



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2019 – 09:08 PM EDT

PDB ID : 6DDN  
Title : The sulfate-binding protein SubI from Mycobacterium tuberculosis H37Rv  
Authors : Meza, A.N.; Balan, A.; Nascimento, A.F.Z.  
Deposited on : 2018-05-10  
Resolution : 2.29 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

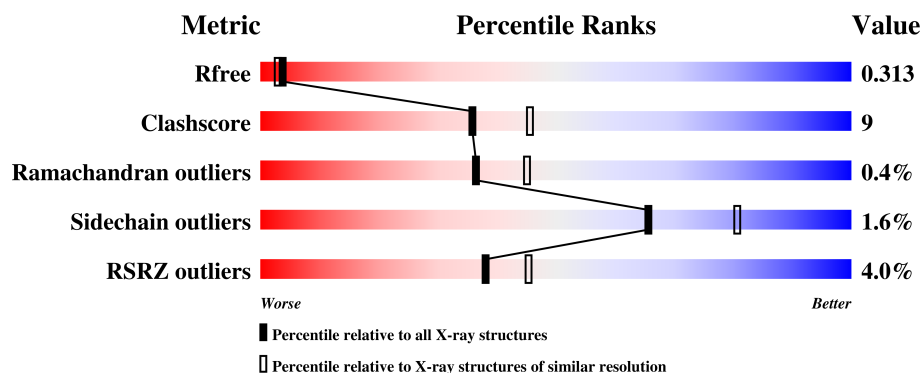
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (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	352	<div> <div>4%</div> <div>67%</div> <div>13%</div> <div>•</div> <div>18%</div> </div>
1	B	352	<div> <div>3%</div> <div>64%</div> <div>17%</div> <div>•</div> <div>18%</div> </div>

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	405	-	-	X	-
3	ACT	A	409	-	-	-	X
4	PEG	A	410	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4563 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 Probable sulfate-binding lipoprotein SubI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	0	1	0
			2166	1377	376	413			
1	B	287	Total	C	N	O	0	2	0
			2168	1378	376	414			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	initiating methionine	UNP P71744
A	6	GLY	-	expression tag	UNP P71744
A	7	SER	-	expression tag	UNP P71744
A	8	SER	-	expression tag	UNP P71744
A	9	HIS	-	expression tag	UNP P71744
A	10	HIS	-	expression tag	UNP P71744
A	11	HIS	-	expression tag	UNP P71744
A	12	HIS	-	expression tag	UNP P71744
A	13	HIS	-	expression tag	UNP P71744
A	14	HIS	-	expression tag	UNP P71744
A	15	SER	-	expression tag	UNP P71744
A	16	SER	-	expression tag	UNP P71744
A	17	GLY	-	expression tag	UNP P71744
A	18	LEU	-	expression tag	UNP P71744
A	19	VAL	-	expression tag	UNP P71744
A	20	PRO	-	expression tag	UNP P71744
A	21	ARG	-	expression tag	UNP P71744
A	22	GLY	-	expression tag	UNP P71744
A	23	SER	-	expression tag	UNP P71744
A	24	HIS	-	expression tag	UNP P71744
A	25	MET	-	expression tag	UNP P71744
A	26	ALA	-	expression tag	UNP P71744
A	27	SER	-	expression tag	UNP P71744
A	28	MET	-	expression tag	UNP P71744
A	29	THR	-	expression tag	UNP P71744

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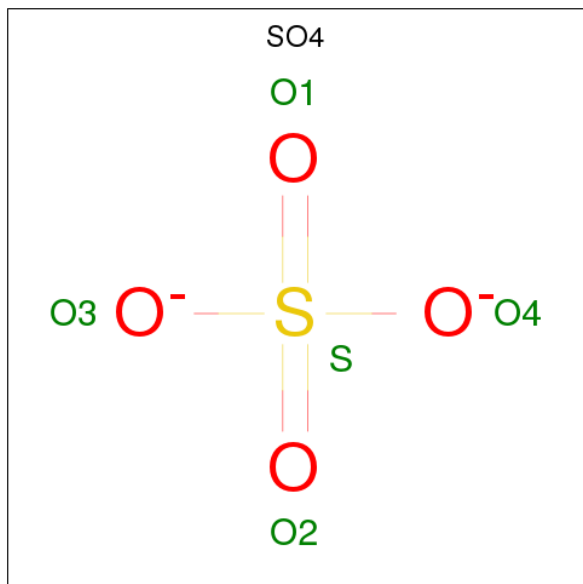
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP P71744
A	31	GLY	-	expression tag	UNP P71744
A	32	GLN	-	expression tag	UNP P71744
A	33	GLN	-	expression tag	UNP P71744
A	34	MET	-	expression tag	UNP P71744
A	35	GLY	-	expression tag	UNP P71744
A	36	ARG	-	expression tag	UNP P71744
A	37	GLY	-	expression tag	UNP P71744
A	38	SER	-	expression tag	UNP P71744
A	39	GLU	-	expression tag	UNP P71744
A	40	PHE	-	expression tag	UNP P71744
B	5	MET	-	initiating methionine	UNP P71744
B	6	GLY	-	expression tag	UNP P71744
B	7	SER	-	expression tag	UNP P71744
B	8	SER	-	expression tag	UNP P71744
B	9	HIS	-	expression tag	UNP P71744
B	10	HIS	-	expression tag	UNP P71744
B	11	HIS	-	expression tag	UNP P71744
B	12	HIS	-	expression tag	UNP P71744
B	13	HIS	-	expression tag	UNP P71744
B	14	HIS	-	expression tag	UNP P71744
B	15	SER	-	expression tag	UNP P71744
B	16	SER	-	expression tag	UNP P71744
B	17	GLY	-	expression tag	UNP P71744
B	18	LEU	-	expression tag	UNP P71744
B	19	VAL	-	expression tag	UNP P71744
B	20	PRO	-	expression tag	UNP P71744
B	21	ARG	-	expression tag	UNP P71744
B	22	GLY	-	expression tag	UNP P71744
B	23	SER	-	expression tag	UNP P71744
B	24	HIS	-	expression tag	UNP P71744
B	25	MET	-	expression tag	UNP P71744
B	26	ALA	-	expression tag	UNP P71744
B	27	SER	-	expression tag	UNP P71744
B	28	MET	-	expression tag	UNP P71744
B	29	THR	-	expression tag	UNP P71744
B	30	GLY	-	expression tag	UNP P71744
B	31	GLY	-	expression tag	UNP P71744
B	32	GLN	-	expression tag	UNP P71744
B	33	GLN	-	expression tag	UNP P71744
B	34	MET	-	expression tag	UNP P71744
B	35	GLY	-	expression tag	UNP P71744

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	ARG	-	expression tag	UNP P71744
B	37	GLY	-	expression tag	UNP P71744
B	38	SER	-	expression tag	UNP P71744
B	39	GLU	-	expression tag	UNP P71744
B	40	PHE	-	expression tag	UNP P71744

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



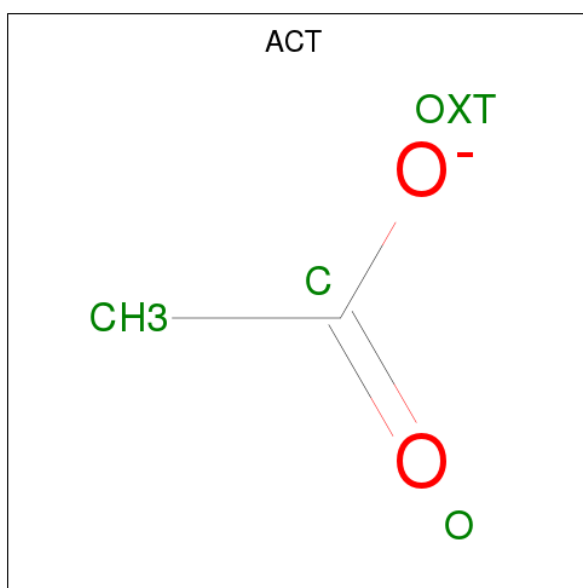
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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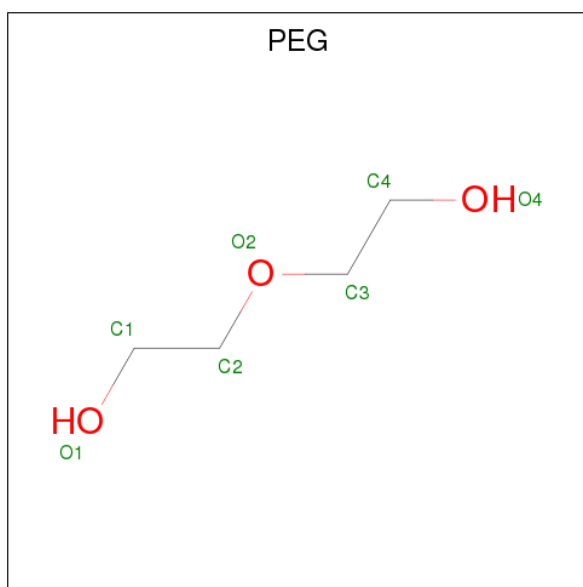
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

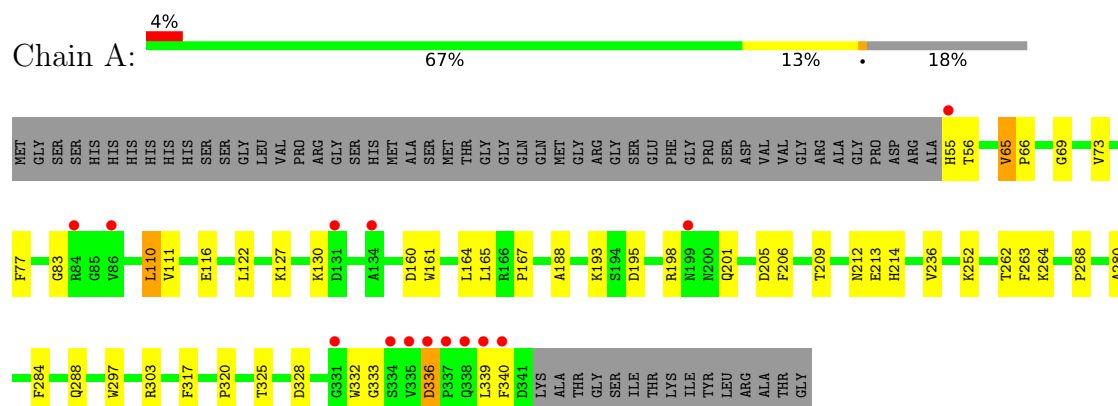
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	59	Total	O	0	0
			59	59		



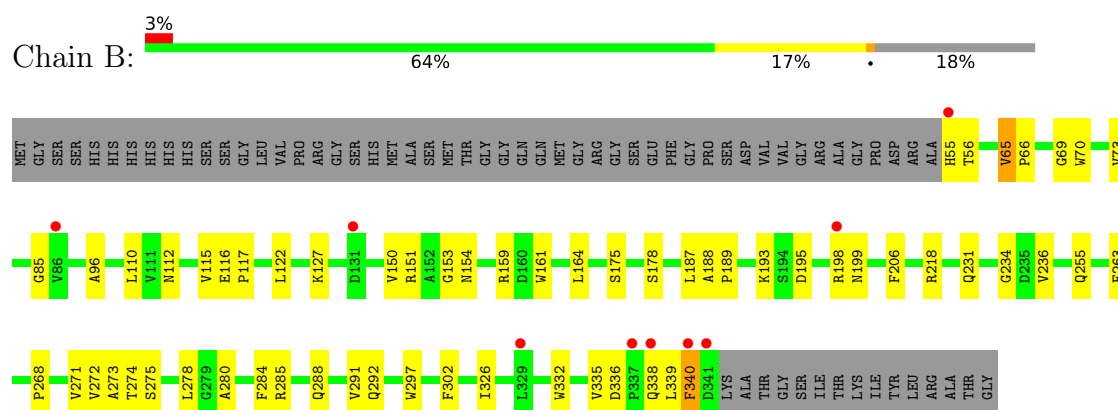
### 3 Residue-property plots [i](#)

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: Probable sulfate-binding lipoprotein SubI



- Molecule 1: Probable sulfate-binding lipoprotein SubI



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	243.73 Å   243.73 Å   243.73 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	46.91 – 2.29 46.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (46.91-2.29) 94.9 (46.91-2.30)	Depositor EDS
$R_{merge}$	0.38	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 2.29 Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.270 , 0.313 0.270 , 0.313	Depositor DCC
$R_{free}$ test set	1338 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0191e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, ACT

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	0.27	0/2226	0.46	0/3046
1	B	0.35	1/2232 (0.0%)	0.48	0/3054
All	All	0.31	1/4458 (0.0%)	0.47	0/6100

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	GLN	CA-CB	-5.02	1.43	1.53

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	2166	0	2118	32	0
1	B	2168	0	2119	43	0
2	A	30	0	0	3	0
2	B	40	0	0	1	0
3	A	12	0	9	0	0
4	A	21	0	30	6	0
4	B	14	0	20	2	0
5	A	53	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	59	0	0	0	0
All	All	4563	0	4296	76	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 9.

All (76) 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:B:187:LEU:HD21	1:B:335:VAL:HG21	1.59	0.82
1:A:195:ASP:O	1:A:198:ARG:NH1	2.21	0.70
1:A:209:THR:HG21	4:A:411:PEG:H12	1.74	0.70
1:A:214:HIS:NE2	4:A:410:PEG:H41	2.08	0.69
1:B:338:GLN:NE2	1:B:338:GLN:O	2.26	0.69
1:B:291:VAL:H	4:B:409:PEG:H12	1.59	0.67
1:A:325:THR:OG1	1:A:328:ASP:OD1	2.14	0.66
1:B:275:SER:HB3	1:B:278:LEU:HD22	1.78	0.64
1:A:164:LEU:HD22	1:A:236:VAL:HG11	1.79	0.63
1:B:122:LEU:HB3	1:B:127:LYS:HB2	1.79	0.63
1:B:117:PRO:CG	1:B:336:ASP:OD2	2.49	0.61
1:B:164:LEU:HD22	1:B:236:VAL:HG11	1.83	0.61
1:A:212[A]:ASN:ND2	5:A:502:HOH:O	2.34	0.60
1:B:110:LEU:HD23	1:B:271:VAL:HA	1.84	0.59
1:A:127:LYS:NZ	5:A:503:HOH:O	2.35	0.59
1:B:336:ASP:O	1:B:339:LEU:HB3	2.03	0.59
1:B:161:TRP:CZ3	1:B:189:PRO:HG3	2.39	0.57
1:B:73:VAL:HG11	1:B:288:GLN:OE1	2.04	0.57
1:A:332:TRP:O	1:A:336:ASP:HB2	2.04	0.57
1:A:160:ASP:HB2	2:A:405:SO4:O2	2.05	0.57
1:B:151:ARG:NH2	1:B:234:GLY:O	2.38	0.56
1:B:110:LEU:HD12	1:B:284:PHE:HD2	1.70	0.55
1:B:338:GLN:HE22	1:B:340:PHE:HE2	1.46	0.55
1:B:175:SER:HB2	1:B:218:ARG:HD2	1.90	0.53
1:A:167:PRO:HG3	4:A:410:PEG:H21	1.91	0.52
1:B:188:ALA:HB2	1:B:263:PHE:HB2	1.93	0.51
1:B:55:HIS:CG	1:B:56:THR:H	2.28	0.51
1:B:272:VAL:HG12	1:B:274:THR:HG22	1.93	0.51
1:B:338:GLN:NE2	1:B:340:PHE:CE2	2.65	0.51
1:A:165:LEU:HD13	4:A:411:PEG:H11	1.93	0.51
1:A:69:GLY:HA3	1:A:297:TRP:CZ3	2.47	0.50
1:B:70:TRP:HE1	1:B:112:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASP:O	1:B:198:ARG:HG3	2.13	0.49
1:A:116:GLU:HA	1:A:268:PRO:HG3	1.94	0.49
1:A:280:ALA:N	2:A:404:SO4:O3	2.37	0.49
1:B:193:LYS:HG3	1:B:206:PHE:CG	2.48	0.49
1:B:69:GLY:HA3	1:B:297:TRP:CZ3	2.49	0.48
1:B:326:ILE:HD11	1:B:335:VAL:HG11	1.95	0.47
1:B:280:ALA:N	2:B:403:SO4:O4	2.46	0.47
1:B:292:GLN:HB2	4:B:409:PEG:H32	1.97	0.47
1:A:188:ALA:HB2	1:A:263:PHE:HB2	1.97	0.47
1:A:213:GLU:OE2	4:A:410:PEG:H42	2.16	0.46
1:A:73:VAL:HG11	1:A:288:GLN:OE1	2.17	0.45
1:B:332:TRP:HE3	1:B:336:ASP:OD1	2.00	0.45
1:A:161:TRP:HD1	2:A:405:SO4:O1	2.00	0.45
4:A:410:PEG:H11	4:A:410:PEG:H32	1.59	0.45
1:B:115:VAL:HB	1:B:117:PRO:HD2	1.98	0.45
1:B:96:ALA:HB3	1:B:178:SER:HA	1.98	0.45
1:A:303:ARG:CZ	1:A:317:PHE:HB3	2.46	0.45
1:B:55:HIS:HB3	1:B:85:GLY:O	2.17	0.45
1:B:117:PRO:HG3	1:B:336:ASP:OD2	2.18	0.44
1:A:111:VAL:HG11	1:A:122:LEU:CD1	2.48	0.44
1:A:262:THR:HG22	1:A:320:PRO:HG3	2.00	0.44
1:A:333:GLY:N	5:A:506:HOH:O	2.40	0.44
1:A:77:PHE:O	1:A:83:GLY:HA3	2.18	0.43
1:B:70:TRP:HE1	1:B:112:ASN:HD22	1.65	0.43
1:B:127:LYS:O	1:B:273:ALA:N	2.43	0.43
1:B:285:ARG:HD2	1:B:285:ARG:C	2.39	0.43
1:B:150:VAL:HG21	1:B:154:ASN:OD1	2.19	0.42
1:B:153:GLY:H	1:B:255:GLN:CD	2.22	0.42
1:B:332:TRP:HA	1:B:335:VAL:CG1	2.49	0.42
1:A:130:LYS:HG3	1:A:130:LYS:H	1.66	0.42
1:A:193:LYS:HG3	1:A:206:PHE:CD2	2.55	0.42
1:A:201:GLN:NE2	1:A:205:ASP:OD1	2.52	0.42
1:A:110:LEU:HD13	1:A:284:PHE:HD2	1.85	0.42
1:A:264:LYS:NZ	5:A:505:HOH:O	2.37	0.42
1:B:116:GLU:HA	1:B:268:PRO:HG3	2.02	0.41
1:B:65:VAL:N	1:B:66:PRO:CD	2.84	0.41
1:A:55:HIS:HB3	1:A:56:THR:H	1.62	0.41
1:B:66:PRO:HA	1:B:302:PHE:CZ	2.56	0.41
1:A:195:ASP:O	1:A:198:ARG:HD2	2.21	0.41
1:B:110:LEU:HD12	1:B:284:PHE:CD2	2.54	0.41
1:B:193:LYS:HG3	1:B:206:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HG3	1:A:206:PHE:CG	2.56	0.40
1:A:65:VAL:N	1:A:66:PRO:CD	2.84	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	286/352 (81%)	275 (96%)	10 (4%)	1 (0%)	43	53
1	B	287/352 (82%)	278 (97%)	8 (3%)	1 (0%)	43	53
All	All	573/704 (81%)	553 (96%)	18 (3%)	2 (0%)	36	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	B	65	VAL

### 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	226/273 (83%)	221 (98%)	5 (2%)	55	72
1	B	227/273 (83%)	225 (99%)	2 (1%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	453/546 (83%)	446 (98%)	7 (2%)	65	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	252	LYS
1	A	336	ASP
1	A	339	LEU
1	A	340	PHE
1	B	159	ARG
1	B	340	PHE

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

Mol	Chain	Res	Type
1	A	231	GLN
1	B	112	ASN

### 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 ⓘ

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	401	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	A	402	-	4,4,4	0.17	0	6,6,6	0.05	0
2	SO4	A	403	-	4,4,4	0.16	0	6,6,6	0.04	0
2	SO4	A	404	-	4,4,4	0.16	0	6,6,6	0.05	0
2	SO4	A	405	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	A	406	-	4,4,4	0.19	0	6,6,6	0.04	0
3	ACT	A	407	-	1,3,3	6.55	1 (100%)	0,3,3	0.00	-
3	ACT	A	408	-	1,3,3	6.87	1 (100%)	0,3,3	0.00	-
3	ACT	A	409	-	1,3,3	6.42	1 (100%)	0,3,3	0.00	-
4	PEG	A	410	-	6,6,6	0.51	0	5,5,5	0.11	0
4	PEG	A	411	-	6,6,6	0.48	0	5,5,5	0.25	0
4	PEG	A	412	-	6,6,6	0.48	0	5,5,5	0.38	0
2	SO4	B	401	-	4,4,4	0.17	0	6,6,6	0.05	0
2	SO4	B	402	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	403	-	4,4,4	0.16	0	6,6,6	0.04	0
2	SO4	B	404	-	4,4,4	0.16	0	6,6,6	0.05	0
2	SO4	B	405	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	B	406	-	4,4,4	0.16	0	6,6,6	0.05	0
2	SO4	B	407	-	4,4,4	0.18	0	6,6,6	0.07	0
2	SO4	B	408	-	4,4,4	0.20	0	6,6,6	0.07	0
4	PEG	B	409	-	6,6,6	0.49	0	5,5,5	0.28	0
4	PEG	B	410	-	6,6,6	0.49	0	5,5,5	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	A	404	-	-	0/0/0/0	0/0/0/0
2	SO4	A	405	-	-	0/0/0/0	0/0/0/0
2	SO4	A	406	-	-	0/0/0/0	0/0/0/0
3	ACT	A	407	-	-	0/0/0/0	0/0/0/0
3	ACT	A	408	-	-	0/0/0/0	0/0/0/0
3	ACT	A	409	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	410	-	-	0/4/4/4	0/0/0/0
4	PEG	A	411	-	-	0/4/4/4	0/0/0/0
4	PEG	A	412	-	-	0/4/4/4	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	403	-	-	0/0/0/0	0/0/0/0
2	SO4	B	404	-	-	0/0/0/0	0/0/0/0
2	SO4	B	405	-	-	0/0/0/0	0/0/0/0
2	SO4	B	406	-	-	0/0/0/0	0/0/0/0
2	SO4	B	407	-	-	0/0/0/0	0/0/0/0
2	SO4	B	408	-	-	0/0/0/0	0/0/0/0
4	PEG	B	409	-	-	0/4/4/4	0/0/0/0
4	PEG	B	410	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	409	ACT	CH3-C	6.42	1.56	1.48
3	A	407	ACT	CH3-C	6.55	1.57	1.48
3	A	408	ACT	CH3-C	6.87	1.57	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	SO4	1	0
2	A	405	SO4	2	0
4	A	410	PEG	4	0
4	A	411	PEG	2	0
2	B	403	SO4	1	0
4	B	409	PEG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/352 (81%)	0.44	14 (4%) 29 37	40, 55, 93, 136	0
1	B	287/352 (81%)	0.45	9 (3%) 49 56	42, 56, 88, 144	0
All	All	574/704 (81%)	0.44	23 (4%) 38 45	40, 56, 93, 144	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PRO	8.3
1	B	340	PHE	5.6
1	A	337	PRO	5.3
1	A	340	PHE	4.5
1	A	336	ASP	3.9
1	B	338	GLN	3.8
1	B	329	LEU	3.6
1	A	86	VAL	3.4
1	A	84	ARG	3.2
1	B	86	VAL	3.0
1	A	134	ALA	2.7
1	A	338	GLN	2.7
1	A	335	VAL	2.6
1	B	55	HIS	2.5
1	B	131	ASP	2.5
1	A	331	GLY	2.4
1	B	341	ASP	2.4
1	B	198	ARG	2.2
1	A	55	HIS	2.2
1	A	131	ASP	2.2
1	A	339	LEU	2.2
1	A	334	SER	2.2
1	A	199	ASN	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( $\text{\AA}^2$ )	Q<0.9
3	ACT	A	409	4/4	0.49	0.42	83,87,87,90	0
4	PEG	B	410	7/7	0.55	0.25	73,78,80,81	0
2	SO4	A	406	5/5	0.74	0.38	131,131,131,133	0
4	PEG	B	409	7/7	0.74	0.18	54,58,68,68	0
2	SO4	B	408	5/5	0.75	0.38	143,144,144,145	0
4	PEG	A	410	7/7	0.80	0.43	72,74,79,79	0
3	ACT	A	408	4/4	0.81	0.21	70,70,73,77	0
4	PEG	A	412	7/7	0.82	0.23	48,60,69,74	0
3	ACT	A	407	4/4	0.82	0.16	68,68,73,82	0
2	SO4	A	405	5/5	0.82	0.36	117,121,123,125	0
4	PEG	A	411	7/7	0.83	0.28	72,76,81,81	0
2	SO4	B	406	5/5	0.83	0.20	119,120,121,123	0
2	SO4	A	404	5/5	0.84	0.19	117,117,120,121	0
2	SO4	B	405	5/5	0.85	0.25	115,117,118,120	0
2	SO4	B	407	5/5	0.86	0.27	132,132,132,133	0
2	SO4	B	402	5/5	0.92	0.10	88,90,93,96	0
2	SO4	B	403	5/5	0.92	0.18	128,128,130,130	0
2	SO4	A	402	5/5	0.94	0.13	62,63,63,63	5
2	SO4	A	403	5/5	0.96	0.11	94,95,96,99	0
2	SO4	B	404	5/5	0.96	0.12	47,47,47,49	5
2	SO4	A	401	5/5	0.98	0.16	48,48,48,49	0
2	SO4	B	401	5/5	0.99	0.16	47,49,56,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.