



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:41 PM UTC

PDB ID : 4DS5 / pdb_00004ds5
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment, DNA duplex, and rCTP in presence of Mg²⁺
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-02-17
Resolution : 1.68 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

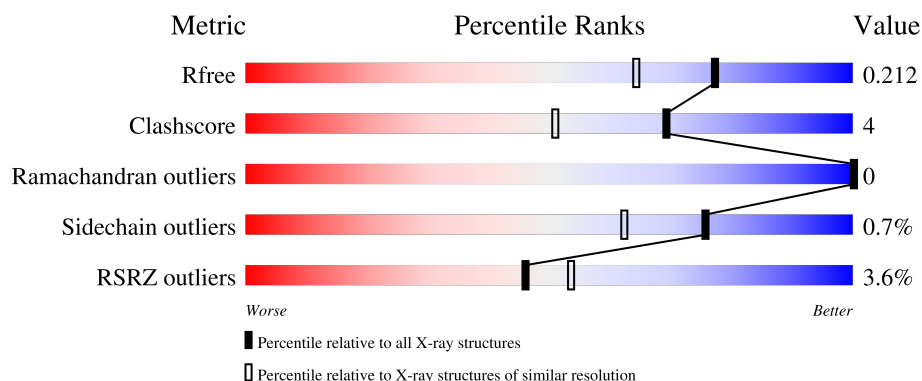
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	592	4% 92% 5%
1	D	592	4% 87% 7% 5%
2	B	9	78% 11% 11%
2	E	9	56% 44%
3	C	13	85% 15%

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Mol	Chain	Length	Quality of chain
3	F	13	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment representing 62%, a yellow segment representing 8%, and a grey segment representing 31%. The percentages are labeled below the bar.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20947 atoms, of which 9809 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	580	Total	C	H	N	O	S	0	2	0
			9391	2963	4731	810	870	17			
1	D	561	Total	C	H	N	O	S	0	20	0
			9228	2914	4655	791	853	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	engineered mutation	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	engineered mutation	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

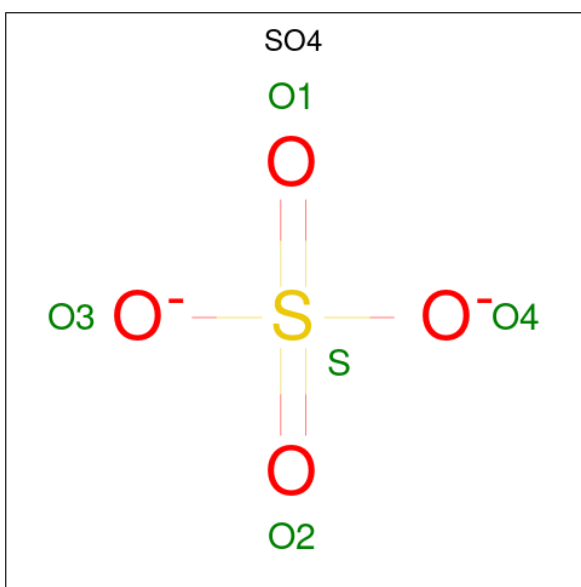
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	0
			356	109	123	47	66	11			
3	F	9	Total	C	H	N	O	P	0	0	0
			291	89	100	40	53	9			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

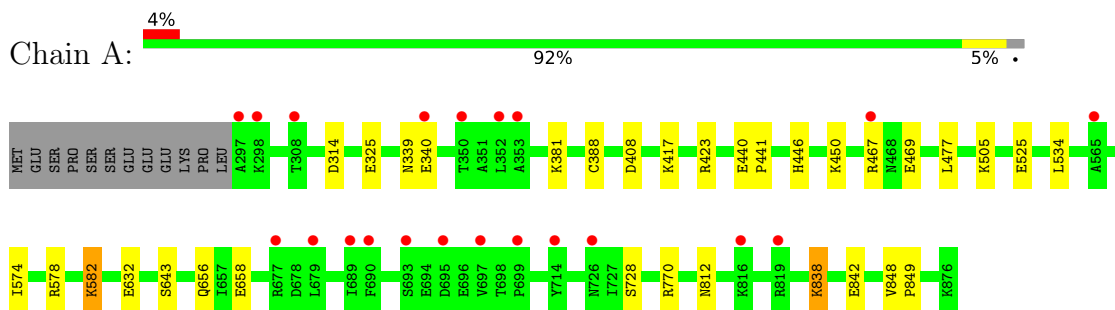
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	356	Total	O	0	0
			356	356		
5	D	601	Total	O	0	0
			601	601		
5	B	30	Total	O	0	0
			30	30		
5	C	46	Total	O	0	0
			46	46		
5	E	31	Total	O	0	0
			31	31		
5	F	54	Total	O	0	0
			54	54		

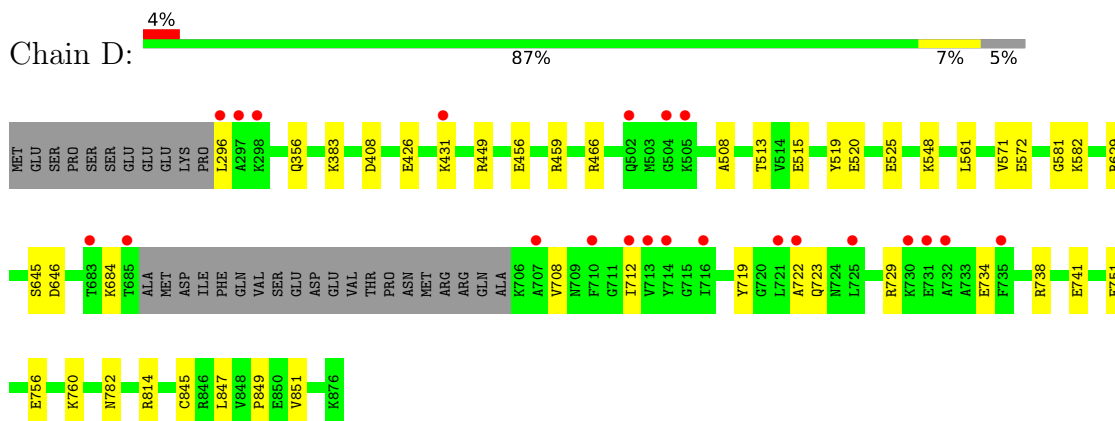
3 Residue-property plots

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.

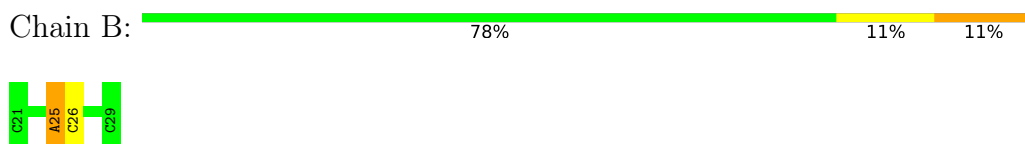
- Molecule 1: DNA polymerase



- Molecule 1: DNA polymerase



- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*C)-3')

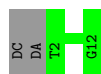


- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*C)-3')



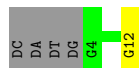
- Molecule 3: DNA (5'-D(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C:  85% 15%



- Molecule 3: DNA (5'-D(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain F:  62% 8% 31%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.88Å 108.86Å 150.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.43 – 1.68 54.43 – 1.68	Depositor EDS
% Data completeness (in resolution range)	86.6 (54.43-1.68) 86.6 (54.43-1.68)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 1.68Å)	Xtriage
Refinement program	PHENIX dev_1026	Depositor
R, R_{free}	0.176 , 0.199 (Not available) , 0.212	Depositor DCC
R_{free} test set	6639 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.1	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	0.96	EDS
Total number of atoms	20947	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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	0.54	0/4750	0.76	0/6418
1	D	0.77	0/4737	0.85	0/6401
2	B	0.52	0/193	1.31	1/294 (0.3%)
2	E	0.55	0/193	1.27	1/294 (0.3%)
3	C	0.48	0/262	1.00	0/404
3	F	0.65	0/215	1.28	0/331
All	All	0.66	0/10350	0.85	2/14142 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	DA	C5'-C4'-C3'	5.73	123.49	114.90
2	E	23	DT	O4'-C1'-N1	-5.42	100.26	108.40

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	4660	4731	4713	31	2
1	D	4573	4655	4546	39	2
2	B	174	100	101	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	174	100	101	3	0
3	C	233	123	124	0	0
3	F	191	100	101	1	0
4	D	15	0	0	0	0
5	A	356	0	0	19	0
5	B	30	0	0	0	0
5	C	46	0	0	0	0
5	D	601	0	0	18	2
5	E	31	0	0	1	0
5	F	54	0	0	1	0
All	All	11138	9809	9686	70	4

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 4.

All (70) 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:D:741:GLU:OE2	5:D:1354:HOH:O	1.85	0.94
1:A:325:GLU:OE1	5:A:1235:HOH:O	1.90	0.89
1:A:656:GLN:OE1	5:A:1201:HOH:O	1.90	0.87
1:D:751:GLU:OE2	5:D:1219:HOH:O	1.93	0.85
1:A:842:GLU:HG2	5:A:1243:HOH:O	1.81	0.80
1:A:582:LYS:HD2	2:B:26:DC:H1'	1.63	0.80
1:A:838:LYS:NZ	5:A:1253:HOH:O	2.18	0.73
1:D:459:ARG:NH1	5:D:1302:HOH:O	2.23	0.71
1:A:388:CYS:SG	5:A:1206:HOH:O	2.14	0.69
1:D:408:ASP:OD1	5:D:1591:HOH:O	2.11	0.68
1:A:417:LYS:O	5:A:1179:HOH:O	2.13	0.67
1:D:708:VAL:HG13	1:D:712:ILE:CD1	2.26	0.66
1:A:469:GLU:CD	1:D:466:ARG:HE	2.04	0.66
1:A:643:SER:O	5:A:1069:HOH:O	2.14	0.65
1:A:842:GLU:OE2	5:A:1243:HOH:O	2.15	0.65
1:A:408:ASP:OD1	5:A:988:HOH:O	2.15	0.64
1:A:658:GLU:OE2	5:A:965:HOH:O	2.15	0.64
1:D:456:GLU:HG2	5:D:1571:HOH:O	1.98	0.63
1:D:581:GLY:HA3	5:D:1575:HOH:O	1.99	0.62
1:A:314:ASP:O	5:A:1226:HOH:O	2.16	0.61
1:D:459:ARG:NH2	5:D:1329:HOH:O	2.33	0.61
1:D:561:LEU:O	1:D:571:VAL:HG11	1.99	0.61
1:A:469:GLU:HG3	1:D:466:ARG:NE	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:VAL:HG13	1:D:712:ILE:HD12	1.85	0.58
1:A:469:GLU:CD	5:A:1246:HOH:O	2.45	0.58
1:D:466:ARG:NH1	5:D:1302:HOH:O	2.03	0.58
2:E:27:DT:OP1	5:E:118:HOH:O	2.17	0.57
1:A:469:GLU:OE1	5:A:1195:HOH:O	2.17	0.57
1:D:520:GLU:CD	5:D:1458:HOH:O	2.50	0.53
1:D:684:LYS:CE	5:D:1563:HOH:O	2.56	0.53
1:D:582:LYS:HE2	2:E:26:DC:O2	2.09	0.52
1:D:561:LEU:HB3	1:D:571:VAL:HG13	1.92	0.52
1:D:508:ALA:O	5:D:1470:HOH:O	2.19	0.51
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.26	0.51
1:A:578:ARG:NH1	2:B:25:DA:H5"	2.27	0.50
1:A:770:ARG:NH2	5:A:1104:HOH:O	2.44	0.50
1:D:684:LYS:NZ	5:D:1563:HOH:O	2.38	0.50
3:F:12:DG:N3	5:F:132:HOH:O	2.34	0.49
1:A:423:ARG:NE	5:A:1221:HOH:O	2.44	0.49
1:D:734:GLU:HB3	1:D:738:ARG:NH1	2.28	0.49
1:A:842:GLU:CG	5:A:1243:HOH:O	2.48	0.49
1:A:467:ARG:HB3	5:D:1551:HOH:O	2.13	0.48
1:D:708:VAL:HG13	1:D:712:ILE:HG13	1.96	0.48
1:A:842:GLU:CD	5:A:1243:HOH:O	2.57	0.47
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.49	0.47
1:A:467:ARG:HD3	5:D:1551:HOH:O	2.15	0.47
1:A:534:LEU:HD11	1:A:574:ILE:HD13	1.98	0.46
1:D:722:ALA:HB2	1:D:729:ARG:HA	1.98	0.46
1:D:814:ARG:CZ	1:D:847[A]:LEU:HD13	2.45	0.46
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.98	0.46
1:D:814:ARG:HG3	1:D:851[B]:VAL:HG11	1.97	0.46
1:D:548:LYS:HE3	5:D:1487:HOH:O	2.17	0.45
1:D:383:LYS:HE3	5:D:1423:HOH:O	2.17	0.45
1:D:645:SER:O	1:D:646:ASP:HB2	2.17	0.45
1:A:446:HIS:CE1	1:A:450:LYS:HD2	2.51	0.45
1:D:296:LEU:HD13	1:D:449:ARG:HD3	1.99	0.45
1:D:756:GLU:OE2	1:D:760:LYS:HE2	2.17	0.44
1:A:440:GLU:N	1:A:441:PRO:HD2	2.33	0.44
1:D:525:GLU:O	5:D:1554:HOH:O	2.21	0.44
1:D:814:ARG:CZ	1:D:847[A]:LEU:CD1	2.95	0.44
1:D:708:VAL:HG13	1:D:712:ILE:CG1	2.47	0.44
1:D:845:CYS:SG	5:D:1382:HOH:O	2.01	0.43
1:D:426:GLU:OE2	1:D:431:LYS:HD3	2.19	0.42
1:A:525:GLU:O	5:A:1222:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LYS:HE3	5:A:1138:HOH:O	2.21	0.41
1:D:629:ARG:NH1	2:E:28:DC:OP2	2.54	0.41
1:A:340:GLU:H	1:A:340:GLU:CD	2.27	0.41
1:D:719:TYR:CE2	1:D:723:GLN:HG3	2.55	0.41
1:A:339:ASN:HB2	1:A:340:GLU:OE1	2.21	0.40

All (4) 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)
5:D:1562:HOH:O	5:D:1567:HOH:O[4_545]	1.45	0.75
5:D:1562:HOH:O	5:D:1564:HOH:O[4_545]	1.86	0.34
1:A:728:SER:OG	1:D:572:GLU:OE2[2_755]	2.12	0.08
1:A:505:LYS:HZ3	1:D:356:GLN:OE1[2_745]	1.59	0.01

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	580/592 (98%)	561 (97%)	19 (3%)	0	100	100
1	D	577/592 (98%)	566 (98%)	11 (2%)	0	100	100
All	All	1157/1184 (98%)	1127 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	497/507 (98%)	492 (99%)	5 (1%)	68	52
1	D	497/507 (98%)	495 (100%)	2 (0%)	84	78
All	All	994/1014 (98%)	987 (99%)	7 (1%)	76	62

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	LEU
1	A	582	LYS
1	A	632	GLU
1	A	812	ASN
1	A	838	LYS
1	D	513	THR
1	D	782	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	GLN
1	D	573	ASN
1	D	782	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	SO4	D	901	-	4,4,4	0.23	0	6,6,6	0.57	0
4	SO4	D	902	-	4,4,4	0.31	0	6,6,6	0.24	0
4	SO4	D	903	-	4,4,4	0.26	0	6,6,6	0.17	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.

No monomer is involved in short contacts.

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	580/592 (97%)	0.46	21 (3%)	46	53	17, 45, 75, 101	1 (0%)
1	D	561/592 (94%)	-0.07	22 (3%)	43	51	7, 27, 53, 73	10 (1%)
2	B	9/9 (100%)	-0.15	0	100	100	28, 33, 47, 65	0
2	E	9/9 (100%)	-0.26	0	100	100	22, 30, 45, 61	0
3	C	11/13 (84%)	-0.29	0	100	100	22, 30, 53, 68	0
3	F	9/13 (69%)	-0.69	0	100	100	17, 21, 36, 46	0
All	All	1179/1228 (96%)	0.18	43 (3%)	46	53	7, 37, 66, 101	11 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	712	ILE	9.1
1	D	713	VAL	5.5
1	D	710	PHE	5.3
1	A	297	ALA	4.7
1	A	353	ALA	4.5
1	A	679	LEU	4.3
1	D	725	LEU	3.2
1	D	735	PHE	3.1
1	A	816	LYS	3.1
1	D	731	GLU	3.1
1	D	722	ALA	3.0
1	D	504	GLY	2.9
1	D	732	ALA	2.8
1	A	714	TYR	2.8
1	D	297	ALA	2.6
1	A	690	PHE	2.6
1	D	716	ILE	2.5
1	D	683	THR	2.5
1	D	502	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	707	ALA	2.4
1	A	677	ARG	2.4
1	A	689	ILE	2.4
1	A	699	PRO	2.4
1	D	714	TYR	2.4
1	A	819	ARG	2.3
1	D	431	LYS	2.3
1	D	296	LEU	2.3
1	A	695	ASP	2.3
1	D	298	LYS	2.3
1	A	565	ALA	2.2
1	A	352	LEU	2.2
1	A	726	ASN	2.2
1	A	298	LYS	2.2
1	D	505	LYS	2.2
1	D	721	LEU	2.2
1	D	730	LYS	2.2
1	A	693	SER	2.2
1	A	697	VAL	2.1
1	D	685	THR	2.1
1	A	467	ARG	2.1
1	A	308	THR	2.1
1	A	350	THR	2.1
1	A	340	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 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($\text{\AA}^2$)	Q<0.9
4	SO4	D	902	5/5	0.86	0.12	39,44,51,51	0
4	SO4	D	903	5/5	0.86	0.11	65,73,77,80	0
4	SO4	D	901	5/5	0.96	0.09	37,38,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.