



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:03 AM JST

PDB ID : 5Y6Q / pdb_00005y6q
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

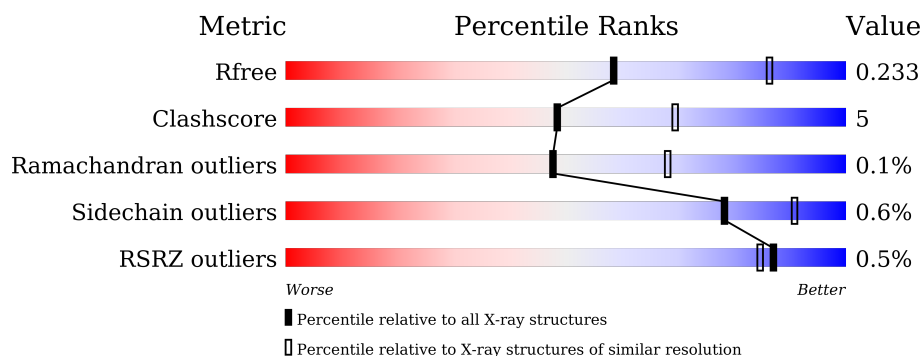
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. 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	
2	B	330	
3	C	775	

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	F5K	C	817	X	-	-	-
5	SO4	C	808	-	-	X	-

2 Entry composition

There are 11 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			

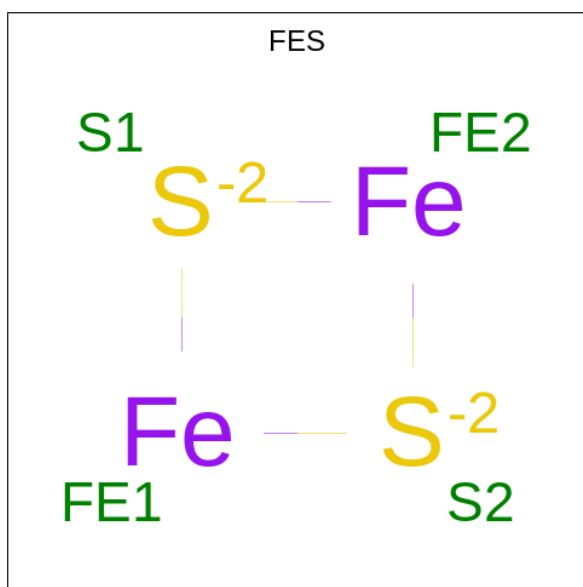
There are 6 discrepancies between the modelled and reference sequences:

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.

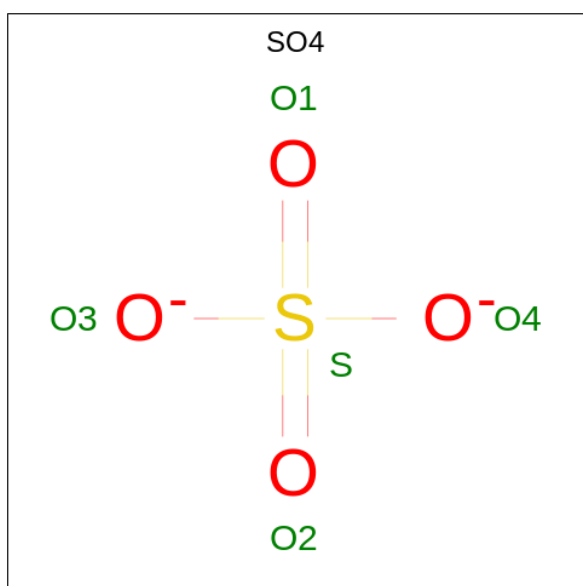
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	748	Total	C	N	O	S	0	0	0
			5646	3537	1003	1085	21			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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 (CCD ID: SO₄) (formula: O₄S).



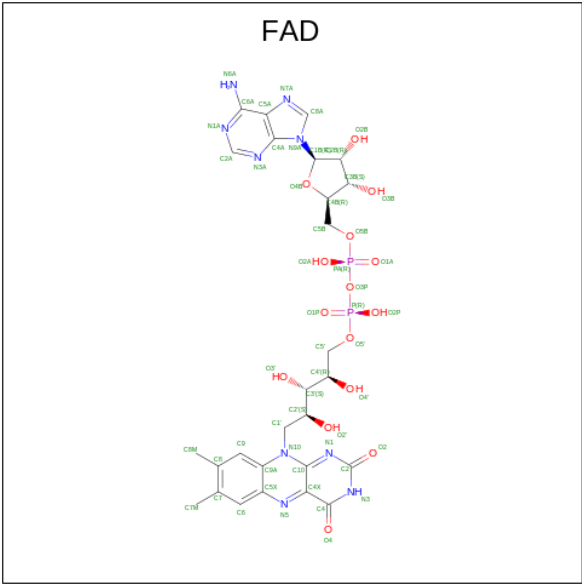
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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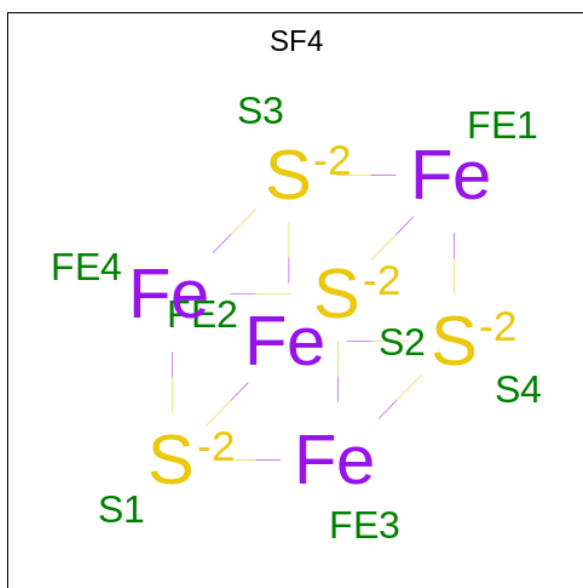
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	B	1	5	4	1	0	0
5	B	1	5	4	1	0	0
5	C	1	5	4	1	0	0
5	C	1	5	4	1	0	0
5	C	1	5	4	1	0	0
5	C	1	5	4	1	0	0
5	C	1	5	4	1	0	0
5	C	1	5	4	1	0	0
5	C	1	5	4	1	0	0
5	C	1	5	4	1	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



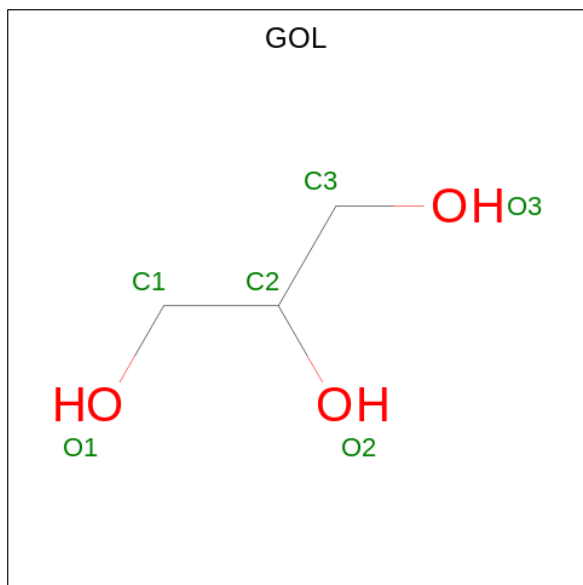
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	53	27	9	15	2	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



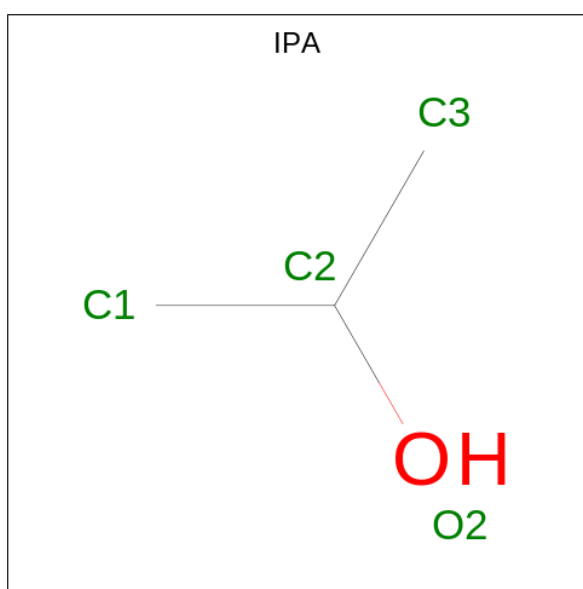
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

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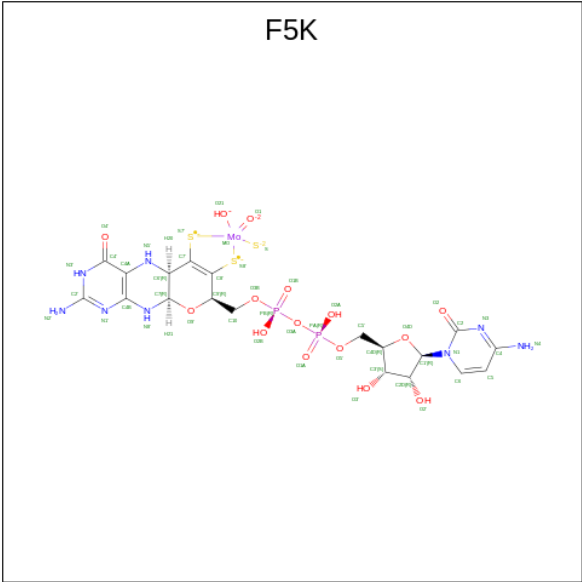
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

- Molecule 10 is Molybdopterin cytosine dinucleotide hydroxy-oxo-sulfido-molybdenum (CCD ID: F5K) (formula: $C_{19}H_{25}MoN_8O_{15}P_2S_3$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	C	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	15	2	3		

- Molecule 11 is water.

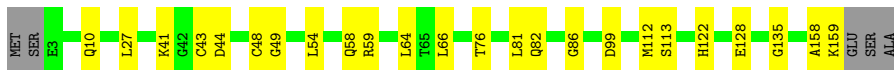
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	56	Total	O	0	0
			56	56		
11	B	111	Total	O	0	0
			111	111		
11	C	340	Total	O	0	0
			340	340		

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.

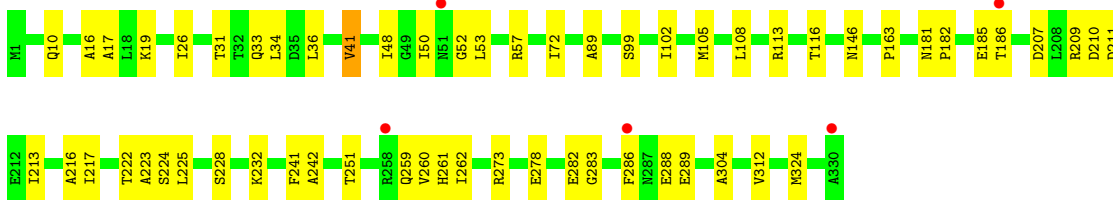
- Molecule 1: Aldehyde oxidase small subunit

Chain A: 



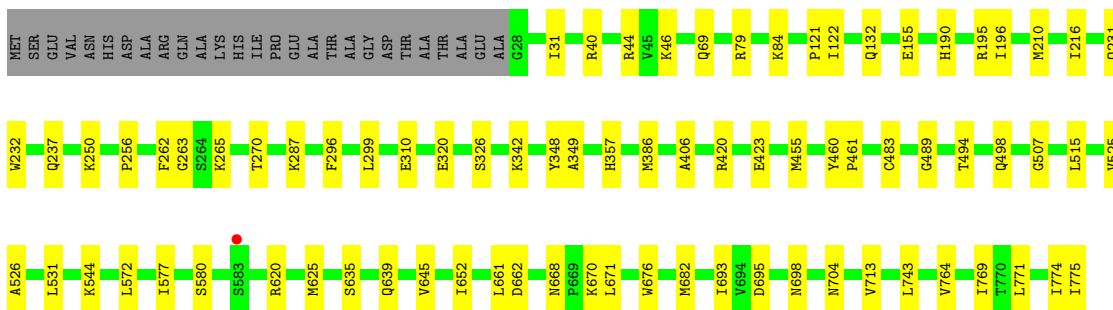
- Molecule 2: Aldehyde oxidase medium subunit

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 46.12 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.12-2.50) 99.1 (46.12-2.50)	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	2211 reflections (4.99%)	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 , 37.7	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, GOL, SO4, F5K, FAD, SF4, IPA

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	0.22	0/1188	0.43	0/1605
2	B	0.25	0/2547	0.47	0/3459
3	C	0.24	0/5757	0.47	0/7830
All	All	0.24	0/9492	0.47	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

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	19	0
2	B	2500	0	2459	40	2
3	C	5646	0	5621	50	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	24	0	32	4	0
9	C	8	0	16	2	0
10	C	48	0	0	1	0
11	A	56	0	0	2	0
11	B	111	0	0	1	0
11	C	340	0	0	1	0
All	All	10044	0	9312	103	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 (103) 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
2:B:273:ARG:HE	2:B:278:GLU:CD	1.98	0.71
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:222:THR:HG23	2:B:225:LEU:H	1.60	0.66
3:C:625:MET:HE1	9:C:816:IPA:H33	1.76	0.66
1:A:59:ARG:NH1	1:A:113:SER:OG	2.29	0.64
1:A:48:CYS:HB2	3:C:210:MET:HE1	1.79	0.63
3:C:620:ARG:HH21	8:C:811:GOL:H31	1.63	0.63
3:C:320:GLU:OE1	11: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	11: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:102:ILE:HA	2:B:105:MET:HE3	1.86	0.57
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
2:B:19:LYS:NZ	2:B:210:ASP:C	2.63	0.56
3:C:232:TRP:HB2	3:C:525:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:48:CYS:SG	1:A:49:GLY:N	2.81	0.54
2:B:52:GLY:H	2:B:57:ARG:HH11	1.56	0.54
2:B:181:ASN:HD21	2:B:185:GLU:HG3	1.73	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
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:CA	2.73	0.51
2:B:216:ALA:O	2:B:217:ILE:HD13	2.10	0.51
2:B:283:GLY:O	11: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
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:420:ARG:HB2	3:C:662:ASP:HB2	1.99	0.45
3:C:483:CYS:O	3:C:515:LEU:HA	2.15	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
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	9:C:815:IPA:H32	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:HA3	2:B:99:SER:HB2	2.00	0.44
3:C:326:SER:HG	3:C:357:HIS:HD1	1.62	0.44
1:A:10:GLN:HG2	11:A:348:HOH:O	2.17	0.43
1:A:43:CYS:SG	1:A:44:ASP:N	2.91	0.43
3:C:40:ARG:NH2	3:C:489:GLY:O	2.50	0.43
3:C:196:ILE:O	3:C:310:GLU:HA	2.18	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:326:SER:OG	3:C:357:HIS:ND1	2.39	0.43
3:C:256:PRO:HB3	8:C:813:GOL:H11	2.01	0.43
2:B:223:ALA:C	2:B:251:THR:HG22	2.44	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
3:C:348:TYR:CE2	3:C:386:MET:HE2	2.54	0.42
1:A:54:LEU:HG	1:A:112:MET:HE3	2.01	0.42
3:C:262:PHE:CD1	3:C:682:MET:HE1	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:HA	3:C:250:LYS:HD3	1.86	0.41
3:C:668:ASN:CG	3:C:671:LEU:HG	2.45	0.41
3:C:231:GLN:HG3	3:C:265:LYS:O	2.21	0.41
3:C:263:GLY:HA2	10:C:817:F5K: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLN:OE1	3:C:580:SER:OG[6_544]	2.09	0.11

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	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%)	48	68
All	All	1230/1267 (97%)	1202 (98%)	27 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	122	ILE

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	126/129 (98%)	126 (100%)	0	100	100
2	B	258/258 (100%)	255 (99%)	3 (1%)	63	83
3	C	590/609 (97%)	587 (100%)	3 (0%)	81	92
All	All	974/996 (98%)	968 (99%)	6 (1%)	78	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	41	VAL
2	B	146	ASN
2	B	186	THR
3	C	46	LYS
3	C	299	LEU
3	C	713	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	14	GLN
1	A	82	GLN
2	B	10	GLN
2	B	33	GLN
2	B	46	GLN
2	B	180	GLN
2	B	183	GLN
2	B	287	ASN
3	C	61	ASN
3	C	99	ASN
3	C	231	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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
5	SO4	B	405	-	4,4,4	0.16	0	6,6,6	0.10	0
10	F5K	C	817	-	43,53,53	4.54	9 (20%)	48,86,86	2.61	6 (12%)
9	IPA	C	815	-	3,3,3	0.51	0	3,3,3	0.34	0
9	IPA	C	816	-	3,3,3	0.53	0	3,3,3	0.38	0
8	GOL	C	814	-	5,5,5	0.39	0	5,5,5	0.27	0
6	FAD	B	401	-	56,58,58	1.43	9 (16%)	81,89,89	1.58	12 (14%)
4	FES	A	202	1	0,4,4	-	-	-	-	-
5	SO4	C	803	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	C	804	-	4,4,4	0.15	0	6,6,6	0.06	0
7	SF4	B	402	2	0,12,12	-	-	-	-	-
8	GOL	C	811	-	5,5,5	0.46	0	5,5,5	0.34	0
4	FES	A	201	1	0,4,4	-	-	-	-	-
5	SO4	C	808	-	4,4,4	0.15	0	6,6,6	0.22	0
5	SO4	C	809	-	4,4,4	0.13	0	6,6,6	0.16	0
5	SO4	A	203	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	C	810	-	4,4,4	0.14	0	6,6,6	0.17	0
8	GOL	C	812	-	5,5,5	0.29	0	5,5,5	0.32	0
8	GOL	B	406	-	5,5,5	0.37	0	5,5,5	0.30	0
8	GOL	C	813	-	5,5,5	0.39	0	5,5,5	0.42	0
5	SO4	C	805	-	4,4,4	0.13	0	6,6,6	0.15	0
8	GOL	B	407	-	5,5,5	0.33	0	5,5,5	0.35	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
5	SO4	C	806	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	C	807	-	4,4,4	0.14	0	6,6,6	0.07	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	813	-	-	2/4/4/4	-
10	F5K	C	817	-	2/2/12/14	10/22/78/78	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FAD	B	401	-	-	0/34/50/50	0/6/6/6
4	FES	A	202	1	-	-	0/1/1/1
8	GOL	B	407	-	-	4/4/4/4	-
8	GOL	C	814	-	-	2/4/4/4	-
8	GOL	C	812	-	-	0/4/4/4	-
7	SF4	B	402	2	-	-	0/6/5/5
8	GOL	C	811	-	-	0/4/4/4	-
4	FES	A	201	1	-	-	0/1/1/1
8	GOL	B	406	-	-	3/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	817	F5K	MO-S8'	18.77	2.66	2.39
10	C	817	F5K	C6'-N5'	-10.34	1.34	1.46
10	C	817	F5K	MO-S7'	10.12	2.53	2.39
10	C	817	F5K	C7-C6'	-9.65	1.46	1.53
10	C	817	F5K	O4'-C4'	7.26	1.37	1.23
10	C	817	F5K	C7-N8'	-6.61	1.34	1.45
10	C	817	F5K	O1-MO	6.49	1.85	1.69
10	C	817	F5K	O9'-C7	-6.21	1.34	1.43
10	C	817	F5K	C4A-C4B	5.37	1.47	1.38
6	B	401	FAD	C9A-C5X	4.71	1.49	1.41
6	B	401	FAD	C5A-C4A	4.34	1.47	1.39
6	B	401	FAD	C8-C7	3.07	1.48	1.40
6	B	401	FAD	C4-N3	-2.89	1.33	1.38
6	B	401	FAD	C8A-N7A	2.52	1.36	1.31
6	B	401	FAD	C5A-C6A	2.48	1.48	1.41
6	B	401	FAD	C5A-N7A	-2.34	1.34	1.39
6	B	401	FAD	C4X-N5	2.20	1.35	1.30
6	B	401	FAD	C2-N3	-2.07	1.34	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	817	F5K	O9'-C7-N8'	14.46	123.43	108.57
10	C	817	F5K	O9'-C7-C6'	6.31	113.18	108.96
6	B	401	FAD	C5A-C4A-N3A	-5.92	119.02	126.75
6	B	401	FAD	N3A-C4A-N9A	4.37	134.29	127.08
10	C	817	F5K	C2'-N1'-C4B	4.26	121.12	113.43
6	B	401	FAD	C2A-N3A-C4A	3.79	120.70	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	817	F5K	O4'-C4'-C4A	-3.70	118.76	127.24
6	B	401	FAD	C4A-C5A-N7A	-3.18	106.74	110.62
6	B	401	FAD	N3A-C2A-N1A	-3.06	123.81	128.60
6	B	401	FAD	P-O3P-PA	-3.05	122.37	132.83
6	B	401	FAD	C4-C4X-N5	2.68	122.05	118.23
6	B	401	FAD	C5A-N7A-C8A	2.58	107.18	103.51
10	C	817	F5K	PB-O3A-PA	-2.41	124.57	132.83
6	B	401	FAD	C4X-C10-N1	-2.38	119.22	124.73
6	B	401	FAD	C1'-C2'-C3'	-2.31	103.34	109.79
6	B	401	FAD	C4A-N9A-C8A	2.18	108.09	105.73
6	B	401	FAD	C6A-C5A-N7A	2.16	136.04	132.02
10	C	817	F5K	C3'-C2D-C1'	2.10	105.42	101.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	C	817	F5K	C7
10	C	817	F5K	C6'

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	407	GOL	O1-C1-C2-C3
8	C	813	GOL	O1-C1-C2-C3
8	C	814	GOL	O1-C1-C2-O2
8	C	814	GOL	O1-C1-C2-C3
10	C	817	F5K	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	817	F5K	PB-O3A-PA-O1A
8	B	406	GOL	O1-C1-C2-O2
8	B	407	GOL	O2-C2-C3-O3
10	C	817	F5K	C10-O3B-PB-O3A
8	B	407	GOL	C1-C2-C3-O3
10	C	817	F5K	C5'-O5'-PA-O1A
10	C	817	F5K	C5'-O5'-PA-O2A
10	C	817	F5K	O3B-C10-C9'-C8'
10	C	817	F5K	PB-O3A-PA-O2A
10	C	817	F5K	O3B-C10-C9'-O9'
10	C	817	F5K	C9'-C10-O3B-PB
8	B	406	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	C	817	F5K	C10-O3B-PB-O1B

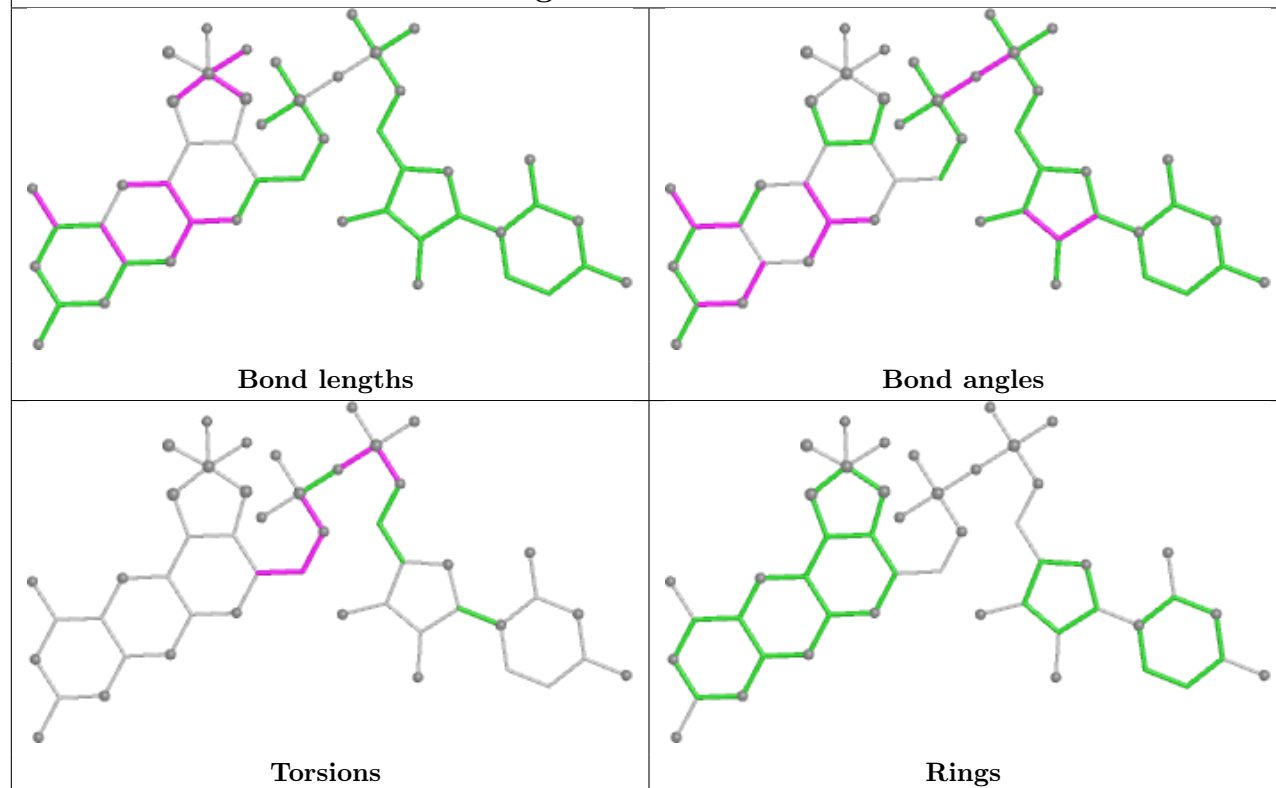
There are no ring outliers.

12 monomers are involved in 15 short contacts:

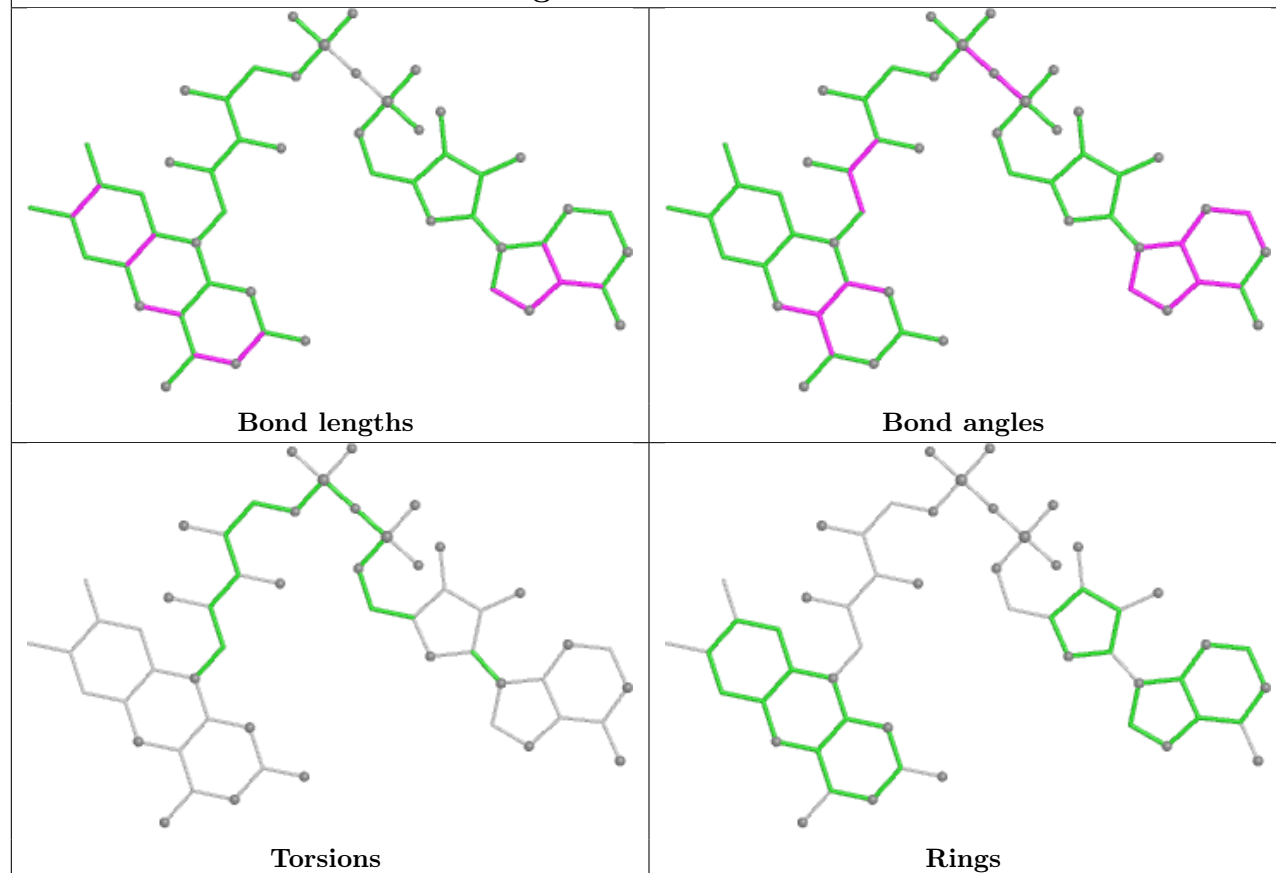
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	817	F5K	1	0
9	C	815	IPA	1	0
9	C	816	IPA	1	0
8	C	814	GOL	1	0
6	B	401	FAD	1	0
8	C	811	GOL	2	0
5	C	808	SO4	3	0
5	A	203	SO4	1	0
8	C	813	GOL	1	0
8	B	407	GOL	1	0
5	B	403	SO4	1	0
5	C	807	SO4	1	0

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.

Ligand F5K C 817



Ligand FAD B 401



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	157/162 (96%)	-0.38	0 100 100	13, 20, 34, 46	1 (0%)
2	B	330/330 (100%)	0.04	5 (1%) 72 68	14, 26, 44, 59	0
3	C	748/775 (96%)	-0.42	1 (0%) 92 90	13, 20, 34, 48	0
All	All	1235/1267 (97%)	-0.29	6 (0%) 87 85	13, 21, 39, 59	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	330	ALA	3.8
2	B	51	ASN	3.1
2	B	258	ARG	2.7
2	B	286	PHE	2.5
3	C	583	SER	2.3
2	B	186	THR	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

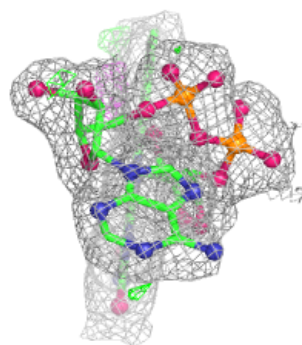
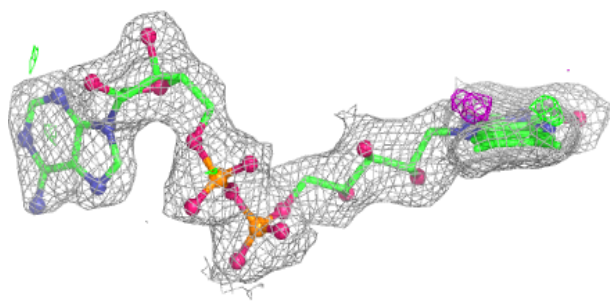
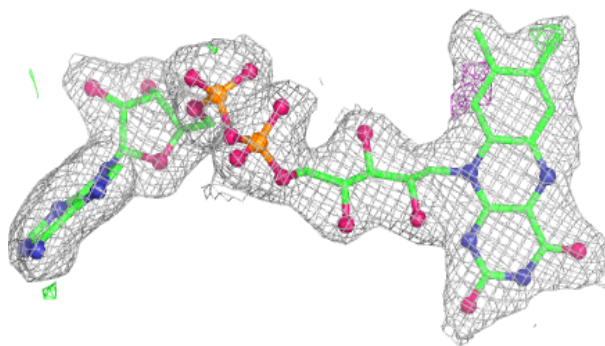
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	810	5/5	0.70	0.16	44,52,56,73	0
5	SO4	B	405	5/5	0.77	0.16	48,56,59,66	0
8	GOL	C	814	6/6	0.77	0.18	25,26,30,31	0
5	SO4	B	404	5/5	0.78	0.18	50,57,72,73	0
5	SO4	C	804	5/5	0.81	0.11	49,55,71,79	0
8	GOL	C	812	6/6	0.84	0.12	34,36,38,39	0
9	IPA	C	816	4/4	0.84	0.16	23,24,25,28	0
8	GOL	C	811	6/6	0.85	0.13	21,24,30,31	0
8	GOL	C	813	6/6	0.85	0.14	18,23,28,34	0
5	SO4	C	805	5/5	0.86	0.17	44,45,60,66	0
5	SO4	C	803	5/5	0.87	0.19	40,47,61,69	0
5	SO4	C	809	5/5	0.90	0.21	37,41,61,63	0
5	SO4	C	806	5/5	0.91	0.18	29,38,53,58	0
5	SO4	B	403	5/5	0.91	0.10	34,38,40,52	0
5	SO4	C	807	5/5	0.93	0.10	39,43,50,52	0
9	IPA	C	815	4/4	0.94	0.09	16,17,19,24	0
8	GOL	B	406	6/6	0.94	0.07	22,26,29,33	0
8	GOL	B	407	6/6	0.95	0.08	22,23,30,31	0
6	FAD	B	401	53/53	0.96	0.06	12,18,26,30	0
5	SO4	A	203	5/5	0.96	0.10	31,33,38,40	0
5	SO4	C	808	5/5	0.96	0.12	31,36,37,52	0
10	F5K	C	817	48/48	0.97	0.09	13,16,23,26	0
7	SF4	B	402	8/8	0.98	0.04	17,21,22,22	0
4	FES	A	202	4/4	0.99	0.04	18,19,19,21	0
4	FES	A	201	4/4	0.99	0.03	18,18,20,22	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.

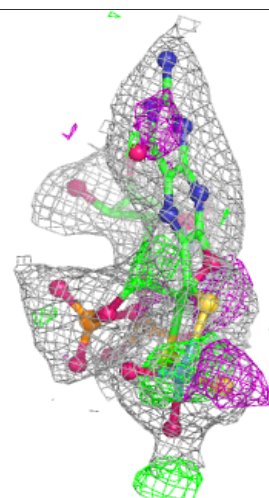
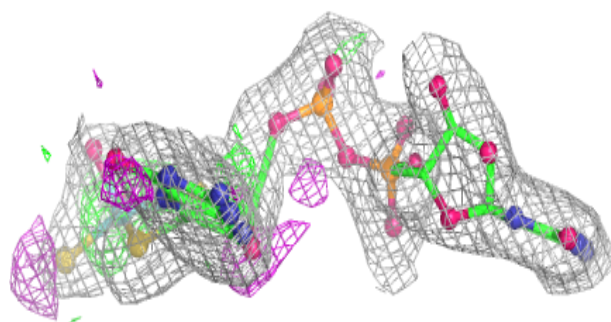
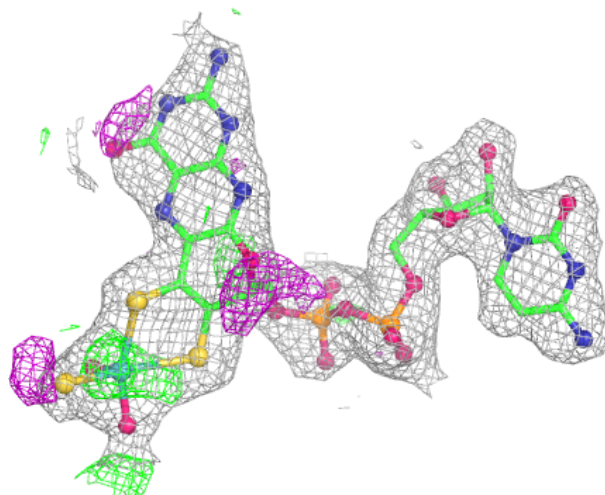
Electron density around FAD B 401:

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



Electron density around F5K C 817:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.