



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 10:22 AM EDT

PDB ID : 9N5B / pdb_00009n5b
Title : RNA polymerase II elongation complex containing 8-oxoG at +1 site, apo form
Authors : Oh, J.; Wang, D.
Deposited on : 2025-02-04
Resolution : 3.10 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

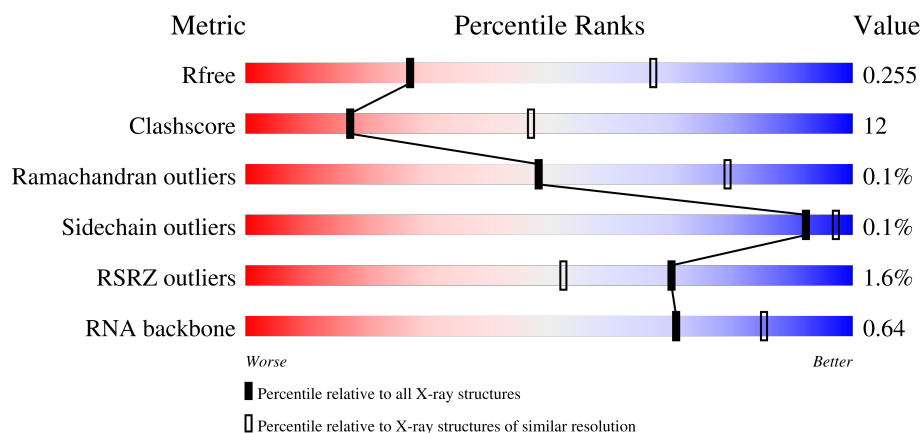
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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	<div> <div>6%</div> <div>56% 33% 11%</div> </div>
2	T	29	<div> <div>24% 66% 10%</div> </div>
3	N	18	<div> <div>6%</div> <div>33% 50% 17%</div> </div>
4	A	1733	<div> <div>2%</div> <div>55% 25% 20%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	 68% 24% 8%
6	C	318	 64% 20% 16%
7	E	215	 68% 31%
8	F	155	 39% 16% 45%
9	H	146	 60% 32% 9%
10	I	122	 68% 29%
11	J	70	 60% 33% 7%
12	K	120	 72% 22% 6%
13	L	70	 43% 19% 39%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29047 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
			195	88	40	59	8			

- 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	0	0
			521	250	80	165	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
			10827	6830	1894	2043	60			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1121	Total	C	N	O	S	0	0	0
			8849	5601	1550	1645	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).

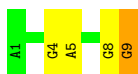
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

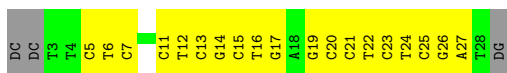
- Molecule 1: RNA

Chain R: 



- Molecule 2: Template strand DNA

Chain T: 



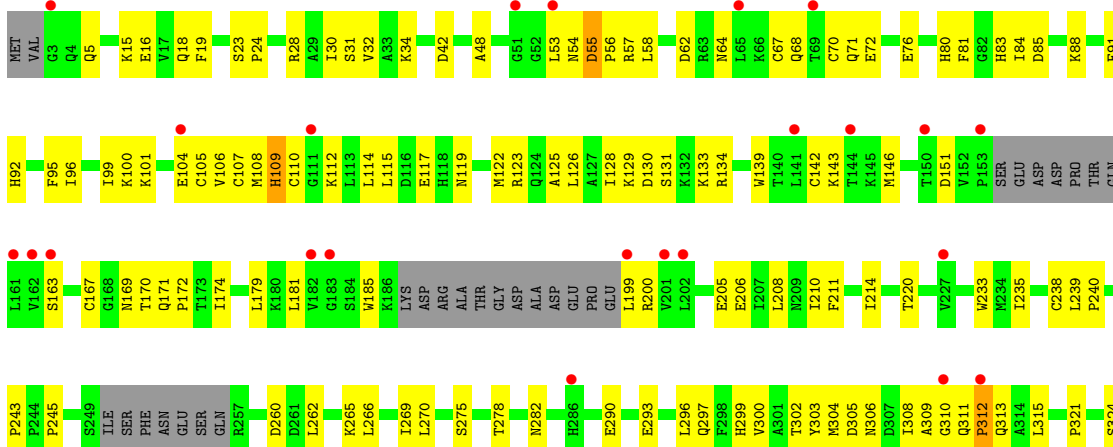
- Molecule 3: Non-template strand DNA

Chain N: 



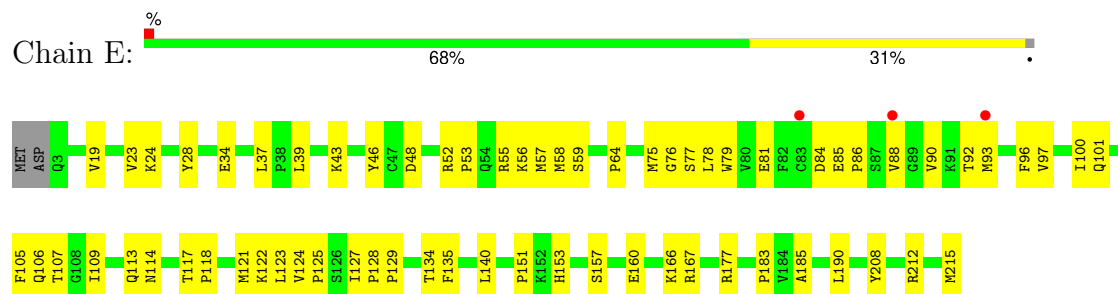
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A: 

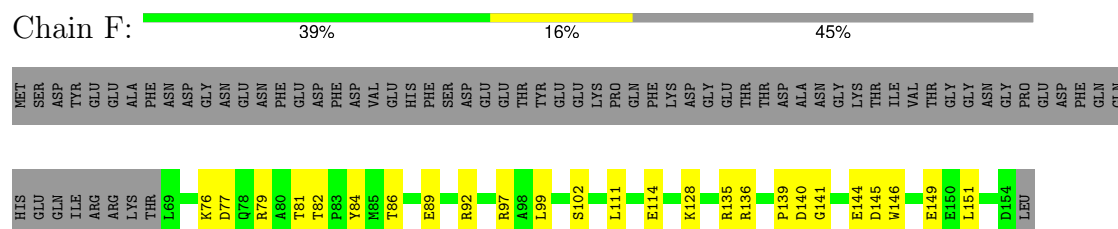




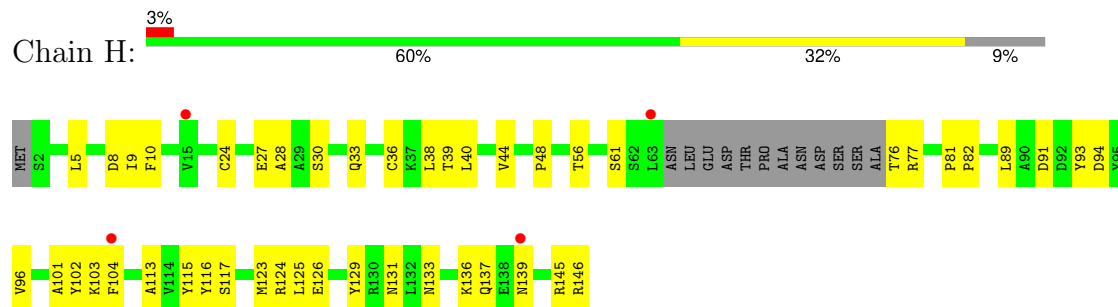
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



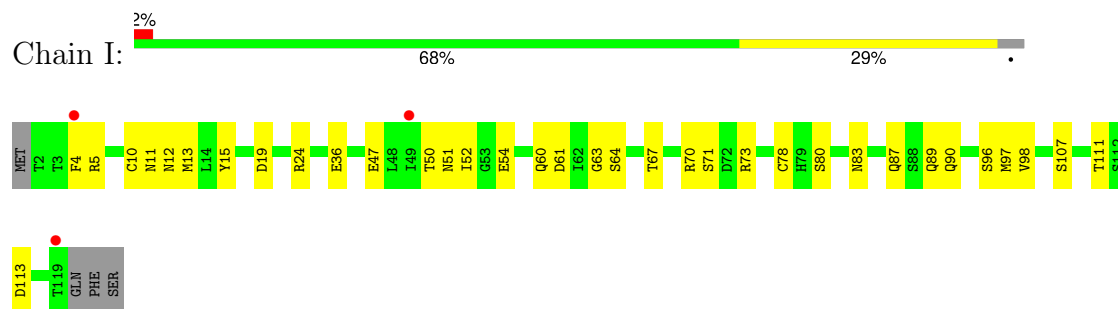
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



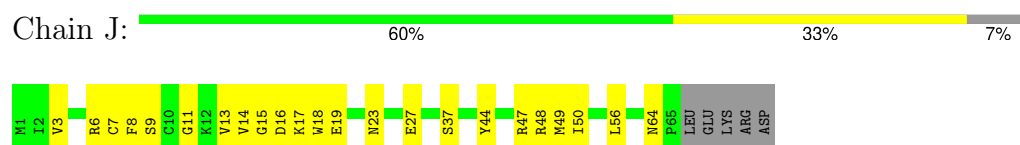
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



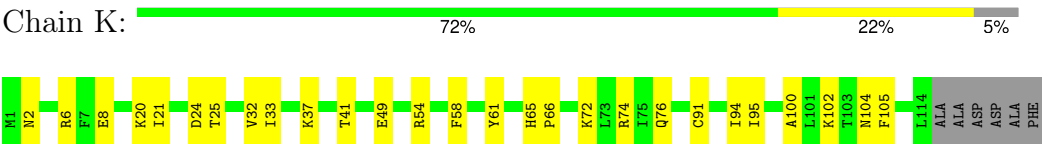
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



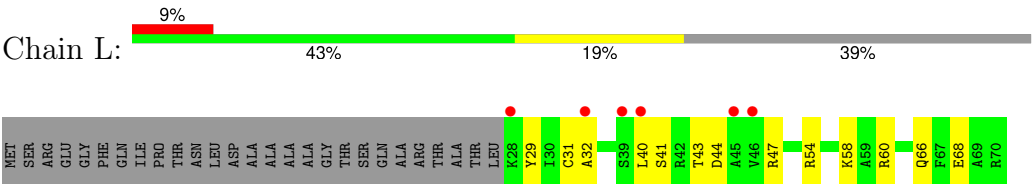
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.84Å 221.72Å 190.84Å 90.00° 97.41° 90.00°	Depositor
Resolution (Å)	46.28 – 3.10 46.28 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.28-3.10) 99.8 (46.28-3.10)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.213 , 0.256 0.214 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29047	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG, MG, 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	0.18	0/219	0.35	0/341
2	T	0.26	0/551	0.51	0/843
3	N	0.25	0/359	0.48	0/553
4	A	0.18	0/11017	0.40	0/14903
5	B	0.18	0/9020	0.39	0/12172
6	C	0.18	0/2139	0.37	0/2899
7	E	0.16	0/1776	0.37	0/2390
8	F	0.16	0/696	0.35	0/943
9	H	0.19	0/1082	0.46	0/1466
10	I	0.17	0/970	0.36	0/1308
11	J	0.17	0/541	0.39	0/727
12	K	0.17	0/937	0.34	0/1265
13	L	0.23	0/339	0.51	0/450
All	All	0.18	0/29646	0.40	0/40260

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	195	0	99	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	521	0	297	13	0
3	N	317	0	166	11	0
4	A	10827	0	10873	319	1
5	B	8849	0	8810	216	0
6	C	2101	0	2056	50	0
7	E	1740	0	1766	48	0
8	F	684	0	692	17	0
9	H	1064	0	1029	33	0
10	I	952	0	897	25	1
11	J	532	0	542	21	0
12	K	919	0	929	20	0
13	L	337	0	352	10	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	29047	0	28508	711	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (711) 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:1224:LEU:HD21	4:A:1240:CYS:HB3	1.57	0.87
4:A:1329:THR:HG22	4:A:1331:SER:H	1.40	0.86
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.09	0.85
4:A:106:VAL:O	4:A:171:GLN:NE2	2.10	0.85
5:B:1099:VAL:HG12	5:B:1103:ILE:HD11	1.62	0.81
4:A:666:ILE:HG23	5:B:1026:LEU:HB2	1.60	0.81
10:I:50:THR:HG22	10:I:52:ILE:H	1.46	0.81
11:J:8:PHE:H	11:J:49:MET:HE3	1.44	0.81
6:C:66:ARG:NH2	11:J:3:VAL:O	2.14	0.80
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.63	0.79
7:E:59:SER:HB3	7:E:81:GLU:HA	1.64	0.79
4:A:108:MET:SD	4:A:171:GLN:NE2	2.55	0.78
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.17	0.77
4:A:91:PHE:H	4:A:297:GLN:HE22	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:46:GLN:OE1	5:B:408:LEU:HD21	1.86	0.74
4:A:575:LYS:HB3	4:A:612:ILE:HD11	1.69	0.74
12:K:100:ALA:O	12:K:104:ASN:ND2	2.19	0.74
5:B:705:MET:HE2	5:B:745:PRO:HB3	1.70	0.73
12:K:32:VAL:HG22	12:K:74:ARG:HG3	1.71	0.73
4:A:636:GLU:OE2	4:A:966:ASN:ND2	2.22	0.72
9:H:36:CYS:HA	9:H:126:GLU:O	1.89	0.72
4:A:806:ARG:NH2	5:B:725:PRO:O	2.22	0.72
4:A:30:ILE:HD12	5:B:1170:THR:HG21	1.71	0.72
5:B:34:ILE:HD13	5:B:747:MET:HE3	1.71	0.72
5:B:822:ASN:O	11:J:48:ARG:NH1	2.23	0.72
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.22	0.71
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.73	0.70
3:N:11:DA:H2'	3:N:12:DG:C8	2.26	0.70
4:A:491:VAL:O	5:B:1150:ARG:NH2	2.25	0.70
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.72	0.70
5:B:519:TRP:CZ2	5:B:705:MET:HE1	2.27	0.70
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.24	0.70
6:C:11:ARG:HH21	6:C:229:TYR:HD2	1.40	0.70
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.74	0.70
4:A:108:MET:HE3	4:A:210:ILE:HD13	1.73	0.70
4:A:1192:LEU:HD11	4:A:1239:ARG:HB3	1.74	0.69
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.74	0.69
4:A:1134:ILE:O	4:A:1138:ILE:HG22	1.92	0.69
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.57	0.69
9:H:40:LEU:HD13	9:H:123:MET:HE3	1.73	0.69
6:C:22:LEU:HG	6:C:25:VAL:HG21	1.75	0.68
4:A:1214:GLU:O	4:A:1218:GLN:NE2	2.27	0.68
4:A:596:THR:HG22	4:A:597:LEU:H	1.57	0.68
5:B:213:ILE:O	5:B:215:GLN:NE2	2.25	0.68
9:H:38:LEU:HD11	9:H:123:MET:HE2	1.76	0.67
6:C:11:ARG:NH2	6:C:206:ASN:OD1	2.27	0.67
7:E:56:LYS:HD3	7:E:84:ASP:HB2	1.75	0.67
4:A:337:ARG:NH2	5:B:1132:GLU:OE1	2.27	0.67
11:J:37:SER:OG	11:J:47:ARG:NH2	2.28	0.67
5:B:101:MET:HG2	5:B:111:ALA:HA	1.75	0.67
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.75	0.67
8:F:82:THR:O	8:F:136:ARG:NH1	2.21	0.67
4:A:433:GLU:OE1	5:B:1108:ARG:NH1	2.28	0.66
4:A:550:LEU:HD21	4:A:561:PRO:HD2	1.76	0.66
11:J:9:SER:OG	11:J:48:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:13:VAL:O	11:J:17:LYS:NZ	2.28	0.66
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.28	0.66
5:B:770:GLN:HE22	5:B:1093:GLN:HE22	1.44	0.66
5:B:792:MET:HG3	5:B:855:PHE:HE1	1.61	0.66
4:A:115:LEU:HD23	4:A:142:CYS:HB3	1.77	0.66
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.28	0.66
4:A:711:ARG:NH2	10:I:87:GLN:OE1	2.28	0.66
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.60	0.66
8:F:128:LYS:NZ	8:F:151:LEU:O	2.26	0.66
4:A:853:ASP:OD1	4:A:855:THR:OG1	2.10	0.65
5:B:276:ILE:HG21	5:B:280:ILE:HD11	1.78	0.65
4:A:821:ARG:O	4:A:825:ILE:HG12	1.95	0.65
5:B:612:GLU:O	5:B:632:ARG:NH2	2.26	0.65
4:A:71:GLN:OE1	5:B:1176:ASN:ND2	2.29	0.65
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.77	0.65
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.30	0.65
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.77	0.65
4:A:1345:ARG:HG2	4:A:1372:VAL:HG12	1.79	0.64
10:I:10:CYS:O	10:I:12:ASN:N	2.31	0.64
4:A:555:ASP:OD1	4:A:648:ASN:ND2	2.30	0.64
4:A:1267:MET:HA	4:A:1271:ILE:HD12	1.79	0.64
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.78	0.64
5:B:198:ASP:OD2	5:B:202:TYR:OH	2.15	0.64
9:H:103:LYS:HB3	9:H:115:TYR:HD1	1.64	0.63
5:B:229:ALA:O	5:B:261:ARG:NH2	2.30	0.63
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.31	0.63
10:I:111:THR:HG22	10:I:113:ASP:H	1.62	0.63
4:A:107:CYS:HA	4:A:171:GLN:HE21	1.64	0.63
4:A:1113:THR:O	4:A:1330:ASN:ND2	2.31	0.63
5:B:299:GLU:OE2	5:B:572:HIS:ND1	2.21	0.63
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.31	0.63
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.31	0.63
5:B:806:THR:HG22	5:B:808:ALA:H	1.64	0.63
5:B:904:ARG:NH1	13:L:66:GLN:O	2.31	0.62
5:B:1187:ASN:ND2	5:B:1190:ASP:O	2.29	0.62
4:A:67:CYS:O	4:A:70:CYS:N	2.30	0.62
4:A:167:CYS:SG	4:A:169:ASN:ND2	2.68	0.62
10:I:63:GLY:O	10:I:70:ARG:NH2	2.33	0.62
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.81	0.62
5:B:260:GLY:O	5:B:267:ARG:NH1	2.29	0.62
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:18:GLN:NE2	4:A:19:PHE:O	2.28	0.62
7:E:77:SER:HB2	7:E:105:PHE:HD2	1.65	0.62
4:A:378:GLU:OE1	4:A:434:ARG:NH1	2.32	0.62
5:B:29:ASP:HB3	5:B:658:ILE:HG12	1.82	0.61
5:B:558:LEU:HB3	5:B:563:MET:HG3	1.82	0.61
2:T:6:DT:H2"	2:T:7:DC:C5	2.35	0.61
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.34	0.61
6:C:143:LEU:HD21	6:C:146:LYS:HE3	1.83	0.61
5:B:522:VAL:HG21	5:B:537:LYS:HB3	1.82	0.61
4:A:72:GLU:HB3	4:A:76:GLU:HB3	1.82	0.61
5:B:766:ARG:HG3	5:B:1022:THR:HG22	1.83	0.61
4:A:100:LYS:O	4:A:104:GLU:N	2.33	0.60
5:B:46:GLN:NE2	5:B:47:GLN:HG2	2.16	0.60
4:A:315:LEU:HA	4:A:321:PRO:HA	1.84	0.60
4:A:562:THR:O	4:A:576:GLN:NE2	2.34	0.60
5:B:69:LEU:HB3	5:B:432:MET:HE1	1.83	0.60
4:A:54:ASN:C	4:A:56:PRO:HD3	2.26	0.60
4:A:269:ILE:HD13	4:A:299:HIS:HB3	1.83	0.60
5:B:629:ASP:HB2	5:B:632:ARG:HD3	1.83	0.60
4:A:1350:LYS:O	4:A:1354:ASN:ND2	2.26	0.60
4:A:134:ARG:NH2	4:A:220:THR:O	2.34	0.60
4:A:596:THR:HG22	4:A:597:LEU:N	2.16	0.60
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.84	0.60
5:B:896:ASP:OD2	13:L:58:LYS:NZ	2.34	0.60
6:C:40:GLU:OE2	6:C:254:LYS:NZ	2.34	0.59
4:A:302:THR:OG1	4:A:306:ASN:OD1	2.19	0.59
4:A:531:ILE:O	4:A:535:THR:OG1	2.19	0.59
4:A:146:MET:SD	4:A:146:MET:N	2.75	0.59
2:T:25:DC:OP1	5:B:857:ARG:NH2	2.35	0.59
5:B:1077:THR:HG22	5:B:1079:LYS:H	1.67	0.59
6:C:93:ASP:O	6:C:127:ARG:NH2	2.35	0.59
4:A:129:LYS:HA	4:A:134:ARG:HH11	1.67	0.59
4:A:1293:SER:OG	4:A:1297:GLU:OE1	2.20	0.59
6:C:54:ASN:ND2	6:C:60:ASP:OD1	2.35	0.58
11:J:8:PHE:CD1	11:J:49:MET:HE1	2.38	0.58
4:A:42:ASP:OD1	4:A:42:ASP:N	2.35	0.58
4:A:903:ASN:O	4:A:907:THR:OG1	2.14	0.58
4:A:1161:THR:HG21	4:A:1166:ASP:HB2	1.85	0.58
7:E:101:GLN:O	7:E:101:GLN:NE2	2.37	0.58
4:A:771:GLU:N	4:A:822:GLU:OE1	2.30	0.58
4:A:704:ALA:HB2	4:A:710:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:262:LEU:O	4:A:266:LEU:HG	2.04	0.58
4:A:337:ARG:HH21	4:A:337:ARG:HG2	1.69	0.58
10:I:60:GLN:NE2	10:I:107:SER:OG	2.30	0.58
4:A:174:ILE:HD11	4:A:181:LEU:HB3	1.87	0.57
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	1.86	0.57
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.66	0.57
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.86	0.57
3:N:12:DG:H1'	3:N:13:DA:N7	2.18	0.57
5:B:175:ARG:HG3	5:B:200:GLY:HA3	1.86	0.57
9:H:5:LEU:HB3	9:H:133:ASN:HB2	1.86	0.57
4:A:329:LEU:HA	4:A:335:ARG:H	1.68	0.57
4:A:392:VAL:HG12	4:A:424:ILE:HD13	1.86	0.57
4:A:170:THR:OG1	4:A:185:TRP:NE1	2.38	0.57
4:A:1235:LYS:HB3	4:A:1237:ILE:HD11	1.86	0.57
5:B:173:MET:O	5:B:176:SER:OG	2.14	0.57
5:B:334:ILE:HG21	5:B:352:ALA:HB2	1.86	0.57
7:E:78:LEU:HD23	7:E:107:THR:HB	1.86	0.57
5:B:905:VAL:HG23	5:B:941:LEU:HD11	1.85	0.57
6:C:142:VAL:HG13	11:J:15:GLY:HA3	1.85	0.57
4:A:744:LYS:HG2	4:A:748:MET:HE2	1.87	0.57
5:B:232:SER:O	5:B:261:ARG:NH2	2.37	0.57
6:C:27:LEU:HD12	6:C:228:PHE:HE2	1.70	0.57
4:A:42:ASP:OD1	4:A:48:ALA:N	2.38	0.56
4:A:587:HIS:HA	4:A:607:ILE:O	2.04	0.56
6:C:88:CYS:HB3	6:C:92:CYS:HB3	1.87	0.56
12:K:8:GLU:O	12:K:37:LYS:HE3	2.05	0.56
4:A:913:LEU:HD22	4:A:915:SER:H	1.69	0.56
4:A:997:LEU:O	4:A:1011:GLN:NE2	2.38	0.56
4:A:1155:ASP:O	4:A:1241:ARG:NH2	2.30	0.56
5:B:629:ASP:O	5:B:632:ARG:NH1	2.38	0.56
5:B:834:ASN:HD22	5:B:1011:ILE:HG22	1.71	0.56
10:I:60:GLN:HE22	10:I:107:SER:HG	1.49	0.56
4:A:68:GLN:NE2	4:A:70:CYS:HB2	2.20	0.56
4:A:105:CYS:SG	4:A:114:LEU:HB2	2.44	0.56
4:A:146:MET:O	4:A:171:GLN:N	2.23	0.56
7:E:93:MET:O	7:E:97:VAL:HG23	2.06	0.56
7:E:101:GLN:HB2	7:E:127:ILE:HG21	1.88	0.56
7:E:157:SER:HB3	7:E:160:GLU:HG3	1.88	0.56
2:T:20:DC:H2'	2:T:21:DC:C6	2.41	0.56
5:B:515:HIS:ND1	5:B:517:THR:OG1	2.34	0.56
5:B:487:THR:OG1	5:B:777:ALA:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:117:GLU:HG2	4:A:123:ARG:HG3	1.87	0.56
4:A:999:VAL:HG12	4:A:1000:LEU:HD12	1.87	0.56
5:B:603:LEU:HB3	5:B:609:ILE:HG13	1.88	0.56
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.19	0.55
5:B:102:VAL:HG13	5:B:112:LEU:HD22	1.88	0.55
7:E:151:PRO:HD2	7:E:153:HIS:HE1	1.69	0.55
4:A:72:GLU:HG3	4:A:76:GLU:HG2	1.86	0.55
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.07	0.55
4:A:392:VAL:HG13	4:A:415:LEU:CD1	2.37	0.55
4:A:391:LEU:HD11	4:A:437:MET:HE1	1.88	0.55
4:A:666:ILE:HD11	5:B:1030:LEU:HD22	1.88	0.55
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.39	0.55
9:H:5:LEU:O	9:H:133:ASN:ND2	2.38	0.55
4:A:1131:ALA:HB3	4:A:1284:MET:HE3	1.87	0.55
5:B:912:ILE:HB	5:B:939:THR:HB	1.89	0.55
5:B:1104:HIS:NE2	5:B:1126:GLY:O	2.36	0.55
4:A:105:CYS:O	4:A:106:VAL:HG23	2.06	0.55
5:B:728:ARG:NH2	5:B:760:ASP:OD2	2.28	0.55
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.89	0.54
5:B:751:VAL:HG23	5:B:812:LEU:HD22	1.90	0.54
6:C:60:ASP:OD2	13:L:60:ARG:NH1	2.40	0.54
5:B:28:GLU:OE1	5:B:807:ARG:NH1	2.39	0.54
5:B:72:GLU:HA	5:B:87:LYS:HA	1.88	0.54
5:B:996:ARG:NH2	6:C:174:ALA:O	2.40	0.54
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.89	0.54
7:E:88:VAL:HG23	7:E:92:THR:HB	1.90	0.54
9:H:44:VAL:HG13	9:H:48:PRO:HA	1.90	0.54
4:A:471:ASN:O	4:A:474:VAL:HG12	2.07	0.54
5:B:881:ASN:HD21	5:B:933:SER:HG	1.55	0.54
4:A:311:GLN:N	4:A:312:PRO:HD3	2.22	0.54
6:C:62:PHE:O	6:C:66:ARG:HG3	2.08	0.54
8:F:128:LYS:HD2	8:F:149:GLU:HA	1.90	0.54
4:A:24:PRO:HB3	4:A:238:CYS:HB3	1.88	0.54
4:A:592:ASP:O	4:A:595:THR:OG1	2.26	0.54
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.88	0.54
4:A:618:GLU:OE2	4:A:620:LYS:HB2	2.07	0.54
4:A:32:VAL:HG12	4:A:32:VAL:O	2.07	0.54
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.89	0.53
6:C:165:LYS:O	12:K:6:ARG:NH1	2.41	0.53
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.37	0.53
5:B:997:GLU:HG2	6:C:39:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.38	0.53
4:A:613:ILE:HG23	9:H:117:SER:HB2	1.90	0.53
4:A:1187:GLN:N	4:A:1187:GLN:OE1	2.41	0.53
5:B:955:THR:OG1	13:L:54:ARG:O	2.25	0.53
7:E:124:VAL:HG23	7:E:125:PRO:HD3	1.90	0.53
4:A:851:HIS:CD2	8:F:139:PRO:HG3	2.43	0.53
5:B:620:ARG:NH2	10:I:89:GLN:OE1	2.42	0.53
5:B:1138:MET:HE2	5:B:1146:PHE:CD2	2.43	0.53
5:B:234:ILE:HD12	5:B:257:LYS:HB3	1.90	0.53
4:A:378:GLU:OE2	4:A:387:ARG:NH2	2.38	0.53
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.90	0.53
6:C:252:GLN:OE1	12:K:102:LYS:NZ	2.34	0.53
11:J:23:ASN:O	11:J:27:GLU:HB3	2.09	0.53
4:A:575:LYS:NZ	4:A:602:ASP:OD2	2.40	0.53
5:B:35:SER:HG	5:B:811:TYR:HH	1.54	0.53
4:A:736:ASN:O	4:A:736:ASN:ND2	2.42	0.53
5:B:287:ARG:NH1	5:B:321:GLY:O	2.41	0.53
4:A:130:ASP:HB3	4:A:133:LYS:HB2	1.90	0.52
7:E:121:MET:O	7:E:124:VAL:HG22	2.10	0.52
4:A:16:GLU:OE2	5:B:1221:SER:N	2.39	0.52
4:A:789:LYS:HG3	10:I:67:THR:HB	1.91	0.52
5:B:680:THR:O	5:B:683:SER:OG	2.25	0.52
4:A:1143:LEU:O	4:A:1147:THR:OG1	2.23	0.52
4:A:1232:ASN:O	4:A:1232:ASN:ND2	2.41	0.52
5:B:1082:MET:HA	6:C:189:THR:HA	1.91	0.52
9:H:89:LEU:HD13	9:H:91:ASP:H	1.74	0.52
4:A:675:THR:OG1	4:A:736:ASN:OD1	2.27	0.52
4:A:34:LYS:HG2	4:A:83:HIS:CE1	2.44	0.52
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.41	0.52
5:B:243:ALA:HA	5:B:251:ILE:HG13	1.90	0.52
6:C:250:THR:O	6:C:254:LYS:HG3	2.08	0.52
6:C:14:SER:OG	6:C:15:LYS:N	2.42	0.52
4:A:122:MET:O	4:A:126:LEU:HG	2.08	0.52
4:A:1398:MET:O	4:A:1401:SER:OG	2.28	0.52
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.92	0.52
7:E:135:PHE:HD2	7:E:140:LEU:HD21	1.74	0.52
3:N:6:DG:H2"	3:N:7:DA:C8	2.45	0.52
4:A:821:ARG:HH21	5:B:514:LEU:HD13	1.75	0.52
9:H:137:GLN:OE1	9:H:139:ASN:ND2	2.43	0.52
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.92	0.52
5:B:936:ASP:OD1	5:B:937:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:900:ASP:HA	4:A:926:GLN:HE22	1.76	0.51
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.92	0.51
5:B:780:VAL:HG11	11:J:56:LEU:HD13	1.93	0.51
4:A:982:THR:HG22	4:A:984:LYS:H	1.75	0.51
8:F:82:THR:HG22	8:F:84:TYR:H	1.75	0.51
4:A:1328:TYR:OH	4:A:1351:GLU:OE1	2.27	0.51
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.92	0.51
3:N:5:DC:N4	3:N:6:DG:O6	2.44	0.51
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.43	0.51
4:A:1220:PHE:HE1	4:A:1224:LEU:HD22	1.75	0.51
4:A:1398:MET:N	4:A:1426:GLU:OE2	2.43	0.51
5:B:760:ASP:OD1	5:B:760:ASP:N	2.34	0.51
4:A:55:ASP:N	4:A:56:PRO:HD3	2.26	0.51
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.10	0.51
7:E:46:TYR:CE1	7:E:58:MET:HG2	2.46	0.51
10:I:50:THR:O	10:I:90:GLN:NE2	2.42	0.51
4:A:278:THR:O	4:A:282:ASN:HB2	2.11	0.51
4:A:585:GLY:N	4:A:609:ASP:OD1	2.40	0.51
7:E:39:LEU:O	7:E:43:LYS:HG3	2.10	0.51
8:F:81:THR:OG1	8:F:144:GLU:OE1	2.25	0.51
4:A:1259:MET:HG2	4:A:1263:ILE:HD13	1.93	0.51
5:B:216:GLU:OE1	5:B:500:THR:OG1	2.25	0.51
5:B:635:ARG:NH1	5:B:742:GLU:OE2	2.43	0.51
7:E:96:PHE:O	7:E:100:ILE:HG12	2.11	0.51
4:A:1021:LEU:O	4:A:1025:ARG:HG3	2.11	0.51
4:A:1076:ALA:HA	4:A:1079:MET:HG3	1.93	0.51
5:B:189:LEU:HD13	5:B:196:PRO:HA	1.93	0.51
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.93	0.51
4:A:308:ILE:HG22	4:A:309:ALA:H	1.76	0.50
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.45	0.50
4:A:443:LEU:HD12	4:A:501:LEU:HD11	1.93	0.50
5:B:1207:LEU:HB3	5:B:1212:ILE:HB	1.93	0.50
4:A:371:ALA:HA	4:A:436:ILE:HG22	1.93	0.50
4:A:514:PRO:HB3	4:A:875:ALA:HB3	1.93	0.50
5:B:736:THR:HG23	5:B:737:THR:HG23	1.93	0.50
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.91	0.50
4:A:602:ASP:HB3	4:A:616:VAL:HG23	1.92	0.50
5:B:69:LEU:HB2	5:B:90:ILE:HB	1.94	0.50
6:C:31:ASN:O	6:C:35:ARG:HG3	2.12	0.50
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.44	0.50
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:49:GLU:HG3	12:K:94:ILE:CG1	2.40	0.50
4:A:108:MET:O	4:A:110:CYS:N	2.45	0.50
4:A:646:PHE:O	4:A:650:GLN:HG3	2.10	0.50
9:H:93:TYR:CD2	9:H:145:ARG:HB2	2.46	0.50
4:A:265:LYS:O	4:A:269:ILE:HG12	2.12	0.50
4:A:960:ILE:HG22	4:A:964:ILE:HD13	1.93	0.50
9:H:133:ASN:OD1	9:H:133:ASN:N	2.45	0.50
4:A:99:ILE:HD12	4:A:211:PHE:HE2	1.77	0.50
4:A:881:GLN:NE2	4:A:958:VAL:O	2.42	0.50
1:R:4:G:H2'	1:R:5:A:C8	2.46	0.50
4:A:1229:SER:OG	4:A:1230:GLU:N	2.45	0.50
5:B:307:ASP:OD2	5:B:392:ARG:NH1	2.44	0.50
5:B:346:GLU:HA	5:B:349:ILE:HD13	1.92	0.50
6:C:244:VAL:HG11	12:K:105:PHE:CZ	2.47	0.50
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.94	0.50
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.47	0.49
6:C:241:ASP:N	6:C:241:ASP:OD1	2.43	0.49
4:A:434:ARG:HE	4:A:437:MET:HE3	1.77	0.49
5:B:46:GLN:CD	5:B:47:GLN:HG2	2.37	0.49
7:E:48:ASP:OD2	7:E:52:ARG:N	2.38	0.49
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.95	0.49
4:A:1074:GLU:O	4:A:1077:THR:OG1	2.28	0.49
6:C:178:PHE:CE1	6:C:230:MET:HE2	2.47	0.49
4:A:57:ARG:HA	4:A:68:GLN:HB3	1.94	0.49
4:A:451:HIS:NE2	4:A:515:GLN:OE1	2.45	0.49
4:A:517:ASN:O	4:A:517:ASN:ND2	2.45	0.49
5:B:635:ARG:HH12	5:B:742:GLU:CD	2.21	0.49
6:C:77:ILE:HG13	6:C:161:LYS:HE3	1.94	0.49
10:I:13:MET:HE2	10:I:15:TYR:CE2	2.47	0.49
2:T:25:DC:P	5:B:942:ARG:HH22	2.36	0.49
6:C:148:ARG:NH1	11:J:64:ASN:O	2.45	0.49
9:H:56:THR:HB	9:H:145:ARG:HB3	1.94	0.49
4:A:853:ASP:OD2	4:A:857:ARG:NH2	2.45	0.49
5:B:578:THR:HG23	5:B:622:LYS:C	2.38	0.49
6:C:246:ARG:O	6:C:250:THR:OG1	2.29	0.49
9:H:8:ASP:OD2	9:H:9:ILE:N	2.42	0.49
4:A:101:LYS:HG3	4:A:139:TRP:CD1	2.48	0.49
4:A:549:MET:HG2	4:A:652:VAL:HG13	1.95	0.49
4:A:1019:CYS:O	4:A:1023:ARG:HG3	2.13	0.49
5:B:997:GLU:CD	5:B:997:GLU:H	2.20	0.49
7:E:128:PRO:N	7:E:129:PRO:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:808:LEU:O	5:B:728:ARG:NH1	2.46	0.48
4:A:979:SER:OG	4:A:980:ASP:N	2.46	0.48
8:F:86:THR:OG1	8:F:89:GLU:HG2	2.13	0.48
9:H:94:ASP:N	9:H:94:ASP:OD1	2.46	0.48
4:A:675:THR:O	4:A:679:ILE:HG13	2.13	0.48
4:A:860:LEU:HD11	4:A:1393:ASN:HB2	1.95	0.48
9:H:5:LEU:HD21	9:H:61:SER:HB2	1.94	0.48
5:B:957:ASN:OD1	5:B:957:ASN:N	2.46	0.48
7:E:121:MET:HE1	7:E:134:THR:HG21	1.95	0.48
10:I:4:PHE:HE1	10:I:13:MET:HG3	1.79	0.48
2:T:11:DC:H2''	2:T:12:DT:C6	2.48	0.48
5:B:100:PRO:HA	5:B:126:SER:HB3	1.95	0.48
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.96	0.48
8:F:140:ASP:OD1	8:F:141:GLY:N	2.47	0.48
4:A:260:ASP:OD2	4:A:328:ARG:NH2	2.46	0.48
5:B:459:TYR:CE2	5:B:469:GLN:HA	2.48	0.48
5:B:944:THR:OG1	5:B:1122:ARG:NH2	2.46	0.48
4:A:939:ASP:OD1	4:A:1023:ARG:NH1	2.47	0.48
5:B:471:LYS:O	5:B:474:SER:N	2.41	0.48
9:H:136:LYS:H	9:H:136:LYS:HD2	1.77	0.48
10:I:61:ASP:O	10:I:64:SER:OG	2.32	0.48
11:J:6:ARG:HD3	11:J:11:GLY:O	2.14	0.48
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.95	0.48
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.96	0.48
4:A:760:GLN:HG2	4:A:765:VAL:HA	1.96	0.48
13:L:47:ARG:NH1	13:L:54:ARG:HE	2.12	0.48
2:T:16:DT:H2'	2:T:17:DG:C8	2.48	0.47
4:A:23:SER:HB3	4:A:233:TRP:CZ2	2.49	0.47
4:A:28:ARG:NH2	4:A:85:ASP:OD1	2.45	0.47
4:A:846:GLU:OE2	4:A:1425:SER:OG	2.31	0.47
12:K:24:ASP:OD1	12:K:25:THR:N	2.46	0.47
3:N:12:DG:H1'	3:N:13:DA:C5	2.49	0.47
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.96	0.47
4:A:540:PHE:HB3	4:A:571:LEU:HG	1.97	0.47
4:A:961:ARG:NH1	4:A:1025:ARG:HH12	2.12	0.47
5:B:519:TRP:CH2	5:B:705:MET:HE1	2.49	0.47
6:C:114:TYR:OH	11:J:19:GLU:OE2	2.22	0.47
11:J:48:ARG:NE	11:J:49:MET:HE2	2.29	0.47
4:A:472:LEU:O	4:A:475:THR:OG1	2.30	0.47
5:B:1002:THR:HG23	5:B:1004:GLU:N	2.27	0.47
4:A:306:ASN:ND2	4:A:313:GLN:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:870:GLU:HG2	7:E:208:TYR:CG	2.49	0.47
4:A:929:LEU:HD21	4:A:983:ILE:HD13	1.96	0.47
5:B:276:ILE:HG22	5:B:278:GLN:H	1.80	0.47
1:R:8:G:H2'	1:R:9:G:C8	2.50	0.47
4:A:5:GLN:HB2	5:B:1175:LEU:HD13	1.96	0.47
4:A:1438:THR:CG2	8:F:92:ARG:HB2	2.45	0.47
5:B:354:ASP:O	5:B:358:LYS:HB2	2.15	0.47
5:B:1135:ARG:O	5:B:1139:ILE:HG13	2.15	0.47
7:E:55:ARG:NH2	7:E:113:GLN:OE1	2.48	0.47
7:E:85:GLU:N	7:E:85:GLU:OE1	2.48	0.47
10:I:97:MET:HE2	10:I:97:MET:HB3	1.87	0.47
11:J:7:CYS:HA	11:J:49:MET:HG3	1.96	0.47
3:N:5:DC:H2'	3:N:6:DG:C8	2.50	0.47
3:N:8:DG:OP2	4:A:143:LYS:NZ	2.37	0.47
5:B:736:THR:OG1	5:B:737:THR:N	2.46	0.47
6:C:251:LEU:O	6:C:255:VAL:HG23	2.14	0.47
9:H:146:ARG:HD2	9:H:146:ARG:H	1.79	0.47
10:I:71:SER:OG	10:I:83:ASN:OD1	2.27	0.47
5:B:225:VAL:HG11	5:B:388:CYS:HB3	1.96	0.47
6:C:18:VAL:HG12	6:C:20:PHE:HD2	1.80	0.47
4:A:672:ASP:OD1	4:A:736:ASN:ND2	2.34	0.47
5:B:100:PRO:O	5:B:180:TYR:OH	2.22	0.47
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.50	0.47
5:B:1219:ASP:OD1	5:B:1219:ASP:N	2.47	0.47
7:E:77:SER:OG	7:E:106:GLN:N	2.48	0.47
10:I:19:ASP:HB3	10:I:24:ARG:HB2	1.97	0.47
11:J:3:VAL:HG11	11:J:18:TRP:HB2	1.97	0.47
4:A:125:ALA:O	4:A:128:ILE:HG22	2.14	0.46
5:B:211:VAL:HG13	5:B:495:LEU:HD23	1.96	0.46
4:A:58:LEU:HA	4:A:58:LEU:HD23	1.56	0.46
4:A:88:LYS:NZ	4:A:205:GLU:HB2	2.30	0.46
4:A:1138:ILE:HG12	4:A:1279:ILE:HG21	1.96	0.46
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.96	0.46
4:A:679:ILE:HG23	4:A:729:ALA:HB1	1.96	0.46
5:B:458:LYS:O	5:B:462:ALA:N	2.40	0.46
5:B:745:PRO:O	5:B:748:ILE:HG12	2.15	0.46
5:B:486:TYR:OH	5:B:1096:ARG:HB3	2.16	0.46
5:B:884:ARG:HH11	5:B:935:ARG:HD3	1.80	0.46
4:A:501:LEU:HD21	5:B:1146:PHE:CD1	2.50	0.46
4:A:866:PHE:H	7:E:208:TYR:HH	1.63	0.46
6:C:33:LEU:HG	6:C:37:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:434:ARG:NH2	4:A:440:ASP:OD2	2.49	0.46
4:A:630:ILE:HG23	4:A:642:CYS:SG	2.56	0.46
4:A:1094:VAL:HA	4:A:1113:THR:HG21	1.98	0.46
5:B:69:LEU:HD12	5:B:432:MET:HE2	1.96	0.46
6:C:33:LEU:O	6:C:37:MET:HG3	2.16	0.46
2:T:14:DG:H2''	2:T:15:DC:C5	2.51	0.46
4:A:1376:THR:HG22	7:E:212:ARG:HH12	1.80	0.46
13:L:31:CYS:SG	13:L:32:ALA:N	2.89	0.46
4:A:290:GLU:HA	4:A:293:GLU:CD	2.41	0.46
4:A:663:SER:OG	5:B:827:ILE:O	2.31	0.46
10:I:78:CYS:SG	10:I:80:SER:OG	2.69	0.46
4:A:446:ARG:HD3	4:A:478:TYR:O	2.16	0.45
4:A:836:TYR:O	4:A:840:ARG:HG3	2.16	0.45
5:B:202:TYR:CD2	5:B:483:LEU:HD11	2.50	0.45
5:B:999:MET:HE2	5:B:1011:ILE:HD12	1.98	0.45
10:I:51:ASN:O	10:I:54:GLU:HG2	2.16	0.45
4:A:15:LYS:HD3	5:B:1218:THR:O	2.16	0.45
4:A:511:ILE:O	4:A:519:PRO:HA	2.15	0.45
4:A:1412:ALA:HA	4:A:1417:GLU:HG3	1.97	0.45
8:F:99:LEU:O	8:F:102:SER:OG	2.31	0.45
5:B:486:TYR:CZ	5:B:1096:ARG:HB3	2.51	0.45
5:B:558:LEU:HD13	5:B:580:VAL:HG11	1.99	0.45
4:A:508:PRO:O	4:A:511:ILE:HG13	2.16	0.45
4:A:1438:THR:HG23	8:F:92:ARG:HB2	1.98	0.45
4:A:199:LEU:HB3	4:A:200:ARG:H	1.58	0.45
4:A:715:GLU:O	4:A:719:VAL:HG23	2.16	0.45
5:B:1000:PRO:HB2	5:B:1072:MET:HE3	1.97	0.45
13:L:29:TYR:HE2	13:L:58:LYS:HG3	1.82	0.45
4:A:110:CYS:SG	4:A:112:LYS:HD2	2.57	0.45
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.98	0.45
4:A:1402:PHE:O	4:A:1403:GLU:HG3	2.15	0.45
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.42	0.45
4:A:1120:LEU:HD21	4:A:1131:ALA:HB2	1.99	0.45
4:A:1428:VAL:HG13	5:B:1151:LEU:CD2	2.46	0.45
5:B:878:GLN:O	5:B:882:THR:N	2.42	0.45
5:B:879:ARG:HB2	5:B:885:MET:HE2	1.98	0.45
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.51	0.45
10:I:96:SER:HB2	10:I:98:VAL:HG23	1.99	0.45
3:N:11:DA:H3'	3:N:12:DG:H2'	1.99	0.45
1:R:4:G:H2'	1:R:5:A:H8	1.82	0.45
4:A:339:ASN:O	4:A:343:LYS:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:698:GLU:HA	5:B:701:ILE:HG12	1.99	0.45
5:B:1084:GLN:HG2	6:C:201:TRP:CH2	2.52	0.45
4:A:100:LYS:HE2	4:A:100:LYS:HB3	1.70	0.45
4:A:598:LEU:HD11	9:H:124:ARG:HB3	1.99	0.45
4:A:1218:GLN:HA	4:A:1221:LYS:HG3	1.99	0.45
2:T:23:DC:H2"	2:T:24:DT:H5'	1.98	0.44
4:A:62:ASP:HB3	4:A:64:ASN:OD1	2.17	0.44
4:A:265:LYS:HG3	4:A:303:TYR:HB2	1.99	0.44
5:B:116:GLU:OE2	5:B:120:ARG:NH1	2.50	0.44
5:B:770:GLN:NE2	5:B:1093:GLN:HE22	2.11	0.44
5:B:904:ARG:NH2	13:L:68:GLU:OE2	2.51	0.44
4:A:666:ILE:HG23	5:B:1026:LEU:CB	2.41	0.44
4:A:1036:ARG:NH1	4:A:1036:ARG:HB2	2.32	0.44
9:H:129:TYR:O	9:H:131:ASN:ND2	2.50	0.44
5:B:863:GLU:OE2	5:B:874:PHE:N	2.47	0.44
9:H:24:CYS:SG	9:H:44:VAL:HG21	2.57	0.44
4:A:549:MET:SD	4:A:577:ILE:HG21	2.57	0.44
4:A:550:LEU:HD23	4:A:556:TRP:CZ2	2.53	0.44
4:A:588:LEU:HB3	4:A:607:ILE:HD12	2.00	0.44
4:A:1157:ASP:HB3	4:A:1160:SER:O	2.16	0.44
8:F:146:TRP:HB3	8:F:151:LEU:HD21	1.98	0.44
11:J:8:PHE:N	11:J:49:MET:HE3	2.22	0.44
4:A:860:LEU:CD1	4:A:1393:ASN:HB2	2.47	0.44
4:A:1030:ARG:HG2	4:A:1034:GLU:OE2	2.18	0.44
4:A:1303:GLU:CD	4:A:1326:ARG:HH12	2.24	0.44
5:B:287:ARG:HG2	5:B:292:ILE:HA	2.00	0.44
6:C:69:LEU:HD12	11:J:6:ARG:HG3	2.00	0.44
12:K:61:TYR:HA	12:K:72:LYS:O	2.18	0.44
4:A:53:LEU:HA	4:A:53:LEU:HD12	1.75	0.44
4:A:68:GLN:HE21	4:A:80:HIS:CD2	2.36	0.44
4:A:239:LEU:HD12	4:A:240:PRO:HD2	2.00	0.44
4:A:1093:LYS:N	4:A:1093:LYS:HD2	2.33	0.44
4:A:296:LEU:O	4:A:300:VAL:HG23	2.18	0.44
4:A:982:THR:HG22	4:A:984:LYS:N	2.33	0.44
5:B:46:GLN:HE22	5:B:47:GLN:HG2	1.83	0.44
5:B:899:ILE:O	5:B:952:VAL:HG21	2.17	0.44
4:A:618:GLU:OE1	4:A:619:LYS:N	2.51	0.44
4:A:648:ASN:O	4:A:652:VAL:HG23	2.17	0.44
4:A:913:LEU:HD21	4:A:981:LEU:O	2.18	0.44
4:A:1317:MET:HA	4:A:1322:ILE:HD11	1.99	0.44
10:I:73:ARG:O	10:I:83:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1434:ALA:HB3	4:A:1436:ILE:HD12	2.00	0.44
5:B:128:LEU:HB3	5:B:167:ILE:HG22	1.99	0.44
9:H:81:PRO:HA	9:H:82:PRO:HD3	1.83	0.44
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	1.99	0.43
5:B:197:PHE:O	5:B:488:TYR:OH	2.27	0.43
6:C:41:ILE:HD11	6:C:172:PRO:HG2	2.00	0.43
7:E:23:VAL:HG12	7:E:28:TYR:HB2	2.00	0.43
4:A:80:HIS:O	4:A:243:PRO:HB3	2.18	0.43
4:A:443:LEU:HB2	4:A:501:LEU:HD11	2.00	0.43
4:A:839:ARG:NH2	4:A:1402:PHE:HA	2.34	0.43
5:B:484:ASN:OD1	5:B:490:SER:OG	2.35	0.43
5:B:1020:ARG:H	5:B:1020:ARG:HG2	1.71	0.43
6:C:17:ASN:OD1	6:C:233:GLU:HG3	2.18	0.43
9:H:30:SER:HB2	9:H:33:GLN:HB3	1.99	0.43
4:A:443:LEU:HD13	5:B:1146:PHE:CZ	2.54	0.43
4:A:765:VAL:CG2	4:A:800:VAL:HB	2.49	0.43
4:A:934:LYS:HE3	4:A:934:LYS:HB2	1.61	0.43
4:A:328:ARG:HD3	5:B:1206:GLU:OE1	2.17	0.43
4:A:767:GLN:NE2	4:A:774:ARG:HG2	2.34	0.43
4:A:1433:MET:HE2	4:A:1433:MET:HB3	1.88	0.43
5:B:1100:ASP:HA	5:B:1103:ILE:HG12	2.00	0.43
9:H:103:LYS:HD3	9:H:104:PHE:N	2.33	0.43
4:A:71:GLN:HE21	5:B:1174:LYS:HB3	1.83	0.43
4:A:275:SER:O	4:A:278:THR:HB	2.18	0.43
4:A:305:ASP:OD1	4:A:306:ASN:N	2.51	0.43
4:A:1128:GLN:HB3	4:A:1304:TRP:CE2	2.53	0.43
5:B:183:GLU:OE1	5:B:183:GLU:N	2.49	0.43
5:B:245:GLU:HG3	5:B:246:LYS:HE2	2.00	0.43
4:A:304:MET:O	4:A:324:SER:HB2	2.18	0.43
4:A:567:LYS:HB2	9:H:96:VAL:HB	2.01	0.43
4:A:800:VAL:HG13	4:A:812:GLU:CD	2.43	0.43
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.18	0.43
5:B:309:GLN:OE1	5:B:392:ARG:NH2	2.51	0.43
12:K:91:CYS:O	12:K:95:ILE:HG13	2.18	0.43
4:A:34:LYS:HE2	4:A:83:HIS:CE1	2.54	0.43
4:A:528:LEU:O	4:A:531:ILE:HG22	2.19	0.43
4:A:939:ASP:OD2	4:A:1023:ARG:HD2	2.19	0.43
5:B:952:VAL:HG22	5:B:966:VAL:HG13	2.01	0.43
11:J:44:TYR:O	11:J:48:ARG:HG3	2.19	0.43
4:A:57:ARG:CA	4:A:68:GLN:HB3	2.49	0.43
4:A:676:MET:O	4:A:680:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1399:ARG:HB3	4:A:1408:ILE:HD13	2.01	0.43
5:B:117:ALA:HA	5:B:122:LEU:HB2	2.00	0.43
5:B:600:LEU:HB3	5:B:615:MET:SD	2.59	0.43
9:H:113:ALA:HA	9:H:125:LEU:O	2.18	0.43
4:A:1081:LEU:HD23	4:A:1081:LEU:HA	1.87	0.43
5:B:30:SER:HB3	5:B:743:ILE:O	2.19	0.43
13:L:40:LEU:HD23	13:L:44:ASP:HB3	1.99	0.43
4:A:1092:LYS:C	4:A:1093:LYS:HD2	2.44	0.43
5:B:210:LYS:NZ	5:B:482:VAL:HG22	2.34	0.43
7:E:19:VAL:O	7:E:23:VAL:HG23	2.19	0.43
9:H:27:GLU:OE1	9:H:39:THR:HG23	2.19	0.43
4:A:96:ILE:O	4:A:99:ILE:HB	2.18	0.42
4:A:1300:LYS:HB2	4:A:1300:LYS:HE2	1.57	0.42
5:B:326:ASP:OD1	5:B:326:ASP:N	2.52	0.42
5:B:492:LEU:O	5:B:496:ARG:HG3	2.19	0.42
6:C:26:ASP:OD1	6:C:26:ASP:N	2.50	0.42
4:A:269:ILE:HD12	4:A:300:VAL:HG22	2.00	0.42
4:A:1134:ILE:HB	4:A:1306:LEU:HD11	2.01	0.42
6:C:39:ALA:HA	6:C:164:ALA:HB3	2.01	0.42
10:I:5:ARG:HD3	10:I:36:GLU:OE2	2.18	0.42
4:A:23:SER:HB3	4:A:233:TRP:CE2	2.53	0.42
4:A:210:ILE:O	4:A:214:ILE:HG12	2.19	0.42
4:A:575:LYS:HB3	4:A:612:ILE:CD1	2.46	0.42
4:A:726:ARG:HD3	4:A:766:GLY:HA3	2.00	0.42
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.49	0.42
5:B:1067:ARG:NE	6:C:194:GLU:OE1	2.47	0.42
4:A:115:LEU:HD12	4:A:119:ASN:HB2	2.01	0.42
4:A:607:ILE:HA	4:A:612:ILE:HA	2.01	0.42
4:A:986:ILE:O	4:A:990:VAL:HG23	2.20	0.42
4:A:1295:THR:HB	4:A:1297:GLU:OE1	2.19	0.42
5:B:522:VAL:CG2	5:B:537:LYS:HB3	2.49	0.42
5:B:851:PHE:O	5:B:974:PRO:HD3	2.20	0.42
4:A:738:LYS:HB2	4:A:740:LEU:HG	2.01	0.42
4:A:1157:ASP:OD2	4:A:1160:SER:HB3	2.19	0.42
5:B:493:SER:OG	5:B:497:ARG:NH2	2.53	0.42
5:B:519:TRP:NE1	5:B:742:GLU:OE1	2.47	0.42
5:B:763:GLN:HG3	5:B:765:PRO:HD2	2.00	0.42
5:B:911:ILE:HD13	5:B:941:LEU:HD23	2.00	0.42
7:E:46:TYR:CD1	7:E:58:MET:HE2	2.55	0.42
4:A:58:LEU:HD21	4:A:80:HIS:O	2.20	0.42
4:A:795:GLU:HG2	5:B:731:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.67	0.42
5:B:58:THR:O	5:B:62:ILE:HG13	2.19	0.42
5:B:651:LEU:H	5:B:651:LEU:HD12	1.84	0.42
7:E:79:TRP:HD1	7:E:100:ILE:HD11	1.83	0.42
12:K:65:HIS:ND1	12:K:66:PRO:HD2	2.34	0.42
3:N:10:DG:H2''	3:N:11:DA:H8	1.85	0.42
13:L:41:SER:N	13:L:44:ASP:OD2	2.52	0.42
2:T:12:DT:H2''	2:T:13:DC:H5'	2.02	0.42
2:T:25:DC:OP2	5:B:942:ARG:NH2	2.41	0.42
4:A:84:ILE:HG23	4:A:239:LEU:HB3	2.01	0.42
4:A:1025:ARG:O	4:A:1035:TYR:OH	2.37	0.42
5:B:1152:MET:HE3	5:B:1152:MET:HB3	1.98	0.42
7:E:177:ARG:HD3	7:E:215:MET:SD	2.60	0.42
8:F:97:ARG:HD2	8:F:97:ARG:HA	1.68	0.42
8:F:135:ARG:NH2	8:F:145:ASP:OD2	2.35	0.42
4:A:388:LEU:HD23	4:A:388:LEU:HA	1.87	0.42
7:E:46:TYR:HD1	7:E:58:MET:HE2	1.83	0.42
4:A:95:PHE:CE2	4:A:1414:ALA:HB2	2.55	0.42
4:A:931:GLU:OE2	4:A:991:LYS:NZ	2.38	0.42
4:A:1217:LYS:HE3	4:A:1228:TRP:CZ3	2.55	0.42
5:B:209:GLU:HB2	5:B:483:LEU:HB2	2.02	0.42
5:B:428:ILE:O	5:B:432:MET:HG2	2.20	0.42
5:B:541:LEU:HD23	5:B:541:LEU:HA	1.92	0.42
5:B:614:SER:OG	5:B:627:PHE:HB2	2.20	0.42
10:I:47:GLU:OE1	10:I:50:THR:HG23	2.20	0.42
12:K:20:LYS:O	12:K:33:ILE:HA	2.20	0.42
4:A:336:ILE:HG21	4:A:1401:SER:HA	2.02	0.41
4:A:463:ILE:HD12	4:A:465:TYR:H	1.85	0.41
4:A:494:SER:O	4:A:498:ARG:HG3	2.19	0.41
5:B:554:ILE:O	5:B:558:LEU:HG	2.20	0.41
5:B:992:ILE:HD11	12:K:66:PRO:HB2	2.02	0.41
5:B:1023:VAL:HG12	5:B:1027:ILE:HD11	2.02	0.41
3:N:15:DA:P	7:E:117:THR:HG21	2.59	0.41
4:A:53:LEU:HB3	4:A:54:ASN:H	1.61	0.41
4:A:310:GLY:C	4:A:312:PRO:HD3	2.45	0.41
5:B:963:PHE:CE2	5:B:965:LYS:HE3	2.55	0.41
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.53	0.41
5:B:1168:LEU:HD21	5:B:1215:ARG:HG2	2.01	0.41
7:E:118:PRO:O	7:E:122:LYS:HG2	2.20	0.41
10:I:60:GLN:NE2	10:I:107:SER:HG	2.11	0.41
5:B:400:HIS:NE2	5:B:517:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:883:LEU:HD12	5:B:884:ARG:H	1.85	0.41
7:E:46:TYR:CD1	7:E:58:MET:HG2	2.56	0.41
7:E:78:LEU:HD21	7:E:109:ILE:HD12	2.02	0.41
7:E:90:VAL:HG13	7:E:123:LEU:HD21	2.02	0.41
11:J:16:ASP:OD1	11:J:16:ASP:N	2.37	0.41
12:K:54:ARG:HE	12:K:54:ARG:HB2	1.59	0.41
2:T:26:DG:H1'	2:T:27:DA:H5'	2.01	0.41
4:A:1128:GLN:O	4:A:1132:LYS:HG3	2.21	0.41
5:B:219:ALA:HB2	5:B:405:ARG:HG2	2.01	0.41
5:B:408:LEU:HD12	5:B:408:LEU:HA	1.80	0.41
5:B:1034:VAL:HG22	5:B:1059:LEU:HB2	2.03	0.41
7:E:64:PRO:HB3	7:E:75:MET:HG2	2.01	0.41
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.01	0.41
4:A:172:PRO:HB3	4:A:185:TRP:CG	2.56	0.41
4:A:845:LEU:O	4:A:1065:GLY:HA3	2.19	0.41
9:H:76:THR:OG1	9:H:77:ARG:N	2.53	0.41
4:A:597:LEU:HD13	9:H:103:LYS:HG3	2.01	0.41
4:A:1195:LEU:HD11	4:A:1267:MET:HE1	2.02	0.41
4:A:1225:PHE:O	4:A:1240:CYS:HA	2.20	0.41
5:B:358:LYS:HA	5:B:366:GLN:HG2	2.01	0.41
5:B:384:ARG:HA	5:B:384:ARG:HD3	1.84	0.41
6:C:268:ASP:OD1	6:C:268:ASP:N	2.54	0.41
9:H:101:ALA:HB2	9:H:116:TYR:CE2	2.55	0.41
4:A:206:GLU:HG3	4:A:210:ILE:HD11	2.03	0.41
5:B:209:GLU:OE2	5:B:788:ARG:NH2	2.46	0.41
5:B:241:ARG:HG2	5:B:253:THR:HG22	2.02	0.41
7:E:166:LYS:HG2	7:E:167:ARG:HD2	2.03	0.41
4:A:1384:VAL:HA	4:A:1389:PHE:HD2	1.85	0.41
5:B:195:CYS:SG	5:B:783:THR:OG1	2.65	0.41
7:E:24:LYS:HE3	7:E:24:LYS:HB2	1.87	0.41
8:F:77:ASP:OD1	8:F:77:ASP:N	2.40	0.41
4:A:151:ASP:CG	4:A:163:SER:H	2.28	0.41
4:A:179:LEU:HD23	4:A:297:GLN:HG3	2.03	0.41
4:A:369:SER:OG	12:K:2:ASN:ND2	2.40	0.41
4:A:1032:LEU:HD23	4:A:1032:LEU:HA	1.84	0.41
4:A:1079:MET:HG2	4:A:1359:ASP:OD2	2.21	0.41
5:B:406:LEU:HD23	5:B:406:LEU:HA	1.87	0.41
6:C:93:ASP:OD1	6:C:122:SER:HB2	2.21	0.41
7:E:46:TYR:OH	7:E:57:MET:HB3	2.21	0.41
7:E:64:PRO:HD3	7:E:76:GLY:HA2	2.03	0.41
8:F:76:LYS:HA	8:F:79:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:982:THR:O	4:A:985:ASP:HB2	2.21	0.41
4:A:1100:ARG:O	4:A:1104:ILE:HG13	2.21	0.41
4:A:1140:HIS:HB2	4:A:1276:VAL:O	2.20	0.41
4:A:1295:THR:HB	4:A:1297:GLU:CD	2.46	0.41
5:B:65:GLU:O	5:B:67:SER:N	2.54	0.41
5:B:418:LYS:HE3	5:B:418:LYS:HB3	1.86	0.41
5:B:1001:PHE:CZ	5:B:1073:TYR:HB2	2.56	0.41
6:C:11:ARG:HD3	6:C:209:TYR:CE1	2.57	0.41
4:A:31:SER:HA	4:A:81:PHE:O	2.21	0.40
4:A:92:HIS:CE1	4:A:304:MET:HE3	2.56	0.40
4:A:108:MET:HB2	4:A:109:HIS:ND1	2.36	0.40
4:A:666:ILE:CD1	5:B:1030:LEU:HD22	2.51	0.40
4:A:924:LYS:O	4:A:927:VAL:HG22	2.20	0.40
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	2.02	0.40
5:B:102:VAL:CG1	5:B:112:LEU:HD22	2.51	0.40
5:B:515:HIS:CE1	5:B:517:THR:HG1	2.34	0.40
5:B:826:ALA:HB3	5:B:1011:ILE:HG12	2.01	0.40
2:T:5:DC:H2''	2:T:6:DT:H5'	2.03	0.40
4:A:492:PRO:HB3	4:A:497:THR:HG22	2.03	0.40
4:A:761:MET:HG3	5:B:1021:MET:HG2	2.03	0.40
4:A:926:GLN:O	4:A:926:GLN:HG3	2.21	0.40
5:B:1038:SER:HB3	5:B:1062:HIS:NE2	2.37	0.40
9:H:10:PHE:HB3	9:H:28:ALA:HB1	2.03	0.40
9:H:103:LYS:HB3	9:H:115:TYR:CD1	2.49	0.40
4:A:270:LEU:HD23	4:A:270:LEU:HA	1.92	0.40
4:A:302:THR:HA	4:A:305:ASP:O	2.21	0.40
4:A:818:MET:HG3	5:B:514:LEU:O	2.21	0.40
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.22	0.40
4:A:1428:VAL:HG22	5:B:1147:LEU:HD11	2.03	0.40
6:C:149:LYS:HE3	6:C:149:LYS:HB3	1.89	0.40
8:F:111:LEU:HD12	8:F:114:GLU:O	2.21	0.40
3:N:15:DA:OP2	7:E:117:THR:HG21	2.21	0.40
4:A:964:ILE:O	4:A:968:GLN:HG3	2.21	0.40
4:A:1207:LEU:HD23	4:A:1207:LEU:HA	1.92	0.40
7:E:34:GLU:O	7:E:37:LEU:HD23	2.22	0.40
7:E:46:TYR:HD2	7:E:53:PRO:CB	2.34	0.40
4:A:909:ASP:HB3	4:A:912:LEU:HG	2.03	0.40
4:A:971:PHE:O	4:A:973:ILE:N	2.54	0.40
4:A:1345:ARG:HG2	4:A:1372:VAL:CG1	2.50	0.40
6:C:29:MET:HE3	6:C:29:MET:HB2	1.92	0.40
7:E:86:PRO:O	7:E:114:ASN:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:920:LEU:O	10:I:24:ARG:NH2[4_546]	2.16	0.04

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	
4	A	1371/1733 (79%)	1292 (94%)	76 (6%)	3 (0%)	44	74
5	B	1101/1224 (90%)	1027 (93%)	74 (7%)	0	100	100
6	C	265/318 (83%)	256 (97%)	9 (3%)	0	100	100
7	E	211/215 (98%)	196 (93%)	15 (7%)	0	100	100
8	F	84/155 (54%)	81 (96%)	3 (4%)	0	100	100
9	H	129/146 (88%)	115 (89%)	14 (11%)	0	100	100
10	I	116/122 (95%)	105 (90%)	10 (9%)	1 (1%)	14	45
11	J	63/70 (90%)	60 (95%)	3 (5%)	0	100	100
12	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3493/4173 (84%)	3280 (94%)	209 (6%)	4 (0%)	48	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	109	HIS
10	I	11	ASN
4	A	312	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1193/1520 (78%)	1191 (100%)	2 (0%)	92	96
5	B	955/1061 (90%)	955 (100%)	0	100	100
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%)	36 (97%)	1 (3%)	40	67
All	All	3072/3657 (84%)	3069 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	131	SER
4	A	805	LEU
13	L	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	118	HIS
4	A	171	GLN
4	A	209	ASN
4	A	282	ASN
4	A	297	GLN
4	A	390	GLN
4	A	394	ASN
4	A	435	HIS

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Mol	Chain	Res	Type
4	A	510	GLN
4	A	603	ASN
4	A	698	GLN
4	A	741	ASN
4	A	968	GLN
4	A	1106	ASN
4	A	1124	HIS
4	A	1187	GLN
4	A	1387	HIS
4	A	1427	ASN
5	B	667	GLN
5	B	842	ASN
5	B	881	ASN
5	B	1093	GLN
7	E	63	ASN
9	H	33	GLN
9	H	139	ASN
12	K	92	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 ⓘ

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	$\# Z > 2$
2	8OG	T	19	2	22,25,26	4.25	17 (77%)	26,37,40	2.43	9 (34%)

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	8OG	T	19	2	-	6/7/21/22	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	8OG	C8-N7	7.31	1.51	1.38
2	T	19	8OG	C8-N9	6.57	1.52	1.40
2	T	19	8OG	C4-N3	6.43	1.49	1.34
2	T	19	8OG	C2-N3	6.28	1.48	1.33
2	T	19	8OG	C2-N2	5.83	1.47	1.34
2	T	19	8OG	C5-N7	4.61	1.45	1.37
2	T	19	8OG	C2-N1	4.55	1.48	1.37
2	T	19	8OG	O4'-C1'	-4.51	1.32	1.42
2	T	19	8OG	C6-N1	4.47	1.47	1.38
2	T	19	8OG	O3'-C3'	3.98	1.51	1.43
2	T	19	8OG	C4-N9	3.96	1.46	1.39
2	T	19	8OG	C2'-C1'	3.69	1.62	1.52
2	T	19	8OG	C5-C4	3.66	1.42	1.37
2	T	19	8OG	C5-C6	3.54	1.52	1.41
2	T	19	8OG	C5'-C4'	-3.23	1.41	1.51
2	T	19	8OG	O6-C6	-2.38	1.19	1.23
2	T	19	8OG	C3'-C4'	2.16	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	8OG	C2-N3-C4	7.14	124.60	112.30
2	T	19	8OG	N1-C2-N3	-4.28	115.50	123.32
2	T	19	8OG	N9-C4-N3	4.17	131.34	126.13
2	T	19	8OG	O6-C6-C5	-3.88	117.89	127.26
2	T	19	8OG	N2-C2-N1	3.46	124.06	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	8OG	C5-C6-N1	3.25	121.05	112.13
2	T	19	8OG	O8-C8-N9	2.38	129.24	126.00
2	T	19	8OG	N7-C8-N9	-2.33	104.02	106.61
2	T	19	8OG	C2-N1-C6	-2.32	120.91	125.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	8OG	O4'-C1'-N9-C8
2	T	19	8OG	C2'-C1'-N9-C8
2	T	19	8OG	O4'-C4'-C5'-O5'
2	T	19	8OG	C3'-C4'-C5'-O5'
2	T	19	8OG	C2'-C1'-N9-C4
2	T	19	8OG	O4'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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%)	-0.15	0 100 100	70, 82, 137, 137	0
2	T	25/29 (86%)	0.75	0 100 100	71, 185, 229, 244	0
3	N	15/18 (83%)	0.97	1 (6%) 25 15	169, 211, 234, 237	0
4	A	1385/1733 (79%)	0.01	28 (2%) 64 45	39, 77, 154, 266	0
5	B	1121/1224 (91%)	-0.10	13 (1%) 76 60	37, 69, 128, 195	0
6	C	267/318 (83%)	-0.26	1 (0%) 89 77	41, 66, 98, 133	0
7	E	213/215 (99%)	0.13	3 (1%) 73 56	58, 104, 168, 202	0
8	F	86/155 (55%)	-0.18	0 100 100	60, 84, 118, 174	0
9	H	133/146 (91%)	0.29	4 (3%) 52 33	71, 103, 145, 175	0
10	I	118/122 (96%)	0.02	3 (2%) 58 39	50, 84, 119, 137	0
11	J	65/70 (92%)	-0.35	0 100 100	50, 61, 95, 123	0
12	K	114/120 (95%)	-0.36	0 100 100	44, 72, 101, 138	0
13	L	43/70 (61%)	0.94	6 (13%) 7 4	63, 128, 178, 218	0
All	All	3594/4229 (84%)	-0.03	59 (1%) 70 52	37, 76, 149, 266	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	H	139	ASN	5.0
5	B	714	GLU	4.2
5	B	335	GLY	3.9
13	L	45	ALA	3.8
4	A	69	THR	3.6
13	L	46	VAL	3.5
7	E	93	MET	3.4
4	A	182	VAL	3.4
4	A	141	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	A	1257	ASP	3.0
5	B	733	HIS	2.9
4	A	161	LEU	2.9
4	A	144	THR	2.8
4	A	1081	LEU	2.8
13	L	32	ALA	2.8
4	A	104	GLU	2.8
9	H	63	LEU	2.7
5	B	473	MET	2.6
5	B	73	GLN	2.6
4	A	111	GLY	2.6
4	A	65	LEU	2.5
13	L	40	LEU	2.5
10	I	119	THR	2.5
4	A	1002	GLY	2.5
4	A	202	LEU	2.5
9	H	15	VAL	2.4
4	A	53	LEU	2.4
5	B	250	PHE	2.3
4	A	162	VAL	2.3
4	A	163	SER	2.3
7	E	83	CYS	2.3
10	I	49	ILE	2.3
4	A	310	GLY	2.3
5	B	246	LYS	2.3
4	A	312	PRO	2.2
13	L	39	SER	2.2
4	A	153	PRO	2.2
10	I	4	PHE	2.2
4	A	286	HIS	2.2
9	H	104	PHE	2.2
4	A	199	LEU	2.1
7	E	88	VAL	2.1
4	A	227	VAL	2.1
4	A	3	GLY	2.1
13	L	28	LYS	2.1
4	A	847	ASP	2.1
3	N	16	DA	2.1
4	A	150	THR	2.1
5	B	138	GLU	2.1
4	A	51	GLY	2.0
4	A	183	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
6	C	96	SER	2.0
5	B	676	VAL	2.0
5	B	502	ILE	2.0
5	B	1191	ILE	2.0
5	B	162	SER	2.0
5	B	446	LEU	2.0
4	A	201	VAL	2.0
4	A	1001	ARG	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	8OG	T	19	23/24	0.89	0.12	75,94,132,135	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	L	101	1/1	0.93	0.11	200,200,200,200	0
14	ZN	A	1801	1/1	0.94	0.09	217,217,217,217	0
15	MG	A	1803	1/1	0.96	0.06	76,76,76,76	0
14	ZN	B	1301	1/1	0.98	0.04	121,121,121,121	0
14	ZN	I	202	1/1	0.99	0.06	139,139,139,139	0
14	ZN	A	1802	1/1	0.99	0.02	108,108,108,108	0
14	ZN	I	201	1/1	0.99	0.03	93,93,93,93	0
14	ZN	C	401	1/1	1.00	0.03	82,82,82,82	0
14	ZN	J	101	1/1	1.00	0.05	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.