Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2026 – 09:39 am BST

PDB ID	:	5ODQ / pdb_00005odq
Title	:	Heterodisulfide reductase / [NiFe]-hydrogenase complex from Methanothermococcus thermolithotrophicus soaked with bromoethanesulfonate.
Authors	:	Wagner, T.; Koch, J.; Ermler, U.; Shima, S.
Deposited on	:	2017-07-06
Resolution	:	2.15 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:

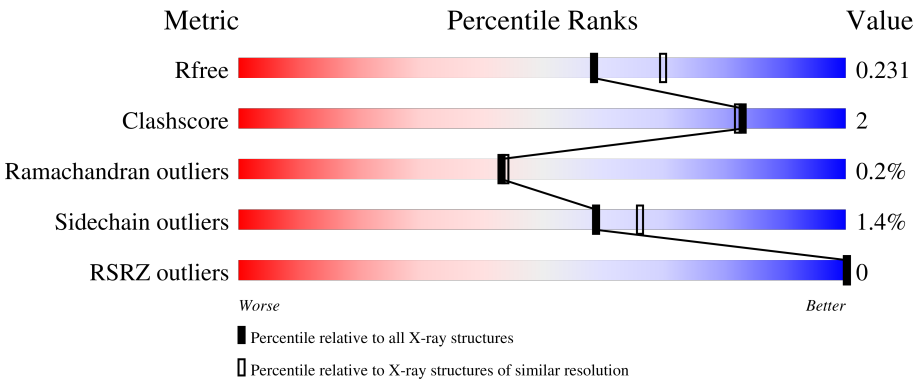
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	92% 7%
1	G	654	92% 7%
2	B	291	93% 6%
2	H	291	93% 7%
3	C	184	91% 9% •

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Mol	Chain	Length	Quality of chain
3	I	184	90% 9%
4	D	140	93% 5%
4	J	140	94%
5	E	299	92% 7%
5	K	299	90% 9%
6	F	473	88% 7% 5%
6	L	473	86% 8% 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
9	SF4	A	707	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 32417 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

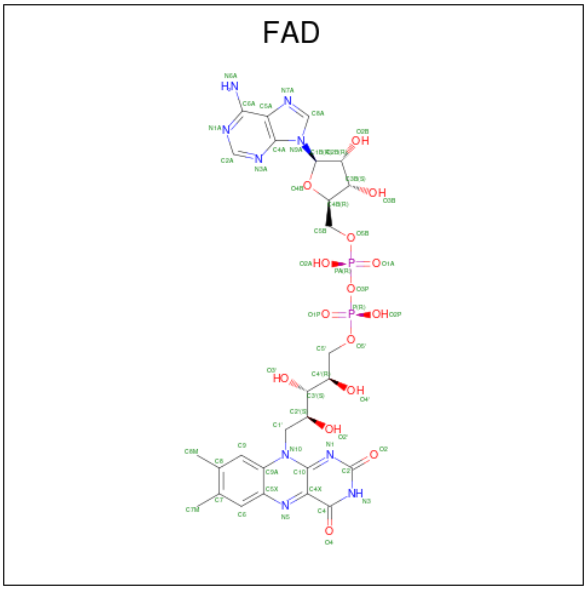
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	298	2258	1425	369	445	19	0	0	0
5	K	298	2266	1430	372	445	19	0	1	0

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

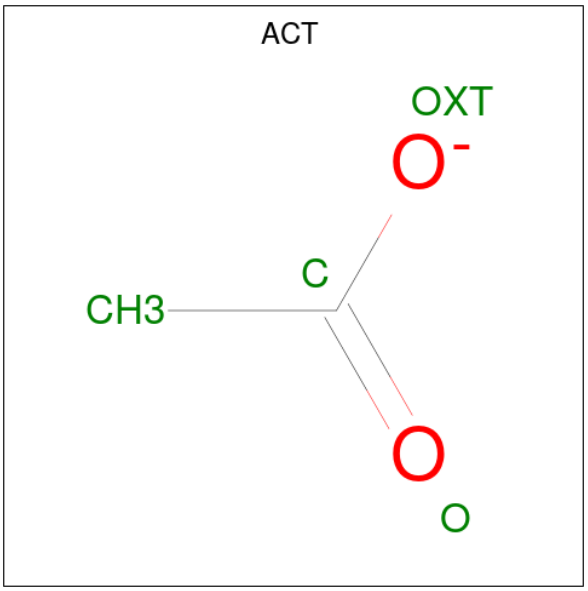
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	447	3521	2230	600	672	19	0	0	0
6	L	447	3521	2230	600	672	19	0	0	0

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



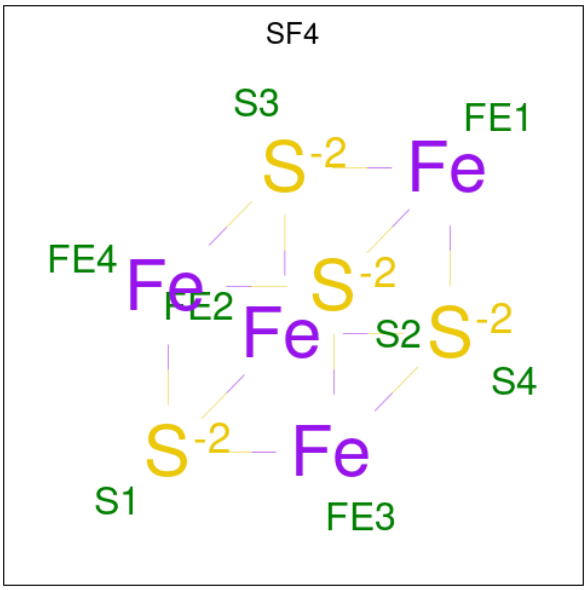
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	53	27	9	15	2	0	0
7	G	1	53	27	9	15	2	0	0

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



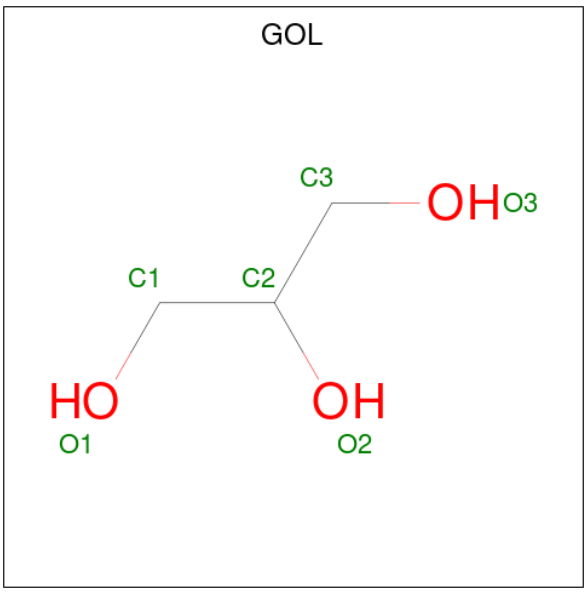
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	4	2	2	0	0
			Total	C	O		
8	A	1	4	2	2	0	0
			Total	C	O		
8	D	1	4	2	2	0	0
			Total	C	O		
8	G	1	4	2	2	0	0
			Total	C	O		
8	G	1	4	2	2	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



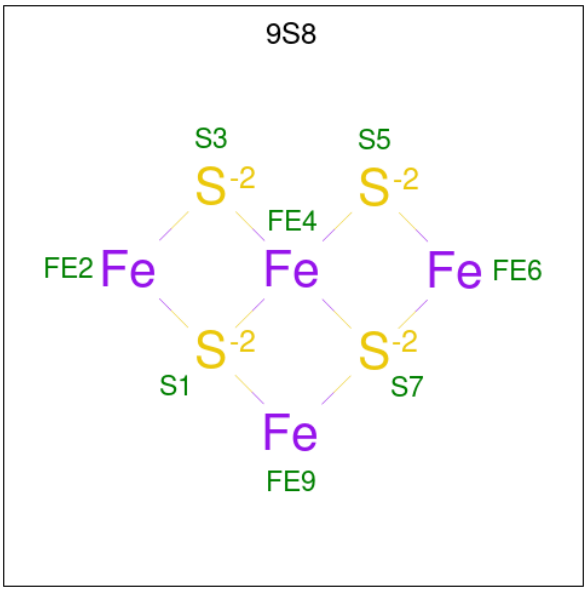
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	A	1	8	4	4	0	0
9	A	1	8	4	4	0	0
9	A	1	8	4	4	0	0
9	A	1	8	4	4	0	0
9	A	1	8	4	4	0	0
9	A	1	8	4	4	0	0
9	C	1	8	4	4	0	0
9	C	1	8	4	4	0	0
9	E	1	8	4	4	0	0
9	E	1	8	4	4	0	0
9	E	1	8	4	4	0	0
9	G	1	8	4	4	0	0
9	G	1	8	4	4	0	0
9	G	1	8	4	4	0	0
9	G	1	8	4	4	0	0
9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

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



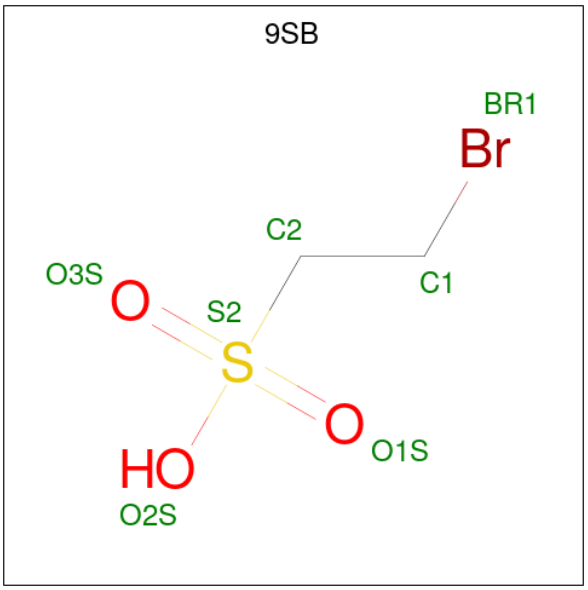
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
10	A	1	6	3	3		0	0
			Total	C	O			
10	A	1	6	3	3		0	0
			Total	C	O			
10	G	1	6	3	3		0	0
			Total	C	O			
10	H	1	6	3	3		0	0
			Total	C	O			
10	K	1	6	3	3		0	0

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



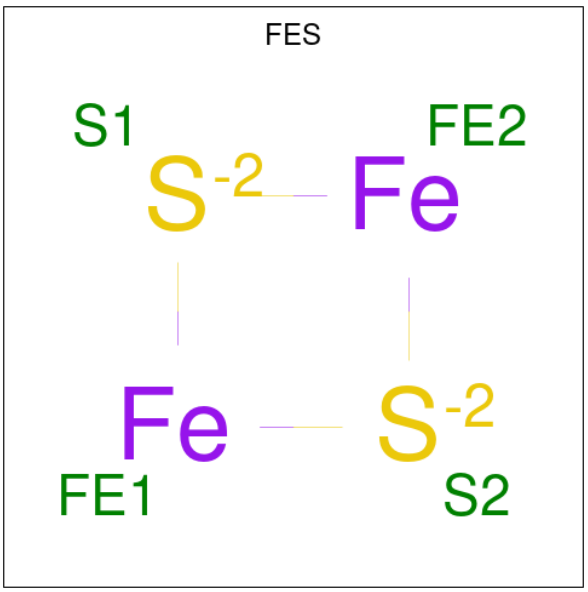
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	B	1	8	4	4	0	0
			Total	Fe	S		
11	B	1	8	4	4	0	0
			Total	Fe	S		
11	H	1	8	4	4	0	0
			Total	Fe	S		
11	H	1	8	4	4	0	0

- Molecule 12 is 2-bromanylethanesulfonic acid (CCD ID: 9SB) (formula: $C_2H_5BrO_3S$).



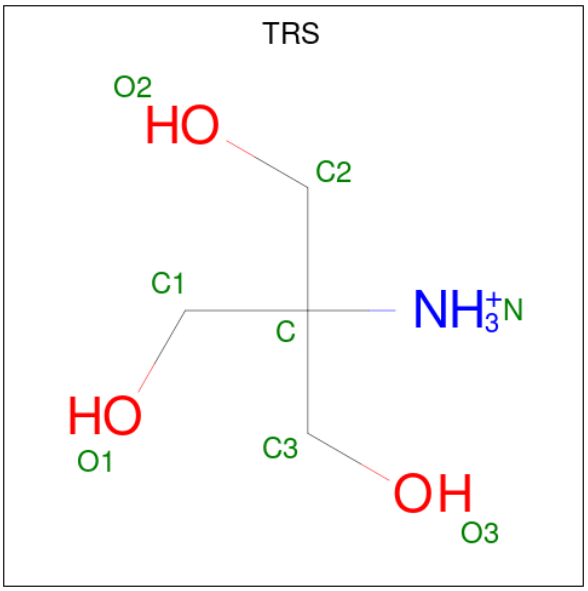
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	O	S		
12	B	1	7	1	2	3	1	0	0
			Total	Br	C	O	S		
12	B	1	7	1	2	3	1	0	0
			Total	Br	C	O	S		
12	H	1	7	1	2	3	1	0	0
			Total	Br	C	O	S		
12	H	1	7	1	2	3	1	0	0

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



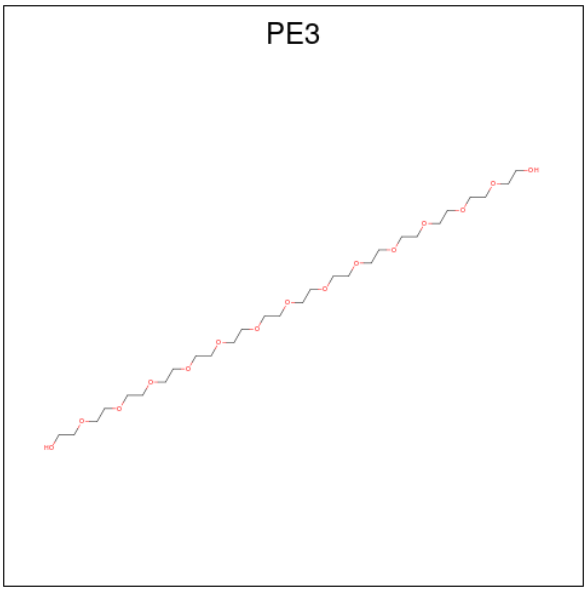
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
13	D	1	4	2	2	0	0
			Total	Fe	S		
13	J	1	4	2	2	0	0

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



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

- Molecule 15 is 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
			Total	C	O			
15	G	1	14	9	5		0	0

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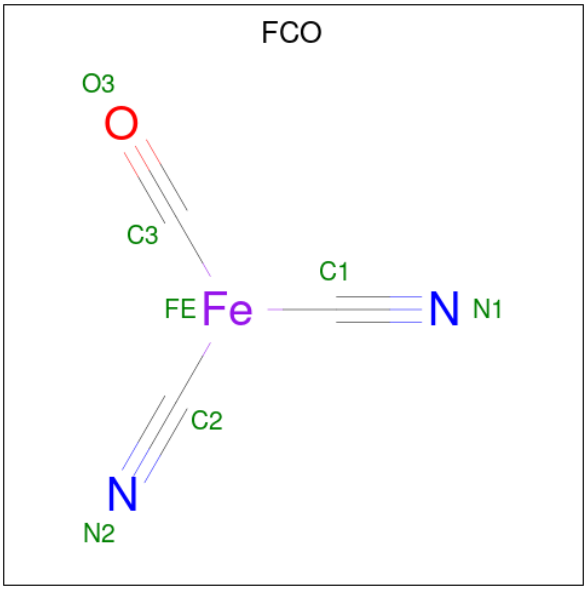
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	L	1	9	6	3	0	0

- 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
			Total	Fe		
16	G	1	1	1	0	0
			Total	Fe		
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 water.

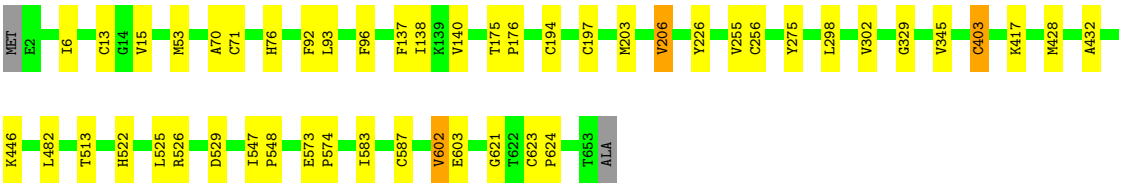
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	171	171	171	0	0
			Total	O		
19	B	43	43	43	0	0
			Total	O		
19	C	45	45	45	0	0
			Total	O		
19	D	37	37	37	0	0
			Total	O		
19	E	61	61	61	0	0
			Total	O		
19	F	92	92	92	0	0
			Total	O		
19	G	166	166	166	0	0
			Total	O		
19	H	24	24	24	0	0
			Total	O		
19	I	31	31	31	0	0
			Total	O		
19	J	47	47	47	0	0
			Total	O		
19	K	75	75	75	0	0
			Total	O		
19	L	125	125	125	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.

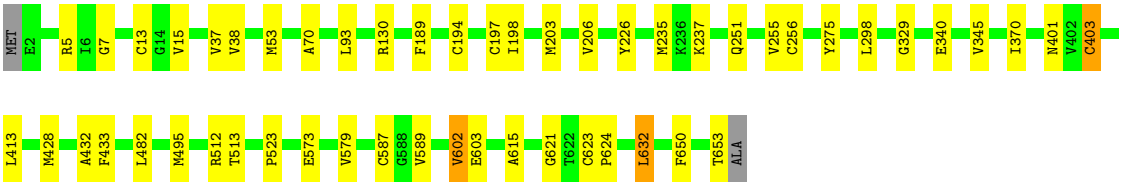
• Molecule 1: Heterodisulfide reductase, subunit A

Chain A: 92% 7%



• Molecule 1: Heterodisulfide reductase, subunit A

Chain G: 92% 7%

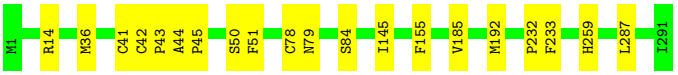


• Molecule 2: Heterodisulfide reductase, subunit B

Chain B: 93% 6%

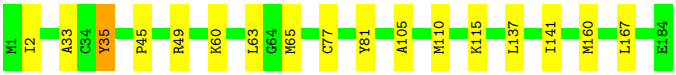
• Molecule 2: Heterodisulfide reductase, subunit B

Chain H: 93% 7%



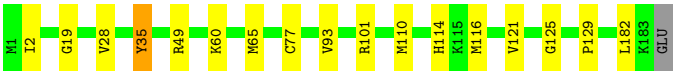
• Molecule 3: Heterodisulfide reductase, subunit C

Chain C: 91% 9%



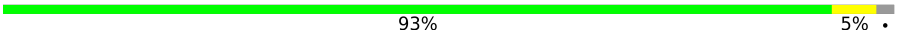
• Molecule 3: Heterodisulfide reductase, subunit C

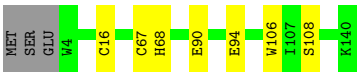
Chain I:



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

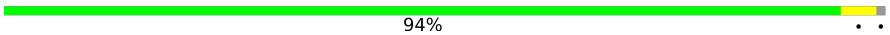
Chain D:





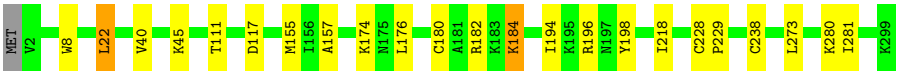
• Molecule 4: Methyl-viologen reducing hydrogenase, subunit D

Chain J:



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

Chain E:

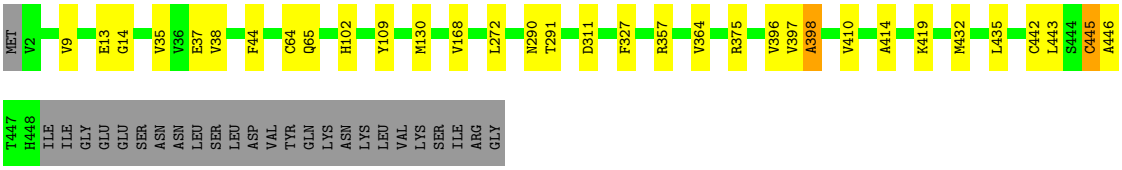


• Molecule 5: Methyl-viologen reducing hydrogenase, subunit G

Chain K:

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

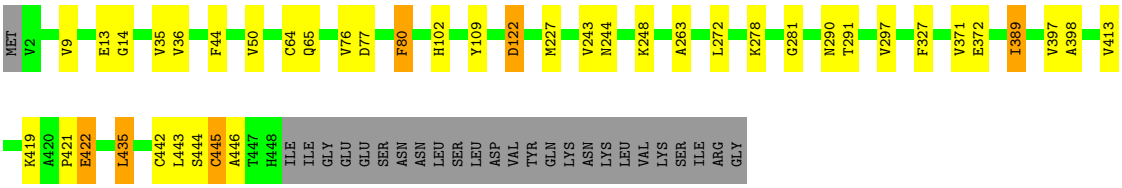
Chain F:



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

Chain L:

86%
8%
• 5%


MET
V2
V9
E13
G14
V35
V36
F44
V50
C64
Q65
V76
D77
F80
H102
Y109
D122
M227
V243
N244
K248
A263
L272
K278
G281
N290
T291
V297
F327
V371
E372
I389
V397
A398
V413
K419
A420
P421
E422
L435
C442
L443
S444
C445
A446
T447
H448
ILE
ILE
GLY
GLU
GLU
SER
ASN
ASN
LEU
SER
LEU
ASP
VAL
TYR
GLN
LYS
ASN
LYS
LEU
VAL
LYS
SER
ILE
ARG
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	366.32Å 97.35Å 133.28Å 90.00° 108.37° 90.00°	Depositor
Resolution (Å)	48.68 – 2.15 48.68 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.68-2.15) 100.0 (48.68-2.15)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.196 , 0.219 0.210 , 0.231	Depositor DCC
R_{free} test set	12098 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 23.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.037 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32417	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: FES, 9SB, TRS, FAD, NI, 9S8, ACT, FE, FCO, PE3, GOL, SF4

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	0.66	1/5071 (0.0%)	0.98	9/6853 (0.1%)
1	G	0.65	1/5071 (0.0%)	1.00	10/6853 (0.1%)
2	B	0.61	0/2277	1.01	3/3070 (0.1%)
2	H	0.62	0/2277	1.01	3/3070 (0.1%)
3	C	0.61	0/1447	0.97	0/1946
3	I	0.60	0/1437	0.97	0/1934
4	D	0.62	0/1123	1.00	0/1508
4	J	0.60	0/1132	0.98	0/1520
5	E	0.64	1/2297 (0.0%)	1.00	4/3113 (0.1%)
5	K	0.64	1/2308 (0.0%)	1.01	3/3127 (0.1%)
6	F	0.63	0/3590	1.06	8/4853 (0.2%)
6	L	0.62	0/3590	1.07	11/4853 (0.2%)
All	All	0.63	4/31620 (0.0%)	1.01	51/42700 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	155	MET	SD-CE	-6.30	1.63	1.79
5	K	155	MET	SD-CE	-6.10	1.64	1.79
1	G	53	MET	SD-CE	-5.18	1.66	1.79
1	A	53	MET	SD-CE	-5.06	1.66	1.79

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	22	LEU	N-CA-C	-8.22	102.70	112.89
5	E	22	LEU	N-CA-C	-8.07	102.88	112.89
5	K	176	LEU	N-CA-C	7.57	120.42	111.71
5	E	176	LEU	N-CA-C	7.51	120.35	111.71
6	L	9	VAL	N-CA-C	-6.97	100.59	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	9	VAL	N-CA-C	-6.91	100.67	109.30
6	L	80	PHE	N-CA-C	-6.85	98.08	109.24
6	L	397	VAL	N-CA-C	6.62	117.38	107.51
1	G	275	TYR	N-CA-C	6.61	118.25	108.60
6	F	44	PHE	CA-CB-CG	6.42	120.22	113.80
6	F	327	PHE	N-CA-C	-6.38	104.37	111.71
6	L	327	PHE	N-CA-C	-6.38	104.37	111.71
6	L	444	SER	N-CA-C	-6.30	104.50	111.36
6	L	44	PHE	CA-CB-CG	6.29	120.09	113.80
6	F	419	LYS	N-CA-C	-6.25	104.62	112.93
1	G	345	VAL	N-CA-C	-6.11	106.79	111.62
2	B	41	CYS	N-CA-C	-6.10	102.05	110.35
1	G	251	GLN	N-CA-C	-5.98	104.88	111.82
6	L	419	LYS	N-CA-C	-5.90	105.08	112.93
1	A	93	LEU	N-CA-C	-5.87	105.43	112.59
1	A	345	VAL	N-CA-C	-5.81	107.03	111.62
2	H	41	CYS	N-CA-C	-5.73	102.55	110.35
6	L	109	TYR	N-CA-C	5.65	118.29	111.40
6	F	397	VAL	N-CA-C	5.64	115.92	107.51
6	F	109	TYR	N-CA-C	5.63	118.27	111.40
6	L	122	ASP	N-CA-C	-5.61	106.56	113.41
2	B	121	HIS	N-CA-C	-5.60	100.11	109.24
1	A	275	TYR	N-CA-C	5.48	115.47	108.24
1	A	15	VAL	N-CA-C	-5.44	107.98	113.20
1	G	432	ALA	N-CA-C	-5.43	100.89	108.54
1	A	428	MET	N-CA-C	-5.40	105.81	112.72
1	G	93	LEU	N-CA-C	-5.38	106.03	112.59
1	A	432	ALA	N-CA-C	-5.37	100.97	108.54
6	F	364	VAL	N-CA-C	-5.37	99.43	107.37
1	G	428	MET	N-CA-C	-5.35	105.87	112.72
1	A	573	GLU	N-CA-C	5.33	117.34	109.50
2	H	259	HIS	N-CA-C	-5.24	101.98	110.32
1	A	6	ILE	N-CA-C	5.23	116.50	108.71
1	A	329	GLY	N-CA-C	5.21	120.44	111.47
1	G	329	GLY	N-CA-C	5.18	120.38	111.47
1	G	401	ASN	N-CA-C	5.13	121.72	110.80
2	B	259	HIS	N-CA-C	-5.10	102.21	110.32
1	G	15	VAL	N-CA-C	-5.09	108.31	113.20
2	H	185	VAL	N-CA-C	5.05	112.97	108.63
6	L	281	GLY	N-CA-C	5.05	118.16	111.70
5	E	45	LYS	N-CA-C	5.04	116.85	111.36
6	F	396	VAL	N-CA-C	-5.03	99.71	106.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	196	ARG	N-CA-C	-5.03	103.04	110.48
6	L	413	VAL	N-CA-C	-5.01	105.82	110.53
1	G	433	PHE	N-CA-C	5.01	119.39	113.28
5	K	45	LYS	N-CA-C	5.00	116.81	111.36

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	4974	32	0
1	G	4979	0	4974	26	0
2	B	2236	0	2243	11	0
2	H	2236	0	2243	15	0
3	C	1426	0	1441	11	0
3	I	1416	0	1435	14	0
4	D	1097	0	1068	5	0
4	J	1106	0	1074	5	0
5	E	2258	0	2265	12	0
5	K	2266	0	2278	16	0
6	F	3521	0	3503	15	0
6	L	3521	0	3503	18	0
7	A	53	0	31	1	0
7	G	53	0	31	2	0
8	A	8	0	6	2	0
8	D	4	0	3	0	0
8	G	8	0	6	0	0
9	A	48	0	0	5	0
9	C	16	0	0	0	0
9	E	24	0	0	1	0
9	G	48	0	0	3	0
9	I	16	0	0	0	0
9	K	24	0	0	1	0
10	A	12	0	16	1	0
10	G	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	6	0	8	0	0
10	K	6	0	8	0	0
11	B	16	0	0	0	0
11	H	16	0	0	0	0
12	B	14	0	0	0	0
12	H	14	0	0	0	0
13	D	4	0	0	0	0
13	J	4	0	0	0	0
14	D	8	0	12	0	0
15	F	9	0	10	0	0
15	G	14	0	16	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	A	171	0	0	0	0
19	B	43	0	0	0	0
19	C	45	0	0	0	0
19	D	37	0	0	0	0
19	E	61	0	0	0	0
19	F	92	0	0	0	0
19	G	166	0	0	0	0
19	H	24	0	0	0	0
19	I	31	0	0	0	0
19	J	47	0	0	0	0
19	K	75	0	0	0	0
19	L	125	0	0	0	0
All	All	32417	0	31166	150	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 (150) 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	1.34	1.07
2:H:51:PHE:CZ	3:I:114:HIS:HB3	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG21	1:A:302:VAL:CG2	2.11	0.81
1:A:255:VAL:CG2	1:A:302:VAL:HG21	2.10	0.79
2:H:145:ILE:HD13	2:H:287:LEU:HD11	1.66	0.78
6:L:263:ALA:HB2	6:L:278:LYS:HG2	1.66	0.77
1:G:403:CYS:HB2	9:G:707:SF4:S3	2.28	0.73
1:A:255:VAL:CG1	1:A:298:LEU:HB3	2.18	0.73
1:A:547:ILE:HD12	7:A:701:FAD:C2	2.24	0.68
6:L:227:MET:HE2	6:L:372:GLU:HG2	1.77	0.65
1:A:255:VAL:HG12	1:A:298:LEU:HB3	1.79	0.64
5:K:40:VAL:HG13	5:K:41:LEU:HG	1.79	0.63
1:G:7:GLY:HA2	1:G:38:VAL:HG13	1.80	0.62
2:H:51:PHE:HZ	3:I:114:HIS:HB3	1.61	0.62
10:G:712:GOL:H2	3:I:35:TYR:HA	1.81	0.62
1:A:623:CYS:SG	1:A:624:PRO:HD3	2.40	0.60
6:L:77:ASP:O	6:L:80:PHE:O	2.18	0.60
6:F:414:ALA:HB2	6:F:432:MET:HE3	1.83	0.60
3:C:60:LYS:HG2	3:C:65:MET:HE3	1.83	0.60
6:F:272:LEU:HD11	6:F:446:ALA:HB1	1.84	0.60
1:A:403:CYS:HB2	9:A:704:SF4:S1	2.42	0.59
1:A:417:LYS:HB3	8:A:702:ACT:H2	1.85	0.58
6:L:272:LEU:HD11	6:L:446:ALA:HB1	1.85	0.58
2:B:145:ILE:HD12	2:B:287:LEU:HD11	1.85	0.57
1:A:525:LEU:O	1:A:526:ARG:HG3	2.05	0.56
3:I:60:LYS:HG2	3:I:65:MET:HE3	1.85	0.56
5:E:184:LYS:HE2	9:E:303:SF4:S2	2.45	0.56
1:G:194:CYS:HB2	1:G:197:CYS:SG	2.45	0.56
2:H:78:CYS:SG	2:H:232:PRO:HD2	2.46	0.56
6:F:35:VAL:HG21	6:F:272:LEU:CD2	2.36	0.56
2:B:78:CYS:SG	2:B:232:PRO:HD2	2.48	0.54
1:G:255:VAL:HG12	1:G:298:LEU:HB3	1.90	0.54
4:J:90:GLU:HB2	5:K:280:LYS:HE2	1.89	0.54
6:L:35:VAL:HG21	6:L:272:LEU:HD22	1.90	0.54
2:B:2:LYS:HE3	2:B:72:VAL:HG11	1.90	0.53
3:C:63:LEU:HD23	3:C:65:MET:HE2	1.90	0.53
5:E:8:TRP:CH2	5:E:40:VAL:HB	2.44	0.53
6:F:442:CYS:SG	6:F:445:CYS:HB2	2.49	0.52
6:L:244:ASN:ND2	6:L:248:LYS:HB3	2.25	0.52
1:A:137:PHE:CD2	8:A:703:ACT:H3	2.45	0.52
2:B:77:VAL:HA	2:B:122:PHE:CD1	2.44	0.52
1:G:370:ILE:C	1:G:370:ILE:HD12	2.35	0.52
1:A:255:VAL:HG11	1:A:298:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:CYS:HA	9:G:709:SF4:S4	2.50	0.51
4:D:90:GLU:OE2	5:E:280:LYS:NZ	2.35	0.51
2:H:45:PRO:HD3	2:H:84:SER:HB2	1.92	0.51
6:L:435:LEU:C	6:L:435:LEU:HD13	2.36	0.51
1:A:525:LEU:C	1:A:526:ARG:HG3	2.35	0.51
6:L:35:VAL:HG21	6:L:272:LEU:CD2	2.41	0.51
2:H:51:PHE:HZ	3:I:114:HIS:CB	2.24	0.50
2:H:51:PHE:CE1	3:I:110:MET:HE3	2.46	0.50
6:L:422:GLU:H	6:L:422:GLU:CD	2.17	0.50
5:K:278:LYS:HB3	6:L:389:ILE:HD11	1.93	0.50
2:H:43:PRO:O	2:H:44:ALA:C	2.54	0.50
10:A:711:GOL:H2	3:C:35:TYR:HA	1.94	0.49
1:G:623:CYS:SG	1:G:624:PRO:HD3	2.52	0.49
1:A:602:VAL:CG2	1:A:603:GLU:N	2.74	0.49
6:F:35:VAL:HG21	6:F:272:LEU:HD22	1.95	0.49
1:G:226:TYR:CZ	1:G:615:ALA:HB1	2.47	0.49
5:K:184:LYS:HE2	9:K:303:SF4:S4	2.53	0.49
1:G:602:VAL:CG2	1:G:603:GLU:N	2.75	0.49
1:A:203:MET:O	1:A:206:VAL:HG12	2.14	0.48
4:J:87:MET:HG3	5:K:257:CYS:SG	2.54	0.48
1:G:587:CYS:HB2	5:K:218:ILE:HG22	1.96	0.48
6:L:13:GLU:HB3	6:L:442:CYS:HA	1.95	0.48
4:D:16:CYS:HB3	4:D:108:SER:HA	1.96	0.48
6:L:421:PRO:HD2	6:L:422:GLU:OE2	2.13	0.48
6:L:243:VAL:HG22	6:L:297:VAL:HG12	1.95	0.48
6:F:13:GLU:HB3	6:F:442:CYS:HA	1.95	0.47
1:G:621:GLY:C	1:G:624:PRO:HD2	2.39	0.47
1:A:548:PRO:HB3	1:G:523:PRO:O	2.14	0.47
4:J:53:LYS:HD3	5:K:293:PHE:CE1	2.50	0.47
5:K:127:PRO:HD3	6:L:36:VAL:HB	1.96	0.47
1:G:5:ARG:HE	1:G:37:VAL:HG21	1.80	0.47
6:F:435:LEU:C	6:F:435:LEU:HD13	2.39	0.47
1:G:130:ARG:NH1	1:G:653:THR:OG1	2.47	0.47
2:H:51:PHE:CD1	3:I:110:MET:HE3	2.49	0.47
1:A:621:GLY:C	1:A:624:PRO:HD2	2.39	0.47
3:C:137:LEU:O	3:C:141:ILE:HG12	2.15	0.47
4:D:94:GLU:HB3	5:E:281:ILE:HD12	1.96	0.47
1:G:482:LEU:HD23	3:I:2:ILE:HB	1.96	0.47
2:B:158:PRO:HG3	3:C:81:TYR:CE1	2.50	0.46
6:F:410:VAL:HG22	6:F:432:MET:HE2	1.97	0.46
5:K:97:LEU:HD21	5:K:281:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:579:VAL:HG22	1:G:632:LEU:HG	1.97	0.46
1:A:583:ILE:O	5:E:174:LYS:HA	2.15	0.46
1:A:76:HIS:CD2	9:A:707:SF4:S1	3.09	0.45
4:D:16:CYS:HB2	4:D:67:CYS:SG	2.55	0.45
1:A:13:CYS:HB2	9:A:707:SF4:S2	2.56	0.45
2:B:59:LEU:HD22	3:C:160:MET:HE3	1.98	0.45
6:L:64:CYS:CB	17:L:504:FCO:C1	2.94	0.45
1:G:495:MET:CE	7:G:701:FAD:H1'1	2.46	0.45
6:L:442:CYS:SG	6:L:445:CYS:HB2	2.56	0.45
5:E:228:CYS:HB2	5:E:229:PRO:HD3	1.99	0.45
1:G:370:ILE:HD12	1:G:370:ILE:O	2.16	0.45
6:L:50:VAL:HG22	6:L:76:VAL:HG22	1.99	0.45
1:A:138:ILE:HG22	1:A:140:VAL:HG13	1.99	0.44
3:I:19:GLY:HA3	3:I:28:VAL:HG21	1.99	0.44
5:K:228:CYS:HB2	5:K:229:PRO:HD3	2.00	0.44
1:G:650:PHE:CD1	4:J:57:GLU:HB3	2.53	0.44
2:B:211:MET:HE3	3:C:45:PRO:HB2	1.99	0.44
1:A:522:HIS:CE1	1:G:198:ILE:HD11	2.52	0.44
2:B:245:ILE:HG23	2:B:249:PHE:CD2	2.53	0.44
2:B:249:PHE:CD1	2:B:249:PHE:N	2.82	0.44
2:H:14:ARG:NH2	3:I:129:PRO:O	2.51	0.44
6:F:14:GLY:HA3	6:F:443:LEU:HB2	1.99	0.44
2:B:2:LYS:HE3	2:B:72:VAL:CG1	2.49	0.43
1:G:235:MET:HE3	1:G:237:LYS:HG2	2.00	0.43
6:F:375:ARG:C	6:F:398:ALA:HB1	2.43	0.43
2:B:55:THR:HA	3:C:167:LEU:HD13	2.01	0.43
6:L:14:GLY:HA3	6:L:443:LEU:HB2	1.99	0.43
1:G:13:CYS:HB2	9:G:706:SF4:S3	2.58	0.43
2:H:42:CYS:SG	2:H:43:PRO:C	3.02	0.43
2:H:51:PHE:HZ	3:I:114:HIS:CG	2.37	0.43
1:A:526:ARG:HB3	1:A:529:ASP:HB2	2.01	0.42
3:C:105:ALA:HA	3:C:110:MET:HG3	2.01	0.42
5:K:152:ASN:ND2	5:K:155:MET:HB2	2.34	0.42
1:A:92:PHE:CZ	1:A:574:PRO:HD2	2.54	0.42
1:A:256:CYS:HA	9:A:706:SF4:S2	2.59	0.42
1:A:446:LYS:HD3	3:C:33:ALA:HB2	2.01	0.42
5:E:180:CYS:SG	5:E:182:ARG:HG3	2.59	0.42
2:H:50:SER:HB3	3:I:101:ARG:HD3	2.01	0.42
4:J:68:HIS:HA	4:J:106:TRP:HB3	2.01	0.42
6:F:410:VAL:CG2	6:F:432:MET:HE2	2.49	0.42
1:G:226:TYR:CD1	1:G:226:TYR:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:589:VAL:HA	5:K:259:ASP:OD2	2.20	0.42
1:A:226:TYR:CD1	1:A:226:TYR:N	2.88	0.41
1:A:482:LEU:HD23	3:C:2:ILE:HB	2.01	0.41
5:K:146:ILE:HG22	5:K:151:PRO:HB3	2.01	0.41
5:K:273:LEU:HB3	5:K:274:PRO:HD3	2.02	0.41
4:D:68:HIS:HA	4:D:106:TRP:HB3	2.02	0.41
1:A:587:CYS:HB2	5:E:218:ILE:HG22	2.03	0.41
2:H:79:ASN:OD1	2:H:155:PHE:HB2	2.20	0.41
2:H:155:PHE:CD1	2:H:155:PHE:C	2.97	0.41
1:A:76:HIS:NE2	9:A:707:SF4:S1	2.93	0.41
6:F:37:GLU:HG2	6:F:38:VAL:N	2.36	0.41
1:A:194:CYS:HB3	1:A:197:CYS:HB2	1.93	0.41
1:G:189:PHE:CE2	7:G:701:FAD:C4	3.04	0.41
1:G:203:MET:O	1:G:206:VAL:HG12	2.21	0.41
5:K:194:ILE:HG13	5:K:273:LEU:CD1	2.51	0.41
5:E:117:ASP:OD1	5:E:117:ASP:N	2.55	0.40
5:K:155:MET:HE2	5:K:171:LEU:HD22	2.03	0.40
5:E:194:ILE:HG13	5:E:273:LEU:CD1	2.50	0.40
6:F:64:CYS:CB	17:F:504:FCO:C1	2.99	0.40
3:I:116:MET:HE2	3:I:182:LEU:HD12	2.02	0.40
5:E:198:TYR:HA	6:F:357:ARG:HH22	1.85	0.40
3:I:121:VAL:O	3:I:125:GLY:HA2	2.21	0.40
1:A:175:THR:HB	1:A:176:PRO:CD	2.51	0.40
5:E:22:LEU:HD21	5:E:157:ALA:HB2	2.04	0.40
6:F:168:VAL:HG23	6:F:357:ARG:HE	1.87	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%)	626 (96%)	22 (3%)	2 (0%)	36 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	650/654 (99%)	627 (96%)	22 (3%)	1 (0%)	43	44
2	B	289/291 (99%)	273 (94%)	16 (6%)	0	100	100
2	H	289/291 (99%)	275 (95%)	14 (5%)	0	100	100
3	C	182/184 (99%)	178 (98%)	4 (2%)	0	100	100
3	I	181/184 (98%)	179 (99%)	2 (1%)	0	100	100
4	D	135/140 (96%)	129 (96%)	6 (4%)	0	100	100
4	J	136/140 (97%)	130 (96%)	6 (4%)	0	100	100
5	E	296/299 (99%)	281 (95%)	15 (5%)	0	100	100
5	K	297/299 (99%)	282 (95%)	15 (5%)	0	100	100
6	F	445/473 (94%)	430 (97%)	13 (3%)	2 (0%)	30	26
6	L	445/473 (94%)	431 (97%)	12 (3%)	2 (0%)	30	26
All	All	3995/4082 (98%)	3841 (96%)	147 (4%)	7 (0%)	43	44

All (7) 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	71	CYS
1	A	70	ALA
1	G	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%)	535 (99%)	5 (1%)	70	77
1	G	540/541 (100%)	532 (98%)	8 (2%)	57	64
2	B	242/242 (100%)	239 (99%)	3 (1%)	63	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	242/242 (100%)	239 (99%)	3 (1%)	63	70
3	C	157/157 (100%)	153 (98%)	4 (2%)	42	45
3	I	156/157 (99%)	152 (97%)	4 (3%)	40	43
4	D	116/119 (98%)	116 (100%)	0	100	100
4	J	117/119 (98%)	117 (100%)	0	100	100
5	E	255/256 (100%)	252 (99%)	3 (1%)	63	70
5	K	256/256 (100%)	252 (98%)	4 (2%)	55	61
6	F	386/410 (94%)	380 (98%)	6 (2%)	55	61
6	L	386/410 (94%)	377 (98%)	9 (2%)	44	49
All	All	3393/3450 (98%)	3344 (99%)	49 (1%)	59	66

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	206	VAL
1	A	403	CYS
1	A	513	THR
1	A	602	VAL
2	B	192	MET
2	B	233	PHE
2	B	249	PHE
3	C	35	TYR
3	C	49	ARG
3	C	77	CYS
3	C	115	LYS
5	E	111	THR
5	E	184	LYS
5	E	238	CYS
6	F	65	GLN
6	F	102	HIS
6	F	130	MET
6	F	290	ASN
6	F	311	ASP
6	F	445	CYS
1	G	340	GLU
1	G	403	CYS
1	G	413	LEU
1	G	512	ARG

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Mol	Chain	Res	Type
1	G	513	THR
1	G	573	GLU
1	G	602	VAL
1	G	632	LEU
2	H	36	MET
2	H	192	MET
2	H	233	PHE
3	I	35	TYR
3	I	49	ARG
3	I	77	CYS
3	I	93	VAL
5	K	111	THR
5	K	113	THR
5	K	238	CYS
5	K	280	LYS
6	L	65	GLN
6	L	102	HIS
6	L	122	ASP
6	L	290	ASN
6	L	371	VAL
6	L	389	ILE
6	L	422	GLU
6	L	435	LEU
6	L	445	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	229	ASN
1	A	410	ASN
1	A	459	GLN
2	B	116	ASN
2	B	128	ASN
2	B	154	HIS
3	C	109	ASN
6	F	403	ASN
1	G	61	HIS
1	G	109	HIS
1	G	306	ASN
1	G	401	ASN
1	G	410	ASN

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Mol	Chain	Res	Type
2	H	90	HIS
2	H	116	ASN
2	H	254	ASN
3	I	10	ASN
3	I	109	ASN
6	L	260	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
15	PE3	F	502	-	8,8,42	0.49	0	7,7,41	0.37	0
9	SF4	A	705	1	0,12,12	-	-	-		
9	SF4	E	303	5	0,12,12	-	-	-		
12	9SB	H	303	-	6,6,6	3.26	1 (16%)	7,8,8	1.64	2 (28%)
9	SF4	I	202	3	0,12,12	-	-	-		
9	SF4	A	704	1	0,12,12	-	-	-		
9	SF4	I	201	3	0,12,12	-	-	-		
10	GOL	K	304	-	5,5,5	0.32	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	GOL	G	712	-	5,5,5	0.25	0	5,5,5	0.17	0
8	ACT	A	703	-	3,3,3	1.00	0	3,3,3	0.91	0
12	9SB	B	304	-	6,6,6	3.13	1 (16%)	7,8,8	1.68	2 (28%)
9	SF4	G	711	1	0,12,12	-	-	-		
13	FES	D	201	4	0,4,4	-	-	-		
12	9SB	H	304	-	6,6,6	3.13	1 (16%)	7,8,8	1.71	2 (28%)
8	ACT	A	702	-	3,3,3	0.93	0	3,3,3	0.97	0
10	GOL	A	711	-	5,5,5	0.25	0	5,5,5	0.55	0
9	SF4	C	201	3	0,12,12	-	-	-		
9	SF4	G	707	1	0,12,12	-	-	-		
10	GOL	H	305	-	5,5,5	0.35	0	5,5,5	0.28	0
9	SF4	E	301	5	0,12,12	-	-	-		
17	FCO	L	504	6	1,6,6	4.26	1 (100%)	-		
7	FAD	A	701	-	56,58,58	1.45	9 (16%)	81,89,89	1.77	19 (23%)
7	FAD	G	701	-	56,58,58	1.43	9 (16%)	81,89,89	1.73	19 (23%)
9	SF4	A	707	1	0,12,12	-	-	-		
13	FES	J	200	4	0,4,4	-	-	-		
9	SF4	E	302	5	0,12,12	-	-	-		
11	9S8	B	302	2	2,10,10	2.92	1 (50%)	-		
11	9S8	B	301	2	2,10,10	3.93	2 (100%)	-		
9	SF4	G	710	1	0,12,12	-	-	-		
9	SF4	K	303	5	0,12,12	-	-	-		
14	TRS	D	203	-	7,7,7	0.28	0	9,9,9	0.43	0
12	9SB	B	303	-	6,6,6	3.33	1 (16%)	7,8,8	1.65	3 (42%)
11	9S8	H	301	2	2,10,10	4.60	2 (100%)	-		
11	9S8	H	302	2	2,10,10	2.97	2 (100%)	-		
9	SF4	A	709	1	0,12,12	-	-	-		
9	SF4	G	709	1	0,12,12	-	-	-		
9	SF4	G	708	1	0,12,12	-	-	-		
9	SF4	A	708	1	0,12,12	-	-	-		
10	GOL	A	710	-	5,5,5	0.31	0	5,5,5	0.41	0
17	FCO	F	504	6	1,6,6	3.68	1 (100%)	-		
9	SF4	A	706	1	0,12,12	-	-	-		
8	ACT	D	202	-	3,3,3	0.99	0	3,3,3	0.98	0
15	PE3	L	502	-	8,8,42	0.47	0	7,7,41	0.21	0
9	SF4	C	202	3	0,12,12	-	-	-		
8	ACT	G	703	-	3,3,3	0.96	0	3,3,3	0.96	0
15	PE3	G	702	-	13,13,42	0.50	0	12,12,41	0.17	0
8	ACT	G	704	-	3,3,3	1.06	0	3,3,3	0.95	0
9	SF4	G	706	1,16	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SF4	K	301	5	0,12,12	-	-	-		
9	SF4	K	302	5	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PE3	F	502	-	-	3/6/6/40	-
9	SF4	A	705	1	-	-	0/6/5/5
9	SF4	E	303	5	-	-	0/6/5/5
12	9SB	H	303	-	-	0/3/4/4	-
9	SF4	I	202	3	-	-	0/6/5/5
9	SF4	A	704	1	-	-	0/6/5/5
9	SF4	I	201	3	-	-	0/6/5/5
10	GOL	G	712	-	-	2/4/4/4	-
12	9SB	B	304	-	-	0/3/4/4	-
9	SF4	G	711	1	-	-	0/6/5/5
13	FES	D	201	4	-	-	0/1/1/1
12	9SB	H	304	-	-	3/3/4/4	-
10	GOL	A	711	-	-	0/4/4/4	-
9	SF4	C	201	3	-	-	0/6/5/5
9	SF4	G	707	1	-	-	0/6/5/5
10	GOL	H	305	-	-	4/4/4/4	-
9	SF4	E	301	5	-	-	0/6/5/5
7	FAD	A	701	-	-	2/34/50/50	0/6/6/6
7	FAD	G	701	-	-	4/34/50/50	0/6/6/6
9	SF4	A	707	1	-	-	0/6/5/5
13	FES	J	200	4	-	-	0/1/1/1
14	TRS	D	203	-	-	7/9/9/9	-
9	SF4	E	302	5	-	-	0/6/5/5
11	9S8	B	301	2	-	-	0/3/3/3
9	SF4	G	710	1	-	-	0/6/5/5
9	SF4	K	303	5	-	-	0/6/5/5
11	9S8	B	302	2	-	-	0/3/3/3
12	9SB	B	303	-	-	3/3/4/4	-
11	9S8	H	301	2	-	-	0/3/3/3
11	9S8	H	302	2	-	-	0/3/3/3
9	SF4	A	709	1	-	-	0/6/5/5
9	SF4	G	709	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	G	708	1	-	-	0/6/5/5
9	SF4	A	708	1	-	-	0/6/5/5
10	GOL	A	710	-	-	0/4/4/4	-
9	SF4	A	706	1	-	-	0/6/5/5
15	PE3	L	502	-	-	2/6/6/40	-
9	SF4	C	202	3	-	-	0/6/5/5
9	SF4	K	302	5	-	-	0/6/5/5
15	PE3	G	702	-	-	6/11/11/40	-
9	SF4	G	706	1,16	-	-	0/6/5/5
9	SF4	K	301	5	-	-	0/6/5/5
10	GOL	K	304	-	-	0/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	303	9SB	C2-S2	-7.92	1.66	1.77
12	H	303	9SB	C2-S2	-7.74	1.66	1.77
12	B	304	9SB	C2-S2	-7.38	1.67	1.77
12	H	304	9SB	C2-S2	-7.37	1.67	1.77
11	H	301	9S8	S3-FE4	-5.86	2.11	2.24
7	A	701	FAD	C9A-C5X	5.57	1.50	1.41
7	G	701	FAD	C9A-C5X	5.42	1.50	1.41
11	B	301	9S8	S3-FE4	-5.06	2.13	2.24
17	L	504	FCO	O3-C3	4.26	1.21	1.16
7	G	701	FAD	C5A-C4A	4.13	1.46	1.39
11	B	302	9S8	S3-FE4	-4.04	2.15	2.24
7	A	701	FAD	C5A-C4A	4.02	1.46	1.39
17	F	504	FCO	O3-C3	3.68	1.21	1.16
11	H	302	9S8	S3-FE4	-3.62	2.16	2.24
7	A	701	FAD	C8-C7	3.52	1.49	1.40
7	G	701	FAD	C8-C7	3.49	1.49	1.40
11	H	301	9S8	S5-FE4	-2.81	2.18	2.24
7	G	701	FAD	C5A-C6A	2.81	1.48	1.41
7	G	701	FAD	C8A-N7A	2.68	1.36	1.31
7	A	701	FAD	C5A-C6A	2.62	1.48	1.41
7	A	701	FAD	C8A-N7A	2.37	1.36	1.31
7	A	701	FAD	C5X-N5	-2.31	1.35	1.39
11	B	301	9S8	S5-FE4	-2.29	2.19	2.24
7	A	701	FAD	C4-N3	-2.28	1.34	1.38
7	G	701	FAD	C4X-N5	2.28	1.35	1.30
7	A	701	FAD	C4X-N5	2.26	1.35	1.30
7	G	701	FAD	C5X-N5	-2.24	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	701	FAD	C5A-N7A	-2.17	1.34	1.39
7	G	701	FAD	C4-N3	-2.16	1.34	1.38
11	H	302	9S8	S5-FE4	-2.13	2.19	2.24
7	G	701	FAD	C5A-N7A	-2.02	1.35	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	701	FAD	C5A-C4A-N3A	-6.08	118.82	126.75
7	G	701	FAD	C5A-C4A-N3A	-5.98	118.94	126.75
7	A	701	FAD	N3A-C4A-N9A	5.01	135.33	127.08
7	G	701	FAD	N3A-C4A-N9A	4.68	134.79	127.08
7	G	701	FAD	C2A-N3A-C4A	4.36	122.05	111.75
7	G	701	FAD	N3A-C2A-N1A	-4.31	121.86	128.60
7	A	701	FAD	C2A-N3A-C4A	4.31	121.93	111.75
7	A	701	FAD	N3A-C2A-N1A	-4.22	122.00	128.60
7	A	701	FAD	P-O3P-PA	-3.72	120.05	132.83
7	G	701	FAD	P-O3P-PA	-3.18	121.90	132.83
7	A	701	FAD	C4A-N9A-C8A	3.14	109.14	105.73
7	G	701	FAD	C4A-C5A-N7A	-3.02	106.94	110.62
12	H	304	9SB	O3S-S2-C2	3.01	110.54	106.92
7	G	701	FAD	C4A-N9A-C8A	3.01	108.99	105.73
7	A	701	FAD	C5A-N7A-C8A	2.95	107.70	103.51
7	G	701	FAD	C5A-N7A-C8A	2.94	107.69	103.51
7	A	701	FAD	C4X-C10-N1	-2.88	118.05	124.73
7	A	701	FAD	C4A-C5A-N7A	-2.79	107.22	110.62
7	A	701	FAD	N9A-C8A-N7A	-2.79	110.09	113.91
7	G	701	FAD	N9A-C8A-N7A	-2.78	110.12	113.91
7	G	701	FAD	O4-C4-C4X	-2.70	119.43	126.60
7	A	701	FAD	O4-C4-C4X	-2.69	119.46	126.60
7	G	701	FAD	C4X-C10-N1	-2.67	118.53	124.73
12	B	304	9SB	O2S-S2-C2	2.64	110.05	105.77
12	H	303	9SB	O2S-S2-C2	2.64	110.04	105.77
12	B	303	9SB	O2S-S2-C2	2.59	109.96	105.77
7	A	701	FAD	C4-N3-C2	-2.46	121.09	125.64
7	G	701	FAD	C6A-C5A-N7A	2.45	136.58	132.02
12	H	303	9SB	O3S-S2-C2	2.43	109.84	106.92
7	G	701	FAD	C4-C4X-N5	2.42	121.67	118.23
7	A	701	FAD	O2-C2-N1	-2.41	117.83	121.83
12	B	304	9SB	O1S-S2-C2	2.38	109.78	106.92
7	G	701	FAD	O2-C2-N1	-2.34	117.94	121.83
7	G	701	FAD	C4-N3-C2	-2.32	121.36	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	701	FAD	C10-N1-C2	2.30	121.51	116.90
7	G	701	FAD	C10-N1-C2	2.29	121.47	116.90
7	A	701	FAD	C4X-C10-N10	2.28	119.82	116.48
7	A	701	FAD	C4X-C4-N3	2.28	118.97	113.19
7	G	701	FAD	C4X-C4-N3	2.27	118.96	113.19
12	B	303	9SB	O1S-S2-C2	2.23	109.60	106.92
7	A	701	FAD	O4'-C4'-C3'	2.20	114.46	109.10
12	H	304	9SB	O2S-S2-C2	2.18	109.29	105.77
7	G	701	FAD	C4X-C10-N10	2.14	119.60	116.48
7	A	701	FAD	C6A-C5A-N7A	2.12	135.98	132.02
7	A	701	FAD	C4-C4X-N5	2.12	121.25	118.23
12	B	303	9SB	O3S-S2-C2	2.01	109.34	106.92
7	G	701	FAD	C2A-N1A-C6A	2.01	122.21	118.77

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	701	FAD	PA-O3P-P-O5'
12	H	304	9SB	C1-C2-S2-O1S
12	H	304	9SB	C1-C2-S2-O2S
12	H	304	9SB	C1-C2-S2-O3S
14	D	203	TRS	C1-C-C3-O3
14	D	203	TRS	N-C-C3-O3
15	G	702	PE3	O31-C32-C33-O34
15	F	502	PE3	O31-C32-C33-O34
10	G	712	GOL	O1-C1-C2-O2
15	L	502	PE3	O34-C35-C36-O37
10	G	712	GOL	O1-C1-C2-C3
10	H	305	GOL	O1-C1-C2-C3
10	H	305	GOL	C1-C2-C3-O3
15	G	702	PE3	O37-C38-C39-O40
10	H	305	GOL	O1-C1-C2-O2
14	D	203	TRS	C2-C-C1-O1
15	F	502	PE3	O34-C35-C36-O37
15	G	702	PE3	C35-C36-O37-C38
15	G	702	PE3	C38-C39-O40-C41
15	G	702	PE3	C32-C33-O34-C35
10	H	305	GOL	O2-C2-C3-O3
14	D	203	TRS	C3-C-C1-O1
14	D	203	TRS	C2-C-C3-O3
7	G	701	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
12	B	303	9SB	C1-C2-S2-O1S
12	B	303	9SB	C1-C2-S2-O3S
12	B	303	9SB	C1-C2-S2-O2S
15	G	702	PE3	C29-C30-O31-C32
7	A	701	FAD	O4B-C4B-C5B-O5B
14	D	203	TRS	C1-C-C2-O2
15	F	502	PE3	C29-C30-O31-C32
7	G	701	FAD	O4B-C4B-C5B-O5B
14	D	203	TRS	N-C-C1-O1
7	A	701	FAD	C2B-C1B-N9A-C8A
7	G	701	FAD	C5'-O5'-P-O1P
15	L	502	PE3	C39-C38-O37-C36

There are no ring outliers.

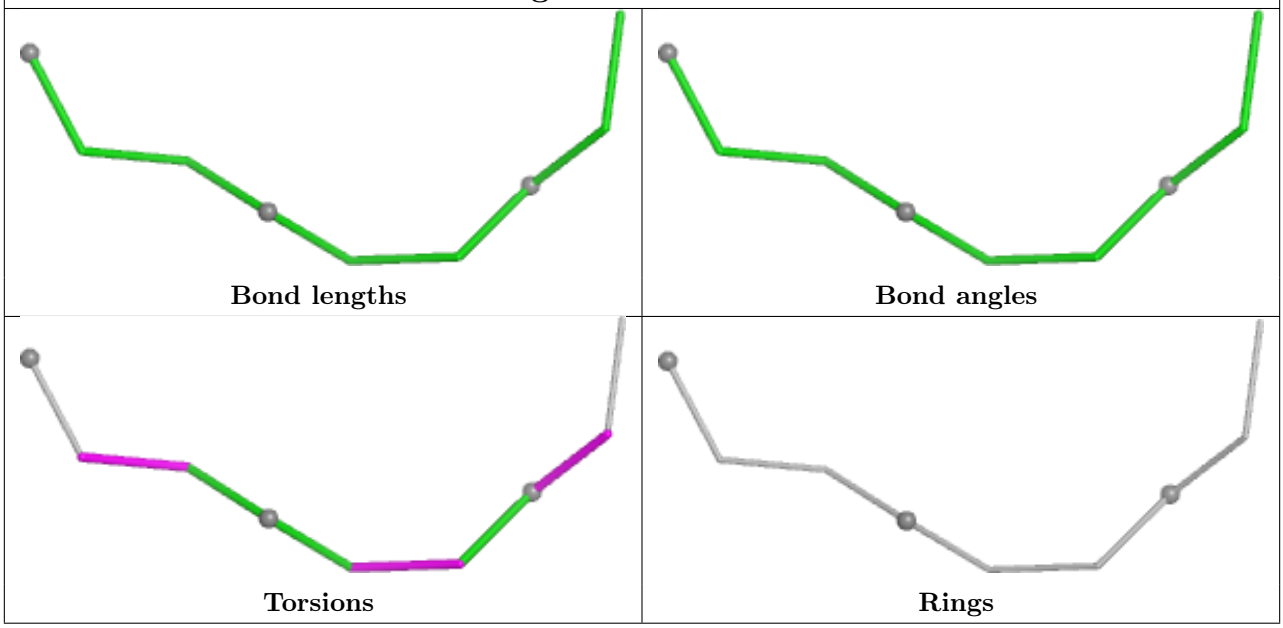
16 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	303	SF4	1	0
9	A	704	SF4	1	0
10	G	712	GOL	1	0
8	A	703	ACT	1	0
8	A	702	ACT	1	0
10	A	711	GOL	1	0
9	G	707	SF4	1	0
17	L	504	FCO	1	0
7	A	701	FAD	1	0
7	G	701	FAD	2	0
9	A	707	SF4	3	0
9	K	303	SF4	1	0
9	G	709	SF4	1	0
17	F	504	FCO	1	0
9	A	706	SF4	1	0
9	G	706	SF4	1	0

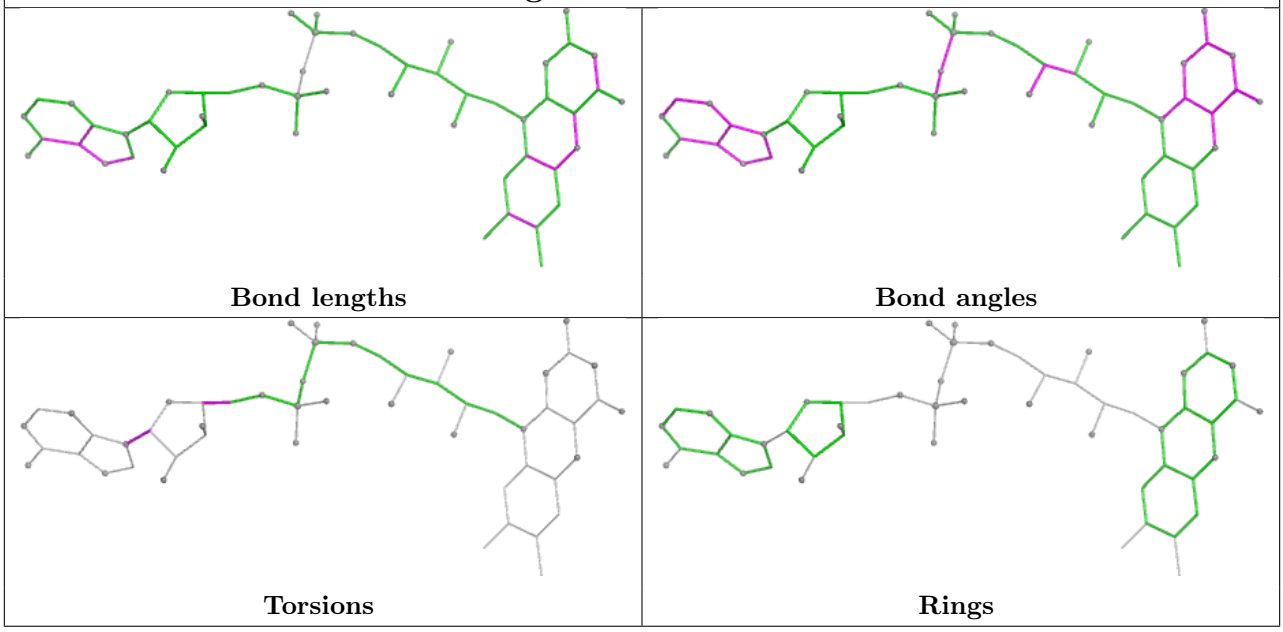
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

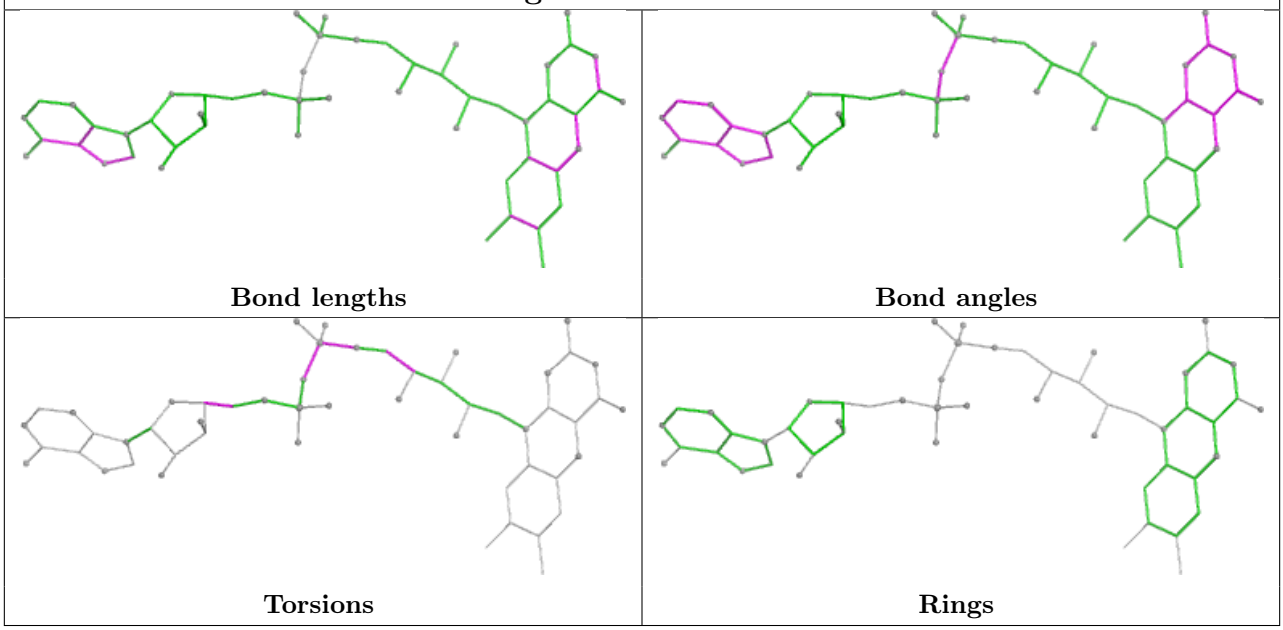
Ligand PE3 F 502



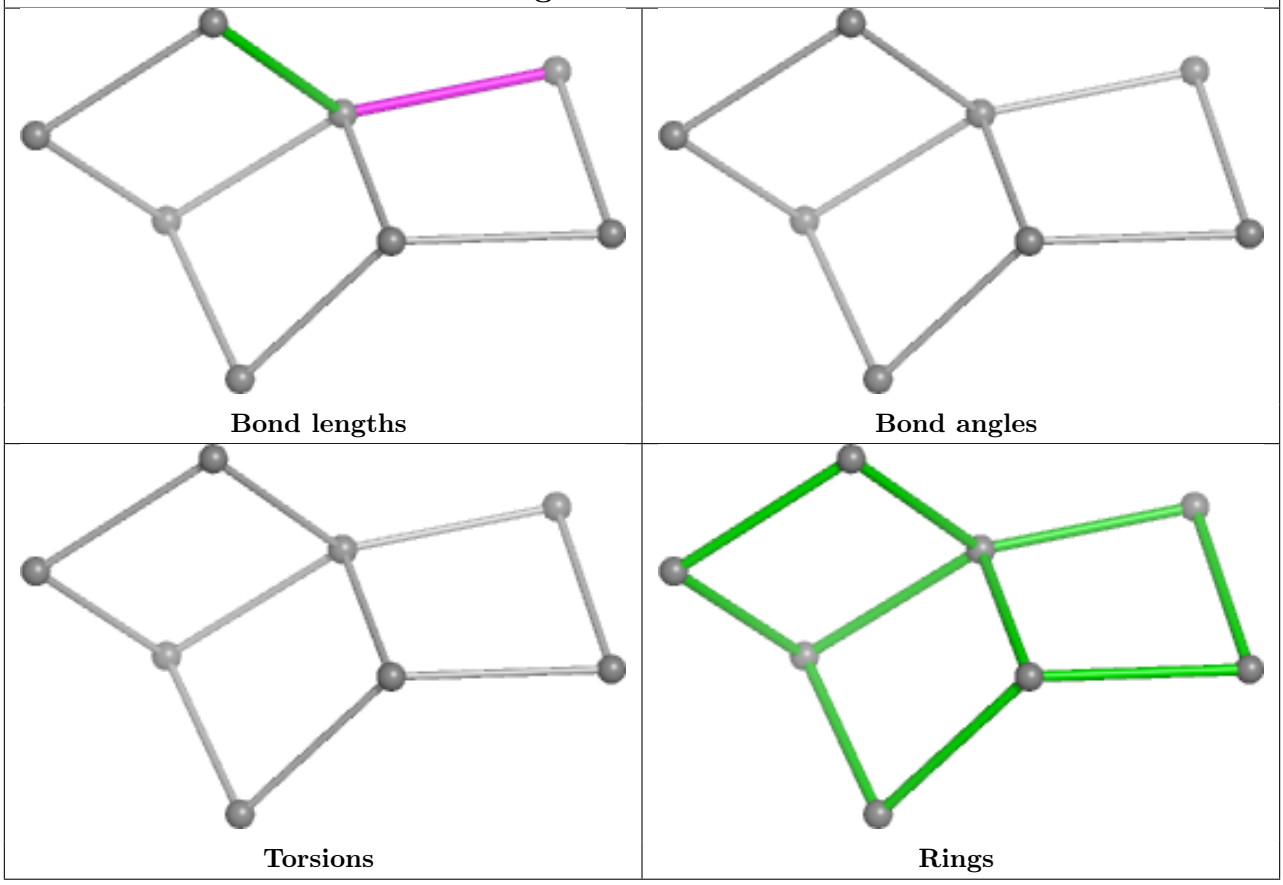
Ligand FAD A 701



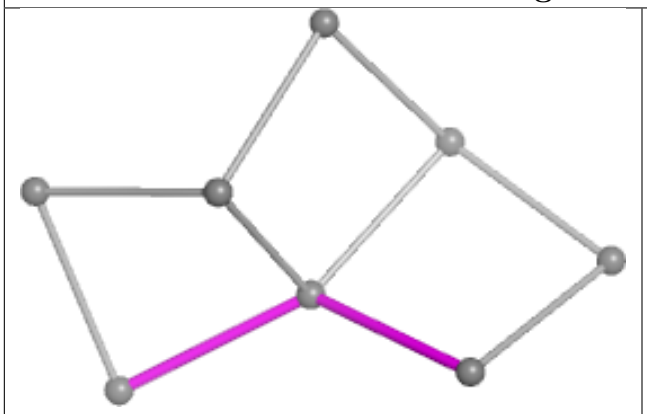
Ligand FAD G 701



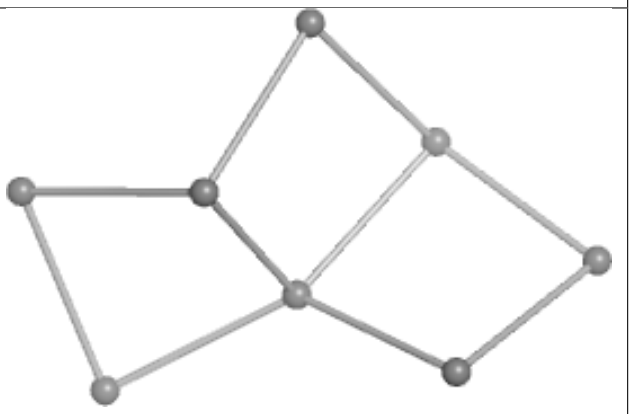
Ligand 9S8 B 302



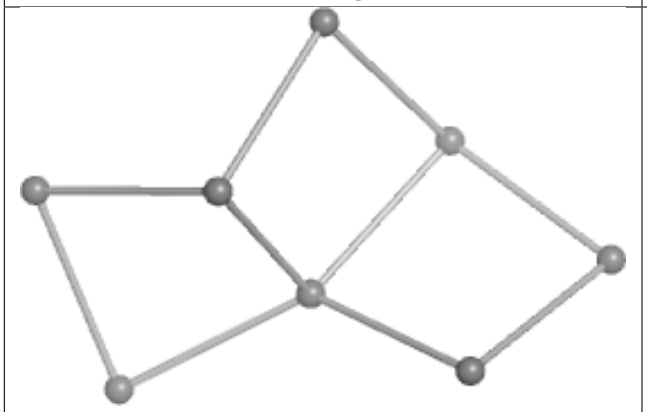
Ligand 9S8 B 301



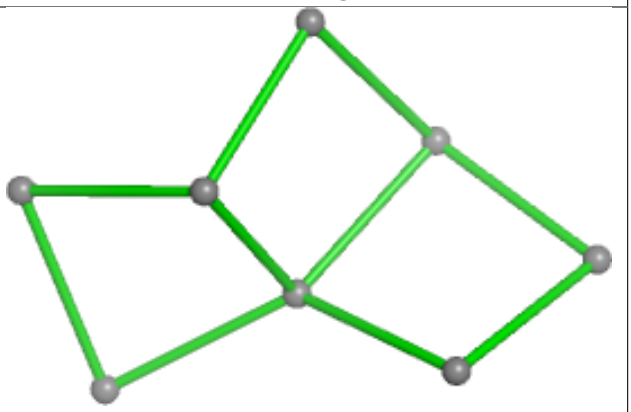
Bond lengths



Bond angles

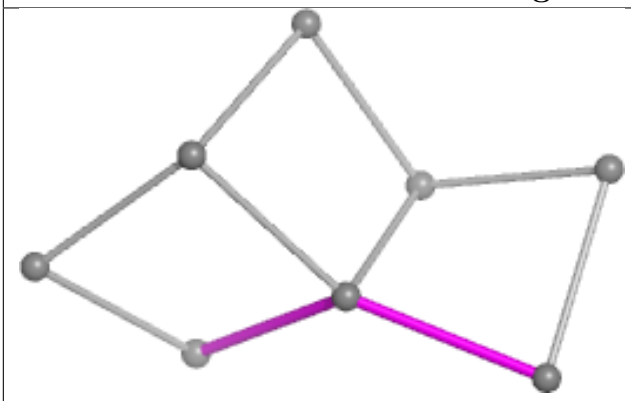


Torsions

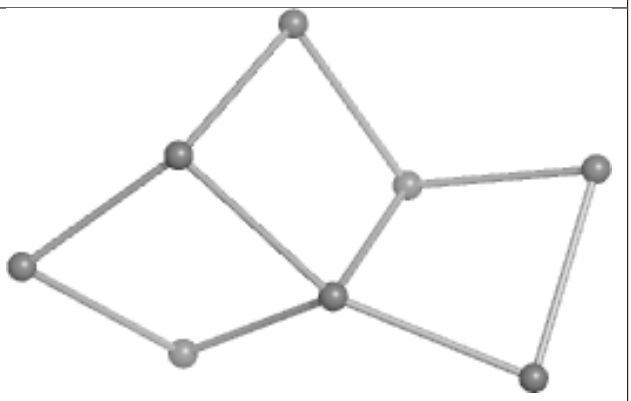


Rings

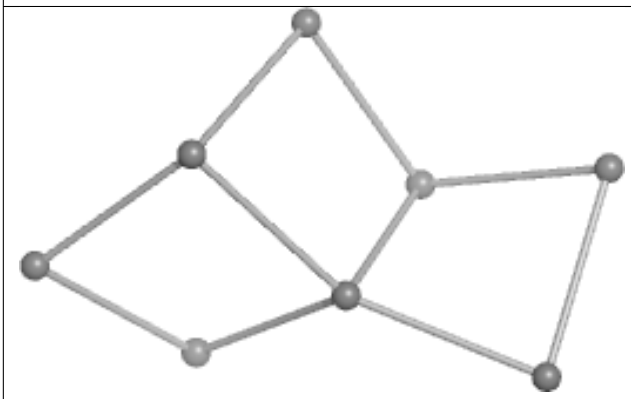
Ligand 9S8 H 301



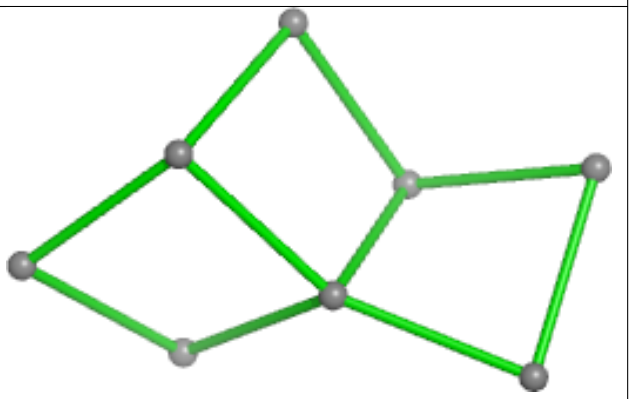
Bond lengths



Bond angles

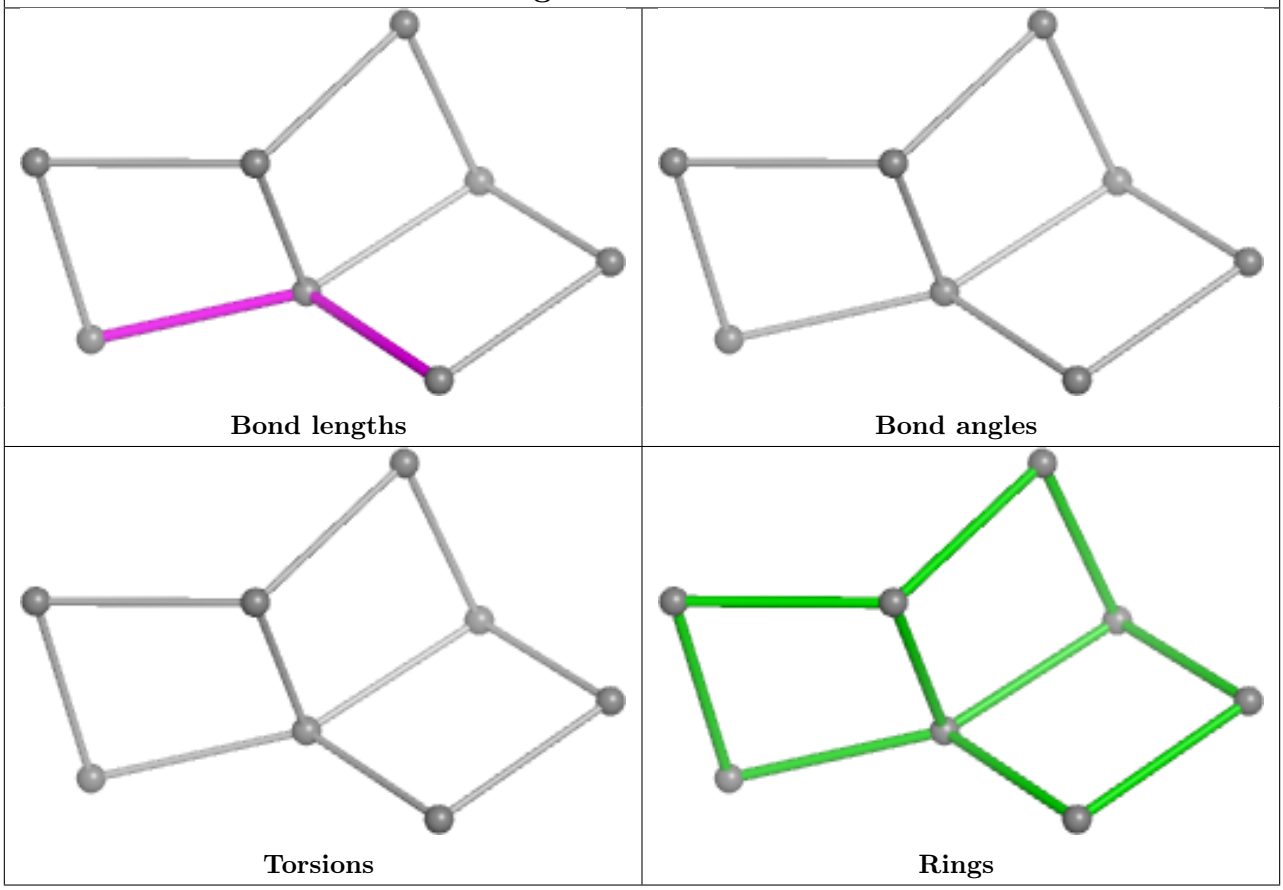


Torsions

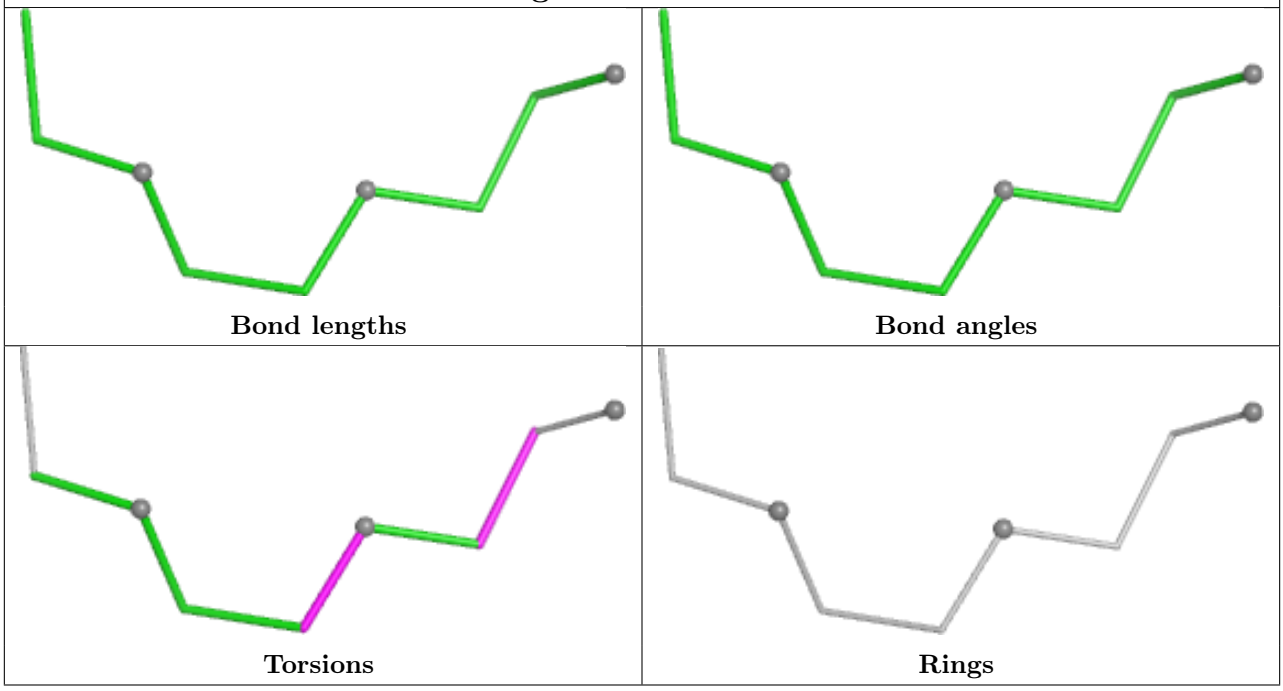


Rings

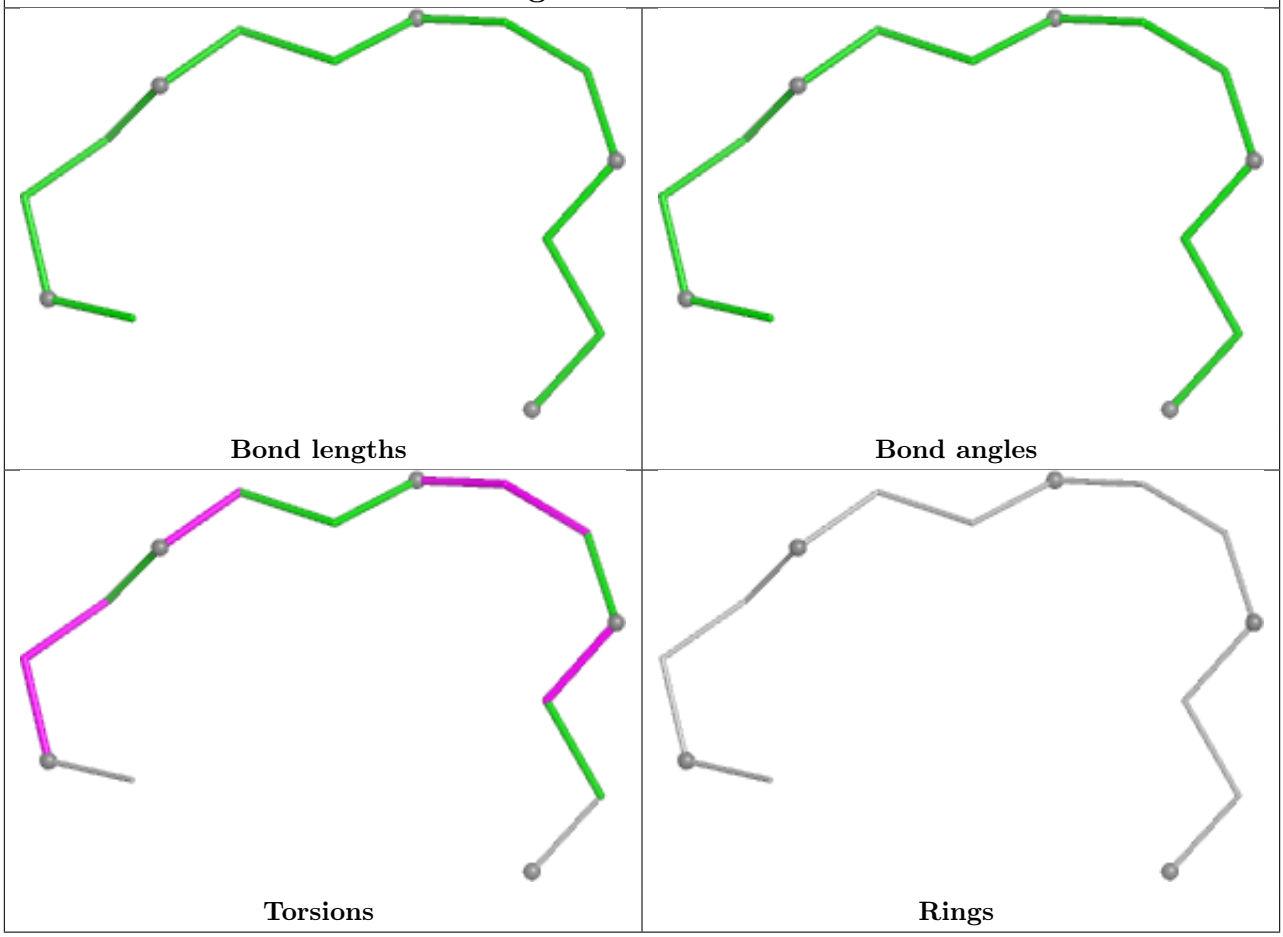
Ligand 9S8 H 302



Ligand PE3 L 502



Ligand PE3 G 702



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%)	-1.56	0	100	100	8, 24, 82, 132	0
1	G	652/654 (99%)	-1.52	0	100	100	9, 27, 75, 103	0
2	B	291/291 (100%)	-1.45	0	100	100	19, 36, 61, 80	0
2	H	291/291 (100%)	-1.38	0	100	100	21, 39, 72, 101	0
3	C	184/184 (100%)	-1.58	0	100	100	13, 29, 53, 70	0
3	I	183/184 (99%)	-1.52	0	100	100	12, 31, 60, 94	0
4	D	137/140 (97%)	-1.68	0	100	100	13, 23, 44, 73	0
4	J	138/140 (98%)	-1.50	0	100	100	16, 26, 45, 79	0
5	E	298/299 (99%)	-1.51	0	100	100	17, 32, 65, 93	0
5	K	298/299 (99%)	-1.54	0	100	100	10, 26, 58, 74	1 (0%)
6	F	447/473 (94%)	-1.53	0	100	100	15, 31, 58, 78	0
6	L	447/473 (94%)	-1.58	0	100	100	10, 27, 54, 97	0
All	All	4018/4082 (98%)	-1.53	0	100	100	8, 29, 64, 132	1 (0%)

There are no RSRZ outliers to report.

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
8	ACT	D	202	4/4	0.98	0.05	40,40,40,40	0
15	PE3	L	502	9/43	0.98	0.04	39,43,46,47	0
8	ACT	G	703	4/4	0.99	0.03	42,42,42,43	0
8	ACT	G	704	4/4	0.99	0.04	36,36,36,36	0
9	SF4	A	705	8/8	0.99	0.04	116,117,117,118	0
10	GOL	A	711	6/6	0.99	0.03	21,24,24,27	0
10	GOL	G	712	6/6	0.99	0.03	26,27,28,29	0
10	GOL	H	305	6/6	0.99	0.05	37,37,38,39	0
10	GOL	K	304	6/6	0.99	0.05	54,55,56,56	0
12	9SB	B	304	7/7	0.99	0.04	67,68,70,72	0
14	TRS	D	203	8/8	0.99	0.03	35,36,37,39	0
15	PE3	F	502	9/43	0.99	0.04	40,41,41,42	0
15	PE3	G	702	14/43	0.99	0.04	33,40,56,57	0
8	ACT	A	702	4/4	0.99	0.03	28,29,29,30	0
9	SF4	C	202	8/8	1.00	0.01	16,17,18,18	0
9	SF4	E	301	8/8	1.00	0.02	26,28,29,29	0
9	SF4	E	302	8/8	1.00	0.02	25,27,28,30	0
9	SF4	E	303	8/8	1.00	0.01	28,29,31,33	0
9	SF4	G	706	8/8	1.00	0.01	21,23,24,26	0
9	SF4	G	707	8/8	1.00	0.01	9,10,11,11	0
9	SF4	G	708	8/8	1.00	0.01	52,52,53,53	0
9	SF4	G	709	8/8	1.00	0.01	52,53,53,54	0
9	SF4	G	710	8/8	1.00	0.01	19,23,23,25	0
9	SF4	G	711	8/8	1.00	0.02	21,24,25,26	0
9	SF4	I	201	8/8	1.00	0.01	11,13,14,14	0
9	SF4	I	202	8/8	1.00	0.01	15,16,18,19	0
9	SF4	K	301	8/8	1.00	0.02	15,16,19,20	0
9	SF4	K	302	8/8	1.00	0.01	17,19,20,21	0
9	SF4	K	303	8/8	1.00	0.01	19,21,22,23	0
10	GOL	A	710	6/6	1.00	0.02	23,24,24,26	0
7	FAD	A	701	53/53	1.00	0.02	9,14,23,26	0
8	ACT	A	703	4/4	1.00	0.03	27,29,29,30	0
9	SF4	A	704	8/8	1.00	0.01	6,9,10,10	0
7	FAD	G	701	53/53	1.00	0.02	10,14,22,26	0
11	9S8	B	301	8/8	1.00	0.01	22,25,27,28	0
11	9S8	B	302	8/8	1.00	0.01	20,24,24,25	0
11	9S8	H	301	8/8	1.00	0.02	31,32,34,34	0

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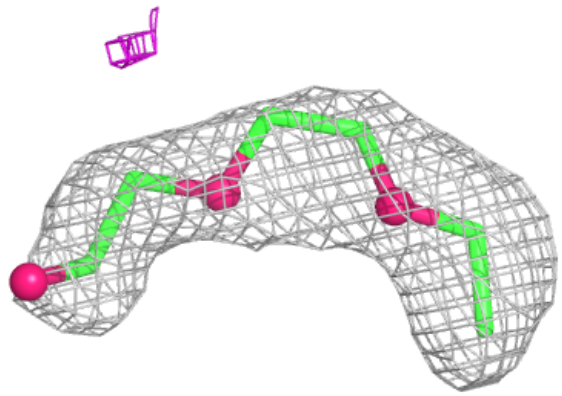
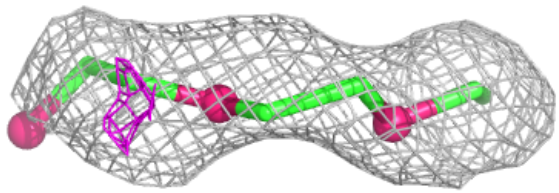
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	9S8	H	302	8/8	1.00	0.01	25,27,28,29	0
12	9SB	B	303	7/7	1.00	0.03	44,45,54,60	0
9	SF4	A	706	8/8	1.00	0.01	59,60,61,61	0
12	9SB	H	303	7/7	1.00	0.02	59,60,64,67	0
12	9SB	H	304	7/7	1.00	0.03	61,62,65,67	0
13	FES	D	201	4/4	1.00	0.01	16,17,18,18	0
13	FES	J	200	4/4	1.00	0.01	16,20,20,21	0
9	SF4	A	707	8/8	1.00	0.01	8,9,10,10	0
9	SF4	A	708	8/8	1.00	0.01	15,17,17,19	0
9	SF4	A	709	8/8	1.00	0.02	23,25,27,28	0
9	SF4	C	201	8/8	1.00	0.01	12,13,14,14	0
16	FE	F	503	1/1	1.00	0.01	16,16,16,16	0
16	FE	G	705	1/1	1.00	0.02	22,22,22,22	1
16	FE	L	503	1/1	1.00	0.01	12,12,12,12	0
17	FCO	F	504	7/7	1.00	0.02	15,17,20,21	0
17	FCO	L	504	7/7	1.00	0.01	12,15,18,19	0
18	NI	F	505	1/1	1.00	0.01	20,20,20,20	0
18	NI	L	505	1/1	1.00	0.01	13,13,13,13	0

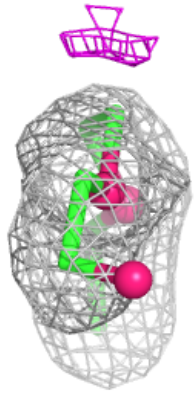
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE3 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)

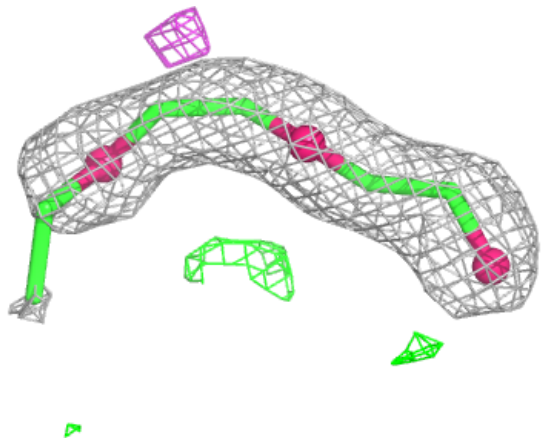


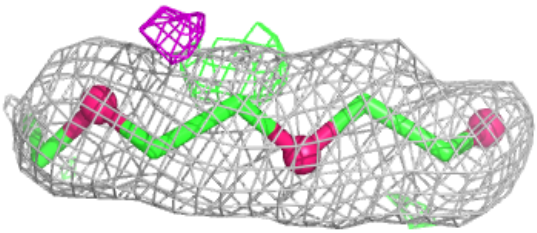


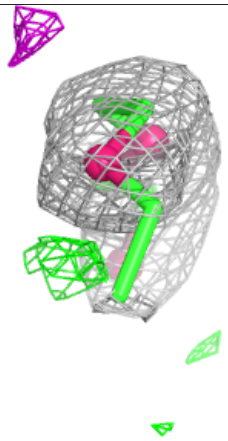


Electron density around PE3 F 502:

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

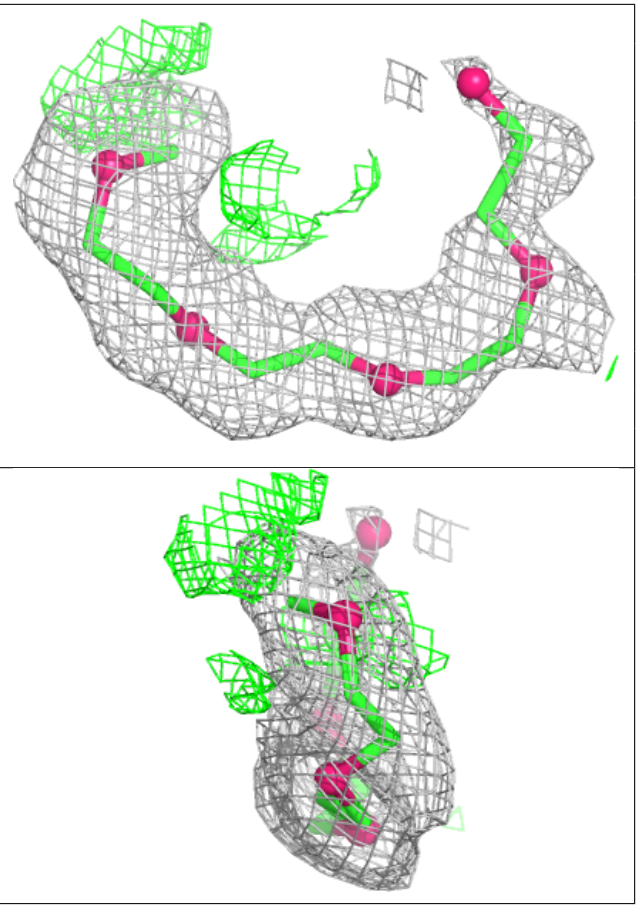






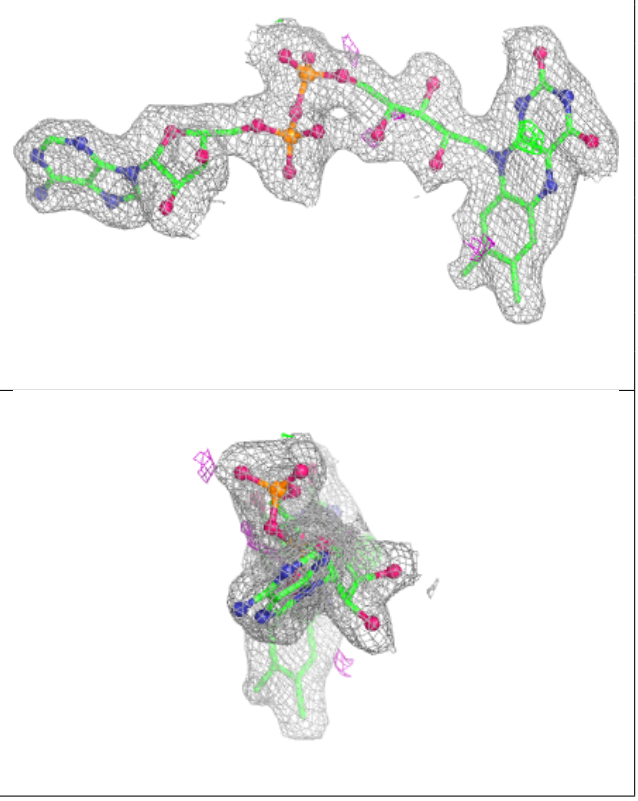
Electron density around PE3 G 702:

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



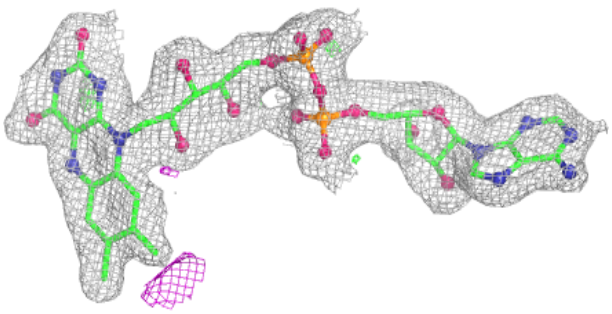
Electron density around FAD A 701:

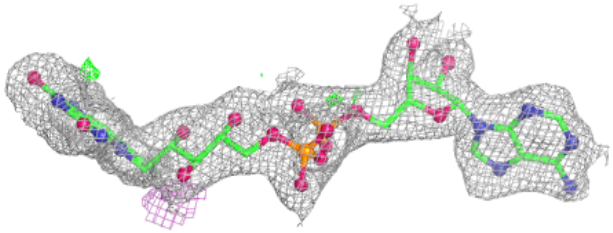
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

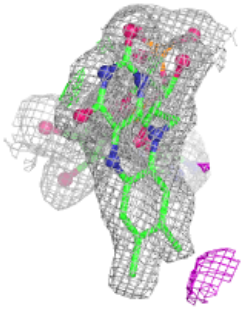


Electron density around FAD G 701:

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

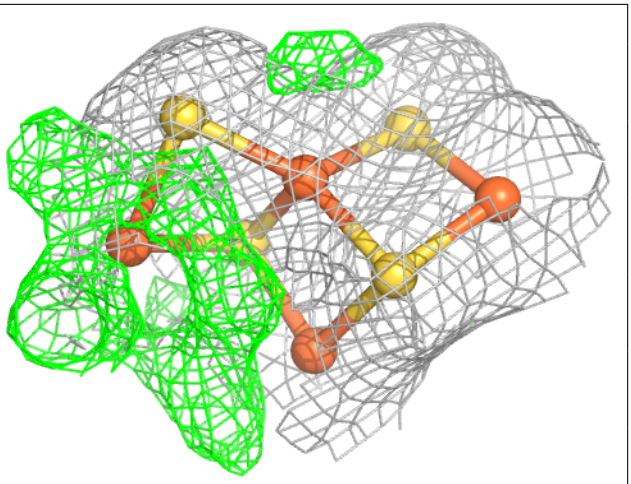


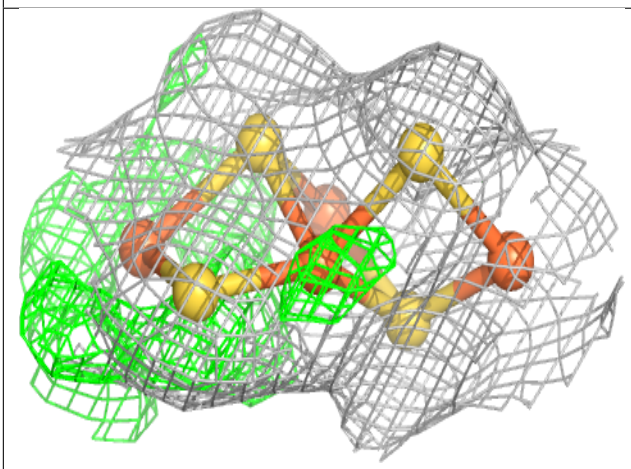


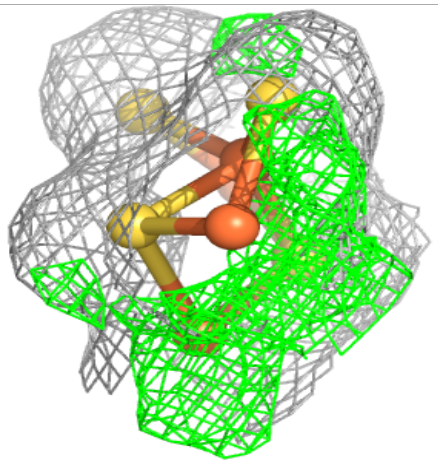


Electron density around 9S8 B 301:

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

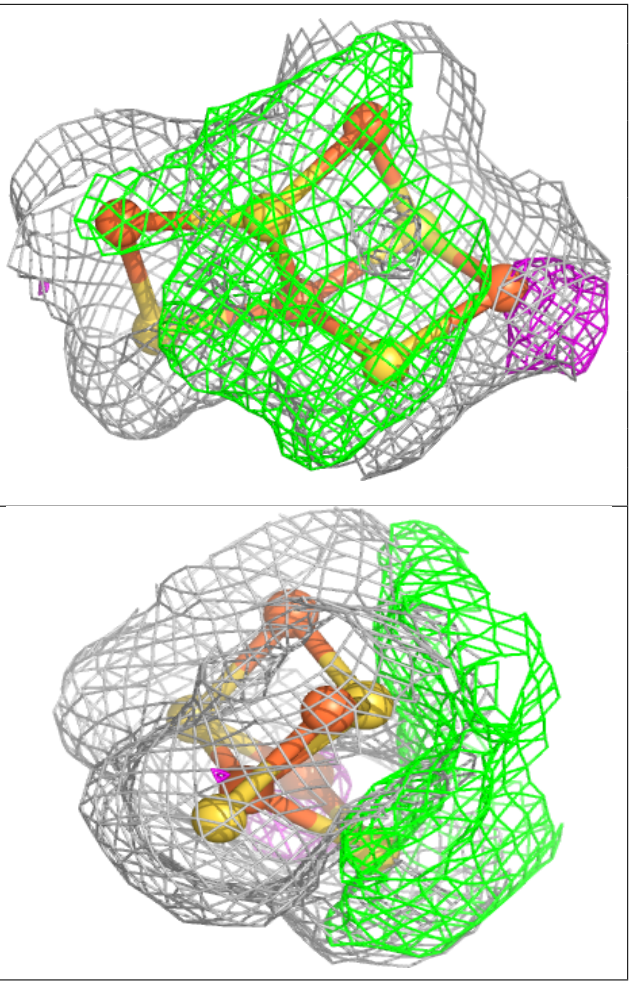






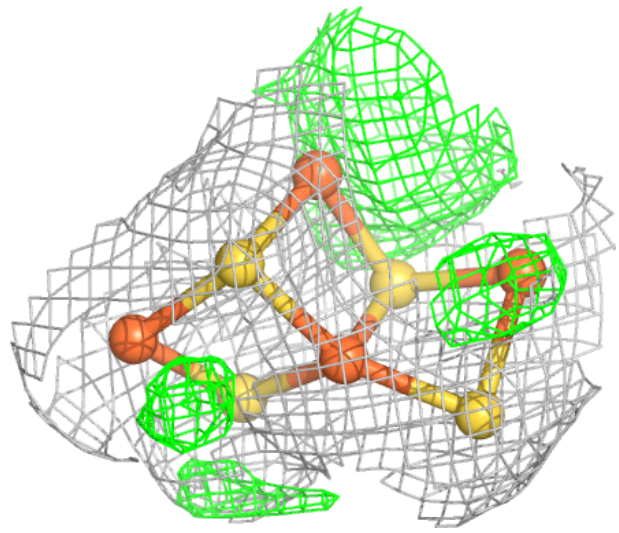
Electron density around 9S8 B 302:

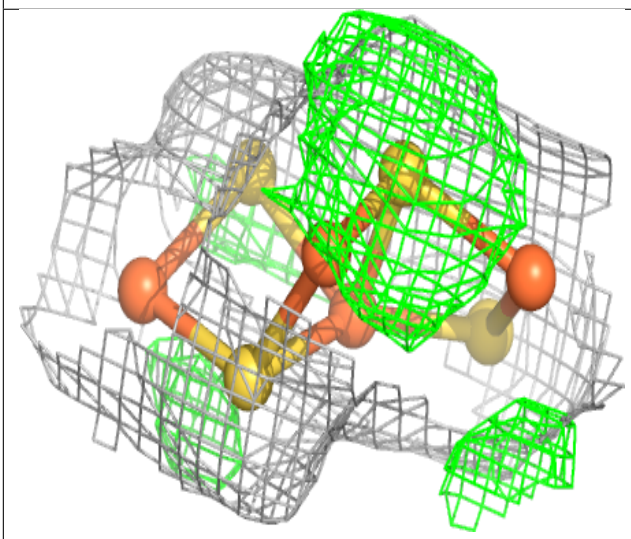
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

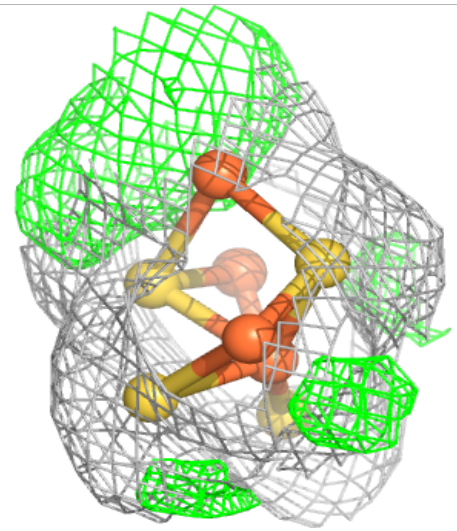


Electron density around 9S8 H 301:

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

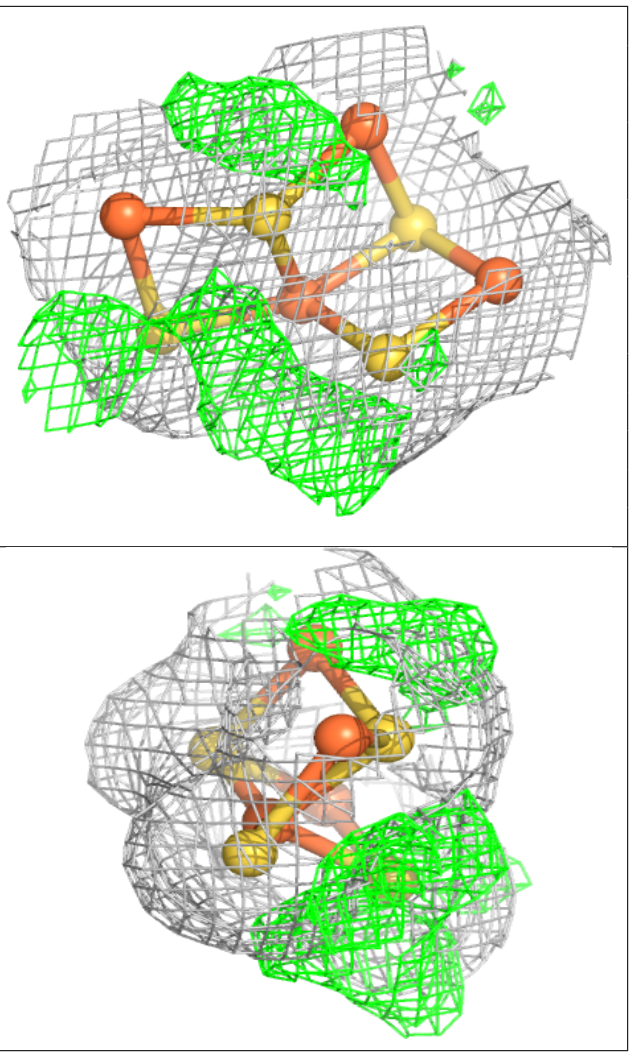






Electron density around 9S8 H 302:

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



6.5 Other polymers (i)

There are no such residues in this entry.