



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:22 PM UTC

PDB ID : 1S5J / pdb_00001s5j
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

<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>.

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

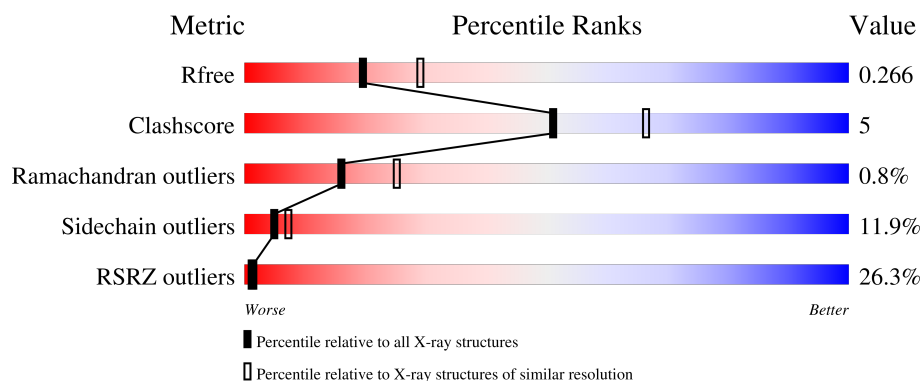
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of 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	847	

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
			Total	C	N	O	S			
1	A	727	5936	3870	958	1096	12	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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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 (CCD ID: MG) (formula: Mg).

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

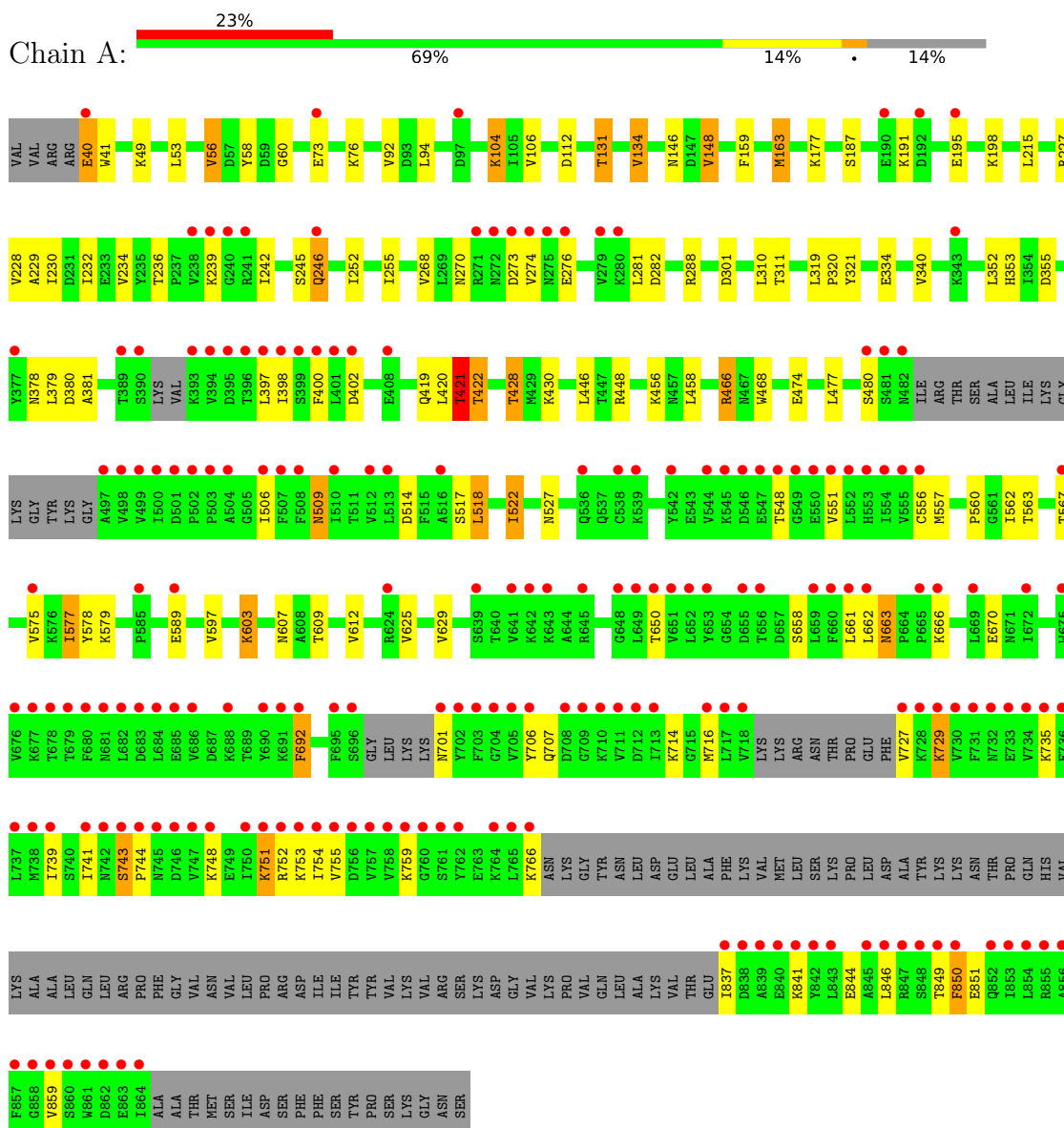
- Molecule 4 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA polymerase I



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 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.40) 99.4 (30.00-2.40)	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 , 0.266	Depositor DCC
R_{free} test set	3011 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	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 [i](#)

5.1 Standard geometry [i](#)

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	0.75	1/6063 (0.0%)	0.89	1/8200 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	VAL	CA-CB	5.19	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	THR	N-CA-CB	-5.74	102.24	110.80

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	5936	0	6025	62	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	62	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 (62) 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:603:LYS:HZ2	1:A:607:ASN:CG	2.08	0.62
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:HD3	1:A:104:LYS:H	1.67	0.58
1:A:522:ILE:HD11	1:A:629:VAL:HA	1.85	0.58
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: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:HG22	1:A:548:THR:O	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:H	1:A:104:LYS:CD	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:751:LYS:HZ1	1:A:754:ILE:HD13	1.75	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:662:LEU:O	1:A:663:ASN:C	2.57	0.47
1:A:228:VAL:HG13	1:A:228:VAL:O	2.13	0.47
1:A:92:VAL:CG1	1:A:148:VAL:HG11	2.45	0.46
1:A:625:VAL:O	1:A:629:VAL:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ILE:HG13	1:A:753:LYS:HZ2	1.81	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:739:ILE:CG1	1:A:753:LYS:HZ2	2.29	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:419:GLN:C	1:A:421:THR:H	2.25	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: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:112:ASP:OD1	1:A:112:ASP:C	2.64	0.41
1:A:268:VAL:CG2	1:A:288:ARG:HG2	2.50	0.41
1:A:311:THR:CG2	1:A:353:HIS:HE2	2.33	0.41
1:A:320:PRO:HA	1:A:340:VAL:HG11	2.01	0.41
1:A:850:PHE:O	1:A:850:PHE:CD2	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 ⓘ

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	715/847 (84%)	660 (92%)	49 (7%)	6 (1%)	16	25

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 ⓘ

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%)	575 (88%)	78 (12%)	5 7

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	49	LYS
1	A	56	VAL
1	A	73	GLU
1	A	104	LYS
1	A	106	VAL
1	A	131	THR
1	A	134	VAL
1	A	146	ASN
1	A	148	VAL
1	A	163	MET
1	A	177	LYS
1	A	187	SER
1	A	191	LYS
1	A	195	GLU
1	A	198	LYS
1	A	215	LEU
1	A	230	ILE
1	A	234	VAL

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Mol	Chain	Res	Type
1	A	236	THR
1	A	242	ILE
1	A	246	GLN
1	A	273	ASP
1	A	276	GLU
1	A	281	LEU
1	A	282	ASP
1	A	334	GLU
1	A	352	LEU
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
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	556	CYS
1	A	557	MET
1	A	562	ILE
1	A	575	VAL
1	A	577	ILE
1	A	579	LYS
1	A	589	GLU
1	A	603	LYS
1	A	609	THR
1	A	612	VAL
1	A	650	THR
1	A	658	SER
1	A	661	LEU
1	A	666	LYS
1	A	670	GLU

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Mol	Chain	Res	Type
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	751	LYS
1	A	759	LYS
1	A	766	LYS
1	A	837	ILE
1	A	841	LYS
1	A	844	GLU
1	A	851	GLU
1	A	859	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	146	ASN
1	A	246	GLN
1	A	270	ASN
1	A	272	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	681	ASN
1	A	701	ASN
1	A	852	GLN

5.3.3 RNA ⓘ

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](#)

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	0.30	0	6,6,6	0.19	0
2	SO4	A	887	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	A	891	-	4,4,4	0.35	0	6,6,6	0.22	0
2	SO4	A	885	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	A	884	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SO4	A	888	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	A	889	-	4,4,4	0.43	0	6,6,6	0.94	0
2	SO4	A	890	-	4,4,4	0.31	0	6,6,6	0.16	0
2	SO4	A	886	-	4,4,4	0.23	0	6,6,6	0.08	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 [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, 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%)	1.19	191 (26%) 1 1	23, 50, 114, 131	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	864	ILE	8.8
1	A	718	VAL	8.8
1	A	846	LEU	8.2
1	A	727	VAL	8.2
1	A	850	PHE	8.0
1	A	717	LEU	7.0
1	A	741	ILE	6.7
1	A	758	VAL	6.6
1	A	859	VAL	6.5
1	A	498	VAL	6.2
1	A	730	VAL	6.2
1	A	757	VAL	6.1
1	A	499	VAL	6.1
1	A	837	ILE	6.1
1	A	397	LEU	5.8
1	A	396	THR	5.8
1	A	753	LYS	5.7
1	A	765	LEU	5.5
1	A	497	ALA	5.4
1	A	839	ALA	5.2
1	A	696	SER	5.2
1	A	398	ILE	5.2
1	A	732	ASN	5.2
1	A	734	VAL	5.2
1	A	703	PHE	5.1
1	A	736	GLU	5.0
1	A	762	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	548	THR	4.9
1	A	401	LEU	4.9
1	A	742	ASN	4.9
1	A	842	TYR	4.7
1	A	737	LEU	4.7
1	A	843	LEU	4.7
1	A	716	MET	4.7
1	A	546	ASP	4.6
1	A	731	PHE	4.6
1	A	549	GLY	4.5
1	A	650	THR	4.4
1	A	508	PHE	4.4
1	A	400	PHE	4.3
1	A	845	ALA	4.3
1	A	500	ILE	4.3
1	A	661	LEU	4.3
1	A	389	THR	4.2
1	A	706	TYR	4.2
1	A	755	VAL	4.2
1	A	711	VAL	4.1
1	A	728	LYS	4.1
1	A	538	CYS	4.1
1	A	747	VAL	4.1
1	A	690	TYR	4.1
1	A	750	ILE	4.1
1	A	395	ASP	4.0
1	A	754	ILE	3.9
1	A	739	ILE	3.9
1	A	680	PHE	3.9
1	A	506	ILE	3.8
1	A	710	LYS	3.8
1	A	729	LYS	3.8
1	A	274	VAL	3.8
1	A	624	ARG	3.8
1	A	390	SER	3.8
1	A	272	ASN	3.7
1	A	482	ASN	3.7
1	A	393	LYS	3.7
1	A	394	VAL	3.7
1	A	240	GLY	3.7
1	A	507	PHE	3.7
1	A	648	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	503	PRO	3.7
1	A	683	ASP	3.7
1	A	701	ASN	3.6
1	A	651	VAL	3.6
1	A	862	ASP	3.6
1	A	681	ASN	3.6
1	A	677	LYS	3.5
1	A	744	PRO	3.5
1	A	705	VAL	3.5
1	A	860	SER	3.5
1	A	273	ASP	3.5
1	A	551	VAL	3.5
1	A	682	LEU	3.5
1	A	545	LYS	3.5
1	A	695	PHE	3.5
1	A	760	GLY	3.4
1	A	743	SER	3.4
1	A	841	LYS	3.4
1	A	863	GLU	3.4
1	A	542	TYR	3.3
1	A	639	SER	3.3
1	A	691	LYS	3.3
1	A	662	LEU	3.3
1	A	684	LEU	3.3
1	A	641	VAL	3.3
1	A	659	LEU	3.2
1	A	239	LYS	3.2
1	A	756	ASP	3.2
1	A	555	VAL	3.2
1	A	649	LEU	3.2
1	A	745	ASN	3.2
1	A	481	SER	3.1
1	A	692	PHE	3.1
1	A	838	ASP	3.1
1	A	686	VAL	3.1
1	A	748	LYS	3.1
1	A	759	LYS	3.1
1	A	738	MET	3.1
1	A	861	TRP	3.1
1	A	847	ARG	3.0
1	A	764	LYS	3.0
1	A	343	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	567	THR	3.0
1	A	761	SER	3.0
1	A	513	LEU	2.9
1	A	643	LYS	2.9
1	A	751	LYS	2.9
1	A	854	LEU	2.9
1	A	399	SER	2.9
1	A	275	ASN	2.9
1	A	709	GLY	2.9
1	A	733	GLU	2.9
1	A	516	ALA	2.8
1	A	704	GLY	2.8
1	A	653	TYR	2.8
1	A	652	LEU	2.8
1	A	669	LEU	2.8
1	A	550	GLU	2.8
1	A	645	ARG	2.8
1	A	512	VAL	2.7
1	A	735	LYS	2.7
1	A	857	PHE	2.7
1	A	702	TYR	2.7
1	A	547	GLU	2.7
1	A	766	LYS	2.7
1	A	480	SER	2.7
1	A	665	PRO	2.6
1	A	672	ILE	2.6
1	A	544	VAL	2.6
1	A	676	VAL	2.6
1	A	195	GLU	2.6
1	A	276	GLU	2.6
1	A	642	LYS	2.6
1	A	502	PRO	2.6
1	A	849	THR	2.6
1	A	660	PHE	2.5
1	A	858	GLY	2.5
1	A	853	ILE	2.5
1	A	852	GLN	2.5
1	A	855	ARG	2.5
1	A	678	THR	2.5
1	A	556	CYS	2.5
1	A	713	ILE	2.5
1	A	712	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	246	GLN	2.4
1	A	752	ARG	2.4
1	A	848	SER	2.4
1	A	585	PRO	2.4
1	A	377	TYR	2.4
1	A	271	ARG	2.4
1	A	241	ARG	2.4
1	A	552	LEU	2.4
1	A	73	GLU	2.4
1	A	554	ILE	2.3
1	A	501	ASP	2.3
1	A	238	VAL	2.3
1	A	190	GLU	2.3
1	A	589	GLU	2.3
1	A	856	ALA	2.3
1	A	840	GLU	2.3
1	A	675	TRP	2.3
1	A	685	GLU	2.3
1	A	280	LYS	2.3
1	A	402	ASP	2.2
1	A	656	THR	2.2
1	A	688	LYS	2.2
1	A	746	ASP	2.2
1	A	279	VAL	2.2
1	A	510	ILE	2.2
1	A	192	ASP	2.2
1	A	40	GLU	2.2
1	A	504	ALA	2.2
1	A	553	HIS	2.2
1	A	408	GLU	2.2
1	A	666	LYS	2.1
1	A	655	ASP	2.1
1	A	536	GLN	2.1
1	A	708	ASP	2.1
1	A	679	THR	2.0
1	A	575	VAL	2.0
1	A	539	LYS	2.0
1	A	97	ASP	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 [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, 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(Å ²)	Q<0.9
2	SO4	A	888	5/5	0.48	0.16	120,120,120,120	0
2	SO4	A	887	5/5	0.67	0.14	91,92,92,92	0
2	SO4	A	886	5/5	0.75	0.12	104,104,104,104	0
2	SO4	A	889	5/5	0.75	0.27	58,59,64,65	0
2	SO4	A	890	5/5	0.79	0.30	77,77,79,80	0
2	SO4	A	891	5/5	0.81	0.32	78,78,80,80	0
3	MG	A	892	1/1	0.82	0.10	49,49,49,49	0
2	SO4	A	885	5/5	0.84	0.20	122,122,122,123	0
2	SO4	A	884	5/5	0.85	0.15	74,74,76,78	0
2	SO4	A	883	5/5	0.96	0.16	59,59,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.