



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 PM UTC

PDB ID : 6US5 / pdb_00006us5
Title : DNA polymerase I Large Fragment from *Bacillus stearothermophilus* with DNA template, 3'-amino primer, dGpNHpp analog, and Mn²⁺
Authors : Zhang, W.; Lelyveld, V.S.; Szostak, J.W.
Deposited on : 2019-10-24
Resolution : 2.25 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

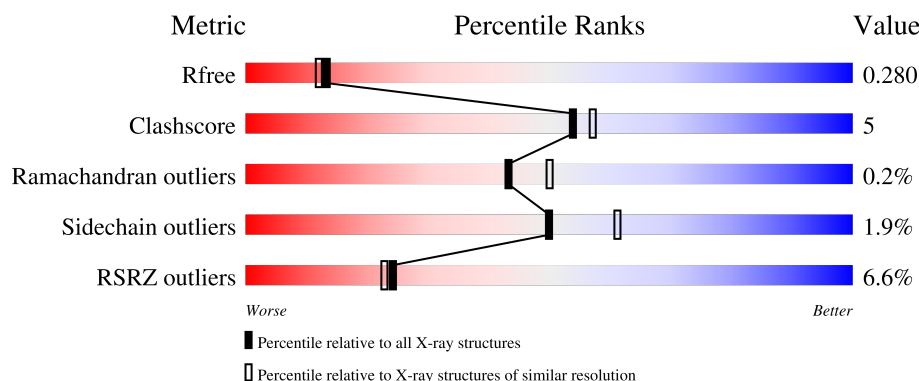
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	579	13% 90% 9%
1	D	579	13% 83% 16%
2	B	9	67% 22% 11%
2	E	9	67% 22% 11%
3	C	13	69% 31%

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Mol	Chain	Length	Quality of chain
3	F	13	 69% 31%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10640 atoms, of which 0 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 I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4646	2955	807	867	17			
1	D	579	Total	C	N	O	S	0	0	0
			4646	2955	807	867	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	710	TYR	PHE	engineered mutation	UNP D9N168
A	713	VAL	PRO	variant	UNP D9N168
D	710	TYR	PHE	engineered mutation	UNP D9N168
D	713	VAL	PRO	variant	UNP D9N168

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*GP*AP*TP*CP*AP*GP*(C42))-3').

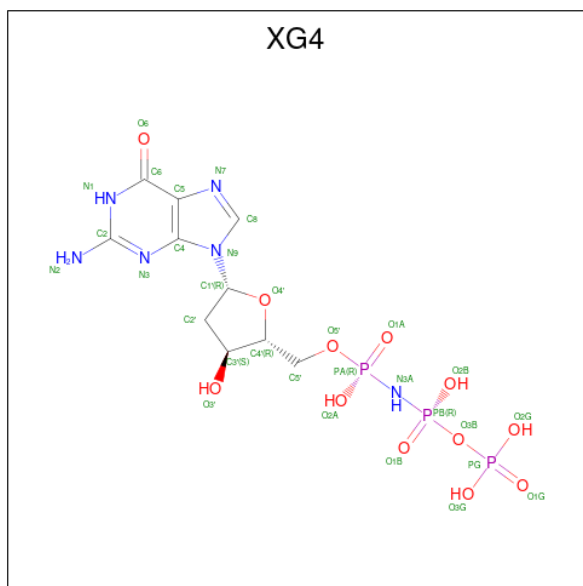
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			182	87	37	50	8			
2	E	9	Total	C	N	O	P	0	0	0
			182	87	37	50	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	1
			246	116	46	72	12			
3	F	13	Total	C	N	O	P	0	0	1
			229	106	41	70	12			

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}]p

hosphoryl]guanosine (CCD ID: XG4) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	234	Total	O	0	0
			234	234		
7	B	14	Total	O	0	0
			14	14		
7	C	27	Total	O	0	0
			27	27		
7	D	112	Total	O	0	0
			112	112		
7	E	7	Total	O	0	0
			7	7		

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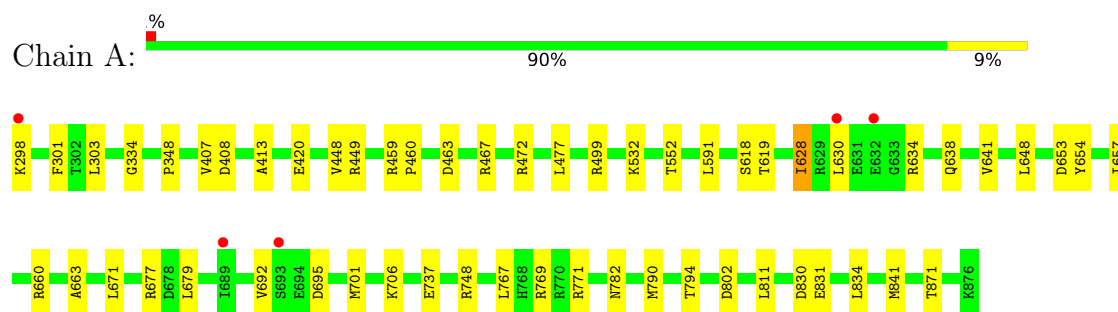
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	16	Total	O	0	0
			16	16		

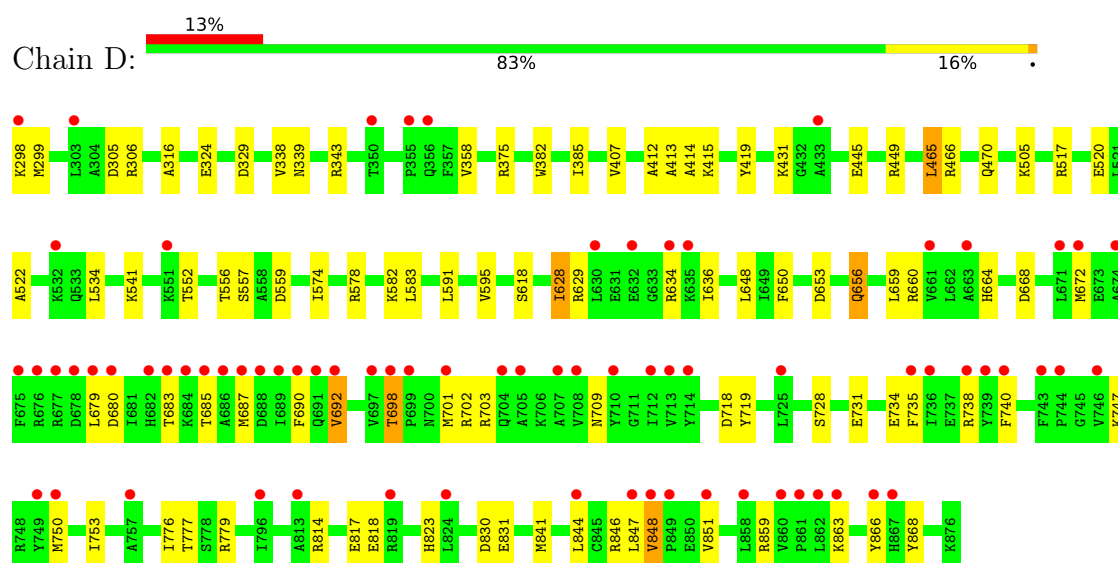
3 Residue-property plots [i](#)

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.

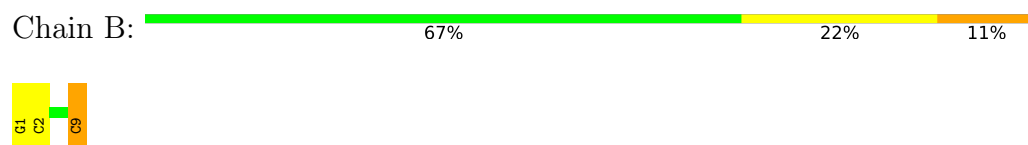
• Molecule 1: DNA polymerase I



• Molecule 1: DNA polymerase I



• Molecule 2: DNA (5'-D(*GP*CP*GP*AP*TP*CP*AP*GP*(C42))-3')



• Molecule 2: DNA (5'-D(*GP*CP*GP*AP*TP*CP*AP*GP*(C42))-3')

Chain E:  67% 22% 11%



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

Chain C:  69% 31%



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

Chain F:  69% 31%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.76Å 108.81Å 149.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.06 – 2.25 47.06 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.06-2.25) 98.3 (47.06-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.224 , 0.278 0.224 , 0.280	Depositor DCC
R_{free} test set	3609 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10640	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: C42, MN, XG4, 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	0.12	0/4730	0.30	0/6393
1	D	0.12	0/4730	0.31	0/6393
2	B	0.20	0/183	0.41	0/281
2	E	0.20	0/183	0.37	0/281
3	C	0.18	0/275	0.34	0/423
3	F	0.17	0/255	0.32	0/393
All	All	0.13	0/10356	0.31	0/14164

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	A	4646	0	4705	31	0
1	D	4646	0	4705	61	0
2	B	182	0	103	3	0
2	E	182	0	103	6	0
3	C	246	0	135	6	0
3	F	229	0	123	3	0
4	A	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	31	0	13	3	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	0	0	0
6	C	5	0	0	1	0
6	D	10	0	0	1	0
7	A	234	0	0	2	0
7	B	14	0	0	0	0
7	C	27	0	0	0	0
7	D	112	0	0	2	0
7	E	7	0	0	0	0
7	F	16	0	0	0	0
All	All	10640	0	9900	99	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 5.

All (99) 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)
2:B:9:C42:O4'	2:B:9:C42:C1'	1.64	1.22
2:E:9:C42:O4'	2:E:9:C42:C1'	1.64	1.20
1:D:830:ASP:OD1	2:E:9:C42:N	2.22	0.73
1:D:702:ARG:NH2	4:D:901:XG4:O3G	2.23	0.71
1:D:324:GLU:O	1:D:375:ARG:NH2	2.25	0.70
1:D:740:PHE:HB3	1:D:747:LYS:HD2	1.76	0.68
1:A:830:ASP:OD1	2:B:9:C42:N	2.27	0.67
1:A:706:LYS:HD2	4:A:901:XG4:HN3A	1.61	0.66
1:A:552:THR:HB	3:C:13:DA:H1'	1.79	0.65
1:D:629:ARG:NH1	2:E:9:C42:O1P	2.32	0.63
1:D:683:THR:HG23	1:D:702:ARG:HH11	1.65	0.61
1:D:414:ALA:HB1	1:D:419:TYR:HB3	1.81	0.61
1:D:517:ARG:NH1	1:D:520:GLU:OE2	2.33	0.61
1:A:660:ARG:NH2	7:A:1001:HOH:O	2.27	0.60
1:D:728:SER:OG	1:D:731:GLU:CB	2.50	0.60
1:D:728:SER:OG	1:D:731:GLU:HB2	2.02	0.59
1:D:650:PHE:HD1	1:D:868:TYR:HB3	1.69	0.58
1:A:532:LYS:HE2	3:C:13:DA:C8	2.40	0.56
1:D:465:LEU:HD12	1:D:470:GLN:HB2	1.87	0.56
1:D:648:LEU:HB2	1:D:841:MET:HE3	1.88	0.56
1:A:769:ARG:NH1	1:A:802:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:VAL:HG13	1:D:385:ILE:HG23	1.88	0.55
1:D:306:ARG:NH2	6:D:903:SO4:O2	2.40	0.55
1:A:653:ASP:HB3	1:A:831:GLU:HG2	1.91	0.53
1:D:664:HIS:O	1:D:859:ARG:NH1	2.42	0.52
1:D:299:MET:HE3	1:D:449:ARG:HG2	1.92	0.52
1:D:653:ASP:HB3	1:D:831:GLU:HG2	1.92	0.52
1:A:790:MET:O	1:A:794:THR:HG23	2.10	0.51
1:D:656:GLN:HB2	1:D:659:LEU:HB2	1.91	0.51
1:D:734:GLU:HA	1:D:734:GLU:OE1	2.11	0.51
1:A:407:VAL:HG11	1:A:413:ALA:HB2	1.93	0.51
1:D:776:ILE:HG23	1:D:777:THR:HG23	1.91	0.51
3:F:10:DC:H2''	3:F:11:DG:C8	2.46	0.50
1:D:466:ARG:NH2	7:D:1007:HOH:O	2.44	0.50
1:A:619:THR:HG22	3:C:7:DG:H3'	1.94	0.50
1:D:628:ILE:HA	1:D:634:ARG:HG3	1.94	0.49
1:D:648:LEU:HD12	1:D:841:MET:HG3	1.94	0.49
1:A:811:LEU:HD21	1:A:834:LEU:HD21	1.93	0.49
1:D:814:ARG:HB3	1:D:847:LEU:HD11	1.93	0.49
1:A:767:LEU:HD12	1:A:802:ASP:HB3	1.95	0.49
1:A:677:ARG:HB2	1:A:679:LEU:HG	1.93	0.49
1:A:641:VAL:HG12	1:A:871:THR:HG22	1.94	0.48
1:D:466:ARG:NH2	7:D:1009:HOH:O	2.46	0.48
1:D:698:THR:HG23	1:D:701:MET:HE3	1.96	0.48
3:C:10:DC:N4	6:C:101:SO4:O2	2.41	0.48
1:D:685:THR:HG21	1:D:709:ASN:OD1	2.13	0.48
1:D:692:VAL:HG21	1:D:701:MET:SD	2.54	0.48
1:A:648:LEU:HD12	1:A:841:MET:HG3	1.95	0.47
1:D:445:GLU:HG2	1:D:449:ARG:HD2	1.97	0.47
1:D:522:ALA:O	1:D:541:LYS:NZ	2.42	0.47
4:D:901:XG4:O4'	2:E:9:C42:H2'2	2.14	0.47
1:A:420:GLU:HB3	1:D:779:ARG:HH22	1.79	0.47
1:D:557:SER:OG	1:D:559:ASP:OD1	2.29	0.46
1:D:683:THR:HG23	1:D:702:ARG:NH1	2.30	0.46
1:A:692:VAL:HG21	1:A:701:MET:HE1	1.98	0.46
1:D:431:LYS:HA	1:D:431:LYS:HD2	1.73	0.46
1:D:668:ASP:O	1:D:672:MET:HG2	2.15	0.46
1:A:301:PHE:HB3	1:A:448:VAL:HG11	1.98	0.46
1:D:591:LEU:O	1:D:595:VAL:HG23	2.15	0.46
1:D:338:VAL:HG22	1:D:343:ARG:HG2	1.97	0.46
1:D:618:SER:O	3:F:7:DG:H4'	2.17	0.45
1:D:718:ASP:OD1	1:D:719:TYR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LEU:HD12	1:A:591:LEU:HA	1.86	0.45
1:D:412:ALA:HA	1:D:415:LYS:HE2	1.99	0.45
4:D:901:XG4:HN1	3:F:3:DC:H42	1.65	0.45
1:D:329:ASP:H	1:D:382:TRP:CD1	2.36	0.44
1:A:298:LYS:HB3	1:A:449:ARG:HH21	1.82	0.44
1:D:629:ARG:HE	1:D:703:ARG:HD3	1.83	0.44
3:C:12:DC:O3'	3:C:13:DA:H3'	2.18	0.44
1:A:771:ARG:HD3	1:A:794:THR:HG21	1.99	0.44
2:B:1:DG:H1'	2:B:2:DC:H5'	1.99	0.44
1:A:663:ALA:HB2	1:A:671:LEU:HG	2.00	0.43
1:A:748:ARG:NH1	7:A:1013:HOH:O	2.43	0.43
1:D:556:THR:O	1:D:578:ARG:NH1	2.44	0.43
1:D:628:ILE:HG22	2:E:8:DG:H5''	1.99	0.43
1:A:618:SER:O	3:C:7:DG:H4'	2.19	0.43
1:D:690:PHE:CD2	1:D:701:MET:HG3	2.54	0.42
1:A:408:ASP:OD1	1:A:408:ASP:N	2.52	0.42
1:A:334:GLY:HA2	1:A:348:PRO:HD3	2.00	0.42
1:D:844:LEU:O	1:D:848:VAL:HG13	2.19	0.42
1:D:582:LYS:HG2	2:E:7:DA:H5'	2.01	0.42
1:A:628:ILE:HA	1:A:634:ARG:HG3	2.01	0.41
1:A:654:TYR:HB3	1:A:657:ILE:HB	2.01	0.41
1:D:534:LEU:HD11	1:D:574:ILE:HD13	2.02	0.41
1:D:650:PHE:CZ	1:D:866:TYR:HD1	2.38	0.41
1:D:848:VAL:HA	1:D:851:VAL:HG12	2.01	0.41
1:D:583:LEU:HD22	1:D:636:ILE:HD12	2.02	0.41
1:D:817:GLU:HG3	1:D:818:GLU:H	1.84	0.41
1:D:680:ASP:CG	1:D:702:ARG:HH12	2.29	0.41
1:D:680:ASP:HB3	1:D:683:THR:OG1	2.19	0.41
1:D:407:VAL:HG11	1:D:413:ALA:HB2	2.01	0.41
1:D:660:ARG:HH22	1:D:863:LYS:HB3	1.86	0.41
1:A:499:ARG:NH2	1:A:638:GLN:O	2.54	0.41
1:D:735:PHE:HA	1:D:738:ARG:HG2	2.03	0.41
1:A:459:ARG:HB3	1:A:460:PRO:HD3	2.03	0.41
1:D:750:MET:HA	1:D:753:ILE:HG22	2.02	0.41
1:A:463:ASP:O	1:A:467:ARG:HG3	2.22	0.40
1:D:316:ALA:HB2	1:D:339:ASN:HB3	2.02	0.40
1:D:679:LEU:HD23	1:D:679:LEU:H	1.86	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	
1	A	577/579 (100%)	565 (98%)	11 (2%)	1 (0%)	43	50
1	D	577/579 (100%)	555 (96%)	21 (4%)	1 (0%)	43	50
All	All	1154/1158 (100%)	1120 (97%)	32 (3%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	628	ILE
1	A	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	495/495 (100%)	488 (99%)	7 (1%)	59	70
1	D	495/495 (100%)	483 (98%)	12 (2%)	43	54
All	All	990/990 (100%)	971 (98%)	19 (2%)	50	61

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	472	ARG
1	A	477	LEU
1	A	630	LEU

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Mol	Chain	Res	Type
1	A	695	ASP
1	A	737	GLU
1	A	782	ASN
1	D	298	LYS
1	D	305	ASP
1	D	465	LEU
1	D	505	LYS
1	D	552	THR
1	D	656	GLN
1	D	687	MET
1	D	692	VAL
1	D	698	THR
1	D	823	HIS
1	D	846	ARG
1	D	848	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	GLN
1	A	579	GLN
1	A	755	GLN
1	A	768	HIS
1	A	821	GLN
1	D	656	GLN
1	D	768	HIS
1	D	793	ASN

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	C42	E	9	3,2	17,20,21	4.25	7 (41%)	20,28,31	1.52	5 (25%)
2	C42	B	9	3,2	17,20,21	4.20	7 (41%)	20,28,31	1.32	2 (10%)

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	C42	E	9	3,2	-	0/7/21/22	0/2/2/2
2	C42	B	9	3,2	-	0/7/21/22	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	C42	O4'-C1'	10.07	1.64	1.42
2	E	9	C42	O4'-C1'	10.00	1.64	1.42
2	E	9	C42	C4-N4	7.73	1.52	1.33
2	B	9	C42	C4-N4	7.65	1.52	1.33
2	E	9	C42	C2'-C1'	-7.53	1.31	1.52
2	B	9	C42	C2'-C1'	-7.27	1.32	1.52
2	E	9	C42	O4'-C4'	-6.91	1.29	1.45
2	B	9	C42	O4'-C4'	-6.88	1.29	1.45
2	E	9	C42	C2-N1	-3.45	1.32	1.40
2	B	9	C42	C2-N1	-3.35	1.33	1.40
2	B	9	C42	C4'-C3'	2.29	1.57	1.52
2	E	9	C42	C4'-C3'	2.27	1.57	1.52
2	E	9	C42	C6-C5	2.21	1.40	1.35
2	B	9	C42	C6-C5	2.17	1.40	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	C42	O2-C2-N3	-2.70	118.07	122.33
2	E	9	C42	C2'-C1'-N1	-2.59	107.33	113.81
2	E	9	C42	C1'-C2'-C3'	2.51	107.68	102.93
2	E	9	C42	O2-C2-N3	-2.41	118.53	122.33
2	B	9	C42	N1-C2-N3	2.39	122.96	118.80
2	E	9	C42	N1-C2-N3	2.24	122.69	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	9	C42	O4'-C1'-N1	2.06	111.53	107.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	9	C42	4	0
2	B	9	C42	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
4	XG4	A	901	5	32,33,33	3.66	16 (50%)	46,52,52	1.77	10 (21%)
6	SO4	A	904	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	D	904	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	A	903	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	906	-	4,4,4	0.23	0	6,6,6	0.06	0
4	XG4	D	901	5	32,33,33	3.66	16 (50%)	46,52,52	1.79	9 (19%)
6	SO4	D	903	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	905	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	C	101	-	4,4,4	0.24	0	6,6,6	0.09	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	XG4	A	901	5	-	3/19/34/34	0/3/3/3
4	XG4	D	901	5	-	4/19/34/34	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	XG4	O6-C6	8.90	1.40	1.23
4	A	901	XG4	O6-C6	8.86	1.40	1.23
4	D	901	XG4	C2'-C3'	-7.97	1.32	1.52
4	A	901	XG4	C2'-C3'	-7.96	1.32	1.52
4	D	901	XG4	O4'-C4'	-7.17	1.29	1.45
4	D	901	XG4	O4'-C1'	7.15	1.58	1.42
4	A	901	XG4	O4'-C4'	-7.13	1.29	1.45
4	A	901	XG4	O4'-C1'	7.12	1.58	1.42
4	D	901	XG4	PB-O3B	5.46	1.65	1.59
4	A	901	XG4	C1'-N9	-5.28	1.34	1.48
4	D	901	XG4	C1'-N9	-5.19	1.35	1.48
4	A	901	XG4	PB-O3B	5.06	1.65	1.59
4	D	901	XG4	C2-N2	5.01	1.45	1.34
4	A	901	XG4	C2-N2	4.98	1.45	1.34
4	A	901	XG4	PB-O1B	3.89	1.52	1.46
4	A	901	XG4	C3'-C4'	3.72	1.62	1.53
4	D	901	XG4	C3'-C4'	3.65	1.62	1.53
4	A	901	XG4	PB-N3A	3.63	1.72	1.63
4	D	901	XG4	PB-N3A	3.48	1.72	1.63
4	D	901	XG4	PA-N3A	3.42	1.72	1.63
4	A	901	XG4	C6-N1	-3.30	1.32	1.38
4	A	901	XG4	PA-O1A	3.24	1.51	1.46
4	D	901	XG4	PB-O1B	3.24	1.51	1.46
4	D	901	XG4	PA-O1A	3.17	1.51	1.46
4	D	901	XG4	C6-N1	-3.13	1.33	1.38
4	A	901	XG4	PA-N3A	2.99	1.71	1.63
4	D	901	XG4	PA-O5'	2.52	1.66	1.57
4	A	901	XG4	PA-O5'	2.51	1.66	1.57
4	A	901	XG4	PB-O2B	-2.47	1.50	1.56
4	A	901	XG4	C2-N1	-2.37	1.31	1.37
4	D	901	XG4	PB-O2B	-2.34	1.50	1.56
4	D	901	XG4	C2-N1	-2.23	1.32	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	XG4	C5-C4-N3	-6.29	118.38	128.39
4	A	901	XG4	C5-C4-N3	-6.23	118.47	128.39
4	D	901	XG4	C2-N3-C4	5.06	121.02	112.30
4	A	901	XG4	C2-N3-C4	5.01	120.92	112.30
4	D	901	XG4	N9-C4-N3	4.21	134.37	125.95
4	A	901	XG4	N9-C4-N3	4.20	134.34	125.95
4	A	901	XG4	O1B-PB-N3A	-2.52	108.06	111.77
4	A	901	XG4	C4-C5-N7	-2.45	106.79	110.67
4	D	901	XG4	C4-C5-N7	-2.42	106.84	110.67
4	D	901	XG4	O1A-PA-N3A	-2.34	108.32	111.77
4	A	901	XG4	C8-N7-C5	2.31	108.38	104.26
4	D	901	XG4	O6-C6-C5	-2.31	120.44	126.53
4	D	901	XG4	C8-N7-C5	2.24	108.26	104.26
4	D	901	XG4	C2-N1-C6	-2.12	121.27	125.11
4	A	901	XG4	C6-C5-N7	2.08	134.08	130.29
4	A	901	XG4	O6-C6-C5	-2.07	121.06	126.53
4	D	901	XG4	C5-C6-N1	2.02	118.39	113.25
4	A	901	XG4	C5-C6-N1	2.01	118.38	113.25
4	A	901	XG4	C2-N1-C6	-2.01	121.47	125.11

There are no chirality outliers.

All (7) torsion outliers are listed below:

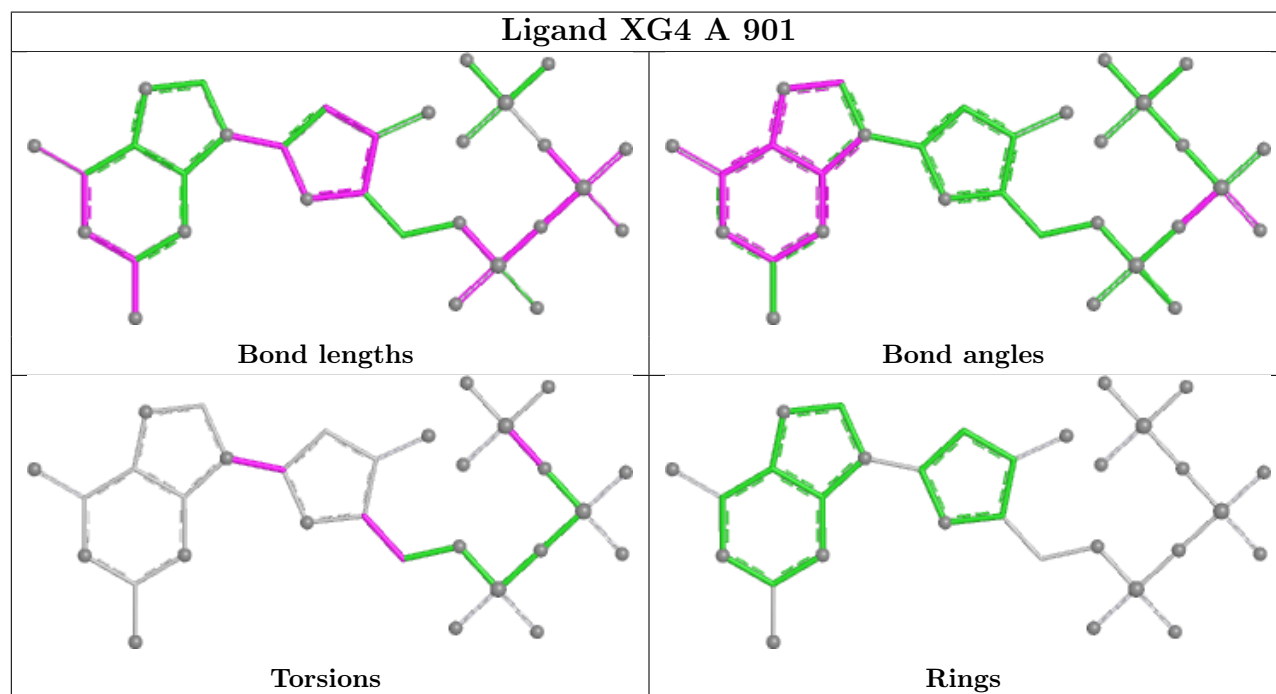
Mol	Chain	Res	Type	Atoms
4	D	901	XG4	C5'-O5'-PA-O2A
4	D	901	XG4	C5'-O5'-PA-N3A
4	D	901	XG4	PA-N3A-PB-O1B
4	D	901	XG4	C5'-O5'-PA-O1A
4	A	901	XG4	C3'-C4'-C5'-O5'
4	A	901	XG4	PB-O3B-PG-O2G
4	A	901	XG4	O4'-C1'-N9-C4

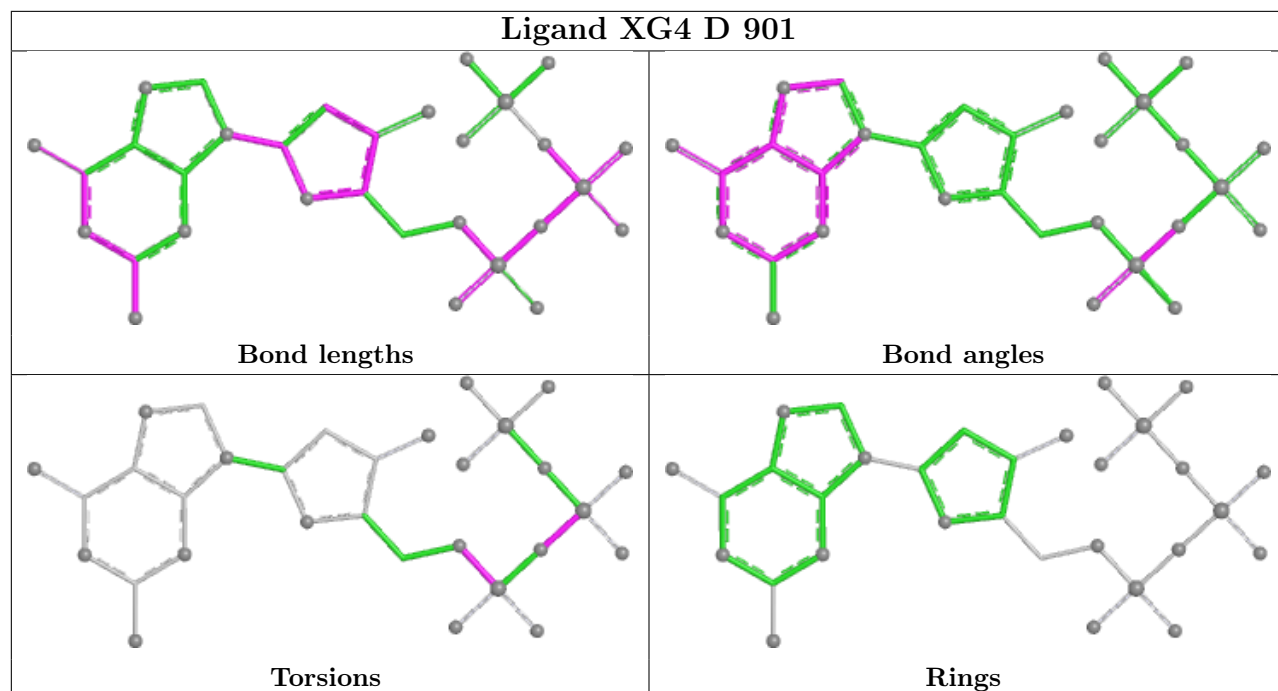
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	XG4	1	0
4	D	901	XG4	3	0
6	D	903	SO4	1	0
6	C	101	SO4	1	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	A	579/579 (100%)	0.11	5 (0%) 81 82	20, 37, 66, 91	0
1	D	579/579 (100%)	0.93	74 (12%) 7 7	29, 57, 102, 146	0
2	B	8/9 (88%)	-0.50	0 100 100	32, 38, 48, 53	0
2	E	8/9 (88%)	-0.54	0 100 100	38, 40, 45, 50	0
3	C	13/13 (100%)	-0.26	0 100 100	25, 35, 75, 110	0
3	F	13/13 (100%)	-0.26	0 100 100	33, 43, 94, 109	0
All	All	1200/1202 (99%)	0.49	79 (6%) 24 23	20, 47, 85, 146	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	686	ALA	6.6
1	D	671	LEU	5.3
1	D	689	ILE	5.2
1	D	708	VAL	4.8
1	D	688	ASP	4.4
1	D	692	VAL	4.3
1	D	861	PRO	4.1
1	D	679	LEU	4.0
1	D	707	ALA	4.0
1	D	712	ILE	4.0
1	D	663	ALA	3.8
1	D	739	TYR	3.8
1	A	298	LYS	3.6
1	D	735	PHE	3.6
1	D	687	MET	3.5
1	D	738	ARG	3.5
1	A	630	LEU	3.5
1	D	713	VAL	3.4
1	D	685	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	675	PHE	3.3
1	D	677	ARG	3.3
1	D	690	PHE	3.3
1	D	844	LEU	3.3
1	D	532	LYS	3.3
1	D	743	PHE	3.3
1	D	862	LEU	3.2
1	D	714	TYR	3.2
1	D	697	VAL	3.2
1	D	750	MET	3.1
1	D	661	VAL	3.0
1	D	433	ALA	3.0
1	D	749	TYR	2.9
1	D	303	LEU	2.9
1	D	860	VAL	2.8
1	D	704	GLN	2.8
1	D	682	HIS	2.7
1	A	632	GLU	2.7
1	D	866	TYR	2.7
1	D	683	THR	2.6
1	D	298	LYS	2.6
1	D	701	MET	2.6
1	D	630	LEU	2.5
1	D	848	VAL	2.5
1	D	736	ILE	2.5
1	D	680	ASP	2.5
1	D	632	GLU	2.4
1	D	740	PHE	2.4
1	D	634	ARG	2.4
1	D	867	HIS	2.4
1	D	699	PRO	2.3
1	D	746	VAL	2.3
1	D	849	PRO	2.3
1	D	796	ILE	2.3
1	D	691	GLN	2.3
1	D	710	TYR	2.3
1	D	813	ALA	2.3
1	D	824	LEU	2.2
1	D	847	LEU	2.2
1	D	551	LYS	2.2
1	D	858	LEU	2.2
1	D	744	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	684	LYS	2.2
1	D	725	LEU	2.2
1	D	698	THR	2.2
1	D	674	ALA	2.2
1	D	851	VAL	2.1
1	D	635	LYS	2.1
1	D	356	GLN	2.1
1	D	350	THR	2.1
1	D	676	ARG	2.1
1	A	689	ILE	2.1
1	D	672	MET	2.1
1	D	819	ARG	2.1
1	D	705	ALA	2.1
1	D	863	LYS	2.1
1	D	678	ASP	2.1
1	D	355	PRO	2.0
1	A	693	SER	2.0
1	D	757	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	C42	E	9	19/20	0.90	0.11	31,43,56,75	0
2	C42	B	9	19/20	0.93	0.08	21,32,43,43	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

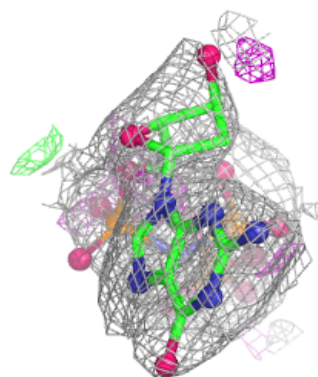
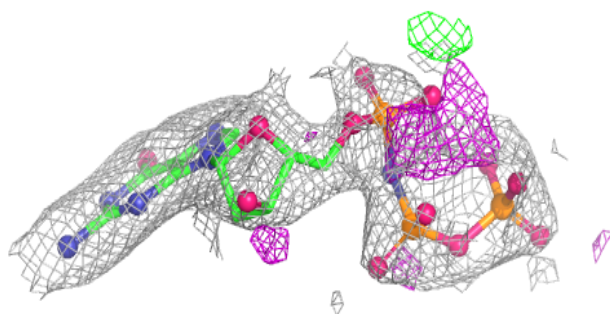
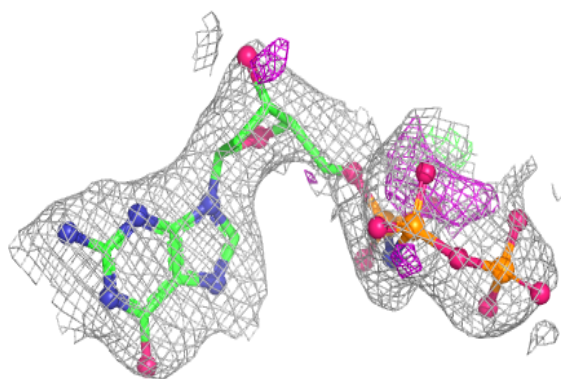
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

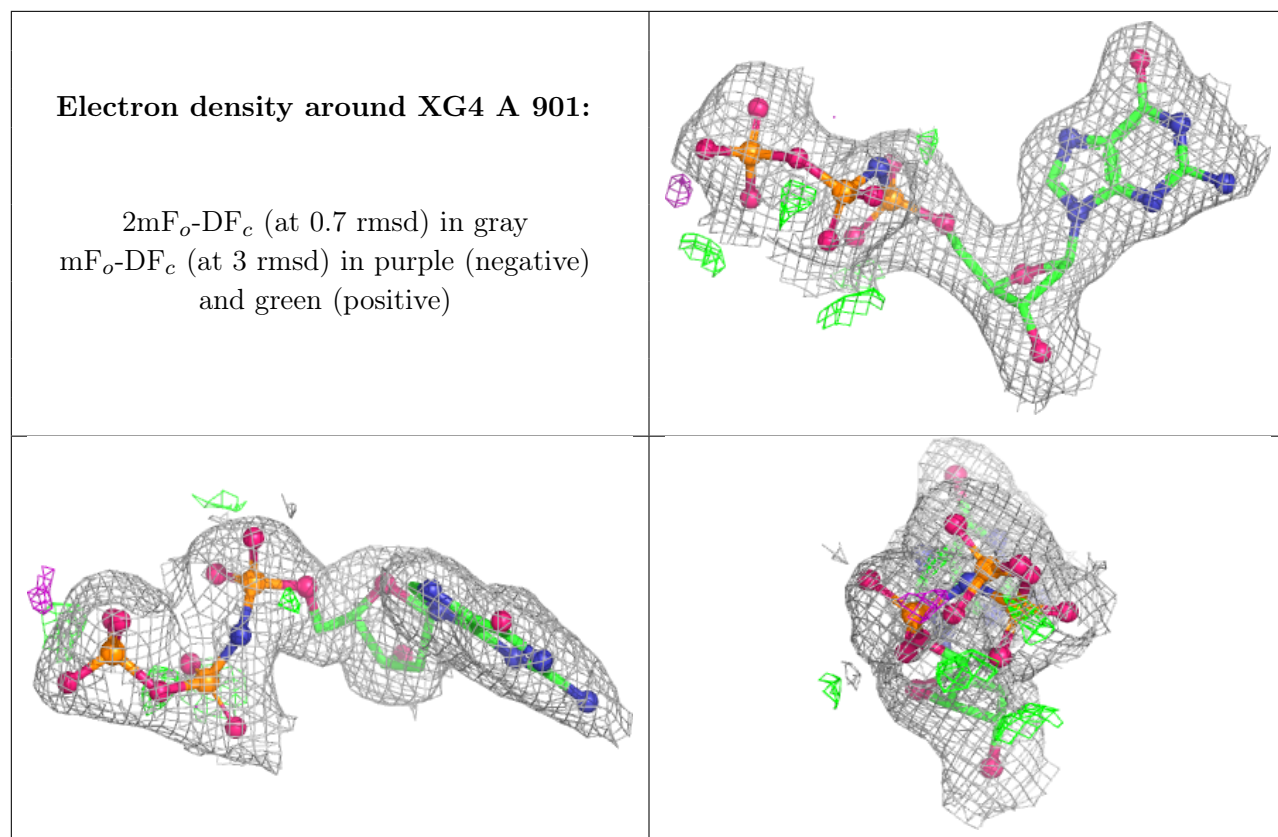
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	C	101	5/5	0.59	0.14	81,89,111,119	0
6	SO4	A	905	5/5	0.69	0.14	61,75,90,110	0
6	SO4	A	904	5/5	0.70	0.11	96,107,116,124	0
6	SO4	D	903	5/5	0.70	0.15	57,59,65,66	5
4	XG4	D	901	31/31	0.78	0.12	54,72,108,117	0
6	SO4	A	906	5/5	0.79	0.14	63,70,100,105	0
5	MN	D	902	1/1	0.80	0.15	134,134,134,134	0
5	MN	A	902	1/1	0.86	0.12	93,93,93,93	0
6	SO4	D	904	5/5	0.88	0.15	39,46,48,55	5
6	SO4	A	903	5/5	0.92	0.11	46,47,65,80	0
4	XG4	A	901	31/31	0.95	0.08	21,29,60,70	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.

Electron density around XG4 D 901:

2mF_o-DF_c (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.