Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 07:58 PM EDT

PDB ID	:	4KHN
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	:	2013-04-30
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

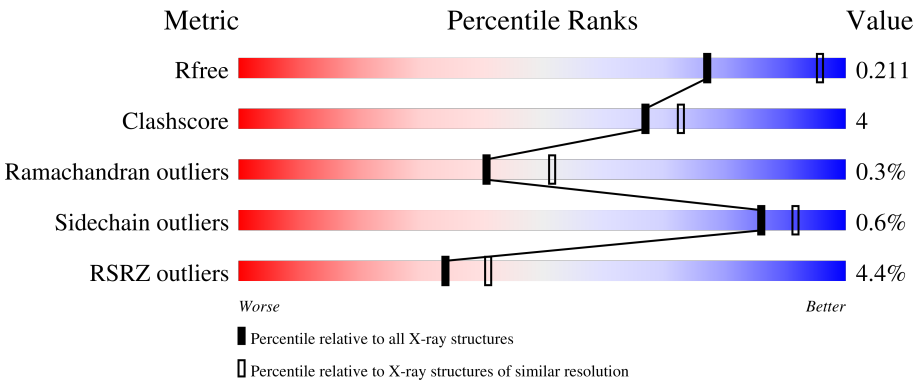
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	3% 92% 8%
1	B	903	6% 83% 13% •
2	C	18	6% 94% 6%
2	E	18	6% 89% 11%

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Mol	Chain	Length	Quality of chain
3	D	13	92% 8%
3	F	13	77% 23%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 15657 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
			Total	C	N	O	S			
1	A	901	7198	4640	1199	1326	33	0	2	0
1	B	870	6730	4352	1113	1235	30	0	1	0

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
			Total	C	N	O	P			
2	C	18	365	174	69	105	17	0	0	0
2	E	18	365	174	69	105	17	0	0	0

- 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
			Total	C	N	O	P			
3	D	13	263	126	48	77	12	0	0	0

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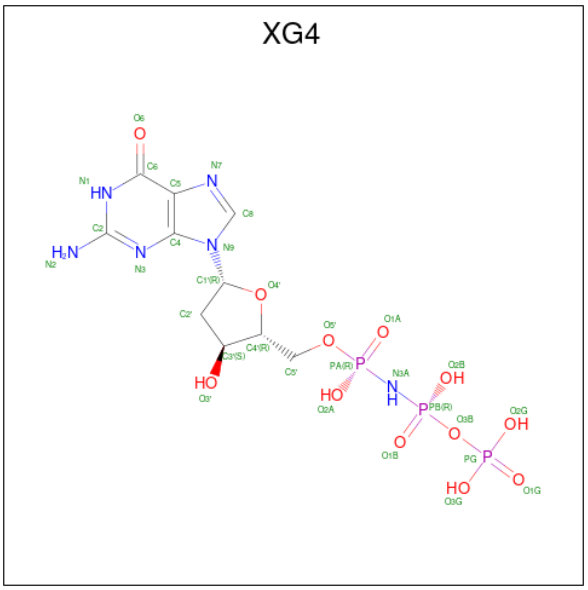
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	13	263	126	48	77	12	0	0	0

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]guanosine (three-letter code: XG4) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

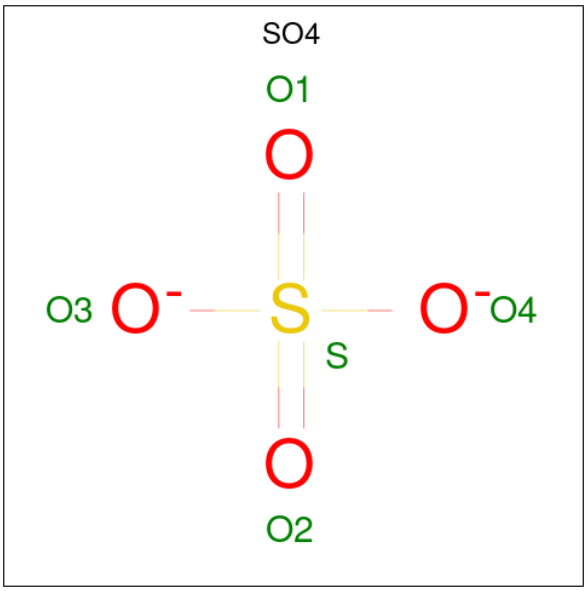


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	6	12	3	0	0
4	C	1	31	10	6	12	3	0	0
4	B	1	31	10	6	12	3	0	0
4	B	1	31	10	6	12	3	0	0

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

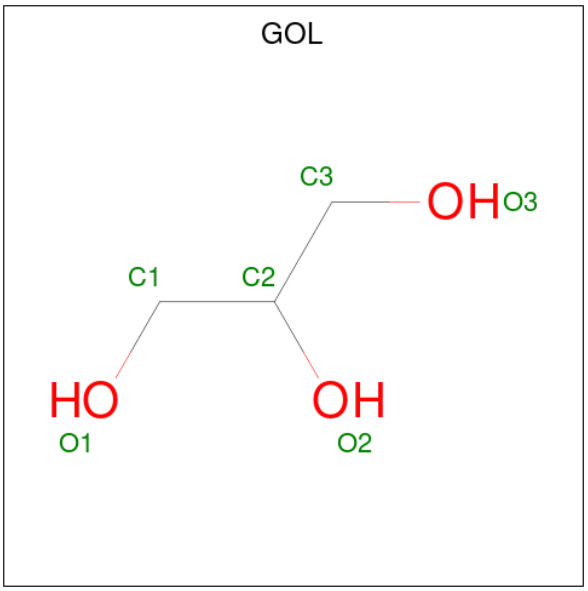
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

- Molecule 9 is water.

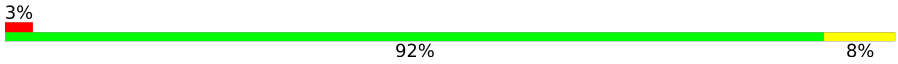
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	228	Total O 228 228	0	0
9	C	23	Total O 23 23	0	0
9	D	17	Total O 17 17	0	0
9	E	6	Total O 6 6	0	0
9	F	3	Total O 3 3	0	0
9	B	27	Total O 27 27	0	0

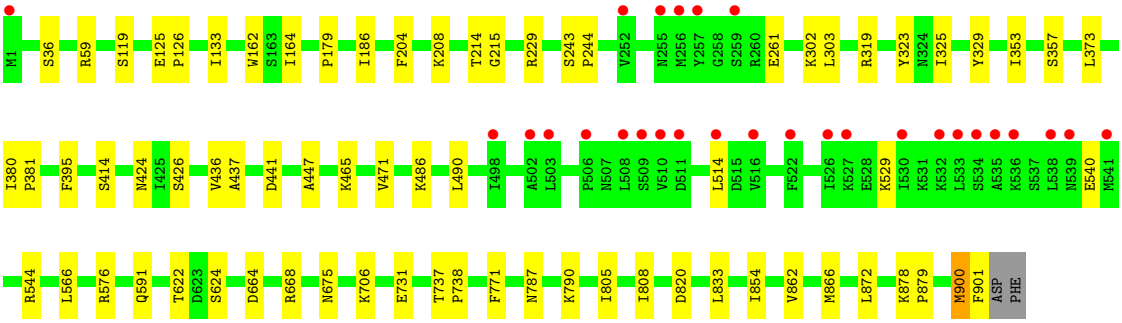
3 Residue-property plots (i)

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

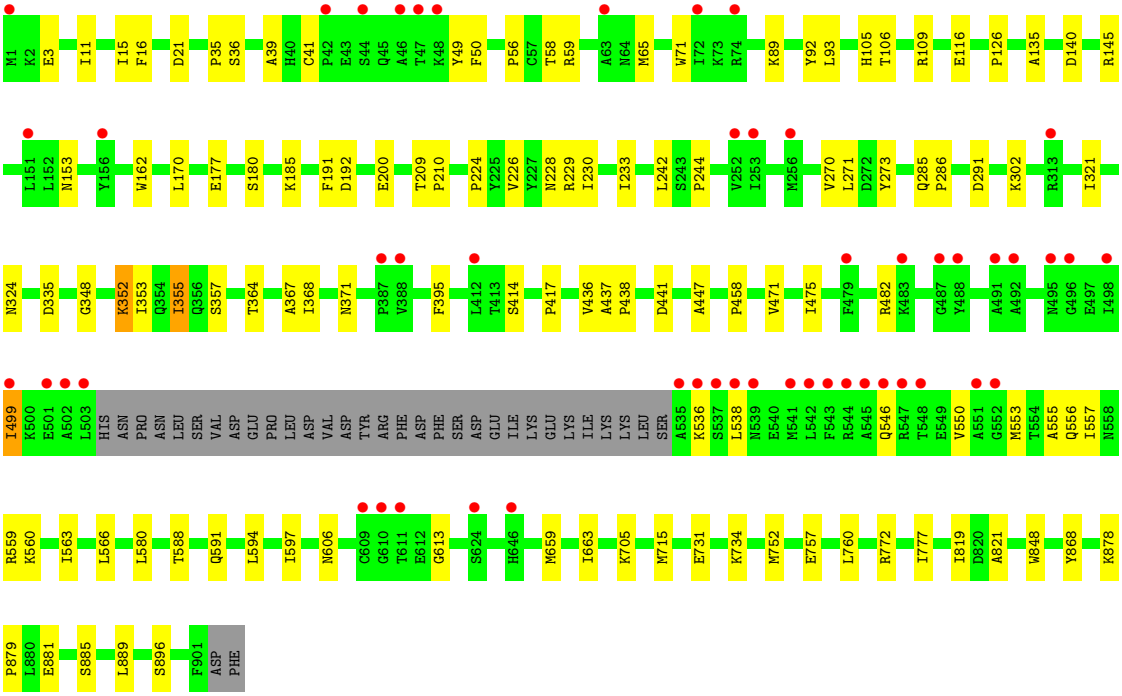
Chain A:





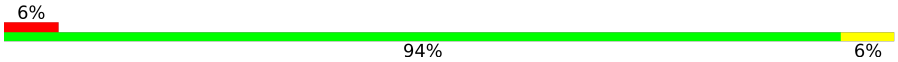
• Molecule 1: DNA polymerase

Chain B:



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

Chain C:



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

Chain E:

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

Chain D:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.26Å 119.35Å 148.03Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	35.33 – 2.55 35.33 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.33-2.55) 95.5 (35.33-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1363)	Depositor
R, R_{free}	0.168 , 0.211 0.168 , 0.211	Depositor DCC
R_{free} test set	4149 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15657	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, NA, XG4, GOL, 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	0.48	0/7382	0.59	1/9996 (0.0%)
1	B	0.43	0/6904	0.56	1/9388 (0.0%)
2	C	0.47	0/409	1.02	0/629
2	E	0.48	0/409	1.05	1/629 (0.2%)
3	D	0.45	0/294	1.05	1/452 (0.2%)
3	F	0.43	0/294	1.09	3/452 (0.7%)
All	All	0.46	0/15692	0.64	7/21546 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	821	ALA	C-N-CD	5.98	140.96	128.40
1	A	900	MET	CB-CG-SD	-5.85	94.86	112.40
3	F	108	DC	C1'-O4'-C4'	-5.29	104.81	110.10
2	E	18	DG	C8-N9-C4	-5.26	104.30	106.40
3	F	108	DC	O4'-C1'-N1	5.11	111.58	108.00
3	D	115	DC	C1'-O4'-C4'	-5.06	105.04	110.10
3	F	115	DC	C1'-O4'-C4'	-5.02	105.08	110.10

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	7198	0	6994	38	0
1	B	6730	0	6330	72	0
2	C	365	0	203	1	0
2	E	365	0	203	1	0
3	D	263	0	148	0	0
3	F	263	0	148	1	0
4	A	31	0	13	0	0
4	B	62	0	26	2	0
4	C	31	0	13	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	25	0	0	0	0
6	B	5	0	0	0	0
7	A	12	0	16	3	0
8	A	1	0	0	0	0
9	A	228	0	0	1	0
9	B	27	0	0	0	0
9	C	23	0	0	0	0
9	D	17	0	0	0	0
9	E	6	0	0	0	0
9	F	3	0	0	0	0
All	All	15657	0	14094	114	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 (114) 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:B:395:PHE:HB2	1:B:591:GLN:HG3	1.61	0.82
1:B:560:LYS:NZ	4:B:1002:XG4:O3G	2.22	0.72
1:B:153:ASN:ND2	1:B:192:ASP:O	2.22	0.71
1:A:833:LEU:HD13	1:A:866:MET:HG2	1.73	0.70
1:A:514:LEU:HD21	1:A:529:LYS:HG2	1.74	0.69
1:B:546:GLN:HE21	1:B:550:VAL:HG23	1.59	0.68
1:A:664:ASP:OD2	1:A:668:ARG:NH1	2.26	0.68
7:A:1008:GOL:H31	4:C:101:XG4:HN3A	1.59	0.67
1:A:486:LYS:HE2	1:A:490:LEU:HD11	1.79	0.64
1:B:170:LEU:HA	1:B:177:GLU:HG3	1.80	0.63
1:A:820:ASP:OD1	1:A:820:ASP:N	2.33	0.62
1:A:668:ARG:HD2	9:A:1290:HOH:O	1.98	0.61
1:B:417:PRO:HG2	1:B:563:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1008:GOL:O3	7:A:1008:GOL:O1	2.18	0.60
1:A:395:PHE:HB2	1:A:591:GLN:HB2	1.86	0.58
1:B:475:ILE:HD12	1:B:566:LEU:HD23	1.86	0.58
1:A:303:LEU:HD21	1:A:319:ARG:HG3	1.86	0.57
1:B:35:PRO:HG3	1:B:65:MET:HG2	1.86	0.55
1:A:900:MET:HE2	1:A:901:PHE:N	2.21	0.55
1:B:36:SER:OG	1:B:59:ARG:NH1	2.39	0.55
1:B:471:VAL:HG13	1:B:566:LEU:HD21	1.88	0.54
1:B:41:CYS:HB3	1:B:58:THR:HG22	1.90	0.54
1:B:209:THR:HG21	1:B:244:PRO:HG3	1.89	0.53
1:B:606:ASN:OD1	1:B:613:GLY:N	2.42	0.53
1:A:186:ILE:HD13	1:A:325:ILE:HD13	1.91	0.53
1:B:367:ALA:O	1:B:371:ASN:ND2	2.32	0.53
1:B:109:ARG:HD2	1:B:140:ASP:OD1	2.09	0.52
1:B:15:ILE:HD13	1:B:92:TYR:CE2	2.45	0.52
1:A:303:LEU:HD23	1:A:323:TYR:HB2	1.90	0.52
1:A:36:SER:OG	1:A:59:ARG:NH1	2.42	0.51
1:B:291:ASP:OD1	1:B:302:LYS:HA	2.10	0.51
1:B:226:VAL:O	1:B:230:ILE:HG12	2.10	0.51
1:A:436:VAL:HG12	1:A:437:ALA:O	2.10	0.51
1:B:50:PHE:HD1	1:B:56:PRO:HA	1.77	0.50
1:B:105:HIS:CE1	1:B:106:THR:HG23	2.47	0.50
1:B:482:ARG:HB2	1:B:559:ARG:HB3	1.92	0.50
1:A:465:LYS:NZ	1:A:675:ASN:OD1	2.44	0.49
1:B:145:ARG:HH11	1:B:185:LYS:HA	1.78	0.49
1:B:436:VAL:HG12	1:B:437:ALA:O	2.12	0.49
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.96	0.48
1:A:787:ASN:HB3	1:A:790:LYS:HB3	1.96	0.47
1:A:133:ILE:HG13	1:A:229:ARG:HG2	1.97	0.47
1:B:50:PHE:CD1	1:B:56:PRO:HA	2.50	0.47
1:B:482:ARG:NE	1:B:560:LYS:HB2	2.30	0.47
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.95	0.47
1:B:555:ALA:HB1	1:B:559:ARG:NH1	2.29	0.47
1:B:659:MET:O	1:B:663:ILE:HG13	2.15	0.47
1:A:540:GLU:HG3	1:A:544:ARG:HE	1.79	0.47
1:B:553:MET:O	1:B:556:GLN:HG3	2.13	0.47
1:B:731:GLU:OE1	1:B:731:GLU:N	2.44	0.47
1:B:109:ARG:HG2	1:B:210:PRO:HA	1.97	0.47
1:B:353:ILE:CD1	1:B:357:SER:HB2	2.45	0.47
4:B:1002:XG4:O2G	4:B:1002:XG4:O2B	2.33	0.46
1:A:706:LYS:HE3	2:C:7:DA:N3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:VAL:HG13	1:A:566:LEU:HD21	1.97	0.46
1:A:771:PHE:CZ	1:A:872:LEU:HB2	2.51	0.46
1:B:772:ARG:HG2	1:B:868:TYR:CG	2.51	0.46
1:B:116:GLU:HG2	1:B:324:ASN:ND2	2.31	0.45
1:B:546:GLN:NE2	1:B:550:VAL:HG23	2.27	0.45
1:B:752:MET:HG2	1:B:760:LEU:HD22	1.97	0.45
1:B:458:PRO:HG2	1:B:588:THR:HG22	1.98	0.45
1:B:438:PRO:HG2	1:B:441:ASP:OD2	2.16	0.45
1:B:777:ILE:HD13	1:B:848:TRP:HZ2	1.81	0.45
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.98	0.45
2:E:8:DA:H5"	1:B:705:LYS:HD3	1.98	0.44
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.48	0.44
1:A:353:ILE:HD12	1:A:357:SER:HB2	1.99	0.44
1:A:854:ILE:HD13	1:A:862:VAL:HG21	2.00	0.44
1:B:39:ALA:HB2	1:B:71:TRP:HH2	1.83	0.44
1:B:499:ILE:HD12	1:B:538:LEU:HD22	1.99	0.44
1:B:553:MET:O	1:B:557:ILE:HG13	2.18	0.44
1:B:597:ILE:HD12	1:B:597:ILE:HA	1.76	0.44
1:B:353:ILE:HD13	1:B:357:SER:HB2	2.00	0.43
1:B:126:PRO:HB2	1:B:224:PRO:HB2	2.00	0.43
1:B:273:TYR:OH	1:B:335:ASP:HA	2.19	0.43
1:B:499:ILE:HD13	1:B:499:ILE:HA	1.85	0.43
1:A:862:VAL:O	1:A:866:MET:HG3	2.19	0.43
1:A:179:PRO:HG2	1:A:329:TYR:CE2	2.54	0.43
1:B:49:TYR:CZ	1:B:59:ARG:HD3	2.54	0.43
1:B:352:LYS:HE3	1:B:352:LYS:HB2	1.63	0.43
1:B:757:GLU:HB2	1:B:889:LEU:HD22	2.01	0.43
1:B:878:LYS:HB3	1:B:879:PRO:HD3	2.00	0.43
3:F:113:DT:H5'	1:B:734:LYS:HG2	2.00	0.43
1:B:3:GLU:HG3	1:B:21:ASP:HA	2.00	0.43
1:B:594:LEU:HD12	1:B:594:LEU:HA	1.86	0.43
1:B:881:GLU:O	1:B:885:SER:HB3	2.18	0.43
7:A:1008:GOL:H32	4:C:101:XG4:N7	2.34	0.42
1:B:126:PRO:O	1:B:228:ASN:ND2	2.52	0.42
1:B:191:PHE:CZ	1:B:200:GLU:HG2	2.54	0.42
1:B:270:VAL:O	1:B:271:LEU:HD23	2.19	0.42
1:B:15:ILE:O	1:B:15:ILE:HD12	2.19	0.42
1:A:731:GLU:OE1	1:A:731:GLU:N	2.48	0.42
1:A:737:THR:HA	1:A:738:PRO:HD3	1.89	0.42
1:A:214:THR:OG1	1:A:215:GLY:N	2.52	0.42
1:B:162:TRP:CD1	1:B:321:ILE:HB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:O	1:A:576:ARG:HD3	2.20	0.42
1:B:229:ARG:O	1:B:233:ILE:HG12	2.19	0.42
1:A:162:TRP:CH2	1:A:164:ILE:HG13	2.55	0.41
1:A:878:LYS:HB3	1:A:879:PRO:HD3	2.02	0.41
1:B:89:LYS:O	1:B:93:LEU:HG	2.20	0.41
1:B:285:GLN:HA	1:B:286:PRO:HD3	1.89	0.41
1:A:125:GLU:HA	1:A:126:PRO:HD2	1.90	0.41
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.56	0.41
1:A:373:LEU:HD12	1:A:380:ILE:HG22	2.03	0.41
1:B:364:THR:O	1:B:368:ILE:HG13	2.20	0.41
1:B:226:VAL:HG12	1:B:242:LEU:HD11	2.02	0.41
1:A:302:LYS:HE2	1:A:323:TYR:CZ	2.55	0.41
1:B:555:ALA:HB1	1:B:559:ARG:HH12	1.85	0.41
1:B:580:LEU:HD12	1:B:580:LEU:HA	1.81	0.41
1:A:243:SER:HA	1:A:244:PRO:HD2	1.83	0.40
1:B:11:ILE:HB	1:B:16:PHE:CE1	2.56	0.40
1:A:805:ILE:HD13	1:A:808:ILE:HD12	2.03	0.40
1:B:715:MET:HE2	1:B:715:MET:HB2	1.98	0.40
1:B:348:GLY:HA3	1:B:355:ILE:HD13	2.04	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	901/903 (100%)	870 (97%)	28 (3%)	3 (0%)	41 51
1	B	867/903 (96%)	832 (96%)	32 (4%)	3 (0%)	41 51
All	All	1768/1806 (98%)	1702 (96%)	60 (3%)	6 (0%)	41 51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	355	ILE
1	B	414	SER
1	B	819	ILE
1	A	414	SER
1	A	622	THR
1	A	424	ASN

5.3.2 Protein sidechains (i)

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	749/798 (94%)	745 (100%)	4 (0%)	88 93
1	B	663/798 (83%)	658 (99%)	5 (1%)	81 88
All	All	1412/1596 (88%)	1403 (99%)	9 (1%)	86 92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	A	261	GLU
1	A	426	SER
1	A	624	SER
1	B	180	SER
1	B	352	LYS
1	B	499	ILE
1	B	536	LYS
1	B	896	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	B	546	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
6	SO4	A	1005	-	4,4,4	0.15	0	6,6,6	0.11	0
4	XG4	B	1001	-	29,33,33	1.62	3 (10%)	35,52,52	1.26	5 (14%)
4	XG4	B	1002	5	29,33,33	1.54	4 (13%)	35,52,52	1.41	5 (14%)
6	SO4	A	1003	-	4,4,4	0.16	0	6,6,6	0.14	0
6	SO4	B	1003	-	4,4,4	0.13	0	6,6,6	0.16	0
4	XG4	A	1001	-	29,33,33	1.67	3 (10%)	35,52,52	1.15	4 (11%)
4	XG4	C	101	5	29,33,33	1.41	3 (10%)	35,52,52	1.67	8 (22%)
6	SO4	A	1006	-	4,4,4	0.12	0	6,6,6	0.13	0
6	SO4	A	1007	-	4,4,4	0.14	0	6,6,6	0.09	0
6	SO4	A	1004	-	4,4,4	0.14	0	6,6,6	0.18	0
7	GOL	A	1008	-	5,5,5	0.23	0	5,5,5	0.96	0
7	GOL	A	1009	-	5,5,5	0.40	0	5,5,5	0.30	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	B	1001	-	-	11/15/34/34	0/3/3/3
4	XG4	B	1002	5	-	7/15/34/34	0/3/3/3
4	XG4	A	1001	-	-	5/15/34/34	0/3/3/3
4	XG4	C	101	5	-	8/15/34/34	0/3/3/3
7	GOL	A	1008	-	-	2/4/4/4	-
7	GOL	A	1009	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	XG4	PA-N3A	4.71	1.75	1.63
4	A	1001	XG4	PA-N3A	4.68	1.75	1.63
4	A	1001	XG4	PB-N3A	4.65	1.75	1.63
4	B	1001	XG4	PB-N3A	4.63	1.75	1.63
4	B	1002	XG4	PB-N3A	4.50	1.75	1.63
4	C	101	XG4	PA-N3A	4.04	1.73	1.63
4	B	1002	XG4	PA-N3A	4.00	1.73	1.63
4	C	101	XG4	PB-N3A	3.60	1.72	1.63
4	A	1001	XG4	C6-N1	-3.20	1.33	1.37
4	C	101	XG4	C6-N1	-2.51	1.34	1.37
4	B	1002	XG4	C6-N1	-2.42	1.34	1.37
4	B	1001	XG4	C6-N1	-2.25	1.34	1.37
4	B	1002	XG4	PB-O3B	2.20	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101	XG4	O1A-PA-N3A	-4.58	105.03	111.77
4	B	1002	XG4	C2'-C1'-N9	-3.91	105.25	114.27
4	C	101	XG4	C2'-C1'-N9	-3.81	105.48	114.27
4	B	1001	XG4	PB-O3B-PG	-3.36	120.79	132.62
4	A	1001	XG4	PB-O3B-PG	-2.84	122.63	132.62
4	C	101	XG4	PB-O3B-PG	-2.54	123.68	132.62
4	B	1001	XG4	C5-C6-N1	2.49	118.35	113.95
4	B	1002	XG4	C5-C6-N1	2.47	118.31	113.95
4	B	1002	XG4	PB-O3B-PG	-2.42	124.08	132.62
4	B	1002	XG4	O6-C6-C5	-2.40	119.68	124.37
4	C	101	XG4	C5-C6-N1	2.40	118.19	113.95
4	C	101	XG4	O1B-PB-N3A	-2.38	108.26	111.77
4	A	1001	XG4	C5-C6-N1	2.35	118.09	113.95
4	C	101	XG4	O2B-PB-O3B	2.34	112.45	104.64
4	C	101	XG4	C8-N7-C5	2.34	107.45	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	XG4	C8-N7-C5	2.32	107.42	102.99
4	B	1001	XG4	C8-N7-C5	2.23	107.24	102.99
4	B	1001	XG4	O6-C6-C5	-2.15	120.17	124.37
4	B	1001	XG4	O1A-PA-N3A	-2.12	108.64	111.77
4	C	101	XG4	O3B-PG-O1G	-2.10	99.52	111.19
4	A	1001	XG4	C2'-C3'-C4'	2.09	107.11	102.76
4	B	1002	XG4	C8-N7-C5	2.08	106.96	102.99

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	XG4	PA-N3A-PB-O1B
4	A	1001	XG4	PB-O3B-PG-O3G
4	C	101	XG4	PB-N3A-PA-O1A
4	C	101	XG4	PA-N3A-PB-O1B
4	C	101	XG4	PG-O3B-PB-O1B
4	C	101	XG4	PG-O3B-PB-O2B
4	C	101	XG4	PB-O3B-PG-O2G
4	B	1001	XG4	PB-N3A-PA-O1A
4	B	1001	XG4	C5'-O5'-PA-O1A
4	B	1001	XG4	C5'-O5'-PA-O2A
4	B	1001	XG4	PA-N3A-PB-O1B
4	B	1001	XG4	PG-O3B-PB-O1B
4	B	1002	XG4	PA-N3A-PB-O1B
4	B	1002	XG4	PG-O3B-PB-O1B
4	B	1002	XG4	PG-O3B-PB-O2B
4	B	1002	XG4	PB-O3B-PG-O2G
7	A	1009	GOL	O1-C1-C2-C3
4	B	1001	XG4	O4'-C4'-C5'-O5'
4	A	1001	XG4	C3'-C4'-C5'-O5'
7	A	1008	GOL	O1-C1-C2-C3
7	A	1009	GOL	O1-C1-C2-O2
4	A	1001	XG4	O4'-C4'-C5'-O5'
4	B	1001	XG4	C3'-C4'-C5'-O5'
7	A	1008	GOL	O1-C1-C2-O2
4	B	1002	XG4	PB-N3A-PA-O5'
4	A	1001	XG4	PB-O3B-PG-O1G
4	B	1002	XG4	PB-N3A-PA-O1A
4	B	1001	XG4	PG-O3B-PB-O2B
4	C	101	XG4	C5'-O5'-PA-O2A
4	B	1001	XG4	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
4	C	101	XG4	PB-O3B-PG-O3G
4	B	1002	XG4	PB-O3B-PG-O3G
4	C	101	XG4	C5'-O5'-PA-O1A
4	B	1001	XG4	PB-N3A-PA-O5'
4	B	1001	XG4	C5'-O5'-PA-N3A

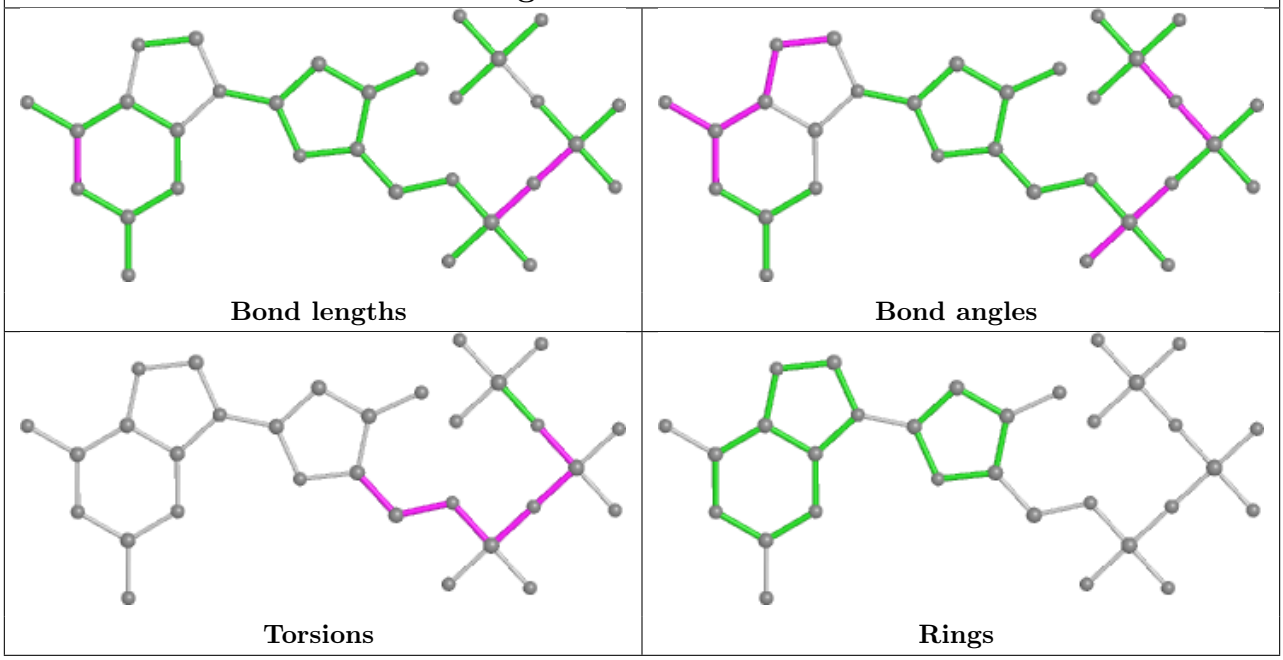
There are no ring outliers.

3 monomers are involved in 5 short contacts:

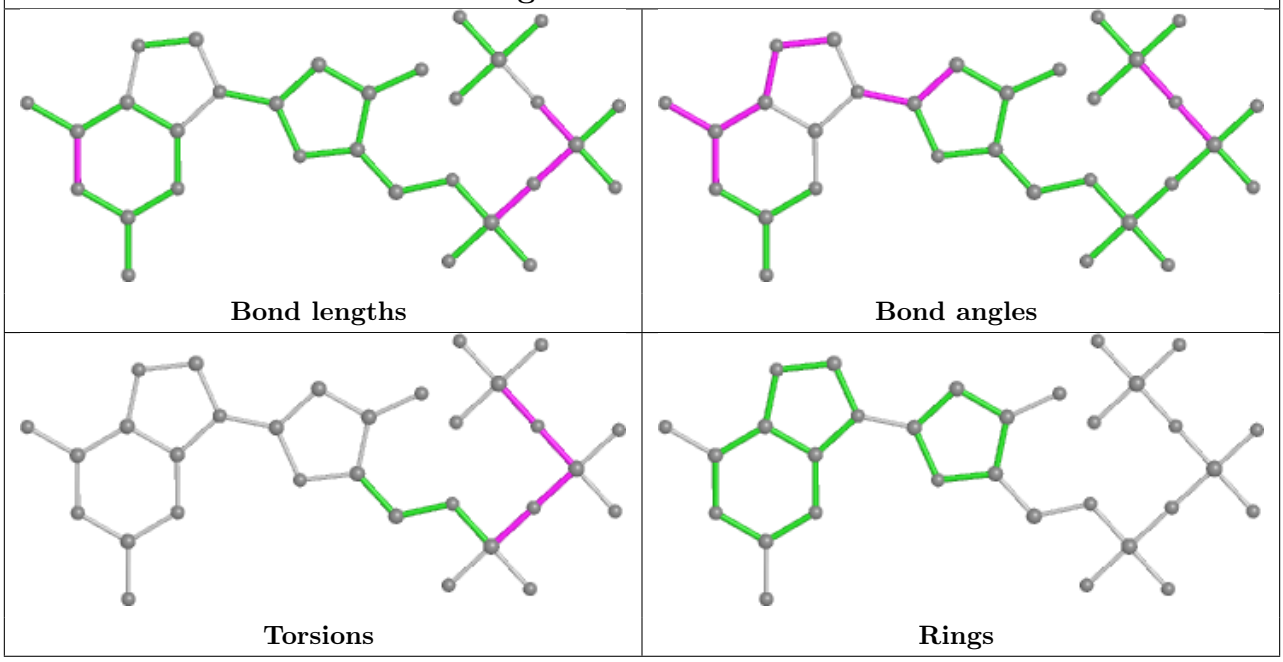
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	XG4	2	0
4	C	101	XG4	2	0
7	A	1008	GOL	3	0

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 then 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.

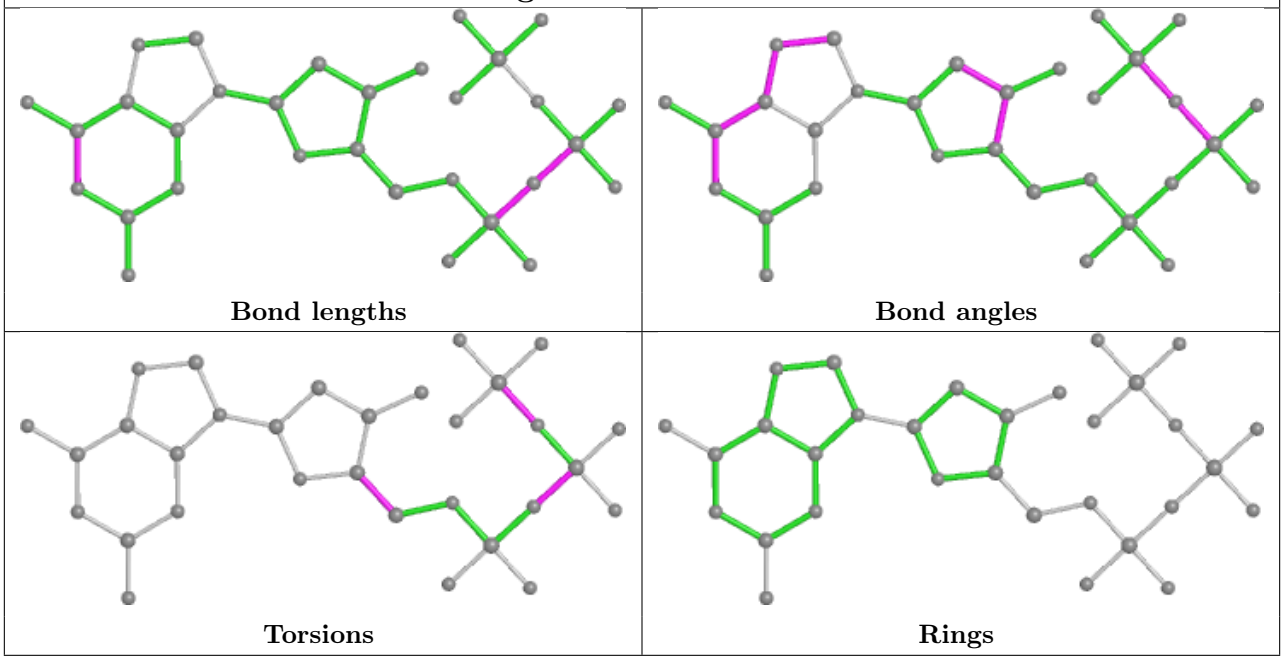
Ligand XG4 B 1001



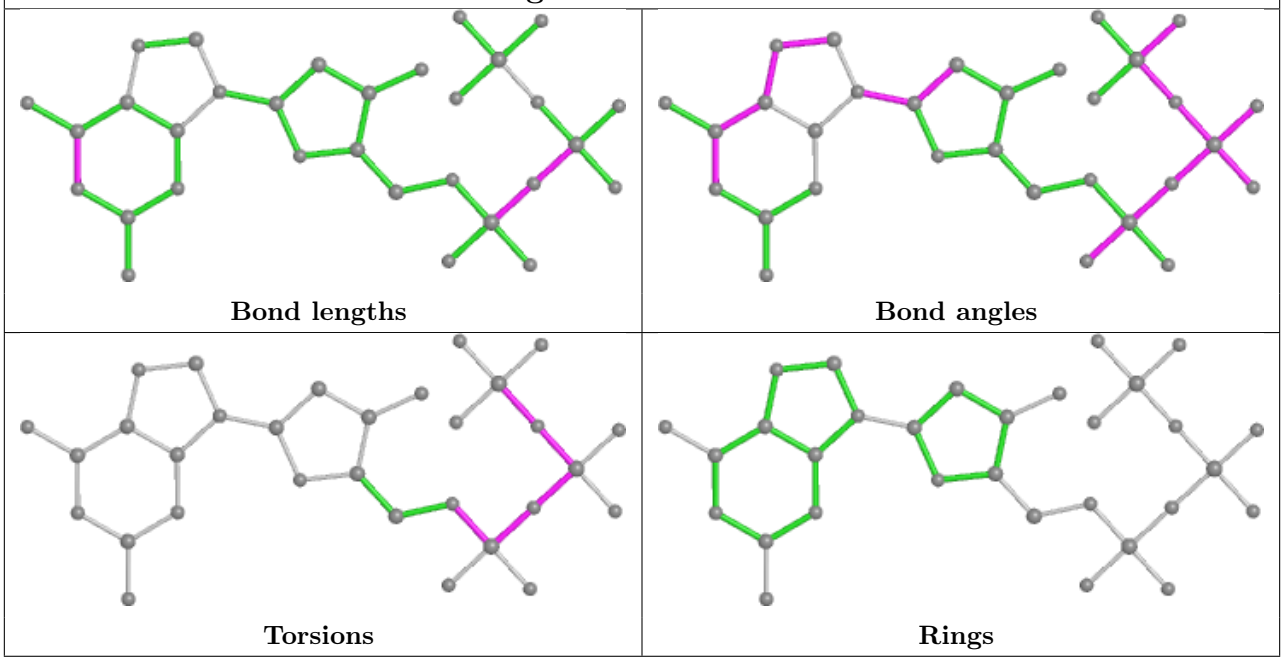
Ligand XG4 B 1002



Ligand XG4 A 1001



Ligand XG4 C 101



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(Å^2)	Q<0.9
1	A	901/903 (99%)	-0.15	28 (3%)	49	56	27, 46, 85, 118	0
1	B	870/903 (96%)	0.17	51 (5%)	22	26	44, 81, 113, 135	0
2	C	18/18 (100%)	0.07	1 (5%)	24	29	29, 44, 118, 128	0
2	E	18/18 (100%)	-0.47	1 (5%)	24	29	50, 66, 118, 126	0
3	D	13/13 (100%)	-0.00	0	100	100	33, 42, 109, 113	0
3	F	13/13 (100%)	-0.07	0	100	100	55, 70, 111, 118	0
All	All	1833/1868 (98%)	0.01	81 (4%)	34	41	27, 62, 109, 135	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	TYR	7.3
1	B	548	THR	6.3
1	A	535	ALA	6.0
1	B	542	LEU	5.9
1	B	543	PHE	5.8
1	A	538	LEU	5.1
1	B	551	ALA	4.9
1	B	496	GLY	4.8
1	A	259	SER	4.6
1	A	516	VAL	4.6
1	A	533	LEU	4.4
1	B	541	MET	4.4
1	B	492	ALA	4.4
1	A	256	MET	4.0
1	B	499	ILE	3.9
1	B	488	TYR	3.9
1	B	72	ILE	3.8
1	B	1	MET	3.8
1	B	552	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	526	ILE	3.6
2	C	1	DT	3.5
1	A	255	ASN	3.5
1	B	46	ALA	3.4
1	B	538	LEU	3.3
1	B	42	PRO	3.3
1	A	534	SER	3.3
1	B	44	SER	3.2
1	B	47	THR	3.2
1	B	388	VAL	3.2
1	A	508	LEU	3.2
1	B	256	MET	3.1
1	B	252	VAL	3.1
1	B	544	ARG	3.0
1	B	74	ARG	3.0
1	B	498	ILE	2.9
1	B	479	PHE	2.9
1	B	624	SER	2.9
1	B	502	ALA	2.9
1	A	1	MET	2.8
1	B	537	SER	2.8
1	B	539	ASN	2.8
1	B	545	ALA	2.7
1	A	503	LEU	2.6
1	B	547	ARG	2.6
1	A	530	ILE	2.6
1	B	501	GLU	2.6
1	A	252	VAL	2.6
1	B	503	LEU	2.6
1	B	151	LEU	2.5
1	A	498	ILE	2.5
1	A	514	LEU	2.5
1	B	491	ALA	2.5
1	B	535	ALA	2.5
1	B	253	ILE	2.4
1	B	546	GLN	2.4
1	A	509	SER	2.4
1	A	510	VAL	2.4
1	B	483	LYS	2.4
1	B	48	LYS	2.4
1	B	387	PRO	2.4
1	A	506	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	156	TYR	2.4
1	B	611	THR	2.3
1	A	539	ASN	2.3
1	A	541	MET	2.3
1	A	502	ALA	2.3
1	B	609	CYS	2.3
1	A	527	LYS	2.2
1	B	610	GLY	2.2
1	B	63	ALA	2.2
1	A	532	LYS	2.1
1	B	646	HIS	2.1
1	A	536	LYS	2.1
2	E	18	DG	2.1
1	B	536	LYS	2.1
1	A	522	PHE	2.0
1	B	495	ASN	2.0
1	B	487	GLY	2.0
1	B	313	ARG	2.0
1	A	511	ASP	2.0
1	B	412	LEU	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 monosaccharides 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(Å^2)	Q<0.9
7	GOL	A	1009	6/6	0.84	0.23	66,73,73,73	0
4	XG4	B	1001	31/31	0.88	0.16	68,100,242,271	0
6	SO4	A	1007	5/5	0.89	0.17	136,137,137,139	0

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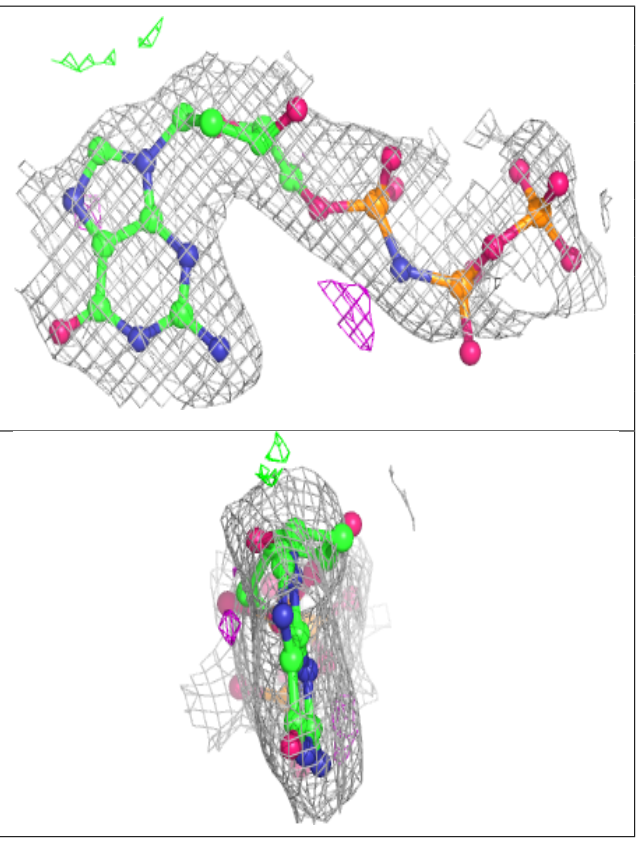
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	1008	6/6	0.90	0.25	44,50,62,69	0
6	SO4	A	1005	5/5	0.91	0.11	114,116,118,118	0
4	XG4	B	1002	31/31	0.93	0.19	47,59,112,307	0
6	SO4	B	1003	5/5	0.94	0.14	93,95,98,98	0
6	SO4	A	1006	5/5	0.94	0.18	109,110,111,113	0
6	SO4	A	1004	5/5	0.94	0.15	94,95,96,103	0
8	NA	A	1010	1/1	0.95	0.21	46,46,46,46	0
4	XG4	A	1001	31/31	0.96	0.14	37,58,206,206	0
4	XG4	C	101	31/31	0.97	0.21	19,31,68,136	0
5	CA	B	1004	1/1	0.97	0.31	82,82,82,82	0
6	SO4	A	1003	5/5	0.99	0.15	47,47,48,53	0
5	CA	A	1002	1/1	1.00	0.22	42,42,42,42	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.

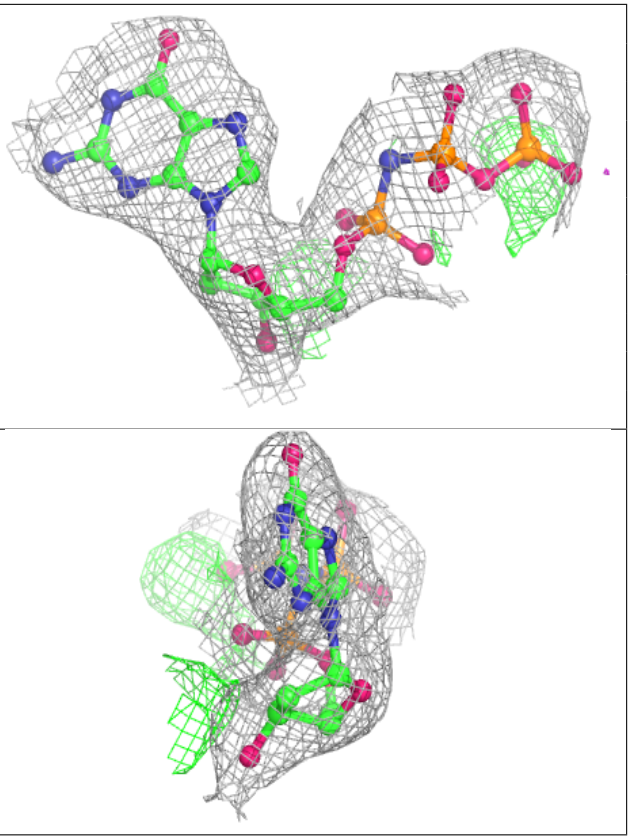
Electron density around XG4 B 1001:

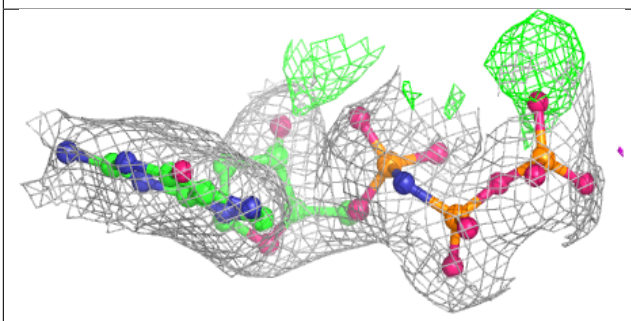
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XG4 B 1002:

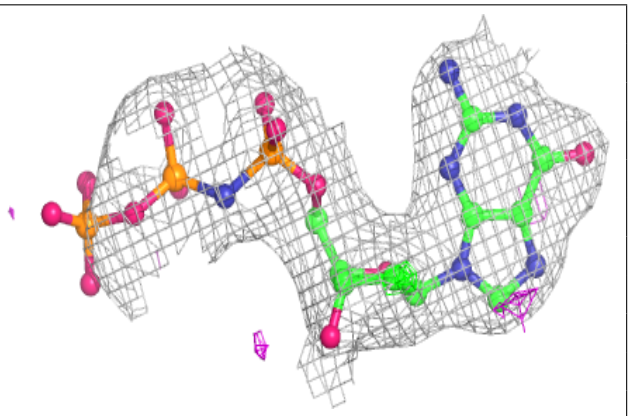
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

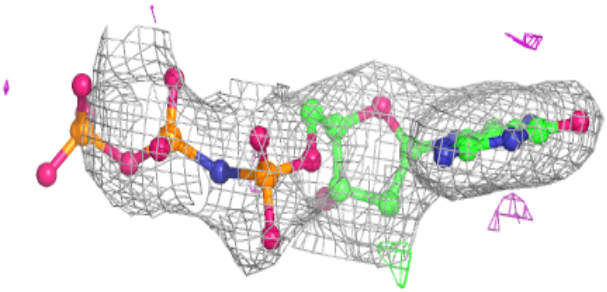


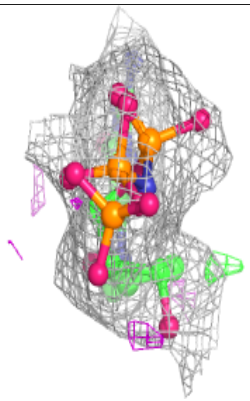


Electron density around XG4 A 1001:

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

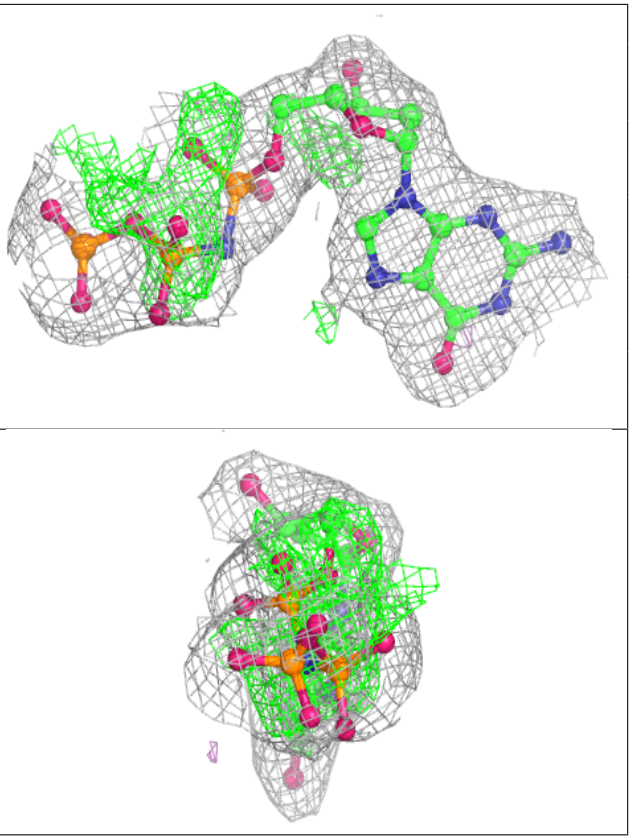






Electron density around XG4 C 101:

$2mF_o$-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.