



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:57 pm BST

PDB ID : 4I9Q
Title : Crystal structure of the ternary complex of the D714A mutant of RB69 DNA polymerase
Authors : Guja, K.E.; Jacewicz, A.; Trzemecka, A.; Plochocka, D.; Yakubovskaya, E.; Bebenek, A.; Garcia-Diaz, M.
Deposited on : 2012-12-05
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

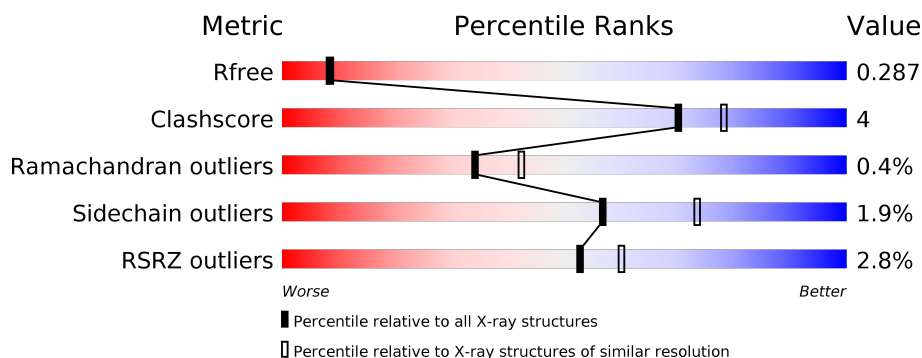
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	903	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	903	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>••</div> </div> </div>
2	D	18	<div> <div>11%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>6%</div> </div> </div>
2	T	18	<div> <div>17%</div> <div> <div></div> <div>72%</div> <div>28%</div> </div> </div>
3	C	13	<div> <div></div> <div>100%</div> </div>
3	P	13	<div> <div></div> <div> <div>69%</div> <div>31%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15929 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	846	Total	C	N	O	S	0	17	0
			6980	4482	1161	1306	31			
1	B	873	Total	C	N	O	S	0	15	0
			7168	4602	1194	1339	33			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	567	ALA	TYR	ENGINEERED MUTATION	UNP Q38087
A	714	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	567	ALA	TYR	ENGINEERED MUTATION	UNP Q38087
B	714	ALA	ASP	ENGINEERED MUTATION	UNP Q38087

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	1	0
			386	184	74	110	18			
2	D	17	Total	C	N	O	P	0	0	0
			343	164	64	99	16			

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

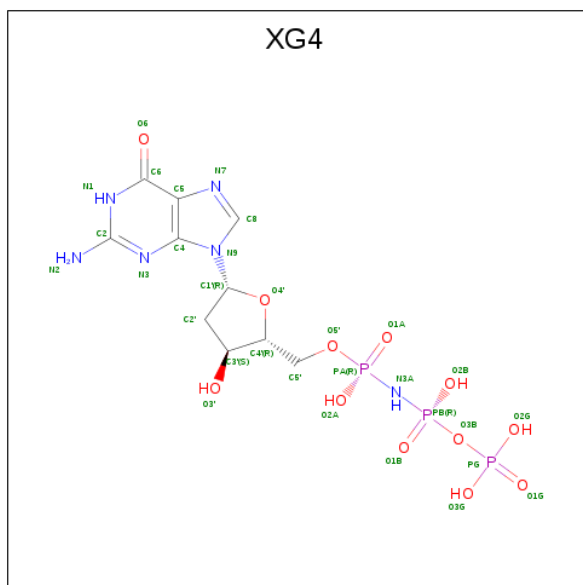
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}p
hosphoryl]guanosine (three-letter code: XG4) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0
6	A	1	Total Na 1 1	0	0

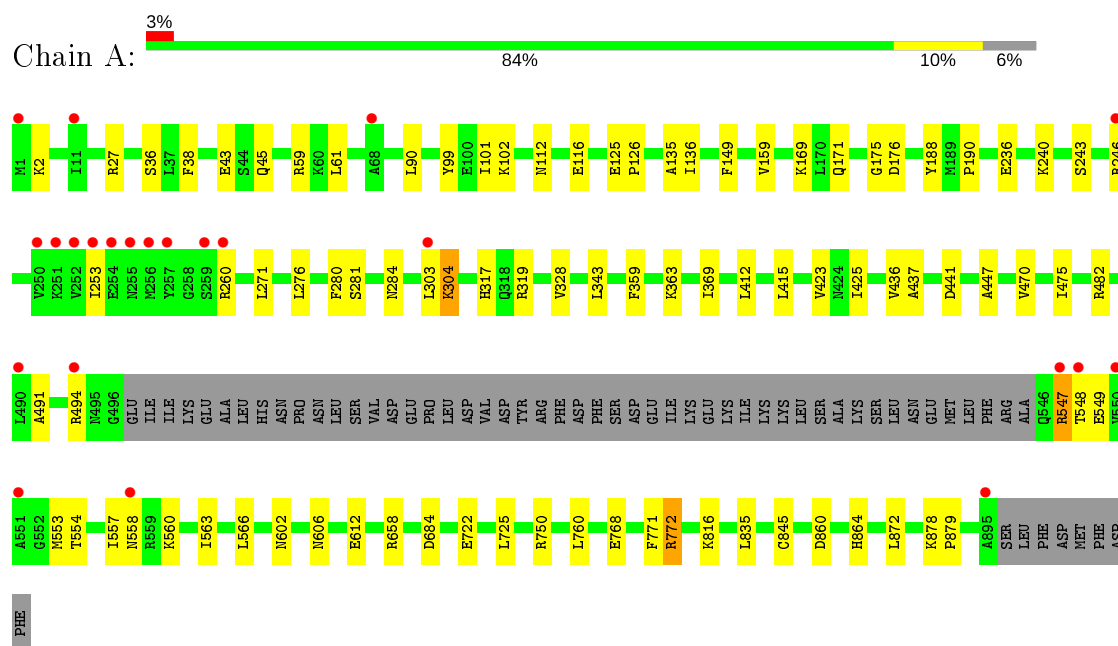
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	216	Total O 216 216	0	0
7	T	27	Total O 27 27	0	0
7	B	135	Total O 135 135	0	0
7	P	9	Total O 9 9	0	0
7	D	9	Total O 9 9	0	0
7	C	2	Total O 2 2	0	0

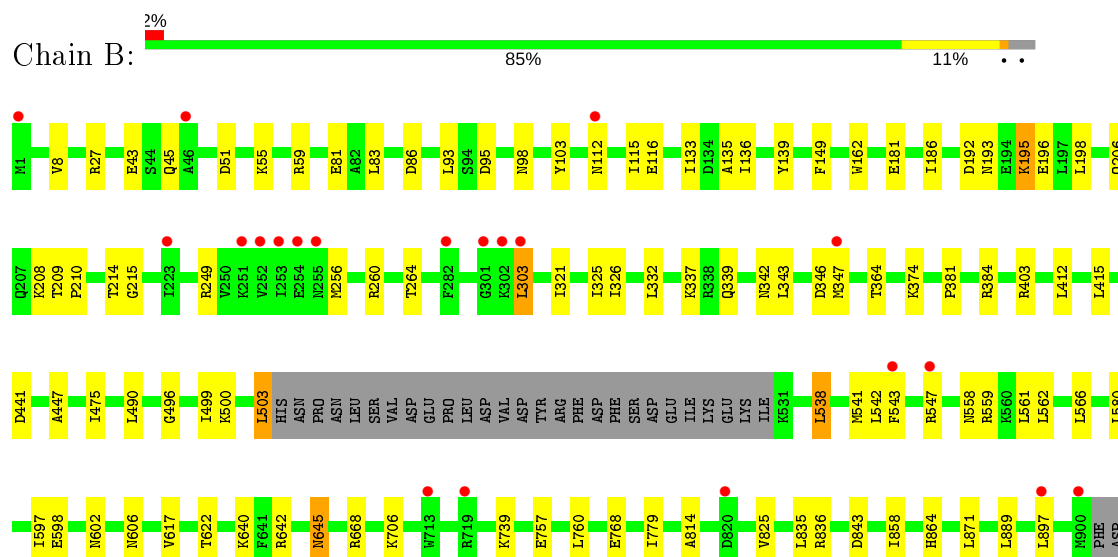
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



• Molecule 1: DNA polymerase

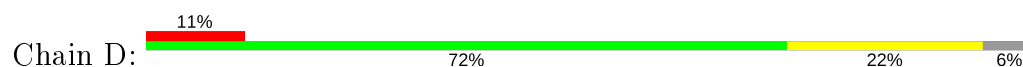


PHE

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



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



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



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



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.78 Å 119.41 Å 146.02 Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	38.40 – 2.30 38.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.40-2.30) 94.4 (38.40-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1227)	Depositor
R, R_{free}	0.252 , 0.287 0.252 , 0.287	Depositor DCC
R_{free} test set	5526 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 17.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15929	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, XG4

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	0.22	0/7189	0.38	0/9717
1	B	0.21	0/7375	0.38	0/9965
2	D	0.44	0/384	0.91	0/590
2	T	0.44	0/433	1.16	1/666 (0.2%)
3	C	0.44	0/294	1.07	0/452
3	P	0.44	0/294	1.07	0/452
All	All	0.24	0/15969	0.49	1/21842 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	DC	OP1-P-OP2	12.85	138.87	119.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6980	0	6900	48	0
1	B	7168	0	7091	55	0
2	D	343	0	192	3	0
2	T	386	0	214	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	263	0	148	0	0
3	P	263	0	148	3	0
4	A	62	0	26	4	0
4	B	62	0	26	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	216	0	0	3	0
7	B	135	0	0	6	0
7	C	2	0	0	0	0
7	D	9	0	0	0	0
7	P	9	0	0	0	0
7	T	27	0	0	1	0
All	All	15929	0	14745	108	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 4.

All (108) 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:A:547:ARG:O	1:A:549:GLU:N	2.22	0.70
2:T:16:DG:H2''	2:T:17:DC:H2'	1.73	0.69
1:B:195:LYS:H	1:B:195:LYS:HZ2	1.41	0.68
1:A:768:GLU:O	1:A:772:ARG:NH2	2.29	0.66
1:A:549:GLU:O	1:A:553:MET:N	2.31	0.64
1:B:412:LEU:HD13	1:B:415:LEU:HD13	1.81	0.62
1:B:543:PHE:O	1:B:547:ARG:NH2	2.32	0.62
1:B:95:ASP:OD1	1:B:374:LYS:NZ	2.27	0.62
1:B:503:LEU:HD12	1:B:538:LEU:HB3	1.82	0.61
1:B:668:ARG:NH1	7:B:1164:HOH:O	2.33	0.61
1:A:253:ILE:HB	1:A:260:ARG:HB2	1.82	0.61
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.83	0.60
1:A:475:ILE:HD12	1:A:566:LEU:HD23	1.84	0.59
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.86	0.58
1:A:59:ARG:HD2	4:A:1002:XG4:H4'	1.86	0.58
1:B:645:ASN:OD1	1:B:645:ASN:N	2.33	0.58
1:A:243:SER:O	1:A:246:ARG:NH1	2.38	0.56
1:A:602:ASN:O	1:A:606:ASN:ND2	2.33	0.55
1:B:260:ARG:NH2	2:D:2:DC:OP2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:HD12	1:B:198:LEU:HD21	1.90	0.54
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.89	0.53
1:B:739:LYS:NZ	7:B:1167:HOH:O	2.41	0.53
1:A:343:LEU:HD22	1:A:558:ASN:HD22	1.72	0.53
1:B:303:LEU:HD11	1:B:326:ILE:HB	1.89	0.53
1:A:491:ALA:HA	1:A:494:ARG:HH21	1.74	0.52
1:B:343:LEU:HD22	1:B:558:ASN:HB3	1.92	0.52
1:B:339:GLN:OE1	1:B:342:ASN:ND2	2.38	0.52
1:B:193:ASN:HD21	1:B:196[B]:GLU:HG2	1.75	0.51
1:B:779:ILE:HB	1:B:871:LEU:HD21	1.93	0.51
1:B:186:ILE:HD13	1:B:325:ILE:HD13	1.93	0.50
1:B:27:ARG:NH2	7:B:1194:HOH:O	2.42	0.50
1:A:280:PHE:HB3	1:A:558:ASN:ND2	2.26	0.50
1:B:602:ASN:O	1:B:606:ASN:ND2	2.34	0.50
1:B:8:VAL:HG11	1:B:93:LEU:HD11	1.94	0.49
1:A:90:LEU:HD11	1:A:363:LYS:HD2	1.95	0.49
1:A:482:ARG:NH1	7:A:1229:HOH:O	2.45	0.49
1:B:214:THR:OG1	1:B:215:GLY:N	2.45	0.49
1:B:475:ILE:HD12	1:B:566:LEU:HD23	1.95	0.49
1:A:2:LYS:HE3	1:A:101:ILE:HA	1.94	0.48
1:B:136:ILE:HB	1:B:149:PHE:HB2	1.95	0.48
2:T:17:DC:H42	3:P:103:DG:H1	1.60	0.48
2:D:15:DC:H2''	2:D:16:DG:C8	2.49	0.48
1:A:2:LYS:HE3	1:A:102:LYS:H	1.78	0.48
1:B:112[A]:ASN:HB2	1:B:139:TYR:HB3	1.96	0.47
1:B:836:ARG:NH1	1:B:864:HIS:O	2.43	0.47
1:A:2:LYS:HE2	1:A:99:TYR:HE1	1.79	0.47
1:A:112[B]:ASN:HD22	1:A:328:VAL:HG13	1.79	0.47
1:B:496:GLY:O	1:B:500:LYS:N	2.36	0.47
1:B:86:ASP:OD1	1:B:86:ASP:N	2.40	0.47
1:B:347:MET:HE3	1:B:562:LEU:HD13	1.97	0.46
1:B:757:GLU:HB2	1:B:889:LEU:HD22	1.97	0.46
1:B:115:ILE:HG22	1:B:136:ILE:HG12	1.96	0.46
1:B:112[B]:ASN:HD22	1:B:332:LEU:HG	1.79	0.46
1:A:38:PHE:HE1	4:A:1002:XG4:C4	2.29	0.46
1:B:181:GLU:N	1:B:181:GLU:OE1	2.42	0.46
1:A:554:THR:HA	1:A:557:ILE:HG22	1.98	0.45
1:A:136:ILE:HB	1:A:149:PHE:HB2	1.98	0.45
1:A:169:LYS:HB2	1:A:175:GLY:HA3	1.97	0.45
1:A:359:PHE:HB3	2:T:3[A]:DA:C4	2.52	0.45
1:A:36:SER:HB2	4:A:1002:XG4:H1'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:104:DC:H2"	3:P:105:DG:C8	2.51	0.44
1:B:103:TYR:OH	1:B:346:ASP:OD1	2.28	0.44
1:B:499:ILE:HG21	1:B:541:MET:O	2.17	0.44
1:B:249:ARG:HG3	1:B:264:THR:HB	2.00	0.44
1:A:188:TYR:CE2	1:A:190:PRO:HG3	2.53	0.44
1:B:193:ASN:ND2	1:B:196[B]:GLU:HG2	2.32	0.44
1:B:83:LEU:HD23	1:B:381:PRO:HA	1.99	0.44
1:A:658:ARG:NH1	7:A:1174:HOH:O	2.36	0.43
1:A:281:SER:O	7:A:1102:HOH:O	2.21	0.43
1:A:116:GLU:HB2	1:A:135:ALA:HB3	2.01	0.43
1:A:725:LEU:HD11	1:A:750:ARG:HB2	2.00	0.43
1:A:303:LEU:HD12	1:A:304:LYS:HZ3	1.83	0.43
1:A:271:LEU:HB3	1:A:276:LEU:HD11	2.00	0.43
1:A:369:ILE:HG23	1:A:470:VAL:HG21	2.00	0.43
1:A:176:ASP:HA	1:A:319:ARG:HH21	1.82	0.43
1:A:36:SER:O	4:A:1002:XG4:H8	2.18	0.43
1:B:337:LYS:HE2	1:B:337:LYS:HB3	1.85	0.43
1:A:835:LEU:HD13	1:A:845:CYS:HA	2.00	0.43
1:A:482:ARG:CZ	1:A:560:LYS:HD3	2.49	0.43
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.54	0.42
1:B:162:TRP:CD1	1:B:321:ILE:HB	2.55	0.42
1:B:706:LYS:HE3	2:D:7:DA:N3	2.34	0.42
1:B:51:ASP:OD1	1:B:55:LYS:N	2.47	0.42
1:B:499:ILE:HD13	1:B:541:MET:O	2.19	0.42
1:A:436:VAL:HG12	1:A:437:ALA:O	2.20	0.42
1:B:116:GLU:HB2	1:B:135:ALA:HB3	2.02	0.42
1:B:45:GLN:NE2	7:B:1129:HOH:O	2.53	0.42
1:B:597:ILE:HA	1:B:597:ILE:HD12	1.92	0.42
1:A:284:ASN:ND2	3:P:113:DT:OP2	2.31	0.42
1:A:125:GLU:HA	1:A:126:PRO:HD3	1.90	0.42
1:A:860:ASP:O	1:A:864:HIS:ND1	2.51	0.42
1:A:236:GLU:O	1:A:240[A]:LYS:HD3	2.20	0.41
1:B:59:ARG:HD2	4:B:1002:XG4:H5'A	2.02	0.41
1:B:81:GLU:HB2	1:B:384:ARG:HH22	1.84	0.41
2:T:10:DC:OP2	7:T:104:HOH:O	2.22	0.41
1:B:209:THR:HA	1:B:210:PRO:HD3	1.85	0.41
1:B:403:ARG:NH1	7:B:1154:HOH:O	2.41	0.41
1:A:423:VAL:HB	1:A:425:ILE:HG13	2.02	0.41
1:B:347:MET:HE3	1:B:364:THR:HG21	2.01	0.41
1:A:771:PHE:CE1	1:A:872:LEU:HD22	2.56	0.41
1:B:814:ALA:HB1	1:B:858:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:LYS:HB3	1:A:879:PRO:HD3	2.03	0.40
1:A:171:GLN:HE22	1:A:303:LEU:HD11	1.87	0.40
1:B:43:GLU:CD	1:B:43:GLU:H	2.24	0.40
1:A:280:PHE:HB3	1:A:558:ASN:HD21	1.86	0.40
1:B:208:LYS:NZ	7:B:1160:HOH:O	2.46	0.40
1:B:598:GLU:HG3	1:B:617:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	859/903 (95%)	830 (97%)	26 (3%)	3 (0%)	41	50
1	B	884/903 (98%)	848 (96%)	32 (4%)	4 (0%)	29	35
All	All	1743/1806 (96%)	1678 (96%)	58 (3%)	7 (0%)	34	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	548	THR
1	A	547	ARG
1	A	612	GLU
1	B	542	LEU
1	B	897	LEU
1	B	256	MET
1	B	622	THR

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	761/798 (95%)	750 (99%)	11 (1%)	67	81
1	B	779/798 (98%)	760 (98%)	19 (2%)	49	66
All	All	1540/1596 (96%)	1510 (98%)	30 (2%)	57	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	43	GLU
1	A	45	GLN
1	A	61	LEU
1	A	304	LYS
1	A	563	ILE
1	A	684	ASP
1	A	722	GLU
1	A	760	LEU
1	A	772	ARG
1	A	816	LYS
1	B	98	ASN
1	B	195	LYS
1	B	206[A]	GLN
1	B	206[B]	GLN
1	B	303	LEU
1	B	490	LEU
1	B	503	LEU
1	B	538	LEU
1	B	559	ARG
1	B	561	LEU
1	B	580	LEU
1	B	640	LYS
1	B	642	ARG
1	B	645	ASN
1	B	760	LEU
1	B	768	GLU

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Mol	Chain	Res	Type
1	B	825	VAL
1	B	835	LEU
1	B	843	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	389	GLN
1	A	444	ASN
1	A	493	GLN
1	A	558	ASN
1	A	818	ASN
1	B	193	ASN
1	B	376	GLN
1	B	582	ASN
1	B	679	HIS

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](#)

Of 8 ligands modelled in this entry, 4 are 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	$\# Z > 2$
4	XG4	B	1001	5	29,33,33	1.70	4 (13%)	35,52,52	1.91	9 (25%)
4	XG4	A	1002	-	29,33,33	1.69	4 (13%)	35,52,52	1.86	6 (17%)
4	XG4	B	1002	-	29,33,33	1.75	5 (17%)	35,52,52	1.79	7 (20%)
4	XG4	A	1001	5,6	29,33,33	1.70	5 (17%)	35,52,52	1.95	10 (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
4	XG4	B	1001	5	-	7/15/34/34	0/3/3/3
4	XG4	A	1002	-	-	7/15/34/34	0/3/3/3
4	XG4	B	1002	-	-	4/15/34/34	0/3/3/3
4	XG4	A	1001	5,6	-	4/15/34/34	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	XG4	PB-N3A	4.70	1.75	1.63
4	B	1002	XG4	PA-N3A	4.66	1.75	1.63
4	B	1002	XG4	PB-N3A	4.64	1.75	1.63
4	A	1002	XG4	PA-N3A	4.59	1.75	1.63
4	A	1001	XG4	PB-N3A	4.52	1.75	1.63
4	B	1001	XG4	PB-N3A	4.51	1.75	1.63
4	A	1001	XG4	PA-N3A	4.51	1.75	1.63
4	B	1001	XG4	PA-N3A	4.40	1.74	1.63
4	B	1002	XG4	C6-C5	4.20	1.48	1.41
4	B	1001	XG4	C6-C5	4.17	1.48	1.41
4	A	1001	XG4	C6-C5	4.03	1.48	1.41
4	A	1002	XG4	C6-C5	3.19	1.46	1.41
4	B	1002	XG4	C5-C4	2.59	1.47	1.40
4	A	1002	XG4	C5-C4	2.51	1.47	1.40
4	B	1001	XG4	C5-C4	2.39	1.47	1.40
4	A	1001	XG4	C5-C4	2.38	1.47	1.40
4	B	1002	XG4	PB-O3B	2.12	1.61	1.59
4	A	1001	XG4	PB-O3B	2.03	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	XG4	C2-N3-C4	5.30	121.41	115.36
4	B	1002	XG4	C2-N3-C4	4.92	120.97	115.36
4	B	1001	XG4	C2-N3-C4	4.87	120.92	115.36
4	A	1001	XG4	C2-N3-C4	4.79	120.83	115.36
4	A	1002	XG4	C6-N1-C2	4.25	122.69	115.93
4	A	1002	XG4	N3-C2-N1	-4.07	121.80	127.22
4	B	1002	XG4	C5-C6-N1	-4.04	117.91	123.43
4	B	1001	XG4	C6-N1-C2	3.96	122.23	115.93
4	A	1001	XG4	C6-N1-C2	3.96	122.22	115.93
4	B	1001	XG4	C6-C5-C4	-3.91	117.06	120.80
4	A	1001	XG4	C6-C5-C4	-3.88	117.09	120.80
4	A	1001	XG4	C5-C6-N1	-3.87	118.14	123.43
4	B	1002	XG4	C6-N1-C2	3.86	122.06	115.93
4	B	1001	XG4	C5-C6-N1	-3.85	118.17	123.43
4	A	1002	XG4	C6-C5-C4	-3.57	117.39	120.80
4	A	1001	XG4	C2'-C1'-N9	-3.56	106.06	114.27
4	A	1002	XG4	C5-C6-N1	-3.47	118.69	123.43
4	B	1001	XG4	N3-C2-N1	-3.34	122.76	127.22
4	A	1001	XG4	N3-C2-N1	-3.33	122.78	127.22
4	B	1002	XG4	C6-C5-C4	-3.09	117.85	120.80
4	B	1002	XG4	PG-O3B-PB	-3.01	122.03	132.62
4	B	1002	XG4	N3-C2-N1	-2.96	123.27	127.22
4	B	1001	XG4	C2'-C1'-N9	-2.88	107.62	114.27
4	B	1001	XG4	PG-O3B-PB	-2.80	122.75	132.62
4	A	1001	XG4	PG-O3B-PB	-2.72	123.05	132.62
4	B	1001	XG4	C4-C5-N7	-2.58	106.71	109.40
4	A	1001	XG4	O2B-PB-O3B	2.56	113.17	104.64
4	A	1002	XG4	PG-O3B-PB	-2.39	124.19	132.62
4	B	1002	XG4	C4-C5-N7	-2.34	106.96	109.40
4	A	1001	XG4	C4-C5-N7	-2.34	106.96	109.40
4	B	1001	XG4	O2B-PB-O3B	2.27	112.23	104.64
4	A	1001	XG4	O3G-PG-O2G	2.05	115.49	107.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	XG4	PB-N3A-PA-O1A
4	B	1001	XG4	C5'-O5'-PA-O2A
4	B	1001	XG4	C5'-O5'-PA-N3A
4	B	1001	XG4	PA-N3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	B	1001	XG4	PG-O3B-PB-O1B
4	B	1001	XG4	PG-O3B-PB-O2B
4	B	1002	XG4	PB-N3A-PA-O1A
4	B	1002	XG4	C5'-O5'-PA-O2A
4	A	1002	XG4	PB-N3A-PA-O1A
4	A	1002	XG4	C5'-O5'-PA-O2A
4	A	1002	XG4	C5'-O5'-PA-N3A
4	A	1002	XG4	O4'-C4'-C5'-O5'
4	A	1001	XG4	PB-N3A-PA-O1A
4	A	1001	XG4	PA-N3A-PB-O1B
4	A	1001	XG4	PG-O3B-PB-O1B
4	A	1001	XG4	PG-O3B-PB-O2B
4	A	1002	XG4	C3'-C4'-C5'-O5'
4	B	1002	XG4	C5'-O5'-PA-O1A
4	A	1002	XG4	C5'-O5'-PA-O1A
4	B	1002	XG4	C5'-O5'-PA-N3A
4	B	1001	XG4	C5'-O5'-PA-O1A
4	A	1002	XG4	PA-N3A-PB-O3B

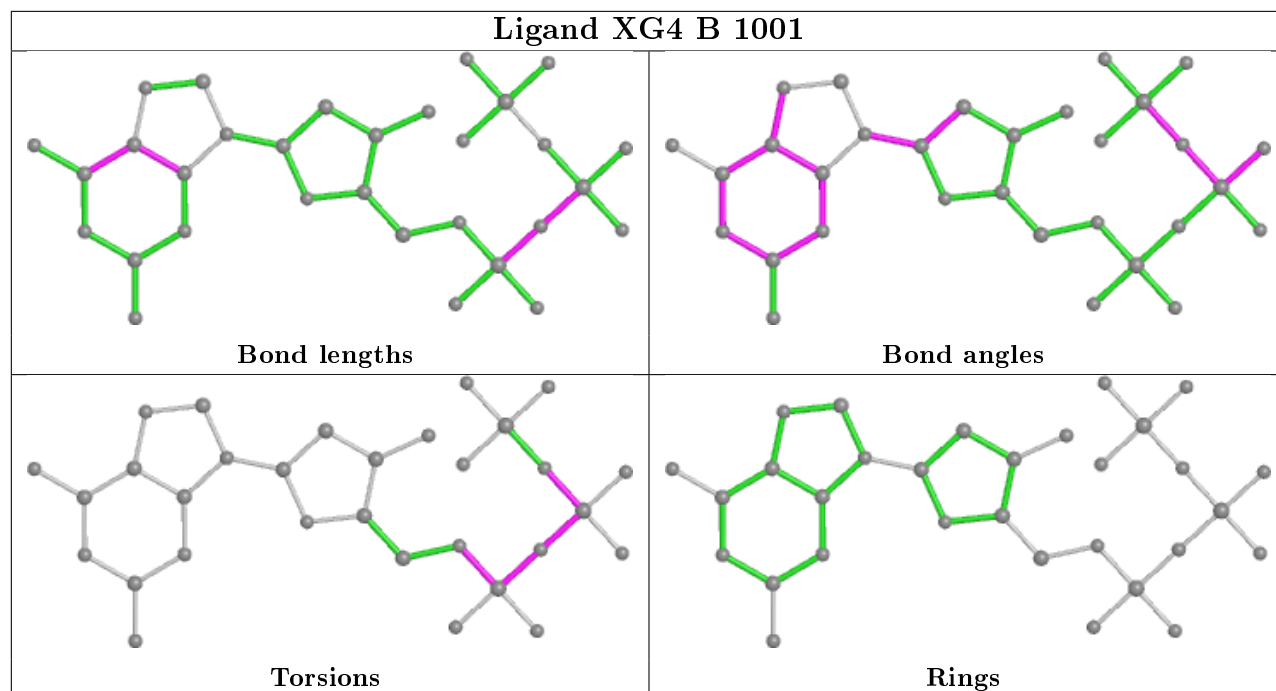
There are no ring outliers.

2 monomers are involved in 5 short contacts:

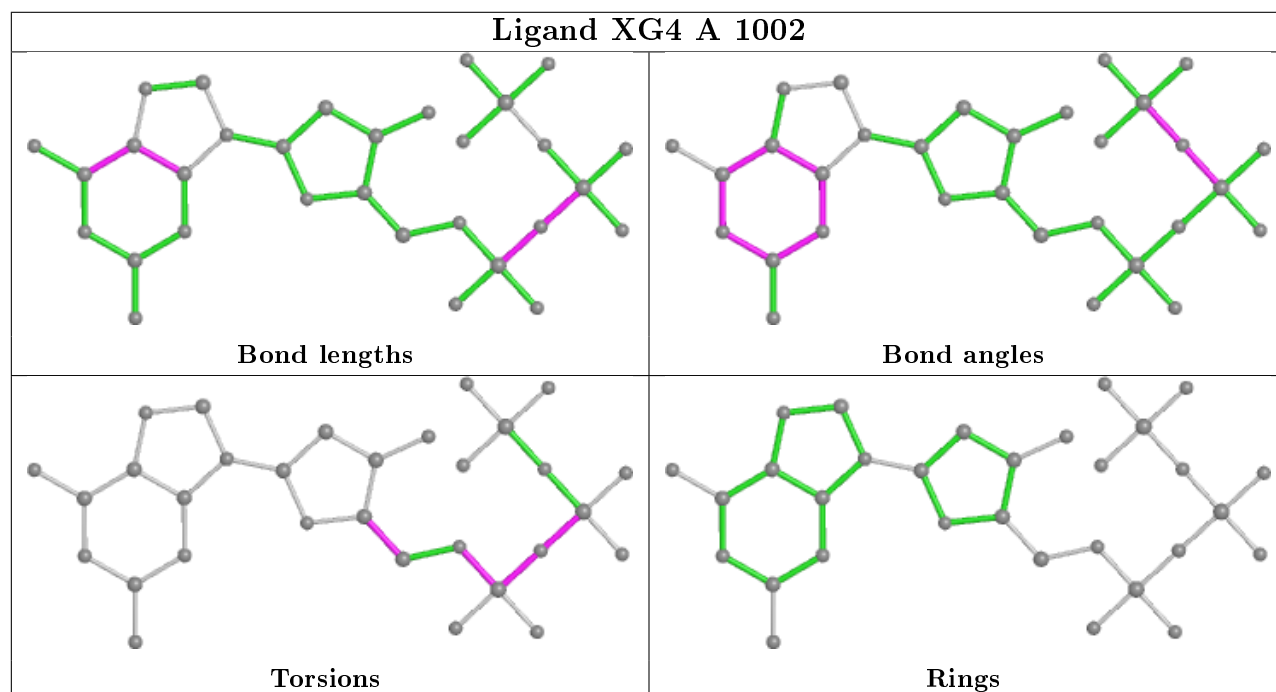
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	XG4	4	0
4	B	1002	XG4	1	0

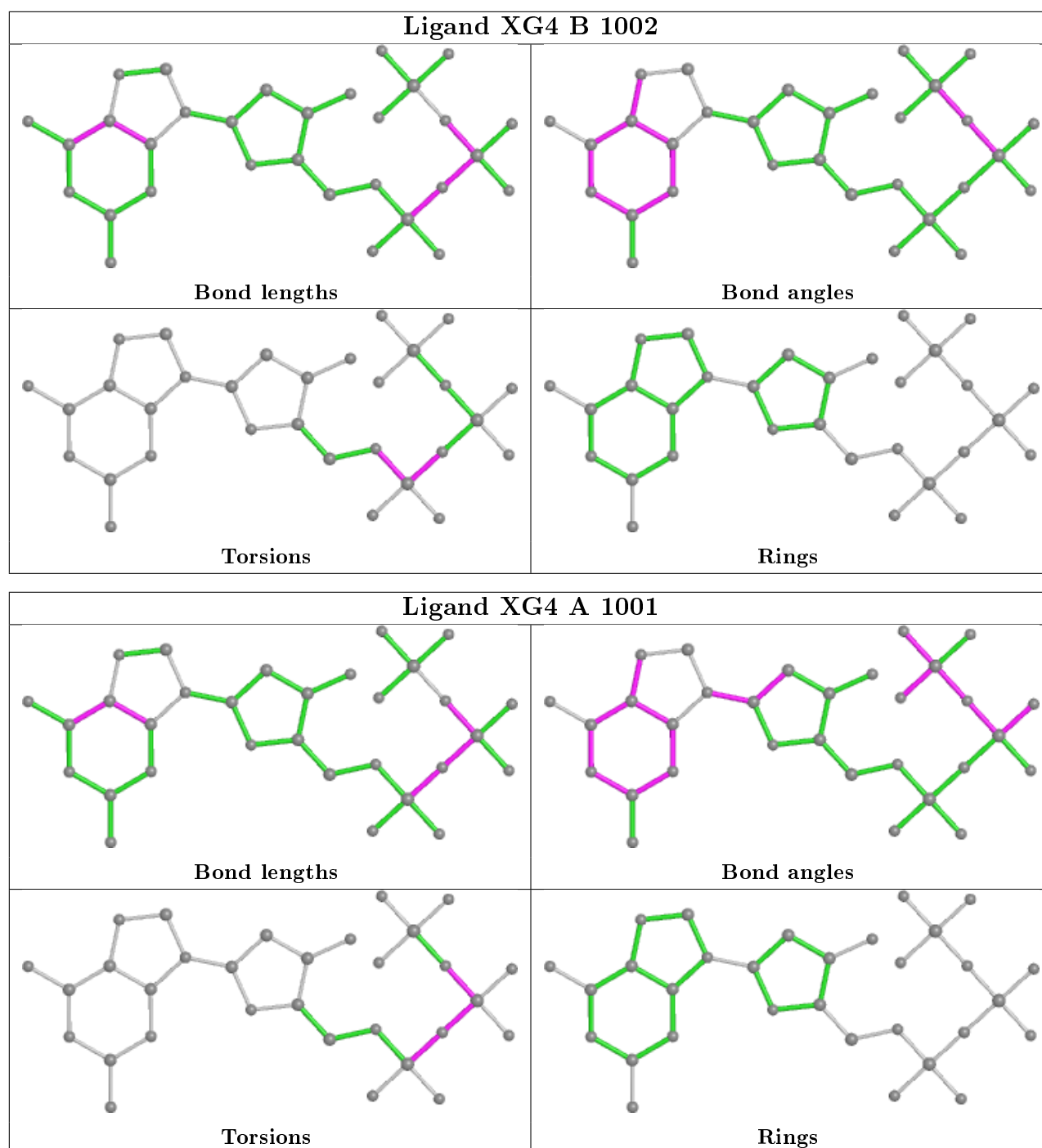
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand XG4 B 1001



Ligand XG4 A 1002





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	846/903 (93%)	0.11	23 (2%) 54 62	16, 32, 59, 81	0
1	B	873/903 (96%)	0.22	21 (2%) 59 66	24, 40, 60, 86	0
2	D	17/18 (94%)	-0.06	2 (11%) 4 6	34, 43, 95, 95	0
2	T	18/18 (100%)	0.16	3 (16%) 1 2	21, 32, 83, 87	0
3	C	13/13 (100%)	-0.54	0 100 100	32, 42, 89, 94	0
3	P	13/13 (100%)	-0.41	0 100 100	25, 33, 82, 87	0
All	All	1780/1868 (95%)	0.15	49 (2%) 53 60	16, 37, 62, 95	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	VAL	5.9
1	A	253	ILE	4.5
1	B	302	LYS	4.5
1	A	551	ALA	4.4
1	A	558	ASN	4.0
1	A	490	LEU	3.6
1	B	254	GLU	3.5
1	B	543	PHE	3.4
2	T	3[A]	DA	3.4
1	B	253	ILE	3.2
1	B	303	LEU	3.2
1	A	257	TYR	3.0
1	B	547	ARG	3.0
1	A	303	LEU	2.9
1	B	301	GLY	2.8
1	A	547	ARG	2.8
1	A	1	MET	2.8
2	T	2	DC	2.8
1	A	255	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	1	DT	2.7
1	A	251	LYS	2.6
1	A	254	GLU	2.6
1	B	223	ILE	2.6
1	B	719	ARG	2.6
1	A	260	ARG	2.5
1	A	250	VAL	2.5
1	B	713	TRP	2.5
1	B	820	ASP	2.5
1	B	282	PHE	2.4
1	A	68	ALA	2.4
1	B	347	MET	2.4
1	A	252	VAL	2.3
1	B	46	ALA	2.3
1	A	494	ARG	2.3
1	A	895	ALA	2.3
1	A	548	THR	2.3
1	B	112[A]	ASN	2.3
1	B	255	ASN	2.3
1	A	256	MET	2.3
1	B	900	MET	2.2
1	A	550	VAL	2.1
1	A	246	ARG	2.1
2	T	1	DT	2.1
1	A	11	ILE	2.1
1	B	251	LYS	2.1
2	D	2	DC	2.0
1	B	1	MET	2.0
1	B	897	LEU	2.0
1	A	259	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

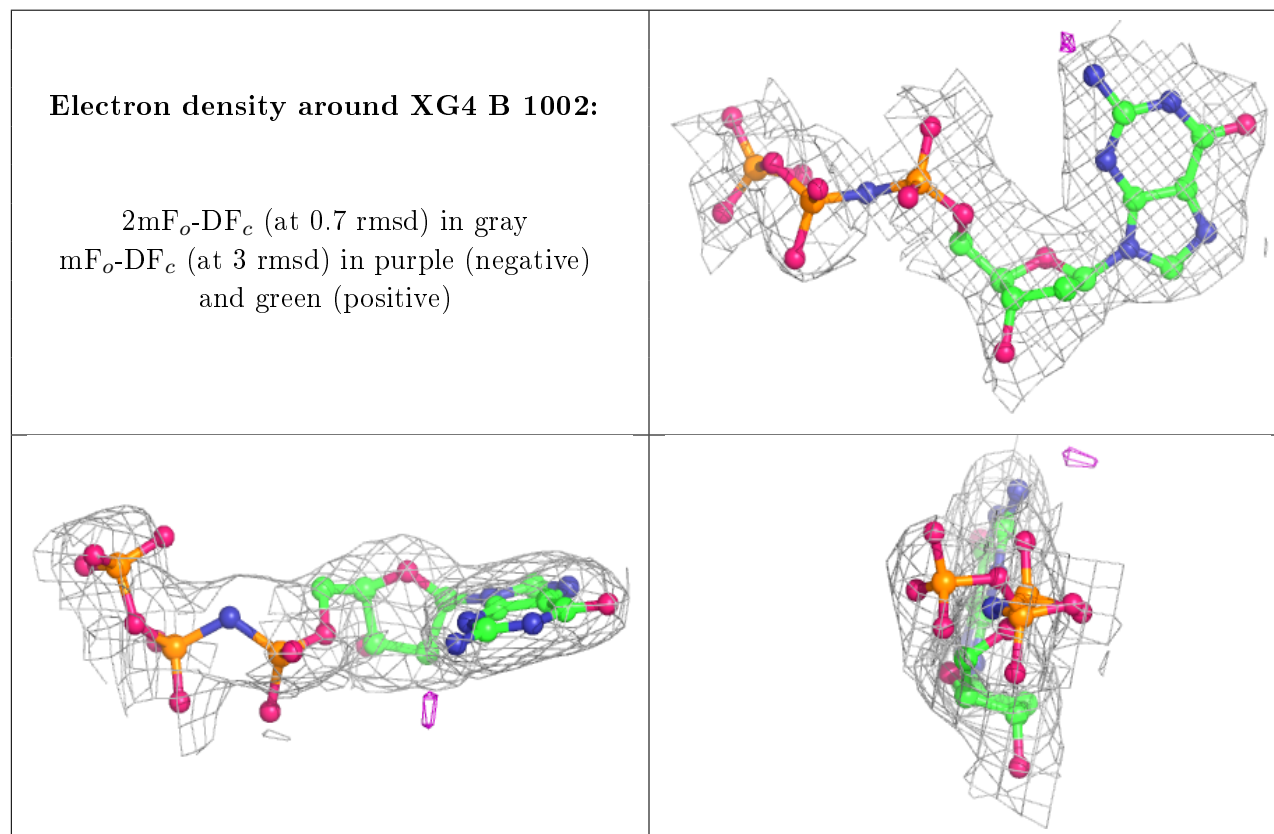
There are no carbohydrates in this entry.

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. 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.

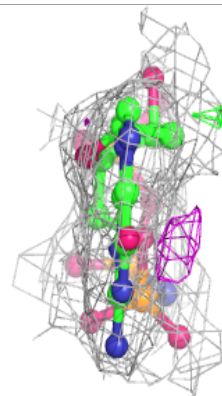
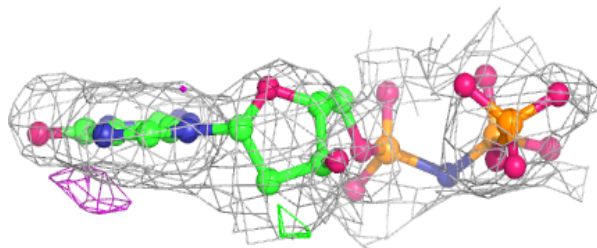
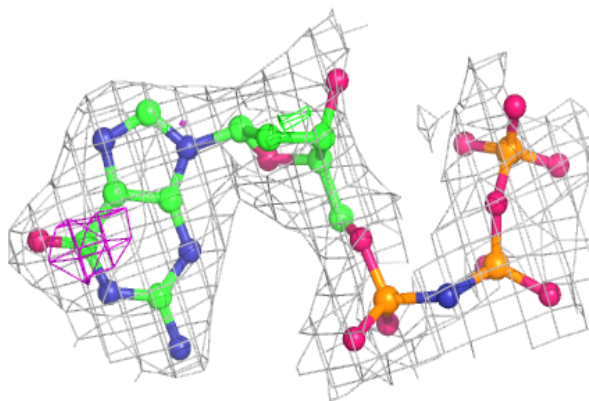
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NA	B	1004	1/1	0.82	0.20	59,59,59,59	0
4	XG4	B	1002	31/31	0.88	0.14	32,45,117,136	0
4	XG4	A	1002	31/31	0.88	0.16	21,53,138,139	0
5	CA	B	1003	1/1	0.90	0.07	78,78,78,78	0
6	NA	A	1004	1/1	0.90	0.12	44,44,44,44	0
4	XG4	A	1001	31/31	0.94	0.14	14,24,52,59	0
5	CA	A	1003	1/1	0.95	0.09	51,51,51,51	0
4	XG4	B	1001	31/31	0.95	0.11	22,29,42,60	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.

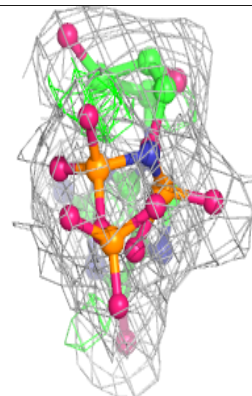
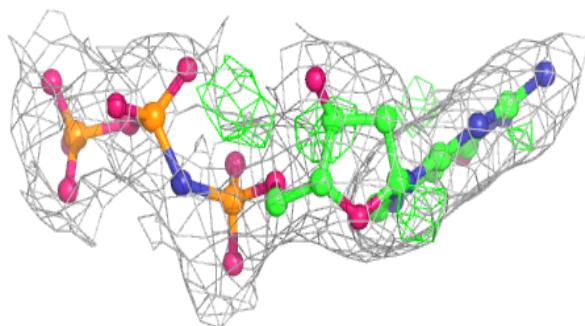
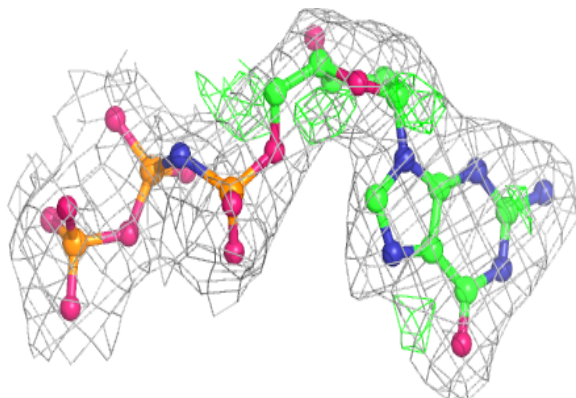


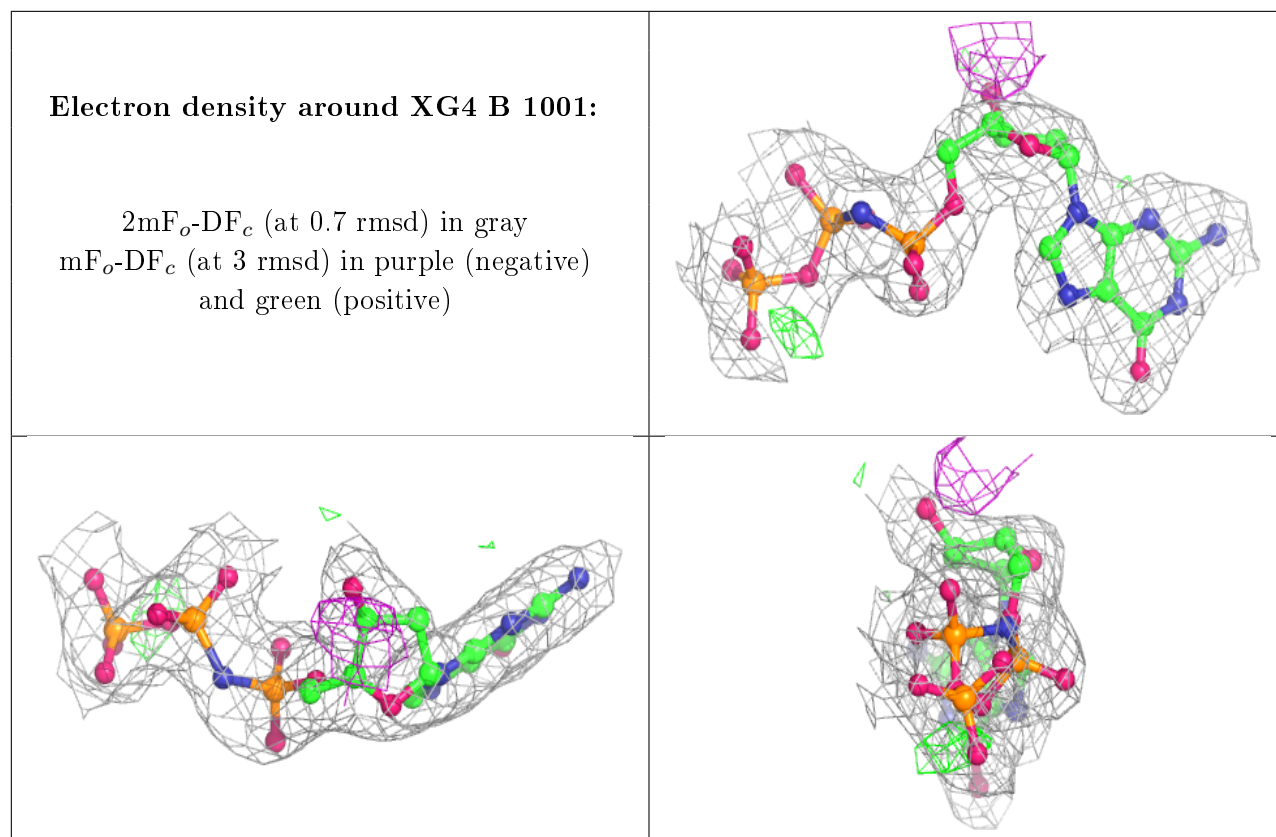
Electron density around XG4 A 1002:

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

**Electron density around XG4 A 1001:**

$2mF_o-DF_c$ (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.