



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:00 PM UTC

PDB ID : 6BM4 / pdb_00006bm4
Title : Pol II elongation complex with an abasic lesion at i-1 position,soaking UMP-NPP
Authors : Wang, W.; Wang, D.
Deposited on : 2017-11-13
Resolution : 2.95 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

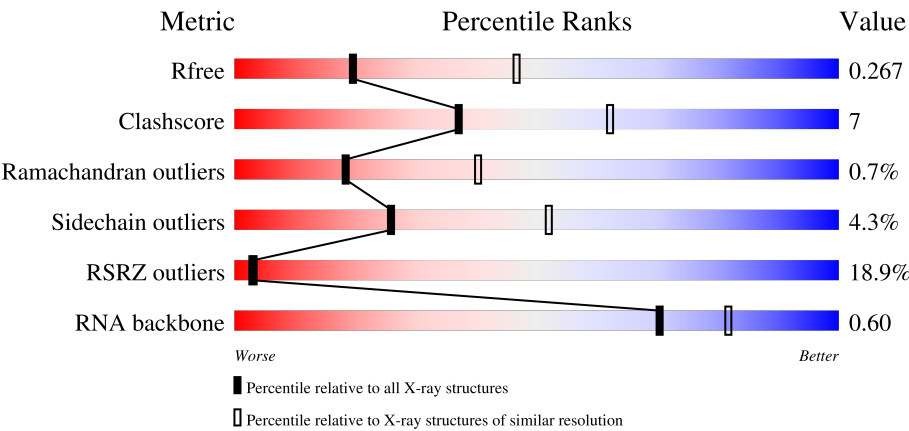
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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	18% 61% 16% • 21%
2	B	1224	14% 69% 19% • 10%
3	C	318	6% 67% 16% • 16%
4	E	215	28% 87% 11% •

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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	R	9	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 28274 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	1372	Total	C	N	O	S	0	0	0
			10784	6802	1887	2034	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8726	5526	1530	1615	55			

- 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 DNA (5'-D(P*CP*AP*(3DR)P*CP*TP*CP*TP*TP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	12	Total	C	N	O	P	0	0	0
			233	111	38	72	12			

- Molecule 12 is a RNA chain called RNA (5'-R(*AP*UP*CP*AP*AP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		

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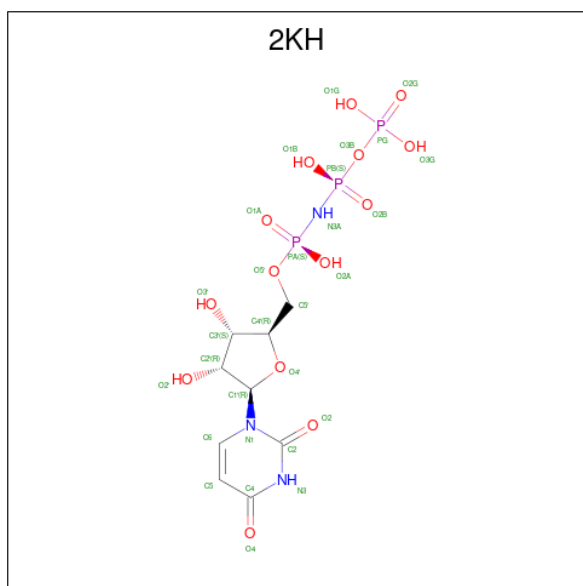
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Zn	0	0
			1	1		
13	C	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	L	1	Total	Zn	0	0
			1	1		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 15 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]uridine (CCD ID: 2KH) (formula: C₉H₁₆N₃O₁₄P₃).

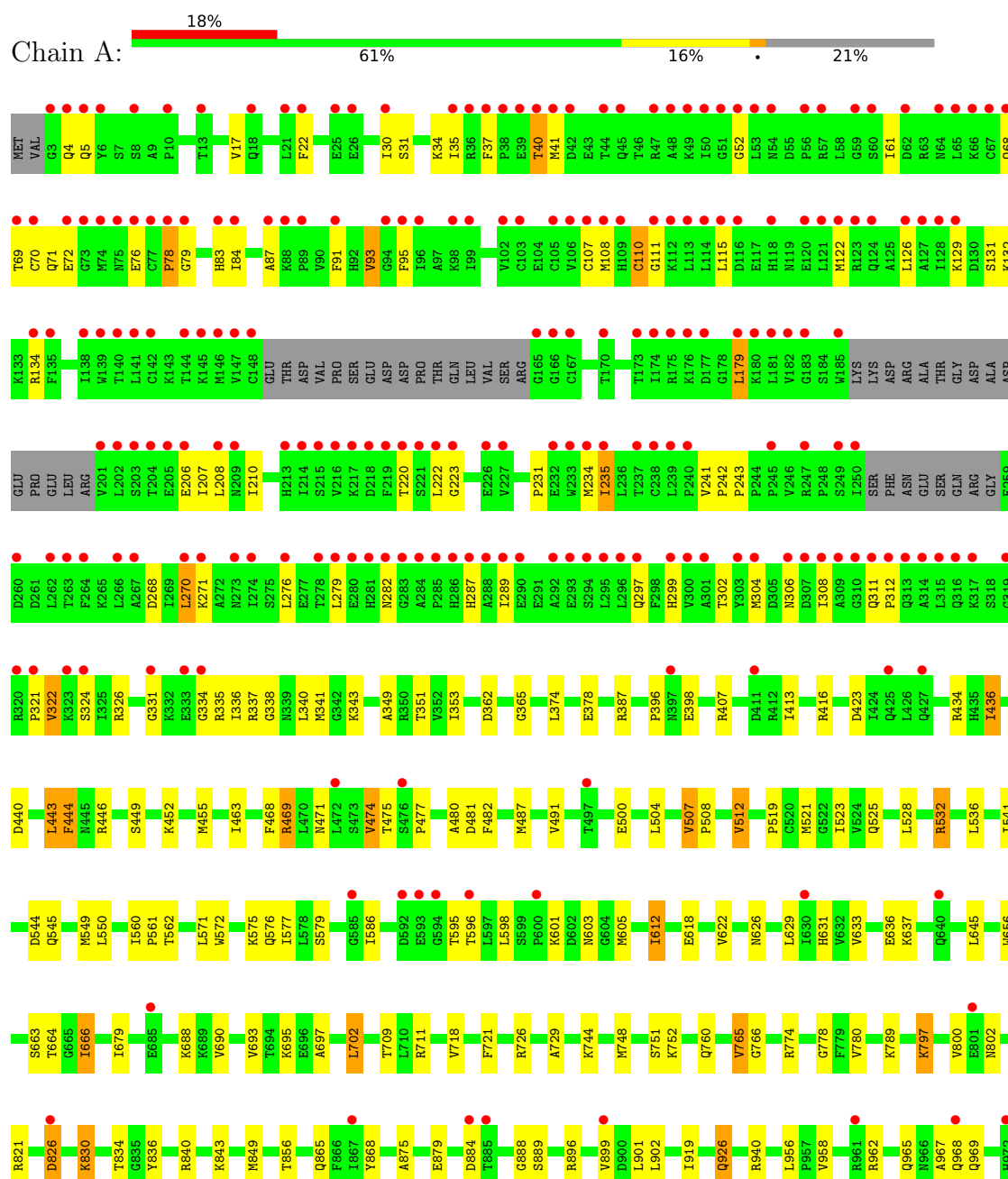


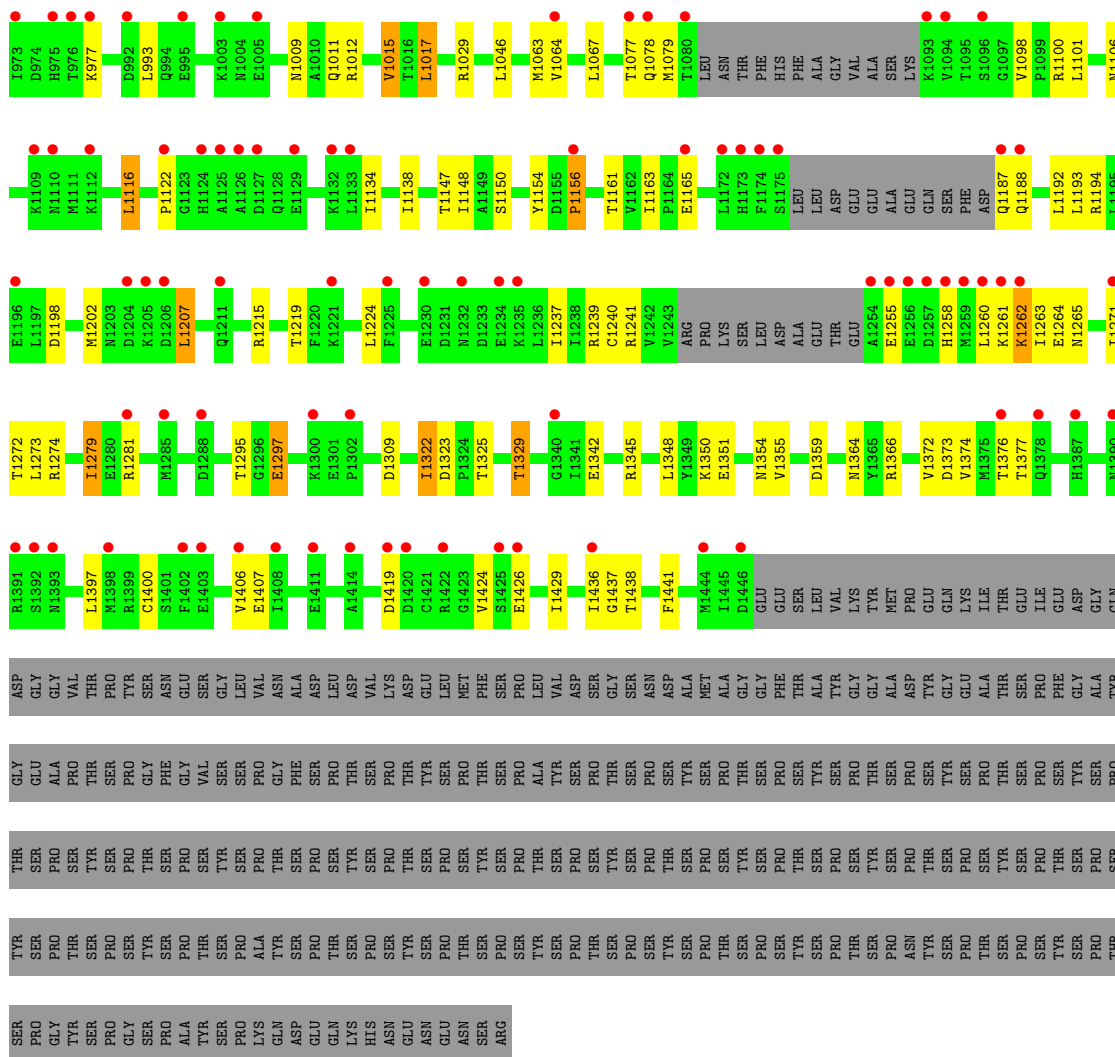
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

3 Residue-property plots

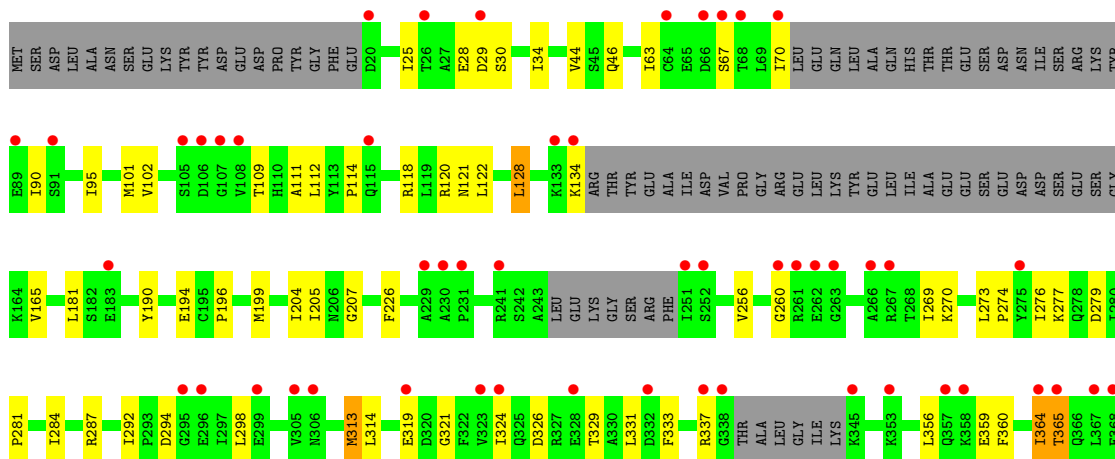
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

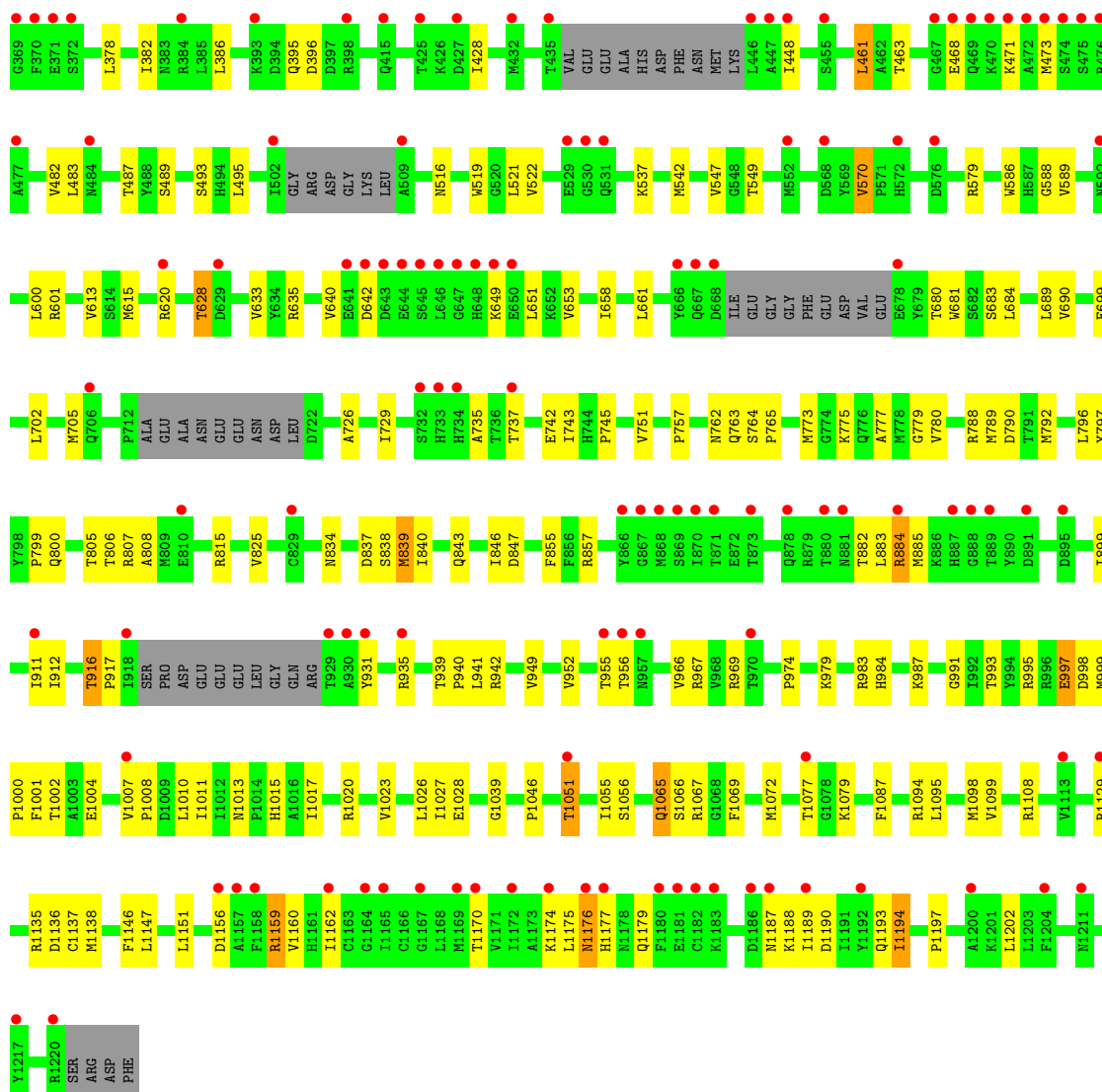
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



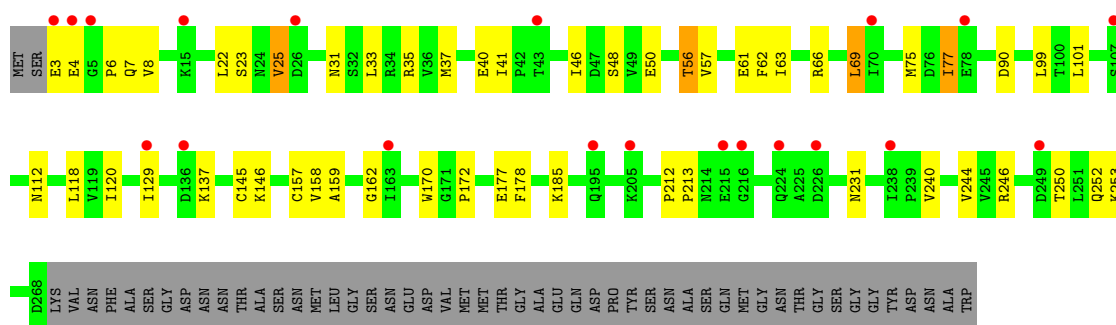


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

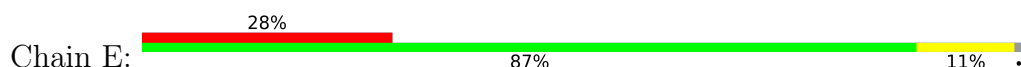


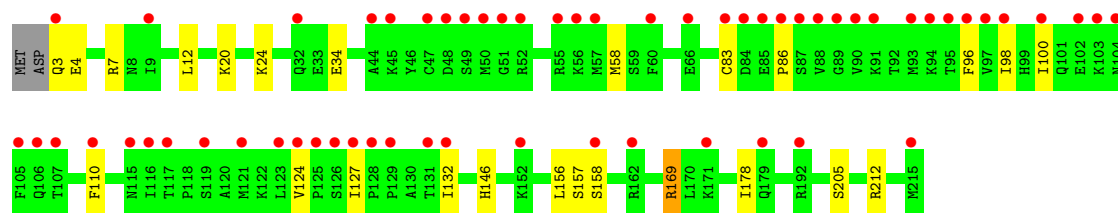


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

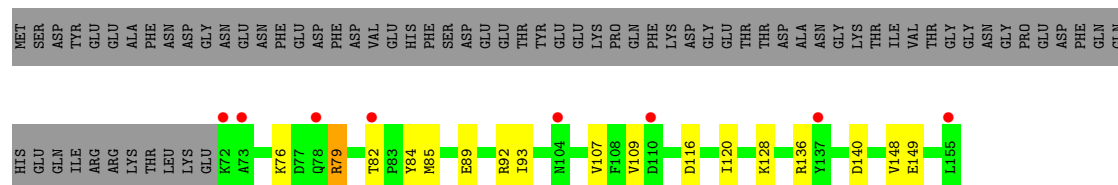


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

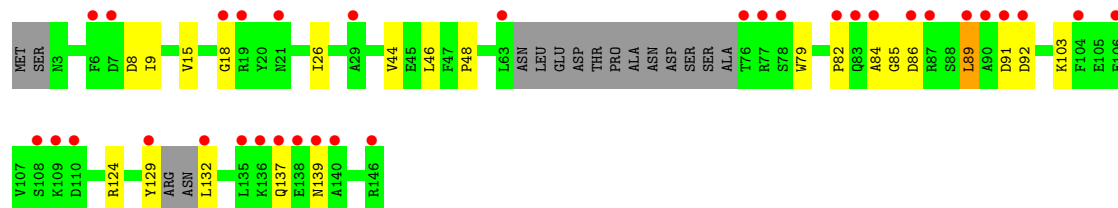
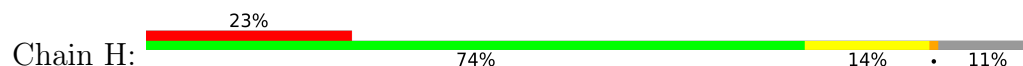




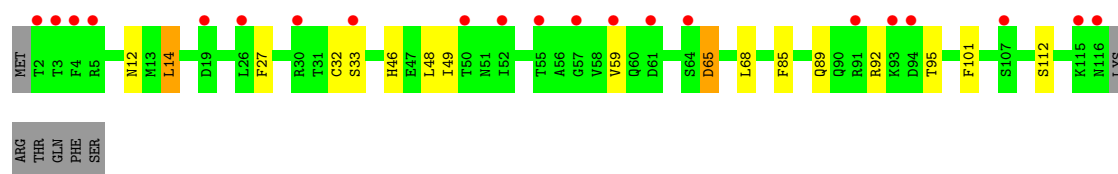
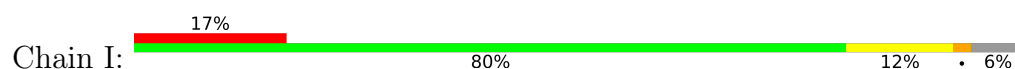
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



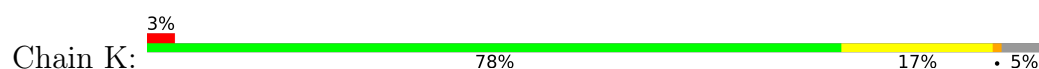
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

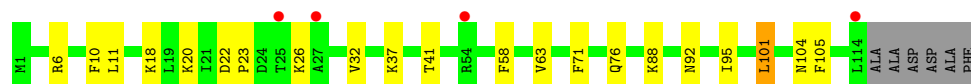


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

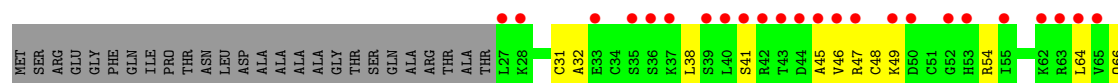


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

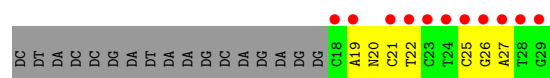




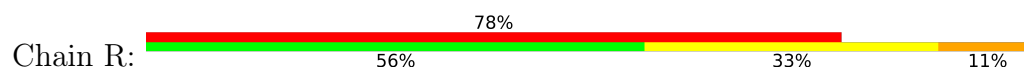
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: DNA (5'-D(P*CP*AP*(3DR)P*CP*TP*CP*TP*TP*GP*AP*TP*G)-3')



- Molecule 12: RNA (5'-R(*AP*UP*CP*AP*AP*GP*AP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.72Å 220.43Å 193.15Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	55.61 – 2.95 55.61 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.0 (55.61-2.95) 86.9 (55.61-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.234 , 0.260 0.241 , 0.267	Depositor DCC
R_{free} test set	6426 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	28274	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: 2KH, MG, 3DR, ZN

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	0/10975	0.70	4/14838 (0.0%)
2	B	0.26	0/8896	0.70	2/11996 (0.0%)
3	C	0.27	0/2133	0.72	0/2891
4	E	0.25	0/1780	0.71	0/2395
5	F	0.25	0/691	0.71	0/933
6	H	0.27	0/1060	0.70	0/1434
7	I	0.25	0/953	0.68	2/1284 (0.2%)
8	J	0.26	0/541	0.66	0/727
9	K	0.24	0/937	0.64	0/1265
10	L	0.24	0/353	0.63	1/468 (0.2%)
11	T	0.15	0/246	0.30	0/374
12	R	0.05	0/218	0.11	0/339
All	All	0.26	0/28783	0.69	9/38944 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	GLN	CB-CA-C	-6.14	109.48	116.54
10	L	45	ALA	CB-CA-C	-5.52	110.23	116.63
2	B	570	VAL	CA-C-N	5.36	124.99	119.05
2	B	570	VAL	C-N-CA	5.36	124.99	119.05
1	A	71	GLN	CB-CA-C	-5.31	110.01	117.23
1	A	1098	VAL	CB-CA-C	-5.25	108.78	114.35
1	A	507	VAL	CB-CA-C	-5.11	108.94	114.35
7	I	65	ASP	CA-C-N	5.09	124.75	119.56
7	I	65	ASP	C-N-CA	5.09	124.75	119.56

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	10784	0	10873	182	0
2	B	8726	0	8760	144	0
3	C	2095	0	2051	39	0
4	E	1744	0	1772	13	0
5	F	679	0	701	12	0
6	H	1043	0	1015	11	0
7	I	935	0	886	12	0
8	J	532	0	542	13	0
9	K	919	0	929	13	0
10	L	351	0	375	7	0
11	T	233	0	133	6	0
12	R	194	0	99	4	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	2	0	0	0	0
15	B	29	0	15	1	0
All	All	28274	0	28151	398	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 (398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.63	0.80
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.67	0.74
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.70	0.74
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.70	0.73
3:C:66:ARG:NH2	8:J:3:VAL:O	2.21	0.73
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.72	0.72
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.57	0.70
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.73	0.70
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.69
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.73	0.69
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.73	0.69
3:C:50:GLU:HG2	10:L:66:GLN:HG2	1.75	0.69
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.74	0.69
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.75	0.69
1:A:40:THR:HG22	1:A:41:MET:HG3	1.76	0.68
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.76	0.68
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.22	0.67
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.75	0.67
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.76	0.66
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.28	0.66
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.76	0.66
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.77	0.66
5:F:82:THR:HG22	5:F:84:TYR:H	1.60	0.66
1:A:134:ARG:NH1	1:A:220:THR:O	2.29	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.78	0.65
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.79	0.65
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.30	0.65
1:A:306:ASN:ND2	1:A:321:PRO:O	2.29	0.65
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.78	0.65
1:A:469:ARG:NH2	2:B:991:GLY:O	2.30	0.64
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.62	0.64
1:A:4:GLN:OE1	2:B:1159:ARG:NH1	2.29	0.64
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.80	0.64
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.80	0.64
2:B:463:THR:HG22	11:T:27:DA:H2"	1.80	0.63
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.80	0.63
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.80	0.63
7:I:32:CYS:SG	7:I:33:SER:N	2.72	0.63
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.80	0.63
8:J:37:SER:OG	8:J:47:ARG:NH2	2.32	0.63
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.81	0.62
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.81	0.62
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.82	0.62
3:C:48:SER:HB3	3:C:158:VAL:HB	1.81	0.62
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.65	0.62
2:B:882:THR:HB	2:B:885:MET:HE2	1.81	0.61
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:7:A:H2'	12:R:8:G:H8	1.64	0.61
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.82	0.61
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.67	0.60
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.83	0.60
1:A:1122:PRO:HD3	1:A:1323:ASP:HB2	1.83	0.60
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.34	0.60
3:C:145:CYS:SG	3:C:146:LYS:N	2.74	0.60
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.84	0.60
4:E:4:GLU:OE1	4:E:7:ARG:NH2	2.32	0.59
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.83	0.59
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.35	0.59
5:F:76:LYS:O	5:F:79:ARG:NH1	2.34	0.59
1:A:68:GLN:O	1:A:70:CYS:N	2.34	0.59
1:A:888:GLY:O	1:A:940:ARG:NH2	2.36	0.59
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.82	0.59
1:A:1325:THR:OG1	4:E:146:HIS:O	2.20	0.59
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.85	0.59
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.84	0.58
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.36	0.58
1:A:834:THR:HG21	1:A:1077:THR:HA	1.85	0.58
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.69	0.58
6:H:129:TYR:O	6:H:132:LEU:N	2.37	0.58
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.86	0.57
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.86	0.57
1:A:34:LYS:H	1:A:34:LYS:HD3	1.70	0.57
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.87	0.56
1:A:331:GLY:HA2	1:A:334:GLY:H	1.70	0.56
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.87	0.56
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.05	0.56
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.87	0.56
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.69	0.56
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.38	0.56
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.87	0.56
5:F:82:THR:O	5:F:136:ARG:NH1	2.30	0.56
1:A:110:CYS:SG	1:A:111:GLY:N	2.77	0.56
1:A:532:ARG:HE	1:A:536:LEU:HD21	1.70	0.56
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.86	0.56
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.87	0.56
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.39	0.55
6:H:91:ASP:OD1	6:H:92:ASP:N	2.38	0.55
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.89	0.55
1:A:595:THR:OG1	1:A:603:ASN:OD1	2.24	0.55
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.88	0.55
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.46	0.55
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.87	0.55
6:H:89:LEU:H	6:H:89:LEU:HD13	1.71	0.55
1:A:512:VAL:HA	1:A:519:PRO:HA	1.87	0.55
1:A:744:LYS:HE2	1:A:748:MET:HE3	1.89	0.55
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.88	0.55
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.88	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.89	0.55
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.42	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.40	0.54
2:B:287:ARG:NH1	2:B:321:GLY:O	2.40	0.54
6:H:137:GLN:HG3	6:H:139:ASN:H	1.71	0.54
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.90	0.54
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.89	0.54
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.89	0.54
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.90	0.54
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.89	0.54
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.90	0.54
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.88	0.54
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.73	0.54
2:B:101:MET:HG2	2:B:111:ALA:HA	1.90	0.54
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.90	0.53
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.38	0.53
2:B:680:THR:O	2:B:683:SER:OG	2.27	0.53
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.89	0.53
1:A:626:ASN:O	1:A:631:HIS:ND1	2.32	0.53
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.42	0.52
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.91	0.52
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.31	0.52
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.91	0.52
3:C:33:LEU:HG	3:C:37:MET:HE2	1.90	0.52
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.43	0.52
3:C:3:GLU:HG3	3:C:4:GLU:HG3	1.90	0.52
6:H:8:ASP:OD1	6:H:9:ILE:N	2.41	0.52
2:B:287:ARG:NH1	2:B:324:ILE:O	2.42	0.52
10:L:68:GLU:O	10:L:70:ARG:N	2.42	0.52
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.43	0.52
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:VAL:HG23	1:A:1067:LEU:HD23	1.91	0.51
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.43	0.51
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.91	0.51
2:B:487:THR:OG1	2:B:777:ALA:O	2.25	0.51
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.92	0.51
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.93	0.51
2:B:30:SER:OG	2:B:743:ILE:O	2.27	0.51
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.92	0.51
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.92	0.51
1:A:544:ASP:OD1	1:A:545:GLN:N	2.42	0.51
3:C:3:GLU:N	9:K:104:ASN:HD21	2.09	0.51
1:A:1116:LEU:HD22	1:A:1329:THR:HB	1.93	0.50
4:E:20:LYS:NZ	4:E:34:GLU:O	2.35	0.50
1:A:562:THR:O	1:A:576:GLN:NE2	2.44	0.50
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.94	0.50
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.93	0.50
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.93	0.50
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.12	0.50
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.43	0.50
1:A:802:ASN:OD1	2:B:729:ILE:N	2.39	0.50
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.39	0.50
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.94	0.50
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.93	0.50
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.93	0.50
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.94	0.50
6:H:85:GLY:HA2	6:H:86:ASP:HB3	1.93	0.49
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.93	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
4:E:83:CYS:HB2	4:E:110:PHE:HE1	1.77	0.49
10:L:48:CYS:SG	10:L:49:LYS:N	2.85	0.49
1:A:596:THR:C	1:A:598:LEU:H	2.19	0.49
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.93	0.49
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.94	0.49
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.94	0.49
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.95	0.49
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.94	0.49
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.46	0.49
1:A:1134:ILE:HD13	1:A:1322:ILE:HG22	1.94	0.49
6:H:89:LEU:HD23	6:H:91:ASP:H	1.78	0.49
1:A:337:ARG:NH1	11:T:19:DA:OP1	2.34	0.48
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:PRO:HB2	2:B:284:ILE:HG12	1.94	0.48
1:A:1207:LEU:HD23	1:A:1274:ARG:HD2	1.95	0.48
11:T:26:DG:H1	12:R:3:C:H42	1.60	0.48
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.94	0.48
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.93	0.48
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.95	0.48
1:A:541:ILE:HD12	1:A:577:ILE:HG12	1.95	0.48
1:A:95:PHE:HB3	1:A:234:MET:HE2	1.96	0.48
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.95	0.48
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.79	0.48
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.79	0.48
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.48
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.95	0.48
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.78	0.48
2:B:601:ARG:HA	2:B:615:MET:HE1	1.95	0.48
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.95	0.48
3:C:22:LEU:HD22	9:K:101:LEU:HD21	1.95	0.47
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.47
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.47	0.47
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.96	0.47
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.79	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.49	0.47
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.95	0.47
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.95	0.47
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.95	0.47
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.49	0.47
2:B:579:ARG:HA	2:B:589:VAL:HA	1.96	0.47
2:B:586:TRP:CD1	2:B:588:GLY:H	2.33	0.47
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.96	0.47
2:B:857:ARG:NH2	11:T:25:DC:OP1	2.47	0.47
1:A:446:ARG:HB2	1:A:487:MET:HE2	1.96	0.47
1:A:1364:ASN:OD1	1:A:1366:ARG:NH1	2.47	0.47
1:A:528:LEU:HD23	1:A:751:SER:HA	1.97	0.47
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.96	0.47
1:A:1064:VAL:HA	1:A:1067:LEU:HB3	1.96	0.46
1:A:107:CYS:SG	1:A:108:MET:N	2.89	0.46
1:A:826:ASP:O	1:A:830:LYS:HB2	2.15	0.46
1:A:1163:ILE:HG22	1:A:1165:GLU:H	1.80	0.46
2:B:378:LEU:O	2:B:382:ILE:HG12	2.15	0.46
3:C:40:GLU:O	3:C:250:THR:HG21	2.15	0.46
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:843:GLN:HB2	2:B:993:THR:HB	1.96	0.46
2:B:471:LYS:HA	2:B:473:MET:HE2	1.96	0.46
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.97	0.46
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.97	0.46
2:B:120:ARG:HB2	2:B:122:LEU:HG	1.98	0.46
2:B:956:THR:HG22	10:L:46:VAL:HG11	1.98	0.46
1:A:856:THR:HB	1:A:865:GLN:HB2	1.97	0.46
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.97	0.46
1:A:690:VAL:HG13	1:A:718:VAL:HG22	1.97	0.46
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.97	0.46
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.51	0.46
7:I:14:LEU:HD13	7:I:27:PHE:HB3	1.98	0.46
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.98	0.45
1:A:78:PRO:HB2	1:A:79:GLY:H	1.56	0.45
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.64	0.45
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.81	0.45
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.98	0.45
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.81	0.45
2:B:1175:LEU:C	2:B:1177:HIS:H	2.24	0.45
5:F:107:VAL:HG12	5:F:109:VAL:H	1.80	0.45
1:A:115:LEU:HB2	1:A:122:MET:HE3	1.98	0.45
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.78	0.45
1:A:962:ARG:HA	1:A:965:GLN:HG2	1.97	0.45
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.45
5:F:85:MET:HE1	5:F:148:VAL:HG13	1.99	0.45
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.99	0.45
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.98	0.45
15:B:1302:2KH:H10	15:B:1302:2KH:H14	1.60	0.45
1:A:774:ARG:HG3	1:A:797:LYS:HZ2	1.82	0.45
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.17	0.45
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.98	0.45
3:C:56:THR:HG21	3:C:63:ILE:HD11	1.99	0.45
1:A:396:PRO:C	1:A:398:GLU:H	2.25	0.45
1:A:695:LYS:HE3	1:A:695:LYS:HB2	1.81	0.45
1:A:235:ILE:H	1:A:235:ILE:HG13	1.55	0.44
1:A:1154:TYR:CE1	1:A:1156:PRO:HG3	2.52	0.44
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.81	0.44
1:A:711:ARG:NH2	7:I:95:THR:OG1	2.49	0.44
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.82	0.44
1:A:633:VAL:HG11	1:A:645:LEU:HD22	1.98	0.44
2:B:757:PRO:HG2	2:B:984:HIS:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:SER:OG	1:A:664:THR:N	2.51	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.82	0.44
1:A:179:LEU:HD22	1:A:297:GLN:HG3	2.00	0.44
1:A:443:LEU:HD12	2:B:1146:PHE:CE1	2.51	0.44
1:A:1260:LEU:HD12	1:A:1263:ILE:HD12	2.00	0.44
3:C:62:PHE:O	3:C:66:ARG:HG3	2.18	0.44
4:E:157:SER:OG	4:E:158:SER:N	2.50	0.44
9:K:10:PHE:HA	9:K:37:LYS:HB3	1.99	0.44
2:B:1039:GLY:HA2	8:J:51:LEU:HD22	2.00	0.44
1:A:336:ILE:HA	1:A:340:LEU:HD12	2.00	0.44
1:A:343:LYS:HE2	2:B:1151:LEU:HA	1.98	0.44
1:A:446:ARG:NH2	12:R:9:A:O2'	2.51	0.44
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.99	0.44
11:T:22:DT:H3	12:R:7:A:H2	1.66	0.44
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.53	0.44
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.99	0.44
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.00	0.44
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.98	0.44
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.99	0.44
1:A:93:VAL:HG12	1:A:304:MET:HE3	2.00	0.44
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.99	0.44
1:A:477:PRO:HG3	1:A:521:MET:HE2	2.00	0.44
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.51	0.44
3:C:99:LEU:HB3	3:C:120:ILE:HD13	2.00	0.44
6:H:84:ALA:HB3	6:H:86:ASP:HB3	2.00	0.44
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.99	0.43
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.43
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.00	0.43
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.00	0.43
3:C:112:ASN:ND2	8:J:19:GLU:OE2	2.51	0.43
9:K:88:LYS:O	9:K:92:ASN:ND2	2.47	0.43
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.18	0.43
2:B:256:VAL:HG11	2:B:382:ILE:HD13	2.00	0.43
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.54	0.43
9:K:63:VAL:HG22	9:K:71:PHE:HB3	2.01	0.43
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.84	0.43
2:B:118:ARG:HG3	2:B:204:ILE:HD13	2.00	0.43
2:B:199:MET:SD	2:B:199:MET:N	2.78	0.43
2:B:883:LEU:O	2:B:885:MET:N	2.52	0.43
1:A:471:ASN:O	1:A:474:VAL:HG12	2.18	0.43
2:B:493:SER:OG	2:B:775:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:792:MET:HE3	2:B:855:PHE:HE1	1.83	0.43
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.19	0.43
10:L:31:CYS:SG	10:L:32:ALA:N	2.92	0.43
2:B:806:THR:HG22	2:B:808:ALA:H	1.84	0.43
1:A:31:SER:HB2	1:A:83:HIS:HB3	2.00	0.43
8:J:8:PHE:H	8:J:49:MET:HE3	1.84	0.43
1:A:541:ILE:N	1:A:572:TRP:O	2.43	0.43
1:A:1255:GLU:HB3	1:A:1258:HIS:CE1	2.54	0.43
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.23	0.43
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.33	0.43
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.19	0.43
3:C:22:LEU:HB3	3:C:25:VAL:HG21	2.01	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.01	0.42
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.99	0.42
3:C:69:LEU:O	8:J:6:ARG:HD2	2.19	0.42
1:A:560:ILE:HB	6:H:79:TRP:H	1.84	0.42
2:B:805:THR:HG21	2:B:815:ARG:HD3	2.01	0.42
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.52	0.42
2:B:1000:PRO:HB2	2:B:1072:MET:HE3	2.01	0.42
1:A:1017:LEU:HB2	4:E:205:SER:C	2.44	0.42
1:A:1215:ARG:HD3	1:A:1272:THR:O	2.19	0.42
2:B:34:ILE:HG23	2:B:542:MET:HE3	2.01	0.42
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	2.02	0.42
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.19	0.42
1:A:1373:ASP:HA	1:A:1376:THR:HG22	2.00	0.42
3:C:8:VAL:HG11	9:K:105:PHE:CD1	2.55	0.42
2:B:1162:ILE:HG12	2:B:1194:ILE:HD12	2.02	0.42
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.87	0.42
4:E:124:VAL:HG13	4:E:132:ILE:HB	2.02	0.42
1:A:108:MET:O	1:A:110:CYS:N	2.50	0.42
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.60	0.42
1:A:129:LYS:HA	1:A:134:ARG:HH21	1.85	0.42
1:A:206:GLU:O	1:A:210:ILE:HG12	2.20	0.42
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.85	0.42
2:B:789:MET:HE1	2:B:967:ARG:HB2	2.02	0.42
2:B:884:ARG:HD3	2:B:884:ARG:HA	1.88	0.42
1:A:84:ILE:HD12	1:A:270:LEU:HG	2.02	0.42
1:A:1262:LYS:O	1:A:1265:ASN:HB3	2.20	0.42
2:B:114:PRO:HG2	2:B:181:LEU:HD11	2.01	0.42
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.55	0.42
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PRO:HA	1:A:234:MET:HG3	2.02	0.41
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.93	0.41
1:A:349:ALA:HB2	1:A:374:LEU:HD11	2.02	0.41
1:A:449:SER:HB3	2:B:1137:CYS:SG	2.61	0.41
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.18	0.41
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.03	0.41
2:B:487:THR:HG22	2:B:489:SER:H	1.85	0.41
1:A:131:SER:HB3	1:A:223:GLY:HA2	2.02	0.41
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.02	0.41
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.02	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.01	0.41
1:A:1436:ILE:O	1:A:1438:THR:N	2.53	0.41
5:F:76:LYS:O	5:F:79:ARG:HD3	2.20	0.41
1:A:70:CYS:O	1:A:72:GLU:HG2	2.20	0.41
1:A:575:LYS:O	1:A:579:SER:OG	2.36	0.41
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.53	0.41
4:E:169:ARG:HG3	5:F:140:ASP:HB3	2.03	0.41
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.03	0.41
1:A:72:GLU:CD	2:B:1175:LEU:HB2	2.46	0.41
1:A:780:VAL:HG22	2:B:699:GLU:OE2	2.20	0.41
1:A:1147:THR:HB	7:I:48:LEU:HD12	2.03	0.41
2:B:364:ILE:HG13	2:B:365:THR:OG1	2.20	0.41
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.02	0.41
1:A:575:LYS:HB3	1:A:612:ILE:HD13	2.03	0.41
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.02	0.41
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.20	0.41
2:B:939:THR:HA	2:B:940:PRO:HD3	1.85	0.41
5:F:93:ILE:HD13	5:F:93:ILE:HA	1.93	0.41
1:A:444:PHE:HD1	1:A:444:PHE:HA	1.72	0.41
1:A:507:VAL:HG13	1:A:521:MET:HE1	2.02	0.41
1:A:1207:LEU:HD22	1:A:1273:LEU:HD23	2.03	0.41
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.55	0.41
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.03	0.41
9:K:22:ASP:HA	9:K:23:PRO:HD3	1.90	0.41
1:A:500:GLU:O	1:A:504:LEU:HB2	2.21	0.41
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.21	0.41
3:C:75:MET:O	3:C:246:ARG:NH2	2.48	0.41
1:A:571:LEU:HD12	6:H:46:LEU:HD11	2.03	0.40
1:A:843:LYS:HD3	1:A:843:LYS:HA	1.94	0.40
1:A:849:MET:HB3	1:A:1063:MET:SD	2.61	0.40
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:O	2:B:67:SER:OG	2.36	0.40
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.73	0.40
5:F:128:LYS:HD2	5:F:149:GLU:HA	2.03	0.40
1:A:311:GLN:N	1:A:312:PRO:HD2	2.36	0.40
1:A:967:ALA:C	1:A:969:GLN:H	2.29	0.40
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.03	0.40
2:B:298:LEU:HD22	2:B:314:LEU:HD13	2.03	0.40
4:E:24:LYS:HE3	4:E:24:LYS:HB2	1.89	0.40
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.56	0.40
1:A:423:ASP:OD1	1:A:423:ASP:N	2.54	0.40
1:A:752:LYS:HG2	2:B:1015:HIS:O	2.22	0.40
1:A:1261:LYS:HB2	1:A:1261:LYS:HE3	1.88	0.40
2:B:270:LYS:HB3	2:B:279:ASP:HB3	2.03	0.40
2:B:916:THR:HA	2:B:917:PRO:HD3	1.84	0.40
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.39	0.40
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.03	0.40
1:A:965:GLN:HA	1:A:968:GLN:HG2	2.04	0.40
2:B:600:LEU:HB3	2:B:615:MET:SD	2.61	0.40
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.21	0.40
5:F:116:ASP:O	5:F:120:ILE:HG13	2.22	0.40
2:B:773:MET:SD	2:B:987:LYS:HB3	2.62	0.40
2:B:999:MET:HE3	2:B:1011:ILE:HG13	2.03	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	1358/1733 (78%)	1248 (92%)	100 (7%)	10 (1%)	18	40
2	B	1077/1224 (88%)	1005 (93%)	64 (6%)	8 (1%)	18	40
3	C	264/318 (83%)	246 (93%)	17 (6%)	1 (0%)	30	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	211/215 (98%)	200 (95%)	10 (5%)	1 (0%)	24	49
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
6	H	124/146 (85%)	106 (86%)	16 (13%)	2 (2%)	7	21
7	I	113/122 (93%)	101 (89%)	12 (11%)	0	100	100
8	J	63/70 (90%)	60 (95%)	3 (5%)	0	100	100
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	14	34
10	L	42/70 (60%)	35 (83%)	5 (12%)	2 (5%)	2	3
All	All	3446/4173 (83%)	3187 (92%)	234 (7%)	25 (1%)	18	40

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
2	B	1046	PRO
1	A	110	CYS
1	A	322	VAL
1	A	1437	GLY
2	B	337	ARG
2	B	468	GLU
4	E	86	PRO
10	L	69	ALA
1	A	282	ASN
2	B	277	LYS
2	B	884	ARG
2	B	1108	ARG
3	C	90	ASP
10	L	41	SER
1	A	40	THR
1	A	958	VAL
2	B	1017	ILE
9	K	26	LYS
1	A	69	THR
1	A	1156	PRO
1	A	1279	ILE
6	H	18	GLY
6	H	82	PRO
2	B	260	GLY

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	1196/1520 (79%)	1136 (95%)	60 (5%)	22	47
2	B	952/1061 (90%)	910 (96%)	42 (4%)	25	51
3	C	234/274 (85%)	226 (97%)	8 (3%)	32	58
4	E	195/197 (99%)	190 (97%)	5 (3%)	40	65
5	F	74/137 (54%)	73 (99%)	1 (1%)	59	77
6	H	114/128 (89%)	109 (96%)	5 (4%)	25	51
7	I	109/116 (94%)	107 (98%)	2 (2%)	51	72
8	J	60/65 (92%)	57 (95%)	3 (5%)	22	47
9	K	99/102 (97%)	94 (95%)	5 (5%)	21	47
10	L	39/57 (68%)	38 (97%)	1 (3%)	40	65
All	All	3072/3657 (84%)	2940 (96%)	132 (4%)	26	52

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	61	ILE
1	A	93	VAL
1	A	126	LEU
1	A	132	LYS
1	A	179	LEU
1	A	208	LEU
1	A	222	LEU
1	A	235	ILE
1	A	270	LEU
1	A	271	LYS
1	A	287	HIS
1	A	308	ILE
1	A	322	VAL
1	A	335	ARG
1	A	351	THR

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Mol	Chain	Res	Type
1	A	436	ILE
1	A	443	LEU
1	A	444	PHE
1	A	452	LYS
1	A	463	ILE
1	A	469	ARG
1	A	474	VAL
1	A	475	THR
1	A	481	ASP
1	A	512	VAL
1	A	532	ARG
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	629	LEU
1	A	666	ILE
1	A	688	LYS
1	A	702	LEU
1	A	765	VAL
1	A	797	LYS
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	884	ASP
1	A	896	ARG
1	A	919	ILE
1	A	926	GLN
1	A	977	LYS
1	A	1015	VAL
1	A	1017	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1207	LEU
1	A	1262	LYS
1	A	1295	THR
1	A	1297	GLU
1	A	1322	ILE
1	A	1329	THR
1	A	1350	LYS
1	A	1354	ASN
1	A	1374	VAL
1	A	1377	THR

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Mol	Chain	Res	Type
1	A	1400	CYS
1	A	1407	GLU
2	B	46	GLN
2	B	70	ILE
2	B	90	ILE
2	B	109	THR
2	B	128	LEU
2	B	134	LYS
2	B	313	MET
2	B	319	GLU
2	B	331	LEU
2	B	364	ILE
2	B	365	THR
2	B	396	ASP
2	B	461	LEU
2	B	482	VAL
2	B	483	LEU
2	B	547	VAL
2	B	549	THR
2	B	570	VAL
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	916	THR
2	B	931	TYR
2	B	983	ARG
2	B	997	GLU
2	B	1007	VAL
2	B	1028	GLU
2	B	1051	THR
2	B	1065	GLN
2	B	1099	VAL
2	B	1147	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1176	ASN
2	B	1188	LYS
2	B	1189	ILE

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Mol	Chain	Res	Type
2	B	1194	ILE
2	B	1202	LEU
3	C	25	VAL
3	C	56	THR
3	C	69	LEU
3	C	77	ILE
3	C	137	LYS
3	C	240	VAL
3	C	244	VAL
3	C	253	LYS
4	E	3	GLN
4	E	98	ILE
4	E	127	ILE
4	E	156	LEU
4	E	169	ARG
5	F	79	ARG
6	H	15	VAL
6	H	26	ILE
6	H	89	LEU
6	H	103	LYS
6	H	124	ARG
7	I	14	LEU
7	I	59	VAL
8	J	3	VAL
8	J	5	VAL
8	J	13	VAL
9	K	11	LEU
9	K	18	LYS
9	K	20	LYS
9	K	32	VAL
9	K	101	LEU
10	L	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	109	HIS
1	A	316	GLN
1	A	394	ASN
1	A	525	GLN
1	A	736	ASN

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Mol	Chain	Res	Type
1	A	965	GLN
1	A	1008	GLN
2	B	60	GLN
2	B	449	ASN
2	B	513	GLN
2	B	531	GLN
2	B	762	ASN
2	B	770	GLN
2	B	862	GLN
2	B	951	GLN
2	B	984	HIS
2	B	1065	GLN
2	B	1093	GLN
2	B	1176	ASN
2	B	1177	HIS
3	C	112	ASN
3	C	131	HIS
3	C	140	ASN
4	E	153	HIS
5	F	104	ASN
7	I	90	GLN
9	K	104	ASN
9	K	112	GLN

5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	9	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	3DR	T	20	11	8,11,12	1.26	1 (12%)	7,14,17	1.46	1 (14%)

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	3DR	T	20	11	-	2/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	20	3DR	O4'-C4'	-2.26	1.40	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	20	3DR	O4'-C4'-C3'	2.88	107.96	103.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	20	3DR	O4'-C4'-C5'-O5'
11	T	20	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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
15	2KH	B	1302	14	29,30,30	3.54	14 (48%)	41,47,47	1.59	4 (9%)

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
15	2KH	B	1302	14	-	13/19/38/38	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1302	2KH	O4'-C1'	8.84	1.62	1.42
15	B	1302	2KH	C2'-C1'	-7.36	1.30	1.53
15	B	1302	2KH	O4'-C4'	-7.36	1.28	1.45
15	B	1302	2KH	C2-N1	5.75	1.47	1.38
15	B	1302	2KH	C2-N3	5.71	1.47	1.38
15	B	1302	2KH	C6-C5	5.59	1.48	1.35
15	B	1302	2KH	PA-O1A	4.03	1.52	1.46
15	B	1302	2KH	PB-O2B	3.51	1.51	1.46
15	B	1302	2KH	O2'-C2'	2.69	1.49	1.43
15	B	1302	2KH	O3'-C3'	-2.55	1.36	1.43
15	B	1302	2KH	C4-N3	2.24	1.42	1.38
15	B	1302	2KH	PB-O1B	-2.07	1.51	1.56
15	B	1302	2KH	C1'-N1	-2.02	1.41	1.47
15	B	1302	2KH	PA-N3A	2.02	1.68	1.63

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1302	2KH	C4-N3-C2	-5.31	120.02	126.61
15	B	1302	2KH	N3-C2-N1	4.14	120.28	114.89
15	B	1302	2KH	C5-C4-N3	3.75	120.05	114.80
15	B	1302	2KH	O4-C4-C5	-3.02	119.96	125.16

There are no chirality outliers.

All (13) torsion outliers are listed below:

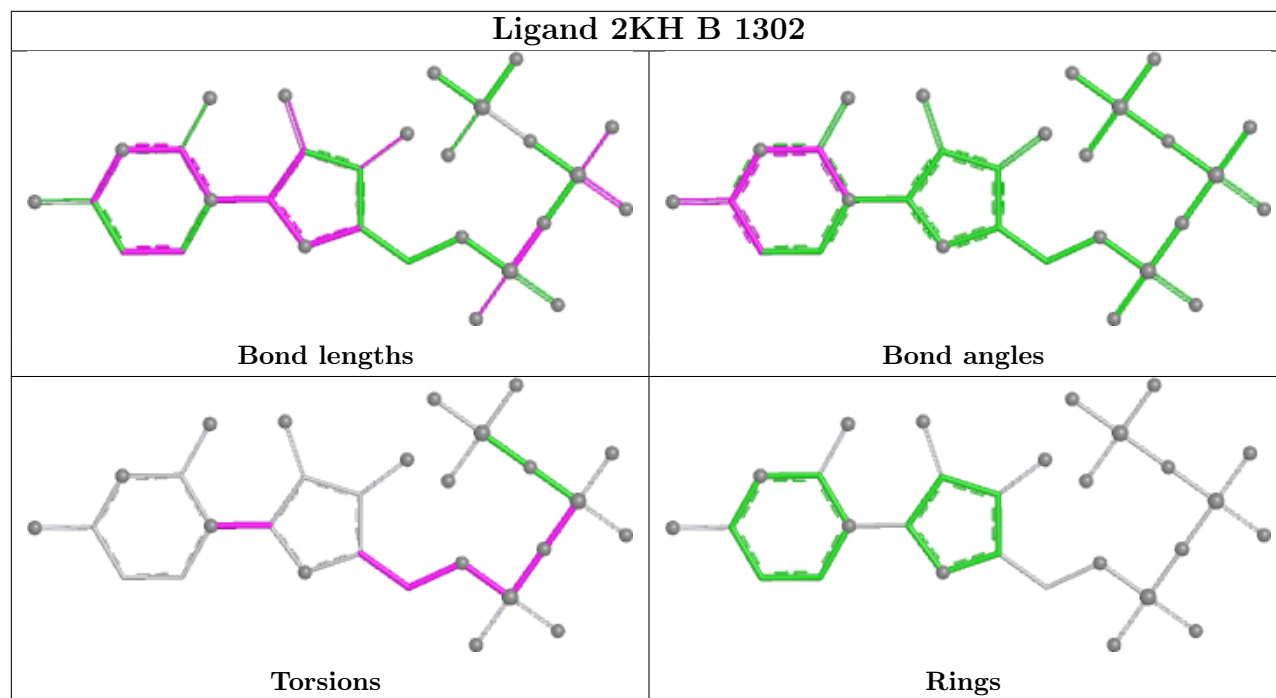
Mol	Chain	Res	Type	Atoms
15	B	1302	2KH	PB-N3A-PA-O1A
15	B	1302	2KH	C5'-O5'-PA-O2A
15	B	1302	2KH	PA-N3A-PB-O2B
15	B	1302	2KH	O4'-C4'-C5'-O5'
15	B	1302	2KH	O4'-C1'-N1-C6
15	B	1302	2KH	O4'-C1'-N1-C2
15	B	1302	2KH	C2'-C1'-N1-C6
15	B	1302	2KH	C3'-C4'-C5'-O5'
15	B	1302	2KH	C5'-O5'-PA-O1A
15	B	1302	2KH	C5'-O5'-PA-N3A
15	B	1302	2KH	C2'-C1'-N1-C2
15	B	1302	2KH	C4'-C5'-O5'-PA
15	B	1302	2KH	PA-N3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1302	2KH	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1372/1733 (79%)	1.09	308 (22%) 2 2	16, 58, 161, 242	0
2	B	1097/1224 (89%)	0.82	169 (15%) 5 5	13, 46, 119, 225	0
3	C	266/318 (83%)	0.55	20 (7%) 20 18	19, 45, 85, 171	0
4	E	213/215 (99%)	1.40	60 (28%) 1 1	35, 86, 172, 234	0
5	F	84/155 (54%)	0.71	8 (9%) 14 12	35, 58, 109, 179	0
6	H	130/146 (89%)	1.48	33 (25%) 1 1	42, 84, 147, 206	0
7	I	115/122 (94%)	1.08	21 (18%) 3 3	20, 61, 101, 114	0
8	J	65/70 (92%)	0.28	2 (3%) 51 44	22, 36, 82, 159	0
9	K	114/120 (95%)	0.36	4 (3%) 47 40	20, 49, 90, 108	0
10	L	44/70 (62%)	2.41	24 (54%) 0 0	26, 88, 182, 231	0
11	T	11/29 (37%)	3.57	11 (100%) 0 0	133, 138, 177, 179	0
12	R	9/9 (100%)	2.24	7 (77%) 0 0	111, 125, 150, 151	0
All	All	3520/4211 (83%)	0.98	667 (18%) 3 3	13, 55, 149, 242	0

All (667) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	J	65	PRO	8.9
1	A	250	ILE	8.8
1	A	65	LEU	8.5
2	B	477	ALA	8.3
1	A	182	VAL	7.7
2	B	474	SER	7.7
10	L	45	ALA	7.5
1	A	179	LEU	7.4
2	B	733	HIS	7.4
10	L	27	LEU	7.3
1	A	312	PRO	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	266	ALA	6.8
2	B	646	LEU	6.6
2	B	918	ILE	6.5
1	A	147	VAL	6.4
2	B	446	LEU	6.2
1	A	98	LYS	6.2
1	A	174	ILE	6.1
1	A	64	ASN	6.0
1	A	49	LYS	6.0
10	L	46	VAL	6.0
3	C	205	LYS	5.8
1	A	397	ASN	5.8
2	B	1183	LYS	5.8
2	B	643	ASP	5.7
1	A	60	SER	5.7
2	B	929	THR	5.6
10	L	41	SER	5.6
4	E	98	ILE	5.6
1	A	177	ASP	5.5
1	A	227	VAL	5.5
11	T	19	DA	5.5
10	L	40	LEU	5.5
2	B	1170	THR	5.5
2	B	1189	ILE	5.5
2	B	476	ARG	5.4
2	B	472	ALA	5.3
6	H	84	ALA	5.3
1	A	1174	PHE	5.3
1	A	249	SER	5.3
1	A	183	GLY	5.3
2	B	251	ILE	5.3
2	B	648	HIS	5.2
1	A	181	LEU	5.2
2	B	471	LYS	5.2
5	F	73	ALA	5.2
1	A	113	LEU	5.1
7	I	3	THR	5.1
2	B	502	ILE	5.1
6	H	19	ARG	5.1
4	E	95	THR	5.1
1	A	1234	GLU	5.0
2	B	509	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	5.0
10	L	35	SER	4.9
1	A	1446	ASP	4.9
6	H	92	ASP	4.9
10	L	64	LEU	4.9
10	L	53	HIS	4.9
2	B	261	ARG	4.9
1	A	221	SER	4.8
1	A	238	CYS	4.8
1	A	141	LEU	4.8
1	A	1256	GLU	4.8
6	H	136	LYS	4.8
6	H	83	GLN	4.8
1	A	73	GLY	4.7
4	E	123	LEU	4.6
1	A	56	PRO	4.6
1	A	1125	ALA	4.6
11	T	24	DT	4.6
1	A	69	THR	4.6
2	B	889	THR	4.6
1	A	142	CYS	4.6
2	B	267	ARG	4.6
10	L	36	SER	4.6
2	B	1217	TYR	4.5
1	A	112	LYS	4.5
1	A	185	TRP	4.5
1	A	975	HIS	4.5
1	A	208	LEU	4.5
2	B	866	TYR	4.5
6	H	129	TYR	4.5
1	A	1261	LYS	4.4
2	B	881	ASN	4.4
1	A	1257	ASP	4.4
1	A	310	GLY	4.4
2	B	262	GLU	4.4
2	B	275	TYR	4.4
6	H	139	ASN	4.3
1	A	316	GLN	4.3
4	E	52	ARG	4.3
1	A	50	ILE	4.3
1	A	274	ILE	4.3
2	B	878	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	ALA	4.3
2	B	576	ASP	4.3
3	C	4	GLU	4.3
7	I	116	ASN	4.3
1	A	91	PHE	4.3
2	B	447	ALA	4.3
1	A	74	MET	4.2
2	B	241	ARG	4.2
1	A	235	ILE	4.2
1	A	234	MET	4.2
6	H	86	ASP	4.2
2	B	370	PHE	4.2
1	A	1258	HIS	4.2
2	B	641	GLU	4.2
1	A	1262	LYS	4.1
4	E	90	VAL	4.1
1	A	233	TRP	4.1
1	A	128	ILE	4.1
1	A	70	CYS	4.1
4	E	83	CYS	4.1
1	A	129	LYS	4.1
4	E	93	MET	4.1
1	A	115	LEU	4.0
1	A	144	THR	4.0
2	B	20	ASP	4.0
2	B	647	GLY	4.0
11	T	18	DC	4.0
11	T	25	DC	4.0
1	A	286	HIS	4.0
4	E	127	ILE	4.0
1	A	1133	LEU	4.0
1	A	425	GLN	4.0
1	A	44	THR	4.0
1	A	240	PRO	4.0
4	E	125	PRO	4.0
1	A	1422	ARG	3.9
10	L	42	ARG	3.9
6	H	63	LEU	3.9
2	B	868	MET	3.9
1	A	1080	THR	3.9
1	A	146	MET	3.9
4	E	105	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
6	H	76	THR	3.9
7	I	2	THR	3.9
1	A	826	ASP	3.9
1	A	1187	GLN	3.9
1	A	596	THR	3.9
1	A	79	GLY	3.8
2	B	467	GLY	3.8
1	A	66	LYS	3.8
1	A	237	THR	3.8
2	B	867	GLY	3.8
1	A	1259	MET	3.8
1	A	103	CYS	3.8
1	A	4	GLN	3.8
1	A	1393	ASN	3.8
4	E	115	ASN	3.8
1	A	108	MET	3.8
2	B	252	SER	3.8
2	B	299	GLU	3.8
1	A	201	VAL	3.8
1	A	216	VAL	3.8
6	H	137	GLN	3.8
2	B	887	HIS	3.8
1	A	1126	ALA	3.8
1	A	239	LEU	3.8
1	A	973	ILE	3.7
1	A	6	TYR	3.7
1	A	315	LEU	3.7
4	E	215	MET	3.7
2	B	263	GLY	3.7
1	A	106	VAL	3.7
1	A	295	LEU	3.7
1	A	333	GLU	3.7
5	F	72	LYS	3.7
1	A	62	ASP	3.7
4	E	87	SER	3.6
2	B	229	ALA	3.6
1	A	323	LYS	3.6
1	A	1403	GLU	3.6
1	A	220	THR	3.6
5	F	155	LEU	3.6
2	B	531	GLN	3.6
2	B	1177	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	45	GLN	3.6
1	A	219	PHE	3.6
12	R	1	A	3.6
1	A	263	THR	3.6
1	A	105	CYS	3.5
1	A	1378	GLN	3.5
4	E	85	GLU	3.5
6	H	106	GLU	3.5
1	A	122	MET	3.5
2	B	134	LYS	3.5
3	C	15	LYS	3.5
1	A	48	ALA	3.5
3	C	78	GLU	3.5
2	B	367	LEU	3.5
1	A	287	HIS	3.5
3	C	163	ILE	3.5
2	B	734	HIS	3.5
2	B	957	ASN	3.5
2	B	1167	GLY	3.5
1	A	472	LEU	3.5
6	H	135	LEU	3.5
1	A	109	HIS	3.5
2	B	435	THR	3.5
7	I	55	THR	3.5
2	B	230	ALA	3.5
1	A	59	GLY	3.4
7	I	57	GLY	3.4
2	B	67	SER	3.4
2	B	475	SER	3.4
1	A	5	GLN	3.4
4	E	9	ILE	3.4
11	T	28	DT	3.4
1	A	41	MET	3.4
1	A	317	LYS	3.4
2	B	473	MET	3.4
11	T	29	DG	3.4
1	A	972	HIS	3.4
2	B	737	THR	3.4
1	A	37	PHE	3.4
1	A	54	ASN	3.4
2	B	1180	PHE	3.4
6	H	90	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
12	R	9	A	3.4
1	A	138	ILE	3.4
1	A	992	ASP	3.4
2	B	1211	ASN	3.4
1	A	3	GLY	3.4
1	A	52	GLY	3.4
2	B	323	VAL	3.4
1	A	39	GLU	3.4
1	A	72	GLU	3.4
2	B	357	GLN	3.4
1	A	266	LEU	3.3
2	B	870	ILE	3.3
3	C	238	ILE	3.3
4	E	55	ARG	3.3
6	H	146	ARG	3.3
4	E	152	LYS	3.3
1	A	270	LEU	3.3
7	I	91	ARG	3.3
1	A	215	SER	3.3
1	A	1425	SER	3.3
4	E	100	ILE	3.3
2	B	365	THR	3.3
1	A	8	SER	3.3
2	B	884	ARG	3.2
1	A	313	GLN	3.2
1	A	1078	GLN	3.2
4	E	117	THR	3.2
1	A	38	PRO	3.2
11	T	23	DC	3.2
1	A	1172	LEU	3.2
2	B	1220	ARG	3.2
7	I	5	ARG	3.2
6	H	138	GLU	3.2
1	A	977	LYS	3.2
1	A	1211	GLN	3.2
10	L	43	THR	3.2
11	T	22	DT	3.2
1	A	867	ILE	3.2
4	E	158	SER	3.2
1	A	42	ASP	3.2
2	B	895	ASP	3.2
6	H	89	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
4	E	89	GLY	3.2
2	B	871	THR	3.2
3	C	3	GLU	3.2
4	E	129	PRO	3.2
1	A	77	CYS	3.1
2	B	105	SER	3.1
1	A	1127	ASP	3.1
1	A	284	ALA	3.1
1	A	1173	HIS	3.1
2	B	345	LYS	3.1
3	C	249	ASP	3.1
4	E	84	ASP	3.1
1	A	21	LEU	3.1
11	T	21	DC	3.1
10	L	37	LYS	3.1
2	B	372	SER	3.1
2	B	432	MET	3.1
10	L	63	ARG	3.1
2	B	931	TYR	3.1
2	B	427	ASP	3.1
1	A	36	ARG	3.1
2	B	89	GLU	3.1
1	A	267	ALA	3.0
1	A	1110	ASN	3.0
3	C	226	ASP	3.0
6	H	110	ASP	3.0
4	E	86	PRO	3.0
1	A	976	THR	3.0
4	E	110	PHE	3.0
2	B	645	SER	3.0
1	A	111	GLY	3.0
1	A	166	GLY	3.0
1	A	53	LEU	3.0
1	A	1005	GLU	3.0
2	B	810	GLU	3.0
2	B	68	THR	3.0
1	A	264	PHE	3.0
1	A	1124	HIS	3.0
1	A	319	GLY	3.0
10	L	62	LYS	3.0
7	I	33	SER	3.0
4	E	107	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	529	GLU	3.0
1	A	51	GLY	2.9
1	A	68	GLN	2.9
1	A	1188	GLN	2.9
4	E	179	GLN	2.9
1	A	1387	HIS	2.9
4	E	124	VAL	2.9
7	I	4	PHE	2.9
10	L	49	LYS	2.9
4	E	48	ASP	2.9
1	A	1175	SER	2.9
6	H	140	ALA	2.9
2	B	935	ARG	2.9
6	H	77	ARG	2.9
1	A	121	LEU	2.9
1	A	1255	GLU	2.9
2	B	29	ASP	2.9
4	E	162	ARG	2.9
10	L	39	SER	2.9
1	A	35	ILE	2.9
2	B	364	ILE	2.9
1	A	67	CYS	2.9
1	A	283	GLY	2.8
1	A	1271	ILE	2.8
2	B	1162	ILE	2.8
4	E	116	ILE	2.8
2	B	295	GLY	2.8
1	A	1411	GLU	2.8
3	C	215	GLU	2.8
2	B	1176	ASN	2.8
1	A	96	ILE	2.8
1	A	214	ILE	2.8
1	A	222	LEU	2.8
2	B	629	ASP	2.8
1	A	94	GLY	2.8
1	A	1109	LYS	2.8
1	A	127	ALA	2.8
1	A	75	ASN	2.8
1	A	120	GLU	2.8
1	A	290	GLU	2.8
1	A	1406	VAL	2.8
1	A	1254	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	289	ILE	2.8
1	A	281	HIS	2.8
2	B	869	SER	2.8
6	H	108	SER	2.8
1	A	321	PRO	2.8
4	E	128	PRO	2.8
1	A	1196	GLU	2.7
1	A	148	CYS	2.7
2	B	1157	ALA	2.7
4	E	96	PHE	2.7
1	A	114	LEU	2.7
1	A	204	THR	2.7
1	A	1376	THR	2.7
2	B	1077	THR	2.7
5	F	82	THR	2.7
1	A	1391	ARG	2.7
1	A	1230	GLU	2.7
2	B	678	GLU	2.7
1	A	288	ALA	2.7
1	A	1112	LYS	2.7
4	E	94	LYS	2.7
1	A	140	THR	2.7
1	A	170	THR	2.7
2	B	642	ASP	2.7
1	A	324	SER	2.7
5	F	78	GLN	2.7
8	J	26	GLN	2.7
4	E	66	GLU	2.7
1	A	271	LYS	2.7
4	E	47	CYS	2.7
4	E	131	THR	2.7
1	A	245	PRO	2.7
1	A	411	ASP	2.7
2	B	66	ASP	2.7
1	A	1129	GLU	2.7
1	A	1235	LYS	2.7
2	B	133	LYS	2.7
1	A	299	HIS	2.7
1	A	273	ASN	2.7
1	A	278	THR	2.7
1	A	218	ASP	2.7
1	A	1300	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
6	H	29	ALA	2.6
1	A	334	GLY	2.6
1	A	1436	ILE	2.6
1	A	175	ARG	2.6
1	A	102	VAL	2.6
1	A	126	LEU	2.6
1	A	205	GLU	2.6
1	A	311	GLN	2.6
1	A	801	GLU	2.6
2	B	415	GLN	2.6
10	L	33	GLU	2.6
6	H	109	LYS	2.6
1	A	13	THR	2.6
2	B	448	ILE	2.6
10	L	65	VAL	2.6
2	B	1181	GLU	2.6
6	H	104	PHE	2.6
1	A	1420	ASP	2.6
1	A	600	PRO	2.6
1	A	300	VAL	2.6
1	A	1285	MET	2.6
2	B	468	GLU	2.6
1	A	1390	ASN	2.6
1	A	123	ARG	2.5
4	E	119	SER	2.5
7	I	107	SER	2.5
2	B	470	LYS	2.5
11	T	26	DG	2.5
1	A	280	GLU	2.5
2	B	319	GLU	2.5
2	B	368	GLU	2.5
4	E	60	PHE	2.5
4	E	192	ARG	2.5
7	I	93	LYS	2.5
1	A	262	LEU	2.5
4	E	121	MET	2.5
4	E	88	VAL	2.5
1	A	593	GLU	2.5
7	I	30	ARG	2.5
2	B	332	ASP	2.5
2	B	568	ASP	2.5
1	A	1096	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	455	SER	2.5
4	E	126	SER	2.5
1	A	78	PRO	2.5
1	A	1122	PRO	2.5
2	B	338	GLY	2.5
3	C	70	ILE	2.5
12	R	4	G	2.5
1	A	95	PHE	2.5
1	A	232	GLU	2.5
1	A	124	GLN	2.5
1	A	297	GLN	2.5
2	B	880	THR	2.5
1	A	247	ARG	2.5
1	A	217	LYS	2.5
1	A	1206	ASP	2.5
1	A	1288	ASP	2.5
10	L	44	ASP	2.5
1	A	1260	LEU	2.5
1	A	594	GLY	2.5
1	A	1225	PHE	2.5
2	B	183	GLU	2.5
1	A	314	ALA	2.5
1	A	320	ARG	2.5
3	C	195	GLN	2.5
2	B	955	THR	2.5
3	C	43	THR	2.5
7	I	115	LYS	2.5
1	A	209	ASN	2.5
5	F	104	ASN	2.5
1	A	1204	ASP	2.4
6	H	82	PRO	2.4
1	A	899	VAL	2.4
2	B	1164	GLY	2.4
1	A	139	TRP	2.4
1	A	135	PHE	2.4
1	A	685	GLU	2.4
1	A	1165	GLU	2.4
1	A	301	ALA	2.4
2	B	1200	ALA	2.4
2	B	956	THR	2.4
1	A	282	ASN	2.4
1	A	107	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1419	ASP	2.4
2	B	260	GLY	2.4
6	H	6	PHE	2.4
1	A	173	THR	2.4
4	E	57	MET	2.4
4	E	132	ILE	2.4
5	F	110	ASP	2.4
1	A	145	LYS	2.4
2	B	1158	PHE	2.4
7	I	64	SER	2.4
4	E	3	GLN	2.4
2	B	666	TYR	2.4
1	A	1408	ILE	2.4
2	B	1165	ILE	2.4
1	A	10	PRO	2.4
2	B	108	VAL	2.4
10	L	52	GLY	2.4
9	K	54	ARG	2.4
1	A	476	SER	2.4
2	B	91	SER	2.4
3	C	107	SER	2.4
2	B	873	THR	2.4
2	B	231	PRO	2.4
1	A	176	LYS	2.3
4	E	97	VAL	2.3
2	B	891	ASP	2.3
1	A	206	GLU	2.3
1	A	995	GLU	2.3
1	A	640	GLN	2.3
2	B	115	GLN	2.3
1	A	1392	SER	2.3
2	B	970	THR	2.3
2	B	911	ILE	2.3
1	A	1132	LYS	2.3
4	E	45	LYS	2.3
2	B	306	ASN	2.3
3	C	216	GLY	2.3
1	A	260	ASP	2.3
2	B	644	GLU	2.3
7	I	61	ASP	2.3
2	B	1182	CYS	2.3
2	B	469	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	106	GLN	2.3
1	A	83	HIS	2.3
1	A	497	THR	2.3
1	A	1003	LYS	2.3
1	A	1093	LYS	2.3
4	E	103	LYS	2.3
2	B	337	ARG	2.3
2	B	1113	VAL	2.3
2	B	369	GLY	2.3
1	A	22	PHE	2.3
1	A	1414	ALA	2.3
1	A	1444	MET	2.3
2	B	1156	ASP	2.3
6	H	91	ASP	2.3
1	A	630	ILE	2.3
2	B	1174	LYS	2.3
10	L	28	LYS	2.3
1	A	285	PRO	2.3
1	A	331	GLY	2.3
1	A	1340	GLY	2.3
2	B	107	GLY	2.3
11	T	27	DA	2.3
2	B	296	GLU	2.3
1	A	279	LEU	2.3
1	A	296	LEU	2.3
6	H	7	ASP	2.3
2	B	649	LYS	2.3
4	E	91	LYS	2.3
1	A	47	ARG	2.3
7	I	50	THR	2.3
2	B	1192	TYR	2.3
4	E	51	GLY	2.3
2	B	371	GLU	2.2
2	B	650	GLU	2.2
4	E	102	GLU	2.2
1	A	1221	LYS	2.2
2	B	353	LYS	2.2
2	B	668	ASP	2.2
2	B	1186	ASP	2.2
1	A	99	ILE	2.2
1	A	308	ILE	2.2
1	A	1094	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1156	PRO	2.2
1	A	223	GLY	2.2
1	A	585	GLY	2.2
2	B	552	MET	2.2
2	B	1169	MET	2.2
1	A	76	GLU	2.2
1	A	309	ALA	2.2
3	C	129	ILE	2.2
7	I	52	ILE	2.2
1	A	884	ASP	2.2
10	L	47	ARG	2.2
1	A	1077	THR	2.2
5	F	137	TYR	2.2
6	H	78	SER	2.2
1	A	1232	ASN	2.2
1	A	427	GLN	2.2
4	E	32	GLN	2.2
2	B	572	HIS	2.2
10	L	50	ASP	2.2
2	B	1051	THR	2.2
1	A	167	CYS	2.2
1	A	303	TYR	2.2
2	B	732	SER	2.2
6	H	18	GLY	2.2
2	B	358	LYS	2.2
1	A	1426	GLU	2.2
2	B	384	ARG	2.2
2	B	398	ARG	2.2
6	H	87	ARG	2.2
12	R	3	C	2.2
2	B	888	GLY	2.2
2	B	64	CYS	2.2
2	B	1204	PHE	2.2
7	I	26	LEU	2.2
1	A	226	GLU	2.2
1	A	293	GLU	2.2
1	A	134	ARG	2.1
1	A	1281	ARG	2.1
2	B	70	ILE	2.1
2	B	324	ILE	2.1
2	B	1172	ILE	2.1
10	L	55	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	18	GLN	2.1
1	A	968	GLN	2.1
2	B	1007	VAL	2.1
1	A	304	MET	2.1
1	A	88	LYS	2.1
2	B	393	LYS	2.1
3	C	5	GLY	2.1
1	A	202	LEU	2.1
2	B	829	CYS	2.1
1	A	26	GLU	2.1
2	B	1129	ARG	2.1
2	B	592	ASN	2.1
1	A	89	PRO	2.1
1	A	1205	LYS	2.1
3	C	136	ASP	2.1
7	I	94	ASP	2.1
1	A	165	GLY	2.1
2	B	26	THR	2.1
1	A	1402	PHE	2.1
6	H	132	LEU	2.1
1	A	30	ILE	2.1
2	B	667	GLN	2.1
1	A	213	HIS	2.1
2	B	1187	ASN	2.1
4	E	104	ASN	2.1
12	R	2	U	2.1
1	A	276	LEU	2.1
1	A	307	ASP	2.1
1	A	592	ASP	2.1
3	C	26	ASP	2.1
9	K	114	LEU	2.1
1	A	885	THR	2.1
1	A	57	ARG	2.1
4	E	44	ALA	2.1
1	A	294	SER	2.1
4	E	49	SER	2.1
2	B	706	GLN	2.1
3	C	224	GLN	2.1
1	A	118	HIS	2.1
1	A	1398	MET	2.1
2	B	530	GLY	2.1
2	B	106	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	930	ALA	2.1
1	A	25	GLU	2.1
2	B	328	GLU	2.1
4	E	171	LYS	2.0
1	A	1064	VAL	2.0
1	A	1302	PRO	2.0
2	B	620	ARG	2.0
12	R	6	G	2.0
1	A	292	ALA	2.0
7	I	19	ASP	2.0
4	E	50	MET	2.0
1	A	203	SER	2.0
12	R	7	A	2.0
1	A	306	ASN	2.0
1	A	961	ARG	2.0
2	B	484	ASN	2.0
6	H	21	ASN	2.0
1	A	84	ILE	2.0
1	A	40	THR	2.0
2	B	425	THR	2.0
9	K	25	THR	2.0
9	K	27	ALA	2.0
1	A	116	ASP	2.0
4	E	56	LYS	2.0
2	B	305	VAL	2.0
7	I	59	VAL	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	3DR	T	20	11/12	0.80	0.24	149,156,161,183	0

6.3 Carbohydrates [i](#)

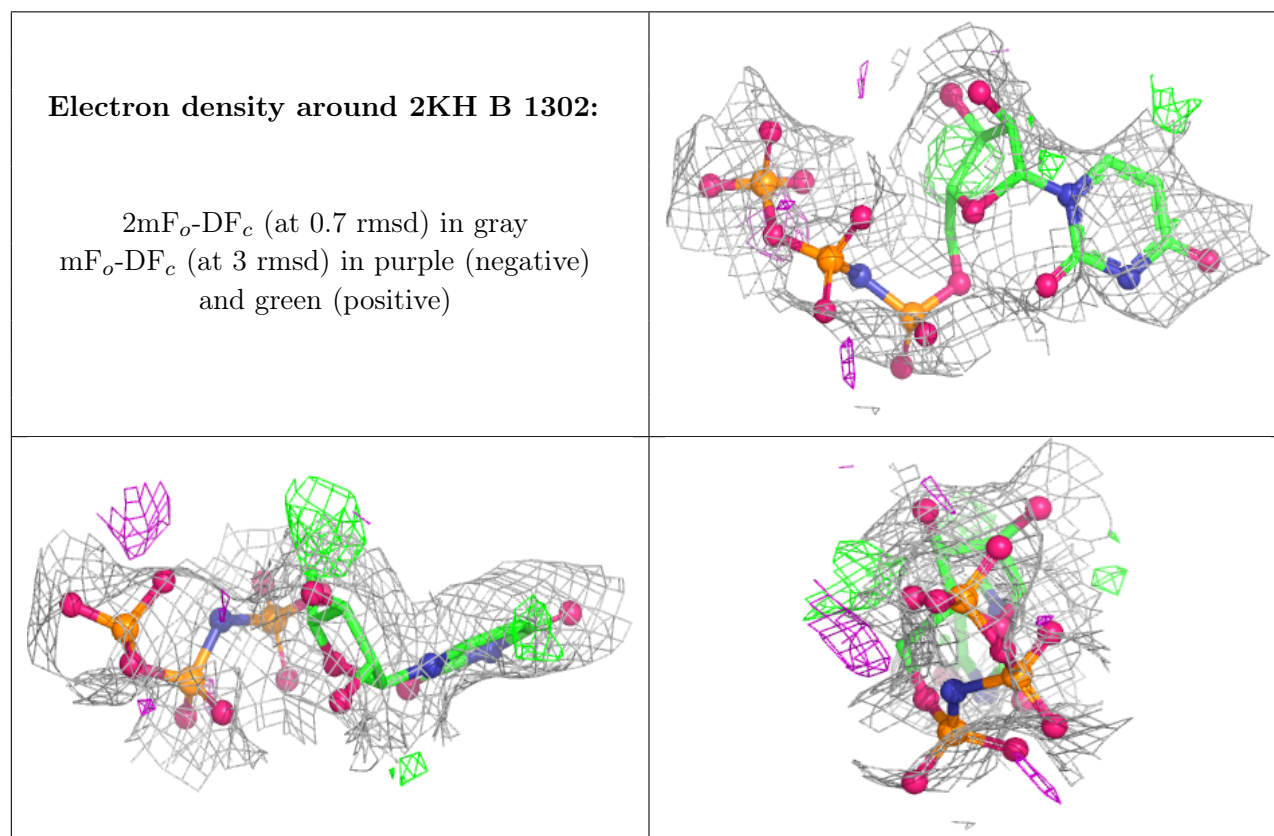
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	2KH	B	1302	29/29	0.66	0.22	101,150,192,196	0
13	ZN	A	1802	1/1	0.94	0.08	80,80,80,80	0
14	MG	A	1804	1/1	0.94	0.09	36,36,36,36	0
13	ZN	A	1801	1/1	0.94	0.07	136,136,136,136	0
13	ZN	J	101	1/1	0.99	0.02	34,34,34,34	0
13	ZN	L	101	1/1	0.99	0.02	70,70,70,70	0
13	ZN	B	1301	1/1	0.99	0.04	93,93,93,93	0
13	ZN	I	202	1/1	0.99	0.03	34,34,34,34	0
14	MG	A	1803	1/1	1.00	0.03	9,9,9,9	0
13	ZN	I	201	1/1	1.00	0.03	49,49,49,49	0
13	ZN	C	401	1/1	1.00	0.02	41,41,41,41	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.