



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2026 – 12:51 am BST

PDB ID : 5ODR / pdb_00005odr
Title : Heterodisulfide reductase / [NiFe]-hydrogenase complex from Methanothermococcus thermolithotrophicus soaked with heterodisulfide for 2 minutes.
Authors : Wagner, T.; Koch, J.; Ermler, U.; Shima, S.
Deposited on : 2017-07-06
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

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

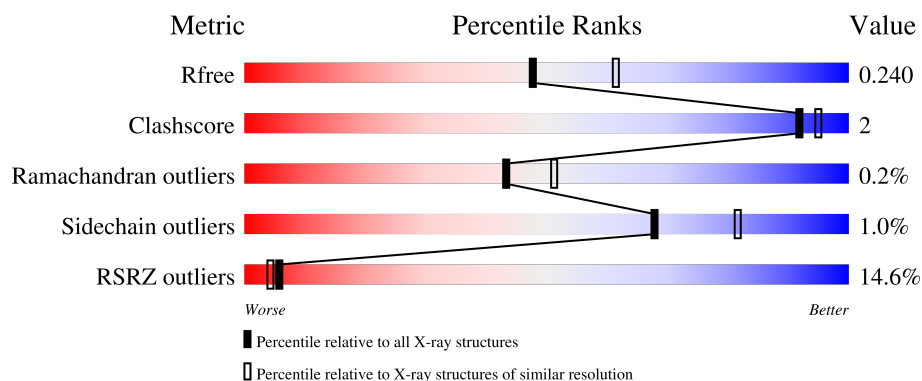
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	654	<div> <div>16%</div> <div>93%</div> <div>6%</div> </div>
1	G	654	<div> <div>18%</div> <div>92%</div> <div>7%</div> </div>
2	B	291	<div> <div>9%</div> <div>97%</div> <div>.</div> </div>
2	H	291	<div> <div>50%</div> <div>91%</div> <div>9%</div> </div>
3	C	184	<div> <div>11%</div> <div>97%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	184	
4	D	140	
4	J	140	
5	E	299	
5	K	299	
6	F	473	
6	L	473	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	9S8	B	302	-	-	X	-
11	COM	B	303	-	X	-	-
8	SF4	G	706	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32577 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heterodisulfide reductase, subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	0	0	0
			4979	3142	845	943	49			
1	G	652	Total	C	N	O	S	0	0	0
			4979	3142	845	943	49			

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

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

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

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

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

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

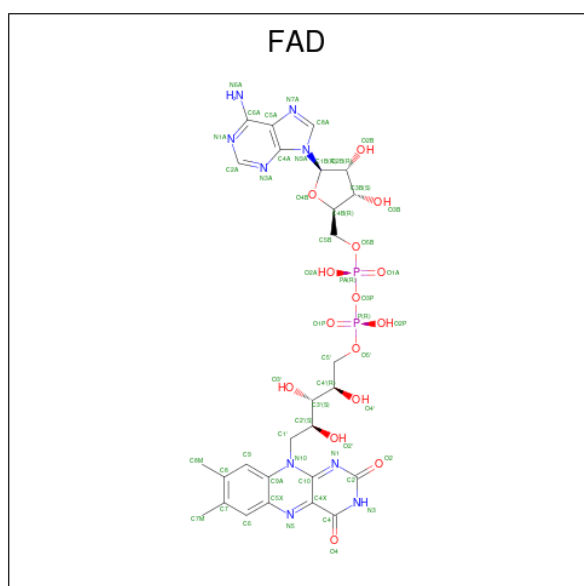
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

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

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

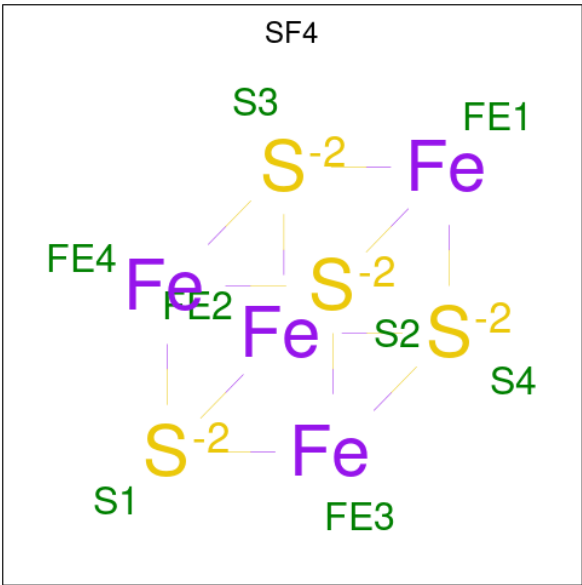
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	447	Total 3521	C 2230	N 600	O 672	S 19	0	0	0
6	L	447	Total 3521	C 2230	N 600	O 672	S 19	0	0	0

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



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

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



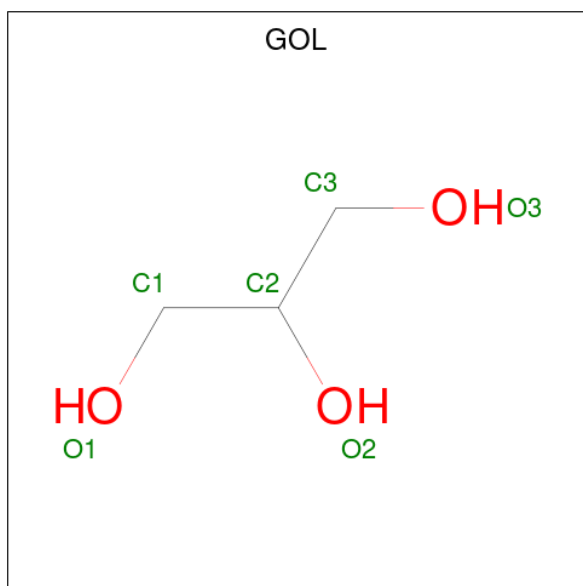
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Fe	S	0	0
8	A	1	8	4	4	0	0
8	A	1	Total	Fe	S	0	0
8	A	1	8	4	4	0	0
8	A	1	Total	Fe	S	0	0
8	A	1	8	4	4	0	0
8	A	1	Total	Fe	S	0	0
8	A	1	8	4	4	0	0
8	C	1	Total	Fe	S	0	0
8	C	1	8	4	4	0	0
8	E	1	Total	Fe	S	0	0
8	E	1	8	4	4	0	0
8	E	1	Total	Fe	S	0	0
8	E	1	8	4	4	0	0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

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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



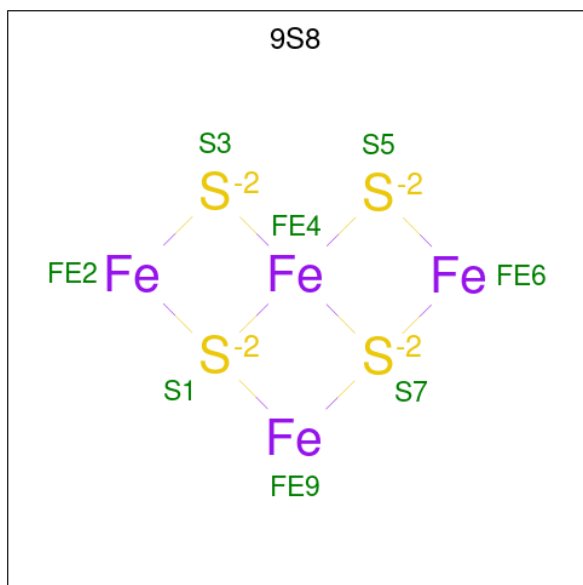
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		

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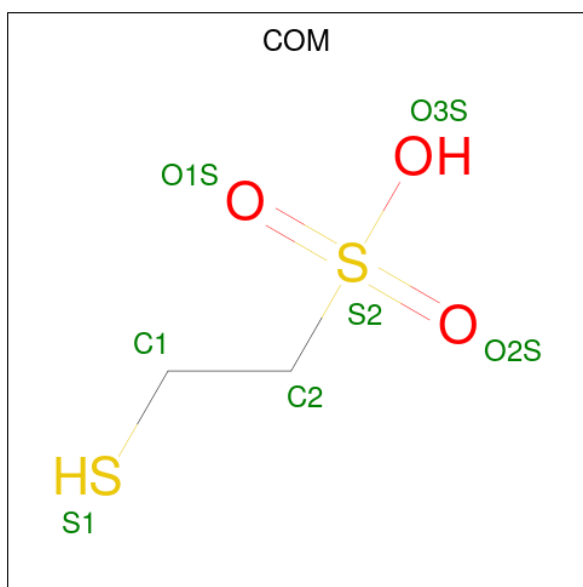
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			6	3	3		
9	I	1	Total	C	O	0	0
			6	3	3		
9	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe_4S_4).



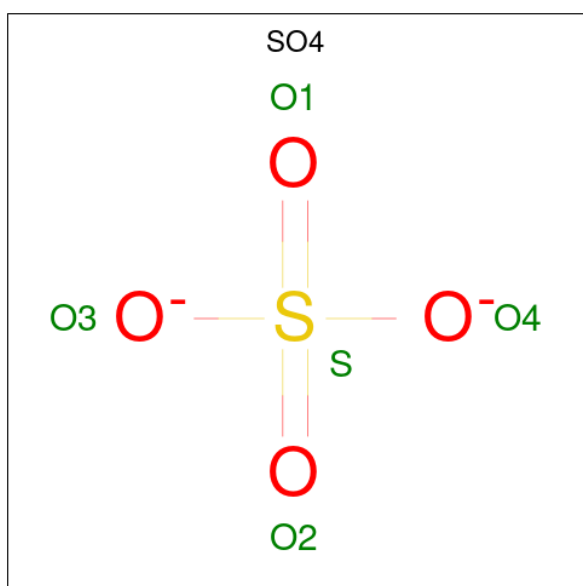
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			8	4	4		
10	B	1	Total	Fe	S	0	0
			8	4	4		
10	H	1	Total	Fe	S	0	0
			8	4	4		
10	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 11 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $\text{C}_2\text{H}_6\text{O}_3\text{S}_2$).



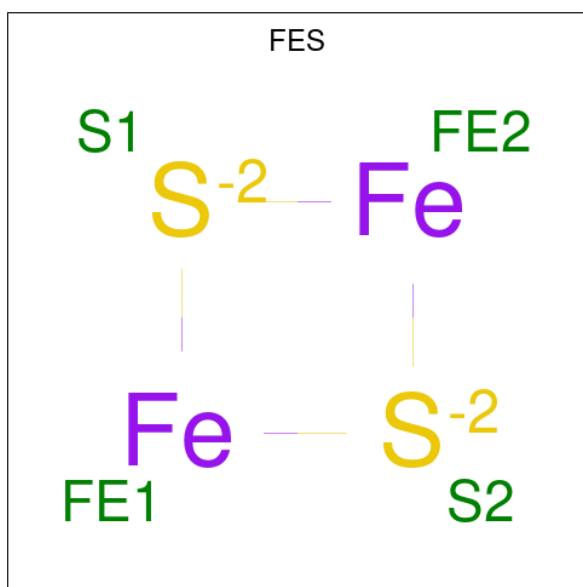
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	O	S	0	0
			7	2	3	2		
11	H	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



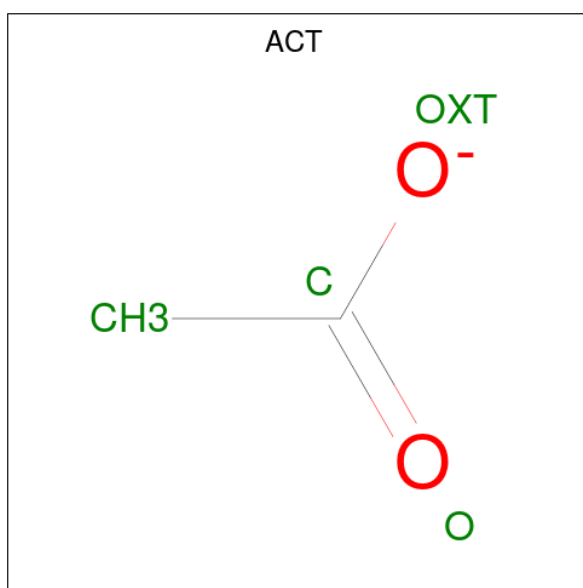
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 14 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



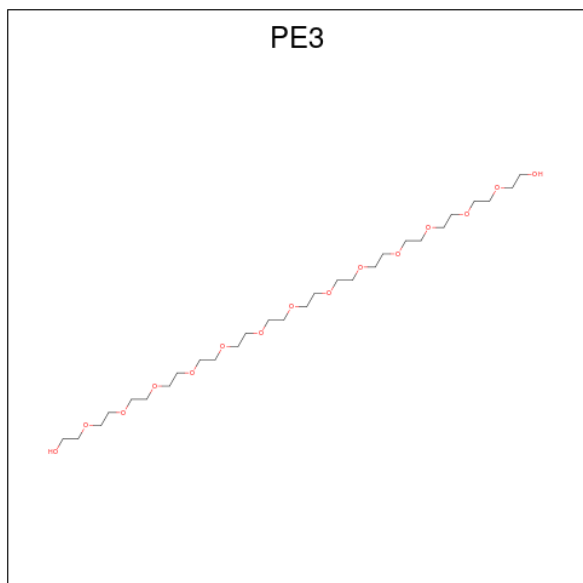
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			4	2	2		
14	E	1	Total	C	O	0	0
			4	2	2		

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

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

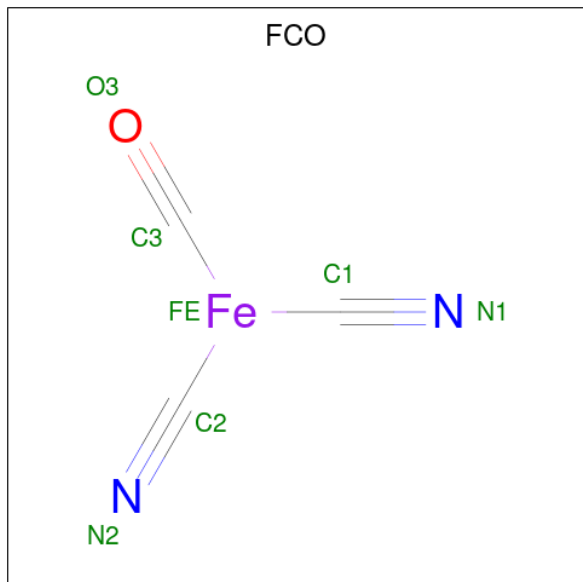


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	F	1	Total	C	O	0	0
			9	6	3		
15	F	1	Total	C	O	0	0
			13	8	5		
15	G	1	Total	C	O	0	0
			10	7	3		
15	L	1	Total	C	O	0	0
			9	6	3		

- 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	G	1	Total	Fe	0	0
			1	1		
16	L	1	Total	Fe	0	0
			1	1		

- Molecule 17 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O).

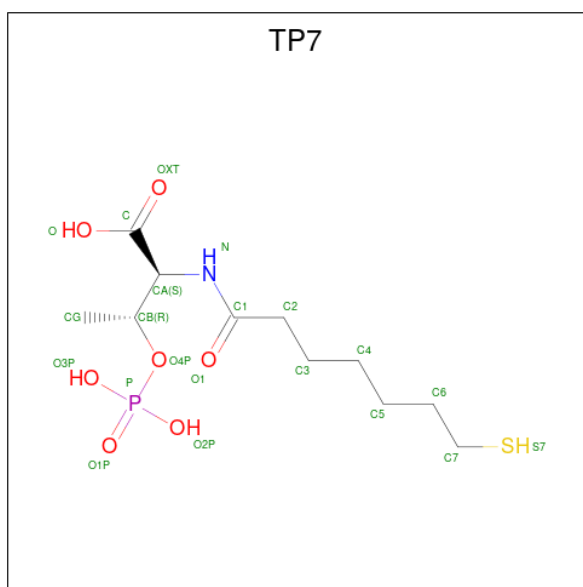


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	F	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
17	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 18 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

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



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

- Molecule 20 is water.

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

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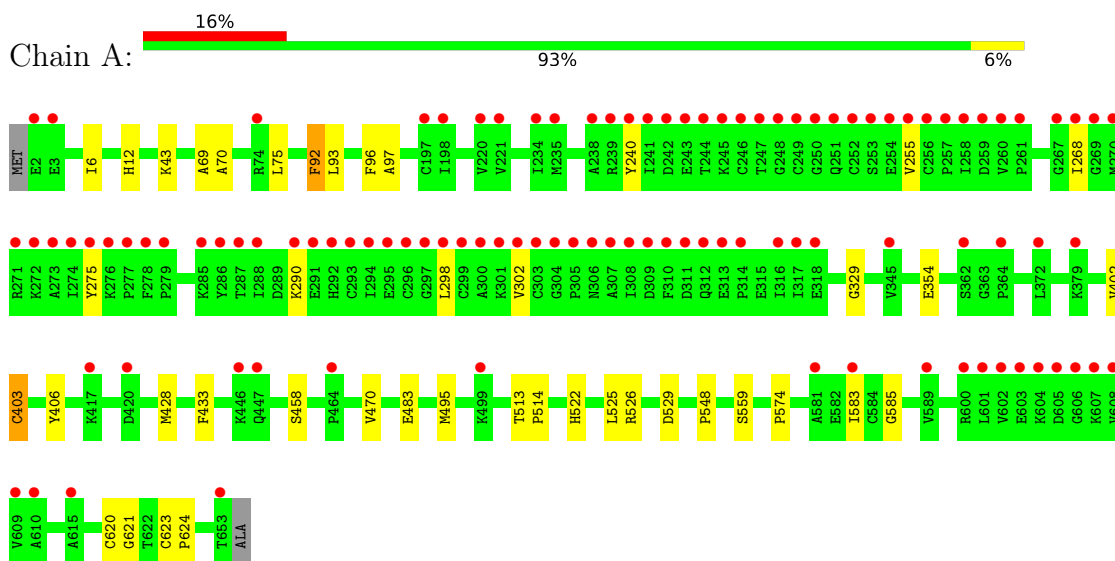
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	L	132	Total 132	O 132	0	0

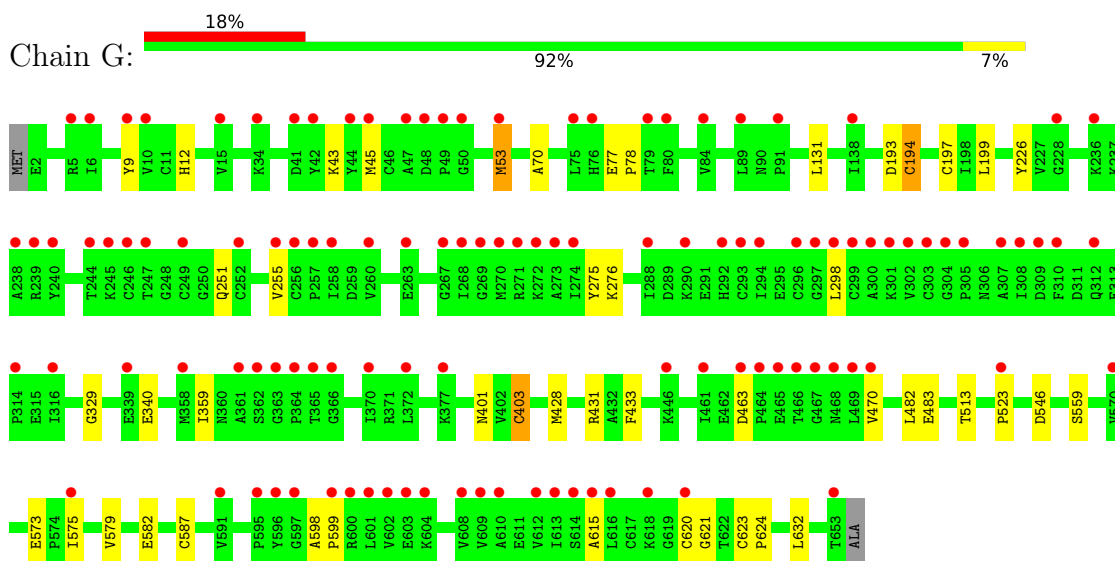
3 Residue-property plots [i](#)

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.

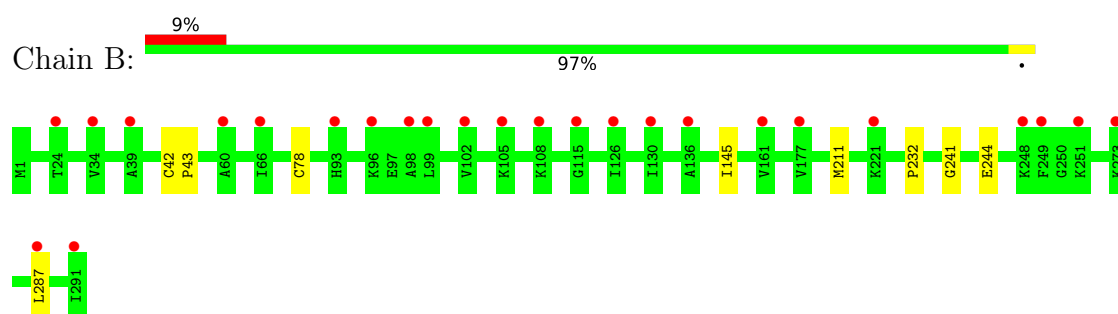
- Molecule 1: Heterodisulfide reductase, subunit A



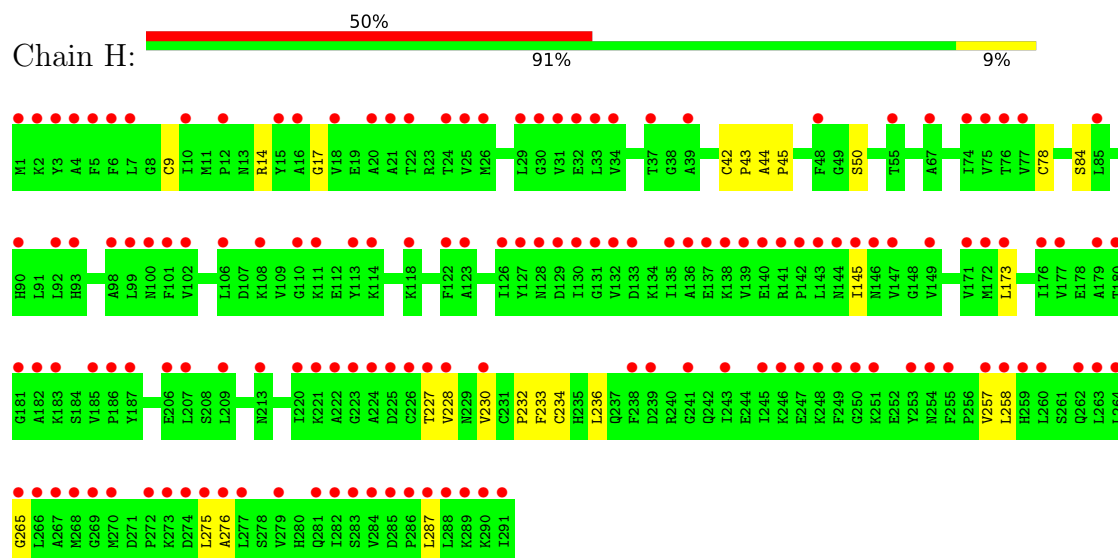
- Molecule 1: Heterodisulfide reductase, subunit A



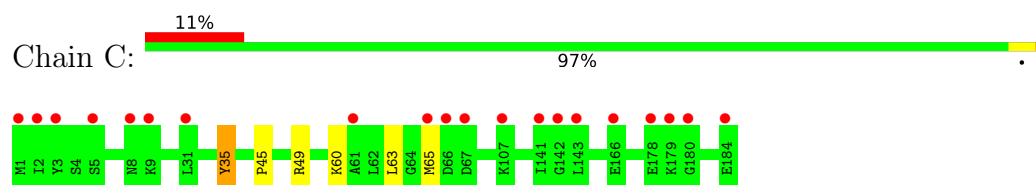
- Molecule 2: Heterodisulfide reductase, subunit B



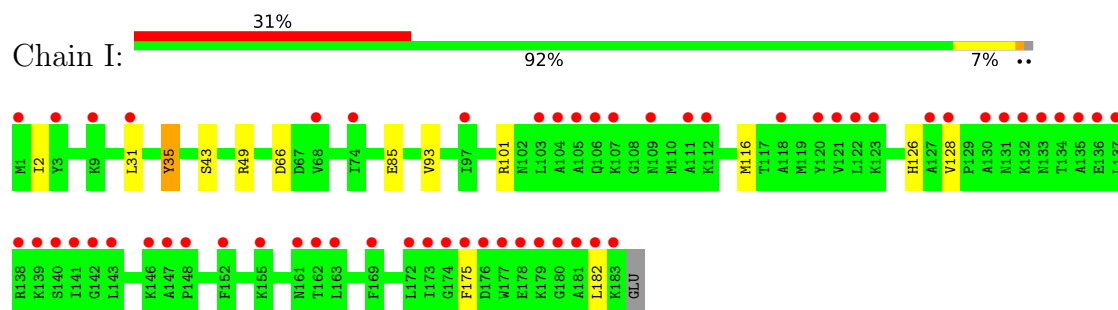
- Molecule 2: Heterodisulfide reductase, subunit B



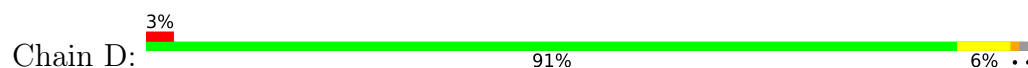
- Molecule 3: Heterodisulfide reductase, subunit C



- Molecule 3: Heterodisulfide reductase, subunit C

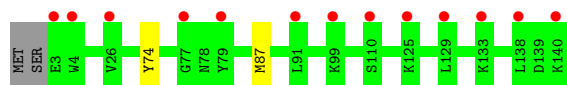


- Molecule 4: Methyl-viologen reducing hydrogenase, subunit D

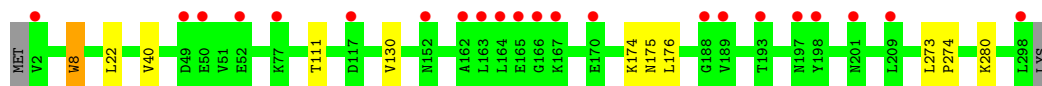




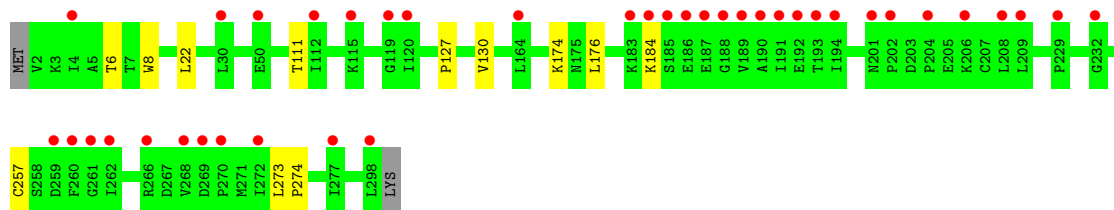
- Molecule 4: Methyl-viologen reducing hydrogenase, subunit D



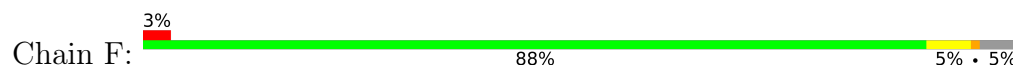
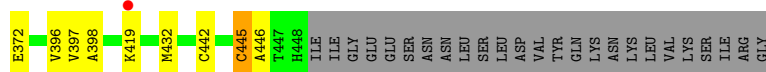
- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G



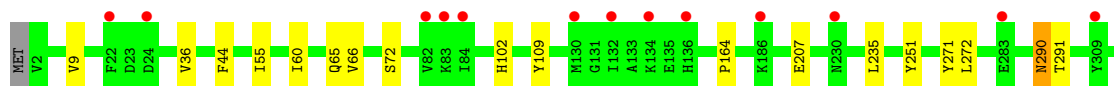
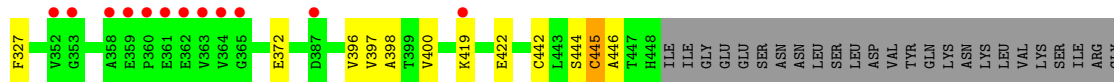
- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G



- 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	366.22Å 96.92Å 134.45Å 90.00° 108.30° 90.00°	Depositor
Resolution (Å)	90.26 – 2.20 90.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (90.26-2.20) 99.1 (90.26-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.204 , 0.225 0.218 , 0.240	Depositor DCC
R_{free} test set	11246 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32577	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, NI, SF4, GOL, 9S8, PE3, FES, SO4, TP7, FCO, ACT, 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	0.63	0/5071	0.96	7/6853 (0.1%)
1	G	0.64	2/5071 (0.0%)	0.97	12/6853 (0.2%)
2	B	0.61	0/2277	0.98	0/3070
2	H	0.61	0/2277	0.97	1/3070 (0.0%)
3	C	0.62	0/1447	0.95	0/1946
3	I	0.62	0/1437	0.94	0/1934
4	D	0.57	0/1123	1.00	2/1508 (0.1%)
4	J	0.58	0/1132	0.96	0/1520
5	E	0.59	0/2288	0.97	3/3102 (0.1%)
5	K	0.61	0/2299	0.98	3/3116 (0.1%)
6	F	0.61	0/3590	1.04	11/4853 (0.2%)
6	L	0.60	0/3590	1.04	13/4853 (0.3%)
All	All	0.61	2/31602 (0.0%)	0.98	52/42678 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	53	MET	SD-CE	-8.24	1.58	1.79
1	G	276	LYS	CA-C	5.67	1.57	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	397	VAL	N-CA-C	7.76	118.68	106.88
6	L	397	VAL	N-CA-C	7.75	118.65	106.88
1	A	275	TYR	N-CA-C	7.67	118.73	108.38
5	E	22	LEU	N-CA-C	-7.44	102.85	112.23
5	K	22	LEU	N-CA-C	-7.31	103.03	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	4979	0	4975	27	0
1	G	4979	0	4974	22	0
2	B	2236	0	2243	5	0
2	H	2236	0	2243	16	0
3	C	1426	0	1441	4	0
3	I	1416	0	1435	11	0
4	D	1097	0	1068	5	0
4	J	1106	0	1074	2	0
5	E	2249	0	2252	5	0
5	K	2257	0	2265	5	0
6	F	3521	0	3503	6	0
6	L	3521	0	3503	7	0
7	A	53	0	31	0	0
7	G	53	0	31	0	0
8	A	48	0	0	1	0
8	C	16	0	0	0	0
8	E	24	0	0	0	0
8	G	48	0	0	2	0
8	I	16	0	0	0	0
8	K	24	0	0	0	0
9	A	12	0	16	2	0
9	D	6	0	8	0	0
9	I	12	0	16	1	0
9	K	6	0	8	0	0
10	B	16	0	0	3	0
10	H	16	0	0	0	0
11	B	7	0	6	0	0
11	H	7	0	5	0	0
12	B	5	0	0	0	0
13	D	4	0	0	0	0
13	J	4	0	0	0	0
14	D	4	0	3	0	0
14	E	4	0	3	0	0
14	F	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	G	4	0	3	0	0
15	F	22	0	27	0	0
15	G	10	0	10	0	0
15	L	9	0	10	0	0
16	F	1	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
17	F	7	0	0	1	0
17	L	7	0	0	1	0
18	F	1	0	0	0	0
18	L	1	0	0	0	0
19	H	21	0	19	0	0
20	A	198	0	0	0	0
20	B	52	0	0	1	0
20	C	48	0	0	0	0
20	D	46	0	0	0	0
20	E	86	0	0	0	0
20	F	137	0	0	0	0
20	G	181	0	0	0	0
20	H	24	0	0	0	0
20	I	35	0	0	1	0
20	J	54	0	0	0	0
20	K	87	0	0	0	0
20	L	132	0	0	0	0
All	All	32577	0	31175	100	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 2.

The worst 5 of 100 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG21	1:A:302:VAL:HG21	1.47	0.96
10:B:302:9S8:S5	10:B:302:9S8:S1	2.73	0.86
10:B:302:9S8:S1	20:B:402:HOH:O	2.42	0.77
3:I:35:TYR:HA	9:I:203:GOL:H2	1.65	0.76
2:B:145:ILE:HD12	2:B:287:LEU:HD11	1.68	0.74

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	650/654 (99%)	629 (97%)	20 (3%)	1 (0%)	43	51
1	G	650/654 (99%)	629 (97%)	19 (3%)	2 (0%)	36	42
2	B	289/291 (99%)	274 (95%)	15 (5%)	0	100	100
2	H	289/291 (99%)	278 (96%)	11 (4%)	0	100	100
3	C	182/184 (99%)	182 (100%)	0	0	100	100
3	I	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
4	D	135/140 (96%)	130 (96%)	5 (4%)	0	100	100
4	J	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
5	E	295/299 (99%)	285 (97%)	10 (3%)	0	100	100
5	K	296/299 (99%)	285 (96%)	11 (4%)	0	100	100
6	F	445/473 (94%)	431 (97%)	11 (2%)	3 (1%)	18	19
6	L	445/473 (94%)	431 (97%)	12 (3%)	2 (0%)	30	34
All	All	3993/4082 (98%)	3865 (97%)	120 (3%)	8 (0%)	43	51

5 of 8 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	540/541 (100%)	537 (99%)	3 (1%)	78	89
1	G	540/541 (100%)	535 (99%)	5 (1%)	70	84
2	B	242/242 (100%)	242 (100%)	0	100	100
2	H	242/242 (100%)	241 (100%)	1 (0%)	84	92
3	C	157/157 (100%)	155 (99%)	2 (1%)	61	76
3	I	156/157 (99%)	153 (98%)	3 (2%)	50	66
4	D	116/119 (98%)	115 (99%)	1 (1%)	70	84
4	J	117/119 (98%)	117 (100%)	0	100	100
5	E	254/256 (99%)	252 (99%)	2 (1%)	73	85
5	K	255/256 (100%)	252 (99%)	3 (1%)	63	78
6	F	386/410 (94%)	379 (98%)	7 (2%)	51	68
6	L	386/410 (94%)	379 (98%)	7 (2%)	51	68
All	All	3391/3450 (98%)	3357 (99%)	34 (1%)	68	81

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	L	72	SER
6	L	102	HIS
6	L	422	GLU
6	F	351	ILE
6	F	290	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	459	GLN
2	H	229	ASN
2	H	154	HIS
2	H	254	ASN
2	B	254	ASN

5.3.3 RNA ⓘ

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 55 ligands modelled in this entry, 5 are monoatomic - leaving 50 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SF4	C	202	3	0,12,12	-	-	-		
15	PE3	F	503	-	12,12,42	0.47	0	11,11,41	0.28	0
7	FAD	G	704	-	56,58,58	1.40	8 (14%)	81,89,89	1.69	19 (23%)
8	SF4	A	707	1	0,12,12	-	-	-		
12	SO4	B	304	-	4,4,4	0.17	0	6,6,6	0.08	0
9	GOL	K	304	-	5,5,5	0.35	0	5,5,5	0.41	0
10	9S8	B	301	2	2,10,10	3.98	1 (50%)	-		
15	PE3	L	502	-	8,8,42	0.50	0	7,7,41	0.18	0
8	SF4	K	301	5	0,12,12	-	-	-		
11	COM	B	303	-	6,6,6	1.30	1 (16%)	7,8,8	2.71	4 (57%)
8	SF4	G	707	1	0,12,12	-	-	-		
14	ACT	D	202	-	3,3,3	1.04	0	3,3,3	0.96	0
17	FCO	L	504	6	1,6,6	4.04	1 (100%)	-		
17	FCO	F	506	6	1,6,6	3.97	1 (100%)	-		
19	TP7	H	304	-	19,20,20	0.69	0	24,26,26	0.94	0
8	SF4	G	706	1	0,12,12	-	-	-		
10	9S8	H	301	2	2,10,10	3.44	2 (100%)	-		
8	SF4	I	202	3	0,12,12	-	-	-		
8	SF4	K	303	5	0,12,12	-	-	-		
7	FAD	A	701	-	56,58,58	1.45	9 (16%)	81,89,89	1.70	19 (23%)
9	GOL	I	203	-	5,5,5	0.23	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	ACT	E	301	-	3,3,3	1.07	0	3,3,3	1.00	0
8	SF4	A	703	1	0,12,12	-	-	-		
13	FES	D	201	4	0,4,4	-	-	-		
9	GOL	A	709	-	5,5,5	0.36	0	5,5,5	0.70	0
8	SF4	A	704	1	0,12,12	-	-	-		
8	SF4	G	709	1	0,12,12	-	-	-		
9	GOL	I	204	-	5,5,5	0.36	0	5,5,5	0.19	0
10	9S8	B	302	2	2,10,10	3.16	1 (50%)	-		
8	SF4	C	201	3	0,12,12	-	-	-		
9	GOL	A	708	-	5,5,5	0.31	0	5,5,5	0.35	0
11	COM	H	303	-	6,6,6	1.38	2 (33%)	7,8,8	2.63	4 (57%)
13	FES	J	200	4	0,4,4	-	-	-		
14	ACT	F	504	-	3,3,3	1.10	0	3,3,3	0.97	0
8	SF4	A	702	1	0,12,12	-	-	-		
8	SF4	A	705	1	0,12,12	-	-	-		
8	SF4	G	710	1	0,12,12	-	-	-		
8	SF4	A	706	1	0,12,12	-	-	-		
8	SF4	I	201	3	0,12,12	-	-	-		
8	SF4	K	302	5	0,12,12	-	-	-		
8	SF4	E	304	5	0,12,12	-	-	-		
9	GOL	D	203	-	5,5,5	0.33	0	5,5,5	0.37	0
8	SF4	G	705	1,16	0,12,12	-	-	-		
8	SF4	E	302	5	0,12,12	-	-	-		
15	PE3	G	701	-	9,9,42	0.50	0	8,8,41	0.20	0
10	9S8	H	302	2	2,10,10	3.26	2 (100%)	-		
8	SF4	G	708	1	0,12,12	-	-	-		
8	SF4	E	303	5	0,12,12	-	-	-		
15	PE3	F	502	-	8,8,42	0.47	0	7,7,41	0.28	0
14	ACT	G	702	-	3,3,3	1.10	0	3,3,3	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SF4	C	202	3	-	-	0/6/5/5
15	PE3	F	503	-	-	7/10/10/40	-
7	FAD	G	704	-	-	1/34/50/50	0/6/6/6
8	SF4	A	707	1	-	-	0/6/5/5
9	GOL	K	304	-	-	0/4/4/4	-
15	PE3	L	502	-	-	2/6/6/40	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	9S8	B	301	2	-	-	0/3/3/3
8	SF4	K	301	5	-	-	0/6/5/5
11	COM	B	303	-	-	3/4/4/4	-
8	SF4	G	707	1	-	-	0/6/5/5
19	TP7	H	304	-	-	1/24/24/24	-
8	SF4	G	706	1	-	-	0/6/5/5
10	9S8	H	301	2	-	-	0/3/3/3
10	9S8	H	302	2	-	-	0/3/3/3
8	SF4	I	202	3	-	-	0/6/5/5
8	SF4	K	303	5	-	-	0/6/5/5
7	FAD	A	701	-	-	2/34/50/50	0/6/6/6
9	GOL	I	203	-	-	2/4/4/4	-
8	SF4	A	703	1	-	-	0/6/5/5
13	FES	D	201	4	-	-	0/1/1/1
9	GOL	A	709	-	-	2/4/4/4	-
8	SF4	A	704	1	-	-	0/6/5/5
8	SF4	G	709	1	-	-	0/6/5/5
9	GOL	I	204	-	-	2/4/4/4	-
10	9S8	B	302	2	-	-	0/3/3/3
9	GOL	A	708	-	-	0/4/4/4	-
8	SF4	C	201	3	-	-	0/6/5/5
13	FES	J	200	4	-	-	0/1/1/1
8	SF4	A	702	1	-	-	0/6/5/5
8	SF4	A	705	1	-	-	0/6/5/5
8	SF4	G	710	1	-	-	0/6/5/5
8	SF4	A	706	1	-	-	0/6/5/5
8	SF4	I	201	3	-	-	0/6/5/5
8	SF4	K	302	5	-	-	0/6/5/5
8	SF4	E	304	5	-	-	0/6/5/5
9	GOL	D	203	-	-	2/4/4/4	-
8	SF4	G	705	1,16	-	-	0/6/5/5
8	SF4	E	302	5	-	-	0/6/5/5
15	PE3	G	701	-	-	3/7/7/40	-
11	COM	H	303	-	-	0/4/4/4	-
8	SF4	G	708	1	-	-	0/6/5/5
8	SF4	E	303	5	-	-	0/6/5/5
15	PE3	F	502	-	-	4/6/6/40	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	301	9S8	S3-FE4	-5.40	2.12	2.24
7	A	701	FAD	C9A-C5X	5.38	1.50	1.41
7	G	704	FAD	C9A-C5X	5.04	1.49	1.41
10	B	302	9S8	S3-FE4	-4.32	2.14	2.24
7	A	701	FAD	C5A-C4A	4.23	1.46	1.39

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	704	FAD	C5A-C4A-N3A	-6.03	118.88	126.75
7	A	701	FAD	C5A-C4A-N3A	-5.94	119.00	126.75
7	G	704	FAD	N3A-C4A-N9A	4.79	134.98	127.08
7	A	701	FAD	N3A-C4A-N9A	4.55	134.57	127.08
7	A	701	FAD	C2A-N3A-C4A	4.09	121.41	111.75

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	709	GOL	C1-C2-C3-O3
9	D	203	GOL	O1-C1-C2-C3
9	I	204	GOL	O1-C1-C2-C3
11	B	303	COM	S1-C1-C2-S2
15	F	502	PE3	O31-C32-C33-O34

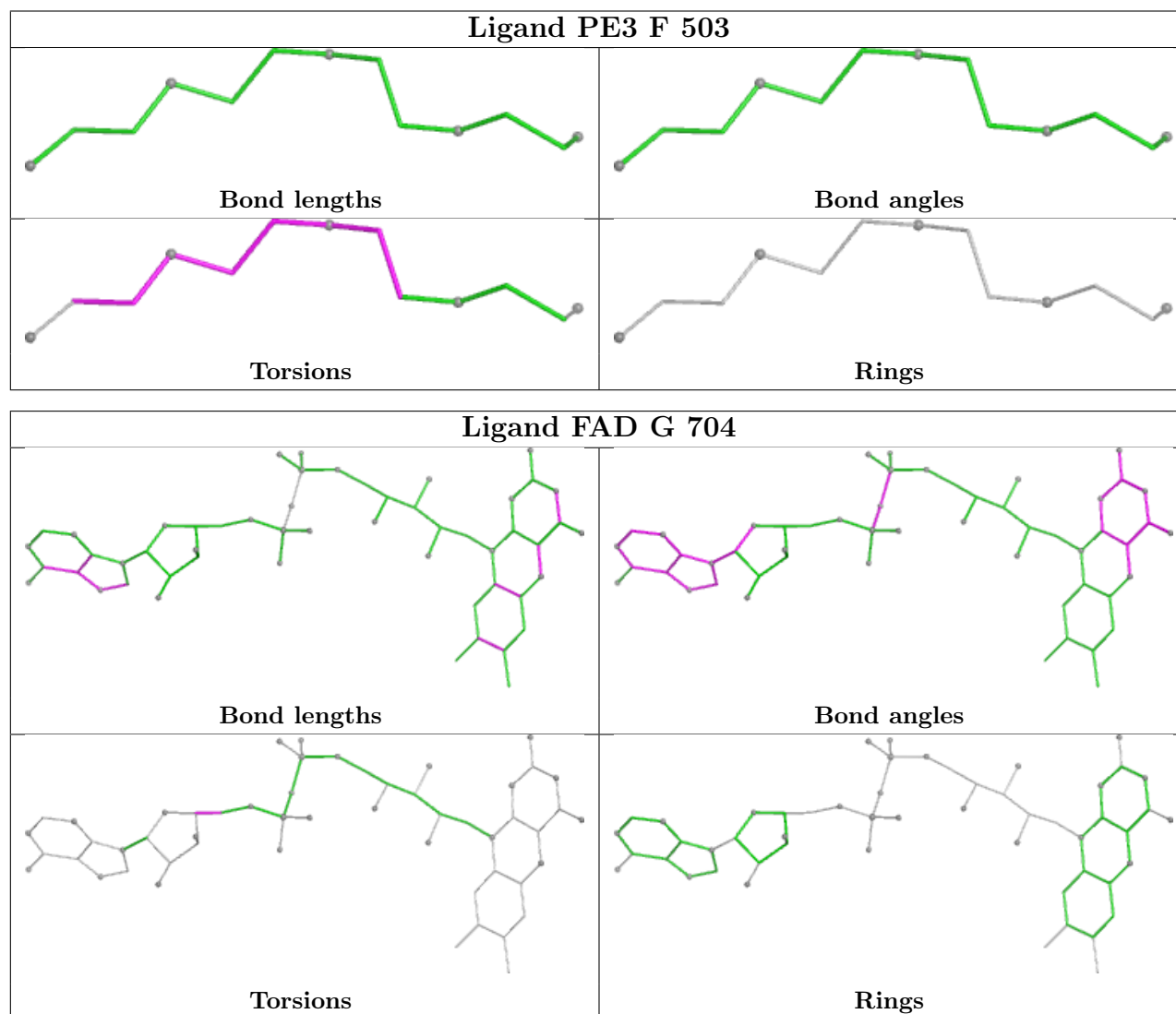
There are no ring outliers.

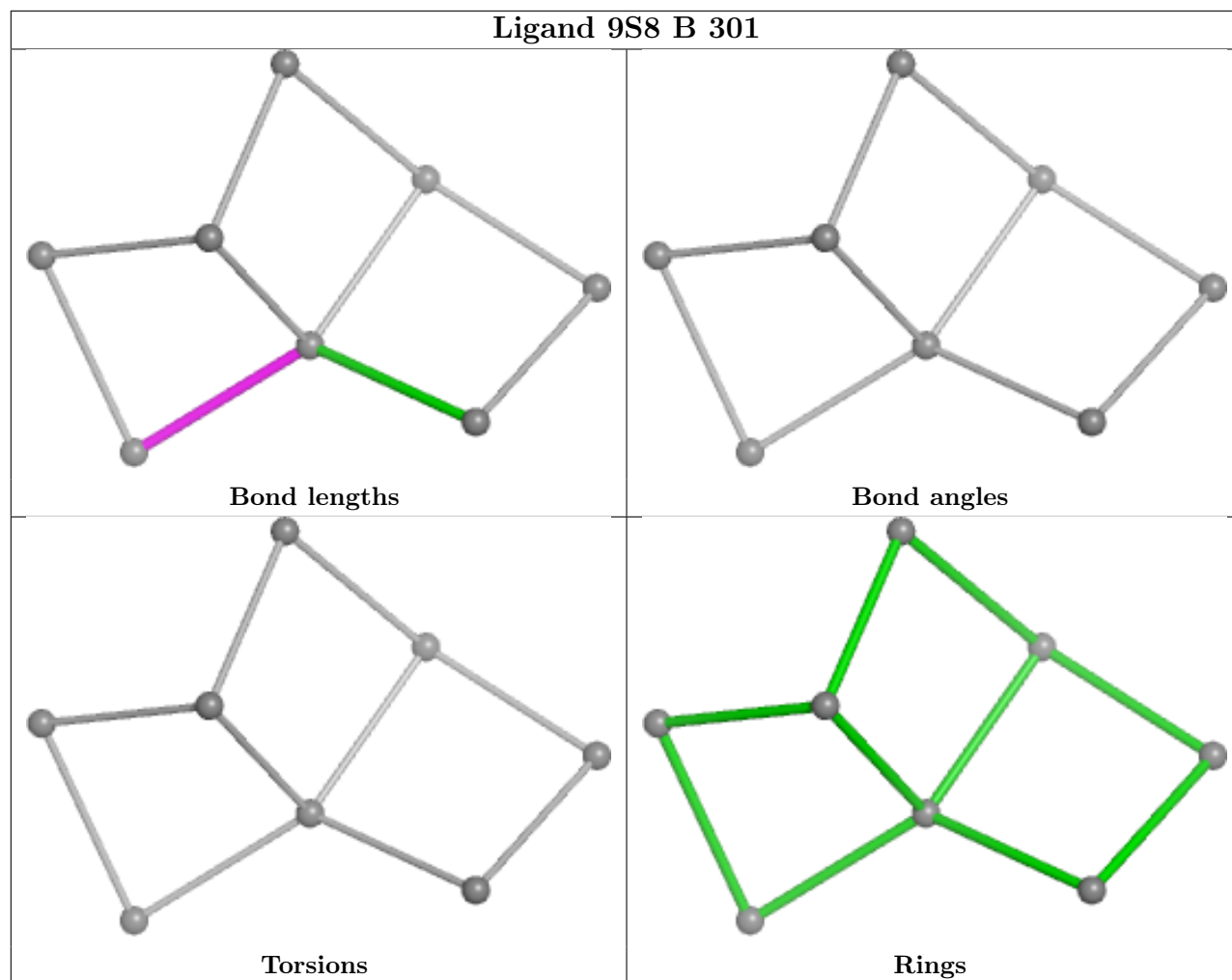
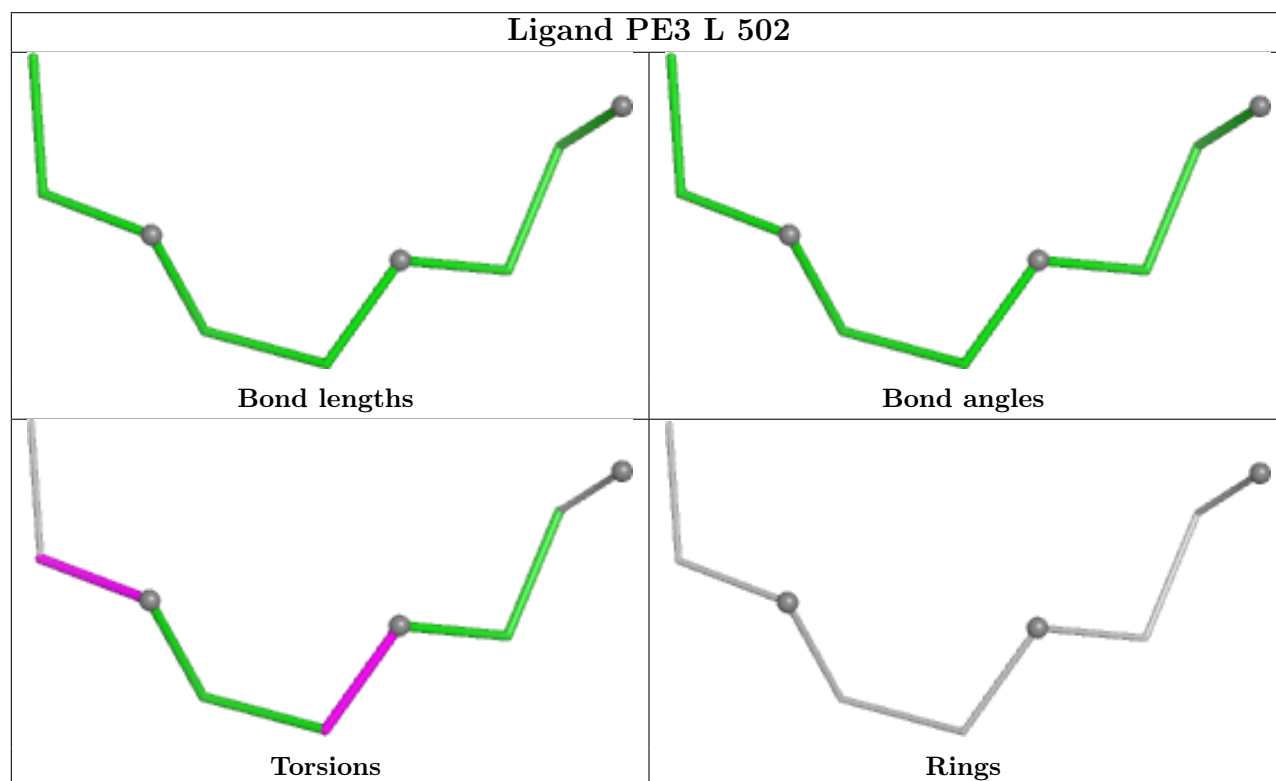
8 monomers are involved in 11 short contacts:

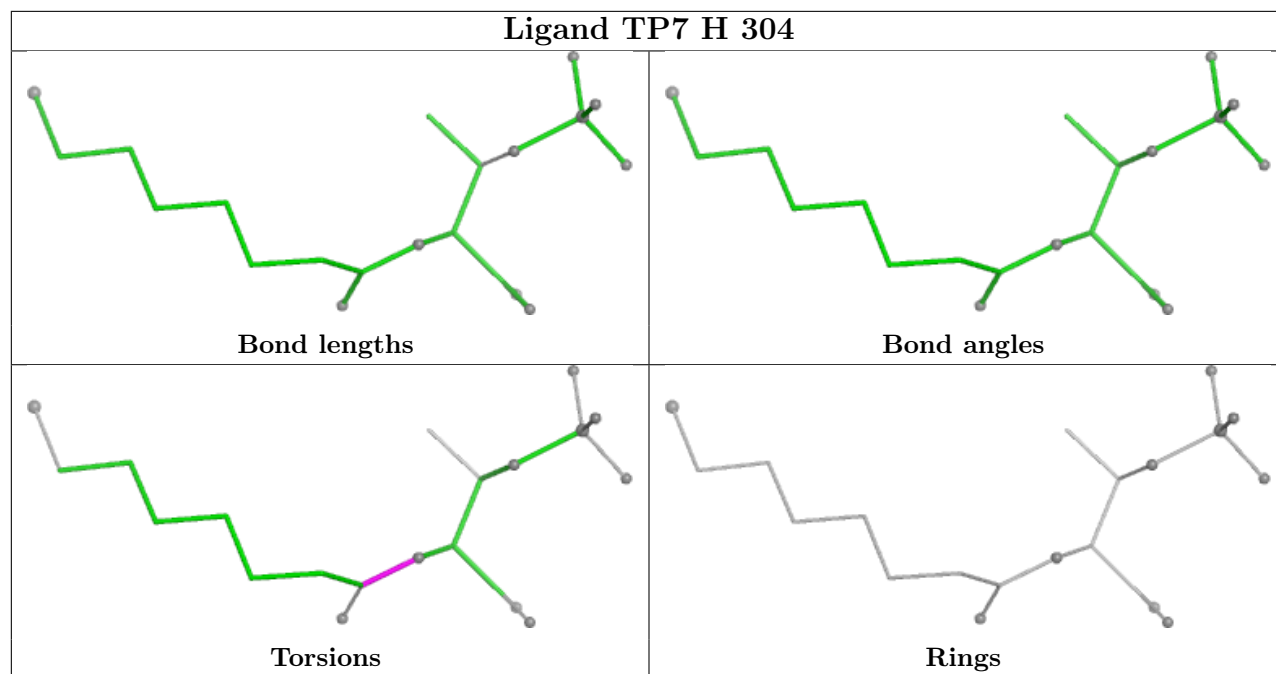
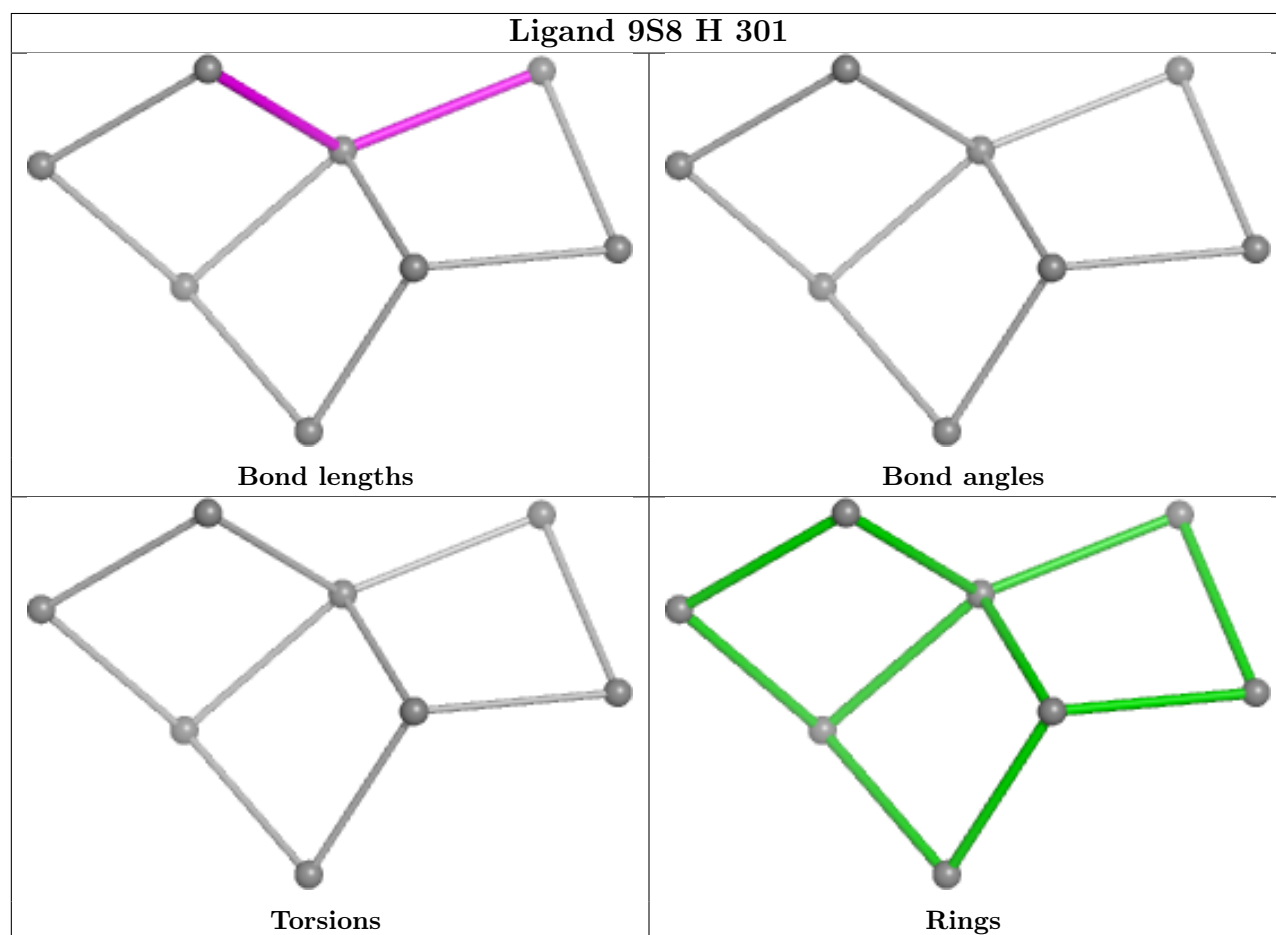
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	504	FCO	1	0
17	F	506	FCO	1	0
8	G	706	SF4	2	0
9	I	203	GOL	1	0
9	A	709	GOL	1	0
10	B	302	9S8	3	0
9	A	708	GOL	1	0
8	A	702	SF4	1	0

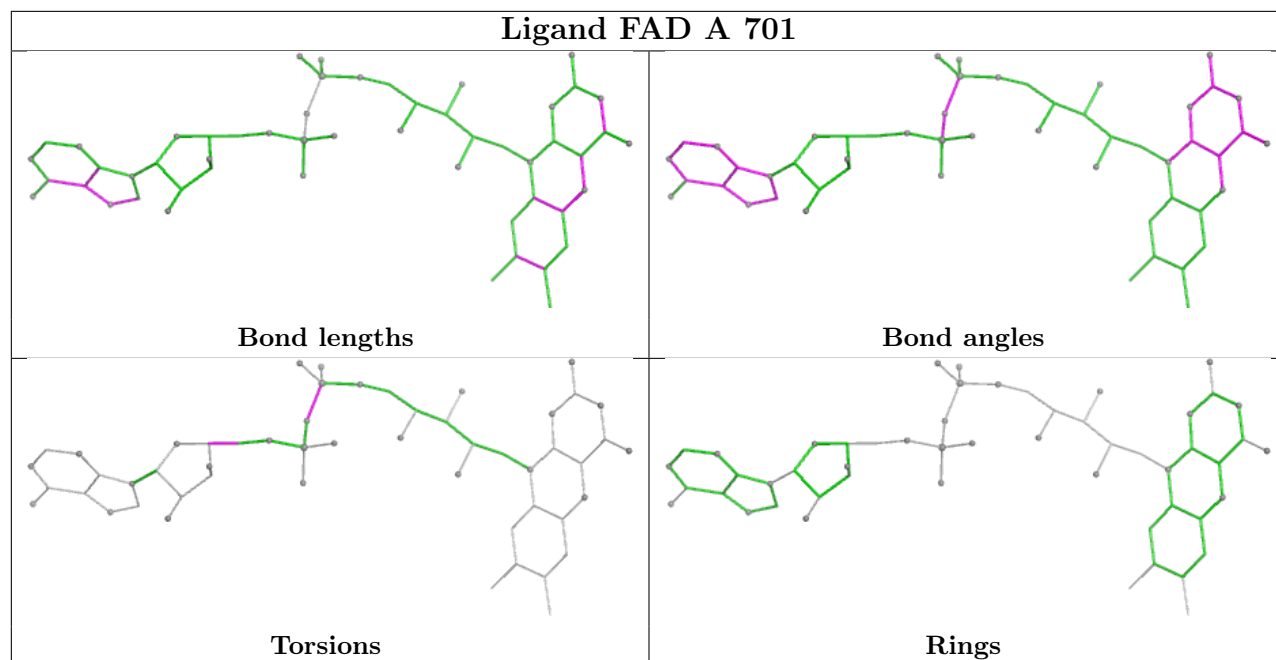
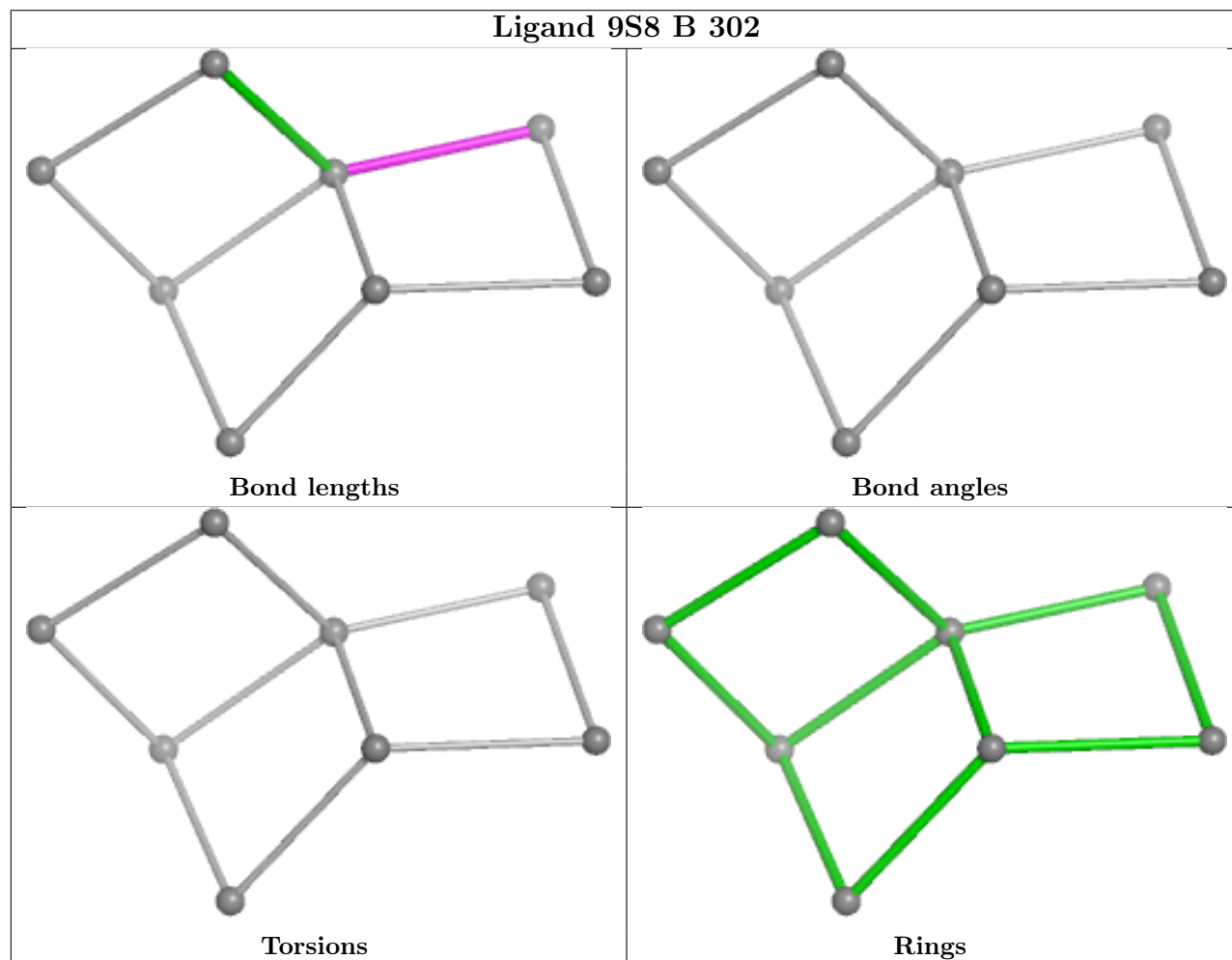
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

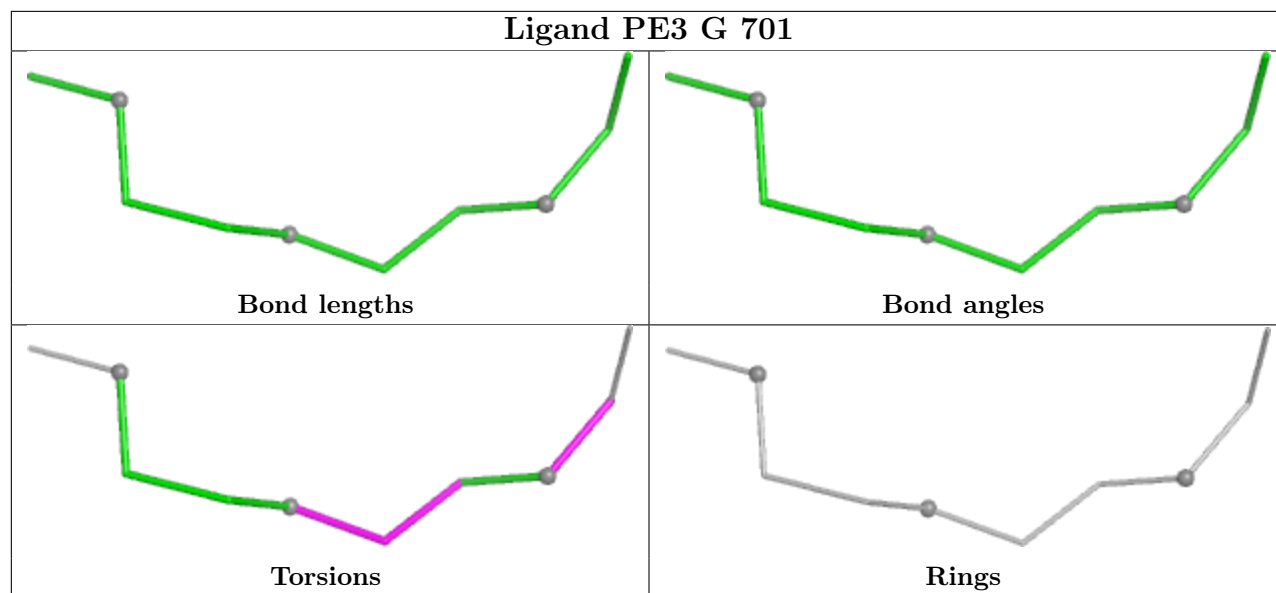
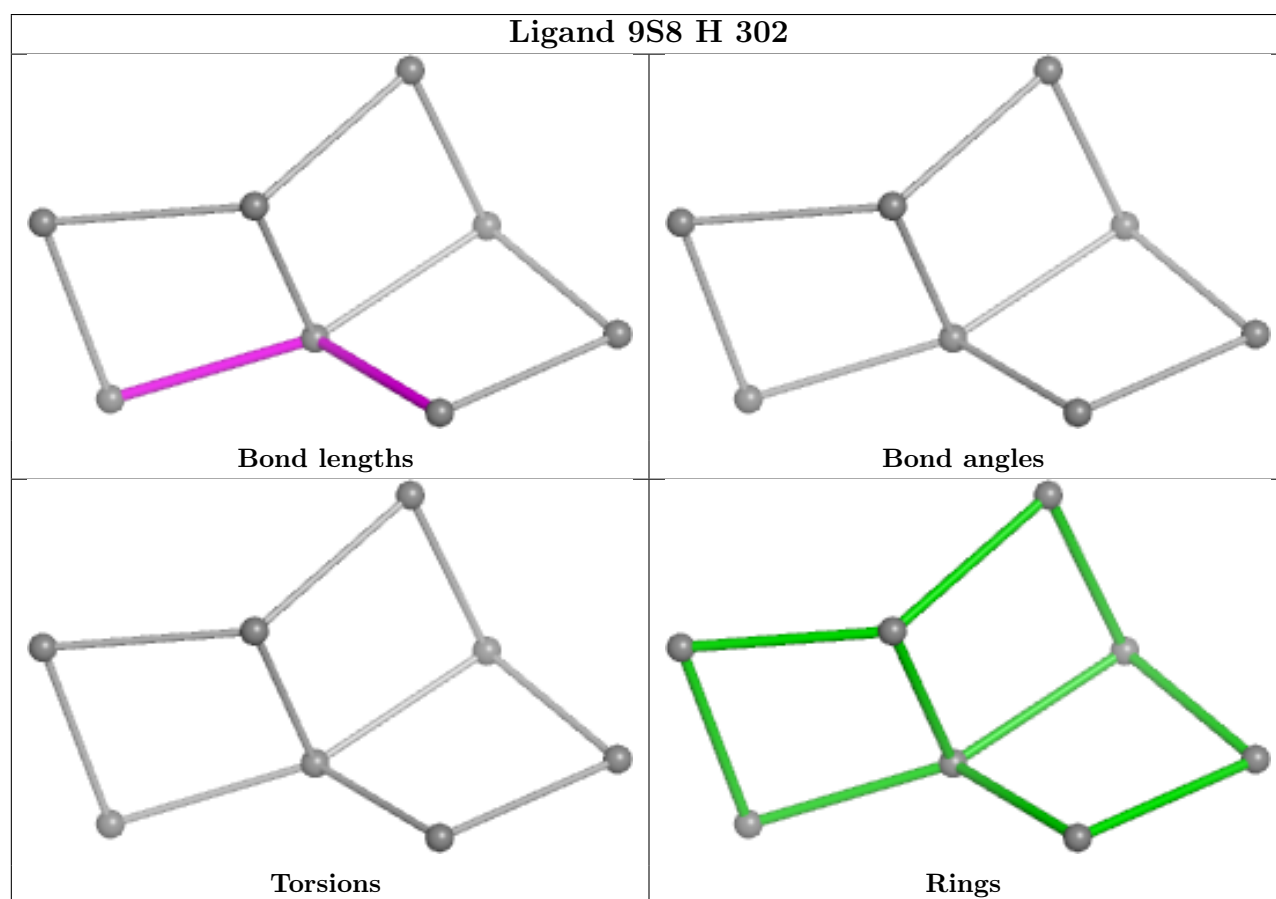
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

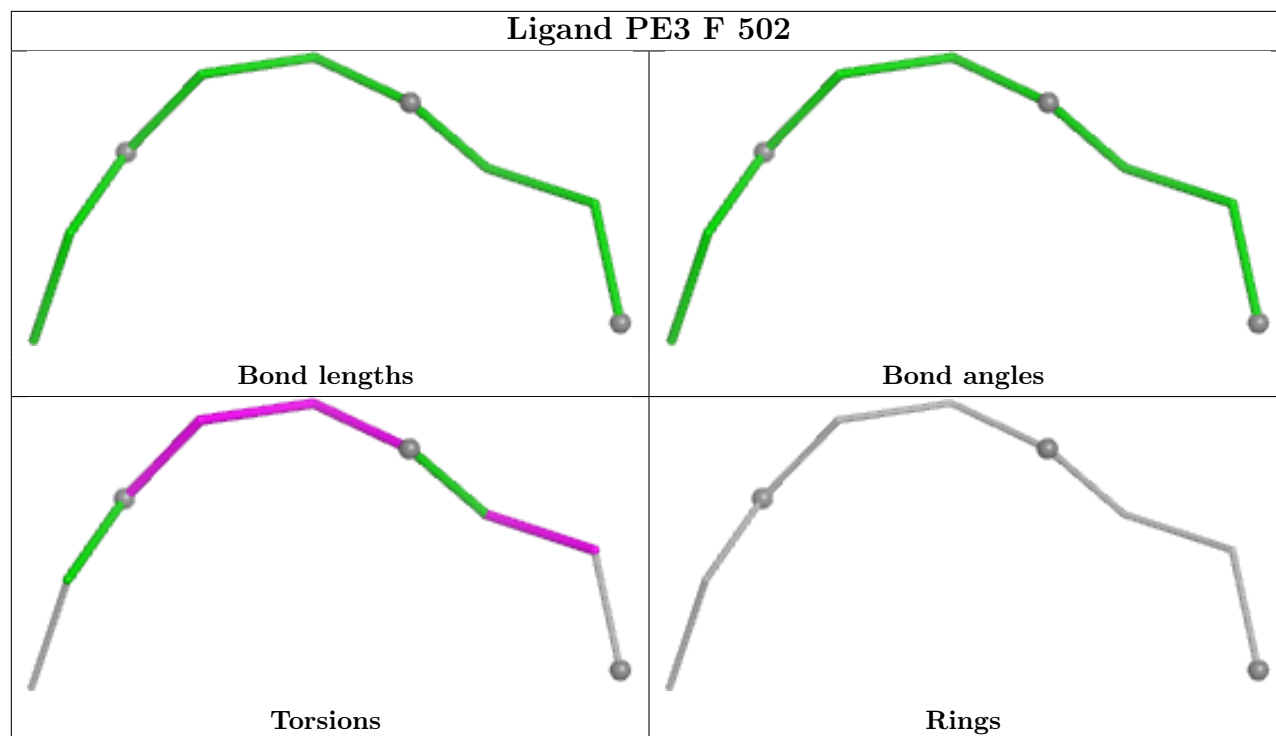












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	652/654 (99%)	0.90	105 (16%) 4 3	25, 44, 135, 185	0
1	G	652/654 (99%)	1.02	115 (17%) 4 3	24, 44, 108, 142	0
2	B	291/291 (100%)	0.99	25 (8%) 16 14	33, 53, 76, 88	0
2	H	291/291 (100%)	2.11	145 (49%) 0 0	44, 75, 123, 151	0
3	C	184/184 (100%)	0.98	20 (10%) 10 8	29, 49, 73, 88	0
3	I	183/184 (99%)	1.46	57 (31%) 1 1	28, 57, 105, 124	0
4	D	137/140 (97%)	0.28	4 (2%) 53 50	28, 38, 58, 88	0
4	J	138/140 (98%)	1.13	13 (9%) 14 11	33, 43, 63, 100	0
5	E	297/299 (99%)	0.62	22 (7%) 20 18	29, 43, 78, 101	0
5	K	297/299 (99%)	0.80	39 (13%) 7 5	23, 42, 79, 103	1 (0%)
6	F	447/473 (94%)	0.36	16 (3%) 46 43	27, 41, 69, 87	0
6	L	447/473 (94%)	0.62	25 (5%) 30 27	24, 42, 69, 109	0
All	All	4016/4082 (98%)	0.91	586 (14%) 6 4	23, 46, 96, 185	1 (0%)

The worst 5 of 586 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	266	LEU	6.4
2	H	263	LEU	6.2
1	A	252	CYS	6.0
1	A	258	ILE	6.0
1	A	294	ILE	5.9

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
14	ACT	G	702	4/4	0.46	0.27	88,90,90,91	0
14	ACT	D	202	4/4	0.60	0.27	75,75,76,76	0
9	GOL	I	204	6/6	0.71	0.17	52,52,54,54	0
14	ACT	E	301	4/4	0.74	0.21	56,59,60,60	0
9	GOL	A	709	6/6	0.77	0.24	61,63,64,65	0
15	PE3	G	701	10/43	0.78	0.25	63,69,76,78	0
15	PE3	L	502	9/43	0.79	0.23	61,66,69,70	0
12	SO4	B	304	5/5	0.80	0.12	74,76,76,77	0
9	GOL	I	203	6/6	0.80	0.20	54,55,58,58	0
9	GOL	K	304	6/6	0.80	0.23	67,69,70,71	0
19	TP7	H	304	21/21	0.80	0.17	72,78,84,85	0
8	SF4	A	703	8/8	0.82	0.17	176,177,177,177	0
15	PE3	F	503	13/43	0.83	0.20	63,64,72,73	0
15	PE3	F	502	9/43	0.84	0.23	74,74,76,77	0
9	GOL	D	203	6/6	0.85	0.16	58,63,64,65	0
8	SF4	A	704	8/8	0.86	0.12	132,134,134,134	0
9	GOL	A	708	6/6	0.88	0.16	58,59,59,60	0
10	9S8	H	301	8/8	0.91	0.11	65,71,77,78	0
8	SF4	G	708	8/8	0.93	0.08	102,102,104,104	0
11	COM	H	303	7/7	0.94	0.10	53,56,61,64	0
11	COM	B	303	7/7	0.94	0.12	65,66,67,69	0
14	ACT	F	504	4/4	0.94	0.09	40,42,44,46	0
8	SF4	K	303	8/8	0.96	0.07	47,48,49,52	0
10	9S8	B	301	8/8	0.96	0.06	39,43,47,47	0
10	9S8	B	302	8/8	0.96	0.06	41,43,47,47	0
7	FAD	G	704	53/53	0.96	0.08	25,31,46,52	0
8	SF4	G	707	8/8	0.96	0.07	72,73,75,75	0
7	FAD	A	701	53/53	0.96	0.08	25,31,45,49	0
8	SF4	G	709	8/8	0.96	0.06	39,41,45,46	0
16	FE	G	703	1/1	0.96	0.09	28,28,28,28	1
8	SF4	G	710	8/8	0.96	0.07	35,41,43,43	0
10	9S8	H	302	8/8	0.97	0.05	56,58,61,61	0

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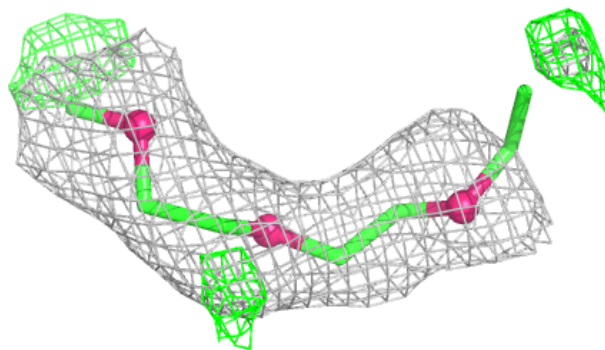
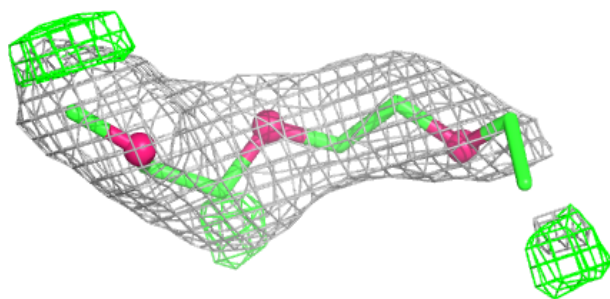
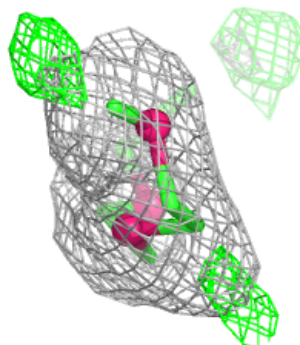
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SF4	G	705	8/8	0.97	0.05	38,42,45,47	0
8	SF4	K	301	8/8	0.98	0.05	29,30,31,33	0
8	SF4	K	302	8/8	0.98	0.06	38,40,40,41	0
8	SF4	A	707	8/8	0.98	0.05	42,44,46,48	0
8	SF4	C	201	8/8	0.98	0.05	33,34,36,36	0
8	SF4	E	303	8/8	0.98	0.05	42,44,47,49	0
8	SF4	A	706	8/8	0.98	0.04	38,40,42,43	0
8	SF4	I	201	8/8	0.98	0.04	32,33,35,35	0
8	SF4	I	202	8/8	0.98	0.05	38,42,42,43	0
13	FES	D	201	4/4	0.98	0.05	34,35,36,39	0
17	FCO	F	506	7/7	0.98	0.08	28,28,32,32	0
13	FES	J	200	4/4	0.98	0.06	36,38,39,41	0
8	SF4	G	706	8/8	0.99	0.04	26,27,28,29	0
8	SF4	C	202	8/8	0.99	0.04	38,38,41,41	0
8	SF4	E	302	8/8	0.99	0.06	38,40,41,42	0
16	FE	F	505	1/1	0.99	0.02	29,29,29,29	0
8	SF4	A	705	8/8	0.99	0.03	29,33,33,33	0
8	SF4	E	304	8/8	0.99	0.05	45,46,50,51	0
17	FCO	L	504	7/7	0.99	0.08	26,28,30,31	0
18	NI	F	507	1/1	0.99	0.04	31,31,31,31	0
18	NI	L	505	1/1	0.99	0.07	31,31,31,31	0
8	SF4	A	702	8/8	0.99	0.04	27,28,29,29	0
16	FE	L	503	1/1	1.00	0.02	29,29,29,29	0

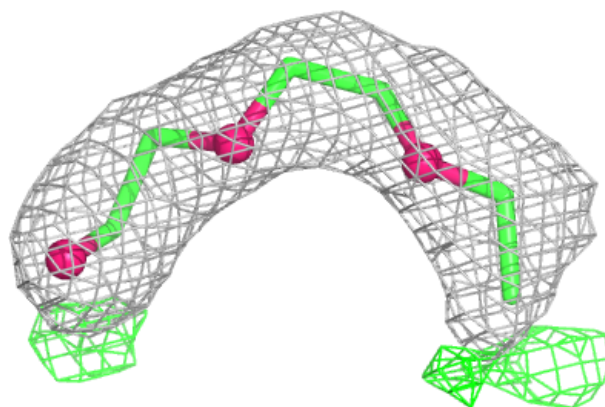
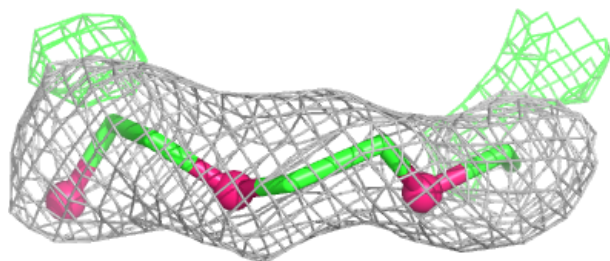
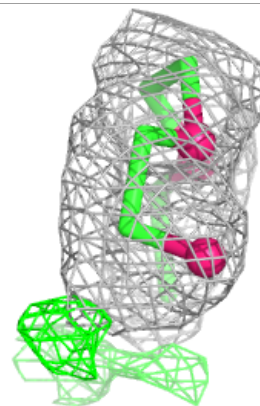
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE3 G 701:

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

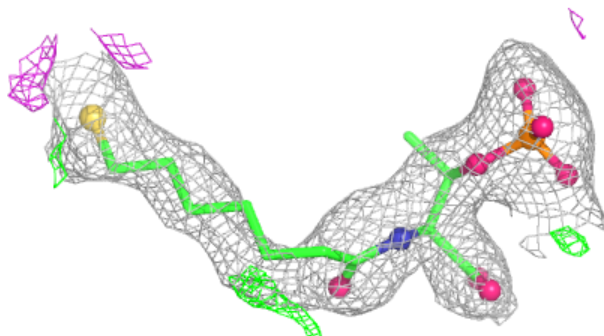
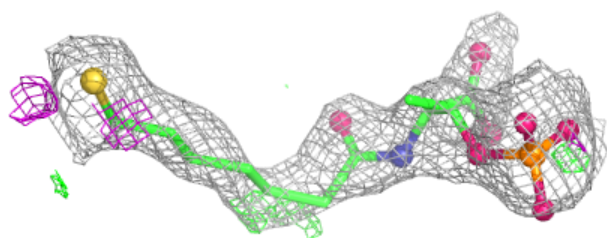
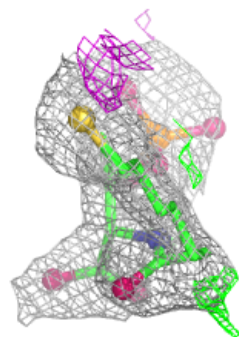
**Electron density around PE3 L 502:**

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

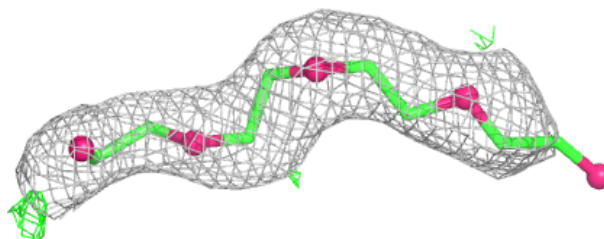
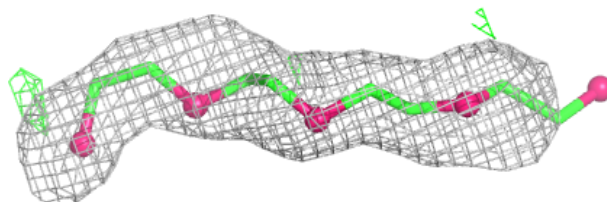
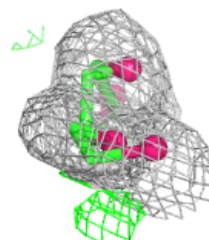


Electron density around TP7 H 304:

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

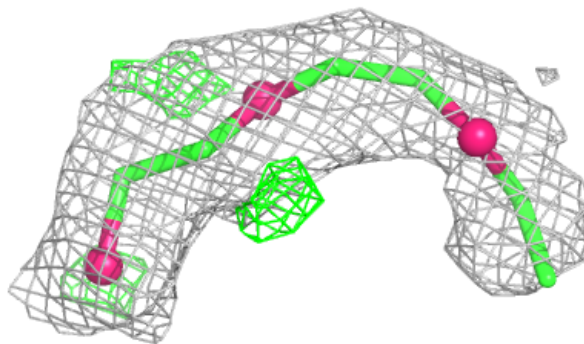
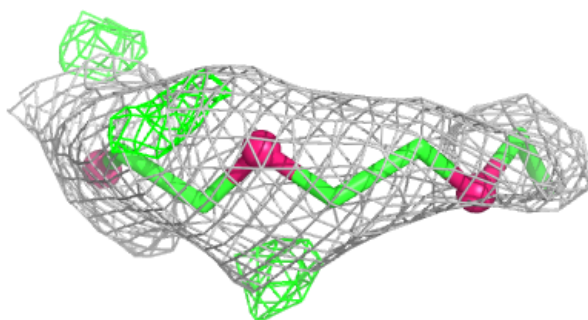
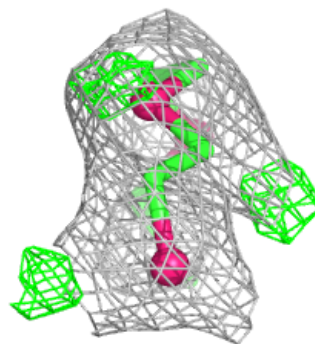
**Electron density around PE3 F 503:**

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



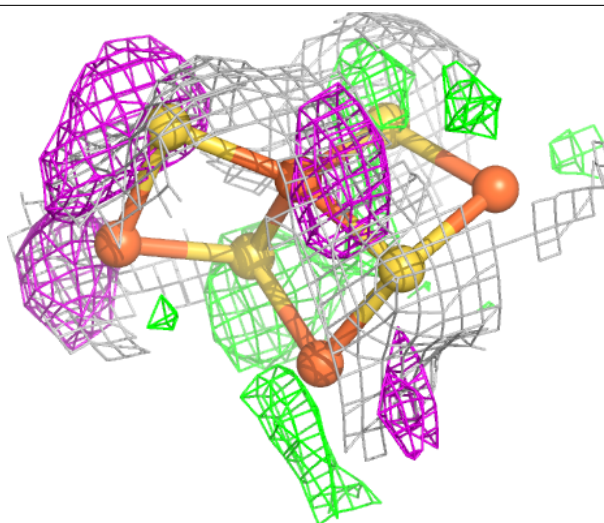
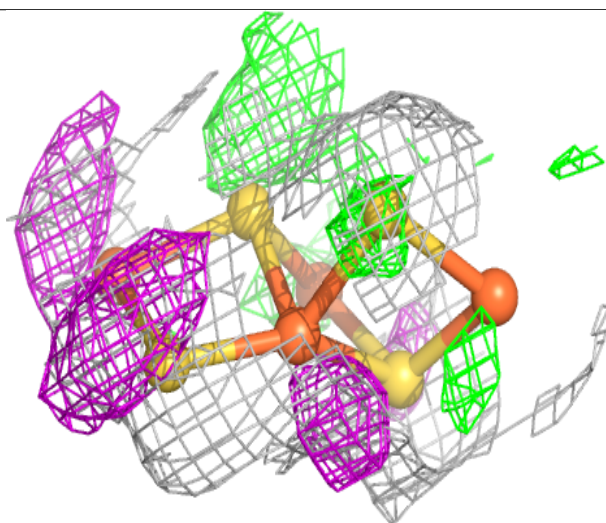
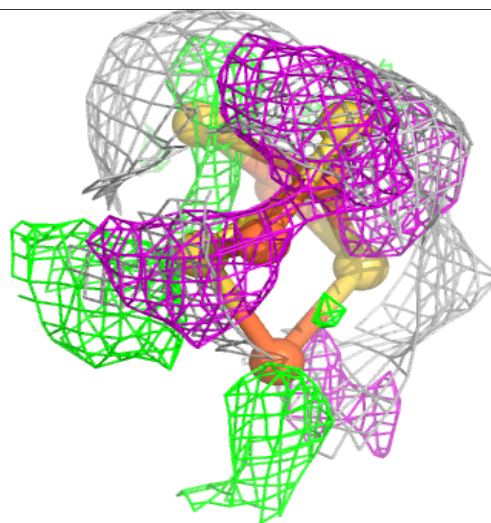
Electron density around PE3 F 502:

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



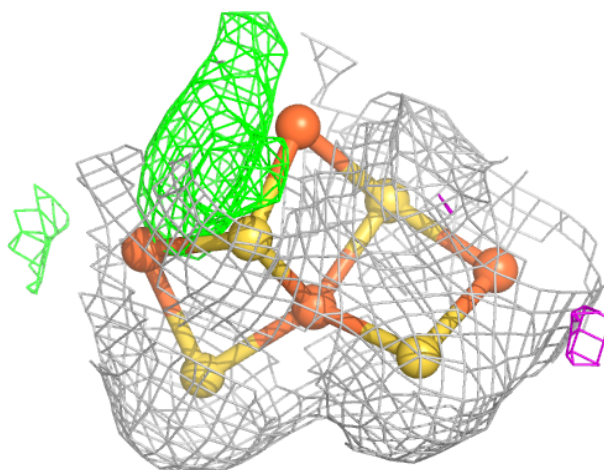
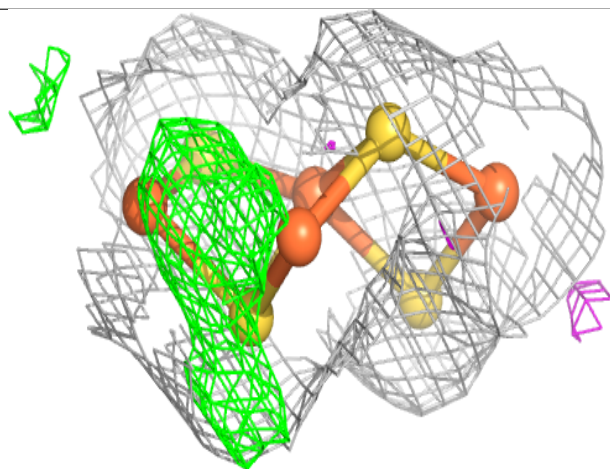
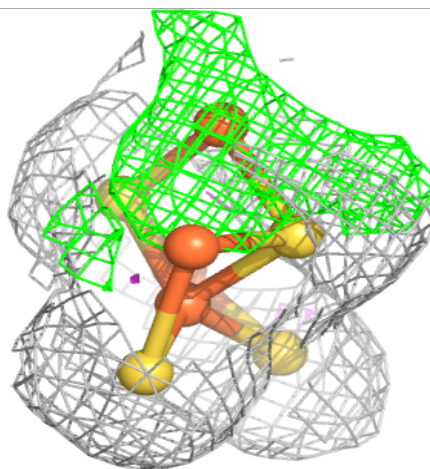
Electron density around 9S8 H 301:

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



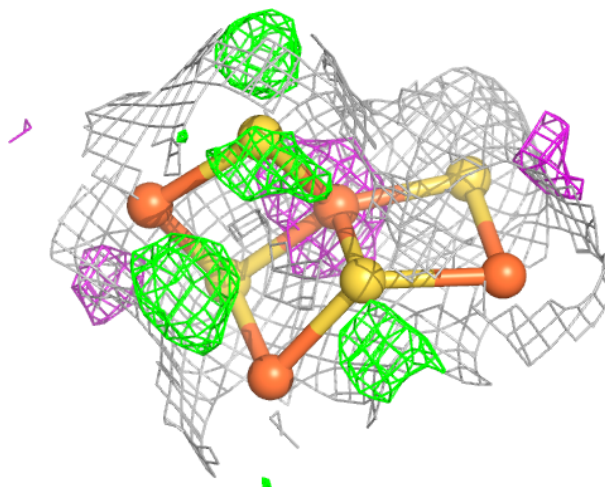
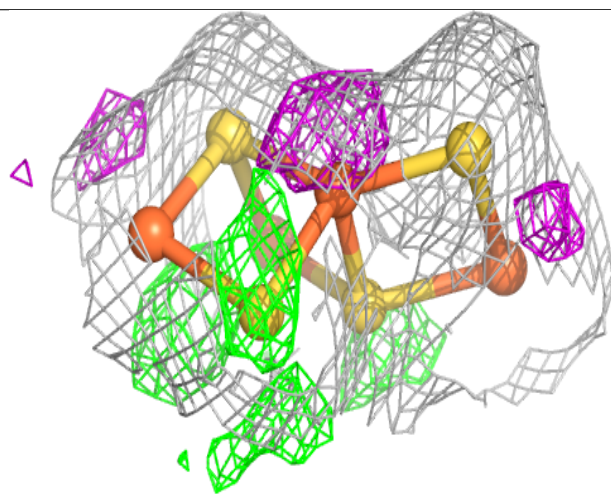
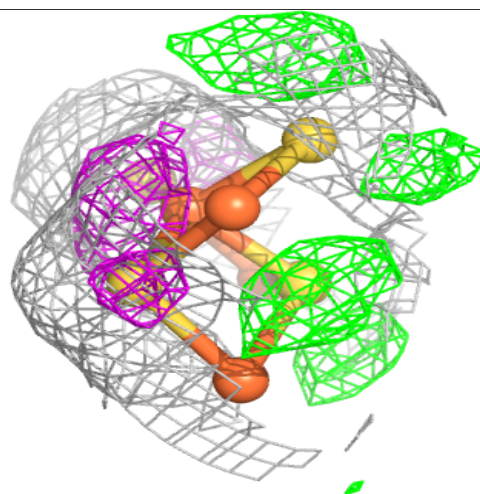
Electron density around 9S8 B 301:

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



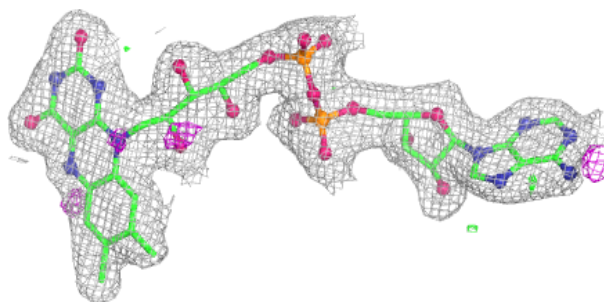
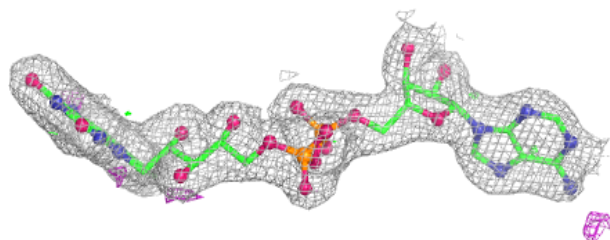
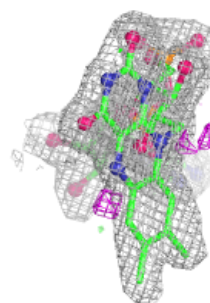
Electron density around 9S8 B 302:

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

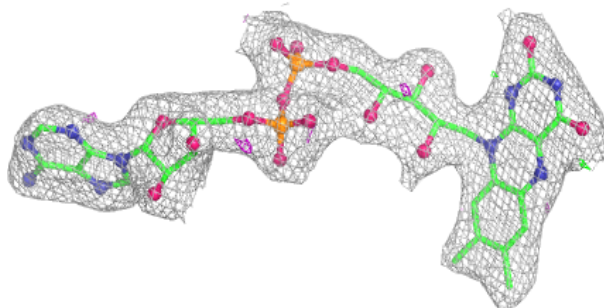
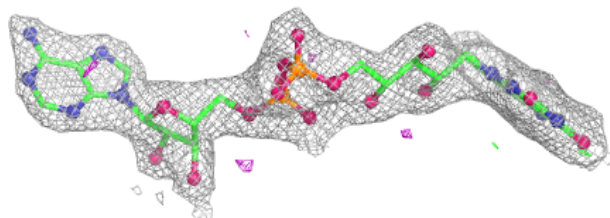
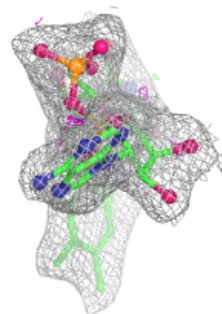


Electron density around FAD G 704:

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

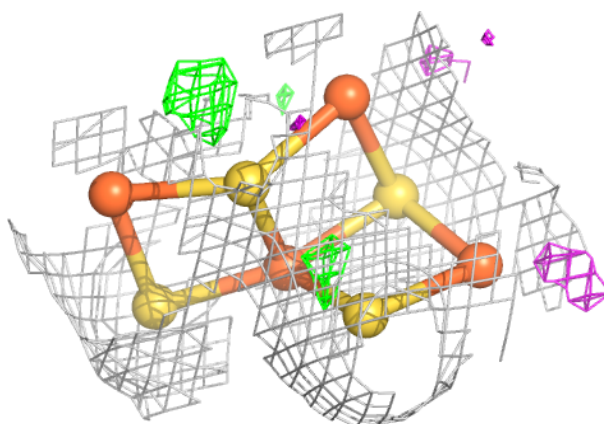
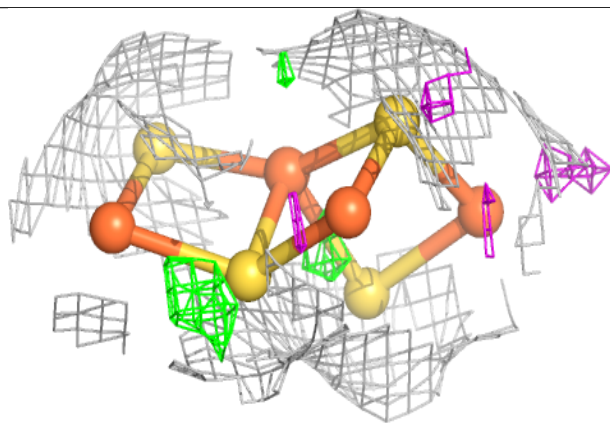
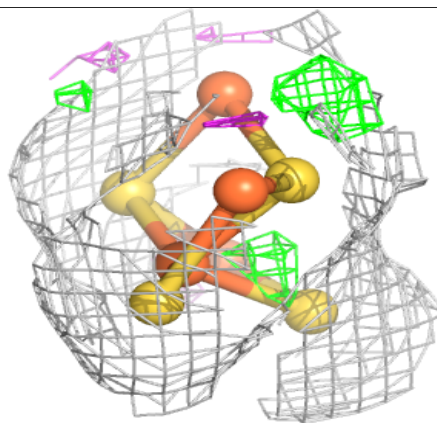
**Electron density around FAD A 701:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.