Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 02:03 PM EDT

PDB ID	:	7RIW
Title	:	RNA polymerase II elongation complex scaffold 2, without polyamide
Authors	:	Oh, J.; Dervan, P.B.; Wang, D.
Deposited on	:	2021-07-20
Resolution	:	3.20 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:

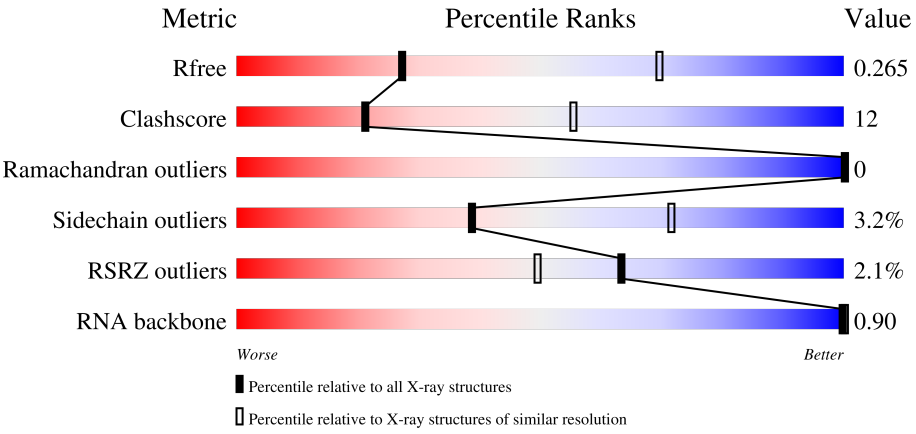
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	10	50% 40% 10%
2	T	30	7% 30% 57% 13%
3	A	1733	2% 57% 22% 20%
4	B	1224	% 63% 27% 8%

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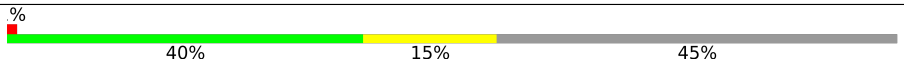
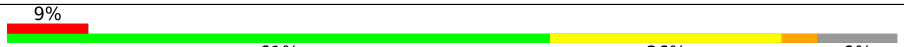
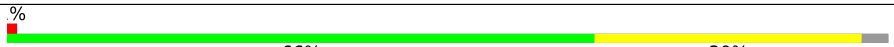
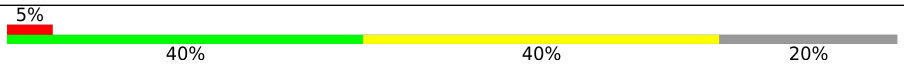
Mol	Chain	Length	Quality of chain
5	C	318	
6	E	215	
7	F	155	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	20	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29078 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			193	87	38	60	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			524	251	85	162	26			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1384	Total	C	N	O	S	0	0	0
			10827	6830	1895	2042	60			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1126	Total	C	N	O	S	0	0	0
			8871	5614	1554	1650	53			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	16	Total	C	N	O	P	0	0	0
			334	157	71	90	16			

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	R	1	Total Mg 1 1	0	0

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

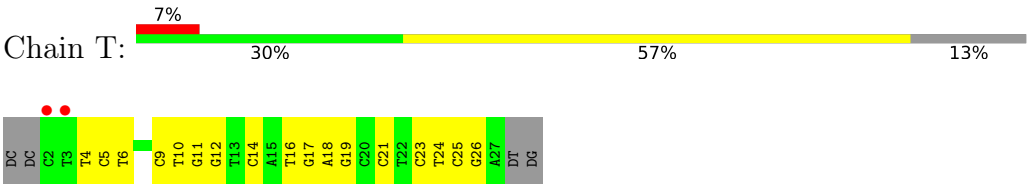
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	2	Total Zn 2 2	0	0
15	B	1	Total Zn 1 1	0	0
15	C	1	Total Zn 1 1	0	0
15	I	2	Total Zn 2 2	0	0
15	J	1	Total Zn 1 1	0	0
15	L	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

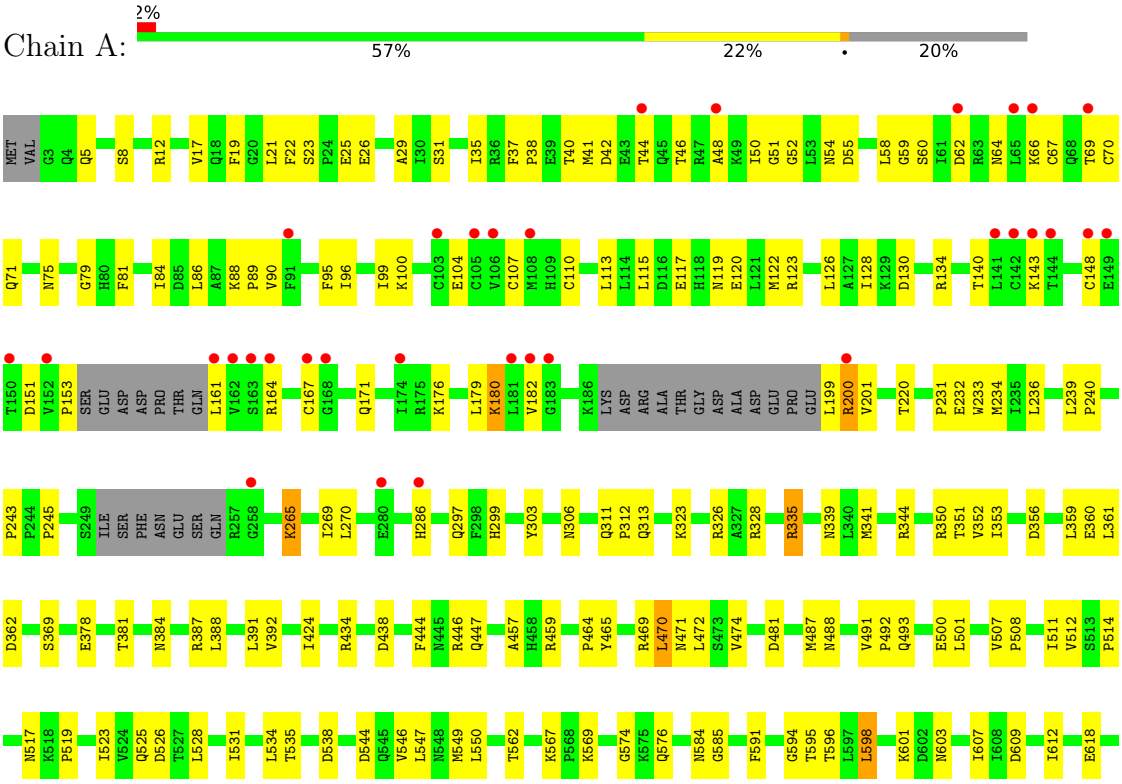
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

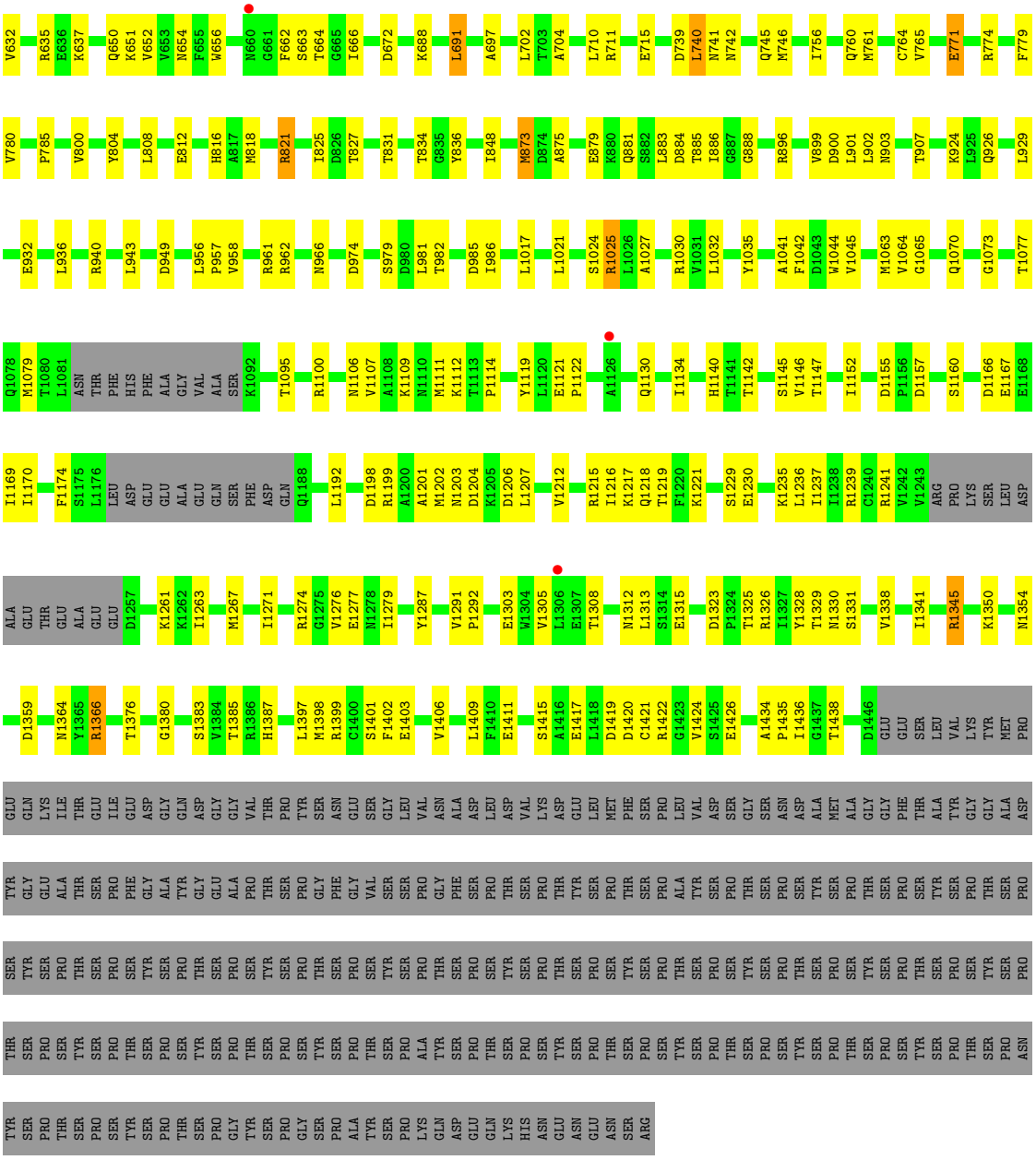
• Molecule 1: RNA

• Molecule 2: Template strand DNA



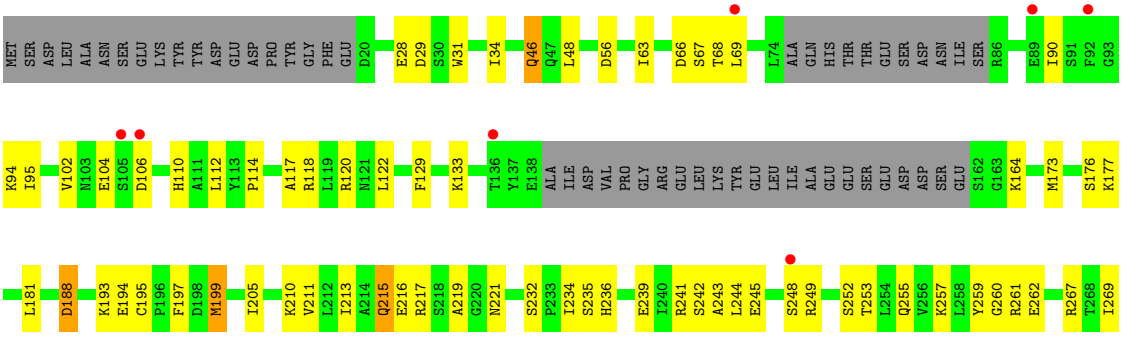
• Molecule 3: DNA-directed RNA polymerase II subunit RPB1

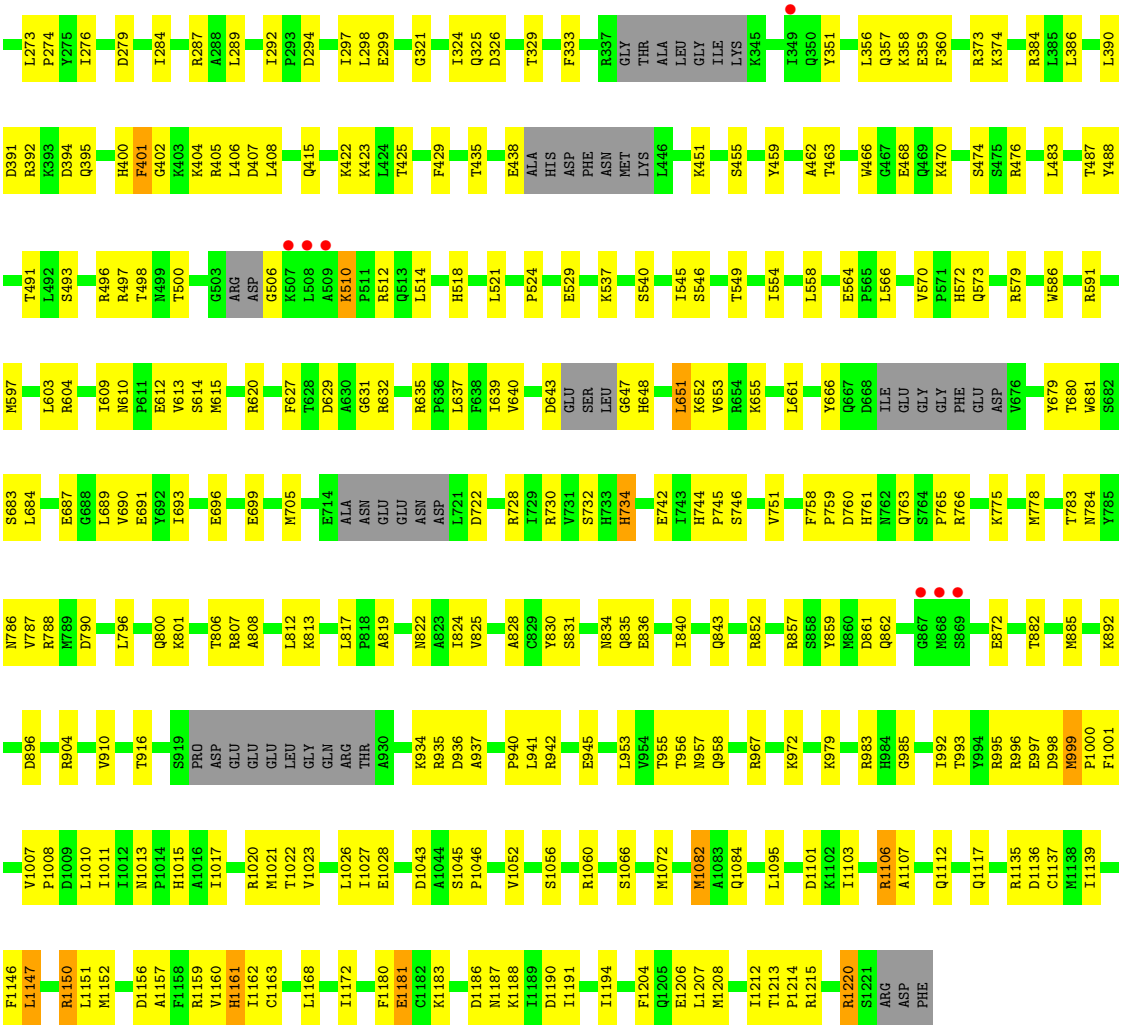




• Molecule 4: DNA-directed RNA polymerase II subunit RPB2

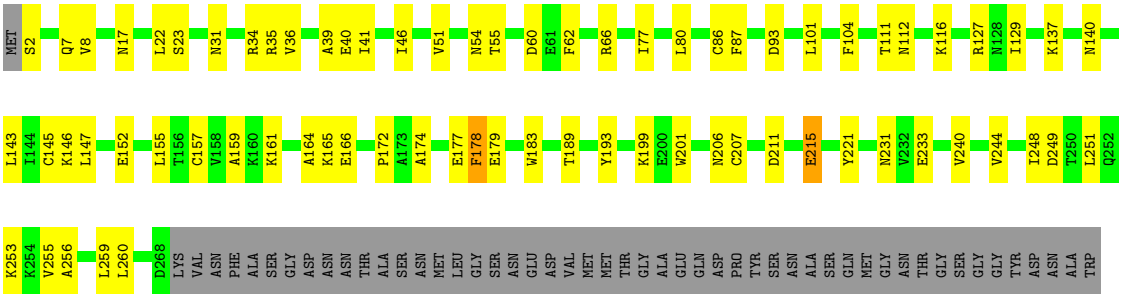
Chain B:





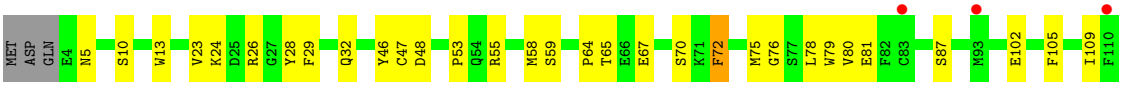
• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C:

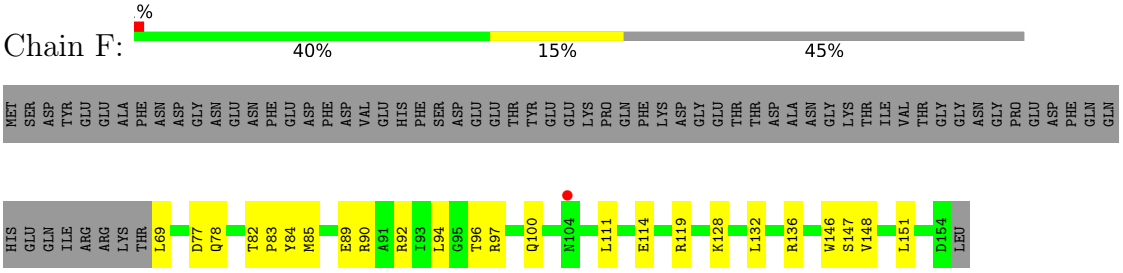


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC1

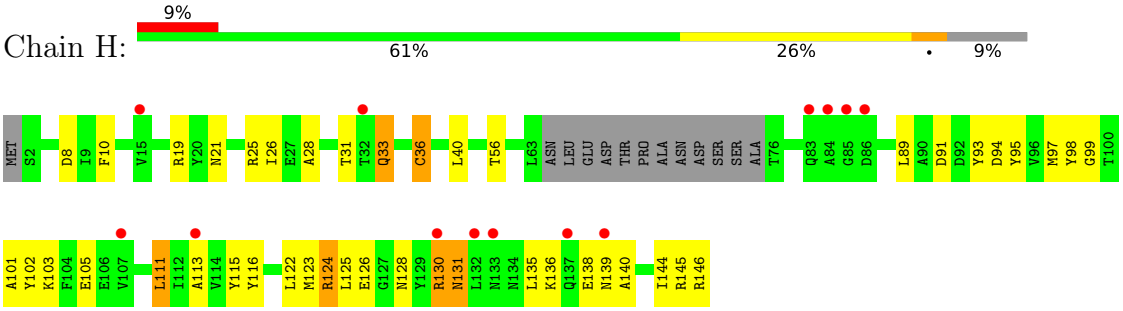
Chain E:



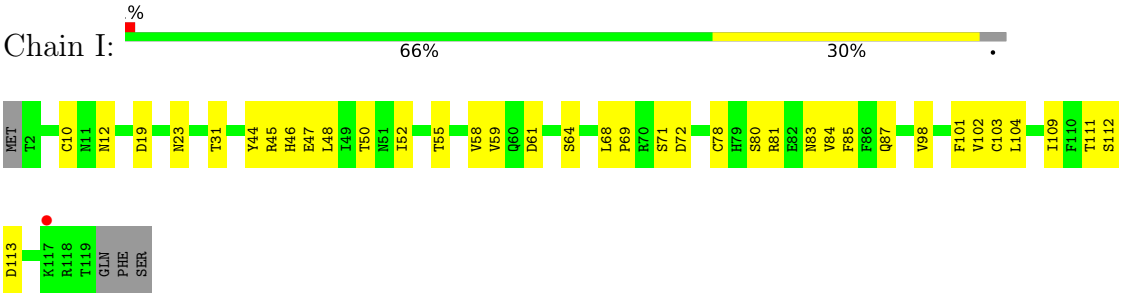
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC2



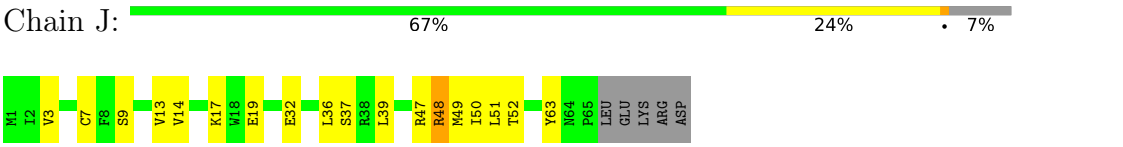
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



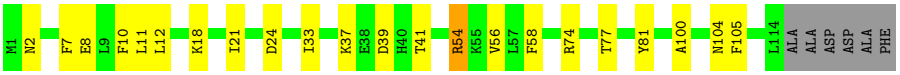
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



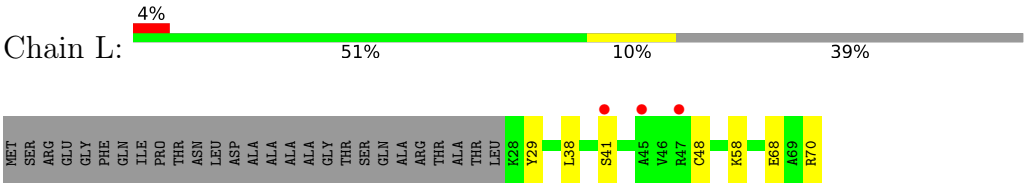
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



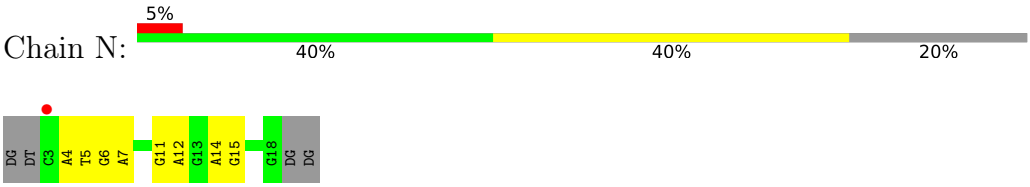
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



• Molecule 13: Non-template strand DNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	165.01Å 222.44Å 192.30Å 90.00° 99.61° 90.00°	Depositor
Resolution (Å)	47.80 – 3.20 47.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.80-3.20) 99.8 (47.81-3.20)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.228 , 0.265 0.228 , 0.265	Depositor DCC
R_{free} test set	1944 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29078	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	R	0.31	0/216	0.92	0/336
2	T	0.63	0/583	1.07	0/896
3	A	0.27	0/11019	0.45	0/14906
4	B	0.27	0/9042	0.45	0/12203
5	C	0.28	0/2139	0.45	0/2899
6	E	0.26	0/1767	0.44	0/2378
7	F	0.25	0/696	0.44	0/943
8	H	0.26	0/1082	0.48	0/1466
9	I	0.29	0/970	0.48	0/1308
10	J	0.24	0/541	0.46	0/727
11	K	0.27	0/937	0.44	0/1265
12	L	0.28	0/339	0.47	0/450
13	N	0.62	0/377	0.83	0/580
All	All	0.29	0/29708	0.49	0/40357

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	193	0	99	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	524	0	296	25	0
3	A	10827	0	10873	280	0
4	B	8871	0	8820	251	0
5	C	2101	0	2056	53	0
6	E	1731	0	1758	36	0
7	F	684	0	692	15	0
8	H	1064	0	1029	35	0
9	I	952	0	898	31	0
10	J	532	0	542	14	0
11	K	919	0	929	25	0
12	L	337	0	352	6	0
13	N	334	0	178	9	0
14	R	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	29078	0	28522	693	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 12.

All (693) 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)
3:A:1329:THR:HG22	3:A:1331:SER:H	1.09	1.10
4:B:570:VAL:HG23	4:B:573:GLN:HB2	1.43	0.98
3:A:122:MET:O	3:A:126:LEU:HD12	1.68	0.92
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.08	0.89
3:A:444:PHE:HE2	3:A:470:LEU:HD23	1.38	0.88
5:C:41:ILE:HG23	5:C:172:PRO:HG2	1.54	0.88
4:B:843:GLN:HG2	4:B:993:THR:HB	1.57	0.87
3:A:444:PHE:CZ	3:A:487:MET:SD	2.68	0.87
3:A:1329:THR:HG22	3:A:1331:SER:N	1.90	0.86
1:R:10:C:N3	2:T:19:DG:N1	2.26	0.84
3:A:122:MET:O	3:A:126:LEU:CD1	2.26	0.84
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.13	0.83
3:A:42:ASP:HA	3:A:50:ILE:HB	1.62	0.82
4:B:570:VAL:CG2	4:B:573:GLN:HB2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:10:C:O2	2:T:19:DG:N2	2.15	0.80
4:B:882:THR:HG22	4:B:934:LYS:HB2	1.66	0.78
4:B:211:VAL:HG21	4:B:483:LEU:HD23	1.66	0.77
4:B:612:GLU:O	4:B:632:ARG:NH2	2.15	0.76
3:A:444:PHE:CE2	3:A:470:LEU:HD23	2.20	0.76
2:T:14:DC:H42	13:N:6:DG:H1	1.35	0.75
3:A:1328:TYR:CZ	3:A:1350:LYS:HD2	2.20	0.75
8:H:31:THR:O	8:H:33:GLN:NE2	2.19	0.75
2:T:10:DT:H2"	2:T:11:DG:C8	2.22	0.74
3:A:335:ARG:NH1	4:B:1206:GLU:OE1	2.20	0.74
4:B:358:LYS:HG3	4:B:359:GLU:HG2	1.69	0.74
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.68	0.74
4:B:995:ARG:NH1	4:B:997:GLU:OE1	2.21	0.74
4:B:1172:ILE:HG22	4:B:1181:GLU:OE2	1.88	0.73
3:A:884:ASP:HB3	3:A:896:ARG:HH22	1.52	0.73
9:I:59:VAL:HG23	9:I:61:ASP:H	1.53	0.73
4:B:1056:SER:HB3	4:B:1066:SER:HB2	1.70	0.73
4:B:852:ARG:NH2	12:L:70:ARG:O	2.16	0.73
3:A:771:GLU:OE2	4:B:510:LYS:NZ	2.23	0.72
4:B:941:LEU:HD13	4:B:942:ARG:N	2.04	0.72
11:K:10:PHE:HD1	11:K:11:LEU:CD1	2.03	0.72
2:T:24:DT:OP1	4:B:857:ARG:NH2	2.23	0.71
3:A:326:ARG:HG3	3:A:1406:VAL:HG11	1.72	0.71
4:B:896:ASP:OD2	12:L:58:LYS:NZ	2.23	0.71
3:A:444:PHE:CE2	3:A:487:MET:SD	2.84	0.71
3:A:879:GLU:OE2	3:A:962:ARG:NH2	2.22	0.71
11:K:100:ALA:O	11:K:104:ASN:ND2	2.23	0.71
4:B:998:ASP:OD1	5:C:35:ARG:NH2	2.24	0.70
3:A:472:LEU:HD21	4:B:835:GLN:HB3	1.73	0.70
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.73	0.70
3:A:117:GLU:HG2	3:A:123:ARG:HD3	1.71	0.70
3:A:664:THR:HG21	4:B:1017:ILE:HG21	1.74	0.70
11:K:10:PHE:CD1	11:K:11:LEU:CD1	2.74	0.70
3:A:356:ASP:HB2	3:A:469:ARG:HE	1.57	0.69
6:E:127:ILE:HG22	6:E:129:PRO:HD2	1.74	0.69
3:A:353:ILE:HD13	3:A:487:MET:HG3	1.73	0.69
2:T:10:DT:O2	13:N:11:DG:N2	2.25	0.69
3:A:739:ASP:OD2	8:H:19:ARG:NH1	2.25	0.69
3:A:666:ILE:HG23	4:B:1026:LEU:HB2	1.74	0.69
3:A:1409:LEU:HD23	4:B:1207:LEU:HD21	1.75	0.69
3:A:153:PRO:HA	3:A:161:LEU:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:LEU:HB2	3:A:926:GLN:HG2	1.75	0.68
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.59	0.68
4:B:232:SER:O	4:B:261:ARG:NH2	2.25	0.68
9:I:44:TYR:HE2	9:I:46:HIS:HB2	1.59	0.68
4:B:822:ASN:O	10:J:48:ARG:NH1	2.27	0.67
3:A:29:ALA:O	4:B:1183:LYS:NZ	2.28	0.67
4:B:778:MET:O	4:B:796:LEU:HD13	1.94	0.67
3:A:134:ARG:NH2	3:A:220:THR:O	2.28	0.67
3:A:119:ASN:HB3	3:A:122:MET:HB2	1.77	0.67
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.77	0.66
4:B:287:ARG:NH2	4:B:294:ASP:OD2	2.27	0.66
10:J:9:SER:OG	10:J:48:ARG:NH2	2.28	0.66
9:I:10:CYS:SG	9:I:31:THR:OG1	2.54	0.66
4:B:882:THR:OG1	4:B:885:MET:SD	2.53	0.66
4:B:1187:ASN:ND2	4:B:1190:ASP:O	2.23	0.66
4:B:261:ARG:HE	4:B:262:GLU:HG3	1.59	0.66
4:B:287:ARG:NH1	4:B:324:ILE:O	2.29	0.66
3:A:1239:ARG:HH12	3:A:1241:ARG:HH12	1.43	0.66
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.29	0.65
3:A:873:MET:SD	3:A:873:MET:N	2.70	0.65
4:B:488:TYR:HE2	4:B:813:LYS:HB2	1.60	0.65
9:I:80:SER:OG	9:I:103:CYS:SG	2.53	0.65
3:A:525:GLN:HB2	4:B:1015:HIS:CD2	2.31	0.65
4:B:470:LYS:O	4:B:474:SER:OG	2.14	0.65
4:B:661:LEU:HD11	4:B:684:LEU:HD11	1.79	0.65
3:A:704:ALA:HB2	3:A:710:LEU:HD13	1.79	0.64
5:C:35:ARG:NH1	11:K:41:THR:OG1	2.30	0.64
4:B:213:ILE:O	4:B:215:GLN:NE2	2.29	0.64
6:E:158:SER:OG	6:E:162:ARG:NH1	2.29	0.64
3:A:1422:ARG:NH1	4:B:1220:ARG:NH1	2.45	0.64
3:A:974:ASP:O	8:H:136:LYS:NZ	2.30	0.64
3:A:761:MET:HG3	4:B:1021:MET:HG2	1.79	0.64
8:H:36:CYS:HA	8:H:126:GLU:O	1.98	0.64
3:A:1420:ASP:OD1	3:A:1422:ARG:NH2	2.30	0.64
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.80	0.64
3:A:1364:ASN:OD1	3:A:1366:ARG:NH1	2.30	0.64
13:N:5:DT:H2"	13:N:6:DG:C8	2.33	0.63
3:A:446:ARG:NH1	3:A:447:GLN:O	2.31	0.63
4:B:102:VAL:HG22	4:B:112:LEU:HB2	1.80	0.63
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.81	0.63
10:J:37:SER:OG	10:J:47:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:525:GLN:NE2	4:B:836:GLU:OE1	2.32	0.63
3:A:711:ARG:NH2	9:I:87:GLN:OE1	2.31	0.62
5:C:86:CYS:SG	5:C:87:PHE:N	2.71	0.62
4:B:483:LEU:HD11	4:B:491:THR:HG23	1.79	0.62
3:A:79:GLY:HA3	3:A:243:PRO:HG3	1.81	0.62
3:A:584:ASN:O	3:A:637:LYS:NZ	2.26	0.62
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.80	0.62
3:A:514:PRO:HB3	3:A:875:ALA:HB3	1.82	0.62
6:E:24:LYS:NZ	6:E:32:GLN:OE1	2.33	0.62
4:B:193:LYS:HB3	4:B:787:VAL:HG11	1.82	0.61
3:A:323:LYS:HE2	3:A:328:ARG:HB2	1.81	0.61
6:E:28:TYR:HE2	6:E:76:GLY:HA2	1.64	0.61
3:A:567:LYS:NZ	8:H:93:TYR:O	2.33	0.61
3:A:54:ASN:HA	3:A:58:LEU:HD12	1.83	0.61
3:A:903:ASN:O	3:A:907:THR:OG1	2.16	0.61
3:A:1239:ARG:HH22	3:A:1241:ARG:HH22	1.48	0.61
5:C:2:SER:OG	11:K:104:ASN:OD1	2.19	0.61
4:B:241:ARG:HG3	4:B:253:THR:HG22	1.83	0.61
6:E:143:ASN:ND2	6:E:145:THR:OG1	2.34	0.61
4:B:221:ASN:OD1	4:B:243:ALA:N	2.28	0.61
4:B:261:ARG:O	4:B:267:ARG:NH1	2.34	0.61
5:C:36:VAL:HG13	5:C:40:GLU:HB2	1.83	0.60
4:B:604:ARG:NH1	4:B:691:GLU:OE2	2.30	0.60
4:B:862:GLN:OE1	4:B:957:ASN:ND2	2.35	0.60
3:A:84:ILE:HD11	3:A:239:LEU:HD23	1.83	0.60
4:B:56:ASP:OD2	4:B:177:LYS:NZ	2.31	0.60
3:A:51:GLY:HA2	3:A:55:ASP:HB3	1.84	0.60
3:A:306:ASN:ND2	3:A:313:GLN:O	2.34	0.60
5:C:39:ALA:HB1	5:C:165:LYS:HG2	1.84	0.60
10:J:13:VAL:O	10:J:17:LYS:NZ	2.27	0.60
4:B:705:MET:HE2	4:B:745:PRO:HB3	1.84	0.60
12:L:68:GLU:HG2	12:L:70:ARG:H	1.67	0.60
4:B:219:ALA:HB2	4:B:405:ARG:HD3	1.84	0.59
4:B:210:LYS:HE3	4:B:462:ALA:HA	1.84	0.59
2:T:9:DC:H2"	2:T:10:DT:H5"	1.83	0.59
3:A:546:VAL:O	3:A:550:LEU:HD23	2.01	0.59
3:A:562:THR:O	3:A:576:GLN:NE2	2.35	0.59
4:B:435:THR:HG22	4:B:435:THR:O	2.02	0.59
4:B:287:ARG:HG2	4:B:292:ILE:HA	1.84	0.59
4:B:824:ILE:HG22	4:B:1008:PRO:HA	1.83	0.59
8:H:56:THR:HB	8:H:145:ARG:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:808:LEU:O	4:B:728:ARG:NH1	2.35	0.59
3:A:836:TYR:OH	3:A:1403:GLU:OE2	2.15	0.58
3:A:1398:MET:N	3:A:1426:GLU:OE2	2.37	0.58
4:B:892:LYS:NZ	4:B:904:ARG:O	2.27	0.58
4:B:680:THR:O	4:B:683:SER:OG	2.21	0.58
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.84	0.58
3:A:547:LEU:HD22	11:K:58:PHE:HD1	1.68	0.58
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.85	0.58
4:B:66:ASP:OD2	4:B:422:LYS:NZ	2.35	0.58
6:E:67:GLU:O	6:E:70:SER:OG	2.22	0.58
3:A:821:ARG:NH1	4:B:524:PRO:O	2.36	0.58
3:A:179:LEU:HD23	3:A:297:GLN:HG3	1.86	0.58
4:B:260:GLY:HA3	4:B:267:ARG:HD2	1.85	0.58
4:B:1168:LEU:HD21	4:B:1213:THR:OG1	2.03	0.58
8:H:103:LYS:HB3	8:H:115:TYR:HD1	1.69	0.58
3:A:1166:ASP:HA	3:A:1169:ILE:HD13	1.85	0.58
3:A:1276:VAL:HG12	3:A:1277:GLU:H	1.68	0.58
4:B:857:ARG:NH1	4:B:945:GLU:OE2	2.36	0.58
3:A:632:VAL:HG13	3:A:962:ARG:HD3	1.86	0.57
4:B:325:GLN:NE2	9:I:12:ASN:OD1	2.37	0.57
3:A:715:GLU:OE2	3:A:774:ARG:NH1	2.33	0.57
3:A:1345:ARG:HH11	6:E:200:ARG:NH1	2.02	0.57
5:C:51:VAL:HA	5:C:155:LEU:HB3	1.85	0.57
5:C:174:ALA:HB3	5:C:233:GLU:HG2	1.87	0.57
10:J:17:LYS:HB3	10:J:39:LEU:HD13	1.86	0.57
3:A:369:SER:OG	11:K:2:ASN:ND2	2.31	0.57
3:A:1323:ASP:OD1	3:A:1325:THR:OG1	2.18	0.57
9:I:78:CYS:SG	9:I:80:SER:OG	2.62	0.57
3:A:472:LEU:HD13	4:B:835:GLN:HE21	1.70	0.57
4:B:744:HIS:ND1	4:B:746:SER:OG	2.34	0.57
4:B:778:MET:C	4:B:796:LEU:HD13	2.24	0.57
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.86	0.57
13:N:6:DG:H2'	13:N:7:DA:C8	2.40	0.57
3:A:666:ILE:CG2	4:B:1026:LEU:HB2	2.35	0.57
4:B:834:ASN:O	4:B:1013:ASN:ND2	2.37	0.57
4:B:326:ASP:OD1	4:B:329:THR:OG1	2.14	0.57
3:A:848:ILE:HB	3:A:1065:GLY:HA3	1.87	0.57
3:A:1276:VAL:HB	3:A:1279:ILE:HD13	1.86	0.57
4:B:825:VAL:HG23	4:B:1010:LEU:HB3	1.86	0.57
3:A:50:ILE:HG23	3:A:52:GLY:H	1.70	0.56
3:A:151:ASP:OD1	3:A:164:ARG:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:517:ASN:OD1	3:A:1364:ASN:ND2	2.38	0.56
3:A:765:VAL:HG13	3:A:800:VAL:HB	1.85	0.56
3:A:873:MET:HG2	3:A:957:PRO:HG3	1.85	0.56
4:B:766:ARG:NH1	4:B:985:GLY:O	2.38	0.56
4:B:643:ASP:O	4:B:647:GLY:N	2.38	0.56
4:B:979:LYS:HG2	4:B:1095:LEU:HD12	1.87	0.56
4:B:1191:ILE:HD12	4:B:1191:ILE:O	2.06	0.56
4:B:1023:VAL:O	4:B:1027:ILE:HG13	2.06	0.56
4:B:373:ARG:HA	4:B:566:LEU:HD23	1.86	0.56
8:H:101:ALA:HB2	8:H:116:TYR:HE2	1.70	0.56
9:I:111:THR:HG22	9:I:113:ASP:H	1.70	0.56
3:A:523:ILE:HG22	3:A:528:LEU:HD13	1.87	0.56
9:I:55:THR:HG21	9:I:109:ILE:HG21	1.88	0.56
3:A:23:SER:OG	3:A:25:GLU:OE1	2.23	0.56
9:I:71:SER:OG	9:I:83:ASN:OD1	2.23	0.56
3:A:100:LYS:O	3:A:104:GLU:N	2.39	0.55
3:A:1218:GLN:OE1	3:A:1221:LYS:NZ	2.39	0.55
3:A:88:LYS:HG2	3:A:89:PRO:HD2	1.88	0.55
3:A:1329:THR:HG22	3:A:1330:ASN:N	2.21	0.55
1:R:3:C:H2'	1:R:4:G:C8	2.42	0.55
5:C:31:ASN:OD1	5:C:34:ARG:NH1	2.38	0.55
6:E:47:CYS:HA	6:E:53:PRO:HA	1.87	0.55
3:A:666:ILE:HG23	4:B:1026:LEU:CB	2.36	0.55
5:C:41:ILE:CG2	5:C:172:PRO:HG2	2.32	0.55
4:B:840:ILE:HB	4:B:1011:ILE:HB	1.87	0.55
3:A:110:CYS:HB2	3:A:167:CYS:HB2	1.88	0.55
3:A:472:LEU:HD11	4:B:835:GLN:HG3	1.87	0.55
6:E:136:ASN:OD1	6:E:138:ALA:N	2.32	0.55
2:T:16:DT:H2'	2:T:17:DG:C8	2.42	0.55
6:E:133:GLU:HB3	6:E:135:PHE:HE1	1.72	0.55
4:B:299:GLU:OE2	4:B:572:HIS:ND1	2.27	0.55
4:B:1213:THR:O	4:B:1213:THR:HG23	2.07	0.55
3:A:981:LEU:HD11	3:A:1042:PHE:HB2	1.88	0.55
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.88	0.54
4:B:118:ARG:NH2	4:B:194:GLU:OE2	2.36	0.54
4:B:235:SER:HG	4:B:236:HIS:CE1	2.25	0.54
9:I:19:ASP:O	9:I:23:ASN:N	2.41	0.54
4:B:29:ASP:OD2	4:B:655:LYS:NZ	2.39	0.54
4:B:173:MET:O	4:B:176:SER:OG	2.16	0.54
3:A:471:ASN:O	3:A:474:VAL:HG12	2.08	0.54
5:C:145:CYS:SG	5:C:146:LYS:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:44:THR:OG1	3:A:46:THR:OG1	2.24	0.54
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.90	0.54
3:A:59:GLY:HA2	3:A:67:CYS:SG	2.48	0.54
3:A:1329:THR:CG2	3:A:1331:SER:H	2.00	0.54
6:E:171:LYS:HB3	6:E:174:GLN:HG3	1.89	0.54
4:B:68:THR:HA	4:B:90:ILE:O	2.08	0.54
5:C:7:GLN:HB2	5:C:23:SER:HB2	1.90	0.54
10:J:7:CYS:HA	10:J:49:MET:HG3	1.88	0.54
3:A:306:ASN:ND2	3:A:313:GLN:OE1	2.41	0.54
4:B:287:ARG:NH1	4:B:321:GLY:O	2.40	0.54
4:B:459:TYR:O	4:B:463:THR:OG1	2.20	0.54
4:B:603:LEU:HB3	4:B:609:ILE:HG13	1.89	0.54
7:F:85:MET:HG3	7:F:89:GLU:HG3	1.90	0.54
3:A:378:GLU:OE1	3:A:434:ARG:NE	2.36	0.54
3:A:526:ASP:HB2	4:B:835:GLN:NE2	2.23	0.54
5:C:112:ASN:ND2	10:J:19:GLU:OE2	2.41	0.54
5:C:179:GLU:OE1	5:C:206:ASN:ND2	2.41	0.53
6:E:55:ARG:HA	6:E:58:MET:HG3	1.89	0.53
8:H:111:LEU:HA	8:H:128:ASN:HB2	1.90	0.53
3:A:122:MET:O	3:A:126:LEU:HD13	2.09	0.53
8:H:105:GLU:OE1	8:H:124:ARG:NH1	2.41	0.53
3:A:569:LYS:HE3	5:C:221:TYR:HD1	1.73	0.53
3:A:901:LEU:HA	3:A:907:THR:HG23	1.90	0.53
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.89	0.53
5:C:77:ILE:HG13	5:C:161:LYS:HE3	1.90	0.53
3:A:113:LEU:HD23	3:A:113:LEU:H	1.73	0.53
3:A:1130:GLN:O	3:A:1134:ILE:HG12	2.07	0.53
4:B:840:ILE:HG12	4:B:992:ILE:HG22	1.90	0.53
5:C:256:ALA:O	5:C:260:LEU:HG	2.08	0.53
4:B:1186:ASP:OD1	4:B:1188:LYS:NZ	2.37	0.53
3:A:21:LEU:HD11	3:A:95:PHE:HE1	1.73	0.53
4:B:806:THR:HG22	4:B:808:ALA:H	1.72	0.53
4:B:1043:ASP:OD1	4:B:1045:SER:OG	2.22	0.53
3:A:1411:GLU:OE2	3:A:1415:SER:OG	2.27	0.53
4:B:1060:ARG:NH2	5:C:199:LYS:O	2.38	0.53
2:T:11:DG:H2"	2:T:12:DG:H8	1.72	0.53
3:A:1215:ARG:O	3:A:1219:THR:OG1	2.24	0.53
6:E:28:TYR:HA	6:E:64:PRO:HA	1.90	0.53
3:A:1119:TYR:HB3	3:A:1326:ARG:HH11	1.72	0.52
5:C:55:THR:HG1	5:C:152:GLU:H	1.53	0.52
8:H:128:ASN:OD1	8:H:131:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:883:LEU:HD11	3:A:1017:LEU:HD21	1.90	0.52
3:A:1167:GLU:O	3:A:1170:ILE:HG12	2.07	0.52
4:B:629:ASP:O	4:B:632:ARG:NH1	2.42	0.52
3:A:881:GLN:HA	3:A:961:ARG:HH22	1.74	0.52
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.91	0.52
2:T:9:DC:H4'	2:T:10:DT:OP1	2.09	0.52
4:B:639:ILE:HD11	4:B:691:GLU:HB2	1.89	0.52
5:C:35:ARG:NH1	11:K:39:ASP:OD2	2.37	0.52
3:A:182:VAL:HG12	3:A:201:VAL:HG12	1.91	0.52
3:A:547:LEU:HD22	11:K:58:PHE:CD1	2.45	0.52
3:A:549:MET:HG2	3:A:652:VAL:HG13	1.90	0.52
4:B:788:ARG:NH1	4:B:790:ASP:OD2	2.43	0.52
6:E:161:LYS:NZ	6:E:193:GLY:O	2.39	0.52
3:A:472:LEU:CD1	4:B:835:GLN:HE21	2.22	0.52
9:I:50:THR:HG22	9:I:52:ILE:H	1.75	0.52
3:A:569:LYS:NZ	5:C:221:TYR:O	2.40	0.52
3:A:1328:TYR:OH	3:A:1350:LYS:HD2	2.08	0.52
6:E:87:SER:HA	6:E:115:ASN:HB3	1.91	0.52
6:E:147:HIS:HB3	6:E:150:VAL:HG23	1.92	0.52
11:K:10:PHE:HE1	11:K:11:LEU:HD13	1.72	0.52
4:B:637:LEU:HD12	4:B:693:ILE:HG13	1.92	0.52
4:B:679:TYR:OH	4:B:687:GLU:OE1	2.23	0.52
2:T:25:DC:H2"	2:T:26:DG:H5"	1.92	0.51
3:A:961:ARG:NH1	3:A:1025:ARG:HH22	2.08	0.51
6:E:5:ASN:O	6:E:5:ASN:ND2	2.43	0.51
3:A:38:PRO:HB3	3:A:270:LEU:HB3	1.91	0.51
3:A:128:ILE:HG23	3:A:134:ARG:HB2	1.92	0.51
3:A:881:GLN:NE2	3:A:958:VAL:O	2.31	0.51
4:B:216:GLU:OE1	4:B:500:THR:OG1	2.29	0.51
4:B:681:TRP:CH2	4:B:690:VAL:HG11	2.45	0.51
2:T:18:DA:H2'	2:T:19:DG:H8	1.75	0.51
3:A:1350:LYS:O	3:A:1354:ASN:ND2	2.37	0.51
4:B:1147:LEU:HD22	4:B:1151:LEU:CD2	2.40	0.51
3:A:491:VAL:O	4:B:1150:ARG:NH2	2.44	0.51
3:A:1313:LEU:HD12	3:A:1338:VAL:HG11	1.93	0.51
4:B:297:ILE:HG22	4:B:298:LEU:HD23	1.93	0.51
4:B:896:ASP:OD2	12:L:29:TYR:OH	2.26	0.51
6:E:10:SER:O	6:E:13:TRP:HB3	2.11	0.51
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.93	0.51
11:K:10:PHE:HD1	11:K:11:LEU:HD12	1.76	0.51
3:A:1152:ILE:HB	9:I:44:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:120:GLU:OE1	3:A:123:ARG:NH2	2.45	0.50
3:A:598:LEU:O	8:H:122:LEU:HD12	2.11	0.50
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.92	0.50
4:B:28:GLU:OE1	4:B:807:ARG:NH1	2.44	0.50
4:B:400:HIS:NE2	4:B:699:GLU:OE1	2.44	0.50
4:B:996:ARG:NH2	5:C:174:ALA:O	2.43	0.50
3:A:888:GLY:O	3:A:940:ARG:NH2	2.45	0.50
2:T:14:DC:N4	13:N:6:DG:H1	2.06	0.50
3:A:1107:VAL:HG22	3:A:1383:SER:HB3	1.93	0.50
4:B:415:GLN:OE1	4:B:476:ARG:NH1	2.38	0.50
3:A:1398:MET:O	3:A:1401:SER:OG	2.30	0.50
9:I:98:VAL:HG11	9:I:113:ASP:HB2	1.94	0.50
2:T:11:DG:H2"	2:T:12:DG:C8	2.45	0.50
3:A:1146:VAL:HG12	3:A:1201:ALA:HB1	1.93	0.50
4:B:117:ALA:HA	4:B:122:LEU:HB2	1.93	0.50
4:B:245:GLU:O	4:B:249:ARG:NH2	2.45	0.50
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.94	0.50
5:C:8:VAL:HG11	11:K:105:PHE:HD1	1.77	0.50
3:A:350:ARG:NH1	3:A:488:ASN:OD1	2.45	0.50
3:A:1063:MET:SD	3:A:1436:ILE:HD12	2.52	0.50
3:A:1142:THR:O	3:A:1145:SER:OG	2.30	0.50
4:B:129:PHE:HB3	4:B:164:LYS:HB3	1.93	0.49
4:B:1082:MET:HA	5:C:189:THR:HA	1.94	0.49
3:A:1385:THR:HG23	3:A:1387:HIS:H	1.78	0.49
3:A:62:ASP:O	3:A:64:ASN:ND2	2.45	0.49
3:A:1376:THR:HG22	6:E:212:ARG:HH12	1.77	0.49
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.93	0.49
3:A:96:ILE:HA	3:A:99:ILE:HD12	1.94	0.49
4:B:1135:ARG:NH2	4:B:1136:ASP:OD1	2.41	0.49
7:F:128:LYS:NZ	7:F:148:VAL:O	2.33	0.49
9:I:19:ASP:O	9:I:23:ASN:HA	2.12	0.49
1:R:10:C:N4	2:T:19:DG:O6	2.31	0.49
3:A:1229:SER:OG	3:A:1230:GLU:N	2.46	0.49
4:B:394:ASP:OD1	4:B:395:GLN:N	2.44	0.49
3:A:378:GLU:OE2	3:A:387:ARG:NH2	2.32	0.49
6:E:185:ALA:HA	6:E:190:LEU:HD23	1.93	0.49
3:A:351:THR:OG1	3:A:352:VAL:N	2.46	0.49
3:A:672:ASP:N	3:A:672:ASP:OD1	2.44	0.49
3:A:949:ASP:OD1	3:A:949:ASP:N	2.45	0.49
3:A:1157:ASP:OD1	3:A:1160:SER:N	2.45	0.49
4:B:800:GLN:NE2	10:J:52:THR:OG1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:538:ASP:OD2	8:H:21:ASN:N	2.36	0.49
3:A:800:VAL:HG13	3:A:812:GLU:HB3	1.95	0.49
4:B:205:ILE:HG21	4:B:462:ALA:HB2	1.95	0.49
7:F:82:THR:O	7:F:136:ARG:NH1	2.20	0.49
11:K:8:GLU:O	11:K:37:LYS:HE3	2.13	0.49
3:A:362:ASP:OD1	3:A:459:ARG:NH1	2.42	0.49
3:A:585:GLY:N	3:A:609:ASP:OD1	2.42	0.49
4:B:493:SER:OG	4:B:775:LYS:HE2	2.13	0.49
4:B:640:VAL:HA	4:B:651:LEU:HA	1.95	0.49
3:A:1206:ASP:O	3:A:1274:ARG:NH1	2.43	0.48
3:A:360:GLU:OE2	3:A:651:LYS:NZ	2.40	0.48
4:B:487:THR:HG21	4:B:819:ALA:HB2	1.94	0.48
4:B:570:VAL:HG23	4:B:570:VAL:O	2.13	0.48
4:B:652:LYS:HB3	4:B:689:LEU:HD22	1.95	0.48
4:B:759:PRO:HD2	4:B:1046:PRO:HB3	1.95	0.48
2:T:5:DC:H2"	2:T:6:DT:C6	2.48	0.48
3:A:662:PHE:O	4:B:828:ALA:HA	2.12	0.48
4:B:197:PHE:CD1	4:B:817:LEU:HD11	2.48	0.48
4:B:760:ASP:OD1	4:B:760:ASP:N	2.40	0.48
4:B:828:ALA:O	4:B:834:ASN:ND2	2.39	0.48
5:C:66:ARG:NH2	10:J:3:VAL:O	2.41	0.48
3:A:1079:MET:HA	3:A:1359:ASP:OD2	2.14	0.48
4:B:239:GLU:HG2	4:B:255:GLN:HB3	1.95	0.48
4:B:261:ARG:HG3	4:B:262:GLU:H	1.78	0.48
4:B:402:GLY:HA3	4:B:696:GLU:HG2	1.95	0.48
4:B:786:ASN:OD1	4:B:967:ARG:NH2	2.47	0.48
3:A:67:CYS:O	3:A:71:GLN:NE2	2.47	0.48
3:A:512:VAL:HA	3:A:519:PRO:HA	1.96	0.48
4:B:69:LEU:HD21	4:B:425:THR:HG23	1.95	0.48
4:B:274:PRO:HG2	4:B:359:GLU:HB3	1.96	0.48
7:F:114:GLU:OE2	7:F:119:ARG:NH2	2.46	0.48
3:A:756:ILE:O	3:A:760:GLN:HG3	2.14	0.48
4:B:1001:PHE:HE1	5:C:178:PHE:HB3	1.79	0.48
6:E:180:ARG:NH2	6:E:192:ARG:HB2	2.28	0.48
3:A:697:ALA:HA	3:A:702:LEU:HG	1.96	0.48
6:E:65:THR:HG23	6:E:67:GLU:H	1.79	0.48
8:H:113:ALA:HA	8:H:125:LEU:O	2.13	0.48
9:I:61:ASP:O	9:I:64:SER:OG	2.25	0.48
3:A:1111:MET:HG3	3:A:1114:PRO:HG3	1.96	0.48
3:A:1279:ILE:HG23	3:A:1308:THR:HB	1.96	0.48
3:A:339:ASN:HB3	4:B:1117:GLN:HE22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.96	0.47
4:B:546:SER:OG	4:B:631:GLY:N	2.46	0.47
7:F:97:ARG:HD2	7:F:97:ARG:HA	1.67	0.47
3:A:901:LEU:N	3:A:926:GLN:OE1	2.33	0.47
4:B:217:ARG:NH1	4:B:407:ASP:OD1	2.47	0.47
4:B:289:LEU:HD21	4:B:356:LEU:HD12	1.95	0.47
4:B:496:ARG:NH2	4:B:540:SER:O	2.47	0.47
5:C:215:GLU:OE1	5:C:215:GLU:N	2.46	0.47
4:B:554:ILE:O	4:B:558:LEU:HG	2.14	0.47
4:B:1152:MET:O	4:B:1157:ALA:HB2	2.13	0.47
7:F:77:ASP:OD1	7:F:78:GLN:N	2.46	0.47
3:A:232:GLU:HG3	3:A:233:TRP:CD1	2.49	0.47
3:A:508:PRO:HA	3:A:511:ILE:HG13	1.96	0.47
3:A:1212:VAL:O	3:A:1216:ILE:HG22	2.14	0.47
3:A:1041:ALA:O	3:A:1045:VAL:HG23	2.14	0.47
3:A:1235:LYS:HB3	3:A:1237:ILE:HD11	1.96	0.47
4:B:31:TRP:CE3	4:B:34:ILE:HD12	2.49	0.47
9:I:19:ASP:O	9:I:23:ASN:CA	2.63	0.47
3:A:40:THR:HG23	3:A:41:MET:H	1.79	0.47
3:A:1198:ASP:O	3:A:1202:MET:HG2	2.14	0.47
4:B:199:MET:SD	4:B:199:MET:N	2.79	0.47
7:F:97:ARG:NH1	7:F:100:GLN:OE1	2.39	0.47
1:R:3:C:H2'	1:R:4:G:H8	1.78	0.47
3:A:1140:HIS:ND1	3:A:1276:VAL:O	2.42	0.47
4:B:122:LEU:HD22	4:B:958:GLN:HG3	1.97	0.47
4:B:360:PHE:HE2	4:B:374:LYS:HB3	1.78	0.47
4:B:1213:THR:HG21	4:B:1215:ARG:NH2	2.30	0.47
5:C:46:ILE:HA	5:C:159:ALA:HA	1.96	0.47
10:J:14:VAL:HB	10:J:50:ILE:HD11	1.96	0.47
4:B:728:ARG:HD2	4:B:730:ARG:HH21	1.79	0.47
5:C:104:PHE:CD1	5:C:152:GLU:HB3	2.49	0.47
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.50	0.47
9:I:45:ARG:NH1	9:I:47:GLU:OE2	2.48	0.47
4:B:1147:LEU:HD22	4:B:1151:LEU:HD22	1.97	0.47
1:R:2:U:H2'	1:R:3:C:C6	2.50	0.47
3:A:86:LEU:HD21	3:A:239:LEU:HB2	1.97	0.47
3:A:424:ILE:HD12	3:A:424:ILE:O	2.15	0.47
4:B:620:ARG:NH1	9:I:68:LEU:HD21	2.29	0.47
4:B:1020:ARG:HB2	4:B:1022:THR:HG23	1.97	0.47
5:C:80:LEU:HD22	5:C:129:ILE:HD12	1.97	0.47
3:A:231:PRO:HA	3:A:234:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:69:LEU:HD13	4:B:429:PHE:HB2	1.97	0.46
4:B:260:GLY:HA3	4:B:267:ARG:HA	1.98	0.46
4:B:614:SER:OG	4:B:627:PHE:HB2	2.15	0.46
11:K:54:ARG:H	11:K:54:ARG:HD2	1.80	0.46
2:T:18:DA:H2'	2:T:19:DG:C8	2.50	0.46
3:A:1147:THR:HB	9:I:48:LEU:HD12	1.97	0.46
3:A:1402:PHE:O	3:A:1403:GLU:HG3	2.16	0.46
4:B:242:SER:OG	4:B:252:SER:OG	2.26	0.46
4:B:357:GLN:HA	4:B:374:LYS:NZ	2.31	0.46
4:B:778:MET:HB3	4:B:796:LEU:CD1	2.46	0.46
4:B:1106:ARG:HG3	4:B:1107:ALA:N	2.30	0.46
4:B:635:ARG:NH1	4:B:742:GLU:OE2	2.42	0.46
4:B:1084:GLN:HG2	5:C:201:TRP:CH2	2.51	0.46
3:A:199:LEU:HB3	3:A:200:ARG:H	1.52	0.46
3:A:328:ARG:HD3	4:B:1206:GLU:OE1	2.14	0.46
3:A:966:ASN:HB3	3:A:1044:TRP:HH2	1.81	0.46
4:B:401:PHE:HD2	4:B:521:LEU:HD12	1.79	0.46
4:B:488:TYR:CE2	4:B:813:LYS:HB2	2.46	0.46
5:C:244:VAL:O	5:C:248:ILE:HG13	2.16	0.46
3:A:825:ILE:HD13	4:B:512:ARG:HB2	1.98	0.46
4:B:983:ARG:NH2	4:B:1028:GLU:OE1	2.46	0.46
5:C:251:LEU:O	5:C:255:VAL:HG23	2.15	0.46
9:I:83:ASN:HA	9:I:104:LEU:HG	1.97	0.46
3:A:265:LYS:HG3	3:A:303:TYR:HB2	1.98	0.46
3:A:961:ARG:HH11	3:A:1025:ARG:HH22	1.63	0.46
5:C:249:ASP:OD2	5:C:253:LYS:NZ	2.39	0.46
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.81	0.46
2:T:21:DC:OP1	3:A:344:ARG:NH1	2.35	0.46
3:A:31:SER:O	4:B:1183:LYS:NZ	2.44	0.46
3:A:500:GLU:OE2	3:A:1438:THR:HG21	2.15	0.46
4:B:830:TYR:CZ	4:B:1000:PRO:HD3	2.50	0.46
10:J:32:GLU:OE1	10:J:32:GLU:N	2.46	0.46
3:A:464:PRO:HG2	3:A:465:TYR:HD1	1.81	0.46
3:A:741:ASN:O	3:A:745:GLN:HG3	2.16	0.46
3:A:899:VAL:HG13	3:A:929:LEU:HD13	1.98	0.46
5:C:17:ASN:HA	5:C:240:VAL:HG11	1.98	0.46
3:A:19:PHE:HZ	3:A:1397:LEU:HD21	1.81	0.45
3:A:491:VAL:H	4:B:1150:ARG:HH22	1.64	0.45
3:A:827:THR:O	3:A:831:THR:OG1	2.34	0.45
4:B:423:LYS:NZ	4:B:468:GLU:OE1	2.42	0.45
3:A:90:VAL:HG13	3:A:236:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:534:LEU:O	3:A:574:GLY:HA3	2.15	0.45
3:A:1438:THR:HG23	7:F:92:ARG:HB2	1.97	0.45
6:E:136:ASN:OD1	6:E:137:GLU:N	2.49	0.45
7:F:83:PRO:HA	7:F:146:TRP:CZ3	2.52	0.45
3:A:5:GLN:O	4:B:1159:ARG:NH2	2.46	0.45
4:B:63:ILE:O	4:B:67:SER:HB3	2.16	0.45
3:A:546:VAL:O	3:A:550:LEU:CD2	2.65	0.45
3:A:1021:LEU:HD11	3:A:1025:ARG:HH11	1.82	0.45
3:A:492:PRO:O	3:A:493:GLN:NE2	2.48	0.45
3:A:746:MET:SD	4:B:1015:HIS:ND1	2.90	0.45
4:B:390:LEU:HD13	4:B:392:ARG:NH2	2.31	0.45
4:B:564:GLU:OE2	4:B:591:ARG:NE	2.40	0.45
3:A:388:LEU:HD23	3:A:388:LEU:HA	1.83	0.45
6:E:177:ARG:O	6:E:212:ARG:NH2	2.50	0.45
7:F:83:PRO:HG2	7:F:84:TYR:HD1	1.81	0.45
3:A:381:THR:OG1	3:A:384:ASN:ND2	2.50	0.45
3:A:666:ILE:HD13	4:B:1052:VAL:HG11	1.99	0.45
3:A:804:TYR:O	4:B:761:HIS:ND1	2.50	0.45
3:A:924:LYS:HE3	3:A:924:LYS:HB2	1.83	0.45
4:B:620:ARG:HH12	9:I:68:LEU:HD21	1.80	0.45
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.82	0.45
2:T:4:DT:H4'	2:T:5:DC:OP1	2.17	0.45
2:T:17:DG:H21	4:B:506:GLY:HA3	1.82	0.45
3:A:607:ILE:HG12	3:A:612:ILE:HA	1.99	0.45
3:A:1424:VAL:HG22	3:A:1436:ILE:HD11	1.99	0.45
4:B:48:LEU:HD23	4:B:173:MET:SD	2.56	0.45
4:B:408:LEU:HD12	4:B:408:LEU:HA	1.83	0.45
5:C:111:THR:HB	5:C:147:LEU:HB2	1.99	0.45
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.97	0.45
3:A:12:ARG:O	4:B:1194:ILE:HG22	2.17	0.45
3:A:269:ILE:HD13	3:A:299:HIS:HB3	1.99	0.45
3:A:311:GLN:N	3:A:312:PRO:HD2	2.31	0.45
3:A:464:PRO:O	11:K:2:ASN:HB3	2.16	0.45
3:A:663:SER:O	3:A:742:ASN:ND2	2.49	0.45
6:E:120:ALA:O	6:E:124:VAL:HG23	2.17	0.45
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.99	0.45
3:A:107:CYS:SG	3:A:171:GLN:NE2	2.90	0.45
4:B:406:LEU:HD23	4:B:406:LEU:HA	1.81	0.45
4:B:1162:ILE:HD13	4:B:1194:ILE:HD13	1.99	0.45
9:I:84:VAL:HG12	9:I:102:VAL:HB	1.99	0.45
4:B:784:ASN:HB3	10:J:63:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:807:ARG:H	4:B:1045:SER:HB3	1.82	0.44
6:E:79:TRP:HB2	6:E:105:PHE:CE1	2.52	0.44
4:B:579:ARG:HB3	4:B:586:TRP:NE1	2.32	0.44
4:B:570:VAL:HG21	4:B:573:GLN:CD	2.38	0.44
4:B:830:TYR:O	4:B:831:SER:OG	2.30	0.44
4:B:861:ASP:OD1	4:B:862:GLN:N	2.42	0.44
7:F:132:LEU:O	7:F:148:VAL:HG23	2.17	0.44
11:K:18:LYS:HD3	11:K:18:LYS:O	2.18	0.44
8:H:98:TYR:OH	8:H:138:GLU:OE2	2.33	0.44
8:H:130:ARG:H	8:H:130:ARG:HD2	1.81	0.44
3:A:69:THR:N	3:A:71:GLN:HE22	2.16	0.44
4:B:955:THR:OG1	4:B:956:THR:N	2.51	0.44
3:A:1121:GLU:HG2	3:A:1122:PRO:HD2	2.00	0.44
9:I:81:ARG:O	9:I:83:ASN:ND2	2.50	0.44
3:A:115:LEU:HB3	3:A:122:MET:HG2	2.00	0.44
4:B:104:GLU:OE2	4:B:120:ARG:NH2	2.42	0.44
5:C:116:LYS:HD3	5:C:140:ASN:HA	1.99	0.44
3:A:834:THR:HG21	3:A:1077:THR:HA	2.00	0.44
3:A:982:THR:HG23	3:A:985:ASP:H	1.83	0.44
4:B:610:ASN:HB3	4:B:613:VAL:HG23	2.00	0.44
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.52	0.44
3:A:1109:LYS:HD3	13:N:7:DA:H5'	1.99	0.43
4:B:521:LEU:HD23	4:B:635:ARG:HD3	2.00	0.43
7:F:128:LYS:NZ	7:F:151:LEU:O	2.51	0.43
3:A:1207:LEU:HD23	3:A:1207:LEU:HA	1.85	0.43
4:B:653:VAL:HG12	4:B:689:LEU:HB3	2.00	0.43
4:B:872:GLU:HG2	4:B:916:THR:HB	2.00	0.43
6:E:26:ARG:HH12	6:E:133:GLU:CD	2.22	0.43
8:H:102:TYR:CZ	8:H:115:TYR:HB3	2.53	0.43
13:N:11:DG:H2'	13:N:12:DA:C8	2.53	0.43
3:A:140:THR:HA	3:A:143:LYS:HE3	2.00	0.43
3:A:1267:MET:HA	3:A:1271:ILE:HD13	2.00	0.43
4:B:63:ILE:HG13	4:B:95:ILE:HD12	1.99	0.43
4:B:195:CYS:SG	4:B:783:THR:OG1	2.70	0.43
4:B:604:ARG:NH2	4:B:613:VAL:O	2.24	0.43
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.53	0.43
3:A:37:PHE:HB2	3:A:52:GLY:HA3	2.00	0.43
3:A:932:GLU:O	3:A:936:LEU:HG	2.18	0.43
3:A:1434:ALA:O	3:A:1436:ILE:N	2.51	0.43
4:B:435:THR:HG23	4:B:438:GLU:HB2	2.00	0.43
4:B:859:TYR:OH	4:B:941:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:941:LEU:CD1	4:B:942:ARG:O	2.66	0.43
4:B:46:GLN:H	4:B:46:GLN:HG3	1.60	0.43
4:B:405:ARG:CZ	4:B:632:ARG:HG2	2.48	0.43
4:B:234:ILE:HD12	4:B:257:LYS:HB3	1.99	0.43
4:B:751:VAL:HG23	4:B:812:LEU:HD22	2.00	0.43
4:B:1150:ARG:HA	4:B:1150:ARG:HD3	1.70	0.43
3:A:531:ILE:O	3:A:535:THR:OG1	2.29	0.43
5:C:62:PHE:HE2	5:C:66:ARG:HD2	1.84	0.43
3:A:444:PHE:CE1	3:A:487:MET:HB3	2.53	0.43
3:A:900:ASP:O	3:A:907:THR:OG1	2.37	0.43
8:H:136:LYS:H	8:H:136:LYS:HG2	1.66	0.43
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.51	0.43
13:N:4:DA:H4'	13:N:5:DT:OP1	2.18	0.43
3:A:60:SER:OG	3:A:66:LYS:O	2.32	0.43
3:A:779:PHE:CE1	3:A:785:PRO:HD3	2.54	0.43
3:A:986:ILE:HD11	3:A:1032:LEU:HD21	2.00	0.43
3:A:1199:ARG:HG2	3:A:1236:LEU:HD23	2.00	0.43
4:B:498:THR:OG1	4:B:537:LYS:HG3	2.18	0.43
3:A:1399:ARG:NH2	3:A:1417:GLU:OE1	2.52	0.42
7:F:96:THR:O	7:F:100:GLN:HG3	2.19	0.42
4:B:935:ARG:HE	4:B:935:ARG:HB2	1.68	0.42
4:B:1159:ARG:HD3	4:B:1161:HIS:HE1	1.84	0.42
4:B:408:LEU:HD22	4:B:545:ILE:HD12	2.01	0.42
6:E:72:PHE:HB2	6:E:75:MET:HG2	1.99	0.42
6:E:197:LYS:HE2	6:E:199:ILE:HD11	2.00	0.42
8:H:26:ILE:HD12	8:H:26:ILE:HA	1.90	0.42
3:A:885:THR:HG23	3:A:1024:SER:HB3	2.01	0.42
4:B:284:ILE:HD13	4:B:333:PHE:HD2	1.84	0.42
4:B:910:VAL:HA	4:B:940:PRO:HA	2.01	0.42
5:C:54:ASN:ND2	5:C:60:ASP:OD1	2.52	0.42
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.54	0.42
3:A:1341:ILE:HD13	3:A:1380:GLY:HA2	2.02	0.42
4:B:1159:ARG:HD3	4:B:1161:HIS:CE1	2.54	0.42
11:K:12:LEU:HD12	11:K:12:LEU:H	1.84	0.42
3:A:130:ASP:O	3:A:134:ARG:HB3	2.20	0.42
3:A:457:ALA:O	3:A:507:VAL:HG23	2.19	0.42
3:A:591:PHE:HD2	3:A:595:THR:HB	1.84	0.42
4:B:758:PHE:HB3	4:B:761:HIS:CD2	2.55	0.42
6:E:78:LEU:HD22	6:E:109:ILE:HD13	2.02	0.42
3:A:351:THR:HB	4:B:1103:ILE:HG13	2.01	0.42
3:A:472:LEU:HD21	4:B:835:GLN:CB	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:601:LYS:HB2	3:A:603:ASN:OD1	2.20	0.42
3:A:848:ILE:HG22	3:A:1064:VAL:HG23	2.01	0.42
3:A:1070:GLN:HE22	4:B:1137:CYS:HA	1.83	0.42
3:A:1073:GLY:O	3:A:1077:THR:HG23	2.19	0.42
3:A:1095:THR:HG21	3:A:1112:LYS:HB2	2.00	0.42
4:B:188:ASP:OD1	4:B:188:ASP:N	2.53	0.42
6:E:46:TYR:CE2	6:E:58:MET:HA	2.54	0.42
8:H:111:LEU:HA	8:H:111:LEU:HD23	1.88	0.42
3:A:501:LEU:HD21	4:B:1146:PHE:CD1	2.54	0.42
3:A:956:LEU:HD23	3:A:956:LEU:HA	1.91	0.42
3:A:1027:ALA:HB3	3:A:1030:ARG:HG3	2.02	0.42
3:A:1419:ASP:OD1	3:A:1426:GLU:HG2	2.20	0.42
4:B:620:ARG:HH11	9:I:68:LEU:HD11	1.84	0.42
6:E:23:VAL:O	6:E:28:TYR:HB2	2.19	0.42
7:F:111:LEU:HD12	7:F:111:LEU:O	2.20	0.42
9:I:72:ASP:OD1	9:I:72:ASP:N	2.53	0.42
3:A:549:MET:HE1	3:A:656:TRP:HD1	1.85	0.42
4:B:835:GLN:OE1	4:B:1013:ASN:ND2	2.53	0.42
4:B:972:LYS:NZ	4:B:1101:ASP:OD1	2.52	0.42
5:C:8:VAL:HG22	5:C:22:LEU:HD12	2.02	0.42
8:H:99:GLY:O	8:H:140:ALA:HB3	2.19	0.42
3:A:176:LYS:HE3	3:A:176:LYS:HB2	1.78	0.42
3:A:392:VAL:CG1	3:A:424:ILE:HG12	2.49	0.42
3:A:528:LEU:HD12	3:A:528:LEU:HA	1.87	0.42
3:A:780:VAL:HG12	4:B:699:GLU:OE2	2.19	0.42
4:B:778:MET:CB	4:B:796:LEU:CD1	2.98	0.42
5:C:253:LYS:HE3	5:C:253:LYS:HB2	1.79	0.42
2:T:23:DC:H2'	2:T:24:DT:H6	1.84	0.41
3:A:67:CYS:HB3	3:A:70:CYS:HB3	2.02	0.41
3:A:392:VAL:HG11	3:A:424:ILE:HG12	2.02	0.41
3:A:740:LEU:H	3:A:740:LEU:HD23	1.84	0.41
4:B:259:TYR:OH	4:B:279:ASP:OD2	2.23	0.41
5:C:101:LEU:HB3	5:C:155:LEU:HD12	2.02	0.41
3:A:526:ASP:HB2	4:B:835:GLN:HE22	1.84	0.41
3:A:1263:ILE:O	3:A:1267:MET:HG3	2.20	0.41
2:T:23:DC:H2'	2:T:24:DT:C6	2.55	0.41
3:A:107:CYS:HB2	3:A:148:CYS:HB2	2.01	0.41
4:B:996:ARG:HG3	4:B:1007:VAL:HG21	2.01	0.41
5:C:101:LEU:HD23	5:C:155:LEU:HD11	2.02	0.41
8:H:105:GLU:HG2	8:H:113:ALA:HB3	2.01	0.41
2:T:11:DG:C2	2:T:12:DG:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:42:ASP:OD2	3:A:48:ALA:HB3	2.20	0.41
3:A:339:ASN:HB3	4:B:1117:GLN:NE2	2.35	0.41
3:A:818:MET:HG3	4:B:514:LEU:O	2.19	0.41
4:B:273:LEU:HB2	4:B:276:ILE:HB	2.02	0.41
4:B:493:SER:OG	4:B:497:ARG:NH2	2.53	0.41
4:B:732:SER:HB3	4:B:734:HIS:CE1	2.56	0.41
8:H:135:LEU:HD23	8:H:135:LEU:HA	1.95	0.41
12:L:29:TYR:CE1	12:L:41:SER:HB2	2.56	0.41
3:A:591:PHE:HA	3:A:595:THR:HG21	2.03	0.41
3:A:691:LEU:HD23	3:A:691:LEU:HA	1.87	0.41
3:A:1291:VAL:HG22	3:A:1292:PRO:HD2	2.03	0.41
3:A:1303:GLU:CD	3:A:1326:ARG:HH12	2.24	0.41
4:B:260:GLY:O	4:B:267:ARG:NH1	2.52	0.41
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.55	0.41
3:A:26:GLU:OE2	4:B:1215:ARG:NH1	2.49	0.41
3:A:356:ASP:OD1	3:A:359:LEU:HB2	2.21	0.41
3:A:1328:TYR:OH	3:A:1350:LYS:CD	2.68	0.41
4:B:766:ARG:HG3	4:B:1022:THR:HG22	2.02	0.41
5:C:211:ASP:N	5:C:211:ASP:OD1	2.43	0.41
3:A:361:LEU:HA	3:A:471:ASN:HD22	1.86	0.41
3:A:1435:PRO:O	3:A:1436:ILE:HD13	2.21	0.41
4:B:1159:ARG:HG2	4:B:1160:VAL:N	2.35	0.41
5:C:93:ASP:O	5:C:127:ARG:NH2	2.43	0.41
13:N:14:DA:H2"	13:N:15:DG:N7	2.36	0.41
3:A:598:LEU:HD22	8:H:25:ARG:NH2	2.35	0.41
4:B:46:GLN:OE1	4:B:408:LEU:HD21	2.21	0.41
4:B:936:ASP:OD1	4:B:937:ALA:N	2.54	0.41
4:B:1204:PHE:O	4:B:1208:MET:HG3	2.20	0.41
5:C:259:LEU:HD12	5:C:259:LEU:HA	1.77	0.41
7:F:90:ARG:O	7:F:94:LEU:HG	2.21	0.41
11:K:21:ILE:HG12	11:K:33:ILE:HG12	2.03	0.41
3:A:594:GLY:O	3:A:596:THR:N	2.50	0.41
3:A:650:GLN:O	3:A:654:ASN:ND2	2.53	0.41
3:A:1199:ARG:O	3:A:1203:ASN:ND2	2.29	0.41
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	2.02	0.41
4:B:244:LEU:HB2	4:B:248:SER:O	2.21	0.41
5:C:177:GLU:HB2	5:C:231:ASN:HB3	2.03	0.41
8:H:95:TYR:HE1	8:H:97:MET:HE2	1.85	0.41
3:A:1166:ASP:O	3:A:1169:ILE:HB	2.19	0.41
4:B:114:PRO:HG2	4:B:181:LEU:HD11	2.02	0.41
4:B:451:LYS:O	4:B:455:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:549:THR:OG1	4:B:610:ASN:ND2	2.53	0.41
5:C:46:ILE:HG21	5:C:157:CYS:HB3	2.03	0.41
9:I:68:LEU:HD23	9:I:68:LEU:HA	1.90	0.41
3:A:35:ILE:O	3:A:84:ILE:HG22	2.21	0.40
3:A:180:LYS:HD3	3:A:180:LYS:HA	1.92	0.40
3:A:1217:LYS:HB2	3:A:1217:LYS:HE3	1.90	0.40
6:E:153:HIS:C	6:E:154:ILE:HD12	2.42	0.40
8:H:89:LEU:HD13	8:H:91:ASP:O	2.21	0.40
2:T:9:DC:H2'	2:T:10:DT:H71	2.02	0.40
3:A:974:ASP:OD1	3:A:974:ASP:N	2.44	0.40
4:B:597:MET:HE1	4:B:615:MET:HB3	2.03	0.40
4:B:778:MET:HB3	4:B:796:LEU:HD12	2.04	0.40
5:C:166:GLU:HG3	11:K:10:PHE:HZ	1.86	0.40
6:E:59:SER:HA	6:E:80:VAL:O	2.20	0.40
9:I:52:ILE:HD13	9:I:52:ILE:HA	1.90	0.40
2:T:18:DA:C2'	2:T:19:DG:H5"	2.52	0.40
3:A:688:LYS:HE2	3:A:688:LYS:HB2	1.81	0.40
4:B:801:LYS:O	10:J:52:THR:HB	2.22	0.40
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.52	0.40
3:A:17:VAL:HG23	3:A:1421:CYS:SG	2.62	0.40
3:A:387:ARG:O	3:A:391:LEU:HG	2.21	0.40
3:A:1287:TYR:CD1	3:A:1305:VAL:HG21	2.56	0.40
4:B:1212:ILE:O	4:B:1214:PRO:HD3	2.21	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	
3	A	1370/1733 (79%)	1307 (95%)	63 (5%)	0	100	100
4	B	1106/1224 (90%)	1066 (96%)	40 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	265/318 (83%)	256 (97%)	9 (3%)	0	100	100
6	E	210/215 (98%)	199 (95%)	11 (5%)	0	100	100
7	F	84/155 (54%)	84 (100%)	0	0	100	100
8	H	129/146 (88%)	118 (92%)	11 (8%)	0	100	100
9	I	116/122 (95%)	110 (95%)	6 (5%)	0	100	100
10	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
11	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3496/4173 (84%)	3349 (96%)	147 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	
3	A	1194/1520 (79%)	1157 (97%)	37 (3%)	40	72
4	B	955/1061 (90%)	919 (96%)	36 (4%)	33	67
5	C	235/274 (86%)	231 (98%)	4 (2%)	60	83
6	E	193/197 (98%)	187 (97%)	6 (3%)	40	72
7	F	73/137 (53%)	71 (97%)	2 (3%)	44	75
8	H	116/128 (91%)	107 (92%)	9 (8%)	12	43
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	60/65 (92%)	59 (98%)	1 (2%)	60	83
11	K	99/102 (97%)	97 (98%)	2 (2%)	55	80
12	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3072/3657 (84%)	2975 (97%)	97 (3%)	39	71

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	8	SER
3	A	22	PHE
3	A	75	ASN
3	A	81	PHE
3	A	180	LYS
3	A	200	ARG
3	A	265	LYS
3	A	286	HIS
3	A	335	ARG
3	A	341	MET
3	A	438	ASP
3	A	470	LEU
3	A	481	ASP
3	A	544	ASP
3	A	598	LEU
3	A	618	GLU
3	A	635	ARG
3	A	691	LEU
3	A	740	LEU
3	A	764	CYS
3	A	771	GLU
3	A	816	HIS
3	A	821	ARG
3	A	873	MET
3	A	979	SER
3	A	1025	ARG
3	A	1035	TYR
3	A	1100	ARG
3	A	1106	ASN
3	A	1155	ASP
3	A	1174	PHE
3	A	1204	ASP
3	A	1261	LYS
3	A	1312	ASN
3	A	1315	GLU
3	A	1345	ARG
3	A	1366	ARG
4	B	46	GLN
4	B	94	LYS
4	B	106	ASP
4	B	110	HIS
4	B	133	LYS
4	B	188	ASP

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Mol	Chain	Res	Type
4	B	199	MET
4	B	215	GLN
4	B	351	TYR
4	B	384	ARG
4	B	391	ASP
4	B	401	PHE
4	B	404	LYS
4	B	466	TRP
4	B	510	LYS
4	B	518	HIS
4	B	529	GLU
4	B	648	HIS
4	B	651	LEU
4	B	666	TYR
4	B	722	ASP
4	B	734	HIS
4	B	953	LEU
4	B	999	MET
4	B	1072	MET
4	B	1082	MET
4	B	1106	ARG
4	B	1112	GLN
4	B	1147	LEU
4	B	1150	ARG
4	B	1156	ASP
4	B	1161	HIS
4	B	1163	CYS
4	B	1180	PHE
4	B	1181	GLU
4	B	1220	ARG
5	C	137	LYS
5	C	178	PHE
5	C	193	TYR
5	C	215	GLU
6	E	29	PHE
6	E	48	ASP
6	E	72	PHE
6	E	81	GLU
6	E	102	GLU
6	E	177	ARG
7	F	69	LEU
7	F	147	SER

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Mol	Chain	Res	Type
8	H	33	GLN
8	H	36	CYS
8	H	94	ASP
8	H	111	LEU
8	H	124	ARG
8	H	130	ARG
8	H	131	ASN
8	H	139	ASN
8	H	146	ARG
10	J	48	ARG
11	K	54	ARG
11	K	81	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	71	GLN
3	A	339	ASN
4	B	794	ASN
4	B	1117	GLN
6	E	143	ASN
8	H	33	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	R	9/10 (90%)	-0.45	0 100 100	81, 87, 139, 143	0
2	T	26/30 (86%)	-0.05	2 (7%) 13 7	87, 164, 246, 261	0
3	A	1384/1733 (79%)	-0.02	36 (2%) 56 40	47, 94, 162, 198	0
4	B	1126/1224 (91%)	-0.01	14 (1%) 79 67	41, 81, 131, 176	0
5	C	267/318 (83%)	-0.21	0 100 100	55, 84, 119, 158	0
6	E	212/215 (98%)	0.01	6 (2%) 53 37	76, 130, 181, 195	0
7	F	86/155 (55%)	-0.12	1 (1%) 79 67	68, 99, 142, 176	0
8	H	133/146 (91%)	0.54	13 (9%) 7 4	89, 124, 164, 195	0
9	I	118/122 (96%)	-0.27	1 (0%) 86 78	63, 98, 128, 144	0
10	J	65/70 (92%)	-0.30	0 100 100	57, 75, 110, 127	0
11	K	114/120 (95%)	-0.14	0 100 100	57, 89, 115, 134	0
12	L	43/70 (61%)	0.53	3 (6%) 16 9	61, 146, 189, 198	0
13	N	16/20 (80%)	0.19	1 (6%) 20 11	153, 205, 239, 242	0
All	All	3599/4233 (85%)	-0.03	77 (2%) 63 49	41, 92, 162, 261	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	105	CYS	4.5
4	B	869	SER	4.5
3	A	183	GLY	4.3
3	A	103	CYS	4.0
4	B	867	GLY	4.0
3	A	69	THR	4.0
6	E	93	MET	3.8
8	H	133	ASN	3.8
3	A	106	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
3	A	200	ARG	3.7
7	F	104	ASN	3.7
3	A	182	VAL	3.6
8	H	86	ASP	3.6
3	A	163	SER	3.6
6	E	121	MET	3.5
3	A	168	GLY	3.4
8	H	85	GLY	3.4
8	H	32	THR	3.4
3	A	144	THR	3.4
8	H	107	VAL	3.4
3	A	149	GLU	3.3
4	B	507	LYS	3.3
4	B	69	LEU	3.2
6	E	83	CYS	3.2
3	A	174	ILE	3.1
4	B	106	ASP	3.0
6	E	128	PRO	3.0
4	B	868	MET	2.9
3	A	142	CYS	2.9
3	A	143	LYS	2.9
3	A	150	THR	2.9
3	A	1126	ALA	2.8
12	L	47	ARG	2.8
8	H	83	GLN	2.8
3	A	162	VAL	2.8
8	H	139	ASN	2.7
4	B	89	GLU	2.7
8	H	84	ALA	2.7
3	A	164	ARG	2.6
12	L	45	ALA	2.6
4	B	136	THR	2.6
12	L	41	SER	2.6
4	B	509	ALA	2.5
3	A	181	LEU	2.5
2	T	3	DT	2.5
3	A	280	GLU	2.5
13	N	3	DC	2.4
3	A	48	ALA	2.4
3	A	62	ASP	2.4
3	A	65	LEU	2.3
3	A	161	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
8	H	113	ALA	2.3
3	A	286	HIS	2.3
3	A	152	VAL	2.3
4	B	508	LEU	2.2
3	A	148	CYS	2.2
2	T	2	DC	2.2
3	A	258	GLY	2.2
3	A	66	LYS	2.2
4	B	105	SER	2.2
8	H	137	GLN	2.1
9	I	117	LYS	2.1
3	A	660	ASN	2.1
3	A	167	CYS	2.1
3	A	91	PHE	2.1
4	B	349	ILE	2.1
3	A	108	MET	2.1
3	A	1306	LEU	2.1
8	H	15	VAL	2.1
4	B	92	PHE	2.0
8	H	130	ARG	2.0
4	B	248	SER	2.0
6	E	110	PHE	2.0
3	A	141	LEU	2.0
8	H	132	LEU	2.0
6	E	118	PRO	2.0
3	A	44	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	ZN	A	1802	1/1	0.78	0.11	135,135,135,135	0
15	ZN	A	1801	1/1	0.88	0.17	205,205,205,205	0
14	MG	R	2001	1/1	0.88	0.11	104,104,104,104	0
15	ZN	L	101	1/1	0.89	0.14	215,215,215,215	0
15	ZN	B	1301	1/1	0.95	0.09	149,149,149,149	0
15	ZN	J	101	1/1	0.98	0.18	63,63,63,63	0
15	ZN	I	201	1/1	0.98	0.10	112,112,112,112	0
15	ZN	C	401	1/1	0.99	0.10	91,91,91,91	0
15	ZN	I	202	1/1	0.99	0.12	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.