



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:26 AM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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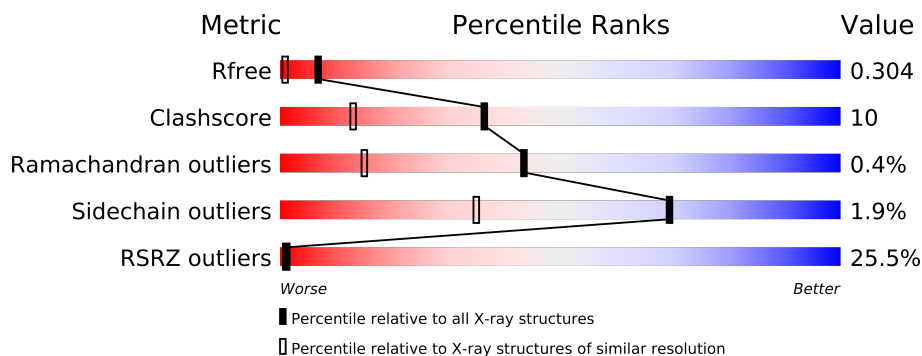
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (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  $\geq 3$ , 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	338	
1	B	338	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	401	-	X
2	SO4	A	402	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5773 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 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<sub>4</sub>S).



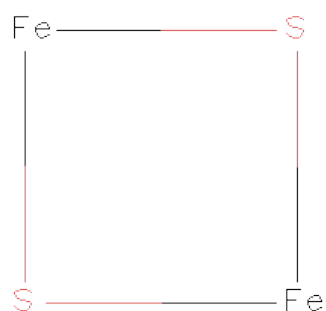
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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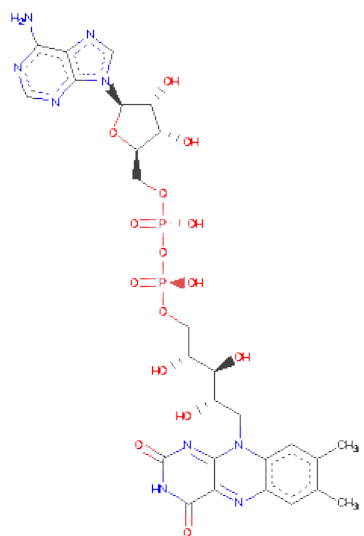
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



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

- Molecule 5 is water.

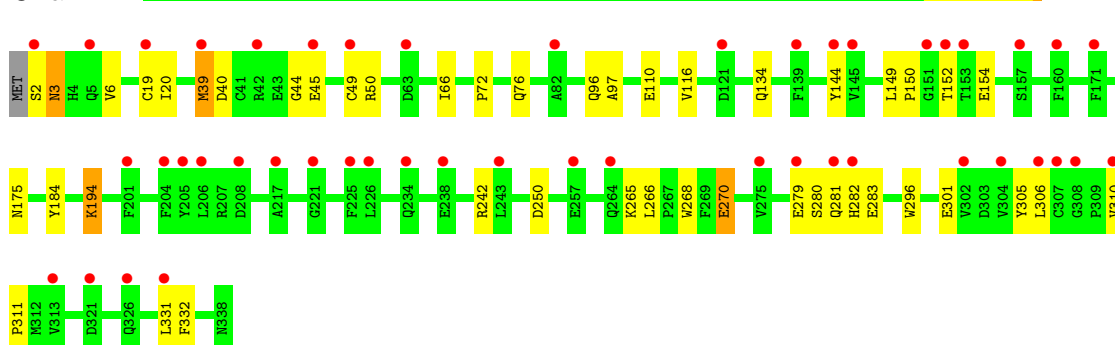
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	283	Total O 283 283	0	0
5	B	81	Total O 81 81	0	0

### 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.

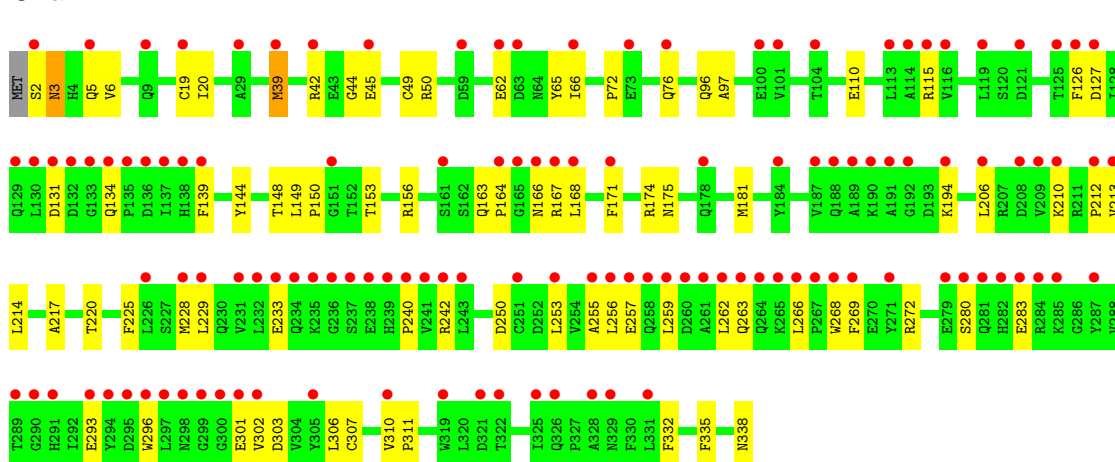
- Molecule 1: Benzoate 1,2-Dioxygenase Reductase

Chain A:



- Molecule 1: Benzoate 1,2-Dioxygenase Reductase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.56 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 109435 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5773	0	5092	108	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 10.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:279:GLU:HG3	5:A:761:HOH:O	1.93	0.68
1:A:3:ASN:HD21	1:A:19:CYS:HB3	1.57	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:B:210:LYS:CD	2:B:404:SO4:O1	2.57	0.51
1:A:281:GLN:NE2	1:B:338:ASN:HA	2.26	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:282:HIS:CE1	1:B:338:ASN:O	2.65	0.49
1:A:250:ASP:OD1	1:A:283:GLU:OE2	2.30	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:B:144:TYR:CD2	4:B:601:FAD:HM72	2.51	0.45
1:A:149:LEU:HB3	1:A:152:THR:CG2	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:166:ASN:C	1:B:168:LEU:N	2.70	0.45
1:A:50:ARG:HE	1:A:96:GLN:NE2	1.93	0.44
1:A:242:ARG:HD3	1:A:296:TRP:CE2	2.52	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:B:126:PHE:CE2	1:B:171:PHE:HB2	2.55	0.42
1:A:265:LYS:HG2	1:A:265:LYS:O	2.19	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:B:229:LEU:HB3	1:B:262:LEU:HD13	2.04	0.40
1:A:39:MET:HG2	3:A:500:FES:S1	2.60	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

### 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	335/338 (99%)	331 (99%)	2 (1%)	2 (1%)	33	9
1	B	335/338 (99%)	323 (96%)	11 (3%)	1 (0%)	50	20
All	All	670/676 (99%)	654 (98%)	13 (2%)	3 (0%)	43	15

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 ⓘ

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%)	73	41
1	B	287/288 (100%)	281 (98%)	6 (2%)	66	30
All	All	574/576 (100%)	563 (98%)	11 (2%)	69	35

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
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 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 ⓘ

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	0.32	0	6,6,6	0.09	0
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	402	-	4,4,4	0.22	0	6,6,6	0.10	0
3	FES	A	500	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	A	501	-	58,58,58	2.66	26 (44%)	85,89,89	2.03	21 (24%)
2	SO4	B	403	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	B	404	-	4,4,4	0.33	0	6,6,6	0.09	0
3	FES	B	600	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	B	601	-	58,58,58	2.38	17 (29%)	85,89,89	2.36	18 (21%)

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	0/0/1/1
4	FAD	A	501	-	-	0/34/50/50	0/1/6/6
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	0/0/1/1
4	FAD	B	601	-	-	0/34/50/50	0/1/6/6

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	FAD	C1'-C2'	9.75	1.60	1.51
4	A	501	FAD	C1'-C2'	7.13	1.58	1.51
4	A	501	FAD	PA-O3P	-6.09	1.48	1.59
4	B	601	FAD	P-O3P	5.95	1.70	1.59
4	A	501	FAD	C9A-N10	5.85	1.47	1.38
4	B	601	FAD	PA-O3P	-5.76	1.49	1.59
4	A	501	FAD	C8A-N9A	5.44	1.44	1.36
4	A	501	FAD	C4A-N9A	-5.20	1.30	1.37
4	A	501	FAD	P-O2P	-4.72	1.33	1.55
4	A	501	FAD	C4-C4X	-4.48	1.33	1.41
4	B	601	FAD	C9A-N10	4.37	1.45	1.38
4	A	501	FAD	C4X-C10	4.09	1.48	1.40
4	B	601	FAD	C8A-N9A	4.04	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	FAD	C5'-C4'	3.96	1.58	1.51
4	A	501	FAD	C4X-N5	3.93	1.44	1.36
4	A	501	FAD	P-O3P	3.60	1.66	1.59
4	A	501	FAD	C2B-C1B	-3.36	1.48	1.53
4	B	601	FAD	C5X-N5	3.21	1.40	1.35
4	A	501	FAD	C4A-N3A	-3.01	1.31	1.35
4	A	501	FAD	C10-N10	-3.00	1.32	1.38
4	B	601	FAD	O4-C4	2.85	1.30	1.24
4	A	501	FAD	C4-N3	2.80	1.41	1.37
4	B	601	FAD	O4B-C1B	2.60	1.45	1.41
4	A	501	FAD	C2A-N3A	2.58	1.37	1.32
4	B	601	FAD	C4-N3	2.49	1.41	1.37
4	A	501	FAD	C2'-C3'	-2.45	1.48	1.53
4	A	501	FAD	O4'-C4'	-2.42	1.37	1.43
4	B	601	FAD	O5'-C5'	-2.40	1.34	1.44
4	A	501	FAD	C8M-C8	-2.38	1.45	1.51
4	A	501	FAD	O2-C2	2.33	1.28	1.23
4	B	601	FAD	C4A-N9A	-2.29	1.34	1.37
4	A	501	FAD	O5B-C5B	-2.28	1.35	1.44
4	B	601	FAD	PA-O1A	-2.26	1.42	1.51
4	A	501	FAD	C5'-C4'	2.26	1.55	1.51
4	B	601	FAD	C4'-C3'	-2.25	1.48	1.53
4	A	501	FAD	PA-O2A	-2.23	1.45	1.55
4	B	601	FAD	C2A-N3A	2.22	1.36	1.32
4	B	601	FAD	C2-N3	2.14	1.41	1.37
4	A	501	FAD	C2-N1	-2.08	1.30	1.35
4	A	501	FAD	PA-O5B	2.07	1.68	1.59
4	A	501	FAD	O4B-C4B	-2.06	1.40	1.45
4	A	501	FAD	C9A-C5X	2.04	1.46	1.42
4	B	601	FAD	O4'-C4'	-2.01	1.38	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	FAD	N3A-C2A-N1A	-10.95	119.56	128.71
4	B	601	FAD	C2-N1-C10	8.38	123.43	114.98
4	B	601	FAD	C4X-N5-C5X	7.47	125.08	116.69
4	A	501	FAD	C4X-C10-N1	-6.83	115.91	122.73
4	B	601	FAD	C4X-C10-N10	-6.71	117.16	120.51
4	A	501	FAD	C2-N1-C10	6.54	121.57	114.98
4	A	501	FAD	N3A-C2A-N1A	-6.00	123.69	128.71
4	A	501	FAD	O4B-C1B-N9A	-5.65	103.18	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	FAD	C4X-C10-N10	4.53	122.77	120.51
4	B	601	FAD	O4B-C1B-N9A	-4.41	104.34	108.44
4	B	601	FAD	N3A-C4A-N9A	4.30	133.19	125.43
4	A	501	FAD	C4-C4X-C10	3.79	123.06	116.95
4	B	601	FAD	C9A-N10-C10	3.70	125.40	121.77
4	A	501	FAD	C10-C4X-N5	-3.52	116.17	120.45
4	A	501	FAD	C4X-N5-C5X	3.34	120.45	116.69
4	B	601	FAD	C5A-C4A-N3A	-3.33	118.46	125.70
4	A	501	FAD	C9-C8-C7	-2.94	115.17	119.88
4	A	501	FAD	C4-N3-C2	-2.70	119.84	125.39
4	B	601	FAD	P-O3P-PA	-2.63	123.98	131.68
4	B	601	FAD	C2A-N3A-C4A	2.62	121.48	114.01
4	B	601	FAD	C4A-C5A-N7A	-2.60	107.30	109.52
4	A	501	FAD	C5X-C9A-N10	-2.58	114.27	116.80
4	A	501	FAD	N3A-C4A-N9A	2.57	130.07	125.43
4	B	601	FAD	O2B-C2B-C1B	2.40	118.48	111.23
4	B	601	FAD	N7A-C8A-N9A	-2.39	107.59	114.36
4	B	601	FAD	C2'-C1'-N10	-2.31	109.38	112.45
4	A	501	FAD	C5A-C4A-N3A	-2.29	120.71	125.70
4	B	601	FAD	N1-C10-N10	2.27	121.94	115.97
4	B	601	FAD	C9A-C5X-N5	-2.24	118.93	122.37
4	B	601	FAD	C10-C4X-N5	-2.20	117.79	120.45
4	A	501	FAD	C1'-N10-C9A	2.14	120.95	118.87
4	A	501	FAD	C6-C5X-C9A	-2.11	116.10	119.02
4	B	601	FAD	O2P-P-O1P	2.10	123.95	112.21
4	A	501	FAD	C4B-O4B-C1B	2.09	112.02	109.75
4	A	501	FAD	C6-C7-C8	2.05	123.16	119.88
4	A	501	FAD	C1'-C2'-C3'	2.04	115.67	109.82
4	A	501	FAD	C8-C9-C9A	2.04	123.92	119.81
4	A	501	FAD	O2'-C2'-C3'	-2.03	104.00	109.05
4	A	501	FAD	N1-C10-N10	2.01	121.26	115.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	337/338 (99%)	1.05	47 (13%) 4 3	9, 10, 13, 16	1 (0%)
1	B	337/338 (99%)	1.86	125 (37%) 1 1	8, 10, 13, 16	1 (0%)
All	All	674/676 (99%)	1.45	172 (25%) 1 1	8, 10, 13, 16	2 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	GLN	8.5
1	B	268	TRP	7.8
1	B	282	HIS	7.4
1	A	2	SER	6.6
1	B	132	ASP	6.5
1	B	2	SER	6.2
1	B	257	GLU	6.1
1	B	133	GLY	6.1
1	B	264	GLN	6.0
1	B	261	ALA	5.7
1	B	241	VAL	5.5
1	B	232	LEU	5.1
1	B	138	HIS	5.0
1	B	135	PRO	4.9
1	B	136	ASP	4.9
1	B	168	LEU	4.8
1	B	280	SER	4.6
1	B	234	GLN	4.6
1	B	266	LEU	4.5
1	B	267	PRO	4.5
1	B	235	LYS	4.5
1	B	137	ILE	4.4
1	B	300	GLY	4.4
1	B	190	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	238	GLU	4.3
1	B	188	GLN	4.3
1	B	258	GLN	4.3
1	B	187	VAL	4.3
1	B	269	PHE	4.3
1	B	166	ASN	4.2
1	B	165	GLY	4.2
1	B	295	ASP	4.1
1	B	293	GLU	4.0
1	B	119	LEU	4.0
1	B	115	ARG	4.0
1	B	236	GLY	3.9
1	B	294	TYR	3.9
1	B	208	ASP	3.8
1	B	231	VAL	3.8
1	B	213	VAL	3.7
1	B	209	VAL	3.5
1	B	265	LYS	3.5
1	B	192	GLY	3.5
1	B	114	ALA	3.4
1	B	262	LEU	3.4
1	B	184	TYR	3.4
1	B	42	ARG	3.4
1	B	240	PRO	3.4
1	B	191	ALA	3.3
1	B	116	VAL	3.3
1	B	210	LYS	3.3
1	B	287	TYR	3.3
1	B	121	ASP	3.2
1	B	113	LEU	3.2
1	B	62	GLU	3.2
1	B	329	ASN	3.2
1	B	63	ASP	3.2
1	B	229	LEU	3.2
1	B	134	GLN	3.1
1	B	279	GLU	3.1
1	B	228	MET	3.1
1	B	302	VAL	3.1
1	B	326	GLN	3.0
1	B	239	HIS	3.0
1	B	283	GLU	3.0
1	B	260	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	313	VAL	3.0
1	A	310	VAL	3.0
1	B	256	LEU	3.0
1	B	237	SER	2.9
1	A	145	VAL	2.9
1	B	322	THR	2.9
1	B	151	GLY	2.9
1	A	205	TYR	2.9
1	B	328	ALA	2.9
1	B	271	TYR	2.9
1	B	194	LYS	2.8
1	B	76	GLN	2.8
1	B	298	ASN	2.8
1	A	264	GLN	2.8
1	B	319	TRP	2.8
1	A	144	TYR	2.8
1	B	290	GLY	2.8
1	B	301	GLU	2.8
1	A	206	LEU	2.7
1	B	212	PRO	2.7
1	B	19	CYS	2.7
1	B	263	GLN	2.7
1	B	285	LYS	2.7
1	B	5	GLN	2.7
1	B	131	ASP	2.7
1	B	130	LEU	2.6
1	A	217	ALA	2.6
1	A	307	CYS	2.6
1	B	167	ARG	2.6
1	A	234	GLN	2.6
1	A	306	LEU	2.6
1	B	171	PHE	2.6
1	B	29	ALA	2.6
1	B	164	PRO	2.6
1	A	19	CYS	2.6
1	B	289	THR	2.5
1	A	304	VAL	2.5
1	B	178	GLN	2.5
1	B	39	MET	2.5
1	B	284	ARG	2.5
1	A	45	GLU	2.5
1	B	73	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	42	ARG	2.5
1	A	243	LEU	2.5
1	B	127	ASP	2.5
1	B	226	LEU	2.5
1	B	297	LEU	2.5
1	A	201	PHE	2.5
1	B	126	PHE	2.5
1	A	49	CYS	2.5
1	A	279	GLU	2.5
1	A	226	LEU	2.5
1	A	63	ASP	2.4
1	B	104	THR	2.4
1	B	331	LEU	2.4
1	B	161	SER	2.4
1	A	139	PHE	2.4
1	A	257	GLU	2.4
1	A	281	GLN	2.4
1	B	253	LEU	2.4
1	A	151	GLY	2.4
1	B	45	GLU	2.4
1	A	321	ASP	2.3
1	B	243	LEU	2.3
1	B	66	ILE	2.3
1	B	9	GLN	2.3
1	B	305	TYR	2.3
1	A	39	MET	2.3
1	B	299	GLY	2.3
1	B	206	LEU	2.3
1	B	325	ILE	2.3
1	A	275	VAL	2.3
1	A	171	PHE	2.3
1	A	152	THR	2.3
1	A	153	THR	2.3
1	B	101	VAL	2.2
1	A	160	PHE	2.2
1	A	225	PHE	2.2
1	A	308	GLY	2.2
1	B	139	PHE	2.2
1	B	255	ALA	2.2
1	A	204	PHE	2.2
1	B	100	GLU	2.2
1	B	296	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	321	ASP	2.2
1	B	291	HIS	2.2
1	A	238	GLU	2.1
1	B	259	LEU	2.1
1	A	326	GLN	2.1
1	B	242	ARG	2.1
1	B	189	ALA	2.1
1	A	331	LEU	2.1
1	B	233	GLU	2.1
1	A	121	ASP	2.1
1	A	82	ALA	2.1
1	B	59	ASP	2.1
1	A	221	GLY	2.1
1	A	282	HIS	2.1
1	B	129	GLN	2.1
1	A	302	VAL	2.0
1	A	157	SER	2.0
1	B	251	CYS	2.0
1	A	208	ASP	2.0
1	A	5	GLN	2.0
1	B	310	VAL	2.0
1	B	125	THR	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 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	401	5/5	0.20	7.10	28,29,29,29	0
2	SO4	A	402	5/5	0.22	3.78	26,28,28,28	0
4	FAD	B	601	53/53	0.17	1.20	17,18,20,23	0
4	FAD	A	501	53/53	0.16	0.90	7,13,20,20	0
2	SO4	B	403	5/5	0.16	0.74	33,33,33,33	0
3	FES	B	600	4/4	0.18	0.39	13,14,15,15	0
3	FES	A	500	4/4	0.17	0.14	11,12,13,13	0
2	SO4	B	404	5/5	0.23	-0.37	34,34,34,34	0
2	SO4	A	400	5/5	0.10	-1.21	33,33,34,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.