



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 09:23 am BST

PDB ID : 4NBQ
Title : Structure of the polynucleotide phosphorylase (CBU_0852) from *Coxiella burnetii*
Authors : Rudolph, M.J.; Cheung, J.; Franklin, M.C.; Cassidy, M.; Gary, E.; Burshteyn, F.; Love, J.
Deposited on : 2013-10-23
Resolution : 2.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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 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

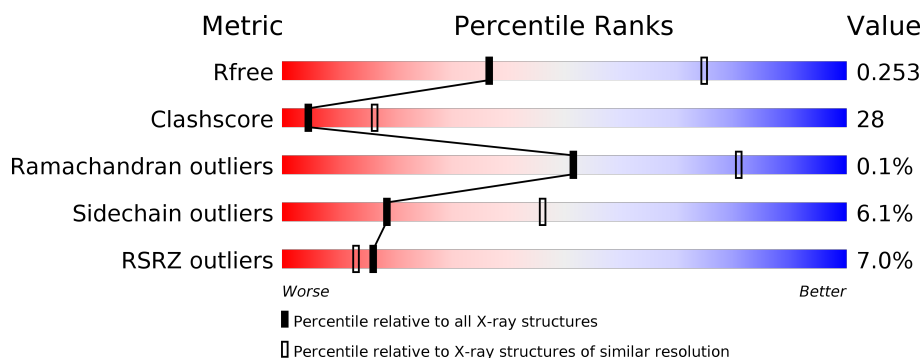
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 ≥ 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	715	<div> <div>5%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	715	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>37%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	715	<div> <div>9%</div> <div> <div></div> <div>44%</div> <div>38%</div> <div>•</div> <div>15%</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
2	SO4	A	701	-	-	X	-
2	SO4	B	701	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14928 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 Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	Se	0	1	0
			5072	3189	891	973	3	16			
1	B	668	Total	C	N	O	S	Se	0	0	0
			5121	3220	892	990	3	16			
1	C	607	Total	C	N	O	S	Se	0	0	0
			4658	2930	815	895	3	15			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	EXPRESSION TAG	UNP Q83D87
A	-17	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-16	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-15	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-14	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-13	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-12	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-11	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-10	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-9	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-8	HIS	-	EXPRESSION TAG	UNP Q83D87
A	-7	GLU	-	EXPRESSION TAG	UNP Q83D87
A	-6	ASN	-	EXPRESSION TAG	UNP Q83D87
A	-5	LEU	-	EXPRESSION TAG	UNP Q83D87
A	-4	TYR	-	EXPRESSION TAG	UNP Q83D87
A	-3	PHE	-	EXPRESSION TAG	UNP Q83D87
A	-2	GLN	-	EXPRESSION TAG	UNP Q83D87
A	-1	SER	-	EXPRESSION TAG	UNP Q83D87
A	0	ALA	-	EXPRESSION TAG	UNP Q83D87
B	-18	MSE	-	EXPRESSION TAG	UNP Q83D87
B	-17	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-16	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-15	HIS	-	EXPRESSION TAG	UNP Q83D87

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-13	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-12	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-11	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-10	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-9	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-8	HIS	-	EXPRESSION TAG	UNP Q83D87
B	-7	GLU	-	EXPRESSION TAG	UNP Q83D87
B	-6	ASN	-	EXPRESSION TAG	UNP Q83D87
B	-5	LEU	-	EXPRESSION TAG	UNP Q83D87
B	-4	TYR	-	EXPRESSION TAG	UNP Q83D87
B	-3	PHE	-	EXPRESSION TAG	UNP Q83D87
B	-2	GLN	-	EXPRESSION TAG	UNP Q83D87
B	-1	SER	-	EXPRESSION TAG	UNP Q83D87
B	0	ALA	-	EXPRESSION TAG	UNP Q83D87
C	-18	MSE	-	EXPRESSION TAG	UNP Q83D87
C	-17	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-16	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-15	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-14	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-13	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-12	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-11	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-10	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-9	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-8	HIS	-	EXPRESSION TAG	UNP Q83D87
C	-7	GLU	-	EXPRESSION TAG	UNP Q83D87
C	-6	ASN	-	EXPRESSION TAG	UNP Q83D87
C	-5	LEU	-	EXPRESSION TAG	UNP Q83D87
C	-4	TYR	-	EXPRESSION TAG	UNP Q83D87
C	-3	PHE	-	EXPRESSION TAG	UNP Q83D87
C	-2	GLN	-	EXPRESSION TAG	UNP Q83D87
C	-1	SER	-	EXPRESSION TAG	UNP Q83D87
C	0	ALA	-	EXPRESSION TAG	UNP Q83D87

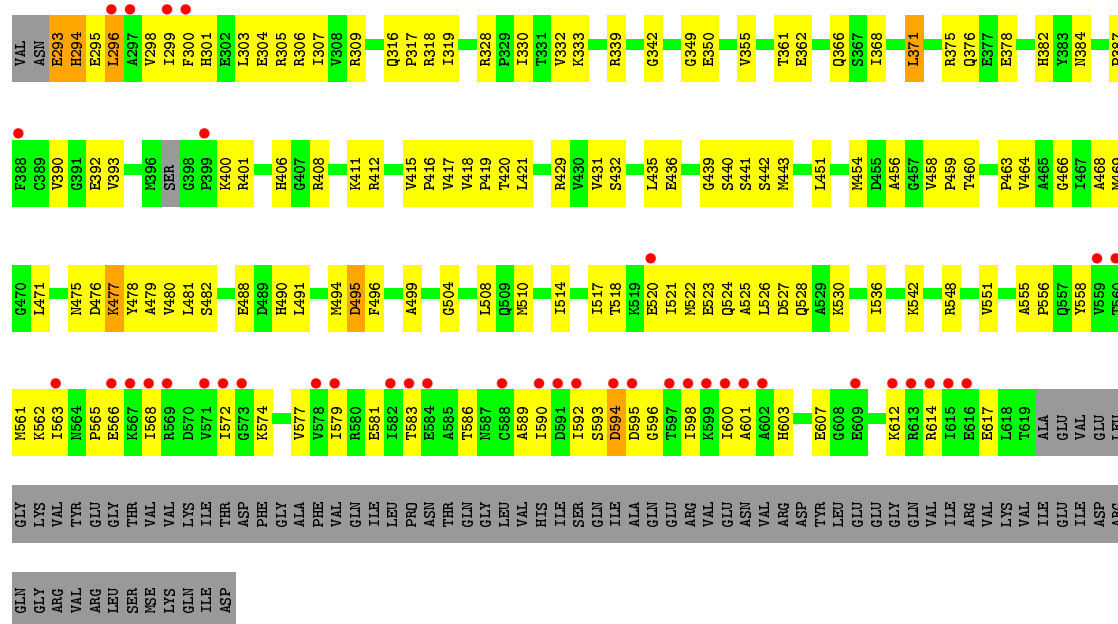
- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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	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		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	O 9	0	0
3	B	3	Total 3	O 3	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.71Å 111.36Å 219.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.91 49.63 – 2.91	Depositor EDS
% Data completeness (in resolution range)	94.3 (49.63-2.91) 94.1 (49.63-2.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.208 , 0.260 0.203 , 0.253	Depositor DCC
R_{free} test set	2590 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14928	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.29	0/5124	0.56	1/6887 (0.0%)
1	B	0.26	0/5173	0.51	0/6959
1	C	0.25	0/4714	0.48	0/6348
All	All	0.27	0/15011	0.52	1/20194 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	VAL	CB-CA-C	-6.76	98.56	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	SER	Peptide
1	A	678	LYS	Peptide
1	A	689	ARG	Peptide
1	C	235	PRO	Peptide

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	5072	0	5156	297	3
1	B	5121	0	5203	296	2
1	C	4658	0	4737	298	0
2	A	35	0	0	3	0
2	B	20	0	0	4	0
2	C	10	0	0	0	0
3	A	9	0	0	1	0
3	B	3	0	0	1	0
All	All	14928	0	15096	847	3

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 28.

The worst 5 of 847 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:C:241:LEU:HD23	1:C:244:TRP:HE1	1.20	1.03
1:A:654:ILE:HG22	1:A:657:ILE:HG22	1.42	1.02
1:B:623:GLU:O	1:B:628:TYR:OH	1.75	1.01
1:A:633:VAL:HG23	1:A:642:VAL:HA	1.39	1.00
1:B:660:GLU:OE2	1:B:668:TYR:OH	1.80	0.99

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:OD2	1:B:661:ARG:NH1[4_445]	1.96	0.24
1:A:284:ARG:O	1:B:653:HIS:NE2[2_555]	2.10	0.10
1:A:227:GLY:O	1:A:661:ARG:NH1[2_555]	2.17	0.03

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	640/715 (90%)	606 (95%)	33 (5%)	1 (0%)	47	77
1	B	650/715 (91%)	617 (95%)	32 (5%)	1 (0%)	47	77
1	C	599/715 (84%)	547 (91%)	52 (9%)	0	100	100
All	All	1889/2145 (88%)	1770 (94%)	117 (6%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	ILE
1	B	627	VAL

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	543/577 (94%)	508 (94%)	35 (6%)	17	44
1	B	550/577 (95%)	516 (94%)	34 (6%)	18	45
1	C	499/577 (86%)	471 (94%)	28 (6%)	21	50
All	All	1592/1731 (92%)	1495 (94%)	97 (6%)	18	46

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	263	THR

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Mol	Chain	Res	Type
1	B	527	ASP
1	C	371	LEU
1	B	343	SER
1	B	383	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	541	ASN
1	B	673	GLN
1	C	382	HIS
1	B	535	HIS
1	C	366	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](#)

13 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	706	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	C	702	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	A	702	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	703	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	B	703	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	B	704	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	704	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	A	707	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	B	702	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	C	701	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	705	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	B	701	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	701	-	4,4,4	0.13	0	6,6,6	0.18	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.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	703	SO4	1	0
2	B	702	SO4	1	0
2	A	705	SO4	1	0
2	B	701	SO4	2	0
2	A	701	SO4	2	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 [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, 95th 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 ²)	Q<0.9
1	A	643/715 (89%)	0.17	33 (5%) 28 24	32, 53, 133, 198	0
1	B	652/715 (91%)	0.30	37 (5%) 23 20	37, 75, 123, 156	0
1	C	592/715 (82%)	0.52	63 (10%) 6 5	43, 83, 139, 184	0
All	All	1887/2145 (87%)	0.32	133 (7%) 16 13	32, 73, 132, 198	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	597	THR	6.2
1	C	571	VAL	6.1
1	B	575	GLY	6.0
1	C	583	THR	6.0
1	C	591	ASP	5.4

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, 95th 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(\AA^2)	Q<0.9
2	SO4	B	703	5/5	0.85	0.24	95,106,109,110	0
2	SO4	A	705	5/5	0.86	0.22	140,142,143,143	0
2	SO4	A	706	5/5	0.88	0.35	149,150,153,154	0
2	SO4	C	702	5/5	0.88	0.28	136,137,137,137	0
2	SO4	B	702	5/5	0.89	0.21	139,140,140,140	0
2	SO4	A	702	5/5	0.90	0.13	112,116,117,120	0
2	SO4	B	701	5/5	0.91	0.19	119,121,123,123	0
2	SO4	A	707	5/5	0.93	0.30	122,125,127,128	0
2	SO4	C	701	5/5	0.93	0.12	103,106,110,110	0
2	SO4	A	704	5/5	0.95	0.14	95,101,102,105	0
2	SO4	A	701	5/5	0.95	0.12	82,84,86,89	0
2	SO4	A	703	5/5	0.96	0.15	71,74,79,82	0
2	SO4	B	704	5/5	0.97	0.09	96,99,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.