Full wwPDB X-ray Structure Validation Report (i)

Nov 30, 2022 – 06:21 pm GMT

PDB ID	:	5G5H
Title	:	Escherichia coli Periplasmic Aldehyde Oxidase R440H mutant
Authors	:	Correia, M.A.S.; Otrelo-Cardoso, A.R.; Romao, M.J.; Santos-Silva, T.
Deposited on	:	2016-05-25
Resolution	:	2.30 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:

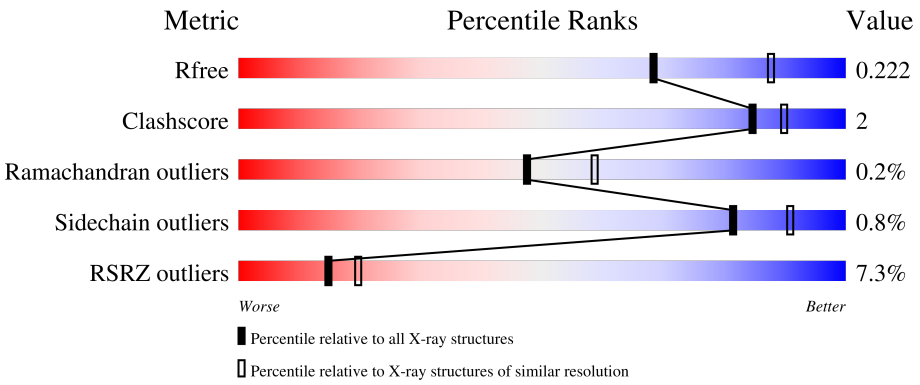
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	229	6% 74% . 24%
2	B	318	11% 95% . .
3	C	732	6% 95% 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	MCN	C	1732	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 9954 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 Aldehyde oxidoreductase iron-sulfur-binding subunit PaoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1272	781	226	252	13	0	0	0

- Molecule 2 is a protein called Aldehyde oxidoreductase FAD-binding subunit PaoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	316	2368	1490	432	438	8	0	0	0

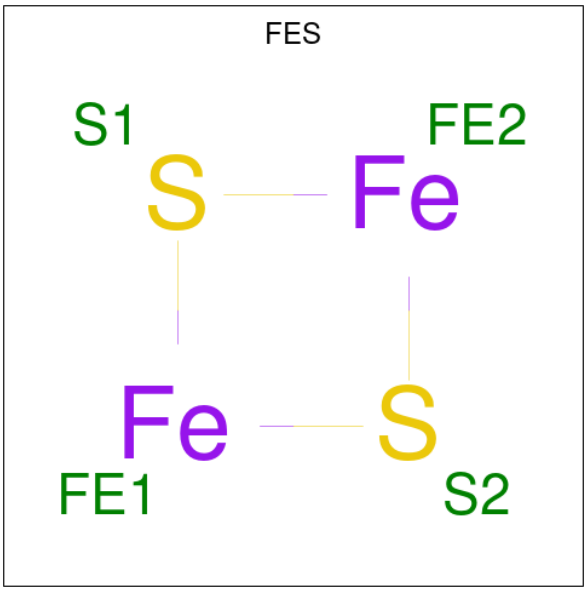
- Molecule 3 is a protein called Aldehyde oxidoreductase molybdenum-binding subunit PaoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	730	5488	3425	978	1059	26	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	VAL	ALA	conflict	UNP P77489
C	391	GLY	ASP	conflict	UNP P77489
C	440	HIS	ARG	engineered mutation	UNP P77489

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

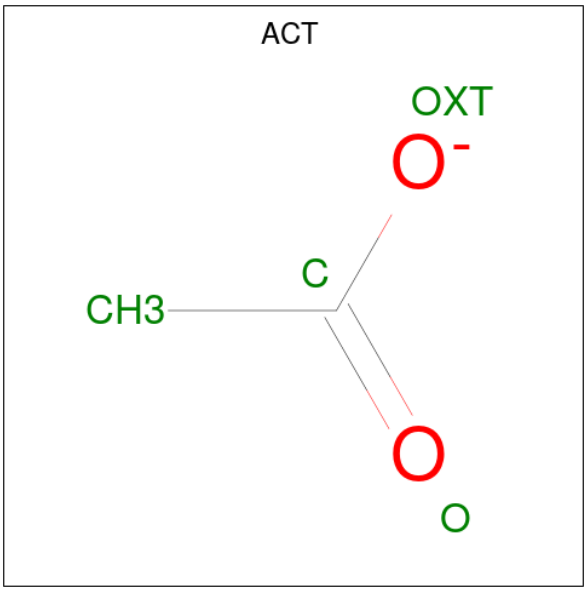


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	A	1	4	2	2	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
5	A	1	1	1	0	0
			Total	I		
5	B	3	3	3	0	0
			Total	I		
5	C	4	4	4	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

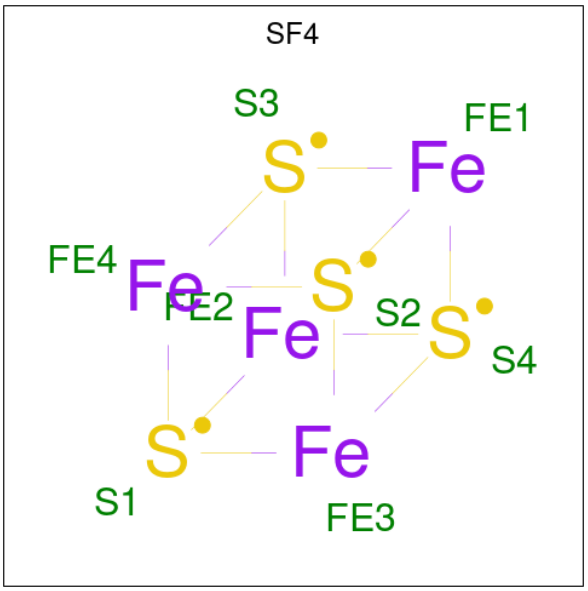


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	C	1	4	2	2	0	0
			Total	C	O		
6	C	1	4	2	2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

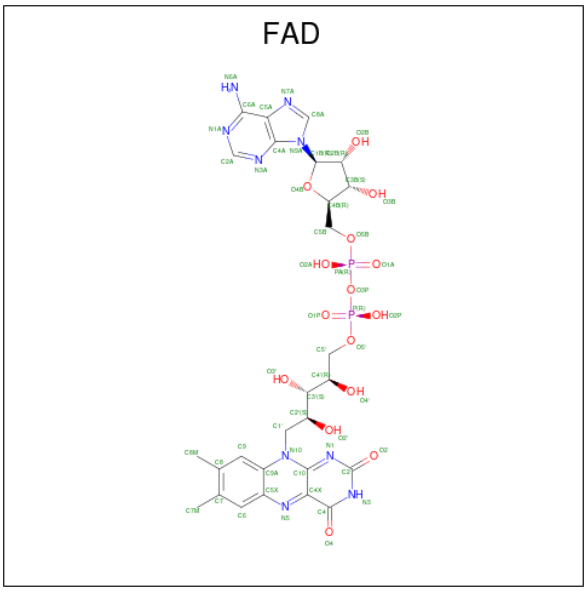
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	A	1	1	1	0	0
			Total	Cl		
7	B	3	3	3	0	0
			Total	Cl		
7	C	6	6	6	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



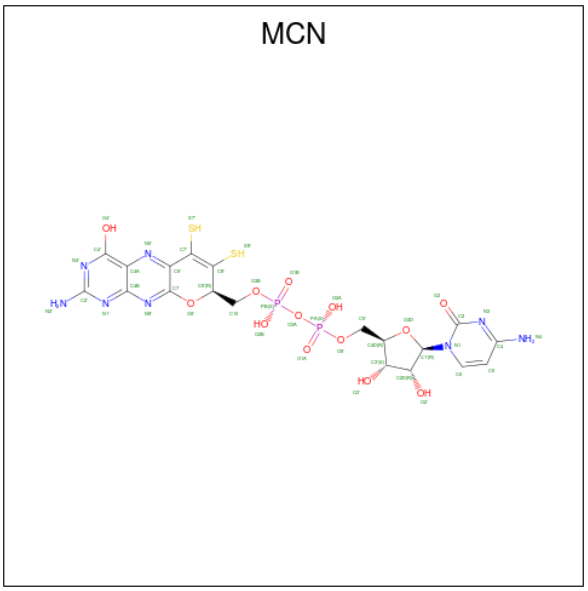
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



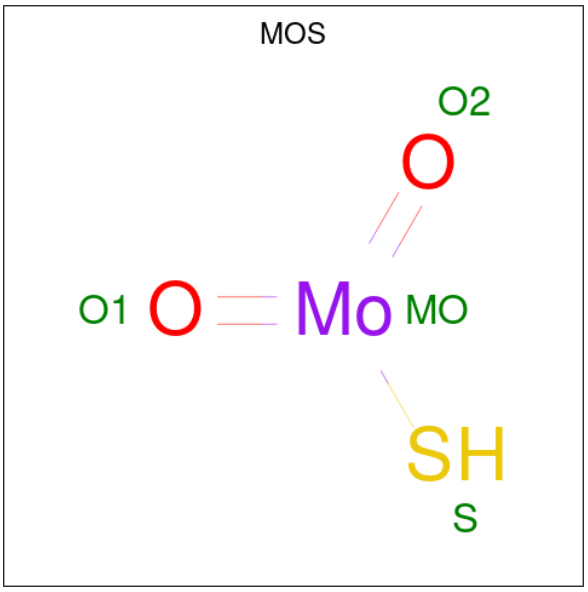
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	53	27	9	15	2	0	0

- Molecule 10 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).



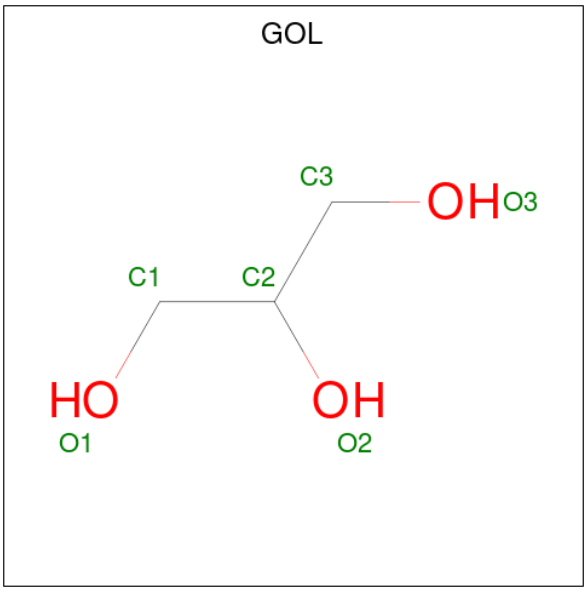
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
10	C	1	44	19	8	13	2	2	0	0

- Molecule 11 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Mo	O	S		
11	C	1	4	1	2	1	0	0

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	C	1	6	3	3	0	0
			Total	C	O		
12	C	1	6	3	3	0	0
			Total	C	O		
12	C	1	6	3	3	0	0

- Molecule 13 is water.

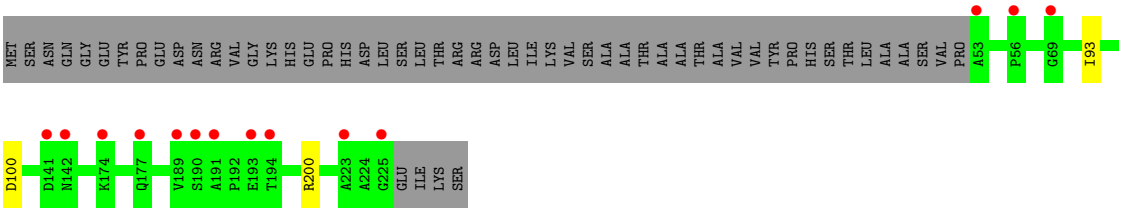
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	111	111	111	0	0
			Total	O		
13	B	155	155	155	0	0
			Total	O		
13	C	395	395	395	0	0

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.

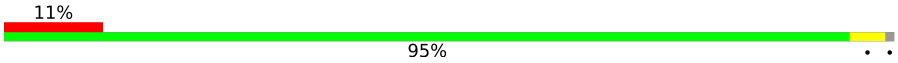
• Molecule 1: Aldehyde oxidoreductase iron-sulfur-binding subunit PaoA

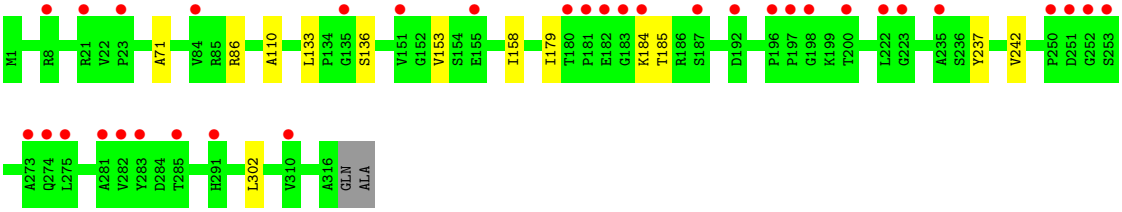
Chain A:



• Molecule 2: Aldehyde oxidoreductase FAD-binding subunit PaoB

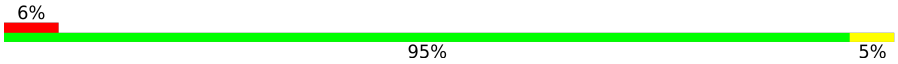
Chain B:

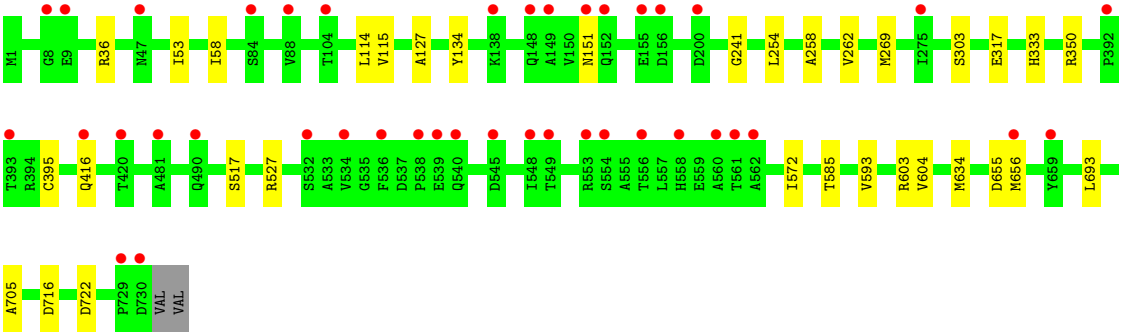




• Molecule 3: Aldehyde oxidoreductase molybdenum-binding subunit PaoC

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.84Å 78.26Å 151.73Å 90.00° 99.93° 90.00°	Depositor
Resolution (Å)	48.27 – 2.30 48.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.27-2.30) 98.0 (48.27-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.164 , 0.220 0.173 , 0.222	Depositor DCC
R_{free} test set	2811 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9954	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, MCN, IOD, ACT, SF4, FAD, CSD, MOS, CL, GOL

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	0.46	0/1288	0.74	2/1748 (0.1%)
2	B	0.43	0/2412	0.67	0/3281
3	C	0.47	0/5597	0.70	2/7602 (0.0%)
All	All	0.46	0/9297	0.70	4/12631 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	527	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	200	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	200	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	C	603	ARG	NE-CZ-NH1	5.11	122.85	120.30

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	1272	0	1263	1	0
2	B	2368	0	2413	5	0
3	C	5488	0	5435	16	0
4	A	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	3	0	0	0	0
5	C	4	0	0	1	0
6	A	4	0	3	0	0
6	C	8	0	6	1	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	6	0	0	0	0
8	B	8	0	0	0	0
9	B	53	0	31	0	0
10	C	44	0	11	22	0
11	C	4	0	0	0	0
12	C	18	0	24	1	0
13	A	111	0	0	0	0
13	B	155	0	0	0	0
13	C	395	0	0	0	0
All	All	9954	0	9186	43	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 (43) 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)
10:C:1732:MCN:C2D	10:C:1732:MCN:C1'	1.79	1.60
10:C:1732:MCN:C4D	10:C:1732:MCN:C3'	1.76	1.59
10:C:1732:MCN:C4A	10:C:1732:MCN:C4B	1.78	1.58
10:C:1732:MCN:N3	10:C:1732:MCN:C2	1.70	1.50
10:C:1732:MCN:C6'	10:C:1732:MCN:N5'	1.86	1.38
10:C:1732:MCN:C7'	10:C:1732:MCN:S7'	2.12	1.36
10:C:1732:MCN:C1'	10:C:1732:MCN:C3'	2.35	1.02
10:C:1732:MCN:C4B	10:C:1732:MCN:C4'	2.49	0.90
3:C:655:ASP:HB2	5:C:1734:IOD:I	2.42	0.90
10:C:1732:MCN:C2	10:C:1732:MCN:C4	2.53	0.86
10:C:1732:MCN:C3'	10:C:1732:MCN:O4D	2.29	0.81
10:C:1732:MCN:C4A	10:C:1732:MCN:N8'	2.46	0.77
10:C:1732:MCN:C2D	10:C:1732:MCN:O4D	2.35	0.74
10:C:1732:MCN:C4A	10:C:1732:MCN:C6'	2.68	0.71
3:C:269:MET:SD	6:C:1743:ACT:H3	2.31	0.70
10:C:1732:MCN:N5'	10:C:1732:MCN:C7'	2.56	0.68
10:C:1732:MCN:N5'	10:C:1732:MCN:C7	2.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1732:MCN:C6'	10:C:1732:MCN:S7'	2.84	0.64
10:C:1732:MCN:C2D	10:C:1732:MCN:C4D	2.63	0.61
10:C:1732:MCN:C4D	10:C:1732:MCN:O3'	2.45	0.61
3:C:114:LEU:HD22	3:C:254:LEU:HB3	1.88	0.55
3:C:317:GLU:HA	12:C:1745:GOL:H31	1.89	0.54
3:C:593:VAL:HG22	3:C:705:ALA:HB1	1.90	0.54
10:C:1732:MCN:C4A	10:C:1732:MCN:C7	2.88	0.51
2:B:153:VAL:HB	2:B:158:ILE:HG22	1.91	0.51
3:C:114:LEU:HD23	3:C:258:ALA:HB2	1.92	0.51
3:C:517:SER:HB3	3:C:572:ILE:HD13	1.93	0.51
3:C:58:ILE:HD13	3:C:134:TYR:HB3	1.93	0.51
2:B:71:ALA:HB1	2:B:110:ALA:HB2	1.93	0.50
10:C:1732:MCN:N3	10:C:1732:MCN:N1	2.50	0.49
10:C:1732:MCN:C4B	10:C:1732:MCN:N5'	2.62	0.48
3:C:722:ASP:OD1	3:C:722:ASP:N	2.45	0.47
3:C:585:THR:HB	3:C:693:LEU:HD22	1.97	0.47
3:C:258:ALA:O	3:C:262:VAL:HG22	2.16	0.46
10:C:1732:MCN:C2D	10:C:1732:MCN:N1	2.69	0.46
3:C:604:VAL:HG21	3:C:634[B]:MET:HG3	1.99	0.44
2:B:242:VAL:HG23	2:B:302:LEU:HD23	2.00	0.43
3:C:303:SER:HA	3:C:333:HIS:O	2.20	0.42
3:C:53:ILE:HD13	3:C:114:LEU:HD13	2.02	0.42
3:C:115:VAL:HG21	3:C:127:ALA:HA	2.01	0.42
2:B:133:LEU:HD22	2:B:136:SER:HB3	2.01	0.41
2:B:179:ILE:HG22	2:B:185:THR:HG22	2.02	0.41
1:A:93:ILE:HD11	3:C:36:ARG:HD3	2.03	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	171/229 (75%)	165 (96%)	6 (4%)	0	100	100
2	B	314/318 (99%)	308 (98%)	6 (2%)	0	100	100
3	C	730/732 (100%)	707 (97%)	21 (3%)	2 (0%)	41	50
All	All	1215/1279 (95%)	1180 (97%)	33 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
3	C	350	ARG

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	139/186 (75%)	138 (99%)	1 (1%)	84	92
2	B	243/244 (100%)	240 (99%)	3 (1%)	71	84
3	C	566/565 (100%)	562 (99%)	4 (1%)	84	92
All	All	948/995 (95%)	940 (99%)	8 (1%)	81	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
2	B	86	ARG
2	B	184	LYS
2	B	237	TYR
3	C	151	ASN
3	C	416	GLN
3	C	656	MET
3	C	716	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
2	B	126	ASN
3	C	42	HIS
3	C	281	HIS
3	C	550	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
3	CSD	C	395	3	3,7,8	0.92	0	1,8,10	2.55	1 (100%)

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
3	CSD	C	395	3	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	395	CSD	OD1-SG-CB	-2.55	100.68	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	395	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
12	GOL	C	1744	-	5,5,5	0.36	0	5,5,5	0.41	0
6	ACT	A	1229	-	3,3,3	0.79	0	3,3,3	0.61	0
6	ACT	C	1742	-	3,3,3	0.77	0	3,3,3	0.66	0
11	MOS	C	1733	3,10	0,3,3	-	-	-		
10	MCN	C	1732	11	41,48,48	9.91	29 (70%)	49,74,74	5.30	32 (65%)
4	FES	A	1226	1	0,4,4	-	-	-		
12	GOL	C	1745	-	5,5,5	0.34	0	5,5,5	0.53	0
8	SF4	B	1317	2	0,12,12	-	-	-		
6	ACT	C	1743	-	3,3,3	0.77	0	3,3,3	1.20	0
9	FAD	B	1318	-	53,58,58	1.97	15 (28%)	68,89,89	1.99	22 (32%)
12	GOL	C	1746	-	5,5,5	0.66	0	5,5,5	0.99	0
4	FES	A	1227	1	0,4,4	-	-	-		

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
12	GOL	C	1744	-	-	2/4/4/4	-
10	MCN	C	1732	11	-	3/22/54/54	0/5/5/5
4	FES	A	1226	1	-	-	0/1/1/1
12	GOL	C	1745	-	-	0/4/4/4	-
8	SF4	B	1317	2	-	-	0/6/5/5
9	FAD	B	1318	-	-	0/30/50/50	0/6/6/6
12	GOL	C	1746	-	-	3/4/4/4	-
4	FES	A	1227	1	-	-	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1732	MCN	C6'-N5'	37.47	1.86	1.32
10	C	1732	MCN	C10-C9'	-22.09	1.22	1.52
10	C	1732	MCN	C4A-C4B	21.53	1.78	1.40
10	C	1732	MCN	C2-N3	16.94	1.70	1.36
10	C	1732	MCN	C6'-C7	16.88	1.68	1.43
10	C	1732	MCN	O9'-C7	12.64	1.50	1.35
10	C	1732	MCN	C2-N1	11.33	1.64	1.40
10	C	1732	MCN	O2-C2	-10.10	1.05	1.23
10	C	1732	MCN	C3'-C4D	9.27	1.76	1.53
10	C	1732	MCN	C2D-C1'	8.21	1.79	1.53
10	C	1732	MCN	C4B-N8'	-7.90	1.21	1.36
10	C	1732	MCN	O9'-C9'	7.83	1.59	1.44
10	C	1732	MCN	C5'-C4D	-7.30	1.28	1.51
10	C	1732	MCN	C5-C4	7.18	1.59	1.42
10	C	1732	MCN	C2'-N2'	6.97	1.47	1.33
10	C	1732	MCN	O2'-C2D	-6.32	1.28	1.43
10	C	1732	MCN	C8'-C7'	-6.19	0.98	1.35
10	C	1732	MCN	O4D-C1'	-6.06	1.27	1.42
9	B	1318	FAD	C9A-C5X	5.83	1.50	1.41
10	C	1732	MCN	O5'-C5'	-4.99	1.25	1.44
9	B	1318	FAD	C5X-N5	-4.81	1.30	1.39
10	C	1732	MCN	C4-N3	4.71	1.44	1.34
10	C	1732	MCN	PB-O1B	-4.05	1.36	1.50
10	C	1732	MCN	C4B-N1'	4.05	1.44	1.36
10	C	1732	MCN	C6-C5	3.87	1.44	1.35
9	B	1318	FAD	C4A-N3A	-3.49	1.30	1.35
9	B	1318	FAD	C2-N1	-3.46	1.28	1.36
10	C	1732	MCN	C2'-N3'	3.43	1.41	1.35
9	B	1318	FAD	C4-N3	-3.41	1.32	1.38
10	C	1732	MCN	C4-N4	-3.26	1.26	1.33
9	B	1318	FAD	PA-O2A	-3.21	1.40	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1732	MCN	C3'-C2D	-3.07	1.44	1.53
9	B	1318	FAD	O4'-C4'	-2.91	1.37	1.43
9	B	1318	FAD	P-O1P	-2.76	1.41	1.50
9	B	1318	FAD	C8-C7	2.71	1.47	1.40
10	C	1732	MCN	PA-O1A	2.69	1.60	1.50
10	C	1732	MCN	O3B-C10	2.61	1.54	1.44
9	B	1318	FAD	PA-O1A	-2.59	1.41	1.50
9	B	1318	FAD	O4-C4	-2.42	1.19	1.23
9	B	1318	FAD	C5A-N7A	-2.32	1.31	1.39
9	B	1318	FAD	P-O2P	-2.29	1.44	1.55
9	B	1318	FAD	C2-N3	-2.23	1.33	1.39
10	C	1732	MCN	O3'-C3'	-2.12	1.38	1.43
9	B	1318	FAD	C6-C5X	-2.04	1.36	1.40

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1732	MCN	C7-N8'-C4B	13.60	128.18	116.61
10	C	1732	MCN	C5-C4-N3	-12.67	99.77	121.33
10	C	1732	MCN	N1-C2-N3	-12.12	96.74	118.81
10	C	1732	MCN	N2'-C2'-N1'	-9.69	101.99	117.79
10	C	1732	MCN	C5-C4-N4	-8.37	107.39	120.57
10	C	1732	MCN	C4-N3-C2	-7.94	107.44	120.25
10	C	1732	MCN	C4B-C4A-N5'	-7.56	113.29	122.41
10	C	1732	MCN	O2-C2-N3	-7.48	110.16	122.33
10	C	1732	MCN	C4D-O4D-C1'	7.47	125.97	109.47
10	C	1732	MCN	C4A-C4B-N8'	-7.45	109.64	121.71
10	C	1732	MCN	O4'-C4'-C4A	-7.40	105.81	119.67
10	C	1732	MCN	O4D-C4D-C3'	-7.24	90.79	105.11
10	C	1732	MCN	N1'-C2'-N3'	-7.07	117.79	127.22
10	C	1732	MCN	N4-C4-N3	-6.41	106.72	117.97
9	B	1318	FAD	C10-N1-C2	5.15	127.19	116.90
10	C	1732	MCN	O4D-C1'-N1	5.04	119.88	108.36
10	C	1732	MCN	C3'-C2D-C1'	-4.75	92.40	101.43
9	B	1318	FAD	C4-C4X-N5	4.57	124.73	118.23
9	B	1318	FAD	C4A-C5A-N7A	-4.36	104.86	109.40
10	C	1732	MCN	N2'-C2'-N3'	-4.28	110.60	117.25
9	B	1318	FAD	O2-C2-N1	-4.09	115.05	121.83
10	C	1732	MCN	C4A-C4B-N1'	-3.84	115.49	121.71
10	C	1732	MCN	C2D-C3'-C4D	3.75	109.93	102.64
9	B	1318	FAD	O2-C2-N3	3.66	125.76	118.65
10	C	1732	MCN	O2'-C2D-C3'	3.59	123.43	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1318	FAD	O4-C4-C4X	-3.57	117.14	126.60
10	C	1732	MCN	O5'-C5'-C4D	3.55	121.21	108.99
10	C	1732	MCN	C5'-C4D-C3'	3.54	128.46	115.18
10	C	1732	MCN	O4D-C1'-C2D	-3.53	98.95	106.64
9	B	1318	FAD	N3A-C2A-N1A	-3.48	123.24	128.68
10	C	1732	MCN	C1'-N1-C6	3.31	128.07	120.84
9	B	1318	FAD	C4X-C10-N10	3.30	121.30	116.48
10	C	1732	MCN	O3'-C3'-C2D	3.25	122.33	111.82
10	C	1732	MCN	O2A-PA-O1A	3.25	128.29	112.24
10	C	1732	MCN	O3'-C3'-C4D	-3.14	101.96	111.05
9	B	1318	FAD	C4X-C4-N3	2.99	120.79	113.19
9	B	1318	FAD	C4X-C10-N1	-2.88	118.05	124.73
9	B	1318	FAD	C1B-N9A-C4A	-2.81	121.71	126.64
9	B	1318	FAD	C9A-N10-C10	-2.66	116.62	120.77
9	B	1318	FAD	C1'-N10-C9A	2.65	124.93	120.51
9	B	1318	FAD	C5'-C4'-C3'	2.60	117.22	112.20
9	B	1318	FAD	O3B-C3B-C2B	2.55	120.08	111.82
10	C	1732	MCN	C1'-N1-C2	-2.50	112.84	118.42
9	B	1318	FAD	C2A-N1A-C6A	2.46	122.96	118.75
9	B	1318	FAD	C5A-C6A-N6A	2.42	124.04	120.35
9	B	1318	FAD	C4-N3-C2	-2.37	121.26	125.64
9	B	1318	FAD	O4'-C4'-C3'	-2.32	103.46	109.10
10	C	1732	MCN	O3B-PB-O1B	2.31	118.08	109.07
9	B	1318	FAD	C4'-C3'-C2'	2.29	118.12	113.36
9	B	1318	FAD	O2P-P-O1P	2.18	123.03	112.24
9	B	1318	FAD	O2'-C2'-C3'	2.09	114.18	109.10
10	C	1732	MCN	C6'-N5'-C4A	-2.09	112.92	117.26
10	C	1732	MCN	PB-O3A-PA	-2.08	125.68	132.83
10	C	1732	MCN	O4D-C4D-C5'	-2.08	102.53	109.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	1744	GOL	O1-C1-C2-C3
12	C	1746	GOL	C1-C2-C3-O3
10	C	1732	MCN	C3'-C4D-C5'-O5'
10	C	1732	MCN	O4D-C4D-C5'-O5'
12	C	1744	GOL	O1-C1-C2-O2
10	C	1732	MCN	C9'-C10-O3B-PB
12	C	1746	GOL	O2-C2-C3-O3
12	C	1746	GOL	O1-C1-C2-C3

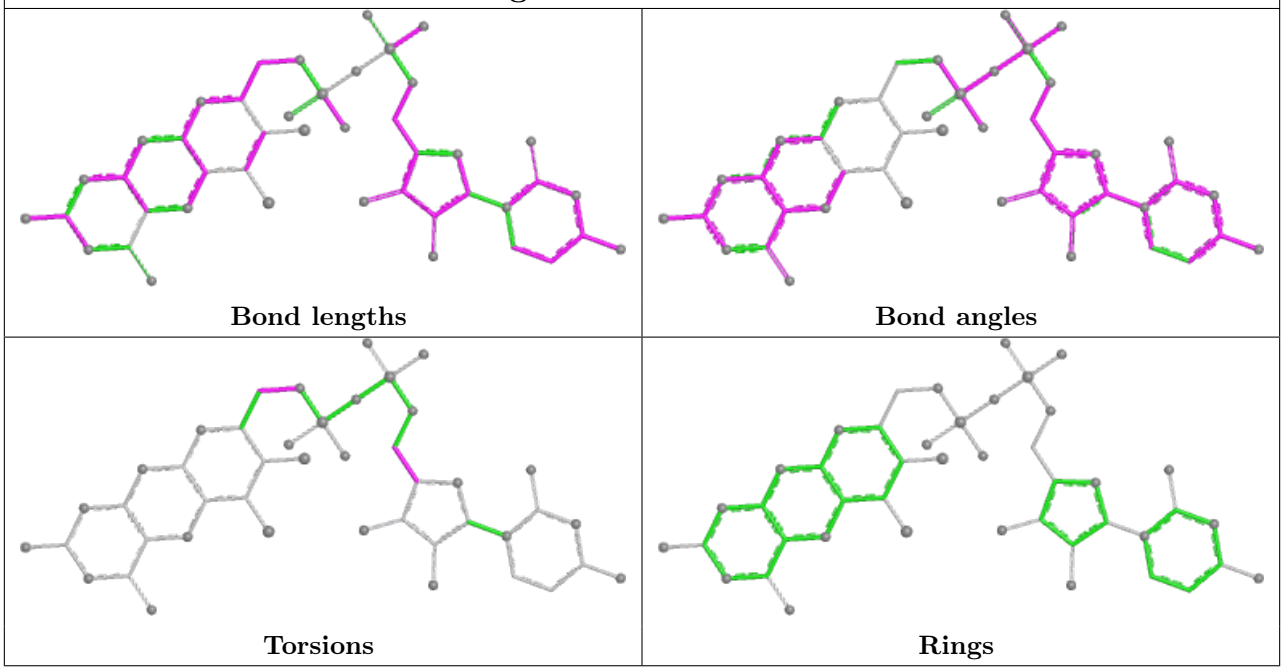
There are no ring outliers.

3 monomers are involved in 24 short contacts:

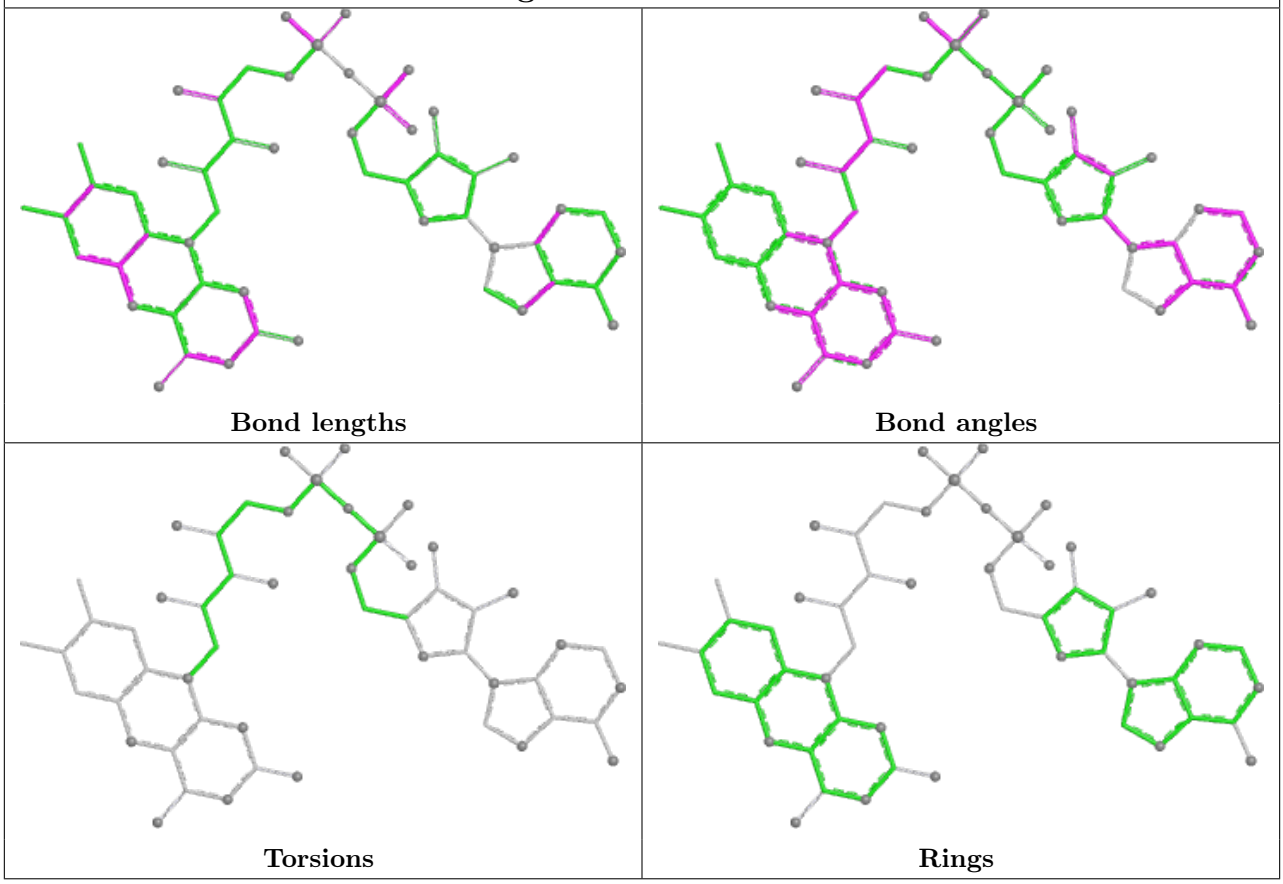
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1732	MCN	22	0
12	C	1745	GOL	1	0
6	C	1743	ACT	1	0

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 MCN C 1732



Ligand FAD B 1318



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	173/229 (75%)	0.74	14 (8%)	12	16	16, 25, 40, 54	0
2	B	316/318 (99%)	0.69	34 (10%)	5	8	18, 29, 45, 68	0
3	C	729/732 (99%)	0.51	41 (5%)	24	30	14, 23, 42, 71	0
All	All	1218/1279 (95%)	0.59	89 (7%)	15	20	14, 25, 43, 71	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	GLY	5.1
3	C	554	SER	4.6
3	C	553	ARG	4.5
3	C	151	ASN	4.4
2	B	181	PRO	4.4
3	C	148	GLN	4.3
2	B	183	GLY	4.3
3	C	556	THR	4.0
2	B	291	HIS	3.9
2	B	21	ARG	3.8
2	B	198	GLY	3.7
3	C	420	THR	3.7
2	B	250	PRO	3.7
2	B	182	GLU	3.7
1	A	189	VAL	3.7
3	C	656	MET	3.7
2	B	135	GLY	3.5
3	C	155	GLU	3.5
2	B	23	PRO	3.5
2	B	180	THR	3.4
3	C	540	GLN	3.2
3	C	539	GLU	3.2
1	A	191	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	549	THR	3.1
2	B	282	VAL	3.1
3	C	729	PRO	3.0
3	C	156	ASP	3.0
3	C	393	THR	2.9
3	C	558	HIS	2.9
2	B	196	PRO	2.9
1	A	223	ALA	2.9
2	B	200	THR	2.9
3	C	88	VAL	2.9
2	B	197	PRO	2.8
2	B	184	LYS	2.8
3	C	730	ASP	2.8
2	B	187	SER	2.8
3	C	200	ASP	2.7
2	B	151	VAL	2.7
3	C	152	GLN	2.7
3	C	562	ALA	2.7
2	B	222	LEU	2.7
2	B	223	GLY	2.7
2	B	285	THR	2.7
1	A	190	SER	2.6
2	B	275	LEU	2.6
3	C	561	THR	2.6
1	A	53	ALA	2.6
2	B	251	ASP	2.6
1	A	225	GLY	2.6
3	C	538	PRO	2.5
2	B	192	ASP	2.5
1	A	177	GLN	2.5
3	C	8	GLY	2.5
2	B	253	SER	2.5
1	A	174	LYS	2.4
1	A	142	ASN	2.4
3	C	138	LYS	2.4
2	B	155	GLU	2.4
1	A	56	PRO	2.4
3	C	149	ALA	2.4
2	B	310	VAL	2.3
3	C	47[A]	ASN	2.3
3	C	560	ALA	2.3
3	C	104	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	281	ALA	2.3
1	A	141	ASP	2.2
3	C	532	SER	2.2
2	B	235	ALA	2.2
3	C	416	GLN	2.2
2	B	252	GLY	2.2
2	B	273	ALA	2.2
3	C	545	ASP	2.1
2	B	274	GLN	2.1
3	C	9[A]	GLU	2.1
3	C	534	VAL	2.1
3	C	392	PRO	2.1
2	B	283	TYR	2.1
3	C	659	TYR	2.1
3	C	536	PHE	2.1
1	A	193	GLU	2.0
3	C	275	ILE	2.0
2	B	84	VAL	2.0
2	B	8	ARG	2.0
3	C	84	SER	2.0
3	C	481	ALA	2.0
3	C	548	ILE	2.0
3	C	490	GLN	2.0
1	A	194	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	CSD	C	395	8/9	0.86	0.24	24,28,39,39	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

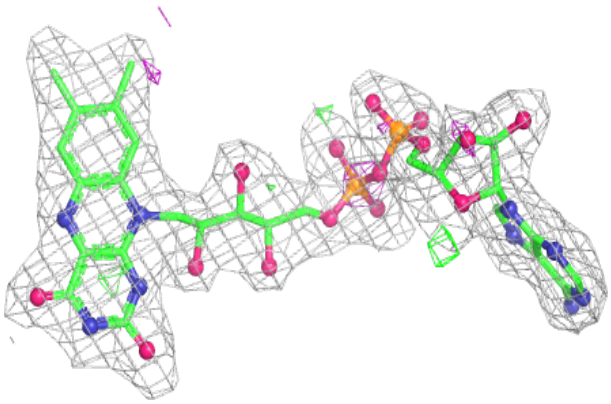
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

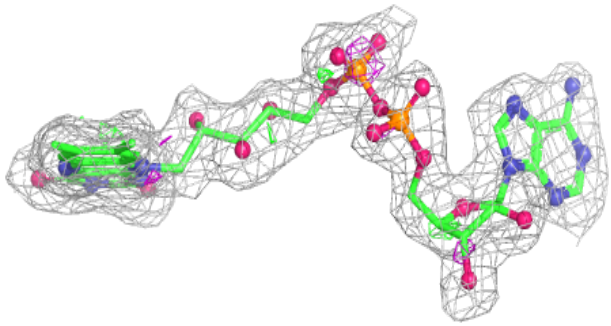
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ACT	A	1229	4/4	0.59	0.21	46,47,48,49	0
12	GOL	C	1745	6/6	0.76	0.26	47,50,53,55	0
12	GOL	C	1744	6/6	0.77	0.28	41,44,46,46	0
6	ACT	C	1742	4/4	0.79	0.23	51,54,55,56	0
7	CL	C	1738	1/1	0.87	0.13	43,43,43,43	0
12	GOL	C	1746	6/6	0.87	0.21	43,45,47,47	0
11	MOS	C	1733	4/4	0.89	0.23	11,14,15,16	1
7	CL	B	1322	1/1	0.89	0.11	50,50,50,50	0
9	FAD	B	1318	53/53	0.91	0.16	15,18,24,25	0
7	CL	C	1740	1/1	0.93	0.12	37,37,37,37	0
6	ACT	C	1743	4/4	0.93	0.29	16,18,18,22	0
8	SF4	B	1317	8/8	0.94	0.09	25,27,30,30	0
7	CL	C	1747	1/1	0.94	0.09	48,48,48,48	0
7	CL	C	1748	1/1	0.94	0.19	26,26,26,26	0
4	FES	A	1227	4/4	0.95	0.08	13,14,15,17	0
10	MCN	C	1732	44/44	0.95	0.14	10,13,16,17	0
4	FES	A	1226	4/4	0.95	0.11	15,17,18,21	0
7	CL	A	1230	1/1	0.97	0.16	10,10,10,10	0
7	CL	C	1739	1/1	0.97	0.08	33,33,33,33	0
5	IOD	B	1320	1/1	0.97	0.06	54,54,54,54	1
7	CL	B	1324	1/1	0.97	0.08	37,37,37,37	0
5	IOD	B	1323	1/1	0.98	0.04	37,37,37,37	1
5	IOD	C	1735	1/1	0.98	0.08	29,29,29,29	1
5	IOD	C	1737	1/1	0.98	0.06	35,35,35,35	1
7	CL	C	1741	1/1	0.99	0.16	22,22,22,22	0
5	IOD	B	1319	1/1	0.99	0.06	36,36,36,36	1
5	IOD	C	1734	1/1	0.99	0.15	33,33,33,33	1
7	CL	B	1321	1/1	0.99	0.20	21,21,21,21	0
5	IOD	A	1228	1/1	0.99	0.12	25,25,25,25	1
5	IOD	C	1736	1/1	1.00	0.06	37,37,37,37	1

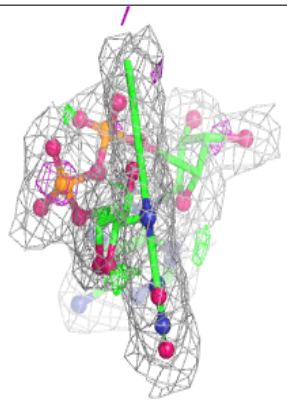
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1318:

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

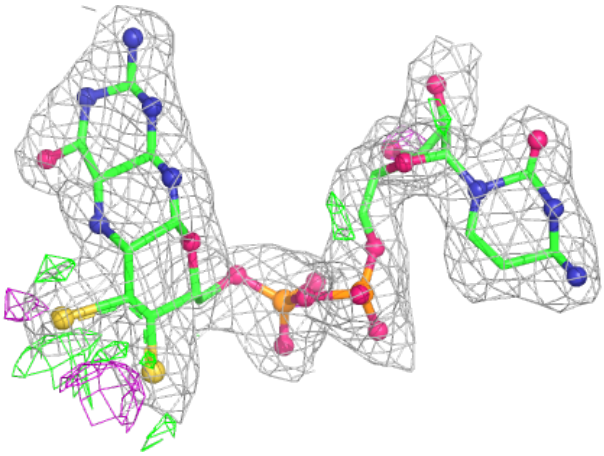


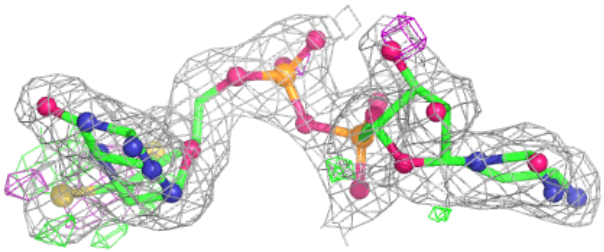


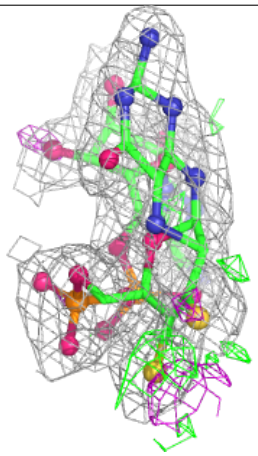


Electron density around MCN C 1732:

$2mF_o$-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.