Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:25 pm BST

PDB ID	:	4A3C
Title	:	RNA Polymerase II initial transcribing complex with a 5nt DNA-RNA hybrid
Authors	:	Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on	:	2011-09-30
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

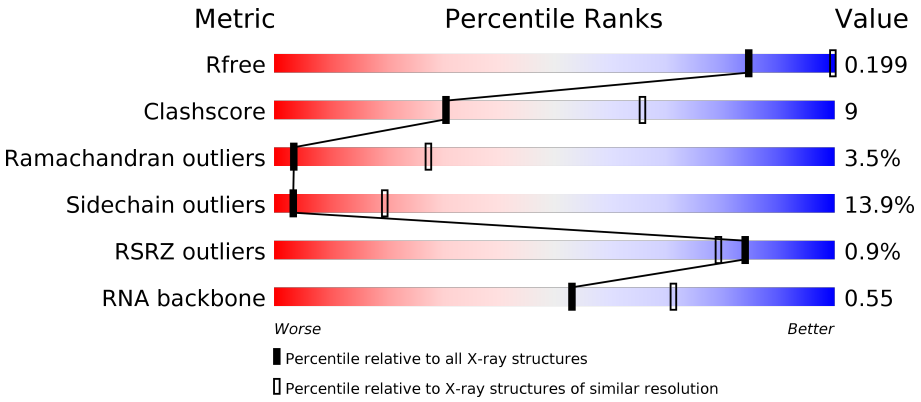
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	A	1732	55% 22% • • 18%
2	B	1224	% 63% 23% • 9%
3	C	318	55% 23% 5% 16%
4	D	221	54% 20% 5% • 19%

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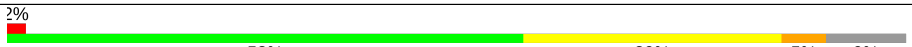
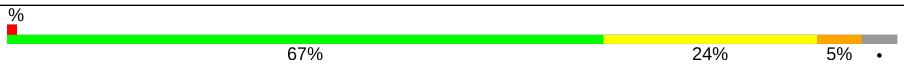
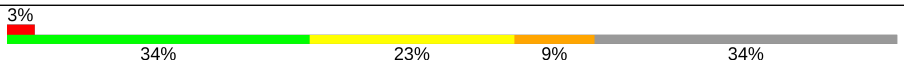
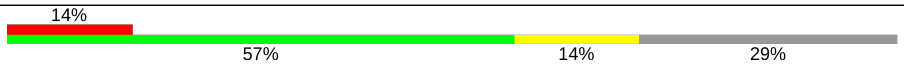
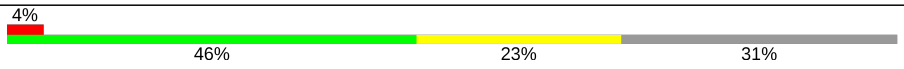
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	5	
15	T	26	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 31858 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	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called NON TEMPLATE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			

- Molecule 14 is a RNA chain called TRANSCRIPT RNA, 5'-R(*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	4	Total	C	N	O	P	0	0	0
			90	40	20	26	4			

- Molecule 15 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	18	Total	Br	C	N	O	P	0	0	0
			365	1	175	58	113	18			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

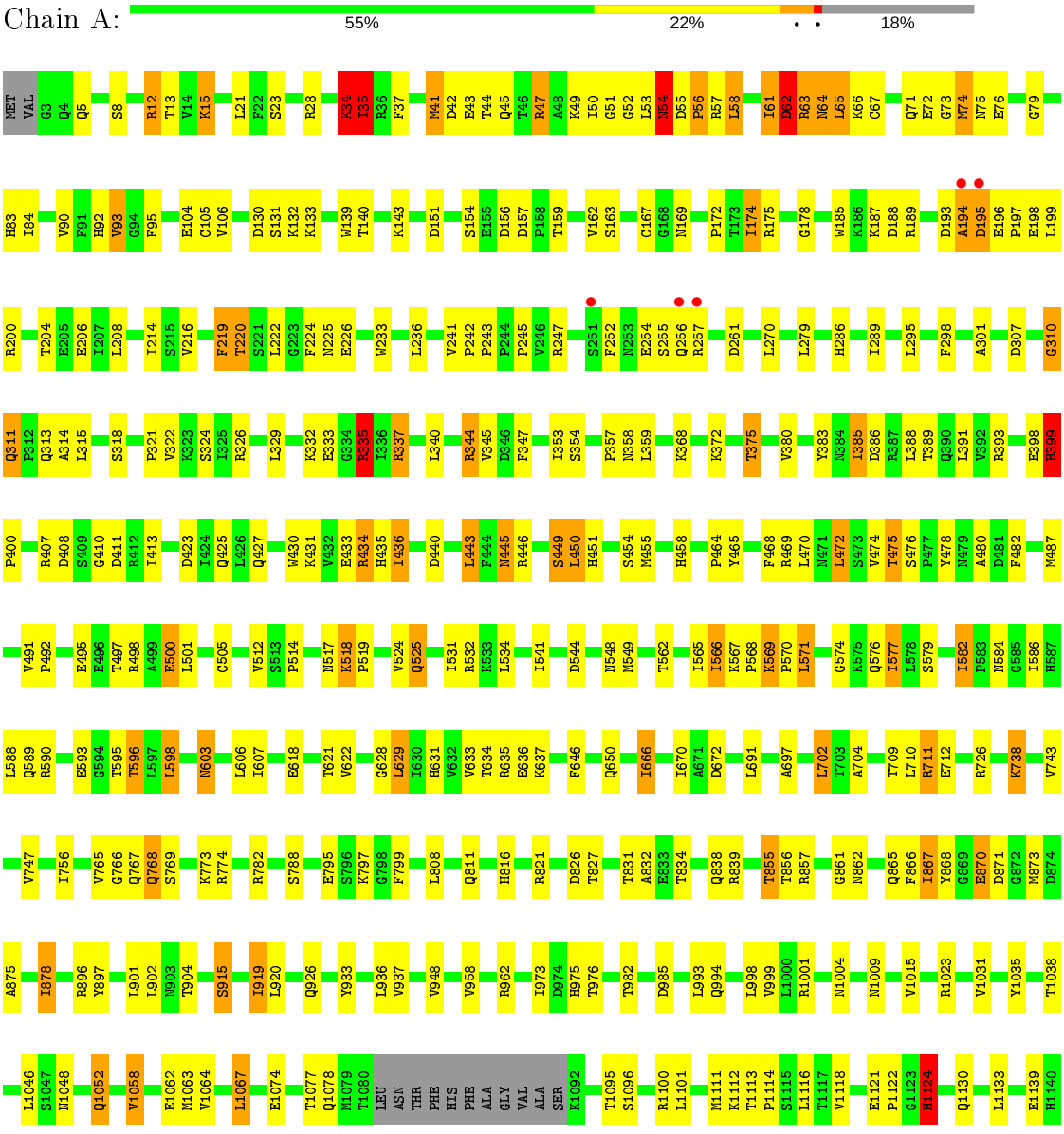
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

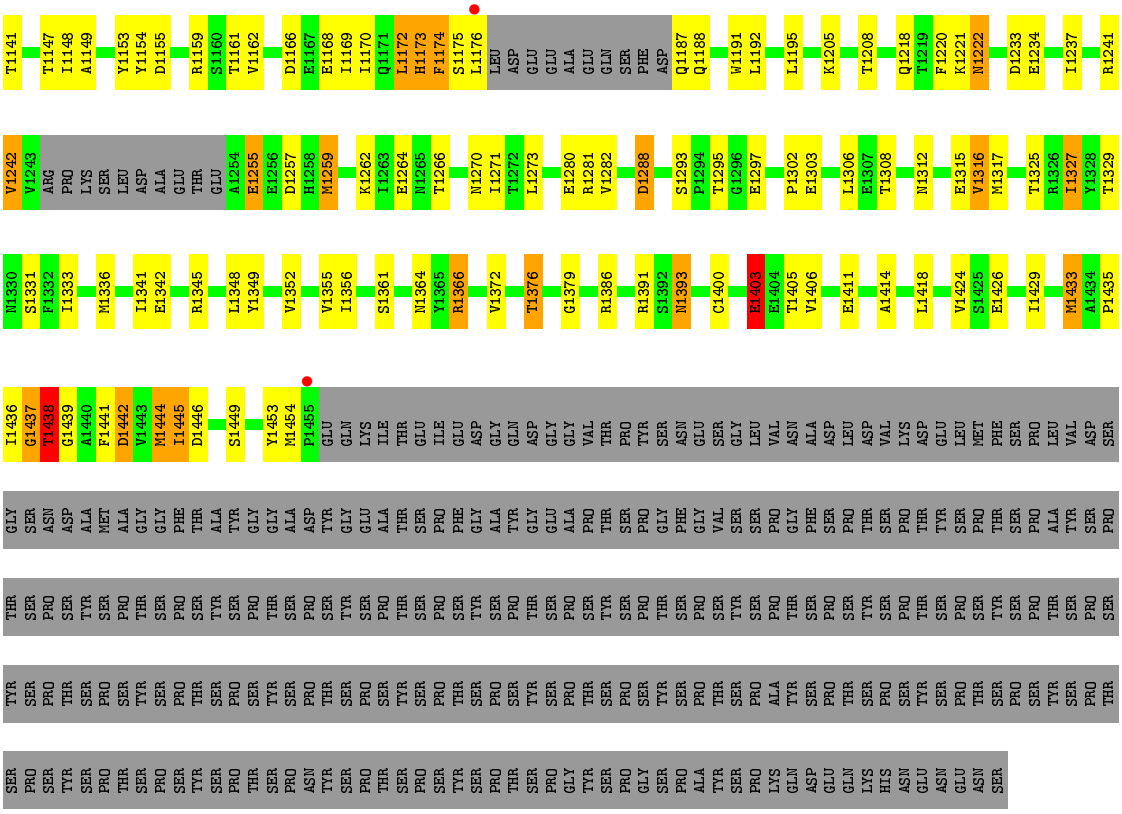
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

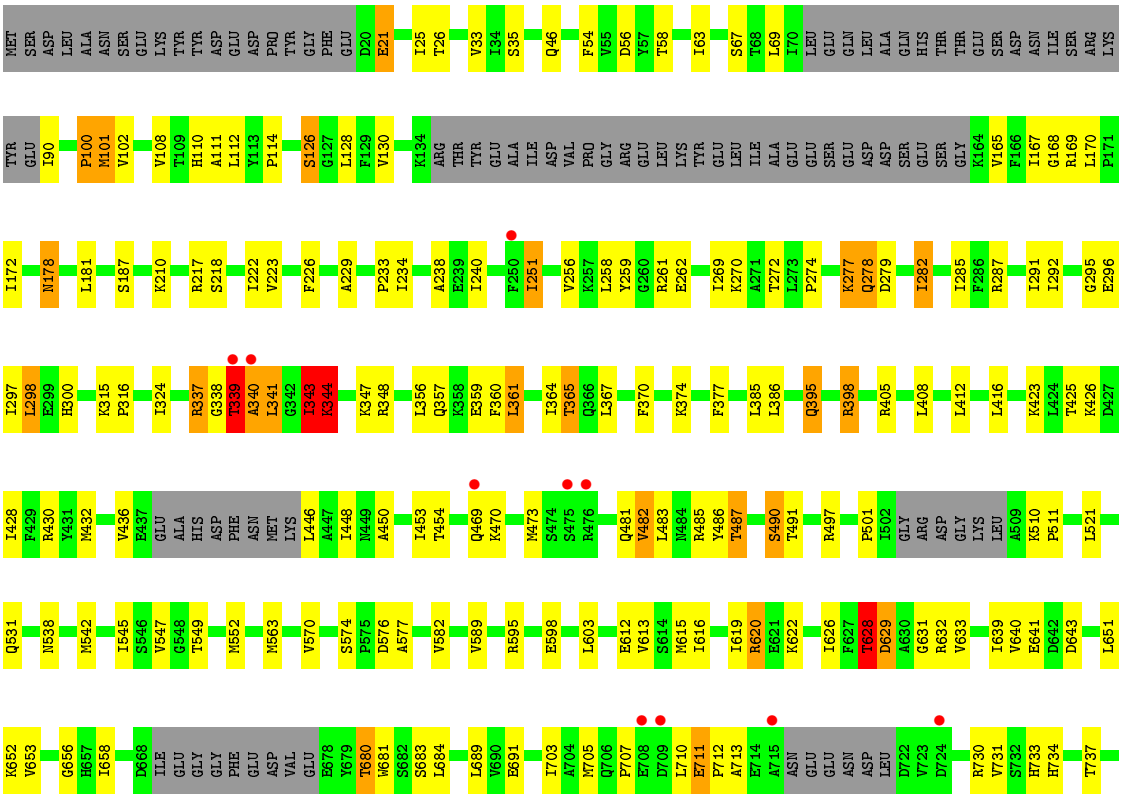
Chain A:

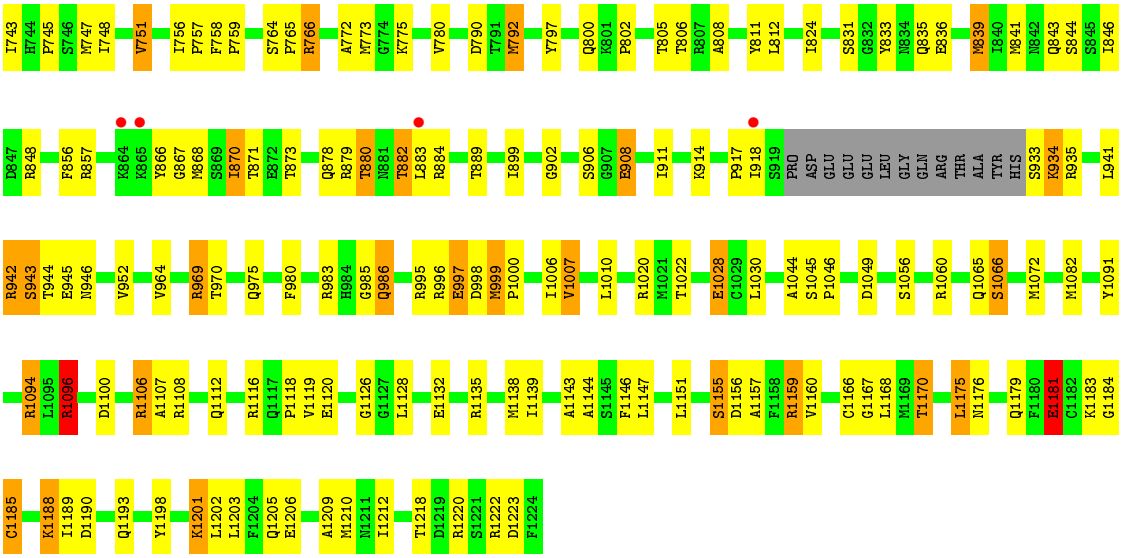




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

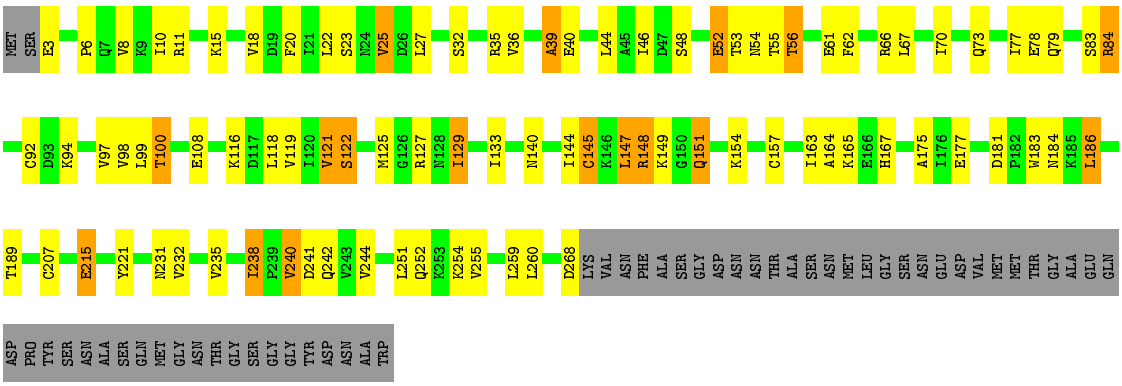
Chain B:





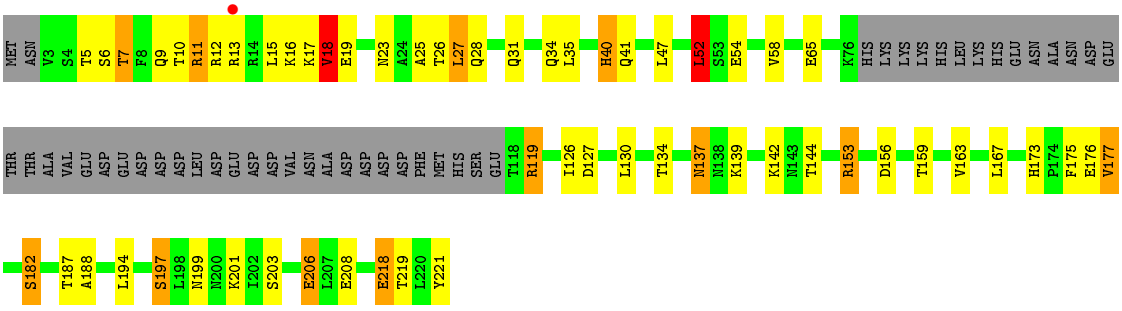
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



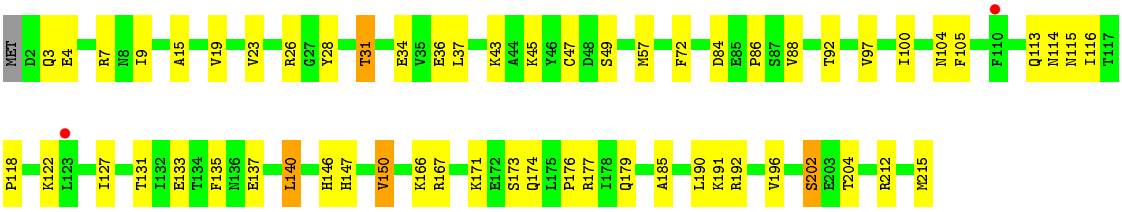
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



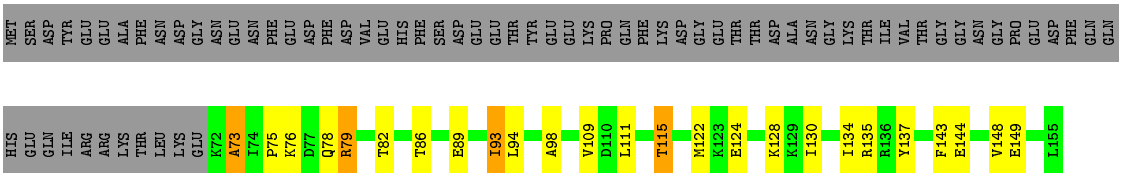
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



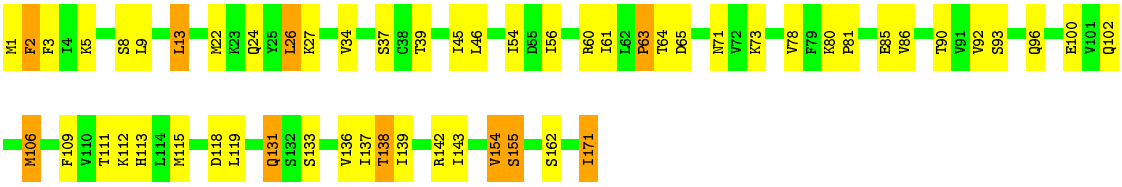
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



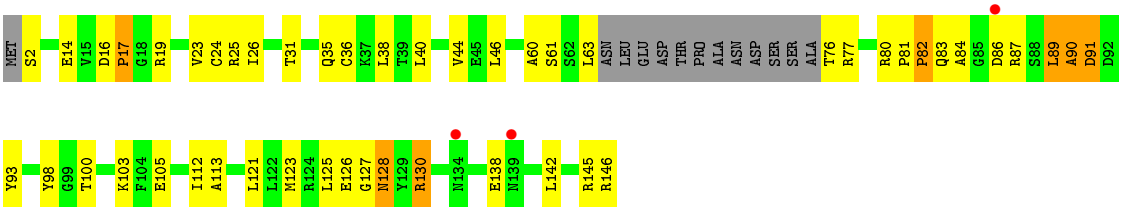
• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



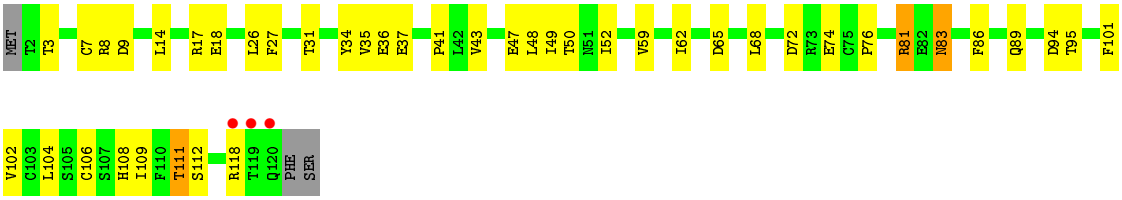
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



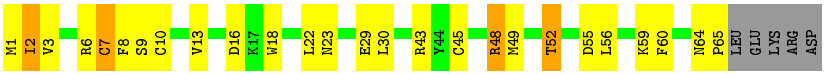
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



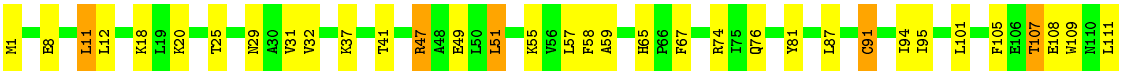
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

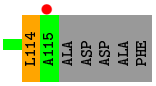
Chain J:



• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

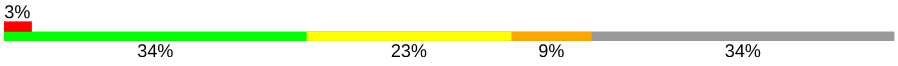
Chain K:

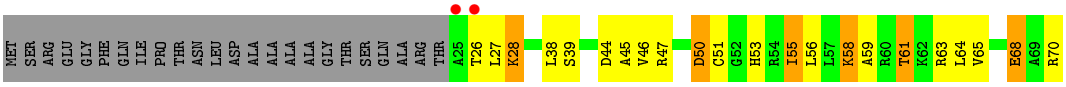




• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

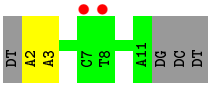
Chain L:





• Molecule 13: NON TEMPLATE DNA

Chain N:



• Molecule 14: TRANSCRIPT RNA, 5'-R(*CP*AP*GP*GP*AP)-3'

Chain P:

• Molecule 15: TEMPLATE DNA

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	221.41Å 393.12Å 282.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.50 49.85 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.85-3.50) 100.0 (49.85-3.50)	Depositor EDS
R_{merge}	0.89	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.158 , 0.184 0.179 , 0.199	Depositor DCC
R_{free} test set	3047 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	97.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 86.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.035 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31858	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: MG, ZN, BRU

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	0.55	0/11374	0.85	9/15383 (0.1%)
2	B	0.51	0/9029	0.81	5/12171 (0.0%)
3	C	0.48	0/2133	0.79	1/2891 (0.0%)
4	D	0.53	0/1444	0.85	2/1935 (0.1%)
5	E	0.48	0/1788	0.74	0/2406
6	F	0.62	0/691	0.83	0/933
7	G	0.53	0/1368	0.82	0/1844
8	H	0.53	0/1086	0.82	0/1470
9	I	0.46	0/989	0.79	0/1331
10	J	0.55	0/541	0.84	0/727
11	K	0.49	0/938	0.73	0/1267
12	L	0.53	0/365	0.96	0/485
13	N	1.18	0/232	1.07	0/356
14	P	1.01	0/101	0.78	0/156
15	T	1.31	1/383 (0.3%)	1.07	1/586 (0.2%)
All	All	0.55	1/32462 (0.0%)	0.83	18/43941 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	14	DC	C1'-N1	5.25	1.56	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	399	HIS	N-CA-CB	6.75	122.74	110.60
4	D	25	ALA	C-N-CA	6.40	137.71	121.70
1	A	56	PRO	C-N-CA	6.27	137.38	121.70
2	B	1184	GLY	C-N-CA	5.95	136.59	121.70
1	A	34	LYS	C-N-CA	5.83	136.27	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	26	THR	N-CA-C	-5.77	95.42	111.00
1	A	54	ASN	C-N-CA	5.69	135.93	121.70
1	A	194	ALA	C-N-CA	5.65	135.83	121.70
2	B	628	THR	C-N-CA	5.51	135.47	121.70
2	B	340	ALA	C-N-CA	5.50	135.46	121.70
1	A	35	ILE	N-CA-CB	5.50	123.44	110.80
1	A	1403	GLU	N-CA-C	5.49	125.83	111.00
2	B	339	THR	C-N-CA	5.46	135.35	121.70
1	A	310	GLY	C-N-CA	5.27	134.87	121.70
15	T	14	DC	O4'-C1'-N1	5.26	111.69	108.00
2	B	1181	GLU	N-CA-C	5.14	124.89	111.00
1	A	311	GLN	N-CA-C	5.11	124.81	111.00
3	C	39	ALA	N-CA-C	5.06	124.67	111.00

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	11174	0	11233	250	0
2	B	8859	0	8901	158	0
3	C	2095	0	2051	61	0
4	D	1434	0	1460	24	0
5	E	1752	0	1776	28	0
6	F	679	0	701	18	0
7	G	1340	0	1357	33	0
8	H	1068	0	1040	25	0
9	I	971	0	927	23	0
10	J	532	0	542	17	0
11	K	920	0	929	28	0
12	L	363	0	386	6	0
13	N	207	0	114	3	0
14	P	90	0	44	0	0
15	T	365	0	204	5	0
16	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31858	0	31665	586	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (586) 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)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.82	1.56
1:A:53:LEU:HD23	1:A:54:ASN:H	1.10	1.14
1:A:855:THR:HG21	1:A:857:ARG:HE	1.18	1.06
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.51	0.91
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.52	0.91
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.52	0.90
10:J:48:ARG:HE	10:J:49:MET:HE2	1.35	0.89
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.55	0.88
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.56	0.86
3:C:98:VAL:H	3:C:122:SER:HB3	1.40	0.84
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.59	0.83
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.60	0.83
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.61	0.81
3:C:66:ARG:NH2	10:J:3:VAL:O	2.14	0.80
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.44	0.80
1:A:53:LEU:HD23	1:A:54:ASN:N	1.94	0.80
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.15	0.79
3:C:148:ARG:H	3:C:151:GLN:HG3	1.48	0.78
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.66	0.78
3:C:46:ILE:H	3:C:46:ILE:HD12	1.49	0.77
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.67	0.76
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.65	0.76
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.68	0.76
1:A:1329:THR:HG22	1:A:1331:SER:H	1.51	0.75
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.27	0.75
7:G:1:MET:SD	7:G:2:PHE:N	2.58	0.75
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.89	0.72
1:A:53:LEU:CD2	1:A:54:ASN:H	1.98	0.72
3:C:32:SER:O	3:C:36:VAL:HG23	1.88	0.72
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.70	0.72
10:J:48:ARG:O	10:J:52:THR:HG23	1.89	0.72
2:B:296:GLU:O	2:B:300:HIS:HD2	1.73	0.71
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.72	0.71
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.71	0.71
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.73	0.71
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.23	0.71
2:B:705:MET:H	2:B:710:LEU:HD12	1.55	0.71
2:B:620:ARG:HE	9:I:89:GLN:HE22	1.39	0.70
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.57	0.70
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.20	0.70
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.58	0.68
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.28	0.68
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.73	0.68
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.76	0.68
8:H:82:PRO:C	8:H:84:ALA:H	1.97	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.67
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.76	0.67
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.59	0.67
1:A:64:ASN:O	1:A:65:LEU:HB3	1.94	0.66
3:C:100:THR:HG22	3:C:119:VAL:HG12	1.77	0.66
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.61	0.66
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.60	0.66
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.76	0.66
4:D:167:LEU:HB3	4:D:177:VAL:HG22	1.78	0.66
12:L:28:LYS:HB2	12:L:39:SER:HA	1.78	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	2.04	0.65
7:G:131:GLN:HG3	7:G:136:VAL:HG22	1.78	0.65
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.78	0.64
12:L:61:THR:HG21	12:L:63:ARG:HE	1.61	0.64
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.78	0.64
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.79	0.64
2:B:839:MET:CE	2:B:980:PHE:HB2	2.27	0.64
11:K:87:LEU:O	11:K:91:CYS:HB2	1.98	0.64
7:G:34:VAL:O	7:G:37:SER:HB3	1.98	0.64
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.63	0.63
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.97	0.63
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.81	0.63
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.99	0.63
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.81	0.63
1:A:315:LEU:HA	1:A:321:PRO:HA	1.81	0.63
1:A:63:ARG:HA	1:A:74:MET:HG3	1.82	0.62
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.82	0.62
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.82	0.62
2:B:806:THR:HG22	2:B:808:ALA:H	1.65	0.62
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.31	0.61
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.82	0.61
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.83	0.61
13:N:2:DA:H61	15:T:16:DT:H3	1.48	0.60
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.83	0.60
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.83	0.60
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.83	0.60
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.35	0.59
1:A:1393:ASN:HD22	1:A:1393:ASN:H	1.50	0.59
3:C:46:ILE:HD13	3:C:67:LEU:O	2.01	0.59
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.84	0.59
6:F:76:LYS:HA	6:F:79:ARG:CD	2.30	0.59
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.68	0.59
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.83	0.59
1:A:866:PHE:O	1:A:867:ILE:HD12	2.03	0.59
1:A:140:THR:HA	1:A:143:LYS:HE2	1.84	0.59
7:G:138:THR:HG22	7:G:139:ILE:H	1.67	0.59
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.85	0.58
3:C:20:PHE:HE2	3:C:22:LEU:HD13	1.67	0.58
7:G:1:MET:CE	7:G:80:LYS:O	2.52	0.58
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.58
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.84	0.58
1:A:586:ILE:HD11	1:A:637:LYS:HG2	1.85	0.58
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.86	0.58
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.85	0.58
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.84	0.58
2:B:839:MET:HE2	2:B:980:PHE:HB2	1.85	0.58
1:A:982:THR:HB	1:A:985:ASP:H	1.69	0.58
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.57
1:A:855:THR:HG21	1:A:857:ARG:NE	2.03	0.57
2:B:713:ALA:HA	2:B:733:HIS:NE2	2.19	0.57
9:I:72:ASP:O	9:I:81:ARG:HG2	2.03	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.86	0.57
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.87	0.57
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.70	0.57
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.85	0.57
1:A:1418:LEU:HD23	2:B:1222:ARG:HD3	1.87	0.57
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.05	0.57
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.87	0.57
1:A:492:PRO:CB	1:A:497:THR:HG22	2.35	0.57
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.86	0.57
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.87	0.57
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.40	0.57
3:C:40:GLU:OE2	3:C:254:LYS:HE3	2.05	0.57
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.87	0.56
3:C:148:ARG:N	3:C:151:GLN:HG3	2.19	0.56
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.86	0.56
7:G:1:MET:HE1	7:G:80:LYS:O	2.05	0.56
2:B:344:LYS:HB3	2:B:347:LYS:HB2	1.86	0.56
4:D:7:THR:HG21	7:G:5:LYS:HZ1	1.70	0.56
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.88	0.56
2:B:210:LYS:HD3	2:B:482:VAL:HG23	1.87	0.56
3:C:100:THR:HG22	3:C:119:VAL:CG1	2.36	0.56
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.40	0.56
11:K:107:THR:O	11:K:111:LEU:HG	2.05	0.56
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.06	0.56
2:B:882:THR:HG21	2:B:935:ARG:HA	1.87	0.56
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.88	0.55
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.71	0.55
1:A:35:ILE:HG13	1:A:56:PRO:HG2	1.88	0.55
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.88	0.55
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.21	0.55
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.22	0.55
12:L:61:THR:HG21	12:L:63:ARG:NE	2.21	0.55
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.06	0.55
2:B:168:GLY:H	2:B:450:ALA:HB1	1.71	0.55
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.55
2:B:882:THR:C	2:B:884:ARG:H	2.10	0.55
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.89	0.55
1:A:216:VAL:O	1:A:220:THR:HB	2.06	0.54
1:A:35:ILE:HG22	1:A:84:ILE:CG2	2.37	0.54
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.90	0.54
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.07	0.54
2:B:780:VAL:HG21	10:J:56:LEU:HD13	1.90	0.54
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.89	0.54
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.07	0.54
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.88	0.54
2:B:1185:CYS:HA	4:D:17:LYS:HD3	1.90	0.54
1:A:55:ASP:N	1:A:56:PRO:HD3	2.22	0.54
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.38	0.54
1:A:55:ASP:H	1:A:56:PRO:HD3	1.72	0.54
1:A:1159:ARG:HE	1:A:1174:PHE:HE2	1.55	0.54
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.89	0.54
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.89	0.54
1:A:56:PRO:CD	1:A:58:LEU:HG	2.38	0.54
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.90	0.53
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.42	0.53
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.91	0.53
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.08	0.53
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.90	0.53
2:B:126:SER:OG	2:B:172:ILE:HD11	2.09	0.53
7:G:111:THR:HG22	7:G:113:HIS:H	1.73	0.53
11:K:12:LEU:HA	11:K:37:LYS:HG3	1.91	0.53
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.90	0.53
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.90	0.53
6:F:128:LYS:HB3	6:F:149:GLU:HA	1.91	0.53
1:A:354:SER:O	1:A:469:ARG:HA	2.09	0.53
1:A:534:LEU:O	1:A:574:GLY:HA3	2.09	0.53
2:B:101:MET:HA	2:B:112:LEU:H	1.74	0.53
2:B:1181:GLU:HG3	2:B:1188:LYS:HG2	1.90	0.53
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.57	0.52
8:H:23:VAL:HG11	8:H:121:LEU:HD22	1.90	0.52
1:A:562:THR:O	1:A:576:GLN:NE2	2.42	0.52
1:A:524:VAL:HG12	1:A:525:GLN:H	1.72	0.52
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.74	0.52
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.92	0.52
6:F:128:LYS:HD3	6:F:148:VAL:O	2.08	0.52
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.92	0.52
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.92	0.52
2:B:745:PRO:O	2:B:748:ILE:HG12	2.10	0.52
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.91	0.52
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.92	0.52
1:A:1386:ARG:HE	1:A:1403:GLU:HG2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.74	0.52
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.91	0.52
1:A:41:MET:CB	1:A:49:LYS:HA	2.40	0.52
1:A:857:ARG:HD3	1:A:861:GLY:O	2.10	0.52
5:E:135:PHE:HB3	5:E:140:LEU:HD21	1.91	0.52
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.40	0.51
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.25	0.51
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.92	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
1:A:541:ILE:HG21	1:A:549:MET:CE	2.40	0.51
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.25	0.51
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.93	0.51
7:G:119:LEU:HD21	7:G:137:ILE:HD12	1.91	0.51
13:N:2:DA:H2"	13:N:3:DA:OP2	2.11	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.93	0.51
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.92	0.51
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.75	0.51
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.92	0.51
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.92	0.51
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.92	0.51
2:B:343:ILE:O	2:B:344:LYS:HB2	2.11	0.51
2:B:542:MET:HE1	2:B:743:ILE:HD12	1.93	0.51
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.93	0.51
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.11	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.93	0.50
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.93	0.50
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.52	0.50
1:A:449:SER:HA	1:A:454:SER:CB	2.41	0.50
1:A:1095:THR:HG21	1:A:1112:LYS:CB	2.41	0.50
9:I:50:THR:HG22	9:I:52:ILE:H	1.76	0.50
13:N:2:DA:N6	15:T:16:DT:H3	2.09	0.50
2:B:870:ILE:HG22	2:B:917:PRO:HG2	1.94	0.50
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.93	0.50
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.92	0.50
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.47	0.50
1:A:15:LYS:HG2	2:B:1220:ARG:HE	1.76	0.50
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.94	0.50
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.47	0.50
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.93	0.50
3:C:46:ILE:H	3:C:46:ILE:CD1	2.22	0.50
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:LEU:HD12	4:D:173:HIS:HB2	1.94	0.50
4:D:13:ARG:NH1	4:D:18:VAL:H	2.10	0.50
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.93	0.50
1:A:35:ILE:HA	1:A:52:GLY:O	2.11	0.49
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.49
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.94	0.49
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.47	0.49
1:A:1147:THR:HB	9:I:48:LEU:HD22	1.94	0.49
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.78	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.93	0.49
2:B:291:ILE:HD12	2:B:291:ILE:H	1.78	0.49
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.48	0.49
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.42	0.49
2:B:841:MET:HG3	2:B:1010:LEU:HD12	1.94	0.49
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.93	0.49
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.77	0.49
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.42	0.49
1:A:443:LEU:HD23	1:A:501:LEU:HD22	1.94	0.49
5:E:176:PRO:O	5:E:212:ARG:HA	2.13	0.49
1:A:194:ALA:HB2	1:A:197:PRO:HB3	1.94	0.49
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.49
4:D:159:THR:O	4:D:163:VAL:HG23	2.12	0.49
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.95	0.49
1:A:868:TYR:CE1	1:A:1064:VAL:HB	2.48	0.49
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.71	0.49
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.95	0.49
1:A:446:ARG:HB2	1:A:487:MET:SD	2.53	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.13	0.49
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.93	0.48
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.93	0.48
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.95	0.48
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.47	0.48
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.93	0.48
1:A:56:PRO:HD3	1:A:58:LEU:HG	1.95	0.48
2:B:773:MET:CE	2:B:985:GLY:HA2	2.43	0.48
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.48	0.48
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.96	0.48
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.77	0.48
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.48	0.48
1:A:933:TYR:O	1:A:937:VAL:HG23	2.13	0.48
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:O	2:B:759:PRO:HD3	2.13	0.48
6:F:111:LEU:H	6:F:111:LEU:HD12	1.79	0.48
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.43	0.48
1:A:646:PHE:O	1:A:650:GLN:HG2	2.13	0.48
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.94	0.48
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.96	0.48
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.94	0.48
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.96	0.48
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.43	0.48
2:B:341:LEU:HD12	2:B:343:ILE:H	1.78	0.48
5:E:15:ALA:O	5:E:19:VAL:HG23	2.13	0.48
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.95	0.48
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.78	0.48
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.44	0.48
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.95	0.48
2:B:510:LYS:N	2:B:511:PRO:HD3	2.29	0.48
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.96	0.48
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.95	0.48
8:H:89:LEU:C	8:H:91:ASP:H	2.16	0.48
9:I:83:ASN:HA	9:I:104:LEU:HG	1.96	0.47
3:C:84:ARG:HD3	11:K:11:LEU:HD21	1.96	0.47
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.62	0.47
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.96	0.47
2:B:1198:TYR:CE1	2:B:1201:LYS:HE3	2.49	0.47
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.97	0.47
2:B:425:THR:HA	2:B:428:ILE:HD12	1.97	0.47
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.96	0.47
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.29	0.47
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.78	0.47
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.96	0.47
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.95	0.47
2:B:613:VAL:HG22	2:B:628:THR:HA	1.96	0.47
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.96	0.47
2:B:933:SER:O	2:B:935:ARG:N	2.47	0.47
1:A:862:ASN:HA	5:E:174:GLN:HA	1.96	0.47
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.50	0.47
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.97	0.47
3:C:56:THR:HG21	3:C:145:CYS:SG	2.55	0.47
4:D:54:GLU:O	4:D:58:VAL:HG23	2.15	0.47
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.78	0.46
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.96	0.46
2:B:800:GLN:HB3	10:J:52:THR:OG1	2.16	0.46
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.80	0.46
1:A:873:MET:C	1:A:1058:VAL:HG22	2.36	0.46
1:A:216:VAL:HG13	1:A:226:GLU:HB3	1.98	0.46
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.97	0.46
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.97	0.46
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.35	0.46
1:A:549:MET:SD	1:A:577:ILE:HD11	2.55	0.46
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.46
2:B:315:LYS:N	2:B:316:PRO:HD2	2.31	0.46
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.98	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.42	0.46
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.96	0.46
7:G:112:LYS:HA	7:G:115:MET:HE3	1.97	0.46
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.81	0.46
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.98	0.46
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.49	0.46
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.48	0.46
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.79	0.46
7:G:100:GLU:HG3	7:G:109:PHE:HB2	1.98	0.46
10:J:64:ASN:HB2	10:J:65:PRO:HD3	1.98	0.46
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.98	0.46
1:A:105:CYS:SG	1:A:139:TRP:HA	2.56	0.46
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.98	0.46
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.97	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
1:A:41:MET:HB3	1:A:49:LYS:HA	1.98	0.46
2:B:54:PHE:HA	2:B:58:THR:HB	1.97	0.46
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.97	0.46
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.97	0.46
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.98	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.46
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.56	0.46
2:B:542:MET:HG3	2:B:747:MET:HB3	1.98	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.15	0.45
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.49	0.45
1:A:79:GLY:H	2:B:1201:LYS:HZ3	1.63	0.45
2:B:295:GLY:H	2:B:298:LEU:HD12	1.81	0.45
2:B:487:THR:HG22	2:B:490:SER:HB3	1.98	0.45
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:VAL:HG12	6:F:124:GLU:HG2	1.98	0.45
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.96	0.45
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.98	0.45
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.97	0.45
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.98	0.45
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.98	0.45
1:A:500:GLU:HG2	2:B:1143:ALA:HA	1.99	0.45
4:D:153:ARG:HG2	4:D:218:GLU:HG3	1.98	0.45
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.97	0.45
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.98	0.45
1:A:541:ILE:HG21	1:A:549:MET:HE1	1.99	0.45
1:A:61:ILE:HG22	1:A:62:ASP:H	1.82	0.45
4:D:47:LEU:HD21	7:G:3:PHE:CD1	2.52	0.45
8:H:35:GLN:HE22	8:H:128:ASN:HD22	1.64	0.45
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.99	0.45
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.98	0.45
2:B:757:PRO:HG2	2:B:1028:GLU:HG3	1.98	0.45
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.98	0.45
4:D:52:LEU:HG	4:D:182:SER:HB3	1.98	0.45
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.16	0.45
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.98	0.45
5:E:97:VAL:HG13	5:E:127:ILE:HG12	1.99	0.45
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.47	0.45
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.99	0.45
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.35	0.45
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.98	0.44
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.53	0.44
8:H:127:GLY:N	8:H:130:ARG:HH21	2.16	0.44
1:A:1187:GLN:HG3	1:A:1188:GLN:HG2	1.99	0.44
1:A:1280:GLU:O	1:A:1282:VAL:HG23	2.17	0.44
1:A:1379:GLY:HA2	5:E:177:ARG:O	2.17	0.44
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.44
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.99	0.44
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.99	0.44
2:B:652:LYS:HB3	2:B:689:LEU:HD23	2.00	0.44
15:T:10:DA:H2"	15:T:11:DG:C8	2.52	0.44
1:A:1220:PHE:HE1	1:A:1271:ILE:HD11	1.83	0.44
1:A:832:ALA:HB1	15:T:18:DT:H2"	2.00	0.44
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.99	0.44
5:E:19:VAL:O	5:E:23:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	2.00	0.44
1:A:62:ASP:HB3	1:A:64:ASN:O	2.17	0.44
2:B:490:SER:HB2	2:B:775:LYS:HA	1.99	0.44
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.44
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.98	0.44
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.99	0.44
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.83	0.44
3:C:18:VAL:HG22	11:K:109:TRP:HZ3	1.82	0.44
3:C:252:GLN:HG2	11:K:95:ILE:HG23	2.00	0.44
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.99	0.44
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.99	0.44
1:A:767:GLN:HA	1:A:799:PHE:HA	1.98	0.44
2:B:908:GLU:HG3	2:B:943:SER:HA	2.00	0.44
5:E:202:SER:OG	5:E:204:THR:HG22	2.18	0.44
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.00	0.44
12:L:68:GLU:HB2	12:L:70:ARG:HD2	2.00	0.44
1:A:242:PRO:HG3	2:B:1209:ALA:HB1	2.00	0.44
1:A:768:GLN:CG	1:A:816:HIS:HA	2.48	0.44
2:B:680:THR:O	2:B:683:SER:HB2	2.18	0.44
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.51	0.44
1:A:743:VAL:O	1:A:747:VAL:HG23	2.18	0.44
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.99	0.44
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.99	0.44
3:C:164:ALA:HA	3:C:167:HIS:O	2.18	0.44
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.00	0.44
5:E:118:PRO:O	5:E:122:LYS:HG2	2.18	0.44
7:G:1:MET:HE3	7:G:80:LYS:O	2.17	0.44
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.90	0.44
1:A:1329:THR:HG22	1:A:1331:SER:N	2.27	0.43
1:A:584:ASN:O	1:A:637:LYS:HE2	2.18	0.43
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.00	0.43
3:C:149:LYS:C	3:C:151:GLN:H	2.21	0.43
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.33	0.43
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.82	0.43
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.43
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.43
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.00	0.43
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.99	0.43
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.83	0.43
7:G:81:PRO:HG3	7:G:106:MET:SD	2.57	0.43
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:LEU:C	1:A:1174:PHE:H	2.22	0.43
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.19	0.43
1:A:982:THR:H	1:A:985:ASP:HB2	1.83	0.43
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.22	0.43
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.52	0.43
1:A:21:LEU:HD11	1:A:1414:ALA:HA	2.00	0.43
1:A:388:LEU:HA	1:A:391:LEU:HD12	2.00	0.43
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.01	0.43
1:A:185:TRP:HE3	1:A:185:TRP:H	1.65	0.43
1:A:194:ALA:HA	1:A:195:ASP:C	2.39	0.43
1:A:933:TYR:HA	1:A:936:LEU:HD12	2.00	0.43
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.84	0.43
1:A:1403:GLU:HG3	15:T:17:DT:H5'	2.00	0.43
3:C:148:ARG:HD3	3:C:149:LYS:HG2	2.01	0.43
3:C:163:ILE:CD1	3:C:165:LYS:HB2	2.40	0.43
5:E:179:GLN:HA	5:E:215:MET:HB2	2.00	0.43
8:H:24:CYS:HB2	8:H:44:VAL:HG21	2.01	0.43
2:B:620:ARG:HE	9:I:89:GLN:NE2	2.10	0.43
4:D:27:LEU:CD1	4:D:173:HIS:HB2	2.47	0.43
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.01	0.43
1:A:856:THR:HB	1:A:865:GLN:HB2	2.01	0.43
3:C:20:PHE:CE2	3:C:22:LEU:HD13	2.51	0.43
2:B:1166:CYS:O	2:B:1168:LEU:N	2.46	0.42
3:C:100:THR:HB	3:C:121:VAL:HG21	2.01	0.42
1:A:598:LEU:HD13	8:H:25:ARG:NH1	2.34	0.42
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.01	0.42
1:A:897:TYR:HB3	1:A:936:LEU:HD13	2.02	0.42
2:B:641:GLU:HG3	2:B:652:LYS:HE2	2.00	0.42
4:D:13:ARG:HH12	4:D:18:VAL:H	1.67	0.42
3:C:10:ILE:HD12	11:K:108:GLU:HB3	2.01	0.42
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.99	0.42
3:C:175:ALA:HB2	10:J:10:CYS:HB2	2.02	0.42
1:A:106:VAL:HG21	1:A:214:ILE:HG12	2.02	0.42
1:A:50:ILE:C	1:A:52:GLY:H	2.22	0.42
1:A:596:THR:HB	1:A:598:LEU:H	1.85	0.42
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.00	0.42
2:B:278:GLN:HB2	2:B:337:ARG:HG2	2.01	0.42
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.01	0.42
2:B:35:SER:HA	2:B:811:TYR:HE1	1.83	0.42
2:B:880:THR:HB	2:B:934:LYS:HD2	2.01	0.42
5:E:43:LYS:O	5:E:47:CYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:154:VAL:HB	7:G:155:SER:H	1.68	0.42
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.18	0.42
8:H:100:THR:HG23	8:H:138:GLU:HA	2.02	0.42
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.02	0.42
1:A:1372:VAL:O	1:A:1376:THR:HB	2.19	0.42
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.01	0.42
2:B:764:SER:HB3	2:B:765:PRO:HD3	2.00	0.42
8:H:2:SER:N	8:H:61:SER:HG	2.18	0.42
9:I:34:TYR:HE2	9:I:36:GLU:HG2	1.85	0.42
1:A:1221:LYS:HB3	1:A:1222:ASN:H	1.68	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.19	0.42
2:B:711:GLU:HB2	2:B:712:PRO:HD3	2.01	0.42
2:B:710:LEU:C	2:B:733:HIS:HB3	2.40	0.42
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.50	0.42
11:K:51:LEU:HD12	11:K:51:LEU:HA	1.89	0.42
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.52	0.42
1:A:42:ASP:O	1:A:44:THR:N	2.53	0.42
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.01	0.42
1:A:1031:VAL:HA	1:A:1035:TYR:CD2	2.55	0.42
1:A:62:ASP:O	1:A:64:ASN:N	2.49	0.42
2:B:101:MET:HB3	2:B:111:ALA:HA	2.00	0.42
2:B:35:SER:HA	2:B:811:TYR:CE1	2.54	0.42
2:B:398:ARG:HH11	2:B:398:ARG:HB2	1.84	0.42
2:B:21:GLU:O	2:B:656:GLY:HA3	2.19	0.42
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	2.18	0.42
2:B:873:THR:O	2:B:914:LYS:HA	2.20	0.42
8:H:63:LEU:HB3	8:H:90:ALA:HB2	2.02	0.42
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.42
4:D:31:GLN:O	4:D:34:GLN:HB2	2.20	0.42
4:D:144:THR:HG21	7:G:46:LEU:HD13	2.02	0.42
9:I:111:THR:HG21	9:I:118:ARG:HD2	2.02	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.90	0.41
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.35	0.41
2:B:361:LEU:O	2:B:374:LYS:HE2	2.18	0.41
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.41
11:K:65:HIS:HE1	11:K:67:PHE:CD1	2.38	0.41
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.16	0.41
1:A:450:LEU:HA	1:A:838:GLN:NE2	2.36	0.41
3:C:73:GLN:O	3:C:129:ILE:HA	2.20	0.41
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.55	0.41
1:A:1288:ASP:HA	1:A:1302:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:711:ARG:H	1.84	0.41
2:B:996:ARG:CG	2:B:1007:VAL:HG11	2.50	0.41
2:B:259:TYR:CE2	2:B:270:LYS:HB2	2.56	0.41
2:B:483:LEU:HD11	2:B:491:THR:HG23	2.01	0.41
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.03	0.41
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.00	0.41
1:A:104:GLU:HG3	1:A:174:ILE:HD12	2.01	0.41
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.56	0.41
1:A:151:ASP:HA	1:A:163:SER:HA	2.01	0.41
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.20	0.41
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.40	0.41
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.85	0.41
3:C:184:ASN:ND2	3:C:189:THR:O	2.54	0.41
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.02	0.41
1:A:1121:GLU:HB3	1:A:1124:HIS:CE1	2.55	0.41
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.86	0.41
2:B:497:ARG:HH22	2:B:775:LYS:HD3	1.85	0.41
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.03	0.41
5:E:135:PHE:HD2	5:E:140:LEU:HD22	1.85	0.41
7:G:13:LEU:HA	7:G:13:LEU:HD23	1.85	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CE2	2.55	0.41
1:A:704:ALA:HB2	1:A:710:LEU:HA	2.03	0.41
8:H:36:CYS:HA	8:H:126:GLU:O	2.21	0.41
4:D:188:ALA:HB2	4:D:208:GLU:HG3	2.02	0.41
1:A:66:LYS:HD2	1:A:71:GLN:HB3	2.03	0.41
2:B:90:ILE:HD12	2:B:432:MET:SD	2.60	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
10:J:45:CYS:O	10:J:48:ARG:HG3	2.21	0.41
11:K:32:VAL:HG22	11:K:74:ARG:HG3	2.01	0.41
11:K:65:HIS:CE1	11:K:67:PHE:CG	3.09	0.41
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.55	0.41
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.03	0.41
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.54	0.41
2:B:33:VAL:HG12	2:B:681:TRP:HZ3	1.85	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.56	0.41
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.56	0.41
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.03	0.41
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.86	0.41
2:B:102:VAL:HG22	2:B:112:LEU:HB2	2.02	0.41
3:C:77:ILE:HA	3:C:129:ILE:HD11	2.03	0.41
3:C:15:LYS:O	3:C:240:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:8:GLU:O	11:K:37:LYS:HD3	2.20	0.41
1:A:1356:ILE:HG23	1:A:1361:SER:HB2	2.03	0.40
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.21	0.40
1:A:35:ILE:HG22	1:A:84:ILE:HG22	2.03	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.03	0.40
2:B:620:ARG:HG3	9:I:62:ILE:HD11	2.03	0.40
2:B:69:LEU:O	2:B:90:ILE:N	2.54	0.40
1:A:37:PHE:CD2	1:A:52:GLY:CA	3.04	0.40
1:A:765:VAL:HG21	1:A:808:LEU:HD11	2.02	0.40
1:A:1139:GLU:HB2	1:A:1282:VAL:HB	2.04	0.40
1:A:132:LYS:HE3	1:A:1411:GLU:OE1	2.21	0.40
2:B:165:VAL:O	2:B:167:ILE:HD12	2.22	0.40
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.87	0.40
2:B:918:ILE:HG12	2:B:935:ARG:HH22	1.86	0.40
3:C:175:ALA:HB3	10:J:43:ARG:NH1	2.35	0.40
3:C:232:VAL:HG21	3:C:244:VAL:HG22	2.03	0.40
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.03	0.40
8:H:82:PRO:O	8:H:84:ALA:N	2.52	0.40
1:A:1376:THR:HG23	5:E:212:ARG:NH2	2.32	0.40
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.02	0.40
3:C:148:ARG:HG3	3:C:149:LYS:H	1.87	0.40
3:C:181:ASP:CG	3:C:186:LEU:HD12	2.42	0.40
1:A:738:LYS:HA	8:H:19:ARG:HH12	1.85	0.40
8:H:89:LEU:O	8:H:91:ASP:N	2.55	0.40
10:J:7:CYS:SG	10:J:49:MET:HE3	2.61	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	1414/1732 (82%)	1230 (87%)	132 (9%)	52 (4%)	3 26
2	B	1095/1224 (90%)	959 (88%)	94 (9%)	42 (4%)	3 25
3	C	264/318 (83%)	245 (93%)	18 (7%)	1 (0%)	34 72
4	D	174/221 (79%)	149 (86%)	17 (10%)	8 (5%)	2 21
5	E	212/215 (99%)	194 (92%)	14 (7%)	4 (2%)	8 40
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	13 50
7	G	169/171 (99%)	159 (94%)	7 (4%)	3 (2%)	8 41
8	H	129/146 (88%)	102 (79%)	20 (16%)	7 (5%)	2 17
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	5 33
10	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1 10
11	K	113/120 (94%)	109 (96%)	3 (3%)	1 (1%)	17 56
12	L	44/70 (63%)	26 (59%)	11 (25%)	7 (16%)	0 2
All	All	3876/4564 (85%)	3398 (88%)	344 (9%)	134 (4%)	3 27

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	72	GLU
1	A	169	ASN
1	A	189	ARG
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	410	GLY
1	A	1403	GLU
1	A	1405	THR
2	B	341	LEU
2	B	344	LYS
2	B	473	MET
2	B	867	GLY
2	B	879	ARG
2	B	943	SER
2	B	1046	PRO
2	B	1157	ALA

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Mol	Chain	Res	Type
2	B	1181	GLU
2	B	1185	CYS
4	D	18	VAL
4	D	199	ASN
8	H	90	ALA
9	I	9	ASP
10	J	6	ARG
10	J	55	ASP
12	L	53	HIS
1	A	43	GLU
1	A	47	ARG
1	A	54	ASN
1	A	58	LEU
1	A	76	GLU
1	A	178	GLY
1	A	195	ASP
1	A	224	PHE
1	A	465	TYR
1	A	628	GLY
1	A	1124	HIS
1	A	1175	SER
2	B	108	VAL
2	B	229	ALA
2	B	251	ILE
2	B	282	ILE
2	B	338	GLY
2	B	629	ASP
2	B	643	ASP
2	B	707	PRO
2	B	711	GLU
2	B	731	VAL
2	B	772	ALA
2	B	880	THR
2	B	1066	SER
2	B	1167	GLY
2	B	1175	LEU
2	B	1176	ASN
2	B	1190	ASP
3	C	215	GLU
4	D	16	LYS
4	D	137	ASN
5	E	45	LYS

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Mol	Chain	Res	Type
7	G	154	VAL
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
9	I	95	THR
12	L	45	ALA
12	L	59	ALA
1	A	35	ILE
1	A	74	MET
1	A	131	SER
1	A	167	CYS
1	A	399	HIS
1	A	1281	ARG
2	B	67	SER
2	B	792	MET
2	B	883	LEU
2	B	1223	ASP
4	D	15	LEU
4	D	52	LEU
4	D	119	ARG
5	E	36	GLU
6	F	73	ALA
8	H	17	PRO
10	J	2	ILE
10	J	30	LEU
11	K	114	LEU
12	L	56	LEU
1	A	156	ASP
1	A	449	SER
1	A	525	GLN
1	A	567	LYS
1	A	569	LYS
1	A	870	GLU
1	A	975	HIS
1	A	1173	HIS
1	A	1438	THR
2	B	262	GLU
2	B	339	THR
2	B	340	ALA
2	B	751	VAL
2	B	942	ARG
4	D	11	ARG

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Mol	Chain	Res	Type
5	E	104	ASN
5	E	137	GLU
7	G	2	PHE
8	H	60	ALA
8	H	128	ASN
12	L	26	THR
12	L	55	ILE
1	A	62	ASP
1	A	958	VAL
1	A	1122	PRO
1	A	1255	GLU
2	B	277	LYS
2	B	1155	SER
9	I	3	THR
10	J	29	GLU
12	L	50	ASP
1	A	73	GLY
1	A	333	GLU
2	B	343	ILE
2	B	619	ILE
2	B	902	GLY
2	B	1096	ARG
1	A	310	GLY
7	G	63	PRO
1	A	61	ILE
1	A	196	GLU
1	A	1437	GLY
1	A	1242	VAL

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
1	A	1240/1519 (82%)	1065 (86%)	175 (14%)	3 19
2	B	966/1061 (91%)	830 (86%)	136 (14%)	3 19
3	C	234/274 (85%)	199 (85%)	35 (15%)	3 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	160/200 (80%)	129 (81%)	31 (19%)	1 7
5	E	196/197 (100%)	174 (89%)	22 (11%)	6 27
6	F	74/137 (54%)	69 (93%)	5 (7%)	16 48
7	G	152/152 (100%)	133 (88%)	19 (12%)	4 23
8	H	117/128 (91%)	105 (90%)	12 (10%)	7 32
9	I	113/116 (97%)	102 (90%)	11 (10%)	8 33
10	J	60/65 (92%)	51 (85%)	9 (15%)	3 17
11	K	99/102 (97%)	86 (87%)	13 (13%)	4 21
12	L	40/57 (70%)	27 (68%)	13 (32%)	0 2
All	All	3451/4008 (86%)	2970 (86%)	481 (14%)	3 20

All (481) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	15	LYS
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	47	ARG
1	A	62	ASP
1	A	63	ARG
1	A	64	ASN
1	A	65	LEU
1	A	67	CYS
1	A	90	VAL
1	A	93	VAL
1	A	157	ASP
1	A	159	THR
1	A	174	ILE
1	A	175	ARG
1	A	188	ASP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	219	PHE
1	A	220	THR

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Mol	Chain	Res	Type
1	A	225	ASN
1	A	252	PHE
1	A	255	SER
1	A	256	GLN
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	289	ILE
1	A	295	LEU
1	A	307	ASP
1	A	313	GLN
1	A	322	VAL
1	A	324	SER
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	375	THR
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	411	ASP
1	A	423	ASP
1	A	425	GLN
1	A	427	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS

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Mol	Chain	Res	Type
1	A	517	ASN
1	A	518	LYS
1	A	532	ARG
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	582	ILE
1	A	593	GLU
1	A	596	THR
1	A	598	LEU
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	711	ARG
1	A	738	LYS
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	896	ARG
1	A	904	THR
1	A	915	SER

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Mol	Chain	Res	Type
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	973	ILE
1	A	976	THR
1	A	998	LEU
1	A	999	VAL
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1038	THR
1	A	1052	GLN
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1096	SER
1	A	1100	ARG
1	A	1116	LEU
1	A	1124	HIS
1	A	1133	LEU
1	A	1170	ILE
1	A	1172	LEU
1	A	1173	HIS
1	A	1174	PHE
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1222	ASN
1	A	1233	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1259	MET
1	A	1264	GLU
1	A	1273	LEU
1	A	1288	ASP
1	A	1293	SER
1	A	1295	THR

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Mol	Chain	Res	Type
1	A	1297	GLU
1	A	1303	GLU
1	A	1308	THR
1	A	1315	GLU
1	A	1316	VAL
1	A	1325	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1453	TYR
1	A	1454	MET
2	B	21	GLU
2	B	25	ILE
2	B	26	THR
2	B	46	GLN
2	B	56	ASP
2	B	63	ILE
2	B	100	PRO
2	B	101	MET
2	B	110	HIS
2	B	126	SER
2	B	178	ASN
2	B	187	SER
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	251	ILE

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	272	THR
2	B	277	LYS
2	B	278	GLN
2	B	279	ASP
2	B	298	LEU
2	B	324	ILE
2	B	337	ARG
2	B	339	THR
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN
2	B	361	LEU
2	B	364	ILE
2	B	365	THR
2	B	367	LEU
2	B	395	GLN
2	B	398	ARG
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	426	LYS
2	B	430	ARG
2	B	436	VAL
2	B	446	LEU
2	B	448	ILE
2	B	453	ILE
2	B	469	GLN
2	B	470	LYS
2	B	481	GLN
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	490	SER
2	B	501	PRO
2	B	531	GLN
2	B	538	ASN
2	B	545	ILE
2	B	547	VAL
2	B	549	THR

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Mol	Chain	Res	Type
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	576	ASP
2	B	595	ARG
2	B	598	GLU
2	B	603	LEU
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	703	ILE
2	B	730	ARG
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	790	ASP
2	B	797	TYR
2	B	831	SER
2	B	835	GLN
2	B	839	MET
2	B	844	SER
2	B	868	MET
2	B	870	ILE
2	B	871	THR
2	B	878	GLN
2	B	882	THR
2	B	889	THR
2	B	906	SER
2	B	908	GLU
2	B	934	LYS
2	B	942	ARG
2	B	944	THR
2	B	946	ASN
2	B	964	VAL
2	B	969	ARG
2	B	970	THR

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1049	ASP
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1094	ARG
2	B	1096	ARG
2	B	1106	ARG
2	B	1112	GLN
2	B	1120	GLU
2	B	1128	LEU
2	B	1138	MET
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1201	LYS
2	B	1202	LEU
2	B	1210	MET
2	B	1212	ILE
3	C	3	GLU
3	C	11	ARG
3	C	23	SER
3	C	25	VAL
3	C	27	LEU
3	C	48	SER
3	C	52	GLU
3	C	53	THR

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Mol	Chain	Res	Type
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	78	GLU
3	C	79	GLN
3	C	83	SER
3	C	84	ARG
3	C	100	THR
3	C	108	GLU
3	C	121	VAL
3	C	122	SER
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	145	CYS
3	C	147	LEU
3	C	148	ARG
3	C	151	GLN
3	C	186	LEU
3	C	215	GLU
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	260	LEU
3	C	268	ASP
4	D	5	THR
4	D	6	SER
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	11	ARG
4	D	12	ARG
4	D	18	VAL
4	D	27	LEU
4	D	35	LEU
4	D	40	HIS
4	D	41	GLN
4	D	52	LEU
4	D	65	GLU
4	D	119	ARG

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Mol	Chain	Res	Type
4	D	126	ILE
4	D	127	ASP
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	153	ARG
4	D	156	ASP
4	D	177	VAL
4	D	182	SER
4	D	187	THR
4	D	197	SER
4	D	201	LYS
4	D	206	GLU
4	D	218	GLU
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	9	ILE
5	E	31	THR
5	E	37	LEU
5	E	49	SER
5	E	57	MET
5	E	72	PHE
5	E	84	ASP
5	E	92	THR
5	E	114	ASN
5	E	115	ASN
5	E	131	THR
5	E	140	LEU
5	E	146	HIS
5	E	150	VAL
5	E	166	LYS
5	E	171	LYS
5	E	173	SER
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	93	ILE

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Mol	Chain	Res	Type
6	F	115	THR
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	39	THR
7	G	64	THR
7	G	65	ASP
7	G	90	THR
7	G	93	SER
7	G	96	GLN
7	G	106	MET
7	G	118	ASP
7	G	131	GLN
7	G	133	SER
7	G	138	THR
7	G	143	ILE
7	G	155	SER
7	G	162	SER
7	G	171	ILE
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	76	THR
8	H	77	ARG
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	112	ILE
8	H	130	ARG
8	H	146	ARG
9	I	7	CYS
9	I	8	ARG
9	I	17	ARG
9	I	31	THR
9	I	35	VAL
9	I	74	GLU
9	I	81	ARG
9	I	83	ASN
9	I	86	PHE
9	I	94	ASP

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Mol	Chain	Res	Type
9	I	111	THR
10	J	2	ILE
10	J	7	CYS
10	J	13	VAL
10	J	16	ASP
10	J	22	LEU
10	J	23	ASN
10	J	48	ARG
10	J	52	THR
10	J	59	LYS
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	41	THR
11	K	47	ARG
11	K	51	LEU
11	K	91	CYS
11	K	101	LEU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
12	L	28	LYS
12	L	38	LEU
12	L	44	ASP
12	L	46	VAL
12	L	47	ARG
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	65	VAL
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	425	GLN

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Mol	Chain	Res	Type
1	A	545	GLN
1	A	548	ASN
1	A	648	ASN
1	A	811	GLN
1	A	994	GLN
1	A	1106	ASN
1	A	1124	HIS
1	A	1265	ASN
1	A	1270	ASN
1	A	1387	HIS
1	A	1390	ASN
1	A	1393	ASN
2	B	47	GLN
2	B	178	ASN
2	B	300	HIS
2	B	465	ASN
2	B	538	ASN
2	B	842	ASN
2	B	1025	HIS
2	B	1062	HIS
2	B	1084	GLN
2	B	1117	GLN
3	C	7	GLN
4	D	9	GLN
4	D	143	ASN
5	E	3	GLN
7	G	71	ASN
7	G	131	GLN
8	H	35	GLN
8	H	137	GLN
9	I	83	ASN
9	I	89	GLN
9	I	114	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/5 (60%)	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)

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	$\#\|Z\| > 2$
15	BRU	T	22	15,14	15,21,22	1.18	1 (6%)	17,30,33	2.46	3 (17%)

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
15	BRU	T	22	15,14	-	2/4/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	3.64	1.43	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	22	BRU	C4-N3-C2	8.73	122.52	115.14
15	T	22	BRU	C5-C4-N3	-4.03	118.81	123.64
15	T	22	BRU	BR-C5-C6	2.33	122.62	117.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	22	BRU	C3'-C4'-C5'-O5'
15	T	22	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	4.93
1	B	351:TYR	C	352:ALA	N	3.22

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	A	1422/1732 (82%)	-0.35	7 (0%) 91 88	48, 96, 156, 222	0
2	B	1115/1224 (91%)	-0.23	14 (1%) 77 71	51, 114, 178, 210	0
3	C	266/318 (83%)	-0.39	0 100 100	71, 100, 140, 168	0
4	D	178/221 (80%)	-0.26	1 (0%) 89 86	75, 112, 164, 183	0
5	E	214/215 (99%)	-0.32	2 (0%) 84 79	75, 130, 176, 189	0
6	F	84/155 (54%)	-0.51	0 100 100	51, 75, 104, 120	0
7	G	171/171 (100%)	-0.33	0 100 100	67, 95, 136, 154	0
8	H	133/146 (91%)	0.16	3 (2%) 60 54	109, 137, 176, 195	0
9	I	119/122 (97%)	-0.19	3 (2%) 57 51	109, 138, 177, 196	0
10	J	65/70 (92%)	-0.43	0 100 100	75, 97, 132, 146	0
11	K	115/120 (95%)	-0.40	1 (0%) 84 79	66, 97, 136, 155	0
12	L	46/70 (65%)	-0.05	2 (4%) 35 31	91, 157, 173, 180	0
13	N	10/14 (71%)	0.48	2 (20%) 1 1	192, 220, 260, 264	0
14	P	4/5 (80%)	-0.15	0 100 100	110, 121, 141, 167	0
15	T	17/26 (65%)	0.33	1 (5%) 22 20	122, 191, 266, 267	0
All	All	3959/4609 (85%)	-0.29	36 (0%) 84 79	48, 106, 172, 267	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	4.2
9	I	119	THR	3.9
1	A	194	ALA	3.4
1	A	1455	PRO	3.3
2	B	883	LEU	3.1
2	B	715	ALA	3.1
13	N	8	DT	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	340	ALA	2.9
4	D	13	ARG	2.9
2	B	709	ASP	2.9
12	L	26	THR	2.8
2	B	339	THR	2.7
12	L	25	ALA	2.7
1	A	251	SER	2.6
9	I	120	GLN	2.6
1	A	257	ARG	2.5
2	B	864	LYS	2.5
1	A	195	ASP	2.5
8	H	139	ASN	2.4
8	H	134	ASN	2.4
11	K	115	ALA	2.4
15	T	7	DT	2.4
2	B	476	ARG	2.4
2	B	918	ILE	2.4
1	A	256	GLN	2.4
5	E	123	LEU	2.3
2	B	250	PHE	2.3
2	B	865	LYS	2.3
2	B	475	SER	2.3
2	B	469	GLN	2.2
13	N	7	DC	2.2
2	B	724	ASP	2.1
9	I	118	ARG	2.1
2	B	708	GLU	2.1
8	H	86	ASP	2.1
5	E	110	PHE	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	BRU	T	22	20/21	0.90	0.12	144,154,161,166	0

6.3 Carbohydrates (i)

There are no carbohydrates 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
16	ZN	L	1071	1/1	0.96	0.06	154,154,154,154	0
16	ZN	I	1122	1/1	0.98	0.04	178,178,178,178	0
16	ZN	A	2456	1/1	0.98	0.07	133,133,133,133	0
17	MG	A	2458	1/1	0.99	0.14	59,59,59,59	0
16	ZN	J	1066	1/1	1.00	0.23	83,83,83,83	0
16	ZN	B	2225	1/1	1.00	0.18	74,74,74,74	0
16	ZN	I	1121	1/1	1.00	0.12	115,115,115,115	0
16	ZN	A	2457	1/1	1.00	0.15	64,64,64,64	0
16	ZN	C	1269	1/1	1.00	0.11	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.