



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:36 pm BST

PDB ID : 4ISB  
Title : Crystal Structure of Apo Mtb FadD10  
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Deposited on : 2013-01-16  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

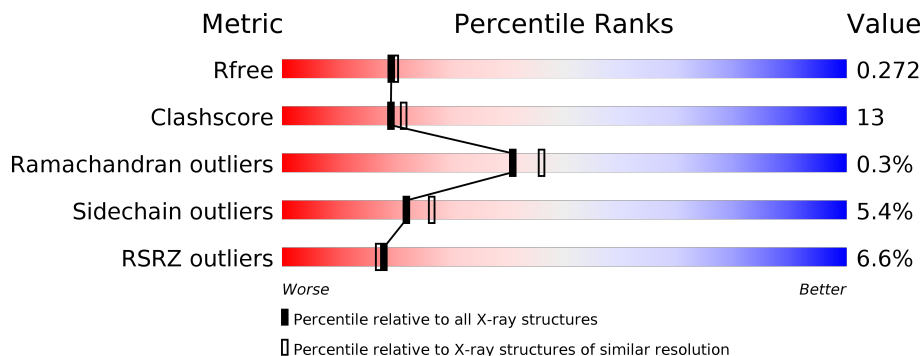
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	541	
1	B	541	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7501 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.

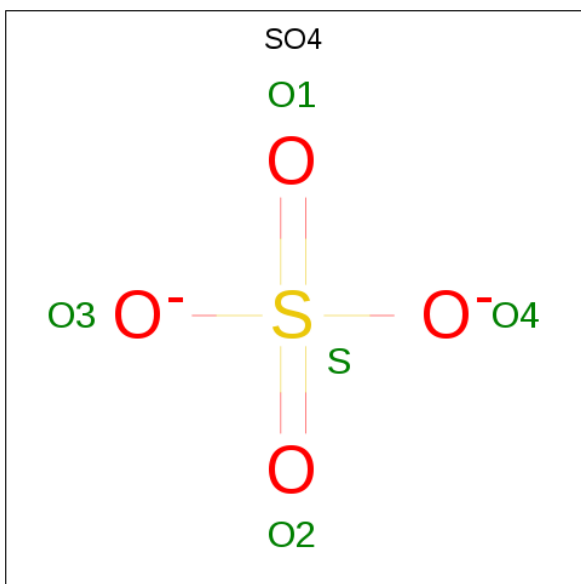
- Molecule 1 is a protein called Long chain fatty acid CoA ligase FadD10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	508	3719	2342	643	715	10	9	0	0	0
1	B	503	3703	2337	638	709	10	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP I6WXG2
B	0	SER	-	EXPRESSION TAG	UNP I6WXG2

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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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	B	1	Total	O	S	0	0
			5	4	1		

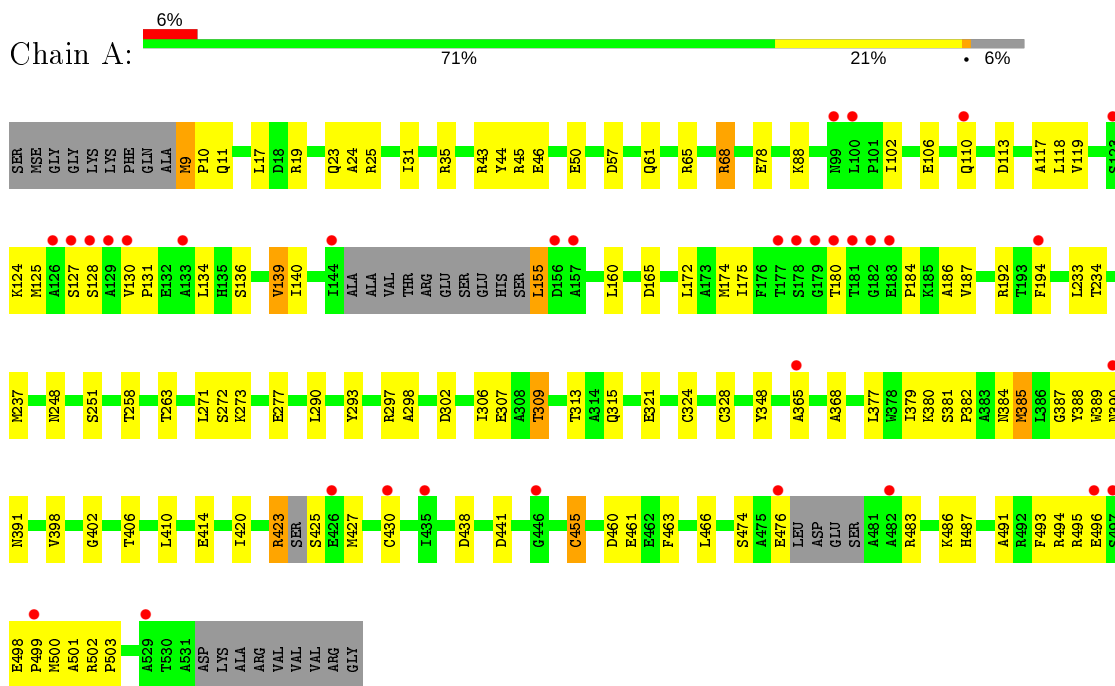
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	25	Total	O	0	0
			25	25		

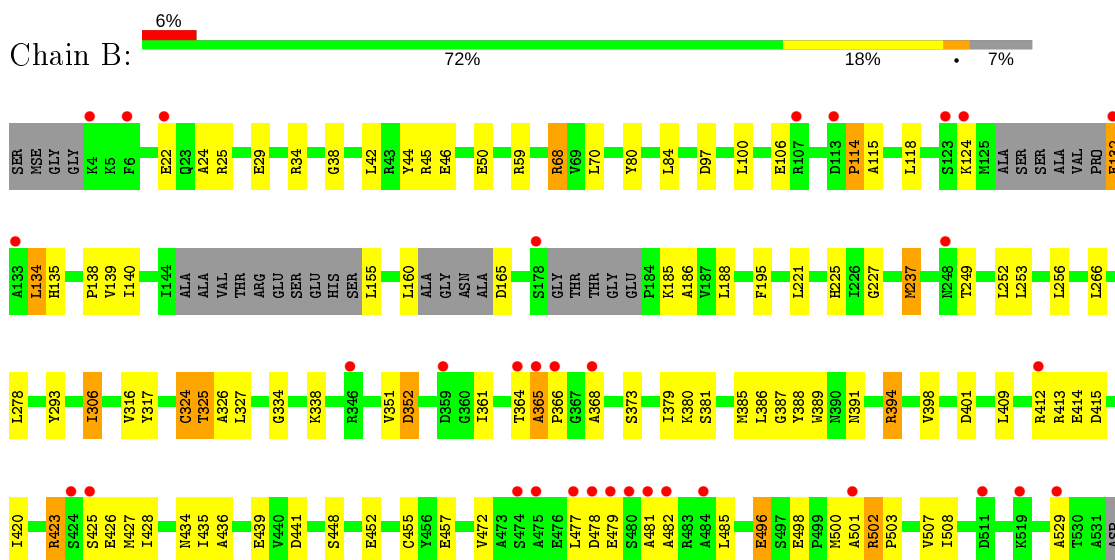
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Long chain fatty acid CoA ligase FadD10



- Molecule 1: Long chain fatty acid CoA ligase FadD10



LYS  
ALA  
ARG  
VAL  
VAL  
VAL  
ARG  
GLY

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.32Å 107.91Å 85.69Å 90.00° 106.92° 90.00°	Depositor
Resolution (Å)	48.89 – 2.20 48.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.89-2.20) 96.7 (48.89-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.227 , 0.273 0.236 , 0.272	Depositor DCC
$R_{free}$ test set	2008 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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

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	0.47	0/3775	0.61	0/5137
1	B	0.48	2/3757 (0.1%)	0.63	1/5104 (0.0%)
All	All	0.47	2/7532 (0.0%)	0.62	1/10241 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	PRO	N-CD	5.39	1.55	1.47
1	B	366	PRO	N-CD	5.27	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	ALA	C-N-CD	5.55	140.06	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3719	0	3737	109	0
1	B	3703	0	3727	86	0
2	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	34	0	0	0	0
3	B	25	0	0	3	0
All	All	7501	0	7464	192	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 13.

All (192) 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:174:MSE:CE	1:A:186:ALA:HB1	1.16	1.61
1:A:174:MSE:CE	1:A:186:ALA:CB	1.98	1.40
1:A:9:MSE:HB3	1:A:10:PRO:CD	1.77	1.13
1:A:127:SER:O	1:A:131:PRO:HD3	1.50	1.11
1:A:174:MSE:HE3	1:A:186:ALA:HB1	1.14	1.10
1:A:174:MSE:HE2	1:A:186:ALA:HB1	1.12	1.10
1:A:430:CYS:SG	1:A:500:MSE:HE3	1.92	1.09
1:A:45:ARG:HG3	1:A:155:LEU:HD13	1.30	1.06
1:A:174:MSE:HE1	1:A:186:ALA:CB	1.85	1.01
1:A:9:MSE:HB3	1:A:10:PRO:HD3	1.44	0.99
1:A:9:MSE:CB	1:A:10:PRO:CD	2.48	0.92
1:B:385:MSE:CE	1:B:387:GLY:O	2.19	0.90
1:A:174:MSE:HE3	1:A:186:ALA:CB	1.81	0.88
1:A:128:SER:O	1:A:131:PRO:HD2	1.75	0.86
1:A:430:CYS:O	1:A:500:MSE:HE2	1.76	0.86
1:B:385:MSE:HE2	1:B:387:GLY:O	1.74	0.86
1:A:119:VAL:HG11	1:A:127:SER:OG	1.75	0.85
1:A:385:MSE:HE1	1:A:387:GLY:O	1.76	0.84
1:B:478:ASP:N	1:B:481:ALA:HB3	1.93	0.84
1:A:9:MSE:HB3	1:A:10:PRO:HD2	1.60	0.84
1:A:9:MSE:CB	1:A:10:PRO:HD3	2.06	0.84
1:A:385:MSE:CE	1:A:387:GLY:O	2.26	0.83
1:B:452:GLU:HG3	1:B:472:VAL:HB	1.62	0.81
1:A:45:ARG:HG3	1:A:155:LEU:CD1	2.08	0.81
1:B:385:MSE:HE2	1:B:387:GLY:C	2.01	0.81
1:A:385:MSE:HE2	1:A:387:GLY:H	1.45	0.80
1:A:496:GLU:OE2	1:A:501:ALA:HB3	1.81	0.80
1:B:415:ASP:HB2	3:B:725:HOH:O	1.82	0.79
1:B:132:GLU:OE1	1:B:135:HIS:HB3	1.82	0.79
1:B:364:THR:CG2	1:B:401:ASP:OD2	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ASP:HB2	1:B:380:LYS:HB3	1.67	0.77
1:B:498:GLU:OE2	1:B:500:MSE:HG2	1.83	0.77
1:B:385:MSE:CE	1:B:387:GLY:C	2.54	0.76
1:B:385:MSE:HE2	1:B:387:GLY:H	1.49	0.76
1:B:22:GLU:HG2	1:B:25:ARG:HH21	1.51	0.76
1:B:364:THR:HG21	1:B:401:ASP:OD2	1.86	0.75
1:A:130:VAL:CG1	1:A:134:LEU:HD12	2.18	0.73
1:B:134:LEU:H	1:B:134:LEU:HD22	1.52	0.73
1:A:117:ALA:HB3	1:A:139:VAL:HB	1.68	0.73
1:A:9:MSE:CG	1:A:10:PRO:HD3	2.19	0.72
1:A:9:MSE:HG2	1:A:10:PRO:HD3	1.74	0.70
1:A:194:PHE:CE1	1:A:233:LEU:HD12	2.27	0.69
1:B:427:MSE:HE3	1:B:434:ASN:HB3	1.75	0.69
1:B:385:MSE:HE2	1:B:387:GLY:N	2.09	0.68
1:A:119:VAL:HG11	1:A:127:SER:CB	2.24	0.67
1:B:385:MSE:HE1	1:B:387:GLY:O	1.93	0.67
1:A:174:MSE:CE	1:A:186:ALA:HB3	2.20	0.65
1:B:435:ILE:HD12	1:B:501:ALA:HA	1.78	0.65
1:B:118:LEU:HD23	1:B:140:ILE:HB	1.79	0.65
1:B:334:GLY:O	1:B:338:LYS:HG3	1.97	0.65
1:A:271:LEU:HD11	1:A:306:ILE:HG13	1.77	0.64
1:B:385:MSE:HE2	1:B:387:GLY:CA	2.28	0.64
1:A:430:CYS:O	1:A:500:MSE:CE	2.45	0.63
1:A:172:LEU:HD23	1:A:194:PHE:CE2	2.33	0.63
1:A:125:MSE:O	1:A:128:SER:OG	2.09	0.63
1:A:119:VAL:CG1	1:A:127:SER:CB	2.76	0.62
1:A:379:ILE:HD12	1:A:406:THR:HG21	1.82	0.62
1:B:364:THR:HG22	1:B:401:ASP:OD2	1.99	0.61
1:A:385:MSE:HE2	1:A:387:GLY:O	2.00	0.60
1:A:124:LYS:HA	1:A:127:SER:HB3	1.83	0.60
1:A:297:ARG:NH1	1:A:298:ALA:O	2.34	0.60
1:B:134:LEU:H	1:B:134:LEU:CD2	2.15	0.60
1:A:385:MSE:CE	1:A:387:GLY:C	2.70	0.59
1:A:234:THR:HA	1:A:237:MSE:HE3	1.83	0.59
1:A:155:LEU:HD23	1:A:160:LEU:HD21	1.85	0.59
1:B:338:LYS:NZ	1:B:415:ASP:OD2	2.36	0.58
1:A:11:GLN:H	1:A:11:GLN:CD	2.06	0.58
1:A:119:VAL:HG13	1:A:127:SER:HB2	1.86	0.58
1:B:413:ARG:HH22	1:B:423:ARG:HH11	1.52	0.57
1:B:253:LEU:HD22	1:B:278:LEU:HD23	1.85	0.57
1:A:45:ARG:CG	1:A:155:LEU:HD13	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:MSE:HE1	1:A:387:GLY:C	2.24	0.57
1:B:68:ARG:NH1	3:B:703:HOH:O	2.37	0.57
1:A:130:VAL:CG1	1:A:134:LEU:CD1	2.82	0.57
1:A:130:VAL:N	1:A:131:PRO:CD	2.68	0.57
1:A:19:ARG:HB2	1:A:237:MSE:HG2	1.87	0.56
1:B:195:PHE:HB3	1:B:237:MSE:CE	2.35	0.56
1:B:195:PHE:HB3	1:B:237:MSE:HE3	1.87	0.56
1:A:321:GLU:O	1:A:385:MSE:HG2	2.06	0.56
1:B:317:TYR:HB3	1:B:327:LEU:HB2	1.88	0.56
1:A:496:GLU:OE2	1:A:501:ALA:CB	2.54	0.55
1:B:46:GLU:O	1:B:50:GLU:HG2	2.06	0.55
1:A:174:MSE:HE2	1:A:186:ALA:CB	2.02	0.55
1:A:263:THR:HG22	1:A:290:LEU:HB3	1.89	0.55
1:B:317:TYR:O	1:B:325:THR:HA	2.08	0.54
1:B:252:LEU:O	1:B:256:LEU:HG	2.06	0.54
1:A:385:MSE:HE2	1:A:387:GLY:N	2.20	0.54
1:B:186:ALA:HB3	1:B:389:TRP:HB3	1.88	0.54
1:B:316:VAL:HB	1:B:325:THR:HB	1.89	0.54
1:B:351:VAL:HG13	1:B:381:SER:HB2	1.89	0.54
1:A:128:SER:C	1:A:131:PRO:HD2	2.28	0.54
1:A:483:ARG:HA	1:A:486:LYS:HE2	1.90	0.54
1:B:428:ILE:HG23	1:B:457:GLU:HG3	1.90	0.54
1:A:174:MSE:HE1	1:A:186:ALA:HB3	1.86	0.53
1:A:430:CYS:SG	1:A:500:MSE:CE	2.83	0.53
1:A:414:GLU:H	1:A:414:GLU:CD	2.12	0.53
1:A:127:SER:O	1:A:130:VAL:HB	2.09	0.53
1:A:130:VAL:HG12	1:A:134:LEU:HD12	1.89	0.53
1:B:482:ALA:HB1	1:B:508:ILE:CD1	2.38	0.53
1:A:119:VAL:CG1	1:A:127:SER:OG	2.52	0.52
1:A:24:ALA:HA	1:A:44:TYR:HB3	1.91	0.52
1:A:365:ALA:HB3	1:A:368:ALA:HB2	1.92	0.52
1:B:134:LEU:N	1:B:134:LEU:CD2	2.73	0.52
1:B:436:ALA:HB3	1:B:439:GLU:HB2	1.92	0.52
1:B:155:LEU:HD11	1:B:160:LEU:HD11	1.91	0.52
1:B:24:ALA:HA	1:B:44:TYR:HB3	1.90	0.52
1:B:188:LEU:HG	1:B:386:LEU:HD12	1.92	0.52
1:A:46:GLU:O	1:A:50:GLU:HG2	2.10	0.51
1:B:385:MSE:HE1	1:B:387:GLY:C	2.29	0.51
1:B:478:ASP:N	1:B:481:ALA:CB	2.70	0.51
1:B:482:ALA:O	1:B:485:LEU:HB3	2.10	0.51
1:B:482:ALA:HB1	1:B:508:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:O	1:A:61:GLN:HG2	2.10	0.51
1:B:373:SER:HA	1:B:412:ARG:HE	1.76	0.51
1:A:194:PHE:CD1	1:A:233:LEU:HD12	2.46	0.51
1:A:328:CYS:HB2	1:A:348:TYR:CZ	2.46	0.51
1:A:174:MSE:HE3	1:A:186:ALA:HB3	1.87	0.50
1:A:251:SER:HA	1:A:277:GLU:OE1	2.12	0.50
1:B:479:GLU:HG2	3:B:724:HOH:O	2.11	0.49
1:A:9:MSE:N	1:A:11:GLN:NE2	2.60	0.49
1:B:441:ASP:OD1	1:B:455:CYS:N	2.46	0.49
1:A:23:GLN:CG	1:A:237:MSE:O	2.61	0.48
1:B:134:LEU:HD23	1:B:134:LEU:O	2.13	0.48
1:A:410:LEU:HD23	1:A:420:ILE:HA	1.96	0.48
1:B:70:LEU:HB2	1:B:114:PRO:HG3	1.95	0.48
1:A:306:ILE:O	1:A:309:THR:HG22	2.14	0.48
1:A:380:LYS:NZ	1:A:402:GLY:HA3	2.29	0.48
1:A:494:ARG:NH2	2:A:602:SO4:S	2.85	0.47
1:A:487:HIS:CD2	1:B:361:ILE:HD12	2.49	0.47
1:B:425:SER:O	1:B:426:GLU:CB	2.61	0.47
1:A:186:ALA:HB3	1:A:389:TRP:HB3	1.97	0.47
1:A:466:LEU:HD21	1:B:409:LEU:HD21	1.97	0.47
1:A:23:GLN:HG3	1:A:237:MSE:O	2.15	0.47
1:A:119:VAL:HG13	1:A:127:SER:CB	2.44	0.47
1:A:19:ARG:CB	1:A:237:MSE:HG2	2.44	0.47
1:A:35:ARG:NH2	1:A:78:GLU:OE1	2.47	0.47
1:B:221:LEU:HD13	1:B:225:HIS:HE1	1.79	0.46
1:A:381:SER:H	1:A:384:ASN:ND2	2.12	0.46
1:A:272:SER:OG	1:A:302:ASP:OD2	2.30	0.46
1:A:493:PHE:O	1:A:496:GLU:HG2	2.16	0.46
1:B:29:GLU:OE1	1:B:45:ARG:NH2	2.32	0.46
1:B:423:ARG:HA	1:B:423:ARG:HH11	1.81	0.46
1:B:478:ASP:H	1:B:481:ALA:HB3	1.78	0.45
1:B:97:ASP:HB3	1:B:100:LEU:HG	1.98	0.45
1:A:102:ILE:HD12	1:A:102:ILE:H	1.82	0.45
1:A:175:ILE:O	1:A:187:VAL:HB	2.17	0.45
1:B:388:TYR:CE2	1:B:398:VAL:HG11	2.51	0.45
1:A:118:LEU:HD23	1:A:140:ILE:HB	1.98	0.44
1:B:34:ARG:HD2	1:B:38:GLY:HA2	1.99	0.44
1:A:463:PHE:CD2	1:B:409:LEU:HD23	2.52	0.44
1:B:452:GLU:OE1	1:B:472:VAL:HG21	2.17	0.44
1:A:493:PHE:CG	1:A:503:PRO:HD3	2.52	0.44
1:B:479:GLU:OE2	1:B:479:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:HIS:ND1	1:B:135:HIS:N	2.60	0.44
1:B:326:ALA:CB	1:B:379:ILE:HD13	2.47	0.44
1:B:124:LYS:HD2	1:B:124:LYS:HA	1.80	0.44
1:B:478:ASP:H	1:B:481:ALA:CB	2.30	0.43
1:A:65:ARG:HH21	1:A:165:ASP:HB3	1.83	0.43
1:B:225:HIS:CE1	1:B:227:GLY:HA3	2.53	0.43
1:B:507:VAL:HG11	1:B:529:ALA:HB1	2.00	0.43
1:A:17:LEU:HD22	1:A:88:LYS:HA	2.01	0.43
1:B:42:LEU:HD21	1:B:50:GLU:HG3	2.00	0.43
1:A:377:LEU:HD22	1:A:410:LEU:HD12	2.01	0.43
1:B:365:ALA:O	1:B:368:ALA:HB2	2.18	0.43
1:A:307:GLU:OE2	1:A:313:THR:OG1	2.36	0.43
1:B:115:ALA:O	1:B:138:PRO:HD2	2.19	0.43
1:A:388:TYR:CE2	1:A:398:VAL:HG11	2.54	0.43
1:A:500:MSE:C	1:A:502:ARG:H	2.21	0.43
1:A:423:ARG:HA	1:A:423:ARG:HD3	1.69	0.43
1:B:306:ILE:HA	1:B:306:ILE:HD13	1.73	0.42
1:B:477:LEU:C	1:B:481:ALA:HB3	2.39	0.42
1:A:441:ASP:OD1	1:A:455:CYS:N	2.53	0.42
1:B:317:TYR:O	1:B:326:ALA:N	2.44	0.42
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.89	0.42
1:B:132:GLU:N	1:B:132:GLU:CD	2.73	0.42
1:A:192:ARG:NH1	1:A:382:PRO:O	2.43	0.42
1:A:491:ALA:O	1:A:495:ARG:HG3	2.20	0.42
1:A:498:GLU:HA	1:A:499:PRO:HD2	1.94	0.42
1:B:266:LEU:O	1:B:293:TYR:HA	2.20	0.41
1:A:293:TYR:CZ	1:A:315:GLN:HB2	2.56	0.41
1:A:425:SER:O	1:A:425:SER:OG	2.32	0.41
1:A:106:GLU:O	1:A:110:GLN:HG3	2.20	0.41
1:A:68:ARG:HH21	1:A:113:ASP:HB3	1.86	0.41
1:B:134:LEU:HD23	1:B:134:LEU:C	2.42	0.41
1:B:22:GLU:CG	1:B:25:ARG:HH21	2.25	0.41
1:B:502:ARG:HA	1:B:503:PRO:HD3	1.84	0.41
1:B:80:TYR:O	1:B:84:LEU:HG	2.21	0.41
1:A:498:GLU:OE2	1:A:499:PRO:HD2	2.20	0.40
1:A:31:ILE:HA	1:A:43:ARG:HA	2.02	0.40
1:A:460:ASP:OD2	1:A:463:PHE:N	2.32	0.40
1:B:185:LYS:HE2	1:B:394:ARG:HG2	2.03	0.40
1:B:496:GLU:OE2	1:B:502:ARG:HG2	2.20	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	500/541 (92%)	488 (98%)	10 (2%)	2 (0%)	34	37
1	B	493/541 (91%)	480 (97%)	12 (2%)	1 (0%)	47	55
All	All	993/1082 (92%)	968 (98%)	22 (2%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	CYS
1	A	324	CYS
1	A	184	PRO

### 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	386/406 (95%)	365 (95%)	21 (5%)	22	26
1	B	386/406 (95%)	365 (95%)	21 (5%)	22	26
All	All	772/812 (95%)	730 (95%)	42 (5%)	22	26

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

Mol	Chain	Res	Type
1	A	9	MSE
1	A	25	ARG
1	A	68	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	136	SER
1	A	139	VAL
1	A	155	LEU
1	A	180	THR
1	A	248	ASN
1	A	258	THR
1	A	273	LYS
1	A	309	THR
1	A	385	MSE
1	A	390	ASN
1	A	391	ASN
1	A	423	ARG
1	A	427	MSE
1	A	438	ASP
1	A	455	CYS
1	A	461	GLU
1	A	474	SER
1	A	476	GLU
1	B	59	ARG
1	B	68	ARG
1	B	106	GLU
1	B	132	GLU
1	B	134	LEU
1	B	139	VAL
1	B	165	ASP
1	B	237	MSE
1	B	249	THR
1	B	306	ILE
1	B	324	CYS
1	B	325	THR
1	B	352	ASP
1	B	391	ASN
1	B	394	ARG
1	B	414	GLU
1	B	420	ILE
1	B	423	ARG
1	B	448	SER
1	B	496	GLU
1	B	502	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	225	HIS
1	B	315	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	603	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	A	601	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	B	601	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	499/541 (92%)	0.47	33 (6%)	18   17	17, 27, 48, 68	0
1	B	494/541 (91%)	0.47	33 (6%)	17   16	17, 30, 50, 70	0
All	All	993/1082 (91%)	0.47	66 (6%)	18   17	17, 29, 49, 70	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	SER	9.7
1	B	132	GLU	7.9
1	A	128	SER	7.8
1	A	182	GLY	7.0
1	B	474	SER	6.0
1	A	129	ALA	5.8
1	A	179	GLY	5.2
1	A	181	THR	4.9
1	A	180	THR	4.6
1	B	480	SER	4.4
1	A	126	ALA	4.3
1	B	424	SER	4.1
1	A	426	GLU	4.0
1	B	178	SER	3.8
1	A	130	VAL	3.8
1	B	481	ALA	3.7
1	B	501	ALA	3.7
1	B	425	SER	3.6
1	A	476	GLU	3.5
1	B	124	LYS	3.5
1	A	497	SER	3.2
1	B	477	LEU	3.2
1	B	4	LYS	3.0
1	A	123	SER	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	110	GLN	2.9
1	B	359	ASP	2.9
1	B	365	ALA	2.9
1	A	183	GLU	2.9
1	B	475	ALA	2.9
1	B	368	ALA	2.8
1	A	178	SER	2.8
1	A	100	LEU	2.8
1	B	366	PRO	2.7
1	A	177	THR	2.7
1	B	478	ASP	2.7
1	B	511	ASP	2.7
1	A	365	ALA	2.6
1	B	484	ALA	2.6
1	A	157	ALA	2.6
1	B	133	ALA	2.6
1	A	499	PRO	2.5
1	B	479	GLU	2.5
1	B	519	LYS	2.4
1	B	6	PHE	2.4
1	A	435	ILE	2.4
1	B	113	ASP	2.4
1	A	99	ASN	2.4
1	A	430	CYS	2.4
1	B	482	ALA	2.3
1	A	194	PHE	2.3
1	B	364	THR	2.2
1	A	496	GLU	2.2
1	A	529	ALA	2.2
1	A	156	ASP	2.2
1	B	107	ARG	2.2
1	B	123	SER	2.2
1	A	482	ALA	2.2
1	A	133	ALA	2.1
1	A	446	GLY	2.1
1	A	144	ILE	2.1
1	B	346	ARG	2.1
1	B	529	ALA	2.1
1	A	390	ASN	2.0
1	B	248	ASN	2.0
1	B	22	GLU	2.0
1	B	412	ARG	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	601	5/5	0.93	0.20	40,41,53,54	0
2	SO4	A	603	5/5	0.94	0.17	39,46,51,52	0
2	SO4	A	602	5/5	0.98	0.11	33,34,36,41	0
2	SO4	A	601	5/5	0.99	0.13	23,26,31,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.