



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 11:49 AM BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

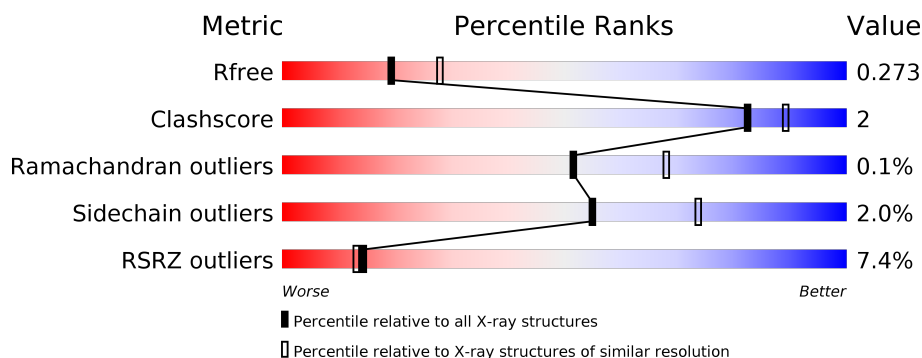
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	654	<div> <div>4%</div> <div>92%</div> <div>8%</div> </div>
1	G	654	<div> <div>10%</div> <div>92%</div> <div>6%</div> </div>
2	B	291	<div> <div>24%</div> <div>93%</div> <div>6%</div> </div>
2	H	291	<div> <div>7%</div> <div>91%</div> <div>8%</div> </div>
3	C	184	<div> <div>17%</div> <div>92%</div> <div>8%</div> </div>
3	I	184	<div> <div>%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	140	 % 91% 6%
4	J	140	 17% 94% 5%
5	E	299	 2% 92% 8%
5	K	299	 7% 92% 7%
6	F	473	 2% 89% 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	GOL	H	304	-	-	-	X
12	COM	H	303	-	X	-	-
15	NFU	F	501	-	-	X	-
7	ACT	A	701	-	-	-	X
7	ACT	G	702	-	-	-	X

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 31986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			4970	3137	844	940	49			
1	G	652	Total	C	N	O	S	0	0	0
			4979	3142	845	943	49			

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

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

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

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

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

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

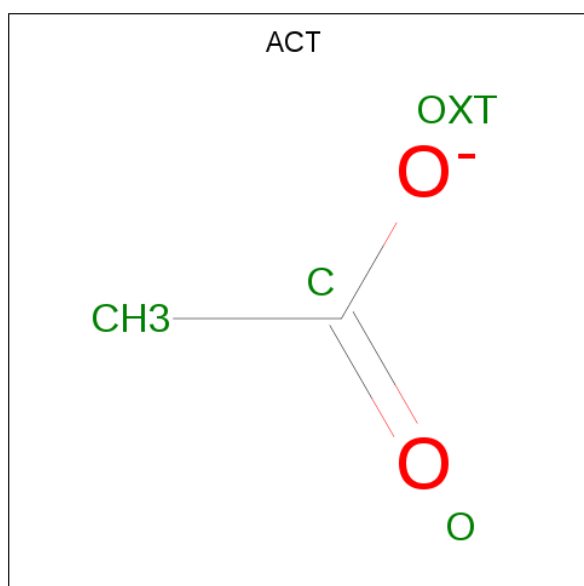
- Molecule 5 is a protein called Methyl-viologen reducing hydrogenase, subunit G.

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

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

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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



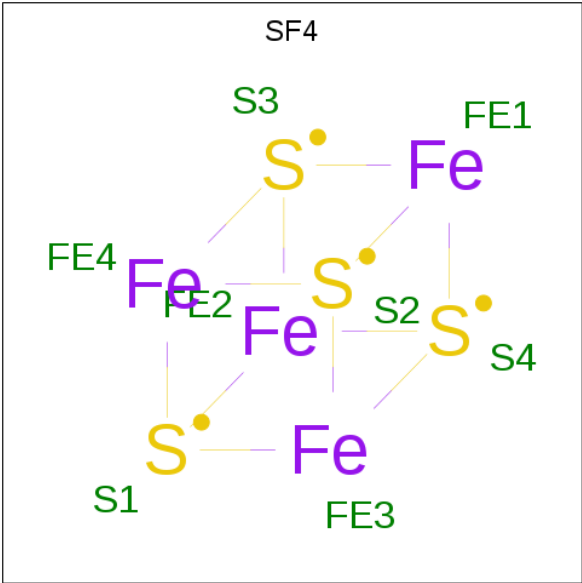
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



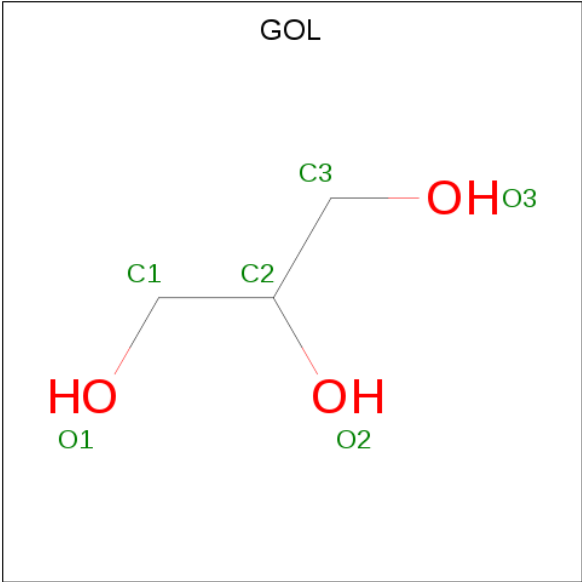
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Fe S	0	0
			8	4 4		
9	A	1	Total	Fe S	0	0
			8	4 4		

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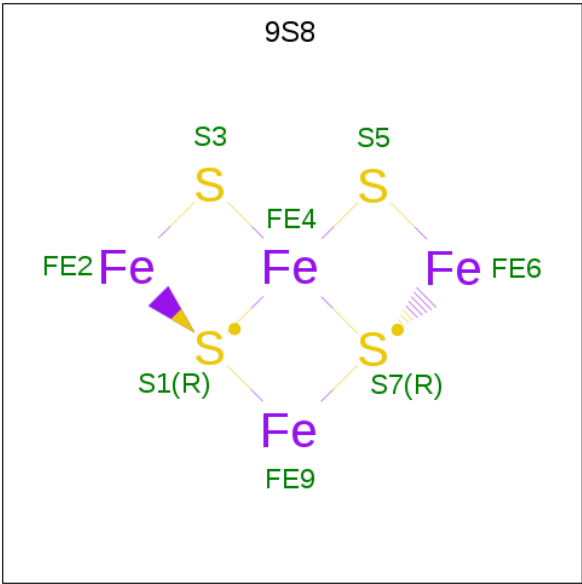
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 8	Fe 4	S 4	0	0
9	A	1	Total 8	Fe 4	S 4	0	0
9	A	1	Total 8	Fe 4	S 4	0	0
9	A	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	E	1	Total 8	Fe 4	S 4	0	0
9	E	1	Total 8	Fe 4	S 4	0	0
9	E	1	Total 8	Fe 4	S 4	0	0
9	G	1	Total 8	Fe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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

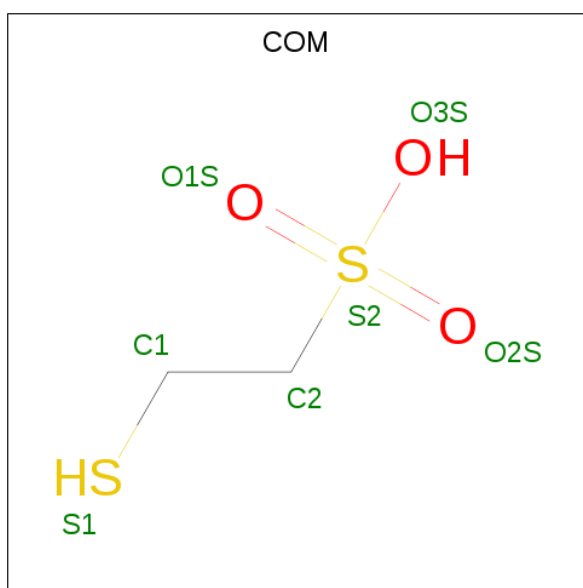
- Molecule 11 is Non-cubane [4Fe-4S]-cluster (three-letter code: 9S8) (formula: Fe<sub>4</sub>S<sub>4</sub>).





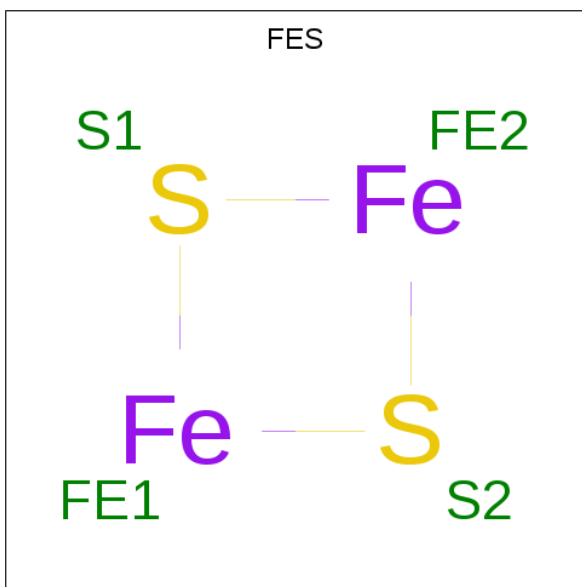
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	H	1	Total	Fe	S	0	0
			8	4	4		
11	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



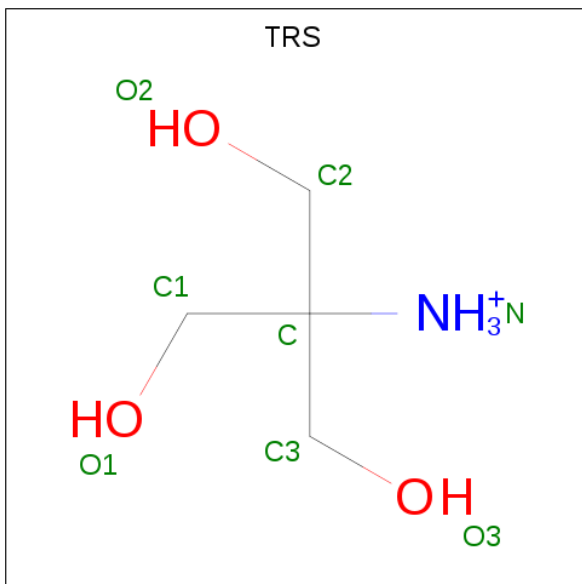
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	O	S	0	0
			7	2	3	2		
12	H	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



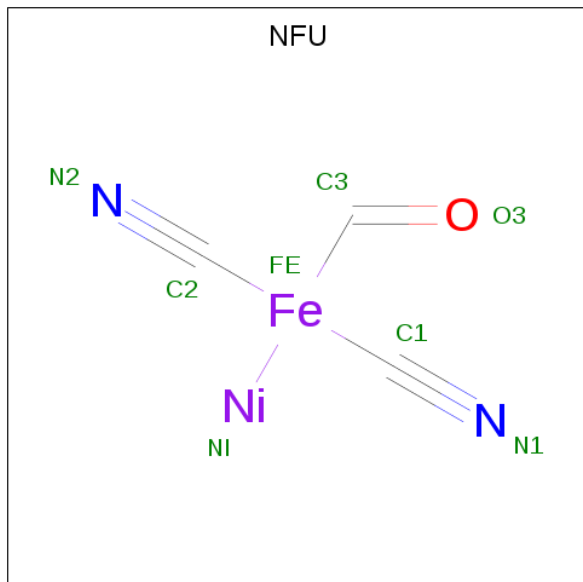
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	Fe	S	0	0
			4	2	2		
13	J	1	Total	Fe	S	0	0
			4	2	2		

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



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

- Molecule 15 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (three-letter code: NFU) (formula:  $C_3HFeN_2NiO$ ).

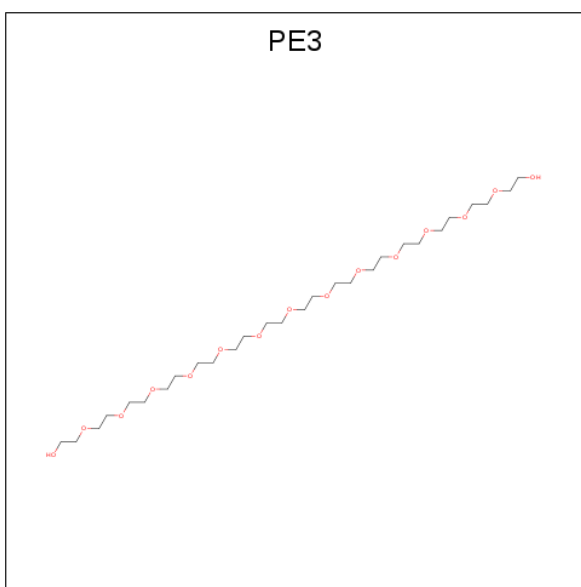


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
15	F	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
15	L	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 17 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDCAOXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula:  $C_{28}H_{58}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	G	1	Total	C	O	0	0
			14	9	5		

- Molecule 18 is water.

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

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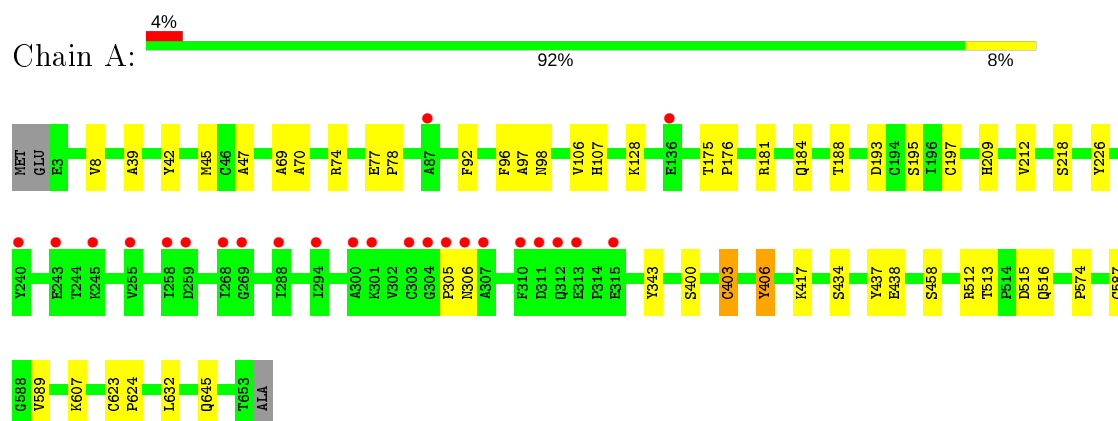
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	62	Total	O	0	0
			62	62		

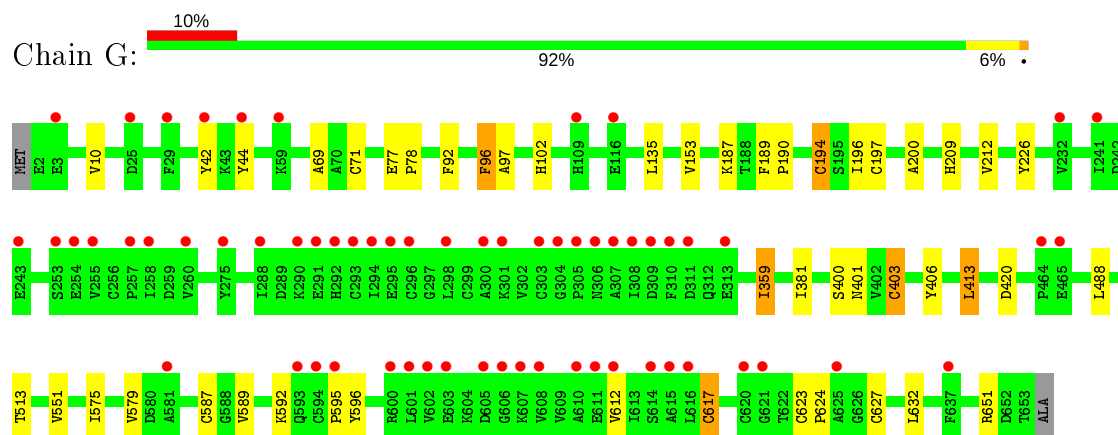
### 3 Residue-property plots [i](#)

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

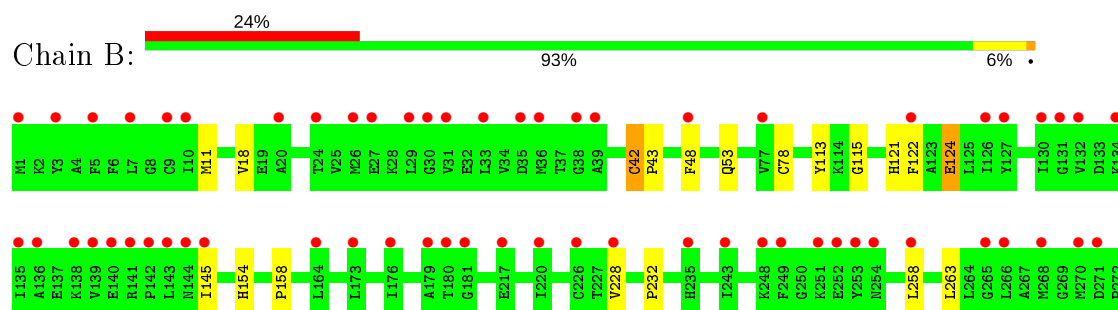
#### • Molecule 1: Heterodisulfide reductase, subunit A

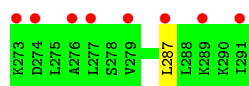


#### • Molecule 1: Heterodisulfide reductase, subunit A

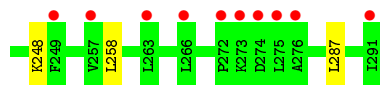
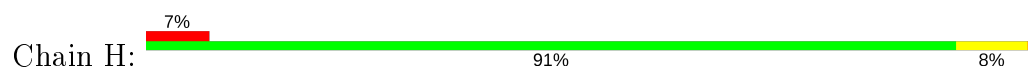


#### • Molecule 2: Heterodisulfide reductase, subunit B

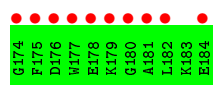
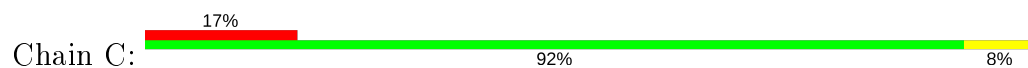




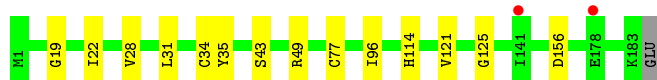
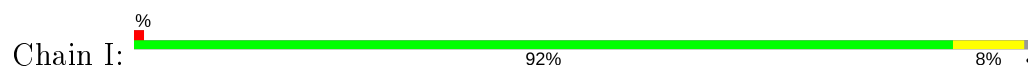
- Molecule 2: Heterodisulfide reductase, subunit B



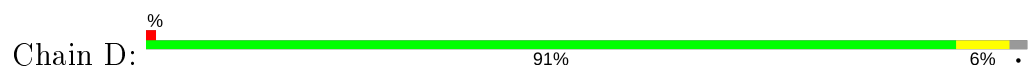
- Molecule 3: Heterodisulfide reductase, subunit C



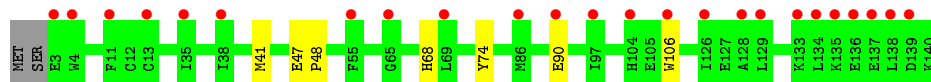
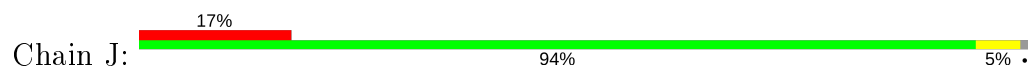
- Molecule 3: Heterodisulfide reductase, subunit C



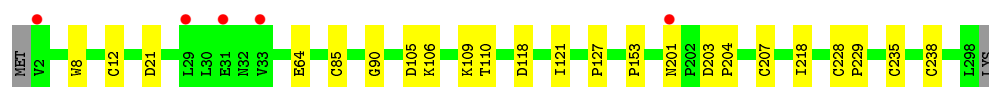
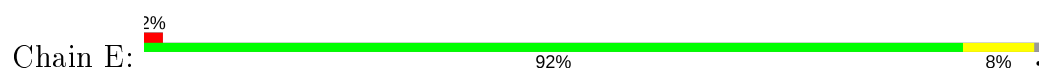
- Molecule 4: Methyl-viologen reducing hydrogenase, subunit D



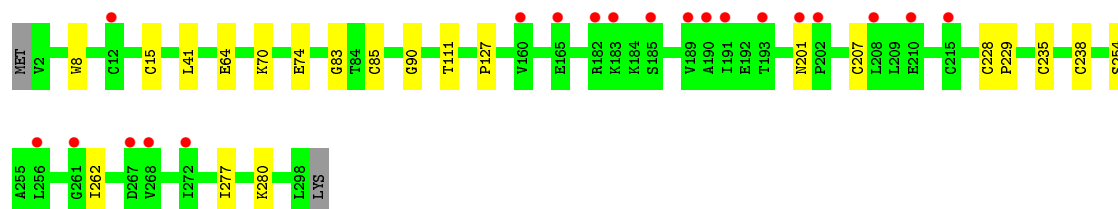
- Molecule 4: Methyl-viologen reducing hydrogenase, subunit D



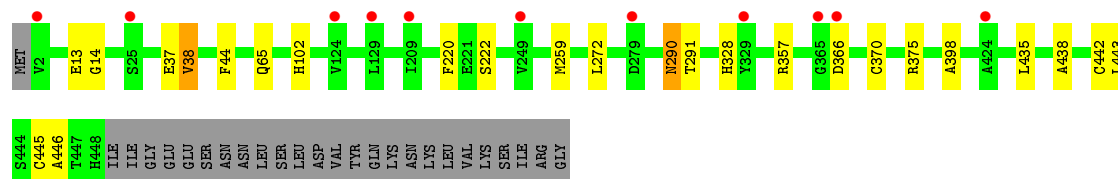
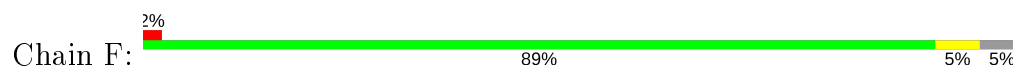
- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G



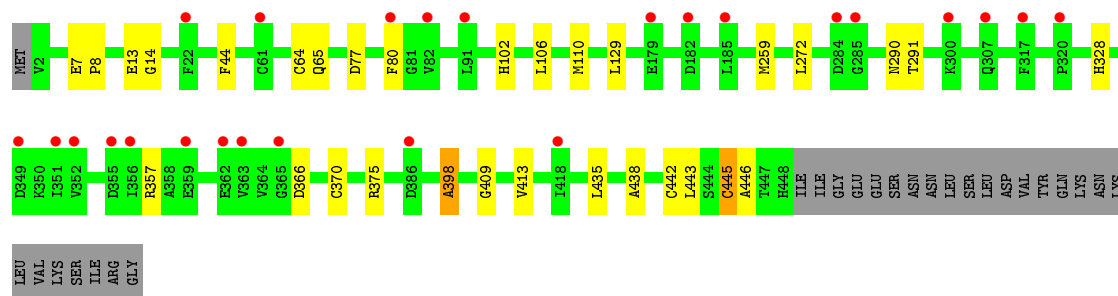
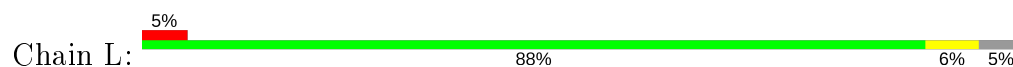
- Molecule 5: Methyl-viologen reducing hydrogenase, subunit G



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	370.53 Å 97.08 Å 135.15 Å 90.00° 109.43° 90.00°	Depositor
Resolution (Å)	48.54 – 2.40 48.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-2.40) 99.9 (48.54-2.40)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.39 Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.202 , 0.241 0.230 , 0.273	Depositor DCC
$R_{free}$ test set	8805 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 68.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.046 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SF4, PE3, NFU, 9S8, FE, ACT, TRS, COM, FAD, FES

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	0.32	0/5062	0.54	0/6841
1	G	0.28	0/5071	0.52	0/6853
2	B	0.20	0/2277	0.41	0/3070
2	H	0.22	0/2277	0.41	0/3070
3	C	0.27	0/1447	0.44	0/1946
3	I	0.27	0/1437	0.44	0/1934
4	D	0.36	0/1123	0.55	0/1508
4	J	0.26	0/1132	0.49	0/1520
5	E	0.31	0/2288	0.53	0/3102
5	K	0.25	0/2299	0.51	0/3116
6	F	0.27	0/3590	0.50	0/4853
6	L	0.25	0/3590	0.48	0/4853
All	All	0.28	0/31593	0.50	0/42666

There are no bond length outliers.

There are no bond angle outliers.

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	4970	0	4967	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4979	0	4974	38	0
2	B	2236	0	2244	12	0
2	H	2236	0	2243	12	1
3	C	1426	0	1441	7	0
3	I	1416	0	1435	7	0
4	D	1097	0	1068	6	0
4	J	1106	0	1074	9	0
5	E	2249	0	2252	9	1
5	K	2257	0	2265	12	0
6	F	3521	0	3503	13	0
6	L	3521	0	3503	13	0
7	A	4	0	3	1	0
7	D	4	0	3	0	0
7	G	4	0	3	0	0
8	A	53	0	31	0	0
8	G	53	0	31	0	0
9	A	48	0	0	0	0
9	C	16	0	0	0	0
9	E	24	0	0	0	0
9	G	48	0	0	1	0
9	I	16	0	0	0	0
9	K	24	0	0	0	0
10	A	12	0	16	0	0
10	G	6	0	8	0	0
10	H	6	0	8	0	0
10	K	6	0	8	0	0
11	B	16	0	0	0	0
11	H	16	0	0	1	0
12	B	7	0	6	1	0
12	H	7	0	6	2	0
13	D	4	0	0	0	0
13	J	4	0	0	0	0
14	D	8	0	12	0	0
15	F	8	0	0	2	0
15	L	8	0	0	1	0
16	F	1	0	0	0	0
16	L	1	0	0	0	0
17	G	14	0	16	0	0
18	A	125	0	0	1	0
18	B	14	0	0	0	0
18	C	19	0	0	0	0
18	D	36	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	E	49	0	0	0	0
18	F	65	0	0	0	0
18	G	87	0	0	1	0
18	H	23	0	0	0	0
18	I	27	0	0	0	0
18	J	5	0	0	0	0
18	K	42	0	0	0	0
18	L	62	0	0	0	0
All	All	31986	0	31120	153	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:HG23	1:A:195:SER:HB2	1.86	0.57
4:J:68:HIS:HA	4:J:106:TRP:HB3	1.84	0.57
1:G:587:CYS:SG	1:G:589:VAL:HG23	2.45	0.56
2:B:78:CYS:SG	2:B:232:PRO:HD2	2.46	0.56
6:F:220:PHE:CE2	6:F:222:SER:HB3	2.40	0.55
3:C:157:LEU:HD23	3:C:157:LEU:C	2.28	0.53
2:H:78:CYS:SG	2:H:232:PRO:HD2	2.49	0.53
4:D:10:GLY:HA2	4:D:63:PHE:O	2.09	0.53
2:H:154:HIS:ND1	12:H:303:COM:S1	2.80	0.52
1:G:579:VAL:HG22	1:G:632:LEU:CD2	2.39	0.52
1:G:153:VAL:HG22	1:G:551:VAL:HG22	1.92	0.52
5:E:106:LYS:HA	5:E:110:THR:OG1	2.10	0.51
2:B:11:MET:HG3	2:B:18:VAL:HB	1.91	0.51
2:H:11:MET:HG3	2:H:18:VAL:HB	1.91	0.51
5:K:70:LYS:O	5:K:74:GLU:HG3	2.11	0.51
1:A:512:ARG:O	4:D:110:SER:HB3	2.11	0.51
5:E:64:GLU:HG2	5:E:127:PRO:HB3	1.92	0.51
2:B:53:GLN:NE2	3:C:23:PRO:HD3	2.25	0.50
4:D:16:CYS:HB2	4:D:67:CYS:SG	2.52	0.50
6:L:435:LEU:C	6:L:435:LEU:HD13	2.32	0.50
2:B:158:PRO:HG3	3:C:81:TYR:CD2	2.47	0.49
1:A:434:SER:HB3	1:A:437:TYR:CE1	2.47	0.49
3:I:121:VAL:O	3:I:125:GLY:HA2	2.12	0.49
1:G:10:VAL:HA	1:G:69:ALA:HB3	1.95	0.48
2:H:42:CYS:SG	2:H:43:PRO:C	2.91	0.48
1:G:77:GLU:N	1:G:78:PRO:CD	2.76	0.48
5:E:105:ASP:O	5:E:109:LYS:HB2	2.13	0.48
1:G:575:ILE:HD12	4:J:41:MET:HG3	1.94	0.48
5:K:41:LEU:HD13	6:L:129:LEU:HD21	1.95	0.48
3:C:157:LEU:HD23	3:C:157:LEU:O	2.13	0.48
1:G:579:VAL:HG22	1:G:632:LEU:HD23	1.95	0.48
5:K:64:GLU:HG3	5:K:127:PRO:HB3	1.96	0.48
3:C:121:VAL:O	3:C:125:GLY:HA2	2.13	0.48
6:F:442:CYS:SG	6:F:445:CYS:CB	2.89	0.48
2:H:51:PHE:CZ	3:I:114:HIS:HB3	2.49	0.48
1:A:305:PRO:O	1:A:306:ASN:OD1	2.31	0.47
1:A:8:VAL:O	1:A:39:ALA:HA	2.14	0.47
1:A:587:CYS:SG	1:A:589:VAL:CG2	3.00	0.47
1:G:92:PHE:CD2	1:G:135:LEU:HB2	2.49	0.47
6:F:442:CYS:HB3	15:F:501:NFU:C2	2.43	0.47
1:A:47:ALA:HA	1:G:200:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:435:LEU:HD13	6:F:435:LEU:C	2.34	0.47
1:G:612:VAL:CG1	1:G:617:CYS:SG	3.02	0.47
2:H:113:TYR:CE2	2:H:115:GLY:HA2	2.49	0.47
1:A:623:CYS:SG	1:A:632:LEU:HD13	2.55	0.47
1:A:400:SER:HB2	1:A:403:CYS:SG	2.54	0.47
5:K:85:CYS:SG	5:K:90:GLY:HA3	2.55	0.47
4:D:17:THR:HG21	4:D:65:GLY:HA3	1.96	0.47
1:G:196:ILE:HG23	1:G:200:ALA:HB2	1.96	0.47
2:B:145:ILE:HD13	2:B:287:LEU:HD11	1.97	0.47
1:G:623:CYS:SG	1:G:624:PRO:HD3	2.55	0.47
1:A:437:TYR:CD1	1:A:437:TYR:N	2.83	0.46
5:K:228:CYS:HB2	5:K:229:PRO:HD3	1.96	0.46
2:B:113:TYR:CE2	2:B:115:GLY:HA2	2.50	0.46
1:G:71:CYS:O	1:G:96:PHE:CE1	2.69	0.46
1:G:69:ALA:HA	1:G:97:ALA:HB3	1.97	0.46
1:A:437:TYR:HD1	1:A:437:TYR:N	2.14	0.46
6:L:13:GLU:HB3	6:L:442:CYS:HA	1.98	0.46
1:G:209:HIS:HB3	1:G:212:VAL:HB	1.97	0.45
6:L:64:CYS:CB	15:L:501:NFU:C1	2.94	0.45
2:B:42:CYS:SG	2:B:43:PRO:C	2.94	0.45
5:E:228:CYS:HB2	5:E:229:PRO:HD3	1.98	0.45
1:A:209:HIS:HB3	1:A:212:VAL:HB	1.98	0.45
6:F:328:HIS:CE1	6:F:438:ALA:HA	2.51	0.45
6:L:328:HIS:CE1	6:L:438:ALA:HA	2.51	0.45
1:G:612:VAL:HG11	1:G:617:CYS:SG	2.57	0.45
1:A:197:CYS:SG	1:G:44:TYR:CD1	3.10	0.45
6:L:14:GLY:HA3	6:L:443:LEU:HB2	1.97	0.45
2:B:154:HIS:ND1	12:B:303:COM:S1	2.89	0.45
6:F:13:GLU:HB3	6:F:442:CYS:HA	1.99	0.44
6:L:106:LEU:HD12	6:L:110:MET:SD	2.57	0.44
1:A:515:ASP:O	1:A:516:GLN:HB2	2.18	0.44
6:L:375:ARG:C	6:L:398:ALA:HB1	2.38	0.44
1:A:188:THR:CG2	1:A:195:SER:HB2	2.47	0.44
1:A:406:TYR:C	1:A:406:TYR:CD1	2.91	0.44
2:B:43:PRO:HB2	2:B:48:PHE:CD1	2.53	0.44
1:A:458:SER:HB2	3:I:43:SER:OG	2.18	0.44
5:K:15:CYS:SG	5:K:83:GLY:HA3	2.58	0.44
1:A:181:ARG:O	1:A:184:GLN:N	2.47	0.44
6:F:14:GLY:HA3	6:F:443:LEU:HB2	1.98	0.44
1:A:128:LYS:HB2	1:A:645:GLN:HG3	1.99	0.44
1:A:69:ALA:HA	1:A:97:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:623:CYS:N	1:G:624:PRO:HD2	2.32	0.44
5:E:85:CYS:SG	5:E:90:GLY:HA3	2.58	0.43
1:A:77:GLU:HB3	1:A:78:PRO:HD3	2.00	0.43
6:L:77:ASP:O	6:L:80:PHE:O	2.36	0.43
2:B:121:HIS:O	2:B:124:GLU:HG3	2.19	0.43
1:A:106:VAL:HG23	1:A:107:HIS:CE1	2.53	0.43
4:J:47:GLU:HB2	4:J:48:PRO:HD2	2.00	0.43
1:G:194:CYS:CB	1:G:197:CYS:SG	3.02	0.42
1:A:42:TYR:HB3	1:A:45:MET:SD	2.59	0.42
2:H:121:HIS:O	2:H:124:GLU:HG3	2.19	0.42
1:A:438:GLU:HG3	18:G:861:HOH:O	2.19	0.42
1:A:417:LYS:HD3	7:A:701:ACT:H2	2.00	0.42
6:F:290:ASN:OD1	6:F:291:THR:HG23	2.19	0.42
4:D:63:PHE:C	4:D:63:PHE:CD2	2.92	0.42
5:E:203:ASP:OD1	5:E:204:PRO:HD2	2.19	0.42
6:F:290:ASN:HB3	6:F:375:ARG:C	2.40	0.42
1:G:592:LYS:HB3	5:K:262:ILE:HG12	2.01	0.42
1:G:400:SER:O	1:G:401:ASN:HB3	2.19	0.41
6:L:7:GLU:HA	6:L:8:PRO:HA	1.89	0.41
4:J:48:PRO:HD2	5:K:254:SER:HB2	2.02	0.41
1:A:175:THR:HB	1:A:176:PRO:CD	2.51	0.41
1:G:381:ILE:HG12	1:G:488:LEU:HB3	2.02	0.41
2:B:263:LEU:C	2:B:263:LEU:HD13	2.41	0.41
1:A:587:CYS:HB2	5:E:218:ILE:HG22	2.02	0.41
1:A:343:TYR:HB3	18:A:840:HOH:O	2.20	0.41
1:G:627:CYS:HB2	1:G:632:LEU:HD12	2.03	0.41
1:A:197:CYS:HB3	9:G:704:SF4:S4	2.60	0.41
3:C:31:LEU:HB3	3:C:96:ILE:HD13	2.03	0.41
3:I:31:LEU:HB3	3:I:96:ILE:HD13	2.03	0.41
2:H:158:PRO:O	2:H:162:LYS:HG2	2.20	0.41
2:H:53:GLN:HB3	3:I:22:ILE:HG22	2.03	0.41
1:A:226:TYR:N	1:A:226:TYR:CD1	2.88	0.41
2:H:228:VAL:HA	2:H:258:LEU:O	2.21	0.41
5:E:21:ASP:HB3	5:E:153:PRO:HG3	2.03	0.41
1:G:189:PHE:HB2	1:G:190:PRO:HA	2.02	0.41
6:L:409:GLY:O	6:L:413:VAL:HG23	2.21	0.41
1:A:77:GLU:N	1:A:78:PRO:CD	2.85	0.40
2:B:228:VAL:HA	2:B:258:LEU:O	2.21	0.40
6:F:272:LEU:HD11	6:F:446:ALA:HB1	2.03	0.40
1:G:226:TYR:CD1	1:G:226:TYR:N	2.88	0.40
6:L:272:LEU:HD11	6:L:446:ALA:HB1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:CYS:SG	1:G:44:TYR:HD1	2.45	0.40
6:F:37:GLU:HG2	6:F:38:VAL:N	2.36	0.40
1:G:153:VAL:CG2	1:G:551:VAL:HG22	2.50	0.40
1:G:623:CYS:N	1:G:624:PRO:CD	2.84	0.40
2:H:38:GLY:HA3	3:I:156:ASP:OD2	2.21	0.40

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

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	649/654 (99%)	619 (95%)	29 (4%)	1 (0%)	47	62
1	G	650/654 (99%)	617 (95%)	33 (5%)	0	100	100
2	B	289/291 (99%)	275 (95%)	14 (5%)	0	100	100
2	H	289/291 (99%)	276 (96%)	13 (4%)	0	100	100
3	C	182/184 (99%)	178 (98%)	4 (2%)	0	100	100
3	I	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
4	D	135/140 (96%)	130 (96%)	5 (4%)	0	100	100
4	J	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
5	E	295/299 (99%)	279 (95%)	16 (5%)	0	100	100
5	K	296/299 (99%)	278 (94%)	18 (6%)	0	100	100
6	F	445/473 (94%)	421 (95%)	22 (5%)	2 (0%)	34	48
6	L	445/473 (94%)	421 (95%)	22 (5%)	2 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3992/4082 (98%)	3804 (95%)	183 (5%)	5 (0%)	51 68

All (5) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	539/541 (100%)	531 (98%)	8 (2%)	65 80
1	G	540/541 (100%)	528 (98%)	12 (2%)	52 71
2	B	242/242 (100%)	239 (99%)	3 (1%)	71 85
2	H	242/242 (100%)	236 (98%)	6 (2%)	47 67
3	C	157/157 (100%)	152 (97%)	5 (3%)	39 59
3	I	156/157 (99%)	152 (97%)	4 (3%)	46 66
4	D	116/119 (98%)	116 (100%)	0	100 100
4	J	117/119 (98%)	117 (100%)	0	100 100
5	E	254/256 (99%)	248 (98%)	6 (2%)	49 68
5	K	255/256 (100%)	249 (98%)	6 (2%)	49 68
6	F	386/410 (94%)	378 (98%)	8 (2%)	53 72
6	L	386/410 (94%)	377 (98%)	9 (2%)	50 70
All	All	3390/3450 (98%)	3323 (98%)	67 (2%)	55 74

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	98	ASN
1	A	193	ASP
1	A	218	SER
1	A	403	CYS
1	A	406	TYR
1	A	513	THR
1	A	607	LYS
2	B	42	CYS
2	B	122	PHE
2	B	124	GLU
3	C	34	CYS
3	C	35	TYR
3	C	49	ARG
3	C	66	ASP
3	C	102	ASN
5	E	8	TRP
5	E	12	CYS
5	E	118	ASP
5	E	207	CYS
5	E	235	CYS
5	E	238	CYS
6	F	44	PHE
6	F	65	GLN
6	F	102	HIS
6	F	259	MET
6	F	290	ASN
6	F	357	ARG
6	F	366	ASP
6	F	370	CYS
1	G	42	TYR
1	G	96	PHE
1	G	102	HIS
1	G	194	CYS
1	G	359	ILE
1	G	403	CYS
1	G	406	TYR
1	G	413	LEU
1	G	420	ASP
1	G	513	THR
1	G	617	CYS
1	G	651	ARG
2	H	42	CYS

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Mol	Chain	Res	Type
2	H	122	PHE
2	H	124	GLU
2	H	133	ASP
2	H	211	MET
2	H	233	PHE
3	I	34	CYS
3	I	35	TYR
3	I	49	ARG
3	I	77	CYS
5	K	8	TRP
5	K	111	THR
5	K	201	ASN
5	K	207	CYS
5	K	235	CYS
5	K	238	CYS
6	L	44	PHE
6	L	65	GLN
6	L	102	HIS
6	L	259	MET
6	L	290	ASN
6	L	357	ARG
6	L	366	ASP
6	L	370	CYS
6	L	445	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	GOL	H	304	-	5,5,5	0.34	0	5,5,5	0.15	0
9	SF4	C	201	3	0,12,12	0.00	-	-		
9	SF4	A	703	1	0,12,12	0.00	-	-		
9	SF4	E	302	5	0,12,12	0.00	-	-		
7	ACT	D	202	-	1,3,3	4.67	1 (100%)	0,3,3	0.00	-
9	SF4	A	706	1	0,12,12	0.00	-	-		
9	SF4	I	201	3	0,12,12	0.00	-	-		
10	GOL	K	304	-	5,5,5	0.42	0	5,5,5	0.36	0
13	FES	D	201	4	0,4,4	0.00	-	-		
9	SF4	A	707	1	0,12,12	0.00	-	-		
9	SF4	K	303	5	0,12,12	0.00	-	-		
12	COM	B	303	-	6,6,6	1.40	2 (33%)	7,8,8	3.01	4 (57%)
9	SF4	G	708	1	0,12,12	0.00	-	-		
9	SF4	E	303	5	0,12,12	0.00	-	-		
9	SF4	I	202	3	0,12,12	0.00	-	-		
10	GOL	A	709	-	5,5,5	0.38	0	5,5,5	0.38	0
11	9S8	B	302	2	2,10,10	1.24	0	-		
11	9S8	B	301	2	2,10,10	0.88	0	-		
7	ACT	A	701	-	1,3,3	4.28	1 (100%)	0,3,3	0.00	-
9	SF4	G	704	1	0,12,12	0.00	-	-		
7	ACT	G	702	-	1,3,3	5.38	1 (100%)	0,3,3	0.00	-
12	COM	H	303	-	6,6,6	1.37	2 (33%)	7,8,8	3.48	4 (57%)
8	FAD	A	702	-	51,58,58	1.85	7 (13%)	60,89,89	2.09	12 (20%)
9	SF4	C	202	3	0,12,12	0.00	-	-		
9	SF4	G	707	1	0,12,12	0.00	-	-		
9	SF4	K	301	5	0,12,12	0.00	-	-		
9	SF4	A	708	1	0,12,12	0.00	-	-		
10	GOL	A	710	-	5,5,5	0.35	0	5,5,5	0.45	0
14	TRS	D	203	-	7,7,7	0.39	0	9,9,9	0.63	0
9	SF4	G	706	1	0,12,12	0.00	-	-		
9	SF4	E	301	5	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SF4	G	709	1	0,12,12	0.00	-	-		
9	SF4	A	705	1	0,12,12	0.00	-	-		
9	SF4	G	705	1	0,12,12	0.00	-	-		
11	9S8	H	302	2	2,10,10	0.85	0	-		
10	GOL	G	710	-	5,5,5	0.32	0	5,5,5	0.42	0
13	FES	J	200	4	0,4,4	0.00	-	-		
15	NFU	L	501	6	2,7,7	0.95	0	-		
9	SF4	K	302	5	0,12,12	0.00	-	-		
8	FAD	G	703	-	51,58,58	1.90	7 (13%)	60,89,89	2.04	14 (23%)
15	NFU	F	501	6	2,7,7	1.48	0	-		
17	PE3	G	701	-	13,13,42	0.58	0	12,12,41	0.25	0
11	9S8	H	301	2	2,10,10	1.65	1 (50%)	-		
9	SF4	A	704	1	0,12,12	0.00	-	-		

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
10	GOL	H	304	-	-	0/4/4/4	-
9	SF4	C	201	3	-	-	0/6/5/5
9	SF4	A	703	1	-	-	0/6/5/5
9	SF4	E	302	5	-	-	0/6/5/5
9	SF4	C	202	3	-	-	0/6/5/5
9	SF4	A	706	1	-	-	0/6/5/5
9	SF4	I	201	3	-	-	0/6/5/5
10	GOL	K	304	-	-	2/4/4/4	-
13	FES	D	201	4	-	-	0/1/1/1
9	SF4	A	707	1	-	-	0/6/5/5
9	SF4	K	303	5	-	-	0/6/5/5
12	COM	B	303	-	-	1/4/4/4	-
9	SF4	G	708	1	-	-	0/6/5/5
9	SF4	E	303	5	-	-	0/6/5/5
9	SF4	I	202	3	-	-	0/6/5/5
10	GOL	A	709	-	-	3/4/4/4	-
11	9S8	B	302	2	-	-	0/3/3/3
11	9S8	B	301	2	-	-	0/3/3/3
9	SF4	G	704	1	-	-	0/6/5/5
12	COM	H	303	-	-	3/4/4/4	-
8	FAD	A	702	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	G	707	1	-	-	0/6/5/5
9	SF4	K	301	5	-	-	0/6/5/5
9	SF4	A	708	1	-	-	0/6/5/5
10	GOL	A	710	-	-	2/4/4/4	-
14	TRS	D	203	-	-	3/9/9/9	-
9	SF4	G	706	1	-	-	0/6/5/5
9	SF4	E	301	5	-	-	0/6/5/5
9	SF4	G	709	1	-	-	0/6/5/5
9	SF4	A	705	1	-	-	0/6/5/5
9	SF4	G	705	1	-	-	0/6/5/5
11	9S8	H	302	2	-	-	0/3/3/3
9	SF4	K	302	5	-	-	0/6/5/5
13	FES	J	200	4	-	-	0/1/1/1
10	GOL	G	710	-	-	4/4/4/4	-
8	FAD	G	703	-	-	1/30/50/50	0/6/6/6
17	PE3	G	701	-	-	6/11/11/40	-
11	9S8	H	301	2	-	-	0/3/3/3
9	SF4	A	704	1	-	-	0/6/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	703	FAD	C4X-C10	9.88	1.48	1.38
8	A	702	FAD	C4X-C10	9.34	1.48	1.38
7	G	702	ACT	CH3-C	5.38	1.55	1.48
7	D	202	ACT	CH3-C	4.67	1.54	1.48
7	A	701	ACT	CH3-C	4.28	1.54	1.48
8	A	702	FAD	C9A-C5X	4.13	1.50	1.42
8	G	703	FAD	C9A-C5X	4.03	1.50	1.42
8	A	702	FAD	C4-C4X	3.69	1.47	1.41
8	A	702	FAD	C8-C7	3.41	1.49	1.40
8	G	703	FAD	C4-C4X	3.31	1.47	1.41
8	G	703	FAD	C8-C7	3.25	1.49	1.40
8	G	703	FAD	C9A-N10	2.96	1.42	1.38
8	G	703	FAD	C1'-N10	-2.42	1.45	1.48
8	A	702	FAD	C5A-C4A	2.39	1.47	1.40
12	B	303	COM	O1S-S2	2.31	1.51	1.45
8	G	703	FAD	C5A-C4A	2.29	1.47	1.40
8	A	702	FAD	C9A-N10	2.20	1.41	1.38
8	A	702	FAD	O4B-C1B	2.17	1.44	1.41
12	H	303	COM	O2S-S2	2.11	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	303	COM	O1S-S2	2.11	1.51	1.45
12	B	303	COM	O2S-S2	2.10	1.51	1.45
11	H	301	9S8	S3-FE4	-2.09	2.20	2.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	702	FAD	C4-N3-C2	8.08	121.97	115.14
8	G	703	FAD	C4-N3-C2	7.84	121.76	115.14
8	A	702	FAD	C1'-N10-C9A	6.78	123.63	118.29
8	G	703	FAD	C4-C4X-C10	-6.17	115.87	119.95
8	A	702	FAD	C4-C4X-C10	-5.49	116.32	119.95
8	G	703	FAD	C1'-N10-C9A	5.49	122.61	118.29
12	H	303	COM	O2S-S2-C2	5.16	113.13	106.92
12	H	303	COM	O3S-S2-O2S	-5.10	98.82	111.27
12	H	303	COM	O3S-S2-C2	4.80	113.53	105.77
12	B	303	COM	O3S-S2-O2S	-4.64	99.94	111.27
12	B	303	COM	O2S-S2-C2	4.14	111.89	106.92
12	B	303	COM	O3S-S2-C2	4.04	112.30	105.77
8	G	703	FAD	P-O3P-PA	-3.78	119.87	132.83
8	A	702	FAD	C4X-N5-C5X	3.76	120.53	116.77
8	G	703	FAD	N3A-C2A-N1A	-3.73	122.85	128.68
8	A	702	FAD	N3A-C2A-N1A	-3.54	123.14	128.68
8	G	703	FAD	C4X-N5-C5X	3.49	120.25	116.77
8	A	702	FAD	C4X-C4-N3	-3.32	118.89	123.43
8	A	702	FAD	C9A-N10-C10	-3.14	117.80	121.91
8	A	702	FAD	C5X-C9A-N10	3.05	119.92	117.72
8	G	703	FAD	C4X-C4-N3	-2.93	119.42	123.43
8	G	703	FAD	C5X-C9A-N10	2.90	119.82	117.72
8	A	702	FAD	P-O3P-PA	-2.89	122.90	132.83
12	H	303	COM	O1S-S2-C2	2.74	110.22	106.92
8	A	702	FAD	C4-C4X-N5	2.71	121.69	118.60
8	G	703	FAD	C10-C4X-N5	2.65	123.09	121.26
12	B	303	COM	O1S-S2-C2	2.62	110.07	106.92
8	G	703	FAD	C4A-C5A-N7A	-2.60	106.69	109.40
8	A	702	FAD	O4'-C4'-C5'	-2.46	104.38	109.92
8	G	703	FAD	C9A-N10-C10	-2.30	118.89	121.91
8	G	703	FAD	C2A-N1A-C6A	2.25	122.61	118.75
8	G	703	FAD	C4X-C10-N10	-2.23	118.00	120.30
8	A	702	FAD	C4A-C5A-N7A	-2.14	107.17	109.40
8	G	703	FAD	C4-C4X-N5	2.14	121.04	118.60

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

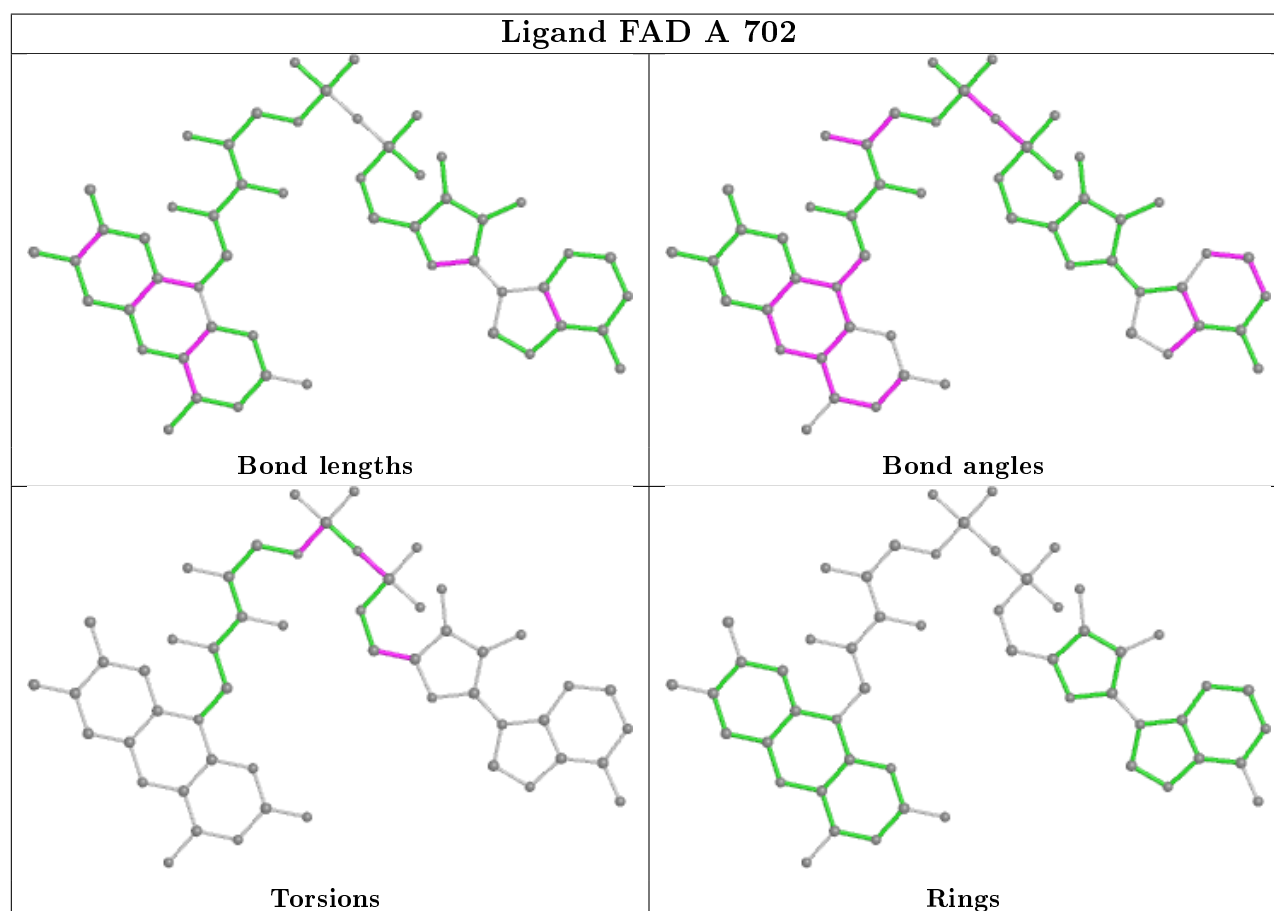
There are no ring outliers.

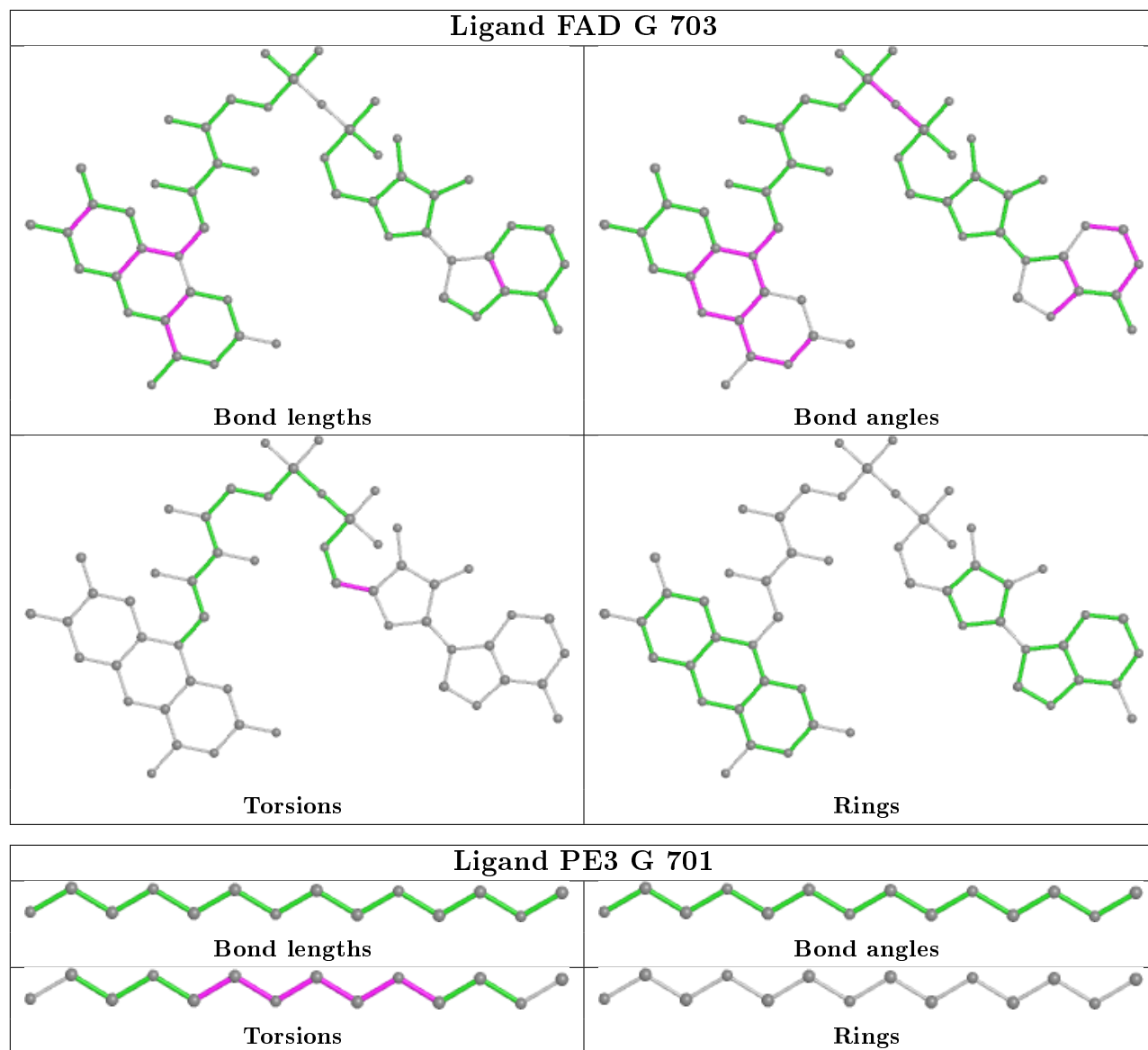
7 monomers are involved in 8 short contacts:

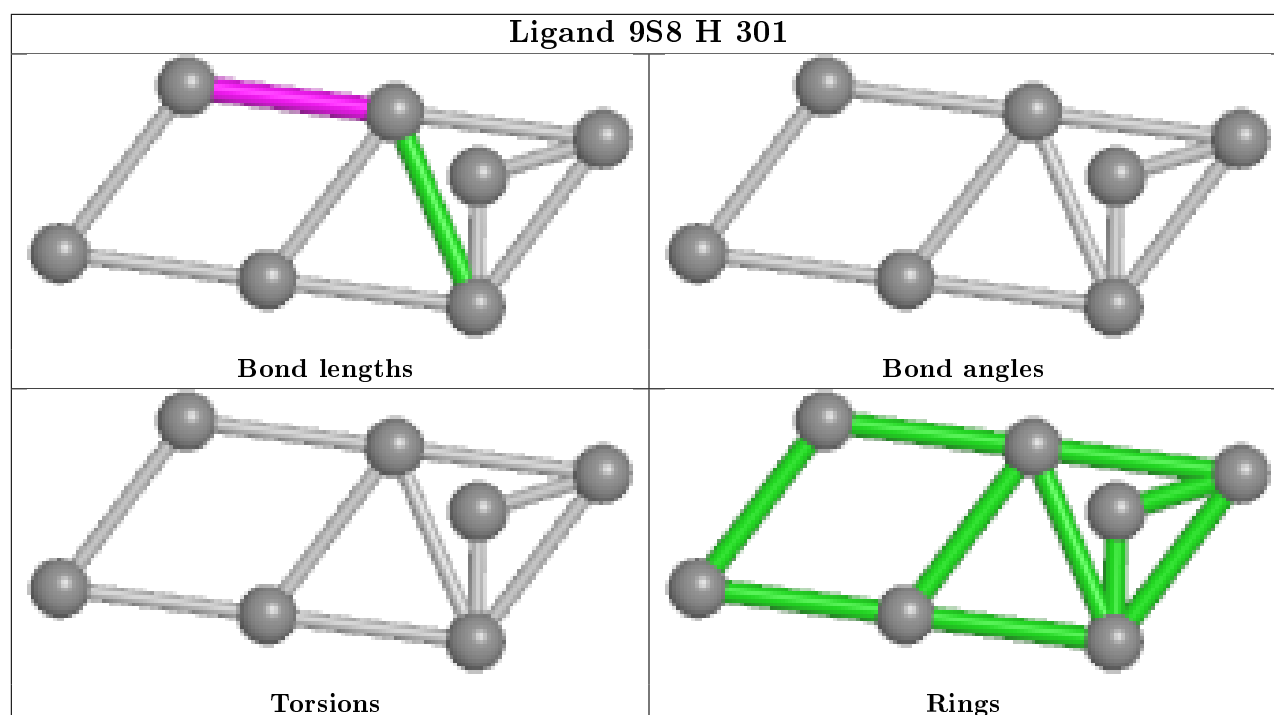
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	303	COM	1	0
7	A	701	ACT	1	0
9	G	704	SF4	1	0
12	H	303	COM	2	0
11	H	302	9S8	1	0
15	L	501	NFU	1	0
15	F	501	NFU	2	0



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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	651/654 (99%)	-0.17	24 (3%) 41 41	15, 43, 106, 161	0
1	G	652/654 (99%)	0.43	63 (9%) 7 7	23, 64, 144, 221	0
2	B	291/291 (100%)	1.24	69 (23%) 0 0	41, 93, 144, 165	0
2	H	291/291 (100%)	0.42	21 (7%) 15 14	37, 68, 105, 132	0
3	C	184/184 (100%)	0.62	32 (17%) 1 1	22, 60, 141, 156	0
3	I	183/184 (99%)	-0.13	2 (1%) 80 79	26, 51, 93, 123	0
4	D	137/140 (97%)	-0.38	2 (1%) 73 72	21, 37, 64, 118	0
4	J	138/140 (98%)	0.90	24 (17%) 1 1	47, 67, 97, 202	0
5	E	297/299 (99%)	-0.21	5 (1%) 70 68	19, 42, 76, 92	0
5	K	297/299 (99%)	0.43	20 (6%) 17 16	28, 62, 122, 165	0
6	F	447/473 (94%)	-0.02	11 (2%) 57 55	26, 52, 85, 102	0
6	L	447/473 (94%)	0.44	25 (5%) 24 23	28, 66, 139, 177	0
All	All	4015/4082 (98%)	0.27	298 (7%) 14 13	15, 58, 123, 221	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	135	ILE	11.3
2	B	136	ALA	10.0
3	C	178	GLU	7.0
1	G	601	LEU	6.9
3	C	181	ALA	6.7
2	B	5	PHE	6.6
1	G	615	ALA	6.4
2	B	140	GLU	6.4
2	B	266	LEU	6.3
2	B	249	PHE	6.2
2	B	30	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	306	ASN	6.0
1	G	606	GLY	6.0
1	G	306	ASN	5.9
2	B	139	VAL	5.9
1	G	293	CYS	5.8
3	C	152	PHE	5.6
1	G	301	LYS	5.5
3	C	146	LYS	5.4
2	B	20	ALA	5.3
2	B	268	MET	5.3
5	K	183	LYS	5.2
2	B	130	ILE	5.1
5	K	190	ALA	5.1
5	K	268	VAL	5.0
1	G	464	PRO	4.9
1	A	307	ALA	4.9
3	C	180	GLY	4.9
3	C	128	VAL	4.9
5	E	2	VAL	4.9
2	B	29	LEU	4.8
4	J	69	LEU	4.7
3	C	132	LYS	4.7
5	K	185	SER	4.7
6	L	355	ASP	4.7
1	A	268	ILE	4.7
3	C	145	GLU	4.6
1	G	298	LEU	4.6
3	C	135	ALA	4.4
3	C	176	ASP	4.4
2	B	132	VAL	4.4
6	L	80	PHE	4.3
2	H	135	ILE	4.3
2	B	144	ASN	4.2
2	B	176	ILE	4.2
2	B	26	MET	4.2
3	C	129	PRO	4.1
4	J	134	LEU	4.1
6	L	185	LEU	4.1
1	G	602	VAL	4.1
2	B	10	ILE	4.1
6	L	365	GLY	4.1
4	J	3	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	39	ALA	4.1
2	B	145	ILE	4.1
3	C	154	GLU	4.0
1	G	291	GLU	4.0
6	F	249	VAL	4.0
5	K	191	ILE	4.0
2	B	1	MET	4.0
3	C	182	LEU	3.9
2	H	143	LEU	3.9
1	A	255	VAL	3.9
1	G	310	PHE	3.9
1	G	258	ILE	3.8
2	B	276	ALA	3.8
1	A	301	LYS	3.8
1	A	240	TYR	3.8
2	B	127	TYR	3.8
4	J	133	LYS	3.8
2	B	35	ASP	3.8
1	A	258	ILE	3.8
1	A	300	ALA	3.8
2	B	77	VAL	3.8
3	C	116	MET	3.7
3	C	123	LYS	3.7
1	G	605	ASP	3.7
3	C	184	GLU	3.7
2	H	274	ASP	3.7
5	K	267	ASP	3.7
1	G	241	ILE	3.6
2	B	291	ILE	3.6
1	G	255	VAL	3.6
3	C	124	TYR	3.6
3	C	179	LYS	3.5
2	B	180	THR	3.5
1	G	614	SER	3.5
1	G	290	LYS	3.5
1	G	603	GLU	3.4
1	A	310	PHE	3.4
1	G	42	TYR	3.4
1	A	269	GLY	3.4
2	B	248	LYS	3.4
2	B	220	ILE	3.4
6	L	351	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
6	L	363	VAL	3.4
2	B	38	GLY	3.3
4	J	65	GLY	3.3
1	G	243	GLU	3.3
3	C	147	ALA	3.3
3	C	175	PHE	3.3
1	G	304	GLY	3.3
6	L	91	LEU	3.2
1	A	288	ILE	3.2
2	H	266	LEU	3.2
4	J	126	ILE	3.2
6	L	356	ILE	3.2
5	E	29	LEU	3.2
2	B	134	LYS	3.2
4	J	128	ALA	3.2
1	G	608	VAL	3.2
2	B	7	LEU	3.2
2	B	279	VAL	3.2
2	B	270	MET	3.1
2	H	276	ALA	3.1
1	G	25	ASP	3.1
5	K	165	GLU	3.1
2	B	179	ALA	3.1
1	G	595	PRO	3.1
4	J	136	GLU	3.1
1	G	610	ALA	3.1
2	H	96	LYS	3.1
1	A	312	GLN	3.0
2	B	33	LEU	3.0
3	C	143	LEU	3.0
6	L	362	GLU	3.0
2	H	273	LYS	3.0
2	B	181	GLY	3.0
1	G	311	ASP	3.0
1	G	607	LYS	3.0
2	B	271	ASP	3.0
3	C	174	GLY	3.0
3	C	127	ALA	3.0
1	G	295	GLU	3.0
1	G	294	ILE	3.0
3	C	151	GLN	3.0
1	G	253	SER	3.0

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Mol	Chain	Res	Type	RSRZ
4	J	106	TRP	3.0
2	H	275	LEU	3.0
2	H	114	LYS	3.0
6	F	124	VAL	3.0
2	H	164	LEU	3.0
1	G	313	GLU	2.9
2	B	126	ILE	2.9
1	G	260	VAL	2.9
5	E	33	VAL	2.9
2	B	131	GLY	2.9
1	A	245	LYS	2.9
6	L	386	ASP	2.9
1	G	600	ARG	2.9
2	B	31	VAL	2.9
2	B	228	VAL	2.9
1	A	87	ALA	2.9
6	L	320	PRO	2.9
6	L	182	ASP	2.9
1	G	625	ALA	2.9
3	C	177	TRP	2.9
2	B	254	ASN	2.8
1	G	308	ILE	2.8
1	G	581	ALA	2.8
2	B	226	CYS	2.8
2	H	20	ALA	2.8
2	B	164	LEU	2.8
1	G	612	VAL	2.8
2	B	265	GLY	2.8
1	G	292	HIS	2.8
6	L	349	ASP	2.8
2	B	289	LYS	2.8
4	J	135	LYS	2.8
6	F	279	ASP	2.8
1	G	307	ALA	2.8
1	A	259	ASP	2.8
1	A	313	GLU	2.7
5	K	201	ASN	2.7
6	F	365	GLY	2.7
4	J	35	ILE	2.7
2	B	287	LEU	2.7
3	C	136	GLU	2.7
2	B	253	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	116	GLU	2.7
4	D	140	LYS	2.7
2	H	257	VAL	2.6
6	L	352	VAL	2.6
2	H	98	ALA	2.6
6	F	2	VAL	2.6
4	J	4	TRP	2.6
6	L	61	CYS	2.6
5	K	202	PRO	2.6
2	B	48	PHE	2.6
6	F	209	ILE	2.6
1	A	305	PRO	2.5
2	B	143	LEU	2.5
6	F	25	SER	2.5
4	J	138	LEU	2.5
1	A	294	ILE	2.5
6	F	424	ALA	2.5
5	K	210	GLU	2.5
6	L	285	GLY	2.5
1	G	620	CYS	2.4
2	H	263	LEU	2.4
6	L	82	VAL	2.4
2	B	3	TYR	2.4
6	L	418	ILE	2.4
2	B	122	PHE	2.4
4	J	55	PHE	2.4
2	B	217	GLU	2.4
1	G	300	ALA	2.4
4	J	11	PHE	2.4
3	C	130	ALA	2.4
2	B	24	THR	2.4
1	A	136	GLU	2.4
1	G	232	VAL	2.3
1	G	288	ILE	2.3
2	B	243	ILE	2.3
2	B	274	ASP	2.3
4	J	97	ILE	2.3
5	K	12	CYS	2.3
5	K	160	VAL	2.3
2	B	141	ARG	2.3
2	B	142	PRO	2.3
3	C	141	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	223	GLY	2.3
4	J	104	HIS	2.3
6	L	307	GLN	2.3
1	G	59	LYS	2.3
1	G	594	CYS	2.3
1	G	29	PHE	2.3
1	G	109	HIS	2.3
2	B	138	LYS	2.3
6	L	300	LYS	2.3
5	K	261	GLY	2.3
2	B	277	LEU	2.3
4	J	129	LEU	2.3
5	K	272	ILE	2.3
6	L	317	PHE	2.3
4	J	139	ASP	2.3
6	F	366	ASP	2.3
3	C	122	LEU	2.3
1	G	275	TYR	2.3
2	H	291	ILE	2.2
4	J	38	ILE	2.2
1	G	637	PHE	2.2
2	B	251	LYS	2.2
3	I	178	GLU	2.2
2	H	67	ALA	2.2
1	G	44	TYR	2.2
2	H	113	TYR	2.2
1	G	303	CYS	2.2
2	B	273	LYS	2.2
3	C	139	LYS	2.2
5	K	256	LEU	2.2
1	A	304	GLY	2.2
2	B	173	LEU	2.2
6	L	179	GLU	2.2
1	G	616	LEU	2.2
1	A	243	GLU	2.2
1	A	315	GLU	2.2
1	A	311	ASP	2.2
1	G	3	GLU	2.2
2	B	9	CYS	2.2
2	B	252	GLU	2.2
6	F	329	TYR	2.1
6	F	129	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	309	ASP	2.1
2	B	27	GLU	2.1
1	G	254	GLU	2.1
4	J	86	MET	2.1
1	A	303	CYS	2.1
1	G	296	CYS	2.1
1	G	621	GLY	2.1
5	K	189	VAL	2.1
5	K	193	THR	2.1
1	G	465	GLU	2.1
4	J	90	GLU	2.1
1	G	305	PRO	2.1
2	B	258	LEU	2.1
5	E	31	GLU	2.1
5	K	208	LEU	2.1
2	B	235	HIS	2.1
6	L	22	PHE	2.1
6	L	284	ASP	2.1
4	D	134	LEU	2.1
3	C	126	HIS	2.1
2	H	249	PHE	2.1
6	L	359	GLU	2.1
1	G	257	PRO	2.0
1	G	611	GLU	2.0
5	E	201	ASN	2.0
2	B	36	MET	2.0
4	J	137	GLU	2.0
3	C	163	LEU	2.0
5	K	182	ARG	2.0
2	H	272	PRO	2.0
1	G	593	GLN	2.0
4	J	13	CYS	2.0
5	K	215	CYS	2.0
2	H	110	GLY	2.0
3	I	141	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	ACT	G	702	4/4	0.66	0.42	108,110,110,110	0
10	GOL	H	304	6/6	0.69	0.44	95,96,99,101	0
7	ACT	A	701	4/4	0.72	0.55	62,66,66,67	0
17	PE3	G	701	14/43	0.74	0.31	50,58,74,76	0
7	ACT	D	202	4/4	0.83	0.34	78,79,80,82	0
10	GOL	K	304	6/6	0.84	0.20	54,55,61,62	0
14	TRS	D	203	8/8	0.86	0.25	41,54,56,61	0
11	9S8	B	302	8/8	0.89	0.14	68,80,86,90	0
10	GOL	A	710	6/6	0.89	0.21	42,49,49,52	0
10	GOL	G	710	6/6	0.91	0.18	46,51,55,59	0
10	GOL	A	709	6/6	0.92	0.15	44,49,50,53	0
12	COM	B	303	7/7	0.92	0.15	62,64,70,75	0
9	SF4	A	707	8/8	0.93	0.09	98,101,104,105	0
9	SF4	G	709	8/8	0.93	0.10	46,52,58,58	0
9	SF4	G	708	8/8	0.94	0.09	61,67,71,72	0
9	SF4	K	303	8/8	0.94	0.11	63,68,75,77	0
9	SF4	G	707	8/8	0.94	0.07	103,106,108,111	0
9	SF4	A	706	8/8	0.94	0.12	34,39,44,45	0
9	SF4	G	704	8/8	0.95	0.11	67,76,84,84	0
9	SF4	K	302	8/8	0.95	0.14	42,50,53,53	0
9	SF4	I	201	8/8	0.95	0.14	25,27,29,29	0
9	SF4	A	708	8/8	0.96	0.09	70,71,79,81	0
11	9S8	H	302	8/8	0.96	0.15	46,51,58,58	0
9	SF4	C	202	8/8	0.96	0.14	29,37,45,47	0
12	COM	H	303	7/7	0.96	0.18	42,46,57,61	0
9	SF4	E	301	8/8	0.96	0.16	18,26,30,32	0
9	SF4	G	706	8/8	0.97	0.07	81,82,85,86	0
9	SF4	I	202	8/8	0.97	0.15	36,37,49,53	0
9	SF4	A	703	8/8	0.97	0.11	13,18,20,24	0
9	SF4	A	705	8/8	0.97	0.12	24,32,36,41	0
9	SF4	G	705	8/8	0.97	0.11	15,17,20,26	0
9	SF4	K	301	8/8	0.97	0.20	37,41,49,50	0

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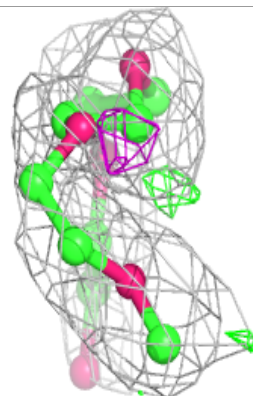
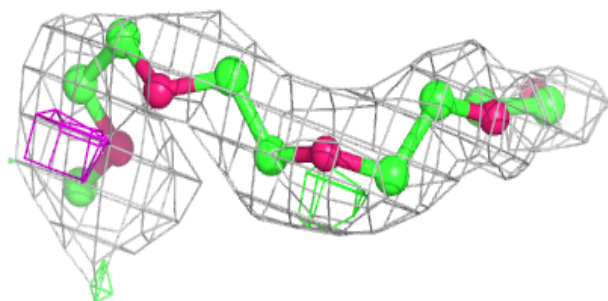
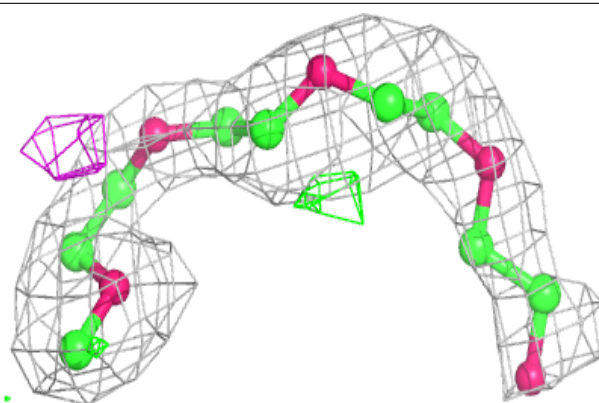
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SF4	E	302	8/8	0.97	0.10	13,24,27,29	0
11	9S8	B	301	8/8	0.97	0.11	57,67,69,74	0
8	FAD	G	703	53/53	0.97	0.15	8,32,52,54	0
8	FAD	A	702	53/53	0.97	0.13	11,27,49,53	0
11	9S8	H	301	8/8	0.97	0.11	41,49,55,59	0
9	SF4	A	704	8/8	0.97	0.09	12,21,28,31	0
9	SF4	C	201	8/8	0.98	0.14	24,27,33,40	0
9	SF4	E	303	8/8	0.98	0.09	10,16,24,27	0
15	NFU	F	501	8/8	0.98	0.17	29,36,39,41	0
13	FES	D	201	4/4	0.99	0.15	20,23,33,36	0
13	FES	J	200	4/4	0.99	0.12	52,54,59,61	0
15	NFU	L	501	8/8	0.99	0.14	28,34,37,41	0
16	FE	L	502	1/1	1.00	0.17	44,44,44,44	0
16	FE	F	502	1/1	1.00	0.10	35,35,35,35	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.

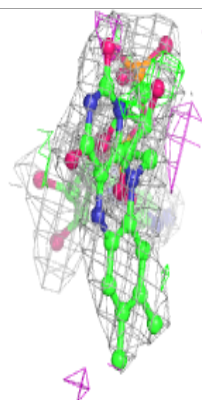
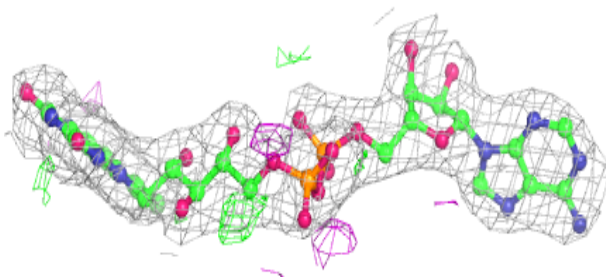
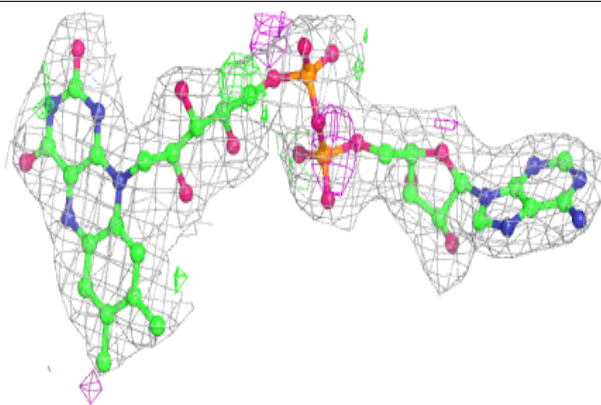
**Electron density around PE3 G 701:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

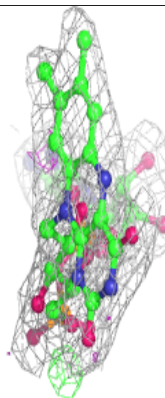
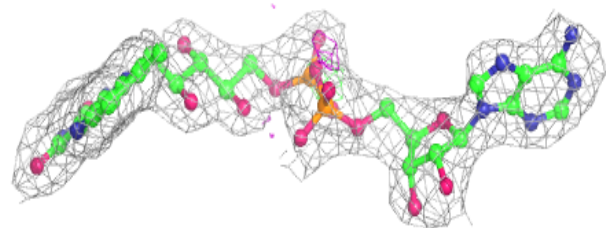
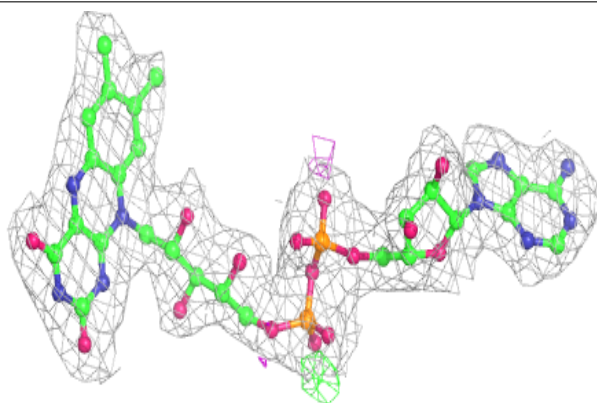


**Electron density around FAD G 703:**

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

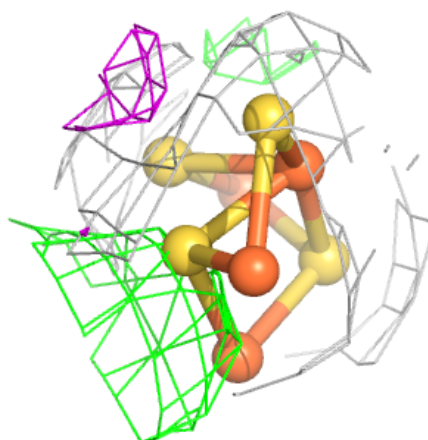
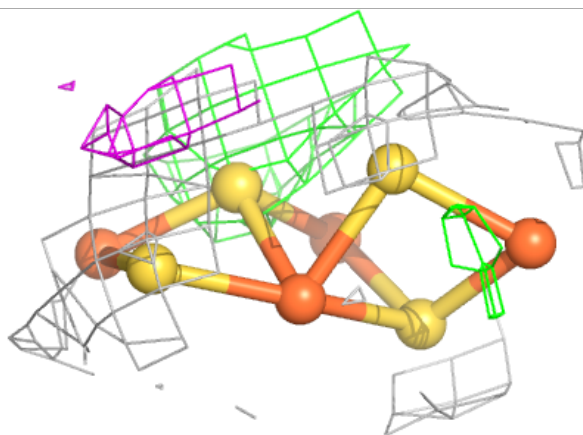
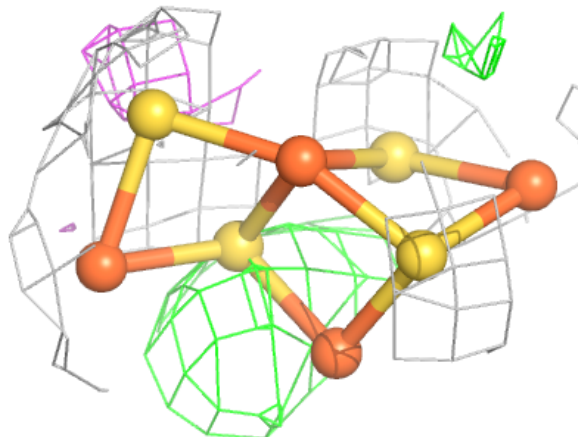
**Electron density around FAD A 702:**

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



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

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.