



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:08 PM UTC

PDB ID : 7KED / pdb_00007ked
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

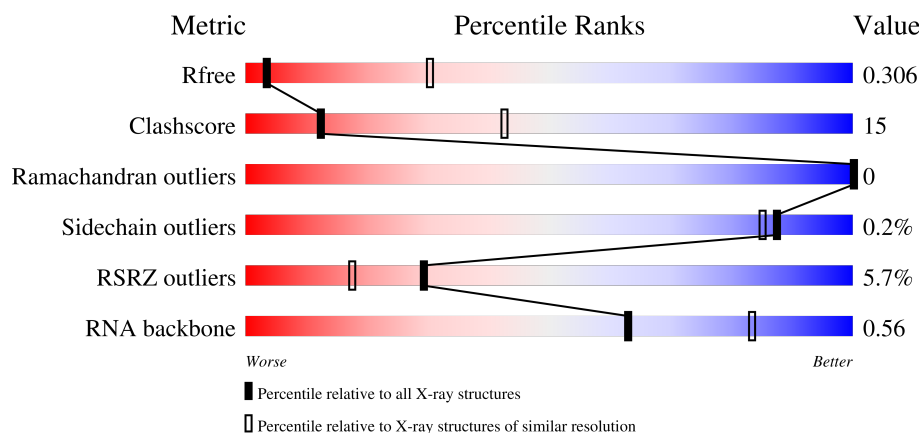
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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	5% 53% 27% 20%
2	B	1224	5% 60% 32% 8%
3	C	318	3% 58% 26% 16%
4	E	215	3% 64% 34% .

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Mol	Chain	Length	Quality of chain
5	F	155	%41%15%45%
6	H	146	6%51%40%9%
7	I	122	3%68%29%.
8	J	70	7%59%34%7%
9	K	120	4%71%24%5%
10	L	70	4%40%21%39%
11	R	10	60%40%
12	T	29	28%34%48%17%
13	N	16	6%6%56%38%

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 (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

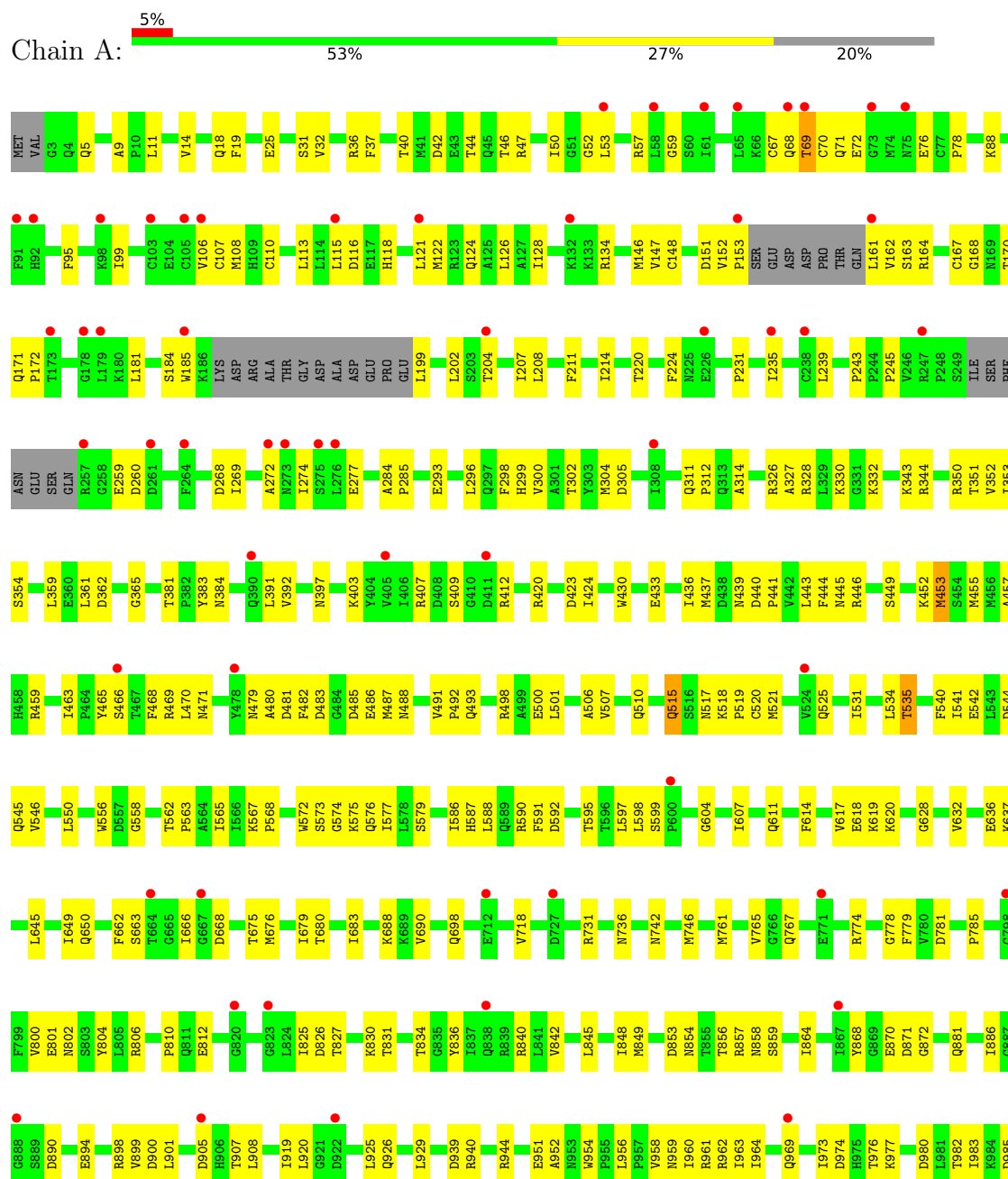
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

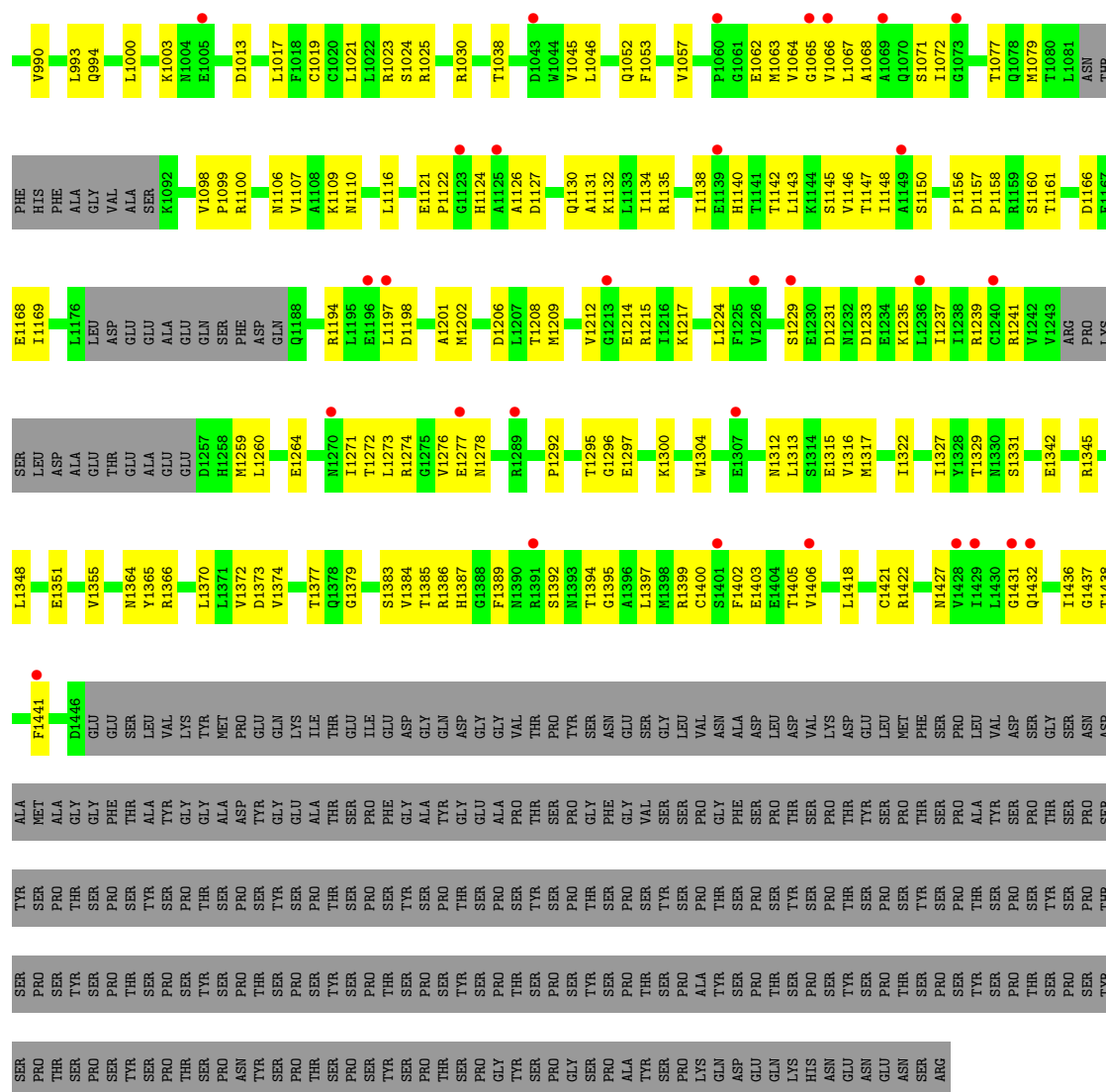
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

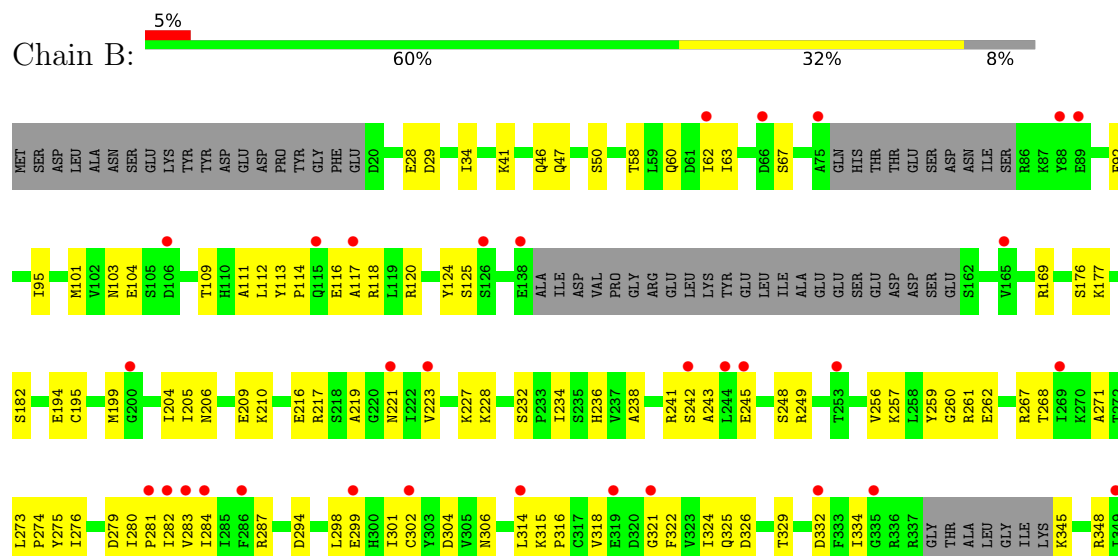
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

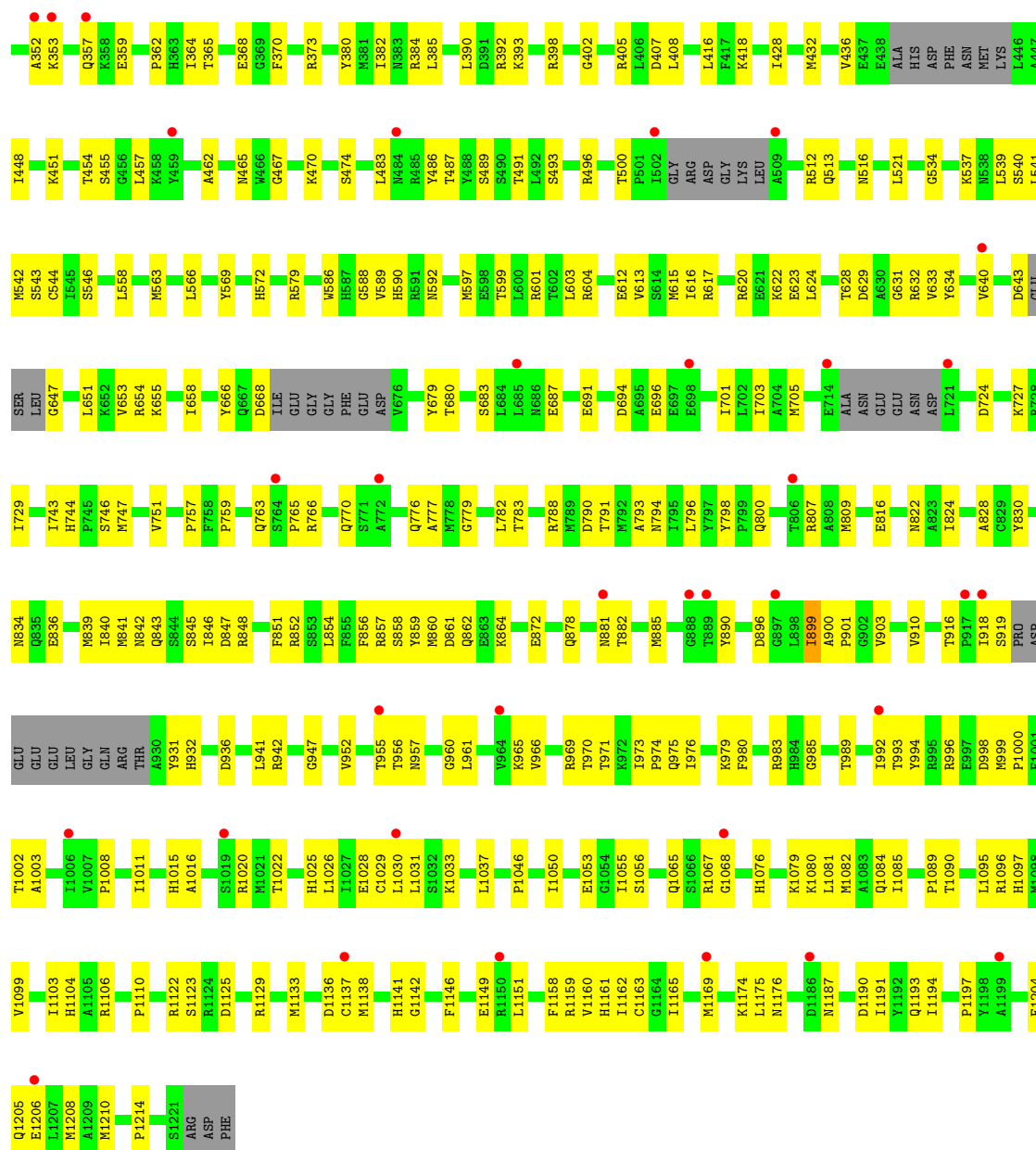
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



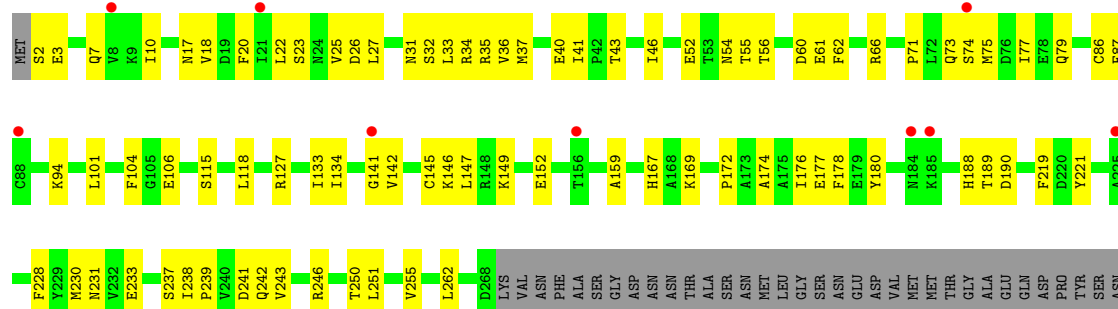


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2





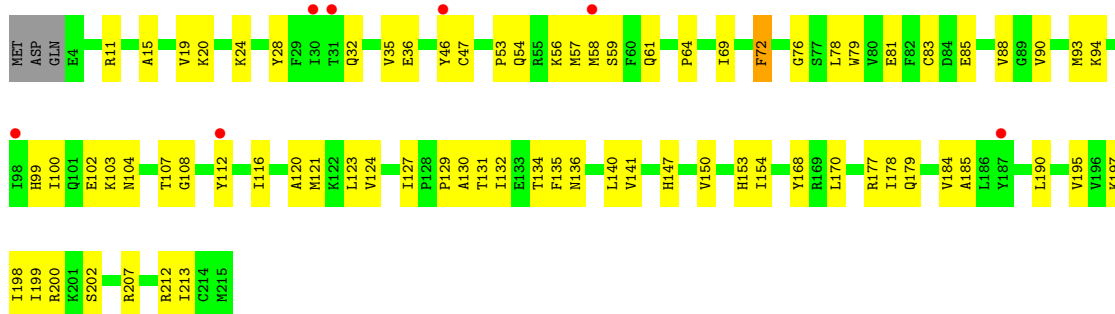
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



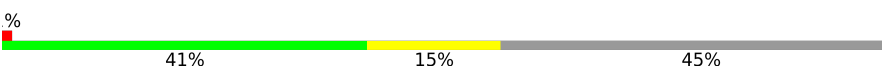
ALA
SER
GLN
MET
GLY
ASN
THR
GLY
SER
GLY
GLY
TYR
ASP
ASN
ALA
TRP

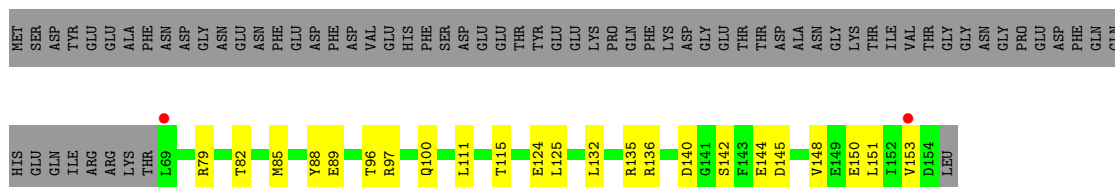
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 

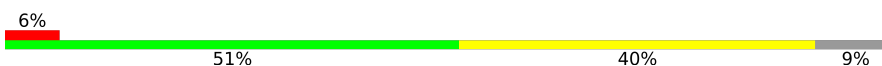


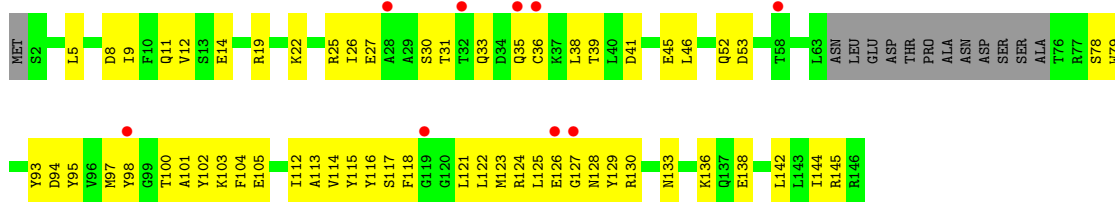
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



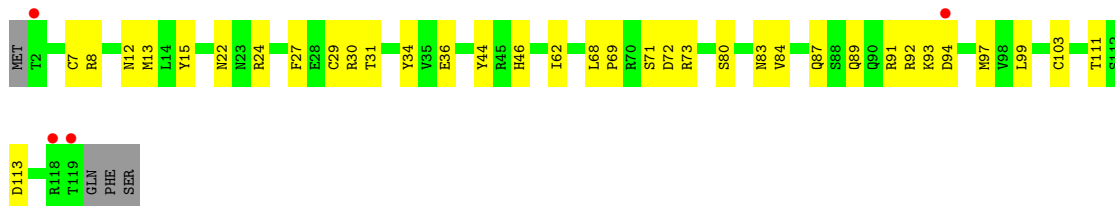
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

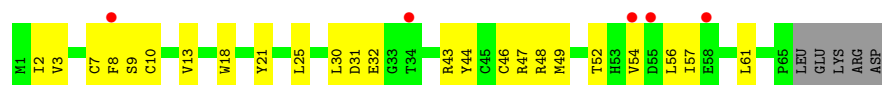


- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

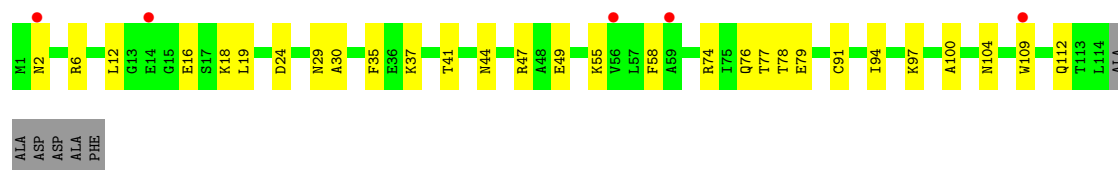
Chain I: 



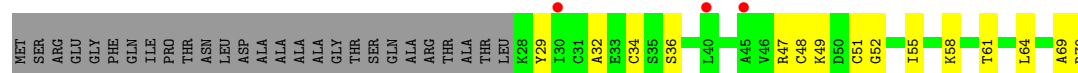
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



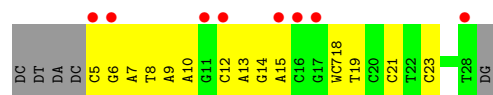
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



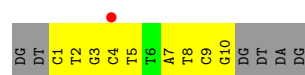
- Molecule 11: RNA



- 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 0.268 , 0.306	Depositor DCC
R_{free} test set	2000 reflections (2.24%)	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)	0.31 , 74.4	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	0.83	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	0.17	0/11012	0.40	0/14897
2	B	0.16	0/9030	0.39	0/12186
3	C	0.16	0/2139	0.38	0/2899
4	E	0.17	0/1767	0.42	0/2378
5	F	0.15	0/696	0.39	0/943
6	H	0.16	0/1082	0.45	0/1466
7	I	0.16	0/970	0.40	0/1308
8	J	0.16	0/541	0.44	0/727
9	K	0.16	0/937	0.38	0/1265
10	L	0.16	0/339	0.42	0/450
11	R	0.16	0/243	0.30	0/378
12	T	0.25	0/524	0.49	0/803
13	N	0.23	0/224	0.55	0/343
All	All	0.16	0/29504	0.40	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	360	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8859	0	8817	304	0
3	C	2101	0	2056	72	0
4	E	1731	0	1758	52	0
5	F	684	0	692	15	0
6	H	1064	0	1029	66	0
7	I	952	0	897	27	0
8	J	532	0	542	20	0
9	K	919	0	929	25	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	11	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	884	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 (884) 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:127:GLY:C	6:H:130:ARG:HH12	1.61	1.07
6:H:128:ASN:N	6:H:130:ARG:HH12	1.57	1.03
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
6:H:38:LEU:HD12	6:H:123:MET:HE2	1.57	0.86
4:E:90:VAL:HG23	4:E:123:LEU:HD11	1.56	0.86
6:H:127:GLY:C	6:H:130:ARG:NH1	2.33	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
1:A:562:THR:O	1:A:576:GLN:NE2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:7:CYS:SG	7:I:8:ARG:N	2.55	0.79
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
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.65	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:THR:HG22	1:A:1331:SER:H	1.56	0.69
2:B:542:MET:HE1	2:B:743:ILE:HG21	1.73	0.69
2:B:896:ASP:OD2	10:L:58:LYS:NZ	2.24	0.69
2:B:1103:ILE:O	2:B:1122:ARG:NH2	2.25	0.69
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
8:J:8:PHE:H	8:J:49:MET:HE3	1.64	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
9:K:91:CYS:HA	9:K:94:ILE:HD12	1.80	0.61
1:A:391:LEU:HD11	1:A:437:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.82	0.61
2:B:955:THR:OG1	2:B:956:THR:N	2.32	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
13:N:7:DA:H2"	13:N:8:DT:H71	1.82	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
2:B:195:CYS:SG	2:B:783:THR:OG1	2.56	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
2:B:1191:ILE:HD12	2:B:1191:ILE:C	2.25	0.59
3:C:46:ILE:O	3:C:169:LYS:NZ	2.33	0.59
4:E:108:GLY:N	4:E:131:THR:O	2.35	0.59
6:H:25:ARG:HH21	6:H:41:ASP:CG	2.10	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
2:B:744:HIS:ND1	2:B:746:SER:OG	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:44:THR:HG1	1:A:46:THR:HG1	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:1187:ASN:HD21	2:B:1190:ASP:C	2.15	0.55
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.89	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
4:E:46:TYR:HB2	4:E:58:MET:HE2	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:34:ILE:HG21	2:B:747:MET:HE3	1.88	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
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.16	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
7:I:13:MET:HE3	7:I:15:TYR:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:597:MET:HE3	2:B:601:ARG:HD2	1.89	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
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:343:LYS:NZ	2:B:1151:LEU:O	2.38	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
2:B:470:LYS:O	2:B:474:SER:OG	2.22	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
1:A:810:PRO:HB2	2:B:705:MET:HE3	1.90	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
1:A:1438:THR:OG1	2:B:1142:GLY:O	2.25	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
2:B:558:LEU:HB3	2:B:563:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:864:LYS:HG2	2:B:872:GLU:CD	2.35	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
6:H:30:SER:OG	6:H:36:CYS:O	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:49:GLU:OE2	9:K:97:LYS:NZ	2.27	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
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
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
1:A:827:THR:O	1:A:831:THR:OG1	2.25	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: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
2:B:878:GLN:O	2:B:882:THR:OG1	2.29	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
1:A:1202:MET:HE2	1:A:1209:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1191:ILE:C	2:B:1191:ILE:CD1	2.86	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
2:B:1169:MET:HE1	2:B:1205:GLN:HG3	1.95	0.49
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.47	0.49
2:B:744:HIS:CE1	2:B:746:SER:HG	2.28	0.49
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
1:A:1386:ARG:HE	1:A:1403:GLU:CD	2.21	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
1:A:618:GLU:OE2	1:A:620:LYS:NZ	2.34	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
6:H:31:THR:C	6:H:33:GLN:H	2.21	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:597:MET:HE1	2:B:615:MET:HB3	1.95	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:1002:THR:OG1	2:B:1003:ALA:N	2.46	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:575:LYS:O	1:A:579:SER:OG	2.32	0.48
1:A:836:TYR:CZ	1:A:840:ARG:HD3	2.49	0.48
1:A:974:ASP:OD2	1:A:977:LYS:NZ	2.32	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:7:GLN:O	3:C:23:SER:OG	2.31	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
2:B:1053:GLU:CD	2:B:1067:ARG:HH12	2.22	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:151:ASP:CG	1:A:163:SER:HA	2.40	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:33:LEU:HG	3:C:37:MET:HE2	1.98	0.45
13:N:2:DT:H2'	13:N:3:DG:N7	2.32	0.45
1:A:531:ILE:O	1:A:535:THR:OG1	2.30	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
3:C:237:SER:C	3:C:238:ILE:HD12	2.42	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
4:E:121:MET:HE1	4:E:134:THR:HG21	1.98	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:941:LEU:HD13	2:B:942:ARG:N	2.32	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
3:C:75:MET:HE1	3:C:239:PRO:HG2	1.98	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
1:A:1345:ARG:HH11	1:A:1373:ASP:CG	2.25	0.44
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.32	0.44
2:B:840:ILE:HG22	2:B:999:MET:HE1	1.99	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
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
2:B:947:GLY:HA3	2:B:970:THR:OG1	2.18	0.44
2:B:104:GLU:CD	2:B:120:ARG:HH22	2.21	0.43
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
4:E:153:HIS:C	4:E:154:ILE:HD12	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:88:LYS:HZ2	1:A:293:GLU:HB3	1.83	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:453:MET:HB2	1:A:453:MET:HE2	1.75	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
2:B:809:MET:HE1	2:B:983:ARG:HH12	1.84	0.43
3:C:115:SER:HB3	3:C:142:VAL:H	1.84	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLN:OE1	2:B:47:GLN:HG2	2.19	0.43
2:B:770:GLN:HG2	2:B:983:ARG:C	2.44	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
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:790:ASP:O	2:B:858:SER:OG	2.24	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:453:MET:HE3	1:A:520:CYS:SG	2.60	0.42
1:A:493:GLN:HB2	2:B:1149:GLU:CD	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1208:THR:OG1	1:A:1231:ASP:OD2	2.33	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
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:248:SER:HA	2:B:418:LYS:HZ1	1.85	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
2:B:896:ASP:OD1	2:B:896:ASP:N	2.43	0.41
7:I:34:TYR:CE2	7:I:36:GLU:HB2	2.47	0.41
1:A:50:ILE:HD12	1:A:50:ILE:C	2.44	0.41
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.56	0.41
2:B:885:MET:HA	2:B:885:MET:HE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:901:PRO:C	2:B:903:VAL:H	2.28	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
5:F:140:ASP:OD1	5:F:142:SER:OG	2.34	0.41
1:A:50:ILE:C	1:A:52:GLY:H	2.29	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:1259:MET:HE3	1:A:1259:MET:HB2	1.76	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
3:C:32:SER:OG	9:K:41:THR:O	2.33	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
6:H:38:LEU:CD1	6:H:123:MET:HE2	2.40	0.41
1:A:40:THR:HA	1:A:53:LEU:HD13	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:GLY:O	2:B:537:LYS:NZ	2.35	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:304:MET:HE1	2:B:1210:MET:HA	2.03	0.40
1:A:973:ILE:HD11	1:A:1038:THR:HG23	2.02	0.40
1:A:1079:MET:HE3	1:A:1079:MET:HB2	1.81	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
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)
6:H:78:SER:OG	6:H:79:TRP:N	2.55	0.40
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	1187 (100%)	5 (0%)	84	81
2	B	955/1061 (90%)	954 (100%)	1 (0%)	88	87
3	C	235/274 (86%)	235 (100%)	0	100	100
4	E	193/197 (98%)	192 (100%)	1 (0%)	81	80
5	F	73/137 (53%)	73 (100%)	0	100	100
6	H	116/128 (91%)	116 (100%)	0	100	100
7	I	110/116 (95%)	110 (100%)	0	100	100
8	J	60/65 (92%)	60 (100%)	0	100	100
9	K	99/102 (97%)	99 (100%)	0	100	100
10	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3070/3657 (84%)	3063 (100%)	7 (0%)	87	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	453	MET
1	A	515	GLN
1	A	535	THR
1	A	899	VAL
2	B	899	ILE
4	E	72	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	306	ASN
1	A	390	GLN
1	A	394	ASN

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Mol	Chain	Res	Type
1	A	654	ASN
1	A	767	GLN
1	A	851	HIS
1	A	953	ASN
1	A	1009	ASN
1	A	1128	GLN
2	B	215	GLN
2	B	465	ASN
2	B	518	HIS
2	B	734	HIS
2	B	761	HIS
2	B	1025	HIS
2	B	1104	HIS
2	B	1176	ASN
2	B	1177	HIS
2	B	1178	ASN
6	H	128	ASN
6	H	139	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	18,23,24	2.12	5 (27%)	23,33,36	1.89	6 (26%)

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	-	1/7/21/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	WC7	C3-C4	7.02	1.46	1.38
12	T	18	WC7	C4-S3	-3.26	1.67	1.72
12	T	18	WC7	C5-S1	-2.43	1.60	1.67
12	T	18	WC7	C1-C2	2.23	1.40	1.35
12	T	18	WC7	C2-C3	-2.16	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	WC7	C8-S3-C4	4.67	96.16	91.38
12	T	18	WC7	C3-C4-S3	-3.91	108.89	111.42
12	T	18	WC7	C5-C4-S3	3.74	128.97	123.13
12	T	18	WC7	C1'-N1-C1	-2.56	116.49	121.53
12	T	18	WC7	C1'-N1-C5	2.38	123.75	119.44
12	T	18	WC7	C2-C1-N1	2.35	125.66	121.84

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 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 [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%)	0.78	87 (6%) 26 16	40, 76, 141, 168	0
2	B	1123/1224 (91%)	0.77	66 (5%) 28 17	41, 67, 108, 132	0
3	C	267/318 (83%)	0.58	9 (3%) 48 27	45, 66, 92, 139	0
4	E	212/215 (98%)	0.72	7 (3%) 49 28	57, 100, 135, 144	0
5	F	86/155 (55%)	0.50	2 (2%) 61 35	61, 79, 105, 118	0
6	H	133/146 (91%)	0.81	9 (6%) 23 15	73, 95, 122, 149	0
7	I	118/122 (96%)	0.66	4 (3%) 48 27	59, 83, 108, 158	0
8	J	65/70 (92%)	0.60	5 (7%) 19 13	43, 55, 79, 80	0
9	K	114/120 (95%)	0.49	5 (4%) 39 22	51, 71, 89, 102	0
10	L	43/70 (61%)	0.87	3 (6%) 22 15	58, 110, 135, 143	0
11	R	10/10 (100%)	0.85	0 100 100	65, 74, 107, 108	0
12	T	23/29 (79%)	1.60	8 (34%) 1 1	60, 125, 295, 301	0
13	N	10/16 (62%)	1.43	1 (10%) 12 10	242, 245, 263, 267	0
All	All	3588/4228 (84%)	0.74	206 (5%) 29 17	40, 74, 131, 301	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	CYS	6.9
1	A	173	THR	4.9
1	A	727	ASP	4.4
4	E	112	TYR	4.4
1	A	1065	GLY	4.4
1	A	91	PHE	4.3
10	L	40	LEU	4.1
1	A	106	VAL	4.0
2	B	640	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	772	ALA	3.9
1	A	667	GLY	3.7
1	A	69	THR	3.7
1	A	1226	VAL	3.6
2	B	117	ALA	3.6
1	A	75	ASN	3.5
2	B	1030	LEU	3.4
1	A	867	ILE	3.4
1	A	275	SER	3.4
1	A	161	LEU	3.3
1	A	405	VAL	3.3
1	A	105	CYS	3.3
2	B	955	THR	3.2
2	B	1186	ASP	3.2
1	A	272	ALA	3.2
1	A	1406	VAL	3.1
2	B	509	ALA	3.1
4	E	31	THR	3.1
1	A	1240	CYS	3.1
2	B	1169	MET	3.1
2	B	1137	CYS	3.1
8	J	55	ASP	3.1
1	A	600	PRO	3.0
7	I	118	ARG	3.0
2	B	335	GLY	3.0
1	A	68	GLN	2.9
1	A	247	ARG	2.9
2	B	106	ASP	2.9
9	K	14	GLU	2.9
2	B	357	GLN	2.9
6	H	36	CYS	2.9
1	A	1139	GLU	2.8
1	A	58	LEU	2.8
1	A	798	GLY	2.8
2	B	286	PHE	2.8
1	A	1125	ALA	2.7
9	K	59	ALA	2.7
6	H	127	GLY	2.7
1	A	1197	LEU	2.7
2	B	897	GLY	2.7
3	C	8	VAL	2.6
1	A	664	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1229	SER	2.6
1	A	411	ASP	2.6
1	A	1432	GLN	2.6
2	B	75	ALA	2.6
3	C	184	ASN	2.6
1	A	264	PHE	2.6
3	C	156	THR	2.6
1	A	905	ASP	2.6
4	E	98	ILE	2.6
1	A	98	LYS	2.6
4	E	58	MET	2.6
1	A	1431	GLY	2.6
2	B	806	THR	2.5
1	A	1429	ILE	2.5
2	B	283	VAL	2.5
1	A	115	LEU	2.5
2	B	721	LEU	2.5
2	B	352	ALA	2.5
1	A	1123	GLY	2.5
2	B	245	GLU	2.5
2	B	299	GLU	2.5
2	B	714	GLU	2.5
8	J	58	GLU	2.5
2	B	88	TYR	2.5
4	E	46	TYR	2.5
1	A	1196	GLU	2.5
12	T	11	DG	2.5
2	B	484	ASN	2.5
9	K	2	ASN	2.5
1	A	238	CYS	2.5
2	B	284	ILE	2.5
2	B	165	VAL	2.5
9	K	56	VAL	2.5
1	A	1441	PHE	2.5
2	B	269	ILE	2.5
12	T	6	DG	2.5
6	H	32	THR	2.5
13	N	4	DC	2.5
4	E	187	TYR	2.5
2	B	502	ILE	2.4
6	H	28	ALA	2.4
1	A	1391	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	820	GLY	2.4
12	T	17	DG	2.4
2	B	1206	GLU	2.4
6	H	119	GLY	2.4
2	B	221	ASN	2.4
1	A	1060	PRO	2.4
3	C	141	GLY	2.4
2	B	244	LEU	2.4
1	A	185	TRP	2.4
9	K	109	TRP	2.4
8	J	34	THR	2.4
1	A	132	LYS	2.4
2	B	685	LEU	2.4
2	B	66	ASP	2.4
6	H	35	GLN	2.3
1	A	92	HIS	2.3
2	B	459	TYR	2.3
3	C	225	ALA	2.3
2	B	321	GLY	2.3
2	B	889	THR	2.3
2	B	764	SER	2.3
3	C	74	SER	2.3
2	B	881	ASN	2.3
1	A	204	THR	2.3
2	B	62	ILE	2.3
2	B	115	GLN	2.3
1	A	466	SER	2.3
1	A	73	GLY	2.3
2	B	917	PRO	2.3
2	B	253	THR	2.3
3	C	185	LYS	2.3
2	B	992	ILE	2.3
6	H	98	TYR	2.3
1	A	1005	GLU	2.3
1	A	1043	ASP	2.3
6	H	58	THR	2.3
12	T	15	DA	2.3
3	C	21	ILE	2.3
1	A	273	ASN	2.2
7	I	119	THR	2.2
2	B	349	ILE	2.2
2	B	302	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	153	PRO	2.2
1	A	823	GLY	2.2
1	A	969	GLN	2.2
1	A	257	ARG	2.2
2	B	138	GLU	2.2
1	A	888	GLY	2.2
12	T	5	DC	2.2
1	A	179	LEU	2.2
7	I	2	THR	2.2
1	A	1270	ASN	2.2
2	B	332	ASP	2.2
1	A	390	GLN	2.2
1	A	838	GLN	2.2
2	B	242	SER	2.2
1	A	478	TYR	2.2
5	F	153	VAL	2.2
2	B	964	VAL	2.2
1	A	1073	GLY	2.2
2	B	1068	GLY	2.2
8	J	8	PHE	2.2
7	I	94	ASP	2.1
1	A	61	ILE	2.1
10	L	30	ILE	2.1
1	A	1149	ALA	2.1
2	B	281	PRO	2.1
2	B	888	GLY	2.1
12	T	28	DT	2.1
5	F	69	LEU	2.1
1	A	1289	ARG	2.1
2	B	1150	ARG	2.1
2	B	1019	SER	2.1
4	E	30	ILE	2.1
1	A	524	VAL	2.1
2	B	223	VAL	2.1
1	A	922	ASP	2.1
1	A	65	LEU	2.1
1	A	712	GLU	2.1
2	B	89	GLU	2.1
2	B	319	GLU	2.1
12	T	16	DC	2.1
1	A	261	ASP	2.1
1	A	1236	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	314	LEU	2.1
1	A	771	GLU	2.1
1	A	1307	GLU	2.1
1	A	308	ILE	2.1
2	B	918	ILE	2.1
1	A	276	LEU	2.1
2	B	200	GLY	2.1
12	T	12	DC	2.1
1	A	235	ILE	2.1
10	L	45	ALA	2.1
1	A	1066	VAL	2.1
1	A	1213	GLY	2.0
1	A	226	GLU	2.0
2	B	282	ILE	2.0
2	B	1199	ALA	2.0
1	A	53	LEU	2.0
1	A	121	LEU	2.0
3	C	88	CYS	2.0
1	A	1428	VAL	2.0
1	A	178	GLY	2.0
2	B	353	LYS	2.0
2	B	1006	ILE	2.0
1	A	1277	GLU	2.0
2	B	698	GLU	2.0
6	H	126	GLU	2.0
1	A	1069	ALA	2.0
1	A	1401	SER	2.0
2	B	126	SER	2.0
8	J	54	VAL	2.0

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

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($\text{\AA}^2$)	Q<0.9
12	WC7	T	18	21/22	0.86	0.12	58,68,101,105	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($\text{\AA}^2$)	Q<0.9
14	ZN	A	1801	1/1	0.91	0.08	165,165,165,165	0
14	ZN	A	1802	1/1	0.94	0.07	129,129,129,129	0
14	ZN	L	101	1/1	0.94	0.10	122,122,122,122	0
14	ZN	B	1301	1/1	0.96	0.07	119,119,119,119	0
15	MG	A	1803	1/1	0.96	0.07	51,51,51,51	0
14	ZN	I	201	1/1	0.98	0.05	78,78,78,78	0
14	ZN	I	202	1/1	0.98	0.06	67,67,67,67	0
14	ZN	C	401	1/1	0.99	0.10	77,77,77,77	0
14	ZN	J	101	1/1	0.99	0.03	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.