



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:10 AM BST

PDB ID : 5Y6Q
Title : Crystal structure of an aldehyde oxidase from *Methylobacillus* sp. KY4400
Authors : Mikami, B.; Uchida, H.
Deposited on : 2017-08-13
Resolution : 2.50 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 ⓘ symbol.

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

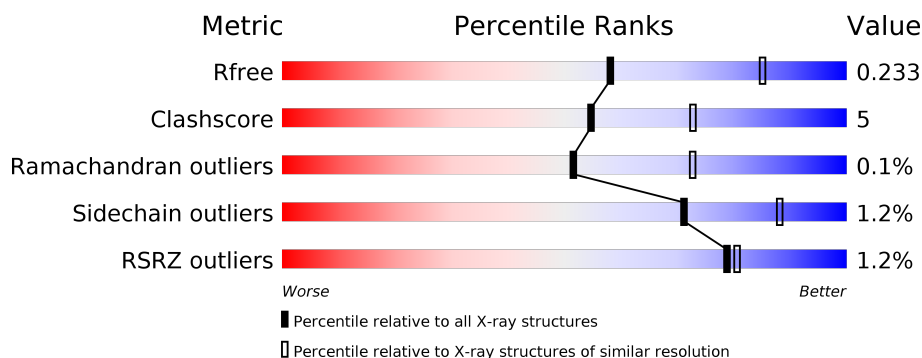
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	162	<div> <div>83%</div> <div>14%</div> <div>.</div> </div>
2	B	330	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
3	C	775	<div> <div>%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>

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
5	SO4	C	808	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10044 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 oxidase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	1	0
			1170	715	207	233	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ARG	PRO	see sequence details	UNP Q84IY0

- Molecule 2 is a protein called Aldehyde oxidase medium subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2500	1557	454	477	12			

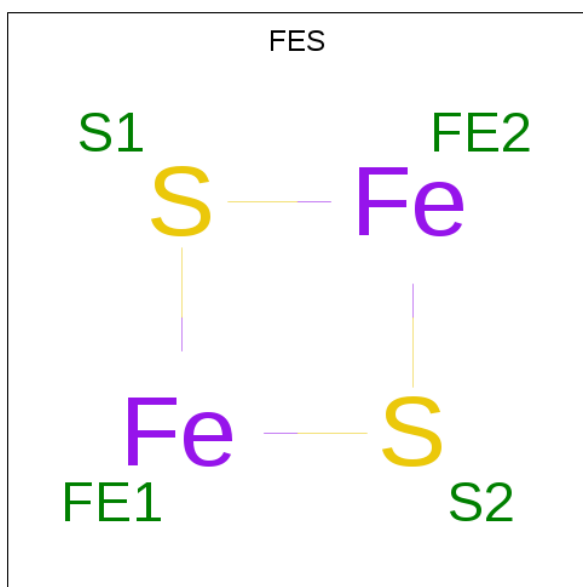
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	PHE	SER	see sequence details	UNP Q84IX9
B	239	TYR	ASN	see sequence details	UNP Q84IX9
B	262	ILE	VAL	see sequence details	UNP Q84IX9
B	270	LYS	GLU	see sequence details	UNP Q84IX9
B	293	GLN	ARG	see sequence details	UNP Q84IX9
B	294	ALA	PRO	see sequence details	UNP Q84IX9

- Molecule 3 is a protein called Aldehyde oxidase large subunit.

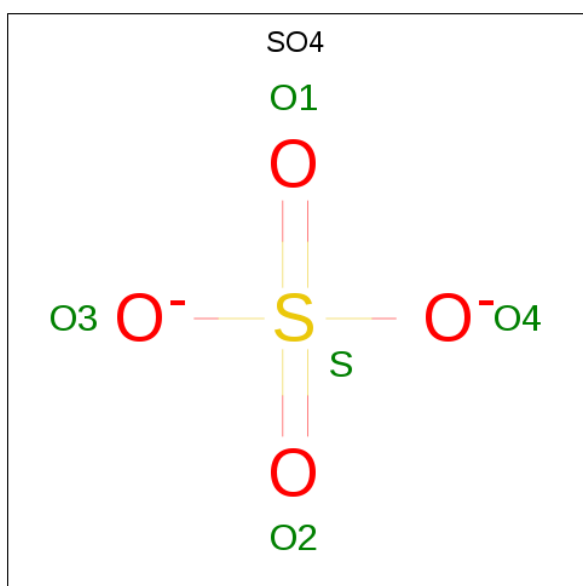
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	748	Total	C	N	O	S	0	0	0
			5646	3537	1003	1085	21			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



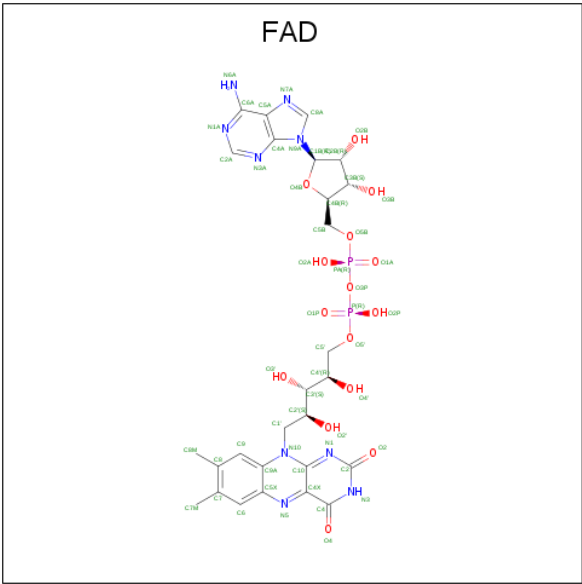
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

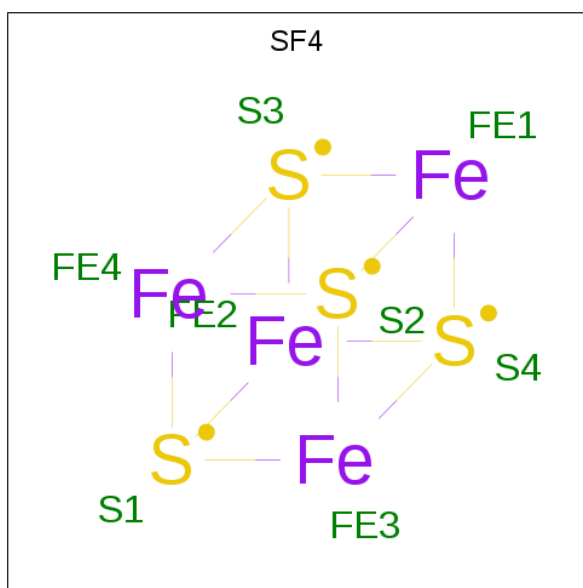
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



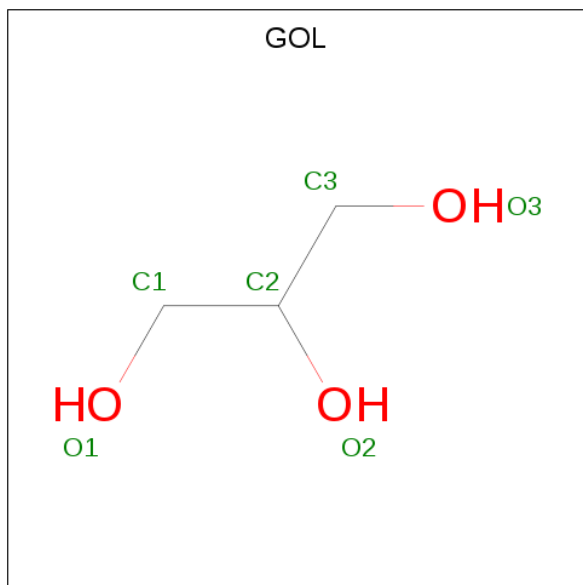
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



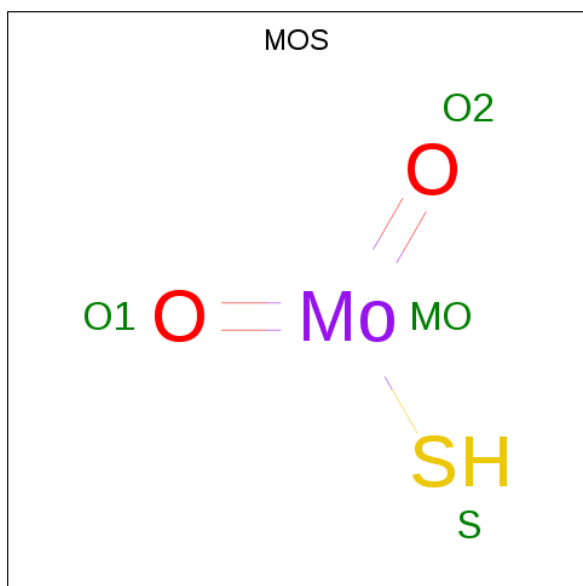
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

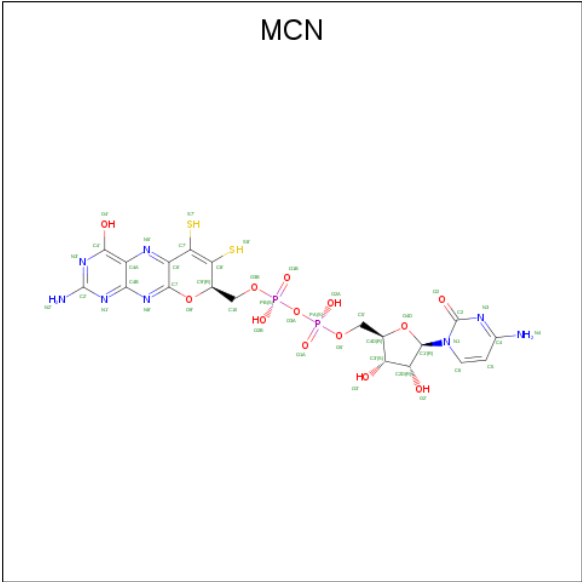
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DIOXOTHIO MOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO_2S).



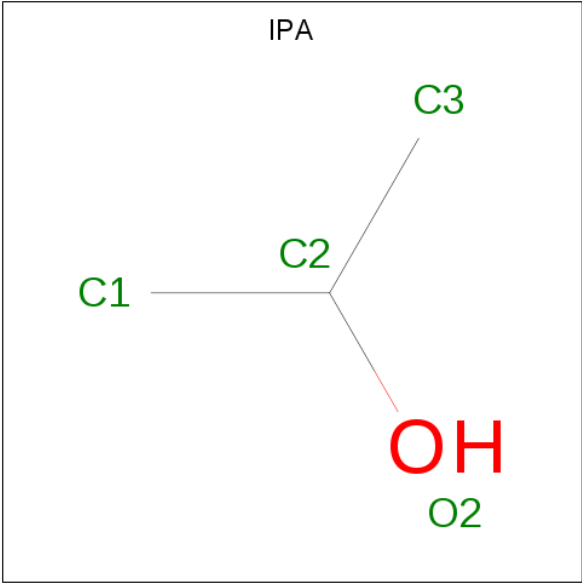
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 10 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $\text{C}_{19}\text{H}_{22}\text{N}_8\text{O}_{13}\text{P}_2\text{S}_2$).



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

- Molecule 11 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	C	1	4	3	1	0	0
11	C	1	Total	C	O	0	0
			4	3	1		


- Molecule 12 is water.

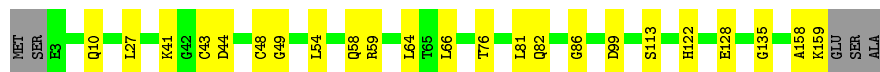
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	56	Total 56	O 56	0	0
12	B	111	Total 111	O 111	0	0
12	C	340	Total 340	O 340	0	0

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.

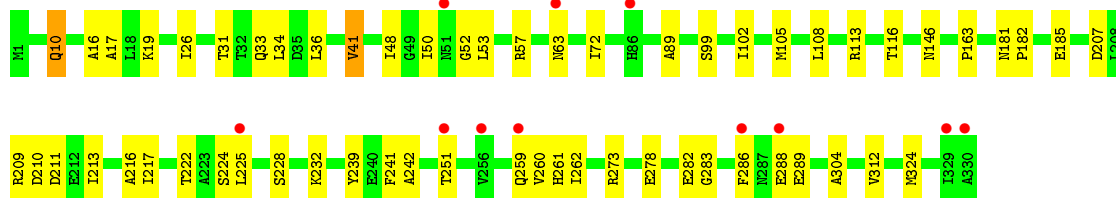
- Molecule 1: Aldehyde oxidase small subunit

Chain A: 




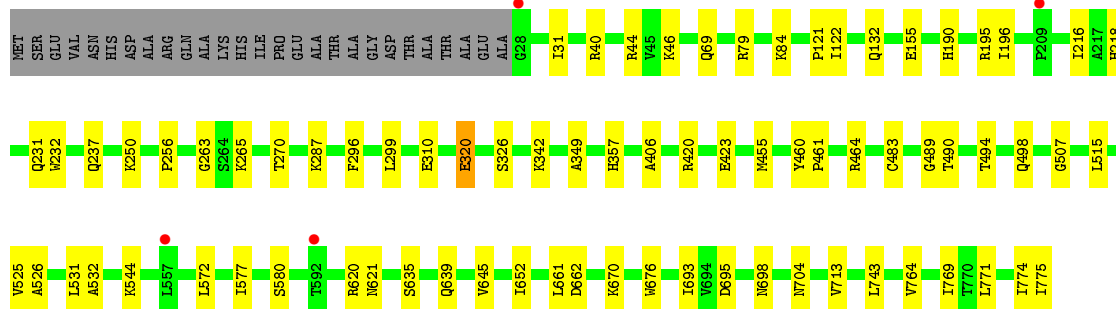
- Molecule 2: Aldehyde oxidase medium subunit

Chain B: 



- Molecule 3: Aldehyde oxidase large subunit

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.97Å 77.97Å 400.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.50 48.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.12-2.50) 99.1 (48.29-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.178 , 0.233 0.178 , 0.233	Depositor DCC
R_{free} test set	2210 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10044	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IPA, MCN, MOS, SF4, SO4, 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	0/1188	0.51	0/1605
2	B	0.32	0/2547	0.50	0/3459
3	C	0.32	0/5757	0.53	0/7830
All	All	0.32	0/9492	0.52	0/12894

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	1170	0	1137	17	0
2	B	2500	0	2459	39	2
3	C	5646	0	5621	46	2
4	A	8	0	0	0	0
5	A	5	0	0	1	0
5	B	15	0	0	1	0
5	C	40	0	0	4	0
6	B	53	0	31	1	0
7	B	8	0	0	0	0
8	B	12	0	16	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	24	0	32	4	0
9	C	4	0	0	1	0
10	C	44	0	18	3	0
11	C	8	0	16	1	0
12	A	56	0	0	2	0
12	B	111	0	0	1	0
12	C	340	0	0	1	0
All	All	10044	0	9330	98	2

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 5.

All (98) 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)
3:C:544:LYS:NZ	5:C:808:SO4:S	2.33	1.01
2:B:273:ARG:NE	2:B:278:GLU:OE2	1.99	0.96
3:C:544:LYS:NZ	5:C:808:SO4:O4	2.01	0.93
2:B:259:GLN:N	2:B:282:GLU:OE2	2.03	0.90
3:C:544:LYS:NZ	5:C:808:SO4:O1	2.12	0.83
2:B:19:LYS:NZ	2:B:210:ASP:O	2.12	0.82
1:A:82:GLN:HB3	1:A:86:GLY:HA2	1.71	0.70
2:B:19:LYS:NZ	2:B:210:ASP:HA	2.08	0.69
2:B:273:ARG:HE	2:B:278:GLU:CD	1.98	0.66
2:B:222:THR:HG23	2:B:225:LEU:H	1.60	0.66
1:A:59:ARG:NH1	1:A:113:SER:OG	2.29	0.64
3:C:620:ARG:HH21	8:C:811:GOL:H31	1.63	0.63
3:C:320:GLU:OE1	12:C:901:HOH:O	2.16	0.63
2:B:224:SER:N	2:B:251:THR:HG22	2.14	0.61
2:B:207:ASP:OD1	2:B:209:ARG:NH2	2.28	0.59
3:C:231:GLN:HE22	3:C:263:GLY:H	1.50	0.59
3:C:342:LYS:HE2	8:C:814:GOL:H11	1.85	0.59
1:A:58:GLN:NE2	12:A:304:HOH:O	2.31	0.58
1:A:27:LEU:HD21	1:A:41:LYS:HB2	1.85	0.58
1:A:64:LEU:HD13	2:B:31:THR:HA	1.85	0.58
2:B:113:ARG:NH2	5:B:403:SO4:O3	2.21	0.57
3:C:195:ARG:NH2	5:C:807:SO4:O2	2.39	0.56
3:C:232:TRP:HB2	3:C:525:VAL:HG23	1.86	0.56
3:C:326:SER:HG	3:C:357:HIS:HD1	1.50	0.56
2:B:163:PRO:HB2	2:B:241:PHE:CD2	2.41	0.56
1:A:54:LEU:HB2	1:A:76:THR:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ILE:HA	2:B:105:MET:HE3	1.88	0.55
1:A:48:CYS:SG	1:A:49:GLY:N	2.81	0.54
2:B:181:ASN:HD21	2:B:185:GLU:HG3	1.73	0.54
2:B:52:GLY:H	2:B:57:ARG:HH11	1.56	0.54
2:B:19:LYS:HZ3	2:B:210:ASP:HA	1.71	0.54
2:B:89:ALA:HB2	2:B:228:SER:HB2	1.90	0.53
3:C:190:HIS:HA	3:C:195:ARG:HH21	1.74	0.53
1:A:122:HIS:HA	1:A:128:GLU:OE2	2.09	0.53
10:C:802:MCN:H6	10:C:802:MCN:O5'	2.09	0.53
3:C:490:THR:HG21	10:C:802:MCN:H102	1.92	0.52
1:A:99:ASP:HB2	3:C:670:LYS:HD3	1.92	0.52
3:C:216:ILE:HG12	3:C:287:LYS:HG2	1.92	0.52
2:B:19:LYS:HZ1	2:B:210:ASP:HA	1.74	0.52
2:B:19:LYS:NZ	2:B:210:ASP:C	2.63	0.51
2:B:19:LYS:NZ	2:B:210:ASP:CA	2.73	0.51
2:B:216:ALA:O	2:B:217:ILE:HD13	2.10	0.51
2:B:283:GLY:O	12:B:501:HOH:O	2.19	0.51
2:B:262:ILE:O	2:B:273:ARG:HD2	2.11	0.50
1:A:99:ASP:OD2	3:C:40:ARG:NH1	2.44	0.50
1:A:66:LEU:HG	2:B:34:LEU:HD11	1.92	0.50
3:C:774:ILE:O	3:C:775:ILE:HG12	2.12	0.49
3:C:69:GLN:HA	3:C:132:GLN:O	2.13	0.49
2:B:288:GLU:HG3	2:B:289:GLU:H	1.79	0.48
8:B:407:GOL:H31	3:C:771:LEU:HG	1.95	0.48
3:C:532:ALA:HB2	10:C:802:MCN:H3'	1.96	0.48
2:B:116:THR:HA	2:B:163:PRO:HD3	1.95	0.47
3:C:526:ALA:HB2	3:C:531:LEU:HD22	1.96	0.47
3:C:31:ILE:HA	3:C:507:GLY:HA2	1.97	0.47
2:B:213:ILE:HD13	2:B:213:ILE:HA	1.76	0.47
3:C:79:ARG:HB3	3:C:155:GLU:HB2	1.96	0.47
3:C:460:TYR:CG	3:C:461:PRO:HD2	2.50	0.47
3:C:645:VAL:HG22	3:C:652:ILE:HG12	1.97	0.47
2:B:33:GLN:HE21	6:B:401:FAD:H3B	1.80	0.46
2:B:16:ALA:HB1	2:B:211:ASP:O	2.16	0.46
2:B:259:GLN:O	2:B:261:HIS:HD2	1.99	0.46
3:C:483:CYS:O	3:C:515:LEU:HA	2.15	0.45
3:C:420:ARG:HB2	3:C:662:ASP:HB2	1.99	0.45
3:C:423:GLU:OE2	3:C:423:GLU:N	2.43	0.45
2:B:17:ALA:HB2	2:B:182:PRO:HB3	1.97	0.45
3:C:661:LEU:HD13	3:C:676:TRP:CD2	2.51	0.45
3:C:635:SER:HB3	3:C:743:LEU:HD22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ILE:HD13	2:B:48:ILE:HB	1.98	0.44
2:B:36:LEU:HB3	2:B:41:VAL:HG22	1.99	0.44
3:C:693:ILE:HG21	11:C:815:IPA:H32	2.00	0.44
1:A:135:GLY:HA3	2:B:99:SER:HB2	2.00	0.44
1:A:10:GLN:HG2	12:A:348:HOH:O	2.17	0.43
1:A:43:CYS:SG	1:A:44:ASP:N	2.91	0.43
3:C:196:ILE:O	3:C:310:GLU:HA	2.18	0.43
3:C:40:ARG:NH2	3:C:489:GLY:O	2.50	0.43
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.88	0.43
2:B:232:LYS:HG3	2:B:242:ALA:HB2	1.99	0.43
3:C:455:MET:HA	3:C:639:GLN:O	2.17	0.43
2:B:304:ALA:HB2	2:B:312:VAL:HG21	2.01	0.43
3:C:256:PRO:HB3	8:C:813:GOL:H11	2.01	0.43
3:C:237:GLN:OE1	8:C:811:GOL:H32	2.19	0.42
3:C:296:PHE:CD1	3:C:704:ASN:HB2	2.54	0.42
2:B:286:PHE:CZ	2:B:324:MET:HA	2.55	0.42
3:C:572:LEU:HD13	3:C:577:ILE:HG12	2.01	0.42
3:C:695:ASP:HB3	3:C:698:ASN:OD1	2.19	0.41
2:B:182:PRO:HD3	2:B:211:ASP:O	2.20	0.41
3:C:121:PRO:HG3	3:C:270:THR:HB	2.02	0.41
3:C:764:VAL:HG21	3:C:769:ILE:HG23	2.03	0.41
3:C:494:THR:O	3:C:498:GLN:HG3	2.20	0.41
3:C:250:LYS:HD3	3:C:250:LYS:HA	1.86	0.41
3:C:231:GLN:HG3	3:C:265:LYS:O	2.21	0.41
3:C:263:GLY:HA2	9:C:801:MOS:O1	2.20	0.41
5:A:203:SO4:O3	3:C:44:ARG:NH1	2.53	0.41
2:B:72:ILE:O	2:B:108:LEU:HG	2.21	0.40
3:C:349:ALA:HB2	3:C:406:ALA:HA	2.01	0.40
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.87	0.40
1:A:158:ALA:HB3	1:A:159:LYS:HE2	2.02	0.40
2:B:50:ILE:O	2:B:53:LEU:HG	2.21	0.40

All (2) 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)
2:B:260:VAL:O	3:C:84:LYS:NZ[7_545]	2.08	0.12
2:B:10:GLN:OE1	3:C:580:SER:OG[6_544]	2.09	0.11

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	156/162 (96%)	150 (96%)	6 (4%)	0	100	100
2	B	328/330 (99%)	317 (97%)	11 (3%)	0	100	100
3	C	746/775 (96%)	735 (98%)	10 (1%)	1 (0%)	51	73
All	All	1230/1267 (97%)	1202 (98%)	27 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	122	ILE

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	126/129 (98%)	126 (100%)	0	100	100
2	B	258/258 (100%)	253 (98%)	5 (2%)	57	80
3	C	590/609 (97%)	583 (99%)	7 (1%)	71	88
All	All	974/996 (98%)	962 (99%)	12 (1%)	71	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	GLN
2	B	41	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	63	ASN
2	B	146	ASN
2	B	239	TYR
3	C	46	LYS
3	C	218	HIS
3	C	299	LEU
3	C	320	GLU
3	C	464	ARG
3	C	621	ASN
3	C	713	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	GLN
2	B	33	GLN
2	B	287	ASN
3	C	231	GLN

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 ⓘ

26 ligands are 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
11	IPA	C	816	-	3,3,3	0.53	0	3,3,3	0.38	0
4	FES	A	201	1	0,4,4	0.00	-	-		
5	SO4	B	405	-	4,4,4	0.16	0	6,6,6	0.10	0
5	SO4	C	804	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	C	810	-	4,4,4	0.14	0	6,6,6	0.17	0
5	SO4	C	808	-	4,4,4	0.15	0	6,6,6	0.22	0
5	SO4	A	203	-	4,4,4	0.14	0	6,6,6	0.09	0
7	SF4	B	402	2	0,12,12	0.00	-	-		
8	GOL	B	406	-	5,5,5	0.37	0	5,5,5	0.30	0
5	SO4	C	806	-	4,4,4	0.14	0	6,6,6	0.10	0
8	GOL	C	813	-	5,5,5	0.39	0	5,5,5	0.42	0
9	MOS	C	801	10	0,3,3	0.00	-	-		
4	FES	A	202	1	0,4,4	0.00	-	-		
8	GOL	B	407	-	5,5,5	0.33	0	5,5,5	0.35	0
5	SO4	C	803	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	C	807	-	4,4,4	0.14	0	6,6,6	0.07	0
6	FAD	B	401	-	51,58,58	1.80	7 (13%)	60,89,89	2.01	13 (21%)
8	GOL	C	811	-	5,5,5	0.46	0	5,5,5	0.34	0
11	IPA	C	815	-	3,3,3	0.51	0	3,3,3	0.34	0
8	GOL	C	814	-	5,5,5	0.39	0	5,5,5	0.27	0
5	SO4	C	805	-	4,4,4	0.13	0	6,6,6	0.15	0
5	SO4	C	809	-	4,4,4	0.13	0	6,6,6	0.16	0
10	MCN	C	802	9	38,48,48	1.15	1 (2%)	40,74,74	1.91	8 (20%)
8	GOL	C	812	-	5,5,5	0.29	0	5,5,5	0.32	0
5	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	C	814	-	-	2/4/4/4	-
8	GOL	B	406	-	-	3/4/4/4	-
4	FES	A	201	1	-	-	0/1/1/1
4	FES	A	202	1	-	-	0/1/1/1
10	MCN	C	802	9	-	10/20/54/54	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	C	812	-	-	0/4/4/4	-
8	GOL	B	407	-	-	4/4/4/4	-
6	FAD	B	401	-	-	0/30/50/50	0/6/6/6
8	GOL	C	811	-	-	0/4/4/4	-
8	GOL	C	813	-	-	2/4/4/4	-
7	SF4	B	402	2	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	401	FAD	C4X-C10	9.25	1.48	1.38
10	C	802	MCN	C4A-C4B	4.14	1.47	1.40
6	B	401	FAD	C4-C4X	3.82	1.47	1.41
6	B	401	FAD	C9A-C5X	3.25	1.49	1.42
6	B	401	FAD	C8-C7	3.07	1.48	1.40
6	B	401	FAD	C5A-C4A	2.34	1.47	1.40
6	B	401	FAD	C1'-N10	-2.21	1.46	1.48
6	B	401	FAD	C2-N3	-2.00	1.34	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	401	FAD	C4-N3-C2	9.19	122.90	115.14
10	C	802	MCN	O9'-C7-N8'	6.55	123.43	115.30
6	B	401	FAD	C4-C4X-C10	-5.32	116.43	119.95
10	C	802	MCN	C2'-N1'-C4B	5.04	121.12	115.36
6	B	401	FAD	C4X-C4-N3	-3.92	118.08	123.43
10	C	802	MCN	N1'-C2'-N3'	-3.81	122.14	127.22
6	B	401	FAD	C4X-N5-C5X	3.77	120.54	116.77
10	C	802	MCN	C2-N3-C4	3.43	119.81	116.34
6	B	401	FAD	N3A-C2A-N1A	-3.12	123.81	128.68
6	B	401	FAD	P-O3P-PA	-3.05	122.37	132.83
6	B	401	FAD	C1'-N10-C10	3.04	121.13	118.41
6	B	401	FAD	C4-C4X-N5	3.02	122.05	118.60
10	C	802	MCN	C3'-C2D-C1'	2.95	105.42	100.98
6	B	401	FAD	C9A-N10-C10	-2.55	118.57	121.91
6	B	401	FAD	C4A-C5A-N7A	-2.55	106.74	109.40
6	B	401	FAD	C5X-C9A-N10	2.44	119.48	117.72
10	C	802	MCN	PB-O3A-PA	-2.41	124.57	132.83
10	C	802	MCN	C2'-N3'-C4'	2.39	122.46	116.43
6	B	401	FAD	C1'-N10-C9A	2.39	120.17	118.29
6	B	401	FAD	C1'-C2'-C3'	-2.31	103.34	109.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	802	MCN	O4'-C4'-N3'	2.25	123.38	117.44

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	813	GOL	O1-C1-C2-C3
8	B	407	GOL	O1-C1-C2-C3
8	C	814	GOL	O1-C1-C2-O2
8	C	814	GOL	O1-C1-C2-C3
10	C	802	MCN	C5'-O5'-PA-O3A
8	C	813	GOL	O1-C1-C2-O2
8	B	406	GOL	O1-C1-C2-C3
8	B	407	GOL	O1-C1-C2-O2
10	C	802	MCN	PB-O3A-PA-O1A
8	B	406	GOL	O1-C1-C2-O2
8	B	407	GOL	O2-C2-C3-O3
10	C	802	MCN	C10-O3B-PB-O3A
8	B	407	GOL	C1-C2-C3-O3
10	C	802	MCN	C5'-O5'-PA-O1A
10	C	802	MCN	C5'-O5'-PA-O2A
10	C	802	MCN	O3B-C10-C9'-C8'
10	C	802	MCN	PB-O3A-PA-O2A
10	C	802	MCN	O3B-C10-C9'-O9'
10	C	802	MCN	C9'-C10-O3B-PB
8	B	406	GOL	O2-C2-C3-O3
10	C	802	MCN	C10-O3B-PB-O1B

There are no ring outliers.

12 monomers are involved in 17 short contacts:

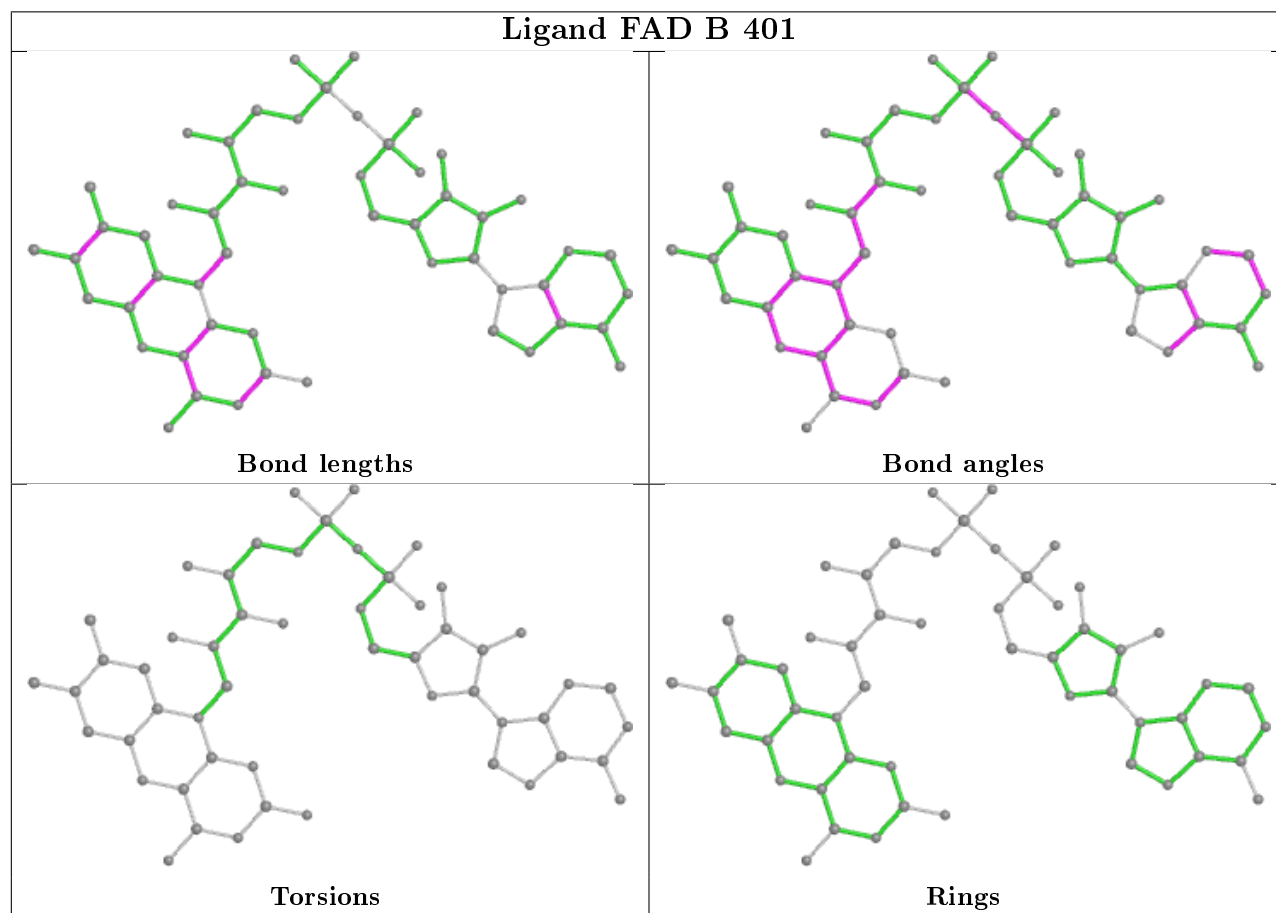
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	808	SO4	3	0
5	A	203	SO4	1	0
8	C	813	GOL	1	0
9	C	801	MOS	1	0
8	B	407	GOL	1	0
5	C	807	SO4	1	0
6	B	401	FAD	1	0
8	C	811	GOL	2	0
11	C	815	IPA	1	0

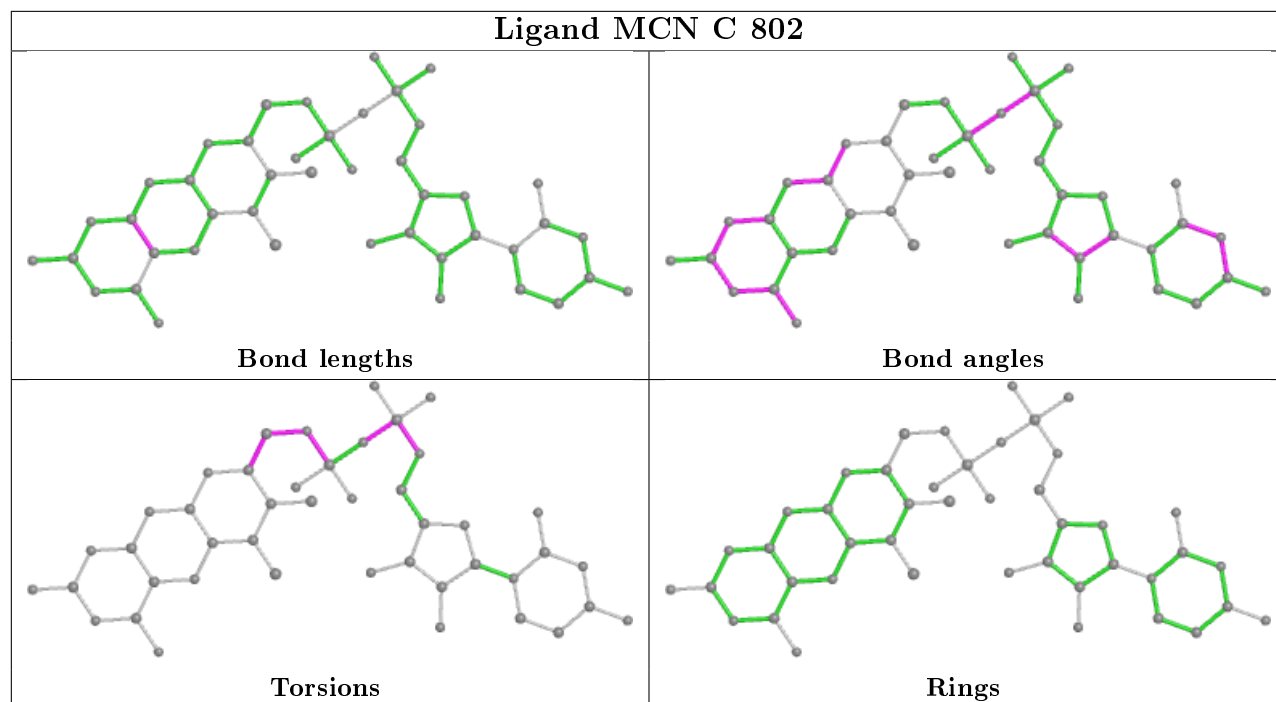
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	814	GOL	1	0
10	C	802	MCN	3	0
5	B	403	SO4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	157/162 (96%)	-0.28	0	100 100	13, 20, 34, 46	0
2	B	330/330 (100%)	-0.09	11 (3%)	46 50	14, 26, 44, 59	0
3	C	748/775 (96%)	-0.31	4 (0%)	91 91	13, 20, 34, 48	0
All	All	1235/1267 (97%)	-0.25	15 (1%)	79 80	13, 21, 39, 59	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	330	ALA	4.1
2	B	286	PHE	3.5
2	B	329	ILE	3.0
2	B	256	VAL	2.9
2	B	288	GLU	2.5
2	B	51	ASN	2.5
3	C	28	GLY	2.3
2	B	225	LEU	2.3
2	B	259	GLN	2.3
3	C	592	THR	2.3
3	C	557	LEU	2.3
2	B	63	ASN	2.1
2	B	251	THR	2.1
3	C	209	PRO	2.1
2	B	86	HIS	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 ⓘ

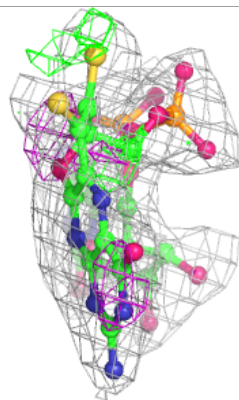
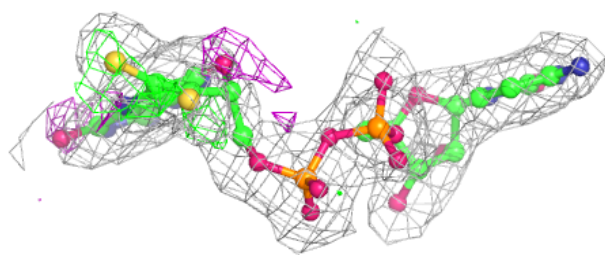
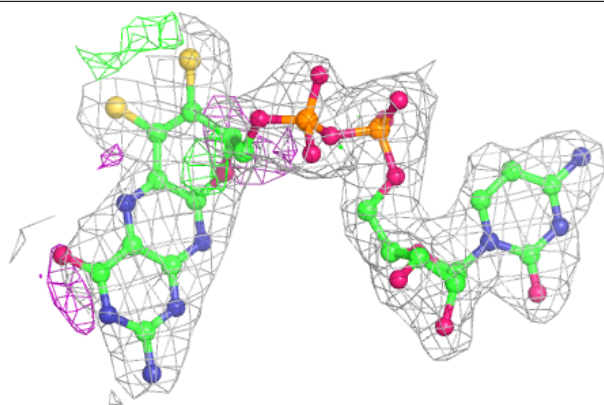
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	C	810	5/5	0.75	0.25	44,52,56,73	0
5	SO4	B	404	5/5	0.83	0.33	50,57,72,73	0
8	GOL	C	814	6/6	0.85	0.27	25,26,30,31	0
8	GOL	C	813	6/6	0.87	0.22	18,23,28,34	0
11	IPA	C	816	4/4	0.89	0.20	23,24,25,28	0
5	SO4	C	803	5/5	0.89	0.36	40,47,61,69	0
8	GOL	C	812	6/6	0.90	0.29	34,36,38,39	0
5	SO4	C	804	5/5	0.90	0.19	49,55,71,79	0
5	SO4	B	405	5/5	0.91	0.26	48,56,59,66	0
5	SO4	C	809	5/5	0.93	0.45	37,41,61,63	0
8	GOL	C	811	6/6	0.93	0.23	21,24,30,31	0
5	SO4	C	805	5/5	0.93	0.31	44,45,60,66	0
8	GOL	B	407	6/6	0.94	0.12	22,23,30,31	0
8	GOL	B	406	6/6	0.95	0.16	22,26,29,33	0
10	MCN	C	802	44/44	0.95	0.15	13,16,19,23	0
5	SO4	C	807	5/5	0.96	0.11	39,43,50,52	0
5	SO4	C	806	5/5	0.96	0.26	29,38,53,58	0
5	SO4	B	403	5/5	0.96	0.11	34,38,40,52	0
11	IPA	C	815	4/4	0.96	0.24	16,17,19,24	0
6	FAD	B	401	53/53	0.97	0.12	12,18,26,30	0
4	FES	A	201	4/4	0.98	0.13	18,18,20,22	0
5	SO4	C	808	5/5	0.98	0.22	31,36,37,52	0
5	SO4	A	203	5/5	0.98	0.12	31,33,38,40	0
7	SF4	B	402	8/8	0.98	0.12	17,21,22,22	0
4	FES	A	202	4/4	0.99	0.16	18,19,19,21	0
9	MOS	C	801	4/4	0.99	0.18	17,23,24,26	0

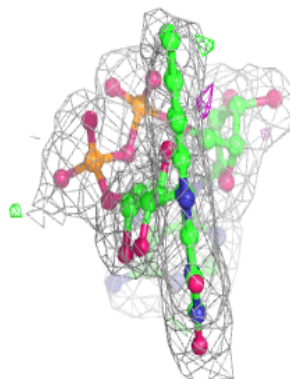
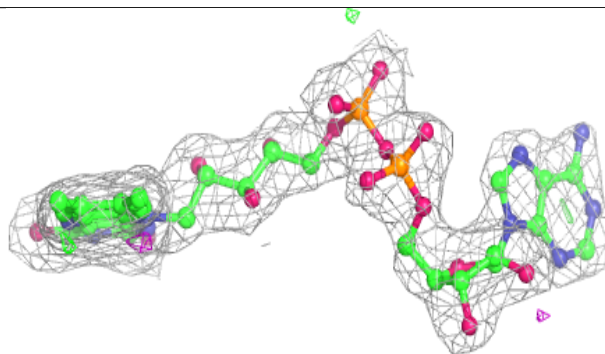
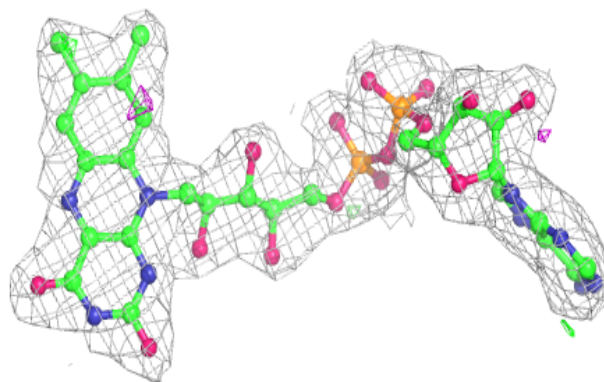
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MCN C 802:

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

**Electron density around FAD B 401:**

$2mF_o-DF_c$ (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.