



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2017 – 07:13 PM EDT

PDB ID : 1S5J
Title : Insight in DNA Replication: The crystal structure of DNA Polymerase B1 from the archaeon *Sulfolobus solfataricus*
Authors : Savino, C.; Federici, L.; Nastopoulos, V.; Johnson, K.A.; Pisani, F.M.; Rossi, M.; Tsernoglou, D.
Deposited on : 2004-01-21
Resolution : 2.40 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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

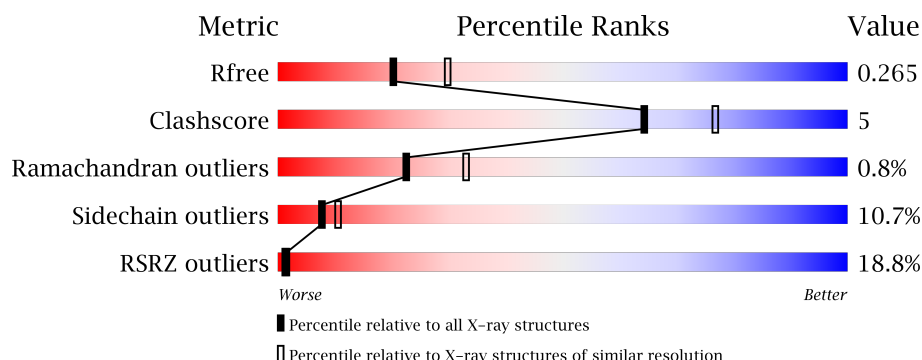
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	847	<div> <div>16%</div> <div>67%</div> <div>17%</div> <div>•</div> <div>14%</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	885	-	-	-	X
2	SO4	A	889	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	890	-	-	-	X
2	SO4	A	891	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6230 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 DNA polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5936	3870	958	1096	12			

- 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		

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.47Å 68.80Å 125.85Å 90.00° 107.94° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.40) 99.5 (29.73-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.272 0.230 , 0.265	Depositor DCC
R_{free} test set	3011 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6230	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.56	0/6063	0.79	31/8200 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ASP	CB-CG-OD1	8.34	125.80	118.30
1	A	93	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	315	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	137	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	316	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	57	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	708	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	657	ASP	CB-CG-OD1	6.02	123.71	118.30
1	A	572	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	261	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	108	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	71	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	501	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	426	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	244	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	395	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	756	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	402	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	534	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	282	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	192	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	273	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	683	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	546	ASP	CB-CG-OD2	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	231	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	746	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	204	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	655	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	687	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	202	ASP	CB-CG-OD2	5.00	122.80	118.30

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	5936	0	6025	58	0
2	A	45	0	0	1	0
3	A	1	0	0	0	0
4	A	248	0	0	5	0
All	All	6230	0	6025	58	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 5.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HE	1:A:421:THR:CG2	1.84	0.90
1:A:239:LYS:HA	1:A:397:LEU:HD22	1.67	0.77
1:A:422:THR:HG21	4:A:957:HOH:O	1.98	0.63
1:A:701:ASN:N	4:A:1087:HOH:O	2.33	0.61
1:A:227:ARG:HE	1:A:421:THR:HG23	1.67	0.59
1:A:567:THR:HG22	4:A:1009:HOH:O	2.02	0.59
1:A:563:THR:O	1:A:567:THR:HG23	2.02	0.59
1:A:104:LYS:H	1:A:104:LYS:HD3	1.67	0.58
1:A:522:ILE:HD11	1:A:629:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD11	1:A:353:HIS:CD2	2.40	0.56
1:A:353:HIS:HE1	1:A:355:ASP:HB2	1.70	0.56
1:A:506:ILE:HG23	1:A:692:PHE:CE1	2.41	0.56
1:A:227:ARG:HE	1:A:421:THR:HG21	1.66	0.56
1:A:232:ILE:HD12	1:A:252:ILE:HD12	1.88	0.55
1:A:603:LYS:HZ2	1:A:607:ASN:CG	2.10	0.55
1:A:40:GLU:HG3	1:A:41:TRP:N	2.22	0.55
1:A:420:LEU:O	1:A:428:THR:HG21	2.06	0.55
1:A:76:LYS:HD3	2:A:889:SO4:O4	2.07	0.54
1:A:548:THR:O	1:A:548:THR:HG22	2.08	0.54
1:A:227:ARG:NE	1:A:421:THR:CG2	2.64	0.53
1:A:735:LYS:NZ	1:A:849:THR:O	2.42	0.53
1:A:509:ASN:O	1:A:663:ASN:HB2	2.08	0.53
1:A:104:LYS:CD	1:A:104:LYS:H	2.22	0.52
1:A:252:ILE:HD11	1:A:321:TYR:CD1	2.45	0.52
1:A:466:ARG:HB3	1:A:468:TRP:CD1	2.45	0.51
1:A:752:ARG:O	1:A:755:VAL:HG12	2.10	0.51
1:A:353:HIS:ND1	1:A:448:ARG:NH2	2.59	0.49
1:A:301:ASP:O	4:A:927:HOH:O	2.20	0.48
1:A:252:ILE:HD11	1:A:321:TYR:HD1	1.78	0.48
1:A:227:ARG:NE	1:A:421:THR:HG23	2.27	0.48
1:A:527:ASN:HD21	1:A:560:PRO:HA	1.79	0.48
1:A:518:LEU:O	1:A:522:ILE:HG23	2.14	0.47
1:A:751:LYS:HZ3	1:A:754:ILE:HG21	1.80	0.47
1:A:228:VAL:O	1:A:228:VAL:HG13	2.13	0.47
1:A:625:VAL:O	1:A:629:VAL:HG23	2.14	0.46
1:A:92:VAL:CG1	1:A:148:VAL:HG11	2.45	0.46
1:A:428:THR:HG23	4:A:1058:HOH:O	2.15	0.46
1:A:270:ASN:HD21	1:A:288:ARG:HD2	1.81	0.46
1:A:727:VAL:N	1:A:846:LEU:HD22	2.31	0.45
1:A:245:SER:HA	1:A:321:TYR:CD2	2.52	0.45
1:A:246:GLN:HE21	1:A:246:GLN:HB2	1.56	0.44
1:A:94:LEU:O	1:A:131:THR:CG2	2.66	0.44
1:A:420:LEU:O	1:A:428:THR:CG2	2.66	0.44
1:A:58:TYR:CE2	1:A:60:GLY:HA2	2.54	0.43
1:A:53:LEU:HD21	1:A:163:MET:CE	2.49	0.42
1:A:662:LEU:O	1:A:663:ASN:C	2.57	0.42
1:A:430:LYS:HB3	1:A:597:VAL:HG11	2.02	0.42
1:A:56:VAL:HG22	1:A:159:PHE:HB2	2.01	0.42
1:A:229:ALA:HA	1:A:310:LEU:O	2.20	0.41
1:A:268:VAL:CG2	1:A:288:ARG:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:HA	1:A:340:VAL:HG11	2.01	0.41
1:A:311:THR:CG2	1:A:353:HIS:HE2	2.33	0.41
1:A:850:PHE:CD2	1:A:850:PHE:O	2.74	0.41
1:A:378:ASN:ND2	1:A:381:ALA:H	2.19	0.41
1:A:397:LEU:HG	1:A:398:ILE:H	1.86	0.41
1:A:232:ILE:HG22	1:A:255:ILE:HG12	2.03	0.41
1:A:577:ILE:HG13	1:A:578:TYR:CD2	2.56	0.40
1:A:743:SER:CB	1:A:744:PRO:HD2	2.52	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	715/847 (84%)	660 (92%)	49 (7%)	6 (1%)	22	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	729	LYS
1	A	850	PHE
1	A	509	ASN
1	A	274	VAL
1	A	663	ASN
1	A	551	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	653/757 (86%)	583 (89%)	70 (11%)	8 10

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	48	ASN
1	A	73	GLU
1	A	97	ASP
1	A	104	LYS
1	A	106	VAL
1	A	131	THR
1	A	146	ASN
1	A	163	MET
1	A	177	LYS
1	A	187	SER
1	A	191	LYS
1	A	195	GLU
1	A	215	LEU
1	A	234	VAL
1	A	236	THR
1	A	246	GLN
1	A	273	ASP
1	A	276	GLU
1	A	281	LEU
1	A	282	ASP
1	A	352	LEU
1	A	366	ARG
1	A	379	LEU
1	A	380	ASP
1	A	400	PHE
1	A	402	ASP
1	A	421	THR
1	A	422	THR
1	A	428	THR
1	A	446	LEU
1	A	456	LYS
1	A	458	LEU
1	A	466	ARG
1	A	474	GLU

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Mol	Chain	Res	Type
1	A	477	LEU
1	A	480	SER
1	A	514	ASP
1	A	517	SER
1	A	518	LEU
1	A	522	ILE
1	A	524	ARG
1	A	556	CYS
1	A	573	PHE
1	A	575	VAL
1	A	577	ILE
1	A	579	LYS
1	A	603	LYS
1	A	609	THR
1	A	650	THR
1	A	658	SER
1	A	666	LYS
1	A	670	GLU
1	A	692	PHE
1	A	706	TYR
1	A	707	GLN
1	A	714	LYS
1	A	716	MET
1	A	729	LYS
1	A	741	ILE
1	A	743	SER
1	A	748	LYS
1	A	759	LYS
1	A	766	LYS
1	A	837	ILE
1	A	840	GLU
1	A	841	LYS
1	A	851	GLU
1	A	859	VAL
1	A	862	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	48	ASN
1	A	146	ASN

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	270	ASN
1	A	378	ASN
1	A	410	ASN
1	A	457	ASN
1	A	509	ASN
1	A	527	ASN
1	A	537	GLN
1	A	587	ASN
1	A	591	GLN
1	A	681	ASN
1	A	701	ASN
1	A	742	ASN
1	A	852	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](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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	883	-	4,4,4	0.21	0	6,6,6	0.20	0
2	SO4	A	884	-	4,4,4	0.18	0	6,6,6	0.35	0
2	SO4	A	885	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	A	886	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	A	887	-	4,4,4	0.20	0	6,6,6	0.12	0
2	SO4	A	888	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	A	889	-	4,4,4	0.42	0	6,6,6	0.88	0
2	SO4	A	890	-	4,4,4	0.28	0	6,6,6	0.20	0
2	SO4	A	891	-	4,4,4	0.31	0	6,6,6	0.20	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	883	-	-	0/0/0/0	0/0/0/0
2	SO4	A	884	-	-	0/0/0/0	0/0/0/0
2	SO4	A	885	-	-	0/0/0/0	0/0/0/0
2	SO4	A	886	-	-	0/0/0/0	0/0/0/0
2	SO4	A	887	-	-	0/0/0/0	0/0/0/0
2	SO4	A	888	-	-	0/0/0/0	0/0/0/0
2	SO4	A	889	-	-	0/0/0/0	0/0/0/0
2	SO4	A	890	-	-	0/0/0/0	0/0/0/0
2	SO4	A	891	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	889	SO4	1	0

5.7 Other polymers

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, 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	727/847 (85%)	0.96	137 (18%) 1 1	23, 50, 114, 131	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	846	LEU	11.7
1	A	718	VAL	10.2
1	A	864	ILE	9.9
1	A	762	TYR	9.1
1	A	498	VAL	8.8
1	A	717	LEU	8.2
1	A	845	ALA	8.1
1	A	839	ALA	7.9
1	A	396	THR	7.8
1	A	837	ILE	7.7
1	A	741	ILE	7.7
1	A	843	LEU	7.6
1	A	842	TYR	7.4
1	A	859	VAL	7.2
1	A	850	PHE	7.1
1	A	400	PHE	7.0
1	A	732	ASN	7.0
1	A	497	ALA	7.0
1	A	482	ASN	7.0
1	A	390	SER	6.7
1	A	727	VAL	6.5
1	A	765	LEU	6.4
1	A	736	GLU	6.3
1	A	759	LYS	6.2
1	A	395	ASP	5.9
1	A	703	PHE	5.8
1	A	240	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	709	GLY	5.7
1	A	838	ASP	5.7
1	A	862	ASP	5.7
1	A	711	VAL	5.6
1	A	758	VAL	5.6
1	A	766	LYS	5.6
1	A	757	VAL	5.6
1	A	753	LYS	5.6
1	A	397	LEU	5.6
1	A	690	TYR	5.5
1	A	863	GLU	5.5
1	A	729	LYS	5.3
1	A	852	GLN	5.3
1	A	548	THR	5.1
1	A	481	SER	5.0
1	A	861	TRP	4.8
1	A	751	LYS	4.7
1	A	728	LYS	4.7
1	A	841	LYS	4.6
1	A	730	VAL	4.6
1	A	708	ASP	4.6
1	A	507	PHE	4.5
1	A	239	LYS	4.5
1	A	272	ASN	4.5
1	A	275	ASN	4.5
1	A	840	GLU	4.5
1	A	706	TYR	4.4
1	A	343	LYS	4.2
1	A	860	SER	4.1
1	A	716	MET	4.1
1	A	740	SER	4.1
1	A	274	VAL	4.1
1	A	731	PHE	4.0
1	A	743	SER	4.0
1	A	667	ASN	3.9
1	A	748	LYS	3.8
1	A	549	GLY	3.8
1	A	550	GLU	3.7
1	A	401	LEU	3.7
1	A	537	GLN	3.6
1	A	752	ARG	3.6
1	A	737	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	742	ASN	3.3
1	A	733	GLU	3.3
1	A	546	ASP	3.3
1	A	551	VAL	3.3
1	A	394	VAL	3.3
1	A	393	LYS	3.2
1	A	734	VAL	3.2
1	A	508	PHE	3.2
1	A	586	ASN	3.2
1	A	276	GLU	3.1
1	A	738	MET	3.1
1	A	754	ILE	3.1
1	A	848	SER	3.1
1	A	273	ASP	3.0
1	A	624	ARG	3.0
1	A	505	GLY	3.0
1	A	241	ARG	3.0
1	A	683	ASP	2.9
1	A	712	ASP	2.9
1	A	755	VAL	2.8
1	A	398	ILE	2.8
1	A	763	GLU	2.8
1	A	844	GLU	2.8
1	A	652	LEU	2.7
1	A	539	LYS	2.7
1	A	399	SER	2.7
1	A	389	THR	2.7
1	A	710	LYS	2.7
1	A	704	GLY	2.6
1	A	761	SER	2.6
1	A	764	LYS	2.6
1	A	760	GLY	2.6
1	A	649	LEU	2.6
1	A	756	ASP	2.6
1	A	585	PRO	2.5
1	A	237	PRO	2.5
1	A	713	ILE	2.5
1	A	851	GLU	2.5
1	A	543	GLU	2.4
1	A	194	GLU	2.4
1	A	589	GLU	2.4
1	A	707	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	689	THR	2.4
1	A	854	LEU	2.4
1	A	433	VAL	2.3
1	A	513	LEU	2.3
1	A	671	ASN	2.3
1	A	651	VAL	2.3
1	A	666	LYS	2.3
1	A	205	GLU	2.2
1	A	847	ARG	2.2
1	A	242	ILE	2.2
1	A	238	VAL	2.2
1	A	536	GLN	2.2
1	A	696	SER	2.2
1	A	702	TYR	2.1
1	A	563	THR	2.1
1	A	739	ILE	2.1
1	A	583	LYS	2.1
1	A	750	ILE	2.1
1	A	344	ASP	2.0
1	A	747	VAL	2.0
1	A	688	LYS	2.0
1	A	670	GLU	2.0
1	A	650	THR	2.0
1	A	310	LEU	2.0
1	A	672	ILE	2.0
1	A	376	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	891	5/5	0.88	0.40	7.00	78,78,80,80	0
2	SO4	A	889	5/5	0.88	0.26	3.37	58,59,64,65	0
2	SO4	A	885	5/5	0.81	0.22	2.45	122,122,122,123	0
2	SO4	A	890	5/5	0.85	0.40	1.84	77,77,79,80	0
3	MG	A	892	1/1	0.78	0.19	-0.19	49,49,49,49	0
2	SO4	A	883	5/5	0.98	0.12	-1.07	59,59,61,61	0
2	SO4	A	886	5/5	0.88	0.17	-1.13	104,104,104,104	0
2	SO4	A	887	5/5	0.90	0.22	-	91,92,92,92	0
2	SO4	A	888	5/5	0.62	0.28	-	120,120,120,120	0
2	SO4	A	884	5/5	0.89	0.17	-	74,74,76,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.