



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:16 PM UTC

PDB ID : 6DSU / pdb_00006dsu
Title : Bst DNA polymerase I pre-insertion complex structure
Authors : Chim, N.; Jackson, L.N.; Chaput, J.C.
Deposited on : 2018-06-14
Resolution : 1.98 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

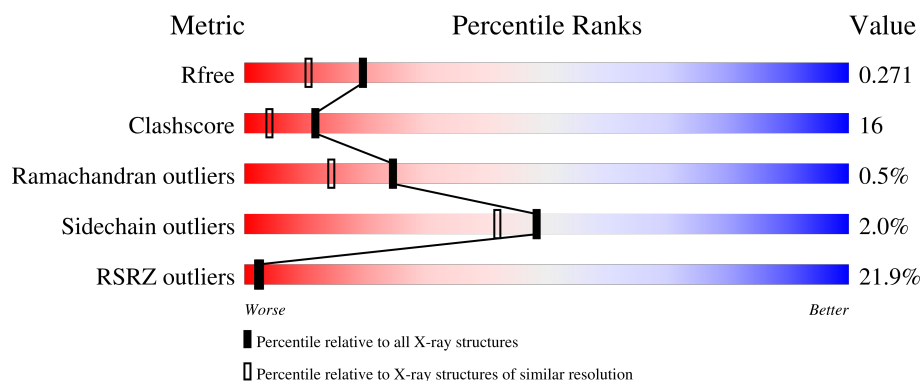
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	P	10	50% 40% 60%
2	T	11	64% 36% 64%
3	A	580	21% 74% 24% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DZ4	A	905	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5496 atoms, of which 13 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 DNA chain called DNA (5'-D(*GP*CP*GP*AP*TP*CP*AP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			

- Molecule 3 is a protein called DNA polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	577	Total	C	N	O	S	0	4	0
			4666	2966	811	873	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	550	THR	SER	conflict	UNP E1C9K5

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

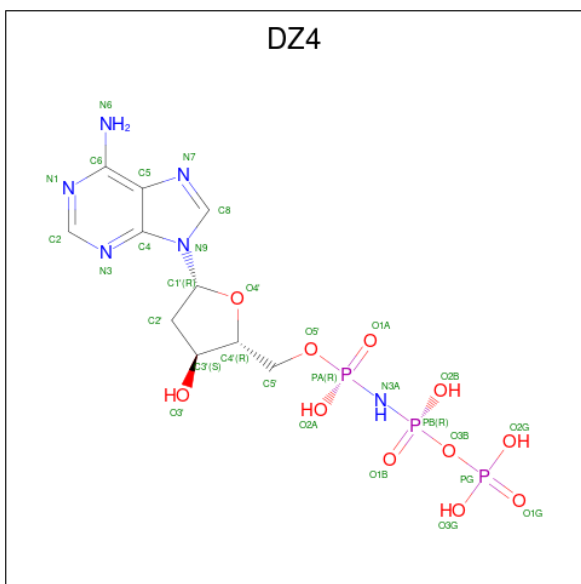
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (CCD ID: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			43	10	13	6	11	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	4	Total	O	0	0
			4	4		
7	T	12	Total	O	0	0
			12	12		
7	A	327	Total	O	0	0
			327	327		

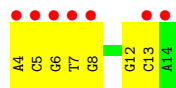
3 Residue-property plots [i](#)

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.

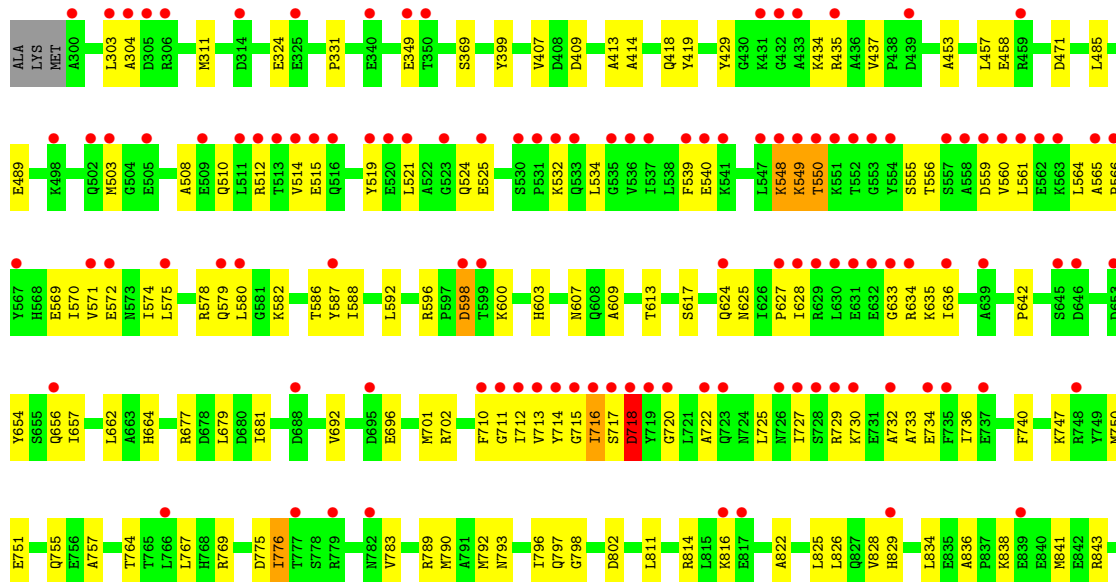
- Molecule 1: DNA (5'-D(*GP*CP*GP*AP*TP*CP*AP*CP*GP*T)-3')

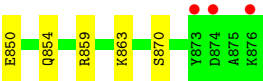


- Molecule 2: DNA (5'-D(P*AP*CP*GP*TP*GP*AP*TP*CP*GP*CP*A)-3')



- Molecule 3: DNA polymerase I





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.44Å 93.39Å 104.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.69 – 1.98 46.69 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.69-1.98) 96.5 (46.69-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.222 , 0.272 0.225 , 0.271	Depositor DCC
R_{free} test set	2007 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: MG, SO4, DZ4

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	P	0.20	0/226	0.40	0/347
2	T	0.23	0/253	0.42	0/388
3	A	0.17	0/4750	0.37	0/6420
All	All	0.18	0/5229	0.37	0/7155

There are no bond length outliers.

There are no bond angle outliers.

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	P	202	0	114	25	0
2	T	226	0	124	13	0
3	A	4666	0	4717	137	0
4	A	1	0	0	0	0
5	A	15	0	0	1	0
6	A	30	13	13	10	0
7	A	327	0	0	11	0
7	P	4	0	0	0	0
7	T	12	0	0	0	0
All	All	5483	13	4968	158	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 16.

All (158) 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)
3:A:508:ALA:O	3:A:512:ARG:HD2	1.51	1.11
3:A:712:ILE:HD13	3:A:716[B]:ILE:HG21	1.48	0.93
3:A:656:GLN:NE2	6:A:905:DZ4:O2B	2.01	0.93
1:P:1:DG:H1	2:T:13:DC:H42	0.97	0.91
3:A:712:ILE:HA	3:A:716[B]:ILE:CG2	2.01	0.89
3:A:715[A]:GLY:O	3:A:789:ARG:NE	2.06	0.88
3:A:628:ILE:HD12	3:A:634:ARG:HG3	1.55	0.87
1:P:6:DC:H42	2:T:8:DG:H1	1.23	0.86
1:P:10:DT:C3'	6:A:905:DZ4:N3	2.41	0.83
3:A:712:ILE:HA	3:A:716[B]:ILE:HG21	1.60	0.83
3:A:534:LEU:HD11	3:A:574:ILE:HD13	1.62	0.82
3:A:692:VAL:HG21	3:A:701:MET:HE1	1.62	0.81
1:P:10:DT:H3'	6:A:905:DZ4:N3	1.96	0.80
3:A:789:ARG:HA	3:A:792:MET:HE3	1.64	0.80
3:A:716[A]:ILE:HG23	3:A:720:GLY:HA3	1.71	0.73
1:P:10:DT:O3'	3:A:829:HIS:HB3	1.87	0.73
3:A:556:THR:O	3:A:578:ARG:NH1	2.20	0.72
3:A:715[A]:GLY:HA2	3:A:789:ARG:HB3	1.70	0.71
3:A:712:ILE:HA	3:A:716[B]:ILE:HG22	1.73	0.70
3:A:587:TYR:HB3	3:A:636:ILE:HD13	1.71	0.70
1:P:9:DG:H2''	3:A:829:HIS:CE1	2.27	0.69
3:A:730:LYS:O	3:A:734:GLU:HG3	1.95	0.67
3:A:716[B]:ILE:HG13	3:A:736:ILE:HD12	1.75	0.67
1:P:10:DT:H4'	3:A:829:HIS:CG	2.30	0.66
3:A:715[B]:GLY:O	3:A:716[B]:ILE:HG23	1.95	0.66
3:A:534:LEU:HD11	3:A:574:ILE:CD1	2.25	0.65
3:A:549:LYS:N	3:A:549:LYS:HD3	2.12	0.65
3:A:503:MET:HE1	3:A:635:LYS:O	1.97	0.65
1:P:6:DC:N3	2:T:8:DG:N2	2.40	0.64
2:T:4:DA:H2''	2:T:5:DC:H5'	1.80	0.64
3:A:715[B]:GLY:C	3:A:716[B]:ILE:HG23	2.25	0.62
3:A:711:GLY:O	3:A:716[B]:ILE:HG22	1.99	0.62
3:A:600:LYS:NZ	7:A:1002:HOH:O	2.29	0.61
3:A:515:GLU:HG2	3:A:519:TYR:CE2	2.35	0.61
3:A:624:GLN:HA	3:A:828:VAL:HG13	1.82	0.61
2:T:6:DG:H2''	2:T:7:DT:H5'	1.83	0.60
3:A:627:PRO:HB2	3:A:633:GLY:C	2.27	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:775:ASP:HB3	3:A:783:VAL:HG12	1.83	0.60
3:A:508:ALA:O	3:A:512:ARG:CD	2.37	0.60
3:A:755:GLN:HG2	7:A:1036:HOH:O	2.01	0.60
3:A:561:LEU:HB2	3:A:575:LEU:HD21	1.83	0.60
3:A:607:ASN:HB3	3:A:617:SER:OG	2.02	0.59
2:T:5:DC:H2'	2:T:6:DG:O4'	2.03	0.59
3:A:627:PRO:HB2	3:A:633:GLY:O	2.03	0.59
3:A:656:GLN:HE22	3:A:681:ILE:HG22	1.66	0.59
1:P:10:DT:H6	1:P:10:DT:O5'	1.86	0.57
1:P:9:DG:H2'	1:P:10:DT:C6	2.40	0.57
1:P:8:DC:H2'	1:P:9:DG:C8	2.40	0.57
1:P:10:DT:H3'	6:A:905:DZ4:C4	2.35	0.57
3:A:662:LEU:HD13	3:A:796:ILE:HD11	1.87	0.57
3:A:811:LEU:HD21	3:A:834:LEU:HD21	1.86	0.57
3:A:740:PHE:HB3	3:A:747:LYS:HD2	1.87	0.56
3:A:429:TYR:O	3:A:435:ARG:HA	2.06	0.56
3:A:717[B]:SER:OG	3:A:789:ARG:HD3	2.06	0.55
3:A:587:TYR:CB	3:A:636:ILE:HD13	2.37	0.55
3:A:789:ARG:HA	3:A:792:MET:CE	2.33	0.55
3:A:715[B]:GLY:C	3:A:716[B]:ILE:CG2	2.80	0.55
3:A:838:LYS:HD2	7:A:1320:HOH:O	2.07	0.55
3:A:539:PHE:CE1	3:A:564:LEU:HD11	2.42	0.54
3:A:656:GLN:HE22	3:A:681:ILE:CG2	2.20	0.54
3:A:825:LEU:O	3:A:826:LEU:HD23	2.08	0.54
3:A:579:GLN:HG3	3:A:580:LEU:N	2.23	0.54
3:A:521:LEU:HD12	3:A:570:ILE:HA	1.90	0.53
3:A:627:PRO:O	3:A:634:ARG:HA	2.09	0.53
3:A:407:VAL:HG11	3:A:413:ALA:HB2	1.91	0.53
3:A:539:PHE:HE1	3:A:564:LEU:HD11	1.75	0.52
3:A:569:GLU:HG3	3:A:572:GLU:OE2	2.09	0.52
3:A:863:LYS:HE3	7:A:1093:HOH:O	2.08	0.52
3:A:822:ALA:CB	3:A:836:ALA:HB2	2.40	0.52
1:P:6:DC:N4	2:T:8:DG:H1	2.00	0.52
3:A:642:PRO:HD3	3:A:870:SER:O	2.10	0.52
3:A:790:MET:HE2	3:A:790:MET:HA	1.92	0.52
3:A:524:GLN:HG2	3:A:525:GLU:N	2.24	0.51
3:A:740:PHE:CD1	3:A:747:LYS:HB2	2.45	0.51
3:A:579:GLN:HG3	3:A:580:LEU:H	1.75	0.51
3:A:692:VAL:HB	3:A:696:GLU:HB2	1.91	0.51
3:A:399:TYR:HB2	3:A:609:ALA:HB1	1.93	0.51
3:A:550:THR:HG23	3:A:555:SER:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:750:MET:SD	3:A:792:MET:HB3	2.51	0.51
3:A:828:VAL:HG12	3:A:829:HIS:ND1	2.26	0.51
3:A:512:ARG:HG3	7:A:1003:HOH:O	2.10	0.50
3:A:732:ALA:O	3:A:736:ILE:HG12	2.11	0.50
3:A:757:ALA:CB	3:A:776:ILE:HD13	2.42	0.50
3:A:548:LYS:HG3	3:A:549:LYS:N	2.27	0.50
3:A:414:ALA:CB	3:A:457:LEU:HD11	2.42	0.50
3:A:434:LYS:HD2	3:A:434:LYS:N	2.27	0.49
3:A:414:ALA:HB1	3:A:419:TYR:HB3	1.94	0.49
3:A:712:ILE:CA	3:A:716[B]:ILE:HG22	2.43	0.48
3:A:716[B]:ILE:O	3:A:716[B]:ILE:HG12	2.12	0.48
1:P:10:DT:O3'	6:A:905:DZ4:N3	2.46	0.48
3:A:654:TYR:HB3	3:A:657:ILE:HB	1.95	0.48
1:P:10:DT:C4'	3:A:829:HIS:CG	2.97	0.48
3:A:822:ALA:HB2	3:A:836:ALA:HB2	1.95	0.48
3:A:565:ALA:N	3:A:566:PRO:CD	2.77	0.48
3:A:414:ALA:HB2	3:A:457:LEU:HD11	1.96	0.47
3:A:613:THR:O	3:A:798:GLY:HA2	2.14	0.47
3:A:596:ARG:HG3	3:A:603:HIS:HD2	1.80	0.47
3:A:725:LEU:O	3:A:727:ILE:HG23	2.15	0.47
2:T:4:DA:H5''	3:A:715[A]:GLY:C	2.40	0.47
3:A:304:ALA:CB	3:A:311:MET:HE1	2.45	0.47
3:A:349:GLU:HG3	7:A:1239:HOH:O	2.15	0.46
1:P:9:DG:H5''	3:A:628:ILE:HG22	1.97	0.46
3:A:764:THR:HA	3:A:769:ARG:O	2.16	0.46
3:A:304:ALA:HB1	3:A:311:MET:HE1	1.97	0.46
3:A:485:LEU:O	3:A:489:GLU:HG3	2.16	0.46
3:A:598:ASP:OD2	3:A:598:ASP:N	2.44	0.46
3:A:716[B]:ILE:O	3:A:716[B]:ILE:CG1	2.64	0.46
1:P:10:DT:H4'	3:A:829:HIS:CB	2.46	0.46
3:A:471:ASP:OD1	3:A:471:ASP:N	2.46	0.46
1:P:10:DT:C2'	6:A:905:DZ4:N3	2.78	0.46
3:A:747:LYS:O	3:A:751:GLU:HG3	2.15	0.45
3:A:588:ILE:O	3:A:592:LEU:HG	2.16	0.45
3:A:582:LYS:O	3:A:586:THR:HB	2.16	0.45
3:A:418:GLN:HA	7:A:1124:HOH:O	2.15	0.45
3:A:790:MET:HE2	3:A:790:MET:CA	2.47	0.45
3:A:843:ARG:HD2	7:A:1240:HOH:O	2.17	0.45
3:A:718:ASP:OD2	3:A:733:ALA:HB2	2.16	0.45
1:P:2:DC:N3	2:T:12:DG:N2	2.52	0.45
3:A:713:VAL:HG21	6:A:905:DZ4:N6	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:656:GLN:NE2	3:A:681:ILE:CG2	2.80	0.44
3:A:767:LEU:HD12	3:A:802:ASP:HB3	1.99	0.44
3:A:510:GLN:O	3:A:514:VAL:HG23	2.18	0.44
1:P:9:DG:O4'	3:A:625:ASN:HA	2.17	0.44
3:A:814:ARG:HG2	7:A:1115:HOH:O	2.17	0.44
3:A:677:ARG:HB2	3:A:679:LEU:HG	1.99	0.43
3:A:664:HIS:ND1	3:A:859:ARG:HG3	2.33	0.43
3:A:757:ALA:HB1	3:A:776:ILE:HD13	2.00	0.43
3:A:789:ARG:C	3:A:790:MET:HE2	2.44	0.43
1:P:2:DC:H42	2:T:12:DG:H1	1.67	0.43
3:A:453:ALA:O	3:A:457:LEU:HG	2.19	0.43
3:A:836:ALA:HB3	3:A:841:MET:CE	2.49	0.43
3:A:717[B]:SER:O	3:A:718:ASP:CB	2.66	0.43
3:A:437:VAL:HG23	7:A:1077:HOH:O	2.19	0.43
3:A:369:SER:OG	3:A:458:GLU:OE2	2.35	0.43
3:A:548:LYS:HB3	3:A:560:VAL:HG22	2.01	0.43
1:P:9:DG:N2	2:T:5:DC:C2	2.86	0.42
3:A:729:ARG:HG3	5:A:904:SO4:O1	2.19	0.42
3:A:816:LYS:HB3	3:A:816:LYS:HE2	1.68	0.42
3:A:550:THR:HG23	3:A:555:SER:CA	2.49	0.42
3:A:722:ALA:HB1	3:A:727:ILE:O	2.20	0.42
3:A:790:MET:HE2	3:A:790:MET:N	2.34	0.42
3:A:850:GLU:O	3:A:854:GLN:HG2	2.19	0.42
3:A:324:GLU:HG3	3:A:331:PRO:HD2	2.02	0.42
3:A:797:GLN:HE22	6:A:905:DZ4:HN6	1.66	0.42
3:A:710:PHE:CZ	3:A:714[A]:TYR:HE1	2.38	0.42
2:T:4:DA:H5'	3:A:715[A]:GLY:O	2.19	0.41
3:A:548:LYS:HB2	3:A:548:LYS:HE3	1.62	0.41
1:P:10:DT:H2'	6:A:905:DZ4:C2	2.49	0.41
3:A:624:GLN:O	3:A:829:HIS:NE2	2.51	0.41
1:P:10:DT:H6	1:P:10:DT:C5'	2.34	0.41
3:A:692:VAL:CG2	3:A:701:MET:HE1	2.42	0.41
1:P:10:DT:H4'	3:A:829:HIS:HB3	2.03	0.41
3:A:409:ASP:HB2	7:A:1066:HOH:O	2.19	0.41
3:A:702:ARG:HH22	6:A:905:DZ4:PG	2.44	0.41
3:A:565:ALA:HA	3:A:571:VAL:HB	2.03	0.40
2:T:5:DC:H5'	2:T:5:DC:C6	2.57	0.40
3:A:414:ALA:HA	3:A:457:LEU:HD11	2.03	0.40
3:A:814:ARG:HD2	3:A:814:ARG:HA	1.94	0.40

There are no symmetry-related clashes.

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	
3	A	579/580 (100%)	551 (95%)	24 (4%)	4 (1%)	18	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	718	ASP
3	A	550	THR
3	A	716[A]	ILE
3	A	716[B]	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	
3	A	497/496 (100%)	487 (98%)	10 (2%)	48	42

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	303	LEU
3	A	532	LYS
3	A	540	GLU
3	A	548	LYS
3	A	549	LYS
3	A	559	ASP
3	A	598	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	718	ASP
3	A	776	ILE
3	A	793	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	656	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
5	SO4	A	903	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	A	904	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	A	902	-	4,4,4	0.23	0	6,6,6	0.07	0
6	DZ4	A	905	4	31,32,32	3.55	16 (51%)	44,50,50	2.90	18 (40%)

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
6	DZ4	A	905	4	-	3/19/34/34	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	905	DZ4	PB-O3B	11.52	1.73	1.59
6	A	905	DZ4	C2'-C3'	-7.08	1.34	1.52
6	A	905	DZ4	PA-O1A	5.69	1.54	1.46
6	A	905	DZ4	O4'-C4'	5.64	1.57	1.45
6	A	905	DZ4	C5'-C4'	-3.95	1.39	1.51
6	A	905	DZ4	C5-C4	-3.89	1.32	1.39
6	A	905	DZ4	C2'-C1'	3.74	1.62	1.52
6	A	905	DZ4	O4'-C1'	-3.72	1.34	1.42
6	A	905	DZ4	PB-O2B	-3.33	1.48	1.56
6	A	905	DZ4	PB-N3A	3.30	1.72	1.63
6	A	905	DZ4	PA-N3A	3.27	1.71	1.63
6	A	905	DZ4	PA-O5'	2.99	1.68	1.57
6	A	905	DZ4	PB-O1B	2.84	1.50	1.46
6	A	905	DZ4	PA-O2A	-2.49	1.50	1.56
6	A	905	DZ4	C6-N6	2.21	1.39	1.34
6	A	905	DZ4	C2-N3	2.18	1.37	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	905	DZ4	C1'-N9-C8	-8.70	96.50	126.95
6	A	905	DZ4	C4-N9-C1'	7.81	157.83	126.50
6	A	905	DZ4	O4'-C1'-N9	7.06	120.65	107.96
6	A	905	DZ4	N3-C2-N1	-5.92	119.62	128.58
6	A	905	DZ4	C5-C4-N3	-5.15	119.63	126.72
6	A	905	DZ4	C2-N3-C4	3.57	120.55	111.83
6	A	905	DZ4	C5-C4-N9	3.51	109.64	105.81
6	A	905	DZ4	N9-C8-N7	-3.39	109.13	113.94
6	A	905	DZ4	C5-N7-C8	2.90	108.01	103.45
6	A	905	DZ4	O2B-PB-O3B	2.70	113.65	104.64
6	A	905	DZ4	O1A-PA-N3A	-2.66	107.85	111.77
6	A	905	DZ4	C4-C5-N7	-2.60	107.61	110.58
6	A	905	DZ4	C4'-O4'-C1'	-2.59	103.36	109.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	905	DZ4	C2'-C1'-N9	-2.48	108.79	114.63
6	A	905	DZ4	C3'-C2'-C1'	2.42	108.52	102.60
6	A	905	DZ4	O2G-PG-O3B	2.42	112.74	104.64
6	A	905	DZ4	O5'-PA-O1A	-2.33	107.36	114.27
6	A	905	DZ4	N3-C4-N9	2.09	130.73	127.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

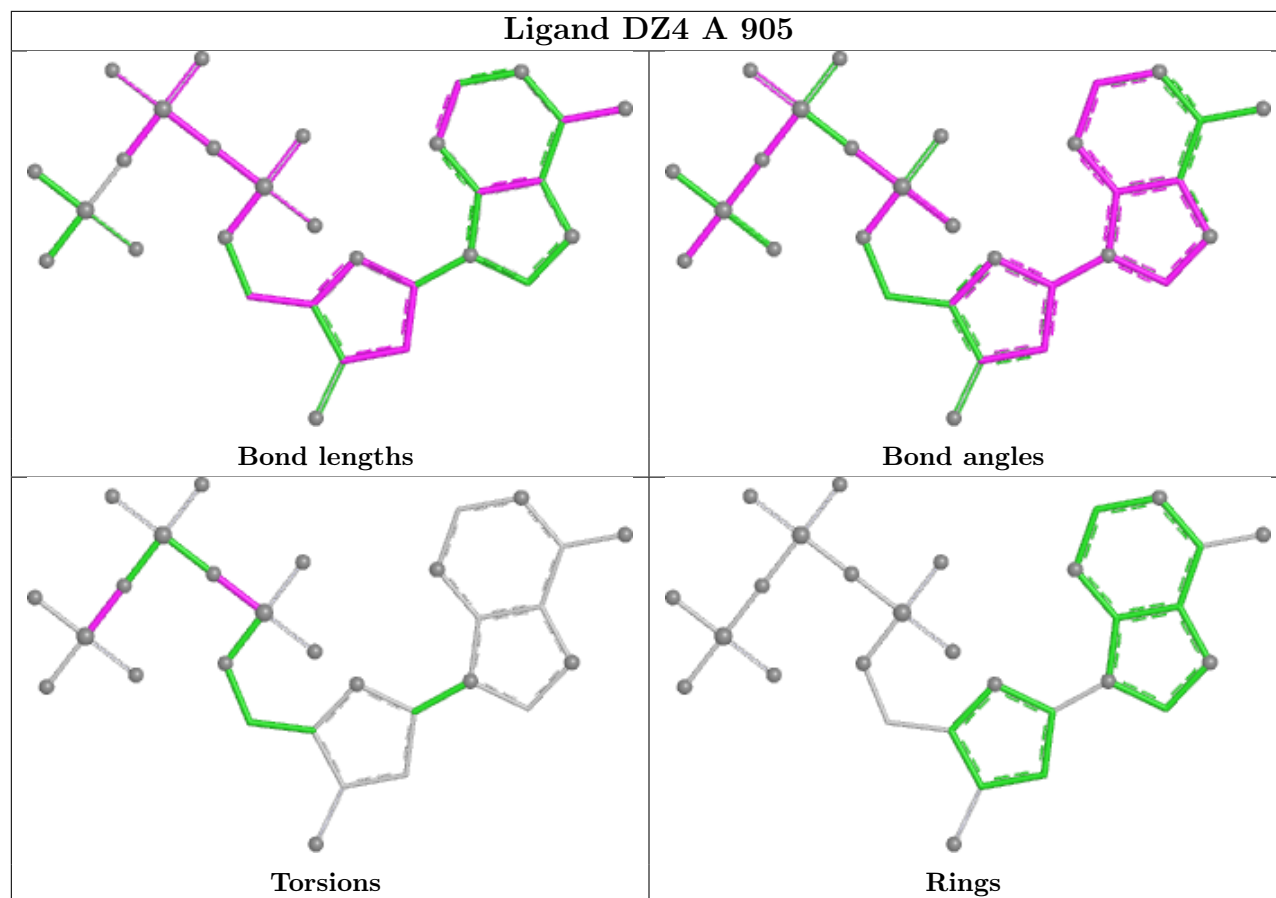
Mol	Chain	Res	Type	Atoms
6	A	905	DZ4	PB-O3B-PG-O2G
6	A	905	DZ4	PB-N3A-PA-O1A
6	A	905	DZ4	PB-O3B-PG-O1G

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	904	SO4	1	0
6	A	905	DZ4	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	P	10/10 (100%)	2.43	5 (50%)  	54, 69, 93, 98	0
2	T	11/11 (100%)	2.66	7 (63%)  	55, 64, 117, 125	0
3	A	577/580 (99%)	1.14	119 (20%)  	15, 33, 70, 103	4 (0%)
All	All	598/601 (99%)	1.19	131 (21%)  	15, 34, 74, 125	4 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	715[A]	GLY	11.1
3	A	550	THR	10.3
3	A	716[A]	ILE	7.8
3	A	512	ARG	7.4
3	A	717[A]	SER	6.8
3	A	628	ILE	6.5
3	A	433	ALA	6.4
3	A	539	PHE	5.6
1	P	1	DG	5.6
3	A	505	GLU	5.1
3	A	547	LEU	4.8
3	A	552	THR	4.8
3	A	300	ALA	4.8
3	A	558	ALA	4.8
3	A	559	ASP	4.6
3	A	719	TYR	4.5
2	T	5	DC	4.3
3	A	553	GLY	4.3
3	A	349	GLU	4.0
3	A	656	GLN	3.9
3	A	730	LYS	3.9
3	A	710	PHE	3.8
3	A	340	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	525	GLU	3.7
3	A	779	ARG	3.7
3	A	305	ASP	3.7
3	A	503	MET	3.7
2	T	14	DA	3.7
2	T	6	DG	3.7
2	T	4	DA	3.6
3	A	714[A]	TYR	3.6
1	P	10	DT	3.5
3	A	523	GLY	3.5
3	A	624	GLN	3.4
3	A	829	HIS	3.4
3	A	718	ASP	3.4
3	A	598	ASP	3.4
3	A	565	ALA	3.4
3	A	630	LEU	3.4
3	A	531	PRO	3.4
3	A	720	GLY	3.3
3	A	536	VAL	3.3
3	A	653	ASP	3.3
3	A	557	SER	3.3
3	A	325	GLU	3.3
3	A	876	LYS	3.3
3	A	303	LEU	3.3
3	A	439	ASP	3.3
3	A	587	TYR	3.2
3	A	511	LEU	3.2
3	A	532	LYS	3.2
3	A	520	GLU	3.2
1	P	9	DG	3.2
3	A	566	PRO	3.1
3	A	432	GLY	3.1
3	A	712	ILE	3.0
3	A	554	TYR	3.0
3	A	575	LEU	3.0
3	A	431	LYS	3.0
3	A	782	ASN	3.0
3	A	599	THR	3.0
2	T	8	DG	2.9
3	A	551	LYS	2.9
3	A	695	ASP	2.9
3	A	839	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	514	VAL	2.9
3	A	636	ILE	2.9
3	A	350	THR	2.8
3	A	713	VAL	2.8
3	A	688	ASP	2.8
2	T	13	DC	2.8
3	A	521	LEU	2.8
3	A	735	PHE	2.8
3	A	513	THR	2.8
3	A	627	PRO	2.8
3	A	728	SER	2.7
3	A	629	ARG	2.7
3	A	722	ALA	2.7
3	A	729	ARG	2.7
3	A	515	GLU	2.7
3	A	631	GLU	2.7
3	A	874	ASP	2.7
3	A	530	SER	2.7
3	A	560	VAL	2.6
3	A	459	ARG	2.6
3	A	632	GLU	2.6
3	A	737	GLU	2.6
1	P	3	DG	2.6
3	A	549	LYS	2.6
3	A	748	ARG	2.6
3	A	645	SER	2.6
3	A	873	TYR	2.5
3	A	734	GLU	2.5
3	A	516	GLN	2.5
3	A	533	GLN	2.5
3	A	535	GLY	2.4
3	A	817	GLU	2.4
3	A	579	GLN	2.4
3	A	304	ALA	2.4
3	A	634	ARG	2.4
2	T	7	DT	2.4
3	A	563	LYS	2.4
3	A	766	LEU	2.3
1	P	2	DC	2.3
3	A	548	LYS	2.3
3	A	777	THR	2.3
3	A	537	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	314	ASP	2.3
3	A	519	TYR	2.3
3	A	571	VAL	2.3
3	A	580	LEU	2.3
3	A	567	TYR	2.2
3	A	502	GLN	2.2
3	A	726	ASN	2.2
3	A	541	LYS	2.2
3	A	562	GLU	2.2
3	A	639	ALA	2.2
3	A	646	ASP	2.2
3	A	509	GLU	2.2
3	A	572	GLU	2.2
3	A	561	LEU	2.2
3	A	633	GLY	2.1
3	A	816	LYS	2.1
3	A	540	GLU	2.1
3	A	435	ARG	2.1
3	A	498	LYS	2.1
3	A	711	GLY	2.1
3	A	723	GLN	2.1
3	A	732	ALA	2.0
3	A	727	ILE	2.0
3	A	306	ARG	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](#)

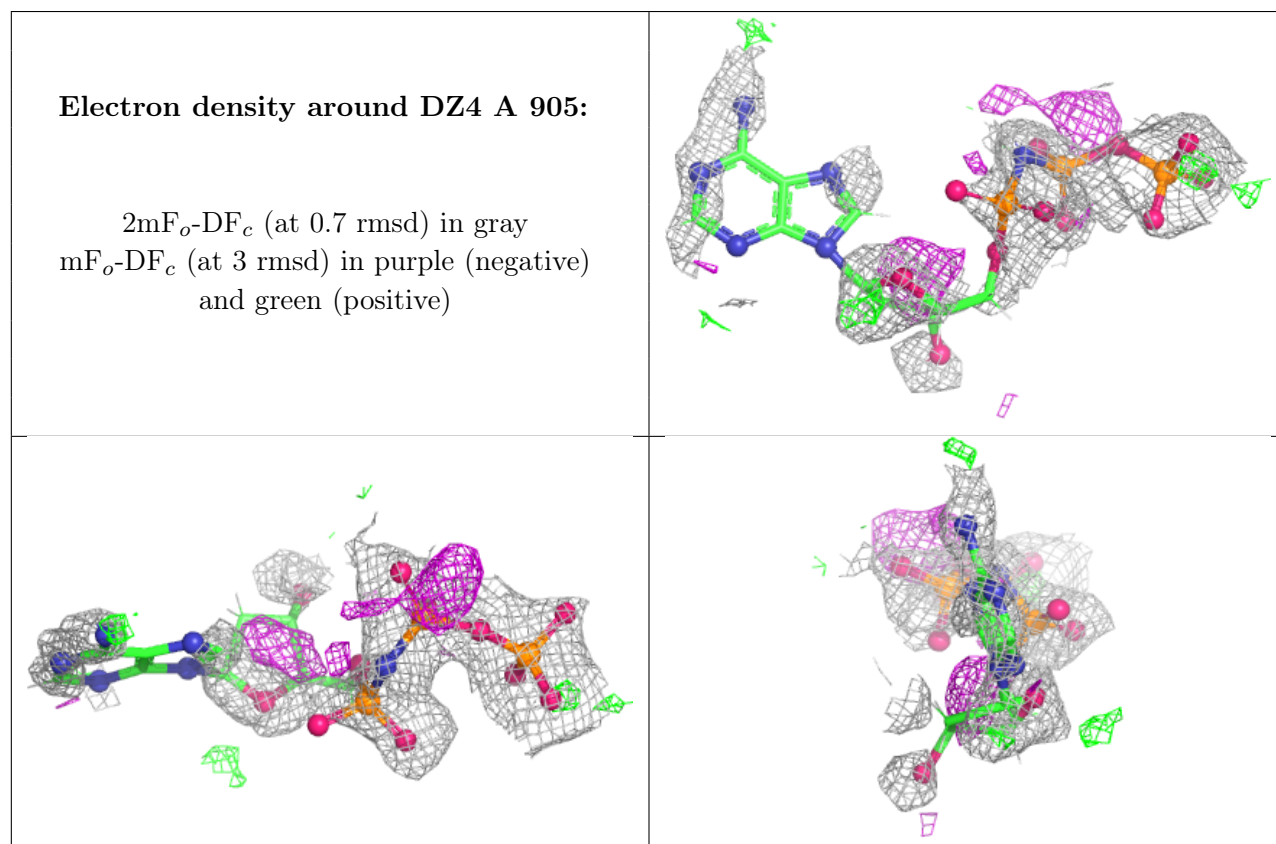
There are no oligosaccharides in this entry.

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
5	SO4	A	904	5/5	0.57	0.17	116,117,120,120	0
6	DZ4	A	905	30/30	0.60	0.25	66,101,136,149	6
5	SO4	A	902	5/5	0.76	0.18	100,101,104,105	0
5	SO4	A	903	5/5	0.78	0.17	89,91,94,97	0
4	MG	A	901	1/1	0.97	0.12	38,38,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.