



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:58 PM EDT

PDB ID : 6UPX / pdb_00006upx
Title : RNA polymerase II elongation complex with 5-guanidinohydantoin lesion in state 1
Authors : Oh, J.; Wang, D.
Deposited on : 2019-10-18
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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

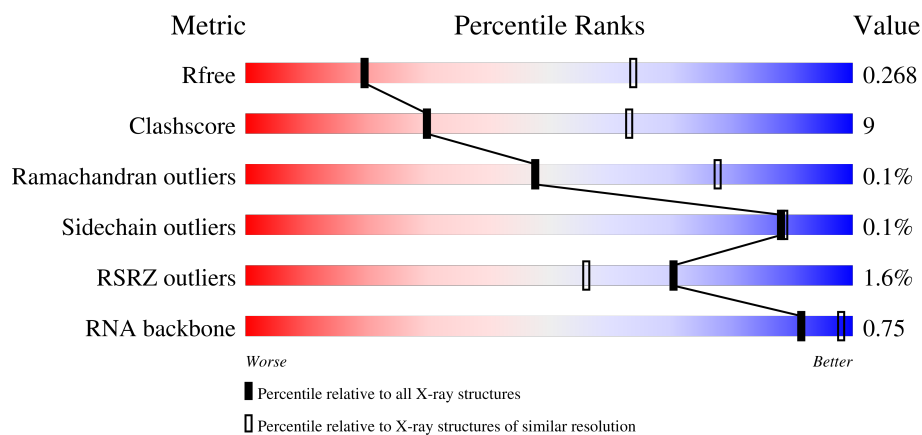
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	R	9	67% 33%
2	T	29	55% 31% 10%
3	N	18	28% 56% 17%
4	A	1733	2% 63% 17% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29092 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	1	0
			538	258	85	169	26			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			317	148	71	83	15			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1385	Total	C	N	O	S	0	0	0
			10841	6838	1899	2044	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1740	1105	307	317	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

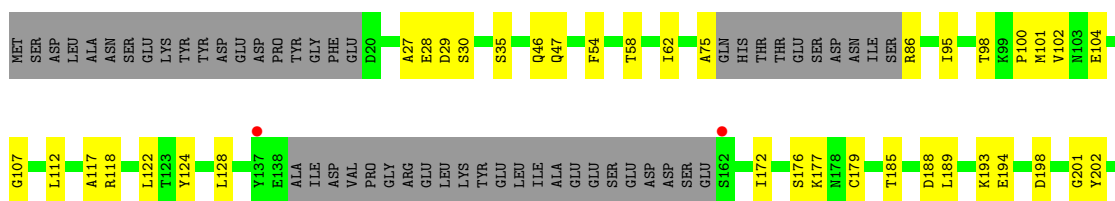
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

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

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

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

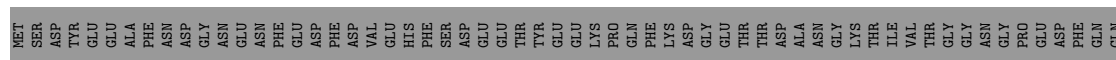
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0





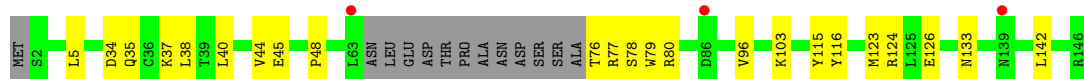
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 48% 8% 45%



- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 2% 75% 16% 9%



- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I: 81% 16% 3%



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 79% 14% 7%



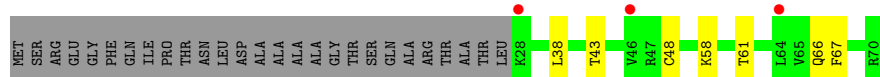
- Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K: 71% 24% 5%



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 4% 51% 10% 39%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.99Å 223.31Å 193.10Å 90.00° 101.03° 90.00°	Depositor
Resolution (Å)	49.30 – 3.40 49.30 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.30-3.40) 99.8 (49.30-3.40)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.220 , 0.266 0.221 , 0.268	Depositor DCC
R_{free} test set	2000 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	86.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 93.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29092	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: MG, G35, 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	R	0.19	0/223	0.31	0/345
2	T	0.27	0/551	0.57	0/843
3	N	0.23	0/359	0.44	0/553
4	A	0.24	1/11033 (0.0%)	0.48	0/14924
5	B	0.23	0/9030	0.45	0/12186
6	C	0.22	0/2139	0.43	0/2899
7	E	0.21	0/1776	0.44	0/2390
8	F	0.21	0/696	0.43	0/943
9	H	0.23	0/1082	0.53	0/1466
10	I	0.22	0/970	0.44	0/1308
11	J	0.23	0/541	0.43	0/727
12	K	0.23	0/937	0.43	0/1265
13	L	0.20	0/339	0.47	0/450
All	All	0.23	1/29676 (0.0%)	0.46	0/40299

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	2
5	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	311	GLN	C-O	-5.73	1.21	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	55	ASP	Peptide
4	A	957	PRO	Peptide
5	B	1106	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	199	0	98	1	0
2	T	538	0	312	9	0
3	N	317	0	166	7	0
4	A	10841	0	10890	226	0
5	B	8859	0	8817	176	0
6	C	2101	0	2056	39	0
7	E	1740	0	1766	22	0
8	F	684	0	692	8	0
9	H	1064	0	1029	20	0
10	I	952	0	897	11	0
11	J	532	0	543	8	0
12	K	919	0	929	26	0
13	L	337	0	353	6	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	1	0	0	0	0
All	All	29092	0	28548	492	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 9.

All (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:873:MET:HE1	4:A:1056:SER:HB2	1.14	1.10
9:H:115:TYR:HE2	9:H:124:ARG:HD3	1.11	1.08
4:A:873:MET:HE1	4:A:1056:SER:CB	1.93	0.98
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.00	0.95
4:A:873:MET:CE	4:A:1056:SER:HB2	1.96	0.95
9:H:115:TYR:CE2	9:H:124:ARG:HD3	2.04	0.93
4:A:873:MET:CE	4:A:1056:SER:CB	2.49	0.90
4:A:780:VAL:HG13	4:A:789:LYS:HE2	1.52	0.88
4:A:1206:ASP:O	4:A:1274:ARG:NH2	2.07	0.87
4:A:164:ARG:NE	4:A:165:GLY:O	2.09	0.84
4:A:443:LEU:HG	4:A:501:LEU:HD11	1.58	0.83
4:A:666:ILE:HD12	4:A:667:GLY:N	1.95	0.81
9:H:115:TYR:HE2	9:H:124:ARG:CD	1.95	0.78
4:A:1207:LEU:HD23	4:A:1274:ARG:NH2	2.01	0.75
5:B:582:VAL:O	5:B:585:VAL:HG12	1.87	0.75
4:A:873:MET:CE	4:A:1056:SER:C	2.60	0.74
4:A:1206:ASP:C	4:A:1274:ARG:HH22	1.97	0.73
4:A:329:LEU:HA	4:A:335:ARG:H	1.55	0.70
4:A:350:ARG:HD2	5:B:1128:LEU:HD11	1.74	0.70
4:A:858:ASN:HD21	4:A:862:ASN:HB2	1.57	0.69
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.74	0.69
2:T:19[B]:G35:H4	4:A:832:ALA:HA	1.75	0.68
5:B:539:LEU:H	5:B:539:LEU:HD23	1.57	0.68
4:A:112:LYS:HE3	4:A:164:ARG:NH2	2.08	0.68
4:A:795:GLU:HG2	5:B:731:VAL:HG11	1.75	0.68
5:B:570:VAL:HG23	5:B:573:GLN:HB3	1.76	0.68
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.76	0.67
4:A:443:LEU:HD11	5:B:1138:MET:HE2	1.76	0.67
4:A:164:ARG:CZ	4:A:165:GLY:O	2.43	0.67
5:B:612:GLU:O	5:B:632:ARG:NH2	2.28	0.67
11:J:9:SER:OG	11:J:48:ARG:NH2	2.27	0.67
8:F:111:LEU:HD23	8:F:111:LEU:H	1.60	0.66
4:A:873:MET:HE2	4:A:1056:SER:C	2.20	0.66
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.77	0.66
9:H:103:LYS:HB3	9:H:115:TYR:HD1	1.61	0.66
4:A:804:TYR:HH	4:A:816:HIS:HE2	1.42	0.66
4:A:879:GLU:OE1	4:A:962:ARG:NH2	2.29	0.65
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.77	0.65
4:A:326:ARG:HG3	4:A:1406:VAL:HG21	1.76	0.65
4:A:471:ASN:O	4:A:474:VAL:HG12	1.96	0.65
5:B:995:ARG:NH1	5:B:997:GLU:OE1	2.29	0.65
4:A:873:MET:HE2	4:A:1056:SER:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.30	0.64
4:A:1363:VAL:HB	4:A:1368:MET:HE2	1.77	0.64
4:A:1207:LEU:HA	4:A:1274:ARG:NH2	2.12	0.64
4:A:378:GLU:OE1	4:A:434:ARG:NH1	2.31	0.63
5:B:1094:ARG:NH2	5:B:1098:MET:SD	2.71	0.63
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.31	0.63
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.81	0.63
4:A:164:ARG:HD2	4:A:165:GLY:N	2.14	0.63
6:C:93:ASP:O	6:C:127:ARG:NH2	2.32	0.63
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.81	0.62
5:B:570:VAL:CG2	5:B:573:GLN:HB3	2.28	0.62
4:A:1207:LEU:HA	4:A:1274:ARG:HH22	1.63	0.62
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.82	0.61
4:A:443:LEU:CD1	5:B:1146:PHE:CZ	2.79	0.61
4:A:873:MET:HE2	4:A:1056:SER:CB	2.28	0.61
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.83	0.61
4:A:446:ARG:NH2	4:A:485:ASP:OD2	2.33	0.61
5:B:705:MET:HE2	5:B:745:PRO:HB3	1.82	0.61
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.83	0.61
4:A:549:MET:HG2	4:A:652:VAL:HG13	1.82	0.61
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.82	0.60
4:A:1100:ARG:NH2	4:A:1351:GLU:OE2	2.33	0.60
5:B:766:ARG:HG2	5:B:1022:THR:HG22	1.84	0.60
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.34	0.60
5:B:834:ASN:O	5:B:1013:ASN:ND2	2.33	0.60
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.84	0.60
5:B:287:ARG:NH1	5:B:324:ILE:O	2.34	0.60
4:A:919:ILE:HD11	4:A:925:LEU:HD12	1.83	0.60
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.35	0.60
4:A:1325:THR:OG1	7:E:146:HIS:O	2.18	0.59
4:A:1342:GLU:OE1	7:E:200:ARG:NH2	2.35	0.59
9:H:76:THR:OG1	9:H:77:ARG:N	2.36	0.59
12:K:10:PHE:CD1	12:K:11:LEU:HD12	2.37	0.59
4:A:434:ARG:NH2	4:A:440:ASP:OD2	2.36	0.59
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.36	0.59
9:H:34:ASP:O	9:H:35:GLN:NE2	2.36	0.59
6:C:258:ILE:HD12	12:K:19:LEU:HD21	1.85	0.58
4:A:562:THR:O	4:A:576:GLN:NE2	2.36	0.58
4:A:901:LEU:HA	4:A:907:THR:HG23	1.84	0.58
5:B:843:GLN:HB2	5:B:993:THR:HB	1.85	0.58
4:A:873:MET:HE2	4:A:1056:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:881:GLN:HA	4:A:961:ARG:HH12	1.68	0.58
4:A:374:LEU:HA	5:B:1107:ALA:HB2	1.85	0.58
4:A:378:GLU:OE2	4:A:387:ARG:NH2	2.36	0.58
5:B:896:ASP:OD2	13:L:58:LYS:NZ	2.36	0.58
4:A:15:LYS:O	5:B:1220:ARG:NH2	2.37	0.58
5:B:904:ARG:NH1	13:L:66:GLN:O	2.37	0.58
5:B:1156:ASP:HB2	5:B:1198:TYR:HB3	1.86	0.58
4:A:353:ILE:HG22	4:A:468:PHE:HB2	1.84	0.58
2:T:19[B]:G35:HI'	4:A:835:GLY:HA3	1.84	0.58
4:A:67:CYS:SG	4:A:68:GLN:N	2.65	0.58
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.35	0.58
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.85	0.57
4:A:575:LYS:NZ	4:A:602:ASP:OD2	2.29	0.57
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.85	0.57
4:A:525:GLN:NE2	5:B:836:GLU:OE1	2.37	0.57
4:A:636:GLU:OE1	4:A:962:ARG:NH1	2.38	0.57
5:B:416:LEU:HD23	5:B:457:LEU:HD23	1.86	0.57
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.35	0.57
5:B:100:PRO:HG3	5:B:172:ILE:HD12	1.87	0.57
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.38	0.57
4:A:182:VAL:HG12	4:A:201:VAL:HA	1.87	0.57
12:K:10:PHE:CE1	12:K:11:LEU:CD1	2.88	0.57
4:A:351:THR:HG22	4:A:352:VAL:N	2.20	0.57
4:A:874:ASP:HB3	4:A:877:HIS:HD2	1.69	0.57
4:A:898:ARG:O	4:A:1029:ARG:NH1	2.38	0.57
5:B:117:ALA:HA	5:B:122:LEU:HB2	1.86	0.57
4:A:95:PHE:O	4:A:99:ILE:N	2.38	0.57
4:A:120:GLU:HG3	4:A:123:ARG:HH21	1.70	0.56
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.88	0.56
5:B:496:ARG:HH12	5:B:541:LEU:HA	1.70	0.56
4:A:59:GLY:HA2	4:A:67:CYS:HB2	1.86	0.56
5:B:118:ARG:NH2	5:B:194:GLU:OE1	2.39	0.56
5:B:176:SER:OG	5:B:177:LYS:N	2.38	0.56
5:B:244:LEU:HD23	5:B:244:LEU:H	1.70	0.56
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.33	0.56
5:B:848:ARG:NH1	11:J:8:PHE:O	2.38	0.56
7:E:78:LEU:HD21	7:E:109:ILE:HD13	1.88	0.56
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.87	0.56
3:N:5:DC:H2'	3:N:6:DG:C8	2.41	0.56
4:A:808:LEU:O	5:B:728:ARG:NH1	2.39	0.56
7:E:18:THR:HG23	7:E:143:ASN:HD22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.87	0.56
8:F:116:ASP:HB3	8:F:119:ARG:HG3	1.87	0.56
4:A:74:MET:O	5:B:1116:ARG:NH2	2.38	0.55
4:A:881:GLN:NE2	4:A:957:PRO:O	2.39	0.55
4:A:30:ILE:HG13	5:B:1170:THR:HG21	1.89	0.55
4:A:1199:ARG:NH1	4:A:1234:GLU:OE2	2.38	0.55
4:A:183:GLY:O	4:A:199:LEU:N	2.39	0.55
5:B:232:SER:O	5:B:261:ARG:NH1	2.35	0.55
6:C:102:GLN:HG2	6:C:154:LYS:HG2	1.89	0.55
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.39	0.55
5:B:118:ARG:NH1	5:B:209:GLU:OE1	2.39	0.55
4:A:151:ASP:OD2	4:A:161:LEU:N	2.39	0.55
4:A:72:GLU:HB3	4:A:76:GLU:HB3	1.88	0.55
11:J:37:SER:OG	11:J:47:ARG:NH2	2.40	0.55
4:A:9:ALA:O	5:B:1193:GLN:NE2	2.38	0.54
5:B:802:PRO:HG2	5:B:805:THR:HG22	1.87	0.54
4:A:147:VAL:HA	4:A:170:THR:HA	1.89	0.54
4:A:1420:ASP:O	5:B:1220:ARG:NH2	2.40	0.54
7:E:20:LYS:NZ	7:E:34:GLU:O	2.41	0.54
7:E:177:ARG:O	7:E:212:ARG:NH2	2.40	0.54
12:K:21:ILE:HG12	12:K:33:ILE:HG23	1.89	0.54
4:A:24:PRO:HB3	4:A:238:CYS:HB3	1.89	0.54
4:A:128:ILE:HG23	4:A:134:ARG:HB2	1.90	0.54
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.41	0.54
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.73	0.54
4:A:756:ILE:HG12	4:A:760:GLN:HE21	1.73	0.54
6:C:196:ASP:OD2	6:C:199:LYS:NZ	2.40	0.54
4:A:873:MET:CE	4:A:1056:SER:HB3	2.35	0.54
7:E:77:SER:HG	7:E:106:GLN:H	1.56	0.54
5:B:102:VAL:HG13	5:B:112:LEU:HB2	1.90	0.53
4:A:1111:MET:HB2	4:A:1114:PRO:HG3	1.89	0.53
12:K:10:PHE:CE1	12:K:11:LEU:HD13	2.43	0.53
5:B:833:TYR:HB2	5:B:840:ILE:HD11	1.88	0.53
3:N:15:DA:OP1	7:E:119:SER:OG	2.24	0.53
4:A:1377:THR:HG23	7:E:176:PRO:HB3	1.90	0.53
5:B:522:VAL:HA	5:B:539:LEU:HA	1.90	0.53
5:B:534:GLY:O	5:B:537:LYS:NZ	2.38	0.53
5:B:629:ASP:O	5:B:632:ARG:NH1	2.42	0.53
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.91	0.53
4:A:903:ASN:O	4:A:907:THR:OG1	2.27	0.53
4:A:1155:ASP:OD2	4:A:1241:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:213:ILE:O	5:B:215:GLN:NE2	2.41	0.53
5:B:1037:LEU:O	11:J:47:ARG:NH1	2.41	0.53
7:E:165:LEU:HD13	7:E:170:LEU:HD12	1.91	0.53
5:B:392:ARG:O	5:B:393:LYS:NZ	2.41	0.53
4:A:860:LEU:HD21	4:A:1394:THR:HA	1.91	0.53
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.91	0.53
5:B:661:LEU:HD11	5:B:684:LEU:HD11	1.91	0.53
2:T:25:DC:OP1	5:B:857:ARG:NH2	2.42	0.52
6:C:35:ARG:NH1	12:K:39:ASP:OD2	2.39	0.52
4:A:524:VAL:HG12	4:A:525:GLN:H	1.74	0.52
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.91	0.52
4:A:151:ASP:OD1	4:A:164:ARG:N	2.43	0.52
12:K:49:GLU:OE2	12:K:97:LYS:NZ	2.34	0.52
3:N:9:DA:H2'	3:N:10:DG:C8	2.45	0.52
4:A:806:ARG:NH1	5:B:725:PRO:O	2.43	0.52
5:B:35:SER:HG	5:B:811:TYR:HH	1.57	0.52
5:B:1163:CYS:HB2	5:B:1187:ASN:HD22	1.74	0.52
4:A:146:MET:HG2	4:A:147:VAL:HG13	1.91	0.52
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.41	0.52
4:A:1329:THR:HG22	4:A:1331:SER:H	1.73	0.52
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.92	0.52
4:A:351:THR:HG21	4:A:466:SER:O	2.10	0.52
4:A:1029:ARG:O	4:A:1033:GLN:HB3	2.09	0.52
4:A:1284:MET:HB3	4:A:1306:LEU:HD23	1.91	0.52
4:A:369:SER:OG	12:K:2:ASN:OD1	2.28	0.51
5:B:334:ILE:HG21	5:B:352:ALA:HB2	1.91	0.51
4:A:146:MET:SD	4:A:146:MET:N	2.76	0.51
4:A:348:SER:HB2	5:B:1128:LEU:HB2	1.92	0.51
5:B:95:ILE:HD11	5:B:128:LEU:HG	1.91	0.51
4:A:153:PRO:HD3	4:A:161:LEU:HD23	1.93	0.51
4:A:602:ASP:HB3	4:A:616:VAL:HG23	1.92	0.51
5:B:185:THR:OG1	5:B:188:ASP:OD1	2.25	0.51
5:B:680:THR:O	5:B:683:SER:OG	2.26	0.51
4:A:901:LEU:N	4:A:926:GLN:OE1	2.37	0.51
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.92	0.51
4:A:362:ASP:OD1	4:A:459:ARG:NH1	2.39	0.51
5:B:46:GLN:HB2	5:B:408:LEU:HD21	1.93	0.51
5:B:955:THR:OG1	5:B:956:THR:N	2.44	0.51
4:A:298:PHE:HE1	4:A:312:PRO:HB2	1.75	0.51
4:A:590:ARG:NH1	4:A:592:ASP:OD1	2.44	0.51
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:867:ILE:HG22	4:A:872:GLY:N	2.26	0.51
6:C:77:ILE:HG13	6:C:161:LYS:HE3	1.92	0.51
7:E:55:ARG:NH2	7:E:137:GLU:OE2	2.43	0.51
4:A:898:ARG:NH1	4:A:930:ASP:OD1	2.36	0.51
4:A:219:PHE:HA	4:A:222:LEU:HD12	1.92	0.50
6:C:248:ILE:HG21	12:K:102:LYS:HB2	1.93	0.50
6:C:66:ARG:NH1	6:C:144:ILE:O	2.44	0.50
4:A:579:SER:HB3	4:A:611:GLN:HA	1.94	0.50
8:F:82:THR:O	8:F:136:ARG:NH1	2.33	0.50
4:A:1132:LYS:HD3	4:A:1135:ARG:HH12	1.76	0.50
6:C:22:LEU:HD11	12:K:101:LEU:HD21	1.92	0.50
5:B:216:GLU:OE1	5:B:500:THR:OG1	2.28	0.50
7:E:124:VAL:HA	7:E:132:ILE:HD13	1.93	0.50
5:B:518:HIS:HB3	5:B:522:VAL:HG12	1.94	0.50
4:A:27:VAL:HA	4:A:30:ILE:HG22	1.92	0.49
4:A:1207:LEU:CA	4:A:1274:ARG:HH22	2.25	0.49
5:B:332:ASP:OD1	5:B:348:ARG:NH2	2.45	0.49
9:H:5:LEU:O	9:H:133:ASN:ND2	2.45	0.49
4:A:575:LYS:HB3	4:A:612:ILE:HD11	1.94	0.49
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.94	0.49
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.93	0.49
4:A:666:ILE:HD12	4:A:666:ILE:C	2.37	0.49
5:B:198:ASP:OD2	5:B:202:TYR:OH	2.28	0.49
5:B:751:VAL:HG23	5:B:812:LEU:HD22	1.94	0.49
4:A:830:LYS:HG3	4:A:1098:VAL:HG21	1.93	0.49
5:B:1072:MET:HE2	5:B:1085:ILE:HG21	1.93	0.49
3:N:9:DA:H2''	3:N:10:DG:H5'	1.95	0.49
5:B:29:ASP:OD2	5:B:655:LYS:NZ	2.36	0.49
5:B:464:GLY:HA2	5:B:480:SER:H	1.76	0.49
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.78	0.49
12:K:40:HIS:HE1	12:K:63:VAL:HG21	1.77	0.49
5:B:351:TYR:CZ	5:B:355:ILE:HD11	2.48	0.49
6:C:54:ASN:OD1	6:C:56:THR:OG1	2.31	0.49
10:I:65:ASP:O	10:I:70:ARG:NH2	2.46	0.49
12:K:24:ASP:HB3	12:K:27:ALA:HB3	1.95	0.49
4:A:979:SER:OG	4:A:980:ASP:N	2.44	0.49
5:B:458:LYS:O	5:B:462:ALA:N	2.45	0.49
4:A:440:ASP:OD1	4:A:498:ARG:NH2	2.46	0.48
4:A:491:VAL:O	5:B:1150:ARG:NH2	2.46	0.48
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.95	0.48
4:A:108:MET:SD	4:A:109:HIS:ND1	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1356:ILE:HG21	4:A:1363:VAL:HG23	1.95	0.48
4:A:1421:CYS:O	4:A:1427:ASN:ND2	2.45	0.48
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.76	0.48
5:B:542:MET:HE1	5:B:743:ILE:HG21	1.95	0.48
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	1.95	0.48
5:B:1169:MET:HE3	5:B:1205:GLN:HG3	1.95	0.48
6:C:165:LYS:O	12:K:6:ARG:NH1	2.43	0.48
4:A:882:SER:O	4:A:1025:ARG:NH1	2.45	0.48
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.95	0.48
5:B:936:ASP:OD1	5:B:938:SER:OG	2.32	0.48
11:J:23:ASN:O	11:J:27:GLU:HB3	2.14	0.48
5:B:273:LEU:HB3	5:B:276:ILE:HD13	1.96	0.48
4:A:306:ASN:HD21	4:A:314:ALA:H	1.62	0.48
4:A:598:LEU:HD21	9:H:124:ARG:HB2	1.95	0.48
9:H:116:TYR:HB2	9:H:123:MET:HB3	1.96	0.48
4:A:1433:MET:HG3	5:B:1144:ALA:HB1	1.95	0.47
5:B:102:VAL:CG1	5:B:112:LEU:HD22	2.44	0.47
6:C:177:GLU:O	6:C:230:MET:HA	2.14	0.47
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.47	0.47
4:A:650:GLN:O	4:A:654:ASN:ND2	2.46	0.47
13:L:43:THR:HG22	13:L:43:THR:O	2.14	0.47
4:A:273:ASN:ND2	4:A:277:GLU:OE2	2.47	0.47
12:K:10:PHE:CD1	12:K:11:LEU:CD1	2.97	0.47
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.95	0.47
3:N:7:DA:H3'	4:A:139:TRP:HH2	1.79	0.47
4:A:261:ASP:HB3	4:A:322:VAL:HG13	1.96	0.47
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.97	0.47
4:A:1116:LEU:HD11	4:A:1313:LEU:HD23	1.96	0.47
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.80	0.47
9:H:123:MET:HE1	9:H:142:LEU:HD13	1.96	0.47
5:B:400:HIS:NE2	5:B:699:GLU:OE1	2.44	0.47
5:B:552:MET:HG3	5:B:553:PRO:HD3	1.96	0.47
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.97	0.47
3:N:2:DC:H2'	3:N:3:DA:C8	2.50	0.47
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.96	0.47
9:H:96:VAL:HA	9:H:142:LEU:O	2.14	0.47
10:I:7:CYS:SG	10:I:9:ASP:N	2.85	0.47
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.97	0.47
5:B:364:ILE:HD13	5:B:585:VAL:HG23	1.96	0.47
9:H:37:LYS:NZ	9:H:126:GLU:OE1	2.41	0.46
4:A:42:ASP:HA	4:A:50:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:81:PHE:CE2	4:A:240:PRO:HB2	2.50	0.46
4:A:591:PHE:HD2	4:A:595:THR:HB	1.80	0.46
4:A:841:LEU:HB3	4:A:1069:ALA:HB1	1.97	0.46
5:B:215:GLN:O	5:B:406:LEU:HA	2.15	0.46
5:B:760:ASP:OD1	5:B:760:ASP:N	2.47	0.46
9:H:44:VAL:HG13	9:H:48:PRO:HA	1.96	0.46
4:A:873:MET:HE3	4:A:1056:SER:C	2.41	0.46
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.36	0.46
6:C:46:ILE:HA	6:C:159:ALA:HA	1.98	0.46
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.98	0.46
2:T:20:DC:H2'	2:T:21:DC:C6	2.51	0.46
2:T:25:DC:H2'	2:T:26:DG:H8	1.80	0.46
4:A:343:LYS:O	5:B:1130:PHE:N	2.45	0.46
4:A:675:THR:HG1	4:A:736:ASN:CG	2.22	0.46
5:B:124:TYR:HH	5:B:179:CYS:HG	1.58	0.46
4:A:58:LEU:HD23	4:A:58:LEU:HA	1.75	0.46
5:B:54:PHE:HA	5:B:58:THR:HB	1.96	0.46
5:B:977:GLY:N	5:B:990:ILE:O	2.49	0.46
7:E:9:ILE:HG22	7:E:39:LEU:HD11	1.98	0.46
10:I:14:LEU:HB3	10:I:27:PHE:HB3	1.97	0.46
2:T:16:DT:H2'	2:T:17:DG:C8	2.50	0.46
4:A:575:LYS:O	4:A:579:SER:OG	2.31	0.46
5:B:75:ALA:O	5:B:86:ARG:N	2.49	0.46
5:B:805:THR:OG1	5:B:1041:GLU:OE1	2.29	0.46
6:C:55:THR:HG1	6:C:152:GLU:H	1.61	0.46
7:E:107:THR:HG23	7:E:131:THR:HG23	1.98	0.46
10:I:2:THR:OG1	10:I:3:THR:N	2.46	0.46
5:B:586:TRP:NE1	5:B:588:GLY:O	2.48	0.46
7:E:22:MET:SD	7:E:26:ARG:NH2	2.82	0.46
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.97	0.46
4:A:75:ASN:OD1	5:B:1116:ARG:NH1	2.48	0.46
4:A:100:LYS:O	4:A:104:GLU:N	2.46	0.46
4:A:179:LEU:HD23	4:A:297:GLN:HG3	1.98	0.46
12:K:114:LEU:HA	12:K:114:LEU:HD23	1.82	0.46
4:A:949:ASP:OD1	4:A:949:ASP:N	2.48	0.45
5:B:260:GLY:O	5:B:267:ARG:NH1	2.40	0.45
4:A:18:GLN:HB2	4:A:1418:LEU:HD12	1.97	0.45
5:B:104:GLU:HB2	5:B:107:GLY:HA3	1.97	0.45
5:B:882:THR:HG23	5:B:934:LYS:HG3	1.98	0.45
5:B:1163:CYS:SG	5:B:1166:CYS:N	2.89	0.45
4:A:353:ILE:HD13	4:A:487:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:957:ASN:OD1	5:B:961:LEU:N	2.49	0.45
9:H:40:LEU:HD21	9:H:142:LEU:HD21	1.97	0.45
4:A:961:ARG:HD2	4:A:1025:ARG:NH2	2.31	0.45
5:B:27:ALA:O	5:B:30:SER:OG	2.34	0.45
5:B:98:THR:HG21	5:B:101:MET:HE2	1.97	0.45
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.99	0.45
9:H:78:SER:OG	9:H:79:TRP:N	2.49	0.45
11:J:1:MET:HB2	11:J:60:PHE:HE2	1.82	0.45
4:A:483:ASP:HB2	5:B:987:LYS:HB2	1.97	0.45
6:C:62:PHE:O	6:C:66:ARG:HG2	2.16	0.45
4:A:848:ILE:HD12	4:A:864:ILE:HG13	1.97	0.45
6:C:86:CYS:SG	6:C:87:PHE:N	2.90	0.45
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.35	0.45
4:A:666:ILE:HG23	5:B:1026:LEU:CB	2.46	0.45
4:A:388:LEU:HD23	4:A:391:LEU:HD12	1.99	0.45
5:B:215:GLN:HG2	5:B:476:ARG:HD2	1.99	0.45
5:B:856:PHE:HE2	5:B:969:ARG:HD3	1.82	0.45
8:F:79:ARG:NH1	8:F:145:ASP:O	2.50	0.45
2:T:22:DT:H2'	2:T:23:DC:H6	1.83	0.44
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.99	0.44
5:B:124:TYR:OH	5:B:179:CYS:SG	2.75	0.44
5:B:209:GLU:OE1	5:B:788:ARG:NH2	2.50	0.44
5:B:393:LYS:HA	5:B:393:LYS:HD3	1.76	0.44
5:B:763:GLN:HG3	5:B:765:PRO:HD2	2.00	0.44
5:B:982:SER:OG	5:B:983:ARG:N	2.49	0.44
9:H:80:ARG:NH2	12:K:79:GLU:OE2	2.49	0.44
2:T:8:DT:H5''	2:T:8:DT:H6	1.82	0.44
4:A:592:ASP:H	4:A:595:THR:HG21	1.83	0.44
4:A:353:ILE:HD12	4:A:470:LEU:HD21	2.00	0.44
11:J:1:MET:HE2	11:J:1:MET:HB3	1.76	0.44
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.99	0.44
5:B:28:GLU:OE1	5:B:807:ARG:NH2	2.51	0.44
5:B:904:ARG:HG2	5:B:948:ILE:HG12	1.99	0.44
4:A:14:VAL:HG11	4:A:1430:LEU:HD22	1.99	0.44
4:A:660:ASN:O	5:B:1082:MET:N	2.50	0.44
4:A:683:ILE:HG21	4:A:801:GLU:HG3	2.00	0.44
7:E:185:ALA:HA	7:E:190:LEU:HD23	2.00	0.44
9:H:40:LEU:HD13	9:H:123:MET:HE3	2.00	0.44
5:B:451:LYS:HA	5:B:454:THR:HB	2.00	0.44
6:C:22:LEU:HG	6:C:25:VAL:HG21	2.00	0.44
7:E:113:GLN:H	7:E:113:GLN:HG2	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:4:G:H2'	1:R:5:A:H8	1.83	0.43
4:A:167:CYS:SG	4:A:168:GLY:N	2.91	0.43
4:A:443:LEU:CD1	5:B:1146:PHE:CE2	3.02	0.43
4:A:1384:VAL:HA	4:A:1389:PHE:HD2	1.83	0.43
5:B:46:GLN:HE22	5:B:496:ARG:HA	1.82	0.43
5:B:1147:LEU:HD13	5:B:1151:LEU:HD22	2.00	0.43
5:B:577:ALA:HB1	5:B:589:VAL:HG22	1.98	0.43
5:B:749:LEU:HB3	5:B:753:ALA:HB3	2.00	0.43
6:C:171:GLY:HA2	6:C:172:PRO:HD3	1.80	0.43
10:I:61:ASP:O	10:I:64:SER:OG	2.34	0.43
3:N:11:DA:H2''	3:N:12:DG:H5'	1.99	0.43
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.99	0.43
4:A:1076:ALA:HA	4:A:1079:MET:HE2	1.99	0.43
4:A:1325:THR:HA	7:E:147:HIS:HA	2.00	0.43
4:A:363:GLN:HA	4:A:459:ARG:O	2.18	0.43
4:A:518:LYS:NZ	4:A:519:PRO:O	2.52	0.43
4:A:113:LEU:HD23	4:A:218:ASP:HB3	1.98	0.43
4:A:134:ARG:NH2	4:A:221:SER:O	2.47	0.43
4:A:353:ILE:HG21	4:A:487:MET:HB2	2.00	0.43
4:A:369:SER:O	4:A:373:THR:OG1	2.35	0.43
4:A:523:ILE:HG23	4:A:527:THR:HB	2.00	0.43
9:H:38:LEU:HD11	9:H:123:MET:HE2	2.01	0.43
4:A:1005:GLU:O	4:A:1009:ASN:ND2	2.37	0.43
4:A:1130:GLN:O	4:A:1134:ILE:HG12	2.19	0.43
5:B:721:LEU:HB3	5:B:722:ASP:H	1.66	0.43
4:A:666:ILE:C	4:A:666:ILE:CD1	2.92	0.43
5:B:615:MET:HG2	5:B:626:ILE:HG23	2.00	0.43
5:B:824:ILE:HG22	5:B:1008:PRO:HA	2.00	0.43
12:K:30:ALA:HA	12:K:75:ILE:O	2.18	0.43
4:A:58:LEU:HD21	4:A:80:HIS:O	2.19	0.42
4:A:868:TYR:CD2	4:A:1058:VAL:HG11	2.54	0.42
12:K:29:ASN:OD1	12:K:77:THR:OG1	2.35	0.42
4:A:585:GLY:H	4:A:609:ASP:HA	1.84	0.42
5:B:230:ALA:O	5:B:261:ARG:NH1	2.53	0.42
5:B:790:ASP:O	5:B:858:SER:OG	2.35	0.42
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.79	0.42
4:A:910:PRO:HA	4:A:916:GLY:HA3	2.00	0.42
4:A:1170:ILE:HD12	4:A:1170:ILE:HA	1.94	0.42
5:B:1060:ARG:NH2	6:C:199:LYS:O	2.52	0.42
4:A:1279:ILE:HG23	4:A:1308:THR:HB	2.01	0.42
10:I:84:VAL:HG12	10:I:102:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:313:MET:HE2	5:B:313:MET:HB3	1.97	0.42
5:B:487:THR:OG1	5:B:777:ALA:O	2.34	0.42
5:B:861:ASP:OD1	5:B:914:LYS:NZ	2.49	0.42
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.49	0.42
8:F:128:LYS:NZ	8:F:148:VAL:O	2.33	0.42
4:A:31:SER:O	5:B:1183:LYS:NZ	2.44	0.42
4:A:632:VAL:HG22	4:A:962:ARG:HD3	2.00	0.42
5:B:1072:MET:HG3	5:B:1085:ILE:HB	2.01	0.42
6:C:34:ARG:HA	6:C:37:MET:HB2	2.01	0.42
10:I:29:CYS:SG	10:I:30:ARG:N	2.93	0.42
11:J:9:SER:HB2	11:J:45:CYS:HB2	2.01	0.42
2:T:22:DT:H2'	2:T:23:DC:C6	2.55	0.42
4:A:30:ILE:HD12	4:A:30:ILE:HA	1.91	0.42
4:A:663:SER:OG	5:B:827:ILE:O	2.28	0.42
4:A:1436:ILE:O	4:A:1440:ALA:N	2.53	0.42
5:B:604:ARG:NH2	5:B:613:VAL:O	2.35	0.42
5:B:835:GLN:HE21	5:B:835:GLN:HB3	1.66	0.42
4:A:99:ILE:HD13	4:A:234:MET:HE3	2.02	0.42
4:A:1436:ILE:HD11	5:B:1144:ALA:HA	2.02	0.42
5:B:58:THR:O	5:B:62:ILE:HG12	2.20	0.42
4:A:92:HIS:HD2	4:A:236:LEU:HD21	1.84	0.42
6:C:143:LEU:HD21	6:C:146:LYS:HE3	2.02	0.42
4:A:946:VAL:HA	7:E:201:LYS:HE3	2.01	0.41
4:A:40:THR:OG1	4:A:41:MET:N	2.53	0.41
4:A:771:GLU:N	4:A:822:GLU:OE1	2.49	0.41
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.68	0.41
6:C:92:CYS:SG	6:C:94:LYS:N	2.88	0.41
5:B:827:ILE:HG23	5:B:1012:ILE:HG13	2.03	0.41
5:B:837:ASP:OD1	5:B:1020:ARG:NH2	2.53	0.41
5:B:879:ARG:HA	5:B:885:MET:HE2	2.02	0.41
5:B:693:ILE:HG21	5:B:701:ILE:HD13	2.03	0.41
6:C:187:LYS:NZ	9:H:45:GLU:OE2	2.36	0.41
4:A:28:ARG:HH21	4:A:238:CYS:HB2	1.85	0.41
4:A:34:LYS:HG2	4:A:83:HIS:CE1	2.55	0.41
4:A:886:ILE:HD11	4:A:943:LEU:HB3	2.03	0.41
4:A:888:GLY:O	4:A:940:ARG:NH2	2.52	0.41
4:A:525:GLN:CD	5:B:836:GLU:OE1	2.63	0.41
4:A:1121:GLU:HB3	4:A:1124:HIS:HB2	2.02	0.41
5:B:817:LEU:HD12	5:B:817:LEU:HA	1.95	0.41
5:B:1162:ILE:HG22	5:B:1169:MET:HB3	2.03	0.41
6:C:8:VAL:HG22	6:C:22:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:201:LYS:H	7:E:201:LYS:HG2	1.55	0.41
10:I:7:CYS:SG	10:I:8:ARG:N	2.93	0.41
4:A:241:VAL:HA	4:A:242:PRO:HD3	1.88	0.41
4:A:1152:ILE:HB	10:I:44:TYR:HB3	2.03	0.41
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.54	0.41
5:B:518:HIS:HB3	5:B:522:VAL:CG1	2.50	0.41
4:A:760:GLN:OE1	4:A:765:VAL:HG23	2.21	0.41
4:A:1303:GLU:CD	4:A:1326:ARG:HH12	2.29	0.41
5:B:654:ARG:HA	5:B:654:ARG:HD3	1.91	0.41
6:C:16:ASP:OD2	6:C:16:ASP:N	2.53	0.41
6:C:154:LYS:HB3	6:C:154:LYS:HE2	1.84	0.41
8:F:77:ASP:OD1	8:F:77:ASP:N	2.54	0.41
5:B:563:MET:HE1	5:B:587:HIS:HB3	2.03	0.41
4:A:420:ARG:O	4:A:424:ILE:HG23	2.22	0.40
4:A:874:ASP:HB3	4:A:877:HIS:CD2	2.52	0.40
4:A:902:LEU:HG	4:A:926:GLN:HG2	2.03	0.40
5:B:461:LEU:O	5:B:480:SER:OG	2.32	0.40
5:B:470:LYS:O	5:B:474:SER:OG	2.38	0.40
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.57	0.40
5:B:1160:VAL:HG11	5:B:1169:MET:SD	2.61	0.40
6:C:2:SER:OG	6:C:3:GLU:N	2.52	0.40
7:E:94:LYS:HB3	7:E:94:LYS:HE2	1.89	0.40
4:A:359:LEU:HA	4:A:359:LEU:HD23	1.84	0.40
4:A:374:LEU:HD23	5:B:1107:ALA:HB2	2.03	0.40
5:B:283:VAL:H	5:B:283:VAL:HG22	1.65	0.40
6:C:60:ASP:HB2	13:L:67:PHE:CZ	2.56	0.40
4:A:367:PRO:HD2	4:A:370:ILE:HD12	2.03	0.40
4:A:474:VAL:HG22	4:A:478:TYR:CE1	2.56	0.40
4:A:882:SER:H	4:A:961:ARG:HH12	1.67	0.40
5:B:47:GLN:NE2	5:B:201:GLY:O	2.54	0.40
5:B:189:LEU:HD23	5:B:189:LEU:HA	1.93	0.40
5:B:415:GLN:OE1	5:B:476:ARG:NH2	2.55	0.40
5:B:797:TYR:HE1	5:B:854:LEU:HG	1.86	0.40
4:A:1366:ARG:H	4:A:1366:ARG:HG2	1.54	0.40
5:B:205:ILE:HG12	5:B:461:LEU:HB3	2.03	0.40
5:B:901:PRO:HA	5:B:949:VAL:HB	2.02	0.40
8:F:82:THR:HG22	8:F:84:TYR:H	1.86	0.40
10:I:29:CYS:SG	10:I:31:THR:N	2.88	0.40
4:A:702:LEU:HD23	4:A:702:LEU:HA	1.96	0.40
6:C:29:MET:HE3	6:C:29:MET:HB2	1.96	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	
4	A	1371/1733 (79%)	1293 (94%)	76 (6%)	2 (0%)	48	78
5	B	1103/1224 (90%)	1056 (96%)	46 (4%)	1 (0%)	48	78
6	C	265/318 (83%)	257 (97%)	8 (3%)	0	100	100
7	E	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
8	F	84/155 (54%)	78 (93%)	6 (7%)	0	100	100
9	H	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
10	I	116/122 (95%)	108 (93%)	8 (7%)	0	100	100
11	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
12	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3495/4173 (84%)	3327 (95%)	165 (5%)	3 (0%)	48	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	1107	ALA
4	A	957	PRO
4	A	958	VAL

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	
4	A	1196/1520 (79%)	1195 (100%)	1 (0%)	88	89
5	B	955/1061 (90%)	954 (100%)	1 (0%)	88	89
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	194/197 (98%)	194 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	110 (100%)	0	100	100
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3075/3657 (84%)	3073 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	985	ASP
5	B	552	MET

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

Mol	Chain	Res	Type
4	A	54	ASN
4	A	64	ASN
4	A	209	ASN
4	A	273	ASN
4	A	358	ASN
4	A	390	GLN
4	A	394	ASN
4	A	447	GLN
4	A	584	ASN
4	A	745	GLN
4	A	757	ASN
4	A	851	HIS
4	A	953	ASN
4	A	1070	GLN
4	A	1110	ASN
4	A	1278	ASN
5	B	47	GLN

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Mol	Chain	Res	Type
5	B	110	HIS
5	B	206	ASN
5	B	350	GLN
5	B	449	ASN
5	B	706	GLN
5	B	835	GLN
5	B	842	ASN
5	B	843	GLN
5	B	862	GLN
5	B	1025	HIS
5	B	1093	GLN
6	C	214	ASN
7	E	114	ASN
10	I	83	ASN

5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

There are no RNA pucker outliers to report.

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

2 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
2	G35	T	19[B]	-	18,23,24	4.81	14 (77%)	18,33,36	2.72	5 (27%)
2	G35	T	19[A]	-	18,23,24	4.76	15 (83%)	18,33,36	1.00	1 (5%)

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
2	G35	T	19[B]	-	-	2/11/41/42	0/2/2/2
2	G35	T	19[A]	-	-	3/11/41/42	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19[B]	G35	C2-N3	9.45	1.49	1.33
2	T	19[A]	G35	C2-N3	9.20	1.49	1.33
2	T	19[B]	G35	O4'-C4'	7.91	1.62	1.45
2	T	19[A]	G35	O4'-C4'	7.56	1.61	1.45
2	T	19[B]	G35	C3'-C4'	-7.50	1.33	1.53
2	T	19[A]	G35	C3'-C4'	-7.15	1.34	1.53
2	T	19[B]	G35	C8-N9	6.96	1.46	1.37
2	T	19[A]	G35	C8-N9	6.65	1.46	1.37
2	T	19[B]	G35	C5-N7	6.38	1.46	1.37
2	T	19[A]	G35	C5-N7	6.34	1.46	1.37
2	T	19[A]	G35	O4'-C1'	-4.99	1.31	1.42
2	T	19[A]	G35	C8-N7	4.93	1.47	1.38
2	T	19[B]	G35	C8-N7	4.74	1.47	1.38
2	T	19[B]	G35	C2-N12	4.71	1.49	1.32
2	T	19[B]	G35	O4'-C1'	-4.67	1.31	1.42
2	T	19[A]	G35	C2-N12	4.63	1.48	1.32
2	T	19[A]	G35	O3'-C3'	3.91	1.51	1.43
2	T	19[B]	G35	C4-N3	3.48	1.48	1.44
2	T	19[A]	G35	C4-N3	2.97	1.47	1.44
2	T	19[A]	G35	O8-C8	-2.92	1.17	1.23
2	T	19[B]	G35	O8-C8	-2.82	1.18	1.23
2	T	19[B]	G35	O3'-C3'	2.82	1.49	1.43
2	T	19[A]	G35	O5-C5	-2.74	1.18	1.23
2	T	19[B]	G35	O5-C5	-2.71	1.18	1.23
2	T	19[B]	G35	C1'-N9	2.61	1.49	1.45
2	T	19[A]	G35	C1'-N9	2.57	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19[B]	G35	C2-N11	-2.47	1.25	1.34
2	T	19[A]	G35	C2-N11	-2.46	1.25	1.34
2	T	19[A]	G35	C2'-C1'	2.21	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19[B]	G35	O4'-C1'-N9	6.98	116.93	108.65
2	T	19[B]	G35	C2'-C1'-N9	-6.94	106.20	115.59
2	T	19[B]	G35	C4'-O4'-C1'	-3.65	100.83	109.51
2	T	19[B]	G35	O4'-C4'-C5'	3.00	118.94	109.33
2	T	19[A]	G35	C2'-C1'-N9	-2.78	111.83	115.59
2	T	19[B]	G35	O4'-C4'-C3'	-2.45	100.06	105.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19[A]	G35	O4'-C1'-N9-C4
2	T	19[A]	G35	O4'-C4'-C5'-O5'
2	T	19[B]	G35	O4'-C1'-N9-C4
2	T	19[A]	G35	C3'-C4'-C5'-O5'
2	T	19[B]	G35	O4'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19[B]	G35	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	-0.14	0 100 100	91, 109, 162, 197	0
2	T	25/29 (86%)	0.30	0 100 100	98, 216, 242, 257	0
3	N	15/18 (83%)	0.25	0 100 100	181, 217, 264, 265	0
4	A	1385/1733 (79%)	0.17	26 (1%) 66 51	55, 106, 186, 282	0
5	B	1123/1224 (91%)	0.12	20 (1%) 67 53	39, 90, 156, 228	0
6	C	267/318 (83%)	-0.03	0 100 100	56, 92, 142, 168	0
7	E	213/215 (99%)	0.13	5 (2%) 61 46	73, 140, 217, 258	0
8	F	86/155 (55%)	-0.11	0 100 100	65, 107, 151, 204	0
9	H	133/146 (91%)	0.18	3 (2%) 61 46	83, 132, 182, 242	0
10	I	118/122 (96%)	0.05	1 (0%) 82 71	77, 114, 149, 183	0
11	J	65/70 (92%)	-0.02	1 (1%) 72 57	52, 86, 119, 133	0
12	K	114/120 (95%)	-0.21	0 100 100	53, 93, 132, 163	0
13	L	43/70 (61%)	0.52	3 (6%) 22 18	69, 152, 210, 259	0
All	All	3596/4229 (85%)	0.12	59 (1%) 70 56	39, 102, 185, 282	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	355	GLY	4.4
4	A	91	PHE	4.3
4	A	141	LEU	4.1
13	L	46	VAL	3.5
9	H	63	LEU	3.4
4	A	105	CYS	3.4
5	B	713	ALA	3.4
5	B	335	GLY	3.2
4	A	885	THR	3.2

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Mol	Chain	Res	Type	RSRZ
5	B	509	ALA	3.2
4	A	312	PRO	3.1
7	E	123	LEU	3.1
7	E	125	PRO	3.1
4	A	1081	LEU	3.0
7	E	93	MET	2.9
5	B	714	GLU	2.9
5	B	721	LEU	2.9
4	A	323	LYS	2.9
5	B	1170	THR	2.9
4	A	153	PRO	2.8
4	A	59	GLY	2.8
13	L	28	LYS	2.8
7	E	98	ILE	2.8
5	B	137	TYR	2.7
5	B	212	LEU	2.7
5	B	869	SER	2.6
10	I	119	THR	2.6
5	B	620	ARG	2.6
5	B	1211	ASN	2.6
4	A	1328	TYR	2.5
4	A	115	LEU	2.5
4	A	161	LEU	2.5
4	A	1332	PHE	2.5
4	A	399	HIS	2.4
5	B	647	GLY	2.4
4	A	103	CYS	2.4
4	A	516	SER	2.4
5	B	162	SER	2.4
5	B	447	ALA	2.3
4	A	1125	ALA	2.3
4	A	152	VAL	2.3
4	A	776	ALA	2.2
5	B	733	HIS	2.2
7	E	128	PRO	2.2
11	J	65	PRO	2.2
9	H	139	ASN	2.2
5	B	446	LEU	2.2
4	A	234	MET	2.2
5	B	230	ALA	2.1
5	B	531	GLN	2.1
13	L	64	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	386	ASP	2.0
4	A	1329	THR	2.0
9	H	86	ASP	2.0
5	B	1113	VAL	2.0
5	B	779	GLY	2.0
4	A	104	GLU	2.0
4	A	320	ARG	2.0
4	A	775	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
2	G35	T	19[A]	22/23	0.68	0.23	143,160,168,174	18
2	G35	T	19[B]	22/23	0.68	0.23	94,158,167,174	18

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
14	ZN	A	1801	1/1	0.91	0.08	258,258,258,258	0
14	ZN	J	101	1/1	0.94	0.15	218,218,218,218	0
14	ZN	B	1301	1/1	0.98	0.04	148,148,148,148	0
14	ZN	A	1802	1/1	0.98	0.04	127,127,127,127	0
14	ZN	L	101	1/1	0.98	0.07	165,165,165,165	0
15	MG	A	1803	1/1	0.98	0.08	83,83,83,83	0
14	ZN	I	201	1/1	0.99	0.03	108,108,108,108	0
14	ZN	C	401	1/1	0.99	0.07	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	I	202	1/1	1.00	0.03	122,122,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.