



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:09 PM GMT

PDB ID : 3T2Z  
Title : Crystal structure of sulfide:quinone oxidoreductase from Acidithiobacillus ferrooxidans  
Authors : Cherney, M.M.; Zhang, Y.; Solomonson, M.; Weiner, J.H.; James, M.N.  
Deposited on : 2011-07-23  
Resolution : 2.30 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](mailto: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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

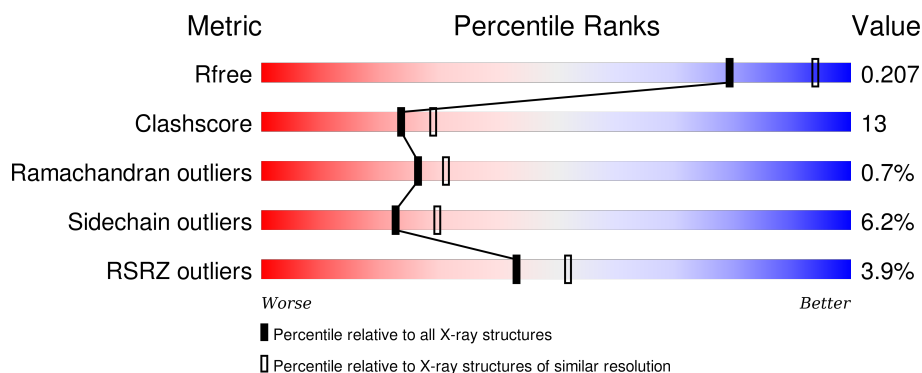
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

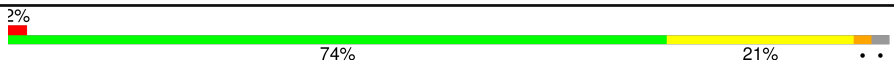
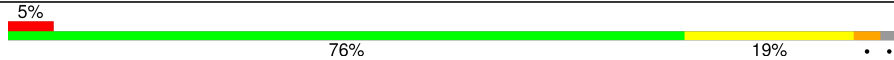
The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	437	
1	B	437	

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
3	BU2	A	502	-	-	X	X
3	BU2	B	501	-	-	-	X
4	SO4	A	437	-	-	X	-
4	SO4	A	438	-	-	-	X
4	SO4	A	439	-	-	-	X
4	SO4	B	437	-	-	-	X
4	SO4	B	439	-	-	-	X
4	SO4	B	440	-	-	-	X
5	H2S	A	440	-	-	X	-
5	H2S	A	441	-	-	-	X
5	H2S	A	443[A]	-	-	-	X
5	H2S	A	445[A]	-	-	-	X
5	H2S	B	445[A]	-	-	-	X
5	H2S	B	447	-	-	-	X
6	S3H	A	442[B]	-	-	-	X
6	S3H	B	442[B]	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7364 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 Sulfide-quinone reductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	2	0
			3277	2103	548	601	25			
1	B	427	Total	C	N	O	S	0	3	0
			3281	2105	548	603	25			

There are 8 discrepancies between the modelled and reference sequences:

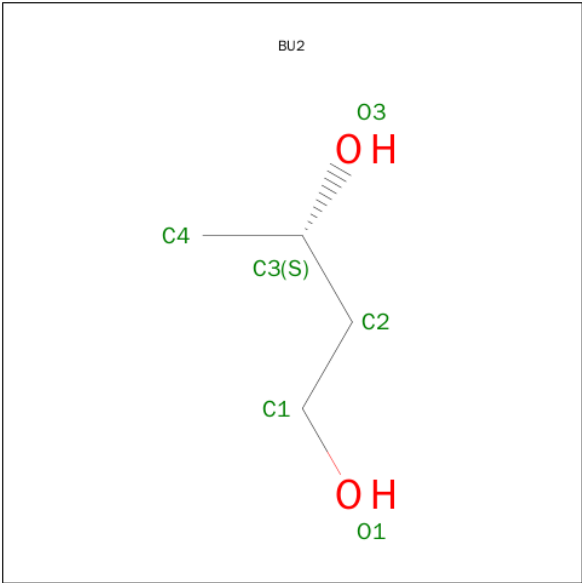
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP B7JBP8
A	-1	ARG	-	EXPRESSION TAG	UNP B7JBP8
A	0	GLY	-	EXPRESSION TAG	UNP B7JBP8
A	1	SER	-	EXPRESSION TAG	UNP B7JBP8
B	-2	MET	-	EXPRESSION TAG	UNP B7JBP8
B	-1	ARG	-	EXPRESSION TAG	UNP B7JBP8
B	0	GLY	-	EXPRESSION TAG	UNP B7JBP8
B	1	SER	-	EXPRESSION TAG	UNP B7JBP8

- 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 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is 1,3-BUTANEDIOL (three-letter code: BU2) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



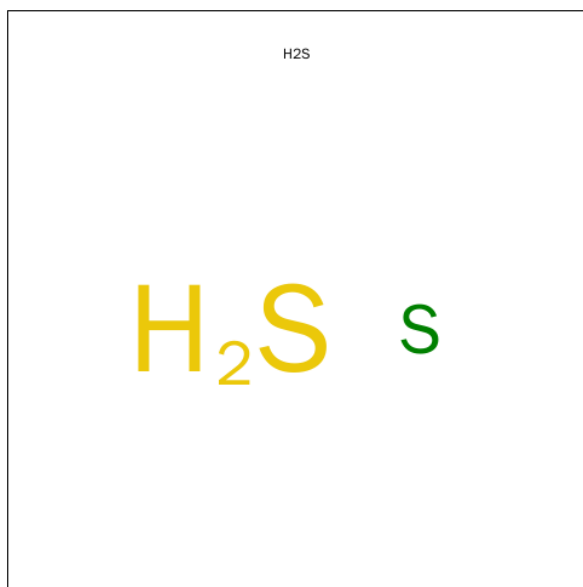
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



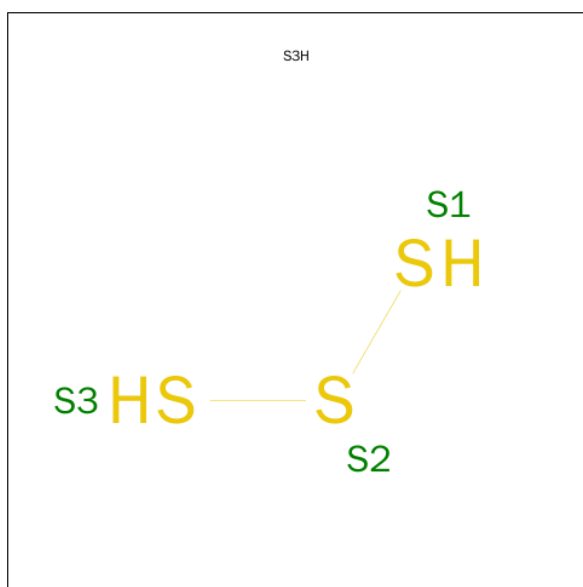
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



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

- Molecule 6 is TRISULFANE (three-letter code: S3H) (formula:  $\text{H}_2\text{S}_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total S 3 3	0	1
6	B	1	Total S 3 3	0	1

- Molecule 7 is water.

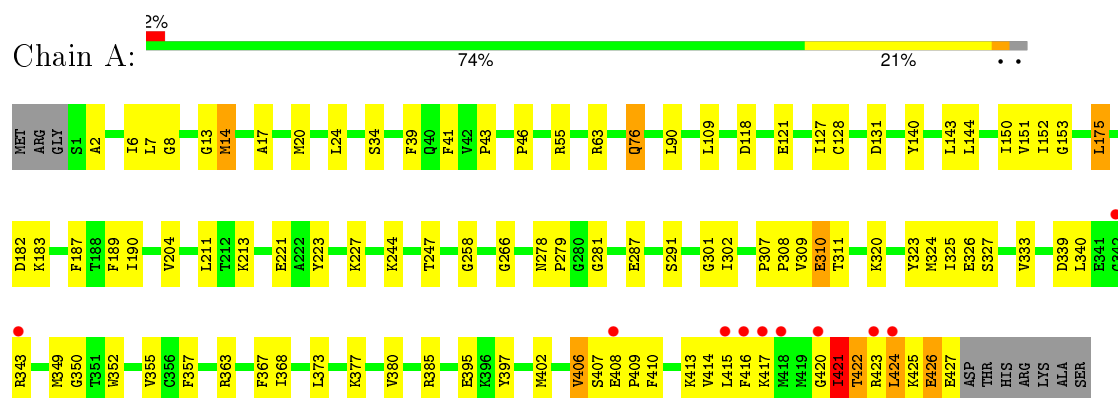
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	308	Total O 308 308	0	0
7	B	309	Total O 309 309	0	0



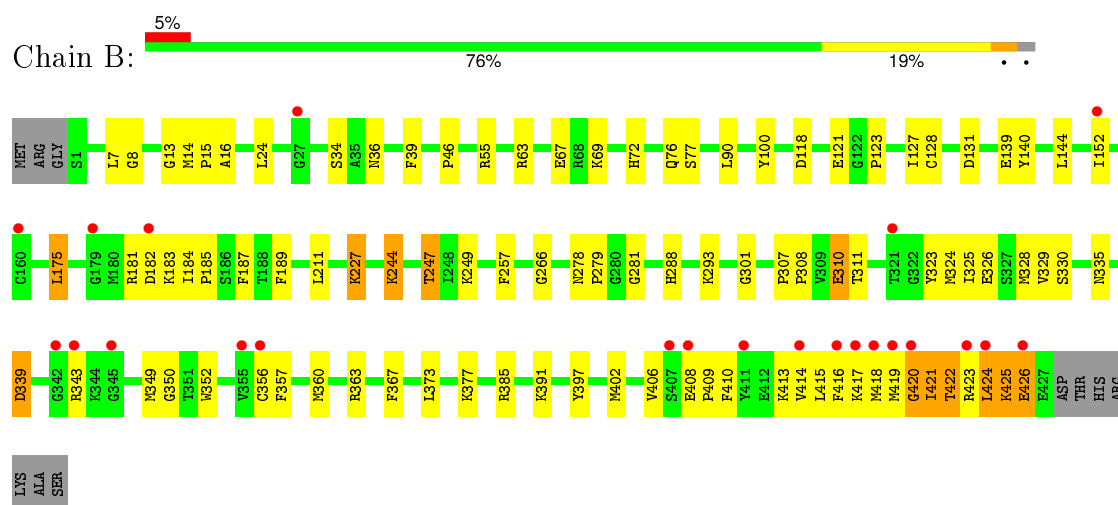
### 3 Residue-property plots [i](#)

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: Sulfide-quinone reductase, putative



- Molecule 1: Sulfide-quinone reductase, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.73 Å   131.73 Å   208.86 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.92 – 2.30 40.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.92-2.30) 100.0 (40.92-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.172   ,   0.212 0.171   ,   0.207	Depositor DCC
$R_{free}$ test set	4110 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 82092 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BU2, SO4, S3H, H2S, 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	0.38	0/3363	0.54	0/4549
1	B	0.37	0/3371	0.53	0/4560
All	All	0.38	0/6734	0.53	0/9109

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	3277	0	3269	92	0
1	B	3281	0	3273	87	0
2	A	53	0	30	1	0
2	B	53	0	30	1	0
3	A	6	0	10	5	0
3	B	6	0	10	3	0
4	A	25	0	0	4	0
4	B	30	0	0	4	0
5	A	5	0	0	3	0
5	B	5	0	0	2	0
6	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	3	0	0	1	0
7	A	308	0	0	6	1
7	B	309	0	0	9	0
All	All	7364	0	6622	176	1

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 13.

All (176) 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:421:ILE:HD12	1:A:423:ARG:HB2	1.49	0.93
1:B:421:ILE:HD12	1:B:423:ARG:HB2	1.52	0.91
1:A:377:LYS:HE2	1:B:424:LEU:HG	1.55	0.89
1:B:63:ARG:NH1	4:B:436:SO4:O1	2.06	0.88
1:B:417:LYS:HD3	1:B:421:ILE:HG21	1.60	0.83
1:A:424:LEU:HG	1:B:377:LYS:HE2	1.63	0.80
1:A:413:LYS:HA	1:A:416:PHE:CE2	2.17	0.80
1:A:310:GLU:HG2	1:A:311:THR:N	1.97	0.79
1:B:310:GLU:HG2	1:B:311:THR:N	1.96	0.78
1:B:247:THR:HG22	7:B:569:HOH:O	1.82	0.78
1:B:413:LYS:HA	1:B:416:PHE:CE2	2.20	0.77
1:A:324:MET:HE3	1:A:352:TRP:CD1	2.21	0.76
1:B:301:GLY:HA2	1:B:325:ILE:HG12	1.68	0.75
1:A:43:PRO:HG2	3:A:502:BU2:HC41	1.70	0.73
1:B:417:LYS:HD3	1:B:421:ILE:CG2	2.19	0.72
1:B:46:PRO:HG3	1:B:127:ILE:HD12	1.70	0.72
1:B:324:MET:HE3	1:B:352:TRP:HA	1.72	0.72
1:B:420:GLY:HA2	1:B:421:ILE:HG12	1.71	0.71
1:A:301:GLY:HA2	1:A:325:ILE:HG12	1.71	0.71
1:B:417:LYS:HA	1:B:421:ILE:HG23	1.73	0.71
1:A:55:ARG:NH2	1:A:131:ASP:OD1	2.24	0.70
1:B:55:ARG:NH2	1:B:131:ASP:OD1	2.23	0.70
1:A:76:GLN:HG2	1:A:90:LEU:HB3	1.74	0.69
1:A:377:LYS:CE	1:B:424:LEU:HG	2.22	0.69
1:A:420:GLY:HA2	1:A:421:ILE:HG12	1.75	0.69
1:B:416:PHE:CD1	1:B:422:THR:HB	2.30	0.67
1:B:181:ARG:N	4:B:440:SO4:O2	2.28	0.66
1:A:424:LEU:HG	1:B:377:LYS:CE	2.24	0.66
1:A:407:SER:N	4:A:437:SO4:O3	2.22	0.66
5:A:445[A]:H2S:S	7:A:620:HOH:O	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASN:ND2	7:B:695:HOH:O	2.28	0.66
1:A:14:MET:HE2	1:A:39:PHE:HB2	1.78	0.66
1:B:8:GLY:O	1:B:13:GLY:HA3	1.97	0.64
1:B:139:GLU:HG2	1:B:257:PHE:HD2	1.61	0.63
1:B:424:LEU:O	1:B:425:LYS:HB2	1.99	0.63
1:B:72:HIS:HD2	7:B:591:HOH:O	1.81	0.63
1:B:244:LYS:HE3	7:B:579:HOH:O	1.99	0.63
1:A:63:ARG:NH2	4:A:439:SO4:O1	2.30	0.62
1:A:408:GLU:HG2	7:A:562:HOH:O	1.98	0.62
1:B:76:GLN:HG2	1:B:90:LEU:HB3	1.83	0.61
1:A:420:GLY:CA	1:A:421:ILE:HG12	2.30	0.60
1:A:8:GLY:O	1:A:13:GLY:HA3	2.01	0.60
1:A:324:MET:HE3	1:A:352:TRP:CG	2.36	0.60
1:B:391:LYS:HD2	3:B:501:BU2:O3	2.01	0.60
1:A:416:PHE:CD1	1:A:422:THR:HB	2.37	0.59
1:A:416:PHE:CE1	1:A:417:LYS:HD2	2.38	0.59
1:B:323:TYR:CE1	1:B:415:LEU:HB2	2.37	0.58
1:A:406:VAL:HG13	1:A:410:PHE:HB2	1.84	0.58
1:A:424:LEU:HG	1:B:377:LYS:CD	2.33	0.58
1:A:324:MET:HE3	1:A:352:TRP:HA	1.84	0.58
1:B:324:MET:CE	1:B:352:TRP:HA	2.34	0.57
1:A:128:CYS:HB2	5:A:440:H2S:S	2.44	0.57
1:A:324:MET:CE	1:A:352:TRP:CD1	2.87	0.57
1:B:118:ASP:HB3	1:B:121:GLU:HG2	1.85	0.57
1:B:421:ILE:HG22	1:B:422:THR:H	1.69	0.56
1:B:416:PHE:CE1	1:B:417:LYS:HE2	2.40	0.56
1:B:357:PHE:CD2	3:B:501:BU2:HC12	2.40	0.56
1:A:343:ARG:NH2	4:A:436:SO4:O1	2.38	0.56
1:A:221:GLU:OE2	1:A:223:TYR:OH	2.19	0.56
1:A:417:LYS:HE3	1:A:423:ARG:HG3	1.87	0.55
1:A:323:TYR:CE1	1:A:415:LEU:HB2	2.42	0.55
1:A:6:ILE:HD13	1:A:17:ALA:HA	1.89	0.55
1:B:326:GLU:HG3	1:B:414:VAL:HG21	1.89	0.55
1:B:417:LYS:HZ2	1:B:423:ARG:HG3	1.71	0.55
1:A:417:LYS:HA	1:A:421:ILE:HG23	1.89	0.54
1:A:426:GLU:CB	1:B:350:GLY:HA2	2.37	0.54
1:B:397:TYR:CE1	1:B:417:LYS:HE3	2.42	0.54
1:A:324:MET:CE	1:A:352:TRP:HA	2.37	0.54
3:A:502:BU2:HC22	7:A:548:HOH:O	2.06	0.54
1:B:140:TYR:OH	1:B:175:LEU:HD13	2.07	0.54
1:B:420:GLY:CA	1:B:421:ILE:HG12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ILE:HG13	1:A:424:LEU:H	1.73	0.53
1:A:421:ILE:HD12	1:A:423:ARG:CB	2.31	0.53
1:B:410:PHE:O	1:B:413:LYS:HB2	2.10	0.52
1:A:118:ASP:HB3	1:A:121:GLU:HG2	1.92	0.52
1:A:287:GLU:O	7:A:596:HOH:O	2.19	0.52
1:B:416:PHE:C	1:B:416:PHE:CD1	2.83	0.52
1:A:20:MET:HE2	1:A:333:VAL:HG22	1.92	0.52
1:B:418:MET:SD	3:B:501:BU2:HC11	2.50	0.51
1:A:408:GLU:N	1:A:409:PRO:HD2	2.25	0.51
1:B:324:MET:HE3	1:B:352:TRP:CD1	2.46	0.51
1:B:410:PHE:HB2	4:B:439:SO4:O2	2.11	0.51
1:B:408:GLU:N	1:B:409:PRO:HD2	2.25	0.51
1:A:424:LEU:HD11	7:B:476:HOH:O	2.10	0.51
1:A:421:ILE:CD1	1:A:423:ARG:HB2	2.33	0.50
1:A:14:MET:HE1	1:A:402:MET:HB3	1.93	0.50
1:A:357:PHE:HB2	3:A:502:BU2:HC12	1.92	0.50
1:A:421:ILE:HB	1:A:423:ARG:N	2.27	0.50
1:A:14:MET:HE2	1:A:39:PHE:CB	2.41	0.50
1:B:416:PHE:CD1	1:B:421:ILE:HG22	2.47	0.49
1:A:424:LEU:HG	1:B:377:LYS:HD2	1.95	0.49
1:A:43:PRO:CG	3:A:502:BU2:HC41	2.40	0.49
1:B:128:CYS:HB2	5:B:441:H2S:S	2.53	0.49
1:A:152:ILE:O	1:A:189:PHE:HA	2.13	0.49
1:B:324:MET:CE	1:B:349:MET:SD	3.01	0.48
1:B:14:MET:HB2	1:B:15:PRO:HD3	1.95	0.48
1:B:266:GLY:HA3	1:B:281:GLY:O	2.13	0.48
1:B:413:LYS:HD3	1:B:416:PHE:CE2	2.47	0.48
1:A:63:ARG:NH1	7:A:653:HOH:O	2.46	0.48
2:A:500:FAD:H9	2:A:500:FAD:O3'	2.14	0.48
1:B:421:ILE:HB	1:B:423:ARG:N	2.29	0.48
1:A:377:LYS:NZ	7:A:512:HOH:O	2.46	0.48
1:A:357:PHE:CD2	3:A:502:BU2:HC12	2.49	0.48
1:B:227:LYS:HD3	7:B:568:HOH:O	2.14	0.48
1:B:324:MET:O	1:B:328:MET:HG3	2.14	0.47
1:B:413:LYS:HA	1:B:416:PHE:CD2	2.49	0.47
1:B:397:TYR:CZ	1:B:417:LYS:HE3	2.49	0.47
1:B:278:ASN:HB2	1:B:279:PRO:CD	2.44	0.47
1:A:324:MET:HE2	1:A:349:MET:HE3	1.97	0.47
1:B:14:MET:HE2	1:B:39:PHE:HB2	1.96	0.47
1:B:363:ARG:HH22	1:B:385:ARG:NH1	2.13	0.47
1:B:397:TYR:CD2	1:B:417:LYS:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:HIS:HB3	1:B:335:ASN:ND2	2.30	0.46
1:A:421:ILE:HD11	7:B:614:HOH:O	2.15	0.46
1:A:363:ARG:HH21	1:A:385:ARG:NH1	2.13	0.46
1:B:324:MET:HE2	1:B:349:MET:SD	2.56	0.46
1:B:421:ILE:HB	1:B:423:ARG:H	1.81	0.46
1:B:14:MET:CE	1:B:402:MET:HB3	2.47	0.46
1:B:14:MET:HE1	1:B:402:MET:HB3	1.96	0.46
1:B:227:LYS:HB2	1:B:227:LYS:NZ	2.31	0.46
1:A:153:GLY:HA3	1:A:190:ILE:O	2.15	0.45
1:A:324:MET:HE2	1:A:349:MET:CE	2.47	0.45
1:B:175:LEU:HD12	1:B:175:LEU:HA	1.85	0.45
1:A:20:MET:HE1	1:A:333:VAL:HA	1.98	0.45
1:A:227:LYS:HE3	1:A:227:LYS:HB2	1.79	0.45
1:A:416:PHE:CE1	1:A:417:LYS:CD	3.00	0.45
1:A:416:PHE:HE1	1:A:417:LYS:HZ2	1.65	0.45
1:A:421:ILE:HB	1:A:423:ARG:H	1.82	0.45
1:B:293:LYS:NZ	7:B:721:HOH:O	2.48	0.45
1:A:421:ILE:CG1	1:A:424:LEU:H	2.30	0.45
1:A:151:VAL:O	1:A:258:GLY:HA2	2.17	0.45
1:A:397:TYR:CE1	1:A:417:LYS:HE2	2.51	0.45
1:B:416:PHE:HD1	1:B:421:ILE:HG22	1.80	0.44
1:B:152:ILE:O	1:B:189:PHE:HA	2.17	0.44
1:B:123:PRO:O	1:B:139:GLU:OE2	2.35	0.44
1:B:416:PHE:HE1	1:B:417:LYS:HZ3	1.62	0.44
1:A:302:ILE:HA	1:A:320:LYS:HD2	2.00	0.44
1:B:182:ASP:OD1	1:B:183:LYS:HD2	2.18	0.44
1:A:326:GLU:HG3	1:A:414:VAL:HG21	1.99	0.44
1:A:143:LEU:HD21	1:A:150:ILE:HD11	1.99	0.44
1:A:410:PHE:HB2	4:A:437:SO4:O3	2.17	0.43
1:A:309:VAL:HB	1:A:373:LEU:HD13	2.00	0.43
1:A:46:PRO:HG3	1:A:127:ILE:HD12	2.00	0.43
1:B:343:ARG:NH2	4:B:437:SO4:O1	2.51	0.43
1:A:416:PHE:HE1	1:A:417:LYS:NZ	2.15	0.43
6:B:442[B]:S3H:S3	5:B:447:H2S:S	3.16	0.43
1:A:355:VAL:HG22	1:A:368:ILE:HG23	2.01	0.43
1:A:420:GLY:C	1:A:421:ILE:HG12	2.39	0.43
1:B:278:ASN:HB2	1:B:279:PRO:HD2	2.00	0.43
1:A:2:ALA:CB	1:A:340:LEU:HD21	2.48	0.43
1:A:182:ASP:OD1	1:A:183:LYS:HD2	2.18	0.43
1:B:414:VAL:O	1:B:418:MET:HG3	2.19	0.43
1:A:327:SER:OG	1:A:349:MET:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ALA:HB2	1:B:329:VAL:HG13	2.01	0.42
1:A:417:LYS:HA	1:A:421:ILE:CG2	2.48	0.42
1:B:55:ARG:HD3	7:B:454:HOH:O	2.19	0.42
1:B:413:LYS:HD3	1:B:416:PHE:HE2	1.85	0.42
1:A:140:TYR:OH	1:A:175:LEU:HD13	2.19	0.42
1:A:417:LYS:HZ1	1:A:423:ARG:HG3	1.84	0.42
1:B:307:PRO:HA	1:B:308:PRO:HD3	1.93	0.42
1:A:367:PHE:HA	1:A:380:VAL:O	2.19	0.41
1:A:278:ASN:HB2	1:A:279:PRO:HD2	2.02	0.41
1:B:67:GLU:C	1:B:69:LYS:H	2.23	0.41
1:A:41:PHE:CD2	1:A:395:GLU:HG3	2.56	0.41
1:B:184:ILE:HA	1:B:185:PRO:HD3	1.91	0.41
2:B:500:FAD:O3'	2:B:500:FAD:H9	2.20	0.41
1:A:2:ALA:CB	1:A:340:LEU:CD2	2.98	0.41
1:A:340:LEU:HA	1:A:340:LEU:HD23	1.70	0.41
1:A:266:GLY:HA3	1:A:281:GLY:O	2.21	0.41
1:A:307:PRO:HA	1:A:308:PRO:HD3	1.93	0.41
1:A:109:LEU:HD13	5:A:440:H2S:S	2.62	0.40
1:B:356[A]:CYS:HB2	1:B:367:PHE:CE1	2.57	0.40
1:A:416:PHE:CD1	1:A:416:PHE:C	2.95	0.40
1:A:350:GLY:HA2	1:B:426:GLU:HB3	2.03	0.40
1:A:426:GLU:O	1:A:427:GLU:HB3	2.21	0.40
1:B:100:TYR:OH	1:B:339:ASP:HB3	2.21	0.40

All (1) 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)
7:A:560:HOH:O	7:A:560:HOH:O[8_666]	2.07	0.13

## 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	427/437 (98%)	410 (96%)	15 (4%)	2 (0%)	34	41
1	B	428/437 (98%)	411 (96%)	13 (3%)	4 (1%)	21	24
All	All	855/874 (98%)	821 (96%)	28 (3%)	6 (1%)	26	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	LYS
1	A	421	ILE
1	B	419	MET
1	B	421	ILE
1	B	425	LYS
1	B	420	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	341/347 (98%)	320 (94%)	21 (6%)	23	30
1	B	342/347 (99%)	321 (94%)	21 (6%)	23	30
All	All	683/694 (98%)	641 (94%)	42 (6%)	23	30

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	14	MET
1	A	24	LEU
1	A	34	SER
1	A	76	GLN
1	A	144	LEU
1	A	175	LEU
1	A	187	PHE
1	A	204	VAL
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	213	LYS
1	A	244	LYS
1	A	247	THR
1	A	291	SER
1	A	310	GLU
1	A	339	ASP
1	A	406	VAL
1	A	421	ILE
1	A	422	THR
1	A	424	LEU
1	A	426	GLU
1	B	7	LEU
1	B	24	LEU
1	B	34	SER
1	B	77	SER
1	B	144	LEU
1	B	175	LEU
1	B	187	PHE
1	B	211	LEU
1	B	227	LYS
1	B	244	LYS
1	B	247	THR
1	B	249	LYS
1	B	310	GLU
1	B	330	SER
1	B	339	ASP
1	B	360	MET
1	B	373	LEU
1	B	406	VAL
1	B	422	THR
1	B	424	LEU
1	B	426	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	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 ⓘ

Of 27 ligands modelled in this entry, 10 are modelled with single atom - leaving 17 for Mogul analysis.

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	$\# Z  > 2$
4	SO4	A	435	-	4,4,4	0.20	0	6,6,6	0.12	0
4	SO4	A	436	-	4,4,4	0.17	0	6,6,6	0.11	0
4	SO4	A	437	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	A	438	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	A	439	-	4,4,4	0.20	0	6,6,6	0.14	0
6	S3H	A	442[B]	1	0,2,2	0.00	-	0,1,1	0.00	-
2	FAD	A	500	-	48,58,58	3.34	22 (45%)	54,89,89	2.54	14 (25%)
3	BU2	A	502	-	5,5,5	0.73	0	4,5,5	1.43	1 (25%)
4	SO4	B	435	-	4,4,4	0.20	0	6,6,6	0.14	0
4	SO4	B	436	-	4,4,4	0.17	0	6,6,6	0.10	0
4	SO4	B	437	-	4,4,4	0.21	0	6,6,6	0.07	0
4	SO4	B	438	-	4,4,4	0.16	0	6,6,6	0.15	0
4	SO4	B	439	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	B	440	-	4,4,4	0.23	0	6,6,6	0.10	0
6	S3H	B	442[B]	1	0,2,2	0.00	-	0,1,1	0.00	-
2	FAD	B	500	-	48,58,58	3.36	23 (47%)	54,89,89	2.53	14 (25%)
3	BU2	B	501	-	5,5,5	0.71	0	4,5,5	1.20	1 (25%)

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
4	SO4	A	435	-	-	0/0/0/0	0/0/0/0
4	SO4	A	436	-	-	0/0/0/0	0/0/0/0
4	SO4	A	437	-	-	0/0/0/0	0/0/0/0
4	SO4	A	438	-	-	0/0/0/0	0/0/0/0
4	SO4	A	439	-	-	0/0/0/0	0/0/0/0
6	S3H	A	442[B]	1	-	0/0/0/0	0/0/0/0
2	FAD	A	500	-	-	0/30/50/50	0/6/6/6
3	BU2	A	502	-	-	0/3/3/3	0/0/0/0
4	SO4	B	435	-	-	0/0/0/0	0/0/0/0
4	SO4	B	436	-	-	0/0/0/0	0/0/0/0
4	SO4	B	437	-	-	0/0/0/0	0/0/0/0
4	SO4	B	438	-	-	0/0/0/0	0/0/0/0
4	SO4	B	439	-	-	0/0/0/0	0/0/0/0
4	SO4	B	440	-	-	0/0/0/0	0/0/0/0
6	S3H	B	442[B]	1	-	0/0/0/0	0/0/0/0
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6
3	BU2	B	501	-	-	0/3/3/3	0/0/0/0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	O2'-C2'	-10.81	1.19	1.43
2	A	500	FAD	O2'-C2'	-10.63	1.19	1.43
2	B	500	FAD	C4X-C10	-2.20	1.36	1.41
2	A	500	FAD	C8M-C8	2.06	1.55	1.51
2	A	500	FAD	C9-C9A	2.18	1.45	1.40
2	B	500	FAD	C8M-C8	2.21	1.55	1.51
2	B	500	FAD	C9-C9A	2.34	1.45	1.40
2	A	500	FAD	C5'-C4'	2.44	1.55	1.51
2	B	500	FAD	C6-C5X	2.49	1.45	1.41
2	B	500	FAD	C5'-C4'	2.52	1.55	1.51
2	A	500	FAD	C6-C7	2.58	1.44	1.37
2	B	500	FAD	C6-C7	2.59	1.44	1.37
2	A	500	FAD	C9-C8	2.74	1.45	1.37
2	B	500	FAD	C9-C8	2.78	1.45	1.37
2	A	500	FAD	C6-C5X	2.81	1.46	1.41
2	A	500	FAD	O4B-C1B	3.12	1.45	1.41
2	B	500	FAD	O4B-C1B	3.31	1.45	1.41
2	A	500	FAD	C9A-N10	3.40	1.43	1.38
2	B	500	FAD	C2A-N1A	3.45	1.40	1.33
2	A	500	FAD	C2A-N1A	3.49	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C8A-N7A	3.53	1.41	1.34
2	A	500	FAD	C6A-N6A	3.54	1.45	1.34
2	B	500	FAD	C6A-N6A	3.59	1.46	1.34
2	A	500	FAD	C8A-N7A	3.60	1.41	1.34
2	B	500	FAD	PA-O1A	3.79	1.65	1.51
2	A	500	FAD	P-O1P	3.80	1.65	1.51
2	A	500	FAD	C2A-N3A	3.81	1.38	1.32
2	A	500	FAD	C10-N10	3.81	1.43	1.39
2	A	500	FAD	PA-O1A	3.82	1.65	1.51
2	B	500	FAD	P-O1P	3.85	1.65	1.51
2	B	500	FAD	C4-C4X	3.86	1.49	1.41
2	B	500	FAD	C9A-N10	3.91	1.44	1.38
2	A	500	FAD	C4-C4X	3.92	1.49	1.41
2	B	500	FAD	C10-N10	3.92	1.43	1.39
2	B	500	FAD	C2A-N3A	3.98	1.39	1.32
2	B	500	FAD	C5X-N5	5.02	1.43	1.35
2	A	500	FAD	C5X-N5	5.66	1.44	1.35
2	A	500	FAD	C4-N3	5.74	1.43	1.33
2	B	500	FAD	C4-N3	5.88	1.44	1.33
2	A	500	FAD	O4-C4	6.51	1.40	1.24
2	B	500	FAD	O4-C4	6.69	1.40	1.24
2	B	500	FAD	C10-N1	7.03	1.47	1.35
2	A	500	FAD	C10-N1	7.12	1.47	1.35
2	B	500	FAD	C4X-N5	7.77	1.45	1.33
2	A	500	FAD	C4X-N5	8.14	1.46	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	N3A-C2A-N1A	-11.65	119.97	128.89
2	A	500	FAD	N3A-C2A-N1A	-11.25	120.28	128.89
2	B	500	FAD	P-O3P-PA	-4.46	120.20	132.73
2	A	500	FAD	P-O3P-PA	-4.18	120.98	132.73
2	A	500	FAD	C4X-C4-N3	-2.62	120.00	123.59
2	B	500	FAD	C4X-C4-N3	-2.57	120.08	123.59
2	A	500	FAD	C4B-O4B-C1B	-2.22	107.28	109.72
2	A	500	FAD	C1B-N9A-C4A	-2.17	123.67	126.94
2	B	500	FAD	C1B-N9A-C4A	-2.09	123.78	126.94
2	B	500	FAD	O4B-C4B-C5B	2.01	116.50	109.32
2	B	500	FAD	O3B-C3B-C2B	2.02	118.39	111.83
2	B	500	FAD	C5X-C9A-N10	2.03	119.16	117.62
2	A	500	FAD	O4B-C4B-C5B	2.11	116.87	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	BU2	O1-C1-C2	2.22	118.78	111.34
2	B	500	FAD	O3B-C3B-C4B	2.25	117.79	111.05
2	A	500	FAD	C5X-C9A-N10	2.59	119.59	117.62
2	B	500	FAD	O3P-P-O5'	2.73	110.19	102.94
3	A	502	BU2	O1-C1-C2	2.73	120.52	111.34
2	A	500	FAD	O3P-P-O5'	2.82	110.41	102.94
2	A	500	FAD	O4'-C4'-C3'	3.06	116.71	109.02
2	A	500	FAD	C1'-N10-C9A	3.14	122.38	118.86
2	B	500	FAD	C1'-N10-C9A	3.25	122.51	118.86
2	A	500	FAD	O2'-C2'-C1'	3.27	117.98	109.94
2	A	500	FAD	O2'-C2'-C3'	3.63	118.14	109.02
2	B	500	FAD	O2'-C2'-C1'	3.72	119.10	109.94
2	B	500	FAD	O2'-C2'-C3'	3.88	118.77	109.02
2	B	500	FAD	C4-N3-C2	5.39	119.90	115.25
2	A	500	FAD	C4-N3-C2	5.86	120.31	115.25
2	A	500	FAD	O4B-C1B-N9A	6.54	121.79	108.10
2	B	500	FAD	O4B-C1B-N9A	7.15	123.06	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	436	SO4	1	0
4	A	437	SO4	2	0
4	A	439	SO4	1	0
2	A	500	FAD	1	0
3	A	502	BU2	5	0
4	B	436	SO4	1	0
4	B	437	SO4	1	0
4	B	439	SO4	1	0
4	B	440	SO4	1	0
6	B	442[B]	S3H	1	0
2	B	500	FAD	1	0
3	B	501	BU2	3	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<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	427/437 (97%)	-0.17	10 (2%) 64 72	35, 48, 83, 156	0
1	B	427/437 (97%)	0.13	23 (5%) 29 38	36, 49, 92, 141	0
All	All	854/874 (97%)	-0.02	33 (3%) 43 52	35, 49, 87, 156	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	LEU	4.5
1	A	423	ARG	4.2
1	B	419	MET	3.9
1	B	343	ARG	3.9
1	B	342	GLY	3.4
1	B	417	LYS	3.3
1	A	424	LEU	3.3
1	A	420	GLY	3.2
1	B	423	ARG	3.2
1	B	418	MET	3.1
1	A	416	PHE	3.0
1	B	407	SER	3.0
1	A	408	GLU	2.9
1	A	418	MET	2.8
1	B	411	TYR	2.8
1	B	355	VAL	2.8
1	B	179	GLY	2.7
1	B	356[A]	CYS	2.6
1	B	426	GLU	2.6
1	B	416	PHE	2.5
1	B	27	GLY	2.4
1	B	408	GLU	2.4
1	A	342	GLY	2.3
1	B	321	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	417	LYS	2.3
1	A	343	ARG	2.3
1	B	182	ASP	2.2
1	A	415	LEU	2.2
1	B	414	VAL	2.2
1	B	345	GLY	2.1
1	B	420	GLY	2.1
1	B	160[A]	CYS	2.0
1	B	152	ILE	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 [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	A	439	5/5	0.74	0.37	8.36	27,44,61,61	5
5	H2S	B	445[A]	1/1	0.97	0.40	8.05	52,52,52,52	1
5	H2S	B	447	1/1	0.94	0.48	6.20	98,98,98,98	0
5	H2S	A	441	1/1	0.89	0.31	5.18	97,97,97,97	0
5	H2S	A	445[A]	1/1	0.96	0.28	4.84	53,53,53,53	1
5	H2S	A	443[A]	1/1	0.92	0.29	4.72	93,93,93,93	1
4	SO4	B	440	5/5	0.90	0.48	4.24	67,82,86,86	5
3	BU2	B	501	6/6	0.76	0.44	3.41	71,93,99,100	0
4	SO4	A	438	5/5	0.91	0.19	3.26	68,81,88,94	5
4	SO4	B	439	5/5	0.92	0.44	3.10	141,144,144,146	5
6	S3H	A	442[B]	3/3	0.96	0.24	2.67	43,43,54,93	3
6	S3H	B	442[B]	3/3	0.96	0.28	2.33	57,57,62,78	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BU2	A	502	6/6	0.90	0.29	2.18	74,79,84,86	0
4	SO4	B	437	5/5	0.86	0.42	1.82	138,140,141,142	5
4	SO4	B	438	5/5	0.92	0.17	1.64	63,88,92,96	5
5	H2S	B	444[A]	1/1	0.95	0.24	1.45	59,59,59,59	1
5	H2S	A	444[A]	1/1	0.96	0.19	1.42	51,51,51,51	1
4	SO4	A	436	5/5	0.96	0.25	1.37	98,99,100,101	5
4	SO4	A	437	5/5	0.94	0.27	1.25	109,113,115,115	5
2	FAD	A	500	53/53	0.97	0.18	0.85	33,42,49,55	0
2	FAD	B	500	53/53	0.97	0.21	0.67	34,44,52,53	0
5	H2S	B	443[A]	1/1	0.98	0.24	0.21	83,83,83,83	1
4	SO4	B	435	5/5	0.79	0.19	-0.53	151,152,155,155	0
5	H2S	A	440	1/1	0.99	0.09	-0.95	52,52,52,52	0
5	H2S	B	441	1/1	0.98	0.10	-1.01	58,58,58,58	0
4	SO4	A	435	5/5	0.94	0.11	-1.09	128,128,133,134	0
4	SO4	B	436	5/5	0.88	0.21	-	92,99,103,108	5

## 6.5 Other polymers

There are no such residues in this entry.