



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:45 AM UTC

PDB ID : 4IR9 / pdb_00004ir9
Title : Polymerase-DNA complex
Authors : Sharma, A.; Nair, D.T.
Deposited on : 2013-01-14
Resolution : 2.33 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

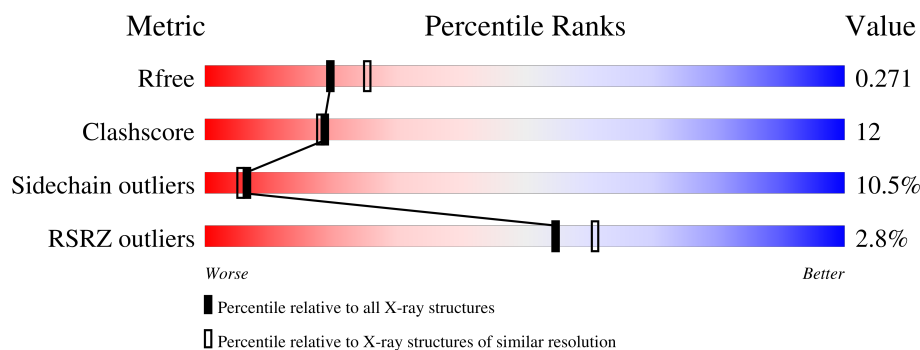
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	B	18	44% 44% 11%
1	G	18	50% 39% 11%
2	C	17	6% 65% 18% 18%
3	H	14	50% 29% 21%
4	A	352	4% 69% 23% 5% .
4	F	352	2% 71% 22% . .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6927 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 DNA chain called DNA (5'-D(P*TP*CP*TP*CP*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	18	Total	C	N	O	P	0	0	0
			362	173	64	108	17			
1	B	18	Total	C	N	O	P	0	0	0
			362	173	64	108	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			344	164	64	100	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	14	Total	C	N	O	P	0	0	0
			284	135	54	82	13			

- Molecule 4 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	342	Total	C	N	O	S	0	0	0
			2687	1695	494	484	14			
4	A	342	Total	C	N	O	S	0	0	0
			2687	1695	494	484	14			

There are 4 discrepancies between the modelled and reference sequences:

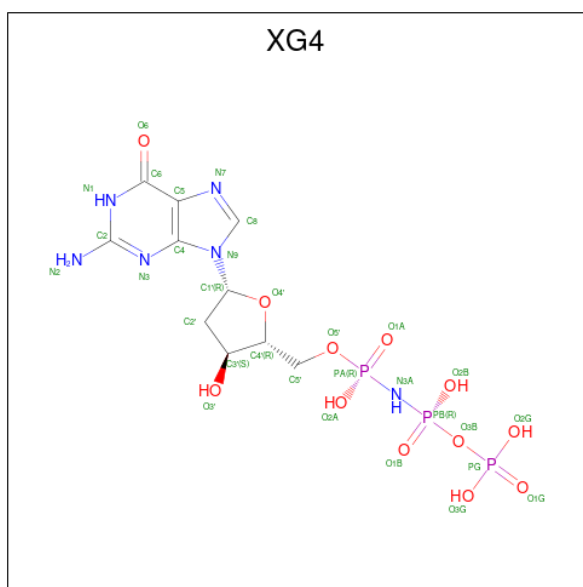
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP Q47155

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	SER	-	expression tag	UNP Q47155
A	0	GLY	-	expression tag	UNP Q47155
A	1	SER	-	expression tag	UNP Q47155

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



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	Mg	0	0
			2	2		
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	20	Total	O	0	0
			20	20		

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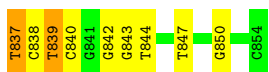
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	7	Total 7	O 7	0	0
7	C	8	Total 8	O 8	0	0
7	H	15	Total 15	O 15	0	0
7	F	63	Total 63	O 63	0	0
7	A	22	Total 22	O 22	0	0

3 Residue-property plots [i](#)

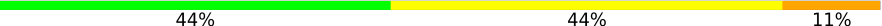
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

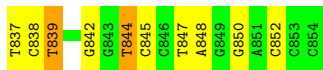
- Molecule 1: DNA (5'-D(P*TP*CP*TP*CP*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3')

Chain G: 



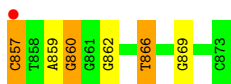
- Molecule 1: DNA (5'-D(P*TP*CP*TP*CP*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3')

Chain B: 



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

Chain C: 



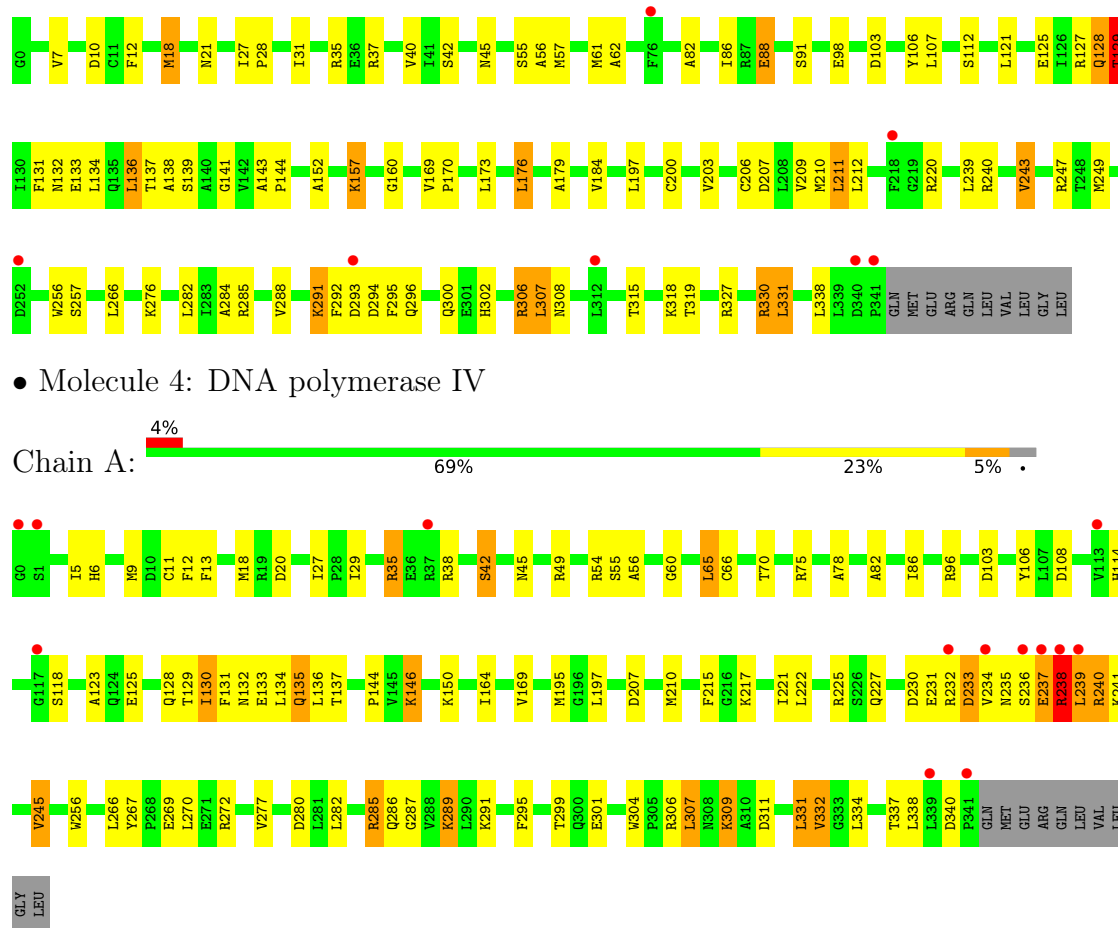
- Molecule 3: DNA (5'-D(P*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3')

Chain H: 



- Molecule 4: DNA polymerase IV

Chain F: 



• Molecule 4: DNA polymerase IV

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.76Å 57.04Å 110.70Å 90.00° 94.76° 90.00°	Depositor
Resolution (Å)	47.66 – 2.33 47.66 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.66-2.33) 99.4 (47.66-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.272 (Not available) , 0.271	Depositor DCC
R_{free} test set	2341 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6927	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: XG4, MG

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	B	0.81	0/404	1.35	5/621 (0.8%)
1	G	0.83	0/404	1.39	7/621 (1.1%)
2	C	0.80	0/385	1.30	3/592 (0.5%)
3	H	0.78	0/318	1.21	4/489 (0.8%)
4	A	0.96	2/2738 (0.1%)	1.10	6/3699 (0.2%)
4	F	1.11	4/2738 (0.1%)	1.17	8/3699 (0.2%)
All	All	0.99	6/6987 (0.1%)	1.18	33/9721 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	1	0
4	F	0	1
All	All	1	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	98	GLU	C-O	-7.32	1.19	1.25
4	A	241	LYS	CA-C	6.14	1.60	1.52
4	F	243	VAL	CA-CB	5.37	1.61	1.54
4	F	7	VAL	C-O	-5.20	1.18	1.24
4	F	243	VAL	C-O	-5.20	1.18	1.24
4	A	169	VAL	C-O	-5.02	1.20	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	837	DT	C5'-C4'-C3'	9.04	128.47	114.90
1	B	839	DT	N1-C1'-C2'	-8.84	100.25	113.50
1	G	850	DG	C2'-C3'-O3'	7.93	123.40	111.50
1	G	837	DT	C5'-C4'-O4'	7.54	120.71	109.40
4	F	128	GLN	N-CA-C	-7.54	100.56	110.43
2	C	857	DC	C5'-C4'-C3'	7.33	125.89	114.90
3	H	863	DT	C4'-C3'-O3'	-7.28	99.08	110.00
4	A	221	ILE	CB-CA-C	-7.19	102.68	111.88
4	F	330	ARG	NE-CZ-NH2	6.61	125.15	119.20
4	F	184	VAL	CB-CA-C	-6.54	102.10	111.19
2	C	866	DT	C4'-C3'-O3'	-6.44	100.34	110.00
1	B	852	DC	C4'-C3'-O3'	-6.33	100.50	110.00
1	G	839	DT	C5'-C4'-C3'	-6.26	105.51	114.90
1	G	847	DT	C2'-C3'-O3'	-6.23	102.16	111.50
3	H	870	DA	C4'-C3'-O3'	-6.18	100.74	110.00
1	B	842	DG	C2'-C3'-O3'	6.11	120.66	111.50
3	H	860	DG	C5'-C4'-C3'	6.00	123.90	114.90
4	F	129	THR	N-CA-CB	5.93	120.50	110.49
4	A	256	TRP	N-CA-C	5.85	117.65	111.28
3	H	863	DT	N1-C2-N3	5.83	123.54	114.80
1	G	844	DT	N1-C2-N3	5.82	123.53	114.80
1	B	844	DT	N1-C2-N3	5.78	123.47	114.80
4	F	88	GLU	N-CA-C	-5.76	105.08	111.36
1	G	844	DT	N1-C2-O2	-5.73	114.61	123.20
4	A	42	SER	O-C-N	5.61	128.09	122.03
4	A	238	ARG	N-CA-C	5.45	117.30	108.41
4	F	296	GLN	N-CA-C	-5.27	103.53	110.33
1	B	850	DG	C2'-C3'-O3'	-5.13	103.81	111.50
4	A	66	CYS	CA-C-N	5.11	125.40	119.47
4	A	66	CYS	C-N-CA	5.11	125.40	119.47
2	C	860	DG	C2'-C3'-O3'	5.07	119.11	111.50
4	F	330	ARG	NE-CZ-NH1	-5.05	116.45	121.50
4	F	18	MET	CB-CG-SD	-5.04	97.58	112.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	837	DT	C4'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	292	PHE	Peptide

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	B	362	0	204	8	0
1	G	362	0	204	13	0
2	C	344	0	192	4	1
3	H	284	0	158	7	0
4	A	2687	0	2739	69	1
4	F	2687	0	2739	64	0
5	A	31	0	13	1	0
5	F	31	0	13	0	0
6	A	2	0	0	0	0
6	F	2	0	0	0	0
7	A	22	0	0	3	0
7	B	7	0	0	0	0
7	C	8	0	0	1	0
7	F	63	0	0	8	0
7	G	20	0	0	4	0
7	H	15	0	0	5	0
All	All	6927	0	6262	155	1

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 12.

All (155) 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)
4:A:18:MET:CE	4:A:45:ASN:HD22	1.67	1.08
4:F:129:THR:N	7:F:550:HOH:O	1.89	1.06
4:F:18:MET:CE	4:F:45:ASN:HD22	1.71	1.02
1:G:837:DT:O3'	7:G:902:HOH:O	1.84	0.94
4:A:129:THR:N	7:A:521:HOH:O	1.96	0.93
4:F:18:MET:HE3	4:F:45:ASN:HD22	1.34	0.90
4:F:157:LYS:NZ	7:F:549:HOH:O	1.99	0.88
4:A:18:MET:HE3	4:A:45:ASN:HD22	1.36	0.86
1:G:838:DC:P	7:G:902:HOH:O	2.32	0.85
3:H:863:DT:O4'	7:H:912:HOH:O	1.94	0.84
4:F:57:MET:HE3	4:F:62:ALA:HA	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:869:DG:N7	7:C:907:HOH:O	2.10	0.83
4:F:57:MET:CE	4:F:62:ALA:HA	2.09	0.82
4:F:129:THR:O	4:F:132:ASN:O	1.97	0.82
2:C:857:DC:H2'	2:C:857:DC:O2	1.78	0.82
4:A:128:GLN:O	4:A:129:THR:OG1	1.96	0.81
4:F:10:ASP:OD2	4:F:137:THR:HG23	1.86	0.76
4:F:291:LYS:O	7:F:523:HOH:O	2.05	0.74
4:F:125:GLU:O	4:F:129:THR:CG2	2.36	0.74
3:H:862:DG:N3	7:H:912:HOH:O	2.21	0.73
4:F:57:MET:HE3	4:F:62:ALA:CA	2.18	0.73
4:F:125:GLU:O	4:F:129:THR:HG23	1.88	0.72
3:H:869:DG:N7	7:H:914:HOH:O	2.22	0.72
3:H:866:DT:O4	7:H:907:HOH:O	2.08	0.71
1:B:838:DC:OP1	4:A:35:ARG:NE	2.25	0.69
3:H:870:DA:N7	7:H:902:HOH:O	2.25	0.68
4:A:233:ASP:OD1	4:A:233:ASP:N	2.27	0.68
1:B:844:DT:H2''	1:B:845:DC:H5'	1.76	0.66
4:F:331:LEU:O	7:F:523:HOH:O	2.14	0.66
4:F:18:MET:HE3	4:F:45:ASN:ND2	2.11	0.65
1:G:843:DG:OP1	4:F:240:ARG:NH1	2.30	0.65
1:G:838:DC:OP1	7:G:902:HOH:O	2.15	0.64
4:A:18:MET:CE	4:A:45:ASN:ND2	2.51	0.64
4:A:96:ARG:C	4:A:234:VAL:HG21	2.22	0.64
4:F:128:GLN:O	4:F:129:THR:HG23	1.99	0.62
4:A:331:LEU:C	4:A:331:LEU:HD23	2.26	0.61
4:F:210:MET:CE	4:F:211:LEU:HD13	2.31	0.61
4:F:294:ASP:OD1	4:F:327:ARG:HD2	2.00	0.61
1:B:847:DT:H2''	1:B:848:DA:OP2	2.01	0.61
4:A:238:ARG:HH12	4:A:240:ARG:CA	2.15	0.60
4:A:129:THR:O	4:A:132:ASN:O	2.19	0.60
1:G:840:DC:H5'	4:F:40:VAL:HG13	1.85	0.59
4:F:331:LEU:N	7:F:523:HOH:O	2.05	0.58
4:F:57:MET:CE	4:F:62:ALA:CA	2.80	0.58
4:A:287:GLY:HA3	4:A:301:GLU:HB3	1.84	0.58
4:A:128:GLN:HA	7:A:521:HOH:O	2.03	0.57
4:A:130:ILE:O	4:A:134:LEU:HB2	2.03	0.57
4:F:300:GLN:NE2	4:F:319:THR:OG1	2.37	0.57
4:A:267:TYR:CG	4:A:309:LYS:HG3	2.40	0.57
1:B:837:DT:H2''	1:B:838:DC:O5'	2.04	0.56
2:C:866:DT:OP2	4:A:285:ARG:NH1	2.35	0.56
1:G:837:DT:C2	4:F:61:MET:HE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:146:LYS:HG3	4:A:230:ASP:OD2	2.06	0.56
1:B:837:DT:H2''	1:B:838:DC:C5'	2.36	0.55
4:A:18:MET:HE3	4:A:45:ASN:ND2	2.16	0.55
4:F:125:GLU:O	4:F:128:GLN:O	2.24	0.55
4:A:75:ARG:NH1	4:A:78:ALA:HB2	2.22	0.55
4:A:231:GLU:O	4:A:232:ARG:HB3	2.07	0.54
4:F:308:ASN:HB2	7:F:538:HOH:O	2.07	0.54
4:A:267:TYR:OH	4:A:307:LEU:HD13	2.08	0.54
4:F:203:VAL:O	4:F:206:CYS:HB2	2.07	0.54
4:A:232:ARG:C	4:A:233:ASP:OD1	2.51	0.54
4:F:302:HIS:HE1	4:F:315:THR:HG21	1.72	0.53
4:A:11:CYS:O	4:A:12:PHE:C	2.52	0.53
4:A:29:ILE:HD13	4:A:70:THR:HB	1.92	0.52
1:B:837:DT:H2''	1:B:838:DC:H5'	1.90	0.52
4:A:125:GLU:O	4:A:128:GLN:O	2.28	0.52
1:G:839:DT:C4	4:F:295:PHE:CE2	2.97	0.51
1:G:837:DT:H2''	1:G:838:DC:C5'	2.40	0.51
4:A:291:LYS:HB3	4:A:331:LEU:HB3	1.91	0.51
4:F:57:MET:HE3	4:F:62:ALA:N	2.26	0.51
4:F:82:ALA:O	4:F:86:ILE:HG23	2.11	0.51
4:A:6:HIS:CE1	4:A:150:LYS:HD2	2.46	0.51
4:F:31:ILE:HD12	4:F:31:ILE:N	2.26	0.50
4:A:280:ASP:O	4:A:282:LEU:HD12	2.11	0.50
4:F:88:GLU:O	4:F:91:SER:OG	2.20	0.50
4:F:35:ARG:NH1	7:F:562:HOH:O	2.44	0.50
4:F:55:SER:O	4:F:56:ALA:HB3	2.12	0.50
4:F:210:MET:HE1	4:F:211:LEU:HD13	1.94	0.50
4:A:146:LYS:NZ	4:A:232:ARG:HH11	2.10	0.50
2:C:859:DA:H2''	2:C:860:DG:C8	2.48	0.49
4:A:96:ARG:CA	4:A:234:VAL:HG21	2.41	0.49
4:A:304:TRP:CD1	4:A:306:ARG:O	2.64	0.49
4:F:306:ARG:O	4:F:307:LEU:C	2.52	0.49
4:A:225:ARG:NH2	4:A:232:ARG:NH2	2.60	0.49
4:A:231:GLU:O	4:A:232:ARG:CB	2.60	0.49
4:A:106:TYR:CE2	4:A:146:LYS:HB2	2.47	0.49
3:H:860:DG:H2''	3:H:861:DG:OP2	2.12	0.48
4:F:210:MET:HE2	4:F:211:LEU:HD13	1.94	0.48
4:A:129:THR:HA	4:A:132:ASN:HB2	1.94	0.48
4:A:238:ARG:NH1	4:A:240:ARG:N	2.61	0.48
4:A:269:GLU:OE1	4:A:272:ARG:HD2	2.13	0.48
4:F:176:LEU:HD12	4:F:200:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:238:ARG:HH12	4:A:240:ARG:N	2.12	0.47
4:F:128:GLN:O	4:F:129:THR:CG2	2.62	0.47
4:F:57:MET:HG3	4:F:61:MET:HE3	1.97	0.47
4:F:132:ASN:O	4:F:133:GLU:HB2	2.15	0.47
4:A:45:ASN:O	4:A:49:ARG:HG3	2.15	0.47
4:A:238:ARG:HH12	4:A:240:ARG:HA	1.80	0.47
4:A:134:LEU:O	4:A:135:GLN:HB2	2.15	0.47
4:F:127:ARG:HD2	4:F:138:ALA:O	2.14	0.47
4:F:27:ILE:HG13	4:F:28:PRO:HD2	1.96	0.46
4:A:20:ASP:OD2	4:A:75:ARG:NH2	2.47	0.46
4:F:57:MET:HE2	4:F:62:ALA:HB2	1.97	0.46
4:F:141:GLY:HA3	4:F:152:ALA:HB3	1.98	0.46
4:A:108:ASP:C	4:A:108:ASP:OD2	2.59	0.46
4:F:212:LEU:HD21	4:F:220:ARG:HB2	1.97	0.46
4:A:235:ASN:O	4:A:237:GLU:N	2.47	0.45
4:A:9:MET:HE3	4:A:137:THR:O	2.17	0.45
4:F:106:TYR:C	4:F:107:LEU:HD23	2.41	0.44
1:G:840:DC:H2'	1:G:840:DC:O5'	2.18	0.44
4:A:289:LYS:HB2	4:A:299:THR:HG22	1.98	0.44
1:G:839:DT:OP2	4:F:330:ARG:NH1	2.37	0.44
1:G:838:DC:C5'	7:G:902:HOH:O	2.65	0.44
4:A:13:PHE:CD2	5:A:401:XG4:H2'A	2.52	0.44
4:A:239:LEU:HD13	4:A:277:VAL:HG13	2.00	0.44
4:F:131:PHE:HA	4:F:136:LEU:O	2.17	0.44
4:F:284:ALA:C	4:F:285:ARG:HG3	2.41	0.44
4:F:210:MET:HE2	4:F:211:LEU:N	2.33	0.43
4:A:195:MET:HE1	4:A:215:PHE:CE1	2.53	0.43
4:A:304:TRP:HD1	4:A:306:ARG:O	2.00	0.43
4:A:82:ALA:O	4:A:86:ILE:HG23	2.18	0.43
4:A:238:ARG:HD2	4:A:238:ARG:HA	1.66	0.43
4:F:143:ALA:HB1	4:F:144:PRO:CD	2.48	0.43
4:F:106:TYR:O	4:F:107:LEU:HD23	2.19	0.43
4:A:285:ARG:HG3	4:A:337:THR:OG1	2.19	0.42
4:F:12:PHE:CD2	4:F:103:ASP:HB3	2.55	0.42
4:F:139:SER:HA	4:F:160:GLY:O	2.19	0.42
3:H:866:DT:OP2	4:F:285:ARG:NH1	2.44	0.42
4:A:146:LYS:HZ3	4:A:232:ARG:HH11	1.67	0.42
1:G:837:DT:H2''	1:G:838:DC:H5'	2.02	0.42
4:F:173:LEU:O	4:F:200:CYS:HB2	2.19	0.42
4:F:249:MET:SD	4:F:249:MET:N	2.93	0.42
4:A:27:ILE:O	4:A:29:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:256:TRP:O	4:F:257:SER:C	2.62	0.42
4:A:55:SER:O	4:A:56:ALA:HB3	2.20	0.42
4:F:179:ALA:O	7:F:534:HOH:O	2.21	0.42
4:A:5:ILE:HD12	4:A:123:ALA:HB2	2.02	0.42
1:B:837:DT:O3'	4:A:35:ARG:NH2	2.51	0.41
1:B:839:DT:H2'	4:A:295:PHE:CZ	2.55	0.41
4:A:286:GLN:NE2	4:A:311:ASP:OD2	2.47	0.41
4:A:144:PRO:HD3	4:A:164:ILE:O	2.21	0.41
4:A:96:ARG:HB3	4:A:234:VAL:HG21	2.03	0.41
4:A:245:VAL:HG23	4:A:270:LEU:HB2	2.03	0.41
4:A:35:ARG:NE	4:A:60:GLY:HA3	2.36	0.41
4:F:169:VAL:HB	4:F:170:PRO:HD3	2.01	0.41
4:A:29:ILE:CD1	4:A:70:THR:HB	2.51	0.41
4:A:331:LEU:HD23	4:A:332:VAL:N	2.36	0.41
4:A:131:PHE:HB3	7:A:521:HOH:O	2.21	0.41
1:G:842:DG:H2'	1:G:843:DG:O4'	2.21	0.40
4:F:21:ASN:OD1	4:F:21:ASN:C	2.64	0.40
4:F:207:ASP:OD2	4:F:209:VAL:HB	2.22	0.40
4:A:11:CYS:SG	4:A:49:ARG:NH2	2.94	0.40
4:F:132:ASN:O	4:F:133:GLU:CB	2.68	0.40
4:A:65:LEU:HD12	4:A:65:LEU:HA	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:862:DG:OP1	4:A:118:SER:OG[2_445]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	
4	A	286/297 (96%)	251 (88%)	35 (12%)	5	4
4	F	286/297 (96%)	261 (91%)	25 (9%)	9	10
All	All	572/594 (96%)	512 (90%)	60 (10%)	6	5

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	37	ARG
4	F	42	SER
4	F	112	SER
4	F	121	LEU
4	F	129	THR
4	F	134	LEU
4	F	136	LEU
4	F	157	LYS
4	F	176	LEU
4	F	197	LEU
4	F	211	LEU
4	F	239	LEU
4	F	243	VAL
4	F	247	ARG
4	F	266	LEU
4	F	276	LYS
4	F	282	LEU
4	F	288	VAL
4	F	291	LYS
4	F	293	ASP
4	F	306	ARG
4	F	307	LEU
4	F	318	LYS
4	F	331	LEU
4	F	338	LEU
4	A	35	ARG
4	A	38	ARG
4	A	42	SER
4	A	54	ARG
4	A	65	LEU
4	A	103	ASP
4	A	114	HIS
4	A	130	ILE

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Mol	Chain	Res	Type
4	A	133	GLU
4	A	135	GLN
4	A	136	LEU
4	A	146	LYS
4	A	197	LEU
4	A	207	ASP
4	A	210	MET
4	A	217	LYS
4	A	222	LEU
4	A	227	GLN
4	A	233	ASP
4	A	236	SER
4	A	237	GLU
4	A	238	ARG
4	A	239	LEU
4	A	240	ARG
4	A	245	VAL
4	A	266	LEU
4	A	285	ARG
4	A	289	LYS
4	A	307	LEU
4	A	309	LYS
4	A	331	LEU
4	A	332	VAL
4	A	334	LEU
4	A	338	LEU
4	A	340	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
4	F	45	ASN
4	F	116	HIS
4	F	124	GLN
4	F	159	ASN
4	F	227	GLN
4	F	296	GLN
4	F	300	GLN
4	A	45	ASN
4	A	84	ASN
4	A	235	ASN
4	A	254	HIS

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Mol	Chain	Res	Type
4	A	308	ASN
4	A	335	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	XG4	A	401	6	32,33,33	1.94	7 (21%)	46,52,52	2.01	12 (26%)
5	XG4	F	401	6	32,33,33	1.72	7 (21%)	46,52,52	2.55	19 (41%)

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
5	XG4	A	401	6	-	5/19/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	XG4	F	401	6	-	4/19/34/34	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	XG4	PB-O1B	4.90	1.53	1.46
5	A	401	XG4	PA-O1A	4.80	1.53	1.46
5	A	401	XG4	PB-O3B	4.32	1.64	1.59
5	F	401	XG4	C5-C4	3.41	1.48	1.38
5	F	401	XG4	PA-O1A	3.32	1.51	1.46
5	A	401	XG4	C5-C4	3.06	1.47	1.38
5	F	401	XG4	C5-N7	-2.89	1.33	1.39
5	A	401	XG4	PA-O2A	-2.82	1.49	1.56
5	F	401	XG4	C4-N9	-2.78	1.31	1.38
5	F	401	XG4	C6-N1	-2.58	1.34	1.38
5	A	401	XG4	C6-N1	-2.54	1.34	1.38
5	F	401	XG4	PA-O2A	-2.52	1.50	1.56
5	A	401	XG4	C5-N7	-2.32	1.34	1.39
5	F	401	XG4	C8-N7	2.16	1.38	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	401	XG4	C5-C4-N3	-6.85	117.49	128.39
5	F	401	XG4	C2-N3-C4	5.99	122.62	112.30
5	F	401	XG4	O1B-PB-N3A	-5.19	104.13	111.77
5	A	401	XG4	O3B-PB-N3A	-4.73	93.48	106.59
5	A	401	XG4	C5-C4-N3	-4.70	120.92	128.39
5	F	401	XG4	O3B-PB-N3A	-4.55	93.98	106.59
5	F	401	XG4	O2B-PB-O3B	4.41	119.36	104.64
5	A	401	XG4	O1B-PB-N3A	4.04	117.71	111.77
5	A	401	XG4	C2-N3-C4	3.96	119.13	112.30
5	A	401	XG4	N9-C4-N3	3.90	133.74	125.95
5	A	401	XG4	O2A-PA-O1A	3.70	117.80	109.87
5	A	401	XG4	O2B-PB-O1B	3.69	117.79	109.87
5	F	401	XG4	O2A-PA-O1A	3.60	117.58	109.87
5	F	401	XG4	C6-C5-N7	3.57	136.78	130.29
5	A	401	XG4	O2B-PB-O3B	3.46	116.19	104.64
5	F	401	XG4	O2B-PB-O1B	3.46	117.28	109.87
5	F	401	XG4	N9-C4-N3	3.41	132.77	125.95
5	F	401	XG4	C4-C5-N7	-3.34	105.37	110.67
5	F	401	XG4	O5'-PA-O1A	-3.04	105.24	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	401	XG4	C2-N1-C6	-3.00	119.68	125.11
5	F	401	XG4	O2G-PG-O1G	2.92	122.21	110.83
5	F	401	XG4	C2'-C1'-N9	-2.86	106.67	113.81
5	F	401	XG4	N2-C2-N3	-2.81	114.18	119.67
5	A	401	XG4	O6-C6-C5	-2.76	119.25	126.53
5	F	401	XG4	O1A-PA-N3A	-2.66	107.85	111.77
5	A	401	XG4	C6-C5-N7	2.64	135.09	130.29
5	A	401	XG4	C2'-C1'-N9	-2.30	108.06	113.81
5	F	401	XG4	N2-C2-N1	2.28	121.57	116.76
5	F	401	XG4	C5-C4-N9	2.28	109.73	105.66
5	F	401	XG4	O4'-C1'-N9	2.08	111.56	107.86
5	A	401	XG4	O1A-PA-N3A	-2.00	108.82	111.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	401	XG4	PB-N3A-PA-O1A
5	F	401	XG4	PA-N3A-PB-O1B
5	F	401	XG4	PB-O3B-PG-O2G
5	A	401	XG4	PB-N3A-PA-O1A
5	A	401	XG4	PA-N3A-PB-O1B
5	A	401	XG4	PB-O3B-PG-O2G
5	F	401	XG4	PB-O3B-PG-O1G
5	A	401	XG4	C5'-O5'-PA-O2A
5	A	401	XG4	PB-O3B-PG-O1G

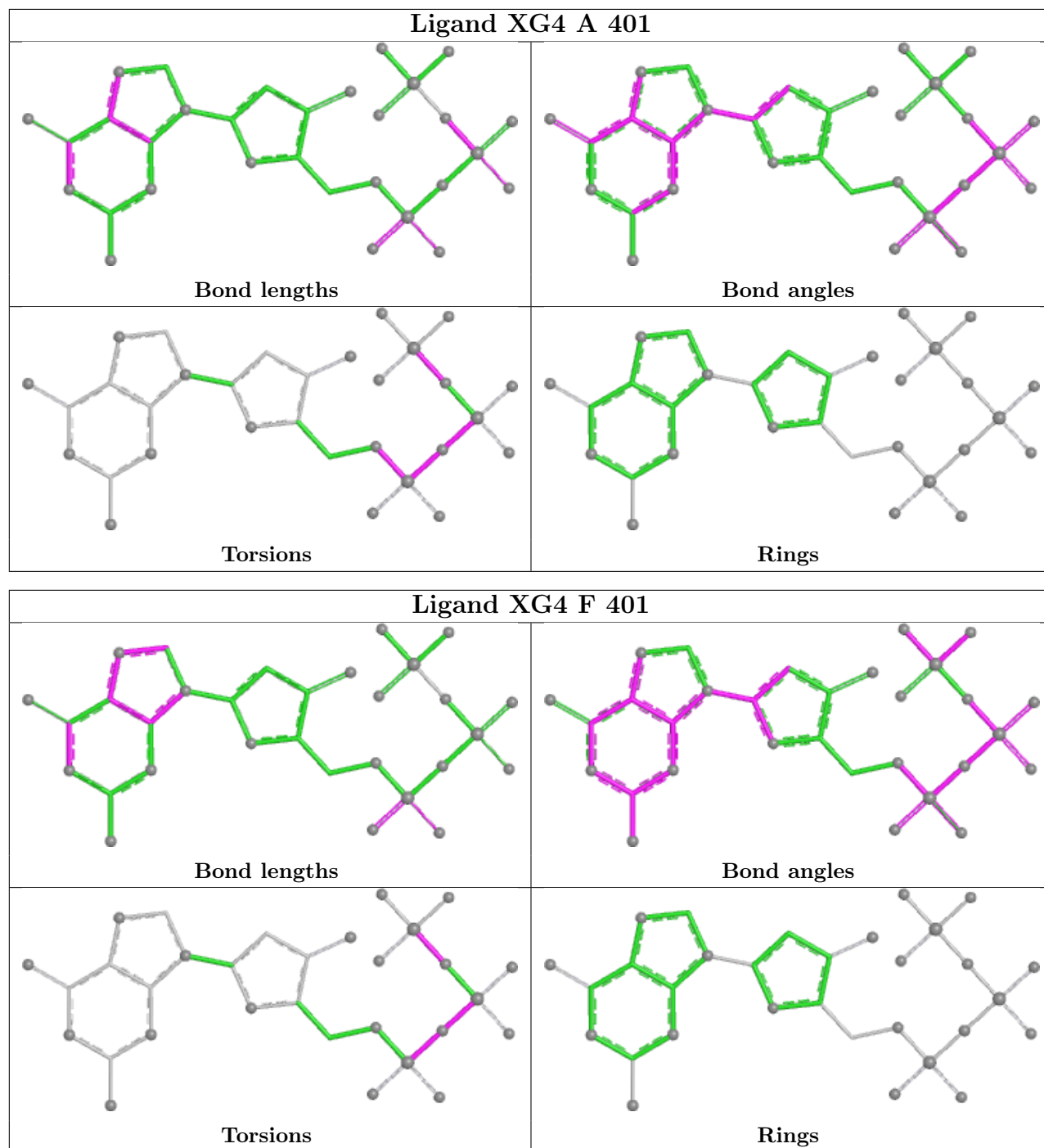
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	B	18/18 (100%)	-0.14	0 100 100	42, 60, 100, 104	0
1	G	18/18 (100%)	-0.44	0 100 100	36, 52, 100, 105	0
2	C	17/17 (100%)	-0.13	1 (5%) 28 33	46, 57, 71, 152	0
3	H	14/14 (100%)	-0.42	0 100 100	35, 52, 88, 110	0
4	A	342/352 (97%)	0.51	13 (3%) 44 50	36, 58, 93, 128	0
4	F	342/352 (97%)	0.32	7 (2%) 65 70	30, 49, 71, 102	0
All	All	751/771 (97%)	0.35	21 (2%) 55 61	30, 54, 86, 152	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	341	PRO	6.7
4	A	234	VAL	5.1
4	F	341	PRO	5.0
4	A	239	LEU	5.0
4	A	0	GLY	4.4
2	C	857	DC	3.7
4	A	237	GLU	3.2
4	A	238	ARG	2.9
4	A	236	SER	2.7
4	F	340	ASP	2.6
4	F	218	PHE	2.5
4	A	117	GLY	2.4
4	F	76	PHE	2.3
4	A	232	ARG	2.3
4	A	113	VAL	2.3
4	F	252	ASP	2.2
4	A	1	SER	2.2
4	A	339	LEU	2.1
4	F	293	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	312	LEU	2.1
4	A	37	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

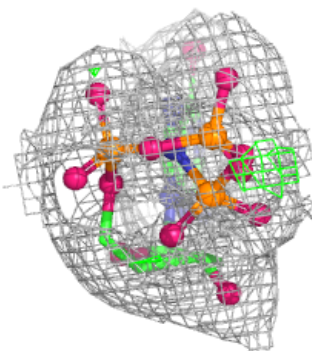
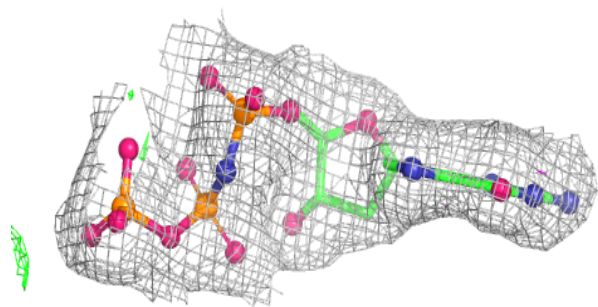
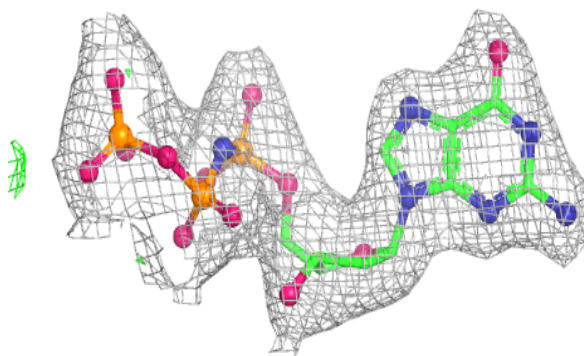
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	403	1/1	0.77	0.14	104,104,104,104	0
5	XG4	A	401	31/31	0.96	0.07	43,51,57,57	0
6	MG	F	403	1/1	0.97	0.11	57,57,57,57	0
5	XG4	F	401	31/31	0.98	0.05	30,32,36,39	0
6	MG	A	402	1/1	0.99	0.03	30,30,30,30	0
6	MG	F	402	1/1	1.00	0.08	20,20,20,20	0

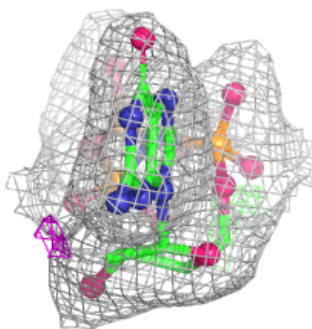
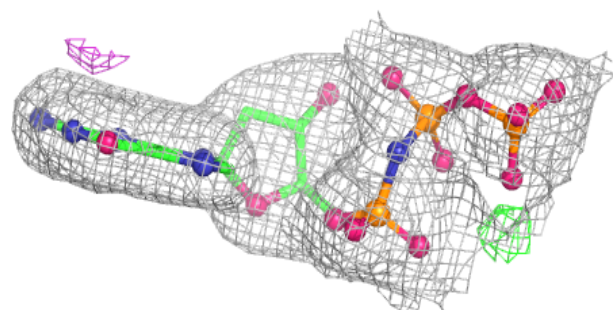
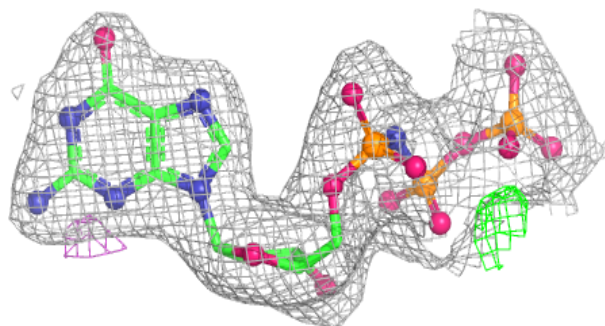
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XG4 A 401:

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

**Electron density around XG4 F 401:**

$2mF_o-DF_c$ (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.