



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:10 AM UTC

PDB ID : 9TP6 / pdb\_00009tp6  
Title : Structure of LolA3 from Porphyromonas gingivalis  
Authors : Jaiman, D.; Persson, K.  
Deposited on : 2025-12-17  
Resolution : 2.32 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

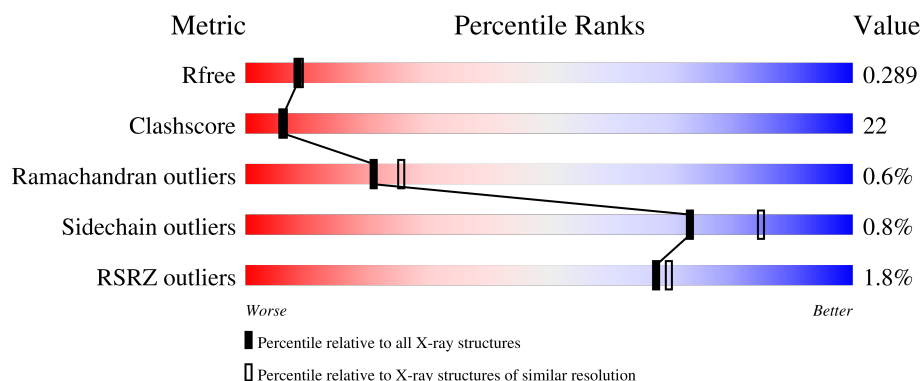
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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))
$R_{free}$	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 of 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	273	<div> <div> <div>0%</div> <div>59%</div> <div>27%</div> <div>12%</div> </div> </div>
1	B	273	<div> <div> <div>0%</div> <div>59%</div> <div>29%</div> <div>12%</div> </div> </div>
1	C	273	<div> <div> <div>3%</div> <div>51%</div> <div>36%</div> <div>12%</div> </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
3	TLA	B	302	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5948 atoms, of which 4 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 Outer membrane lipoprotein-sorting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1963	1232	350	369	12			
1	B	240	Total	C	N	O	S	0	0	0
			1972	1238	351	371	12			
1	C	240	Total	C	N	O	S	0	0	0
			1972	1238	351	371	12			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP B2RJC1
A	-8	HIS	-	expression tag	UNP B2RJC1
A	-7	HIS	-	expression tag	UNP B2RJC1
A	-6	HIS	-	expression tag	UNP B2RJC1
A	-5	HIS	-	expression tag	UNP B2RJC1
A	-4	HIS	-	expression tag	UNP B2RJC1
A	-3	HIS	-	expression tag	UNP B2RJC1
A	-2	GLY	-	expression tag	UNP B2RJC1
A	-1	LYS	-	expression tag	UNP B2RJC1
A	0	PRO	-	expression tag	UNP B2RJC1
A	1	ILE	-	expression tag	UNP B2RJC1
A	2	PRO	-	expression tag	UNP B2RJC1
A	3	ASN	-	expression tag	UNP B2RJC1
A	4	PRO	-	expression tag	UNP B2RJC1
A	5	LEU	-	expression tag	UNP B2RJC1
A	6	LEU	-	expression tag	UNP B2RJC1
A	7	GLY	-	expression tag	UNP B2RJC1
A	8	LEU	-	expression tag	UNP B2RJC1
A	9	ASP	-	expression tag	UNP B2RJC1
A	10	SER	-	expression tag	UNP B2RJC1
A	11	THR	-	expression tag	UNP B2RJC1
A	12	GLU	-	expression tag	UNP B2RJC1
A	13	ASN	-	expression tag	UNP B2RJC1

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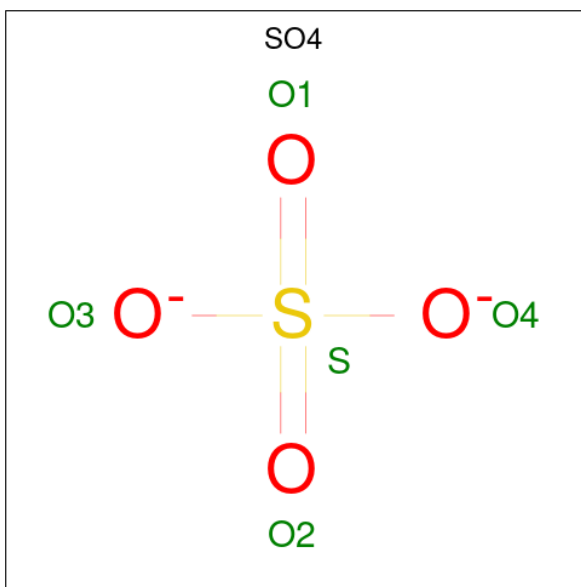
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	-	expression tag	UNP B2RJC1
A	15	TYR	-	expression tag	UNP B2RJC1
A	16	PHE	-	expression tag	UNP B2RJC1
A	17	GLN	-	expression tag	UNP B2RJC1
A	18	GLY	-	expression tag	UNP B2RJC1
A	19	ILE	-	expression tag	UNP B2RJC1
A	20	ASP	-	expression tag	UNP B2RJC1
A	21	PRO	-	expression tag	UNP B2RJC1
A	22	PHE	-	expression tag	UNP B2RJC1
A	23	THR	-	expression tag	UNP B2RJC1
B	-9	MET	-	initiating methionine	UNP B2RJC1
B	-8	HIS	-	expression tag	UNP B2RJC1
B	-7	HIS	-	expression tag	UNP B2RJC1
B	-6	HIS	-	expression tag	UNP B2RJC1
B	-5	HIS	-	expression tag	UNP B2RJC1
B	-4	HIS	-	expression tag	UNP B2RJC1
B	-3	HIS	-	expression tag	UNP B2RJC1
B	-2	GLY	-	expression tag	UNP B2RJC1
B	-1	LYS	-	expression tag	UNP B2RJC1
B	0	PRO	-	expression tag	UNP B2RJC1
B	1	ILE	-	expression tag	UNP B2RJC1
B	2	PRO	-	expression tag	UNP B2RJC1
B	3	ASN	-	expression tag	UNP B2RJC1
B	4	PRO	-	expression tag	UNP B2RJC1
B	5	LEU	-	expression tag	UNP B2RJC1
B	6	LEU	-	expression tag	UNP B2RJC1
B	7	GLY	-	expression tag	UNP B2RJC1
B	8	LEU	-	expression tag	UNP B2RJC1
B	9	ASP	-	expression tag	UNP B2RJC1
B	10	SER	-	expression tag	UNP B2RJC1
B	11	THR	-	expression tag	UNP B2RJC1
B	12	GLU	-	expression tag	UNP B2RJC1
B	13	ASN	-	expression tag	UNP B2RJC1
B	14	LEU	-	expression tag	UNP B2RJC1
B	15	TYR	-	expression tag	UNP B2RJC1
B	16	PHE	-	expression tag	UNP B2RJC1
B	17	GLN	-	expression tag	UNP B2RJC1
B	18	GLY	-	expression tag	UNP B2RJC1
B	19	ILE	-	expression tag	UNP B2RJC1
B	20	ASP	-	expression tag	UNP B2RJC1
B	21	PRO	-	expression tag	UNP B2RJC1
B	22	PHE	-	expression tag	UNP B2RJC1

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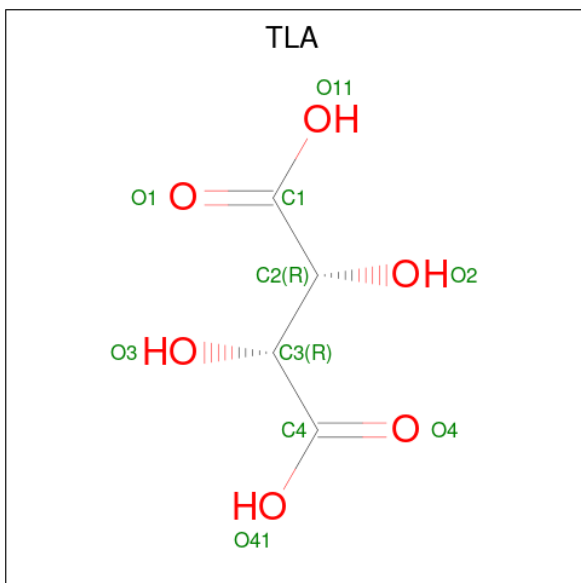
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	THR	-	expression tag	UNP B2RJC1
C	-9	MET	-	initiating methionine	UNP B2RJC1
C	-8	HIS	-	expression tag	UNP B2RJC1
C	-7	HIS	-	expression tag	UNP B2RJC1
C	-6	HIS	-	expression tag	UNP B2RJC1
C	-5	HIS	-	expression tag	UNP B2RJC1
C	-4	HIS	-	expression tag	UNP B2RJC1
C	-3	HIS	-	expression tag	UNP B2RJC1
C	-2	GLY	-	expression tag	UNP B2RJC1
C	-1	LYS	-	expression tag	UNP B2RJC1
C	0	PRO	-	expression tag	UNP B2RJC1
C	1	ILE	-	expression tag	UNP B2RJC1
C	2	PRO	-	expression tag	UNP B2RJC1
C	3	ASN	-	expression tag	UNP B2RJC1
C	4	PRO	-	expression tag	UNP B2RJC1
C	5	LEU	-	expression tag	UNP B2RJC1
C	6	LEU	-	expression tag	UNP B2RJC1
C	7	GLY	-	expression tag	UNP B2RJC1
C	8	LEU	-	expression tag	UNP B2RJC1
C	9	ASP	-	expression tag	UNP B2RJC1
C	10	SER	-	expression tag	UNP B2RJC1
C	11	THR	-	expression tag	UNP B2RJC1
C	12	GLU	-	expression tag	UNP B2RJC1
C	13	ASN	-	expression tag	UNP B2RJC1
C	14	LEU	-	expression tag	UNP B2RJC1
C	15	TYR	-	expression tag	UNP B2RJC1
C	16	PHE	-	expression tag	UNP B2RJC1
C	17	GLN	-	expression tag	UNP B2RJC1
C	18	GLY	-	expression tag	UNP B2RJC1
C	19	ILE	-	expression tag	UNP B2RJC1
C	20	ASP	-	expression tag	UNP B2RJC1
C	21	PRO	-	expression tag	UNP B2RJC1
C	22	PHE	-	expression tag	UNP B2RJC1
C	23	THR	-	expression tag	UNP B2RJC1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



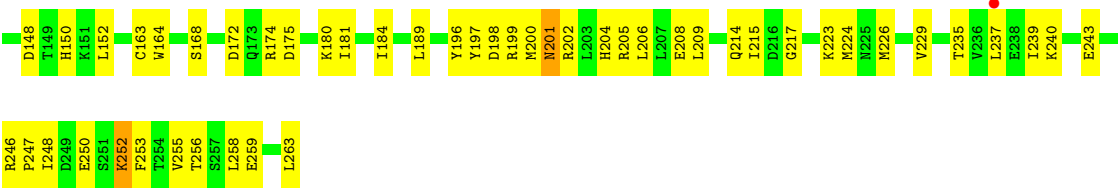
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 14	C 4	H 4	O 6	0	0

- Molecule 4 is water.

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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.11Å 124.11Å 44.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.03 – 2.32 41.03 – 2.32	Depositor EDS
% Data completeness (in resolution range)	88.7 (41.03-2.32) 94.1 (41.03-2.32)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.15 (at 2.32Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, $R_{free}$	0.237 , 0.287 0.239 , 0.289	Depositor DCC
$R_{free}$ test set	1460 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.023 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, TLA

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	0.20	0/2000	0.37	0/2677
1	B	0.07	0/2009	0.22	0/2688
1	C	0.11	0/2009	0.25	0/2688
All	All	0.14	0/6018	0.29	0/8053

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 [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	1963	0	1958	69	0
1	B	1972	0	1969	72	0
1	C	1972	0	1969	120	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	B	10	4	4	2	0
4	A	3	0	0	1	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
All	All	5944	4	5900	263	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 22.

All (263) 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:209:LEU:HD22	1:B:224:MET:HG2	1.28	1.07
1:B:101:ILE:HG13	1:B:144:ASN:HD21	1.29	0.96
1:A:77:LYS:HG2	1:A:96:TRP:CD1	2.04	0.93
1:A:79:ILE:HD13	1:A:94:LEU:HD13	1.53	0.91
1:C:116:LYS:HE2	1:C:118:ARG:HB2	1.51	0.91
1:C:117:THR:HG21	1:C:255:VAL:HG13	1.56	0.86
1:C:79:ILE:HD13	1:C:94:LEU:HB2	1.61	0.82
1:C:246:ARG:HB2	1:C:248:ILE:HD11	1.60	0.81
1:A:77:LYS:CG	1:A:96:TRP:CD1	2.66	0.79
1:C:100:GLN:OE1	1:C:100:GLN:N	2.17	0.77
1:C:126:LYS:H	1:C:126:LYS:HD3	1.50	0.77
1:C:126:LYS:HD3	1:C:126:LYS:N	2.00	0.77
1:A:29:ILE:HD12	1:A:152:LEU:HD13	1.66	0.76
1:B:94:LEU:HD11	1:B:96:TRP:CD1	2.22	0.74
1:B:79:ILE:HD12	1:B:94:LEU:HB2	1.69	0.73
1:C:196:TYR:CE2	1:C:226:MET:HE1	2.25	0.72
1:A:193:ARG:NH1	1:A:195:GLU:OE2	2.25	0.69
1:B:181:ILE:HD12	1:B:197:TYR:CE1	2.28	0.69
1:C:196:TYR:HD2	1:C:205:ARG:HG3	1.57	0.68
1:A:101:ILE:H	1:A:101:ILE:HD12	1.59	0.68
1:A:203:LEU:HG	1:A:229:VAL:HG21	1.77	0.67
1:B:135:PHE:CB	1:B:140:MET:HE2	2.24	0.67
1:C:25:THR:O	1:C:29:ILE:HD13	1.93	0.67
1:A:85:PRO:HG2	1:A:87:ASP:OD1	1.95	0.67
1:A:220:MET:HE1	1:A:239:ILE:HG21	1.76	0.67
1:C:124:SER:HB2	1:C:128:ASP:OD2	1.94	0.66
1:A:97:ASP:HA	1:A:105:ASP:HB3	1.76	0.66
1:B:178:SER:HA	1:B:199:ARG:HH21	1.62	0.64
1:C:252:LYS:HE2	1:C:263:LEU:HA	1.77	0.64
1:A:43:ARG:HH21	1:A:63:ILE:HD11	1.62	0.64
1:C:72:ASP:O	1:C:74:LYS:HD3	1.97	0.64
1:C:200:MET:O	1:C:201:ASN:HB3	1.97	0.63
1:C:256:THR:HA	1:C:259:GLU:OE2	1.99	0.63
1:C:79:ILE:HD11	1:C:258:LEU:HD21	1.81	0.62
1:C:71:LYS:HG3	1:C:71:LYS:O	1.99	0.62
1:C:246:ARG:HB3	1:C:247:PRO:HD2	1.82	0.62
1:A:126:LYS:HD3	1:A:175:ASP:OD1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD13	1:B:95:THR:N	2.15	0.61
1:C:74:LYS:O	1:C:76:LYS:HE3	2.01	0.61
1:B:79:ILE:CD1	1:B:94:LEU:HB2	2.31	0.61
1:C:200:MET:SD	1:C:202:ARG:HB2	2.41	0.60
1:C:196:TYR:CD2	1:C:226:MET:HE1	2.37	0.60
1:C:252:LYS:NZ	1:C:263:LEU:OXT	2.34	0.60
1:B:181:ILE:HD12	1:B:197:TYR:HE1	1.65	0.59
1:A:204:HIS:O	1:A:229:VAL:HG22	2.03	0.59
1:A:110:TYR:CE1	1:A:112:PRO:HA	2.37	0.59
1:C:172:ASP:CG	1:C:174:ARG:HE	2.10	0.59
1:A:43:ARG:NH2	1:A:63:ILE:HD11	2.18	0.58
1:C:28:ASP:O	1:C:28:ASP:OD1	2.19	0.58
1:C:209:LEU:HD21	1:C:224:MET:HE2	1.85	0.58
1:A:34:LYS:NZ	1:A:144:ASN:HA	2.19	0.58
3:B:302:TLA:O1	3:B:302:TLA:O3	2.21	0.58
1:A:49:LYS:HB2	1:A:236:VAL:HB	1.86	0.58
1:C:108:TRP:CD1	1:C:119:ARG:HB3	2.39	0.57
1:C:79:ILE:HD12	1:C:93:PHE:O	2.05	0.57
1:C:62:LEU:HD23	1:C:62:LEU:H	1.68	0.57
1:C:196:TYR:HE2	1:C:226:MET:HE1	1.69	0.57
1:C:67:ILE:HD12	1:C:77:LYS:H	1.69	0.57
1:B:33:VAL:HG21	1:B:184:ILE:HG21	1.87	0.57
1:C:148:ASP:HB2	1:C:150:HIS:CE1	2.39	0.57
1:B:68:ASP:OD1	1:B:76:LYS:HE2	2.05	0.57
1:B:25:THR:HG22	1:B:28:ASP:OD2	2.04	0.56
1:B:131:MET:HA	1:B:131:MET:HE2	1.88	0.56
1:B:224:MET:HE3	1:B:239:ILE:HD11	1.87	0.56
1:A:45:GLU:HG2	1:A:63:ILE:HD12	1.86	0.56
1:B:49:LYS:C	1:B:50:LEU:HD23	2.30	0.56
1:B:200:MET:O	1:B:201:ASN:HB3	2.05	0.56
1:C:180:LYS:HE2	1:C:196:TYR:HE1	1.71	0.55
1:B:207:LEU:HB2	1:B:226:MET:SD	2.47	0.55
1:C:67:ILE:HD13	1:C:69:MET:HG3	1.88	0.55
1:C:117:THR:HG21	1:C:255:VAL:CG1	2.34	0.55
1:C:117:THR:CG2	1:C:258:LEU:HD12	2.36	0.55
1:C:126:LYS:H	1:C:126:LYS:CD	2.17	0.55
1:C:67:ILE:CD1	1:C:77:LYS:H	2.19	0.55
1:C:31:GLN:HG2	1:C:145:VAL:HG21	1.89	0.55
1:B:78:THR:O	1:B:94:LEU:HD22	2.06	0.55
1:B:144:ASN:OD1	1:B:145:VAL:N	2.40	0.55
1:C:174:ARG:C	1:C:199:ARG:HH21	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:GLN:HE21	1:C:217:GLY:C	2.15	0.54
1:C:206:LEU:HD21	1:C:208:GLU:HG3	1.90	0.54
1:C:246:ARG:O	1:C:248:ILE:HD12	2.07	0.54
1:A:168:SER:HB2	1:A:180:LYS:HG2	1.90	0.54
1:B:44:SER:HA	1:B:241:LYS:O	2.08	0.53
1:A:110:TYR:O	1:A:111:LEU:HB2	2.09	0.53
1:B:41:THR:HG22	1:B:67:ILE:HG13	1.89	0.53
1:A:193:ARG:NH2	1:A:206:LEU:HD11	2.23	0.53
1:B:49:LYS:NZ	1:B:59:GLU:OE1	2.41	0.53
1:C:119:ARG:O	1:C:119:ARG:HG3	2.06	0.53
1:B:135:PHE:HB2	1:B:140:MET:HE2	1.89	0.53
1:A:50:LEU:HD12	1:A:58:ARG:NH1	2.24	0.53
1:C:152:LEU:HD11	1:C:164:TRP:CD1	2.44	0.52
1:A:247:PRO:C	1:A:248:ILE:HD12	2.34	0.52
1:A:174:ARG:H	1:A:174:ARG:HD2	1.74	0.52
1:C:107:LYS:O	1:C:119:ARG:HB2	2.09	0.52
1:B:94:LEU:HD11	1:B:96:TRP:NE1	2.24	0.52
1:A:101:ILE:HD12	1:A:101:ILE:N	2.24	0.52
1:C:72:ASP:C	1:C:73:LYS:HG3	2.35	0.52
1:C:111:LEU:H	1:C:111:LEU:HD22	1.75	0.52
1:C:134:ASP:H	1:C:235:THR:HG21	1.74	0.52
1:C:79:ILE:HD13	1:C:94:LEU:CB	2.37	0.52
1:B:41:THR:OG1	1:B:246:ARG:N	2.43	0.52
1:C:98:TYR:HB3	1:C:100:GLN:OE1	2.10	0.52
1:C:239:ILE:C	1:C:240:LYS:HD3	2.36	0.52
1:B:79:ILE:CD1	1:B:94:LEU:HD23	2.40	0.51
1:B:77:LYS:HE3	1:B:96:TRP:CD1	2.45	0.51
1:A:249:ASP:OD2	1:A:250:GLU:N	2.44	0.51
1:C:40:ASP:OD1	1:C:40:ASP:N	2.44	0.51
1:B:92:GLY:O	1:B:109:LEU:HD12	2.11	0.51
1:B:101:ILE:HD12	1:B:101:ILE:N	2.25	0.51
1:C:252:LYS:HE2	1:C:263:LEU:HD22	1.93	0.51
1:C:42:ARG:HB2	1:C:66:SER:HB3	1.92	0.51
1:C:34:LYS:NZ	1:C:142:SER:HB3	2.26	0.51
1:C:180:LYS:HE2	1:C:196:TYR:CE1	2.45	0.51
1:B:69:MET:CE	1:B:77:LYS:HD2	2.41	0.50
1:A:100:GLN:OE1	1:A:103:LYS:HD2	2.11	0.50
1:C:239:ILE:HD12	1:C:239:ILE:N	2.27	0.50
1:A:24:GLN:HA	1:A:24:GLN:OE1	2.10	0.50
1:A:127:LYS:HD2	1:A:176:VAL:HG12	1.94	0.50
1:C:243:GLU:HB3	1:C:246:ARG:HE	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:C	1:B:215:ILE:HD13	2.37	0.50
1:A:77:LYS:HG2	1:A:96:TRP:HD1	1.69	0.50
1:C:250:GLU:HA	1:C:253:PHE:HD2	1.75	0.50
1:A:246:ARG:O	1:A:248:ILE:HD13	2.11	0.49
1:C:109:LEU:HD23	1:C:110:TYR:N	2.27	0.49
1:B:150:HIS:HB3	1:B:166:LEU:HD11	1.94	0.49
1:A:138:ASP:OD2	1:A:143:ARG:NH1	2.45	0.49
1:C:184:ILE:HD12	1:C:184:ILE:N	2.27	0.49
1:A:110:TYR:HE1	1:A:112:PRO:HA	1.76	0.49
1:C:200:MET:O	1:C:201:ASN:CB	2.59	0.49
1:C:101:ILE:HG23	1:C:101:ILE:O	2.13	0.49
1:A:34:LYS:HZ2	1:A:144:ASN:HA	1.76	0.48
1:B:49:LYS:HB2	1:B:236:VAL:HB	1.94	0.48
1:C:214:GLN:C	1:C:215:ILE:HD12	2.38	0.48
1:A:85:PRO:HD2	1:A:88:VAL:CG2	2.43	0.48
1:B:185:ARG:HH21	1:B:187:ASP:CG	2.20	0.48
1:A:65:TYR:HB2	1:A:79:ILE:CG2	2.43	0.48
1:B:69:MET:HE2	1:B:77:LYS:NZ	2.28	0.48
1:A:87:ASP:OD1	1:A:87:ASP:N	2.44	0.48
1:B:66:SER:HA	1:B:77:LYS:O	2.14	0.48
1:A:98:TYR:CD1	1:A:105:ASP:HA	2.48	0.48
1:C:67:ILE:HD11	1:C:77:LYS:HG3	1.96	0.48
1:A:75:ASP:OD1	1:A:98:TYR:HA	2.14	0.48
1:A:79:ILE:CD1	1:A:94:LEU:HD13	2.36	0.48
1:B:101:ILE:HG13	1:B:144:ASN:ND2	2.12	0.47
1:C:114:MET:O	1:C:116:LYS:N	2.47	0.47
1:B:143:ARG:NH2	1:B:147:GLU:HG2	2.29	0.47
1:C:109:LEU:HD22	1:C:111:LEU:HD13	1.95	0.47
1:A:63:ILE:HG23	1:A:63:ILE:O	2.14	0.47
1:A:204:HIS:CD2	1:A:205:ARG:HG3	2.49	0.47
1:A:92:GLY:C	1:A:258:LEU:HD11	2.39	0.47
1:B:41:THR:HG1	1:B:246:ARG:H	1.62	0.47
1:B:79:ILE:HD13	1:B:94:LEU:HD23	1.97	0.47
1:C:67:ILE:HD11	1:C:77:LYS:HB2	1.96	0.47
1:C:72:ASP:O	1:C:73:LYS:HG3	2.15	0.47
1:C:72:ASP:HB3	1:C:74:LYS:NZ	2.29	0.47
1:C:118:ARG:HE	1:C:119:ARG:N	2.13	0.47
1:C:250:GLU:HA	1:C:253:PHE:CD2	2.49	0.47
1:B:148:ASP:HA	1:B:171:LYS:HG3	1.96	0.47
1:C:246:ARG:C	1:C:248:ILE:HD12	2.40	0.47
1:B:180:LYS:HE2	1:B:196:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ILE:HD11	1:C:77:LYS:CB	2.45	0.47
1:C:223:LYS:HE3	1:C:223:LYS:HB2	1.77	0.47
1:B:62:LEU:HD23	1:B:62:LEU:N	2.29	0.46
1:B:135:PHE:HB3	1:B:140:MET:HE2	1.96	0.46
1:B:173:GLN:HA	1:B:199:ARG:NH1	2.30	0.46
1:C:96:TRP:HB3	1:C:98:TYR:HE1	1.80	0.46
1:C:263:LEU:HD13	1:C:263:LEU:C	2.41	0.46
1:C:118:ARG:HE	1:C:119:ARG:H	1.64	0.46
1:A:113:ALA:C	1:A:114:MET:HE2	2.41	0.46
1:C:204:HIS:O	1:C:229:VAL:HG22	2.16	0.46
1:C:206:LEU:HD21	1:C:208:GLU:CD	2.41	0.46
1:A:85:PRO:HD2	1:A:88:VAL:HG22	1.97	0.46
1:C:198:ASP:OD1	1:C:202:ARG:HB3	2.16	0.46
1:B:94:LEU:HD13	1:B:94:LEU:C	2.41	0.46
1:C:60:ARG:HD3	1:C:82:PHE:HE1	1.81	0.46
1:B:185:ARG:NH2	1:B:187:ASP:OD2	2.46	0.45
1:C:252:LYS:CE	1:C:263:LEU:HA	2.42	0.45
1:B:34:LYS:HE2	1:B:142:SER:OG	2.16	0.45
1:B:220:MET:SD	1:B:242:PRO:HB3	2.56	0.45
1:C:53:LYS:HD2	1:C:53:LYS:C	2.41	0.45
1:C:118:ARG:HE	1:C:118:ARG:HA	1.81	0.45
1:C:117:THR:HG23	1:C:258:LEU:HD12	1.97	0.45
1:A:24:GLN:N	4:A:401:HOH:O	2.50	0.45
1:C:78:THR:O	1:C:94:LEU:HD12	2.15	0.45
1:C:168:SER:HB2	1:C:180:LYS:HG2	1.99	0.45
1:C:214:GLN:HE21	1:C:217:GLY:HA2	1.81	0.45
1:B:62:LEU:HD23	1:B:62:LEU:H	1.81	0.45
1:C:197:TYR:HA	1:C:202:ARG:O	2.16	0.45
1:C:209:LEU:HD21	1:C:224:MET:CE	2.46	0.45
1:A:176:VAL:HG21	1:A:205:ARG:HH12	1.82	0.45
1:C:71:LYS:O	1:C:72:ASP:HB2	2.17	0.45
1:B:241:LYS:HB2	1:B:241:LYS:HE3	1.70	0.45
1:C:206:LEU:CD2	1:C:208:GLU:HG3	2.47	0.45
1:A:117:THR:OG1	1:A:259:GLU:OE2	2.34	0.45
1:A:69:MET:HE2	1:A:69:MET:C	2.42	0.44
1:B:182:ALA:HA	1:B:193:ARG:O	2.17	0.44
1:C:67:ILE:HD12	1:C:67:ILE:C	2.42	0.44
1:C:206:LEU:HD21	1:C:208:GLU:CG	2.47	0.44
1:B:115:LYS:HA	1:B:115:LYS:HD2	1.74	0.44
1:B:212:ILE:HD12	1:B:212:ILE:N	2.32	0.44
1:C:174:ARG:O	1:C:199:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HG2	1:A:117:THR:H	1.81	0.44
1:C:181:ILE:HD12	1:C:197:TYR:CE1	2.53	0.44
1:C:172:ASP:OD2	1:C:174:ARG:NE	2.45	0.44
1:A:77:LYS:HD3	1:A:96:TRP:NE1	2.33	0.44
1:A:100:GLN:CD	1:A:103:LYS:HD2	2.43	0.43
1:C:53:LYS:HD2	1:C:54:ARG:N	2.33	0.43
1:C:51:ILE:HA	1:C:56:ALA:O	2.18	0.43
1:A:100:GLN:HG3	1:A:103:LYS:CB	2.48	0.43
1:B:111:LEU:HB2	1:B:114:MET:HB3	2.00	0.43
1:C:76:LYS:HD2	1:C:76:LYS:N	2.34	0.43
1:C:109:LEU:CD2	1:C:111:LEU:HD13	2.48	0.43
1:C:115:LYS:H	1:C:115:LYS:HD2	1.82	0.43
1:B:72:ASP:HB2	1:B:74:LYS:HG2	1.99	0.43
1:B:69:MET:HE3	1:B:77:LYS:HD2	1.99	0.43
1:C:96:TRP:HB3	1:C:98:TYR:CE1	2.54	0.43
1:A:74:LYS:NZ	1:A:99:ASP:OD1	2.41	0.42
1:A:110:TYR:CD2	1:A:259:GLU:HA	2.55	0.42
1:B:79:ILE:HD11	1:B:258:LEU:HD13	2.00	0.42
1:C:45:GLU:HG2	1:C:63:ILE:HG13	2.00	0.42
1:C:42:ARG:HH22	1:C:68:ASP:CG	2.27	0.42
1:A:110:TYR:CE2	1:A:259:GLU:HA	2.54	0.42
1:A:249:ASP:OD2	1:A:251:SER:N	2.51	0.42
1:C:118:ARG:NH2	1:C:119:ARG:HG2	2.33	0.42
1:C:214:GLN:HE21	1:C:217:GLY:CA	2.31	0.42
1:B:72:ASP:C	1:B:73:LYS:HD2	2.44	0.42
1:C:215:ILE:HD12	1:C:215:ILE:N	2.34	0.42
1:B:144:ASN:HB3	1:B:147:GLU:HB2	2.02	0.42
1:C:73:LYS:HD2	1:C:73:LYS:O	2.18	0.42
1:C:189:LEU:N	1:C:189:LEU:HD12	2.34	0.42
1:A:126:LYS:NZ	1:A:172:ASP:OD2	2.49	0.42
1:A:172:ASP:CG	1:A:174:ARG:HD3	2.45	0.42
1:B:73:LYS:HD2	1:B:73:LYS:N	2.34	0.42
1:B:114:MET:HE3	1:B:114:MET:HB2	1.96	0.42
1:B:143:ARG:HH21	1:B:147:GLU:HG2	1.84	0.42
1:C:126:LYS:HG3	1:C:175:ASP:OD1	2.20	0.42
1:A:144:ASN:HB3	1:A:147:GLU:HG3	2.01	0.41
1:B:196:TYR:CE2	1:B:226:MET:HE1	2.55	0.41
1:C:118:ARG:HE	1:C:118:ARG:CA	2.33	0.41
1:C:134:ASP:OD2	1:C:235:THR:HG23	2.20	0.41
1:C:237:LEU:HD23	1:C:237:LEU:HA	1.93	0.41
1:B:143:ARG:HE	1:B:143:ARG:HB3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LEU:C	1:B:263:LEU:HD13	2.45	0.41
1:C:252:LYS:HE2	1:C:263:LEU:CD2	2.51	0.41
1:A:206:LEU:HD21	1:A:208:GLU:CD	2.46	0.41
1:B:126:LYS:O	1:B:176:VAL:HG13	2.20	0.41
1:B:130:PHE:CD2	1:B:140:MET:HE3	2.55	0.41
1:B:204:HIS:HA	1:B:230:GLN:NE2	2.36	0.41
3:B:302:TLA:O41	3:B:302:TLA:O2	2.29	0.41
1:A:69:MET:HE2	1:A:70:GLY:N	2.35	0.41
1:A:100:GLN:HG3	1:A:103:LYS:HB2	2.01	0.41
1:B:168:SER:HB2	1:B:180:LYS:CG	2.50	0.41
1:C:98:TYR:HD2	1:C:103:LYS:HG3	1.85	0.41
1:C:73:LYS:HD2	1:C:73:LYS:C	2.46	0.41
1:C:48:MET:HE3	1:C:50:LEU:HD21	2.03	0.40
1:A:163:CYS:HA	1:A:184:ILE:O	2.20	0.40
1:A:184:ILE:HA	1:A:191:PRO:HA	2.03	0.40
1:A:92:GLY:O	1:A:109:LEU:HD12	2.22	0.40
1:B:226:MET:O	1:B:235:THR:N	2.54	0.40
1:A:79:ILE:HD11	1:A:258:LEU:HD13	2.03	0.40
1:A:180:LYS:HA	1:A:195:GLU:O	2.22	0.40
1:A:194:VAL:HB	1:A:207:LEU:HB3	2.02	0.40
1:C:163:CYS:HA	1:C:184:ILE:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/273 (87%)	219 (92%)	16 (7%)	2 (1%)	16	19
1	B	238/273 (87%)	227 (95%)	11 (5%)	0	100	100
1	C	238/273 (87%)	214 (90%)	22 (9%)	2 (1%)	16	19
All	All	713/819 (87%)	660 (93%)	49 (7%)	4 (1%)	21	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	115	LYS
1	C	201	ASN
1	A	111	LEU
1	A	142	SER

### 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	215/246 (87%)	212 (99%)	3 (1%)	59	75
1	B	216/246 (88%)	216 (100%)	0	100	100
1	C	216/246 (88%)	214 (99%)	2 (1%)	70	83
All	All	647/738 (88%)	642 (99%)	5 (1%)	73	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	THR
1	A	149	THR
1	A	206	LEU
1	C	126	LYS
1	C	252	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	222	GLN
1	A	225	ASN
1	B	186	GLN
1	B	214	GLN
1	C	31	GLN
1	C	150	HIS

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Mol	Chain	Res	Type
1	C	186	GLN
1	C	204	HIS
1	C	214	GLN
1	C	222	GLN
1	C	225	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	303	-	4,4,4	0.66	0	6,6,6	0.08	0
2	SO4	A	302	-	4,4,4	0.66	0	6,6,6	0.08	0
2	SO4	A	301	-	4,4,4	0.66	0	6,6,6	0.08	0
3	TLA	B	302	-	9,9,9	1.31	0	12,12,12	1.39	2 (16%)
2	SO4	B	301	-	4,4,4	0.67	0	6,6,6	0.07	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
3	TLA	B	302	-	-	12/12/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	TLA	O4-C4-C3	-2.53	114.89	121.62
3	B	302	TLA	O1-C1-C2	-2.37	115.32	121.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	TLA	C1-C2-C3-C4
3	B	302	TLA	O1-C1-C2-O2
3	B	302	TLA	O11-C1-C2-O2
3	B	302	TLA	C2-C3-C4-O4
3	B	302	TLA	C2-C3-C4-O41
3	B	302	TLA	O2-C2-C3-O3
3	B	302	TLA	C1-C2-C3-O3
3	B	302	TLA	O2-C2-C3-C4
3	B	302	TLA	O3-C3-C4-O4
3	B	302	TLA	O3-C3-C4-O41
3	B	302	TLA	O1-C1-C2-C3
3	B	302	TLA	O11-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	TLA	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	239/273 (87%)	0.25	3 (1%) 75 76	62, 84, 110, 128	0
1	B	240/273 (87%)	0.30	3 (1%) 75 76	67, 88, 114, 139	0
1	C	240/273 (87%)	0.54	7 (2%) 53 56	77, 102, 134, 163	0
All	All	719/819 (87%)	0.37	13 (1%) 67 70	62, 91, 124, 163	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	3.0
1	C	62	LEU	2.9
1	C	86	GLY	2.7
1	A	67	ILE	2.6
1	C	120	ILE	2.4
1	C	82	PHE	2.3
1	C	25	THR	2.3
1	C	101	ILE	2.3
1	A	93	PHE	2.2
1	A	125	ALA	2.2
1	C	237	LEU	2.2
1	B	219	TRP	2.1
1	B	96	TRP	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 oligosaccharides 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	A	302	5/5	0.72	0.09	95,96,112,113	5
2	SO4	B	301	5/5	0.76	0.16	105,109,126,137	5
2	SO4	A	301	5/5	0.78	0.12	84,90,130,132	5
2	SO4	A	303	5/5	0.84	0.13	70,80,94,105	5
3	TLA	B	302	10/10	0.90	0.10	76,92,117,124	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.