Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:42 PM GMT

PDB ID	:	4A3J
Title	:	RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A 2NT DNA-RNA HYBRID AND SOAKED WITH GMPCPP
Authors	:	Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on	:	2011-09-30
Resolution	:	3.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

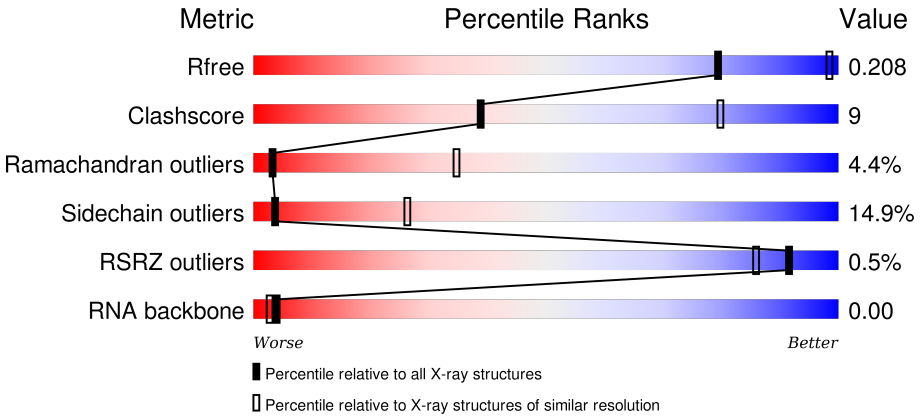
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.70 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.



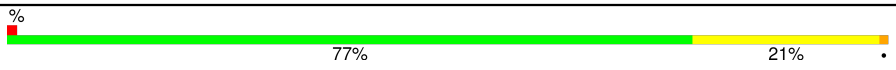
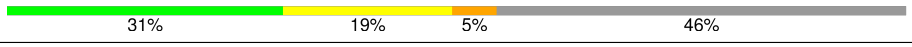
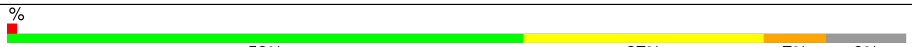
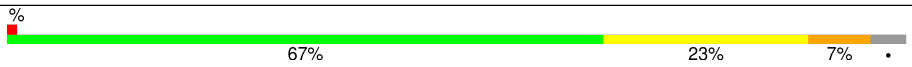
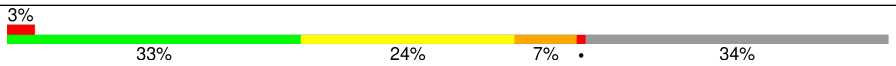
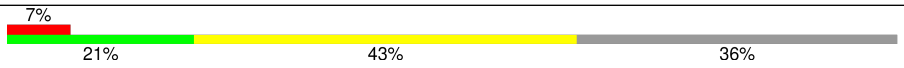
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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. 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	54% 23% • • 18%
2	B	1224	% 63% 23% • • 9%
3	C	318	54% 25% 5% • 16%
4	D	221	47% 29% 5% • 19%

Continued on next page...

Continued from previous page...

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	2	
15	T	27	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	G2P	T	1024	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 31802 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	1425	Total	C	N	O	S	0	0	0
			11197	7051	1958	2126	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 5'-D(*GP*TP*AP*GP*AP*AP*AP*GP*CP*TP*AP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	9	Total	C	N	O	P	0	0	0
			184	89	37	50	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	2	Total	C	N	O	P	0	0	0
			42	19	8	13	2			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*TP*CP*BRUP*AP*CP*CP *TP*GP*AP*AP*CP*AP*AP*CP*TP*AP*AP*CP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	16	Total	Br	C	N	O	P	0	0	0
			325	1	155	57	96	16			

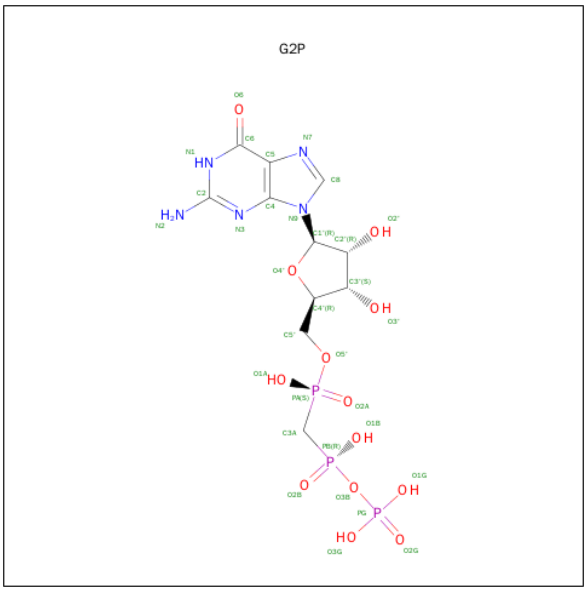
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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		

- Molecule 18 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



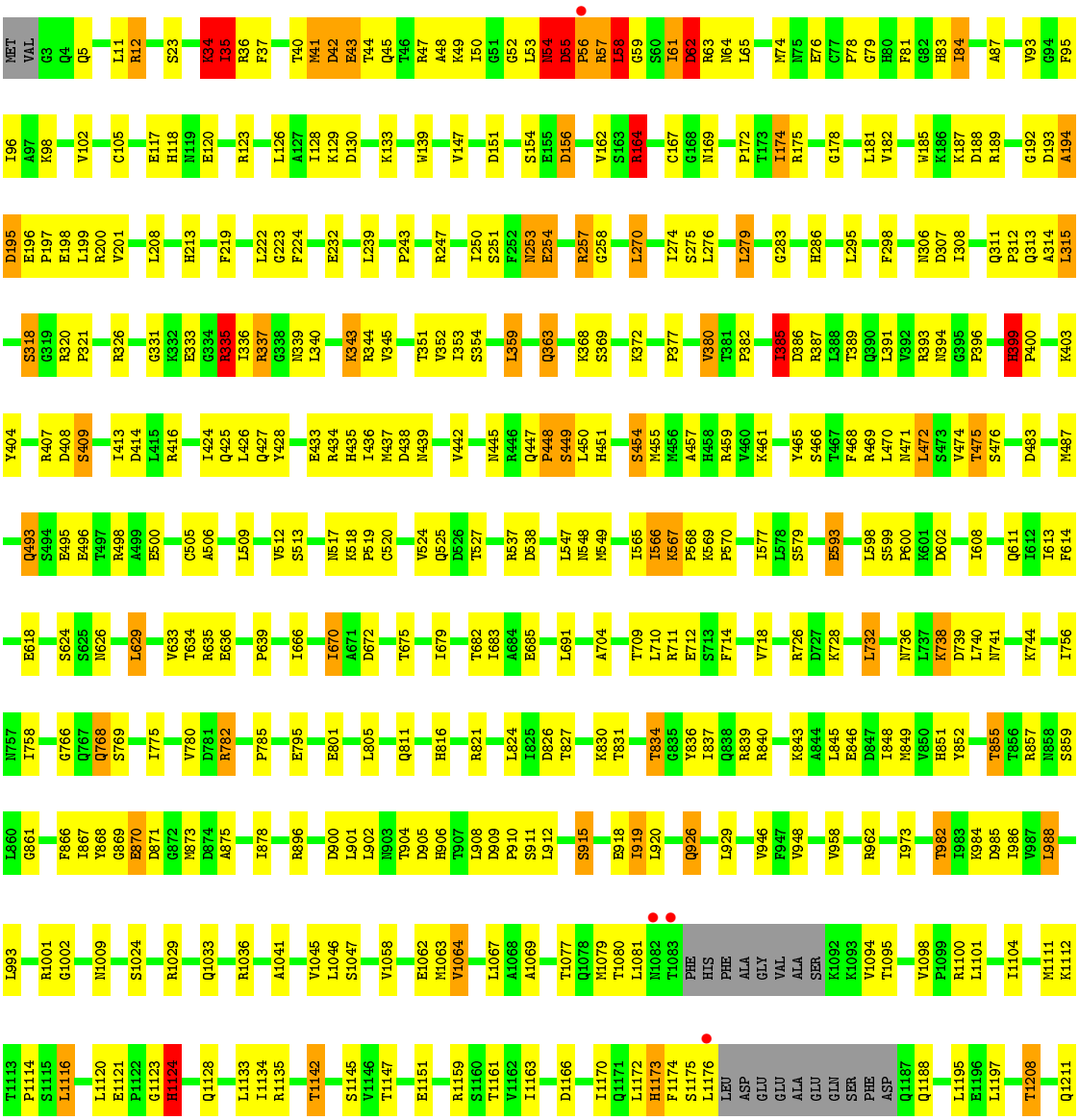
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	T	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

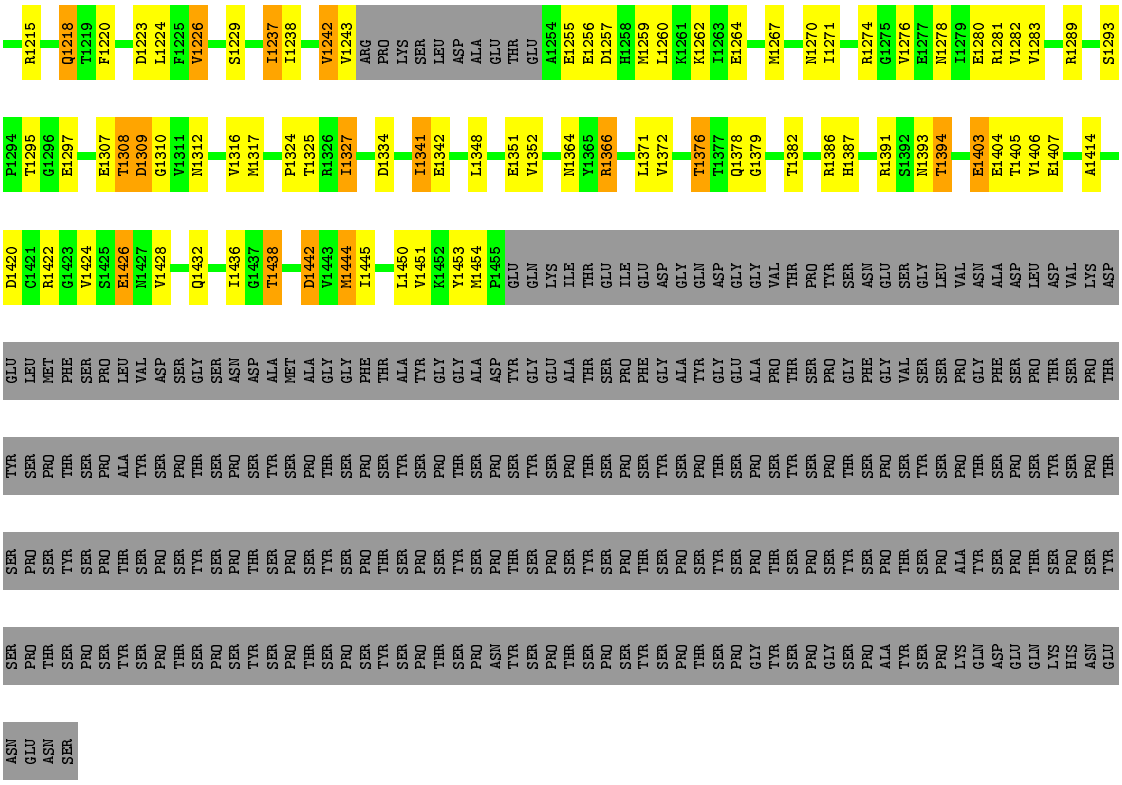
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

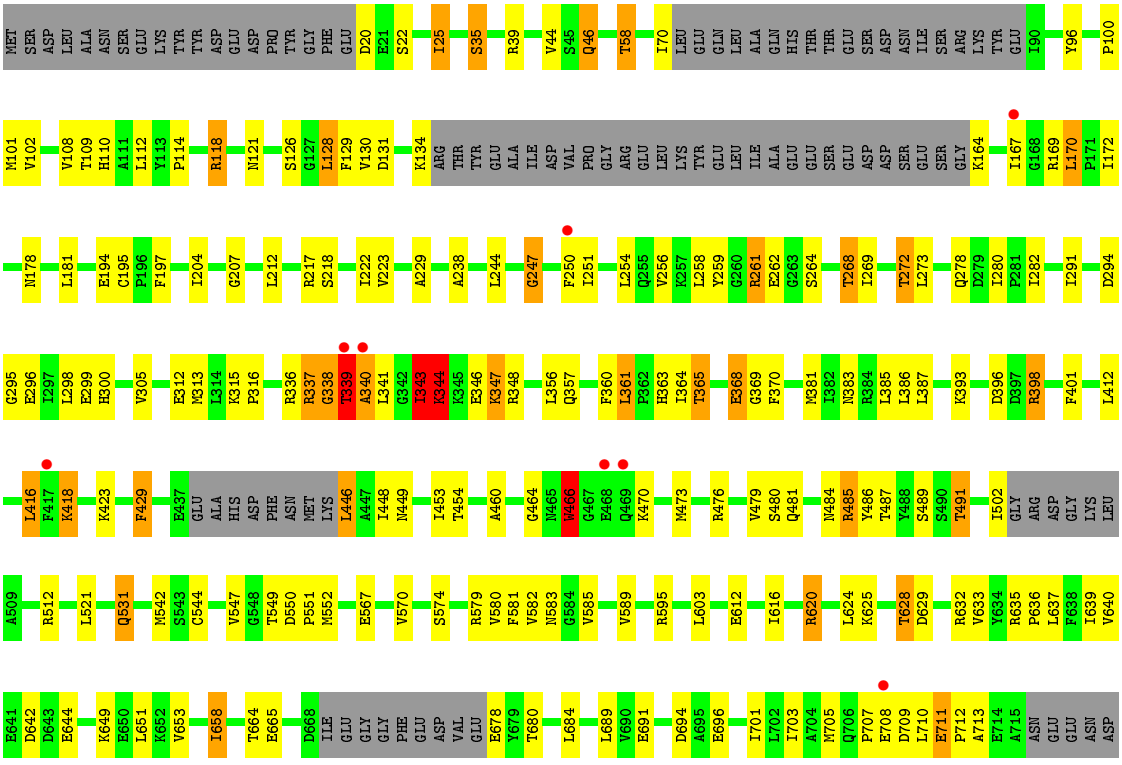
Chain A:

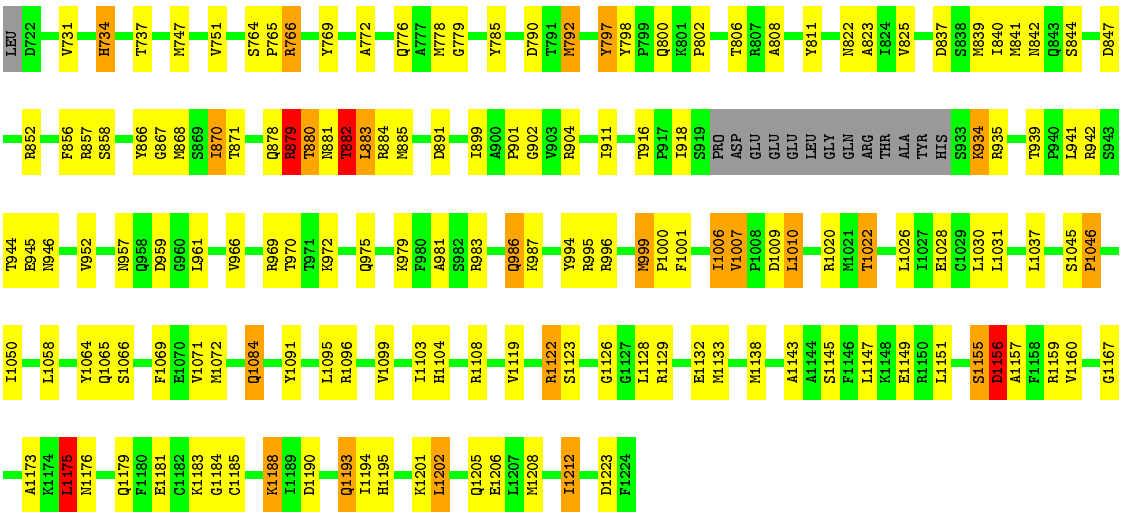




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

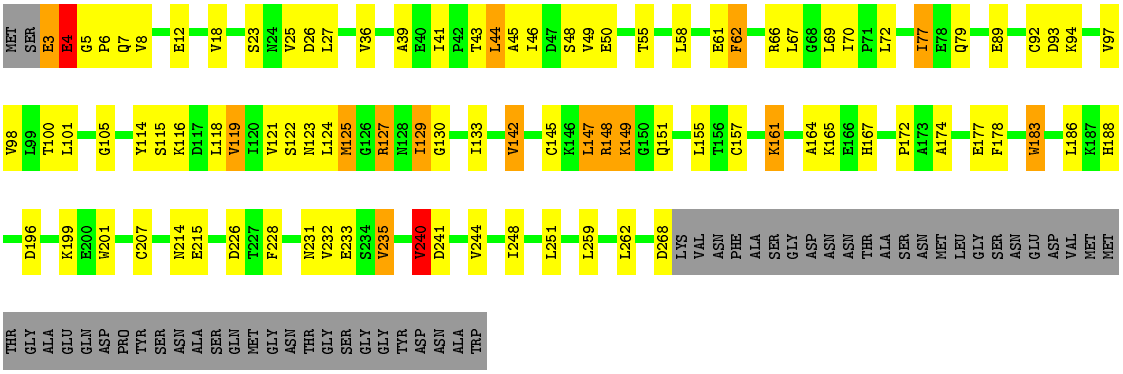
Chain B:





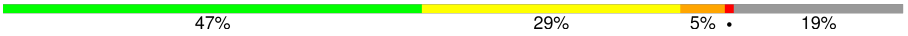
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

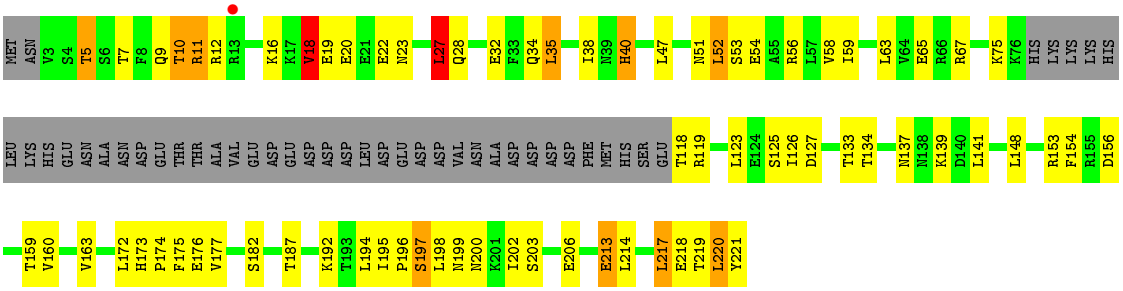
Chain C:



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

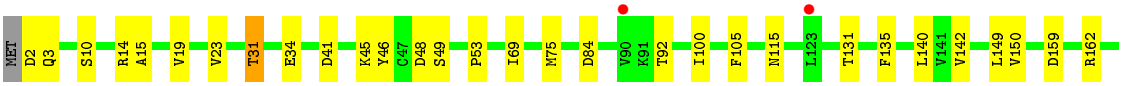
Chain D:

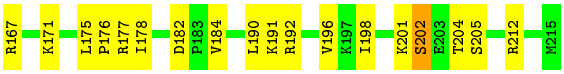




• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

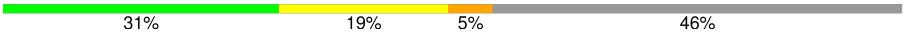
Chain E:

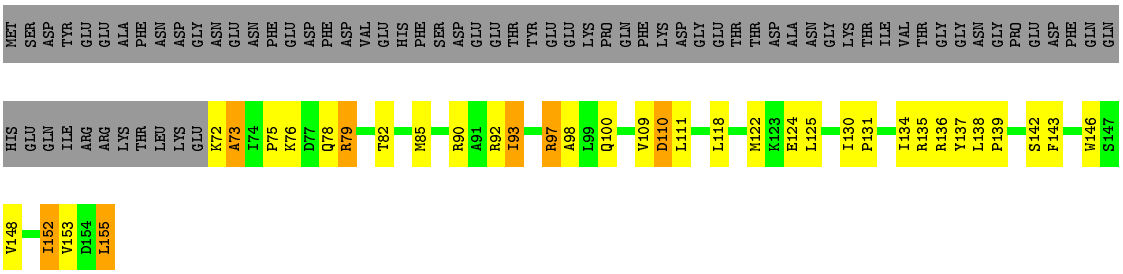




• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

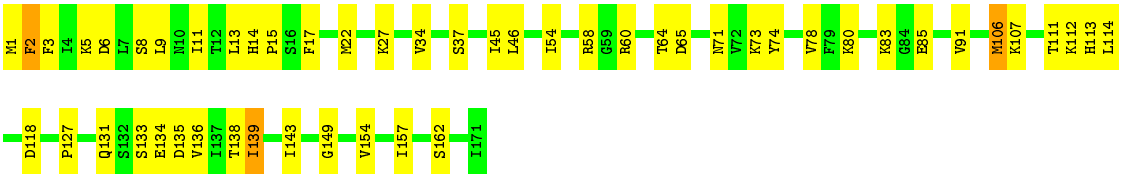
Chain F:





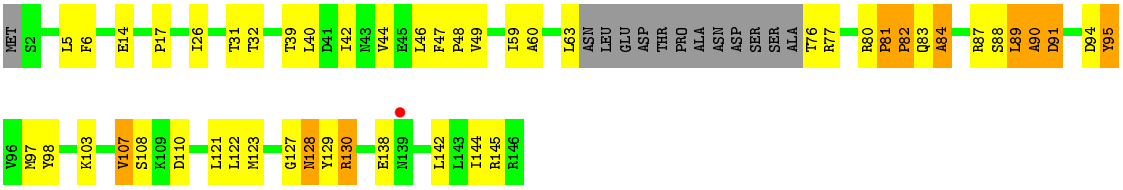
• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



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

Chain H:

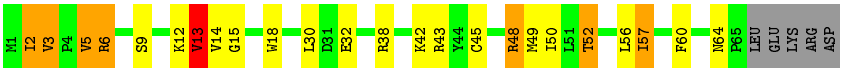


• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:

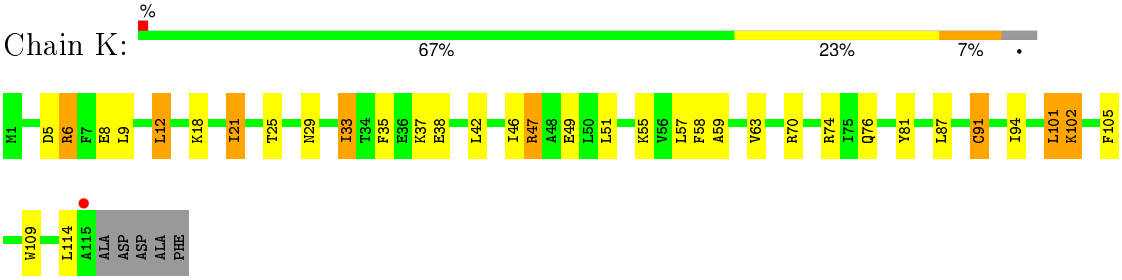
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



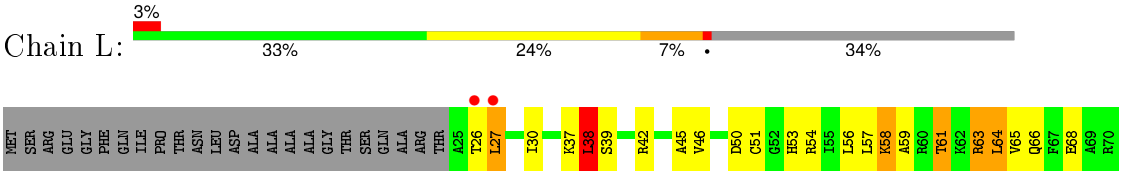
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



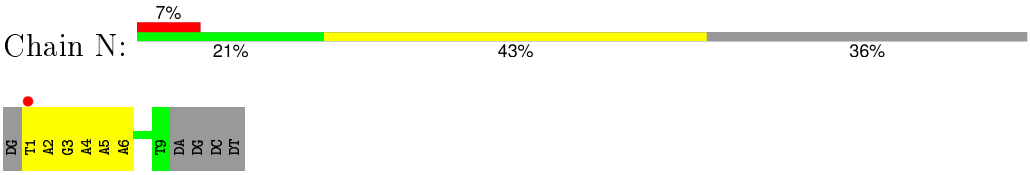
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:



• Molecule 13: 5'-D(*GP*TP*AP*GP*AP*AP*AP*GP*CP*TP*AP*GP*CP*TP)-3'

Chain N:

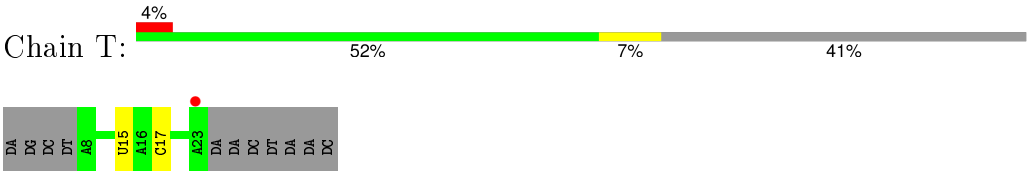


• Molecule 14: 5'-R(*CP*AP)-3'

Chain P:

• Molecule 15: 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*TP*CP*BRUP*AP*CP*CP *TP* GP*AP*AP*CP*AP*AP*CP*TP*AP*AP*CP)-3'

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	223.29Å 392.79Å 282.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 74.11 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.00-3.70) 97.2 (74.11-3.70)	Depositor EDS
R_{merge}	0.65	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.67Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.157 , 0.194 0.180 , 0.208	Depositor DCC
R_{free} test set	2526 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	117.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 111.4	EDS
Estimated twinning fraction	0.040 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.057 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 128365 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31802	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, G2P

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	0/11397	0.86	10/15415 (0.1%)
2	B	0.52	0/9029	0.82	4/12171 (0.0%)
3	C	0.50	0/2133	0.80	1/2891 (0.0%)
4	D	0.54	0/1444	0.85	0/1935
5	E	0.47	0/1788	0.73	0/2406
6	F	0.58	0/691	0.81	0/933
7	G	0.51	0/1368	0.81	0/1844
8	H	0.53	0/1086	0.84	0/1470
9	I	0.46	0/989	0.79	0/1331
10	J	0.52	0/541	0.85	1/727 (0.1%)
11	K	0.50	0/938	0.73	0/1267
12	L	0.54	0/365	0.93	0/485
13	N	1.33	2/207 (1.0%)	1.11	0/318
14	P	1.39	1/46 (2.2%)	0.81	0/69
15	T	1.25	0/340	0.97	0/519
All	All	0.55	3/32362 (0.0%)	0.83	16/43781 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	1	DT	C1'-N1	5.97	1.57	1.49
14	P	9	C	C1'-N1	5.92	1.57	1.48
13	N	1	DT	C3'-O3'	5.27	1.50	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	PRO	C-N-CA	6.46	137.85	121.70
2	B	340	ALA	C-N-CA	6.45	137.81	121.70
1	A	399	HIS	N-CA-CB	6.42	122.16	110.60
2	B	881	ASN	C-N-CA	6.39	137.67	121.70
1	A	34	LYS	C-N-CA	6.35	137.58	121.70
1	A	54	ASN	C-N-CA	6.29	137.43	121.70
1	A	35	ILE	CB-CA-C	5.63	122.87	111.60
1	A	57	ARG	C-N-CA	5.45	135.32	121.70
3	C	183	TRP	N-CA-C	-5.26	96.80	111.00
1	A	35	ILE	N-CA-CB	5.21	122.77	110.80
2	B	339	THR	C-N-CA	5.18	134.66	121.70
1	A	194	ALA	C-N-CA	5.18	134.64	121.70
2	B	1184	GLY	C-N-CA	5.09	134.43	121.70
1	A	223	GLY	C-N-CA	5.06	134.36	121.70
1	A	55	ASP	N-CA-CB	5.03	119.66	110.60
10	J	5	VAL	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

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	11197	0	11257	219	0
2	B	8859	0	8901	158	0
3	C	2095	0	2051	58	0
4	D	1434	0	1460	33	0
5	E	1752	0	1776	21	0
6	F	679	0	701	25	0
7	G	1340	0	1357	33	0
8	H	1068	0	1040	28	0
9	I	971	0	927	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	532	0	542	20	0
11	K	920	0	929	26	0
12	L	363	0	386	9	0
13	N	184	0	103	4	0
14	P	42	0	22	0	0
15	T	325	0	179	2	0
16	A	2	0	0	0	0
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
18	T	32	0	14	0	0
All	All	31802	0	31645	570	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 (570) 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	1.76	1.62
1:A:53:LEU:HD23	1:A:54:ASN:H	1.12	1.15
1:A:855:THR:HG21	1:A:857:ARG:HE	1.23	1.01
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.04	0.93
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.51	0.92
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.36	0.87
3:C:148:ARG:H	3:C:151:GLN:HG3	1.40	0.86
1:A:53:LEU:HD23	1:A:54:ASN:N	1.91	0.86
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.60	0.82
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.42	0.82
12:L:61:THR:HG21	12:L:63:ARG:HE	1.43	0.82
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.61	0.81
3:C:66:ARG:NH2	10:J:3:VAL:O	2.15	0.79
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.64	0.79
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.64	0.78
2:B:338:GLY:HA2	2:B:339:THR:HB	1.65	0.77
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.66	0.77
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.65	0.76
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:O	5:E:23:VAL:HG23	1.86	0.76
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.68	0.75
10:J:48:ARG:O	10:J:52:THR:HG22	1.87	0.75
2:B:882:THR:HG1	2:B:935:ARG:N	1.85	0.74
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.71	0.73
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.69	0.73
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.69	0.73
4:D:220:LEU:H	4:D:220:LEU:HD12	1.53	0.73
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.69	0.73
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.71	0.72
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.71	0.72
1:A:62:ASP:HB3	1:A:65:LEU:HB2	1.71	0.71
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.72	0.71
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.89	0.71
1:A:1077:THR:HG22	1:A:1081:LEU:HD12	1.72	0.71
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.72	0.71
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.31	0.71
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.73	0.71
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.26	0.70
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.27	0.70
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.72	0.69
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.73	0.69
6:F:118:LEU:O	6:F:122:MET:HG3	1.94	0.68
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.74	0.68
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.76	0.68
8:H:127:GLY:HA3	8:H:130:ARG:HH21	1.58	0.68
1:A:41:MET:HB2	1:A:49:LYS:HA	1.76	0.67
10:J:48:ARG:HE	10:J:49:MET:HE2	1.59	0.67
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.76	0.67
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.76	0.66
1:A:866:PHE:O	1:A:867:ILE:HD12	1.96	0.66
1:A:1100:ARG:O	1:A:1104:ILE:HG13	1.96	0.66
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.10	0.65
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.76	0.65
4:D:40:HIS:ND1	7:G:6:ASP:HB3	2.12	0.65
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.79	0.64
2:B:776:GLN:HA	2:B:1096:ARG:HH11	1.61	0.64
1:A:670:ILE:HG13	1:A:805:LEU:HD21	1.77	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.64
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.79	0.64
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:VAL:HG22	4:D:20:GLU:H	1.63	0.64
2:B:916:THR:HB	2:B:935:ARG:HG3	1.80	0.64
7:G:34:VAL:O	7:G:37:SER:HB3	1.98	0.63
3:C:148:ARG:N	3:C:151:GLN:HG3	2.13	0.63
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.79	0.63
1:A:870:GLU:O	5:E:205:SER:HB3	1.98	0.63
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.80	0.63
3:C:50:GLU:HB3	12:L:64:LEU:HD22	1.79	0.63
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.29	0.62
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.35	0.62
3:C:125:MET:SD	3:C:125:MET:N	2.73	0.62
1:A:855:THR:CG2	1:A:857:ARG:HE	2.07	0.62
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.64	0.62
4:D:35:LEU:HD11	4:D:173:HIS:HB3	1.82	0.62
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.35	0.61
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.82	0.61
1:A:343:LYS:HD3	2:B:1156:ASP:HB2	1.82	0.61
2:B:338:GLY:HA2	2:B:339:THR:CB	2.30	0.61
8:H:82:PRO:C	8:H:84:ALA:H	2.02	0.61
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.83	0.61
2:B:296:GLU:O	2:B:300:HIS:HD2	1.83	0.61
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.36	0.61
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.31	0.60
2:B:797:TYR:HB2	2:B:852:ARG:O	2.01	0.60
2:B:1006:ILE:HG23	10:J:43:ARG:HD2	1.83	0.60
3:C:98:VAL:H	3:C:122:SER:HB3	1.66	0.60
3:C:43:THR:HG22	3:C:44:LEU:H	1.64	0.60
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.84	0.60
1:A:855:THR:HG21	1:A:857:ARG:NE	2.05	0.60
9:I:72:ASP:O	9:I:81:ARG:HG2	2.01	0.60
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.17	0.60
1:A:824:LEU:HD11	2:B:765:PRO:HB3	1.84	0.60
3:C:46:ILE:HD13	3:C:67:LEU:O	2.02	0.60
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.67	0.60
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.84	0.59
3:C:142:VAL:HG22	10:J:15:GLY:HA3	1.84	0.59
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.84	0.59
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.84	0.59
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.83	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.84	0.59
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.85	0.58
1:A:827:THR:O	1:A:831:THR:HB	2.03	0.58
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.68	0.58
2:B:705:MET:H	2:B:710:LEU:HD12	1.68	0.58
2:B:642:ASP:HA	2:B:649:LYS:HA	1.86	0.58
8:H:89:LEU:C	8:H:91:ASP:H	2.05	0.58
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.86	0.58
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.86	0.58
3:C:3:GLU:HB3	3:C:7:GLN:HE22	1.69	0.58
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.67	0.58
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.86	0.57
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.04	0.57
2:B:620:ARG:HD2	9:I:62:ILE:HD11	1.85	0.57
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.04	0.57
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.69	0.57
1:A:53:LEU:CD2	1:A:54:ASN:H	2.03	0.57
7:G:114:LEU:HD12	7:G:162:SER:HB2	1.86	0.57
1:A:414:ASP:OD1	1:A:416:ARG:HB2	2.05	0.57
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.86	0.57
2:B:261:ARG:H	2:B:264:SER:HB3	1.70	0.56
11:K:18:LYS:HE3	11:K:38:GLU:HG2	1.87	0.56
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.87	0.56
1:A:472:LEU:O	1:A:475:THR:HB	2.06	0.56
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.88	0.56
2:B:35:SER:HA	2:B:811:TYR:HE1	1.69	0.56
13:N:5:DA:H2"	13:N:6:DA:C8	2.40	0.56
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.87	0.56
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.88	0.56
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.70	0.56
3:C:100:THR:CG2	3:C:119:VAL:HG13	2.36	0.56
1:A:512:VAL:HA	1:A:519:PRO:HA	1.87	0.56
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.85	0.56
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.87	0.56
2:B:35:SER:HA	2:B:811:TYR:CE1	2.41	0.55
1:A:714:PHE:O	1:A:718:VAL:HG23	2.07	0.55
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.42	0.55
6:F:72:LYS:HE3	6:F:142:SER:HB3	1.87	0.55
2:B:806:THR:HG22	2:B:808:ALA:H	1.72	0.55
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.89	0.55
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.89	0.55
2:B:512:ARG:NH1	2:B:531:GLN:O	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.41	0.55
3:C:124:LEU:HD22	3:C:129:ILE:HG22	1.89	0.55
1:A:982:THR:HB	1:A:985:ASP:H	1.72	0.54
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.37	0.54
3:C:165:LYS:O	11:K:6:ARG:NH1	2.40	0.54
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.71	0.54
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.88	0.54
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.71	0.54
11:K:42:LEU:HG	11:K:46:ILE:CD1	2.38	0.54
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.71	0.54
4:D:47:LEU:HD21	7:G:3:PHE:CD1	2.43	0.54
8:H:47:PHE:HB3	8:H:95:TYR:HD2	1.70	0.54
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.08	0.54
3:C:43:THR:HG22	3:C:44:LEU:N	2.23	0.54
6:F:100:GLN:HG2	7:G:15:PRO:HB3	1.90	0.54
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.89	0.54
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.42	0.54
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.38	0.54
1:A:565:ILE:O	1:A:570:PRO:HA	2.08	0.54
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.90	0.54
1:A:900:ASP:HB3	1:A:906:HIS:HB2	1.90	0.54
2:B:542:MET:HG2	2:B:747:MET:HE3	1.89	0.53
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.89	0.53
1:A:353:ILE:HD13	1:A:487:MET:CE	2.38	0.53
11:K:42:LEU:HG	11:K:46:ILE:HD11	1.88	0.53
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.89	0.53
11:K:87:LEU:O	11:K:91:CYS:HB2	2.08	0.53
3:C:172:PRO:O	3:C:235:VAL:HG23	2.08	0.53
5:E:19:VAL:HG22	5:E:140:LEU:HD22	1.90	0.53
1:A:194:ALA:HA	1:A:195:ASP:C	2.28	0.53
1:A:741:ASN:HB3	1:A:744:LYS:HB2	1.90	0.53
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	1.90	0.53
1:A:1224:LEU:HD23	1:A:1226:VAL:HG22	1.89	0.53
2:B:315:LYS:N	2:B:316:PRO:HD2	2.24	0.52
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.91	0.52
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.90	0.52
2:B:344:LYS:HB3	2:B:347:LYS:HB2	1.90	0.52
3:C:100:THR:HG22	3:C:119:VAL:HG13	1.91	0.52
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.90	0.52
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.74	0.52
2:B:880:THR:HB	2:B:934:LYS:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1037:LEU:HD21	2:B:1064:TYR:HE2	1.75	0.52
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.92	0.52
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.91	0.52
9:I:82:GLU:HB3	9:I:104:LEU:HB2	1.92	0.52
3:C:105:GLY:HA3	3:C:149:LYS:O	2.10	0.52
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.44	0.52
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.92	0.52
1:A:451:HIS:HB2	1:A:454:SER:HB2	1.92	0.52
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.91	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.52
3:C:62:PHE:O	3:C:66:ARG:HG3	2.09	0.51
1:A:1077:THR:CG2	1:A:1081:LEU:HD12	2.41	0.51
1:A:55:ASP:H	1:A:56:PRO:HD3	1.75	0.51
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.51
2:B:1181:GLU:HG3	2:B:1188:LYS:HG2	1.92	0.51
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.92	0.51
2:B:291:ILE:HD12	2:B:291:ILE:H	1.75	0.51
4:D:172:LEU:HB2	4:D:177:VAL:HG22	1.92	0.51
1:A:359:LEU:HD13	1:A:363:GLN:HG3	1.93	0.51
2:B:361:LEU:HD11	2:B:381:MET:HE1	1.91	0.51
8:H:5:LEU:HB2	8:H:59:ILE:HG22	1.93	0.51
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.93	0.51
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.45	0.51
1:A:63:ARG:HG3	1:A:74:MET:HG3	1.92	0.51
4:D:40:HIS:CB	7:G:73:LYS:HE3	2.40	0.51
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.73	0.51
7:G:1:MET:CG	7:G:2:PHE:H	2.23	0.51
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.44	0.51
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.92	0.51
1:A:1379:GLY:HA2	5:E:177:ARG:O	2.11	0.51
1:A:831:THR:O	1:A:834:THR:HG22	2.11	0.51
3:C:18:VAL:HG22	11:K:109:TRP:HZ3	1.76	0.51
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.75	0.51
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.72	0.50
1:A:449:SER:HA	1:A:454:SER:HB3	1.92	0.50
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.10	0.50
1:A:1229:SER:HB3	1:A:1237:ILE:H	1.76	0.50
1:A:182:VAL:HB	1:A:201:VAL:HG23	1.92	0.50
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.93	0.50
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.47	0.50
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:91:VAL:HG22	7:G:143:ILE:HD12	1.93	0.50
1:A:982:THR:H	1:A:985:ASP:HB2	1.76	0.50
7:G:1:MET:CG	7:G:2:PHE:N	2.75	0.50
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.93	0.50
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.47	0.50
1:A:857:ARG:HD3	1:A:861:GLY:O	2.11	0.50
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.44	0.50
1:A:387:ARG:NH1	1:A:437:MET:HE1	2.26	0.50
2:B:336:ARG:HH21	2:B:337:ARG:HH21	1.58	0.50
7:G:106:MET:HG2	7:G:107:LYS:N	2.25	0.50
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.12	0.50
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.94	0.50
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.60	0.50
7:G:83:LYS:HD3	7:G:149:GLY:HA2	1.94	0.50
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.93	0.50
13:N:2:DA:H4'	13:N:3:DG:OP1	2.12	0.50
1:A:315:LEU:HA	1:A:321:PRO:HA	1.93	0.50
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.27	0.49
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.93	0.49
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.94	0.49
5:E:15:ALA:O	5:E:19:VAL:HG23	2.11	0.49
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.47	0.49
2:B:840:ILE:CG2	2:B:994:TYR:HD2	2.25	0.49
1:A:471:ASN:O	1:A:474:VAL:HG12	2.13	0.49
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.94	0.49
7:G:111:THR:HG22	7:G:113:HIS:H	1.77	0.49
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.49
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.94	0.49
2:B:792:MET:H	2:B:857:ARG:HA	1.78	0.49
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.48	0.49
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.93	0.49
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.95	0.49
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.20	0.49
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.95	0.49
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.95	0.49
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.46	0.49
13:N:5:DA:H2"	13:N:6:DA:H8	1.76	0.48
2:B:579:ARG:HA	2:B:589:VAL:HG12	1.94	0.48
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.47	0.48
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.95	0.48
1:A:709:THR:HB	1:A:712:GLU:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:HB3	2:B:1201:LYS:HE3	1.95	0.48
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.94	0.48
1:A:337:ARG:NH2	15:T:17:DC:OP1	2.46	0.48
4:D:159:THR:O	4:D:163:VAL:HG23	2.14	0.48
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.96	0.48
4:D:54:GLU:O	4:D:58:VAL:HG23	2.13	0.48
1:A:1220:PHE:HE2	1:A:1267:MET:HG3	1.78	0.48
4:D:220:LEU:H	4:D:220:LEU:CD1	2.22	0.48
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.48
1:A:1135:ARG:HG2	1:A:1282:VAL:HG12	1.95	0.48
9:I:50:THR:HG22	9:I:52:ILE:H	1.78	0.48
2:B:1037:LEU:HD21	2:B:1064:TYR:CE2	2.48	0.48
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.95	0.48
1:A:629:LEU:O	1:A:633:VAL:HG23	2.14	0.48
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.94	0.48
8:H:142:LEU:HG	8:H:144:ILE:HD11	1.95	0.48
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.95	0.48
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.96	0.48
1:A:275:SER:O	1:A:279:LEU:HB2	2.14	0.48
1:A:58:LEU:HB3	1:A:59:GLY:H	1.47	0.48
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.96	0.48
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.55	0.48
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.96	0.47
1:A:352:VAL:HB	2:B:1099:VAL:HG23	1.95	0.47
4:D:7:THR:HG21	7:G:5:LYS:HZ2	1.79	0.47
1:A:98:LYS:O	1:A:102:VAL:HG23	2.13	0.47
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.96	0.47
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.96	0.47
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.96	0.47
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.97	0.47
8:H:81:PRO:CB	8:H:82:PRO:HD3	2.44	0.47
11:K:35:PHE:O	11:K:70:ARG:HA	2.14	0.47
1:A:1172:LEU:C	1:A:1174:PHE:H	2.17	0.47
1:A:306:ASN:OD1	1:A:314:ALA:HB3	2.15	0.47
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.50	0.47
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.97	0.47
2:B:1071:VAL:HG13	2:B:1084:GLN:HG3	1.97	0.47
5:E:159:ASP:HA	5:E:162:ARG:NH1	2.29	0.47
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.97	0.47
1:A:1438:THR:O	6:F:92:ARG:HD2	2.15	0.47
1:A:257:ARG:HB3	1:A:258:GLY:H	1.52	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:CG2	3:C:44:LEU:H	2.27	0.47
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.97	0.47
7:G:106:MET:HG3	7:G:157:ILE:O	2.15	0.47
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.97	0.47
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.15	0.47
1:A:537:ARG:HG2	8:H:121:LEU:HD23	1.95	0.47
1:A:851:HIS:HB3	6:F:139:PRO:HD3	1.96	0.47
4:D:18:VAL:HG22	4:D:20:GLU:N	2.30	0.46
2:B:879:ARG:HG3	2:B:883:LEU:HD23	1.97	0.46
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.97	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.46
8:H:127:GLY:CA	8:H:130:ARG:HH21	2.25	0.46
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.98	0.46
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.97	0.46
2:B:797:TYR:HB3	2:B:798:TYR:HD1	1.81	0.46
13:N:4:DA:H2"	13:N:5:DA:C8	2.51	0.46
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.97	0.46
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.51	0.46
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.98	0.46
2:B:580:VAL:HG13	2:B:624:LEU:HD23	1.97	0.46
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.98	0.46
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.96	0.46
3:C:124:LEU:O	3:C:127:ARG:HG2	2.16	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.49	0.46
3:C:6:PRO:HB2	11:K:101:LEU:HD23	1.98	0.46
6:F:76:LYS:HA	6:F:79:ARG:CD	2.42	0.46
2:B:765:PRO:O	2:B:769:TYR:HD1	1.99	0.46
1:A:709:THR:HG23	9:I:94:ASP:HA	1.98	0.46
10:J:2:ILE:HD12	10:J:57:ILE:HD13	1.98	0.46
1:A:908:LEU:HB3	1:A:912:LEU:HD12	1.98	0.46
2:B:295:GLY:H	2:B:298:LEU:HD12	1.81	0.46
4:D:5:THR:HG21	7:G:74:TYR:OH	2.16	0.46
11:K:55:LYS:HB3	11:K:81:TYR:CE2	2.51	0.45
1:A:726:ARG:CD	1:A:766:GLY:HA3	2.45	0.45
1:A:524:VAL:HG12	1:A:525:GLN:H	1.81	0.45
3:C:58:LEU:HD12	3:C:145:CYS:SG	2.56	0.45
2:B:825:VAL:HG13	2:B:1010:LEU:HB3	1.98	0.45
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.81	0.45
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.83	0.45
3:C:46:ILE:H	3:C:46:ILE:HD12	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:VAL:HB	1:A:1307:GLU:HB2	1.98	0.45
4:D:213:GLU:O	4:D:217:LEU:HD12	2.16	0.45
1:A:826:ASP:HB2	1:A:830:LYS:HD2	1.97	0.45
7:G:138:THR:HG22	7:G:139:ILE:H	1.82	0.45
3:C:164:ALA:HA	3:C:167:HIS:O	2.16	0.45
2:B:823:ALA:O	2:B:825:VAL:HG23	2.16	0.45
1:A:869:GLY:O	5:E:204:THR:HG21	2.17	0.45
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.81	0.45
1:A:382:PRO:HA	1:A:428:TYR:HE1	1.81	0.45
10:J:30:LEU:HD21	10:J:38:ARG:HH12	1.81	0.45
10:J:48:ARG:HE	10:J:49:MET:CE	2.27	0.45
3:C:3:GLU:HB3	3:C:7:GLN:NE2	2.32	0.45
7:G:138:THR:HG22	7:G:139:ILE:N	2.32	0.45
1:A:1450:LEU:HD12	6:F:131:PRO:HG3	1.99	0.45
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.41	0.45
8:H:6:PHE:HB3	8:H:59:ILE:HB	1.98	0.45
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.99	0.45
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.98	0.45
8:H:63:LEU:C	8:H:90:ALA:HB3	2.37	0.45
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.17	0.45
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.99	0.45
10:J:9:SER:OG	10:J:48:ARG:NH2	2.49	0.45
1:A:915:SER:O	1:A:918:GLU:HG3	2.17	0.45
11:K:6:ARG:O	11:K:9:LEU:HD12	2.16	0.44
2:B:295:GLY:O	2:B:299:GLU:HB2	2.18	0.44
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.98	0.44
1:A:185:TRP:HE3	1:A:185:TRP:H	1.65	0.44
2:B:778:MET:HB3	2:B:779:GLY:H	1.64	0.44
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.99	0.44
8:H:47:PHE:CB	8:H:95:TYR:HD2	2.29	0.44
2:B:640:VAL:HA	2:B:651:LEU:HA	2.00	0.44
5:E:176:PRO:O	5:E:212:ARG:HA	2.18	0.44
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.57	0.44
1:A:42:ASP:O	1:A:44:THR:N	2.51	0.44
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.99	0.44
2:B:1201:LYS:HE2	2:B:1205:GLN:HE22	1.82	0.44
7:G:131:GLN:HA	7:G:136:VAL:HG22	2.00	0.44
2:B:291:ILE:HD12	2:B:291:ILE:N	2.33	0.44
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.17	0.44
12:L:61:THR:HG21	12:L:63:ARG:NE	2.22	0.44
4:D:52:LEU:H	4:D:182:SER:HB3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.00	0.44
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.85	0.44
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.33	0.44
1:A:849:MET:HB3	1:A:1063:MET:SD	2.57	0.44
8:H:89:LEU:O	8:H:91:ASP:N	2.48	0.44
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.18	0.44
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.83	0.44
6:F:111:LEU:H	6:F:111:LEU:HD12	1.82	0.44
1:A:780:VAL:O	1:A:782:ARG:HD3	2.18	0.44
4:D:198:LEU:O	4:D:200:ASN:N	2.51	0.44
4:D:18:VAL:HG13	4:D:19:GLU:HA	2.00	0.44
1:A:675:THR:HG21	1:A:736:ASN:HB2	2.00	0.44
1:A:447:GLN:HA	1:A:448:PRO:C	2.37	0.44
4:D:59:ILE:HG21	4:D:141:LEU:HD11	1.99	0.44
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.53	0.44
7:G:1:MET:CE	7:G:80:LYS:O	2.66	0.43
11:K:59:ALA:HA	11:K:74:ARG:O	2.18	0.43
1:A:41:MET:CB	1:A:49:LYS:HA	2.45	0.43
1:A:354:SER:O	1:A:469:ARG:HA	2.18	0.43
2:B:902:GLY:O	12:L:65:VAL:HG11	2.17	0.43
10:J:14:VAL:HG13	10:J:50:ILE:HD11	2.00	0.43
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.20	0.43
2:B:879:ARG:HB3	2:B:880:THR:H	1.51	0.43
11:K:8:GLU:O	11:K:37:LYS:HD3	2.18	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.99	0.43
12:L:61:THR:HB	12:L:63:ARG:HG2	1.99	0.43
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.83	0.43
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.99	0.43
2:B:247:GLY:H	2:B:418:LYS:NZ	2.17	0.43
1:A:442:VAL:O	1:A:457:ALA:HA	2.18	0.43
1:A:1215:ARG:O	1:A:1218:GLN:HG2	2.18	0.43
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
4:D:154:PHE:HB2	4:D:160:VAL:HG22	2.01	0.43
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.83	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
2:B:446:LEU:HD12	2:B:448:ILE:HD11	2.01	0.43
1:A:49:LYS:HD3	1:A:61:ILE:HG13	2.00	0.43
2:B:918:ILE:HG12	2:B:935:ARG:NH2	2.32	0.43
4:D:202:ILE:HD11	4:D:206:GLU:HB3	2.01	0.43
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.84	0.43
1:A:984:LYS:O	1:A:988:LEU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:HA	2:B:112:LEU:H	1.83	0.43
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.99	0.43
1:A:466:SER:HB2	2:B:1099:VAL:HG13	2.01	0.43
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.82	0.43
2:B:1173:ALA:HB1	2:B:1175:LEU:HD23	2.01	0.43
6:F:109:VAL:HG22	6:F:110:ASP:N	2.34	0.43
1:A:1386:ARG:CD	15:T:15:BRU:H2"	2.48	0.43
3:C:101:LEU:HD12	3:C:118:LEU:HG	1.99	0.43
2:B:911:ILE:HD11	2:B:941:LEU:HD13	2.00	0.43
4:D:27:LEU:HD23	4:D:197:SER:HB3	2.00	0.43
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.34	0.43
2:B:957:ASN:HB3	2:B:961:LEU:H	1.82	0.43
4:D:63:LEU:O	4:D:133:THR:HG21	2.18	0.43
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.00	0.43
2:B:343:ILE:O	2:B:344:LYS:HB2	2.19	0.43
1:A:1142:THR:HG22	1:A:1271:ILE:O	2.19	0.43
2:B:167:ILE:HG22	2:B:167:ILE:O	2.18	0.43
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	2.01	0.43
1:A:105:CYS:SG	1:A:139:TRP:HA	2.58	0.43
3:C:149:LYS:HE2	10:J:64:ASN:O	2.18	0.43
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.52	0.43
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.00	0.43
2:B:981:ALA:HB2	2:B:987:LYS:HA	2.00	0.43
1:A:859:SER:HB3	1:A:1394:THR:HG22	2.00	0.43
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.92	0.43
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	2.00	0.42
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	2.01	0.42
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.01	0.42
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.02	0.42
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.73	0.42
6:F:85:MET:O	6:F:155:LEU:HD11	2.19	0.42
2:B:46:GLN:H	2:B:46:GLN:HG3	1.65	0.42
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.02	0.42
1:A:675:THR:HG23	1:A:732:LEU:HD22	2.01	0.42
2:B:842:ASN:HB2	2:B:1009:ASP:HA	2.01	0.42
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.01	0.42
9:I:55:THR:HG21	9:I:109:ILE:HG21	2.01	0.42
2:B:701:ILE:HD11	2:B:703:ILE:HD11	2.01	0.42
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.01	0.42
10:J:57:ILE:O	10:J:60:PHE:HB2	2.19	0.42
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE2	1:A:1058:VAL:HG11	2.54	0.42
8:H:47:PHE:CB	8:H:95:TYR:CD2	3.02	0.42
1:A:1442:ASP:HB2	6:F:137:TYR:CE1	2.51	0.42
1:A:81:PHE:HE1	2:B:1205:GLN:HG2	1.85	0.42
1:A:1159:ARG:HE	1:A:1174:PHE:HE2	1.66	0.42
7:G:127:PRO:HB2	7:G:139:ILE:HD13	2.00	0.42
2:B:254:LEU:HD12	2:B:272:THR:O	2.19	0.42
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.01	0.42
5:E:46:TYR:O	5:E:53:PRO:HA	2.20	0.42
2:B:464:GLY:HA2	2:B:480:SER:HB3	2.01	0.42
6:F:93:ILE:HG21	6:F:148:VAL:HG11	2.01	0.42
1:A:270:LEU:HD12	1:A:274:ILE:HD11	2.01	0.42
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.60	0.42
1:A:568:PRO:HG2	8:H:46:LEU:HD12	2.02	0.42
2:B:130:VAL:HG23	2:B:167:ILE:HD13	2.02	0.42
3:C:4:GLU:HB3	3:C:5:GLY:H	1.51	0.42
1:A:519:PRO:O	1:A:624:SER:HB2	2.19	0.42
6:F:152:ILE:HG13	6:F:152:ILE:H	1.62	0.42
1:A:837:ILE:HG21	1:A:1101:LEU:HD21	2.02	0.41
2:B:383:ASN:O	2:B:387:LEU:HB2	2.20	0.41
1:A:174:ILE:H	1:A:174:ILE:HG13	1.71	0.41
2:B:101:MET:HB3	2:B:109:THR:HG22	2.02	0.41
1:A:445:ASN:HB2	1:A:455:MET:HG2	2.01	0.41
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.19	0.41
2:B:1208:MET:HA	2:B:1212:ILE:O	2.20	0.41
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.01	0.41
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.55	0.41
2:B:785:TYR:HE2	10:J:60:PHE:CE2	2.38	0.41
12:L:38:LEU:O	12:L:39:SER:HB3	2.19	0.41
4:D:153:ARG:HH12	4:D:214:LEU:HD13	1.85	0.41
1:A:1404:GLU:HB3	1:A:1407:GLU:HB2	2.02	0.41
8:H:110:ASP:HB3	8:H:128:ASN:HB2	2.02	0.41
2:B:882:THR:CG2	2:B:935:ARG:HA	2.50	0.41
1:A:679:ILE:HG13	1:A:732:LEU:HD13	2.03	0.41
1:A:1444:MET:HG2	7:G:58:ARG:HB3	2.02	0.41
2:B:996:ARG:NH2	3:C:174:ALA:O	2.53	0.41
1:A:84:ILE:HG13	1:A:239:LEU:HB3	2.02	0.41
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.02	0.41
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.50	0.41
1:A:63:ARG:HA	1:A:74:MET:CG	2.51	0.41
1:A:79:GLY:HA3	1:A:243:PRO:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:THR:CG2	1:A:1077:THR:HG23	2.50	0.41
7:G:111:THR:HB	7:G:114:LEU:HD23	2.03	0.41
3:C:100:THR:HG23	3:C:119:VAL:HG13	2.02	0.41
1:A:1208:THR:H	1:A:1211:GLN:HG2	1.86	0.41
1:A:946:VAL:HG22	5:E:201:LYS:HB3	2.01	0.41
1:A:335:ARG:HA	1:A:339:ASN:HB2	2.02	0.41
3:C:69:LEU:HD23	10:J:6:ARG:HD3	2.02	0.41
1:A:1121:GLU:HG2	1:A:1124:HIS:CE1	2.56	0.41
1:A:909:ASP:C	1:A:911:SER:H	2.23	0.41
2:B:126:SER:HB2	2:B:172:ILE:HD11	2.02	0.41
1:A:95:PHE:HE1	1:A:1414:ALA:HB2	1.86	0.41
1:A:35:ILE:O	1:A:84:ILE:HG22	2.21	0.41
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.56	0.41
2:B:102:VAL:HG13	2:B:112:LEU:HB2	2.02	0.41
3:C:18:VAL:HG22	11:K:109:TRP:CZ3	2.54	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.56	0.41
5:E:202:SER:HB3	5:E:205:SER:H	1.86	0.41
1:A:335:ARG:HD3	2:B:1202:LEU:HD13	2.02	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.56	0.41
3:C:45:ALA:HA	3:C:72:LEU:HD12	2.03	0.41
1:A:118:HIS:CD2	1:A:164:ARG:HB3	2.56	0.41
2:B:398:ARG:HH11	2:B:398:ARG:HB2	1.86	0.41
4:D:10:THR:HG22	4:D:12:ARG:HH12	1.86	0.41
4:D:194:LEU:O	4:D:196:PRO:HD3	2.20	0.41
1:A:55:ASP:N	1:A:56:PRO:HD3	2.35	0.41
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.86	0.41
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.03	0.41
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.02	0.40
1:A:579:SER:HB3	1:A:611:GLN:HA	2.03	0.40
3:C:248:ILE:HD13	11:K:102:LYS:HA	2.04	0.40
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.23	0.40
2:B:806:THR:HG23	2:B:1046:PRO:HD3	2.03	0.40
7:G:1:MET:HE3	7:G:80:LYS:O	2.21	0.40
5:E:100:ILE:HG13	5:E:105:PHE:HD2	1.86	0.40
2:B:856:PHE:CE1	2:B:969:ARG:HG3	2.56	0.40
2:B:295:GLY:N	2:B:298:LEU:HD12	2.37	0.40
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.03	0.40
12:L:27:LEU:HA	12:L:39:SER:HB2	2.03	0.40
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.21	0.40
10:J:32:GLU:CD	10:J:32:GLU:H	2.24	0.40
12:L:57:LEU:HA	12:L:57:LEU:HD23	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:776:GLN:O	2:B:1095:LEU:HA	2.22	0.40
8:H:42:ILE:HG23	8:H:95:TYR:HE2	1.85	0.40
2:B:485:ARG:HD2	2:B:491:THR:HG23	2.04	0.40
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.21	0.40
6:F:76:LYS:HG2	6:F:79:ARG:CZ	2.51	0.40
1:A:901:LEU:HB2	1:A:926:GLN:HG2	2.03	0.40
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.51	0.40
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.03	0.40
1:A:1208:THR:HB	1:A:1211:GLN:H	1.86	0.40
4:D:23:ASN:HA	4:D:28:GLN:O	2.20	0.40
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.87	0.40
2:B:244:LEU:HD11	2:B:250:PHE:HD2	1.86	0.40
1:A:439:ASN:OD1	1:A:459:ARG:HG2	2.22	0.40
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.04	0.40
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.02	0.40
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.54	0.40
2:B:484:ASN:HB3	2:B:486:TYR:CE2	2.57	0.40
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.56	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	1417/1732 (82%)	1205 (85%)	143 (10%)	69 (5%)	3 32
2	B	1095/1224 (90%)	940 (86%)	109 (10%)	46 (4%)	3 36
3	C	264/318 (83%)	238 (90%)	20 (8%)	6 (2%)	8 52
4	D	174/221 (79%)	151 (87%)	9 (5%)	14 (8%)	1 18
5	E	212/215 (99%)	189 (89%)	19 (9%)	4 (2%)	10 55
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	16 63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	169/171 (99%)	150 (89%)	16 (10%)	3 (2%)	11 56
8	H	129/146 (88%)	99 (77%)	19 (15%)	11 (8%)	1 16
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	7 48
10	J	63/70 (90%)	56 (89%)	3 (5%)	4 (6%)	2 26
11	K	113/120 (94%)	105 (93%)	8 (7%)	0	100 100
12	L	44/70 (63%)	27 (61%)	8 (18%)	9 (20%)	0 2
All	All	3879/4564 (85%)	3333 (86%)	376 (10%)	170 (4%)	3 35

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	ALA
1	A	58	LEU
1	A	189	ARG
1	A	193	ASP
1	A	195	ASP
1	A	286	HIS
1	A	311	GLN
1	A	335	ARG
1	A	399	HIS
1	A	448	PRO
1	A	775	ILE
1	A	1341	ILE
1	A	1403	GLU
2	B	340	ALA
2	B	341	LEU
2	B	344	LYS
2	B	473	MET
2	B	707	PRO
2	B	711	GLU
2	B	731	VAL
2	B	751	VAL
2	B	1157	ALA
2	B	1185	CYS
3	C	161	LYS
4	D	18	VAL
4	D	53	SER
4	D	199	ASN
4	D	220	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	81	PRO
10	J	6	ARG
10	J	13	VAL
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG
1	A	61	ILE
1	A	76	GLU
1	A	167	CYS
1	A	251	SER
1	A	257	ARG
1	A	318	SER
1	A	449	SER
1	A	870	GLU
1	A	1405	THR
2	B	108	VAL
2	B	229	ALA
2	B	338	GLY
2	B	339	THR
2	B	369	GLY
2	B	449	ASN
2	B	772	ALA
2	B	792	MET
2	B	867	GLY
2	B	879	ARG
2	B	880	THR
2	B	883	LEU
2	B	1046	PRO
2	B	1066	SER
2	B	1167	GLY
2	B	1176	ASN
4	D	27	LEU
4	D	52	LEU
4	D	119	ARG
4	D	174	PRO
6	F	73	ALA
7	G	139	ILE
7	G	154	VAL
8	H	17	PRO
8	H	82	PRO
8	H	90	ALA
8	H	128	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	3	THR
9	I	95	THR
12	L	37	LYS
12	L	45	ALA
12	L	50	ASP
1	A	62	ASP
1	A	169	ASN
1	A	409	SER
1	A	426	LEU
1	A	465	TYR
1	A	600	PRO
1	A	846	GLU
1	A	852	TYR
1	A	1124	HIS
1	A	1173	HIS
1	A	1255	GLU
1	A	1438	THR
2	B	58	THR
2	B	282	ILE
2	B	343	ILE
2	B	364	ILE
2	B	368	GLU
2	B	1069	PHE
2	B	1143	ALA
2	B	1156	ASP
2	B	1175	LEU
3	C	4	GLU
3	C	240	VAL
4	D	11	ARG
5	E	3	GLN
5	E	45	LYS
5	E	49	SER
7	G	2	PHE
8	H	32	THR
8	H	60	ALA
8	H	83	GLN
8	H	84	ALA
8	H	108	SER
12	L	26	THR
12	L	53	HIS
12	L	59	ALA
1	A	164	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	GLU
1	A	253	ASN
1	A	333	GLU
1	A	569	LYS
1	A	593	GLU
1	A	1002	GLY
1	A	1242	VAL
2	B	713	ALA
2	B	734	HIS
2	B	764	SER
2	B	882	THR
2	B	891	ASP
2	B	1155	SER
2	B	1223	ASP
3	C	149	LYS
3	C	214	ASN
4	D	16	LYS
4	D	22	GLU
4	D	40	HIS
5	E	48	ASP
9	I	105	SER
12	L	63	ARG
1	A	224	PHE
1	A	254	GLU
1	A	312	PRO
1	A	958	VAL
2	B	466	TRP
4	D	192	LYS
10	J	2	ILE
10	J	57	ILE
1	A	40	THR
1	A	156	ASP
1	A	331	GLY
1	A	336	ILE
1	A	910	PRO
1	A	1327	ILE
2	B	901	PRO
4	D	218	GLU
12	L	38	LEU
1	A	283	GLY
1	A	567	LYS
1	A	986	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1123	GLY
8	H	107	VAL
1	A	385	ILE
1	A	639	PRO
1	A	35	ILE
1	A	178	GLY
1	A	380	VAL
1	A	599	SER
2	B	247	GLY
1	A	128	ILE
12	L	46	VAL
1	A	192	GLY
1	A	197	PRO
2	B	870	ILE
3	C	77	ILE

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	1243/1519 (82%)	1043 (84%)	200 (16%)	3 22
2	B	966/1061 (91%)	819 (85%)	147 (15%)	3 25
3	C	234/274 (85%)	198 (85%)	36 (15%)	3 24
4	D	160/200 (80%)	131 (82%)	29 (18%)	2 15
5	E	196/197 (100%)	174 (89%)	22 (11%)	7 39
6	F	74/137 (54%)	63 (85%)	11 (15%)	4 26
7	G	152/152 (100%)	141 (93%)	11 (7%)	18 59
8	H	117/128 (91%)	99 (85%)	18 (15%)	3 24
9	I	113/116 (97%)	105 (93%)	8 (7%)	18 60
10	J	60/65 (92%)	53 (88%)	7 (12%)	7 36
11	K	99/102 (97%)	85 (86%)	14 (14%)	4 29
12	L	40/57 (70%)	28 (70%)	12 (30%)	0 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3454/4008 (86%)	2939 (85%)	515 (15%)	4 26

All (515) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	23	SER
1	A	34	LYS
1	A	36	ARG
1	A	41	MET
1	A	42	ASP
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	50	ILE
1	A	58	LEU
1	A	62	ASP
1	A	64	ASN
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	117	GLU
1	A	120	GLU
1	A	123	ARG
1	A	126	LEU
1	A	129	LYS
1	A	147	VAL
1	A	151	ASP
1	A	156	ASP
1	A	164	ARG
1	A	174	ILE
1	A	175	ARG
1	A	188	ASP
1	A	199	LEU
1	A	200	ARG
1	A	208	LEU
1	A	213	HIS
1	A	232	GLU
1	A	250	ILE
1	A	253	ASN
1	A	270	LEU
1	A	279	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	295	LEU
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	315	LEU
1	A	318	SER
1	A	320	ARG
1	A	335	ARG
1	A	337	ARG
1	A	340	LEU
1	A	343	LYS
1	A	344	ARG
1	A	359	LEU
1	A	363	GLN
1	A	369	SER
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
1	A	391	LEU
1	A	393	ARG
1	A	394	ASN
1	A	408	ASP
1	A	409	SER
1	A	425	GLN
1	A	427	GLN
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	450	LEU
1	A	454	SER
1	A	461	LYS
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	483	ASP
1	A	493	GLN
1	A	496	GLU
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	517	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	LYS
1	A	527	THR
1	A	538	ASP
1	A	549	MET
1	A	566	ILE
1	A	567	LYS
1	A	577	ILE
1	A	593	GLU
1	A	598	LEU
1	A	602	ASP
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	670	ILE
1	A	683	ILE
1	A	685	GLU
1	A	691	LEU
1	A	732	LEU
1	A	738	LYS
1	A	739	ASP
1	A	756	ILE
1	A	758	ILE
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	795	GLU
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	834	THR
1	A	839	ARG
1	A	843	LYS
1	A	848	ILE
1	A	855	THR
1	A	896	ARG
1	A	904	THR
1	A	905	ASP
1	A	915	SER
1	A	919	ILE
1	A	920	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	926	GLN
1	A	929	LEU
1	A	948	VAL
1	A	973	ILE
1	A	982	THR
1	A	988	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1024	SER
1	A	1029	ARG
1	A	1033	GLN
1	A	1036	ARG
1	A	1047	SER
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1079	MET
1	A	1080	THR
1	A	1094	VAL
1	A	1098	VAL
1	A	1116	LEU
1	A	1124	HIS
1	A	1128	GLN
1	A	1133	LEU
1	A	1134	ILE
1	A	1142	THR
1	A	1145	SER
1	A	1147	THR
1	A	1170	ILE
1	A	1173	HIS
1	A	1175	SER
1	A	1176	LEU
1	A	1188	GLN
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1226	VAL
1	A	1237	ILE
1	A	1242	VAL
1	A	1243	VAL
1	A	1256	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1270	ASN
1	A	1274	ARG
1	A	1276	VAL
1	A	1289	ARG
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1309	ASP
1	A	1325	THR
1	A	1334	ASP
1	A	1341	ILE
1	A	1351	GLU
1	A	1366	ARG
1	A	1371	LEU
1	A	1376	THR
1	A	1378	GLN
1	A	1382	THR
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1403	GLU
1	A	1420	ASP
1	A	1422	ARG
1	A	1424	VAL
1	A	1426	GLU
1	A	1432	GLN
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
1	A	1454	MET
2	B	20	ASP
2	B	22	SER
2	B	25	ILE
2	B	35	SER
2	B	44	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	46	GLN
2	B	58	THR
2	B	110	HIS
2	B	118	ARG
2	B	128	LEU
2	B	134	LYS
2	B	170	LEU
2	B	194	GLU
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	251	ILE
2	B	261	ARG
2	B	262	GLU
2	B	268	THR
2	B	272	THR
2	B	278	GLN
2	B	294	ASP
2	B	305	VAL
2	B	312	GLU
2	B	313	MET
2	B	337	ARG
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	347	LYS
2	B	348	ARG
2	B	357	GLN
2	B	361	LEU
2	B	365	THR
2	B	368	GLU
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	401	PHE
2	B	412	LEU
2	B	416	LEU
2	B	418	LYS
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	453	ILE
2	B	466	TRP
2	B	470	LYS
2	B	476	ARG
2	B	481	GLN
2	B	485	ARG
2	B	487	THR
2	B	489	SER
2	B	491	THR
2	B	502	ILE
2	B	531	GLN
2	B	544	CYS
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	567	GLU
2	B	570	VAL
2	B	574	SER
2	B	582	VAL
2	B	595	ARG
2	B	603	LEU
2	B	612	GLU
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	635	ARG
2	B	637	LEU
2	B	644	GLU
2	B	658	ILE
2	B	664	THR
2	B	678	GLU
2	B	680	THR
2	B	694	ASP
2	B	696	GLU
2	B	708	GLU
2	B	709	ASP
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	790	ASP
2	B	797	TYR
2	B	837	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	858	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	884	ARG
2	B	885	MET
2	B	904	ARG
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	946	ASN
2	B	959	ASP
2	B	970	THR
2	B	972	LYS
2	B	975	GLN
2	B	979	LYS
2	B	986	GLN
2	B	995	ARG
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1022	THR
2	B	1028	GLU
2	B	1031	LEU
2	B	1045	SER
2	B	1050	ILE
2	B	1058	LEU
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1122	ARG
2	B	1123	SER
2	B	1128	LEU
2	B	1129	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1133	MET
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1149	GLU
2	B	1156	ASP
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1190	ASP
2	B	1193	GLN
2	B	1195	HIS
2	B	1202	LEU
2	B	1212	ILE
3	C	3	GLU
3	C	4	GLU
3	C	12	GLU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	44	LEU
3	C	48	SER
3	C	49	VAL
3	C	55	THR
3	C	62	PHE
3	C	79	GLN
3	C	89	GLU
3	C	93	ASP
3	C	115	SER
3	C	119	VAL
3	C	121	VAL
3	C	123	ASN
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	142	VAL
3	C	147	LEU
3	C	148	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	161	LYS
3	C	215	GLU
3	C	226	ASP
3	C	228	PHE
3	C	233	GLU
3	C	235	VAL
3	C	240	VAL
3	C	259	LEU
3	C	262	LEU
3	C	268	ASP
4	D	5	THR
4	D	9	GLN
4	D	10	THR
4	D	11	ARG
4	D	18	VAL
4	D	27	LEU
4	D	32	GLU
4	D	34	GLN
4	D	35	LEU
4	D	38	ILE
4	D	51	ASN
4	D	65	GLU
4	D	67	ARG
4	D	75	LYS
4	D	118	THR
4	D	123	LEU
4	D	125	SER
4	D	126	ILE
4	D	127	ASP
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	187	THR
4	D	197	SER
4	D	213	GLU
4	D	217	LEU
4	D	219	THR
4	D	221	TYR
5	E	2	ASP
5	E	10	SER
5	E	14	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	31	THR
5	E	41	ASP
5	E	69	ILE
5	E	75	MET
5	E	84	ASP
5	E	92	THR
5	E	115	ASN
5	E	131	THR
5	E	149	LEU
5	E	150	VAL
5	E	171	LYS
5	E	175	LEU
5	E	182	ASP
5	E	184	VAL
5	E	190	LEU
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	90	ARG
6	F	93	ILE
6	F	97	ARG
6	F	110	ASP
6	F	125	LEU
6	F	138	LEU
6	F	152	ILE
6	F	153	VAL
6	F	155	LEU
7	G	11	ILE
7	G	22	MET
7	G	46	LEU
7	G	64	THR
7	G	65	ASP
7	G	106	MET
7	G	112	LYS
7	G	118	ASP
7	G	133	SER
7	G	134	GLU
7	G	135	ASP
8	H	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	26	ILE
8	H	31	THR
8	H	39	THR
8	H	49	VAL
8	H	76	THR
8	H	77	ARG
8	H	88	SER
8	H	89	LEU
8	H	91	ASP
8	H	94	ASP
8	H	95	TYR
8	H	103	LYS
8	H	107	VAL
8	H	129	TYR
8	H	130	ARG
8	H	138	GLU
8	H	145	ARG
9	I	8	ARG
9	I	21	GLU
9	I	31	THR
9	I	50	THR
9	I	52	ILE
9	I	62	ILE
9	I	92	ARG
9	I	94	ASP
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
10	J	56	LEU
11	K	5	ASP
11	K	6	ARG
11	K	12	LEU
11	K	21	ILE
11	K	25	THR
11	K	29	ASN
11	K	33	ILE
11	K	47	ARG
11	K	51	LEU
11	K	63	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	91	CYS
11	K	101	LEU
11	K	102	LYS
11	K	114	LEU
12	L	27	LEU
12	L	30	ILE
12	L	38	LEU
12	L	42	ARG
12	L	51	CYS
12	L	54	ARG
12	L	56	LEU
12	L	58	LYS
12	L	61	THR
12	L	64	LEU
12	L	66	GLN
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	71	GLN
1	A	253	ASN
1	A	256	GLN
1	A	358	ASN
1	A	425	GLN
1	A	510	GLN
1	A	515	GLN
1	A	548	ASN
1	A	654	ASN
1	A	660	ASN
1	A	736	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	811	GLN
1	A	935	GLN
1	A	968	GLN
1	A	1033	GLN
1	A	1106	ASN
1	A	1128	GLN
1	A	1312	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1390	ASN
2	B	47	GLN
2	B	224	GLN
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	363	HIS
2	B	366	GLN
2	B	484	ASN
2	B	538	ASN
2	B	842	ASN
2	B	975	GLN
2	B	986	GLN
2	B	1025	HIS
3	C	7	GLN
4	D	132	GLN
5	E	8	ASN
7	G	57	GLN
7	G	71	ASN
7	G	158	HIS
8	H	134	ASN
9	I	22	ASN
9	I	51	ASN
9	I	60	GLN
9	I	89	GLN
9	I	108	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	1/2 (50%)	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	15	13,15	13,21,22	2.02	3 (23%)	16,30,33	2.48	3 (18%)

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	15	13,15	-	0/3/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	15	BRU	C6-N1	2.99	1.39	1.35
15	T	15	BRU	C4-N3	3.51	1.39	1.33
15	T	15	BRU	C4-C5	5.50	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	15	BRU	C5-C4-N3	-6.11	117.47	124.00
15	T	15	BRU	O4'-C1'-N1	3.56	113.89	107.72
15	T	15	BRU	C4-N3-C2	6.82	121.14	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	15	BRU	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
18	G2P	T	1024	-	26,34,34	2.63	7 (26%)	33,54,54	3.00	8 (24%)

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
18	G2P	T	1024	-	-	0/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	1024	G2P	C6-C5	2.04	1.45	1.41
18	T	1024	G2P	C2-N2	2.68	1.39	1.34
18	T	1024	G2P	PB-O3B	3.89	1.62	1.58
18	T	1024	G2P	C2-N1	3.95	1.42	1.35
18	T	1024	G2P	C4-N3	4.02	1.42	1.35
18	T	1024	G2P	PA-O5'	6.65	1.64	1.57
18	T	1024	G2P	C6-N1	7.25	1.46	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	1024	G2P	C5-C6-N1	-7.63	113.15	123.59
18	T	1024	G2P	O3G-PG-O1G	-2.27	98.74	107.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	1024	G2P	O2B-PB-C3A	2.20	114.56	109.02
18	T	1024	G2P	O1G-PG-O2G	3.06	120.42	110.58
18	T	1024	G2P	O2A-PA-C3A	3.25	117.19	109.02
18	T	1024	G2P	C4'-O4'-C1'	3.28	113.33	109.72
18	T	1024	G2P	C6-N1-C2	4.67	122.42	115.94
18	T	1024	G2P	PG-O3B-PB	12.49	174.55	132.67

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	A	1425/1732 (82%)	-0.12	4 (0%) 94 90	68, 122, 180, 239	0
2	B	1115/1224 (91%)	0.00	8 (0%) 89 81	71, 135, 194, 224	0
3	C	266/318 (83%)	-0.25	0 100 100	89, 120, 158, 195	0
4	D	178/221 (80%)	-0.11	1 (0%) 90 83	95, 134, 183, 201	0
5	E	214/215 (99%)	-0.09	2 (0%) 85 75	97, 158, 205, 214	0
6	F	84/155 (54%)	-0.32	0 100 100	75, 103, 132, 149	0
7	G	171/171 (100%)	-0.10	0 100 100	94, 119, 151, 181	0
8	H	133/146 (91%)	-0.07	1 (0%) 87 77	135, 163, 198, 220	0
9	I	119/122 (97%)	-0.25	0 100 100	123, 168, 204, 216	0
10	J	65/70 (92%)	-0.20	0 100 100	101, 117, 161, 173	0
11	K	115/120 (95%)	-0.27	1 (0%) 85 75	87, 119, 157, 171	0
12	L	46/70 (65%)	0.04	2 (4%) 39 26	110, 185, 203, 208	0
13	N	9/14 (64%)	0.88	1 (11%) 7 5	236, 246, 283, 284	0
14	P	2/2 (100%)	1.46	0 100 100	216, 216, 216, 220	0
15	T	15/27 (55%)	0.28	1 (6%) 21 12	191, 217, 273, 276	0
All	All	3957/4607 (85%)	-0.10	21 (0%) 91 86	68, 129, 194, 284	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	N	1	DT	4.7
1	A	1176	LEU	3.6
2	B	339	THR	3.2
2	B	708	GLU	3.2
12	L	27	LEU	2.9
15	T	23	DA	2.9
2	B	250	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	469	GLN	2.7
1	A	1083	THR	2.7
2	B	167	ILE	2.7
4	D	13	ARG	2.6
5	E	90	VAL	2.3
1	A	56	PRO	2.3
2	B	340	ALA	2.3
2	B	417	PHE	2.2
2	B	468	GLU	2.1
8	H	139	ASN	2.1
12	L	26	THR	2.1
5	E	123	LEU	2.0
11	K	115	ALA	2.0
1	A	1082	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
15	BRU	T	15	20/21	0.81	0.22	-	214,225,227,233	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
18	G2P	T	1024	32/32	0.67	0.47	3.62	221,226,247,248	0
16	ZN	I	1121	1/1	1.00	0.15	0.38	142,142,142,142	0
16	ZN	C	1269	1/1	1.00	0.20	0.15	96,96,96,96	0
16	ZN	B	2225	1/1	1.00	0.21	0.13	97,97,97,97	0
16	ZN	J	1066	1/1	0.99	0.21	-0.08	95,95,95,95	0
16	ZN	I	1122	1/1	0.98	0.09	-0.62	217,217,217,217	0
16	ZN	A	2457	1/1	1.00	0.18	-0.69	82,82,82,82	0
16	ZN	A	2456	1/1	0.99	0.12	-1.37	157,157,157,157	0
16	ZN	L	1071	1/1	0.98	0.08	-1.69	194,194,194,194	0
17	MG	A	2458	1/1	0.97	0.22	-	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.