Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 07:26 PM EST

PDB ID	:	1KRH
Title	:	X-ray Structure of Benzoate Dioxygenase Reductase
Authors	:	Karlsson, A.; Beharry, Z.M.; Eby, D.M.; Coulter, E.D.; Niedle, E.L.; Kurtz Jr., D.M.; Eklund, H.; Ramaswamy, S.
Deposited on	:	2002-01-09
Resolution	:	1.50 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
http://wwpdb.org/validation/2016/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:

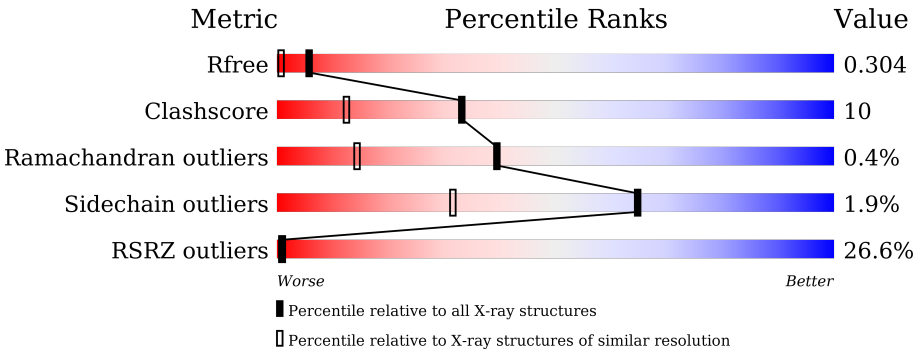
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	12% 86% 12%
1	B	338	41% 76% 23%

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
2	SO4	A	401	-	-	-	X
2	SO4	A	402	-	-	-	X
2	SO4	B	403	-	-	X	-
2	SO4	B	404	-	-	X	-
3	FES	A	500	-	-	X	-
3	FES	B	600	-	-	X	-

2 Entry composition

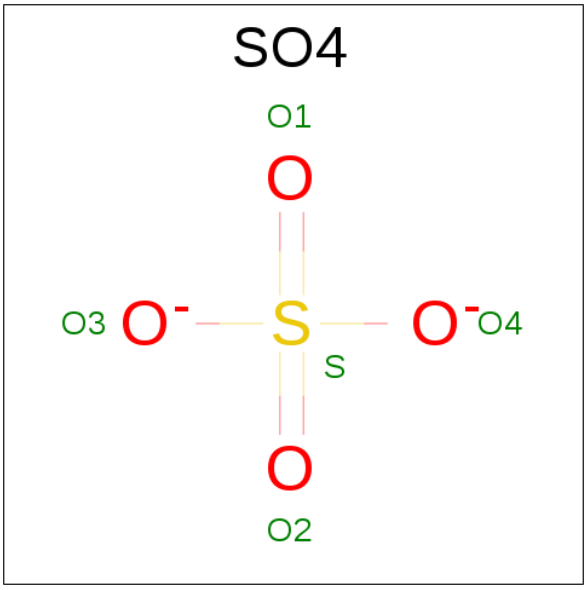
There are 5 unique types of molecules in this entry. The entry contains 5773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Benzoate 1,2-Dioxygenase Reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	3	0	0
			2635	1656	447	515	17			
1	B	337	Total	C	N	O	S	3	0	0
			2635	1656	447	515	17			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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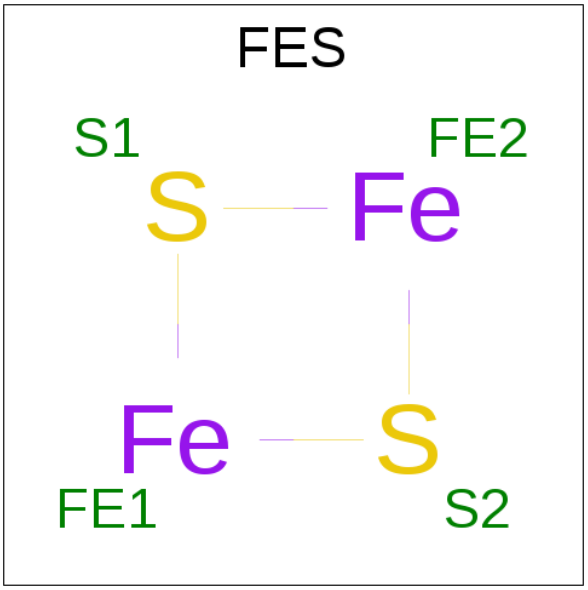
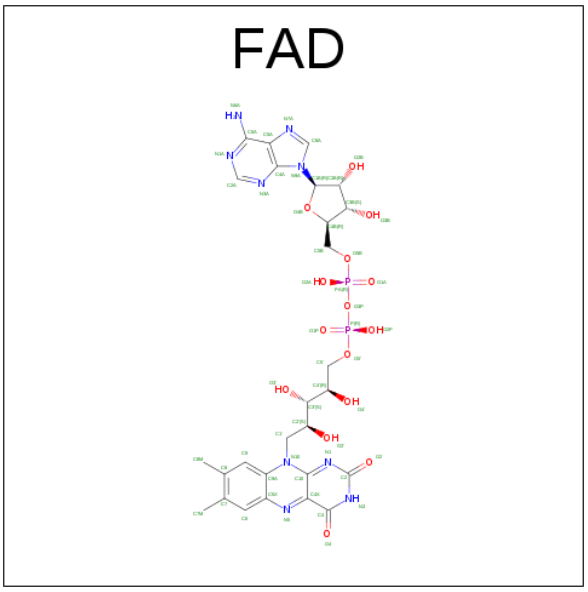
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is water.

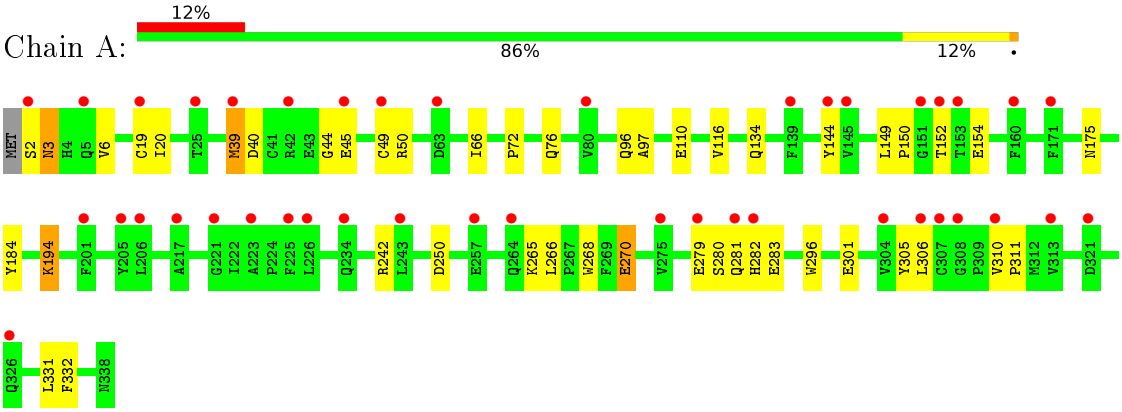
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	283	Total	O	0	0
			283	283		
5	B	81	Total	O	0	0
			81	81		

3 Residue-property plots (i)

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.

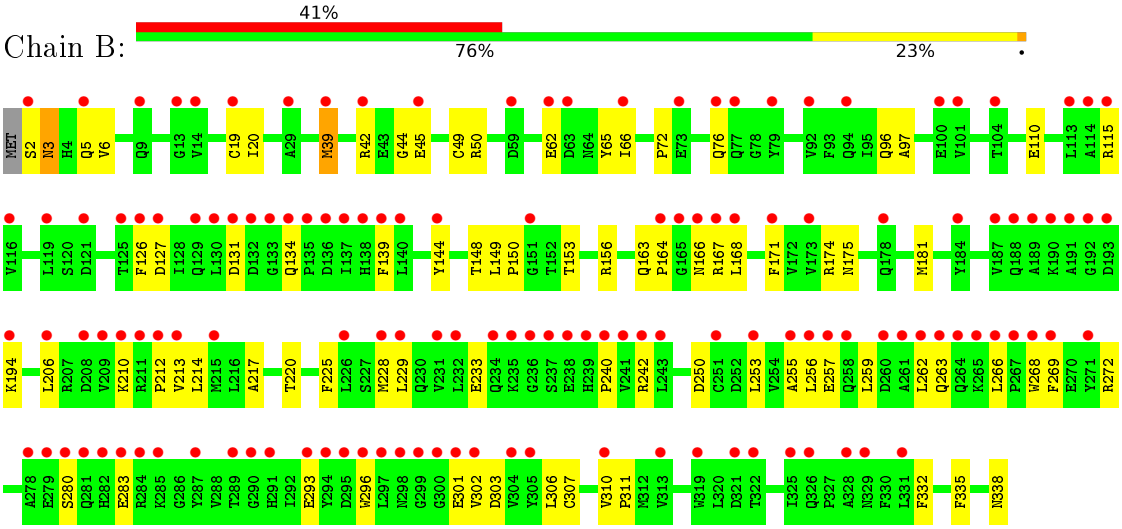
- Molecule 1: Benzoate 1,2-Dioxygenase Reductase

Chain A:



- Molecule 1: Benzoate 1,2-Dioxygenase Reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	94.09Å 100.68Å 153.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 1.50 9.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (9.00-1.50) 94.6 (9.00-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.249 0.301 , 0.304	Depositor DCC
R_{free} test set	5515 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.57 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5773	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/2694	0.62	0/3655
1	B	0.32	0/2694	0.57	0/3655
All	All	0.33	0/5388	0.60	0/7310

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	2635	0	2515	40	0
1	B	2635	0	2515	71	0
2	A	15	0	0	0	0
2	B	10	0	0	6	0
3	A	4	0	0	2	0
3	B	4	0	0	2	0
4	A	53	0	31	1	0
4	B	53	0	31	4	0
5	A	283	0	0	5	0
5	B	81	0	0	2	0
All	All	5773	0	5092	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (108) 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)
1:A:50:ARG:HE	1:A:96:GLN:HE22	1.09	0.95
1:B:50:ARG:HE	1:B:96:GLN:HE22	1.14	0.94
1:A:45:GLU:HG3	1:A:66:ILE:HD11	1.55	0.89
1:B:233:GLU:HA	1:B:268:TRP:HZ2	1.41	0.82
1:B:149:LEU:HA	1:B:181:MET:HE1	1.62	0.81
1:B:110:GLU:H	1:B:134:GLN:HE21	1.27	0.79
1:B:212:PRO:HG3	1:B:240:PRO:HD2	1.66	0.76
1:B:110:GLU:H	1:B:134:GLN:NE2	1.83	0.76
1:B:153:THR:CG2	2:B:403:SO4:O1	2.32	0.76
1:B:156:ARG:HD2	4:B:601:FAD:O4'	1.87	0.73
1:A:152:THR:HG23	1:A:154:GLU:H	1.53	0.72
1:A:45:GLU:HG2	5:A:734:HOH:O	1.90	0.71
1:B:206:LEU:HB2	1:B:228:MET:SD	2.32	0.69
1:A:6:VAL:HG21	1:A:20:ILE:HD12	1.74	0.69
1:A:149:LEU:O	1:A:152:THR:HG22	1.93	0.69
1:A:3:ASN:HD21	1:A:19:CYS:HB3	1.57	0.68
1:A:279:GLU:HG3	5:A:761:HOH:O	1.93	0.68
1:B:149:LEU:HA	1:B:181:MET:CE	2.23	0.68
1:B:6:VAL:HG21	1:B:20:ILE:HD12	1.76	0.68
1:B:153:THR:HG23	2:B:403:SO4:O1	1.93	0.67
1:B:45:GLU:HG2	5:B:650:HOH:O	1.95	0.66
1:B:3:ASN:HD21	1:B:19:CYS:HB3	1.59	0.66
1:B:233:GLU:HA	1:B:268:TRP:CZ2	2.28	0.65
1:B:272:ARG:NH1	1:B:293:GLU:HG2	2.11	0.64
1:B:272:ARG:HH12	1:B:293:GLU:HG2	1.61	0.63
1:B:262:LEU:O	1:B:266:LEU:HB2	1.99	0.63
1:B:210:LYS:HD2	2:B:404:SO4:O1	1.98	0.63
1:B:212:PRO:O	1:B:302:VAL:HG23	2.00	0.62
1:A:110:GLU:H	1:A:134:GLN:HE21	1.49	0.61
1:A:110:GLU:H	1:A:134:GLN:NE2	1.99	0.60
1:B:257:GLU:H	1:B:257:GLU:CD	2.05	0.60
1:B:139:PHE:CE2	1:B:164:PRO:HG3	2.36	0.60
1:A:194:LYS:HG3	5:A:554:HOH:O	2.01	0.59
1:A:2:SER:O	1:A:3:ASN:HB3	2.02	0.59
1:B:272:ARG:HH12	1:B:293:GLU:CG	2.15	0.58
1:B:166:ASN:OD1	1:B:168:LEU:HB3	2.04	0.58
1:B:72:PRO:O	1:B:76:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:SER:O	1:B:3:ASN:HB3	2.04	0.57
1:A:72:PRO:O	1:A:76:GLN:HG3	2.06	0.56
1:B:62:GLU:HA	1:B:65:TYR:CE2	2.41	0.56
1:B:253:LEU:HD13	1:B:256:LEU:HD11	1.89	0.55
1:B:266:LEU:HD13	1:B:268:TRP:CZ2	2.42	0.55
1:B:212:PRO:HA	1:B:240:PRO:O	2.08	0.54
1:B:50:ARG:HE	1:B:96:GLN:NE2	1.96	0.54
1:B:263:GLN:HG3	1:B:269:PHE:O	2.08	0.53
1:B:153:THR:HG21	2:B:403:SO4:O1	2.08	0.53
1:A:266:LEU:HD13	1:A:268:TRP:CZ2	2.43	0.53
1:A:242:ARG:HD3	1:A:296:TRP:CD2	2.43	0.53
1:B:213:VAL:HG12	1:B:214:LEU:N	2.24	0.53
1:B:229:LEU:HB3	1:B:262:LEU:CD1	2.40	0.52
1:B:280:SER:HB3	1:B:283:GLU:CD	2.29	0.52
1:B:50:ARG:NE	1:B:96:GLN:HE22	1.96	0.52
1:B:97:ALA:HB2	5:B:671:HOH:O	2.09	0.52
1:A:281:GLN:NE2	1:B:338:ASN:HA	2.26	0.51
1:B:210:LYS:CD	2:B:404:SO4:O1	2.57	0.51
1:A:44:GLY:HA2	3:A:500:FES:S2	2.52	0.50
1:B:144:TYR:CE2	4:B:601:FAD:HM72	2.47	0.50
1:B:310:VAL:HB	1:B:311:PRO:HD3	1.94	0.50
1:A:250:ASP:OD1	1:A:283:GLU:OE2	2.30	0.49
1:A:282:HIS:CE1	1:B:338:ASN:O	2.65	0.49
1:A:39:MET:HG2	1:A:49:CYS:HB3	1.94	0.49
1:B:45:GLU:HG3	1:B:66:ILE:HD11	1.93	0.49
1:A:97:ALA:HB2	5:A:517:HOH:O	2.12	0.49
1:B:307:CYS:SG	1:B:335:PHE:CE1	3.06	0.49
1:A:242:ARG:HG2	1:A:270:GLU:HG2	1.95	0.49
1:B:302:VAL:HG22	1:B:303:ASP:N	2.28	0.48
1:B:166:ASN:C	1:B:168:LEU:H	2.17	0.47
1:B:115:ARG:NE	1:B:127:ASP:OD2	2.47	0.46
1:B:134:GLN:HB2	1:B:167:ARG:HH22	1.80	0.46
1:B:293:GLU:O	1:B:296:TRP:HB2	2.15	0.46
1:B:174:ARG:N	1:B:220:THR:HG21	2.31	0.46
1:A:50:ARG:NE	1:A:96:GLN:HE22	1.93	0.46
1:B:110:GLU:N	1:B:134:GLN:NE2	2.59	0.46
1:B:39:MET:HG2	1:B:49:CYS:HB3	1.98	0.45
1:A:305:TYR:CE2	1:A:331:LEU:HD12	2.52	0.45
1:A:149:LEU:HB3	1:A:152:THR:CG2	2.47	0.45
1:B:144:TYR:CD2	4:B:601:FAD:HM72	2.51	0.45
1:B:166:ASN:C	1:B:168:LEU:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HD3	1:A:296:TRP:CE2	2.52	0.44
1:A:50:ARG:HE	1:A:96:GLN:NE2	1.93	0.44
1:B:255:ALA:O	1:B:259:LEU:HG	2.17	0.44
1:B:250:ASP:OD1	1:B:283:GLU:OE2	2.35	0.44
1:B:217:ALA:HB2	1:B:225:PHE:CD1	2.53	0.44
1:A:149:LEU:HD23	1:A:152:THR:HG21	1.99	0.43
1:A:150:PRO:HG2	1:A:184:TYR:CE2	2.54	0.43
1:B:306:LEU:O	1:B:332:PHE:HA	2.18	0.43
1:B:131:ASP:O	1:B:134:GLN:HB2	2.19	0.43
1:B:131:ASP:O	1:B:167:ARG:NH2	2.52	0.43
1:B:44:GLY:HA2	3:B:600:FES:S2	2.58	0.42
1:B:39:MET:SD	1:B:42:ARG:HG2	2.60	0.42
1:A:280:SER:HB3	1:A:283:GLU:CD	2.40	0.42
1:A:306:LEU:O	1:A:332:PHE:HA	2.20	0.42
1:B:153:THR:OG1	2:B:403:SO4:O3	2.31	0.42
1:A:242:ARG:HD3	1:A:296:TRP:CG	2.55	0.42
1:A:265:LYS:HG2	1:A:265:LYS:O	2.19	0.42
1:B:126:PHE:CE2	1:B:171:PHE:HB2	2.55	0.42
4:B:601:FAD:H1'1	4:B:601:FAD:H9	1.90	0.41
1:B:242:ARG:HD3	1:B:296:TRP:CG	2.56	0.41
1:A:282:HIS:NE2	1:B:338:ASN:OXT	2.52	0.41
1:B:148:THR:O	1:B:150:PRO:HD3	2.21	0.41
1:A:281:GLN:HE22	1:B:338:ASN:HA	1.85	0.41
1:B:39:MET:HG2	3:B:600:FES:S1	2.61	0.41
1:A:39:MET:HG2	3:A:500:FES:S1	2.60	0.40
1:B:229:LEU:HB3	1:B:262:LEU:HD13	2.04	0.40
1:A:144:TYR:CD2	4:A:501:FAD:HM72	2.55	0.40
1:A:266:LEU:HD13	1:A:268:TRP:CH2	2.57	0.40
1:A:310:VAL:HB	1:A:311:PRO:HD3	2.03	0.40
1:A:116:VAL:HG22	5:A:778:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	335/338 (99%)	331 (99%)	2 (1%)	2 (1%)	30 8
1	B	335/338 (99%)	323 (96%)	11 (3%)	1 (0%)	46 19
All	All	670/676 (99%)	654 (98%)	13 (2%)	3 (0%)	39 14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	B	3	ASN
1	A	40	ASP

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	287/288 (100%)	282 (98%)	5 (2%)	68 37
1	B	287/288 (100%)	281 (98%)	6 (2%)	61 27
All	All	574/576 (100%)	563 (98%)	11 (2%)	65 31

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	MET
1	A	175	ASN
1	A	194	LYS
1	A	270	GLU
1	A	301	GLU
1	B	5	GLN
1	B	39	MET
1	B	163	GLN
1	B	175	ASN
1	B	194	LYS

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Mol	Chain	Res	Type
1	B	301	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	5	GLN
1	A	77	GLN
1	A	96	GLN
1	A	134	GLN
1	A	175	ASN
1	A	188	GLN
1	A	249	GLN
1	A	281	GLN
1	B	3	ASN
1	B	5	GLN
1	B	77	GLN
1	B	96	GLN
1	B	134	GLN
1	B	175	ASN
1	B	188	GLN
1	B	249	GLN
1	B	281	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 carbohydrates in this entry.

5.6 Ligand geometry

9 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	SO4	A	400	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	A	401	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	A	402	-	4,4,4	0.16	0	6,6,6	0.09	0
3	FES	A	500	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	A	501	-	52,58,58	2.54	20 (38%)	52,89,89	2.22	15 (28%)
2	SO4	B	403	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	B	404	-	4,4,4	0.27	0	6,6,6	0.08	0
3	FES	B	600	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	B	601	-	52,58,58	1.84	13 (25%)	52,89,89	2.88	12 (23%)

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	SO4	A	400	-	-	0/0/0/0	0/0/0/0
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	FES	A	500	1	-	0/0/4/4	0/1/1/1
4	FAD	A	501	-	-	0/30/50/50	0/6/6/6
2	SO4	B	403	-	-	0/0/0/0	0/0/0/0
2	SO4	B	404	-	-	0/0/0/0	0/0/0/0
3	FES	B	600	1	-	0/0/4/4	0/1/1/1
4	FAD	B	601	-	-	0/30/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	FAD	C10-N10	-5.87	1.32	1.39
4	A	501	FAD	P-O2P	-4.99	1.33	1.55
4	A	501	FAD	C2-N1	-3.63	1.30	1.38
4	A	501	FAD	C4-C4X	-3.59	1.33	1.41
4	A	501	FAD	C2B-C1B	-3.13	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	FAD	C4A-N3A	-3.11	1.31	1.35
4	A	501	FAD	C2'-C3'	-2.58	1.48	1.53
4	A	501	FAD	C8M-C8	-2.57	1.45	1.51
4	B	601	FAD	C2-N1	-2.54	1.32	1.38
4	B	601	FAD	O5'-C5'	-2.49	1.34	1.44
4	A	501	FAD	O4'-C4'	-2.48	1.37	1.43
4	A	501	FAD	O5B-C5B	-2.37	1.35	1.44
4	B	601	FAD	C4'-C3'	-2.36	1.48	1.53
4	A	501	FAD	PA-O2A	-2.36	1.45	1.55
4	B	601	FAD	PA-O1A	-2.32	1.42	1.51
4	A	501	FAD	O4B-C4B	-2.11	1.40	1.45
4	B	601	FAD	O4'-C4'	-2.05	1.38	1.43
4	A	501	FAD	O3B-C3B	2.03	1.47	1.43
4	B	601	FAD	O4-C4	2.18	1.30	1.24
4	A	501	FAD	PA-O5B	2.21	1.68	1.59
4	A	501	FAD	C5'-C4'	2.32	1.55	1.51
4	B	601	FAD	C2A-N3A	2.50	1.36	1.32
4	B	601	FAD	O4B-C1B	2.87	1.45	1.41
4	A	501	FAD	C2A-N3A	2.90	1.37	1.32
4	B	601	FAD	C5X-N5	3.13	1.40	1.35
4	B	601	FAD	C4X-N5	3.30	1.38	1.33
4	A	501	FAD	C4X-C10	3.88	1.48	1.40
4	B	601	FAD	C5'-C4'	4.11	1.58	1.51
4	B	601	FAD	C9A-N10	4.57	1.45	1.38
4	B	601	FAD	C4-N3	4.63	1.41	1.33
4	A	501	FAD	C4-N3	4.92	1.41	1.33
4	A	501	FAD	C9A-N10	6.12	1.47	1.38
4	A	501	FAD	C4X-N5	7.20	1.44	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	FAD	N3A-C2A-N1A	-11.86	119.56	128.87
4	A	501	FAD	N3A-C2A-N1A	-6.60	123.69	128.87
4	B	601	FAD	N3-C2-N1	-6.17	117.30	127.69
4	A	501	FAD	C4X-C4-N3	-5.00	116.99	123.52
4	B	601	FAD	C4X-C10-N10	-4.62	117.16	120.52
4	A	501	FAD	C5X-C9A-N10	-4.41	114.27	117.58
4	B	601	FAD	C4X-C4-N3	-3.83	118.51	123.52
4	B	601	FAD	C4-C4X-C10	-3.61	117.63	119.94
4	A	501	FAD	N3-C2-N1	-3.08	122.51	127.69
4	B	601	FAD	C5X-C9A-N10	-3.03	115.30	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	FAD	C6-C5X-C9A	-2.73	116.10	119.11
4	A	501	FAD	O4B-C1B-N9A	-2.61	103.18	108.11
4	A	501	FAD	C9-C8-C7	-2.45	115.17	119.97
4	A	501	FAD	C1'-C2'-C3'	2.04	115.67	109.82
4	A	501	FAD	C8M-C8-C7	2.12	125.28	120.73
4	A	501	FAD	C1B-N9A-C4A	2.17	129.23	126.81
4	B	601	FAD	O2P-P-O1P	2.19	123.95	112.56
4	B	601	FAD	O2B-C2B-C1B	2.19	118.48	111.61
4	A	501	FAD	C4B-O4B-C1B	2.24	112.02	109.64
4	B	601	FAD	C1B-N9A-C4A	2.43	129.52	126.81
4	A	501	FAD	C4X-C10-N10	3.10	122.77	120.52
4	A	501	FAD	C4X-N5-C5X	3.16	120.45	116.72
4	B	601	FAD	C4-C4X-N5	4.82	124.56	118.70
4	A	501	FAD	C4-C4X-C10	4.88	123.06	119.94
4	A	501	FAD	C4-N3-C2	5.62	119.84	115.16
4	B	601	FAD	C4X-N5-C5X	7.09	125.08	116.72
4	B	601	FAD	C4-N3-C2	8.20	122.00	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	FES	2	0
4	A	501	FAD	1	0
2	B	403	SO4	4	0
2	B	404	SO4	2	0
3	B	600	FES	2	0
4	B	601	FAD	4	0

5.7 Other polymers

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, 95^{th} 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	337/338 (99%)	1.07	42 (12%) 5 5	9, 10, 13, 16	1 (0%)
1	B	337/338 (99%)	1.93	137 (40%) 0 0	8, 10, 13, 16	1 (0%)
All	All	674/676 (99%)	1.50	179 (26%) 1 1	8, 10, 13, 16	2 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	TRP	8.6
1	B	281	GLN	8.2
1	B	282	HIS	7.6
1	B	133	GLY	6.7
1	A	2	SER	6.7
1	B	132	ASP	6.6
1	B	2	SER	6.4
1	B	257	GLU	5.8
1	B	261	ALA	5.8
1	B	232	LEU	5.7
1	B	135	PRO	5.6
1	B	264	GLN	5.5
1	B	137	ILE	5.4
1	B	138	HIS	5.3
1	B	241	VAL	5.3
1	B	168	LEU	5.2
1	B	266	LEU	5.0
1	B	136	ASP	4.9
1	B	300	GLY	4.8
1	B	234	GLN	4.8
1	B	240	PRO	4.5
1	B	187	VAL	4.5
1	B	166	ASN	4.4
1	B	280	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	269	PHE	4.3
1	B	190	LYS	4.3
1	B	119	LEU	4.2
1	B	115	ARG	4.2
1	B	165	GLY	4.2
1	B	208	ASP	4.1
1	B	294	TYR	4.1
1	B	188	GLN	4.1
1	B	235	LYS	4.1
1	B	114	ALA	4.0
1	B	258	GLN	4.0
1	B	231	VAL	4.0
1	B	295	ASP	3.9
1	B	267	PRO	3.9
1	B	293	GLU	3.9
1	B	265	LYS	3.9
1	B	287	TYR	3.9
1	B	238	GLU	3.8
1	B	113	LEU	3.7
1	B	191	ALA	3.7
1	B	262	LEU	3.6
1	B	329	ASN	3.6
1	B	260	ASP	3.5
1	B	209	VAL	3.5
1	B	302	VAL	3.5
1	B	213	VAL	3.5
1	B	236	GLY	3.4
1	B	184	TYR	3.4
1	B	229	LEU	3.3
1	A	313	VAL	3.3
1	B	62	GLU	3.3
1	B	237	SER	3.2
1	B	42	ARG	3.2
1	B	271	TYR	3.2
1	B	121	ASP	3.2
1	B	279	GLU	3.2
1	B	322	THR	3.2
1	B	301	GLU	3.1
1	B	192	GLY	3.1
1	B	63	ASP	3.1
1	B	239	HIS	3.0
1	B	228	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	151	GLY	3.0
1	A	139	PHE	3.0
1	B	76	GLN	3.0
1	B	253	LEU	3.0
1	B	116	VAL	3.0
1	A	264	GLN	3.0
1	B	256	LEU	3.0
1	B	210	LYS	2.9
1	B	285	LYS	2.9
1	A	144	TYR	2.9
1	B	263	GLN	2.9
1	B	278	ALA	2.9
1	A	310	VAL	2.9
1	B	194	LYS	2.9
1	B	326	GLN	2.9
1	A	217	ALA	2.8
1	A	145	VAL	2.8
1	B	299	GLY	2.8
1	B	134	GLN	2.8
1	B	104	THR	2.8
1	B	328	ALA	2.8
1	B	19	CYS	2.8
1	B	243	LEU	2.8
1	A	49	CYS	2.7
1	A	152	THR	2.7
1	A	153	THR	2.7
1	B	167	ARG	2.7
1	B	164	PRO	2.7
1	A	304	VAL	2.7
1	A	42	ARG	2.7
1	A	205	TYR	2.7
1	A	206	LEU	2.7
1	B	226	LEU	2.7
1	A	234	GLN	2.7
1	A	257	GLU	2.7
1	B	290	GLY	2.7
1	B	29	ALA	2.7
1	B	39	MET	2.7
1	B	283	GLU	2.6
1	B	101	VAL	2.6
1	B	298	ASN	2.6
1	B	5	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	201	PHE	2.6
1	A	307	CYS	2.6
1	B	14	VAL	2.6
1	B	45	GLU	2.6
1	B	206	LEU	2.6
1	B	297	LEU	2.6
1	B	331	LEU	2.6
1	B	126	PHE	2.6
1	A	281	GLN	2.6
1	B	178	GLN	2.6
1	A	45	GLU	2.6
1	B	319	TRP	2.5
1	A	279	GLU	2.5
1	A	63	ASP	2.5
1	A	39	MET	2.5
1	B	127	ASP	2.5
1	B	289	THR	2.5
1	A	226	LEU	2.5
1	A	306	LEU	2.5
1	B	131	ASP	2.5
1	B	212	PRO	2.5
1	B	171	PHE	2.5
1	B	325	ILE	2.5
1	A	321	ASP	2.4
1	A	243	LEU	2.4
1	B	130	LEU	2.4
1	A	151	GLY	2.4
1	B	242	ARG	2.4
1	B	321	ASP	2.4
1	B	140	LEU	2.4
1	B	305	TYR	2.4
1	A	171	PHE	2.4
1	B	296	TRP	2.4
1	A	282	HIS	2.4
1	B	284	ARG	2.4
1	A	326	GLN	2.3
1	B	129	GLN	2.3
1	A	275	VAL	2.3
1	A	225	PHE	2.3
1	B	291	HIS	2.3
1	B	92	VAL	2.3
1	B	211	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	308	GLY	2.3
1	B	77	GLN	2.3
1	B	73	GLU	2.3
1	B	173	VAL	2.3
1	A	160	PHE	2.3
1	B	9	GLN	2.3
1	B	313	VAL	2.3
1	B	189	ALA	2.2
1	B	310	VAL	2.2
1	B	251	CYS	2.2
1	B	59	ASP	2.2
1	B	193	ASP	2.2
1	A	221	GLY	2.2
1	A	223	ALA	2.1
1	A	19	CYS	2.1
1	B	13	GLY	2.1
1	B	100	GLU	2.1
1	A	25	THR	2.1
1	B	94	GLN	2.1
1	B	215	MET	2.1
1	B	139	PHE	2.1
1	B	255	ALA	2.1
1	A	5	GLN	2.0
1	B	79	TYR	2.0
1	A	80	VAL	2.0
1	B	66	ILE	2.0
1	B	144	TYR	2.0
1	B	304	VAL	2.0
1	B	125	THR	2.0

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 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	401	5/5	0.93	0.21	8.92	28,29,29,29	0
2	SO4	A	402	5/5	0.97	0.22	4.29	26,28,28,28	0
4	FAD	B	601	53/53	0.90	0.17	1.23	17,18,20,23	0
4	FAD	A	501	53/53	0.93	0.16	0.96	7,13,20,20	0
2	SO4	B	403	5/5	0.91	0.16	0.82	33,33,33,33	0
3	FES	B	600	4/4	0.98	0.17	0.38	13,14,15,15	0
3	FES	A	500	4/4	0.99	0.17	0.09	11,12,13,13	0
2	SO4	A	400	5/5	0.94	0.13	-	33,33,34,34	0
2	SO4	B	404	5/5	0.90	0.23	-	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.