Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:30 PM GMT

PDB ID : 4A9W
Title : Flavin-containing monooxygenase from Stenotrophomonas maltophilia
Authors : Jensen, C.N.; Cartwright, J.; Hart, S.; Turkenburg, J.P.; Ali, S.T.; Allen, M.J.; Grogan, G.
Deposited on : 2011-11-29
Resolution : 2.72 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683
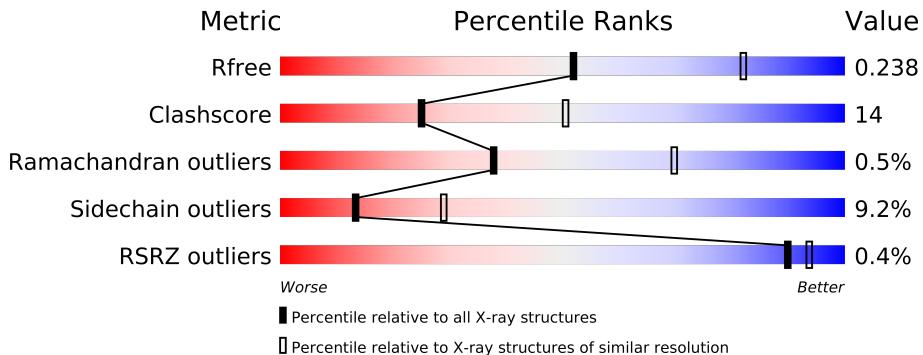
1 Overall quality at a glance ⓘ
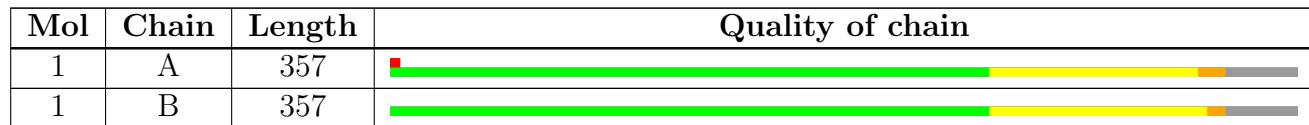
The reported resolution of this entry is 2.72 Å.

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	Percentile Ranks	Value
Rfree		0.238
Clashscore		14
Ramachandran outliers		0.5%
Sidechain outliers		9.2%
RSRZ outliers		0.4%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1770 (2.74-2.70)
Clashscore	79885	2183 (2.74-2.70)
Ramachandran outliers	78287	2147 (2.74-2.70)
Sidechain outliers	78261	2148 (2.74-2.70)
RSRZ outliers	66119	1772 (2.74-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	1359	-	X
3	SO4	A	1360	-	X
3	SO4	B	1359	-	X
3	SO4	B	1361	-	X

2 Entry composition ⓘ
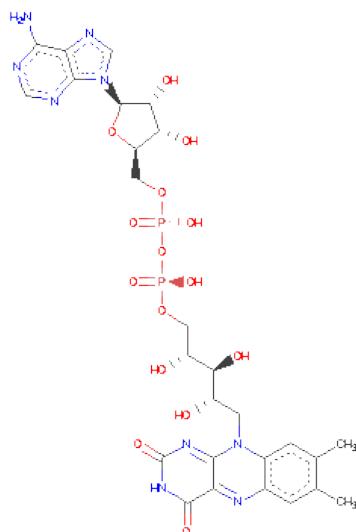
There are 4 unique types of molecules in this entry. The entry contains 5310 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MONOOXYGENASE.
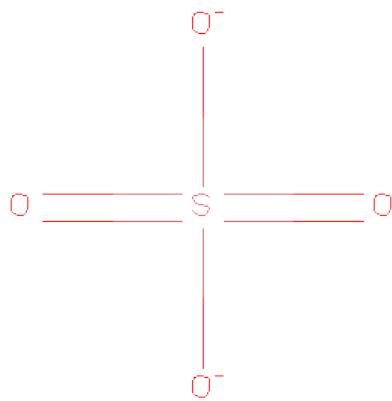
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	1	0
			2503	1603	440	452	8			
1	B	330	Total	C	N	O	S	0	1	0
			2506	1603	443	452	8			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 4 is water.
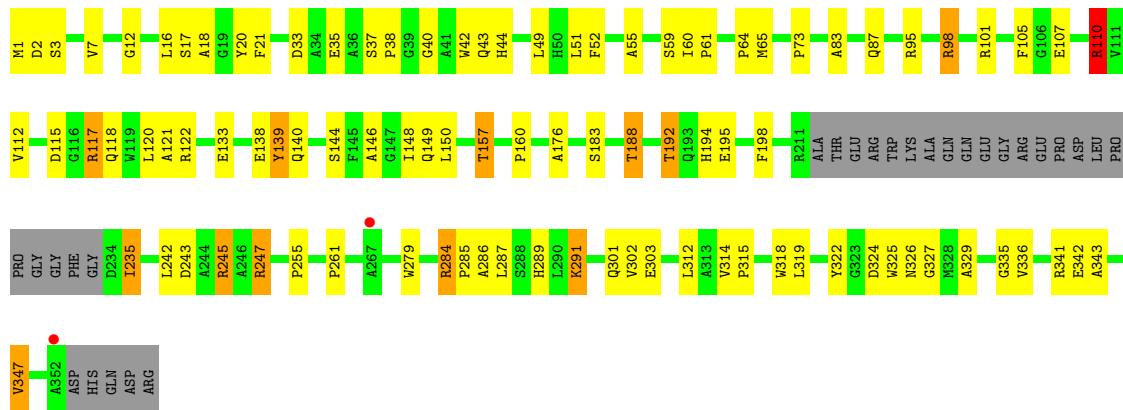
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	40	Total 40	O 40	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
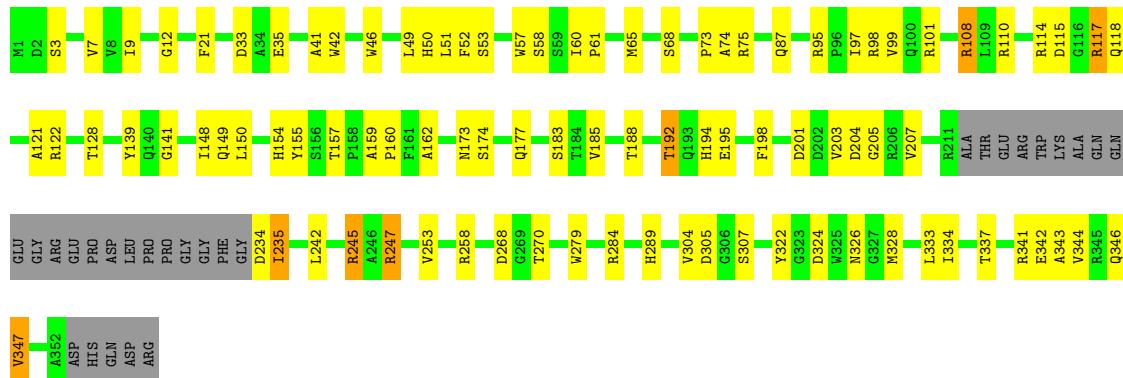
• Molecule 1: MONOOXYGENASE

Chain A:

• Molecule 1: MONOOXYGENASE

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	84.00Å 84.00Å 103.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.75 – 2.72 42.10 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.75-2.72) 100.0 (42.10-2.72)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.182 , 0.238 0.183 , 0.238	Depositor DCC
R_{free} test set	1115 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 2.7	EDS
Estimated twinning fraction	0.013 for -h,-k,l 0.034 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 21799 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5310	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 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: SO4, FAD

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	0.79	0/2578	0.89	4/3524 (0.1%)
1	B	0.78	0/2581	0.88	4/3528 (0.1%)
All	All	0.78	0/5159	0.89	8/7052 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	B	115	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	110	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	247	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	234	ASP	N-CA-C	5.44	125.69	111.00
1	A	247	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	110	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	115	ASP	CB-CG-OD1	5.13	122.92	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243[A]	ASP	Mainchain
1	A	243[B]	ASP	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2503	0	2441	67	0
1	B	2506	0	2447	75	0
2	A	53	0	31	3	0
2	B	53	0	31	4	0
3	A	55	0	0	3	0
3	B	45	0	0	6	0
4	A	55	0	0	6	0
4	B	40	0	0	1	0
All	All	5310	0	4950	140	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (140) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.23	1.01
1:B:141:GLY:N	3:B:1362:SO4:O3	1.91	1.01
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.31	0.95
1:A:157:THR:HG22	1:A:160:PRO:HD3	1.51	0.92
1:B:245:ARG:HG2	1:B:245:ARG:HH11	1.37	0.89
1:B:192:THR:CG2	1:B:194:HIS:O	2.20	0.89
1:B:149:GLN:HE21	1:B:279:TRP:HE1	1.18	0.89
1:A:245:ARG:HG2	1:A:245:ARG:HH11	1.38	0.89
1:B:65:MET:HE1	1:B:73:PRO:HG2	1.56	0.87
1:B:33:ASP:OD1	2:B:1353:FAD:H3B	1.73	0.87
1:B:60:ILE:HB	1:B:61:PRO:HD2	1.57	0.86
1:A:149:GLN:HE21	1:A:279:TRP:HE1	1.22	0.85
1:A:33:ASP:OD1	2:A:1353:FAD:H3B	1.79	0.82
1:A:188:THR:HG23	4:A:2036:HOH:O	1.79	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:284:ARG:HH11	1:A:284:ARG:CG	1.96	0.79
1:B:198:PHE:CD1	1:B:235:ILE:HD12	2.19	0.77
1:A:322:TYR:H	1:A:326:ASN:HD22	1.34	0.73
1:A:157:THR:HG22	1:A:160:PRO:CD	2.21	0.71
1:B:198:PHE:HD1	1:B:235:ILE:HD12	1.56	0.69
1:B:65:MET:HE1	1:B:73:PRO:CG	2.21	0.69
1:B:188:THR:HG23	4:B:2028:HOH:O	1.95	0.66
1:B:192:THR:HG21	1:B:194:HIS:O	1.96	0.65
1:B:305:ASP:OD1	1:B:307:SER:HB3	1.97	0.65
1:B:268:ASP:OD1	1:B:268:ASP:C	2.35	0.65
1:B:65:MET:CE	1:B:73:PRO:CG	2.74	0.64
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.63	0.64
1:A:149:GLN:NE2	1:A:279:TRP:HE1	1.95	0.63
1:A:42:TRP:HZ3	1:A:49:LEU:HD21	1.63	0.63
1:B:154:HIS:HD2	3:B:1355:SO4:O4	1.81	0.62
1:B:343:ALA:O	1:B:347:VAL:HG12	2.00	0.61
1:A:98:ARG:HD2	3:A:1354:SO4:O2	2.00	0.61
1:B:141:GLY:CA	3:B:1362:SO4:O3	2.49	0.60
1:B:117:ARG:HG3	1:B:117:ARG:NH1	2.04	0.59
1:B:117:ARG:HH11	1:B:117:ARG:CG	2.06	0.59
1:A:107:GLU:HG2	4:A:2022:HOH:O	2.02	0.59
1:B:198:PHE:HD1	1:B:235:ILE:CD1	2.16	0.58
1:A:35:GLU:O	1:A:95:ARG:HG3	2.04	0.57
1:A:157:THR:CG2	1:A:160:PRO:HD3	2.32	0.57
1:A:42:TRP:CZ3	1:A:49:LEU:HD21	2.40	0.57
1:B:65:MET:HE3	1:B:73:PRO:HB3	1.87	0.56
1:A:192:THR:HG23	1:A:194:HIS:O	2.05	0.56
1:A:318:TRP:C	1:A:319:LEU:HG	2.24	0.56
1:A:7:VAL:HG23	1:A:121:ALA:HB2	1.87	0.56
1:B:173:ASN:O	1:B:177:GLN:HG3	2.05	0.55
1:A:117:ARG:NH1	1:A:117:ARG:HG3	2.10	0.55
1:A:65:MET:HE3	1:A:73:PRO:HB3	1.89	0.55
1:A:38:PRO:HG2	1:A:83:ALA:HB2	1.89	0.55
1:B:235:ILE:C	1:B:235:ILE:HD13	2.26	0.55
1:A:65:MET:HE1	1:A:73:PRO:HG2	1.90	0.55
1:A:245:ARG:HG2	4:A:2040:HOH:O	2.06	0.54
1:B:110:ARG:HD2	1:B:118:GLN:NE2	2.22	0.54
1:B:322:TYR:H	1:B:326:ASN:HD22	1.55	0.54
1:A:303:GLU:HB3	1:A:312:LEU:HD12	1.90	0.54
1:B:245:ARG:NH1	1:B:245:ARG:HG2	2.16	0.54
1:B:50:HIS:CD2	1:B:74:ALA:HA	2.43	0.53
1:B:97:ILE:HD13	1:B:117:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:PHE:CD2	1:A:120:LEU:HD11	2.44	0.53
1:B:60:ILE:CB	1:B:61:PRO:HD2	2.34	0.52
1:A:343:ALA:O	1:A:347:VAL:HG13	2.09	0.52
1:B:192:THR:HG22	1:B:194:HIS:O	2.06	0.52
1:A:133:GLU:HG3	1:A:286:ALA:HA	1.91	0.52
1:A:55:ALA:HA	1:A:65:MET:HE1	1.92	0.52
1:A:198:PHE:CE1	1:A:235:ILE:HD11	2.44	0.51
1:B:183:SER:OG	1:B:247:ARG:NH2	2.42	0.51
1:A:329:ALA:O	1:A:335:GLY:HA3	2.10	0.51
1:B:35:GLU:O	1:B:95:ARG:HG2	2.10	0.51
1:B:42:TRP:HZ3	1:B:49:LEU:HD21	1.76	0.51
1:B:128:THR:HB	2:B:1353:FAD:C8A	2.41	0.51
1:A:245:ARG:HG2	1:A:245:ARG:NH1	2.15	0.50
1:A:291:LYS:NZ	4:A:2043:HOH:O	2.43	0.50
1:B:61:PRO:HB3	1:B:337:THR:HG23	1.92	0.50
1:B:324:ASP:OD1	1:B:328:MET:O	2.30	0.49
1:A:21:PHE:CZ	1:A:341:ARG:HB2	2.47	0.49
1:A:146:ALA:O	1:B:110:ARG:NH2	2.46	0.49
1:A:65:MET:HE1	1:A:73:PRO:CG	2.43	0.48
1:B:201:ASP:OD2	1:B:245:ARG:NH2	2.47	0.48
1:A:139:TYR:OH	1:A:255:PRO:HB3	2.13	0.48
1:A:183:SER:OG	1:A:247:ARG:NH2	2.47	0.48
1:A:37:SER:HB2	1:A:43:GLN:NE2	2.29	0.47
1:B:12:GLY:H	2:B:1353:FAD:H51A	1.78	0.47
1:A:324:ASP:HA	1:A:327:GLY:O	2.14	0.47
1:B:344:VAL:HA	1:B:347:VAL:HG13	1.95	0.47
1:A:59:SER:HB3	1:A:64:PRO:HA	1.97	0.47
1:B:154:HIS:CD2	3:B:1355:SO4:O4	2.65	0.47
1:B:203:VAL:HG22	1:B:204:ASP:H	1.80	0.47
1:A:118:GLN:CD	1:B:148:ILE:HD11	2.35	0.47
1:A:60:ILE:HB	1:A:61:PRO:CD	2.45	0.47
1:B:235:ILE:O	1:B:235:ILE:HD13	2.15	0.47
1:A:157:THR:O	1:A:160:PRO:HD2	2.15	0.46
1:A:40:GLY:HA2	2:A:1353:FAD:O3B	2.15	0.46
1:B:21:PHE:CZ	1:B:341:ARG:HB2	2.50	0.46
1:B:108:ARG:HB3	1:B:121:ALA:O	2.16	0.46
1:A:138:GLU:O	1:A:139:TYR:O	2.34	0.46
1:B:97:ILE:CD1	1:B:117:ARG:NH2	2.79	0.46
1:B:305:ASP:OD1	1:B:307:SER:CB	2.63	0.46
1:A:342:GLU:HA	1:A:342:GLU:OE1	2.16	0.46
1:A:110:ARG:NE	1:A:118:GLN:NE2	2.64	0.46
1:B:305:ASP:OD1	1:B:307:SER:N	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:342:GLU:O	1:B:346:GLN:HG3	2.15	0.45
1:B:174:SER:HB2	3:B:1361:SO4:O3	2.16	0.45
1:B:46:TRP:HB3	1:B:155:TYR:O	2.16	0.45
1:B:97:ILE:CD1	1:B:117:ARG:HH21	2.30	0.45
1:B:157:THR:HG23	1:B:160:PRO:HD3	1.98	0.45
1:A:60:ILE:HB	1:A:61:PRO:HD3	1.98	0.45
1:A:17:SER:O	1:A:18:ALA:C	2.53	0.45
1:B:60:ILE:HB	1:B:61:PRO:CD	2.36	0.44
1:A:285:PRO:HB2	1:A:287:LEU:HG	2.00	0.44
1:A:148:ILE:HD11	1:B:118:GLN:NE2	2.33	0.44
1:B:21:PHE:HB2	1:B:344:VAL:HG21	1.98	0.44
1:B:58:SER:HB3	1:B:333:LEU:HD13	1.98	0.44
1:A:20:TYR:CD2	1:A:61:PRO:HB2	2.52	0.44
2:A:1353:FAD:N1	2:A:1353:FAD:C2'	2.79	0.44
1:B:65:MET:HE3	1:B:73:PRO:CB	2.48	0.43
1:B:128:THR:HG21	1:B:289:HIS:CE1	2.53	0.43
1:B:75:ARG:NH1	3:B:1358:SO4:O3	2.51	0.43
1:B:342:GLU:HA	1:B:342:GLU:OE1	2.19	0.43
4:A:2029:HOH:O	1:B:114:ARG:HD2	2.19	0.43
1:A:188:THR:CG2	4:A:2036:HOH:O	2.50	0.42
1:B:159:ALA:N	1:B:160:PRO:CD	2.82	0.42
1:A:176:ALA:HB2	1:A:235:ILE:HD12	2.00	0.42
1:B:9:ILE:HG23	1:B:99:VAL:HG21	2.01	0.42
1:B:42:TRP:CZ3	1:B:49:LEU:HD21	2.54	0.42
1:B:198:PHE:CE1	1:B:235:ILE:HD12	2.55	0.42
1:A:101:ARG:NH2	1:A:112:VAL:HG21	2.35	0.42
1:B:53:SER:HB3	1:B:57:TRP:HB2	2.01	0.42
1:A:144:SER:O	1:A:261:PRO:HA	2.20	0.41
1:A:44:HIS:HB3	3:A:1355:SO4:O2	2.20	0.41
1:B:7:VAL:HG23	1:B:121:ALA:HB2	2.01	0.41
1:A:284:ARG:HH11	1:A:284:ARG:HG2	1.80	0.41
1:A:98:ARG:NH1	3:A:1354:SO4:O2	2.39	0.41
1:A:12:GLY:O	1:A:16:LEU:HG	2.20	0.41
1:A:287:LEU:HA	1:A:289:HIS:CE1	2.56	0.41
1:A:110:ARG:HE	1:A:118:GLN:NE2	2.19	0.41
1:A:284:ARG:NH1	1:A:284:ARG:CG	2.66	0.40
1:B:57:TRP:O	1:B:334:ILE:HB	2.22	0.40
1:B:268:ASP:OD1	1:B:270:THR:OG1	2.31	0.40
1:A:301:GLN:HG2	1:A:325:TRP:CE2	2.56	0.40
1:A:314:VAL:HA	1:A:315:PRO:HD3	1.81	0.40
1:B:41:ALA:HB2	2:B:1353:FAD:O2A	2.21	0.40
1:B:162:ALA:HA	1:B:185:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

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	327/357 (92%)	304 (93%)	22 (7%)	1 (0%)	50	81
1	B	327/357 (92%)	303 (93%)	22 (7%)	2 (1%)	33	65
All	All	654/714 (92%)	607 (93%)	44 (7%)	3 (0%)	38	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	TYR
1	B	139	TYR
1	B	205	GLY

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	250/272 (92%)	226 (90%)	24 (10%)	12	27
1	B	250/272 (92%)	228 (91%)	22 (9%)	14	32
All	All	500/544 (92%)	454 (91%)	46 (9%)	13	29

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASP
1	A	3	SER

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Mol	Chain	Res	Type
1	A	51	LEU
1	A	52	PHE
1	A	87	GLN
1	A	98	ARG
1	A	110	ARG
1	A	117	ARG
1	A	122	ARG
1	A	140	GLN
1	A	150	LEU
1	A	157	THR
1	A	188	THR
1	A	192	THR
1	A	195	GLU
1	A	235	ILE
1	A	242	LEU
1	A	245	ARG
1	A	284	ARG
1	A	291	LYS
1	A	302	VAL
1	A	336	VAL
1	A	347	VAL
1	B	3	SER
1	B	51	LEU
1	B	52	PHE
1	B	68	SER
1	B	87	GLN
1	B	98	ARG
1	B	101	ARG
1	B	108	ARG
1	B	117	ARG
1	B	122	ARG
1	B	150	LEU
1	B	192	THR
1	B	195	GLU
1	B	207	VAL
1	B	235	ILE
1	B	242	LEU
1	B	245	ARG
1	B	253	VAL
1	B	258	ARG
1	B	284	ARG
1	B	304	VAL

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Mol	Chain	Res	Type
1	B	347	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	84	GLN
1	A	118	GLN
1	A	140	GLN
1	A	149	GLN
1	A	154	HIS
1	A	326	ASN
1	B	100	GLN
1	B	118	GLN
1	B	149	GLN
1	B	154	HIS
1	B	301	GLN
1	B	326	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

22 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	#$|Z| > 2$
2	FAD	A	1353	-	58,58,58	1.57	7 (12%)	85,89,89	2.58	25 (29%)
3	SO4	A	1354	-	4,4,4	0.09	0	6,6,6	0.22	0
3	SO4	A	1355	-	4,4,4	0.35	0	6,6,6	0.91	1 (16%)
3	SO4	A	1356	-	4,4,4	0.35	0	6,6,6	0.11	0
3	SO4	A	1357	-	4,4,4	0.31	0	6,6,6	0.39	0
3	SO4	A	1358	-	4,4,4	0.47	0	6,6,6	0.55	0
3	SO4	A	1359	-	4,4,4	0.08	0	6,6,6	0.30	0
3	SO4	A	1360	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	A	1361	-	4,4,4	0.39	0	6,6,6	0.79	0
3	SO4	A	1362	-	4,4,4	0.26	0	6,6,6	0.49	0
3	SO4	A	1363	-	4,4,4	0.13	0	6,6,6	0.21	0
3	SO4	A	1364	-	4,4,4	0.36	0	6,6,6	1.00	1 (16%)
2	FAD	B	1353	-	58,58,58	1.93	8 (13%)	85,89,89	2.81	31 (36%)
3	SO4	B	1354	-	4,4,4	0.11	0	6,6,6	0.17	0
3	SO4	B	1355	-	4,4,4	0.30	0	6,6,6	0.63	0
3	SO4	B	1356	-	4,4,4	0.14	0	6,6,6	0.54	0
3	SO4	B	1357	-	4,4,4	0.15	0	6,6,6	0.64	0
3	SO4	B	1358	-	4,4,4	0.21	0	6,6,6	0.25	0
3	SO4	B	1359	-	4,4,4	0.09	0	6,6,6	0.14	0
3	SO4	B	1360	-	4,4,4	0.28	0	6,6,6	0.50	0
3	SO4	B	1361	-	4,4,4	0.26	0	6,6,6	0.70	0
3	SO4	B	1362	-	4,4,4	1.87	2 (50%)	6,6,6	0.32	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
2	FAD	A	1353	-	3/3/9/9	0/34/50/50	0/1/6/6
3	SO4	A	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1357	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1358	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1359	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1360	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1361	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1362	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1363	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1364	-	-	0/0/0/0	0/0/0/0
2	FAD	B	1353	-	3/3/9/9	0/34/50/50	0/1/6/6
3	SO4	B	1354	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1356	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1357	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1358	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1359	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1360	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1361	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1362	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1353	FAD	O4B-C1B	8.28	1.54	1.41
2	A	1353	FAD	O4B-C1B	5.49	1.49	1.41
2	A	1353	FAD	C5X-N5	5.07	1.43	1.35
2	B	1353	FAD	P-O3P	4.43	1.67	1.59
2	B	1353	FAD	C9A-N10	4.03	1.44	1.38
2	B	1353	FAD	P-O1P	4.03	1.66	1.51
2	B	1353	FAD	C1'-C2'	3.58	1.55	1.51
2	A	1353	FAD	C4X-N5	3.45	1.43	1.36
2	B	1353	FAD	C5X-N5	3.22	1.40	1.35
2	A	1353	FAD	P-O1P	2.85	1.62	1.51
2	B	1353	FAD	C4A-N9A	-2.82	1.33	1.37
2	A	1353	FAD	C5'-C4'	2.58	1.55	1.51
2	B	1353	FAD	C4X-N5	2.49	1.41	1.36
3	B	1362	SO4	O2-S	-2.28	1.39	1.47
2	A	1353	FAD	C2'-C3'	2.17	1.58	1.53
2	A	1353	FAD	C2B-C3B	-2.11	1.47	1.53
3	B	1362	SO4	O4-S	-2.08	1.40	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1353	FAD	O4B-C1B-N9A	9.73	117.49	108.44
2	B	1353	FAD	N3A-C2A-N1A	-9.61	120.68	128.71
2	B	1353	FAD	C3B-C2B-C1B	-8.97	86.87	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1353	FAD	C2'-C1'-N10	-8.50	101.18	112.45
2	A	1353	FAD	C3B-C2B-C1B	-8.12	88.20	100.91
2	B	1353	FAD	C4B-O4B-C1B	-7.92	101.15	109.75
2	A	1353	FAD	O4B-C4B-C3B	-7.09	90.79	105.17
2	A	1353	FAD	N3A-C2A-N1A	-6.05	123.65	128.71
2	A	1353	FAD	C2B-C3B-C4B	-6.05	90.60	102.65
2	A	1353	FAD	C4B-O4B-C1B	-6.03	103.20	109.75
2	B	1353	FAD	C2B-C3B-C4B	-5.64	91.41	102.65
2	B	1353	FAD	C2'-C1'-N10	-5.18	105.58	112.45
2	B	1353	FAD	O4B-C4B-C3B	-4.88	95.28	105.17
2	B	1353	FAD	C4X-N5-C5X	4.85	122.14	116.69
2	B	1353	FAD	C2-N1-C10	4.64	119.66	114.98
2	A	1353	FAD	O4B-C1B-N9A	4.63	112.74	108.44
2	A	1353	FAD	O4B-C1B-C2B	-4.22	100.30	106.77
2	A	1353	FAD	O2'-C2'-C3'	4.03	119.08	109.05
2	A	1353	FAD	N3A-C4A-N9A	4.01	132.68	125.43
2	B	1353	FAD	O4B-C4B-C5B	3.97	123.52	109.36
2	A	1353	FAD	C1'-N10-C9A	3.86	122.63	118.87
2	B	1353	FAD	N3A-C4A-N9A	3.69	132.09	125.43
2	A	1353	FAD	C5X-C9A-N10	3.54	120.29	116.80
2	A	1353	FAD	C2-N1-C10	3.50	118.51	114.98
2	B	1353	FAD	C1'-N10-C9A	3.44	122.22	118.87
2	A	1353	FAD	C9A-N10-C10	-3.36	118.47	121.77
2	B	1353	FAD	O4B-C1B-C2B	-3.26	101.77	106.77
2	B	1353	FAD	C4X-C10-N1	-3.26	119.47	122.73
2	A	1353	FAD	O4B-C4B-C5B	3.20	120.77	109.36
2	A	1353	FAD	C4A-C5A-N7A	-3.02	106.93	109.52
2	B	1353	FAD	C4-C4X-C10	2.83	121.52	116.95
2	B	1353	FAD	O3P-PA-O5B	-2.79	90.95	103.41
2	A	1353	FAD	C8A-N9A-C4A	2.77	109.02	106.90
2	B	1353	FAD	C4-N3-C2	-2.64	119.98	125.39
2	B	1353	FAD	O2B-C2B-C1B	2.58	119.02	111.23
2	A	1353	FAD	C6-C5X-N5	2.54	121.94	118.97
2	A	1353	FAD	C8M-C8-C9	-2.50	114.34	120.38
2	B	1353	FAD	O5B-PA-O1A	2.50	119.17	109.37
2	B	1353	FAD	C5X-C9A-N10	2.46	119.22	116.80
2	A	1353	FAD	C4-N3-C2	-2.40	120.47	125.39
2	B	1353	FAD	C9A-N10-C10	-2.39	119.42	121.77
2	B	1353	FAD	C5A-C4A-N3A	-2.38	120.52	125.70
2	A	1353	FAD	O5B-PA-O1A	2.36	118.63	109.37
2	B	1353	FAD	C9A-C5X-N5	-2.35	118.77	122.37
2	B	1353	FAD	P-O3P-PA	-2.33	124.84	131.68

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1353	FAD	C2A-N3A-C4A	2.28	120.51	114.01
2	B	1353	FAD	O3'-C3'-C2'	2.28	114.50	108.74
2	B	1353	FAD	O2B-C2B-C3B	-2.24	104.54	111.83
2	A	1353	FAD	N7A-C8A-N9A	-2.24	108.02	114.36
2	A	1353	FAD	C5A-C4A-N3A	-2.24	120.83	125.70
2	A	1353	FAD	C1B-N9A-C4A	-2.22	122.80	126.64
2	B	1353	FAD	C1B-N9A-C4A	-2.21	122.82	126.64
2	B	1353	FAD	C4A-C5A-N7A	-2.20	107.63	109.52
2	B	1353	FAD	C6-C5X-C9A	2.15	121.99	119.02
3	A	1355	SO4	O2-S-O1	-2.12	102.53	109.53
2	B	1353	FAD	O2'-C2'-C3'	2.07	114.19	109.05
2	A	1353	FAD	O3B-C3B-C4B	2.06	117.16	111.08
3	A	1364	SO4	O2-S-O1	-2.03	102.81	109.53

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1353	FAD	C4B
2	B	1353	FAD	C2'
2	B	1353	FAD	C3B
2	A	1353	FAD	C4B
2	A	1353	FAD	C2'
2	A	1353	FAD	C3B

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	330/357 (92%)	-0.29	2 (0%)	86	91	11, 19, 41, 54	0
1	B	330/357 (92%)	-0.25	0	100	100	10, 23, 39, 60	0
All	All	660/714 (92%)	-0.27	2 (0%)	90	95	10, 21, 40, 60	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	ALA	3.3
1	A	352	ALA	2.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	A	1360	5/5	0.42	13.03	90,96,96,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	1359	5/5	0.21	8.36	65,66,74,74	0
3	SO4	B	1361	5/5	0.14	2.73	45,49,51,55	0
3	SO4	A	1359	5/5	0.17	2.00	59,59,61,64	0
3	SO4	B	1357	5/5	0.17	1.93	45,47,49,55	0
3	SO4	A	1363	5/5	0.18	1.42	62,64,73,76	0
3	SO4	A	1355	5/5	0.16	1.00	36,38,39,39	0
3	SO4	B	1362	5/5	0.20	0.35	60,61,63,64	0
3	SO4	B	1356	5/5	0.15	0.11	57,57,62,66	0
3	SO4	A	1361	5/5	0.20	0.04	37,37,39,41	0
3	SO4	B	1354	5/5	0.13	-0.04	56,60,61,61	0
2	FAD	A	1353	53/53	0.13	-0.08	11,15,17,18	0
2	FAD	B	1353	53/53	0.13	-0.33	13,15,18,19	0
3	SO4	A	1362	5/5	0.12	-0.62	32,33,36,36	0
3	SO4	A	1354	5/5	0.15	-0.65	58,61,63,64	0
3	SO4	B	1360	5/5	0.10	-0.84	31,31,31,32	0
3	SO4	A	1358	5/5	0.12	-1.46	29,30,30,31	0
3	SO4	B	1358	5/5	0.13	-1.47	43,44,44,45	0
3	SO4	A	1357	5/5	0.10	-1.55	31,33,35,35	0
3	SO4	A	1356	5/5	0.12	-1.66	38,40,42,43	0
3	SO4	A	1364	5/5	0.09	-2.22	30,34,37,40	0
3	SO4	B	1355	5/5	0.09	-3.40	32,34,35,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.