Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:54 PM GMT

PDB ID	:	4DS5
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)

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)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
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 (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.
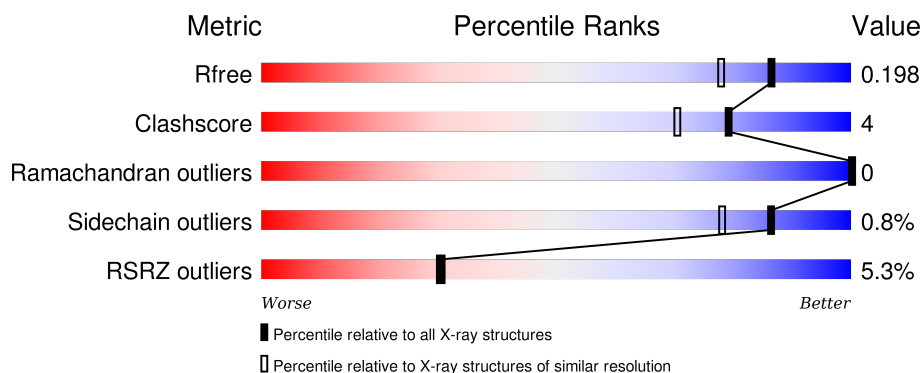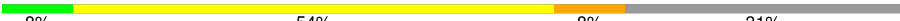

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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 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 <=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	8% 54% 8% 31%

2 Entry composition (i)

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 9391	C 2963	H 4731	N 810	O 870	S 17	0	2	0
1	D	561	Total 9228	C 2914	H 4655	N 791	O 853	S 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	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 274	C 85	H 100	N 29	O 52	P 8	0	0	0
2	E	9	Total 274	C 85	H 100	N 29	O 52	P 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
3	C	11	Total 356	C 109	H 123	N 47	O 66	P 11	0	0	0
3	F	9	Total 291	C 89	H 100	N 40	O 53	P 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 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

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

3 Residue-property plots (i)

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
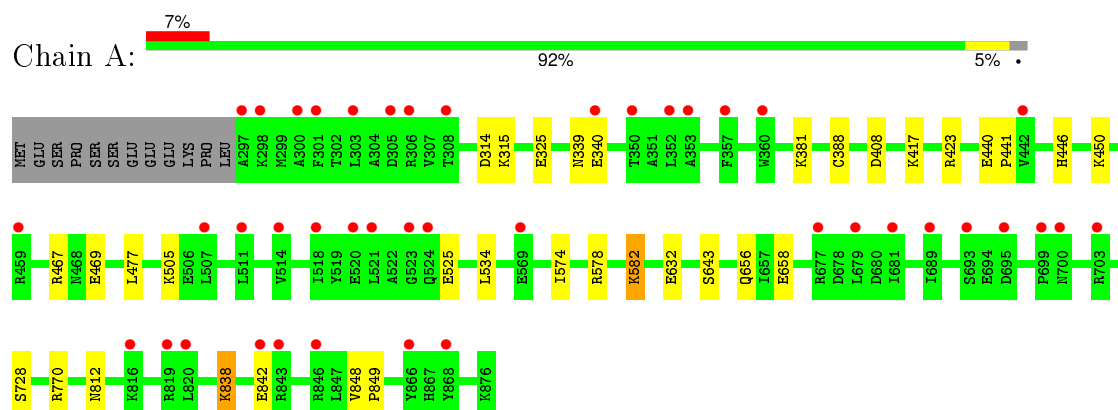
- Molecule 1: DNA polymerase
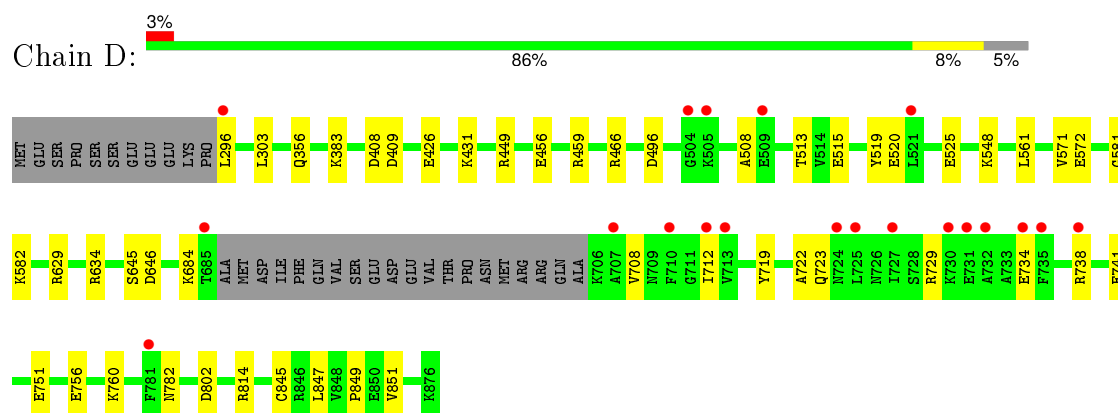
- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*C)-3')
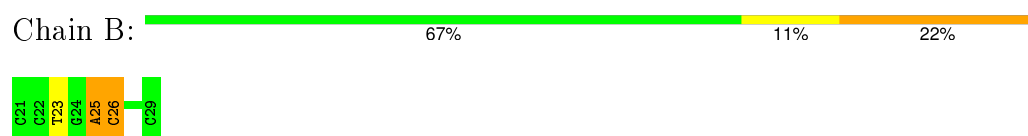
- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*C)-3')

C21 C22 T23 G24 A25 C26 T27 C28 C29

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

Chain C:

| 46% | 38% | 15% |

DC DA T2 G5 A6 G7 T8 C9 A10 G11 G12

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

Chain F:

| 8% | 54% | 8% | 31% |

DC DA DT DG G4 G5 A6 G7 T8 C9 A10 G11 G12
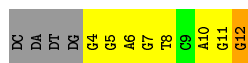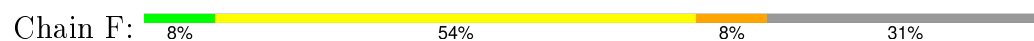
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.55 (at 1.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.176 , 0.199 0.175 , 0.198	Depositor DCC
R_{free} test set	6643 reflections (4.36%)	DCC
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 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 152369 reflections	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.44	0/4750	0.57	0/6418
1	D	0.63	0/4737	0.71	5/6401 (0.1%)
2	B	1.05	0/193	2.05	11/294 (3.7%)
2	E	1.16	1/193 (0.5%)	1.91	3/294 (1.0%)
3	C	1.02	0/262	1.69	6/404 (1.5%)
3	F	1.44	1/215 (0.5%)	2.02	12/331 (3.6%)
All	All	0.62	2/10350 (0.0%)	0.85	37/14142 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	DA	C3'-O3'	-6.33	1.35	1.44
3	F	5	DG	C8-N7	5.47	1.34	1.30

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	23	DT	O4'-C1'-N1	-11.05	100.26	108.00
2	B	25	DA	O4'-C4'-C3'	-9.98	100.01	106.00
2	B	25	DA	O5'-P-OP2	-8.63	97.94	105.70
3	C	8	DT	O4'-C1'-N1	-8.42	102.11	108.00
2	B	25	DA	O5'-P-OP1	7.77	120.02	110.70
2	B	23	DT	O4'-C1'-N1	-7.49	102.76	108.00
3	F	4	DG	O5'-P-OP2	-7.42	99.02	105.70
2	B	26	DC	C6-N1-C2	6.71	122.98	120.30
3	F	8	DT	O4'-C1'-N1	-6.59	103.39	108.00
3	F	6	DA	OP1-P-OP2	-6.56	109.76	119.60
1	D	802	ASP	CB-CG-OD2	6.50	124.15	118.30
2	B	26	DC	C2-N3-C4	-6.45	116.67	119.90
3	C	11	DG	O4'-C1'-N9	-6.38	103.53	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	12	DG	O4'-C1'-N9	6.37	112.46	108.00
3	F	10	DA	O4'-C1'-N9	-6.29	103.60	108.00
2	B	26	DC	O4'-C1'-N1	6.22	112.35	108.00
2	B	26	DC	N3-C4-C5	6.12	124.35	121.90
3	F	4	DG	O4'-C4'-C3'	-6.05	102.08	104.50
2	B	26	DC	C5-C6-N1	-5.85	118.07	121.00
3	F	6	DA	C5-C6-N6	-5.83	119.04	123.70
2	E	23	DT	N3-C4-O4	5.73	123.34	119.90
2	B	26	DC	O4'-C1'-C2'	5.73	110.48	105.90
3	F	7	DG	O4'-C4'-C3'	5.68	109.41	106.00
3	F	5	DG	C2-N3-C4	-5.67	109.07	111.90
1	D	496	ASP	CB-CG-OD1	5.61	123.35	118.30
3	F	6	DA	N1-C6-N6	5.56	121.94	118.60
2	E	23	DT	C5-C4-O4	-5.46	121.08	124.90
3	F	5	DG	N3-C4-N9	-5.45	122.73	126.00
3	C	6	DA	C2-N3-C4	-5.31	107.94	110.60
1	D	634	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	C	5	DG	N3-C4-N9	-5.23	122.86	126.00
2	B	25	DA	C5'-C4'-C3'	5.22	123.49	114.10
1	D	409	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	634	ARG	NE-CZ-NH2	-5.17	117.72	120.30
3	C	9	DC	O4'-C1'-C2'	5.12	110.00	105.90
3	C	8	DT	OP2-P-O3'	5.01	116.23	105.20
3	F	11	DG	O4'-C1'-N9	-5.01	104.50	108.00

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
2	E	174	100	101	3	0
3	C	233	123	124	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	191	100	101	1	0
4	D	15	0	0	0	0
5	A	356	0	0	20	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: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:A:469:GLU:CD	1:D:466:ARG:HE	2.04	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
1:D:708:VAL:HG13	1:D:712:ILE:HD12	1.85	0.58
1:D:466:ARG:NH1	5:D:1302:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:469:GLU:CD	5:A:1246:HOH:O	2.45	0.54
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:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.26	0.51
1:D:508:ALA:O	5:D:1470:HOH:O	2.19	0.51
1:D:684:LYS:NZ	5:D:1563:HOH:O	2.38	0.51
1:A:770:ARG:NH2	5:A:1104:HOH:O	2.44	0.50
1:A:578:ARG:NH1	2:B:25:DA:H5"	2.27	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:520:GLU:CD	5:D:1458:HOH:O	2.50	0.48
1:D:708:VAL:HG13	1:D:712:ILE:HG13	1.96	0.48
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:814:ARG:CZ	1:D:847[A]:LEU:HD13	2.45	0.46
1:D:722:ALA:HB2	1:D:729:ARG:HA	1.98	0.46
1:D:814:ARG:HG3	1:D:851[B]:VAL:HG11	1.97	0.46
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.98	0.46
1:D:548:LYS:HE3	5:D:1487:HOH:O	2.17	0.45
1:D:645:SER:O	1:D:646:ASP:HB2	2.17	0.45
1:D:383:LYS:HE3	5:D:1423:HOH:O	2.17	0.45
1:D:296:LEU:HD13	1:D:449:ARG:HD3	1.99	0.45
1:A:446:HIS:CE1	1:A:450:LYS:HD2	2.51	0.45
1:D:756:GLU:OE2	1:D:760:LYS:HE2	2.17	0.44
1:D:814:ARG:CZ	1:D:847[A]:LEU:CD1	2.95	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: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:315:LYS:NZ	5:A:1171:HOH:O	2.42	0.42
1:A:525:GLU:O	5:A:1222:HOH:O	2.21	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:842:GLU:CD	5:A:1243:HOH:O	2.57	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%)	82　71
1	D	497/507 (98%)	494 (99%)	3 (1%)	90　84
All	All	994/1014 (98%)	986 (99%)	8 (1%)	86　78

All (8) 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	303	LEU
1	D	513	THR
1	D	782	ASN

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

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)

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

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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	0.33	0	6,6,6	0.60	0
4	SO4	D	902	-	4,4,4	0.15	0	6,6,6	0.15	0
4	SO4	D	903	-	4,4,4	0.23	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	D	901	-	-	0/0/0/0	0/0/0/0
4	SO4	D	902	-	-	0/0/0/0	0/0/0/0
4	SO4	D	903	-	-	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.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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($\mathring{A}^2$)	Q<0.9
1	A	580/592 (97%)	0.33	42 (7%)	18	18	21, 41, 68, 94	0
1	D	561/592 (94%)	0.26	20 (3%)	46	49	10, 25, 48, 65	0
2	B	9/9 (100%)	-0.39	0	100	100	26, 30, 45, 60	0
2	E	9/9 (100%)	-0.32	0	100	100	20, 28, 43, 56	0
3	C	11/13 (84%)	-0.36	0	100	100	20, 28, 49, 65	0
3	F	9/13 (69%)	-0.34	0	100	100	16, 20, 34, 42	0
All	All	1179/1228 (96%)	0.27	62 (5%)	30	30	10, 33, 60, 94	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	712	ILE	10.2
1	A	297	ALA	6.1
1	A	353	ALA	5.5
1	D	731	GLU	5.0
1	A	298	LYS	4.8
1	A	521	LEU	4.6
1	A	819	ARG	4.5
1	D	735	PHE	4.5
1	A	303	LEU	4.3
1	A	699	PRO	4.0
1	D	710	PHE	4.0
1	A	357	PHE	3.9
1	D	734	GLU	3.9
1	A	816	LYS	3.6
1	A	352	LEU	3.6
1	D	505	LYS	3.5
1	D	725	LEU	3.5
1	A	677	ARG	3.4
1	D	713	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	509	GLU	3.3
1	A	679	LEU	3.3
1	A	703	ARG	3.2
1	D	296	LEU	3.2
1	A	305	ASP	3.1
1	D	730	LYS	3.0
1	A	842	GLU	3.0
1	A	306	ARG	2.9
1	A	866	TYR	2.9
1	A	523	GLY	2.9
1	D	724	ASN	2.9
1	D	732	ALA	2.8
1	A	846	ARG	2.8
1	D	685	THR	2.7
1	D	504	GLY	2.7
1	A	695	ASP	2.7
1	A	340	GLU	2.6
1	A	689	ILE	2.6
1	A	442	VAL	2.5
1	A	524	GLN	2.5
1	A	518	ILE	2.5
1	A	520	GLU	2.4
1	A	569	GLU	2.3
1	A	300	ALA	2.3
1	A	360	TRP	2.3
1	A	843	ARG	2.3
1	A	511	LEU	2.3
1	D	727	ILE	2.3
1	A	693	SER	2.3
1	D	781	PHE	2.3
1	A	700	ASN	2.2
1	D	707	ALA	2.2
1	D	738	ARG	2.2
1	A	301	PHE	2.2
1	A	514	VAL	2.1
1	A	820	LEU	2.1
1	D	521	LEU	2.1
1	A	868	TYR	2.1
1	A	507	LEU	2.1
1	A	308	THR	2.0
1	A	350	THR	2.0
1	A	459	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	681	ILE	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 carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	D	901	5/5	0.98	0.10	-0.03	37,38,47,49	0
4	SO4	D	902	5/5	0.93	0.10	-0.22	39,44,51,51	0
4	SO4	D	903	5/5	0.93	0.12	-	65,73,77,80	0

6.5 Other polymers (i)

There are no such residues in this entry.