



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:07 PM GMT

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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

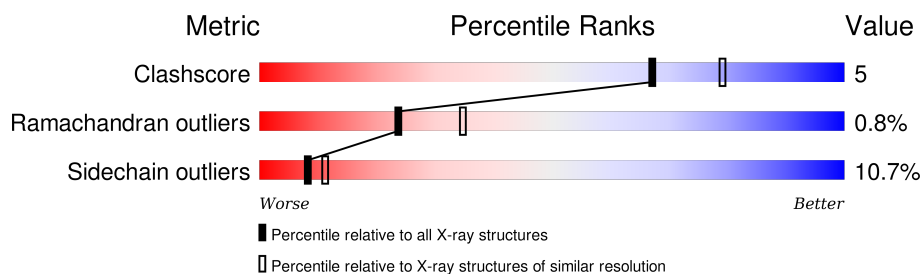
1 Overall quality at a glance

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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	 67% 17% • 14%

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.

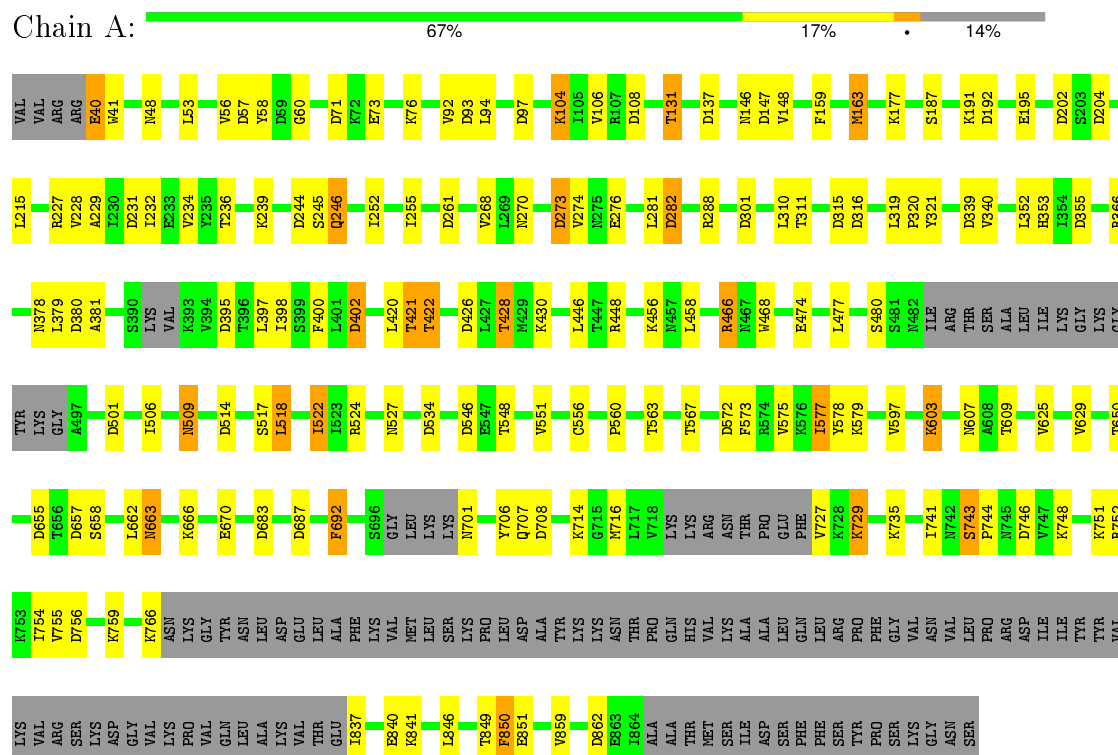
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: DNA polymerase I



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	99.5 (30.00-2.40)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6230	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

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:311:THR:CG2	1:A:353:HIS:HE2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:CG2	1:A:288:ARG:HG2	2.50	0.41
1:A:850:PHE:CD2	1:A:850:PHE:O	2.74	0.41
1:A:320:PRO:HA	1:A:340:VAL:HG11	2.01	0.41
1:A:397:LEU:HG	1:A:398:ILE:H	1.86	0.41
1:A:378:ASN:ND2	1:A:381:ALA:H	2.19	0.41
1:A:232:ILE:HG22	1:A:255:ILE:HG12	2.03	0.41
1:A:743:SER:CB	1:A:744:PRO:HD2	2.52	0.40
1:A:577:ILE:HG13	1:A:578:TYR:CD2	2.56	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%)	24	35

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 11

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	0.39	0	6,6,6	0.22	0
2	SO4	A	884	-	4,4,4	0.14	0	6,6,6	0.55	0
2	SO4	A	885	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	A	886	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	887	-	4,4,4	0.12	0	6,6,6	0.25	0
2	SO4	A	888	-	4,4,4	0.20	0	6,6,6	0.12	0
2	SO4	A	889	-	4,4,4	0.65	0	6,6,6	0.74	0
2	SO4	A	890	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	A	891	-	4,4,4	0.15	0	6,6,6	0.24	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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.