



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:55 pm BST

PDB ID : 4B3H  
Title : Crystal structure of Mycobacterium tuberculosis fatty acid beta- oxidation complex  
Authors : Venkatesan, R.; Wierenga, R.  
Deposited on : 2012-07-24  
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

<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

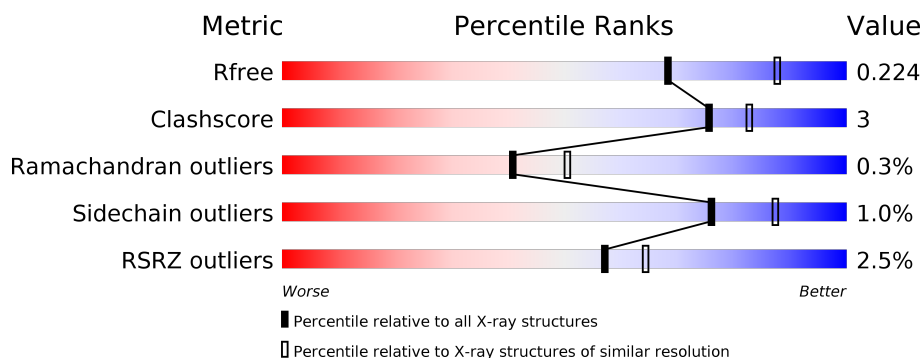
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	736	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> </div>
1	B	736	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	C	403	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
2	D	403	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18048 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 FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	7	0
			5457	3455	937	1043	22			
1	B	728	Total	C	N	O	S	0	10	0
			5441	3449	930	1039	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP O53872
A	-14	GLY	-	expression tag	UNP O53872
A	-13	SER	-	expression tag	UNP O53872
A	-12	SER	-	expression tag	UNP O53872
A	-11	HIS	-	expression tag	UNP O53872
A	-10	HIS	-	expression tag	UNP O53872
A	-9	HIS	-	expression tag	UNP O53872
A	-8	HIS	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	-	expression tag	UNP O53872
A	-4	GLN	-	expression tag	UNP O53872
A	-3	ASP	-	expression tag	UNP O53872
A	-2	PRO	-	expression tag	UNP O53872
A	-1	ASN	-	expression tag	UNP O53872
A	0	SER	-	expression tag	UNP O53872
B	-15	MET	-	expression tag	UNP O53872
B	-14	GLY	-	expression tag	UNP O53872
B	-13	SER	-	expression tag	UNP O53872
B	-12	SER	-	expression tag	UNP O53872
B	-11	HIS	-	expression tag	UNP O53872
B	-10	HIS	-	expression tag	UNP O53872
B	-9	HIS	-	expression tag	UNP O53872
B	-8	HIS	-	expression tag	UNP O53872

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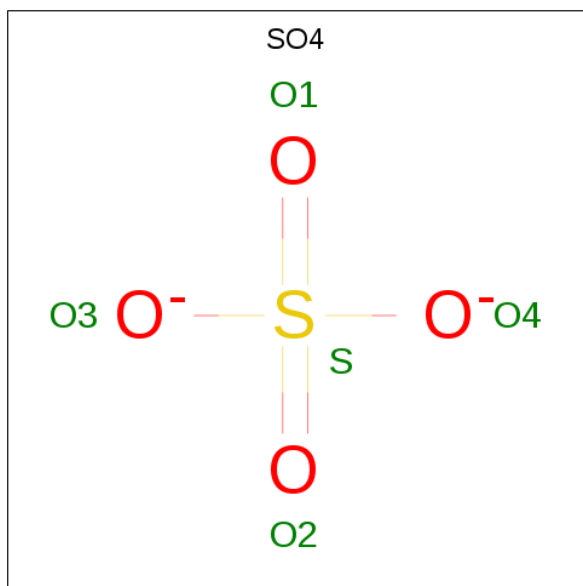
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP O53872
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	398	Total	C	N	O	S	0	4	0
			2950	1843	521	571	15			
2	D	401	Total	C	N	O	S	0	4	0
			2970	1857	525	572	16			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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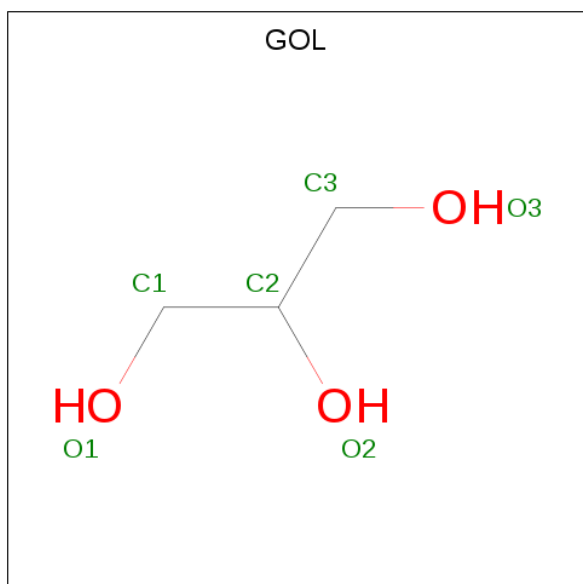
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

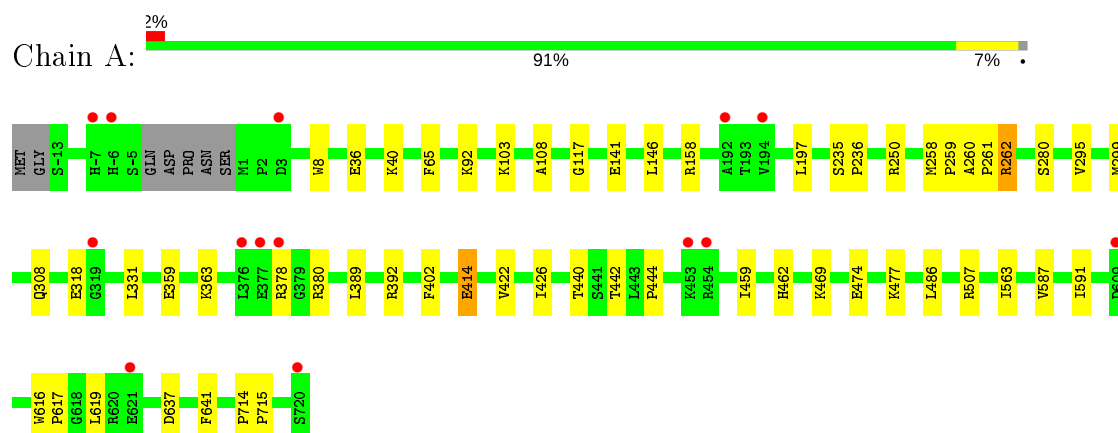
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	329	Total	O	0	0
			329	329		
5	B	351	Total	O	0	0
			351	351		
5	C	202	Total	O	0	0
			202	202		
5	D	144	Total	O	0	0
			144	144		

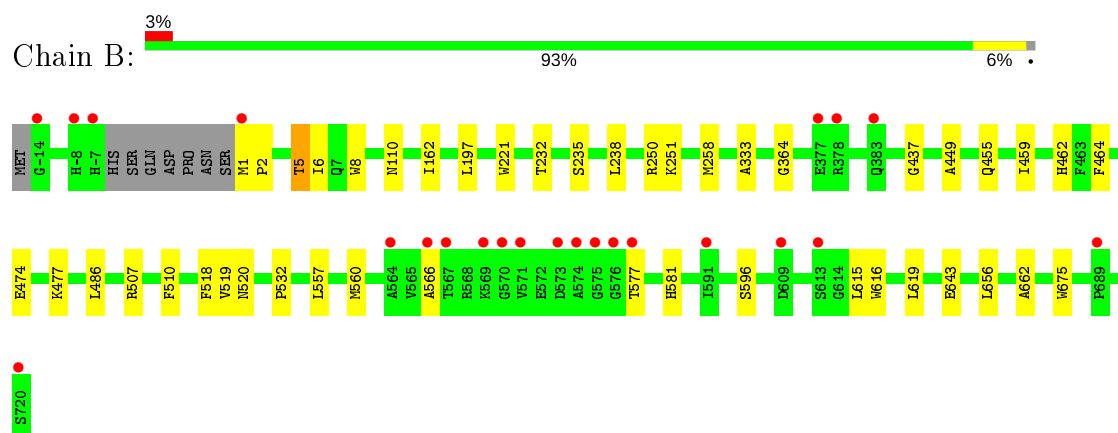
### 3 Residue-property plots [i](#)

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.

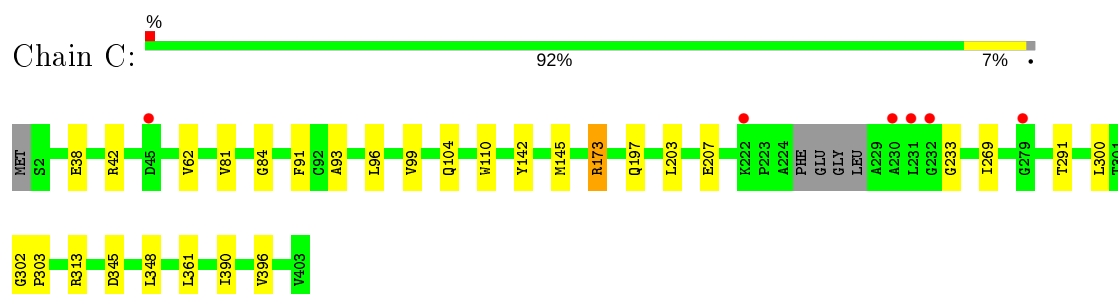
#### • Molecule 1: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB



#### • Molecule 1: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB

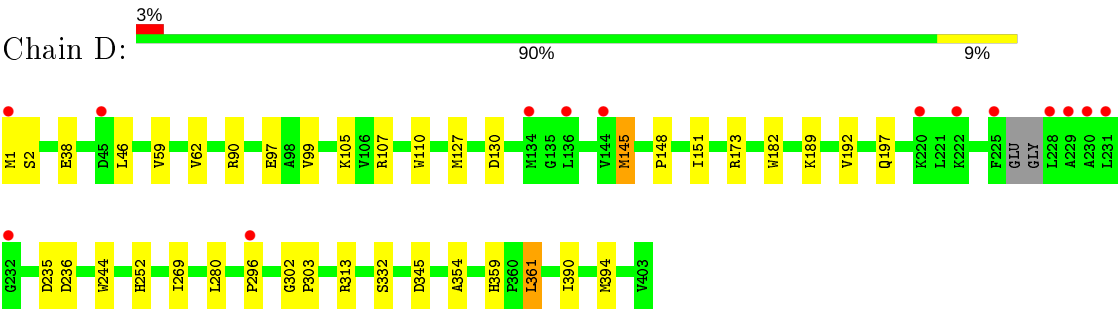


#### • Molecule 2: FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA





● Molecule 2: FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	249.46 Å   134.25 Å   118.40 Å 90.00°   110.74°   90.00°	Depositor
Resolution (Å)	49.94 – 2.30 49.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.94-2.30) 99.8 (49.94-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.195   ,   0.224 0.195   ,   0.224	Depositor DCC
$R_{free}$ test set	8108 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.333 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: GOL, 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	0.39	0/5583	0.49	0/7559
1	B	0.39	1/5575 (0.0%)	0.49	0/7550
2	C	0.39	0/3005	0.53	0/4069
2	D	0.40	2/3025 (0.1%)	0.52	0/4095
All	All	0.39	3/17188 (0.0%)	0.50	0/23273

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	182	TRP	CD2-CE2	5.16	1.47	1.41
1	B	221	TRP	CD2-CE2	5.02	1.47	1.41
2	D	244	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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	5457	0	5483	40	0
1	B	5441	0	5478	25	0
2	C	2950	0	2975	25	0
2	D	2970	0	3005	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	35	0	0	0	0
3	B	45	0	0	0	0
3	C	40	0	0	0	0
3	D	30	0	0	0	0
4	A	24	0	32	0	0
4	B	18	0	24	1	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	329	0	0	4	0
5	B	351	0	0	3	0
5	C	202	0	0	1	0
5	D	144	0	0	1	0
All	All	18048	0	17013	104	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 3.

All (104) 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)
5:B:2189:HOH:O	2:D:197[A]:GLN:NE2	1.63	1.29
1:A:262[B]:ARG:HG3	1:A:262[B]:ARG:HH11	1.05	1.12
1:A:262[B]:ARG:CG	1:A:262[B]:ARG:HH11	1.77	0.95
1:A:262[B]:ARG:HG3	1:A:262[B]:ARG:NH1	1.86	0.82
5:B:2189:HOH:O	2:D:197[A]:GLN:CD	2.02	0.81
2:C:62:VAL:HG12	2:D:62[A]:VAL:HG22	1.64	0.80
1:A:262[A]:ARG:NH2	5:A:2150:HOH:O	1.72	0.79
1:A:250:ARG:HH12	2:D:145:MET:HG2	1.53	0.72
1:B:258[A]:MET:HG2	1:B:675:TRP:HB3	1.72	0.72
1:B:250:ARG:HH12	2:C:145:MET:HG2	1.56	0.70
5:B:2189:HOH:O	2:D:197[A]:GLN:OE1	2.07	0.66
1:A:262[A]:ARG:NH1	5:A:2150:HOH:O	2.30	0.65
1:B:510:PHE:HB2	1:B:656[A]:LEU:HD21	1.78	0.65
2:C:62:VAL:CG1	2:D:62[A]:VAL:HG22	2.27	0.64
1:A:250:ARG:NH1	2:D:145:MET:HG2	2.11	0.64
2:D:302:GLY:N	2:D:303:PRO:HD2	2.13	0.63
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.81	0.62
2:C:38:GLU:O	2:C:42:ARG:HG2	1.98	0.62
2:C:197[B]:GLN:HG2	5:C:2121:HOH:O	2.00	0.62
2:C:84:GLY:HA2	2:D:394:MET:HE3	1.80	0.62
2:D:197[B]:GLN:OE1	5:D:2086:HOH:O	0.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:252:HIS:HE1	2:D:332:SER:H	1.48	0.61
1:A:262[A]:ARG:CZ	5:A:2150:HOH:O	2.30	0.59
1:A:295:VAL:HG12	1:A:299:MET:HE3	1.82	0.59
1:A:295:VAL:CG1	1:A:299:MET:HE3	2.33	0.59
2:C:203:LEU:HD11	2:C:207:GLU:HG3	1.84	0.58
1:A:262[A]:ARG:HB3	1:A:262[A]:ARG:HH11	1.68	0.58
1:B:250:ARG:NH1	2:C:145:MET:HG2	2.18	0.58
2:C:62:VAL:HG12	2:D:62[A]:VAL:CG2	2.34	0.56
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.41	0.56
1:A:262[B]:ARG:CG	1:A:262[B]:ARG:NH1	2.48	0.55
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.88	0.55
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.89	0.55
2:D:62[A]:VAL:HG21	2:D:130:ASP:HA	1.90	0.54
2:C:173:ARG:NH2	2:C:348:LEU:O	2.42	0.53
1:B:251:LYS:HD2	2:C:233:GLY:HA2	1.91	0.52
1:A:402:PHE:CD2	1:A:426:ILE:HG12	2.45	0.52
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.92	0.52
1:B:250:ARG:NH1	2:C:142:TYR:O	2.43	0.52
2:D:148:PRO:HG2	2:D:151:ILE:HD12	1.92	0.51
1:B:5:THR:HG22	1:B:6:ILE:HG13	1.92	0.51
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.47	0.49
2:C:91:PHE:HB2	2:C:390:ILE:CG2	2.43	0.49
2:D:252:HIS:CE1	2:D:332:SER:H	2.30	0.49
2:C:96:LEU:HD23	2:C:396[A]:VAL:HG13	1.94	0.48
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.96	0.48
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.94	0.47
1:B:519:VAL:HG11	1:B:560:MET:SD	2.54	0.47
1:B:507:ARG:HG2	1:B:566:ALA:HB1	1.96	0.47
1:B:557:LEU:HD12	1:B:596:SER:HA	1.96	0.47
1:A:295:VAL:CG1	1:A:299:MET:CE	2.92	0.47
1:B:656[B]:LEU:HD13	1:B:662:ALA:HB2	1.97	0.47
1:A:108:ALA:HB1	1:A:197:LEU:HB3	1.98	0.46
1:A:359:GLU:HG2	1:A:363:LYS:HE2	1.97	0.46
1:B:333:ALA:HB1	1:B:364:GLY:HA3	1.97	0.46
1:B:110:ASN:HA	1:B:197:LEU:HD11	1.98	0.46
1:A:444:PRO:HG3	1:A:507:ARG:HB3	1.98	0.45
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.50	0.45
1:A:258:MET:HG3	1:A:299:MET:HE1	1.97	0.45
1:A:616:TRP:O	1:A:619:LEU:HB2	2.17	0.45
1:A:65:PHE:HB3	1:A:117:GLY:HA2	1.99	0.45
1:B:437:GLY:HA2	1:B:459:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:THR:HG22	2:C:396[B]:VAL:HG22	1.99	0.45
1:A:103:LYS:HE3	5:A:2033:HOH:O	2.17	0.44
2:C:291:THR:HG22	2:C:396[A]:VAL:HG23	1.99	0.44
2:C:110:TRP:CH2	2:D:107:ARG:HD2	2.53	0.44
2:C:93:ALA:HB1	2:C:396[A]:VAL:HG11	2.00	0.44
1:B:616:TRP:O	1:B:619:LEU:HB2	2.18	0.43
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.38	0.43
1:A:442:THR:HG21	1:A:563:ILE:HG12	2.00	0.43
1:A:235:SER:HA	1:A:236:PRO:HD3	1.90	0.42
1:A:459:ILE:HD11	1:A:486:LEU:HD13	2.02	0.42
2:D:90:ARG:HD3	2:D:394:MET:HE2	2.02	0.42
1:A:389:LEU:HA	1:A:392:ARG:NH1	2.35	0.42
1:A:414:GLU:OE2	1:A:440:THR:HG23	2.20	0.42
2:C:81:VAL:CG1	2:D:296:PRO:HD3	2.49	0.42
1:A:331:LEU:HD13	1:A:422:VAL:HG12	2.01	0.42
1:B:477:LYS:HB2	1:B:486:LEU:HD11	2.01	0.42
1:A:258:MET:CG	1:A:299:MET:HE1	2.49	0.42
2:C:99:VAL:HG13	2:C:269:ILE:HD11	2.00	0.42
2:C:302:GLY:N	2:C:303:PRO:CD	2.82	0.41
2:D:390:ILE:HB	2:D:394:MET:HB2	2.01	0.41
1:A:36:GLU:OE2	1:A:40:LYS:HE3	2.19	0.41
1:A:477:LYS:HG3	1:A:486:LEU:HD21	2.02	0.41
1:B:162:ILE:HD12	1:B:238:LEU:HD21	2.02	0.41
1:A:259:PRO:HD2	1:A:295:VAL:HG11	2.02	0.41
2:D:46:LEU:HD12	2:D:280:LEU:HD21	2.02	0.41
1:A:378:ARG:HH21	1:A:380:ARG:HH22	1.67	0.41
2:D:1:MET:HA	2:D:107:ARG:NH2	2.34	0.41
1:A:714:PRO:HA	1:A:715:PRO:HD3	1.98	0.41
2:D:90:ARG:HH21	2:D:97:GLU:CD	2.24	0.41
1:A:260:ALA:HB3	1:A:261:PRO:HD3	2.02	0.41
2:C:104:GLN:OE1	2:D:105:LYS:HG2	2.21	0.41
2:D:59:VAL:HG21	2:D:361:LEU:HB3	2.02	0.41
1:A:616:TRP:HA	1:A:617:PRO:HD3	1.93	0.41
1:B:464:PHE:HD2	4:B:1731:GOL:H2	1.85	0.41
2:D:38:GLU:HG2	2:D:192:VAL:HG21	2.03	0.41
1:A:92:LYS:HD2	1:A:280:SER:OG	2.20	0.40
2:D:354:ALA:HB1	2:D:359:HIS:HB2	2.04	0.40
1:B:232:THR:O	1:B:235:SER:HB3	2.21	0.40
1:B:449:ALA:O	1:B:455:GLN:HG2	2.21	0.40
1:A:587:VAL:O	1:A:591:ILE:HG12	2.21	0.40
1:A:141:GLU:HB2	1:A:146:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ASP:O	1:A:641:PHE:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	732/736 (100%)	709 (97%)	21 (3%)	2 (0%)	41	50
1	B	734/736 (100%)	718 (98%)	16 (2%)	0	100	100
2	C	398/403 (99%)	385 (97%)	12 (3%)	1 (0%)	41	50
2	D	401/403 (100%)	388 (97%)	10 (2%)	3 (1%)	22	26
All	All	2265/2278 (99%)	2200 (97%)	59 (3%)	6 (0%)	41	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	145	MET
2	C	361	LEU
2	D	361	LEU
1	A	414	GLU
2	D	2	SER
1	A	318	GLU

### 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	563/566 (100%)	556 (99%)	7 (1%)	71	84
1	B	562/566 (99%)	558 (99%)	4 (1%)	84	92
2	C	309/310 (100%)	306 (99%)	3 (1%)	76	87
2	D	311/310 (100%)	304 (98%)	7 (2%)	50	67
All	All	1745/1752 (100%)	1724 (99%)	21 (1%)	76	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8[A]	TRP
1	A	8[B]	TRP
1	A	158	ARG
1	A	262[A]	ARG
1	A	262[B]	ARG
1	A	308	GLN
1	A	469	LYS
1	B	5	THR
1	B	8[A]	TRP
1	B	8[B]	TRP
1	B	577	THR
2	C	173	ARG
2	C	300	LEU
2	C	345	ASP
2	D	127[A]	MET
2	D	127[B]	MET
2	D	173	ARG
2	D	189	LYS
2	D	235	ASP
2	D	236	ASP
2	D	345	ASP

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

Mol	Chain	Res	Type
2	D	338	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 ⓘ

39 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	$\# Z  > 2$
3	SO4	D	1404	-	4,4,4	0.34	0	6,6,6	0.15	0
3	SO4	D	1408	-	4,4,4	0.30	0	6,6,6	0.08	0
4	GOL	C	1412	-	5,5,5	0.32	0	5,5,5	0.10	0
3	SO4	A	1724	-	4,4,4	0.33	0	6,6,6	0.10	0
3	SO4	A	1723	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	B	1726	-	4,4,4	0.30	0	6,6,6	0.18	0
4	GOL	A	1728	-	5,5,5	0.36	0	5,5,5	0.30	0
3	SO4	C	1409	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	A	1725	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	A	1726	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SO4	C	1407	-	4,4,4	0.34	0	6,6,6	0.10	0
4	GOL	A	1731	-	5,5,5	0.30	0	5,5,5	0.30	0
3	SO4	C	1410	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	B	1728	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	D	1405	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	D	1409	-	4,4,4	0.33	0	6,6,6	0.05	0
3	SO4	C	1411	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	B	1724	-	4,4,4	0.32	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	1405	-	4,4,4	0.34	0	6,6,6	0.07	0
4	GOL	B	1731	-	5,5,5	0.23	0	5,5,5	0.33	0
3	SO4	B	1723	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	B	1722	-	4,4,4	0.35	0	6,6,6	0.09	0
4	GOL	B	1730	-	5,5,5	0.41	0	5,5,5	0.35	0
3	SO4	B	1721	-	4,4,4	0.29	0	6,6,6	0.06	0
3	SO4	C	1406	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	B	1725	-	4,4,4	0.32	0	6,6,6	0.06	0
3	SO4	D	1407	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	A	1722	-	4,4,4	0.32	0	6,6,6	0.10	0
4	GOL	A	1729	-	5,5,5	0.34	0	5,5,5	0.29	0
4	GOL	B	1732	-	5,5,5	0.29	0	5,5,5	0.23	0
3	SO4	B	1727	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	C	1404	-	4,4,4	0.29	0	6,6,6	0.20	0
4	GOL	D	1410	-	5,5,5	0.33	0	5,5,5	0.36	0
3	SO4	A	1721	-	4,4,4	0.31	0	6,6,6	0.08	0
4	GOL	A	1730	-	5,5,5	0.37	0	5,5,5	0.27	0
3	SO4	D	1406	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SO4	C	1408	-	4,4,4	0.33	0	6,6,6	0.09	0
3	SO4	B	1729	-	4,4,4	0.33	0	6,6,6	0.09	0
3	SO4	A	1727	-	4,4,4	0.32	0	6,6,6	0.11	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
4	GOL	B	1732	-	-	2/4/4/4	-
4	GOL	C	1412	-	-	0/4/4/4	-
4	GOL	B	1730	-	-	0/4/4/4	-
4	GOL	D	1410	-	-	0/4/4/4	-
4	GOL	A	1731	-	-	2/4/4/4	-
4	GOL	A	1728	-	-	4/4/4/4	-
4	GOL	A	1730	-	-	2/4/4/4	-
4	GOL	B	1731	-	-	0/4/4/4	-
4	GOL	A	1729	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1728	GOL	C1-C2-C3-O3
4	B	1732	GOL	C1-C2-C3-O3
4	B	1732	GOL	O2-C2-C3-O3
4	A	1730	GOL	C1-C2-C3-O3
4	A	1730	GOL	O2-C2-C3-O3
4	A	1728	GOL	O1-C1-C2-C3
4	A	1728	GOL	O1-C1-C2-O2
4	A	1728	GOL	O2-C2-C3-O3
4	A	1731	GOL	O1-C1-C2-O2
4	A	1731	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1731	GOL	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	729/736 (99%)	-0.24	14 (1%) 66 73	17, 33, 52, 79	0
1	B	728/736 (98%)	-0.19	23 (3%) 47 54	18, 30, 61, 85	0
2	C	398/403 (98%)	-0.15	6 (1%) 73 79	17, 25, 44, 71	0
2	D	401/403 (99%)	-0.06	14 (3%) 44 51	17, 28, 51, 92	0
All	All	2256/2278 (99%)	-0.18	57 (2%) 57 64	17, 30, 54, 92	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	230	ALA	6.3
2	D	225	PHE	6.1
1	B	1	MET	5.6
2	D	229	ALA	5.5
1	B	577	THR	4.7
1	A	720	SER	4.1
1	A	319	GLY	4.0
1	A	378	ARG	3.9
1	B	-14	GLY	3.7
1	B	573	ASP	3.6
1	B	-7	HIS	3.6
1	B	609	ASP	3.5
2	C	231	LEU	3.2
2	D	231	LEU	3.2
1	B	378	ARG	3.1
1	B	574	ALA	3.1
1	B	564	ALA	3.0
1	B	575	GLY	3.0
1	B	720	SER	3.0
1	B	377	GLU	3.0
1	B	571	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	454	ARG	2.9
1	A	3	ASP	2.8
1	B	576	GLY	2.7
2	D	220	LYS	2.7
2	C	45	ASP	2.6
2	D	144	VAL	2.5
1	A	376	LEU	2.5
1	B	591	ILE	2.4
1	A	377	GLU	2.4
2	D	1	MET	2.4
2	D	134	MET	2.4
2	C	279	GLY	2.4
1	B	-8	HIS	2.3
2	C	232	GLY	2.3
1	B	566	ALA	2.3
1	B	613	SER	2.3
2	D	45	ASP	2.3
1	A	453	LYS	2.3
1	A	-6	HIS	2.3
2	D	296	PRO	2.3
2	D	228	LEU	2.2
1	A	621	GLU	2.2
1	A	-7	HIS	2.2
1	A	192	ALA	2.2
1	A	194	VAL	2.2
1	B	383	GLN	2.2
1	B	569	LYS	2.2
1	B	567	THR	2.1
2	C	222	LYS	2.1
2	D	136	LEU	2.1
2	D	232	GLY	2.1
2	D	222	LYS	2.0
2	C	230	ALA	2.0
1	B	689	PRO	2.0
1	A	609	ASP	2.0
1	B	570	GLY	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. 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
4	GOL	A	1728	6/6	0.69	0.20	49,50,51,52	0
3	SO4	C	1411	5/5	0.74	0.27	43,44,44,44	5
4	GOL	C	1412	6/6	0.77	0.33	46,47,48,48	0
4	GOL	B	1732	6/6	0.78	0.18	60,60,62,62	0
4	GOL	B	1730	6/6	0.81	0.18	32,35,35,37	0
4	GOL	A	1729	6/6	0.82	0.22	33,37,38,38	0
4	GOL	A	1731	6/6	0.82	0.25	46,46,46,48	0
3	SO4	D	1408	5/5	0.83	0.38	40,42,42,43	5
3	SO4	B	1726	5/5	0.84	0.28	54,55,55,56	5
3	SO4	D	1409	5/5	0.84	0.19	75,75,76,78	1
4	GOL	B	1731	6/6	0.88	0.24	43,44,45,47	0
3	SO4	B	1727	5/5	0.88	0.23	54,55,56,57	5
3	SO4	C	1406	5/5	0.89	0.17	61,62,65,65	0
3	SO4	A	1726	5/5	0.89	0.27	50,51,52,52	5
3	SO4	A	1724	5/5	0.91	0.12	51,51,52,53	5
4	GOL	D	1410	6/6	0.91	0.37	46,47,47,47	0
4	GOL	A	1730	6/6	0.92	0.13	39,39,40,40	0
3	SO4	C	1408	5/5	0.92	0.26	45,47,48,48	5
3	SO4	B	1729	5/5	0.92	0.16	29,29,29,30	5
3	SO4	B	1725	5/5	0.93	0.15	47,47,47,48	5
3	SO4	C	1410	5/5	0.93	0.16	65,65,67,67	0
3	SO4	A	1727	5/5	0.93	0.21	32,32,32,32	5
3	SO4	C	1407	5/5	0.94	0.22	65,67,67,67	0
3	SO4	B	1728	5/5	0.95	0.23	61,67,67,67	0
3	SO4	D	1404	5/5	0.95	0.11	60,60,61,62	0
3	SO4	A	1723	5/5	0.95	0.15	60,61,62,62	0
3	SO4	B	1724	5/5	0.95	0.14	49,49,50,50	5
3	SO4	C	1409	5/5	0.96	0.23	64,66,67,67	0
3	SO4	A	1725	5/5	0.96	0.13	64,66,66,66	0
3	SO4	C	1405	5/5	0.96	0.20	51,51,53,53	0
3	SO4	B	1721	5/5	0.97	0.10	33,34,35,35	0
3	SO4	D	1405	5/5	0.97	0.26	56,58,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	1406	5/5	0.97	0.26	51,52,53,54	0
3	SO4	D	1407	5/5	0.98	0.20	56,57,57,58	0
3	SO4	B	1723	5/5	0.98	0.13	57,57,58,58	0
3	SO4	A	1721	5/5	0.98	0.09	36,36,37,37	0
3	SO4	B	1722	5/5	0.98	0.12	42,43,44,45	0
3	SO4	C	1404	5/5	0.99	0.10	35,36,36,37	0
3	SO4	A	1722	5/5	0.99	0.09	35,36,36,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.