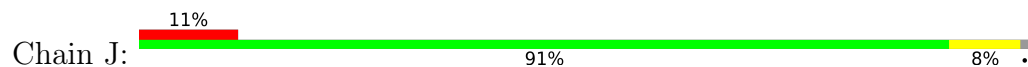
• Molecule 3: Heterodisulfide reductase, subunit C



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



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



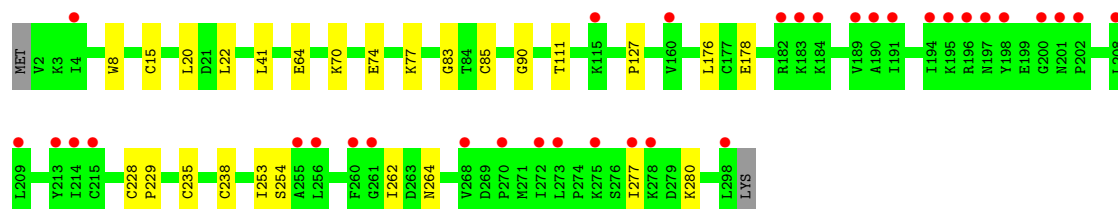
- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

Chain E:  92% 8% .



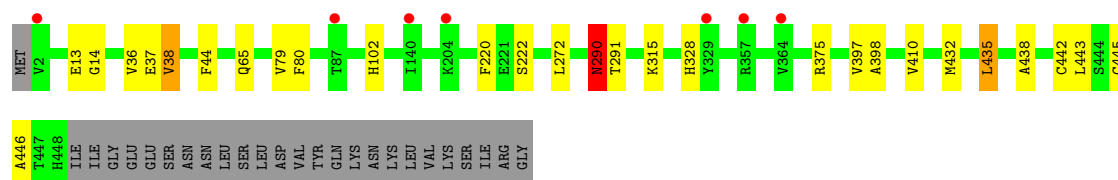
- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

Chain K:  11% 91% 9% .



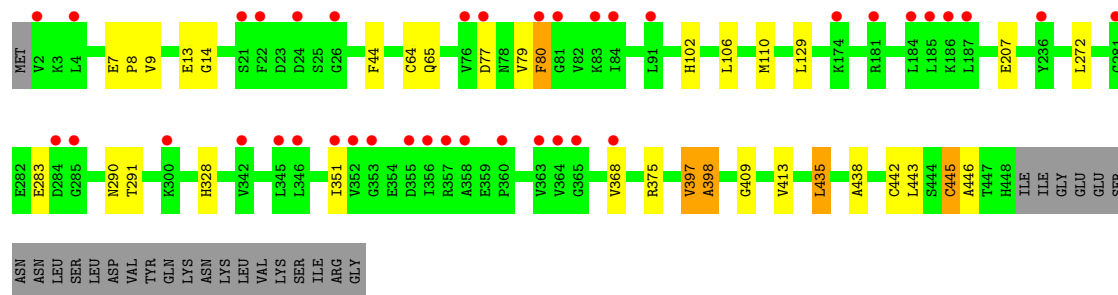
- Molecule 6: Methyl-viologen reducing hydrogenase, subunit A

Chain F:  % 89% 5% 5%



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

Chain L:  8% 87% 6% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	370.53Å 97.08Å 135.15Å 90.00° 109.43° 90.00°	Depositor
Resolution (Å)	48.54 – 2.40 48.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-2.40) 99.9 (48.54-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.202 , 0.241 0.230 , 0.273	Depositor DCC
R_{free} test set	8805 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.046 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31986	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: FE, PE3, TRS, GOL, ACT, 9S8, SF4, FES, NFU, FAD, COM

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	0.59	0/5062	0.96	4/6841 (0.1%)
1	G	0.54	0/5071	0.96	6/6853 (0.1%)
2	B	0.46	0/2277	0.87	0/3070
2	H	0.48	0/2277	0.89	0/3070
3	C	0.51	0/1447	0.88	1/1946 (0.1%)
3	I	0.51	0/1437	0.86	0/1934
4	D	0.64	0/1123	1.03	1/1508 (0.1%)
4	J	0.51	0/1132	0.97	2/1520 (0.1%)
5	E	0.57	0/2288	0.96	3/3102 (0.1%)
5	K	0.51	0/2299	0.95	3/3116 (0.1%)
6	F	0.54	0/3590	0.97	6/4853 (0.1%)
6	L	0.51	0/3590	0.97	6/4853 (0.1%)
All	All	0.54	0/31593	0.95	32/42666 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	275	TYR	N-CA-C	7.41	118.39	108.38
5	E	176	LEU	N-CA-C	7.15	119.98	111.33
5	K	176	LEU	N-CA-C	7.04	119.84	111.33
6	L	397	VAL	N-CA-C	6.76	118.28	107.73
1	G	93	LEU	N-CA-C	-6.37	105.08	112.92
6	L	79	VAL	N-CA-C	-6.33	104.58	110.53
6	L	9	VAL	N-CA-C	-6.30	100.64	109.21
6	F	79	VAL	N-CA-C	-6.28	104.63	110.53
5	K	178	GLU	CB-CG-CD	6.17	123.10	112.60
1	A	275	TYR	N-CA-C	6.14	116.67	108.38
1	A	430	ILE	N-CA-C	-5.74	100.04	108.54
6	F	80	PHE	N-CA-C	-5.69	100.02	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	397	VAL	N-CA-C	5.68	116.59	107.73
6	L	80	PHE	N-CA-C	-5.63	100.12	109.46
6	L	44	PHE	CA-CB-CG	5.55	119.35	113.80
1	G	199	LEU	N-CA-C	5.55	117.19	111.03
1	A	15	VAL	N-CA-C	-5.51	107.90	113.47
6	F	36	VAL	N-CA-C	5.51	116.81	111.91
1	A	13	CYS	N-CA-C	-5.50	103.79	111.39
5	E	19	LEU	N-CA-C	-5.45	105.34	111.28
4	J	32	PRO	N-CA-C	5.38	117.27	110.70
4	J	60	ASP	N-CA-C	-5.35	106.60	113.23
6	F	44	PHE	CA-CB-CG	5.31	119.11	113.80
1	G	193	ASP	N-CA-C	-5.31	103.88	110.41
1	G	193	ASP	CA-CB-CG	5.22	117.82	112.60
5	E	178	GLU	CB-CG-CD	5.21	121.46	112.60
6	F	290	ASN	CA-CB-CG	5.18	117.78	112.60
1	G	433	PHE	N-CA-C	5.14	119.82	113.50
6	L	207	GLU	N-CA-C	-5.13	105.38	111.69
5	K	264	ASN	N-CA-C	-5.12	104.86	111.71
3	C	66	ASP	CA-CB-CG	5.06	117.66	112.60
4	D	43	SER	N-CA-C	-5.04	106.40	112.54

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	4970	0	4967	43	0
1	G	4979	0	4974	40	0
2	B	2236	0	2244	13	0
2	H	2236	0	2243	12	1
3	C	1426	0	1441	8	0
3	I	1416	0	1435	8	0
4	D	1097	0	1068	7	0
4	J	1106	0	1074	10	0
5	E	2249	0	2252	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	2257	0	2265	14	0
6	F	3521	0	3503	14	0
6	L	3521	0	3503	14	0
7	A	4	0	3	1	0
7	D	4	0	3	0	0
7	G	4	0	3	0	0
8	A	53	0	31	0	0
8	G	53	0	31	0	0
9	A	48	0	0	0	0
9	C	16	0	0	0	0
9	E	24	0	0	0	0
9	G	48	0	0	1	0
9	I	16	0	0	0	0
9	K	24	0	0	0	0
10	A	12	0	16	0	0
10	G	6	0	8	0	0
10	H	6	0	8	0	0
10	K	6	0	8	0	0
11	B	16	0	0	0	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	2	0
15	L	8	0	0	1	0
16	F	1	0	0	0	0
16	L	1	0	0	0	0
17	G	14	0	16	0	0
18	A	125	0	0	1	0
18	B	14	0	0	0	0
18	C	19	0	0	0	0
18	D	36	0	0	1	0
18	E	49	0	0	0	0
18	F	65	0	0	0	0
18	G	87	0	0	1	0
18	H	23	0	0	0	0
18	I	27	0	0	0	0
18	J	5	0	0	0	0
18	K	42	0	0	0	0
18	L	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31986	0	31120	170	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 3.

All (170) 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:442:CYS:SG	6:F:445:CYS:HB2	2.00	1.02
11:H:302:9S8:S5	12:H:303:COM:S1	2.75	0.84
1:G:187:LYS:HD2	1:G:413:LEU:HD11	1.60	0.84
1:G:596:TYR:OH	4:J:74:TYR:HA	1.79	0.82
1:G:595:PRO:CG	4:J:74:TYR:O	2.27	0.82
1:G:194:CYS:HB2	1:G:197:CYS:SG	2.21	0.80
6:L:442:CYS:SG	6:L:445:CYS:HB2	2.21	0.80
5:E:109:LYS:HE3	5:E:121:ILE:HD11	1.64	0.78
2:H:145:ILE:HD12	2:H:287:LEU:HD11	1.67	0.77
1:A:623:CYS:SG	1:A:624:PRO:HD3	2.25	0.76
1:A:587:CYS:SG	1:A:589:VAL:HG23	2.28	0.74
1:G:595:PRO:HG2	4:J:74:TYR:O	1.88	0.74
6:F:442:CYS:HB3	15:F:501:NFU:N2	2.05	0.72
1:G:592:LYS:HB2	5:K:262:ILE:HG12	1.73	0.71
1:G:359:ILE:HG21	1:G:413:LEU:HD23	1.79	0.64
1:G:592:LYS:CB	5:K:262:ILE:HG12	2.27	0.64
1:G:595:PRO:HG3	4:J:74:TYR:O	1.96	0.62
5:K:277:ILE:O	5:K:280:LYS:NZ	2.33	0.61
4:D:68:HIS:HA	4:D:106:TRP:HB3	1.83	0.59
1:G:400:SER:HB2	1:G:403:CYS:SG	2.43	0.59
1:A:74:ARG:HD3	18:D:309:HOH:O	2.02	0.59
3:C:19:GLY:HA3	3:C:28:VAL:HG21	1.85	0.59
3:I:19:GLY:HA3	3:I:28:VAL:HG21	1.85	0.58
1:A:92:PHE:CZ	1:A:574:PRO:HD2	2.37	0.58
3:C:157:LEU:C	3:C:157:LEU:HD23	2.28	0.58
4:J:90:GLU:HB2	5:K:280:LYS:HE2	1.86	0.57
1:A:188:THR:HG23	1:A:195:SER:HB2	1.86	0.57
4:J:68:HIS:HA	4:J:106:TRP:HB3	1.84	0.57
6:F:410:VAL:HG22	6:F:432:MET:HE2	1.87	0.56
1:G:587:CYS:SG	1:G:589:VAL:HG23	2.45	0.56
2:B:78:CYS:SG	2:B:232:PRO:HD2	2.46	0.56
6:F:220:PHE:CE2	6:F:222:SER:HB3	2.40	0.55
6:L:435:LEU:C	6:L:435:LEU:HD13	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:CYS:SG	2:H:43:PRO:C	2.91	0.53
2:H:78:CYS:SG	2:H:232:PRO:HD2	2.49	0.53
4:D:10:GLY:HA2	4:D:63:PHE:O	2.09	0.53
2:H:154:HIS:ND1	12:H:303:COM:S1	2.80	0.52
1:G:579:VAL:HG22	1:G:632:LEU:CD2	2.39	0.52
1:G:153:VAL:HG22	1:G:551:VAL:HG22	1.92	0.52
6:F:435:LEU:C	6:F:435:LEU:HD13	2.34	0.52
5:E:106:LYS:HA	5:E:110:THR:OG1	2.10	0.51
2:B:11:MET:HG3	2:B:18:VAL:HB	1.91	0.51
2:H:11:MET:HG3	2:H:18:VAL:HB	1.91	0.51
5:K:70:LYS:O	5:K:74:GLU:HG3	2.11	0.51
1:A:512:ARG:O	4:D:110:SER:HB3	2.11	0.51
5:E:64:GLU:HG2	5:E:127:PRO:HB3	1.92	0.51
2:B:53:GLN:NE2	3:C:23:PRO:HD3	2.25	0.50
2:B:42:CYS:SG	2:B:43:PRO:C	2.94	0.50
4:D:16:CYS:HB2	4:D:67:CYS:SG	2.52	0.50
2:B:158:PRO:HG3	3:C:81:TYR:CD2	2.47	0.49
1:A:434:SER:HB3	1:A:437:TYR:CE1	2.47	0.49
3:I:121:VAL:O	3:I:125:GLY:HA2	2.12	0.49
6:L:375:ARG:C	6:L:398:ALA:HB1	2.38	0.49
1:A:406:TYR:C	1:A:406:TYR:CD1	2.91	0.49
1:G:10:VAL:HA	1:G:69:ALA:HB3	1.95	0.48
1:G:77:GLU:N	1:G:78:PRO:CD	2.76	0.48
5:E:105:ASP:O	5:E:109:LYS:HB2	2.13	0.48
1:G:575:ILE:HD12	4:J:41:MET:HG3	1.94	0.48
5:K:41:LEU:HD13	6:L:129:LEU:HD21	1.95	0.48
3:C:157:LEU:HD23	3:C:157:LEU:O	2.13	0.48
1:G:579:VAL:HG22	1:G:632:LEU:HD23	1.95	0.48
5:K:64:GLU:HG3	5:K:127:PRO:HB3	1.96	0.48
3:C:121:VAL:O	3:C:125:GLY:HA2	2.13	0.48
6:F:442:CYS:SG	6:F:445:CYS:CB	2.89	0.48
2:H:51:PHE:CZ	3:I:114:HIS:HB3	2.49	0.48
1:A:8:VAL:O	1:A:39:ALA:HA	2.14	0.47
1:A:305:PRO:O	1:A:306:ASN:OD1	2.31	0.47
1:A:587:CYS:SG	1:A:589:VAL:CG2	3.00	0.47
1:G:92:PHE:CD2	1:G:135:LEU:HB2	2.49	0.47
6:F:442:CYS:HB3	15:F:501:NFU:C2	2.43	0.47
1:A:47:ALA:HA	1:G:200:ALA:HB1	1.96	0.47
1:G:612:VAL:CG1	1:G:617:CYS:SG	3.02	0.47
2:H:113:TYR:CE2	2:H:115:GLY:HA2	2.49	0.47
1:A:623:CYS:SG	1:A:632:LEU:HD13	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:HB2	1:A:403:CYS:SG	2.54	0.47
4:D:63:PHE:CD2	4:D:63:PHE:C	2.92	0.47
5:K:85:CYS:SG	5:K:90:GLY:HA3	2.55	0.47
4:D:17:THR:HG21	4:D:65:GLY:HA3	1.96	0.47
1:G:196:ILE:HG23	1:G:200:ALA:HB2	1.96	0.47
2:B:145:ILE:HD13	2:B:287:LEU:HD11	1.97	0.47
6:F:290:ASN:HB3	6:F:375:ARG:C	2.40	0.47
1:G:623:CYS:SG	1:G:624:PRO:HD3	2.55	0.47
1:A:437:TYR:CD1	1:A:437:TYR:N	2.83	0.46
5:K:228:CYS:HB2	5:K:229:PRO:HD3	1.96	0.46
2:B:113:TYR:CE2	2:B:115:GLY:HA2	2.50	0.46
2:B:263:LEU:C	2:B:263:LEU:HD13	2.41	0.46
1:G:71:CYS:O	1:G:96:PHE:CE1	2.69	0.46
1:G:69:ALA:HA	1:G:97:ALA:HB3	1.97	0.46
1:A:437:TYR:N	1:A:437:TYR:HD1	2.14	0.46
6:L:13:GLU:HB3	6:L:442:CYS:HA	1.98	0.46
1:G:209:HIS:HB3	1:G:212:VAL:HB	1.97	0.45
6:L:64:CYS:CB	15:L:501:NFU:C1	2.94	0.45
5:E:228:CYS:HB2	5:E:229:PRO:HD3	1.98	0.45
1:A:209:HIS:HB3	1:A:212:VAL:HB	1.98	0.45
6:F:328:HIS:CE1	6:F:438:ALA:HA	2.51	0.45
6:L:328:HIS:CE1	6:L:438:ALA:HA	2.51	0.45
1:G:612:VAL:HG11	1:G:617:CYS:SG	2.57	0.45
1:A:197:CYS:SG	1:G:44:TYR:CD1	3.10	0.45
6:L:14:GLY:HA3	6:L:443:LEU:HB2	1.97	0.45
6:F:13:GLU:HB3	6:F:442:CYS:HA	1.99	0.44
1:G:389:SER:O	1:G:390:ARG:C	2.58	0.44
6:L:106:LEU:HD12	6:L:110:MET:SD	2.57	0.44
1:A:515:ASP:O	1:A:516:GLN:HB2	2.18	0.44
1:A:188:THR:CG2	1:A:195:SER:HB2	2.47	0.44
1:A:189:PHE:C	1:A:189:PHE:CD1	2.96	0.44
1:A:305:PRO:O	1:A:306:ASN:CG	2.60	0.44
1:A:458:SER:HB2	3:I:43:SER:OG	2.18	0.44
2:B:43:PRO:HB2	2:B:48:PHE:CD1	2.53	0.44
5:K:15:CYS:SG	5:K:83:GLY:HA3	2.58	0.44
1:A:181:ARG:O	1:A:184:GLN:N	2.47	0.44
1:A:406:TYR:C	1:A:406:TYR:HD1	2.26	0.44
6:F:14:GLY:HA3	6:F:443:LEU:HB2	1.98	0.44
1:A:69:ALA:HA	1:A:97:ALA:HB3	2.00	0.44
1:A:128:LYS:HB2	1:A:645:GLN:HG3	1.99	0.44
1:G:621:GLY:C	1:G:624:PRO:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:623:CYS:N	1:G:624:PRO:HD2	2.32	0.44
5:E:85:CYS:SG	5:E:90:GLY:HA3	2.58	0.43
1:A:77:GLU:HB3	1:A:78:PRO:HD3	2.00	0.43
6:L:77:ASP:O	6:L:80:PHE:O	2.36	0.43
2:B:121:HIS:O	2:B:124:GLU:HG3	2.19	0.43
1:A:106:VAL:HG23	1:A:107:HIS:CE1	2.53	0.43
1:A:124:MET:HE1	4:D:36:ARG:HB3	2.01	0.43
4:J:47:GLU:HB2	4:J:48:PRO:HD2	2.00	0.43
6:L:397:VAL:O	6:L:398:ALA:C	2.61	0.43
1:A:23:CYS:O	1:A:24:PRO:C	2.62	0.43
1:A:389:SER:O	1:A:390:ARG:C	2.61	0.43
3:C:116:MET:HE2	3:C:182:LEU:HD12	2.01	0.42
1:G:194:CYS:CB	1:G:197:CYS:SG	3.02	0.42
1:A:42:TYR:HB3	1:A:45:MET:SD	2.59	0.42
2:H:121:HIS:O	2:H:124:GLU:HG3	2.19	0.42
1:A:438:GLU:HG3	18:G:861:HOH:O	2.19	0.42
3:I:116:MET:HE2	3:I:182:LEU:HD12	2.00	0.42
1:A:417:LYS:HD3	7:A:701:ACT:H2	2.00	0.42
6:F:290:ASN:OD1	6:F:291:THR:HG23	2.19	0.42
2:B:154:HIS:ND1	12:B:303:COM:S1	2.89	0.42
5:E:203:ASP:OD1	5:E:204:PRO:HD2	2.19	0.42
1:G:592:LYS:HB3	5:K:262:ILE:HG12	2.01	0.42
1:G:400:SER:O	1:G:401:ASN:HB3	2.19	0.41
6:L:7:GLU:HA	6:L:8:PRO:HA	1.89	0.41
4:J:48:PRO:HD2	5:K:254:SER:HB2	2.02	0.41
1:A:175:THR:HB	1:A:176:PRO:CD	2.51	0.41
1:G:381:ILE:HG12	1:G:488:LEU:HB3	2.02	0.41
1:A:587:CYS:HB2	5:E:218:ILE:HG22	2.02	0.41
1:A:343:TYR:HB3	18:A:840:HOH:O	2.20	0.41
1:G:627:CYS:HB2	1:G:632:LEU:HD12	2.03	0.41
1:A:197:CYS:HB3	9:G:704:SF4:S4	2.60	0.41
3:C:31:LEU:HB3	3:C:96:ILE:HD13	2.03	0.41
3:I:31:LEU:HB3	3:I:96:ILE:HD13	2.03	0.41
2:H:53:GLN:HB3	3:I:22:ILE:HG22	2.03	0.41
2:H:158:PRO:O	2:H:162:LYS:HG2	2.20	0.41
5:K:253:ILE:O	5:K:254:SER:C	2.64	0.41
1:A:226:TYR:CD1	1:A:226:TYR:N	2.88	0.41
2:H:228:VAL:HA	2:H:258:LEU:O	2.21	0.41
4:J:16:CYS:SG	4:J:67:CYS:SG	3.18	0.41
5:E:21:ASP:HB3	5:E:153:PRO:HG3	2.03	0.41
1:G:189:PHE:HB2	1:G:190:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:409:GLY:O	6:L:413:VAL:HG23	2.21	0.41
1:A:77:GLU:N	1:A:78:PRO:CD	2.85	0.40
5:K:20:LEU:C	5:K:22:LEU:H	2.29	0.40
2:B:157:LYS:HA	2:B:158:PRO:C	2.47	0.40
2:B:228:VAL:HA	2:B:258:LEU:O	2.21	0.40
6:F:272:LEU:HD11	6:F:446:ALA:HB1	2.03	0.40
1:G:226:TYR:CD1	1:G:226:TYR:N	2.88	0.40
6:L:272:LEU:HD11	6:L:446:ALA:HB1	2.04	0.40
1:A:280:GLN:N	1:A:280:GLN:CD	2.80	0.40
1:A:197:CYS:SG	1:G:44:TYR:HD1	2.45	0.40
6:F:37:GLU:HG2	6:F:38:VAL:N	2.36	0.40
1:G:153:VAL:CG2	1:G:551:VAL:HG22	2.50	0.40
1:G:623:CYS:N	1:G:624:PRO:CD	2.84	0.40
2:H:38:GLY:HA3	3:I:156:ASP:OD2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:201:ASN:N	2:H:248:LYS:O[4_556]	2.11	0.09

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	649/654 (99%)	619 (95%)	29 (4%)	1 (0%)	43	58
1	G	650/654 (99%)	617 (95%)	33 (5%)	0	100	100
2	B	289/291 (99%)	275 (95%)	14 (5%)	0	100	100
2	H	289/291 (99%)	276 (96%)	13 (4%)	0	100	100
3	C	182/184 (99%)	178 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
4	D	135/140 (96%)	130 (96%)	5 (4%)	0	100	100
4	J	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
5	E	295/299 (99%)	279 (95%)	16 (5%)	0	100	100
5	K	296/299 (99%)	278 (94%)	18 (6%)	0	100	100
6	F	445/473 (94%)	421 (95%)	22 (5%)	2 (0%)	30	43
6	L	445/473 (94%)	421 (95%)	22 (5%)	2 (0%)	30	43
All	All	3992/4082 (98%)	3804 (95%)	183 (5%)	5 (0%)	48	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	398	ALA
6	L	398	ALA
6	L	291	THR
1	A	70	ALA
6	F	38	VAL

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	539/541 (100%)	534 (99%)	5 (1%)	70	85
1	G	540/541 (100%)	529 (98%)	11 (2%)	48	70
2	B	242/242 (100%)	241 (100%)	1 (0%)	84	92
2	H	242/242 (100%)	238 (98%)	4 (2%)	53	74
3	C	157/157 (100%)	153 (98%)	4 (2%)	42	64
3	I	156/157 (99%)	152 (97%)	4 (3%)	40	63
4	D	116/119 (98%)	116 (100%)	0	100	100
4	J	117/119 (98%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	254/256 (99%)	251 (99%)	3 (1%)	63	81
5	K	255/256 (100%)	250 (98%)	5 (2%)	48	70
6	F	386/410 (94%)	381 (99%)	5 (1%)	61	80
6	L	386/410 (94%)	378 (98%)	8 (2%)	47	69
All	All	3390/3450 (98%)	3340 (98%)	50 (2%)	57	77

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	SER
1	A	403	CYS
1	A	406	TYR
1	A	513	THR
1	A	607	LYS
2	B	42	CYS
3	C	35	TYR
3	C	49	ARG
3	C	66	ASP
3	C	102	ASN
5	E	8	TRP
5	E	111	THR
5	E	238	CYS
6	F	65	GLN
6	F	102	HIS
6	F	290	ASN
6	F	315	LYS
6	F	435	LEU
1	G	5	ARG
1	G	42	TYR
1	G	194	CYS
1	G	359	ILE
1	G	403	CYS
1	G	413	LEU
1	G	420	ASP
1	G	513	THR
1	G	579	VAL
1	G	617	CYS
1	G	651	ARG
2	H	42	CYS
2	H	87	GLU
2	H	125	LEU

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Mol	Chain	Res	Type
2	H	211	MET
3	I	35	TYR
3	I	49	ARG
3	I	77	CYS
3	I	102	ASN
5	K	8	TRP
5	K	77	LYS
5	K	111	THR
5	K	235	CYS
5	K	238	CYS
6	L	65	GLN
6	L	102	HIS
6	L	283	GLU
6	L	290	ASN
6	L	351	ILE
6	L	368	VAL
6	L	435	LEU
6	L	445	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	229	ASN
1	A	251	GLN
1	A	401	ASN
1	A	459	GLN
2	B	213	ASN
2	B	262	GLN
3	C	109	ASN
5	E	37	HIS
5	E	248	GLN
5	E	264	ASN
1	G	12	HIS
1	G	229	ASN
1	G	292	HIS
1	G	401	ASN
2	H	262	GLN
3	I	106	GLN
3	I	109	ASN
5	K	37	HIS
5	K	248	GLN

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Mol	Chain	Res	Type
5	K	264	ASN
6	L	78	ASN
6	L	394	ASN

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 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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	$\# Z > 2$
9	SF4	G	709	1	0,12,12	-	-	-		
10	GOL	G	710	-	5,5,5	0.33	0	5,5,5	0.46	0
11	9S8	B	302	2	4,10,10	7.00	2 (50%)	-		
11	9S8	B	301	2	4,10,10	6.66	2 (50%)	-		
9	SF4	K	303	5	0,12,12	-	-	-		
7	ACT	D	202	-	3,3,3	1.08	0	3,3,3	1.06	0
17	PE3	G	701	-	13,13,42	0.58	0	12,12,41	0.25	0
9	SF4	C	201	3	0,12,12	-	-	-		
8	FAD	G	703	-	58,58,58	1.51	10 (17%)	85,89,89	1.60	17 (20%)
9	SF4	K	301	5	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SF4	I	201	3	0,12,12	-	-	-		
12	COM	H	303	-	6,6,6	1.40	2 (33%)	8,8,8	2.87	4 (50%)
14	TRS	D	203	-	7,7,7	0.42	0	9,9,9	0.71	0
7	ACT	G	702	-	3,3,3	1.22	0	3,3,3	0.91	0
7	ACT	A	701	-	3,3,3	1.07	0	3,3,3	1.07	0
9	SF4	A	703	1	0,12,12	-	-	-		
9	SF4	A	705	1	0,12,12	-	-	-		
9	SF4	A	708	1	0,12,12	-	-	-		
9	SF4	K	302	5	0,12,12	-	-	-		
9	SF4	A	707	1	0,12,12	-	-	-		
8	FAD	A	702	-	58,58,58	1.57	11 (18%)	85,89,89	1.64	20 (23%)
10	GOL	H	304	-	5,5,5	0.35	0	5,5,5	0.15	0
15	NFU	L	501	6	2,7,7	0.95	0	-		
9	SF4	G	708	1	0,12,12	-	-	-		
9	SF4	G	704	1	0,12,12	-	-	-		
10	GOL	A	709	-	5,5,5	0.39	0	5,5,5	0.39	0
9	SF4	G	705	1	0,12,12	-	-	-		
11	9S8	H	302	2	4,10,10	7.23	2 (50%)	-		
15	NFU	F	501	6	2,7,7	1.49	0	-		
13	FES	D	201	4	0,4,4	-	-	-		
9	SF4	I	202	3	0,12,12	-	-	-		
9	SF4	C	202	3	0,12,12	-	-	-		
9	SF4	E	301	5	0,12,12	-	-	-		
9	SF4	G	707	1	0,12,12	-	-	-		
9	SF4	E	302	5	0,12,12	-	-	-		
11	9S8	H	301	2	4,10,10	6.03	3 (75%)	-		
9	SF4	A	706	1	0,12,12	-	-	-		
10	GOL	K	304	-	5,5,5	0.44	0	5,5,5	0.37	0
9	SF4	E	303	5	0,12,12	-	-	-		
13	FES	J	200	4	0,4,4	-	-	-		
10	GOL	A	710	-	5,5,5	0.36	0	5,5,5	0.48	0
9	SF4	A	704	1	0,12,12	-	-	-		
12	COM	B	303	-	6,6,6	1.43	2 (33%)	8,8,8	2.49	4 (50%)
9	SF4	G	706	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
9	SF4	G	709	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	G	710	-	-	4/4/4/4	-
11	9S8	B	302	2	-	-	0/3/3/3
11	9S8	B	301	2	-	-	0/3/3/3
9	SF4	K	303	5	-	-	0/6/5/5
17	PE3	G	701	-	-	6/11/11/40	-
9	SF4	C	201	3	-	-	0/6/5/5
12	COM	H	303	-	-	3/4/4/4	-
8	FAD	G	703	-	-	1/34/50/50	0/6/6/6
9	SF4	I	201	3	-	-	0/6/5/5
9	SF4	K	301	5	-	-	0/6/5/5
14	TRS	D	203	-	-	3/9/9/9	-
9	SF4	A	703	1	-	-	0/6/5/5
9	SF4	A	705	1	-	-	0/6/5/5
9	SF4	A	708	1	-	-	0/6/5/5
9	SF4	K	302	5	-	-	0/6/5/5
9	SF4	A	707	1	-	-	0/6/5/5
8	FAD	A	702	-	-	4/34/50/50	0/6/6/6
10	GOL	H	304	-	-	0/4/4/4	-
9	SF4	G	708	1	-	-	0/6/5/5
9	SF4	G	704	1	-	-	0/6/5/5
10	GOL	A	709	-	-	3/4/4/4	-
9	SF4	G	705	1	-	-	0/6/5/5
11	9S8	H	302	2	-	-	0/3/3/3
13	FES	D	201	4	-	-	0/1/1/1
9	SF4	I	202	3	-	-	0/6/5/5
9	SF4	C	202	3	-	-	0/6/5/5
9	SF4	E	301	5	-	-	0/6/5/5
9	SF4	G	707	1	-	-	0/6/5/5
9	SF4	E	302	5	-	-	0/6/5/5
11	9S8	H	301	2	-	-	0/3/3/3
9	SF4	A	706	1	-	-	0/6/5/5
10	GOL	K	304	-	-	2/4/4/4	-
9	SF4	E	303	5	-	-	0/6/5/5
13	FES	J	200	4	-	-	0/1/1/1
10	GOL	A	710	-	-	2/4/4/4	-
9	SF4	A	704	1	-	-	0/6/5/5
12	COM	B	303	-	-	1/4/4/4	-
9	SF4	G	706	1	-	-	0/6/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	302	9S8	S1-FE4	-11.25	2.10	2.28
11	B	302	9S8	S1-FE4	-10.28	2.12	2.28
11	B	301	9S8	S1-FE4	-9.83	2.12	2.28
11	B	302	9S8	S7-FE4	-9.35	2.13	2.28
11	H	302	9S8	S7-FE4	-9.00	2.14	2.28
11	B	301	9S8	S7-FE4	-8.89	2.14	2.28
11	H	301	9S8	S1-FE4	-8.67	2.14	2.28
11	H	301	9S8	S7-FE4	-8.05	2.15	2.28
8	A	702	FAD	C9A-C5X	6.01	1.50	1.41
8	G	703	FAD	C9A-C5X	5.89	1.50	1.41
8	A	702	FAD	C5A-C4A	4.57	1.47	1.39
8	G	703	FAD	C5A-C4A	4.43	1.47	1.39
8	A	702	FAD	C8-C7	3.51	1.49	1.40
8	G	703	FAD	C8-C7	3.35	1.49	1.40
8	A	702	FAD	P-O3P	2.70	1.62	1.59
8	A	702	FAD	C5A-C6A	2.64	1.48	1.41
8	A	702	FAD	C4-N3	-2.63	1.33	1.38
8	A	702	FAD	PA-O3P	2.59	1.62	1.59
8	G	703	FAD	C4-N3	-2.56	1.34	1.38
8	G	703	FAD	C5A-N7A	-2.54	1.34	1.39
8	A	702	FAD	C5A-N7A	-2.45	1.34	1.39
8	G	703	FAD	C5A-C6A	2.44	1.47	1.41
8	G	703	FAD	C4X-N5	2.41	1.36	1.30
8	A	702	FAD	C5X-N5	-2.40	1.35	1.39
12	B	303	COM	O1S-S2	2.38	1.51	1.45
8	G	703	FAD	C8A-N7A	2.28	1.36	1.31
12	H	303	COM	O2S-S2	2.18	1.51	1.45
12	H	303	COM	O1S-S2	2.18	1.51	1.45
8	G	703	FAD	C5X-N5	-2.18	1.35	1.39
12	B	303	COM	O2S-S2	2.17	1.51	1.45
11	H	301	9S8	S3-FE4	-2.09	2.20	2.24
8	A	702	FAD	C4X-N5	2.07	1.35	1.30
8	G	703	FAD	PA-O3P	2.03	1.61	1.59
8	A	702	FAD	C8A-N7A	2.01	1.35	1.31

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	702	FAD	C5A-C4A-N3A	-5.55	119.08	126.72
8	G	703	FAD	C5A-C4A-N3A	-5.49	119.16	126.72
12	H	303	COM	O3S-S2-O2S	-5.03	98.82	111.40
8	A	702	FAD	N3A-C4A-N9A	4.81	135.35	127.17
8	G	703	FAD	N3A-C4A-N9A	4.67	135.10	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	303	COM	O3S-S2-O2S	-4.58	99.94	111.40
12	H	303	COM	O2S-S2-C2	4.24	113.13	106.73
12	H	303	COM	O3S-S2-C2	3.84	113.53	106.00
8	G	703	FAD	N3A-C2A-N1A	-3.78	122.85	128.58
8	A	702	FAD	C2A-N3A-C4A	3.71	120.90	111.83
8	G	703	FAD	C2A-N3A-C4A	3.63	120.69	111.83
8	A	702	FAD	N3A-C2A-N1A	-3.59	123.14	128.58
8	G	703	FAD	C4A-N9A-C8A	3.51	109.42	105.74
12	B	303	COM	O2S-S2-C2	3.42	111.89	106.73
8	G	703	FAD	C4A-C5A-N7A	-3.41	106.69	110.58
12	B	303	COM	O3S-S2-C2	3.22	112.30	106.00
8	G	703	FAD	O4-C4-C4X	-3.14	118.24	126.53
8	A	702	FAD	C4A-N9A-C8A	3.09	108.98	105.74
8	A	702	FAD	C4A-C5A-N7A	-2.98	107.17	110.58
8	G	703	FAD	C5A-N7A-C8A	2.94	108.07	103.45
8	G	703	FAD	N9A-C8A-N7A	-2.71	110.09	113.94
8	A	702	FAD	C5A-N7A-C8A	2.67	107.65	103.45
8	A	702	FAD	O4-C4-C4X	-2.64	119.56	126.53
8	A	702	FAD	O4'-C4'-C5'	-2.54	104.38	109.99
8	A	702	FAD	C4-C4X-N5	2.52	121.69	118.21
8	G	703	FAD	C4X-C4-N3	2.42	119.42	113.25
8	G	703	FAD	C9A-C5X-N5	-2.39	119.92	122.45
8	G	703	FAD	C2A-N1A-C6A	2.36	122.61	118.73
8	A	702	FAD	C4X-C10-N1	-2.34	118.85	124.59
8	A	702	FAD	N9A-C8A-N7A	-2.33	110.63	113.94
8	A	702	FAD	O4B-C1B-N9A	2.31	112.53	108.09
12	H	303	COM	O1S-S2-C2	2.31	110.22	106.73
8	A	702	FAD	O2-C2-N1	-2.25	118.07	121.80
8	A	702	FAD	C4X-C4-N3	2.21	118.89	113.25
12	B	303	COM	O1S-S2-C2	2.21	110.07	106.73
8	G	703	FAD	C4-N3-C2	-2.19	121.76	125.64
8	A	702	FAD	C5X-C9A-N10	2.16	119.92	117.97
8	A	702	FAD	C9A-C5X-N5	-2.16	120.17	122.45
8	A	702	FAD	C4X-C10-N10	2.15	119.56	116.48
8	G	703	FAD	C4X-C10-N1	-2.15	119.32	124.59
8	A	702	FAD	C4-N3-C2	-2.07	121.97	125.64
8	G	703	FAD	C4-C4X-N5	2.05	121.04	118.21
8	G	703	FAD	C5X-C9A-N10	2.05	119.82	117.97
8	A	702	FAD	C10-N1-C2	2.03	121.23	116.85
8	G	703	FAD	C6A-C5A-N7A	2.02	135.99	132.09

There are no chirality outliers.

All (29) torsion outliers are listed below:

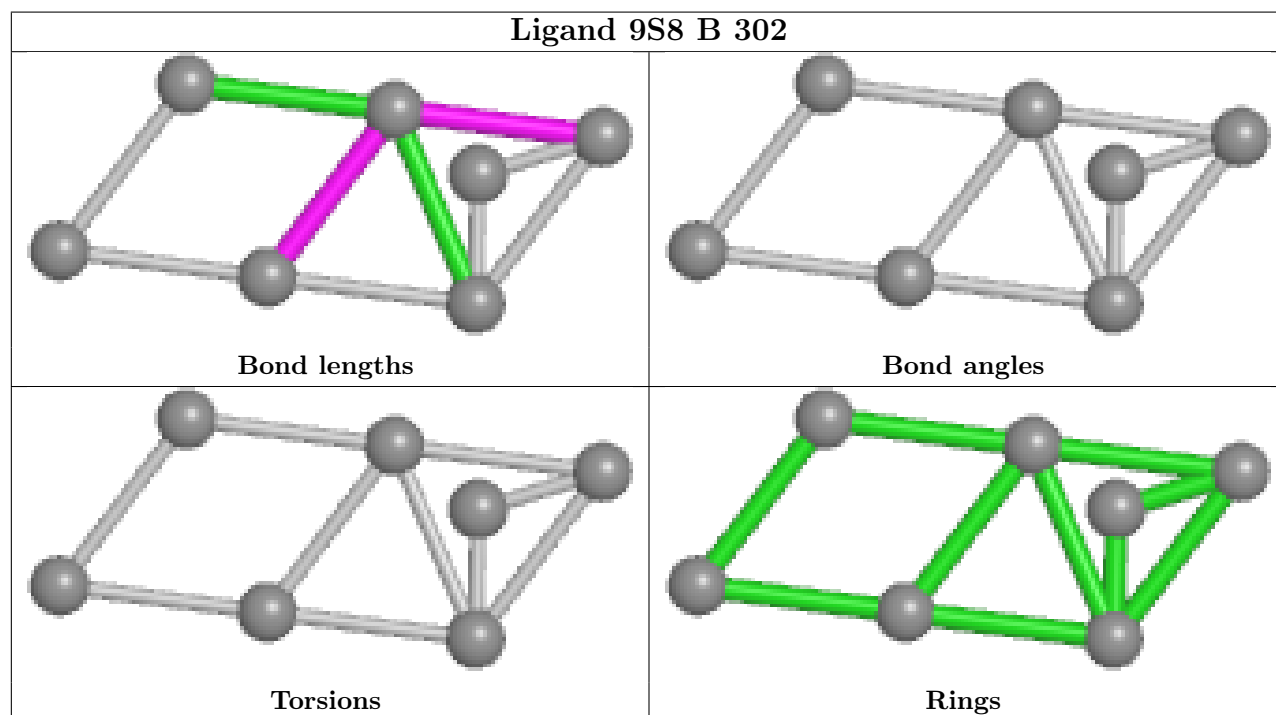
Mol	Chain	Res	Type	Atoms
10	A	709	GOL	C1-C2-C3-O3
10	G	710	GOL	O1-C1-C2-O2
10	G	710	GOL	O1-C1-C2-C3
10	K	304	GOL	C1-C2-C3-O3
12	H	303	COM	C1-C2-S2-O2S
14	D	203	TRS	C2-C-C1-O1
14	D	203	TRS	C3-C-C1-O1
14	D	203	TRS	N-C-C1-O1
17	G	701	PE3	O34-C35-C36-O37
10	A	709	GOL	O1-C1-C2-C3
10	A	709	GOL	O2-C2-C3-O3
10	K	304	GOL	O2-C2-C3-O3
8	A	702	FAD	P-O3P-PA-O5B
17	G	701	PE3	C39-C38-O37-C36
17	G	701	PE3	C36-C35-O34-C33
8	A	702	FAD	C2B-C1B-N9A-C8A
17	G	701	PE3	O31-C32-C33-O34
17	G	701	PE3	C35-C36-O37-C38
8	A	702	FAD	C5'-O5'-P-O1P
12	H	303	COM	S1-C1-C2-S2
12	H	303	COM	C1-C2-S2-O1S
17	G	701	PE3	C32-C33-O34-C35
10	A	710	GOL	O1-C1-C2-C3
10	G	710	GOL	C1-C2-C3-O3
8	G	703	FAD	O4B-C4B-C5B-O5B
10	A	710	GOL	O1-C1-C2-O2
10	G	710	GOL	O2-C2-C3-O3
12	B	303	COM	C1-C2-S2-O3S
8	A	702	FAD	O4B-C1B-N9A-C8A

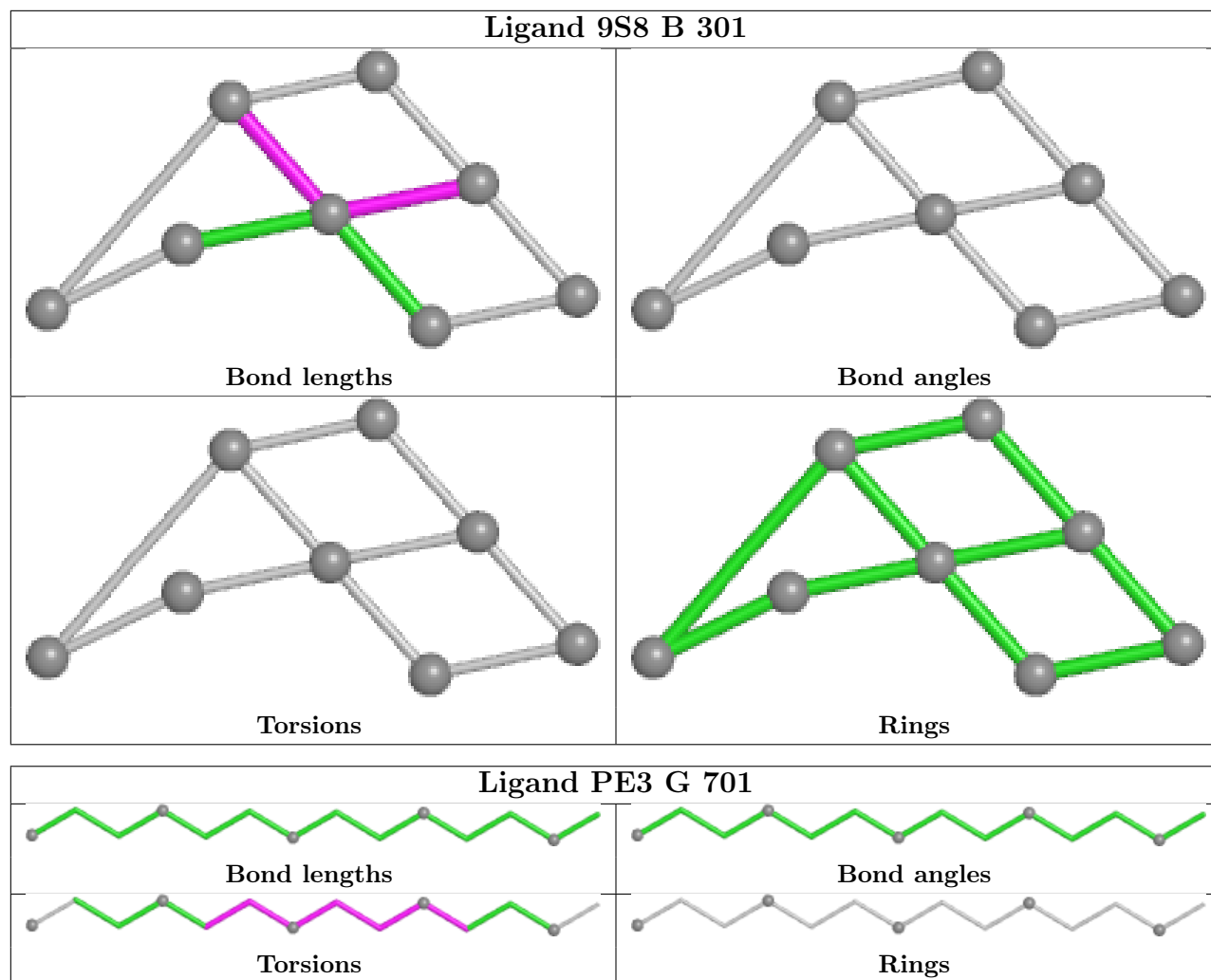
There are no ring outliers.

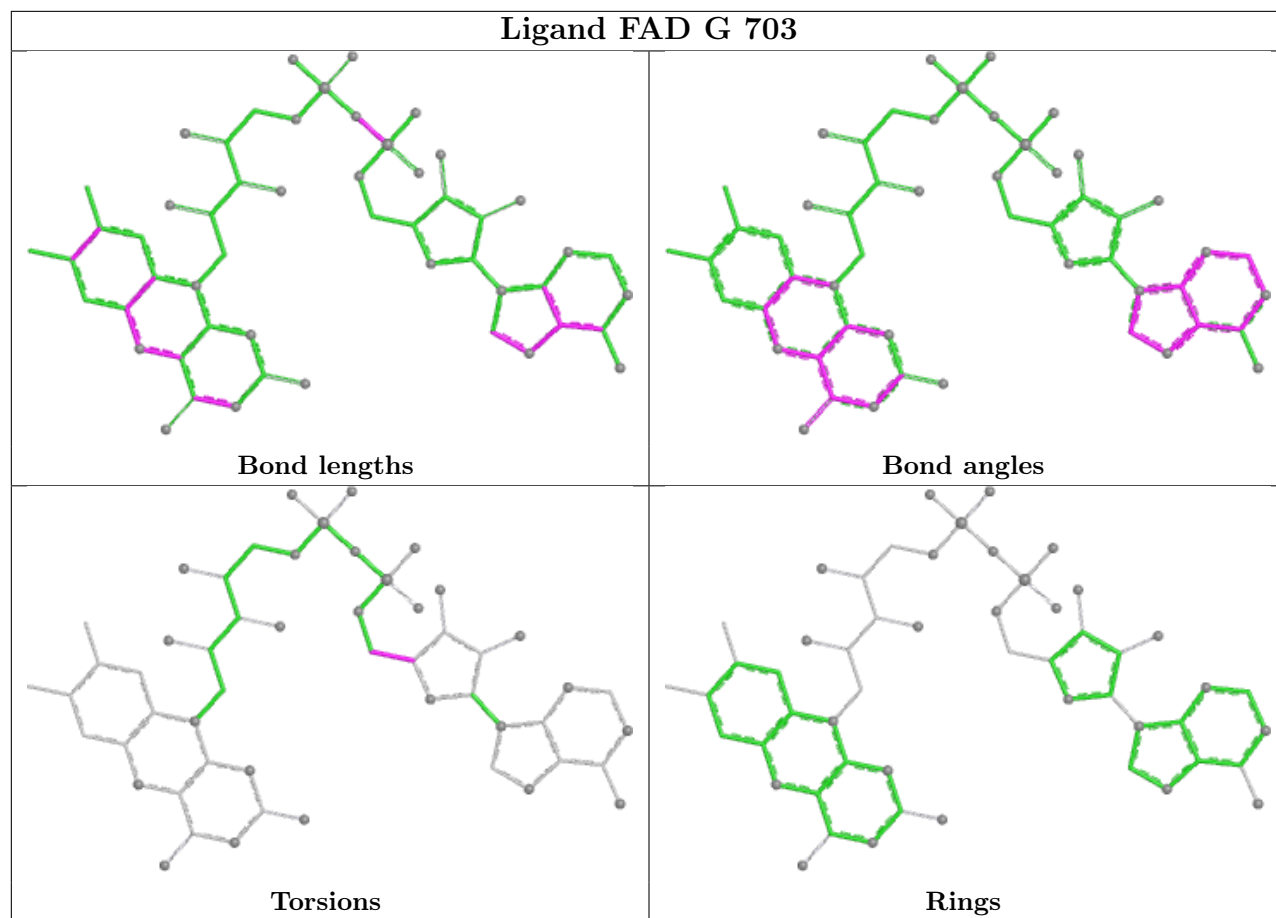
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	303	COM	2	0
7	A	701	ACT	1	0
15	L	501	NFU	1	0
9	G	704	SF4	1	0
11	H	302	9S8	1	0
15	F	501	NFU	2	0
12	B	303	COM	1	0

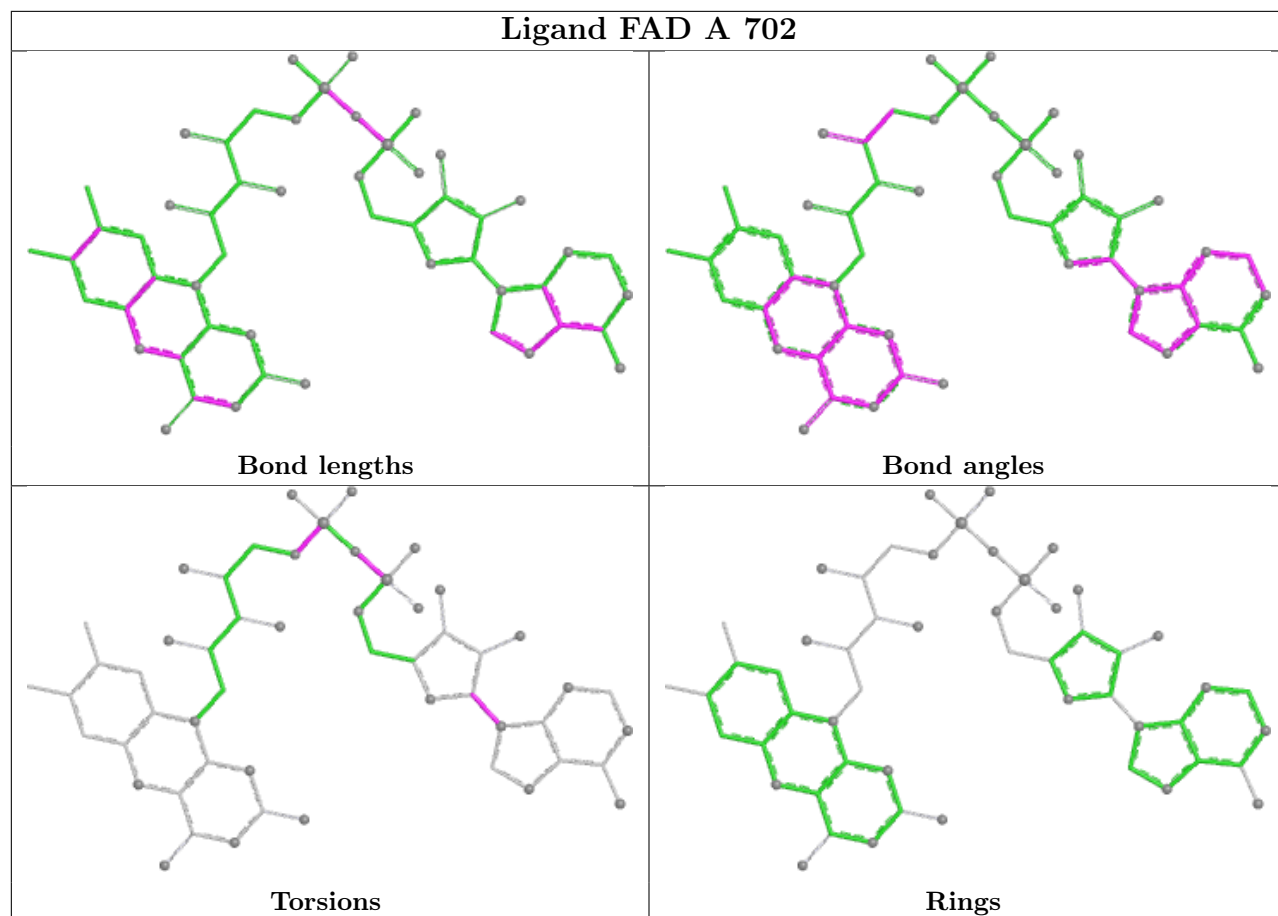
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



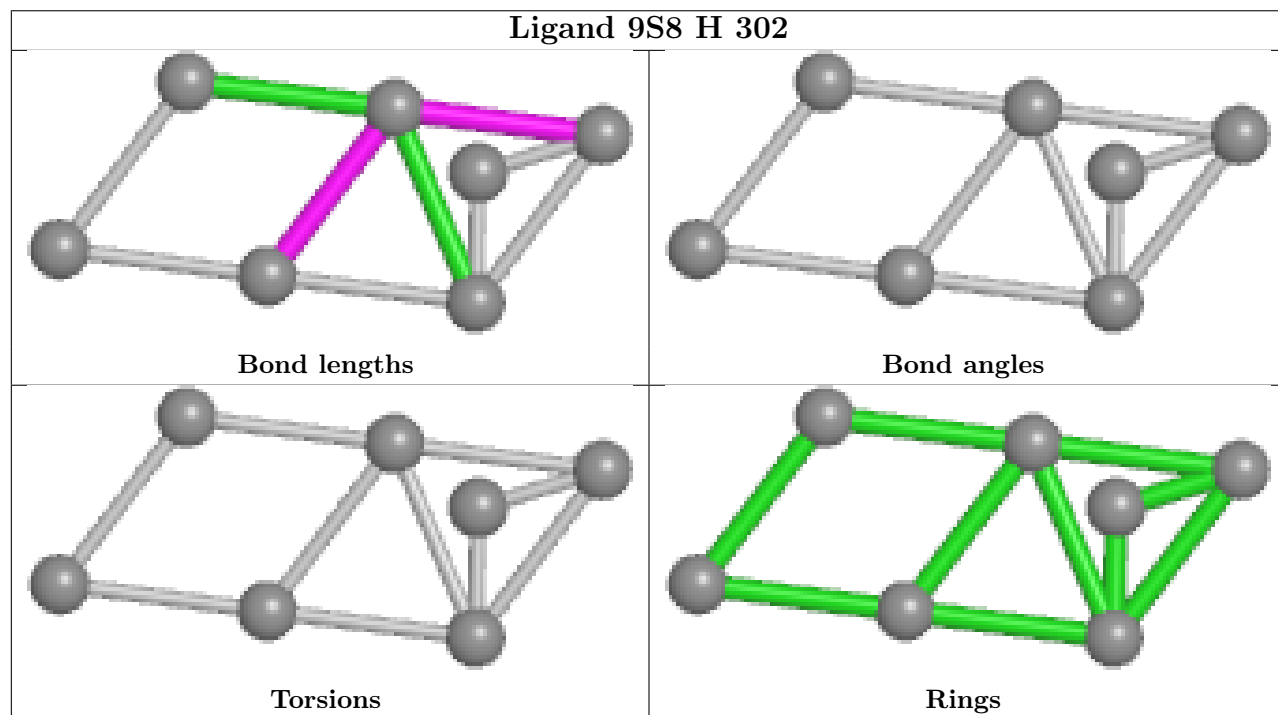


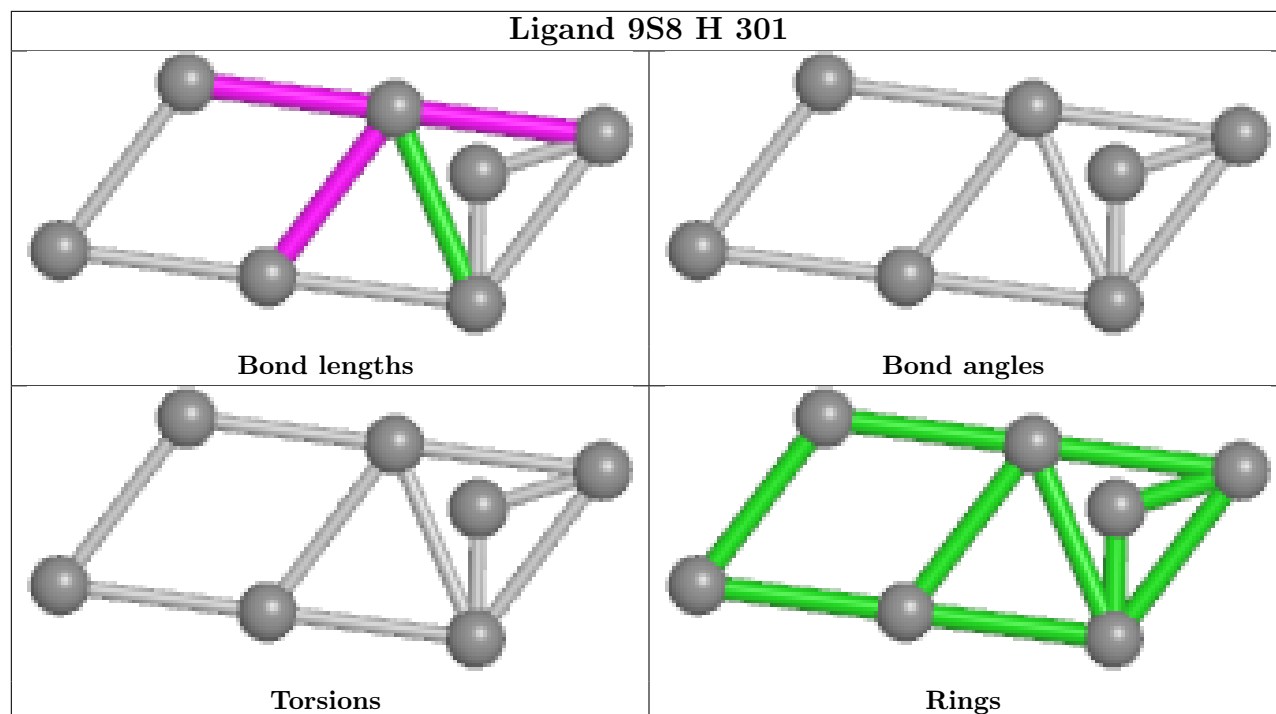


Ligand FAD A 702



Ligand 9S8 H 302





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	651/654 (99%)	0.06	19 (2%) 53 50	15, 43, 106, 161	0
1	G	652/654 (99%)	0.76	84 (12%) 7 5	23, 64, 144, 221	0
2	B	291/291 (100%)	1.48	73 (25%) 1 1	41, 93, 144, 165	0
2	H	291/291 (100%)	0.60	12 (4%) 41 37	37, 68, 105, 132	0
3	C	184/184 (100%)	0.77	27 (14%) 6 4	22, 60, 141, 156	0
3	I	183/184 (99%)	0.31	2 (1%) 78 74	26, 51, 93, 123	0
4	D	137/140 (97%)	-0.38	0 100 100	21, 37, 64, 118	0
4	J	138/140 (98%)	1.14	16 (11%) 9 7	47, 67, 97, 202	0
5	E	297/299 (99%)	-0.04	1 (0%) 90 88	19, 42, 76, 92	0
5	K	297/299 (99%)	0.76	34 (11%) 10 7	28, 62, 122, 165	1 (0%)
6	F	447/473 (94%)	0.22	7 (1%) 70 66	26, 52, 85, 102	0
6	L	447/473 (94%)	0.73	39 (8%) 16 13	28, 66, 139, 177	0
All	All	4015/4082 (98%)	0.52	314 (7%) 19 15	15, 58, 123, 221	1 (0%)

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	5	PHE	6.2
2	B	135	ILE	6.2
1	G	308	ILE	5.2
2	B	10	ILE	5.1
1	G	601	LEU	5.0
2	B	249	PHE	4.9
1	G	302	VAL	4.8
2	B	266	LEU	4.6
2	B	287	LEU	4.4
2	B	77	VAL	4.3
2	B	288	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
6	L	356	ILE	4.2
1	G	610	ALA	4.2
1	G	612	VAL	4.2
1	G	300	ALA	4.1
2	B	291	ILE	4.1
1	G	307	ALA	4.0
3	C	143	LEU	4.0
1	G	595	PRO	3.9
1	G	609	VAL	3.9
6	L	185	LEU	3.8
1	G	297	GLY	3.8
2	B	26	MET	3.8
1	G	298	LEU	3.7
1	G	608	VAL	3.7
5	K	197	ASN	3.7
1	G	258	ILE	3.7
3	C	128	VAL	3.6
1	G	294	ILE	3.6
2	B	220	ILE	3.6
5	K	255	ALA	3.6
2	B	176	ILE	3.6
2	B	29	LEU	3.6
4	J	65	GLY	3.6
5	K	209	LEU	3.6
2	B	136	ALA	3.5
6	L	364	VAL	3.5
3	C	127	ALA	3.5
5	K	298	LEU	3.5
1	G	602	VAL	3.5
2	B	253	TYR	3.5
2	B	228	VAL	3.5
6	L	352	VAL	3.5
1	G	617	CYS	3.5
5	K	256	LEU	3.4
3	C	150	ALA	3.4
6	L	345	LEU	3.4
3	C	141	ILE	3.4
6	L	181	ARG	3.4
2	B	143	LEU	3.4
1	G	248	GLY	3.4
2	B	145	ILE	3.4
2	H	249	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	33	LEU	3.3
3	C	148	PRO	3.3
1	G	310	PHE	3.3
2	B	275	LEU	3.3
2	H	164	LEU	3.3
1	A	308	ILE	3.3
1	G	54	ILE	3.3
2	B	279	VAL	3.3
6	L	80	PHE	3.2
1	G	613	ILE	3.2
6	L	351	ILE	3.2
1	G	615	ALA	3.2
1	G	637	PHE	3.2
1	G	25	ASP	3.2
6	L	187	LEU	3.2
1	G	594	CYS	3.2
3	C	152	PHE	3.2
1	G	304	GLY	3.2
1	G	616	LEU	3.1
2	B	15	TYR	3.1
3	C	147	ALA	3.1
2	B	142	PRO	3.1
4	J	134	LEU	3.1
6	L	363	VAL	3.1
1	G	596	TYR	3.1
2	B	180	THR	3.1
5	K	273	LEU	3.1
2	B	147	VAL	3.1
6	F	2	VAL	3.1
1	G	593	GLN	3.1
1	A	301	LYS	3.1
2	B	248	LYS	3.1
6	L	353	GLY	3.1
2	B	270	MET	3.0
2	B	284	VAL	3.0
2	B	276	ALA	3.0
1	G	314	PRO	3.0
5	K	189	VAL	3.0
4	J	11	PHE	3.0
3	C	142	GLY	3.0
2	H	291	ILE	3.0
1	G	42	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	137	LEU	2.9
4	J	140	LYS	2.9
1	G	299	CYS	2.9
3	C	129	PRO	2.9
5	K	190	ALA	2.9
1	A	310	PHE	2.9
1	G	43	LYS	2.8
1	A	255	VAL	2.8
2	H	275	LEU	2.8
1	A	297	GLY	2.8
1	G	626	GLY	2.8
2	B	108	LYS	2.8
5	K	195	LYS	2.8
1	G	23	CYS	2.8
2	B	173	LEU	2.8
2	H	135	ILE	2.8
3	I	131	ASN	2.8
5	K	261	GLY	2.8
5	K	4	ILE	2.8
2	B	34	VAL	2.8
2	B	257	VAL	2.8
1	G	653	THR	2.8
2	B	24	THR	2.8
2	B	268	MET	2.8
1	G	44	TYR	2.7
1	G	591	VAL	2.7
6	L	77	ASP	2.7
6	L	2	VAL	2.7
3	C	122	LEU	2.7
1	G	625	ALA	2.7
3	C	123	LYS	2.7
3	C	181	ALA	2.7
1	G	241	ILE	2.7
3	C	149	ILE	2.7
2	B	185	VAL	2.7
5	K	278	LYS	2.7
1	G	69	ALA	2.7
4	J	70	GLY	2.7
5	K	194	ILE	2.7
1	G	614	SER	2.7
3	C	124	TYR	2.7
4	J	106	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	620	CYS	2.6
2	B	186	PRO	2.6
4	J	91	LEU	2.6
1	G	70	ALA	2.6
2	H	276	ALA	2.6
1	G	6	ILE	2.6
5	K	202	PRO	2.6
3	C	157	LEU	2.6
2	B	31	VAL	2.6
6	F	329	TYR	2.6
5	K	184	LYS	2.6
3	C	138	ARG	2.6
1	G	46	CYS	2.6
1	G	255	VAL	2.6
1	G	598	ALA	2.6
1	G	9	TYR	2.6
2	B	258	LEU	2.6
1	G	26	VAL	2.6
3	C	179	LYS	2.6
5	K	198	TYR	2.6
1	G	288	ILE	2.5
1	A	302	VAL	2.5
1	G	232	VAL	2.5
5	K	215	CYS	2.5
1	G	464	PRO	2.5
2	B	130	ILE	2.5
4	J	107	ILE	2.5
5	K	272	ILE	2.5
6	L	4	LEU	2.5
2	B	183	LYS	2.5
6	L	186	LYS	2.5
1	A	294	ILE	2.5
2	B	290	LYS	2.5
2	B	144	ASN	2.5
5	K	160	VAL	2.5
5	K	268	VAL	2.5
6	L	342	VAL	2.5
2	B	39	ALA	2.5
3	C	173	ILE	2.5
2	B	277	LEU	2.5
5	K	208	LEU	2.5
6	F	204	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	29	PHE	2.5
6	L	22	PHE	2.5
2	B	132	VAL	2.5
3	C	182	LEU	2.4
6	L	346	LEU	2.4
2	B	262	GLN	2.4
2	B	161	VAL	2.4
1	A	307	ALA	2.4
5	K	115	LYS	2.4
2	B	271	ASP	2.4
2	B	263	LEU	2.4
2	B	167	ALA	2.4
1	A	258	ILE	2.4
6	L	357	ARG	2.4
5	K	213	TYR	2.4
6	L	358	ALA	2.4
1	G	618	LYS	2.4
1	G	461	ILE	2.4
5	K	191	ILE	2.4
5	K	214	ILE	2.4
2	H	277	LEU	2.4
4	J	138	LEU	2.4
1	G	45	MET	2.4
3	C	130	ALA	2.4
4	J	32	PRO	2.3
2	B	30	GLY	2.3
2	B	38	GLY	2.3
6	L	84	ILE	2.3
1	G	623	CYS	2.3
1	G	10	VAL	2.3
4	J	14	ASN	2.3
1	A	288	ILE	2.3
1	G	642	LEU	2.3
2	B	7	LEU	2.3
2	B	106	LEU	2.3
1	G	592	LYS	2.3
6	L	76	VAL	2.3
1	A	420	ASP	2.3
1	G	96	PHE	2.3
1	G	68	VAL	2.3
2	B	16	ALA	2.3
3	C	177	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
5	K	260	PHE	2.3
1	G	570	VAL	2.3
6	F	364	VAL	2.3
6	L	81	GLY	2.2
1	G	575	ILE	2.2
4	J	37	ILE	2.2
1	A	305	PRO	2.2
2	H	279	VAL	2.2
6	L	360	PRO	2.2
6	L	368	VAL	2.2
2	B	265	GLY	2.2
1	G	253	SER	2.2
1	G	583	ILE	2.2
2	B	126	ILE	2.2
2	B	243	ILE	2.2
6	L	24	ASP	2.2
1	A	300	ALA	2.2
1	A	312	GLN	2.2
2	B	138	LYS	2.2
6	L	83	LYS	2.2
1	G	252	CYS	2.2
3	C	180	GLY	2.2
6	L	285	GLY	2.2
6	L	21	SER	2.2
1	G	628	PRO	2.2
2	B	289	LYS	2.2
3	C	165	LYS	2.2
3	C	151	GLN	2.2
1	A	248	GLY	2.2
1	G	256	CYS	2.2
1	G	296	CYS	2.2
6	L	91	LEU	2.2
6	L	365	GLY	2.2
2	B	122	PHE	2.2
2	B	238	PHE	2.2
2	H	138	LYS	2.2
2	B	139	VAL	2.1
2	B	150	HIS	2.1
1	G	621	GLY	2.1
6	F	87	THR	2.1
6	L	281	GLY	2.1
5	K	196	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
5	K	183	LYS	2.1
5	K	270	PRO	2.1
6	L	300	LYS	2.1
2	B	48	PHE	2.1
1	G	37	VAL	2.1
2	B	117	VAL	2.1
1	A	87	ALA	2.1
6	F	140	ILE	2.1
5	K	182	ARG	2.1
4	J	48	PRO	2.1
2	B	255	PHE	2.1
1	G	306	ASN	2.1
5	E	201	ASN	2.1
5	K	201	ASN	2.1
1	G	75	LEU	2.1
1	G	632	LEU	2.1
6	L	184	LEU	2.1
6	F	357	ARG	2.1
1	A	316	ILE	2.1
1	G	611	GLU	2.1
5	K	277	ILE	2.1
1	G	301	LYS	2.1
5	K	275	LYS	2.1
6	L	174	LYS	2.1
1	G	303	CYS	2.1
2	B	226	CYS	2.1
1	G	109	HIS	2.1
3	C	116	MET	2.1
4	J	21	ALA	2.1
1	G	600	ARG	2.1
2	H	29	LEU	2.1
4	J	125	LYS	2.1
6	L	284	ASP	2.1
6	L	355	ASP	2.1
2	B	25	VAL	2.0
2	H	228	VAL	2.0
2	B	141	ARG	2.0
2	B	179	ALA	2.0
3	I	143	LEU	2.0
1	G	633	GLU	2.0
1	G	466	THR	2.0
4	J	4	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
5	K	200	GLY	2.0
6	L	236	TYR	2.0
2	B	36	MET	2.0
1	G	249	CYS	2.0
6	L	26	GLY	2.0
2	H	145	ILE	2.0
1	A	257	PRO	2.0
1	A	314	PRO	2.0
1	G	305	PRO	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(Å ²)	Q<0.9
7	ACT	G	702	4/4	0.46	0.18	108,110,110,110	0
10	GOL	H	304	6/6	0.64	0.27	95,96,99,101	0
7	ACT	A	701	4/4	0.69	0.28	62,66,66,67	0
17	PE3	G	701	14/43	0.69	0.17	50,58,74,76	0
7	ACT	D	202	4/4	0.70	0.24	78,79,80,82	0
10	GOL	K	304	6/6	0.82	0.14	54,55,61,62	0
14	TRS	D	203	8/8	0.86	0.13	41,54,56,61	0
10	GOL	A	710	6/6	0.87	0.14	42,49,49,52	0
10	GOL	G	710	6/6	0.89	0.14	46,51,55,59	0
11	9S8	B	302	8/8	0.90	0.08	68,80,86,90	0
10	GOL	A	709	6/6	0.92	0.10	44,49,50,53	0
9	SF4	A	707	8/8	0.93	0.07	98,101,104,105	0
12	COM	B	303	7/7	0.93	0.11	62,64,70,75	0
9	SF4	G	708	8/8	0.94	0.06	61,67,71,72	0

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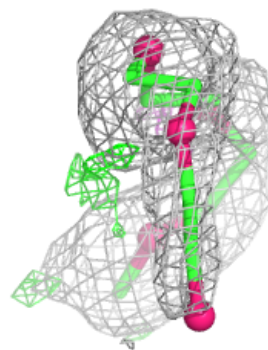
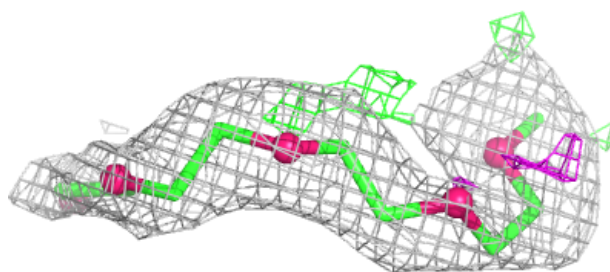
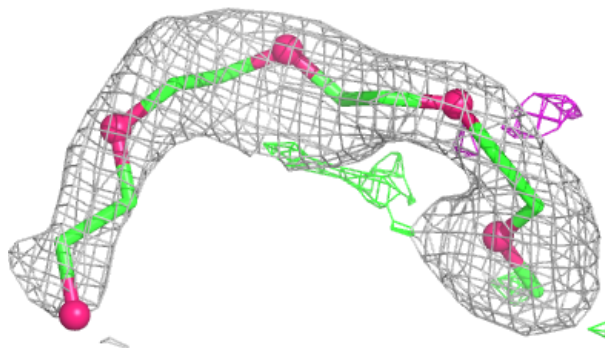
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SF4	G	707	8/8	0.95	0.05	103,106,108,111	0
11	9S8	H	302	8/8	0.95	0.06	46,51,58,58	0
9	SF4	A	708	8/8	0.95	0.06	70,71,79,81	0
12	COM	H	303	7/7	0.95	0.10	42,46,57,61	0
9	SF4	K	303	8/8	0.95	0.06	63,68,75,77	0
9	SF4	G	704	8/8	0.95	0.06	67,76,84,84	0
9	SF4	G	709	8/8	0.96	0.05	46,52,58,58	0
9	SF4	G	706	8/8	0.96	0.05	81,82,85,86	0
9	SF4	A	706	8/8	0.96	0.05	34,39,44,45	0
11	9S8	B	301	8/8	0.96	0.06	57,67,69,74	0
8	FAD	G	703	53/53	0.96	0.08	8,32,52,54	0
11	9S8	H	301	8/8	0.97	0.05	41,49,55,59	0
9	SF4	I	201	8/8	0.97	0.05	25,27,29,29	0
9	SF4	K	302	8/8	0.97	0.04	42,50,53,53	0
9	SF4	A	705	8/8	0.98	0.04	24,32,36,41	0
9	SF4	G	705	8/8	0.98	0.03	15,17,20,26	0
8	FAD	A	702	53/53	0.98	0.06	11,27,49,53	0
9	SF4	A	703	8/8	0.98	0.03	13,18,20,24	0
9	SF4	A	704	8/8	0.98	0.03	12,21,28,31	0
9	SF4	C	201	8/8	0.98	0.04	24,27,33,40	0
9	SF4	C	202	8/8	0.98	0.05	29,37,45,47	0
9	SF4	I	202	8/8	0.98	0.05	36,37,49,53	0
9	SF4	K	301	8/8	0.98	0.05	37,41,49,50	0
9	SF4	E	301	8/8	0.98	0.04	18,26,30,32	0
9	SF4	E	302	8/8	0.98	0.03	13,24,27,29	0
9	SF4	E	303	8/8	0.98	0.03	10,16,24,27	0
13	FES	D	201	4/4	0.99	0.04	20,23,33,36	0
15	NFU	F	501	8/8	0.99	0.07	29,36,39,41	0
13	FES	J	200	4/4	0.99	0.04	52,54,59,61	0
16	FE	F	502	1/1	1.00	0.02	35,35,35,35	0
16	FE	L	502	1/1	1.00	0.06	44,44,44,44	0
15	NFU	L	501	8/8	1.00	0.04	28,34,37,41	0

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

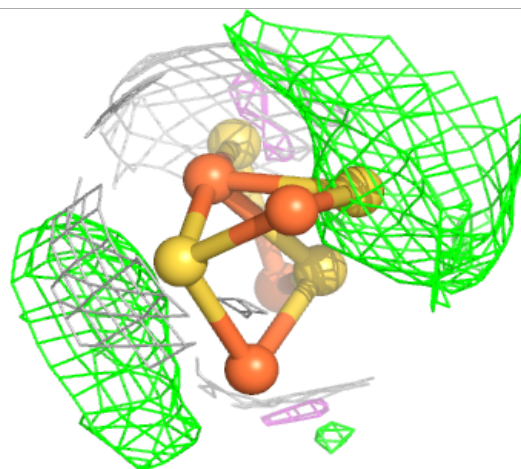
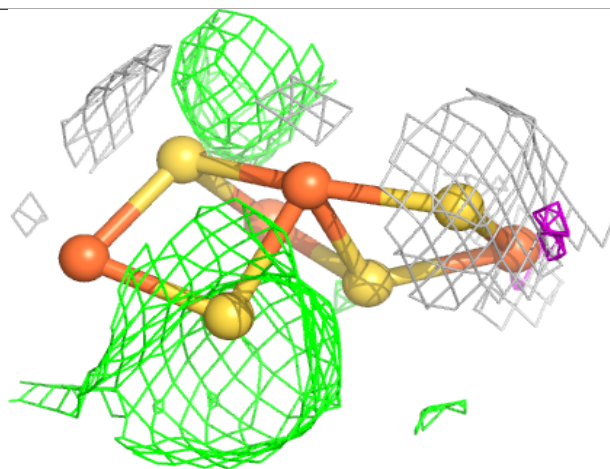
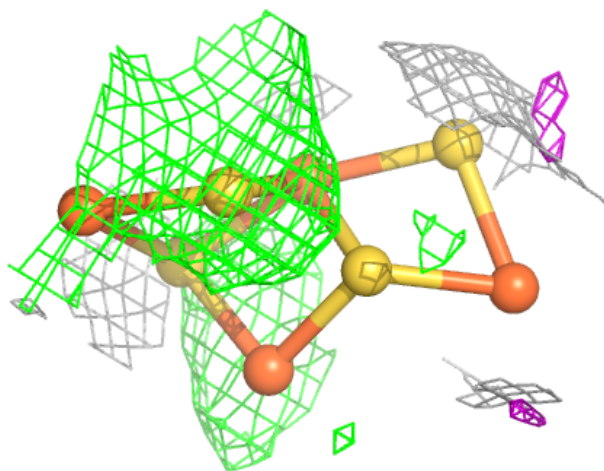
Electron density around PE3 G 701:

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



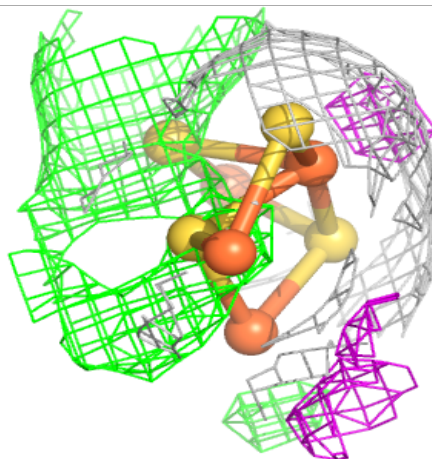
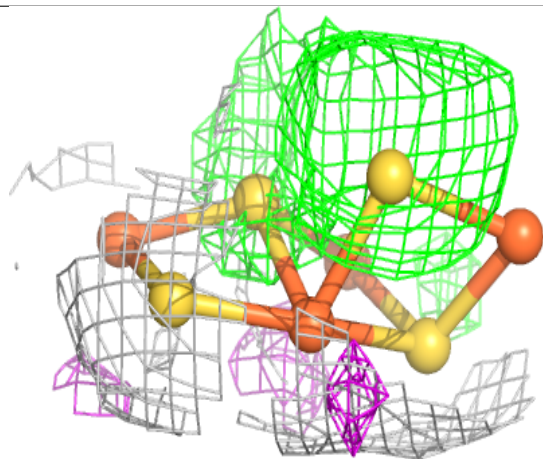
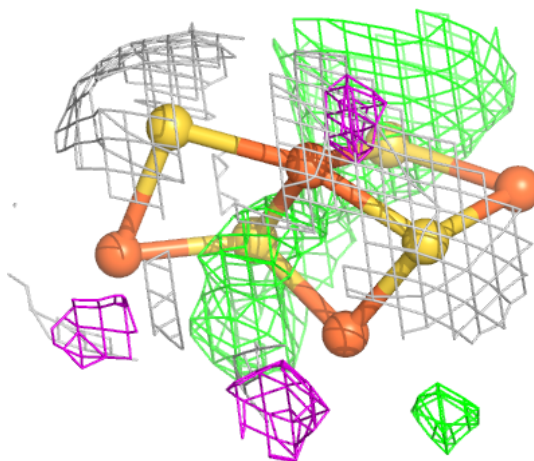
Electron density around 9S8 B 302:

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



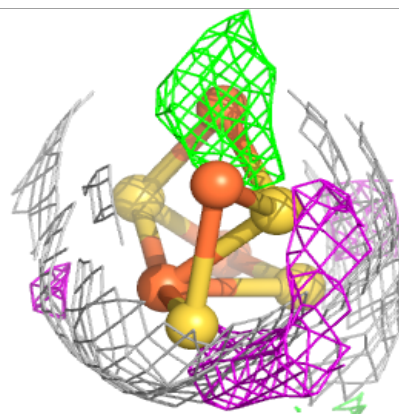
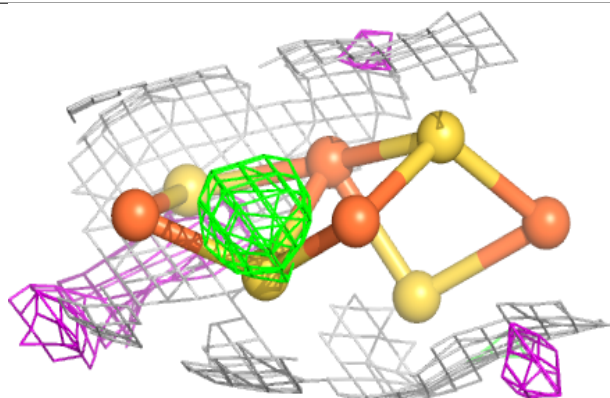
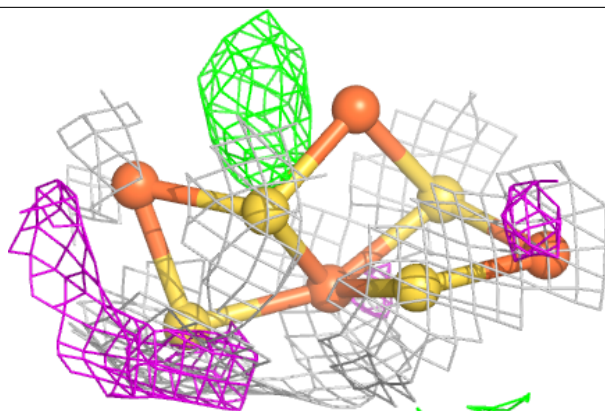
Electron density around 9S8 H 302:

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

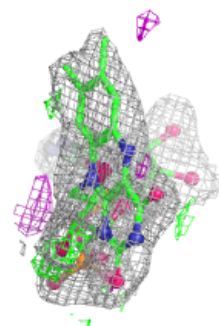
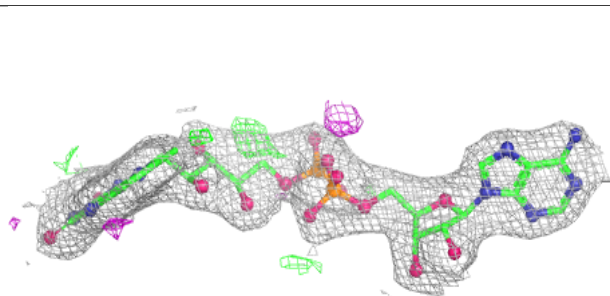
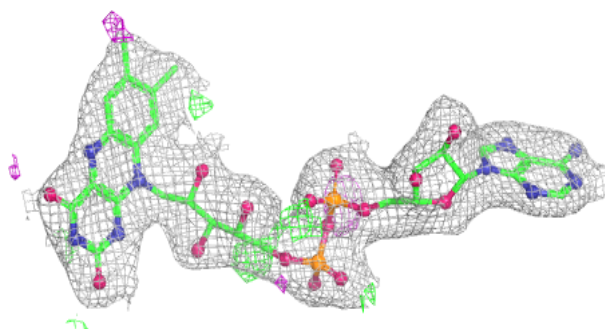


Electron density around 9S8 B 301:

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

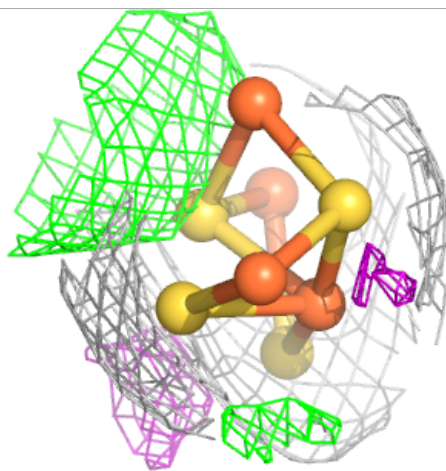
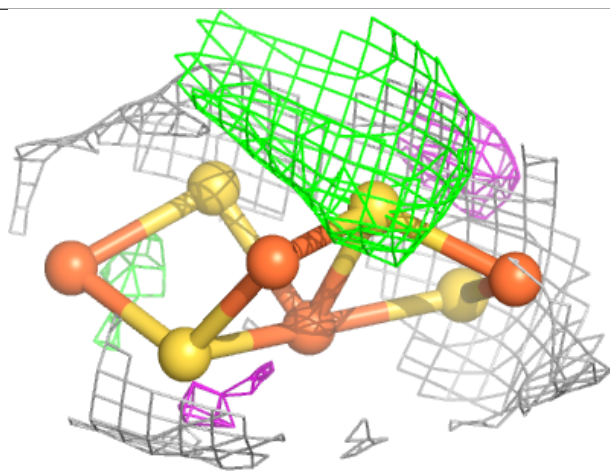
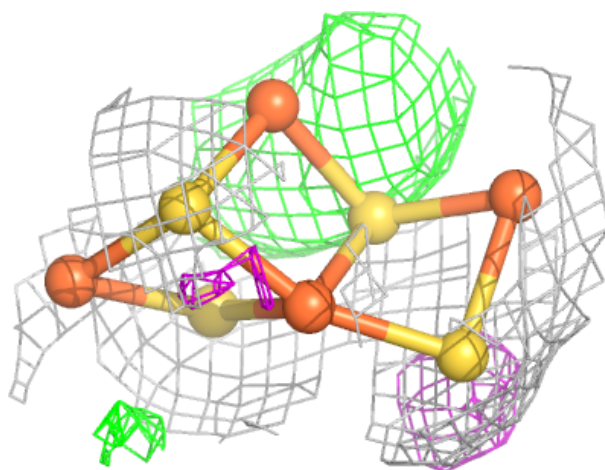
**Electron density around FAD G 703:**

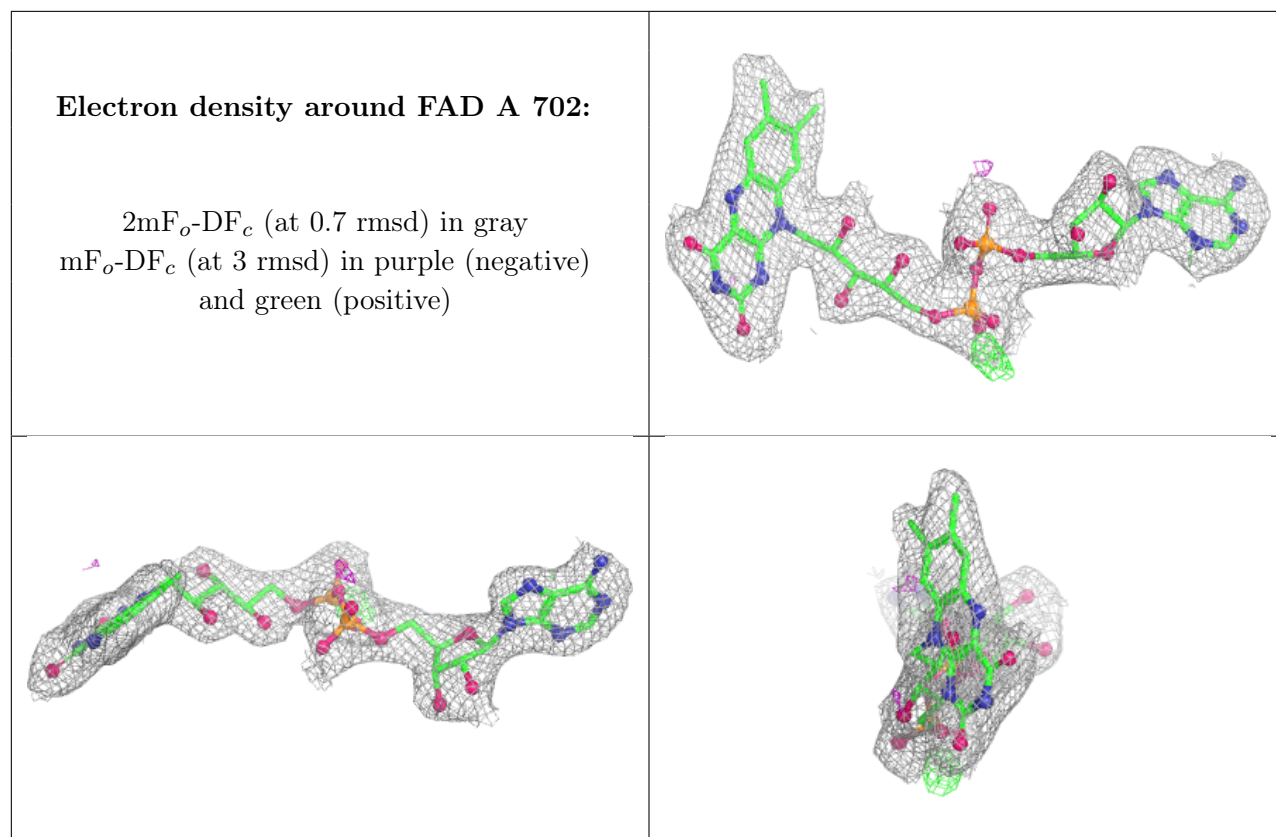
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.