



# Full wwPDB X-ray Structure Validation Report

Apr 29, 2014 – 02:33 AM EDT

PDB ID : 4F8R  
Title : Bacillus DNA Polymerase I Large Fragment complex 7  
Authors : Wang, W.; Beese, L.S.  
Deposited on : 2012-05-17  
Resolution : 1.64 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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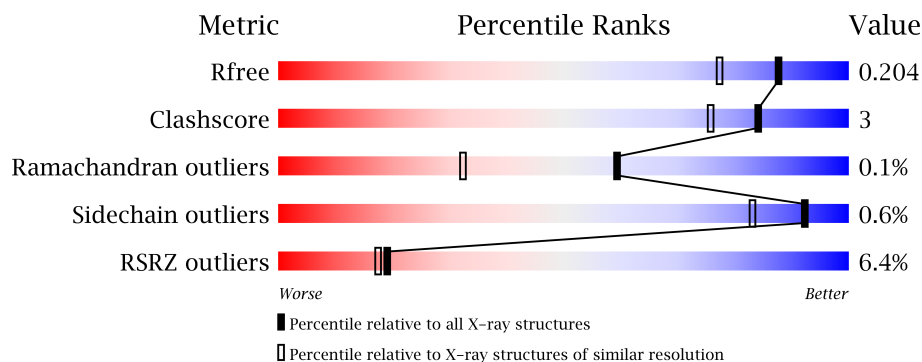
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 1.64 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))
$R_{free}$	66092	1326 (1.66-1.62)
Clashscore	79885	1525 (1.66-1.62)
Ramachandran outliers	78287	1490 (1.66-1.62)
Sidechain outliers	78261	1490 (1.66-1.62)
RSRZ outliers	66119	1326 (1.66-1.62)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	592	
1	D	592	
2	B	9	
2	E	9	
3	C	13	
3	F	13	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21034 atoms, of which 9790 are hydrogens and 0 are deuterium.

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	579	Total	C	H	N	O	S	0	6	0
			9416	2968	4744	814	873	17			
1	D	553	Total	C	H	N	O	S	0	18	0
			9124	2884	4598	781	845	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
A	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
D	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

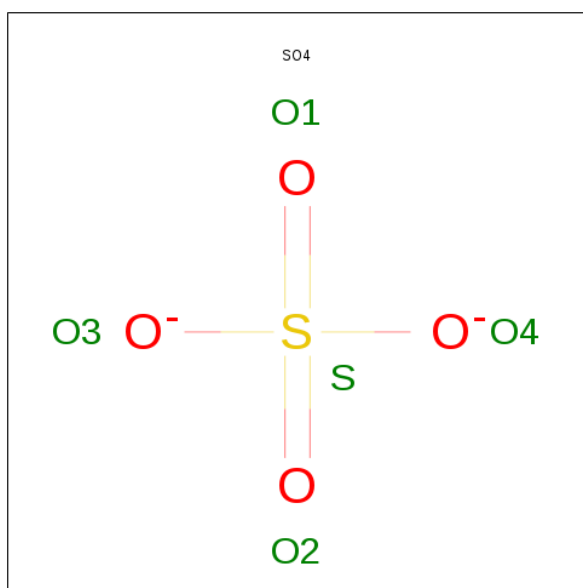
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DDG))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			276	86	100	31	51	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			277	86	100	31	52	8			

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*AP\*TP\*TP\*CP\*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
			341	108	113	42	67	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			381	118	135	47	70	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

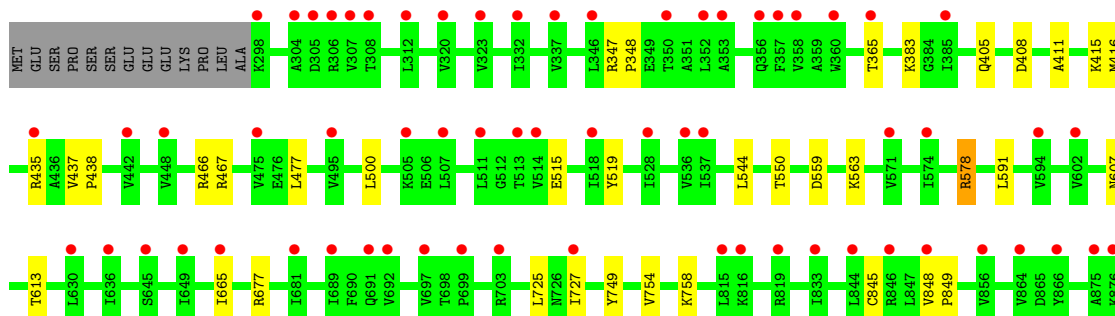
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	406	Total	O	0	0
			406	406		
5	C	59	Total	O	0	0
			59	59		
5	D	620	Total	O	0	0
			620	620		
5	B	29	Total	O	0	0
			29	29		
5	E	26	Total	O	0	0
			26	26		
5	F	54	Total	O	0	0
			54	54		

### 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.

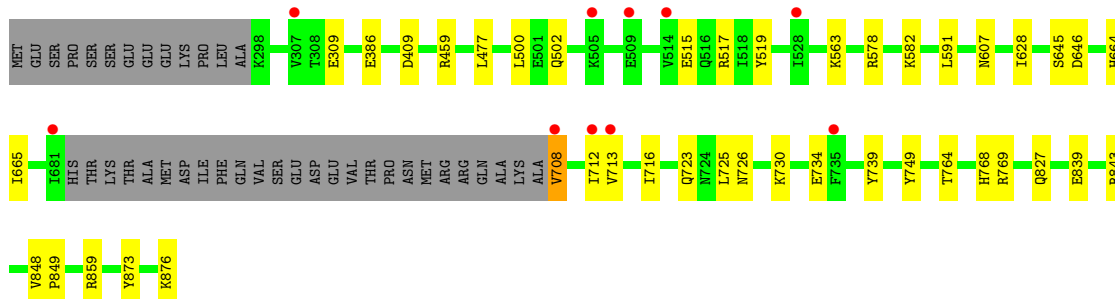
- Molecule 1: DNA polymerase

Chain A: 



- Molecule 1: DNA polymerase

Chain D: 



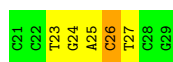
- Molecule 2: DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DDG))-3')

Chain B: 



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

Chain E: 




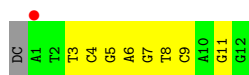
- Molecule 3: DNA (5'-D(\*CP\*AP\*TP\*TP\*CP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*G)-3')

Chain C: 



- Molecule 3: DNA (5'-D(\*CP\*AP\*TP\*TP\*CP\*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, $\alpha$ , $\beta$ , $\gamma$	93.67Å 109.37Å 150.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.98 – 1.64 88.45 – 1.64	Depositor EDS
% Data completeness (in resolution range)	87.7 (30.98-1.64) 87.7 (88.45-1.64)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 1.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, $R_{free}$	0.181 , 0.203 0.182 , 0.204	Depositor DCC
$R_{free}$ test set	7480 reflections (4.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 40.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 165508 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DDG, 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	0.44	0/4785	0.59	2/6466 (0.0%)
1	D	0.61	0/4672	0.69	4/6313 (0.1%)
2	B	0.99	0/173	1.92	9/264 (3.4%)
2	E	1.11	1/173 (0.6%)	2.00	7/264 (2.7%)
3	C	1.08	1/255 (0.4%)	2.29	21/392 (5.4%)
3	F	1.13	0/276	2.02	16/425 (3.8%)
All	All	0.60	2/10334 (0.0%)	0.89	59/14124 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	DA	C3'-O3'	-6.86	1.35	1.44
3	C	5	DG	C3'-O3'	5.67	1.51	1.44

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	DG	N3-C4-N9	-9.55	120.27	126.00
2	E	27	DT	O4'-C4'-C3'	-9.51	100.29	106.00
2	E	23	DT	O4'-C1'-N1	-9.46	101.38	108.00
3	F	8	DT	O4'-C1'-N1	-9.24	101.53	108.00
1	A	578	ARG	NE-CZ-NH2	-8.49	116.06	120.30
3	C	8	DT	O4'-C1'-N1	-8.24	102.23	108.00
2	B	27	DT	O4'-C1'-N1	7.93	113.55	108.00
3	C	11	DG	O4'-C1'-N9	-7.74	102.58	108.00
2	B	27	DT	O4'-C4'-C3'	-7.44	101.53	104.50
2	B	23	DT	N3-C4-O4	7.25	124.25	119.90
3	F	5	DG	N3-C4-C5	7.19	132.19	128.60
2	B	23	DT	O4'-C1'-N1	-7.14	103.00	108.00
3	C	8	DT	N3-C4-O4	6.96	124.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	DG	N9-C4-C5	6.93	108.17	105.40
3	C	2	DT	O4'-C1'-N1	6.86	112.80	108.00
3	C	5	DG	OP2-P-O3'	-6.75	90.35	105.20
1	D	578	ARG	NE-CZ-NH2	-6.73	116.93	120.30
3	F	3	DT	N3-C2-O2	6.63	126.28	122.30
3	F	5	DG	N3-C4-N9	-6.55	122.07	126.00
1	D	843	ARG	NE-CZ-NH2	-6.53	117.03	120.30
3	F	5	DG	OP1-P-OP2	-6.48	109.88	119.60
3	C	7	DG	C2-N3-C4	6.45	115.12	111.90
3	C	8	DT	C5-C4-O4	-6.32	120.47	124.90
2	E	26	DC	O4'-C1'-N1	6.31	112.42	108.00
3	C	4	DC	O5'-P-OP2	-6.30	100.03	105.70
3	C	6	DA	O4'-C1'-C2'	6.30	110.94	105.90
2	B	26	DC	O4'-C1'-N1	6.26	112.38	108.00
3	F	7	DG	C5-N7-C8	6.24	107.42	104.30
3	F	6	DA	O4'-C1'-N9	-6.15	103.69	108.00
3	C	4	DC	C2-N3-C4	6.13	122.97	119.90
3	F	3	DT	N3-C4-O4	6.13	123.58	119.90
3	F	5	DG	C6-N1-C2	6.05	128.73	125.10
3	F	5	DG	O4'-C1'-C2'	6.05	110.74	105.90
3	F	4	DC	O5'-P-OP2	-6.00	100.30	105.70
3	F	3	DT	C5-C4-O4	-5.96	120.73	124.90
3	C	5	DG	C6-N1-C2	5.93	128.66	125.10
3	C	5	DG	N3-C4-C5	5.92	131.56	128.60
2	E	23	DT	N3-C4-O4	5.92	123.45	119.90
3	C	3	DT	N3-C4-O4	5.77	123.36	119.90
2	B	25	DA	C1'-O4'-C4'	-5.76	104.33	110.10
1	D	409	ASP	CB-CG-OD2	5.74	123.47	118.30
3	F	11	DG	O4'-C1'-N9	-5.70	104.01	108.00
3	C	4	DC	N1-C2-N3	-5.61	115.28	119.20
2	B	25	DA	O4'-C1'-N9	5.59	111.91	108.00
3	C	3	DT	C5-C4-O4	-5.44	121.09	124.90
3	C	5	DG	O4'-C4'-C3'	5.40	109.24	106.00
2	E	27	DT	C6-C5-C7	-5.38	119.67	122.90
3	C	5	DG	C8-N9-C1'	5.37	133.99	127.00
3	F	7	DG	N7-C8-N9	-5.34	110.43	113.10
1	D	843	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	E	25	DA	O4'-C4'-C3'	-5.27	102.39	104.50
3	F	9	DC	O4'-C1'-C2'	5.22	110.08	105.90
3	C	7	DG	C5-C6-N1	5.17	114.08	111.50
3	F	3	DT	OP2-P-O3'	5.15	116.53	105.20
2	B	23	DT	C5-C4-O4	-5.11	121.32	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	24	DG	O4'-C1'-C2'	-5.10	101.82	105.90
1	A	578	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	C	5	DG	OP1-P-O3'	5.05	116.32	105.20
2	B	28	DC	C2-N3-C4	5.02	122.41	119.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4672	4744	0	25	0
1	D	4526	4598	0	28	0
2	B	176	100	0	3	0
2	E	177	100	0	1	0
3	C	228	113	0	4	0
3	F	246	135	0	0	0
4	A	15	0	0	0	0
4	D	10	0	0	0	0
5	A	406	0	0	9	0
5	B	29	0	0	0	0
5	C	59	0	0	1	0
5	D	620	0	0	10	1
5	E	26	0	0	0	0
5	F	54	0	0	0	0
All	All	11244	9790	0	58	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:502:GLN:NE2	5:D:1603:HOH:O	2.10	0.84
1:A:845:CYS:SG	5:A:1386:HOH:O	2.36	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:408:ASP:OD1	5:A:1097:HOH:O	1.96	0.81
1:A:466:ARG:NH2	5:A:1403:HOH:O	2.13	0.81
1:D:517:ARG:NH1	5:D:1144:HOH:O	2.20	0.74
1:A:435:ARG:NH1	5:A:1229:HOH:O	2.19	0.74
1:D:607:ASN:OD1	5:D:1378:HOH:O	2.07	0.72
1:A:607[A]:ASN:OD1	5:A:1094:HOH:O	2.07	0.71
1:D:309:GLU:OE2	5:D:1598:HOH:O	2.12	0.67
1:D:873:TYR:O	1:D:876:LYS:HD3	1.96	0.65
2:B:22:DC:H2'	2:B:23:DT:H71	1.78	0.65
1:D:386:GLU:OE1	5:D:1243:HOH:O	2.14	0.65
1:D:664:HIS:HD1	1:D:859:ARG:H	1.45	0.64
3:C:5:DG:H2'	5:C:150:HOH:O	1.96	0.64
1:A:365:THR:O	5:A:1338:HOH:O	2.17	0.58
1:A:665:ILE:HG22	1:A:749:TYR:CE1	2.40	0.56
3:C:5:DG:C2'	3:C:6:DA:OP2	2.51	0.56
1:D:730:LYS:NZ	1:D:734:GLU:OE2	2.38	0.56
1:D:764[B]:THR:CG2	1:D:768:HIS:HA	2.40	0.51
1:A:405:GLN:HG3	1:A:416:MET:HE3	1.93	0.50
1:A:411:ALA:O	1:A:415:LYS:HG2	2.12	0.49
1:D:713:VAL:CG1	1:D:739:TYR:HH	2.25	0.49
1:A:559:ASP:OD1	1:A:563:LYS:NZ	2.45	0.48
1:D:665:ILE:HG22	1:D:749[A]:TYR:CE1	2.48	0.48
1:D:713:VAL:HG12	1:D:739:TYR:HH	1.77	0.48
1:D:764[B]:THR:HG21	5:D:1396:HOH:O	2.14	0.48
1:D:725:LEU:O	1:D:726:ASN:HB2	2.13	0.47
1:D:459:ARG:NH1	5:D:1328:HOH:O	2.38	0.47
1:A:754:VAL:O	1:A:758:LYS:HG3	2.15	0.47
1:A:613:THR:CG2	3:C:5:DG:H4'	2.45	0.46
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.97	0.46
1:D:645:SER:O	1:D:646:ASP:HB2	2.15	0.46
1:A:578:ARG:NH2	2:B:25:DA:H5''	2.31	0.46
1:D:708:VAL:HG12	1:D:712:ILE:CD1	2.46	0.45
1:D:848:VAL:HB	1:D:849:PRO:HD3	1.98	0.45
2:B:21:DC:H2'	2:B:22:DC:C6	2.51	0.45
1:D:563:LYS:NZ	1:D:723:GLN:O	2.50	0.45
1:A:500:LEU:HD21	1:A:591:LEU:HD23	2.00	0.44
1:A:725:LEU:HB2	1:A:727:ILE:HG12	1.99	0.44
1:D:500:LEU:HD11	1:D:591:LEU:HD23	2.00	0.44
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.54	0.43
1:A:467[B]:ARG:HA	5:D:1501:HOH:O	2.19	0.42
1:D:582:LYS:HE2	2:E:26:DC:O2	2.19	0.42
1:A:550:THR:CG2	5:A:1245:HOH:O	2.67	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:764[B]:THR:HA	1:D:769:ARG:O	2.19	0.42
1:A:467[A]:ARG:HA	5:D:1501:HOH:O	2.19	0.42
1:D:764[A]:THR:HA	1:D:769:ARG:O	2.20	0.42
1:D:712:ILE:HA	1:D:716:ILE:HG22	2.00	0.42
1:A:613:THR:HG21	3:C:5:DG:H4'	2.02	0.41
1:D:873:TYR:CE2	1:D:876:LYS:HE2	2.55	0.41
1:D:708:VAL:HG12	1:D:712:ILE:HD11	2.01	0.41
1:D:839[A]:GLU:OE2	5:D:1512:HOH:O	2.21	0.41
1:A:515:GLU:HG2	1:A:519:TYR:CE2	2.56	0.41
1:A:665:ILE:CG2	1:A:749:TYR:CE1	3.04	0.40
1:A:347:ARG:HA	1:A:348:PRO:HD3	2.00	0.40
1:A:383:LYS:NZ	5:A:1266:HOH:O	2.54	0.40
1:A:437:VAL:HA	1:A:438:PRO:HD3	1.95	0.40

All (1) 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	Distance(Å)	Clash(Å)
5:D:1474:HOH:O	5:D:1565:HOH:O[4_545]	2.16	0.04

## 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	583/592 (98%)	571 (98%)	12 (2%)	0	100	100
1	D	567/592 (96%)	557 (98%)	9 (2%)	1 (0%)	56	29
All	All	1150/1184 (97%)	1128 (98%)	21 (2%)	1 (0%)	59	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	628	ILE

### 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	501/507 (99%)	498 (99%)	3 (1%)	92	83
1	D	490/507 (97%)	487 (99%)	3 (1%)	92	83
All	All	991/1014 (98%)	985 (99%)	6 (1%)	92	83

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

Mol	Chain	Res	Type
1	A	477	LEU
1	A	544	LEU
1	A	677	ARG
1	D	477	LEU
1	D	708	VAL
1	D	827	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	GLN
1	A	502	GLN
1	A	573	ASN
1	A	755	GLN
1	A	793	ASN
1	A	797	GLN
1	D	573	ASN
1	D	752	ASN
1	D	755	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	DDG	B	29	3,2	20,22,24	1.47	4 (20%)	27,31,36	6.58	6 (22%)
2	DDG	E	29	3,2	21,23,24	1.59	4 (19%)	28,33,36	6.22	8 (28%)

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	DDG	B	29	3,2	-	0/5/17/19	0/3/3/3
2	DDG	E	29	3,2	-	0/6/18/19	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	DDG	P-OP1	3.86	1.51	1.46
2	B	29	DDG	C2-N2	3.49	1.37	1.32
2	B	29	DDG	C6-N1	3.07	1.41	1.36
2	E	29	DDG	C8-N7	-2.68	1.29	1.34
2	B	29	DDG	C2-N3	-2.62	1.30	1.33
2	E	29	DDG	C4-N9	-2.55	1.34	1.37
2	E	29	DDG	O5'-C5'	-2.41	1.41	1.44
2	B	29	DDG	C8-N7	-2.00	1.30	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	29	DDG	C6-C5-N7	-32.06	129.82	134.14
2	E	29	DDG	C6-C5-N7	-31.60	129.88	134.14
2	B	29	DDG	C6-N1-C2	9.52	125.58	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DDG	N1-C2-N3	3.67	126.74	121.78
2	B	29	DDG	C2-N3-C4	-3.60	110.98	115.30
2	E	29	DDG	C4'-O4'-C1'	3.45	111.49	110.05
2	E	29	DDG	C6-N1-C2	3.40	122.12	120.20
2	E	29	DDG	C2-N3-C4	-3.38	111.24	115.30
2	E	29	DDG	N2-C2-N1	-3.32	114.26	117.82
2	E	29	DDG	O4'-C1'-N9	2.94	112.95	107.66
2	B	29	DDG	C5-C4-N3	2.76	129.24	126.07
2	E	29	DDG	C6-C5-C4	2.11	120.58	117.53
2	B	29	DDG	N1-C2-N3	2.06	124.56	121.78
2	B	29	DDG	O4'-C1'-N9	2.01	111.27	107.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 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	A	901	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	A	902	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	A	903	-	4,4,4	0.07	0	6,6,6	0.12	0
4	SO4	D	901	-	4,4,4	0.27	0	6,6,6	0.32	0
4	SO4	D	902	-	4,4,4	0.12	0	6,6,6	0.16	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
4	SO4	A	901	-	-	0/0/0/0	0/0/0/0
4	SO4	A	902	-	-	0/0/0/0	0/0/0/0
4	SO4	A	903	-	-	0/0/0/0	0/0/0/0
4	SO4	D	901	-	-	0/0/0/0	0/0/0/0
4	SO4	D	902	-	-	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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	579/592 (97%)	0.53	64 (11%) 6 5	17, 36, 59, 77	0
1	D	553/592 (93%)	0.22	10 (1%) 65 67	9, 23, 44, 56	0
2	B	9/9 (100%)	-0.21	0 100 100	22, 29, 52, 65	0
2	E	9/9 (100%)	-0.12	0 100 100	19, 32, 43, 52	0
3	C	11/13 (84%)	-0.36	0 100 100	22, 31, 44, 55	0
3	F	12/13 (92%)	0.06	1 (8%) 11 9	18, 28, 62, 73	0
All	All	1173/1228 (95%)	0.36	75 (6%) 19 17	9, 30, 54, 77	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	ILE	5.2
1	A	298	LYS	5.1
1	D	712	ILE	4.7
1	A	514	VAL	4.5
1	A	816	LYS	4.4
1	A	337	VAL	4.3
1	A	518	ILE	4.3
1	A	692	VAL	4.3
1	A	307	VAL	4.2
1	A	848	VAL	3.8
1	D	514	VAL	3.8
1	A	495	VAL	3.8
1	A	819	ARG	3.7
1	A	697	VAL	3.6
1	A	305	ASP	3.5
1	A	636	ILE	3.4
1	A	353	ALA	3.3
1	A	360	TRP	3.2
1	A	442	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	357	PHE	3.1
1	D	713	VAL	3.1
1	A	864	VAL	3.1
1	D	307	VAL	3.1
1	A	833	ILE	3.1
1	A	691	GLN	3.1
1	A	703	ARG	3.0
1	A	323	VAL	3.0
1	A	866	TYR	3.0
1	A	352	LEU	3.0
1	A	528	ILE	3.0
1	A	537	ILE	2.9
1	A	594	VAL	2.9
1	A	876	LYS	2.9
1	A	320	VAL	2.8
1	A	856	VAL	2.8
1	A	630	LEU	2.7
1	A	681	ILE	2.7
1	D	708	VAL	2.7
1	A	846	ARG	2.7
1	D	509	GLU	2.7
3	F	1	DA	2.7
1	A	511	LEU	2.6
1	A	536	VAL	2.6
1	A	306	ARG	2.6
1	A	507	LEU	2.6
1	A	513	THR	2.5
1	A	475	VAL	2.5
1	A	645	SER	2.5
1	D	681	ILE	2.5
1	A	312	LEU	2.4
1	A	350	THR	2.4
1	A	365	THR	2.4
1	A	571	VAL	2.4
1	D	735[A]	PHE	2.4
1	A	356	GLN	2.3
1	A	649	ILE	2.3
1	A	358	VAL	2.3
1	A	332	ILE	2.3
1	A	875	ALA	2.3
1	A	304	ALA	2.3
1	A	308	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	505	LYS	2.2
1	A	665	ILE	2.2
1	A	505	LYS	2.2
1	A	815	LEU	2.1
1	A	844	LEU	2.1
1	A	574	ILE	2.1
1	A	727	ILE	2.1
1	D	528	ILE	2.1
1	A	699	PRO	2.1
1	A	435	ARG	2.1
1	A	346	LEU	2.0
1	A	448	VAL	2.0
1	A	602	VAL	2.0
1	A	385	ILE	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. 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DDG	E	29	21/22	0.11	0.93	14,20,25,27	0
2	DDG	B	29	20/22	0.10	-0.15	19,23,29,35	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	902	5/5	0.24	1.35	70,73,78,81	0
4	SO4	A	903	5/5	0.24	1.19	53,62,70,75	0
4	SO4	D	901	5/5	0.08	-0.39	37,38,43,46	0
4	SO4	A	902	5/5	0.08	-0.85	41,48,58,65	0
4	SO4	A	901	5/5	0.08	-1.29	36,39,48,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.