



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:02 PM UTC

PDB ID : 5W51 / pdb_00005w51
Title : Pol II elongation complex with an N6-methyladenine-containing template and a matched UMPNPP
Authors : Wang, W.; Wang, D.
Deposited on : 2017-06-13
Resolution : 3.40 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

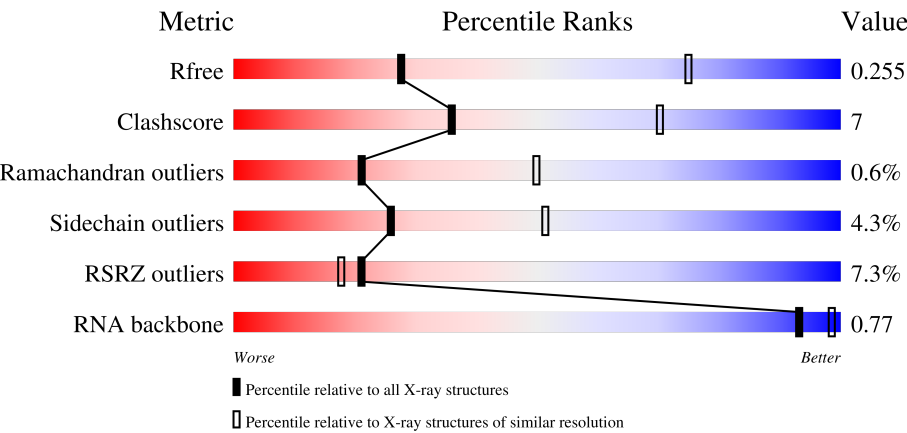
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	7% 61% 17% • 21%
2	B	1224	5% 67% 20% • 11%
3	C	318	2% 67% 15% • 16%
4	E	215	8% 88% 10% ••

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	T	29	
12	N	14	
13	R	9	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 28880 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-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1371	Total	C	N	O	S	0	0	0
			10787	6806	1886	2034	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1089	Total	C	N	O	S	0	0	0
			8657	5485	1517	1601	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	130	Total	C	N	O	S	0	0	0
			1043	660	173	206	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	115	Total	C	N	O	S	0	0	0
			935	575	170	180	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 11 is a DNA chain called 29mer template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	29	Total	C	N	O	P	0	0	0
			588	283	107	170	28			

- Molecule 12 is a DNA chain called 14mer non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 13 is a RNA chain called 9mer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			198	89	42	59	8			

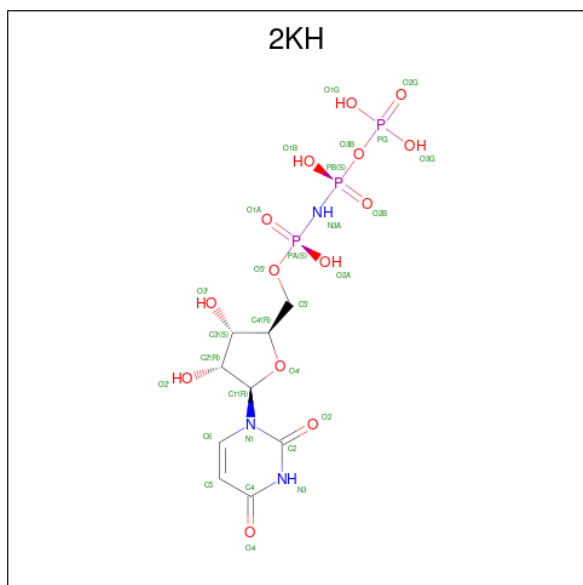
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		
14	C	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	L	1	Total	Zn	0	0
			1	1		

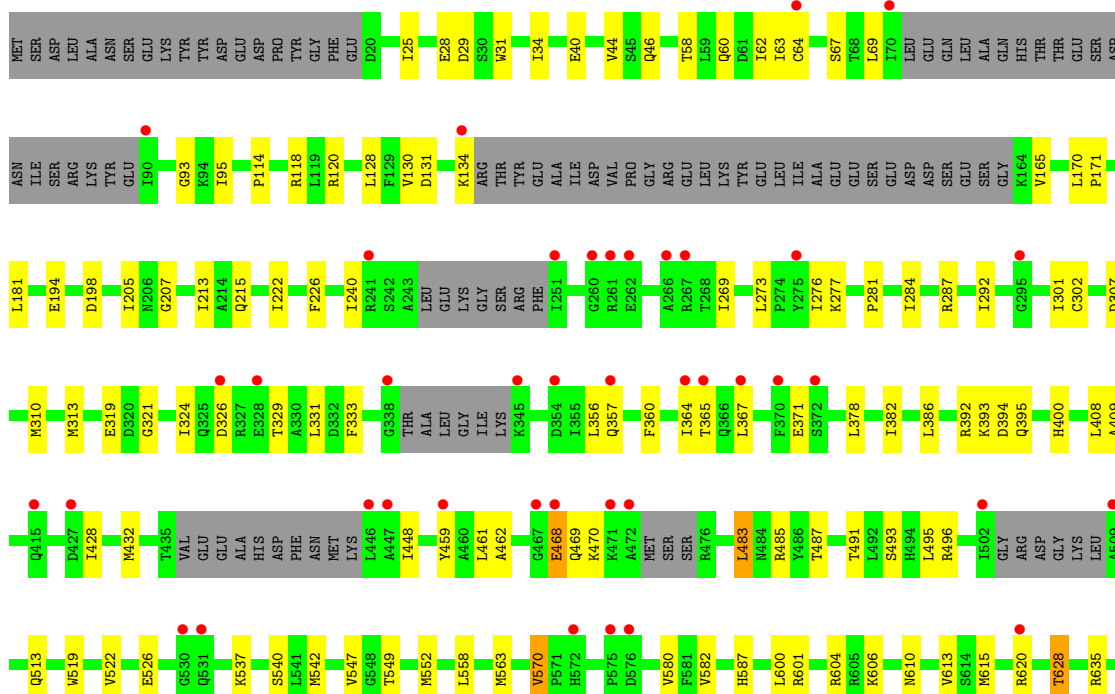
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

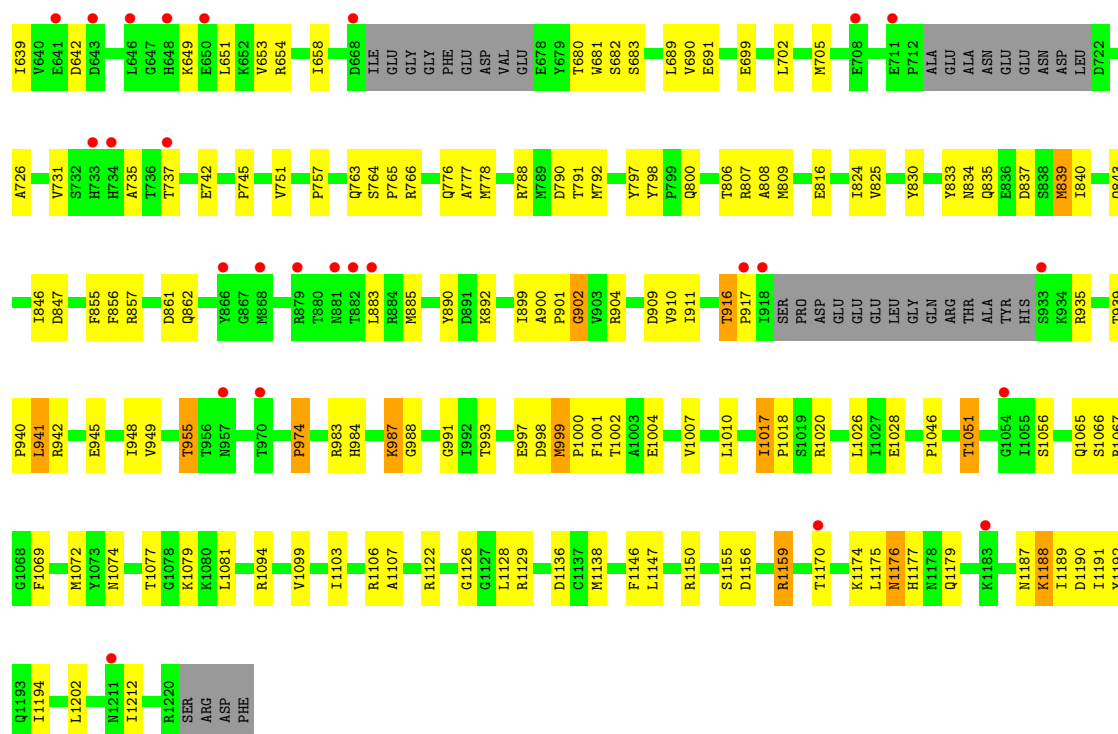
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]uridine (CCD ID: 2KH) (formula: C₉H₁₆N₃O₁₄P₃).

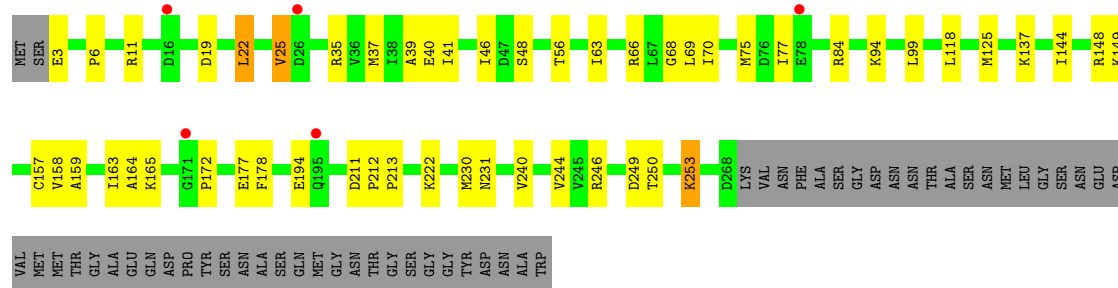


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	A	1	Total	C	N	O	P	0	1
			58	18	6	28	6		

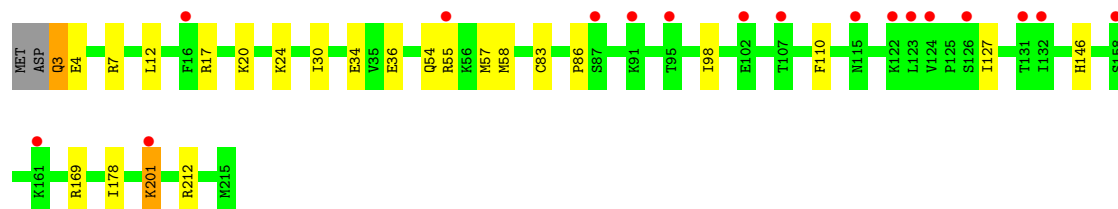
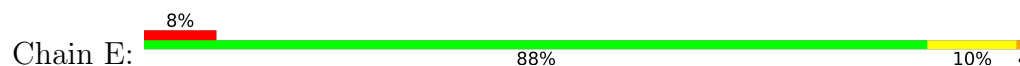




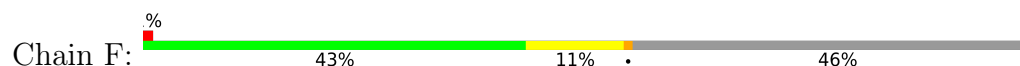
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



MET SER ASP TYR GLU ALA PHE ASN ASP ASP ASP VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU LYS PRO GLN PHE LYS ASP GLY GLU THR THR ASP ASP ASN GLY THR ILE VAL THR GLY GLN ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS GLU K72 K73 I74 P75 P76 R79 T82 P83 Y84 Y88 Y89 R90 I93 R97 Q100 V107 F108 V109 E124 I130 P131 L132 V133 I134 R135 R136 L155

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 12% 71% 18% 11%

MET SER T3 F6 F7 D8 I9 E14 V15 V16 G18 I26 E27 V44 P48 L55 I59 S62 L63 ASN LEU GLU ASP THR PRO ALA ASN ASP SER SER ALA T76 W79 R80 P81 P82 Q83 A84 C85 D86 L89 A90 D91 D92 Y93 K103 I112

L122 Y129 ARG ASN L132 L136 L137 Q137 E138 N139 A140 R145

- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 12% 78% 15% 6%

MET T2 T3 F4 L14 R24 L25 L26 F27 C32 S33 S40 I49 I52 T55 A56 G57 V58 V59 Q60 D61 L68 E74 F85 Q89 Q90 R91 R92 T95 S96 M97 V98 F101 L104 S105 C106 S107 T111 S112 D113 N116 LYS ARG THR

GLN PHE SER

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: % 69% 21% 7%

N1 I2 V3 P4 V5 R6 C7 F8 S9 C10 G11 V14 N23 E27 C45 R48 M49 I50 I51 T52 N64 P65 LEU GLU LYS ARG ASP

- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 74% 19% 5%

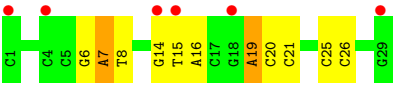
N1 P4 D5 R6 L11 K18 L19 K20 I21 K26 V32 T41 L45 L46 R47 A48 E49 V56 L57 F58 A59 A60 V61 Q76 T77 K84 K88 N92 S93 I94 K97 L101 N104 L114 ALA ASP ASP ALA PHE

- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

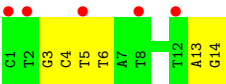
Chain L: 14% 46% 17% 37%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN ASP ALA ALA ALA GLY THR SER GLN ALA ARG THR ALA THR L27 K28 C31 A32 S35 L38 S39 L40 S41 A45 V46 R47 C48 K49 D50 H53 R54 I55 T61 R70

- Molecule 11: 29mer template DNA



• Molecule 12: 14mer non-template DNA



• Molecule 13: 9mer RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.70Å 224.00Å 193.06Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	82.79 – 3.40 82.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	87.1 (82.79-3.40) 87.1 (82.79-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.227 , 0.254 0.230 , 0.255	Depositor DCC
R_{free} test set	4066 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28880	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: ZN, MG, 2KH, 6MA

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	0.27	0/10979	0.71	4/14843 (0.0%)
2	B	0.26	0/8824	0.70	2/11898 (0.0%)
3	C	0.25	0/2133	0.70	0/2891
4	E	0.25	0/1780	0.72	0/2395
5	F	0.26	0/691	0.71	0/933
6	H	0.26	0/1060	0.69	0/1434
7	I	0.23	0/953	0.63	0/1284
8	J	0.25	0/541	0.63	0/727
9	K	0.24	0/937	0.65	0/1265
10	L	0.24	0/353	0.61	0/468
11	T	0.13	0/580	0.28	0/884
12	N	0.17	0/317	0.36	0/488
13	R	0.05	0/223	0.10	0/348
All	All	0.25	0/29371	0.68	6/39858 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	GLN	CB-CA-C	-5.97	109.71	116.63
1	A	1403	GLU	CB-CA-C	-5.69	109.49	117.23
1	A	593	GLU	CB-CA-C	-5.32	110.00	117.23
2	B	570	VAL	CA-C-N	5.31	125.12	119.28
2	B	570	VAL	C-N-CA	5.31	125.12	119.28
1	A	1098	VAL	CB-CA-C	-5.14	108.90	114.35

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	10787	0	10872	180	0
2	B	8657	0	8693	158	0
3	C	2095	0	2051	31	0
4	E	1744	0	1772	12	0
5	F	679	0	701	12	0
6	H	1043	0	1015	14	0
7	I	935	0	887	12	0
8	J	532	0	542	11	0
9	K	919	0	929	17	0
10	L	351	0	375	7	0
11	T	588	0	333	9	0
12	N	284	0	161	3	0
13	R	198	0	99	5	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	A	58	0	32	3	0
All	All	28880	0	28462	414	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 7.

All (414) 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:1239:ARG:HH22	1:A:1241:ARG:HH21	1.29	0.78
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.67	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.69	0.73
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.72	0.72
1:A:42:ASP:HB3	1:A:46:THR:H	1.55	0.71
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HG3	7:I:97:MET:HE3	1.74	0.69
3:C:48:SER:HB3	3:C:158:VAL:HB	1.74	0.69
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.72	0.69
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.74	0.68
3:C:46:ILE:HB	3:C:68:GLY:HA2	1.73	0.68
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.74	0.68
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.76	0.67
2:B:287:ARG:NH1	2:B:324:ILE:O	2.27	0.67
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.77	0.67
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.78	0.66
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.60	0.66
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.28	0.66
3:C:75:MET:O	3:C:246:ARG:NH2	2.29	0.66
2:B:468:GLU:HA	2:B:470:LYS:H	1.60	0.65
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.61	0.65
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.79	0.64
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.78	0.64
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.80	0.64
2:B:604:ARG:HE	2:B:615:MET:HE2	1.63	0.64
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.29	0.64
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.80	0.63
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.64	0.63
4:E:4:GLU:OE1	4:E:7:ARG:NH2	2.30	0.63
1:A:42:ASP:H	1:A:43:GLU:HA	1.64	0.63
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.64	0.63
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.81	0.63
2:B:468:GLU:HG3	2:B:469:GLN:HA	1.81	0.62
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.32	0.62
7:I:32:CYS:SG	7:I:33:SER:N	2.72	0.62
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.81	0.62
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.82	0.62
2:B:496:ARG:NH2	2:B:540:SER:O	2.31	0.61
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.82	0.61
1:A:503:GLN:OE1	5:F:90:ARG:NH2	2.33	0.61
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.82	0.61
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.83	0.61
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.34	0.61
5:F:82:THR:HG22	5:F:84:TYR:H	1.66	0.61
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.31	0.61
1:A:72:GLU:HG3	2:B:1175:LEU:HB2	1.83	0.61
4:E:20:LYS:NZ	4:E:34:GLU:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.65	0.61
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.82	0.60
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.83	0.60
3:C:163:ILE:HG22	3:C:165:LYS:H	1.67	0.60
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.83	0.60
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.34	0.60
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.81	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.84	0.60
1:A:477:PRO:HG3	1:A:521:MET:HE2	1.83	0.60
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.84	0.59
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.84	0.59
10:L:48:CYS:SG	10:L:49:LYS:N	2.74	0.59
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.85	0.59
1:A:544:ASP:OD1	1:A:545:GLN:N	2.36	0.59
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.83	0.58
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.36	0.58
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.36	0.58
1:A:562:THR:O	1:A:576:GLN:NE2	2.37	0.58
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.85	0.58
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.86	0.58
4:E:54:GLN:HG2	4:E:57:MET:HE3	1.85	0.58
1:A:469:ARG:NH2	2:B:991:GLY:O	2.31	0.58
6:H:89:LEU:H	6:H:89:LEU:HD13	1.69	0.58
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.86	0.57
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.86	0.57
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.37	0.57
11:T:14:DG:H2''	11:T:15:DT:H5'	1.86	0.57
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.37	0.57
1:A:34:LYS:H	1:A:34:LYS:HD3	1.70	0.57
1:A:40:THR:HB	1:A:41:MET:HA	1.86	0.57
2:B:487:THR:OG1	2:B:777:ALA:O	2.22	0.57
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.84	0.57
9:K:88:LYS:O	9:K:92:ASN:ND2	2.37	0.57
1:A:49:LYS:HB2	1:A:56:PRO:HD3	1.86	0.57
2:B:60:GLN:NE2	2:B:64:CYS:SG	2.77	0.57
2:B:63:ILE:O	2:B:67:SER:OG	2.19	0.56
6:H:129:TYR:O	6:H:132:LEU:N	2.37	0.56
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.71	0.56
1:A:72:GLU:OE2	2:B:1176:ASN:ND2	2.38	0.56
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.88	0.56
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HB3	2:B:432:MET:HE1	1.87	0.55
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.88	0.55
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.39	0.55
6:H:91:ASP:OD1	6:H:92:ASP:N	2.40	0.55
1:A:115:LEU:HB2	1:A:122:MET:HE3	1.88	0.55
6:H:14:GLU:HB3	6:H:27:GLU:HB3	1.86	0.55
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.89	0.55
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.89	0.54
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.71	0.54
2:B:680:THR:O	2:B:683:SER:OG	2.22	0.54
6:H:93:TYR:HD1	6:H:145:ARG:HB3	1.73	0.54
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.37	0.54
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.90	0.54
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.88	0.54
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.89	0.53
2:B:493:SER:OG	2:B:526:GLU:OE2	2.27	0.53
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.90	0.53
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.72	0.53
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.91	0.53
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.42	0.53
1:A:946:VAL:HG22	4:E:201:LYS:HD3	1.91	0.52
5:F:82:THR:O	5:F:136:ARG:NH1	2.28	0.52
1:A:42:ASP:O	1:A:48:ALA:N	2.41	0.51
2:B:857:ARG:NH2	11:T:25:DC:OP1	2.43	0.51
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.92	0.51
1:A:41:MET:HE2	1:A:43:GLU:HG2	1.92	0.51
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.91	0.51
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.91	0.51
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.93	0.51
1:A:744:LYS:HE2	1:A:748:MET:HE3	1.91	0.51
12:N:3:DG:H2''	12:N:4:DC:H5''	1.91	0.51
1:A:1325:THR:OG1	4:E:146:HIS:O	2.24	0.51
2:B:357:GLN:NE2	2:B:371:GLU:OE1	2.43	0.51
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.92	0.51
8:J:9:SER:OG	8:J:48:ARG:NH2	2.43	0.51
12:N:5:DT:H2''	12:N:6:DT:H71	1.93	0.51
1:A:475:THR:OG1	1:A:480:ALA:O	2.28	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.92	0.51
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.76	0.51
13:R:4:G:H2'	13:R:5:A:H8	1.75	0.51
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.93	0.51
11:T:26:DC:H42	13:R:3:G:H1	1.59	0.51
1:A:4:GLN:NE2	1:A:76:GLU:OE1	2.43	0.51
2:B:563:MET:HE3	2:B:580:VAL:HB	1.94	0.50
8:J:8:PHE:H	8:J:49:MET:HE3	1.76	0.50
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.93	0.50
1:A:134:ARG:NH1	1:A:220:THR:O	2.44	0.50
2:B:806:THR:HG22	2:B:808:ALA:H	1.76	0.50
1:A:67:CYS:H	1:A:71:GLN:HA	1.77	0.50
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.93	0.50
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.94	0.50
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.93	0.50
1:A:528:LEU:HD23	1:A:751:SER:HA	1.94	0.50
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.93	0.50
1:A:1116:LEU:HD23	1:A:1311:VAL:HA	1.94	0.50
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.76	0.50
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.94	0.50
16:A:1805[A]:2KH:O4	11:T:19:6MA:N6	2.35	0.49
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.94	0.49
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.48	0.49
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.94	0.49
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.94	0.49
2:B:400:HIS:NE2	2:B:699:GLU:OE1	2.38	0.49
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.43	0.49
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.93	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.49
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.77	0.49
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.95	0.49
2:B:287:ARG:NH1	2:B:321:GLY:O	2.46	0.49
6:H:8:ASP:OD1	6:H:9:ILE:N	2.45	0.49
12:N:13:DA:H2''	12:N:14:DG:H5'	1.95	0.49
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.77	0.49
3:C:3:GLU:N	9:K:104:ASN:HD21	2.11	0.49
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.13	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.48
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.13	0.48
2:B:651:LEU:O	2:B:654:ARG:NE	2.44	0.48
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.95	0.48
7:I:14:LEU:HD13	7:I:27:PHE:HB3	1.95	0.48
1:A:173:THR:HB	1:A:184:SER:HB3	1.96	0.48
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.94	0.48
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.79	0.48
1:A:752:LYS:NZ	16:A:1805[B]:2KH:O2G	2.39	0.48
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.96	0.48
2:B:776:GLN:NE2	13:R:7:A:O3'	2.47	0.48
1:A:95:PHE:HB3	1:A:234:MET:HE2	1.96	0.48
2:B:213:ILE:O	2:B:215:GLN:NE2	2.47	0.48
6:H:137:GLN:HG3	6:H:139:ASN:H	1.79	0.48
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	1.96	0.47
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.29	0.47
1:A:541:ILE:HD12	1:A:577:ILE:HG12	1.95	0.47
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.95	0.47
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.32	0.47
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.50	0.47
2:B:394:ASP:H	7:I:91:ARG:HG3	1.80	0.47
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.95	0.47
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.96	0.47
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.79	0.47
1:A:560:ILE:HB	6:H:79:TRP:H	1.80	0.47
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	1.96	0.47
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.96	0.47
13:R:4:G:H2'	13:R:5:A:C8	2.50	0.47
10:L:31:CYS:SG	10:L:32:ALA:N	2.88	0.47
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.97	0.47
1:A:826:ASP:O	1:A:830:LYS:HB2	2.15	0.47
1:A:962:ARG:O	1:A:966:ASN:HB2	2.14	0.47
1:A:1353:TYR:HD2	1:A:1368:MET:HE1	1.80	0.47
2:B:620:ARG:HH21	7:I:89:GLN:HE22	1.62	0.47
5:F:107:VAL:HG12	5:F:109:VAL:H	1.79	0.47
1:A:532:ARG:HE	1:A:536:LEU:HD21	1.79	0.47
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.97	0.47
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.96	0.47
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.80	0.47
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.96	0.46
2:B:378:LEU:O	2:B:382:ILE:HG12	2.15	0.46
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.97	0.46
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.97	0.46
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.98	0.46
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.97	0.46
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.97	0.46
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:SER:OG	1:A:664:THR:N	2.47	0.46
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.97	0.46
2:B:788:ARG:NH1	2:B:790:ASP:OD2	2.48	0.46
2:B:806:THR:HB	2:B:809:MET:HG3	1.97	0.46
1:A:51:GLY:HA2	1:A:52:GLY:HA2	1.51	0.46
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.98	0.46
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.48	0.46
2:B:900:ALA:O	2:B:902:GLY:N	2.48	0.46
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.79	0.46
1:A:208:LEU:HD23	1:A:235:ILE:HD13	1.97	0.46
1:A:1064:VAL:HA	1:A:1067:LEU:HB3	1.98	0.46
1:A:1279:ILE:HA	1:A:1310:GLY:HA3	1.98	0.46
2:B:40:GLU:OE2	2:B:682:SER:OG	2.33	0.46
3:C:84:ARG:HD2	9:K:11:LEU:HD21	1.98	0.46
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.98	0.46
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.51	0.45
9:K:21:ILE:HD13	9:K:84:LYS:HE2	1.98	0.45
1:A:346:ASP:O	2:B:1150:ARG:NH1	2.44	0.45
2:B:1175:LEU:C	2:B:1177:HIS:H	2.23	0.45
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.98	0.45
9:K:49:GLU:OE2	9:K:97:LYS:NZ	2.39	0.45
1:A:821:ARG:O	1:A:825:ILE:HG12	2.16	0.45
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.97	0.45
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.45
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.97	0.45
6:H:93:TYR:CD1	6:H:145:ARG:HB3	2.51	0.45
2:B:792:MET:HA	2:B:856:PHE:O	2.17	0.45
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.99	0.45
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.17	0.45
3:C:94:LYS:HG2	3:C:125:MET:HE1	1.98	0.45
1:A:231:PRO:HA	1:A:234:MET:HG3	1.99	0.45
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.97	0.45
1:A:783:THR:HG21	1:A:796:SER:O	2.16	0.45
16:A:1805[A]:2KH:PG	2:B:766:ARG:HH12	2.40	0.45
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.82	0.45
2:B:301:ILE:HD13	2:B:382:ILE:HG21	1.99	0.45
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.64	0.45
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.99	0.45
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.99	0.45
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.98	0.45
1:A:107:CYS:SG	1:A:108:MET:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:ARG:HA	2:B:615:MET:HE1	1.97	0.45
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.52	0.44
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.99	0.44
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.65	0.44
2:B:1067:ARG:NE	3:C:194:GLU:OE1	2.46	0.44
1:A:346:ASP:HB3	2:B:1107:ALA:O	2.16	0.44
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.98	0.44
1:A:977:LYS:HG3	1:A:978:PRO:HD2	1.99	0.44
2:B:757:PRO:HG2	2:B:984:HIS:NE2	2.32	0.44
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.99	0.44
1:A:1281:ARG:NE	1:A:1309:ASP:OD2	2.51	0.44
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.98	0.44
3:C:56:THR:HG21	3:C:63:ILE:HD11	2.00	0.44
2:B:1138:MET:HE2	2:B:1146:PHE:CD1	2.52	0.44
4:E:55:ARG:HA	4:E:58:MET:HE2	1.99	0.44
6:H:6:PHE:HB3	6:H:59:ILE:HB	2.00	0.44
8:J:10:CYS:SG	8:J:11:GLY:N	2.90	0.44
9:K:45:LEU:HG	9:K:94:ILE:HD13	2.00	0.44
1:A:707:GLY:O	1:A:1281:ARG:NH1	2.45	0.44
2:B:459:TYR:HE1	2:B:468:GLU:HB3	1.82	0.44
1:A:483:ASP:HB2	2:B:987:LYS:HG2	2.00	0.44
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.99	0.44
2:B:987:LYS:NZ	13:R:9:G:OP1	2.51	0.44
1:A:402:ALA:HA	1:A:434:ARG:HA	1.99	0.44
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.21	0.44
2:B:902:GLY:HA3	10:L:61:THR:HG22	1.99	0.44
2:B:558:LEU:HB3	2:B:563:MET:SD	2.58	0.43
2:B:916:THR:HA	2:B:917:PRO:HD3	1.88	0.43
8:J:64:ASN:N	8:J:65:PRO:HD2	2.33	0.43
1:A:464:PRO:HB2	9:K:4:PRO:HD3	2.00	0.43
1:A:316:GLN:NE2	1:A:320:ARG:HH12	2.16	0.43
2:B:552:MET:HE3	2:B:552:MET:HA	2.01	0.43
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.52	0.43
1:A:30:ILE:HG23	2:B:1170:THR:HG23	2.00	0.43
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.99	0.43
6:H:83:GLN:HB3	6:H:86:ASP:HB3	2.01	0.43
1:A:206:GLU:O	1:A:210:ILE:HG12	2.18	0.43
1:A:423:ASP:OD1	1:A:423:ASP:N	2.50	0.43
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.00	0.43
1:A:881:GLN:NE2	1:A:958:VAL:O	2.46	0.43
1:A:1287:TYR:OH	1:A:1307:GLU:OE1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.99	0.43
3:C:22:LEU:HD21	9:K:101:LEU:HD21	2.00	0.43
1:A:42:ASP:N	1:A:43:GLU:HA	2.29	0.43
7:I:24:ARG:NH1	7:I:26:LEU:HD21	2.32	0.43
11:T:19:6MA:H2"	11:T:20:DC:C6	2.53	0.43
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	2.01	0.43
2:B:1188:LYS:HE3	2:B:1188:LYS:HB2	1.92	0.43
1:A:860:LEU:HD21	1:A:1394:THR:HA	2.00	0.43
1:A:1132:LYS:HG3	1:A:1135:ARG:HH12	1.83	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.99	0.43
4:E:83:CYS:HB2	4:E:110:PHE:HE1	1.83	0.43
1:A:68:GLN:HA	1:A:69:THR:HA	1.46	0.43
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.34	0.43
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.54	0.43
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.19	0.43
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.19	0.43
2:B:702:LEU:HD21	2:B:735:ALA:HB1	2.00	0.43
2:B:861:ASP:OD1	2:B:862:GLN:N	2.50	0.43
5:F:76:LYS:O	5:F:79:ARG:NH1	2.43	0.43
9:K:56:VAL:HG22	9:K:77:THR:HG22	1.99	0.43
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.42
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.53	0.42
1:A:614:PHE:HB3	6:H:122:LEU:HD21	2.01	0.42
2:B:904:ARG:HG2	2:B:948:ILE:HG12	2.00	0.42
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.91	0.42
8:J:23:ASN:O	8:J:27:GLU:HB3	2.19	0.42
1:A:38:PRO:HA	1:A:270:LEU:HD13	2.00	0.42
1:A:265:LYS:HZ1	1:A:302:THR:HG23	1.84	0.42
2:B:791:THR:OG1	11:T:26:DC:OP1	2.26	0.42
3:C:40:GLU:O	3:C:250:THR:HG21	2.19	0.42
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.01	0.42
2:B:955:THR:HG23	10:L:55:ILE:HA	2.01	0.42
8:J:45:CYS:HB2	8:J:48:ARG:HH21	1.84	0.42
9:K:47:ARG:HD3	9:K:61:TYR:HD1	1.84	0.42
1:A:396:PRO:C	1:A:398:GLU:H	2.26	0.42
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.01	0.42
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.19	0.42
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.55	0.42
8:J:48:ARG:O	8:J:52:THR:OG1	2.24	0.42
1:A:774:ARG:H	1:A:774:ARG:HG2	1.63	0.42
4:E:17:ARG:HH12	4:E:36:GLU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:93:ILE:HD11	5:F:134:ILE:HD11	2.01	0.42
1:A:4:GLN:NE2	2:B:1159:ARG:HB3	2.35	0.42
1:A:1276:VAL:HG11	1:A:1316:VAL:HG22	2.01	0.42
2:B:302:CYS:SG	2:B:310:MET:HE3	2.60	0.42
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.87	0.42
1:A:98:LYS:HB3	1:A:234:MET:HE1	2.01	0.42
1:A:800:VAL:HG13	1:A:812:GLU:CD	2.45	0.42
2:B:468:GLU:CG	2:B:469:GLN:HA	2.47	0.42
2:B:620:ARG:HD2	7:I:68:LEU:HD11	2.02	0.42
2:B:939:THR:HA	2:B:940:PRO:HD3	1.87	0.42
3:C:37:MET:SD	3:C:244:VAL:HG12	2.59	0.42
6:H:89:LEU:HD22	6:H:90:ALA:N	2.34	0.42
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.84	0.42
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.02	0.42
1:A:795:GLU:HG3	2:B:731:VAL:HG21	2.02	0.42
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.55	0.42
1:A:12:ARG:HH11	2:B:1192:TYR:HE1	1.68	0.41
3:C:178:PHE:CE2	3:C:230:MET:HE2	2.55	0.41
3:C:249:ASP:O	3:C:253:LYS:HB2	2.20	0.41
4:E:3:GLN:HB2	4:E:4:GLU:H	1.59	0.41
1:A:527:THR:O	1:A:653:VAL:HG11	2.20	0.41
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	2.03	0.41
2:B:1000:PRO:HB2	2:B:1072:MET:HE3	2.02	0.41
2:B:281:PRO:HB2	2:B:284:ILE:HG12	2.02	0.41
5:F:97:ARG:HE	5:F:124:GLU:CD	2.28	0.41
1:A:1207:LEU:HB3	1:A:1274:ARG:HH11	1.85	0.41
2:B:34:ILE:HG23	2:B:542:MET:HE3	2.01	0.41
2:B:816:GLU:N	2:B:816:GLU:OE1	2.54	0.41
1:A:634:THR:HG1	1:A:642:CYS:HG	1.60	0.41
1:A:642:CYS:O	1:A:645:LEU:HB3	2.20	0.41
2:B:58:THR:O	2:B:62:ILE:HG12	2.20	0.41
2:B:942:ARG:HB2	2:B:945:GLU:HB2	2.03	0.41
1:A:453:MET:HB3	1:A:477:PRO:HB2	2.02	0.41
1:A:941:LYS:HE3	1:A:941:LYS:HB3	1.91	0.41
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.53	0.41
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.02	0.41
2:B:600:LEU:HB3	2:B:615:MET:SD	2.60	0.41
11:T:7:6MA:H2'	11:T:8:DT:H5'	2.02	0.41
1:A:781:ASP:O	1:A:790:ASP:N	2.45	0.41
1:A:889:SER:HA	1:A:1296:GLY:HA3	2.02	0.41
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.02	0.41
2:B:205:ILE:HG21	2:B:462:ALA:HB2	2.02	0.41
1:A:962:ARG:HA	1:A:965:GLN:HG2	2.02	0.41
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.86	0.41
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.21	0.41
1:A:1227:ILE:HD12	1:A:1239:ARG:HH11	1.86	0.41
1:A:1260:LEU:HD12	1:A:1263:ILE:HD12	2.03	0.41
2:B:792:MET:HE3	2:B:855:PHE:HE1	1.86	0.41
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.55	0.41
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.86	0.41
10:L:28:LYS:HA	10:L:39:SER:HA	2.03	0.41
1:A:733:ALA:HB2	1:A:763:ALA:HB2	2.03	0.41
1:A:873:MET:HE1	1:A:1057:VAL:HG22	2.01	0.41
2:B:93:GLY:N	2:B:131:ASP:O	2.53	0.41
1:A:9:ALA:HA	1:A:10:PRO:HD3	1.89	0.40
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.02	0.40
7:I:98:VAL:HG11	7:I:113:ASP:HB2	2.03	0.40
11:T:6:DG:H2"	11:T:7:6MA:H8	2.02	0.40
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.46	0.40
2:B:408:LEU:HB3	2:B:409:ALA:H	1.75	0.40
2:B:843:GLN:HB2	2:B:993:THR:HB	2.04	0.40
1:A:52:GLY:HA3	1:A:53:LEU:HA	1.89	0.40
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	2.03	0.40
2:B:582:VAL:HB	2:B:587:HIS:CE1	2.56	0.40
2:B:1155:SER:OG	2:B:1156:ASP:N	2.54	0.40
5:F:109:VAL:HG11	5:F:124:GLU:HA	2.02	0.40
1:A:35:ILE:HG23	1:A:52:GLY:HA3	2.04	0.40
1:A:226:GLU:HG3	1:A:227:VAL:HG13	2.02	0.40
1:A:678:GLU:HA	1:A:681:GLU:HG2	2.03	0.40
1:A:1128:GLN:HB3	1:A:1304:TRP:NE1	2.36	0.40
1:A:1445:ILE:HG22	5:F:132:LEU:HD23	2.04	0.40
2:B:307:ASP:OD1	2:B:392:ARG:NH1	2.46	0.40
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.52	0.40
3:C:11:ARG:NH2	3:C:19:ASP:OD1	2.55	0.40
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	2.03	0.40
2:B:483:LEU:HD21	2:B:491:THR:HG23	2.03	0.40
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.57	0.40
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.81	0.40
10:L:46:VAL:HA	10:L:47:ARG:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1357/1733 (78%)	1258 (93%)	95 (7%)	4 (0%)	36	65
2	B	1067/1224 (87%)	987 (92%)	71 (7%)	9 (1%)	16	44
3	C	264/318 (83%)	245 (93%)	18 (7%)	1 (0%)	30	59
4	E	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	24	54
5	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
6	H	124/146 (85%)	113 (91%)	9 (7%)	2 (2%)	7	29
7	I	113/122 (93%)	101 (89%)	11 (10%)	1 (1%)	14	42
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	14	42
10	L	42/70 (60%)	34 (81%)	7 (17%)	1 (2%)	4	22
All	All	3435/4173 (82%)	3181 (93%)	234 (7%)	20 (1%)	21	50

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
2	B	902	GLY
2	B	277	LYS
2	B	883	LEU
2	B	1046	PRO
6	H	82	PRO
9	K	26	LYS
1	A	1156	PRO
2	B	1017	ILE
3	C	148	ARG
4	E	86	PRO
1	A	957	PRO
1	A	1221	LYS
2	B	367	LEU

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Mol	Chain	Res	Type
2	B	824	ILE
7	I	33	SER
10	L	41	SER
2	B	901	PRO
6	H	18	GLY
2	B	974	PRO

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	1198/1520 (79%)	1138 (95%)	60 (5%)	22	49
2	B	944/1061 (89%)	901 (95%)	43 (5%)	24	50
3	C	234/274 (85%)	226 (97%)	8 (3%)	32	57
4	E	195/197 (99%)	190 (97%)	5 (3%)	40	61
5	F	74/137 (54%)	72 (97%)	2 (3%)	39	60
6	H	114/128 (89%)	110 (96%)	4 (4%)	32	56
7	I	109/116 (94%)	106 (97%)	3 (3%)	38	60
8	J	60/65 (92%)	57 (95%)	3 (5%)	22	49
9	K	99/102 (97%)	94 (95%)	5 (5%)	21	48
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3066/3657 (84%)	2933 (96%)	133 (4%)	26	51

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	30	ILE
1	A	46	THR
1	A	69	THR
1	A	93	VAL
1	A	126	LEU
1	A	132	LYS

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	208	LEU
1	A	222	LEU
1	A	235	ILE
1	A	271	LYS
1	A	308	ILE
1	A	322	VAL
1	A	335	ARG
1	A	351	THR
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	463	ILE
1	A	470	LEU
1	A	481	ASP
1	A	512	VAL
1	A	532	ARG
1	A	612	ILE
1	A	618	GLU
1	A	666	ILE
1	A	688	LYS
1	A	691	LEU
1	A	702	LEU
1	A	774	ARG
1	A	780	VAL
1	A	783	THR
1	A	797	LYS
1	A	805	LEU
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	885	THR
1	A	899	VAL
1	A	919	ILE
1	A	926	GLN
1	A	934	LYS
1	A	977	LYS
1	A	1017	LEU
1	A	1034	GLU
1	A	1035	TYR
1	A	1116	LEU
1	A	1128	GLN

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Mol	Chain	Res	Type
1	A	1172	LEU
1	A	1230	GLU
1	A	1262	LYS
1	A	1297	GLU
1	A	1322	ILE
1	A	1333	ILE
1	A	1350	LYS
1	A	1374	VAL
1	A	1377	THR
1	A	1400	CYS
1	A	1407	GLU
2	B	46	GLN
2	B	130	VAL
2	B	134	LYS
2	B	222	ILE
2	B	240	ILE
2	B	319	GLU
2	B	331	LEU
2	B	364	ILE
2	B	365	THR
2	B	393	LYS
2	B	468	GLU
2	B	483	LEU
2	B	547	VAL
2	B	549	THR
2	B	570	VAL
2	B	606	LYS
2	B	628	THR
2	B	737	THR
2	B	751	VAL
2	B	764	SER
2	B	797	TYR
2	B	825	VAL
2	B	839	MET
2	B	885	MET
2	B	916	THR
2	B	941	LEU
2	B	955	THR
2	B	983	ARG
2	B	987	LYS
2	B	997	GLU
2	B	999	MET

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Mol	Chain	Res	Type
2	B	1007	VAL
2	B	1028	GLU
2	B	1051	THR
2	B	1099	VAL
2	B	1147	LEU
2	B	1159	ARG
2	B	1176	ASN
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
3	C	22	LEU
3	C	25	VAL
3	C	77	ILE
3	C	137	LYS
3	C	149	LYS
3	C	222	LYS
3	C	240	VAL
3	C	253	LYS
4	E	3	GLN
4	E	98	ILE
4	E	127	ILE
4	E	169	ARG
4	E	201	LYS
5	F	72	LYS
5	F	97	ARG
6	H	15	VAL
6	H	26	ILE
6	H	89	LEU
6	H	103	LYS
7	I	14	LEU
7	I	59	VAL
7	I	111	THR
8	J	3	VAL
8	J	5	VAL
8	J	52	THR
9	K	18	LYS
9	K	20	LYS
9	K	32	VAL
9	K	47	ARG
9	K	101	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	68	GLN
1	A	358	ASN
1	A	439	ASN
1	A	445	ASN
1	A	659	HIS
1	A	742	ASN
1	A	877	HIS
1	A	935	GLN
1	A	966	ASN
1	A	968	GLN
1	A	1048	ASN
1	A	1078	GLN
1	A	1188	GLN
1	A	1390	ASN
2	B	449	ASN
2	B	762	ASN
2	B	770	GLN
2	B	794	ASN
2	B	984	HIS
2	B	1040	ASN
2	B	1093	GLN
2	B	1176	ASN
2	B	1177	HIS
2	B	1195	HIS
3	C	267	GLN
4	E	63	ASN
5	F	104	ASN
6	H	21	ASN
6	H	35	GLN
6	H	128	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	9	G

There are no RNA pucker outliers to report.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	6MA	T	7	12,11	21,24,25	2.63	7 (33%)	27,34,37	2.11	4 (14%)
11	6MA	T	19	11	21,24,25	2.63	7 (33%)	27,34,37	2.07	4 (14%)
11	6MA	T	16	11	21,24,25	2.50	7 (33%)	27,34,37	2.13	6 (22%)

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
11	6MA	T	7	12,11	-	5/9/23/24	0/3/3/3
11	6MA	T	19	11	-	0/9/23/24	0/3/3/3
11	6MA	T	16	11	-	3/9/23/24	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19	6MA	C6-N6	7.74	1.43	1.34
11	T	7	6MA	C6-N6	7.70	1.43	1.34
11	T	16	6MA	C6-N6	7.04	1.42	1.34
11	T	7	6MA	C5-N7	4.76	1.47	1.39
11	T	19	6MA	C5-N7	4.67	1.47	1.39
11	T	16	6MA	C5-N7	4.50	1.47	1.39
11	T	7	6MA	C1'-N9	-3.83	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19	6MA	C1'-N9	-3.74	1.39	1.46
11	T	16	6MA	C1'-N9	-3.70	1.39	1.46
11	T	19	6MA	C8-N9	-3.59	1.31	1.37
11	T	7	6MA	C8-N9	-3.59	1.31	1.37
11	T	16	6MA	C8-N9	-3.49	1.31	1.37
11	T	7	6MA	C4-N9	-2.60	1.32	1.37
11	T	19	6MA	C8-N7	2.57	1.36	1.31
11	T	19	6MA	C4-N9	-2.57	1.32	1.37
11	T	16	6MA	C4-N9	-2.56	1.32	1.37
11	T	19	6MA	C5-C4	2.52	1.43	1.39
11	T	7	6MA	C5-C4	2.50	1.43	1.39
11	T	16	6MA	C8-N7	2.49	1.36	1.31
11	T	7	6MA	C8-N7	2.47	1.36	1.31
11	T	16	6MA	C5-C4	2.23	1.43	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	7	6MA	C4-N9-C8	8.50	114.66	105.74
11	T	19	6MA	C4-N9-C8	8.35	114.50	105.74
11	T	16	6MA	C4-N9-C8	8.22	114.37	105.74
11	T	19	6MA	C6-C5-N7	3.46	136.20	132.43
11	T	7	6MA	C6-C5-N7	3.45	136.19	132.43
11	T	16	6MA	C1-N6-C6	-3.25	119.84	122.85
11	T	16	6MA	C2'-C3'-C4'	2.58	108.04	102.80
11	T	16	6MA	C6-C5-N7	2.49	135.15	132.43
11	T	19	6MA	C4-C5-N7	-2.44	107.79	110.58
11	T	7	6MA	C4-C5-N7	-2.37	107.88	110.58
11	T	19	6MA	N9-C8-N7	-2.08	110.98	113.94
11	T	7	6MA	N9-C8-N7	-2.08	110.98	113.94
11	T	16	6MA	C5-C4-N9	-2.07	103.56	105.81
11	T	16	6MA	C2'-C1'-N9	-2.01	109.90	114.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	7	6MA	C3'-C4'-C5'-O5'
11	T	7	6MA	O4'-C4'-C5'-O5'
11	T	7	6MA	C2'-C1'-N9-C4
11	T	16	6MA	C4'-C5'-O5'-P
11	T	7	6MA	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
11	T	16	6MA	N1-C6-N6-C1
11	T	16	6MA	C5-C6-N6-C1
11	T	7	6MA	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	7	6MA	2	0
11	T	19	6MA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 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$
16	2KH	A	1805[B]	15	29,30,30	2.16	9 (31%)	41,47,47	1.68	7 (17%)
16	2KH	A	1805[A]	15	29,30,30	2.12	11 (37%)	41,47,47	1.72	8 (19%)

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
16	2KH	A	1805[B]	15	-	5/19/38/38	0/2/2/2
16	2KH	A	1805[A]	15	-	6/19/38/38	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1805[B]	2KH	PB-O2B	4.68	1.53	1.46
16	A	1805[A]	2KH	PB-O2B	4.61	1.53	1.46
16	A	1805[B]	2KH	PB-N3A	4.16	1.74	1.63
16	A	1805[B]	2KH	PB-O3B	4.08	1.64	1.59
16	A	1805[A]	2KH	PB-O3B	3.96	1.64	1.59
16	A	1805[A]	2KH	PB-N3A	3.91	1.73	1.63
16	A	1805[B]	2KH	PA-N3A	3.78	1.73	1.63
16	A	1805[A]	2KH	PA-N3A	3.53	1.72	1.63
16	A	1805[A]	2KH	C2-N1	3.41	1.43	1.38
16	A	1805[B]	2KH	C2-N1	3.26	1.43	1.38
16	A	1805[B]	2KH	PA-O1A	3.24	1.51	1.46
16	A	1805[A]	2KH	PA-O1A	3.10	1.50	1.46
16	A	1805[B]	2KH	PB-O1B	-2.60	1.49	1.56
16	A	1805[B]	2KH	PA-O5'	2.49	1.66	1.57
16	A	1805[A]	2KH	PB-O1B	-2.48	1.50	1.56
16	A	1805[A]	2KH	PA-O5'	2.42	1.66	1.57
16	A	1805[A]	2KH	C5'-C4'	2.11	1.57	1.51
16	A	1805[B]	2KH	C5'-C4'	2.04	1.57	1.51
16	A	1805[A]	2KH	C4-N3	2.02	1.42	1.38
16	A	1805[A]	2KH	C2-N3	2.01	1.41	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1805[A]	2KH	O1G-PG-O3B	5.55	123.24	104.64
16	A	1805[B]	2KH	O1G-PG-O3B	5.51	123.10	104.64
16	A	1805[B]	2KH	O3B-PB-N3A	3.82	117.20	106.59
16	A	1805[B]	2KH	O3G-PG-O2G	-3.77	96.14	110.83
16	A	1805[A]	2KH	O3G-PG-O2G	-3.68	96.49	110.83
16	A	1805[A]	2KH	O3B-PB-N3A	3.65	116.72	106.59
16	A	1805[A]	2KH	O2B-PB-N3A	-3.44	106.70	111.77
16	A	1805[B]	2KH	O2B-PB-N3A	-3.25	106.98	111.77
16	A	1805[B]	2KH	N3-C2-N1	2.20	117.76	114.89
16	A	1805[A]	2KH	O2A-PA-O1A	-2.12	105.33	109.87
16	A	1805[A]	2KH	N3-C2-N1	2.11	117.63	114.89
16	A	1805[B]	2KH	O2A-PA-O1A	-2.09	105.38	109.87
16	A	1805[A]	2KH	C4'-O4'-C1'	2.05	113.99	109.47
16	A	1805[B]	2KH	O3G-PG-O3B	2.01	111.39	104.64
16	A	1805[A]	2KH	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

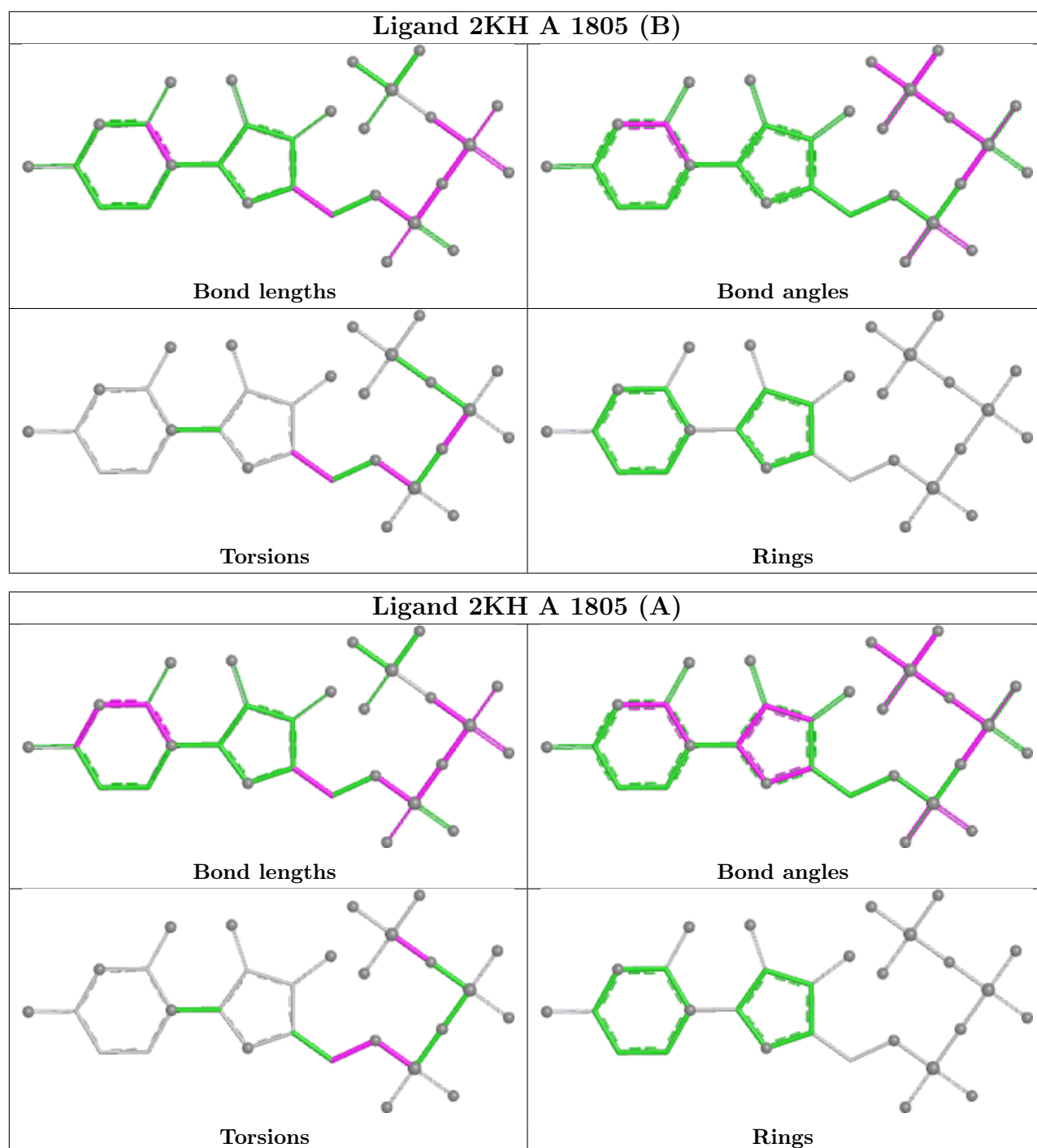
Mol	Chain	Res	Type	Atoms
16	A	1805[A]	2KH	C5'-O5'-PA-O1A
16	A	1805[A]	2KH	C5'-O5'-PA-O2A
16	A	1805[A]	2KH	C4'-C5'-O5'-PA
16	A	1805[A]	2KH	PB-O3B-PG-O1G
16	A	1805[B]	2KH	C5'-O5'-PA-O2A
16	A	1805[B]	2KH	PA-N3A-PB-O2B
16	A	1805[B]	2KH	C3'-C4'-C5'-O5'
16	A	1805[B]	2KH	O4'-C4'-C5'-O5'
16	A	1805[A]	2KH	C5'-O5'-PA-N3A
16	A	1805[B]	2KH	C5'-O5'-PA-O1A
16	A	1805[A]	2KH	PB-O3B-PG-O2G

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1805[B]	2KH	1	0
16	A	1805[A]	2KH	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1371/1733 (79%)	0.65	115 (8%) 17 15	13, 68, 150, 221	0
2	B	1089/1224 (88%)	0.44	67 (6%) 26 21	13, 48, 115, 201	0
3	C	266/318 (83%)	0.26	5 (1%) 66 51	21, 50, 93, 148	0
4	E	213/215 (99%)	0.80	17 (7%) 18 16	44, 95, 174, 201	0
5	F	84/155 (54%)	0.23	2 (2%) 59 45	38, 66, 115, 154	0
6	H	130/146 (89%)	0.88	17 (13%) 7 8	41, 88, 155, 215	0
7	I	115/122 (94%)	0.77	15 (13%) 7 8	35, 70, 119, 149	0
8	J	65/70 (92%)	0.04	1 (1%) 72 57	17, 40, 78, 138	0
9	K	114/120 (95%)	0.05	0 100 100	16, 50, 91, 105	0
10	L	44/70 (62%)	1.46	10 (22%) 2 4	37, 119, 176, 195	0
11	T	26/29 (89%)	1.31	6 (23%) 2 3	45, 185, 246, 273	0
12	N	14/14 (100%)	1.92	5 (35%) 1 1	157, 216, 265, 267	0
13	R	9/9 (100%)	-0.04	0 100 100	30, 43, 91, 92	0
All	All	3540/4225 (83%)	0.55	260 (7%) 21 18	13, 62, 145, 273	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	6.2
2	B	468	GLU	6.0
1	A	54	ASN	5.7
2	B	883	LEU	5.4
1	A	108	MET	5.4
1	A	98	LYS	4.9
1	A	596	THR	4.8
1	A	1378	GLN	4.6
10	L	27	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	105	CYS	4.4
6	H	139	ASN	4.4
6	H	85	GLY	4.4
1	A	49	LYS	4.3
6	H	84	ALA	4.2
2	B	446	LEU	4.1
1	A	176	LYS	4.1
11	T	15	DT	3.9
1	A	1174	PHE	3.9
1	A	826	ASP	3.9
1	A	65	LEU	3.9
10	L	45	ALA	3.8
2	B	338	GLY	3.8
2	B	472	ALA	3.8
1	A	323	LYS	3.8
2	B	881	ASN	3.7
10	L	53	HIS	3.7
1	A	140	THR	3.7
6	H	83	GLN	3.7
10	L	40	LEU	3.7
1	A	322	VAL	3.6
1	A	628	GLY	3.6
1	A	72	GLU	3.6
12	N	1	DC	3.6
1	A	251	SER	3.5
1	A	250	ILE	3.5
2	B	530	GLY	3.5
10	L	46	VAL	3.4
1	A	1173	HIS	3.4
2	B	275	TYR	3.4
2	B	447	ALA	3.4
1	A	50	ILE	3.4
8	J	65	PRO	3.4
2	B	267	ARG	3.4
7	I	52	ILE	3.3
4	E	95	THR	3.3
2	B	918	ILE	3.3
10	L	41	SER	3.3
1	A	171	GLN	3.3
2	B	70	ILE	3.3
4	E	102	GLU	3.3
1	A	310	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	74	MET	3.2
1	A	59	GLY	3.2
1	A	1261	LYS	3.2
2	B	266	ALA	3.2
1	A	828	ALA	3.1
2	B	643	ASP	3.1
1	A	1262	LYS	3.1
3	C	171	GLY	3.1
2	B	1211	ASN	3.1
2	B	415	GLN	3.1
2	B	733	HIS	3.0
2	B	328	GLU	3.0
3	C	78	GLU	3.0
2	B	370	PHE	3.0
1	A	1260	LEU	3.0
3	C	195	GLN	3.0
1	A	1096	SER	3.0
4	E	87	SER	3.0
7	I	105	SER	2.9
1	A	201	VAL	2.9
6	H	82	PRO	2.9
1	A	279	LEU	2.9
1	A	710	LEU	2.9
1	A	145	LYS	2.9
1	A	40	THR	2.9
6	H	81	PRO	2.9
2	B	134	LYS	2.9
1	A	107	CYS	2.8
2	B	260	GLY	2.8
1	A	66	LYS	2.8
1	A	288	ALA	2.8
1	A	1035	TYR	2.8
2	B	459	TYR	2.8
7	I	40	SER	2.8
1	A	76	GLU	2.8
2	B	711	GLU	2.8
1	A	1284	MET	2.8
5	F	73	ALA	2.8
2	B	641	GLU	2.8
2	B	502	ILE	2.8
2	B	576	ASP	2.7
6	H	129	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	251	ILE	2.7
2	B	572	HIS	2.7
1	A	1283	VAL	2.7
2	B	467	GLY	2.7
2	B	261	ARG	2.7
4	E	107	THR	2.7
6	H	135	LEU	2.7
1	A	173	THR	2.7
4	E	123	LEU	2.7
6	H	137	GLN	2.6
2	B	241	ARG	2.6
7	I	60	GLN	2.6
1	A	1407	GLU	2.6
7	I	74	GLU	2.6
1	A	179	LEU	2.6
1	A	1154	TYR	2.6
1	A	1449	SER	2.6
4	E	131	THR	2.6
1	A	830	LYS	2.6
1	A	96	ILE	2.6
11	T	14	DG	2.6
7	I	57	GLY	2.5
2	B	646	LEU	2.5
2	B	326	ASP	2.5
2	B	262	GLU	2.5
6	H	63	LEU	2.5
1	A	101	LYS	2.5
1	A	26	GLU	2.5
2	B	970	THR	2.5
2	B	367	LEU	2.5
2	B	620	ARG	2.5
4	E	55	ARG	2.5
1	A	260	ASP	2.5
3	C	16	ASP	2.5
1	A	1220	PHE	2.5
2	B	531	GLN	2.5
1	A	67	CYS	2.5
1	A	801	GLU	2.5
1	A	1235	LYS	2.5
1	A	79	GLY	2.5
2	B	509	ALA	2.4
4	E	122	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1315	GLU	2.4
1	A	252	PHE	2.4
1	A	1377	THR	2.4
10	L	50	ASP	2.4
7	I	49	ILE	2.4
4	E	201	LYS	2.4
7	I	4	PHE	2.4
1	A	397	ASN	2.4
2	B	668	ASP	2.4
2	B	648	HIS	2.4
1	A	289	ILE	2.4
1	A	143	LYS	2.4
1	A	1188	GLN	2.4
2	B	345	LYS	2.4
1	A	957	PRO	2.4
2	B	365	THR	2.4
7	I	55	THR	2.4
4	E	115	ASN	2.4
1	A	62	ASP	2.4
1	A	1206	ASP	2.4
1	A	1419	ASP	2.4
2	B	866	TYR	2.4
6	H	86	ASP	2.4
2	B	868	MET	2.4
7	I	104	LEU	2.4
10	L	35	SER	2.4
1	A	182	VAL	2.4
2	B	295	GLY	2.3
1	A	1125	ALA	2.3
1	A	146	MET	2.3
1	A	968	GLN	2.3
12	N	5	DT	2.3
12	N	12	DT	2.3
1	A	60	SER	2.3
1	A	249	SER	2.3
4	E	161	LYS	2.3
11	T	1	DC	2.3
1	A	475	THR	2.3
1	A	831	THR	2.3
2	B	734	HIS	2.3
1	A	626	ASN	2.3
1	A	702	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	427	ASP	2.3
1	A	1112	LYS	2.3
1	A	73	GLY	2.3
1	A	69	THR	2.3
1	A	975	HIS	2.3
7	I	107	SER	2.3
2	B	64	CYS	2.3
2	B	1183	LYS	2.3
1	A	1302	PRO	2.3
1	A	1175	SER	2.3
4	E	158	SER	2.3
10	L	31	CYS	2.3
1	A	147	VAL	2.3
1	A	709	THR	2.2
2	B	357	GLN	2.2
1	A	973	ILE	2.2
2	B	1054	GLY	2.2
1	A	139	TRP	2.2
1	A	175	ARG	2.2
2	B	575	PRO	2.2
1	A	1422	ARG	2.2
4	E	124	VAL	2.2
1	A	1150	SER	2.2
1	A	1223	ASP	2.2
3	C	26	ASP	2.2
7	I	61	ASP	2.2
1	A	275	SER	2.2
1	A	316	GLN	2.2
2	B	917	PRO	2.2
7	I	2	THR	2.1
11	T	4	DC	2.1
4	E	126	SER	2.1
6	H	140	ALA	2.1
2	B	879	ARG	2.1
1	A	170	THR	2.1
10	L	38	LEU	2.1
12	N	8	DT	2.1
1	A	48	ALA	2.1
2	B	372	SER	2.1
2	B	650	GLU	2.1
6	H	62	SER	2.1
2	B	354	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	265	LYS	2.1
1	A	705	LYS	2.1
1	A	1322	ILE	2.1
5	F	74	ILE	2.1
1	A	234	MET	2.1
1	A	91	PHE	2.1
1	A	229	SER	2.1
4	E	91	LYS	2.1
1	A	266	LEU	2.1
6	H	55	LEU	2.1
2	B	1170	THR	2.1
11	T	18	DG	2.1
11	T	29	DG	2.1
1	A	1234	GLU	2.1
12	N	2	DT	2.1
2	B	471	LYS	2.1
7	I	116	ASN	2.1
2	B	90	ILE	2.1
4	E	132	ILE	2.1
2	B	708	GLU	2.1
4	E	16	PHE	2.1
2	B	933	SER	2.0
1	A	64	ASN	2.0
1	A	1271	ILE	2.0
2	B	364	ILE	2.0
6	H	132	LEU	2.0
1	A	423	ASP	2.0
1	A	332	LYS	2.0
1	A	1094	VAL	2.0
1	A	215	SER	2.0
1	A	1259	MET	2.0
1	A	1393	ASN	2.0
2	B	957	ASN	2.0
1	A	351	THR	2.0
1	A	1376	THR	2.0
2	B	737	THR	2.0
2	B	882	THR	2.0
6	H	90	ALA	2.0
7	I	3	THR	2.0
1	A	1169	ILE	2.0
6	H	112	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	6MA	T	16	22/23	0.46	0.21	138,145,158,168	0
11	6MA	T	7	22/23	0.61	0.17	227,229,235,237	0
11	6MA	T	19	22/23	0.89	0.14	63,79,96,101	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

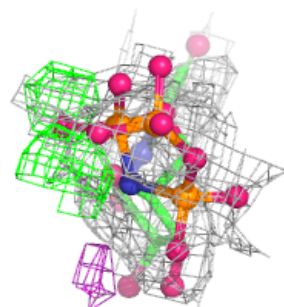
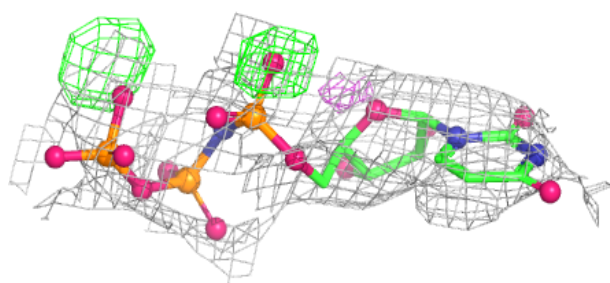
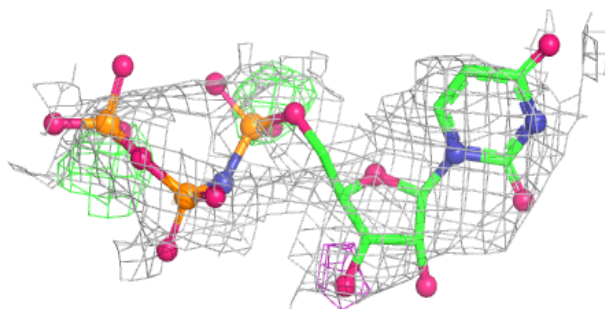
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	2KH	A	1805[A]	29/29	0.84	0.22	79,110,128,143	29
16	2KH	A	1805[B]	29/29	0.84	0.22	113,115,127,136	29
14	ZN	A	1801	1/1	0.95	0.06	150,150,150,150	0
14	ZN	L	101	1/1	0.96	0.05	120,120,120,120	0
15	MG	A	1804	1/1	0.96	0.05	31,31,31,31	0
14	ZN	B	1301	1/1	0.98	0.04	83,83,83,83	0
14	ZN	A	1802	1/1	0.99	0.05	77,77,77,77	0
14	ZN	C	401	1/1	0.99	0.03	51,51,51,51	0
14	ZN	I	201	1/1	0.99	0.04	71,71,71,71	0
14	ZN	J	101	1/1	0.99	0.02	33,33,33,33	0
15	MG	A	1803	1/1	1.00	0.02	11,11,11,11	0
14	ZN	I	202	1/1	1.00	0.02	53,53,53,53	0

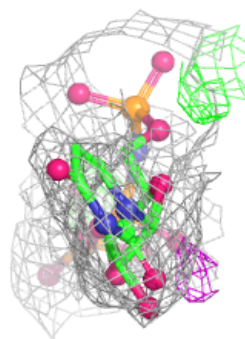
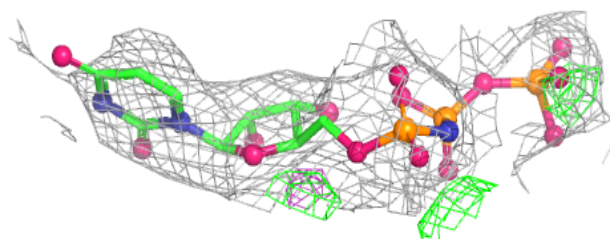
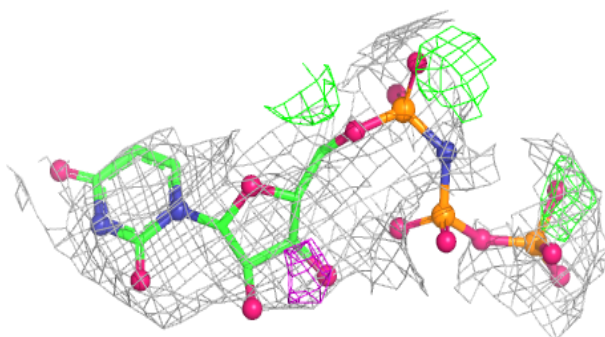
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2KH A 1805 (A):

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

**Electron density around 2KH A 1805 (B):**

$2mF_o-DF_c$ (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.