Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 07:12 PM EDT

PDB ID	:	4DS4
Title	:	Ternary complex of Bacillus DNA Polymerase I Large Fragment, DNA duplex, and rCTP in presence of Mn2+
Authors	:	Wang, W.; Beese, L.S.
Deposited on	:	2012-02-17
Resolution	:	1.68 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

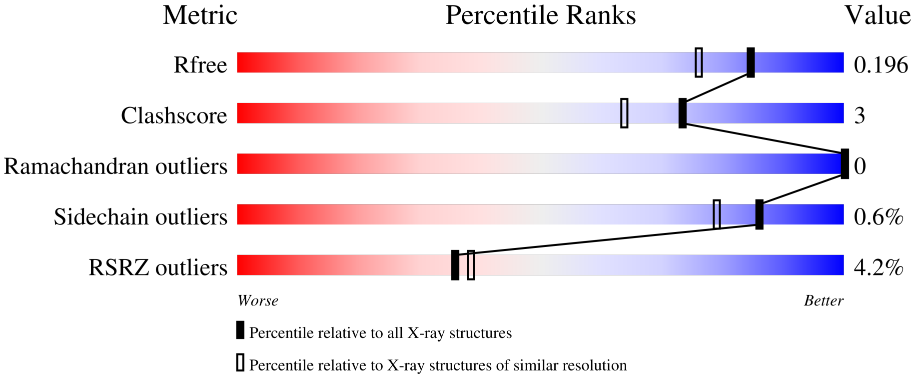
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

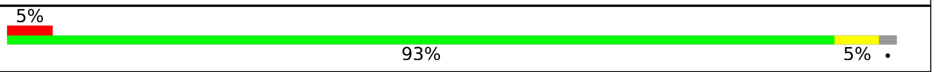
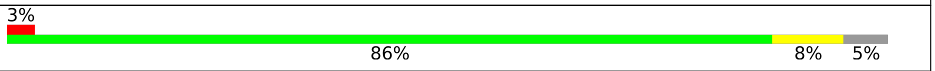
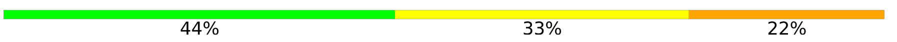
The reported resolution of this entry is 1.68 Å.

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}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 <=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	
1	D	592	
2	B	9	
2	E	9	
3	C	13	

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Mol	Chain	Length	Quality of chain
3	F	13	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20911 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
			Total	C	H	N	O	S			
1	A	580	9391	2963	4731	810	870	17	0	2	0
			Total	C	H	N	O	S			
1	D	561	9228	2914	4655	791	853	15	0	20	0

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	engineered mutation	UNP Q5KWC1
D	598	ALA	ASP	engineered mutation	UNP Q5KWC1
D	823	HIS	ARG	engineered mutation	UNP Q5KWC1

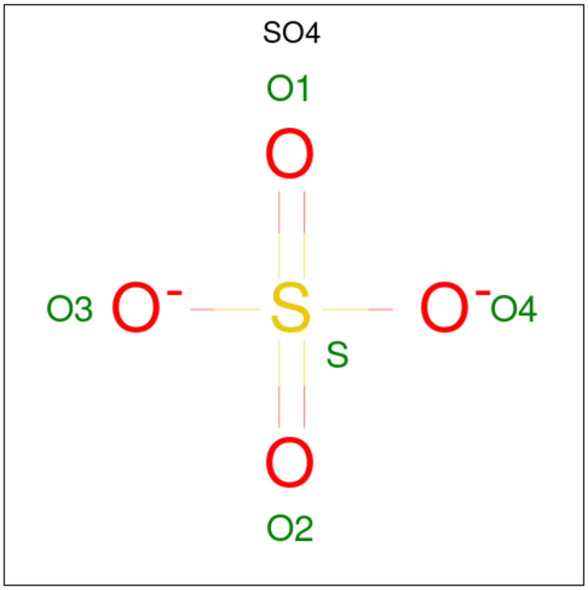
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3').

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

- 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
			Total	C	H	N	O	P			
3	C	11	356	109	123	47	66	11	0	0	0
			Total	C	H	N	O	P			
3	F	9	291	89	100	40	53	9	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

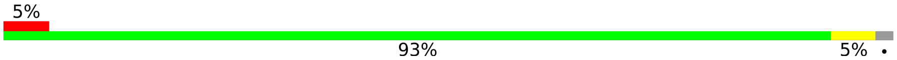
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	354	Total O 354 354	0	0
5	D	570	Total O 570 570	0	0
5	B	28	Total O 28 28	0	0
5	C	47	Total O 47 47	0	0
5	E	29	Total O 29 29	0	0
5	F	54	Total O 54 54	0	0

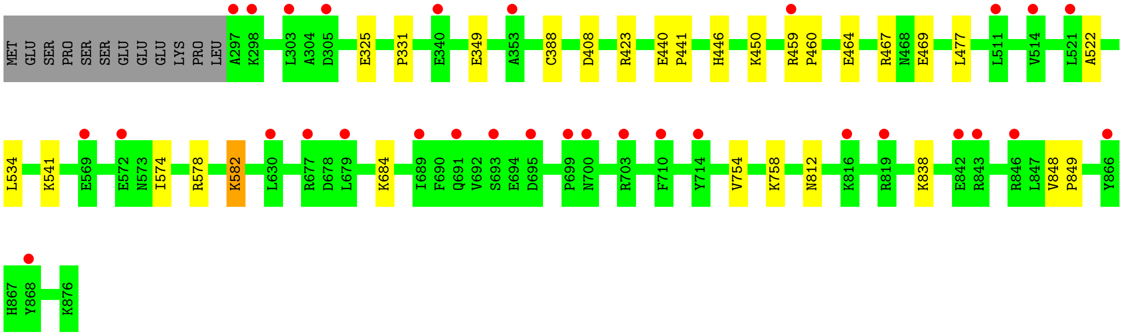
3 Residue-property plots ⓘ

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

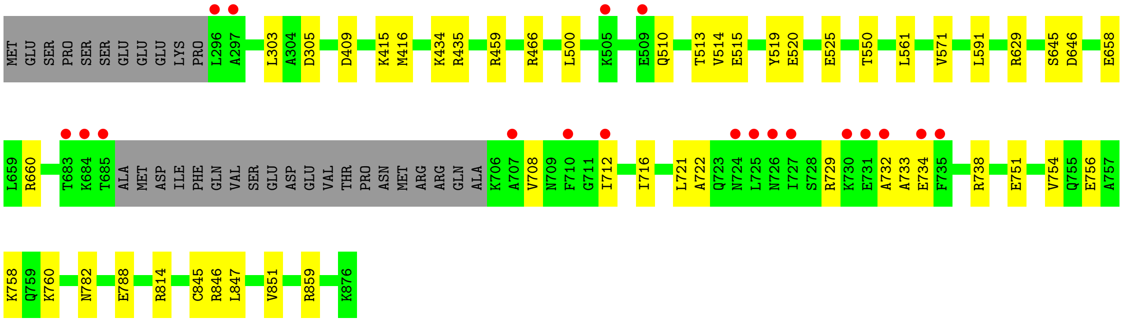
Chain A:





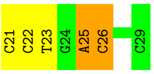
- Molecule 1: DNA polymerase

Chain D:



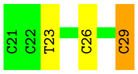
- Molecule 2: DNA (5’-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3’)

Chain B:



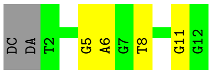
- Molecule 2: DNA (5’-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3’)

Chain E:



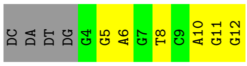
- Molecule 3: DNA (5'-D(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C:



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

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.79Å 108.77Å 150.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.25 – 1.68 64.25 – 1.68	Depositor EDS
% Data completeness (in resolution range)	87.7 (64.25-1.68) 87.7 (64.25-1.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.68Å)	Xtriage
Refinement program	PHENIX dev_1026	Depositor
R, R_{free}	0.174 , 0.199 0.173 , 0.196	Depositor DCC
R_{free} test set	6888 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20911	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, DOC

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	0.43	0/4750	0.57	0/6418
1	D	0.63	0/4737	0.70	4/6401 (0.1%)
2	B	0.91	0/173	1.94	8/264 (3.0%)
2	E	1.09	0/173	1.82	2/264 (0.8%)
3	C	1.04	0/262	1.59	6/404 (1.5%)
3	F	1.30	0/215	1.95	5/331 (1.5%)
All	All	0.60	0/10310	0.81	25/14082 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	23	DT	O4'-C1'-N1	-9.98	101.02	108.00
2	B	25	DA	O4'-C4'-C3'	-9.32	100.41	106.00
3	F	6	DA	OP1-P-OP2	-7.18	108.83	119.60
2	B	25	DA	O5'-P-OP1	6.36	118.33	110.70
3	F	12	DG	O4'-C1'-N9	6.30	112.41	108.00
1	D	660	ARG	NE-CZ-NH1	6.25	123.42	120.30
3	F	10	DA	O4'-C1'-N9	-6.24	103.63	108.00
3	F	8	DT	O4'-C1'-N1	-6.18	103.67	108.00
3	F	5	DG	C2-N3-C4	-5.97	108.92	111.90
3	C	11	DG	O4'-C1'-N9	-5.94	103.84	108.00
3	C	5	DG	C5-C6-N1	-5.76	108.62	111.50
1	D	859	ARG	NE-CZ-NH1	5.75	123.18	120.30
3	C	8	DT	O4'-C1'-N1	-5.74	103.98	108.00
2	B	23	DT	O4'-C1'-N1	-5.67	104.03	108.00
1	D	409	ASP	CB-CG-OD2	5.66	123.40	118.30
2	B	26	DC	O4'-C1'-N1	5.60	111.92	108.00
2	B	25	DA	O5'-P-OP2	-5.43	100.81	105.70
3	C	5	DG	N1-C6-O6	5.38	123.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	DA	C5'-C4'-C3'	5.37	123.77	114.10
2	B	26	DC	O4'-C1'-C2'	5.37	110.19	105.90
1	D	859	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	E	26	DC	N1-C2-O2	-5.15	115.81	118.90
3	C	5	DG	N3-C4-N9	-5.02	122.99	126.00
3	C	6	DA	C5-N7-C8	-5.01	101.39	103.90
2	B	26	DC	C6-N1-C2	5.00	122.30	120.30

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	4660	4731	4713	24	0
1	D	4573	4655	4546	42	0
2	B	174	100	103	3	0
2	E	174	100	103	1	0
3	C	233	123	124	0	0
3	F	191	100	101	1	0
4	D	15	0	0	0	0
5	A	354	0	0	9	2
5	B	28	0	0	0	0
5	C	47	0	0	0	0
5	D	570	0	0	20	2
5	E	29	0	0	0	0
5	F	54	0	0	1	0
All	All	11102	9809	9690	65	2

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 3.

All (65) 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:416:MET:HE3	5:D:1543:HOH:O	1.63	0.96
1:A:388:CYS:SG	5:A:1043:HOH:O	2.23	0.95
1:A:408:ASP:OD1	5:A:1012:HOH:O	1.89	0.91
1:D:845:CYS:SG	5:D:1481:HOH:O	2.29	0.90
1:A:582:LYS:HD2	2:B:26:DC:H1'	1.61	0.82
1:D:846:ARG:HD2	5:D:1535:HOH:O	1.79	0.81
1:D:758:LYS:CE	5:D:1562:HOH:O	2.33	0.77
1:D:788:GLU:OE2	5:D:1562:HOH:O	2.01	0.77
1:D:305:ASP:OD1	5:D:1435:HOH:O	2.03	0.75
1:A:423:ARG:NE	5:A:1239:HOH:O	2.20	0.70
1:D:459:ARG:NH2	5:D:1342:HOH:O	2.25	0.69
1:A:464:GLU:OE1	5:A:1159:HOH:O	2.11	0.69
1:D:751:GLU:OE2	5:D:1267:HOH:O	2.11	0.67
3:F:11:DG:OP1	5:F:144:HOH:O	2.13	0.67
1:D:733:ALA:O	5:D:1522:HOH:O	2.12	0.65
1:A:812:ASN:O	5:A:1073:HOH:O	2.15	0.64
1:D:658:GLU:OE1	5:D:1559:HOH:O	2.15	0.63
1:D:758:LYS:HE2	5:D:1562:HOH:O	1.98	0.63
1:D:758:LYS:NZ	5:D:1562:HOH:O	2.23	0.63
1:D:520:GLU:OE1	5:D:1490:HOH:O	2.16	0.62
1:D:561:LEU:O	1:D:571:VAL:HG11	1.99	0.61
1:D:561:LEU:HB3	1:D:571:VAL:HG13	1.82	0.61
1:D:708:VAL:HG13	1:D:712:ILE:CD1	2.33	0.59
1:A:467:ARG:NH2	5:A:1107:HOH:O	2.35	0.59
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.42	0.55
1:D:708:VAL:HG13	1:D:712:ILE:HD12	1.89	0.53
1:A:459:ARG:HB2	1:A:460:PRO:HD3	1.91	0.52
1:A:534:LEU:HD11	1:A:574:ILE:HD13	1.93	0.51
1:D:520:GLU:CD	5:D:1490:HOH:O	2.48	0.50
1:A:684:LYS:NZ	5:A:1014:HOH:O	2.38	0.49
1:D:734:GLU:HB3	1:D:738:ARG:NH1	2.27	0.49
1:D:721:LEU:HB3	1:D:732:ALA:HB1	1.95	0.48
1:A:469:GLU:HG3	1:D:466:ARG:NE	2.28	0.48
1:A:440:GLU:N	1:A:441:PRO:HD2	2.29	0.48
1:D:814:ARG:HG3	1:D:851[B]:VAL:HG11	1.96	0.48
1:D:415:LYS:NZ	5:D:1318:HOH:O	2.48	0.47
1:A:325:GLU:OE1	5:A:1248:HOH:O	2.20	0.47
1:D:510:GLN:O	1:D:514:VAL:HG23	2.14	0.47
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.96	0.47
1:A:469:GLU:CD	1:D:466:ARG:HE	2.17	0.47
1:D:459:ARG:CZ	5:D:1342:HOH:O	2.62	0.47
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:LEU:HD21	1:D:591:LEU:HD23	1.98	0.45
1:D:645:SER:O	1:D:646:ASP:HB2	2.17	0.45
1:D:756:GLU:OE2	1:D:760:LYS:HE2	2.17	0.45
1:D:525:GLU:O	5:D:1365:HOH:O	2.21	0.45
1:D:550:THR:CG2	5:D:1376:HOH:O	2.65	0.45
1:D:712:ILE:HA	1:D:716:ILE:HG22	1.99	0.45
1:A:469:GLU:CD	1:D:466:ARG:NE	2.70	0.44
1:D:722:ALA:HB2	1:D:729:ARG:HA	2.00	0.44
1:D:754:VAL:CG1	1:D:758:LYS:HE3	2.48	0.43
1:D:814:ARG:CZ	1:D:847[A]:LEU:HD13	2.47	0.43
1:A:446:HIS:NE2	1:A:450:LYS:HD2	2.34	0.43
1:D:629:ARG:HH22	2:E:29:DOC:H5	1.84	0.43
1:A:522:ALA:O	1:A:541:LYS:HE2	2.19	0.42
2:B:21:DC:H2'	2:B:22:DC:C6	2.54	0.42
1:A:578:ARG:NH1	2:B:25:DA:H5"	2.35	0.42
1:A:349:GLU:H	1:A:349:GLU:CD	2.24	0.41
1:A:582:LYS:O	1:A:582:LYS:HG3	2.20	0.41
1:D:708:VAL:HG13	1:D:712:ILE:HG13	2.03	0.41
1:A:446:HIS:CE1	1:A:450:LYS:HD2	2.55	0.41
1:D:435:ARG:NH2	5:D:1428:HOH:O	2.53	0.41
1:A:331:PRO:HG2	5:A:1063:HOH:O	2.21	0.41
1:A:754:VAL:HG12	1:A:758:LYS:HE2	2.02	0.41
1:D:434:LYS:NZ	5:D:1514:HOH:O	2.46	0.41

All (2) 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:A:977:HOH:O	5:D:1176:HOH:O[2_745]	1.72	0.48
5:A:1010:HOH:O	5:D:1088:HOH:O[2_745]	1.99	0.21

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	580/592 (98%)	567 (98%)	13 (2%)	0	100	100
1	D	577/592 (98%)	566 (98%)	11 (2%)	0	100	100
All	All	1157/1184 (98%)	1133 (98%)	24 (2%)	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%)	494 (99%)	3 (1%)	86	79
1	D	497/507 (98%)	494 (99%)	3 (1%)	86	79
All	All	994/1014 (98%)	988 (99%)	6 (1%)	86	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	LEU
1	A	582	LYS
1	A	838	LYS
1	D	303	LEU
1	D	513	THR
1	D	782	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	DOC	B	29	3,2	16,19,20	0.47	0	20,26,29	0.51	0
2	DOC	E	29	3,2	16,19,20	0.82	0	20,26,29	0.90	1 (5%)

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	DOC	B	29	3,2	-	0/7/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	29	DOC	O4'-C4'-C5'	-2.33	105.69	109.52

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	E	29	DOC	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.15	0	6,6,6	0.44	0
4	SO4	D	903	-	4,4,4	0.16	0	6,6,6	0.17	0
4	SO4	D	902	-	4,4,4	0.15	0	6,6,6	0.20	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 ⓘ

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	580/592 (97%)	0.23	31 (5%)	26	28	21, 39, 66, 91	0
1	D	561/592 (94%)	0.18	19 (3%)	45	48	11, 25, 47, 63	0
2	B	8/9 (88%)	-0.44	0	100	100	26, 32, 47, 60	0
2	E	8/9 (88%)	-0.33	0	100	100	20, 28, 44, 57	0
3	C	11/13 (84%)	-0.30	0	100	100	21, 28, 47, 66	0
3	F	9/13 (69%)	-0.25	0	100	100	16, 21, 34, 41	0
All	All	1177/1228 (95%)	0.19	50 (4%)	36	38	11, 32, 59, 91	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	712	ILE	6.2
1	D	731	GLU	5.5
1	D	735	PHE	5.4
1	A	297	ALA	5.2
1	A	298	LYS	4.9
1	A	819	ARG	4.7
1	A	816	LYS	4.3
1	A	699	PRO	4.1
1	A	703	ARG	4.0
1	D	685	THR	3.9
1	D	725	LEU	3.9
1	A	679	LEU	3.8
1	A	630	LEU	3.7
1	A	521	LEU	3.7
1	D	724	ASN	3.7
1	D	727	ILE	3.7
1	D	296	LEU	3.5
1	D	509	GLU	3.5
1	A	695	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	732	ALA	3.3
1	D	734	GLU	3.3
1	A	842	GLU	3.3
1	A	846	ARG	3.1
1	D	710	PHE	3.1
1	D	707	ALA	3.1
1	A	353	ALA	2.9
1	A	714	TYR	2.8
1	A	303	LEU	2.8
1	D	730	LYS	2.7
1	A	689	ILE	2.7
1	A	700	ASN	2.7
1	A	866	TYR	2.6
1	A	569	GLU	2.5
1	D	505	LYS	2.5
1	A	710	PHE	2.4
1	A	340	GLU	2.4
1	D	684	LYS	2.3
1	D	726	ASN	2.3
1	D	297	ALA	2.3
1	A	572	GLU	2.3
1	A	459	ARG	2.2
1	A	693	SER	2.2
1	A	677	ARG	2.2
1	D	683	THR	2.2
1	A	691	GLN	2.1
1	A	868	TYR	2.1
1	A	511	LEU	2.1
1	A	514	VAL	2.0
1	A	843	ARG	2.0
1	A	305	ASP	2.0

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

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, 95^{th} 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	DOC	B	29	18/19	0.98	0.08	28,33,43,43	0
2	DOC	E	29	18/19	0.98	0.10	17,21,29,35	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	SO4	D	903	5/5	0.88	0.14	75,82,85,85	0
4	SO4	D	902	5/5	0.95	0.09	36,44,49,59	0
4	SO4	D	901	5/5	0.98	0.09	33,36,48,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.