Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:41 PM GMT

PDB ID	:	4A3D
Title	:	RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A 6NT DNA-RNA HYBRID
Authors	:	Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on	:	2011-09-30
Resolution	:	3.40 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:

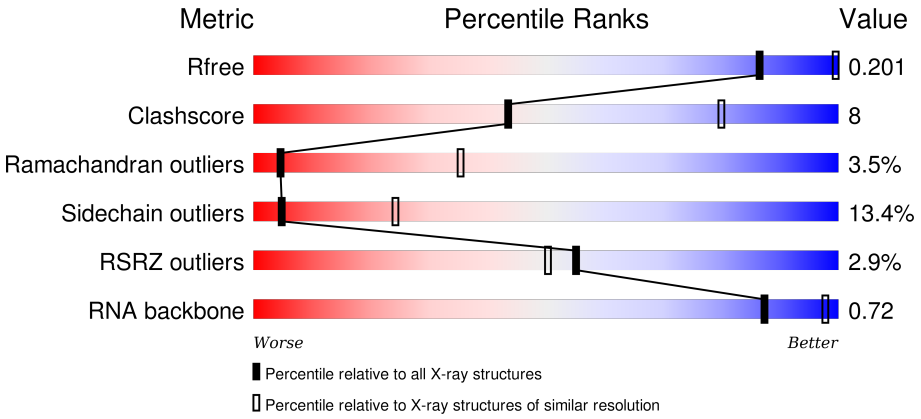
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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	2% 58% 20% • • 18%
2	B	1224	3% 62% 25% • 9%
3	C	318	61% 18% • 16%
4	D	221	2% 56% 20% • 19%

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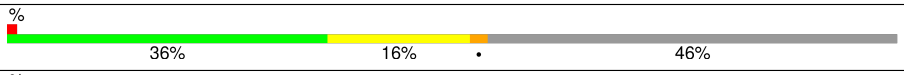
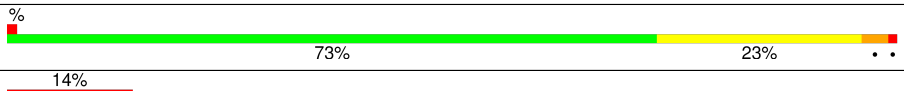
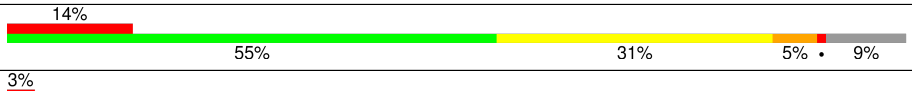
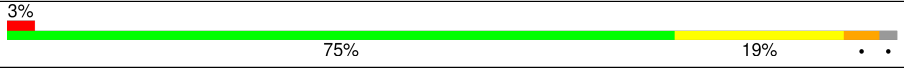
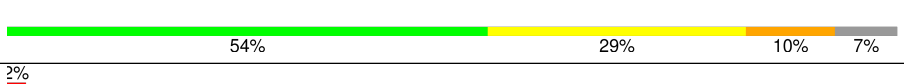
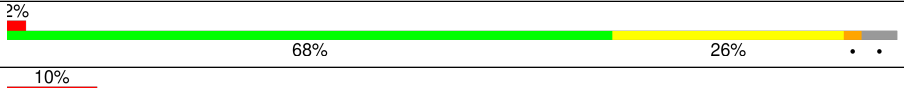
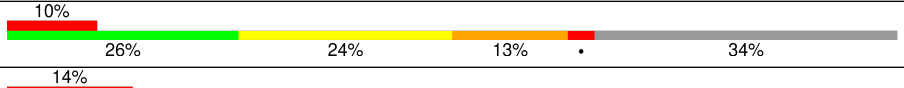
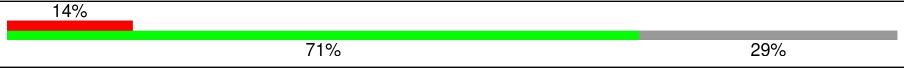
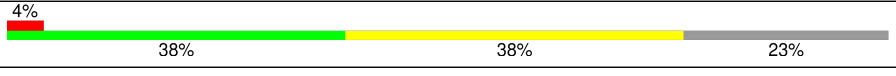
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	6	
15	T	26	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 31937 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 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP *GP*AP*GP*CP*TP)-3'.

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*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	6	Total	C	N	O	P	0	0	0
			130	58	26	40	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	20	Total	Br	C	N	O	P	0	0	0
			404	1	194	63	126	20			

- 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).

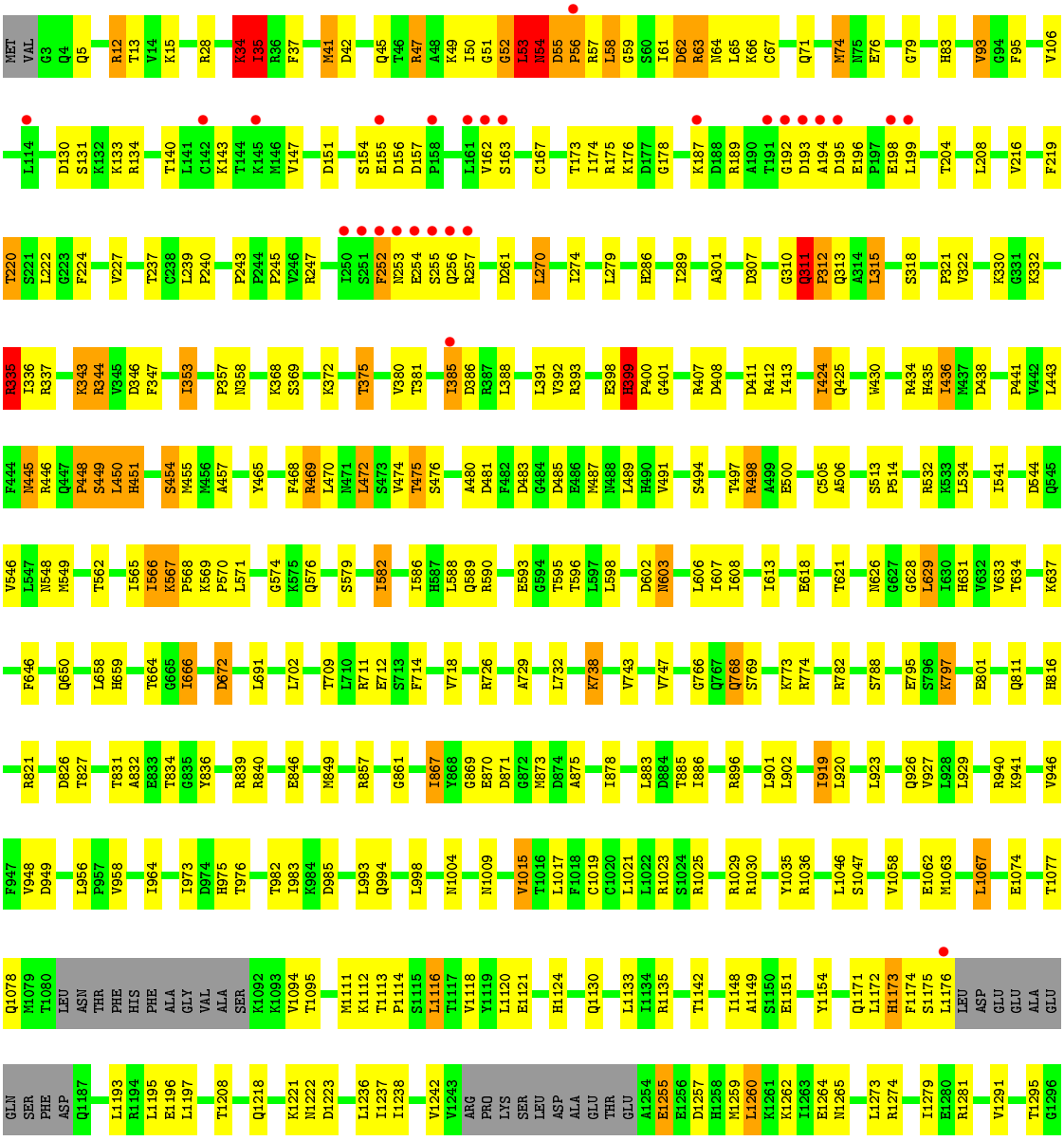
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

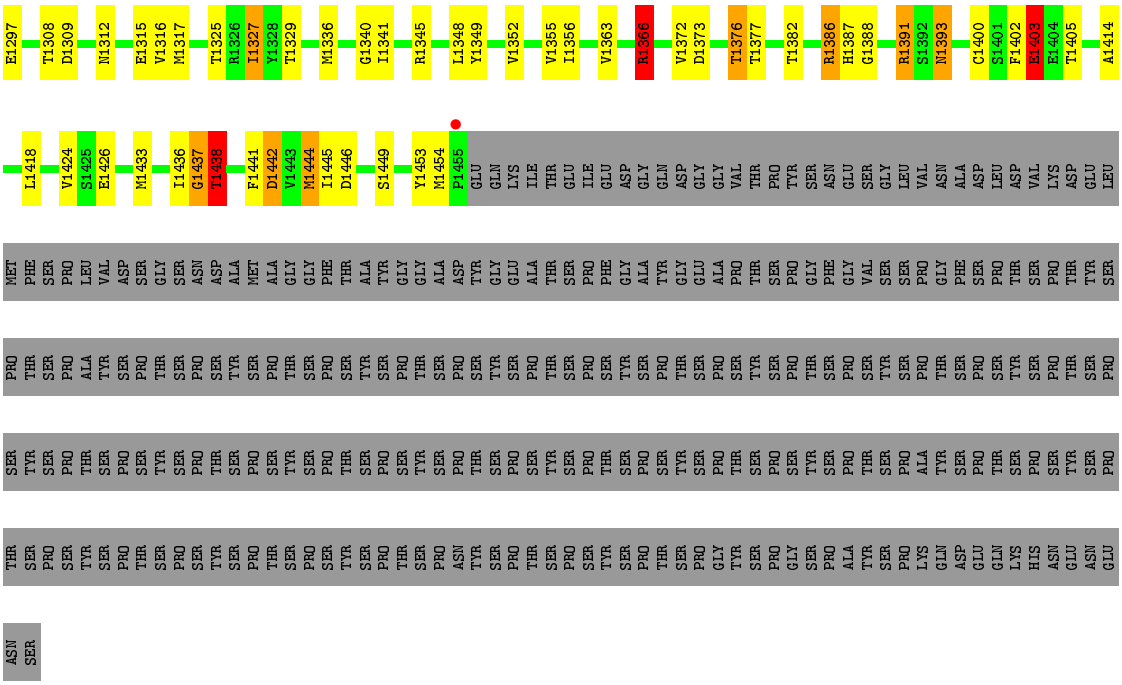
3 Residue-property plots (i)

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

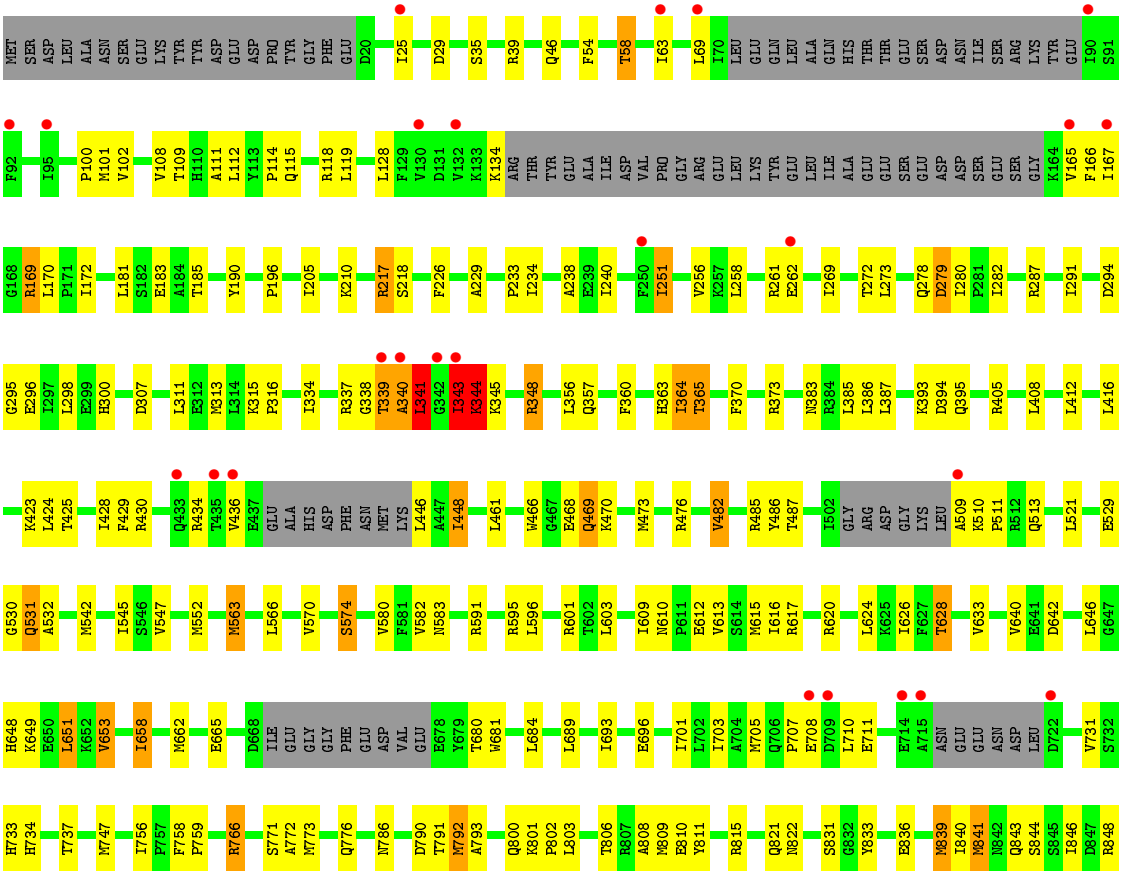
Chain A:

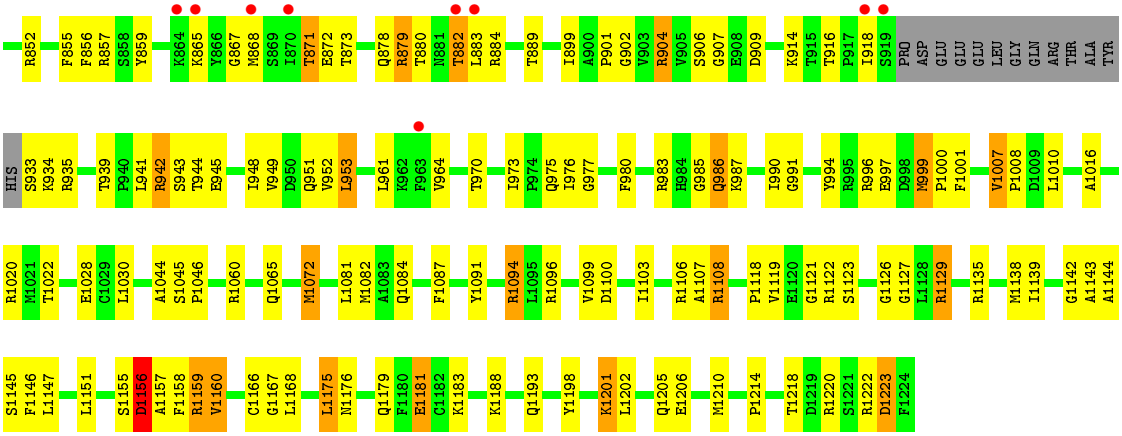




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

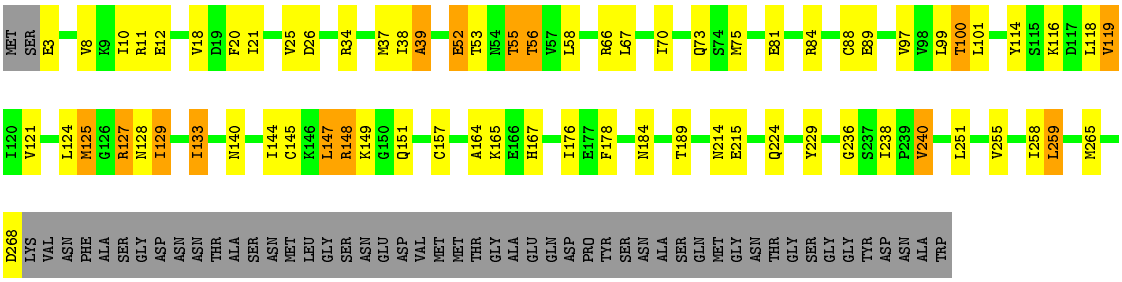
Chain B:





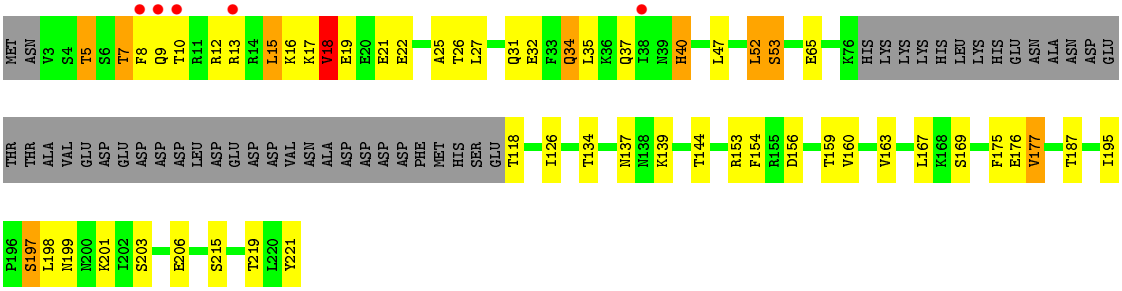
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



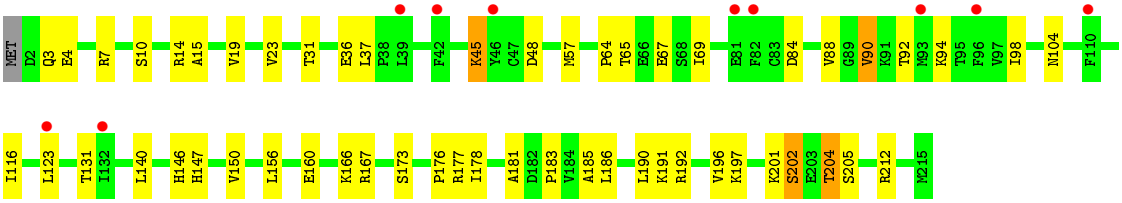
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



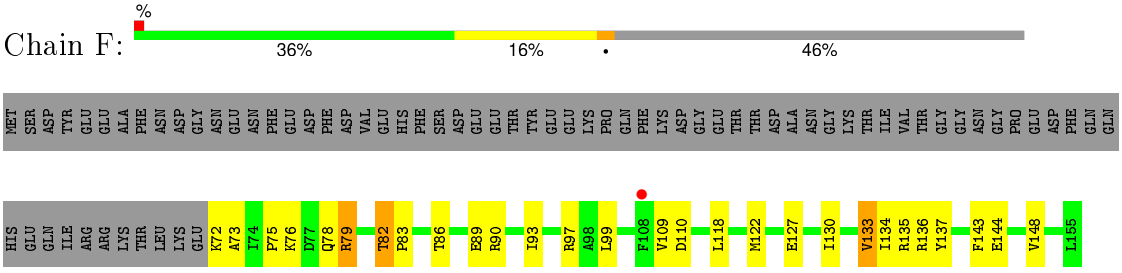
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



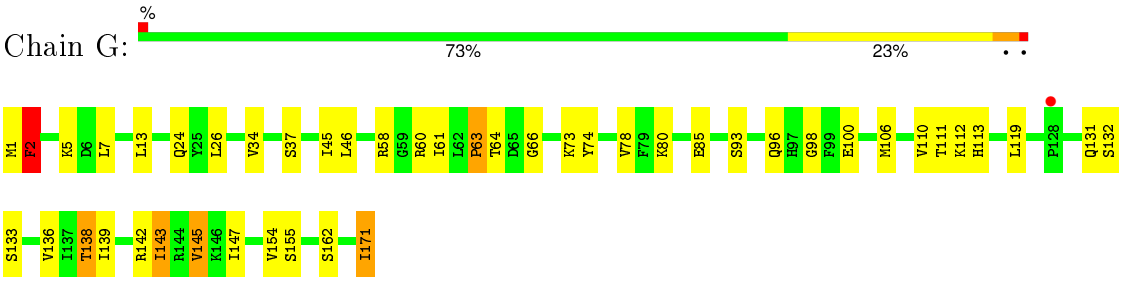
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



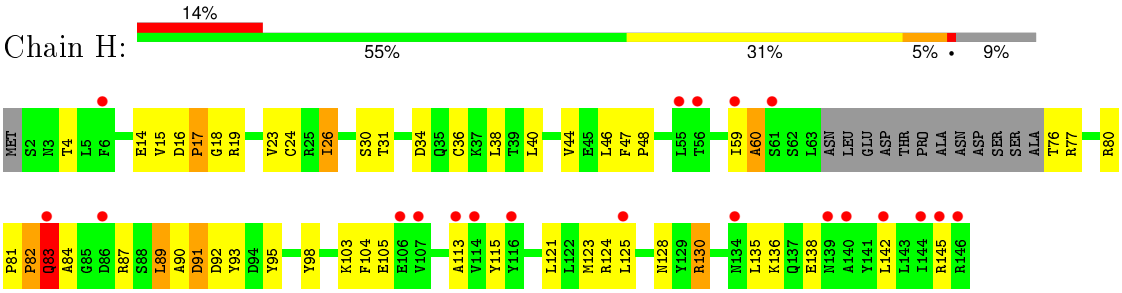
• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



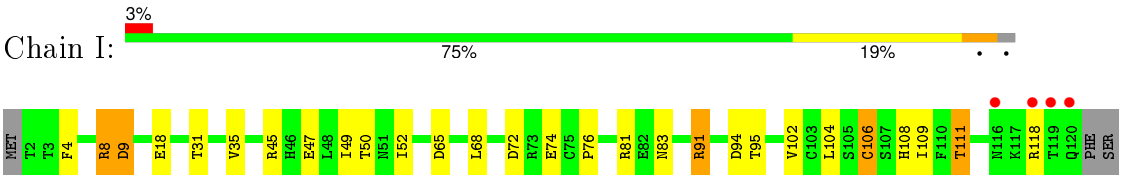
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



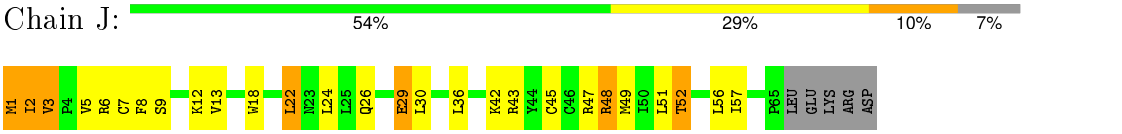
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



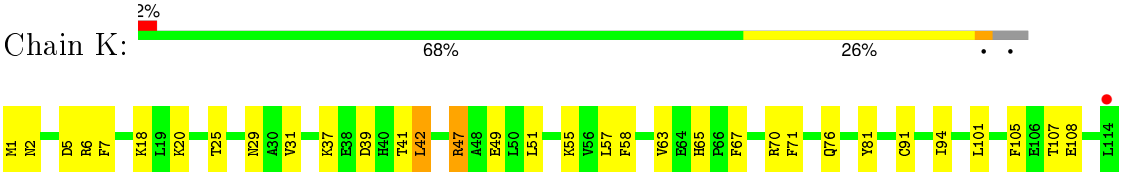
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

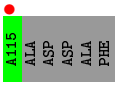
Chain J:



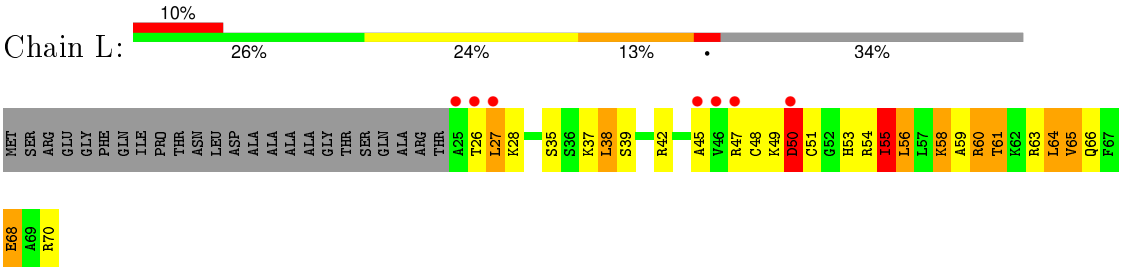
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:

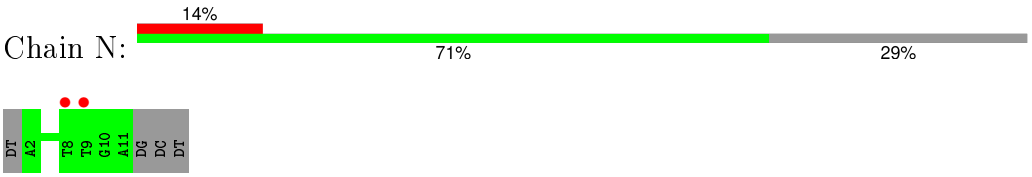




• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

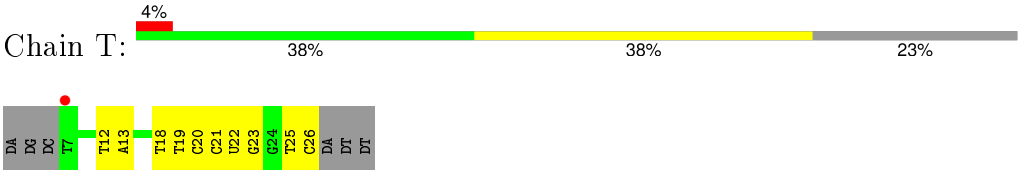


• Molecule 13: NON TEMPLATE DNA 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP *GP*AP*GP*CP*TP)-3'



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

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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	221.91Å 391.36Å 283.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 3.40 49.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.96-3.40) 100.0 (49.96-3.40)	Depositor EDS
R_{merge}	0.93	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.161 , 0.186 0.183 , 0.201	Depositor DCC
R_{free} test set	3331 reflections (2.02%)	DCC
Wilson B-factor (Å^2)	95.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 80.4	EDS
Estimated twinning fraction	0.034 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 168581 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31937	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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

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	0.54	0/11374	0.85	10/15383 (0.1%)
2	B	0.51	0/9029	0.79	4/12171 (0.0%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	D	0.51	0/1444	0.83	2/1935 (0.1%)
5	E	0.48	0/1788	0.71	0/2406
6	F	0.62	0/691	0.81	0/933
7	G	0.52	0/1368	0.81	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.47	0/989	0.78	0/1331
10	J	0.54	0/541	0.88	1/727 (0.1%)
11	K	0.47	0/938	0.71	0/1267
12	L	0.54	0/365	0.95	0/485
13	N	1.07	0/232	1.06	0/356
14	P	1.21	0/145	0.79	0/224
15	T	1.26	1/426 (0.2%)	1.08	0/652
All	All	0.55	1/32549 (0.0%)	0.82	19/44075 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	26	DC	C1'-N1	5.63	1.56	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	399	HIS	N-CA-CB	7.25	123.66	110.60
1	A	34	LYS	C-N-CA	7.21	139.73	121.70
4	D	25	ALA	C-N-CA	6.11	136.98	121.70
1	A	56	PRO	C-N-CA	6.01	136.73	121.70
1	A	35	ILE	N-CA-CB	5.95	124.49	110.80
2	B	340	ALA	C-N-CA	5.70	135.94	121.70
1	A	194	ALA	C-N-CA	5.65	135.83	121.70
1	A	311	GLN	N-CA-C	5.56	126.01	111.00
4	D	26	THR	N-CA-C	-5.52	96.11	111.00
1	A	54	ASN	C-N-CA	5.44	135.31	121.70
3	C	39	ALA	N-CA-C	5.44	125.68	111.00
2	B	628	THR	C-N-CA	5.43	135.29	121.70
3	C	89	GLU	N-CA-C	-5.29	96.73	111.00
1	A	53	LEU	N-CA-CB	5.27	120.94	110.40
1	A	310	GLY	C-N-CA	5.17	134.63	121.70
2	B	1181	GLU	N-CA-C	5.16	124.92	111.00
1	A	1403	GLU	N-CA-C	5.11	124.81	111.00
10	J	5	VAL	N-CA-C	-5.03	97.43	111.00
2	B	1156	ASP	N-CA-C	5.01	124.52	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	11174	0	11233	210	0
2	B	8859	0	8901	164	0
3	C	2095	0	2051	42	0
4	D	1434	0	1460	17	0
5	E	1752	0	1776	26	0
6	F	679	0	701	20	0
7	G	1340	0	1357	28	0
8	H	1068	0	1040	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	971	0	927	15	0
10	J	532	0	542	14	0
11	K	920	0	929	20	0
12	L	363	0	386	16	0
13	N	207	0	114	0	0
14	P	130	0	66	1	0
15	T	404	0	227	8	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
All	All	31937	0	31710	517	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 8.

All (517) 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	1.83	1.53
1:A:53:LEU:HD23	1:A:54:ASN:H	1.03	1.13
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.27	0.94
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.52	0.91
1:A:53:LEU:HD23	1:A:54:ASN:N	1.87	0.89
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.56	0.86
10:J:48:ARG:HE	10:J:49:MET:HE2	1.40	0.86
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.59	0.84
3:C:148:ARG:H	3:C:151:GLN:HG3	1.43	0.82
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.61	0.81
1:A:53:LEU:CD2	1:A:54:ASN:H	1.91	0.80
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.64	0.80
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.77
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.67	0.77
2:B:101:MET:HG2	2:B:111:ALA:HA	1.66	0.76
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.66	0.76
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.68	0.74
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.74
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.70	0.73
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.71	0.72
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.72	0.72
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.72	0.72
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.72	0.72
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.71	0.71
2:B:1198:TYR:CE2	2:B:1201:LYS:HE3	2.25	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.70
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.74	0.69
1:A:140:THR:HA	1:A:143:LYS:HE2	1.75	0.69
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.74	0.69
2:B:563:MET:HE2	2:B:580:VAL:HB	1.73	0.69
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.74	0.69
3:C:259:LEU:HD22	11:K:91:CYS:HB3	1.75	0.68
7:G:138:THR:HG22	7:G:139:ILE:H	1.59	0.68
1:A:61:ILE:HG22	1:A:62:ASP:H	1.58	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.68
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.75	0.68
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.60	0.67
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.76	0.67
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.76	0.67
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.30	0.66
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.75	0.66
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.78	0.66
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.59	0.66
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.61	0.66
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.26	0.65
7:G:1:MET:CE	7:G:80:LYS:O	2.45	0.65
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.64
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.64
3:C:56:THR:HG21	3:C:145:CYS:SG	2.37	0.64
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.64
2:B:806:THR:HG22	2:B:808:ALA:H	1.63	0.64
7:G:1:MET:HE1	7:G:80:LYS:O	1.98	0.64
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.28	0.64
1:A:1402:PHE:CE1	1:A:1403:GLU:HG2	2.33	0.64
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.33	0.63
12:L:28:LYS:HB2	12:L:39:SER:HA	1.80	0.63
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.81	0.63
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.62
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.62
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.62
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.99	0.62
1:A:343:LYS:HD3	2:B:1156:ASP:HB2	1.82	0.61
1:A:448:PRO:O	1:A:449:SER:HB2	2.01	0.61
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.41	0.61
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.81	0.61
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.61
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.81	0.61
2:B:486:TYR:HB3	2:B:1096:ARG:CZ	2.31	0.61
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.83	0.61
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.60
7:G:1:MET:SD	7:G:2:PHE:N	2.63	0.60
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.60
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.36	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.60
3:C:184:ASN:HD21	3:C:189:THR:H	1.50	0.60
2:B:918:ILE:HD13	2:B:935:ARG:HH22	1.65	0.60
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.84	0.60
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.60
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.02	0.59
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.16	0.59
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.59
5:E:202:SER:HB3	5:E:205:SER:H	1.66	0.59
2:B:976:ILE:O	2:B:990:ILE:HB	2.02	0.59
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.58
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.02	0.58
1:A:483:ASP:HB2	2:B:987:LYS:HE3	1.84	0.58
1:A:315:LEU:HA	1:A:321:PRO:HA	1.85	0.58
8:H:82:PRO:C	8:H:84:ALA:H	2.05	0.58
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.86	0.58
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.85	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.58
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.85	0.58
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.38	0.58
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.69	0.58
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.50	0.58
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.84	0.58
2:B:792:MET:HA	2:B:856:PHE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.57
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.57
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.85	0.57
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.87	0.57
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.35	0.57
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.85	0.57
2:B:882:THR:HG1	2:B:935:ARG:N	2.03	0.57
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.39	0.56
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.56
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.88	0.56
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.88	0.56
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.88	0.56
4:D:7:THR:HG21	7:G:5:LYS:HZ1	1.69	0.56
7:G:34:VAL:O	7:G:37:SER:HB3	2.06	0.56
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.88	0.56
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.88	0.55
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.55
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.55
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.88	0.55
1:A:35:ILE:HA	1:A:52:GLY:O	2.07	0.55
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.47	0.55
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.87	0.55
4:D:167:LEU:HB3	4:D:177:VAL:HG22	1.87	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.89	0.55
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.89	0.55
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.89	0.55
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.72	0.55
10:J:1:MET:HB2	10:J:56:LEU:HB2	1.89	0.54
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.54
6:F:89:GLU:O	6:F:93:ILE:HD12	2.06	0.54
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.89	0.54
6:F:109:VAL:HG23	6:F:127:GLU:OE1	2.07	0.54
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.22	0.54
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.54
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.54
7:G:111:THR:HG22	7:G:113:HIS:H	1.72	0.54
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.89	0.54
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.08	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.54
1:A:832:ALA:HB1	15:T:18:DT:H2"	1.89	0.54
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.89	0.54
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.90	0.54
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.54
2:B:343:ILE:O	2:B:344:LYS:HB2	2.07	0.54
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.54
2:B:815:ARG:HH11	2:B:815:ARG:HG3	1.72	0.54
2:B:338:GLY:CA	2:B:339:THR:HB	2.38	0.54
1:A:982:THR:HB	1:A:985:ASP:H	1.73	0.53
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.24	0.53
10:J:24:LEU:O	10:J:30:LEU:HB2	2.08	0.53
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.90	0.53
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.08	0.53
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.91	0.53
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.91	0.53
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.53
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.91	0.53
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.39	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.53
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.91	0.53
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.92	0.53
3:C:164:ALA:HA	3:C:167:HIS:O	2.09	0.52
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.90	0.52
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.44	0.52
1:A:63:ARG:HA	1:A:74:MET:HG3	1.91	0.52
2:B:291:ILE:HD12	2:B:291:ILE:H	1.75	0.52
1:A:55:ASP:H	1:A:56:PRO:HD3	1.75	0.52
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.91	0.52
2:B:873:THR:O	2:B:914:LYS:HA	2.09	0.52
1:A:79:GLY:HA3	1:A:243:PRO:HB2	1.92	0.52
5:E:19:VAL:O	5:E:23:VAL:HG23	2.08	0.52
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.40	0.52
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.45	0.52
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.91	0.52
1:A:494:SER:HB3	1:A:497:THR:OG1	2.10	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
2:B:101:MET:HB3	2:B:109:THR:HG22	1.90	0.51
2:B:166:PHE:HZ	2:B:169:ARG:HG2	1.74	0.51
1:A:646:PHE:O	1:A:650:GLN:HG2	2.10	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.51
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.92	0.51
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.93	0.51
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.51
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.92	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.92	0.51
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.40	0.51
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.45	0.51
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.76	0.51
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.93	0.51
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.51
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.46	0.51
1:A:52:GLY:N	1:A:56:PRO:HB3	2.26	0.51
2:B:773:MET:CE	2:B:985:GLY:HA2	2.40	0.51
5:E:15:ALA:O	5:E:19:VAL:HG23	2.11	0.51
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.94	0.51
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.93	0.50
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.23	0.50
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.93	0.50
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.94	0.50
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.50
1:A:64:ASN:O	1:A:65:LEU:HB3	2.12	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.50
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.52	0.50
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.50
2:B:902:GLY:O	12:L:65:VAL:HG11	2.11	0.50
1:A:940:ARG:HB3	1:A:941:LYS:HE2	1.92	0.50
8:H:89:LEU:C	8:H:91:ASP:H	2.14	0.50
1:A:1444:MET:HB2	6:F:133:VAL:HG12	1.92	0.50
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.47	0.50
2:B:1122:ARG:HB3	15:T:23:DG:OP1	2.12	0.50
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.11	0.50
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.50
1:A:315:LEU:H	1:A:315:LEU:HD12	1.76	0.49
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.11	0.49
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.94	0.49
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.77	0.49
2:B:430:ARG:HB3	2:B:434:ARG:HH21	1.77	0.49
7:G:1:MET:HE3	7:G:80:LYS:O	2.12	0.49
7:G:1:MET:CG	7:G:2:PHE:N	2.76	0.49
2:B:338:GLY:HA2	2:B:339:THR:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:HD1	1:A:256:GLN:HB3	1.78	0.49
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.77	0.49
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.42	0.49
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.49
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.95	0.49
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.95	0.49
2:B:806:THR:HB	2:B:809:MET:HG3	1.94	0.49
2:B:574:SER:HB3	2:B:591:ARG:HE	1.77	0.49
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.49
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	1.95	0.49
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.27	0.49
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.93	0.49
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.49
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.95	0.49
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.33	0.49
10:J:48:ARG:HE	10:J:49:MET:CE	2.19	0.48
2:B:217:ARG:HH21	2:B:405:ARG:HG3	1.78	0.48
1:A:227:VAL:HG12	4:D:15:LEU:HD23	1.95	0.48
2:B:933:SER:O	2:B:935:ARG:N	2.45	0.48
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.95	0.48
8:H:23:VAL:HG11	8:H:121:LEU:HD22	1.95	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.48
2:B:916:THR:O	2:B:935:ARG:HG2	2.12	0.48
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.94	0.48
2:B:693:ILE:HG21	2:B:701:ILE:HD13	1.95	0.48
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.96	0.48
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.95	0.48
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.94	0.48
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.95	0.48
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.79	0.48
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.96	0.48
1:A:216:VAL:O	1:A:220:THR:HB	2.12	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.48
1:A:66:LYS:HB3	1:A:71:GLN:O	2.13	0.48
1:A:738:LYS:HA	8:H:19:ARG:HH12	1.79	0.48
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.48
1:A:55:ASP:N	1:A:56:PRO:HD3	2.28	0.48
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.96	0.48
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.96	0.48
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.96	0.47
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.95	0.47
1:A:12:ARG:HB3	2:B:1218:THR:HB	1.96	0.47
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.96	0.47
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.47
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.96	0.47
2:B:486:TYR:HB3	2:B:1096:ARG:NE	2.28	0.47
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.95	0.47
2:B:542:MET:HG3	2:B:747:MET:HB3	1.95	0.47
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.96	0.47
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.47
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.50	0.47
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.80	0.47
1:A:497:THR:HG22	2:B:1146:PHE:CD1	2.42	0.47
5:E:176:PRO:O	5:E:212:ARG:HA	2.14	0.47
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.14	0.47
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.55	0.47
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.47
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.47
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.97	0.47
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.13	0.47
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.47
1:A:253:ASN:HB3	2:B:935:ARG:NE	2.29	0.47
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.49	0.47
1:A:448:PRO:HG3	15:T:19:DT:O2	2.13	0.46
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.80	0.46
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.97	0.46
2:B:882:THR:C	2:B:884:ARG:H	2.19	0.46
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.46
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.81	0.46
4:D:5:THR:HG21	7:G:74:TYR:OH	2.15	0.46
9:I:83:ASN:HA	9:I:104:LEU:HG	1.98	0.46
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.97	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.16	0.46
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.98	0.46
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.97	0.46
2:B:210:LYS:HD3	2:B:482:VAL:HG13	1.97	0.46
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.97	0.46
2:B:882:THR:HG21	2:B:935:ARG:HA	1.98	0.46
5:E:65:THR:O	5:E:69:ILE:HD12	2.16	0.46
2:B:852:ARG:HH22	12:L:70:ARG:C	2.19	0.46
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.46
2:B:662:MET:HA	2:B:665:GLU:HB2	1.97	0.46
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.15	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.46
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
9:I:72:ASP:O	9:I:81:ARG:HG2	2.16	0.46
2:B:803:LEU:HG	10:J:52:THR:HG21	1.98	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.46
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.45
2:B:291:ILE:HD12	2:B:291:ILE:N	2.30	0.45
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.45
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.99	0.45
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.99	0.45
1:A:1433:MET:HE3	7:G:63:PRO:CB	2.46	0.45
1:A:448:PRO:O	1:A:449:SER:CB	2.63	0.45
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.98	0.45
2:B:901:PRO:O	12:L:60:ARG:HA	2.17	0.45
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.45
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.99	0.45
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.99	0.45
2:B:468:GLU:HG2	2:B:469:GLN:HB2	1.99	0.45
7:G:98:GLY:HA3	7:G:110:VAL:O	2.17	0.45
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.97	0.45
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.45
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.99	0.45
4:D:31:GLN:O	4:D:34:GLN:HB2	2.17	0.45
1:A:254:GLU:H	2:B:935:ARG:HH21	1.65	0.45
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.97	0.45
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.98	0.45
1:A:35:ILE:HG13	1:A:56:PRO:HG2	1.99	0.45
1:A:743:VAL:O	1:A:747:VAL:HG23	2.16	0.45
9:I:50:THR:HG22	9:I:52:ILE:H	1.81	0.45
3:C:148:ARG:N	3:C:151:GLN:HG3	2.22	0.44
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.44
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.83	0.44
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.53	0.44
1:A:869:GLY:O	5:E:204:THR:HG21	2.18	0.44
1:A:347:PHE:H	2:B:1107:ALA:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.99	0.44
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.98	0.44
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.15	0.44
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.99	0.44
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.44
3:C:34:ARG:HA	3:C:37:MET:HE2	2.00	0.44
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.66	0.44
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.44
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.44
2:B:365:THR:HG21	2:B:370:PHE:CG	2.51	0.44
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.00	0.44
3:C:55:THR:HB	3:C:151:GLN:HA	1.99	0.44
1:A:1148:ILE:HA	9:I:49:ILE:HD12	2.00	0.44
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.65	0.44
15:T:12:DT:H2'	15:T:13:DA:C8	2.52	0.44
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.99	0.44
4:D:7:THR:HG23	7:G:7:LEU:HD23	1.99	0.44
14:P:8:G:H2'	14:P:9:G:H8	1.81	0.44
1:A:270:LEU:HD12	1:A:274:ILE:HD11	1.98	0.44
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.00	0.44
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.53	0.44
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.00	0.44
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.83	0.44
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.99	0.44
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.98	0.44
2:B:865:LYS:HB2	2:B:961:LEU:HD21	2.00	0.44
1:A:62:ASP:HB2	1:A:65:LEU:HD22	1.99	0.43
1:A:449:SER:HA	1:A:454:SER:HB3	1.98	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.53	0.43
15:T:21:DC:H2'	15:T:22:BRU:H6	2.00	0.43
1:A:344:ARG:HG2	2:B:1127:GLY:O	2.18	0.43
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.43
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.48	0.43
1:A:449:SER:HA	1:A:454:SER:CB	2.49	0.43
1:A:41:MET:HB3	1:A:49:LYS:HA	2.00	0.43
15:T:19:DT:H2'	15:T:20:DC:C6	2.54	0.43
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.43
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.43
2:B:167:ILE:O	2:B:167:ILE:HG22	2.18	0.43
7:G:93:SER:OG	7:G:100:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
1:A:239:LEU:HD12	1:A:240:PRO:HD2	2.01	0.43
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.54	0.43
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.35	0.43
1:A:1025:ARG:O	1:A:1035:TYR:HE2	2.02	0.43
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.43
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.92	0.43
1:A:1438:THR:HB	2:B:1142:GLY:O	2.19	0.43
8:H:4:THR:HA	8:H:60:ALA:HB2	2.00	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.43
1:A:450:LEU:HG	1:A:450:LEU:H	1.71	0.43
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.83	0.43
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.43
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.84	0.43
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.43
6:F:82:THR:HG22	6:F:83:PRO:HD2	2.01	0.43
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.49	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.43
12:L:49:LYS:O	12:L:50:ASP:HB2	2.19	0.43
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.19	0.43
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.01	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG13	2.00	0.43
2:B:115:GLN:O	2:B:119:LEU:HD12	2.19	0.43
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.01	0.42
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.01	0.42
2:B:424:LEU:HD11	2:B:448:ILE:HG22	2.01	0.42
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.42
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.01	0.42
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.42
2:B:226:PHE:HA	2:B:395:GLN:CG	2.49	0.42
2:B:831:SER:HG	2:B:994:TYR:HE2	1.64	0.42
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.42
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.84	0.42
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.42
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.99	0.42
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.42
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.42
1:A:598:LEU:HA	1:A:598:LEU:HD23	1.83	0.42
3:C:148:ARG:HG3	3:C:151:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ILE:HG21	1:A:549:MET:CE	2.49	0.42
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	2.01	0.42
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.02	0.42
2:B:165:VAL:O	2:B:167:ILE:HD12	2.20	0.42
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.20	0.42
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.52	0.42
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.42
2:B:792:MET:HG2	2:B:855:PHE:CZ	2.55	0.42
2:B:383:ASN:O	2:B:387:LEU:HB2	2.19	0.42
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.52	0.42
1:A:1221:LYS:HB3	1:A:1222:ASN:H	1.72	0.42
1:A:58:LEU:HB3	1:A:59:GLY:H	1.45	0.42
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.12	0.42
12:L:38:LEU:HD21	12:L:48:CYS:HA	2.02	0.42
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.02	0.42
6:F:99:LEU:HD23	7:G:66:GLY:HA2	2.01	0.42
3:C:99:LEU:HB3	3:C:118:LEU:HD22	2.01	0.41
2:B:69:LEU:HD11	2:B:425:THR:HG23	2.01	0.41
3:C:99:LEU:HD12	3:C:118:LEU:HB3	2.02	0.41
15:T:25:DT:H2'	15:T:25:DT:H6	1.64	0.41
2:B:311:LEU:HB3	9:I:4:PHE:HE2	1.85	0.41
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.87	0.41
5:E:156:LEU:HD23	5:E:160:GLU:HB3	2.03	0.41
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.84	0.41
2:B:425:THR:HA	2:B:428:ILE:HD12	2.01	0.41
11:K:39:ASP:OD1	11:K:41:THR:HB	2.20	0.41
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.41
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.41
2:B:205:ILE:HD13	2:B:461:LEU:HB3	2.02	0.41
8:H:82:PRO:HB2	8:H:83:GLN:H	1.65	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.78	0.41
5:E:10:SER:O	5:E:14:ARG:HG3	2.19	0.41
1:A:37:PHE:O	1:A:53:LEU:HB2	2.21	0.41
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.02	0.41
1:A:133:LYS:HE3	1:A:1391:ARG:HH12	1.85	0.41
1:A:1196:GLU:HA	1:A:1236:LEU:O	2.21	0.41
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.41
1:A:1094:VAL:HG22	1:A:1113:THR:HB	2.02	0.41
1:A:567:LYS:HA	1:A:568:PRO:C	2.41	0.41
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.86	0.41
9:I:111:THR:HG21	9:I:118:ARG:HD2	2.03	0.41
2:B:841:MET:HG2	2:B:1010:LEU:HD12	2.01	0.41
12:L:27:LEU:HD22	12:L:37:LYS:HE3	2.02	0.41
1:A:1418:LEU:HD23	2:B:1222:ARG:HD3	2.03	0.41
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.56	0.41
1:A:626:ASN:O	1:A:631:HIS:ND1	2.53	0.41
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.85	0.41
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.02	0.41
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.41
2:B:899:ILE:HG21	2:B:949:VAL:HG21	2.03	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
2:B:509:ALA:O	2:B:511:PRO:HD3	2.20	0.41
2:B:953:LEU:HD11	12:L:55:ILE:HG22	2.03	0.41
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.03	0.41
2:B:1082:MET:HA	3:C:189:THR:HA	2.03	0.41
2:B:341:LEU:HD11	2:B:343:ILE:HB	2.02	0.41
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.85	0.41
10:J:22:LEU:O	10:J:26:GLN:HG2	2.20	0.41
2:B:100:PRO:HG3	2:B:172:ILE:HG13	2.03	0.41
2:B:871:THR:HG22	2:B:872:GLU:H	1.86	0.41
1:A:311:GLN:O	1:A:312:PRO:C	2.59	0.41
10:J:48:ARG:NE	10:J:49:MET:HE2	2.22	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
3:C:125:MET:HB2	3:C:127:ARG:NE	2.36	0.41
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.21	0.41
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.51	0.41
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.41
10:J:43:ARG:O	10:J:47:ARG:HG3	2.21	0.41
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.03	0.41
1:A:93:VAL:HG22	1:A:301:ALA:HA	2.04	0.40
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.86	0.40
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.03	0.40
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.40
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.36	0.40
8:H:104:PHE:CE1	8:H:136:LYS:HG3	2.57	0.40
4:D:154:PHE:HB2	4:D:160:VAL:HG22	2.04	0.40
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.03	0.40
9:I:8:ARG:O	9:I:9:ASP:CB	2.69	0.40
6:F:89:GLU:C	6:F:93:ILE:HD12	2.42	0.40
2:B:904:ARG:NH1	12:L:66:GLN:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:ILE:HG13	11:K:42:LEU:HD21	2.03	0.40
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.82	0.40
1:A:1402:PHE:CE1	1:A:1403:GLU:CG	3.04	0.40
1:A:982:THR:H	1:A:985:ASP:HB2	1.86	0.40
2:B:1129:ARG:HB3	15:T:21:DC:OP1	2.22	0.40
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.03	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%)	1236 (87%)	126 (9%)	52 (4%)	4 33
2	B	1095/1224 (90%)	968 (88%)	85 (8%)	42 (4%)	4 32
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	24 67
4	D	174/221 (79%)	148 (85%)	17 (10%)	9 (5%)	2 23
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	10 49
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100 100
7	G	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	11 50
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1 15
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	7 42
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	3 25
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100 100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0 1
All	All	3876/4564 (85%)	3413 (88%)	328 (8%)	135 (4%)	4 35

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	189	ARG
1	A	195	ASP
1	A	257	ARG
1	A	318	SER
1	A	399	HIS
1	A	449	SER
1	A	628	GLY
1	A	1377	THR
1	A	1403	GLU
1	A	1405	THR
2	B	108	VAL
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	473	MET
2	B	531	GLN
2	B	772	ALA
2	B	867	GLY
2	B	943	SER
2	B	1046	PRO
2	B	1181	GLU
4	D	18	VAL
4	D	53	SER
4	D	199	ASN
9	I	9	ASP
9	I	95	THR
12	L	50	ASP
12	L	53	HIS
1	A	47	ARG
1	A	54	ASN
1	A	167	CYS
1	A	178	GLY
1	A	193	ASP
1	A	224	PHE
1	A	286	HIS
1	A	332	LYS
1	A	672	ASP
1	A	1175	SER
1	A	1281	ARG
2	B	262	GLU

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Mol	Chain	Res	Type
2	B	282	ILE
2	B	339	THR
2	B	341	LEU
2	B	466	TRP
2	B	707	PRO
2	B	731	VAL
2	B	792	MET
2	B	879	ARG
2	B	1175	LEU
2	B	1176	ASN
4	D	16	LYS
4	D	52	LEU
4	D	169	SER
5	E	36	GLU
7	G	2	PHE
8	H	17	PRO
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
8	H	90	ALA
10	J	6	ARG
12	L	45	ALA
12	L	56	LEU
1	A	335	ARG
1	A	975	HIS
1	A	1173	HIS
2	B	58	THR
2	B	340	ALA
2	B	343	ILE
2	B	711	GLU
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
4	D	22	GLU
5	E	45	LYS
5	E	48	ASP
7	G	154	VAL
8	H	18	GLY
12	L	59	ALA
1	A	42	ASP
1	A	52	GLY
1	A	74	MET

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Mol	Chain	Res	Type
1	A	465	TYR
1	A	569	LYS
1	A	846	GLU
1	A	958	VAL
1	A	1255	GLU
1	A	1437	GLY
1	A	1438	THR
2	B	648	HIS
2	B	883	LEU
2	B	942	ARG
2	B	1108	ARG
2	B	1155	SER
3	C	88	CYS
9	I	91	ARG
10	J	29	GLU
12	L	26	THR
12	L	55	ILE
12	L	64	LEU
1	A	156	ASP
1	A	311	GLN
1	A	336	ILE
1	A	567	LYS
1	A	1171	GLN
1	A	1366	ARG
2	B	251	ILE
2	B	469	GLN
2	B	880	THR
2	B	907	GLY
2	B	1223	ASP
4	D	21	GLU
8	H	60	ALA
8	H	128	ASN
10	J	2	ILE
1	A	35	ILE
1	A	55	ASP
1	A	155	GLU
1	A	885	THR
3	C	214	ASN
4	D	15	LEU
1	A	196	GLU
1	A	1388	GLY
5	E	90	VAL

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Mol	Chain	Res	Type
7	G	63	PRO
2	B	364	ILE
1	A	192	GLY
1	A	312	PRO
2	B	1121	GLY
1	A	448	PRO
2	B	1214	PRO
8	H	59	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	1240/1519 (82%)	1062 (86%)	178 (14%)	4 21
2	B	966/1061 (91%)	842 (87%)	124 (13%)	5 26
3	C	234/274 (85%)	206 (88%)	28 (12%)	6 29
4	D	160/200 (80%)	129 (81%)	31 (19%)	2 8
5	E	196/197 (100%)	175 (89%)	21 (11%)	8 35
6	F	74/137 (54%)	67 (90%)	7 (10%)	11 41
7	G	152/152 (100%)	135 (89%)	17 (11%)	7 32
8	H	117/128 (91%)	103 (88%)	14 (12%)	6 29
9	I	113/116 (97%)	106 (94%)	7 (6%)	23 63
10	J	60/65 (92%)	49 (82%)	11 (18%)	2 10
11	K	99/102 (97%)	87 (88%)	12 (12%)	6 28
12	L	40/57 (70%)	27 (68%)	13 (32%)	0 2
All	All	3451/4008 (86%)	2988 (87%)	463 (13%)	5 24

All (463) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR

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Mol	Chain	Res	Type
1	A	15	LYS
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	45	GLN
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	93	VAL
1	A	106	VAL
1	A	131	SER
1	A	134	ARG
1	A	147	VAL
1	A	157	ASP
1	A	173	THR
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	237	THR
1	A	252	PHE
1	A	255	SER
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	289	ILE
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU
1	A	322	VAL
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	411	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	532	ARG
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	596	THR
1	A	602	ASP
1	A	603	ASN
1	A	618	GLU

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	634	THR
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	738	LYS
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	797	LYS
1	A	801	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	849	MET
1	A	867	ILE
1	A	886	ILE
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	949	ASP
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	998	LEU
1	A	1009	ASN
1	A	1015	VAL
1	A	1029	ARG
1	A	1030	ARG
1	A	1047	SER
1	A	1058	VAL
1	A	1062	GLU

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Mol	Chain	Res	Type
1	A	1067	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1273	LEU
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS

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Mol	Chain	Res	Type
1	A	1403	GLU
1	A	1426	GLU
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	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	118	ARG
2	B	134	LYS
2	B	169	ARG
2	B	183	GLU
2	B	185	THR
2	B	217	ARG
2	B	218	SER
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN
2	B	365	THR
2	B	393	LYS
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	436	VAL
2	B	446	LEU
2	B	448	ILE

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Mol	Chain	Res	Type
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	529	GLU
2	B	531	GLN
2	B	547	VAL
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	596	LEU
2	B	601	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	646	LEU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	696	GLU
2	B	708	GLU
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	771	SER
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	801	LYS
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	868	MET
2	B	871	THR

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Mol	Chain	Res	Type
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	906	SER
2	B	909	ASP
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	951	GLN
2	B	953	LEU
2	B	964	VAL
2	B	970	THR
2	B	973	ILE
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1094	ARG
2	B	1106	ARG
2	B	1123	SER
2	B	1129	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS

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Mol	Chain	Res	Type
2	B	1193	GLN
2	B	1201	LYS
2	B	1202	LEU
2	B	1210	MET
2	B	1220	ARG
2	B	1223	ASP
3	C	3	GLU
3	C	12	GLU
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	81	GLU
3	C	84	ARG
3	C	100	THR
3	C	101	LEU
3	C	119	VAL
3	C	121	VAL
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	147	LEU
3	C	148	ARG
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	12	ARG
4	D	13	ARG
4	D	17	LYS
4	D	18	VAL

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Mol	Chain	Res	Type
4	D	27	LEU
4	D	32	GLU
4	D	34	GLN
4	D	35	LEU
4	D	40	HIS
4	D	47	LEU
4	D	52	LEU
4	D	53	SER
4	D	65	GLU
4	D	118	THR
4	D	126	ILE
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	187	THR
4	D	197	SER
4	D	201	LYS
4	D	215	SER
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	31	THR
5	E	37	LEU
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	84	ASP
5	E	92	THR
5	E	104	ASN
5	E	131	THR
5	E	140	LEU
5	E	146	HIS
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	178	ILE
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL

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Mol	Chain	Res	Type
5	E	202	SER
5	E	204	THR
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	110	ASP
6	F	133	VAL
7	G	2	PHE
7	G	13	LEU
7	G	24	GLN
7	G	26	LEU
7	G	60	ARG
7	G	61	ILE
7	G	64	THR
7	G	96	GLN
7	G	106	MET
7	G	112	LYS
7	G	133	SER
7	G	138	THR
7	G	143	ILE
7	G	145	VAL
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	34	ASP
8	H	76	THR
8	H	77	ARG
8	H	83	GLN
8	H	89	LEU
8	H	91	ASP
8	H	92	ASP
8	H	103	LYS
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	8	ARG
9	I	31	THR

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Mol	Chain	Res	Type
9	I	35	VAL
9	I	74	GLU
9	I	94	ASP
9	I	106	CYS
9	I	111	THR
10	J	1	MET
10	J	2	ILE
10	J	3	VAL
10	J	7	CYS
10	J	12	LYS
10	J	13	VAL
10	J	22	LEU
10	J	29	GLU
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	70	ARG
11	K	101	LEU
11	K	107	THR
12	L	27	LEU
12	L	35	SER
12	L	38	LEU
12	L	42	ARG
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	56	LEU
12	L	58	LYS
12	L	60	ARG
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 (33) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	253	ASN
1	A	399	HIS
1	A	425	GLN
1	A	545	GLN
1	A	548	ASN
1	A	603	ASN
1	A	994	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1173	HIS
1	A	1270	ASN
1	A	1390	ASN
1	A	1393	ASN
2	B	46	GLN
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	449	ASN
2	B	842	ASN
2	B	975	GLN
2	B	1025	HIS
2	B	1117	GLN
3	C	184	ASN
4	D	37	GLN
4	D	143	ASN
5	E	3	GLN
7	G	71	ASN
7	G	102	GLN
8	H	35	GLN
8	H	83	GLN
9	I	83	ASN
9	I	89	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/6 (83%)	1 (20%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	G

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	13,21,22	1.07	1 (7%)	16,30,33	3.73	4 (25%)

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	-	0/3/21/22	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	2.91	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	22	BRU	C5-C4-N3	-8.62	114.80	124.00
15	T	22	BRU	C2'-C1'-N1	-2.43	108.25	114.16
15	T	22	BRU	O4'-C1'-N1	4.41	115.35	107.72
15	T	22	BRU	C4-N3-C2	11.05	124.80	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	22	BRU	1	0

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)

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	1422/1732 (82%)	0.04	28 (1%) 68 62	52, 96, 155, 215	0
2	B	1115/1224 (91%)	0.13	34 (3%) 54 49	56, 111, 174, 201	0
3	C	266/318 (83%)	-0.07	0 100 100	68, 97, 135, 165	0
4	D	178/221 (80%)	0.09	5 (2%) 56 52	77, 110, 162, 182	0
5	E	214/215 (99%)	0.14	10 (4%) 35 32	72, 129, 170, 191	0
6	F	84/155 (54%)	-0.16	1 (1%) 81 75	55, 76, 106, 122	0
7	G	171/171 (100%)	0.10	1 (0%) 90 86	65, 96, 135, 153	0
8	H	133/146 (91%)	0.87	20 (15%) 3 3	110, 136, 175, 195	0
9	I	119/122 (97%)	0.16	4 (3%) 49 44	107, 137, 173, 189	0
10	J	65/70 (92%)	-0.22	0 100 100	73, 94, 129, 142	0
11	K	115/120 (95%)	-0.10	2 (1%) 73 67	63, 95, 135, 151	0
12	L	46/70 (65%)	0.82	7 (15%) 3 3	92, 161, 182, 184	0
13	N	10/14 (71%)	0.52	2 (20%) 1 2	158, 184, 239, 246	0
14	P	6/6 (100%)	-0.25	0 100 100	75, 90, 111, 138	0
15	T	19/26 (73%)	0.33	1 (5%) 30 27	105, 152, 246, 248	0
All	All	3963/4610 (85%)	0.10	115 (2%) 55 50	52, 105, 168, 248	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	SER	7.2
1	A	1176	LEU	6.9
1	A	194	ALA	5.8
12	L	26	THR	5.6
9	I	119	THR	5.2
1	A	257	ARG	5.0
12	L	25	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	195	ASP	4.6
12	L	27	LEU	4.4
1	A	256	GLN	4.2
2	B	883	LEU	4.2
11	K	115	ALA	4.1
1	A	1455	PRO	4.1
2	B	918	ILE	4.1
2	B	709	ASP	4.0
2	B	715	ALA	3.9
2	B	865	LYS	3.7
1	A	191	THR	3.6
1	A	192	GLY	3.6
8	H	139	ASN	3.4
5	E	110	PHE	3.3
9	I	120	GLN	3.3
2	B	340	ALA	3.3
2	B	864	LYS	3.2
9	I	118	ARG	3.2
2	B	868	MET	3.1
8	H	86	ASP	3.0
4	D	9	GLN	3.0
8	H	83	GLN	3.0
2	B	708	GLU	3.0
4	D	38	ILE	3.0
8	H	107	VAL	2.9
8	H	134	ASN	2.9
2	B	250	PHE	2.9
2	B	132	VAL	2.9
2	B	339	THR	2.8
1	A	255	SER	2.8
1	A	193	ASP	2.8
2	B	167	ILE	2.8
12	L	50	ASP	2.8
4	D	8	PHE	2.8
8	H	142	LEU	2.8
2	B	92	PHE	2.8
1	A	252	PHE	2.8
1	A	253	ASN	2.8
8	H	146	ARG	2.8
5	E	39	LEU	2.7
1	A	142	CYS	2.7
2	B	509	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	69	LEU	2.6
12	L	47	ARG	2.6
8	H	144	ILE	2.6
7	G	128	PRO	2.6
12	L	45	ALA	2.6
2	B	342	GLY	2.5
13	N	8	DT	2.5
6	F	108	PHE	2.5
8	H	125	LEU	2.5
1	A	155	GLU	2.5
4	D	13	ARG	2.5
1	A	250	ILE	2.5
2	B	130	VAL	2.5
2	B	343	ILE	2.5
1	A	163	SER	2.4
2	B	90	ILE	2.4
1	A	114	LEU	2.4
15	T	7	DT	2.4
2	B	165	VAL	2.4
1	A	56	PRO	2.4
8	H	59	ILE	2.4
1	A	187	LYS	2.3
2	B	433	GLN	2.3
5	E	93	MET	2.3
8	H	140	ALA	2.3
11	K	114	LEU	2.3
8	H	56	THR	2.3
1	A	145	LYS	2.3
2	B	95	ILE	2.3
1	A	161	LEU	2.3
5	E	82	PHE	2.3
2	B	870	ILE	2.3
8	H	114	VAL	2.3
8	H	106	GLU	2.3
8	H	61	SER	2.3
8	H	145	ARG	2.2
2	B	963	PHE	2.2
9	I	116	ASN	2.2
1	A	162	VAL	2.2
1	A	254	GLU	2.2
1	A	199	LEU	2.2
2	B	714	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	722	ASP	2.2
5	E	123	LEU	2.2
5	E	46	TYR	2.2
8	H	113	ALA	2.2
13	N	9	DT	2.2
2	B	25	ILE	2.2
1	A	158	PRO	2.1
2	B	919	SER	2.1
2	B	882	THR	2.1
8	H	116	TYR	2.1
1	A	385	ILE	2.1
5	E	96	PHE	2.1
2	B	436	VAL	2.1
5	E	81	GLU	2.1
5	E	42	PHE	2.1
12	L	46	VAL	2.1
1	A	198	GLU	2.1
2	B	262	GLU	2.1
2	B	435	THR	2.0
5	E	132	ILE	2.0
8	H	6	PHE	2.0
8	H	55	LEU	2.0
2	B	63	ILE	2.0
4	D	10	THR	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	22	20/21	0.96	0.13	-	107,109,114,121	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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
16	ZN	J	1066	1/1	0.98	0.23	0.16	91,91,91,91	0
16	ZN	B	2225	1/1	0.99	0.19	0.01	77,77,77,77	0
16	ZN	I	1121	1/1	0.99	0.12	-0.05	121,121,121,121	0
16	ZN	A	2457	1/1	0.99	0.14	-0.96	67,67,67,67	0
16	ZN	C	1269	1/1	0.99	0.10	-1.22	88,88,88,88	0
16	ZN	A	2456	1/1	1.00	0.07	-2.34	133,133,133,133	0
16	ZN	I	1122	1/1	0.98	0.04	-2.43	182,182,182,182	0
16	ZN	L	1071	1/1	0.99	0.06	-2.74	163,163,163,163	0
17	MG	A	2458	1/1	1.00	0.17	-	64,64,64,64	0

6.5 Other polymers

There are no such residues in this entry.