



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2021 – 01:09 PM EDT

PDB ID : 7KED
Title : RNA polymerase II elongation complex with unnatural base dTPT3
Authors : Oh, J.; Wang, W.; Wang, D.
Deposited on : 2020-10-10
Resolution : 3.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

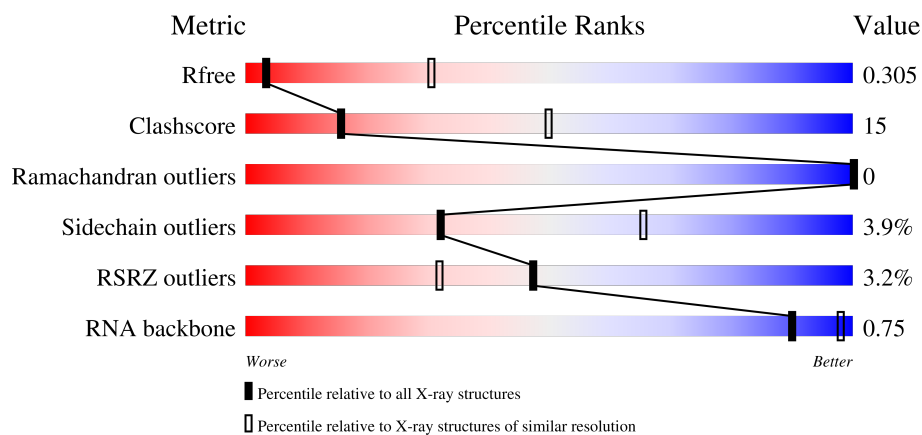
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>3%</div> <div>52% 26% . 20%</div> </div>
2	B	1224	<div> <div>2%</div> <div>61% 30% . 8%</div> </div>
3	C	318	<div> <div>58% 25% . 16%</div> </div>
4	E	215	<div> <div>3%</div> <div>63% 33% ..</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	<div><div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div></div><div>41%14%45%</div></div>
6	H	146	<div><div><div></div><div></div><div></div></div><div>10%</div><div><div></div><div></div><div></div></div><div>48%42%9%</div></div>
7	I	122	<div><div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div></div><div>67%25%</div></div>
8	J	70	<div><div><div></div><div></div><div></div></div><div></div><div><div></div><div></div><div></div></div><div>59%31%7%</div></div>
9	K	120	<div><div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div></div><div>65%30%5%</div></div>
10	L	70	<div><div><div></div><div></div><div></div></div><div>7%</div><div><div></div><div></div><div></div></div><div>39%21%39%</div></div>
11	R	10	<div><div><div></div><div></div><div></div></div><div></div><div><div></div><div></div><div></div></div><div>60%40%</div></div>
12	T	29	<div><div><div></div><div></div><div></div></div><div>17%</div><div><div></div><div></div><div></div></div><div>34%48%17%</div></div>
13	N	16	<div><div><div></div><div></div><div></div></div><div></div><div><div></div><div></div><div></div></div><div>6%56%38%</div></div>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28916 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1384	Total	C	N	O	S	0	0	0
			10820	6827	1894	2039	60			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 12 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	24	Total	C	N	O	P	0	0	0
			490	235	87	142	24	2		

- Molecule 13 is a DNA chain called Non template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			202	97	32	63	10			

- Molecule 14 is ZINC ION (three-letter code: 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

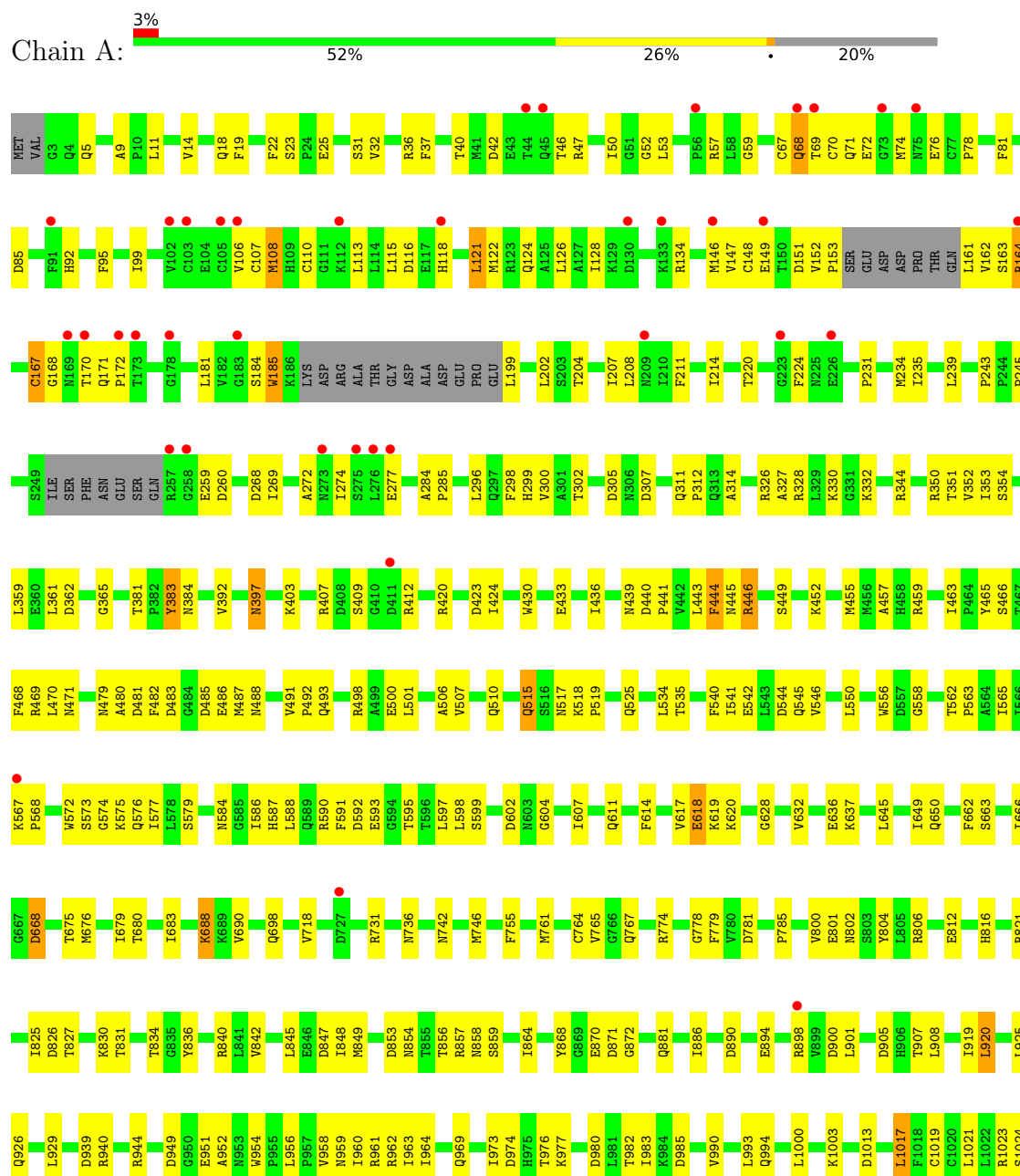
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

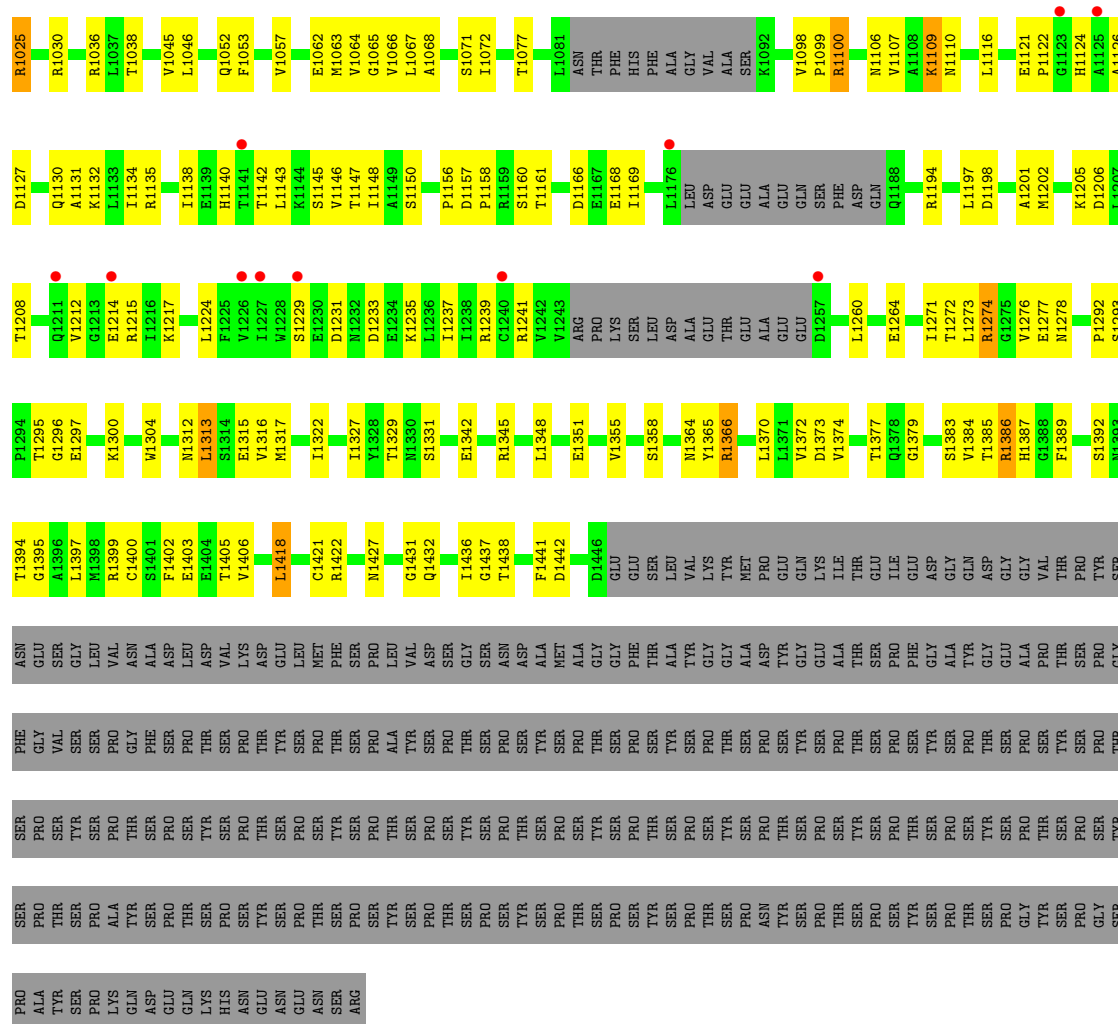
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

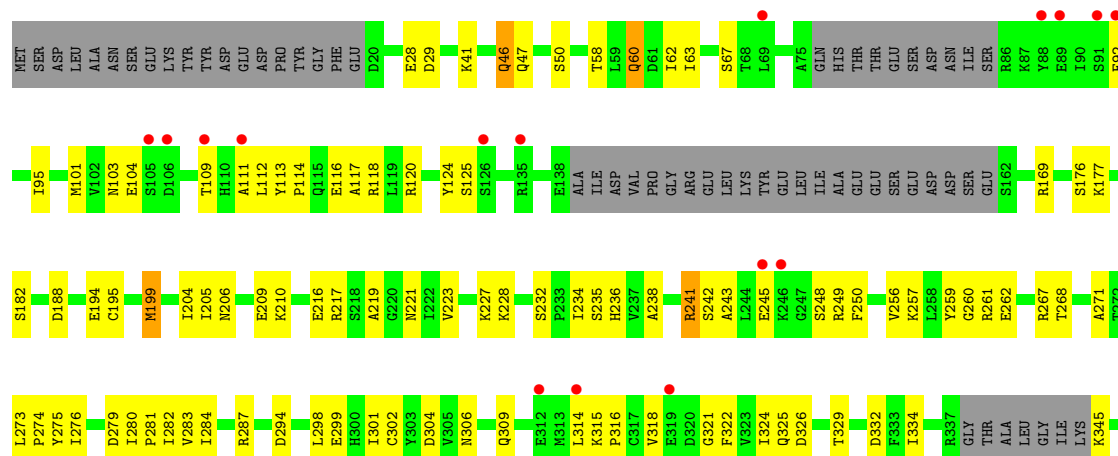
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

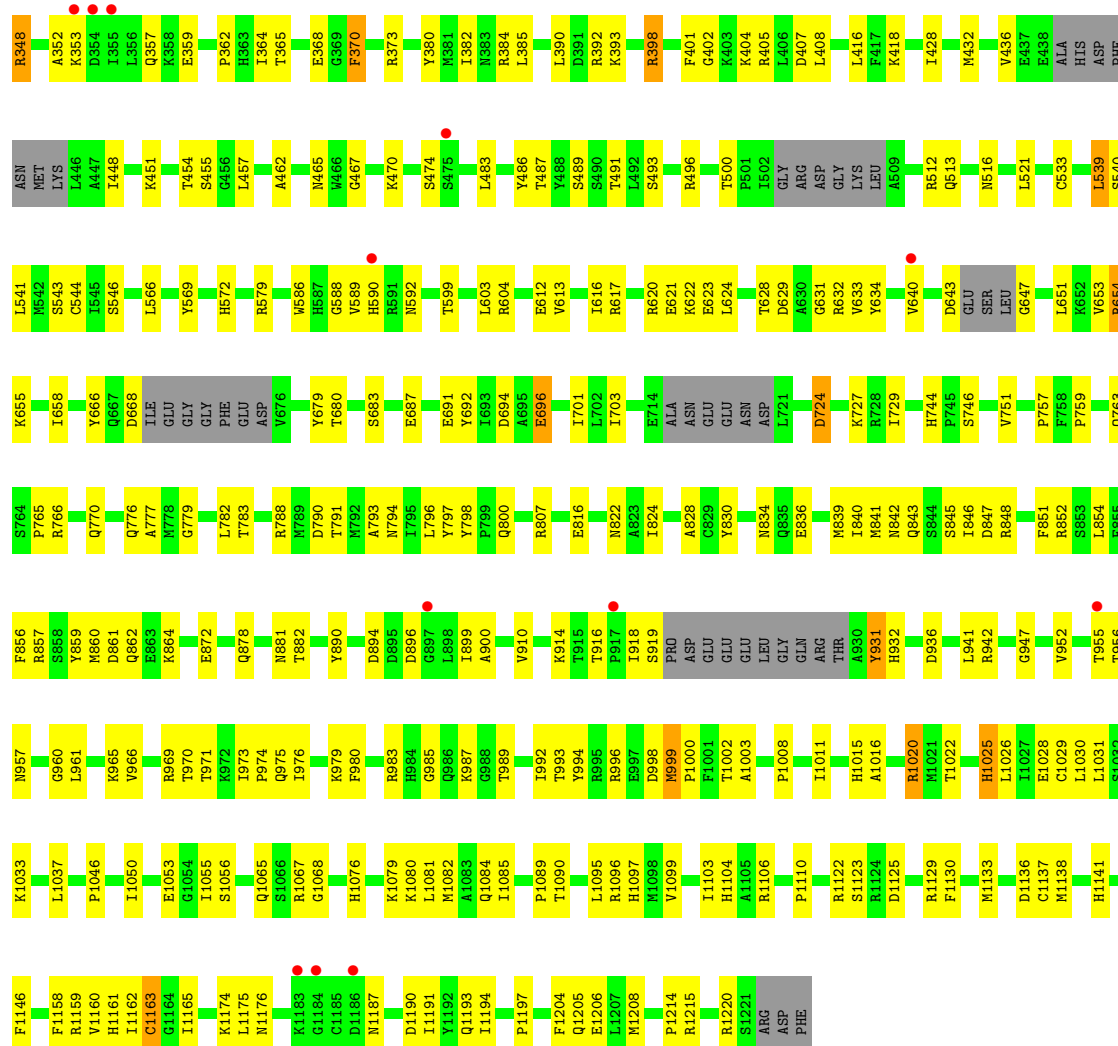
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





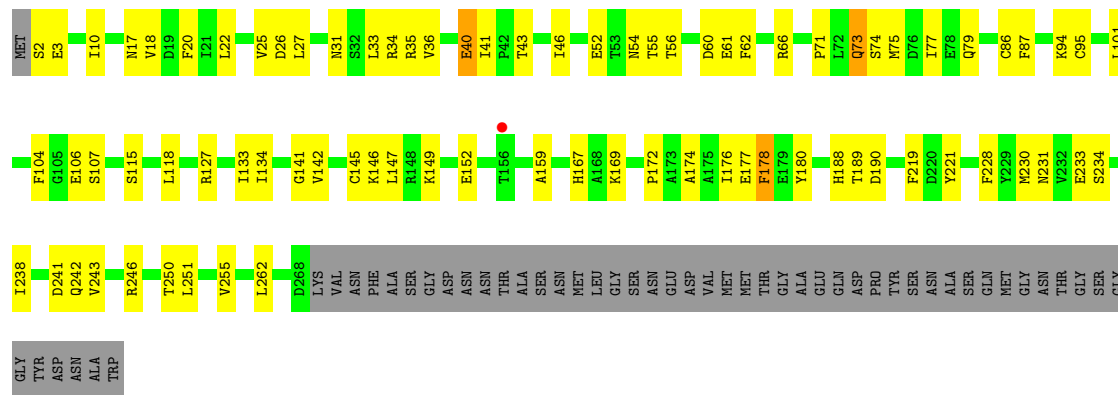
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2





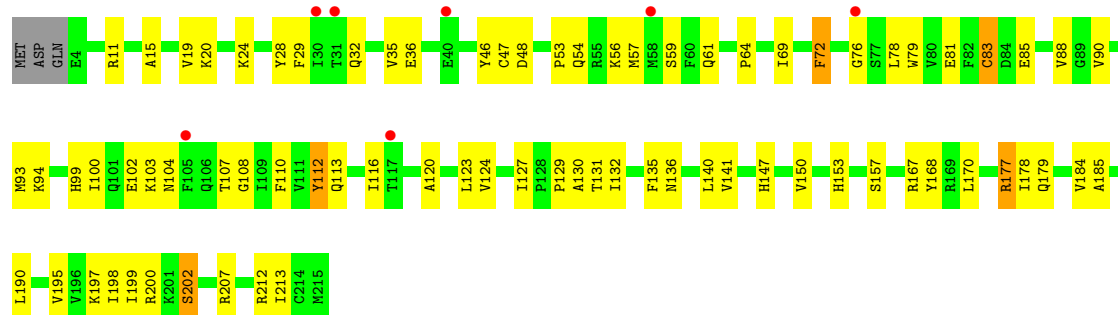
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 58% 25% 16%

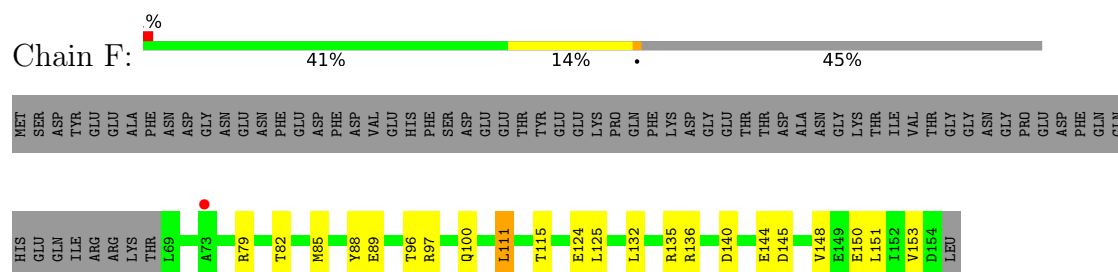


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

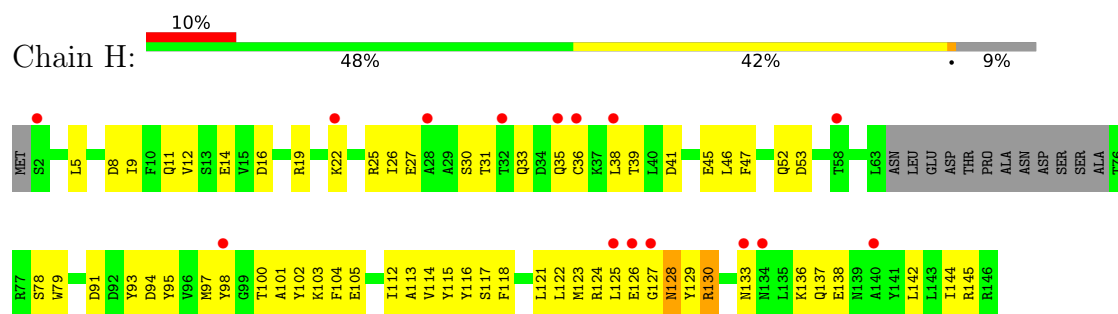
Chain E: 3% 63% 33%



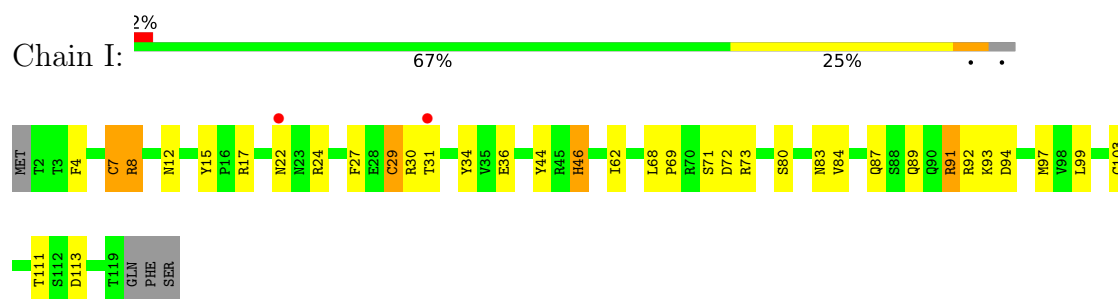
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



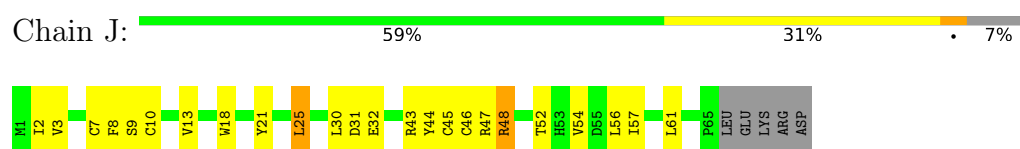
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



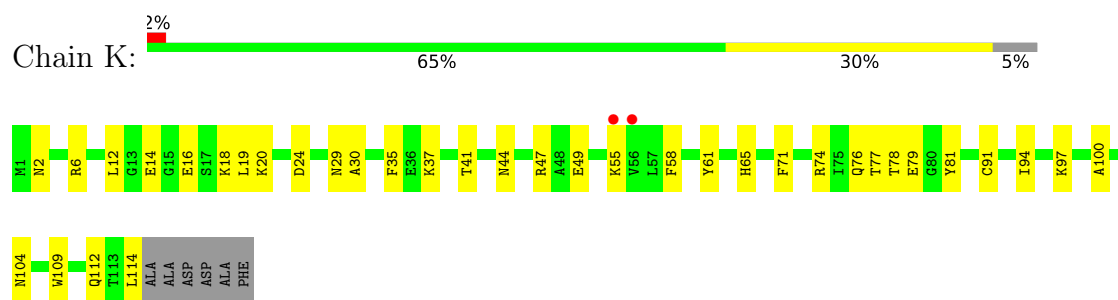
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



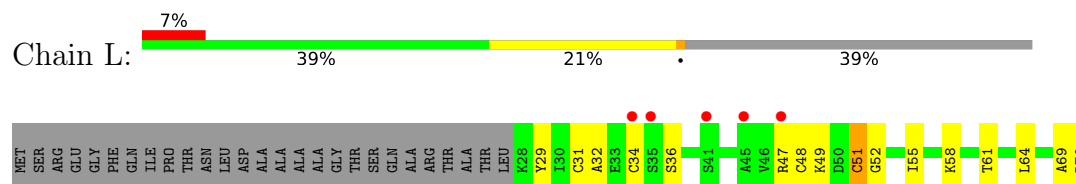
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



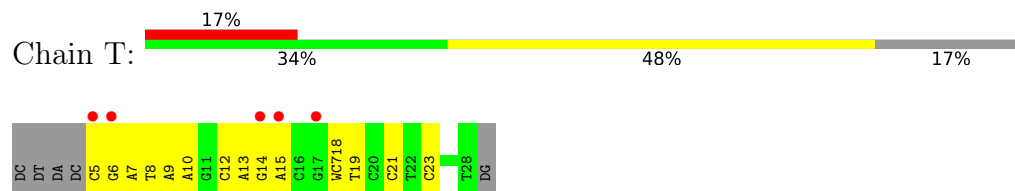
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



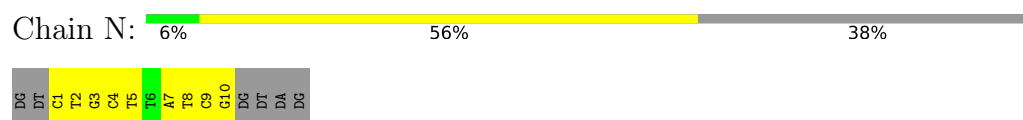
- Molecule 11: RNA



- Molecule 12: Template strand DNA



- Molecule 13: Non template strand DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.89Å 223.01Å 194.70Å 90.00° 101.60° 90.00°	Depositor
Resolution (Å)	82.60 – 3.60 82.60 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (82.60-3.60) 97.3 (82.60-3.60)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.266 , 0.305 0.266 , 0.305	Depositor DCC
R_{free} test set	1833 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	28916	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: ZN, MG, WC7

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/11012	0.46	0/14897
2	B	0.25	0/9030	0.46	0/12186
3	C	0.26	0/2139	0.48	0/2899
4	E	0.27	0/1767	0.46	0/2378
5	F	0.25	0/696	0.45	0/943
6	H	0.27	0/1082	0.52	0/1466
7	I	0.28	0/970	0.47	0/1308
8	J	0.25	0/541	0.51	0/727
9	K	0.25	0/937	0.45	0/1265
10	L	0.27	0/339	0.48	0/450
11	R	0.33	0/243	0.94	0/378
12	T	0.63	0/524	0.98	0/803
13	N	0.59	0/224	1.13	0/343
All	All	0.27	0/29504	0.50	0/40043

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	A	10820	0	10866	342	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8859	0	8817	286	0
3	C	2101	0	2056	67	0
4	E	1731	0	1758	49	0
5	F	684	0	692	14	0
6	H	1064	0	1029	67	0
7	I	952	0	897	26	0
8	J	532	0	542	19	0
9	K	919	0	929	24	0
10	L	337	0	352	14	0
11	R	216	0	110	2	0
12	T	490	0	259	18	0
13	N	202	0	115	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	28916	0	28422	842	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 15.

All (842) 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)
6:H:128:ASN:N	6:H:130:ARG:HH12	1.57	1.03
6:H:127:GLY:C	6:H:130:ARG:HH12	1.61	1.02
10:L:32:ALA:HB3	10:L:55:ILE:HD13	1.42	1.01
2:B:1191:ILE:HD12	2:B:1191:ILE:O	1.63	0.98
1:A:42:ASP:HB2	1:A:50:ILE:HG23	1.47	0.95
6:H:127:GLY:HA3	6:H:130:ARG:HH22	1.33	0.91
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.55	0.88
1:A:1206:ASP:HB3	1:A:1274:ARG:HH22	1.38	0.86
4:E:90:VAL:HG23	4:E:123:LEU:HD11	1.56	0.86
2:B:112:LEU:HD21	2:B:117:ALA:HB2	1.60	0.83
1:A:840:ARG:HH21	1:A:1384:VAL:HG23	1.44	0.82
6:H:127:GLY:C	6:H:130:ARG:NH1	2.33	0.81
1:A:562:THR:O	1:A:576:GLN:NE2	2.15	0.79
7:I:7:CYS:SG	7:I:8:ARG:N	2.55	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1082:MET:HA	3:C:189:THR:HA	1.63	0.79
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.15	0.79
1:A:890:ASP:OD2	1:A:940:ARG:NH1	2.15	0.78
2:B:496:ARG:HH22	2:B:541:LEU:HA	1.48	0.78
6:H:127:GLY:CA	6:H:130:ARG:HH22	1.96	0.78
1:A:443:LEU:HG	1:A:501:LEU:HD11	1.66	0.78
7:I:44:TYR:HE2	7:I:46:HIS:HB2	1.48	0.77
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.67	0.77
2:B:1159:ARG:HH12	2:B:1175:LEU:HD11	1.50	0.76
2:B:878:GLN:HB2	2:B:881:ASN:HB3	1.68	0.76
2:B:612:GLU:O	2:B:632:ARG:NH2	2.19	0.76
2:B:788:ARG:NH1	2:B:790:ASP:OD2	2.19	0.76
9:K:44:ASN:OD1	9:K:47:ARG:NH2	2.17	0.75
1:A:108:MET:SD	1:A:171:GLN:NE2	2.60	0.75
6:H:130:ARG:H	6:H:130:ARG:HD2	1.50	0.75
2:B:332:ASP:OD1	2:B:348:ARG:NH2	2.20	0.75
1:A:542:GLU:O	1:A:546:VAL:HG23	1.85	0.74
1:A:439:ASN:HA	1:A:459:ARG:HG2	1.69	0.74
2:B:800:GLN:NE2	8:J:52:THR:OG1	2.18	0.73
6:H:128:ASN:CA	6:H:130:ARG:HH12	2.01	0.73
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.21	0.73
1:A:446:ARG:HH21	1:A:480:ALA:HA	1.52	0.73
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.70	0.73
6:H:93:TYR:HD2	6:H:145:ARG:HB2	1.52	0.73
1:A:859:SER:O	1:A:1422:ARG:NH1	2.19	0.73
9:K:16:GLU:OE1	9:K:37:LYS:NZ	2.21	0.72
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.71	0.72
1:A:362:ASP:OD1	1:A:459:ARG:NH1	2.23	0.72
4:E:112:TYR:CE1	4:E:116:ILE:HG22	2.24	0.72
2:B:643:ASP:O	2:B:647:GLY:N	2.23	0.71
1:A:1364:ASN:OD1	1:A:1366:ARG:NH1	2.24	0.71
6:H:36:CYS:HA	6:H:126:GLU:O	1.91	0.71
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.24	0.71
1:A:153:PRO:HA	1:A:161:LEU:HB2	1.73	0.71
2:B:287:ARG:NH1	2:B:324:ILE:O	2.24	0.70
6:H:98:TYR:OH	6:H:138:GLU:OE2	2.07	0.70
2:B:228:LYS:HG3	2:B:234:ILE:HG13	1.72	0.70
4:E:102:GLU:O	4:E:104:ASN:ND2	2.24	0.70
7:I:73:ARG:O	7:I:83:ASN:ND2	2.24	0.69
1:A:1329:THR:HG22	1:A:1331:SER:H	1.56	0.69
2:B:1103:ILE:O	2:B:1122:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:95:TYR:HD2	6:H:144:ILE:HD13	1.55	0.69
2:B:798:TYR:OH	3:C:66:ARG:NH2	2.26	0.69
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	1.76	0.68
2:B:896:ASP:OD2	10:L:58:LYS:NZ	2.24	0.68
3:C:66:ARG:NH1	8:J:3:VAL:O	2.26	0.68
2:B:345:LYS:O	2:B:348:ARG:NH1	2.26	0.68
1:A:960:ILE:HG22	1:A:964:ILE:HD13	1.76	0.68
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.74	0.68
4:E:177:ARG:O	4:E:212:ARG:NH2	2.26	0.68
2:B:103:ASN:OD1	2:B:169:ARG:NH2	2.27	0.67
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.26	0.67
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.75	0.67
7:I:34:TYR:HE2	7:I:36:GLU:HB2	1.60	0.67
2:B:103:ASN:ND2	2:B:109:THR:OG1	2.28	0.67
6:H:100:THR:HG23	6:H:138:GLU:HA	1.75	0.67
2:B:260:GLY:O	2:B:267:ARG:NH1	2.28	0.67
1:A:517:ASN:OD1	1:A:1364:ASN:ND2	2.27	0.66
5:F:82:THR:O	5:F:136:ARG:NH1	2.22	0.66
2:B:67:SER:HB3	2:B:92:PHE:HD1	1.59	0.66
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.78	0.66
1:A:840:ARG:HD2	1:A:1402:PHE:HZ	1.60	0.66
2:B:539:LEU:HD12	2:B:543:SER:OG	1.94	0.66
8:J:43:ARG:NH2	8:J:46:CYS:SG	2.68	0.66
6:H:22:LYS:NZ	6:H:45:GLU:OE1	2.24	0.66
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.25	0.66
1:A:550:LEU:HD22	1:A:577:ILE:HD13	1.78	0.66
1:A:1127:ASP:O	1:A:1131:ALA:N	2.28	0.66
2:B:41:LYS:NZ	2:B:544:CYS:SG	2.69	0.66
1:A:50:ILE:HD13	1:A:52:GLY:H	1.60	0.65
1:A:881:GLN:HE21	1:A:956:LEU:HB2	1.61	0.65
1:A:900:ASP:O	1:A:907:THR:OG1	2.12	0.65
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.79	0.65
1:A:848:ILE:HG21	1:A:1370:LEU:HD21	1.78	0.65
2:B:724:ASP:HB2	2:B:727:LYS:HE3	1.77	0.65
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.26	0.65
2:B:1056:SER:OG	2:B:1067:ARG:NH2	2.29	0.65
1:A:663:SER:O	1:A:742:ASN:ND2	2.23	0.65
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.29	0.65
4:E:178:ILE:N	4:E:213:ILE:O	2.30	0.65
1:A:1132:LYS:HE2	1:A:1135:ARG:HH11	1.62	0.65
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:SER:HB3	2:B:169:ARG:HB3	1.79	0.65
1:A:204:THR:HA	1:A:207:ILE:HD12	1.79	0.64
2:B:546:SER:OG	2:B:631:GLY:N	2.29	0.64
1:A:974:ASP:OD2	1:A:976:THR:OG1	2.15	0.64
1:A:1024:SER:O	1:A:1030:ARG:NH1	2.29	0.64
2:B:931:TYR:HD2	2:B:932:HIS:H	1.42	0.64
1:A:412:ARG:NH1	1:A:433:GLU:OE2	2.30	0.64
6:H:128:ASN:CA	6:H:130:ARG:NH1	2.59	0.64
2:B:620:ARG:NE	7:I:89:GLN:HE22	1.96	0.64
2:B:975:GLN:HG2	2:B:976:ILE:H	1.63	0.64
13:N:1:DC:H2'	13:N:2:DT:H71	1.80	0.64
3:C:174:ALA:HB3	3:C:233:GLU:HB3	1.80	0.63
9:K:100:ALA:O	9:K:104:ASN:ND2	2.30	0.63
6:H:105:GLU:HB3	6:H:113:ALA:HB3	1.80	0.63
1:A:383:TYR:HB3	5:F:115:THR:HB	1.81	0.63
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.81	0.63
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.31	0.63
2:B:744:HIS:ND1	2:B:746:SER:OG	2.31	0.63
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.28	0.63
2:B:899:ILE:HG12	2:B:900:ALA:H	1.64	0.63
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.32	0.63
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.80	0.63
2:B:955:THR:OG1	2:B:956:THR:N	2.32	0.63
1:A:25:GLU:OE1	1:A:25:GLU:N	2.27	0.62
2:B:29:ASP:OD2	2:B:655:LYS:NZ	2.31	0.62
2:B:1033:LYS:HB2	2:B:1089:PRO:HD2	1.81	0.62
1:A:1138:ILE:HD11	1:A:1316:VAL:HG13	1.82	0.62
2:B:199:MET:SD	2:B:199:MET:N	2.72	0.62
1:A:18:GLN:HB2	1:A:1418:LEU:HD12	1.80	0.62
1:A:50:ILE:CD1	1:A:52:GLY:H	2.12	0.62
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.32	0.62
4:E:47:CYS:HA	4:E:53:PRO:HB3	1.81	0.62
6:H:35:GLN:N	6:H:35:GLN:OE1	2.32	0.62
12:T:15:DA:H5''	12:T:15:DA:H8	1.65	0.62
6:H:114:VAL:HG12	6:H:125:LEU:HB3	1.81	0.62
6:H:12:VAL:HG12	6:H:53:ASP:H	1.64	0.61
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.81	0.61
6:H:38:LEU:HD12	6:H:123:MET:HE2	1.81	0.61
9:K:91:CYS:HA	9:K:94:ILE:HD12	1.80	0.61
3:C:36:VAL:HG23	3:C:40:GLU:HB3	1.83	0.61
4:E:46:TYR:HE1	4:E:57:MET:HB3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.82	0.61
2:B:195:CYS:SG	2:B:783:THR:OG1	2.56	0.61
1:A:106:VAL:O	1:A:171:GLN:NE2	2.33	0.61
2:B:245:GLU:O	2:B:249:ARG:NH2	2.34	0.61
2:B:384:ARG:NH2	2:B:623:GLU:OE2	2.34	0.61
10:L:51:CYS:SG	10:L:52:GLY:N	2.74	0.61
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.83	0.61
2:B:101:MET:HG2	2:B:111:ALA:HA	1.83	0.61
2:B:304:ASP:OD1	2:B:306:ASN:ND2	2.28	0.61
2:B:236:HIS:HB3	2:B:385:LEU:HD11	1.82	0.60
2:B:613:VAL:HG22	2:B:628:THR:HG22	1.82	0.60
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.82	0.60
1:A:466:SER:HB3	2:B:1103:ILE:HD12	1.83	0.60
1:A:445:ASN:OD1	1:A:449:SER:OG	2.19	0.60
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.34	0.60
2:B:232:SER:OG	2:B:234:ILE:O	2.19	0.60
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.82	0.60
1:A:1166:ASP:OD1	1:A:1194:ARG:NH2	2.27	0.60
2:B:176:SER:OG	2:B:177:LYS:N	2.33	0.60
6:H:118:PHE:CZ	6:H:142:LEU:HD12	2.36	0.60
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.36	0.60
1:A:550:LEU:HD12	1:A:556:TRP:CE2	2.36	0.60
1:A:825:ILE:HD12	2:B:513:GLN:HG3	1.83	0.60
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.33	0.60
1:A:167:CYS:SG	1:A:168:GLY:N	2.75	0.60
4:E:127:ILE:HG22	4:E:129:PRO:HD2	1.83	0.60
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.84	0.60
4:E:197:LYS:HE2	4:E:199:ILE:HD11	1.84	0.60
4:E:108:GLY:N	4:E:131:THR:O	2.35	0.59
3:C:31:ASN:OD1	3:C:34:ARG:NH1	2.32	0.59
4:E:46:TYR:OH	4:E:56:LYS:N	2.34	0.59
4:E:59:SER:HB3	4:E:81:GLU:HA	1.83	0.59
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.84	0.59
3:C:169:LYS:NZ	10:L:69:ALA:O	2.24	0.59
6:H:103:LYS:HB3	6:H:115:TYR:HD1	1.67	0.59
1:A:352:VAL:HG21	2:B:1099:VAL:HG12	1.84	0.59
2:B:301:ILE:HD13	2:B:382:ILE:HG21	1.82	0.59
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.85	0.59
1:A:767:GLN:HE21	1:A:774:ARG:HG2	1.68	0.59
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.85	0.59
1:A:1110:ASN:ND2	13:N:1:DC:OP2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1053:GLU:OE2	2:B:1067:ARG:NH1	2.36	0.58
5:F:111:LEU:HD23	5:F:111:LEU:H	1.67	0.58
2:B:830:TYR:OH	2:B:998:ASP:O	2.21	0.58
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.36	0.58
3:C:73:GLN:HG2	3:C:133:ILE:HD11	1.85	0.58
13:N:1:DC:H2"	13:N:2:DT:H5"	1.84	0.58
1:A:354:SER:OG	1:A:469:ARG:NH1	2.36	0.58
2:B:679:TYR:OH	2:B:687:GLU:OE1	2.16	0.58
1:A:1421:CYS:O	1:A:1427:ASN:ND2	2.36	0.58
4:E:112:TYR:HE1	4:E:116:ILE:HG22	1.68	0.58
1:A:148:CYS:SG	1:A:164:ARG:NH1	2.76	0.58
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.83	0.58
8:J:9:SER:OG	8:J:48:ARG:NH2	2.36	0.58
1:A:1116:LEU:HD11	1:A:1327:ILE:HD11	1.85	0.58
1:A:1142:THR:O	1:A:1145:SER:OG	2.22	0.58
6:H:129:TYR:H	6:H:130:ARG:NH1	2.02	0.58
1:A:420:ARG:NH2	1:A:423:ASP:OD1	2.35	0.58
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.37	0.58
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.36	0.58
6:H:128:ASN:HA	6:H:130:ARG:NH1	2.18	0.58
1:A:381:THR:OG1	1:A:384:ASN:ND2	2.37	0.57
6:H:123:MET:HE1	6:H:142:LEU:HD11	1.85	0.57
1:A:440:ASP:OD2	1:A:498:ARG:NH2	2.37	0.57
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.86	0.57
2:B:242:SER:HB3	2:B:362:PRO:HD2	1.84	0.57
1:A:765:VAL:HG13	1:A:800:VAL:HB	1.85	0.57
1:A:592:ASP:N	1:A:595:THR:OG1	2.34	0.57
1:A:1235:LYS:HB3	1:A:1237:ILE:HD11	1.86	0.57
1:A:951:GLU:O	1:A:954:TRP:NE1	2.37	0.57
1:A:1013:ASP:HB3	4:E:207:ARG:HB2	1.85	0.57
2:B:486:TYR:CE2	2:B:1096:ARG:HB3	2.40	0.57
9:K:49:GLU:OE2	9:K:97:LYS:NZ	2.27	0.57
2:B:851:PHE:CD1	2:B:980:PHE:HE2	2.22	0.57
3:C:71:PRO:HG3	8:J:13:VAL:HG11	1.87	0.57
10:L:47:ARG:NE	10:L:52:GLY:O	2.37	0.57
1:A:1121:GLU:HB3	1:A:1124:HIS:HB2	1.86	0.57
4:E:195:VAL:HG22	4:E:213:ILE:HG13	1.85	0.57
6:H:127:GLY:O	6:H:130:ARG:NH1	2.38	0.57
2:B:223:VAL:HG11	2:B:380:TYR:HE2	1.69	0.56
2:B:315:LYS:HB3	2:B:316:PRO:HD3	1.87	0.56
2:B:822:ASN:O	8:J:48:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:20:LYS:HD2	4:E:35:VAL:HA	1.87	0.56
6:H:115:TYR:HE2	6:H:124:ARG:HG3	1.71	0.56
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.39	0.56
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.39	0.56
2:B:586:TRP:NE1	2:B:588:GLY:O	2.36	0.56
6:H:8:ASP:OD1	6:H:129:TYR:OH	2.18	0.56
1:A:761:MET:HA	1:A:804:TYR:HB2	1.88	0.56
2:B:770:GLN:O	2:B:770:GLN:NE2	2.38	0.56
4:E:46:TYR:HH	4:E:56:LYS:H	1.54	0.56
2:B:766:ARG:NH1	2:B:985:GLY:O	2.39	0.56
1:A:147:VAL:HG23	1:A:171:GLN:HG2	1.87	0.56
1:A:840:ARG:NE	1:A:1384:VAL:O	2.37	0.56
2:B:169:ARG:N	2:B:454:THR:OG1	2.38	0.56
2:B:852:ARG:HH21	2:B:971:THR:HG21	1.70	0.56
4:E:85:GLU:HB2	4:E:88:VAL:HG12	1.87	0.56
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.86	0.56
1:A:50:ILE:HD13	1:A:52:GLY:N	2.20	0.56
1:A:767:GLN:HE22	1:A:774:ARG:HE	1.53	0.56
1:A:1278:ASN:HB2	1:A:1312:ASN:HB2	1.86	0.56
3:C:46:ILE:O	3:C:169:LYS:NZ	2.33	0.56
3:C:241:ASP:OD1	3:C:242:GLN:N	2.38	0.56
1:A:806:ARG:NH2	2:B:727:LYS:O	2.38	0.56
6:H:128:ASN:O	6:H:128:ASN:ND2	2.37	0.56
1:A:9:ALA:CB	2:B:1191:ILE:HD13	2.36	0.55
1:A:361:LEU:HG	1:A:507:VAL:HG11	1.88	0.55
1:A:446:ARG:NH2	1:A:479:ASN:O	2.39	0.55
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.38	0.55
1:A:128:ILE:HG23	1:A:134:ARG:HB2	1.87	0.55
1:A:172:PRO:HB3	1:A:185:TRP:HB2	1.88	0.55
7:I:29:CYS:SG	7:I:31:THR:N	2.78	0.55
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.87	0.55
2:B:1082:MET:HG3	3:C:190:ASP:H	1.71	0.55
6:H:14:GLU:HB3	6:H:27:GLU:HB3	1.89	0.55
7:I:87:GLN:HG2	7:I:99:LEU:HD23	1.87	0.55
1:A:95:PHE:O	1:A:99:ILE:N	2.37	0.55
1:A:901:LEU:HA	1:A:907:THR:HG23	1.88	0.55
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.40	0.55
7:I:22:ASN:HB3	7:I:24:ARG:HG3	1.89	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.89	0.55
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.88	0.55
11:R:3:C:H2'	11:R:4:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:9:DA:H2''	12:T:10:DA:C8	2.41	0.55
3:C:115:SER:HB3	3:C:142:VAL:HG12	1.89	0.55
12:T:6:DG:H2''	12:T:7:DA:H8	1.71	0.55
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.89	0.55
2:B:1191:ILE:HD12	2:B:1191:ILE:C	2.25	0.55
6:H:25:ARG:HH21	6:H:41:ASP:CG	2.10	0.55
1:A:481:ASP:HB2	1:A:483:ASP:OD2	2.07	0.55
2:B:1159:ARG:HD3	2:B:1161:HIS:CE1	2.42	0.55
2:B:326:ASP:O	2:B:329:THR:OG1	2.25	0.54
2:B:451:LYS:O	2:B:455:SER:HB3	2.06	0.54
12:T:8:DT:H2'	12:T:9:DA:C8	2.42	0.54
1:A:153:PRO:HB3	1:A:161:LEU:HD13	1.88	0.54
1:A:492:PRO:O	1:A:493:GLN:NE2	2.40	0.54
1:A:1168:GLU:HG3	1:A:1169:ILE:HD12	1.88	0.54
2:B:334:ILE:HG12	2:B:352:ALA:HB2	1.90	0.54
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.26	0.54
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.36	0.54
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.41	0.54
2:B:390:LEU:HD13	2:B:392:ARG:NH2	2.23	0.54
5:F:125:LEU:HD11	5:F:153:VAL:HG21	1.90	0.54
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.90	0.54
3:C:2:SER:OG	3:C:3:GLU:N	2.40	0.54
1:A:134:ARG:NH2	1:A:220:THR:O	2.36	0.54
1:A:351:THR:OG1	1:A:352:VAL:N	2.41	0.54
1:A:353:ILE:HD11	1:A:485:ASP:HB2	1.90	0.54
2:B:496:ARG:NH2	2:B:541:LEU:HA	2.21	0.54
3:C:79:GLN:HB3	3:C:127:ARG:HH11	1.72	0.54
4:E:46:TYR:OH	4:E:54:GLN:O	2.14	0.54
1:A:525:GLN:HB2	2:B:1015:HIS:CD2	2.43	0.54
2:B:326:ASP:OD1	2:B:326:ASP:N	2.41	0.54
2:B:824:ILE:HG22	2:B:1008:PRO:HA	1.90	0.54
7:I:80:SER:OG	7:I:103:CYS:SG	2.66	0.54
1:A:827:THR:O	1:A:831:THR:OG1	2.25	0.53
2:B:245:GLU:HA	2:B:249:ARG:HH22	1.73	0.53
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.90	0.53
2:B:861:ASP:OD1	2:B:862:GLN:N	2.41	0.53
12:T:5:DC:H1'	12:T:6:DG:C8	2.42	0.53
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.40	0.53
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.41	0.53
1:A:1312:ASN:ND2	1:A:1315:GLU:OE2	2.25	0.53
6:H:5:LEU:HG	6:H:133:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:THR:N	1:A:985:ASP:OD2	2.40	0.53
7:I:29:CYS:SG	7:I:30:ARG:N	2.81	0.53
1:A:944:ARG:NH2	1:A:1296:GLY:O	2.28	0.53
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.91	0.53
7:I:15:TYR:O	7:I:27:PHE:HA	2.08	0.53
2:B:287:ARG:NH1	2:B:321:GLY:O	2.41	0.53
1:A:146:MET:SD	1:A:146:MET:N	2.81	0.53
1:A:675:THR:OG1	1:A:736:ASN:OD1	2.24	0.53
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.91	0.53
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.44	0.53
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.74	0.53
1:A:980:ASP:OD1	1:A:980:ASP:N	2.42	0.53
6:H:12:VAL:HG23	6:H:26:ILE:HG23	1.89	0.53
1:A:1100:ARG:NH2	1:A:1351:GLU:OE2	2.42	0.53
1:A:1150:SER:OG	1:A:1264:GLU:OE2	2.18	0.53
1:A:848:ILE:HD13	1:A:858:ASN:HB3	1.91	0.53
2:B:957:ASN:OD1	2:B:961:LEU:N	2.42	0.53
4:E:24:LYS:NZ	4:E:32:GLN:OE1	2.42	0.53
2:B:1065:GLN:OE1	2:B:1068:GLY:N	2.42	0.52
2:B:1020:ARG:HB2	2:B:1022:THR:HG23	1.92	0.52
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.44	0.52
1:A:540:PHE:HZ	6:H:121:LEU:HD11	1.74	0.52
2:B:248:SER:HA	2:B:418:LYS:NZ	2.25	0.52
9:K:12:LEU:HD12	9:K:12:LEU:H	1.74	0.52
9:K:30:ALA:HB2	9:K:76:GLN:HB2	1.91	0.52
9:K:78:THR:HG22	9:K:79:GLU:H	1.73	0.52
1:A:1066:VAL:HG11	2:B:1136:ASP:O	2.10	0.52
3:C:94:LYS:HA	3:C:127:ARG:HH22	1.74	0.52
13:N:2:DT:H2'	13:N:3:DG:C8	2.44	0.52
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.09	0.52
2:B:210:LYS:HE2	2:B:462:ALA:HA	1.91	0.52
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.91	0.52
8:J:31:ASP:OD1	8:J:32:GLU:N	2.43	0.52
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.91	0.52
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.92	0.52
3:C:62:PHE:HE2	3:C:66:ARG:HD2	1.75	0.52
1:A:618:GLU:OE1	1:A:619:LYS:N	2.42	0.52
2:B:680:THR:O	2:B:683:SER:OG	2.21	0.52
6:H:142:LEU:HD22	6:H:144:ILE:HD11	1.91	0.52
12:T:15:DA:H5''	12:T:15:DA:C8	2.44	0.52
1:A:332:LYS:NZ	12:T:19:DT:OP2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH1	12:T:21:DC:OP1	2.27	0.52
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.92	0.52
6:H:8:ASP:OD2	6:H:9:ILE:N	2.43	0.52
1:A:359:LEU:HD11	1:A:469:ARG:HB2	1.91	0.52
4:E:108:GLY:O	4:E:132:ILE:HA	2.10	0.52
6:H:93:TYR:CD2	6:H:145:ARG:HB2	2.40	0.52
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.91	0.51
12:T:6:DG:H2"	12:T:7:DA:C8	2.45	0.51
1:A:71:GLN:OE1	2:B:1176:ASN:N	2.43	0.51
1:A:463:ILE:HD12	1:A:465:TYR:H	1.74	0.51
2:B:617:ARG:HG3	2:B:624:LEU:HD12	1.93	0.51
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.91	0.51
1:A:544:ASP:OD1	1:A:545:GLN:N	2.43	0.51
2:B:116:GLU:OE2	2:B:120:ARG:NH1	2.43	0.51
1:A:449:SER:HB3	2:B:1137:CYS:SG	2.51	0.51
2:B:63:ILE:HG13	2:B:95:ILE:HD13	1.93	0.51
2:B:842:ASN:O	2:B:845:SER:OG	2.26	0.51
4:E:168:TYR:HB3	4:E:170:LEU:HG	1.91	0.51
1:A:455:MET:O	2:B:1141:HIS:HE1	1.94	0.51
1:A:506:ALA:O	1:A:510:GLN:HG2	2.11	0.51
1:A:515:GLN:HB2	1:A:1071:SER:HB3	1.93	0.51
1:A:679:ILE:O	1:A:683:ILE:HG12	2.10	0.51
1:A:690:VAL:HG13	1:A:718:VAL:HG22	1.93	0.51
3:C:86:CYS:SG	3:C:87:PHE:N	2.82	0.51
6:H:104:PHE:HE1	6:H:136:LYS:HB3	1.74	0.51
1:A:848:ILE:HD12	1:A:864:ILE:HG13	1.93	0.51
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.93	0.51
1:A:802:ASN:OD1	2:B:729:ILE:N	2.24	0.51
2:B:219:ALA:O	2:B:241:ARG:NH1	2.44	0.51
3:C:26:ASP:OD1	3:C:26:ASP:N	2.42	0.51
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.93	0.51
2:B:487:THR:OG1	2:B:777:ALA:O	2.28	0.51
1:A:1067:LEU:O	1:A:1071:SER:OG	2.24	0.50
2:B:275:TYR:CE2	2:B:359:GLU:HG3	2.46	0.50
4:E:99:HIS:O	4:E:103:LYS:HB2	2.11	0.50
7:I:111:THR:HG22	7:I:113:ASP:H	1.77	0.50
10:L:32:ALA:CB	10:L:55:ILE:HD13	2.29	0.50
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.51	0.50
2:B:402:GLY:O	2:B:405:ARG:NH1	2.45	0.50
1:A:901:LEU:O	1:A:920:LEU:HD23	2.12	0.50
1:A:905:ASP:OD1	1:A:905:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:THR:HB	1:A:1297:GLU:HG2	1.93	0.50
1:A:70:CYS:O	1:A:71:GLN:HG2	2.10	0.50
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.46	0.50
2:B:1187:ASN:HD21	2:B:1190:ASP:C	2.15	0.50
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.94	0.50
1:A:397:ASN:O	1:A:397:ASN:ND2	2.35	0.50
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.93	0.50
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.77	0.50
1:A:974:ASP:OD2	1:A:977:LYS:NZ	2.32	0.50
1:A:1062:GLU:OE2	5:F:88:TYR:OH	2.28	0.50
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.47	0.50
2:B:398:ARG:H	2:B:398:ARG:CZ	2.25	0.50
2:B:899:ILE:HG12	2:B:900:ALA:N	2.26	0.50
7:I:71:SER:OG	7:I:83:ASN:OD1	2.17	0.50
1:A:1206:ASP:H	1:A:1274:ARG:HH12	1.60	0.50
2:B:67:SER:HB3	2:B:92:PHE:CD1	2.44	0.50
8:J:21:TYR:O	8:J:25:LEU:HD23	2.11	0.50
1:A:1436:ILE:HG22	1:A:1437:GLY:H	1.77	0.49
2:B:257:LYS:NZ	2:B:279:ASP:OD2	2.29	0.49
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.94	0.49
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.77	0.49
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.93	0.49
6:H:105:GLU:O	6:H:113:ALA:N	2.42	0.49
2:B:402:GLY:HA3	2:B:696:GLU:HG2	1.94	0.49
2:B:890:TYR:CE2	2:B:910:VAL:HG11	2.47	0.49
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.12	0.49
2:B:794:ASN:HA	2:B:854:LEU:O	2.12	0.49
4:E:94:LYS:HE2	4:E:123:LEU:HD13	1.93	0.49
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.47	0.49
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.95	0.49
7:I:72:ASP:N	7:I:72:ASP:OD1	2.45	0.49
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.52	0.49
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.93	0.49
3:C:177:GLU:O	3:C:230:MET:HA	2.13	0.49
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.47	0.49
10:L:34:CYS:SG	10:L:36:SER:OG	2.68	0.49
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.44	0.49
2:B:221:ASN:OD1	2:B:243:ALA:N	2.46	0.49
2:B:353:LYS:O	2:B:357:GLN:NE2	2.29	0.49
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.47	0.49
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.13	0.49
1:A:959:ASN:OD1	1:A:961:ARG:HB3	2.13	0.49
2:B:124:TYR:HB2	2:B:204:ILE:HB	1.95	0.49
3:C:2:SER:OG	9:K:104:ASN:OD1	2.30	0.49
1:A:1351:GLU:O	1:A:1355:VAL:HG13	2.13	0.49
8:J:2:ILE:HG12	8:J:3:VAL:H	1.78	0.49
1:A:746:MET:SD	2:B:1015:HIS:ND1	2.80	0.49
1:A:1116:LEU:HD21	1:A:1316:VAL:HG11	1.95	0.49
1:A:1148:ILE:HD11	1:A:1198:ASP:HB2	1.94	0.49
12:T:9:DA:H2"	12:T:10:DA:H8	1.78	0.49
1:A:802:ASN:ND2	2:B:729:ILE:O	2.37	0.48
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.94	0.48
5:F:135:ARG:NH2	5:F:145:ASP:OD2	2.28	0.48
8:J:54:VAL:HG12	8:J:56:LEU:HG	1.94	0.48
1:A:465:TYR:CD1	2:B:976:ILE:HG13	2.48	0.48
2:B:496:ARG:NH2	2:B:540:SER:O	2.46	0.48
2:B:1103:ILE:O	2:B:1122:ARG:HD2	2.13	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.48
1:A:550:LEU:HD12	1:A:556:TRP:NE1	2.28	0.48
1:A:668:ASP:OD2	1:A:742:ASN:N	2.40	0.48
1:A:919:ILE:HD11	1:A:925:LEU:HD12	1.96	0.48
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.78	0.48
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.95	0.48
2:B:1002:THR:OG1	2:B:1003:ALA:N	2.46	0.48
2:B:1029:CYS:SG	2:B:1090:THR:OG1	2.51	0.48
12:T:5:DC:H1'	12:T:6:DG:N7	2.28	0.48
1:A:452:LYS:O	2:B:1141:HIS:NE2	2.44	0.48
1:A:9:ALA:HB2	2:B:1191:ILE:HD13	1.95	0.48
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.79	0.48
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.48	0.48
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.48
1:A:836:TYR:CZ	1:A:840:ARG:HD3	2.49	0.48
4:E:69:ILE:HA	4:E:72:PHE:O	2.14	0.48
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.49	0.48
12:T:14:DG:H2"	12:T:15:DA:H8	1.79	0.48
1:A:311:GLN:N	1:A:312:PRO:HD3	2.28	0.48
3:C:31:ASN:O	3:C:35:ARG:HG3	2.13	0.48
2:B:301:ILE:HG21	2:B:314:LEU:HD11	1.95	0.47
2:B:325:GLN:OE1	7:I:12:ASN:ND2	2.47	0.47
2:B:599:THR:O	2:B:603:LEU:HG	2.14	0.47
2:B:770:GLN:HG2	2:B:983:ARG:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:29:ASN:OD1	9:K:77:THR:OG1	2.25	0.47
11:R:3:C:H2'	11:R:4:G:H8	1.79	0.47
6:H:127:GLY:CA	6:H:130:ARG:NH2	2.72	0.47
1:A:668:ASP:N	1:A:668:ASP:OD1	2.47	0.47
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.49	0.47
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	1.95	0.47
1:A:1260:LEU:HD12	1:A:1260:LEU:HA	1.78	0.47
2:B:365:THR:HG21	2:B:370:PHE:HD1	1.79	0.47
2:B:861:ASP:OD1	2:B:914:LYS:NZ	2.39	0.47
3:C:55:THR:OG1	3:C:152:GLU:N	2.47	0.47
3:C:145:CYS:SG	3:C:146:LYS:N	2.87	0.47
4:E:79:TRP:HD1	4:E:100:ILE:HD11	1.79	0.47
5:F:85:MET:HB2	5:F:151:LEU:HB3	1.96	0.47
1:A:211:PHE:HA	1:A:214:ILE:HG12	1.95	0.47
1:A:108:MET:SD	1:A:108:MET:N	2.88	0.47
1:A:944:ARG:HH12	1:A:1292:PRO:HB3	1.80	0.47
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.96	0.47
4:E:127:ILE:HB	4:E:130:ALA:HB3	1.95	0.47
2:B:29:ASP:HB3	2:B:658:ILE:HG21	1.96	0.47
2:B:104:GLU:OE1	2:B:120:ARG:NH2	2.38	0.47
1:A:46:THR:HG22	1:A:47:ARG:H	1.80	0.47
1:A:272:ALA:HB3	1:A:296:LEU:HD23	1.96	0.47
1:A:365:GLY:O	1:A:468:PHE:HA	2.15	0.47
1:A:598:LEU:O	6:H:122:LEU:HD12	2.14	0.47
1:A:881:GLN:OE1	1:A:959:ASN:HA	2.14	0.47
1:A:1208:THR:OG1	1:A:1231:ASP:OD2	2.33	0.47
1:A:1427:ASN:OD1	1:A:1432:GLN:NE2	2.48	0.47
2:B:616:ILE:HD11	2:B:696:GLU:HB3	1.97	0.47
2:B:864:LYS:HG2	2:B:872:GLU:CD	2.35	0.47
4:E:15:ALA:O	4:E:19:VAL:HG23	2.14	0.47
6:H:11:GLN:NE2	6:H:52:GLN:OE1	2.47	0.47
8:J:10:CYS:SG	8:J:43:ARG:NH2	2.87	0.47
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.96	0.47
1:A:1045:VAL:HG12	1:A:1046:LEU:HD12	1.96	0.47
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.14	0.47
2:B:843:GLN:N	2:B:994:TYR:O	2.40	0.47
10:L:48:CYS:SG	10:L:49:LYS:N	2.88	0.47
1:A:565:ILE:HD13	6:H:97:MET:HG2	1.97	0.47
6:H:101:ALA:HB2	6:H:116:TYR:HE2	1.79	0.47
10:L:34:CYS:SG	10:L:51:CYS:HB3	2.54	0.47
1:A:116:ASP:HB3	1:A:118:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD12	1:A:277:GLU:HB2	1.97	0.46
1:A:542:GLU:O	1:A:546:VAL:CG2	2.59	0.46
9:K:18:LYS:HD3	9:K:18:LYS:O	2.15	0.46
2:B:1163:CYS:SG	2:B:1165:ILE:N	2.89	0.46
3:C:74:SER:HB3	3:C:77:ILE:HD13	1.96	0.46
6:H:129:TYR:N	6:H:130:ARG:NH1	2.62	0.46
8:J:7:CYS:SG	8:J:8:PHE:N	2.88	0.46
8:J:57:ILE:O	8:J:61:LEU:HG	2.15	0.46
2:B:470:LYS:O	2:B:474:SER:OG	2.22	0.46
3:C:27:LEU:HD13	3:C:228:PHE:CE2	2.50	0.46
1:A:19:PHE:CE2	2:B:1214:PRO:HB3	2.51	0.46
1:A:148:CYS:O	1:A:168:GLY:HA3	2.15	0.46
1:A:662:PHE:O	2:B:828:ALA:HA	2.15	0.46
2:B:205:ILE:HG22	2:B:206:ASN:OD1	2.16	0.46
4:E:11:ARG:CZ	4:E:141:VAL:HG21	2.46	0.46
6:H:105:GLU:OE1	6:H:115:TYR:OH	2.19	0.46
9:K:58:PHE:HD2	9:K:74:ARG:HE	1.62	0.46
1:A:147:VAL:HG21	1:A:170:THR:HA	1.97	0.46
1:A:224:PHE:CE1	1:A:231:PRO:HB3	2.51	0.46
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.16	0.46
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.98	0.46
2:B:841:MET:O	2:B:993:THR:HA	2.16	0.46
3:C:251:LEU:O	3:C:255:VAL:HG23	2.16	0.46
1:A:14:VAL:N	1:A:1432:GLN:OE1	2.49	0.46
6:H:128:ASN:N	6:H:130:ARG:NH1	2.42	0.46
1:A:1374:VAL:O	1:A:1377:THR:HG22	2.15	0.46
1:A:407:ARG:NH2	1:A:409:SER:OG	2.49	0.46
1:A:466:SER:OG	9:K:2:ASN:ND2	2.41	0.46
3:C:167:HIS:CG	10:L:70:ARG:HG2	2.51	0.46
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.45
1:A:628:GLY:O	1:A:632:VAL:HG23	2.16	0.45
1:A:1166:ASP:OD2	1:A:1194:ARG:NE	2.38	0.45
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.16	0.45
1:A:1379:GLY:HA3	4:E:179:GLN:HG2	1.98	0.45
1:A:1395:GLY:O	1:A:1399:ARG:NH2	2.43	0.45
2:B:579:ARG:NH2	2:B:622:LYS:O	2.49	0.45
2:B:941:LEU:HD22	2:B:942:ARG:H	1.81	0.45
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.98	0.45
1:A:825:ILE:HD13	2:B:512:ARG:HB3	1.98	0.45
1:A:1143:LEU:O	1:A:1147:THR:OG1	2.32	0.45
2:B:569:TYR:CZ	2:B:589:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.81	0.45
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.52	0.45
2:B:483:LEU:CD2	2:B:491:THR:HG23	2.46	0.45
2:B:996:ARG:NH2	3:C:174:ALA:O	2.49	0.45
4:E:112:TYR:HB2	4:E:136:ASN:HA	1.98	0.45
12:T:12:DC:H1'	12:T:13:DA:C8	2.51	0.45
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.98	0.45
2:B:235:SER:OG	2:B:236:HIS:ND1	2.49	0.45
4:E:93:MET:SD	4:E:120:ALA:HB1	2.56	0.45
3:C:41:ILE:HG13	3:C:172:PRO:HG2	1.99	0.45
5:F:132:LEU:O	5:F:148:VAL:HG23	2.17	0.45
1:A:894:GLU:O	1:A:898:ARG:HB3	2.16	0.45
6:H:104:PHE:CE2	6:H:114:VAL:HG23	2.51	0.45
1:A:107:CYS:HB3	1:A:110:CYS:HB2	1.98	0.45
1:A:663:SER:HB2	2:B:1085:ILE:HA	1.98	0.45
3:C:134:ILE:HG23	3:C:141:GLY:HA2	1.98	0.45
4:E:32:GLN:NE2	4:E:36:GLU:OE2	2.31	0.45
1:A:71:GLN:OE1	2:B:1175:LEU:N	2.49	0.45
1:A:326:ARG:NE	1:A:1406:VAL:HG11	2.31	0.45
2:B:1191:ILE:C	2:B:1191:ILE:CD1	2.86	0.45
13:N:2:DT:H2'	13:N:3:DG:N7	2.32	0.45
1:A:544:ASP:HB2	9:K:47:ARG:NH1	2.31	0.45
1:A:1157:ASP:HB3	1:A:1160:SER:O	2.16	0.45
1:A:1276:VAL:HG12	1:A:1277:GLU:H	1.82	0.45
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.82	0.45
3:C:34:ARG:HD3	3:C:178:PHE:HD1	1.82	0.45
3:C:55:THR:OG1	3:C:152:GLU:O	2.35	0.45
4:E:83:CYS:SG	4:E:88:VAL:HG11	2.57	0.45
6:H:95:TYR:CD2	6:H:144:ILE:HD13	2.44	0.45
6:H:114:VAL:CG1	6:H:125:LEU:HB3	2.45	0.45
1:A:269:ILE:HD11	1:A:300:VAL:HA	2.00	0.44
5:F:96:THR:O	5:F:100:GLN:HG2	2.17	0.44
13:N:3:DG:H2''	13:N:4:DC:C6	2.53	0.44
1:A:36:ARG:HB3	1:A:37:PHE:CD1	2.52	0.44
1:A:1109:LYS:H	1:A:1109:LYS:HG2	1.59	0.44
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.51	0.44
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.98	0.44
2:B:828:ALA:HB2	2:B:1085:ILE:HG21	2.00	0.44
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.52	0.44
1:A:121:LEU:O	1:A:124:GLN:HG2	2.17	0.44
1:A:901:LEU:N	1:A:926:GLN:OE1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:HA	1:A:1030:ARG:HH11	1.83	0.44
2:B:1084:GLN:NE2	3:C:189:THR:OG1	2.50	0.44
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.99	0.44
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.44	0.44
7:I:44:TYR:CE2	7:I:46:HIS:HB2	2.39	0.44
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.99	0.44
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.99	0.44
1:A:575:LYS:O	1:A:579:SER:OG	2.32	0.44
1:A:856:THR:HG22	1:A:864:ILE:HB	2.00	0.44
1:A:990:VAL:O	1:A:994:GLN:HG3	2.17	0.44
1:A:1003:LYS:HE2	1:A:1003:LYS:HB2	1.80	0.44
1:A:1019:CYS:HB3	1:A:1023:ARG:HH21	1.83	0.44
1:A:1386:ARG:HE	1:A:1403:GLU:CD	2.21	0.44
2:B:176:SER:O	2:B:182:SER:HB3	2.17	0.44
2:B:261:ARG:NH1	2:B:262:GLU:HG3	2.32	0.44
2:B:629:ASP:O	2:B:632:ARG:NH1	2.50	0.44
2:B:941:LEU:HD13	2:B:942:ARG:N	2.32	0.44
2:B:1191:ILE:O	2:B:1191:ILE:CD1	2.52	0.44
3:C:241:ASP:HB3	9:K:109:TRP:NE1	2.32	0.44
4:E:107:THR:HA	4:E:131:THR:HB	2.00	0.44
1:A:587:HIS:NE2	1:A:969:GLN:HG3	2.32	0.44
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.24	0.44
2:B:653:VAL:O	2:B:654:ARG:NE	2.45	0.44
2:B:976:ILE:HD12	2:B:992:ILE:HA	2.00	0.44
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.76	0.44
1:A:403:LYS:HB3	1:A:403:LYS:HE3	1.74	0.44
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	2.00	0.44
2:B:393:LYS:HA	2:B:393:LYS:HD3	1.83	0.44
2:B:816:GLU:O	8:J:56:LEU:HD21	2.18	0.44
2:B:1159:ARG:NH1	2:B:1175:LEU:HD11	2.26	0.44
1:A:579:SER:HB3	1:A:611:GLN:HA	1.99	0.44
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.99	0.44
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.18	0.44
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.32	0.44
2:B:1037:LEU:HD21	8:J:44:TYR:HD2	1.82	0.44
3:C:17:ASN:HB3	3:C:233:GLU:HG3	1.99	0.44
3:C:46:ILE:HA	3:C:159:ALA:HA	2.00	0.44
6:H:30:SER:OG	6:H:33:GLN:O	2.36	0.44
6:H:31:THR:C	6:H:33:GLN:H	2.21	0.44
1:A:449:SER:O	2:B:1133:MET:HG2	2.18	0.44
1:A:731:ARG:HA	1:A:731:ARG:HD3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:947:GLY:HA3	2:B:970:THR:OG1	2.18	0.44
2:B:493:SER:HA	2:B:751:VAL:HG11	1.99	0.43
2:B:776:GLN:OE1	2:B:1097:HIS:NE2	2.50	0.43
2:B:1123:SER:OG	12:T:23:DC:OP2	2.35	0.43
1:A:274:ILE:HD12	1:A:274:ILE:HA	1.85	0.43
1:A:688:LYS:HD3	1:A:688:LYS:HA	1.83	0.43
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.99	0.43
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.19	0.43
1:A:849:MET:HB2	1:A:1063:MET:SD	2.59	0.43
1:A:122:MET:O	1:A:126:LEU:HG	2.18	0.43
1:A:767:GLN:NE2	1:A:774:ARG:HG2	2.32	0.43
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.18	0.43
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	2.00	0.43
2:B:299:GLU:OE1	2:B:572:HIS:HB3	2.18	0.43
2:B:465:ASN:O	2:B:467:GLY:N	2.51	0.43
6:H:38:LEU:HD12	6:H:123:MET:CE	2.47	0.43
1:A:208:LEU:HD23	1:A:235:ILE:HD11	2.00	0.43
1:A:501:LEU:HD13	1:A:501:LEU:HA	1.86	0.43
1:A:1068:ALA:O	1:A:1072:ILE:HG13	2.18	0.43
1:A:1107:VAL:HG22	1:A:1383:SER:HB3	2.00	0.43
2:B:209:GLU:O	2:B:483:LEU:N	2.41	0.43
2:B:283:VAL:HG11	2:B:318:VAL:HA	2.00	0.43
2:B:539:LEU:H	2:B:539:LEU:HD23	1.83	0.43
2:B:957:ASN:OD1	2:B:960:GLY:N	2.51	0.43
2:B:1162:ILE:HD13	2:B:1194:ILE:HD13	2.00	0.43
3:C:219:PHE:CE2	3:C:221:TYR:HA	2.53	0.43
6:H:103:LYS:HA	6:H:103:LYS:HD2	1.73	0.43
1:A:328:ARG:NE	2:B:1206:GLU:OE1	2.52	0.43
1:A:675:THR:O	1:A:679:ILE:HG13	2.19	0.43
3:C:246:ARG:O	3:C:250:THR:OG1	2.25	0.43
7:I:94:ASP:OD1	7:I:94:ASP:N	2.51	0.43
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.48	0.43
1:A:886:ILE:HG22	1:A:952:ALA:HB2	1.99	0.43
2:B:590:HIS:NE2	2:B:592:ASN:O	2.43	0.43
1:A:259:GLU:OE1	1:A:260:ASP:N	2.51	0.43
1:A:567:LYS:HB3	1:A:568:PRO:HD3	2.01	0.43
1:A:698:GLN:HA	7:I:97:MET:O	2.19	0.43
1:A:870:GLU:OE2	1:A:1365:TYR:OH	2.28	0.43
1:A:1017:LEU:HA	1:A:1017:LEU:HD23	1.76	0.43
2:B:640:VAL:HA	2:B:651:LEU:HA	2.00	0.43
3:C:115:SER:HB3	3:C:142:VAL:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:SER:OG	3:C:141:GLY:HA3	2.19	0.43
13:N:4:DC:H2"	13:N:5:DT:H5"	2.01	0.43
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.34	0.43
2:B:216:GLU:OE1	2:B:500:THR:OG1	2.36	0.43
2:B:483:LEU:HD21	2:B:491:THR:HG23	1.99	0.43
2:B:1053:GLU:CD	2:B:1067:ARG:HH12	2.22	0.43
2:B:852:ARG:HD2	2:B:973:ILE:HG22	2.00	0.43
3:C:104:PHE:HD2	3:C:106:GLU:HG3	1.83	0.43
4:E:28:TYR:CZ	4:E:78:LEU:HB2	2.53	0.43
6:H:102:TYR:CE2	6:H:117:SER:HB2	2.53	0.43
9:K:55:LYS:O	9:K:78:THR:OG1	2.35	0.43
1:A:113:LEU:HG	1:A:115:LEU:O	2.19	0.43
2:B:46:GLN:OE1	2:B:47:GLN:HG2	2.19	0.43
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.32	0.43
1:A:181:LEU:HB2	1:A:202:LEU:HD13	2.01	0.42
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.81	0.42
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.51	0.42
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.54	0.42
2:B:298:LEU:O	2:B:302:CYS:N	2.44	0.42
2:B:1104:HIS:CD2	2:B:1122:ARG:HG3	2.54	0.42
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.48	0.42
7:I:69:PRO:O	7:I:84:VAL:HG23	2.19	0.42
1:A:9:ALA:HB1	2:B:1191:ILE:HD13	2.00	0.42
2:B:839:MET:HG2	2:B:989:THR:O	2.20	0.42
2:B:1084:GLN:NE2	3:C:190:ASP:O	2.45	0.42
6:H:112:ILE:HG22	6:H:127:GLY:O	2.19	0.42
12:T:7:DA:C6	12:T:8:DT:C4	3.07	0.42
1:A:598:LEU:HB3	6:H:25:ARG:NH1	2.34	0.42
2:B:373:ARG:HA	2:B:566:LEU:HD23	2.01	0.42
2:B:451:LYS:O	2:B:455:SER:CB	2.67	0.42
2:B:680:THR:N	2:B:683:SER:OG	2.53	0.42
2:B:859:TYR:O	2:B:965:LYS:HA	2.19	0.42
2:B:1079:LYS:HA	3:C:180:TYR:OH	2.19	0.42
1:A:974:ASP:OD1	1:A:974:ASP:N	2.51	0.42
1:A:1140:HIS:NE2	1:A:1272:THR:HG22	2.34	0.42
2:B:918:ILE:HG23	2:B:919:SER:H	1.84	0.42
6:H:19:ARG:HE	6:H:19:ARG:HB3	1.66	0.42
8:J:30:LEU:HD23	8:J:30:LEU:HA	1.86	0.42
1:A:152:VAL:O	1:A:162:VAL:N	2.49	0.42
1:A:471:ASN:OD1	1:A:650:GLN:NE2	2.41	0.42
1:A:1229:SER:OG	1:A:1233:ASP:OD1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:THR:O	2:B:62:ILE:HG12	2.20	0.42
2:B:271:ALA:N	2:B:280:ILE:O	2.42	0.42
2:B:872:GLU:HG2	2:B:916:THR:HB	2.00	0.42
7:I:62:ILE:HD12	7:I:62:ILE:HA	1.94	0.42
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.82	0.42
1:A:676:MET:O	1:A:680:THR:HG22	2.20	0.42
1:A:1021:LEU:HD11	1:A:1025:ARG:HH11	1.84	0.42
2:B:487:THR:HG22	2:B:489:SER:H	1.84	0.42
4:E:59:SER:HB2	4:E:79:TRP:CH2	2.54	0.42
2:B:274:PRO:HG2	2:B:359:GLU:HB3	2.01	0.42
1:A:599:SER:HB2	1:A:614:PHE:CE2	2.55	0.42
4:E:20:LYS:HB3	4:E:35:VAL:HG22	2.02	0.42
5:F:79:ARG:NH2	5:F:150:GLU:OE1	2.51	0.42
1:A:50:ILE:HD13	1:A:52:GLY:HA3	2.02	0.42
1:A:1313:LEU:HD23	1:A:1313:LEU:HA	1.83	0.42
2:B:432:MET:O	2:B:436:VAL:HG22	2.20	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	2.02	0.42
2:B:1081:LEU:HD23	2:B:1081:LEU:HA	1.87	0.42
10:L:55:ILE:HD12	10:L:55:ILE:O	2.20	0.42
12:T:12:DC:H4'	12:T:13:DA:OP1	2.20	0.42
13:N:7:DA:H4'	13:N:8:DT:OP1	2.20	0.42
1:A:31:SER:OG	1:A:32:VAL:N	2.53	0.41
1:A:71:GLN:NE2	2:B:1176:ASN:HB3	2.35	0.41
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.41
1:A:1215:ARG:NH1	1:A:1273:LEU:HA	2.35	0.41
1:A:1397:LEU:HA	1:A:1400:CYS:SG	2.60	0.41
2:B:791:THR:O	2:B:857:ARG:HA	2.20	0.41
2:B:878:GLN:O	2:B:882:THR:OG1	2.29	0.41
3:C:176:ILE:HA	3:C:231:ASN:O	2.19	0.41
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.02	0.41
1:A:834:THR:HG21	1:A:1077:THR:HG22	2.02	0.41
1:A:864:ILE:HG21	1:A:1374:VAL:HG23	2.02	0.41
1:A:1342:GLU:OE1	4:E:200:ARG:NH2	2.53	0.41
2:B:50:SER:HB2	2:B:408:LEU:HD23	2.02	0.41
2:B:634:TYR:HA	2:B:694:ASP:HA	2.02	0.41
3:C:149:LYS:HE3	3:C:149:LYS:HB3	1.93	0.41
6:H:46:LEU:HD23	6:H:46:LEU:HA	1.88	0.41
1:A:446:ARG:HD3	1:A:487:MET:HG2	2.02	0.41
1:A:592:ASP:HB2	1:A:604:GLY:H	1.86	0.41
1:A:1126:ALA:HA	1:A:1304:TRP:CD1	2.55	0.41
2:B:273:LEU:HB2	2:B:276:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:ASP:OD1	2:B:896:ASP:N	2.43	0.41
6:H:30:SER:OG	6:H:36:CYS:O	2.28	0.41
7:I:34:TYR:CE2	7:I:36:GLU:HB2	2.47	0.41
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.56	0.41
1:A:618:GLU:OE2	1:A:620:LYS:NZ	2.34	0.41
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.53	0.41
2:B:1081:LEU:HD13	2:B:1085:ILE:HD11	2.03	0.41
4:E:64:PRO:HG3	4:E:76:GLY:HA2	2.02	0.41
1:A:11:LEU:HA	2:B:1193:GLN:O	2.20	0.41
1:A:42:ASP:HA	1:A:50:ILE:HG13	2.03	0.41
1:A:50:ILE:HD12	1:A:50:ILE:O	2.20	0.41
1:A:471:ASN:ND2	1:A:650:GLN:OE1	2.47	0.41
1:A:881:GLN:NE2	1:A:958:VAL:O	2.41	0.41
1:A:1019:CYS:CB	1:A:1023:ARG:HH21	2.33	0.41
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	2.02	0.41
2:B:1050:ILE:HD13	2:B:1050:ILE:HA	1.81	0.41
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.20	0.41
3:C:43:THR:HG21	3:C:172:PRO:HB3	2.03	0.41
3:C:62:PHE:CE2	3:C:66:ARG:HD2	2.54	0.41
1:A:591:PHE:HB3	1:A:595:THR:HB	2.02	0.41
1:A:781:ASP:OD2	7:I:91:ARG:NH1	2.53	0.41
1:A:963:ILE:HD11	1:A:1052:GLN:OE1	2.20	0.41
1:A:1387:HIS:NE2	13:N:2:DT:OP1	2.53	0.41
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.54	0.41
2:B:368:GLU:OE1	2:B:368:GLU:N	2.54	0.41
2:B:666:TYR:O	2:B:668:ASP:N	2.53	0.41
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.85	0.41
2:B:1106:ARG:NH1	2:B:1125:ASP:O	2.54	0.41
9:K:19:LEU:HD23	9:K:19:LEU:HA	1.77	0.41
9:K:19:LEU:HD21	9:K:35:PHE:CD2	2.56	0.41
1:A:525:GLN:OE1	2:B:836:GLU:HG2	2.21	0.41
1:A:573:SER:O	1:A:577:ILE:HG22	2.21	0.41
2:B:860:MET:SD	2:B:861:ASP:N	2.94	0.41
2:B:942:ARG:HD3	2:B:942:ARG:HA	1.79	0.41
1:A:40:THR:HA	1:A:53:LEU:HD13	2.02	0.41
1:A:151:ASP:CG	1:A:163:SER:HA	2.40	0.41
1:A:840:ARG:HH12	1:A:1106:ASN:HD21	1.69	0.41
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.50	0.41
1:A:1384:VAL:HA	1:A:1389:PHE:CD2	2.56	0.41
2:B:46:GLN:HB2	2:B:408:LEU:HD21	2.02	0.41
2:B:60:GLN:OE1	2:B:95:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.03	0.41
2:B:322:PHE:CZ	7:I:30:ARG:HD2	2.56	0.41
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	2.03	0.41
2:B:1158:PHE:CD2	2:B:1160:VAL:HG22	2.56	0.41
3:C:73:GLN:HE22	3:C:75:MET:HB2	1.86	0.41
6:H:25:ARG:NH2	6:H:41:ASP:OD2	2.53	0.41
6:H:94:ASP:N	6:H:94:ASP:OD1	2.51	0.41
7:I:92:ARG:HH11	7:I:93:LYS:NZ	2.18	0.41
12:T:6:DG:C2	12:T:7:DA:C5	3.09	0.41
13:N:9:DC:H2''	13:N:10:DG:C8	2.55	0.41
1:A:57:ARG:CB	1:A:68:GLN:HB3	2.50	0.41
1:A:327:ALA:HA	1:A:330:LYS:HB3	2.03	0.41
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.03	0.41
1:A:826:ASP:OD2	1:A:830:LYS:NZ	2.54	0.41
1:A:868:TYR:O	1:A:872:GLY:N	2.46	0.41
1:A:1300:LYS:O	1:A:1300:LYS:HG3	2.21	0.41
2:B:841:MET:SD	2:B:846:ILE:HD11	2.61	0.41
3:C:10:ILE:HG21	9:K:112:GLN:HG3	2.03	0.41
6:H:142:LEU:HD22	6:H:144:ILE:CD1	2.50	0.41
1:A:11:LEU:HA	2:B:1193:GLN:HB3	2.02	0.40
1:A:115:LEU:HD13	1:A:115:LEU:HA	1.94	0.40
1:A:284:ALA:HB1	1:A:285:PRO:HD2	2.02	0.40
1:A:441:PRO:HG2	1:A:498:ARG:HG2	2.02	0.40
1:A:908:LEU:HD12	1:A:983:ILE:HD11	2.03	0.40
1:A:1214:GLU:HA	1:A:1217:LYS:HD3	2.04	0.40
1:A:1271:ILE:HG22	1:A:1273:LEU:HD23	2.03	0.40
6:H:39:THR:O	6:H:123:MET:HA	2.21	0.40
1:A:973:ILE:HD11	1:A:1038:THR:HG23	2.02	0.40
1:A:1134:ILE:O	1:A:1138:ILE:HB	2.22	0.40
1:A:1392:SER:HB2	1:A:1394:THR:HG23	2.03	0.40
3:C:33:LEU:HA	3:C:36:VAL:HG12	2.03	0.40
12:T:7:DA:H2'	12:T:8:DT:H6	1.87	0.40
2:B:408:LEU:HD12	2:B:408:LEU:HA	1.83	0.40
2:B:651:LEU:HD13	2:B:653:VAL:HG23	2.03	0.40
2:B:1031:LEU:HD13	2:B:1055:ILE:HD12	2.03	0.40
4:E:135:PHE:CD2	4:E:140:LEU:HD11	2.56	0.40
5:F:135:ARG:HA	5:F:144:GLU:O	2.22	0.40
6:H:78:SER:OG	6:H:79:TRP:N	2.55	0.40
1:A:407:ARG:HD2	1:A:430:TRP:CH2	2.56	0.40
1:A:1053:PHE:O	1:A:1057:VAL:HG23	2.21	0.40
2:B:282:ILE:H	2:B:282:ILE:HG12	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:O	1:A:199:LEU:HG	2.22	0.40
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.56	0.40
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.57	0.40
1:A:870:GLU:OE1	4:E:202:SER:HB2	2.22	0.40
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.57	0.40
2:B:428:ILE:HD11	2:B:448:ILE:CD1	2.52	0.40
2:B:757:PRO:HG3	2:B:1028:GLU:OE1	2.22	0.40
6:H:130:ARG:H	6:H:130:ARG:CD	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1370/1733 (79%)	1258 (92%)	112 (8%)	0	100	100
2	B	1103/1224 (90%)	1026 (93%)	77 (7%)	0	100	100
3	C	265/318 (83%)	250 (94%)	15 (6%)	0	100	100
4	E	210/215 (98%)	196 (93%)	14 (7%)	0	100	100
5	F	84/155 (54%)	76 (90%)	8 (10%)	0	100	100
6	H	129/146 (88%)	118 (92%)	11 (8%)	0	100	100
7	I	116/122 (95%)	107 (92%)	9 (8%)	0	100	100
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100	100
10	L	41/70 (59%)	38 (93%)	3 (7%)	0	100	100
All	All	3493/4173 (84%)	3233 (93%)	260 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1192/1520 (78%)	1145 (96%)	47 (4%)	32	65
2	B	955/1061 (90%)	925 (97%)	30 (3%)	40	71
3	C	235/274 (86%)	229 (97%)	6 (3%)	46	74
4	E	193/197 (98%)	182 (94%)	11 (6%)	20	55
5	F	73/137 (53%)	71 (97%)	2 (3%)	44	73
6	H	116/128 (91%)	110 (95%)	6 (5%)	23	58
7	I	110/116 (95%)	103 (94%)	7 (6%)	17	52
8	J	60/65 (92%)	57 (95%)	3 (5%)	24	59
9	K	99/102 (97%)	92 (93%)	7 (7%)	14	48
10	L	37/57 (65%)	35 (95%)	2 (5%)	22	57
All	All	3070/3657 (84%)	2949 (96%)	121 (4%)	32	65

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	23	SER
1	A	68	GLN
1	A	74	MET
1	A	81	PHE
1	A	85	ASP
1	A	92	HIS
1	A	108	MET
1	A	121	LEU
1	A	149	GLU
1	A	164	ARG
1	A	167	CYS
1	A	185	TRP
1	A	234	MET
1	A	307	ASP
1	A	383	TYR

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Mol	Chain	Res	Type
1	A	397	ASN
1	A	444	PHE
1	A	446	ARG
1	A	515	GLN
1	A	584	ASN
1	A	593	GLU
1	A	602	ASP
1	A	618	GLU
1	A	668	ASP
1	A	688	LYS
1	A	755	PHE
1	A	764	CYS
1	A	816	HIS
1	A	821	ARG
1	A	847	ASP
1	A	920	LEU
1	A	949	ASP
1	A	1017	LEU
1	A	1025	ARG
1	A	1036	ARG
1	A	1100	ARG
1	A	1109	LYS
1	A	1205	LYS
1	A	1274	ARG
1	A	1293	SER
1	A	1313	LEU
1	A	1358	SER
1	A	1366	ARG
1	A	1386	ARG
1	A	1418	LEU
1	A	1442	ASP
2	B	46	GLN
2	B	60	GLN
2	B	188	ASP
2	B	199	MET
2	B	241	ARG
2	B	250	PHE
2	B	309	GLN
2	B	348	ARG
2	B	370	PHE
2	B	398	ARG
2	B	401	PHE

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Mol	Chain	Res	Type
2	B	404	LYS
2	B	533	CYS
2	B	539	LEU
2	B	621	GLU
2	B	654	ARG
2	B	692	TYR
2	B	696	GLU
2	B	724	ASP
2	B	797	TYR
2	B	894	ASP
2	B	931	TYR
2	B	987	LYS
2	B	999	MET
2	B	1020	ARG
2	B	1025	HIS
2	B	1130	PHE
2	B	1163	CYS
2	B	1215	ARG
2	B	1220	ARG
3	C	40	GLU
3	C	73	GLN
3	C	95	CYS
3	C	107	SER
3	C	178	PHE
3	C	234	SER
4	E	29	PHE
4	E	48	ASP
4	E	72	PHE
4	E	83	CYS
4	E	110	PHE
4	E	112	TYR
4	E	113	GLN
4	E	157	SER
4	E	167	ARG
4	E	177	ARG
4	E	202	SER
5	F	111	LEU
5	F	140	ASP
6	H	16	ASP
6	H	47	PHE
6	H	91	ASP
6	H	128	ASN

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Mol	Chain	Res	Type
6	H	130	ARG
6	H	137	GLN
7	I	4	PHE
7	I	7	CYS
7	I	8	ARG
7	I	17	ARG
7	I	29	CYS
7	I	46	HIS
7	I	91	ARG
8	J	25	LEU
8	J	45	CYS
8	J	48	ARG
9	K	14	GLU
9	K	20	LYS
9	K	61	TYR
9	K	65	HIS
9	K	71	PHE
9	K	81	TYR
9	K	114	LEU
10	L	31	CYS
10	L	51	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	767	GLN
2	B	215	GLN
2	B	1025	HIS
2	B	1104	HIS
2	B	1176	ASN
2	B	1177	HIS
4	E	104	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	6	G
11	R	8	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	$\# Z > 2$
12	WC7	T	18	12	17,23,24	1.77	3 (17%)	17,33,36	1.62	4 (23%)

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
12	WC7	T	18	12	-	1/4/21/22	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	WC7	C5-C4	4.97	1.48	1.40
12	T	18	WC7	C5-S1	-3.86	1.60	1.67
12	T	18	WC7	C1-C2	2.67	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	WC7	C3-C4-S3	-4.77	108.89	111.74
12	T	18	WC7	C6-C3-C4	2.37	113.71	108.07
12	T	18	WC7	C2-C1-N1	2.23	125.66	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	WC7	C6-C3-C2	-2.11	129.36	136.72

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	T	18	WC7	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1384/1733 (79%)	0.16	49 (3%) 44 29	40, 76, 141, 168	0
2	B	1123/1224 (91%)	0.10	28 (2%) 57 41	41, 67, 108, 132	0
3	C	267/318 (83%)	-0.03	1 (0%) 92 86	45, 66, 92, 139	0
4	E	212/215 (98%)	0.28	7 (3%) 46 31	57, 100, 135, 144	0
5	F	86/155 (55%)	0.13	1 (1%) 79 66	61, 79, 105, 118	0
6	H	133/146 (91%)	0.68	15 (11%) 5 3	73, 95, 122, 149	0
7	I	118/122 (96%)	0.26	2 (1%) 70 55	59, 83, 108, 158	0
8	J	65/70 (92%)	-0.25	0 100 100	43, 55, 79, 80	0
9	K	114/120 (95%)	-0.10	2 (1%) 68 53	51, 71, 89, 102	0
10	L	43/70 (61%)	0.62	5 (11%) 4 3	58, 110, 135, 143	0
11	R	10/10 (100%)	0.47	0 100 100	65, 74, 107, 108	0
12	T	23/29 (79%)	1.22	5 (21%) 0 0	60, 125, 295, 301	0
13	N	10/16 (62%)	1.03	0 100 100	242, 245, 263, 267	0
All	All	3588/4228 (84%)	0.15	115 (3%) 47 32	40, 74, 131, 301	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	VAL	6.2
1	A	103	CYS	6.0
1	A	173	THR	5.8
12	T	6	DG	5.7
6	H	32	THR	4.8
1	A	91	PHE	4.6
6	H	36	CYS	4.5
12	T	5	DC	4.4
1	A	275	SER	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	106	ASP	4.3
1	A	1226	VAL	4.2
2	B	1186	ASP	4.1
1	A	69	THR	4.0
1	A	169	ASN	3.6
1	A	1229	SER	3.6
6	H	28	ALA	3.6
6	H	126	GLU	3.6
1	A	178	GLY	3.5
1	A	1240	CYS	3.5
10	L	35	SER	3.4
1	A	164	ARG	3.4
1	A	68	GLN	3.2
2	B	89	GLU	3.1
6	H	127	GLY	3.1
6	H	58	THR	3.1
2	B	126	SER	3.1
2	B	354	ASP	3.0
6	H	140	ALA	3.0
6	H	133	ASN	3.0
1	A	105	CYS	2.9
2	B	897	GLY	2.9
1	A	1211	GLN	2.9
1	A	209	ASN	2.9
1	A	1227	ILE	2.9
6	H	35	GLN	2.8
1	A	273	ASN	2.8
4	E	30	ILE	2.8
4	E	31	THR	2.8
1	A	102	VAL	2.8
12	T	14	DG	2.8
2	B	246	LYS	2.8
6	H	98	TYR	2.7
1	A	130	ASP	2.7
1	A	172	PRO	2.7
1	A	112	LYS	2.7
2	B	353	LYS	2.6
1	A	1141	THR	2.6
1	A	170	THR	2.6
1	A	73	GLY	2.6
2	B	312	GLU	2.6
6	H	125	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	355	ILE	2.5
2	B	955	THR	2.5
1	A	1176	LEU	2.5
1	A	133	LYS	2.5
1	A	567	LYS	2.4
1	A	56	PRO	2.4
1	A	411	ASP	2.4
6	H	38	LEU	2.4
1	A	75	ASN	2.4
10	L	47	ARG	2.4
2	B	88	TYR	2.3
1	A	258	GLY	2.3
2	B	105	SER	2.3
4	E	58	MET	2.3
2	B	314	LEU	2.3
1	A	1123	GLY	2.3
1	A	1125	ALA	2.3
2	B	135	ARG	2.3
12	T	17	DG	2.3
7	I	31	THR	2.3
1	A	1214	GLU	2.3
2	B	1184	GLY	2.3
2	B	475	SER	2.2
12	T	15	DA	2.2
6	H	134	ASN	2.2
9	K	56	VAL	2.2
7	I	22	ASN	2.2
1	A	276	LEU	2.2
1	A	44	THR	2.2
2	B	109	THR	2.2
2	B	245	GLU	2.2
1	A	898	ARG	2.2
10	L	45	ALA	2.2
4	E	40	GLU	2.2
1	A	146	MET	2.2
4	E	117	THR	2.2
3	C	156	THR	2.1
2	B	92	PHE	2.1
10	L	34	CYS	2.1
10	L	41	SER	2.1
1	A	183	GLY	2.1
2	B	917	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	45	GLN	2.1
2	B	590	HIS	2.1
1	A	1257	ASP	2.1
2	B	69	LEU	2.1
2	B	640	VAL	2.1
2	B	111	ALA	2.1
1	A	149	GLU	2.1
1	A	226	GLU	2.1
2	B	91	SER	2.1
4	E	105	PHE	2.0
6	H	2	SER	2.0
1	A	727	ASP	2.0
1	A	118	HIS	2.0
2	B	319	GLU	2.0
6	H	22	LYS	2.0
9	K	55	LYS	2.0
1	A	277	GLU	2.0
2	B	1183	LYS	2.0
4	E	76	GLY	2.0
5	F	73	ALA	2.0
1	A	223	GLY	2.0
1	A	257	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(\AA^2)	Q<0.9
12	WC7	T	18	21/22	0.92	0.32	58,68,101,105	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
14	ZN	L	101	1/1	0.76	0.08	122,122,122,122	0
14	ZN	A	1802	1/1	0.82	0.07	129,129,129,129	0
15	MG	A	1803	1/1	0.83	0.32	51,51,51,51	0
14	ZN	A	1801	1/1	0.88	0.07	165,165,165,165	0
14	ZN	B	1301	1/1	0.92	0.08	119,119,119,119	0
14	ZN	I	201	1/1	0.97	0.08	78,78,78,78	0
14	ZN	I	202	1/1	0.97	0.06	67,67,67,67	0
14	ZN	J	101	1/1	0.98	0.14	46,46,46,46	0
14	ZN	C	401	1/1	0.99	0.06	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.