Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2026 – 12:57 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 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

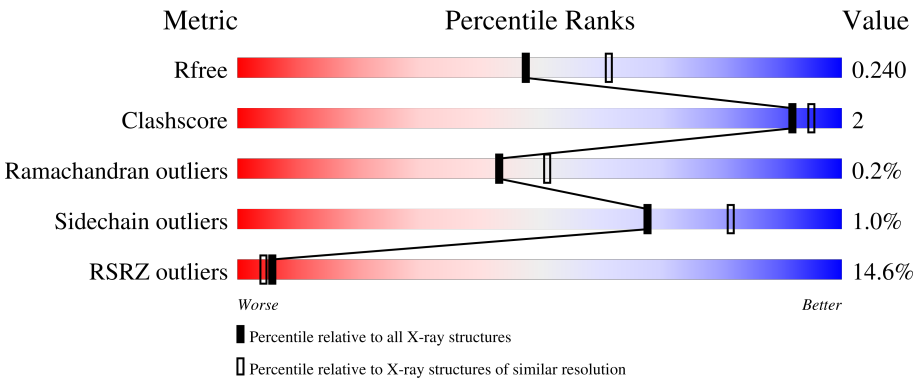
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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 <=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	16% 93% 6%
1	G	654	18% 92% 7%
2	B	291	9% 97% .
2	H	291	50% 91% 9%
3	C	184	11% 97% . .

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Mol	Chain	Length	Quality of chain
3	I	184	31% 92% 7%
4	D	140	3% 91% 6%
4	J	140	9% 97%
5	E	299	7% 96%
5	K	299	13% 95%
6	F	473	3% 88% 5% 5%
6	L	473	5% 88% 6% 5%

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

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

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	652	4979	3142	845	943	49	0	0	0
1	G	652	4979	3142	845	943	49	0	0	0

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

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

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

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

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

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

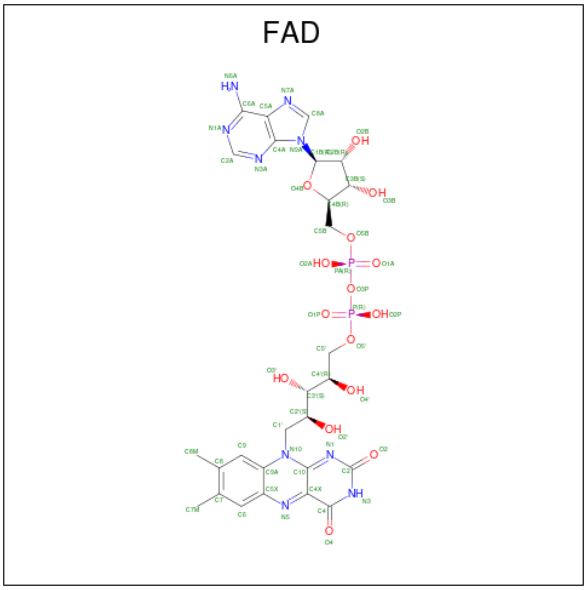
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

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

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

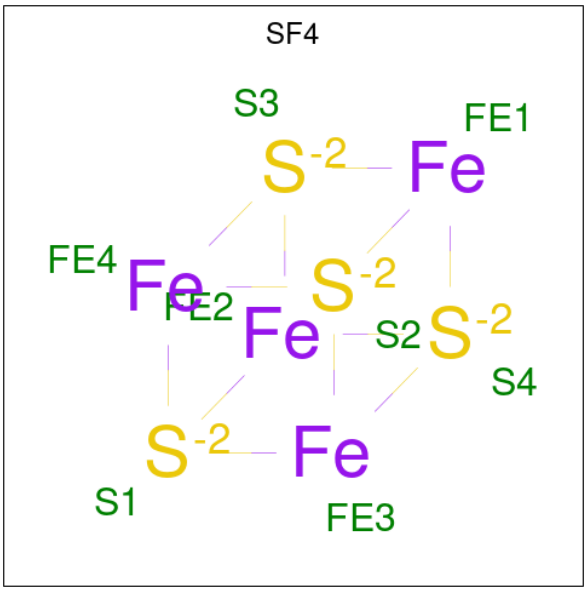
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	447	3521	2230	600	672	19	0	0	0
6	L	447	3521	2230	600	672	19	0	0	0

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



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

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



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

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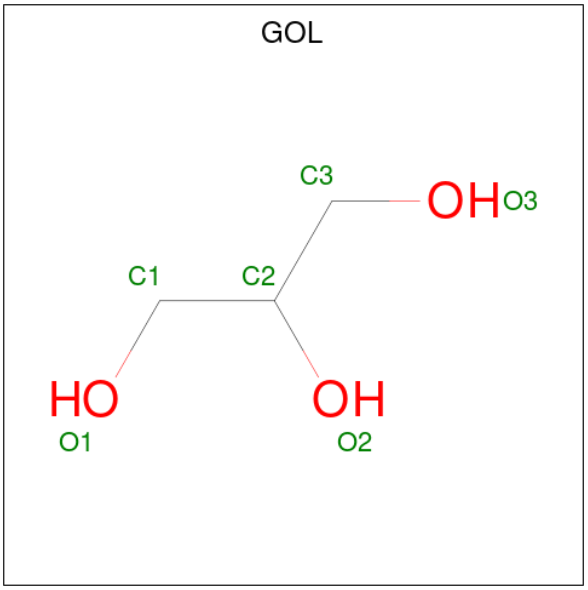
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	Fe	S		0	0
			8	4	4			
8	G	1	Total	Fe	S		0	0
			8	4	4			
8	G	1	Total	Fe	S		0	0
			8	4	4			
8	I	1	Total	Fe	S		0	0
			8	4	4			
8	I	1	Total	Fe	S		0	0
			8	4	4			
8	K	1	Total	Fe	S		0	0
			8	4	4			
8	K	1	Total	Fe	S		0	0
			8	4	4			
8	K	1	Total	Fe	S		0	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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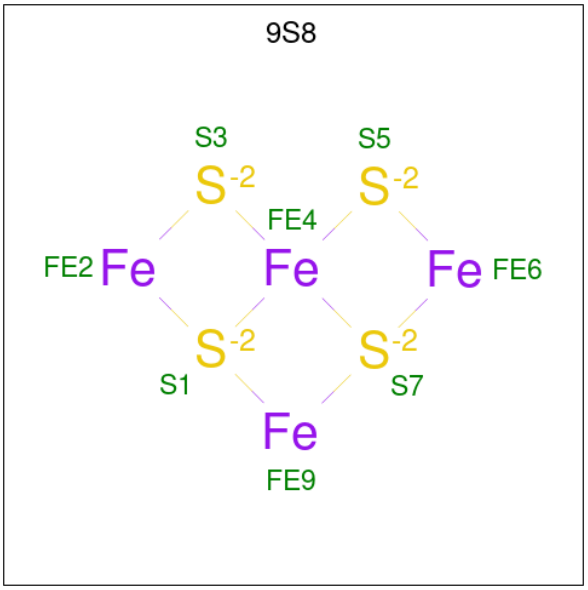
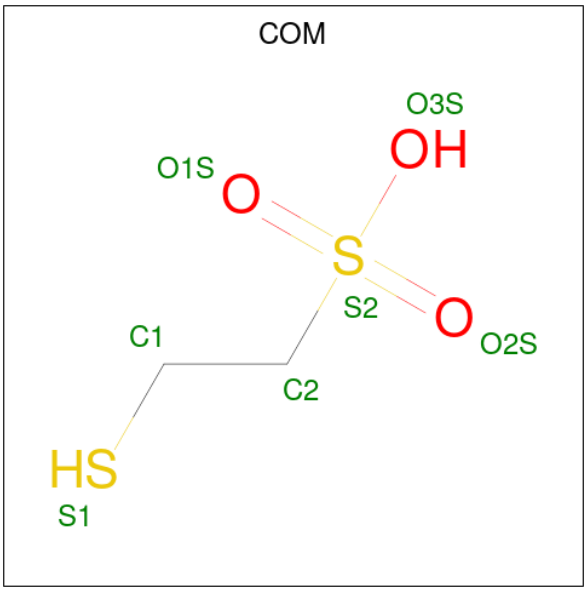
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	K	1	Total C O 6 3 3	0	0

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



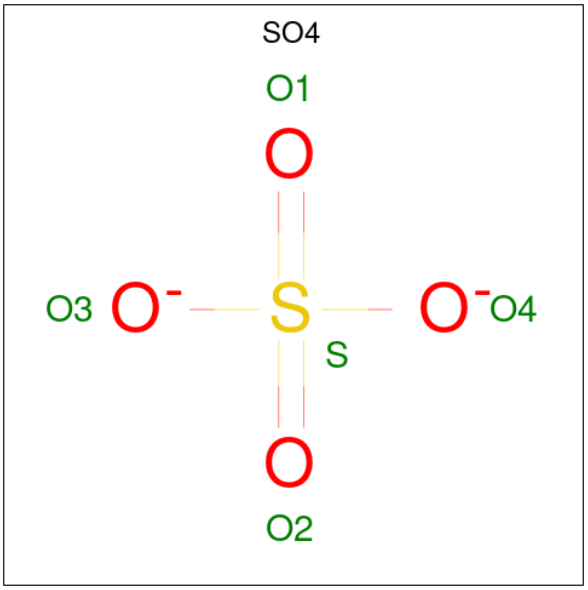
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 8 4 4	0	0
10	B	1	Total Fe S 8 4 4	0	0
10	H	1	Total Fe S 8 4 4	0	0
10	H	1	Total Fe S 8 4 4	0	0

- Molecule 11 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



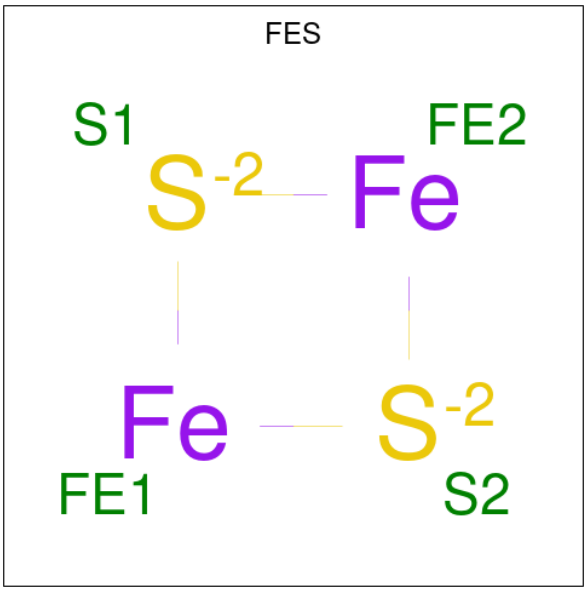
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
11	B	1	7	2	3	2	0	0
			Total	C	O	S		
11	H	1	7	2	3	2	0	0

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



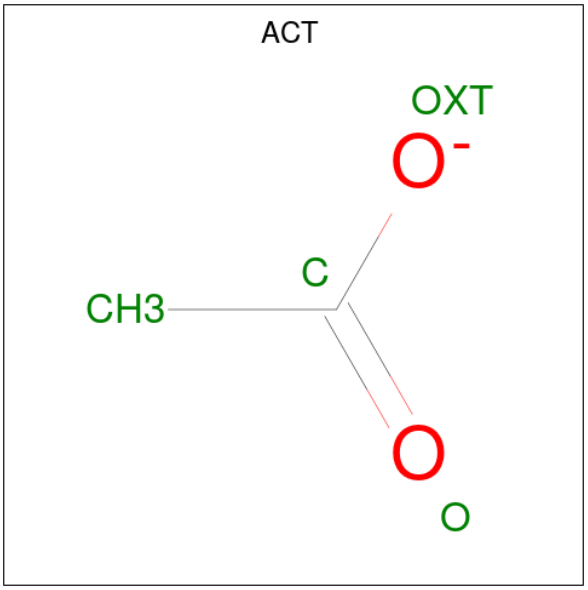
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
12	B	1	5	4	1	0	0

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



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

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



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

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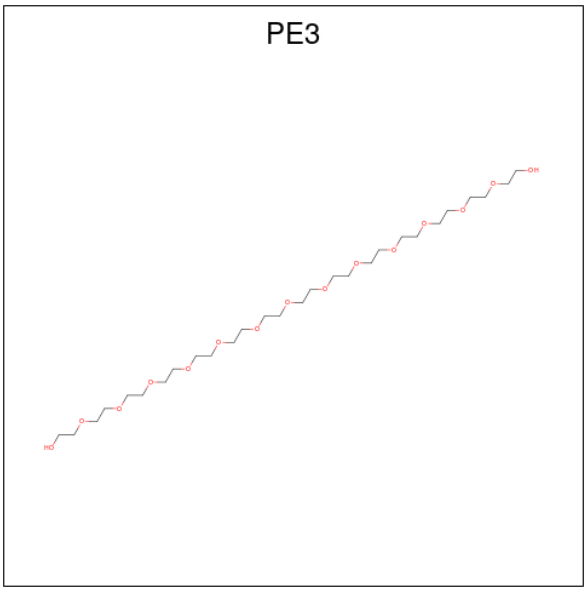
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	F	1	4	2	2	0	0
14	G	1	4	2	2	0	0

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

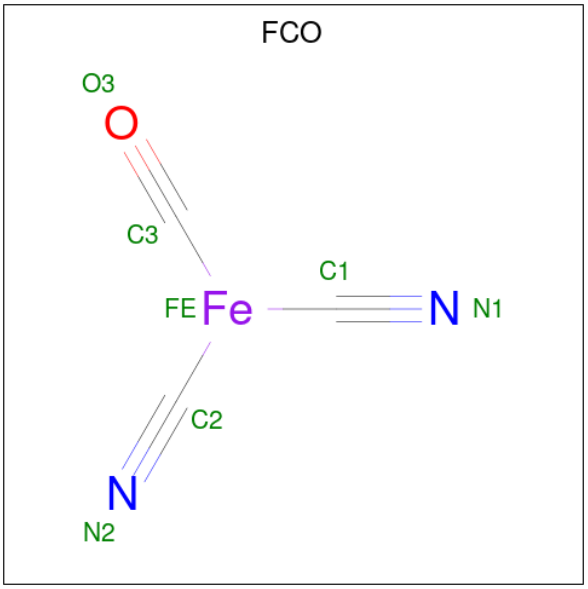


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	F	1	9	6	3	0	0
15	F	1	13	8	5	0	0
15	G	1	10	7	3	0	0
15	L	1	9	6	3	0	0

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

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

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

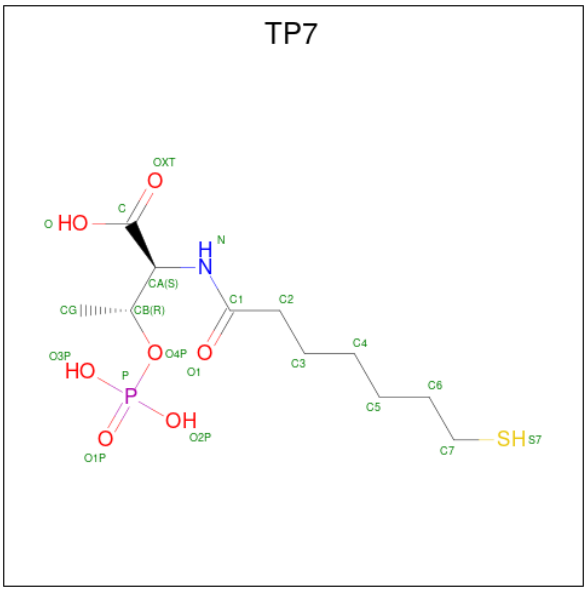


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
17	F	1	7	3	1	2	1	0	0
			Total	C	Fe	N	O		
17	L	1	7	3	1	2	1	0	0

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

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

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



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

- Molecule 20 is water.

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

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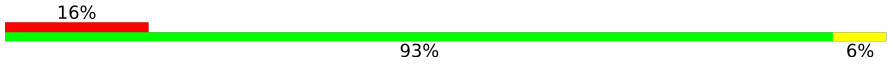
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	L	132	132	132	0	0

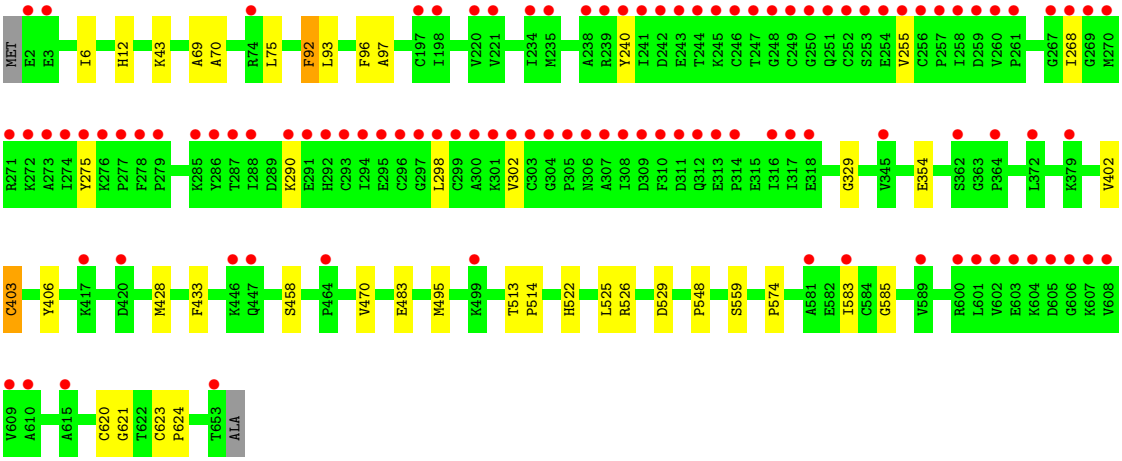
3 Residue-property plots (i)

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

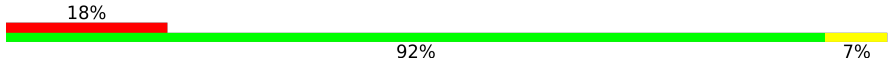
Chain A:

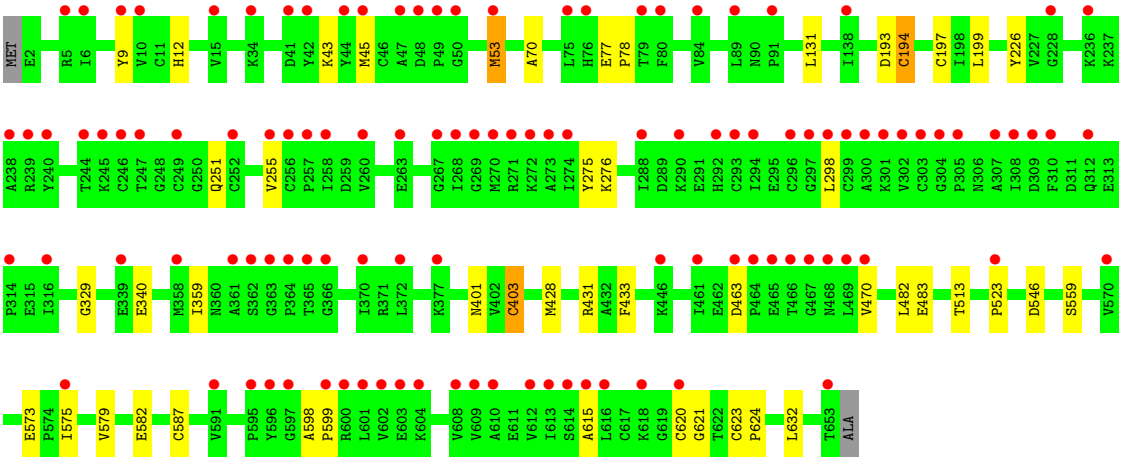




• Molecule 1: Heterodisulfide reductase, subunit A

Chain G:





• Molecule 2: Heterodisulfide reductase, subunit B

Chain B: 9% 97%

M1 T24 V34 A39 C42 P43 A60 I66 C78 H93 K96 E97 A98 L99 V102 K105 K108 G115 I126 I130 A136 I145 V161 V177 M211 K221 P232 G241 E244 K248 F249 G250 K251 K273

L287 I291

- Molecule 2: Heterodisulfide reductase, subunit B

Chain H: 50% 91% 9%

M1 K2 Y3 A4 F5 F6 L7 G8 C9 I10 M11 P12 N13 R14 Y15 A16 G17 V18 E19 A20 A21 T22 R23 T24 V25 M26 L29 G30 V31 E32 L33 V34 T37 G38 A39 C42 P43 A44 P45 F48 G49 S50 T55 A67 I74 V75 T76 V77 C78 S84 L85

H90 L91 L92 H93 A98 L99 N100 F101 V102 L106 D107 K108 V109 G110 K111 E112 Y113 K114 K118 F122 A123 I126 Y127 N128 D129 I130 G131 V132 D133 K134 I135 A136 E137 K138 V139 E140 R141 P142 L143 N144 I145 N146 V147 G148 V149 V171 M172 L173 I176 V177 E178 A179 T180

G181 A182 K183 S184 V185 P186 Y187 E206 L207 S208 L209 N213 I220 K221 A222 G223 A224 D225 C226 T227 V228 N229 V230 C231 P232 F233 C234 H235 L236 Q237 F238 D239 R240 G241 Q242 I243 E244 I245 K246 E247 K248 F249 G250 K251 E252 Y253 N254 F255 P256 V257 L258 H259 L260 S261 Q262 L263 L264

G265 L266 A267 M268 G269 M270 D271 P272 K273 D274 L275 A276 L277 S278 V279 H280 Q281 I282 S283 V284 D285 P286 L287 L288 K289 K290 I291

- Molecule 3: Heterodisulfide reductase, subunit C

Chain C: 11% 97%

M1 I2 Y3 S4 S5 N8 K9 L31 Y35 P45 R49 K60 A61 L62 L63 G64 M65 D66 D67 K107 I141 G142 L143 E166 E178 K179 G180 E184

- Molecule 3: Heterodisulfide reductase, subunit C

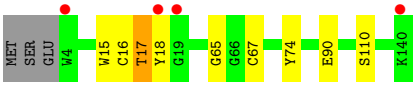
Chain I: 31% 92% 7%

M1 I2 Y3 K9 L31 Y35 S43 R49 D66 D67 V68 I74 E85 V93 I97 R101 N102 L103 A104 A105 Q106 K107 G108 N109 M110 A111 K112 M116 T117 A118 M119 Y120 V121 L122 K123 H126 A127 V128 F129 A130 N131 K132 N133 T134 A135 E136 L137

R138 K139 S140 I141 G142 L143 K146 A147 P148 F152 K155 N161 T162 L163 F169 L172 I173 G174 F175 D176 W177 E178 K179 G180 A181 L182 K183 GLU

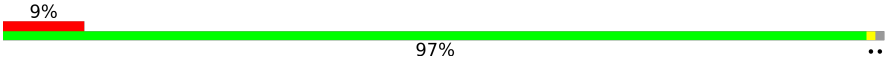
- Molecule 4: Methyl-viologen reducing hydrogenase, subunit D

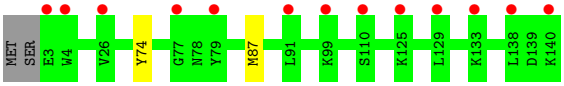
Chain D: 3% 91% 6%



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

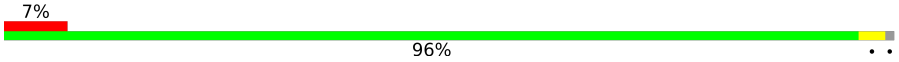
Chain J:

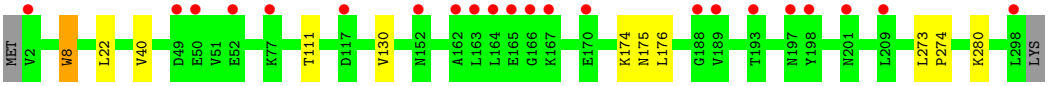




• Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

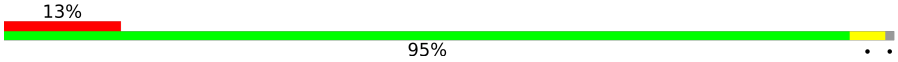
Chain E:

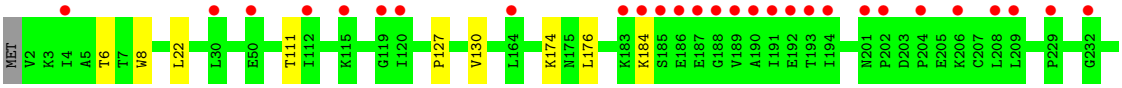


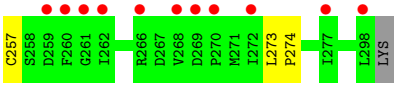


• Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

Chain K:

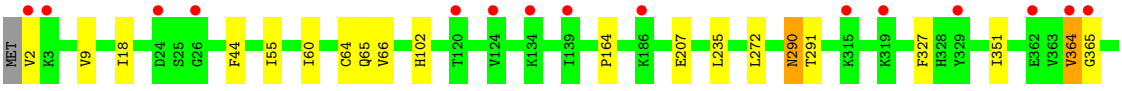


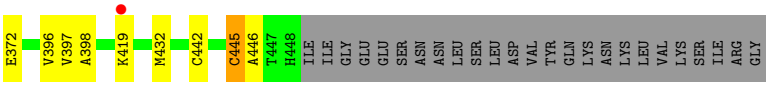




• Molecule 6: Methyl-viologen reducing hydrogenase, subunit A

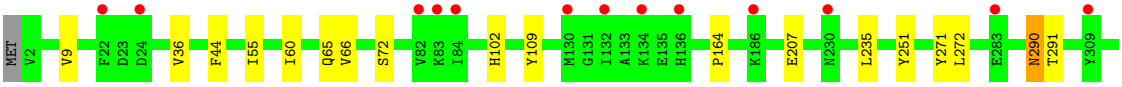
Chain F:

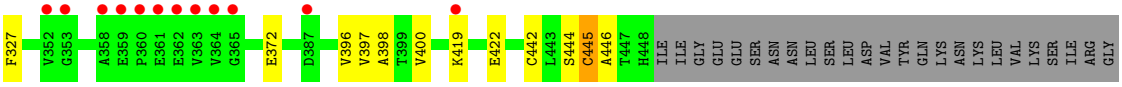




• Molecule 6: Methyl-viologen reducing hydrogenase, subunit A

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	366.22Å 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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
6	F	44	PHE	CA-CB-CG	7.25	121.05	113.80
6	L	44	PHE	CA-CB-CG	7.19	120.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	176	LEU	N-CA-C	7.07	119.84	111.71
6	F	9	VAL	N-CA-C	-6.98	100.57	109.30
5	K	176	LEU	N-CA-C	6.96	119.72	111.71
6	L	9	VAL	N-CA-C	-6.95	100.62	109.30
6	F	327	PHE	N-CA-C	-6.80	103.94	111.82
6	F	290	ASN	CA-CB-CG	6.35	118.95	112.60
6	L	290	ASN	CA-CB-CG	6.33	118.93	112.60
6	L	327	PHE	N-CA-C	-6.33	104.48	111.82
6	L	60	ILE	N-CA-C	-6.17	104.49	110.72
6	F	60	ILE	N-CA-C	-6.00	104.66	110.72
6	F	419	LYS	N-CA-C	-5.92	105.15	112.72
1	A	433	PHE	N-CA-C	5.82	120.45	113.23
1	G	433	PHE	N-CA-C	5.79	120.41	113.23
5	K	130	VAL	N-CA-C	-5.76	103.77	110.05
1	G	329	GLY	N-CA-C	5.72	121.32	111.47
1	G	199	LEU	N-CA-C	5.72	117.32	111.14
1	G	194	CYS	N-CA-C	-5.71	102.84	110.55
6	F	364	VAL	N-CA-C	-5.63	99.04	107.37
1	A	93	LEU	N-CA-C	-5.53	105.85	112.59
6	L	419	LYS	N-CA-C	-5.50	105.68	112.72
1	A	428	MET	N-CA-C	-5.50	105.68	112.72
1	G	428	MET	N-CA-C	-5.48	105.70	112.72
5	E	130	VAL	N-CA-C	-5.46	104.09	110.05
6	F	55	ILE	N-CA-C	-5.42	107.15	111.81
6	L	207	GLU	N-CA-C	-5.40	105.47	111.36
6	L	55	ILE	N-CA-C	-5.37	107.19	111.81
2	H	234	CYS	N-CA-C	-5.33	105.56	111.36
6	F	207	GLU	N-CA-C	-5.32	105.56	111.36
1	A	6	ILE	N-CA-C	5.30	116.60	108.71
1	G	463	ASP	N-CA-C	-5.29	99.01	108.47
4	D	15	TRP	N-CA-C	5.28	119.63	111.56
6	L	444	SER	N-CA-C	-5.20	105.69	111.36
1	G	193	ASP	N-CA-C	-5.17	103.86	110.53
4	D	18	TYR	N-CA-C	-5.17	105.77	111.71
1	G	251	GLN	N-CA-C	-5.12	105.88	111.82
6	L	271	TYR	N-CA-C	-5.12	106.98	113.18
1	G	275	TYR	N-CA-C	5.11	116.75	109.14
6	F	396	VAL	N-CA-C	-5.09	99.63	106.85
6	L	396	VAL	N-CA-C	-5.08	99.64	106.85
1	G	546	ASP	CA-C-N	5.07	124.39	120.33
1	G	546	ASP	C-N-CA	5.07	124.39	120.33
6	L	109	TYR	N-CA-C	5.04	117.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	401	ASN	N-CA-C	5.04	121.54	110.80
1	A	329	GLY	N-CA-C	5.01	120.09	111.47
1	A	92	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	7	0	6	0	0
11	H	7	0	5	0	0
12	B	5	0	0	0	0
13	D	4	0	0	0	0
13	J	4	0	0	0	0
14	D	4	0	3	0	0
14	E	4	0	3	0	0
14	F	4	0	3	0	0
14	G	4	0	3	0	0
15	F	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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:226:TYR:CZ	1:G:615:ALA:HB1	2.28	0.68
1:A:403:CYS:HB2	8:A:702:SF4:S1	2.36	0.66
10:B:302:9S8:S1	10:B:302:9S8:FE4	1.90	0.63
2:H:42:CYS:SG	2:H:43:PRO:C	2.89	0.56
1:G:598:ALA:HB3	1:G:599:PRO:HD3	1.87	0.55
2:H:257:VAL:C	2:H:258:LEU:HD12	2.31	0.55
1:A:525:LEU:C	1:A:526:ARG:HG3	2.31	0.55
4:D:17:THR:HG21	4:D:65:GLY:HA3	1.88	0.55
4:D:16:CYS:HB2	4:D:67:CYS:SG	2.48	0.54
6:F:272:LEU:HD11	6:F:446:ALA:HB1	1.90	0.54
1:A:255:VAL:CG2	1:A:302:VAL:HG21	2.30	0.53
1:G:470:VAL:CG1	1:G:483:GLU:HG2	2.39	0.53
1:A:12:HIS:HB2	1:A:43:LYS:HA	1.90	0.52
1:G:403:CYS:HB2	8:G:706:SF4:S3	2.50	0.52
1:A:470:VAL:CG1	1:A:483:GLU:HG2	2.39	0.51
2:H:50:SER:HB3	3:I:101:ARG:HD3	1.92	0.51
3:I:116:MET:HE2	3:I:182:LEU:HD22	1.92	0.50
2:H:228:VAL:HA	2:H:258:LEU:O	2.10	0.50
6:F:18:ILE:HG21	6:F:432:MET:HE2	1.94	0.50
1:G:45:MET:HE1	1:G:53:MET:HE2	1.92	0.50
1:A:623:CYS:SG	1:A:624:PRO:HD3	2.52	0.50
1:G:9:TYR:CD1	1:G:53:MET:HE3	2.47	0.50
1:A:458:SER:HB2	3:I:43:SER:OG	2.12	0.49
6:F:442:CYS:SG	6:F:445:CYS:HB2	2.52	0.49
3:C:63:LEU:HD23	3:C:65:MET:HE2	1.95	0.49
4:J:87:MET:HG3	5:K:257:CYS:SG	2.53	0.49
1:A:470:VAL:HG11	1:A:483:GLU:HG2	1.95	0.49
2:B:78:CYS:SG	2:B:232:PRO:HD2	2.53	0.48
3:I:31:LEU:HD12	3:I:31:LEU:C	2.38	0.48
1:G:623:CYS:SG	1:G:624:PRO:HD3	2.53	0.48
2:H:173:LEU:HD21	2:H:230:VAL:HG11	1.95	0.48
2:H:265:GLY:HA3	2:H:275:LEU:HD21	1.96	0.48
1:A:255:VAL:HG21	1:A:302:VAL:CG2	2.32	0.47
1:A:514:PRO:HA	4:D:110:SER:HB2	1.96	0.47
1:A:525:LEU:O	1:A:526:ARG:HG3	2.14	0.47
1:G:482:LEU:HD23	3:I:2:ILE:HB	1.96	0.47
1:A:75:LEU:HD13	1:A:522:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:470:VAL:HG11	1:G:483:GLU:HG2	1.97	0.47
6:L:442:CYS:SG	6:L:445:CYS:HB2	2.55	0.47
5:K:273:LEU:HB3	5:K:274:PRO:HD3	1.97	0.47
3:I:175:PHE:HD1	3:I:182:LEU:HD12	1.80	0.46
5:K:127:PRO:HD3	6:L:36:VAL:HB	1.98	0.46
2:H:227:THR:CG2	2:H:257:VAL:HG13	2.47	0.45
4:D:90:GLU:HB3	5:E:280:LYS:HE3	1.99	0.45
2:H:145:ILE:CD1	2:H:287:LEU:HD11	2.47	0.45
3:I:66:ASP:HB3	20:I:302:HOH:O	2.17	0.45
1:A:526:ARG:HB3	1:A:529:ASP:HB2	2.00	0.44
1:A:548:PRO:HB3	1:G:523:PRO:O	2.18	0.44
2:H:17:GLY:HA3	2:H:276:ALA:HB3	2.00	0.44
1:A:92:PHE:CZ	1:A:574:PRO:HD2	2.52	0.44
1:A:255:VAL:HG12	1:A:298:LEU:HB3	1.99	0.44
1:G:621:GLY:C	1:G:624:PRO:HD2	2.43	0.44
6:F:66:VAL:HG22	6:F:164:PRO:HG3	2.00	0.43
2:B:211:MET:HE3	3:C:45:PRO:HB2	2.01	0.43
1:A:268:ILE:HD11	1:A:354:GLU:HB3	2.01	0.43
1:A:621:GLY:C	1:A:624:PRO:HD2	2.43	0.43
9:A:708:GOL:H31	3:I:85:GLU:O	2.18	0.43
1:G:582:GLU:O	5:K:174:LYS:HG3	2.19	0.43
1:G:255:VAL:HG12	1:G:298:LEU:HB3	2.01	0.43
1:G:579:VAL:HG22	1:G:632:LEU:HD13	2.01	0.43
6:L:235:LEU:HA	6:L:372:GLU:HB2	2.01	0.43
2:B:241:GLY:HA2	2:B:244:GLU:OE1	2.19	0.43
1:G:194:CYS:HB2	1:G:197:CYS:SG	2.59	0.43
1:A:583:ILE:O	5:E:174:LYS:HA	2.19	0.43
3:C:60:LYS:HG2	3:C:65:MET:HE3	2.01	0.43
1:G:620:CYS:HB3	4:J:74:TYR:CG	2.54	0.42
1:A:69:ALA:HA	1:A:97:ALA:HB3	2.01	0.42
1:A:402:VAL:HG21	1:A:495:MET:HE3	2.01	0.42
6:F:235:LEU:HA	6:F:372:GLU:HB2	2.01	0.42
2:H:14:ARG:HD3	3:I:128:VAL:HG11	2.01	0.42
9:A:709:GOL:H2	3:C:35:TYR:HA	2.01	0.42
1:A:240:TYR:CE2	1:A:290:LYS:HG3	2.54	0.42
5:E:273:LEU:HB3	5:E:274:PRO:HD3	2.00	0.42
1:G:131:LEU:HD22	1:G:131:LEU:N	2.34	0.42
6:L:272:LEU:HD11	6:L:446:ALA:HB1	2.01	0.42
1:A:620:CYS:HB3	4:D:74:TYR:CG	2.55	0.42
2:H:9:CYS:SG	3:I:126:HIS:HB3	2.60	0.42
1:A:559:SER:HB2	1:G:559:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:TRP:CH2	5:E:40:VAL:HB	2.55	0.41
2:H:236:LEU:C	2:H:236:LEU:HD23	2.45	0.41
1:G:12:HIS:HB2	1:G:43:LYS:HA	2.02	0.41
6:L:66:VAL:HG22	6:L:164:PRO:HG3	2.02	0.41
1:A:585:GLY:HA3	5:E:175:ASN:OD1	2.21	0.41
1:G:77:GLU:N	1:G:78:PRO:CD	2.83	0.41
1:G:587:CYS:HA	5:K:184:LYS:HE3	2.02	0.41
2:H:45:PRO:HD3	2:H:84:SER:HB2	2.02	0.41
2:H:145:ILE:HD12	2:H:287:LEU:HD11	2.02	0.41
6:F:64:CYS:CB	17:F:506:FCO:C1	2.99	0.40
2:H:43:PRO:O	2:H:44:ALA:C	2.63	0.40
2:B:42:CYS:SG	2:B:43:PRO:C	3.04	0.40
6:L:272:LEU:HD11	6:L:400:VAL:HA	2.03	0.40
6:L:442:CYS:HB3	17:L:504:FCO:N2	2.37	0.40
1:A:406:TYR:C	1:A:406:TYR:CD1	2.99	0.40
2:H:78:CYS:SG	2:H:232:PRO:HD2	2.62	0.40
1:G:431:ARG:HD2	8:G:706:SF4:S1	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	398	ALA
6	L	398	ALA
6	F	291	THR
6	L	291	THR
1	A	70	ALA
1	G	70	ALA
1	G	575	ILE
6	F	365	GLY

5.3.2 Protein sidechains (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	403	CYS
1	A	513	THR
3	C	35	TYR
3	C	49	ARG
4	D	17	THR
5	E	8	TRP
5	E	111	THR
6	F	2	VAL
6	F	65	GLN
6	F	102	HIS
6	F	290	ASN
6	F	351	ILE
6	F	364	VAL
6	F	445	CYS
1	G	340	GLU
1	G	359	ILE
1	G	403	CYS
1	G	513	THR
1	G	573	GLU
2	H	233	PHE
3	I	35	TYR
3	I	49	ARG
3	I	93	VAL
5	K	6	THR
5	K	8	TRP
5	K	111	THR
6	L	65	GLN
6	L	72	SER
6	L	102	HIS
6	L	251	TYR
6	L	290	ASN

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Mol	Chain	Res	Type
6	L	422	GLU
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	192	ASN
1	A	229	ASN
1	A	412	GLN
2	B	13	ASN
2	B	95	ASN
2	B	128	ASN
2	B	254	ASN
3	C	109	ASN
3	C	133	ASN
5	E	28	ASN
6	F	260	ASN
6	F	427	GLN
1	G	262	ASN
1	G	306	ASN
1	G	459	GLN
2	H	90	HIS
2	H	154	HIS
2	H	229	ASN
2	H	254	ASN
3	I	109	ASN
3	I	133	ASN
6	L	93	ASN
6	L	97	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	701	FAD	C5A-C4A	4.23	1.46	1.39
7	G	704	FAD	C5A-C4A	4.21	1.46	1.39
10	H	302	9S8	S3-FE4	-4.08	2.15	2.24
10	H	301	9S8	S3-FE4	-4.06	2.15	2.24
17	L	504	FCO	O3-C3	4.04	1.21	1.16
17	F	506	FCO	O3-C3	3.97	1.21	1.16
7	G	704	FAD	C8-C7	3.49	1.49	1.40
7	A	701	FAD	C8-C7	3.28	1.49	1.40
10	H	301	9S8	S5-FE4	-2.69	2.18	2.24
7	A	701	FAD	C5A-C6A	2.58	1.48	1.41
7	G	704	FAD	C8A-N7A	2.48	1.36	1.31
7	A	701	FAD	C4X-N5	2.47	1.35	1.30
7	A	701	FAD	C8A-N7A	2.46	1.36	1.31
7	G	704	FAD	C5A-C6A	2.46	1.47	1.41
7	G	704	FAD	C5A-N7A	-2.45	1.34	1.39
7	G	704	FAD	C4X-N5	2.42	1.35	1.30
11	H	303	COM	O2S-S2	2.20	1.51	1.45
7	A	701	FAD	C5A-N7A	-2.19	1.34	1.39
7	G	704	FAD	C4-N3	-2.17	1.34	1.38
10	H	302	9S8	S5-FE4	-2.14	2.19	2.24
7	A	701	FAD	C4-N3	-2.11	1.34	1.38
11	H	303	COM	O1S-S2	2.11	1.51	1.45
7	A	701	FAD	C5X-N5	-2.10	1.35	1.39
11	B	303	COM	O1S-S2	2.00	1.50	1.45

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
7	G	704	FAD	C2A-N3A-C4A	4.05	121.31	111.75
11	B	303	COM	O3S-S2-C2	4.03	112.28	105.77
11	H	303	COM	O3S-S2-O1S	-3.99	101.52	111.27
11	H	303	COM	O3S-S2-C2	3.98	112.20	105.77
7	A	701	FAD	N3A-C2A-N1A	-3.96	122.40	128.60
7	G	704	FAD	N3A-C2A-N1A	-3.93	122.45	128.60
11	B	303	COM	O3S-S2-O2S	-3.89	101.76	111.27
7	A	701	FAD	C4A-C5A-N7A	-3.27	106.63	110.62
7	G	704	FAD	C4A-C5A-N7A	-3.04	106.92	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	701	FAD	C5A-N7A-C8A	3.03	107.82	103.51
11	B	303	COM	O1S-S2-C2	2.98	110.50	106.92
7	A	701	FAD	P-O3P-PA	-2.97	122.64	132.83
7	G	704	FAD	C5A-N7A-C8A	2.90	107.62	103.51
7	G	704	FAD	P-O3P-PA	-2.89	122.91	132.83
7	G	704	FAD	C4A-N9A-C8A	2.85	108.81	105.73
7	A	701	FAD	O4-C4-C4X	-2.80	119.18	126.60
7	A	701	FAD	C4A-N9A-C8A	2.73	108.69	105.73
7	A	701	FAD	C4X-C10-N1	-2.68	118.50	124.73
11	H	303	COM	O2S-S2-C2	2.66	110.12	106.92
7	G	704	FAD	O4-C4-C4X	-2.63	119.63	126.60
7	A	701	FAD	O2-C2-N1	-2.58	117.56	121.83
11	B	303	COM	O2S-S2-C2	2.56	110.00	106.92
7	A	701	FAD	N9A-C8A-N7A	-2.54	110.44	113.91
11	H	303	COM	O1S-S2-C2	2.51	109.94	106.92
7	G	704	FAD	C4X-C10-N1	-2.51	118.92	124.73
7	G	704	FAD	N9A-C8A-N7A	-2.50	110.49	113.91
7	G	704	FAD	C4-C4X-N5	2.47	121.74	118.23
7	A	701	FAD	C4-N3-C2	-2.40	121.21	125.64
7	A	701	FAD	C6A-C5A-N7A	2.32	136.35	132.02
7	A	701	FAD	C4X-C10-N10	2.32	119.87	116.48
7	A	701	FAD	C4-C4X-N5	2.29	121.49	118.23
7	G	704	FAD	O2-C2-N1	-2.29	118.04	121.83
7	A	701	FAD	C10-N1-C2	2.28	121.46	116.90
7	A	701	FAD	C4X-C4-N3	2.27	118.96	113.19
7	G	704	FAD	C4X-C4-N3	2.26	118.92	113.19
7	G	704	FAD	C4-N3-C2	-2.19	121.60	125.64
7	G	704	FAD	O4B-C1B-N9A	2.11	112.22	108.06
7	G	704	FAD	C2A-N1A-C6A	2.10	122.37	118.77
7	A	701	FAD	C2A-N1A-C6A	2.05	122.29	118.77
7	G	704	FAD	C10-N1-C2	2.04	120.97	116.90
7	G	704	FAD	C6A-C5A-N7A	2.03	135.81	132.02

There are no chirality outliers.

All (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

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

There are no ring outliers.

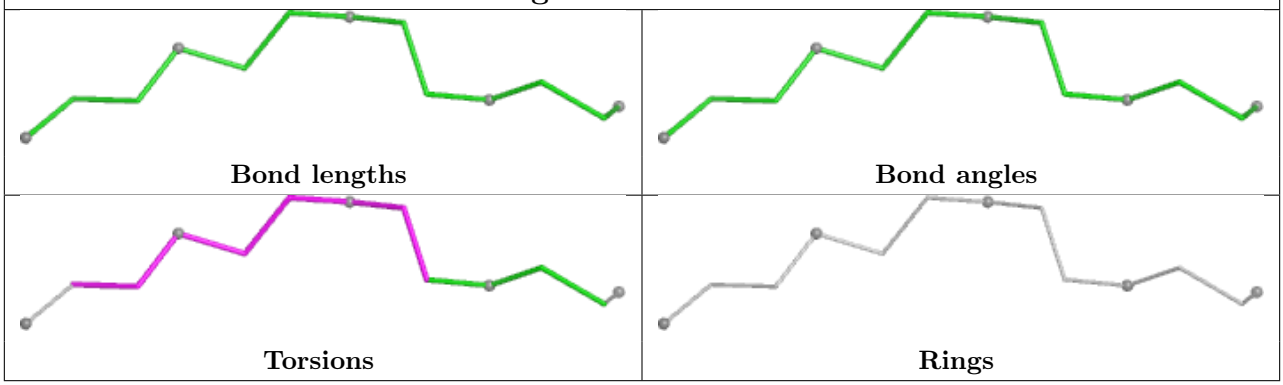
8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

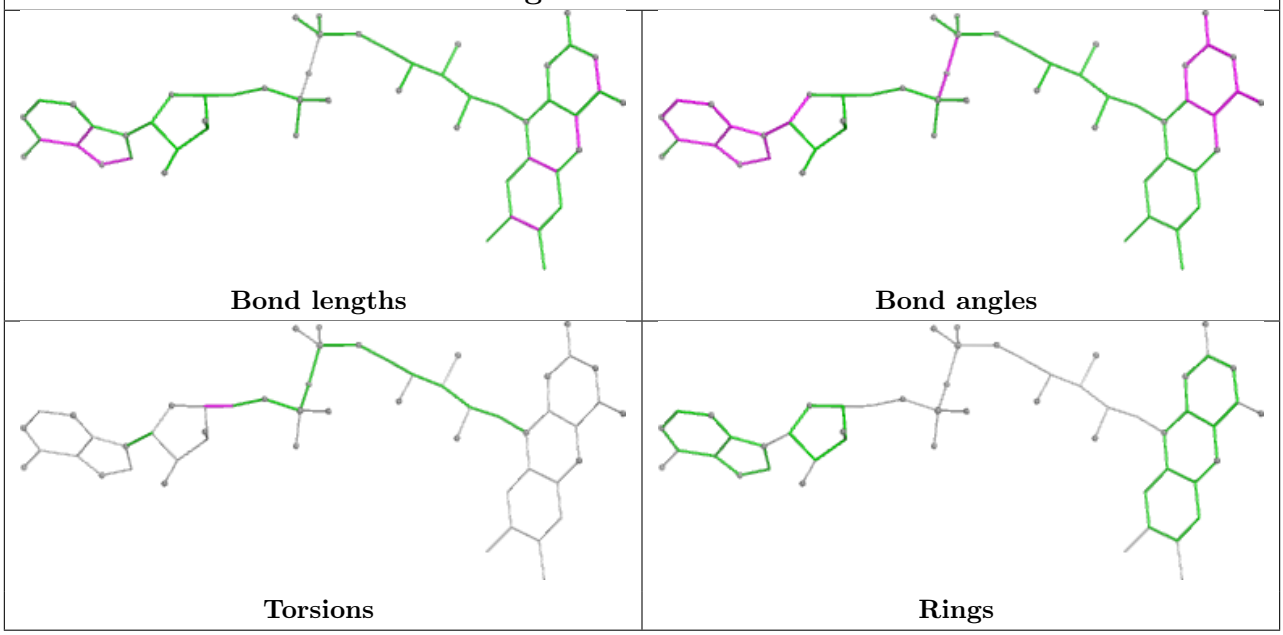
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

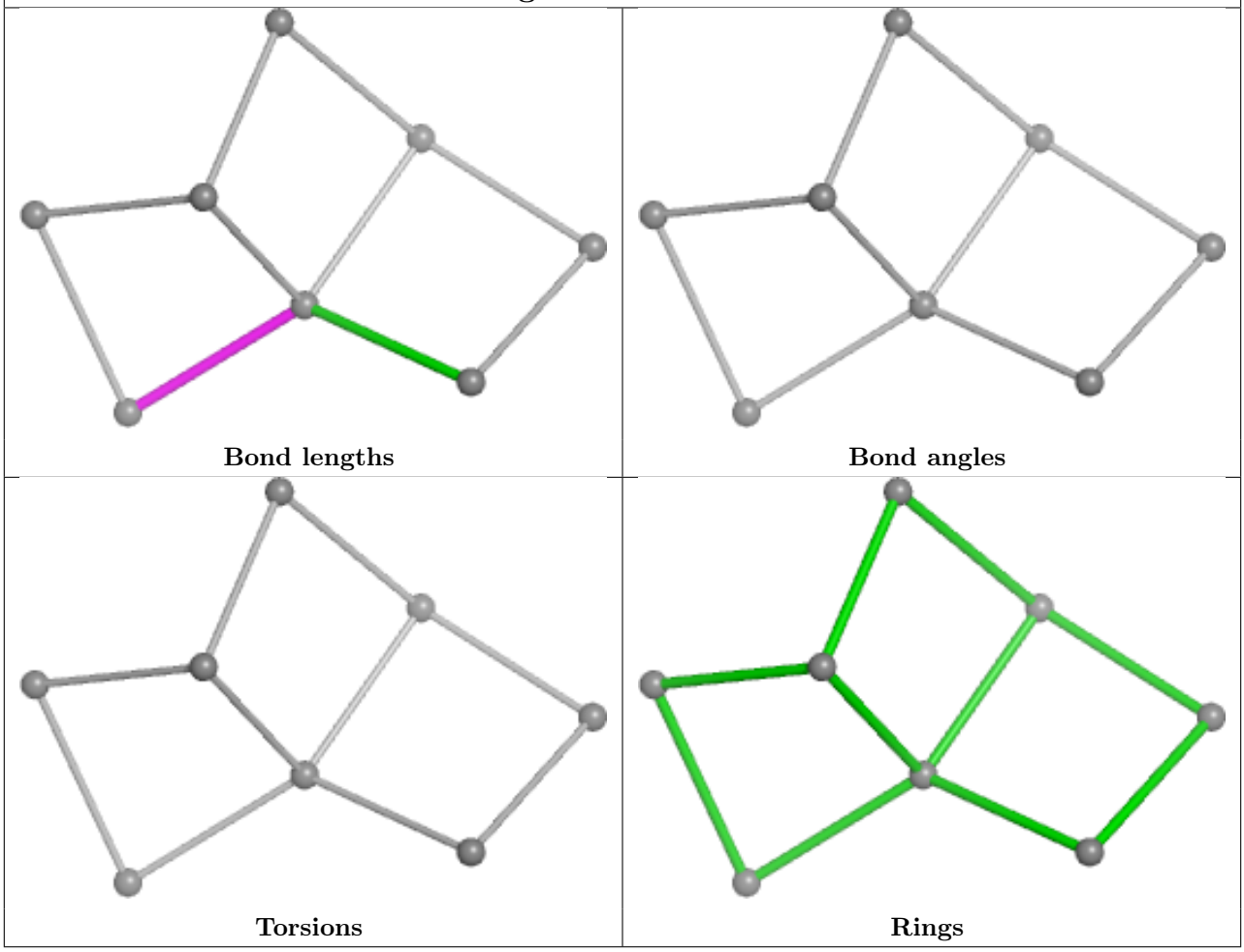
Ligand PE3 F 503



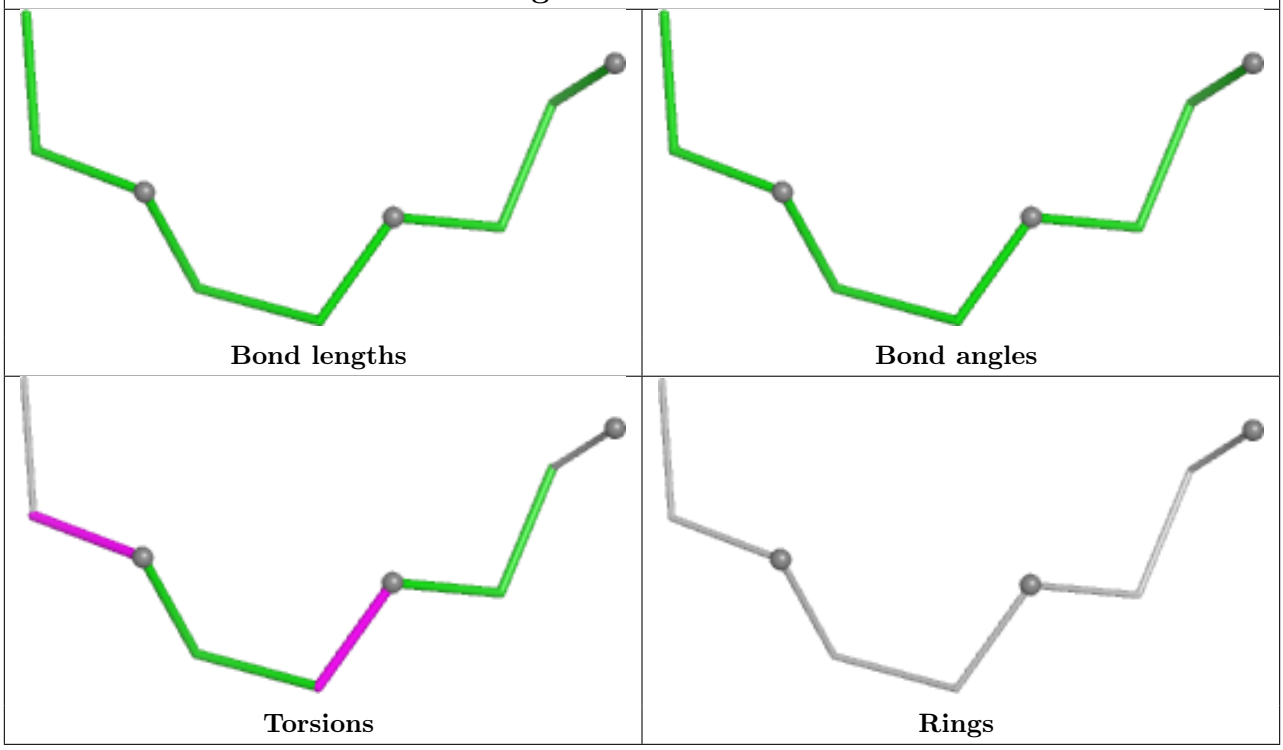
Ligand FAD G 704



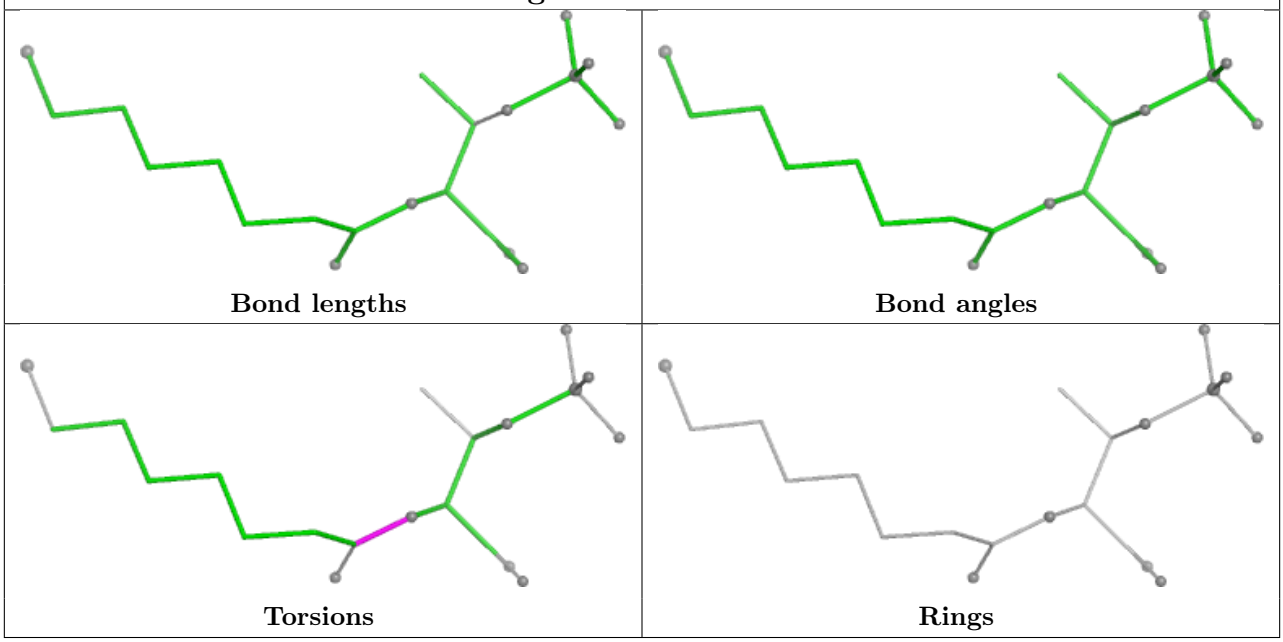
Ligand 9S8 B 301



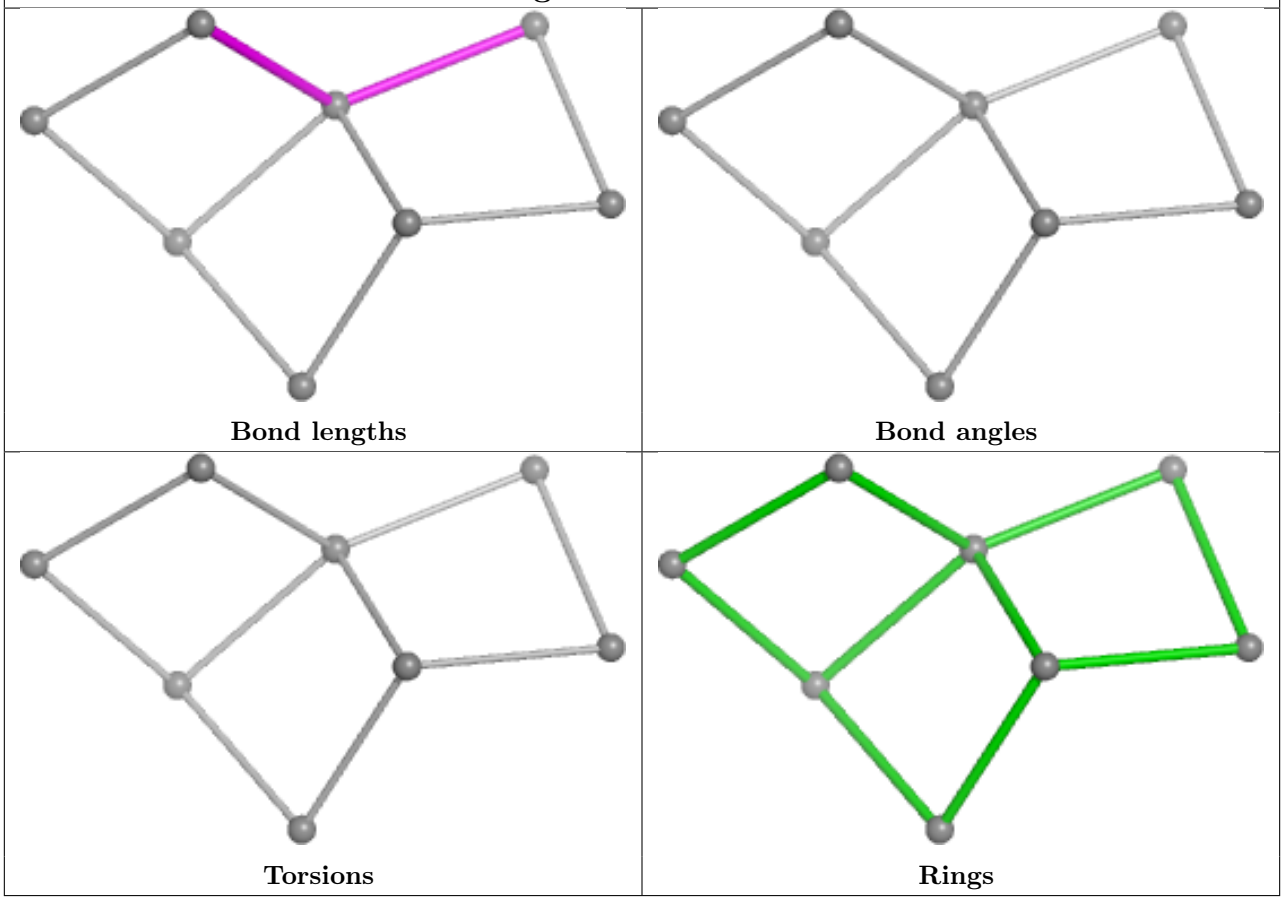
Ligand PE3 L 502



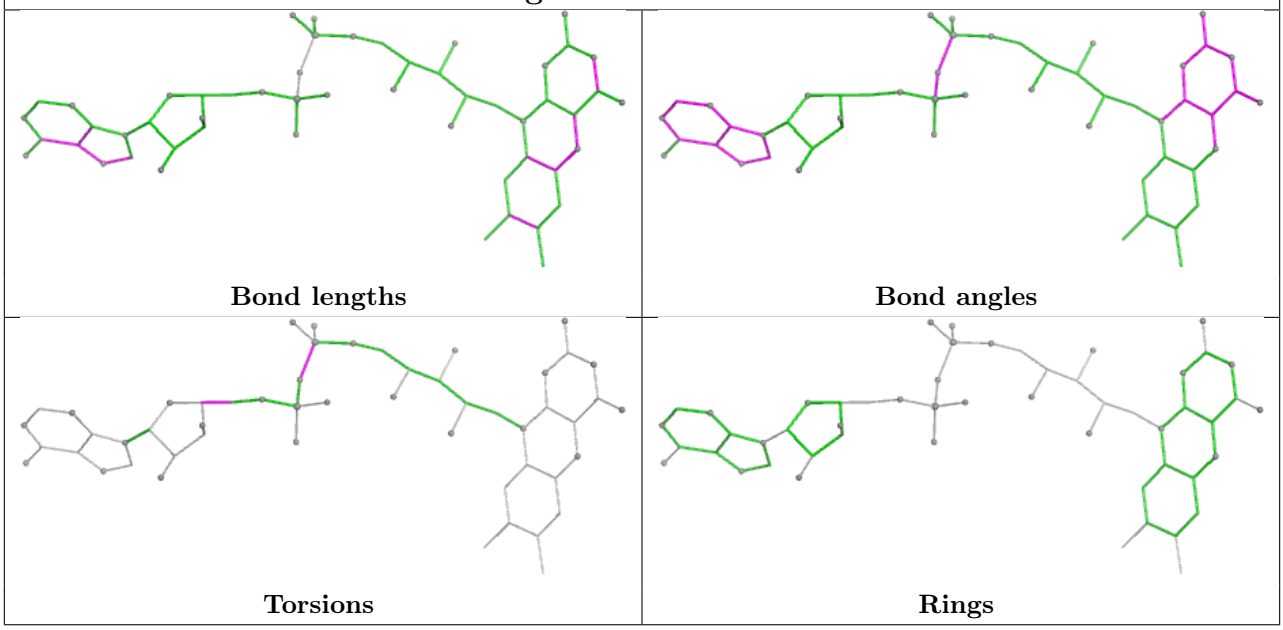
Ligand TP7 H 304



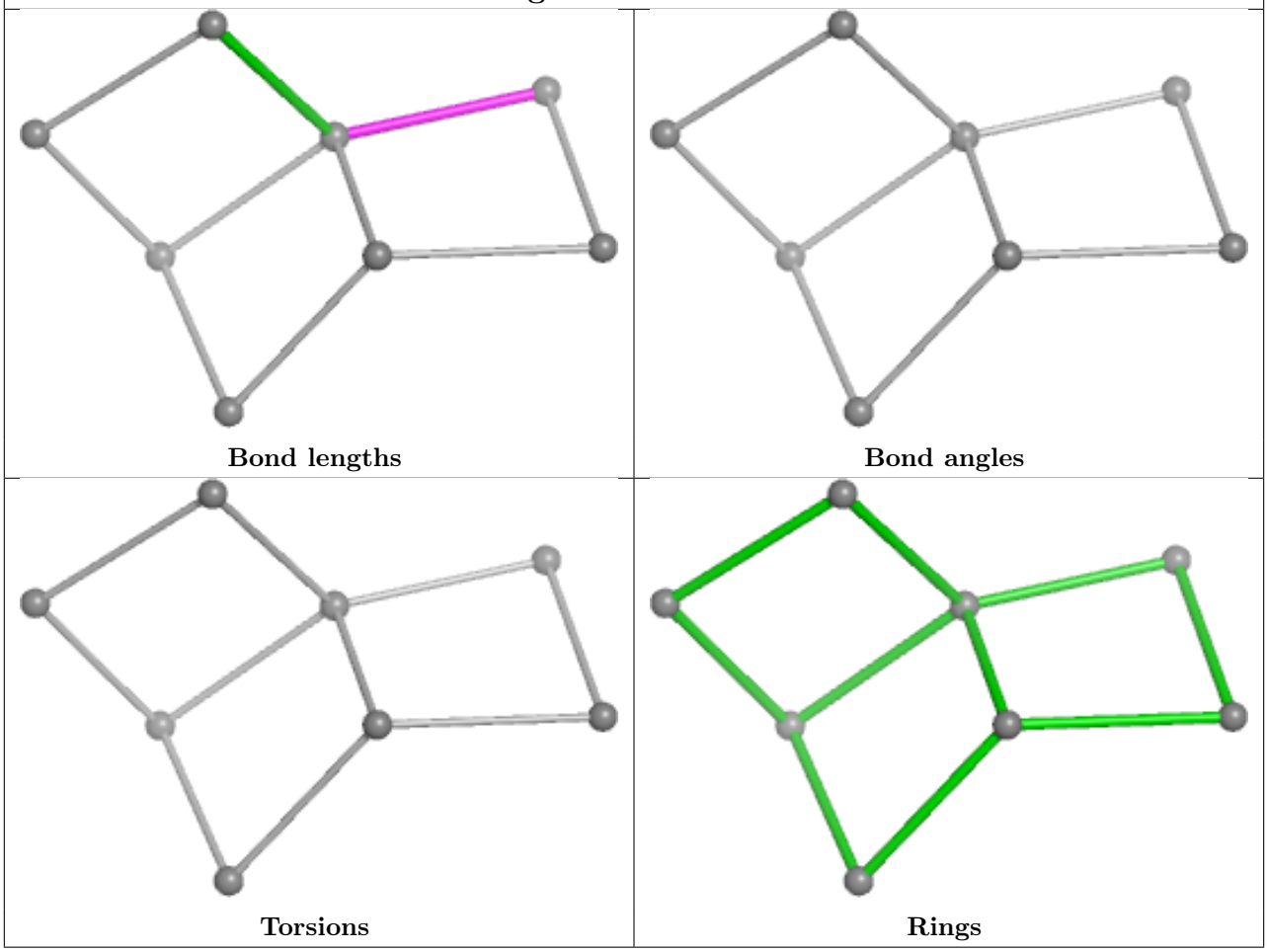
Ligand 9S8 H 301



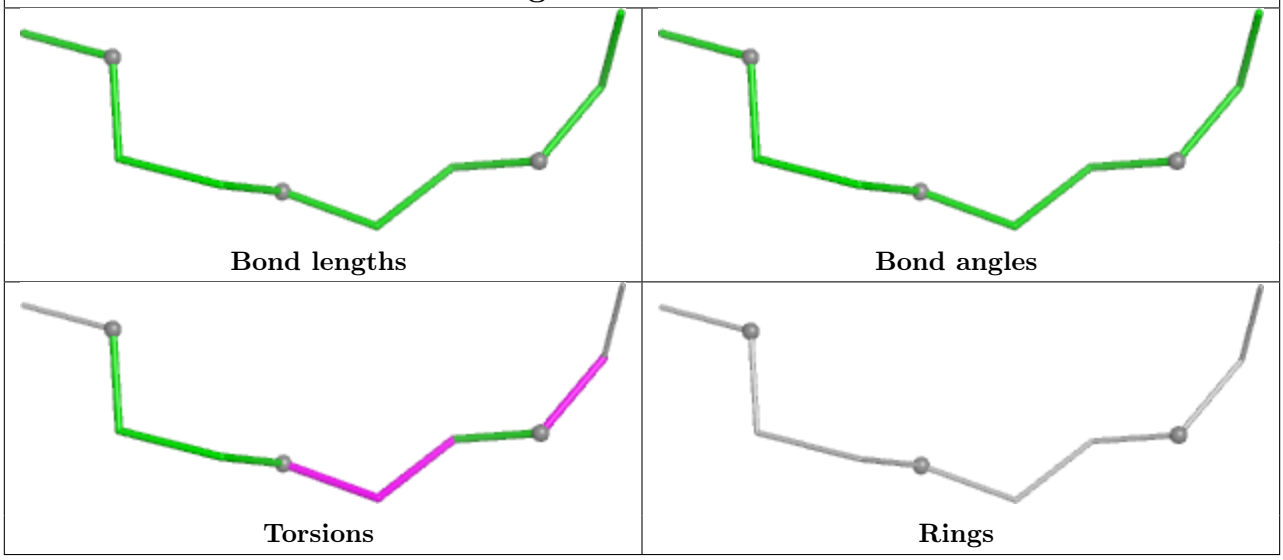
Ligand FAD A 701



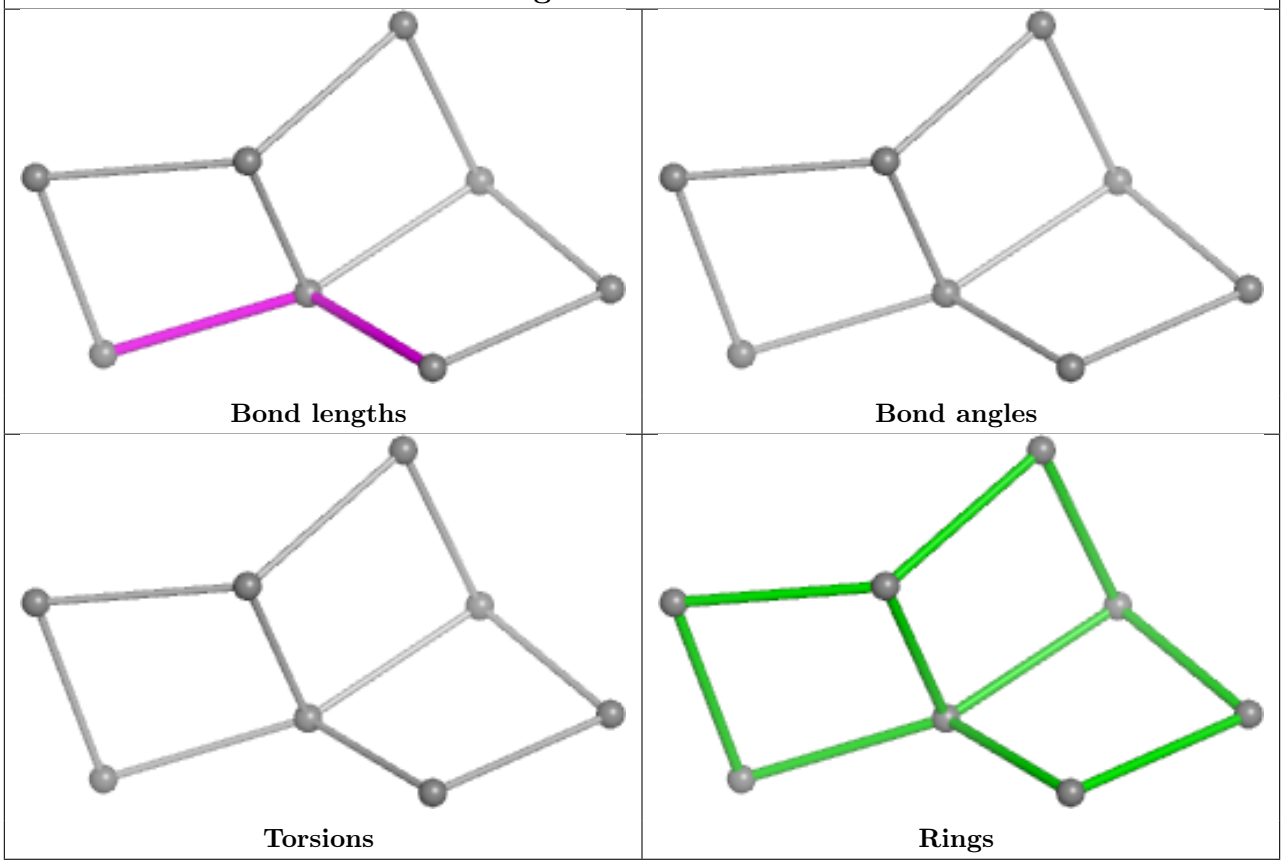
Ligand 9S8 B 302



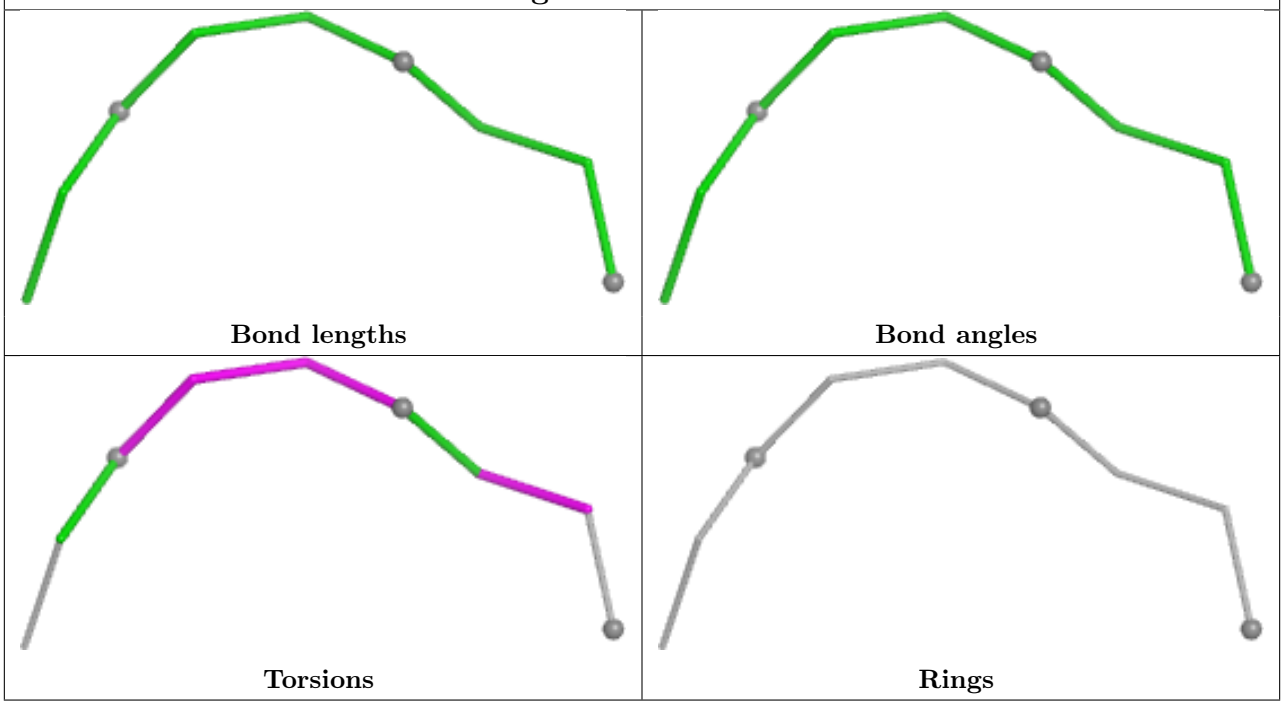
Ligand PE3 G 701



Ligand 9S8 H 302



Ligand PE3 F 502



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%)

All (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
2	H	142	PRO	5.7
1	A	249	CYS	5.7
6	L	364	VAL	5.7
1	A	308	ILE	5.5
3	I	177	TRP	5.5
2	H	291	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	255	VAL	5.4
6	L	363	VAL	5.3
1	A	299	CYS	5.3
1	A	302	VAL	5.3
2	H	279	VAL	5.2
1	G	308	ILE	5.2
1	A	307	ALA	5.0
1	G	570	VAL	5.0
1	G	602	VAL	5.0
6	F	2	VAL	4.9
2	H	75	VAL	4.8
1	G	653	THR	4.8
1	A	298	LEU	4.7
2	H	277	LEU	4.7
1	A	310	PHE	4.7
1	A	269	GLY	4.7
2	H	176	ILE	4.6
1	G	613	ILE	4.6
1	A	653	THR	4.5
1	G	599	PRO	4.5
1	A	364	PRO	4.4
3	I	183	LYS	4.4
1	A	240	TYR	4.4
3	C	9	LYS	4.4
1	A	246	CYS	4.3
4	J	140	LYS	4.3
2	H	132	VAL	4.3
1	G	361	ALA	4.3
1	G	464	PRO	4.3
2	H	143	LEU	4.3
1	A	290	LYS	4.3
2	H	287	LEU	4.2
2	H	262	GLN	4.2
1	A	248	GLY	4.2
6	F	365	GLY	4.2
1	A	253	SER	4.2
1	A	257	PRO	4.2
1	G	297	GLY	4.2
5	K	189	VAL	4.2
1	A	305	PRO	4.2
2	H	29	LEU	4.2
1	A	256	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	301	LYS	4.1
1	G	615	ALA	4.1
6	F	362	GLU	4.1
5	K	191	ILE	4.1
3	I	181	ALA	4.1
5	K	190	ALA	4.1
3	I	180	GLY	4.1
2	H	270	MET	4.1
1	A	241	ILE	4.1
3	I	135	ALA	4.0
1	A	268	ILE	4.0
1	G	258	ILE	4.0
1	G	316	ILE	4.0
1	A	372	LEU	4.0
2	H	145	ILE	4.0
1	A	303	CYS	4.0
3	I	137	LEU	4.0
2	H	265	GLY	3.9
1	A	292	HIS	3.9
1	A	602	VAL	3.9
1	G	255	VAL	3.9
1	A	250	GLY	3.9
2	H	249	PHE	3.9
1	A	608	VAL	3.9
1	G	302	VAL	3.9
2	H	108	LYS	3.8
6	F	364	VAL	3.8
1	G	300	ALA	3.8
1	A	605	ASP	3.8
5	K	193	THR	3.8
2	H	33	LEU	3.8
2	H	135	ILE	3.7
1	G	50	GLY	3.7
2	H	25	VAL	3.7
2	H	4	ALA	3.7
2	H	268	MET	3.7
3	I	130	ALA	3.7
1	A	316	ILE	3.7
2	H	226	CYS	3.7
2	H	248	LYS	3.7
2	H	180	THR	3.7
2	H	272	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	80	PHE	3.7
2	H	282	ILE	3.7
1	G	269	GLY	3.7
1	A	306	ASN	3.7
2	H	243	ILE	3.6
1	A	197	CYS	3.6
1	A	276	LYS	3.6
1	G	294	ILE	3.6
3	I	141	ILE	3.6
3	I	182	LEU	3.6
3	I	179	LYS	3.6
2	H	136	ALA	3.6
2	H	258	LEU	3.6
5	E	167	LYS	3.5
1	A	244	THR	3.5
1	G	362	SER	3.5
1	A	297	GLY	3.5
5	K	260	PHE	3.5
1	G	48	ASP	3.5
1	G	15	VAL	3.5
1	A	275	TYR	3.5
2	H	286	PRO	3.5
2	H	139	VAL	3.5
2	H	110	GLY	3.5
2	H	173	LEU	3.5
2	H	264	LEU	3.4
5	E	298	LEU	3.4
5	E	162	ALA	3.4
1	A	274	ILE	3.4
1	A	245	LYS	3.4
1	G	609	VAL	3.4
6	L	361	GLU	3.4
3	I	127	ALA	3.4
1	G	469	LEU	3.3
1	A	243	GLU	3.3
1	G	76	HIS	3.3
2	B	93	HIS	3.3
5	K	187	GLU	3.3
1	G	307	ALA	3.3
6	L	365	GLY	3.3
1	G	616	LEU	3.3
1	G	268	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	465	GLU	3.3
2	H	2	LYS	3.3
2	H	224	ALA	3.3
5	K	188	GLY	3.3
1	G	6	ILE	3.3
1	G	79	THR	3.3
2	H	144	ASN	3.3
2	B	108	LYS	3.3
1	A	247	THR	3.3
1	A	238	ALA	3.2
2	H	269	GLY	3.2
1	A	604	LYS	3.2
2	B	291	ILE	3.2
6	F	419	LYS	3.2
1	A	293	CYS	3.2
1	A	296	CYS	3.2
6	F	120	THR	3.2
1	A	300	ALA	3.2
2	H	267	ALA	3.2
1	A	259	ASP	3.2
3	I	131	ASN	3.2
1	G	298	LEU	3.2
5	K	120	ILE	3.2
5	K	272	ILE	3.2
3	C	178	GLU	3.2
6	L	186	LYS	3.2
3	C	31	LEU	3.2
3	C	3	TYR	3.2
1	A	312	GLN	3.2
1	A	288	ILE	3.2
3	C	1	MET	3.2
2	H	5	PHE	3.1
1	A	260	VAL	3.1
1	G	364	PRO	3.1
1	G	604	LYS	3.1
2	H	289	LYS	3.1
3	I	175	PHE	3.1
2	H	185	VAL	3.1
2	H	253	TYR	3.1
2	H	245	ILE	3.1
1	G	466	THR	3.1
1	G	309	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
3	I	133	ASN	3.1
2	H	276	ALA	3.1
2	H	34	VAL	3.1
2	H	230	VAL	3.1
2	H	284	VAL	3.1
1	G	372	LEU	3.1
3	I	172	LEU	3.1
1	A	270	MET	3.1
1	G	299	CYS	3.1
1	G	310	PHE	3.1
2	H	141	ARG	3.1
2	H	111	LYS	3.1
2	H	290	LYS	3.1
3	I	140	SER	3.0
2	H	288	LEU	3.0
1	G	296	CYS	3.0
2	H	207	LEU	3.0
3	I	136	GLU	3.0
3	I	163	LEU	3.0
5	E	164	LEU	3.0
2	H	126	ILE	3.0
2	H	76	THR	3.0
1	A	251	GLN	3.0
1	A	314	PRO	3.0
6	L	360	PRO	3.0
3	I	143	LEU	3.0
5	K	268	VAL	3.0
5	K	298	LEU	3.0
2	H	22	THR	3.0
4	J	110	SER	3.0
1	A	311	ASP	3.0
1	A	254	GLU	3.0
4	J	26	VAL	2.9
1	A	317	ILE	2.9
1	G	370	ILE	2.9
1	G	42	TYR	2.9
2	H	238	PHE	2.9
1	A	601	LEU	2.9
1	G	610	ALA	2.9
1	A	272	LYS	2.9
1	G	461	ILE	2.9
1	A	309	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	607	LYS	2.9
2	H	118	LYS	2.9
3	I	132	LYS	2.9
2	H	222	ALA	2.9
1	A	609	VAL	2.9
1	G	305	PRO	2.9
1	G	292	HIS	2.9
1	G	75	LEU	2.9
2	B	39	ALA	2.9
2	B	249	PHE	2.9
1	G	614	SER	2.8
1	G	9	TYR	2.8
1	A	615	ALA	2.8
2	H	67	ALA	2.8
3	C	61	ALA	2.8
2	H	77	VAL	2.8
1	G	249	CYS	2.8
3	I	134	THR	2.8
1	A	499	LYS	2.8
1	G	618	LYS	2.8
2	H	138	LYS	2.8
2	H	183	LYS	2.8
1	A	420	ASP	2.8
2	H	100	ASN	2.8
2	H	225	ASP	2.8
2	H	12	PRO	2.8
2	H	177	VAL	2.8
3	I	155	LYS	2.8
4	J	133	LYS	2.8
6	F	315	LYS	2.8
1	G	244	THR	2.8
2	H	130	ILE	2.8
3	C	141	ILE	2.8
1	G	366	GLY	2.8
1	G	597	GLY	2.8
1	G	601	LEU	2.8
1	A	285	LYS	2.8
3	I	112	LYS	2.8
3	I	139	LYS	2.8
3	I	146	LYS	2.8
1	G	470	VAL	2.8
1	G	612	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	5	ARG	2.8
1	G	595	PRO	2.8
5	E	165	GLU	2.8
2	H	113	TYR	2.8
3	I	103	LEU	2.8
1	G	270	MET	2.8
2	B	98	ALA	2.8
1	A	278	PHE	2.8
2	H	223	GLY	2.7
4	J	3	GLU	2.7
5	E	50	GLU	2.7
1	G	34	LYS	2.7
1	G	377	LYS	2.7
3	I	123	LYS	2.7
2	H	147	VAL	2.7
3	C	8	ASN	2.7
3	I	74	ILE	2.7
5	K	4	ILE	2.7
2	H	250	GLY	2.7
3	I	174	GLY	2.7
1	A	279	PRO	2.7
1	G	49	PRO	2.7
3	I	107	LYS	2.7
2	H	7	LEU	2.7
3	I	122	LEU	2.7
3	I	147	ALA	2.7
3	I	152	PHE	2.7
2	H	37	THR	2.7
2	H	285	ASP	2.7
2	H	131	GLY	2.7
3	C	2	ILE	2.7
2	H	251	LYS	2.7
3	C	184	GLU	2.7
2	B	99	LEU	2.7
2	H	275	LEU	2.7
1	A	610	ALA	2.7
2	H	123	ALA	2.7
3	I	3	TYR	2.7
1	G	290	LYS	2.7
2	B	24	THR	2.7
2	H	221	LYS	2.7
3	I	178	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	91	PRO	2.7
1	A	235	MET	2.7
2	H	260	LEU	2.7
5	E	209	LEU	2.7
2	H	21	ALA	2.6
3	I	111	ALA	2.6
4	D	18	TYR	2.6
1	G	608	VAL	2.6
2	H	31	VAL	2.6
5	E	152	ASN	2.6
5	E	197	ASN	2.6
6	L	352	VAL	2.6
5	E	166	GLY	2.6
5	K	262	ILE	2.6
1	G	45	MET	2.6
1	A	291	GLU	2.6
5	K	266	ARG	2.6
2	H	102	VAL	2.6
3	I	1	MET	2.6
5	K	202	PRO	2.6
1	G	603	GLU	2.6
2	H	146	ASN	2.6
1	A	606	GLY	2.6
2	H	15	TYR	2.6
3	I	120	TYR	2.6
5	E	193	THR	2.6
5	K	194	ILE	2.6
2	H	106	LEU	2.6
4	J	129	LEU	2.6
5	K	164	LEU	2.6
6	L	362	GLU	2.6
1	G	463	ASP	2.6
3	C	66	ASP	2.6
5	E	201	ASN	2.6
2	H	1	MET	2.6
1	A	304	GLY	2.6
1	G	274	ILE	2.6
2	H	283	SER	2.6
2	H	99	LEU	2.5
2	H	48	PHE	2.5
1	G	260	VAL	2.5
3	C	5	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	179	LYS	2.5
5	K	115	LYS	2.5
5	K	183	LYS	2.5
1	A	583	ILE	2.5
6	F	139	ILE	2.5
6	L	230	ASN	2.5
2	H	181	GLY	2.5
2	H	273	LYS	2.5
5	K	229	PRO	2.5
1	G	365	THR	2.5
2	H	93	HIS	2.5
1	G	245	LYS	2.5
2	B	96	LYS	2.5
6	F	24	ASP	2.5
1	G	257	PRO	2.5
2	H	281	GLN	2.5
1	G	339	GLU	2.5
3	I	121	VAL	2.5
5	K	50	GLU	2.5
3	I	173	ILE	2.5
1	A	286	TYR	2.5
1	A	446	LYS	2.5
6	F	186	LYS	2.5
2	H	16	ALA	2.5
1	A	3	GLU	2.4
1	G	600	ARG	2.4
5	E	189	VAL	2.4
1	G	596	TYR	2.4
2	B	221	LYS	2.4
2	B	248	LYS	2.4
2	B	251	LYS	2.4
2	B	273	LYS	2.4
2	H	133	ASP	2.4
5	K	269	ASP	2.4
1	A	313	GLU	2.4
3	C	180	GLY	2.4
6	L	353	GLY	2.4
1	A	287	THR	2.4
5	E	2	VAL	2.4
3	I	9	LYS	2.4
5	K	259	ASP	2.4
3	I	118	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	114	LYS	2.4
1	A	220	VAL	2.4
3	C	143	LEU	2.4
1	G	240	TYR	2.4
2	H	3	TYR	2.4
3	I	109	ASN	2.4
6	L	387	ASP	2.4
1	G	267	GLY	2.4
2	H	98	ALA	2.4
3	I	104	ALA	2.4
2	H	55	THR	2.4
5	K	184	LYS	2.4
1	G	256	CYS	2.4
1	G	303	CYS	2.4
2	H	26	MET	2.4
2	H	209	LEU	2.4
2	H	140	GLU	2.4
6	L	283	GLU	2.4
2	H	129	ASP	2.3
3	I	176	ASP	2.3
5	E	49	ASP	2.3
1	G	523	PRO	2.3
2	H	20	ALA	2.3
1	G	358	MET	2.3
1	G	84	VAL	2.3
1	G	288	ILE	2.3
2	B	177	VAL	2.3
2	H	74	ILE	2.3
2	H	122	PHE	2.3
5	K	277	ILE	2.3
3	I	138	ARG	2.3
2	H	247	GLU	2.3
5	K	192	GLU	2.3
1	A	242	ASP	2.3
5	E	117	ASP	2.3
2	H	186	PRO	2.3
1	G	467	GLY	2.3
1	G	271	ARG	2.3
2	H	220	ILE	2.3
1	A	603	GLU	2.3
2	B	102	VAL	2.3
2	H	171	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	166	GLU	2.3
6	F	124	VAL	2.3
2	H	92	LEU	2.3
1	A	417	LYS	2.3
2	H	246	LYS	2.3
3	I	161	ASN	2.3
6	L	24	ASP	2.3
6	L	419	LYS	2.3
5	K	270	PRO	2.3
4	D	19	GLY	2.3
5	E	198	TYR	2.3
5	K	261	GLY	2.3
6	F	26	GLY	2.3
1	G	247	THR	2.3
1	A	74	ARG	2.3
1	G	312	GLN	2.3
5	E	170	GLU	2.3
2	H	6	PHE	2.3
2	H	18	VAL	2.3
2	H	101	PHE	2.3
4	J	138	LEU	2.3
2	H	182	ALA	2.3
4	J	4	TRP	2.3
2	H	227	THR	2.3
1	A	234	ILE	2.3
1	G	138	ILE	2.3
3	C	107	LYS	2.3
6	F	3	LYS	2.3
6	L	83	LYS	2.3
2	B	161	VAL	2.3
1	G	620	CYS	2.2
2	H	213	ASN	2.2
1	A	239	ARG	2.2
1	A	271	ARG	2.2
1	G	363	GLY	2.2
2	H	172	MET	2.2
1	A	273	ALA	2.2
1	A	295	GLU	2.2
2	B	60	ALA	2.2
2	H	259	HIS	2.2
6	L	136	HIS	2.2
5	K	185	SER	2.2

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Mol	Chain	Res	Type	RSRZ
5	K	201	ASN	2.2
1	A	277	PRO	2.2
1	G	53	MET	2.2
4	J	77	GLY	2.2
2	H	90	HIS	2.2
1	G	236	LYS	2.2
2	B	136	ALA	2.2
4	D	140	LYS	2.2
5	E	77	LYS	2.2
5	K	206	LYS	2.2
1	G	575	ILE	2.2
5	E	163	LEU	2.2
5	K	209	LEU	2.2
2	H	255	PHE	2.2
3	I	169	PHE	2.2
1	G	238	ALA	2.2
1	G	273	ALA	2.2
2	H	39	ALA	2.2
6	L	358	ALA	2.2
4	D	4	TRP	2.2
2	B	126	ILE	2.2
1	A	221	VAL	2.2
3	C	67	ASP	2.2
2	B	105	LYS	2.2
2	H	137	GLU	2.2
4	J	125	LYS	2.2
5	K	186	GLU	2.2
1	A	267	GLY	2.2
5	K	119	GLY	2.2
1	G	252	CYS	2.2
1	A	362	SER	2.2
3	I	105	ALA	2.2
2	B	66	ILE	2.1
5	K	30	LEU	2.1
1	G	41	ASP	2.1
2	H	228	VAL	2.1
2	H	239	ASP	2.1
2	H	274	ASP	2.1
1	A	2	GLU	2.1
1	A	261	PRO	2.1
3	I	148	PRO	2.1
6	L	359	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	115	GLY	2.1
3	I	142	GLY	2.1
5	E	188	GLY	2.1
2	H	179	ALA	2.1
1	G	89	LEU	2.1
2	B	287	LEU	2.1
6	L	134	LYS	2.1
2	H	128	ASN	2.1
2	H	206	GLU	2.1
1	A	345	VAL	2.1
2	H	257	VAL	2.1
1	A	447	GLN	2.1
1	G	228	GLY	2.1
1	G	304	GLY	2.1
3	C	142	GLY	2.1
5	K	232	GLY	2.1
3	I	162	THR	2.1
1	G	47	ALA	2.1
1	G	272	LYS	2.1
1	G	301	LYS	2.1
3	C	65	MET	2.1
6	F	134	LYS	2.1
6	F	319	LYS	2.1
2	H	32	GLU	2.1
2	H	85	LEU	2.1
5	K	208	LEU	2.1
1	G	468	ASN	2.1
4	J	79	TYR	2.1
6	F	329	TYR	2.1
6	L	132	ILE	2.1
1	G	591	VAL	2.1
5	K	204	PRO	2.1
1	A	600	ARG	2.1
1	G	293	CYS	2.1
1	A	581	ALA	2.1
5	E	52	GLU	2.1
1	A	198	ILE	2.1
6	L	84	ILE	2.1
2	H	127	TYR	2.1
1	A	589	VAL	2.1
1	G	10	VAL	2.1
3	I	128	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
6	L	82	VAL	2.1
2	H	30	GLY	2.1
2	H	241	GLY	2.1
6	L	22	PHE	2.1
1	G	446	LYS	2.0
4	J	99	LYS	2.0
2	H	24	THR	2.0
1	A	318	GLU	2.0
1	G	314	PRO	2.0
1	G	44	TYR	2.0
2	H	187	TYR	2.0
6	L	309	TYR	2.0
1	G	239	ARG	2.0
2	B	34	VAL	2.0
2	H	149	VAL	2.0
3	I	68	VAL	2.0
1	G	263	GLU	2.0
6	L	130	MET	2.0
1	G	246	CYS	2.0
3	I	106	GLN	2.0
2	H	254	ASN	2.0
3	I	31	LEU	2.0
4	J	91	LEU	2.0
1	A	464	PRO	2.0
2	B	130	ILE	2.0
2	H	10	ILE	2.0
3	I	97	ILE	2.0
5	K	112	ILE	2.0
1	A	379	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(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
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

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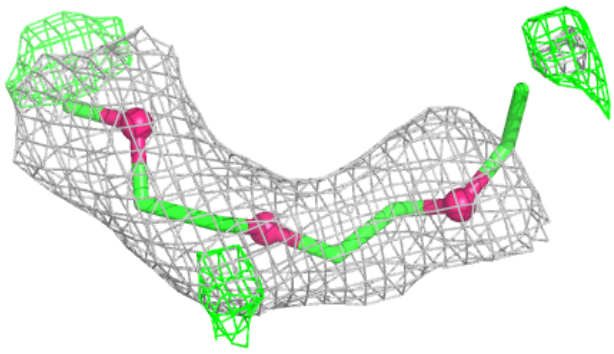
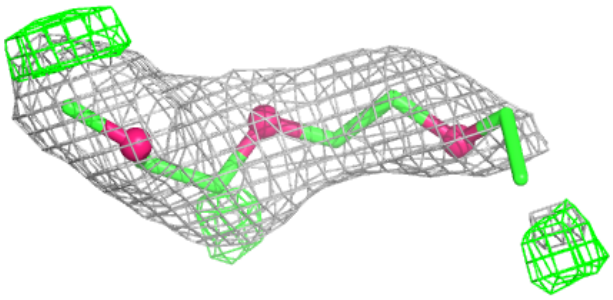
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SF4	E	303	8/8	0.98	0.05	42,44,47,49	0
8	SF4	A	706	8/8	0.98	0.04	38,40,42,43	0
8	SF4	I	201	8/8	0.98	0.04	32,33,35,35	0
8	SF4	I	202	8/8	0.98	0.05	38,42,42,43	0
13	FES	D	201	4/4	0.98	0.05	34,35,36,39	0
17	FCO	F	506	7/7	0.98	0.08	28,28,32,32	0
13	FES	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

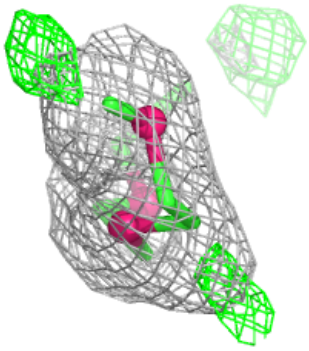
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

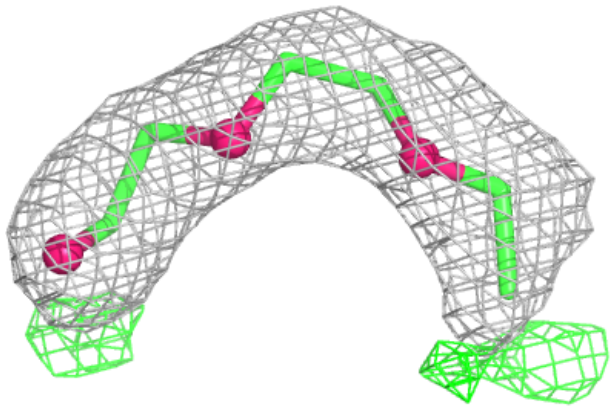


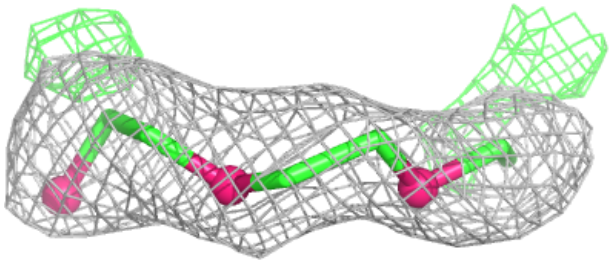


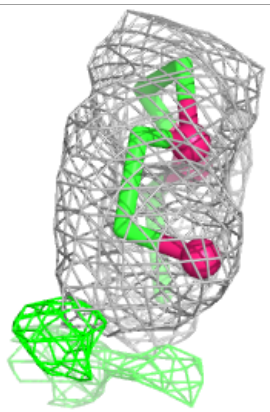


Electron density around PE3 L 502:

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

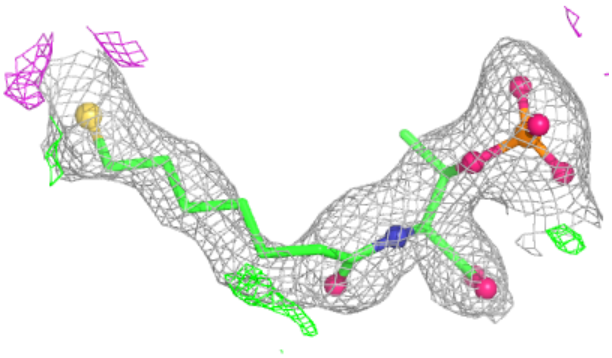


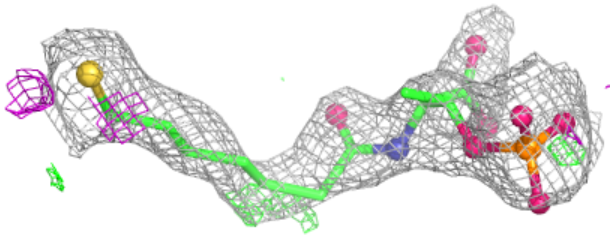


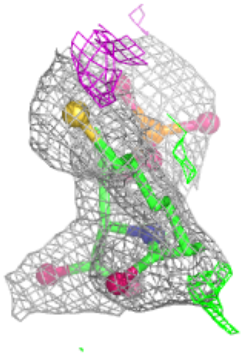


Electron density around TP7 H 304:

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

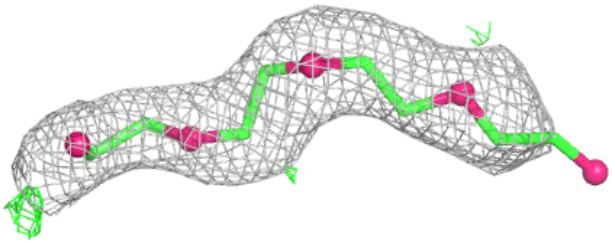


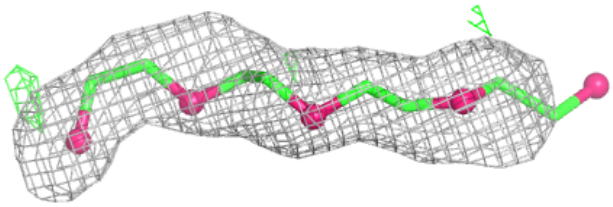


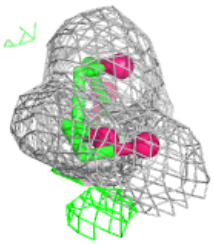


Electron density around PE3 F 503:

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

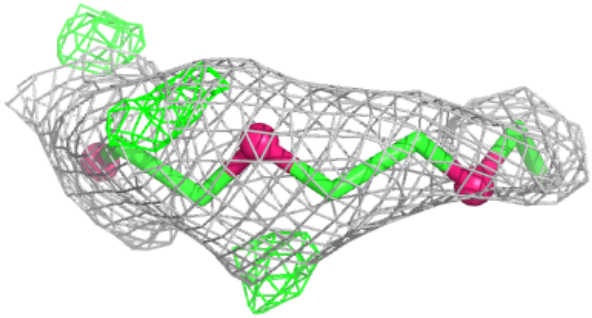


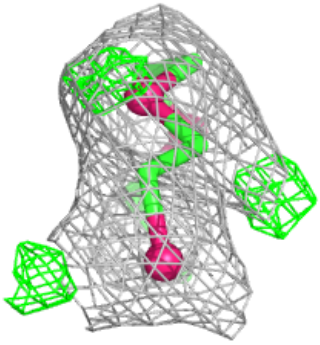




Electron density around PE3 F 502:

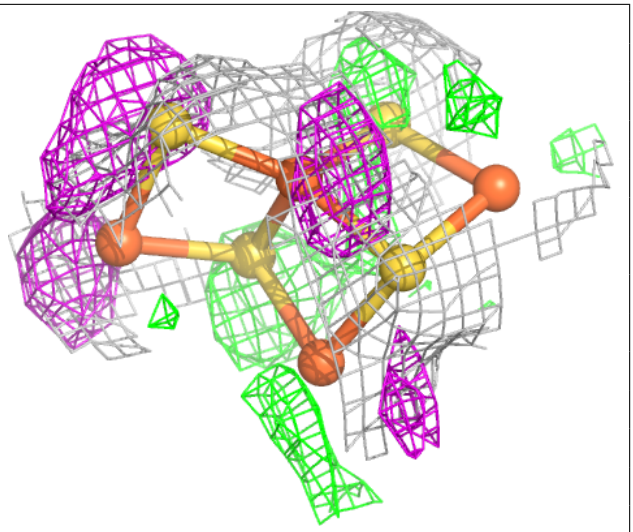
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

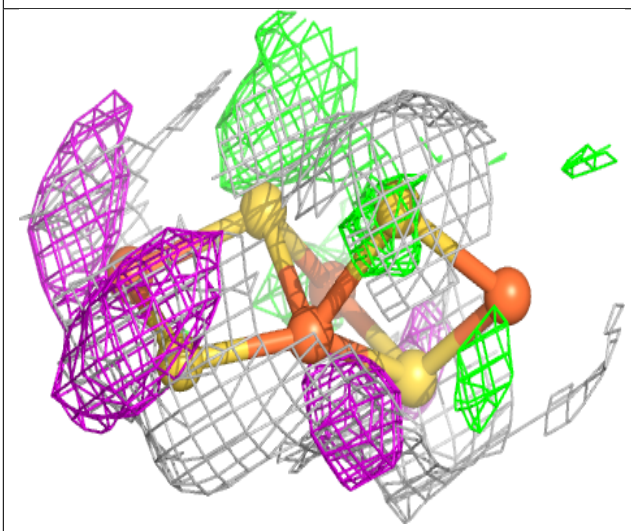


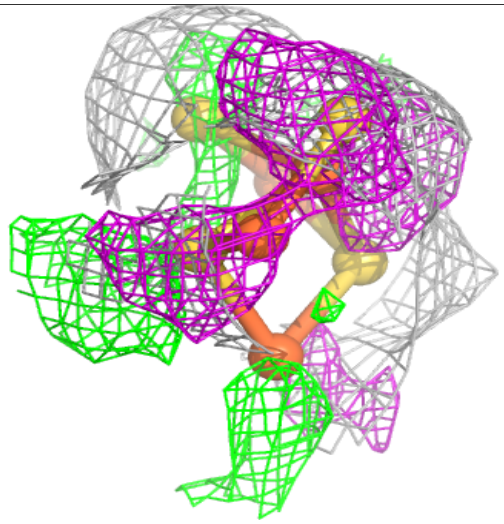


Electron density around 9S8 H 301:

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

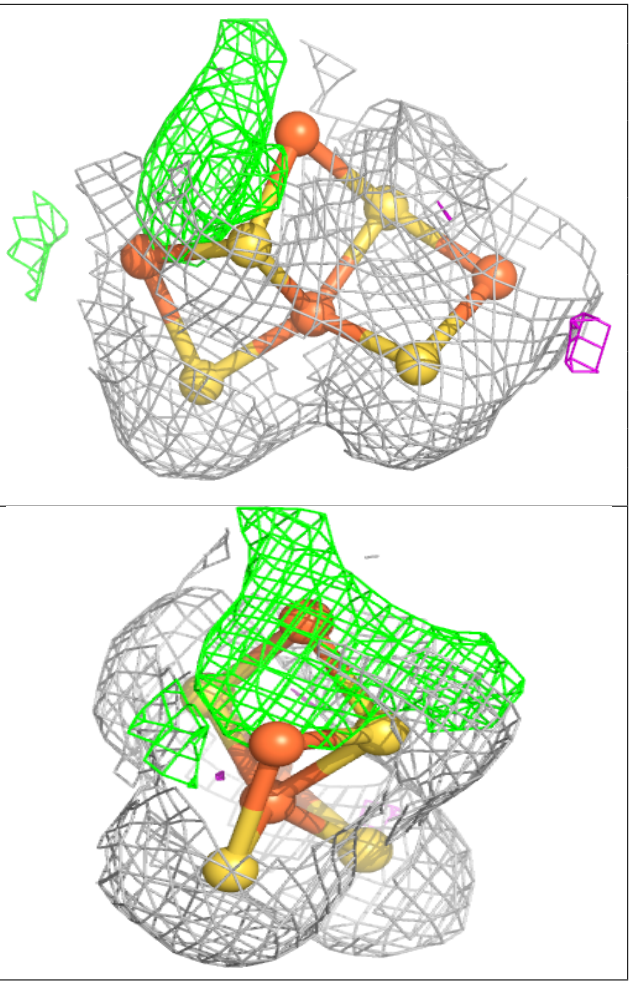






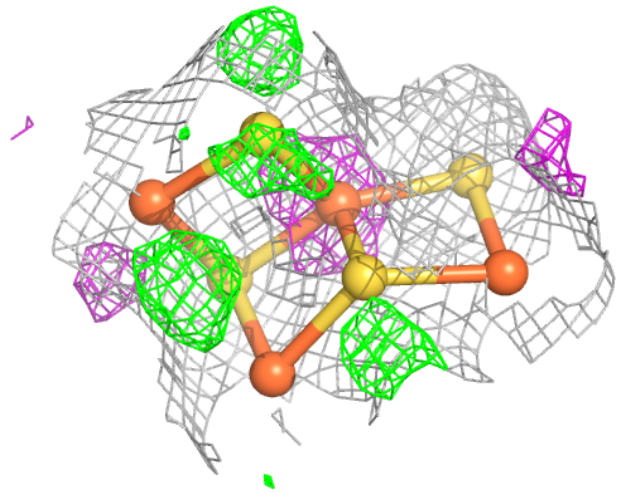
Electron density around 9S8 B 301:

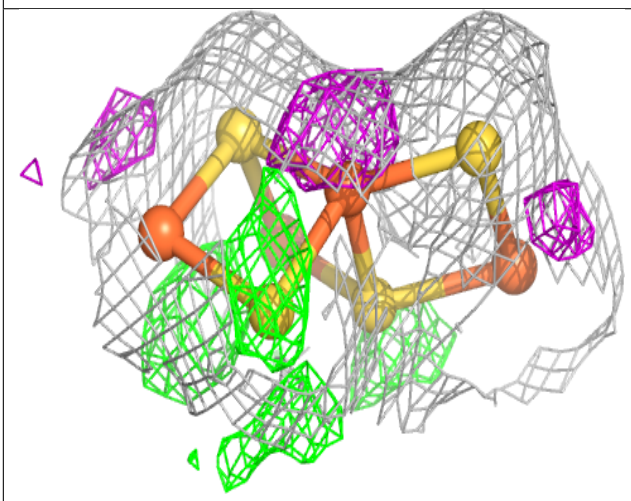
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

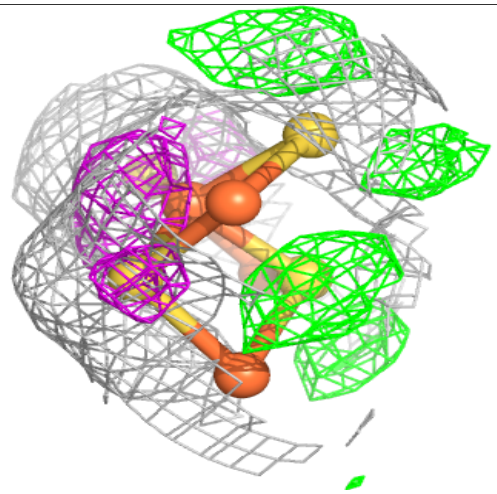


Electron density around 9S8 B 302:

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

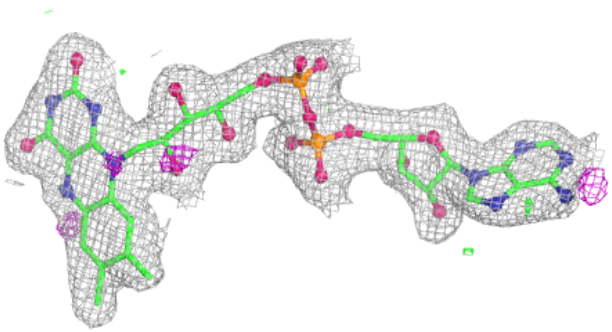


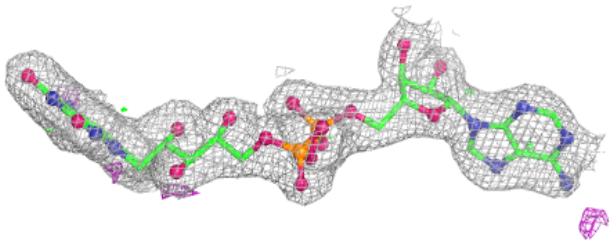


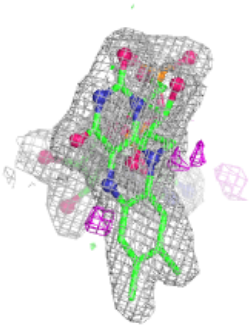


Electron density around FAD G 704:

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

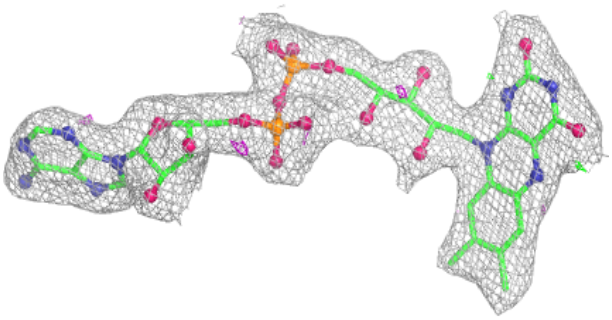


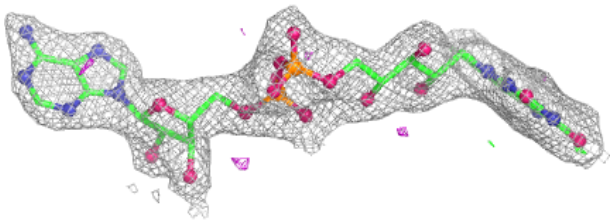


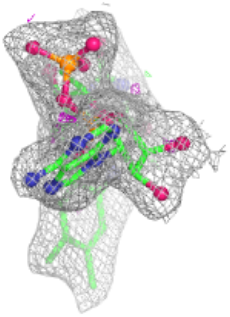


Electron density around FAD A 701:

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

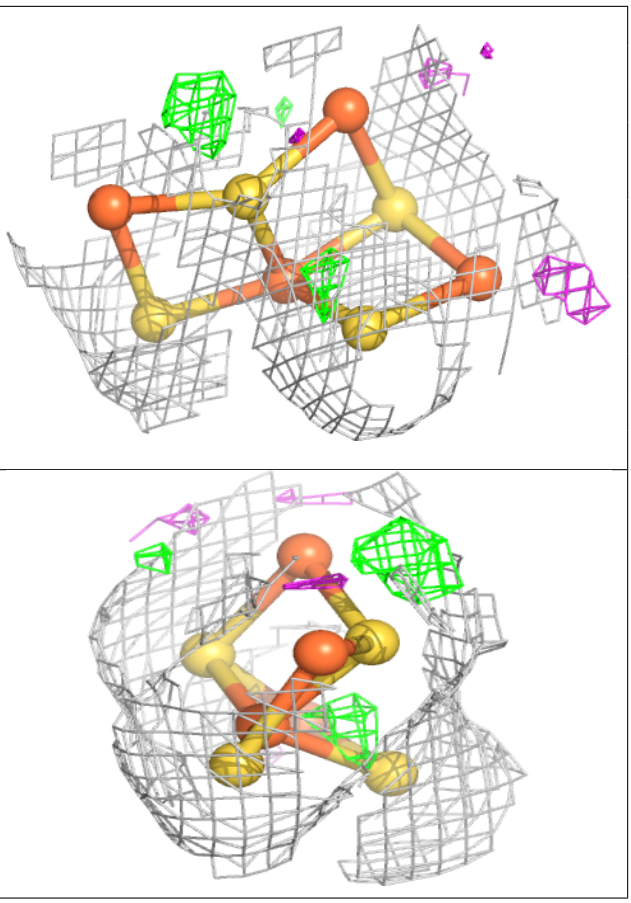






Electron density around 9S8 H 302:

$2mF_o$-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.