Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:43 pm BST

PDB ID	:	4A3M
Title	:	RNA Polymerase II initial transcribing complex with a 4nt DNA-RNA hybrid and soaked with AMPCPP
Authors	:	Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on	:	2011-09-30
Resolution	:	3.90 Å(reported)

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

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

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

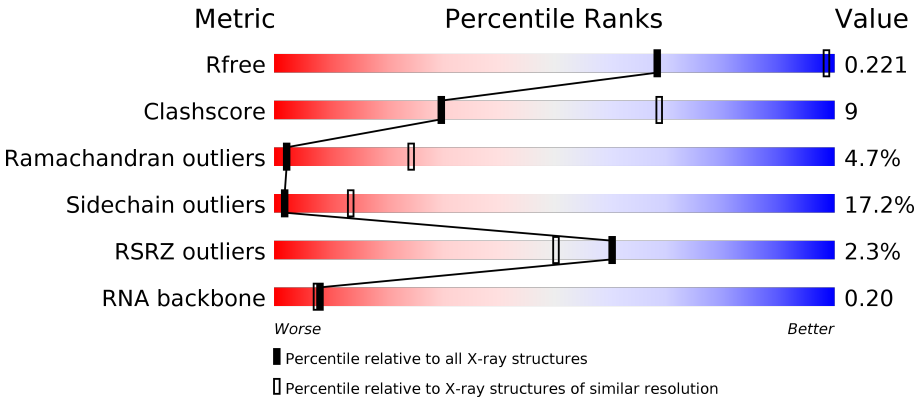
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1732	2% 51% 26% 5% 18%
2	B	1224	2% 60% 25% 6% 9%
3	C	318	48% 30% 5% 16%
4	D	221	% 53% 24% 19%

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Mol	Chain	Length	Quality of chain
5	E	215	2% 70% 27%
6	F	155	37% 13% 5% 46%
7	G	171	% 66% 27% 6%
8	H	146	8% 57% 28% 5% 9%
9	I	122	% 72% 20% 5%
10	J	70	50% 33% 6% 7%
11	K	120	% 64% 27% 5%
12	L	70	11% 33% 23% 9% 34%
13	N	14	14% 50% 14% 36%
14	P	4	25% 75%
15	T	26	4% 27% 38% 35%

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
16	APC	A	2455	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 31868 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 RPABC1.

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 RPABC2.

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 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 RPABC3.

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 RPABC5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	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 RPABC4.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	9	Total	C	N	O	P	0	0	0
			183	89	34	52	8			

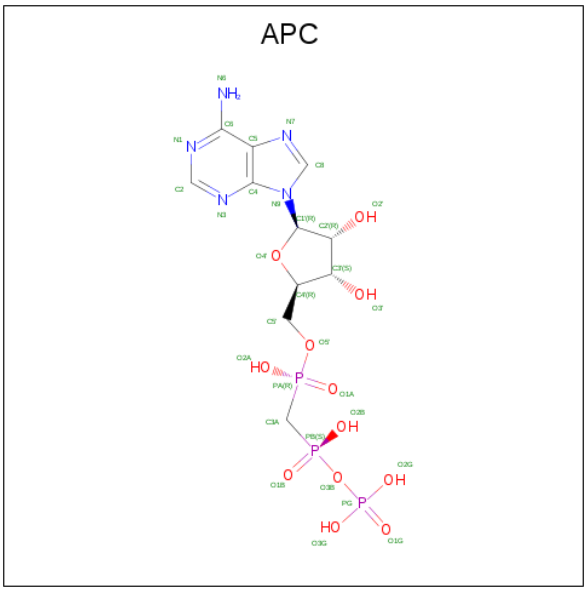
- Molecule 14 is a RNA chain called 5'-R(*AP*GP*GP*A)-3'.

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

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*T P*TP*TP* TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	17	Total	Br	C	N	O	P	0	0	0
			345	1	165	56	106	17			

- Molecule 16 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

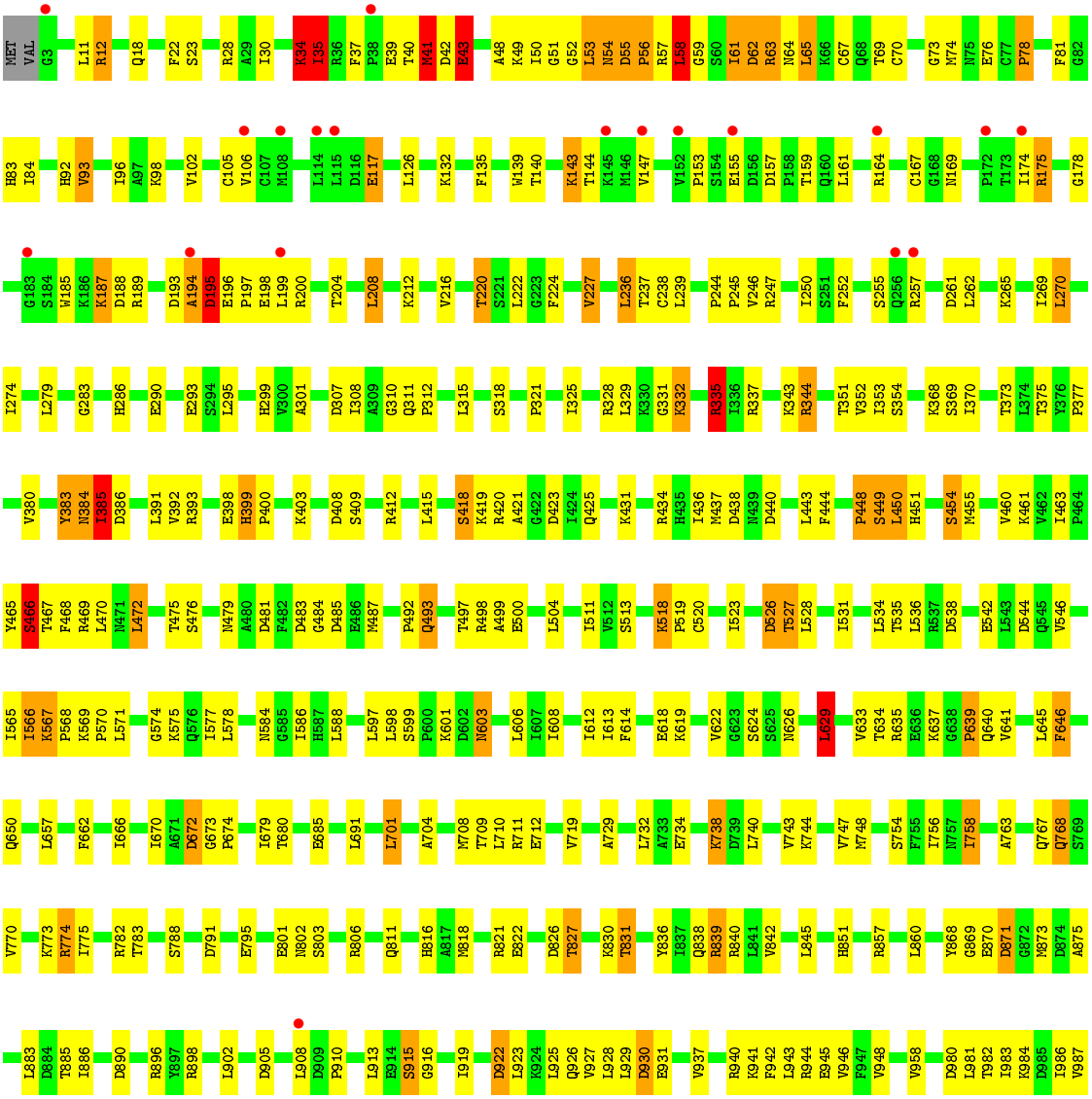
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Mg 1 1	0	0

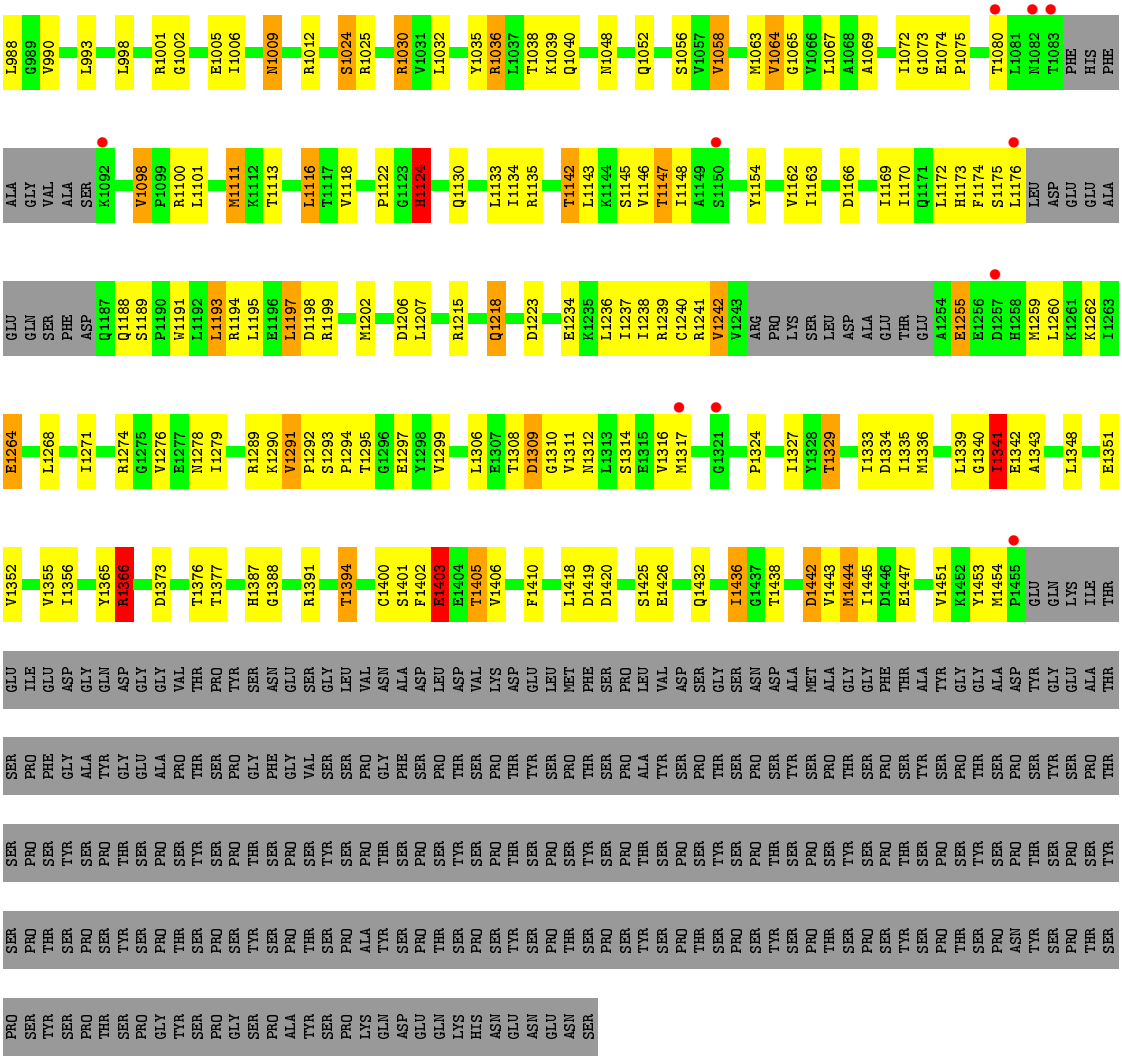
3 Residue-property plots (i)

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

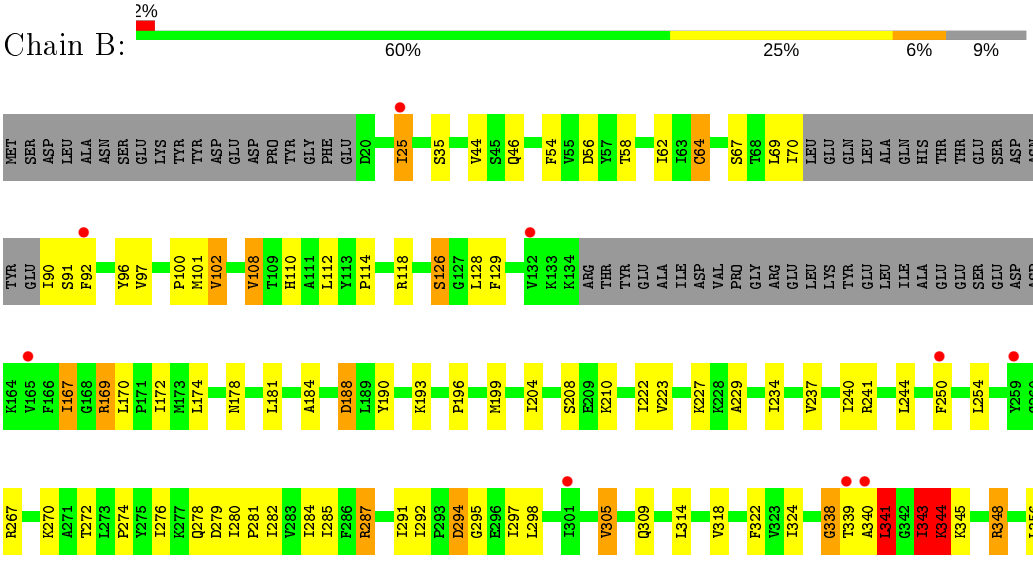
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

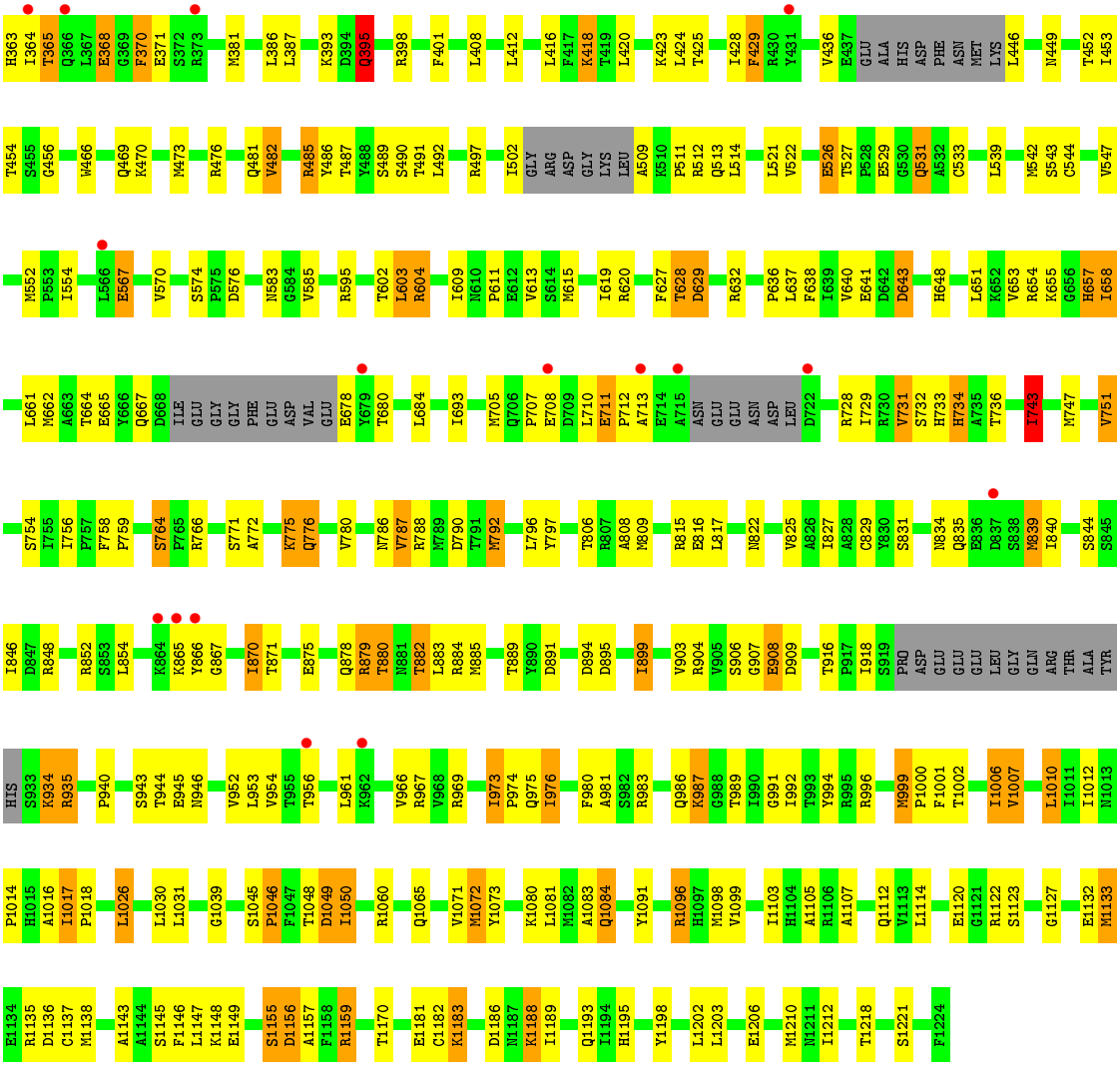
Chain A: 





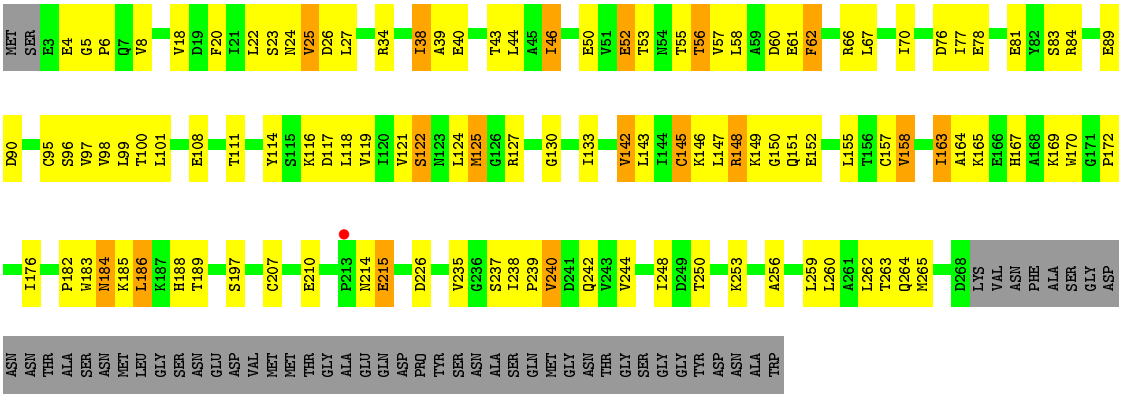
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





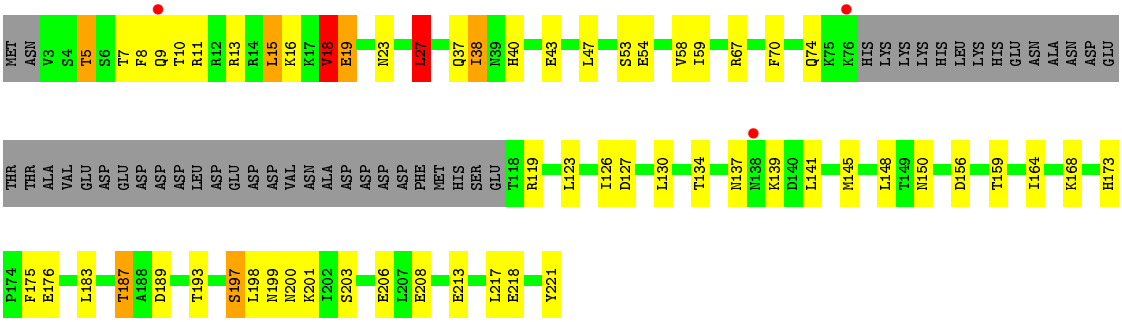
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



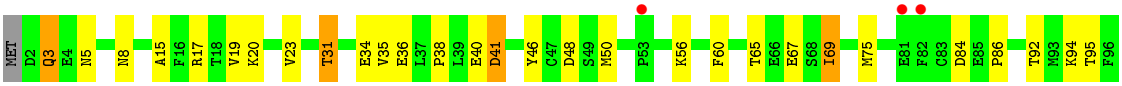
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



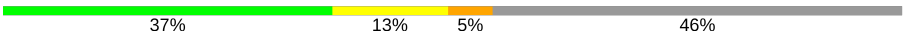
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

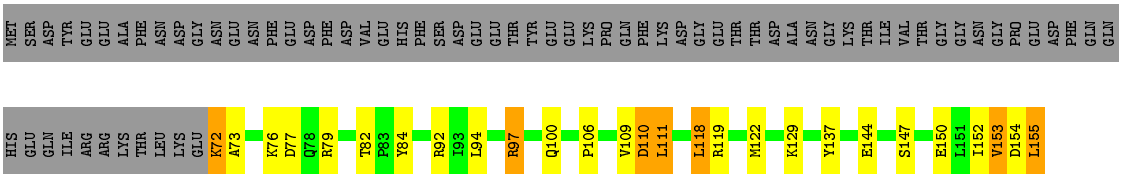
Chain E:



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

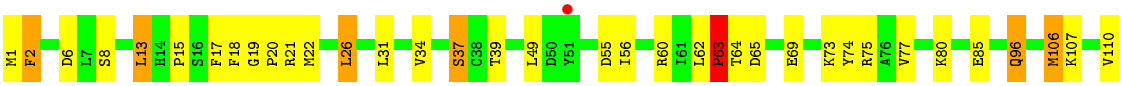
Chain F:





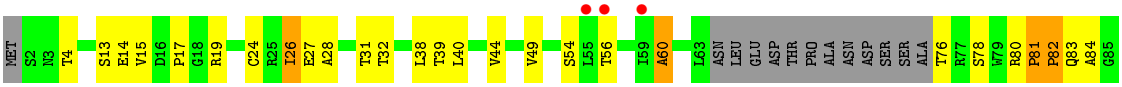
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

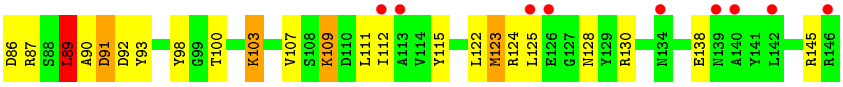
Chain G:



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

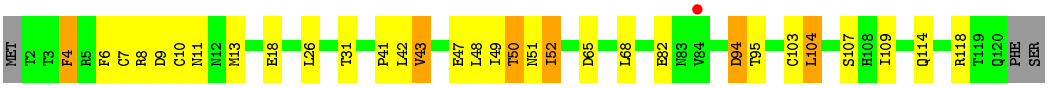
Chain H:





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

Chain I:

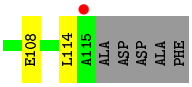


• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5

Chain J:

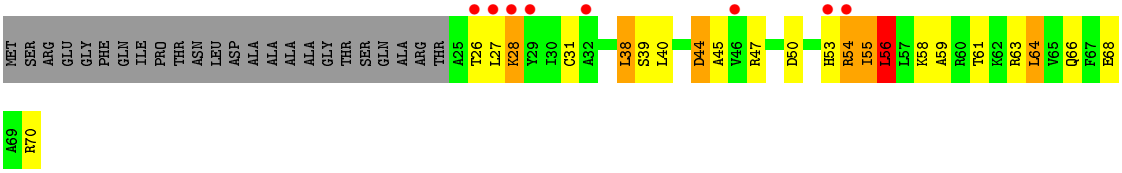
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



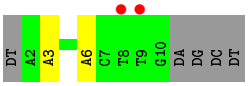
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

Chain L:



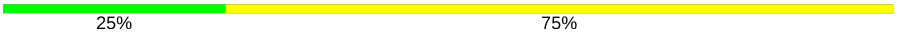
• Molecule 13: 5'-D(*AP*AP*GP*TP*AP*CP*TP)-3'

Chain N:



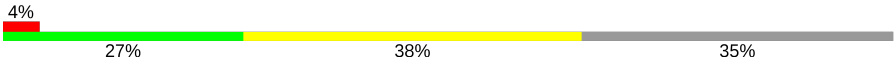
• Molecule 14: 5'-R(*AP*GP*GP*A)-3'

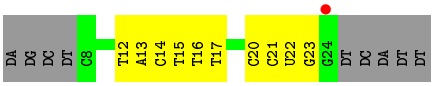
Chain P:



• Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP* TP*TP*CP* CP*BRUP*GP*GP*TP*CP*AP*TP*T)-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	222.27Å 392.99Å 282.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.65 – 3.90 58.65 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.65-3.90) 99.2 (58.65-3.90)	Depositor EDS
R_{merge}	0.87	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.154 , 0.190 0.187 , 0.221	Depositor DCC
R_{free} test set	2247 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	131.7	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 140.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.057 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.047 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31868	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, APC, 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	0/11397	0.86	7/15415 (0.0%)
2	B	0.52	0/9029	0.82	1/12171 (0.0%)
3	C	0.50	0/2133	0.80	0/2891
4	D	0.54	0/1444	0.85	0/1935
5	E	0.46	0/1788	0.73	0/2406
6	F	0.59	0/691	0.83	0/933
7	G	0.52	0/1368	0.82	1/1844 (0.1%)
8	H	0.53	0/1086	0.87	0/1470
9	I	0.45	0/989	0.78	0/1331
10	J	0.55	0/541	0.83	0/727
11	K	0.50	0/938	0.76	0/1267
12	L	0.51	0/365	0.91	0/485
13	N	1.32	1/205 (0.5%)	1.16	0/315
14	P	0.85	0/101	0.83	0/156
15	T	1.35	0/361	1.10	1/552 (0.2%)
All	All	0.55	1/32436 (0.0%)	0.84	10/43898 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	3	DA	C3'-O3'	5.74	1.51	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	PRO	C-N-CA	6.96	139.11	121.70
1	A	34	LYS	C-N-CA	5.83	136.27	121.70
1	A	399	HIS	N-CA-CB	5.59	120.66	110.60
1	A	35	ILE	N-CA-CB	5.49	123.43	110.80
1	A	194	ALA	C-N-CA	5.49	135.42	121.70
7	G	63	PRO	N-CA-C	5.48	126.35	112.10
2	B	338	GLY	C-N-CA	5.38	135.16	121.70
1	A	55	ASP	N-CA-CB	5.20	119.96	110.60
1	A	35	ILE	CB-CA-C	5.07	121.75	111.60
15	T	23	DG	O4'-C4'-C3'	-5.01	102.50	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain

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	246	0
2	B	8859	0	8901	176	0
3	C	2095	0	2051	61	0
4	D	1434	0	1460	22	0
5	E	1752	0	1776	27	0
6	F	679	0	701	19	0
7	G	1340	0	1357	31	0
8	H	1068	0	1040	22	0
9	I	971	0	927	14	0
10	J	532	0	542	16	0
11	K	920	0	929	19	0
12	L	363	0	386	6	0
13	N	183	0	104	2	0
14	P	90	0	44	1	0
15	T	345	0	192	10	0
16	A	31	0	14	2	0
17	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	31868	0	31681	594	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 (594) 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)
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.41	1.02
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.47	0.96
3:C:46:ILE:H	3:C:46:ILE:HD12	1.38	0.87
2:B:1017:ILE:H	2:B:1017:ILE:HD13	1.41	0.86
10:J:48:ARG:O	10:J:52:THR:HG22	1.76	0.85
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.59	0.84
1:A:450:LEU:H	1:A:450:LEU:HD12	1.42	0.83
13:N:6:DA:H61	15:T:12:DT:H3	1.25	0.81
3:C:163:ILE:HD11	3:C:165:LYS:HB2	1.62	0.81
1:A:41:MET:HB2	1:A:49:LYS:HA	1.64	0.79
1:A:1193:LEU:HD21	1:A:1264:GLU:HB3	1.65	0.79
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.78
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.64	0.78
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.67	0.77
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.68	0.75
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.68	0.75
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.69	0.75
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.23	0.73
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.70	0.73
6:F:118:LEU:O	6:F:122:MET:HG3	1.88	0.73
3:C:46:ILE:H	3:C:46:ILE:CD1	2.03	0.72
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.71	0.71
15:T:16:DT:H2'	15:T:17:DT:H5"	1.72	0.71
1:A:679:ILE:HG13	1:A:732:LEU:HD12	1.73	0.70
8:H:4:THR:HA	8:H:60:ALA:HB2	1.73	0.70
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.75	0.69
1:A:40:THR:HG22	1:A:41:MET:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.73	0.69
2:B:64:CYS:HA	2:B:67:SER:HB3	1.74	0.69
7:G:1:MET:CG	7:G:2:PHE:H	2.06	0.68
1:A:315:LEU:HA	1:A:321:PRO:HA	1.75	0.68
1:A:216:VAL:O	1:A:220:THR:HB	1.94	0.68
2:B:244:LEU:HD11	2:B:250:PHE:HD2	1.57	0.68
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.76	0.68
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.76	0.68
7:G:26:LEU:HB3	7:G:56:ILE:HD11	1.76	0.68
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.76	0.67
3:C:46:ILE:HD13	3:C:67:LEU:O	1.93	0.67
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.30	0.67
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.77	0.67
1:A:629:LEU:O	1:A:633:VAL:HG23	1.94	0.66
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.77	0.66
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.61	0.66
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.78	0.66
1:A:352:VAL:HB	2:B:1099:VAL:HG23	1.78	0.66
5:E:197:LYS:HG3	5:E:211:TYR:CE1	2.31	0.66
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.76	0.66
2:B:822:ASN:O	10:J:48:ARG:NH1	2.28	0.65
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.79	0.65
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.79	0.65
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.77	0.65
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.78	0.64
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.31	0.64
2:B:512:ARG:HD3	2:B:533:CYS:O	1.98	0.64
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.78	0.64
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.80	0.64
6:F:100:GLN:HG2	7:G:15:PRO:HB3	1.80	0.64
1:A:140:THR:HA	1:A:143:LYS:HD3	1.80	0.64
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.98	0.63
10:J:8:PHE:H	10:J:49:MET:HE3	1.62	0.63
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.33	0.63
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.64	0.63
4:D:40:HIS:ND1	7:G:6:ASP:HB3	2.14	0.63
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.63	0.62
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.64	0.62
7:G:34:VAL:O	7:G:37:SER:HB3	1.99	0.62
11:K:21:ILE:HG23	11:K:33:ILE:CG1	2.28	0.62
1:A:873:MET:HG3	1:A:1056:SER:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:LEU:C	8:H:91:ASP:H	2.01	0.62
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.38	0.61
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.63	0.61
1:A:262:LEU:HD21	1:A:325:ILE:HG12	1.82	0.61
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.82	0.61
2:B:880:THR:HB	2:B:934:LYS:HD2	1.83	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.35	0.61
12:L:40:LEU:HD13	12:L:44:ASP:HB2	1.82	0.61
15:T:15:DT:H2'	15:T:16:DT:C6	2.35	0.60
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.83	0.60
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.83	0.60
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.83	0.60
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.32	0.60
1:A:827:THR:O	1:A:831:THR:HB	2.01	0.60
2:B:234:ILE:HG21	2:B:237:VAL:HG22	1.84	0.60
1:A:227:VAL:HG12	4:D:15:LEU:HD23	1.83	0.59
1:A:35:ILE:O	1:A:84:ILE:HG22	2.02	0.59
1:A:41:MET:CB	1:A:49:LYS:HA	2.31	0.59
2:B:291:ILE:HD12	2:B:291:ILE:H	1.67	0.59
4:D:5:THR:HG21	7:G:74:TYR:OH	2.01	0.59
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.84	0.59
4:D:54:GLU:O	4:D:58:VAL:HG23	2.03	0.59
8:H:82:PRO:C	8:H:84:ALA:H	2.03	0.59
5:E:3:GLN:HE21	5:E:5:ASN:HB2	1.67	0.59
7:G:13:LEU:HD22	7:G:17:PHE:HD2	1.68	0.59
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.83	0.59
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.85	0.59
1:A:986:ILE:O	1:A:990:VAL:HG23	2.04	0.58
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.68	0.58
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.84	0.58
1:A:567:LYS:HA	1:A:568:PRO:C	2.23	0.58
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.85	0.58
1:A:499:ALA:HB2	6:F:118:LEU:HD11	1.85	0.58
1:A:98:LYS:O	1:A:102:VAL:HG23	2.04	0.58
7:G:129:SER:HB3	7:G:138:THR:HG23	1.85	0.58
1:A:709:THR:HB	1:A:712:GLU:H	1.69	0.57
3:C:56:THR:HG22	3:C:57:VAL:H	1.69	0.57
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.86	0.57
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.86	0.57
3:C:56:THR:HG22	3:C:57:VAL:HG22	1.86	0.57
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:MET:SD	7:G:2:PHE:N	2.74	0.57
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.70	0.57
1:A:860:LEU:HD21	1:A:1394:THR:HA	1.87	0.57
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.25	0.57
1:A:923:LEU:H	1:A:923:LEU:HD12	1.70	0.56
5:E:15:ALA:O	5:E:19:VAL:HG23	2.05	0.56
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.86	0.56
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.87	0.56
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.86	0.56
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.87	0.56
1:A:1451:VAL:HG13	7:G:20:PRO:HB3	1.86	0.56
10:J:57:ILE:O	10:J:60:PHE:HB2	2.05	0.56
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.40	0.56
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.86	0.56
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.06	0.56
1:A:448:PRO:O	1:A:449:SER:HB2	2.06	0.56
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.86	0.56
1:A:175:ARG:HH12	1:A:199:LEU:HD21	1.69	0.56
2:B:128:LEU:HB3	2:B:167:ILE:HD12	1.88	0.56
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.88	0.56
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.87	0.56
1:A:1343:ALA:HB2	5:E:150:VAL:HG13	1.86	0.55
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.19	0.55
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.88	0.55
5:E:190:LEU:HD12	5:E:214:CYS:HB2	1.88	0.55
1:A:78:PRO:O	1:A:245:PRO:HG2	2.07	0.55
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.86	0.55
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.87	0.55
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.05	0.55
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.88	0.55
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.89	0.55
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.87	0.55
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.72	0.55
15:T:16:DT:H2'	15:T:17:DT:C5'	2.36	0.55
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.07	0.55
1:A:392:VAL:HG13	1:A:415:LEU:HD21	1.88	0.55
2:B:492:LEU:HB2	2:B:751:VAL:HG11	1.88	0.55
1:A:578:LEU:HD23	1:A:612:ILE:HD11	1.89	0.54
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.87	0.54
11:K:18:LYS:HE3	11:K:38:GLU:HG2	1.89	0.54
1:A:1215:ARG:O	1:A:1218:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ARG:HH22	2:B:775:LYS:HD3	1.72	0.54
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.89	0.54
2:B:174:LEU:HD11	2:B:204:ILE:HD12	1.90	0.54
1:A:851:HIS:HE1	1:A:857:ARG:HB2	1.73	0.54
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.90	0.54
8:H:13:SER:HB2	8:H:27:GLU:HB3	1.89	0.54
1:A:63:ARG:HG3	1:A:74:MET:HG3	1.90	0.54
2:B:1006:ILE:HG23	10:J:43:ARG:HD2	1.89	0.54
10:J:7:CYS:O	10:J:11:GLY:HA2	2.08	0.54
2:B:788:ARG:O	2:B:967:ARG:NH1	2.41	0.54
8:H:100:THR:HG23	8:H:138:GLU:HA	1.90	0.54
2:B:244:LEU:CD1	2:B:250:PHE:HD2	2.19	0.53
3:C:66:ARG:NH2	10:J:3:VAL:O	2.41	0.53
1:A:1172:LEU:C	1:A:1174:PHE:H	2.11	0.53
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.90	0.53
2:B:295:GLY:H	2:B:298:LEU:HD13	1.73	0.53
2:B:916:THR:HB	2:B:935:ARG:HG3	1.90	0.53
2:B:281:PRO:HD2	2:B:284:ILE:HD13	1.91	0.53
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.43	0.53
4:D:59:ILE:HG21	4:D:141:LEU:HD11	1.90	0.53
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.90	0.53
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.39	0.53
10:J:24:LEU:HD21	10:J:38:ARG:HD2	1.91	0.53
3:C:183:TRP:HB2	3:C:185:LYS:HE2	1.90	0.53
15:T:16:DT:C2'	15:T:17:DT:H5"	2.38	0.53
3:C:124:LEU:O	3:C:127:ARG:HG2	2.08	0.53
15:T:13:DA:H4'	15:T:14:DC:OP1	2.09	0.53
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.90	0.53
13:N:6:DA:N6	15:T:12:DT:H3	2.02	0.53
1:A:981:LEU:HD23	1:A:1039:LYS:HD2	1.89	0.52
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.72	0.52
2:B:425:THR:HA	2:B:428:ILE:HD12	1.91	0.52
1:A:153:PRO:HA	1:A:161:LEU:HA	1.91	0.52
1:A:35:ILE:HG22	1:A:270:LEU:HD21	1.91	0.52
2:B:654:ARG:H	2:B:657:HIS:CE1	2.27	0.52
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	1.91	0.52
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.90	0.52
1:A:1025:ARG:HA	1:A:1030:ARG:HH11	1.75	0.52
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.92	0.52
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.92	0.52
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:54:ASN:H	1.73	0.52
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.91	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.25	0.52
1:A:885:THR:OG1	1:A:1024:SER:HB2	2.09	0.52
2:B:497:ARG:NH2	2:B:775:LYS:HD3	2.25	0.52
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.91	0.52
3:C:62:PHE:O	3:C:66:ARG:HG3	2.09	0.52
2:B:711:GLU:CB	2:B:712:PRO:HD3	2.40	0.51
3:C:163:ILE:CD1	3:C:165:LYS:HB2	2.36	0.51
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.09	0.51
1:A:637:LYS:HB3	1:A:641:VAL:CG1	2.41	0.51
5:E:97:VAL:HG13	5:E:127:ILE:HG12	1.91	0.51
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.40	0.51
1:A:335:ARG:HH12	2:B:1114:LEU:HD21	1.75	0.51
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.74	0.51
2:B:865:LYS:HD2	2:B:961:LEU:HD21	1.93	0.51
6:F:111:LEU:H	6:F:111:LEU:HD12	1.74	0.51
1:A:942:PHE:O	1:A:945:GLU:HB2	2.10	0.51
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.91	0.51
1:A:937:VAL:O	1:A:941:LYS:HG2	2.11	0.51
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.92	0.51
1:A:743:VAL:O	1:A:747:VAL:HG23	2.11	0.51
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.46	0.51
3:C:125:MET:SD	3:C:125:MET:N	2.84	0.51
4:D:27:LEU:HD23	4:D:197:SER:HB3	1.92	0.51
8:H:103:LYS:HB3	8:H:115:TYR:HD2	1.76	0.51
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.76	0.50
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	1.93	0.50
6:F:79:ARG:NH2	6:F:150:GLU:OE2	2.44	0.50
9:I:103:CYS:HB3	9:I:107:SER:H	1.76	0.50
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.51	0.50
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.92	0.50
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.93	0.50
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.93	0.50
1:A:929:LEU:HD21	1:A:983:ILE:HG12	1.94	0.50
2:B:509:ALA:O	2:B:511:PRO:HD3	2.11	0.50
2:B:542:MET:HG2	2:B:747:MET:HB3	1.92	0.50
3:C:20:PHE:HE2	3:C:22:LEU:HD13	1.77	0.50
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.94	0.50
2:B:882:THR:HB	2:B:934:LYS:C	2.32	0.50
1:A:1341:ILE:HD12	1:A:1376:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.94	0.50
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.12	0.50
2:B:852:ARG:HG2	2:B:973:ILE:HG13	1.92	0.50
1:A:984:LYS:O	1:A:988:LEU:HB2	2.12	0.50
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.92	0.50
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.93	0.49
1:A:542:GLU:O	1:A:546:VAL:HG23	2.12	0.49
1:A:62:ASP:HB3	1:A:65:LEU:HB2	1.94	0.49
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.32	0.49
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.93	0.49
2:B:542:MET:HE3	2:B:743:ILE:HD13	1.93	0.49
1:A:466:SER:HB3	2:B:1103:ILE:HD12	1.93	0.49
2:B:758:PHE:HZ	2:B:1031:LEU:HD13	1.77	0.49
4:D:8:PHE:HB2	4:D:38:ILE:HD12	1.94	0.49
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.94	0.49
1:A:1329:THR:HG23	1:A:1335:ILE:HG12	1.94	0.49
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.94	0.49
1:A:332:LYS:H	1:A:337:ARG:HB2	1.78	0.49
1:A:738:LYS:HD3	1:A:740:LEU:HD21	1.94	0.49
2:B:806:THR:HG22	2:B:808:ALA:H	1.77	0.49
3:C:146:LYS:HD2	10:J:57:ILE:HG12	1.95	0.49
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.13	0.49
1:A:373:THR:HG21	2:B:1105:ALA:CB	2.41	0.49
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.76	0.49
1:A:472:LEU:O	1:A:475:THR:HG22	2.12	0.49
1:A:927:VAL:O	1:A:931:GLU:HB2	2.13	0.49
2:B:1017:ILE:H	2:B:1017:ILE:CD1	2.10	0.49
4:D:127:ASP:HA	4:D:130:LEU:HD12	1.94	0.49
7:G:106:MET:HG2	7:G:107:LYS:N	2.26	0.49
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.27	0.49
2:B:343:ILE:O	2:B:344:LYS:HB2	2.11	0.49
4:D:126:ILE:HG21	4:D:145:MET:HB3	1.95	0.49
7:G:1:MET:CG	7:G:2:PHE:N	2.75	0.49
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.93	0.49
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.94	0.49
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.49
2:B:613:VAL:HG22	2:B:628:THR:HA	1.94	0.49
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.95	0.49
11:K:12:LEU:HD22	11:K:16:GLU:HB3	1.95	0.49
1:A:940:ARG:O	1:A:944:ARG:HG3	2.12	0.49
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ILE:HD12	3:C:165:LYS:H	1.76	0.49
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.95	0.48
2:B:62:ILE:HG12	2:B:418:LYS:HD3	1.94	0.48
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.95	0.48
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.94	0.48
2:B:270:LYS:NZ	2:B:281:PRO:HG3	2.27	0.48
2:B:848:ARG:HH12	2:B:996:ARG:HD3	1.78	0.48
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.95	0.48
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.28	0.48
7:G:151:ILE:HD11	7:G:160:ILE:HD11	1.93	0.48
7:G:49:LEU:HD11	7:G:77:VAL:HG23	1.94	0.48
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.95	0.48
1:A:1163:ILE:HD13	1:A:1194:ARG:HD2	1.95	0.48
1:A:194:ALA:HA	1:A:195:ASP:C	2.34	0.48
2:B:280:ILE:HB	2:B:285:ILE:HD11	1.94	0.48
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.95	0.48
1:A:440:ASP:O	1:A:460:VAL:HG23	2.13	0.48
2:B:827:ILE:HG23	2:B:1012:ILE:HG13	1.95	0.48
2:B:908:GLU:HG3	2:B:943:SER:HA	1.96	0.48
3:C:40:GLU:HA	3:C:163:ILE:HD13	1.95	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:HD2	1.96	0.48
3:C:164:ALA:HA	3:C:167:HIS:O	2.14	0.48
9:I:50:THR:HG22	9:I:52:ILE:H	1.78	0.48
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.13	0.48
1:A:492:PRO:CB	1:A:497:THR:HG22	2.43	0.48
2:B:638:PHE:HB3	2:B:651:LEU:HD23	1.96	0.48
3:C:146:LYS:HB2	10:J:57:ILE:HD11	1.94	0.48
3:C:165:LYS:O	11:K:6:ARG:NH1	2.44	0.48
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.48
11:K:87:LEU:O	11:K:91:CYS:HB2	2.14	0.47
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.96	0.47
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.96	0.47
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.48	0.47
7:G:19:GLY:O	7:G:22:MET:HB2	2.14	0.47
1:A:534:LEU:O	1:A:574:GLY:HA3	2.14	0.47
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.97	0.47
5:E:19:VAL:O	5:E:23:VAL:HG23	2.13	0.47
7:G:96:GLN:HG3	7:G:96:GLN:H	1.48	0.47
1:A:344:ARG:HG2	2:B:1127:GLY:O	2.14	0.47
2:B:758:PHE:HE1	2:B:1050:ILE:HD13	1.79	0.47
1:A:448:PRO:CG	16:A:2455:APC:H2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:GLU:H	2:B:567:GLU:HG2	1.44	0.47
2:B:796:LEU:HD12	2:B:852:ARG:O	2.13	0.47
5:E:20:LYS:HD3	5:E:35:VAL:HA	1.97	0.47
1:A:246:VAL:O	1:A:328:ARG:NH1	2.39	0.47
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.97	0.47
6:F:147:SER:H	6:F:150:GLU:HG2	1.78	0.47
1:A:270:LEU:HD12	1:A:274:ILE:HD11	1.97	0.47
3:C:6:PRO:HB2	11:K:101:LEU:HD23	1.95	0.47
8:H:89:LEU:O	8:H:91:ASP:N	2.47	0.47
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.79	0.47
11:K:45:LEU:HD21	11:K:94:ILE:HG21	1.96	0.47
15:T:21:DC:H2'	15:T:22:BRU:H6	1.95	0.47
1:A:518:LYS:HE2	1:A:624:SER:O	2.15	0.47
3:C:55:THR:HB	3:C:152:GLU:H	1.80	0.47
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.14	0.47
1:A:535:THR:HG22	1:A:575:LYS:HA	1.97	0.47
3:C:250:THR:HA	3:C:253:LYS:HD2	1.96	0.47
4:D:189:ASP:O	4:D:193:THR:HB	2.15	0.47
1:A:62:ASP:C	1:A:64:ASN:H	2.17	0.47
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.96	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB2	1.97	0.47
1:A:1025:ARG:O	1:A:1035:TYR:HE2	1.98	0.46
1:A:352:VAL:HG12	1:A:467:THR:HG22	1.98	0.46
2:B:780:VAL:HB	2:B:817:LEU:HD23	1.97	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.47	0.46
3:C:256:ALA:HA	3:C:259:LEU:HD23	1.97	0.46
2:B:487:THR:HG23	2:B:490:SER:H	1.80	0.46
1:A:806:ARG:HH21	2:B:729:ILE:HG13	1.80	0.46
9:I:6:PHE:HB3	9:I:11:ASN:O	2.16	0.46
2:B:341:LEU:HD12	2:B:343:ILE:H	1.79	0.46
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.98	0.46
1:A:12:ARG:HB3	2:B:1218:THR:HG21	1.97	0.46
2:B:449:ASN:HD22	2:B:452:THR:HG23	1.81	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.98	0.46
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.98	0.46
3:C:169:LYS:HE3	3:C:170:TRP:CH2	2.50	0.46
1:A:1142:THR:HG22	1:A:1271:ILE:O	2.16	0.46
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.81	0.46
2:B:126:SER:CB	2:B:172:ILE:HD11	2.46	0.46
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.97	0.46
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:LYS:HB3	11:K:34:THR:HB	1.97	0.46
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.50	0.46
1:A:255:SER:HB2	2:B:918:ILE:HD11	1.96	0.46
1:A:869:GLY:O	5:E:204:THR:HG21	2.15	0.46
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.97	0.46
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.98	0.46
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.98	0.46
3:C:56:THR:HG21	3:C:145:CYS:SG	2.55	0.46
7:G:62:LEU:HD11	7:G:69:GLU:HB2	1.98	0.46
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.97	0.45
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.97	0.45
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.98	0.45
1:A:528:LEU:HD21	1:A:619:LYS:HG3	1.98	0.45
2:B:664:THR:HG23	2:B:678:GLU:N	2.31	0.45
3:C:244:VAL:O	3:C:248:ILE:HG13	2.16	0.45
4:D:176:GLU:OE2	4:D:201:LYS:HE2	2.15	0.45
6:F:82:THR:HG22	6:F:84:TYR:HB2	1.98	0.45
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.96	0.45
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.98	0.45
1:A:1189:SER:HB3	1:A:1242:VAL:H	1.81	0.45
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.99	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.97	0.45
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.98	0.45
2:B:1133:MET:O	2:B:1136:ASP:HB2	2.17	0.45
1:A:873:MET:C	1:A:1058:VAL:HG22	2.37	0.45
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.99	0.45
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.47	0.45
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.98	0.45
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.49	0.45
1:A:70:CYS:SG	1:A:70:CYS:O	2.74	0.45
1:A:744:LYS:O	1:A:748:MET:HG3	2.17	0.45
1:A:1268:LEU:HD22	9:I:48:LEU:HD21	1.98	0.45
2:B:54:PHE:HA	2:B:58:THR:HB	1.98	0.45
1:A:448:PRO:HG3	16:A:2455:APC:H2	1.98	0.45
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.82	0.45
2:B:839:MET:CE	2:B:980:PHE:HB2	2.47	0.45
2:B:882:THR:C	2:B:884:ARG:H	2.20	0.45
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.99	0.45
3:C:52:GLU:HA	12:L:64:LEU:HD21	1.99	0.45
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.99	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LYS:HD3	2:B:482:VAL:HG13	1.99	0.44
2:B:627:PHE:HB3	2:B:629:ASP:HB2	1.98	0.44
3:C:100:THR:CG2	3:C:119:VAL:HG13	2.47	0.44
9:I:82:GLU:HG2	9:I:104:LEU:HD13	1.98	0.44
1:A:484:GLY:H	2:B:989:THR:HG23	1.83	0.44
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.98	0.44
3:C:184:ASN:HD21	3:C:189:THR:H	1.63	0.44
3:C:172:PRO:O	3:C:235:VAL:HG23	2.17	0.44
8:H:103:LYS:HB3	8:H:115:TYR:CD2	2.52	0.44
1:A:1006:ILE:HD13	5:E:164:LEU:HA	1.98	0.44
1:A:851:HIS:CE1	1:A:857:ARG:HB2	2.53	0.44
1:A:928:LEU:HB3	1:A:987:VAL:HG11	2.00	0.44
3:C:70:ILE:HG12	3:C:142:VAL:HG11	2.00	0.44
6:F:153:VAL:HG12	6:F:155:LEU:HD12	1.99	0.44
12:L:31:CYS:HA	12:L:56:LEU:HD23	1.99	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	2.00	0.44
1:A:353:ILE:HD13	1:A:487:MET:CE	2.47	0.44
2:B:1083:ALA:HA	2:B:1084:GLN:HE21	1.82	0.44
7:G:112:LYS:HE2	7:G:120:THR:HG22	1.99	0.44
1:A:18:GLN:NE2	1:A:1418:LEU:HD12	2.32	0.44
5:E:124:VAL:O	5:E:132:ILE:HD12	2.18	0.44
5:E:17:ARG:HA	5:E:20:LYS:HD2	1.99	0.44
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	2.00	0.44
1:A:1276:VAL:HG21	1:A:1316:VAL:HG22	1.99	0.44
1:A:332:LYS:H	1:A:337:ARG:CB	2.31	0.44
4:D:27:LEU:HD23	4:D:197:SER:CB	2.47	0.44
1:A:1197:LEU:HD11	1:A:1238:ILE:HD12	2.00	0.44
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.99	0.44
4:D:213:GLU:O	4:D:217:LEU:HG	2.18	0.44
9:I:4:PHE:HE2	9:I:13:MET:HB2	1.83	0.44
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.86	0.43
1:A:383:TYR:O	1:A:384:ASN:HB3	2.17	0.43
2:B:424:LEU:HD22	2:B:453:ILE:HD11	2.00	0.43
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.18	0.43
1:A:883:LEU:HD13	1:A:943:LEU:HD22	2.00	0.43
2:B:776:GLN:HA	2:B:1096:ARG:HD3	2.00	0.43
8:H:109:LYS:HD3	8:H:111:LEU:HB2	2.00	0.43
8:H:93:TYR:HA	8:H:145:ARG:HB3	2.00	0.43
1:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.43
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.00	0.43
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HG3	7:G:60:ARG:HA	2.00	0.43
1:A:58:LEU:HB3	1:A:59:GLY:H	1.39	0.43
2:B:1016:ALA:HB3	2:B:1017:ILE:HD13	2.01	0.43
6:F:72:LYS:HZ3	6:F:72:LYS:N	2.16	0.43
1:A:265:LYS:O	1:A:269:ILE:HG13	2.18	0.43
2:B:69:LEU:HB2	2:B:90:ILE:HG22	1.99	0.43
3:C:96:SER:HB2	3:C:158:VAL:HG12	2.00	0.43
6:F:106:PRO:HG2	7:G:18:PHE:C	2.38	0.43
6:F:82:THR:HG22	6:F:84:TYR:H	1.83	0.43
1:A:418:SER:O	1:A:420:ARG:N	2.52	0.43
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.39	0.43
1:A:922:ASP:HB3	1:A:925:LEU:HD12	2.00	0.43
3:C:240:VAL:O	3:C:244:VAL:HG23	2.18	0.43
7:G:132:SER:HB3	7:G:135:ASP:H	1.83	0.43
1:A:747:VAL:HG21	1:A:758:ILE:HD12	2.01	0.43
1:A:84:ILE:HG13	1:A:239:LEU:HB3	2.00	0.43
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.99	0.43
1:A:945:GLU:HB3	5:E:201:LYS:HE3	1.99	0.43
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.49	0.43
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.19	0.43
1:A:140:THR:O	1:A:143:LYS:HG2	2.18	0.43
1:A:767:GLN:NE2	1:A:774:ARG:HB2	2.34	0.43
2:B:1017:ILE:HG12	2:B:1018:PRO:HD3	2.01	0.43
2:B:227:LYS:HG3	2:B:395:GLN:HG3	1.99	0.43
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.01	0.43
3:C:4:GLU:HB3	3:C:5:GLY:H	1.57	0.43
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.00	0.43
1:A:1406:VAL:HG12	1:A:1410:PHE:CE2	2.54	0.43
1:A:450:LEU:H	1:A:450:LEU:CD1	2.13	0.43
1:A:673:GLY:N	1:A:674:PRO:HD2	2.33	0.43
5:E:135:PHE:HB3	5:E:140:LEU:HD11	2.01	0.43
1:A:105:CYS:SG	1:A:139:TRP:HA	2.59	0.43
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.54	0.43
1:A:639:PRO:HD2	1:A:640:GLN:H	1.83	0.43
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.33	0.43
2:B:67:SER:HB2	2:B:92:PHE:HD2	1.84	0.43
1:A:135:PHE:HE1	1:A:222:LEU:HD23	1.84	0.42
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.58	0.42
1:A:325:ILE:HD12	2:B:1210:MET:HG3	1.99	0.42
5:E:5:ASN:HA	5:E:8:ASN:ND2	2.34	0.42
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	2.01	0.42
2:B:825:VAL:HG22	2:B:1010:LEU:HB2	2.01	0.42
2:B:114:PRO:HG3	2:B:181:LEU:HD11	2.01	0.42
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.01	0.42
3:C:182:PRO:HD2	3:C:210:GLU:CD	2.39	0.42
1:A:1116:LEU:HD12	1:A:1311:VAL:HA	2.01	0.42
1:A:531:ILE:HD13	1:A:622:VAL:HG21	2.00	0.42
1:A:586:ILE:HD11	1:A:633:VAL:HA	2.01	0.42
1:A:672:ASP:HB3	1:A:674:PRO:HD2	2.00	0.42
1:A:818:MET:HA	2:B:514:LEU:HB3	2.02	0.42
2:B:365:THR:HG21	2:B:370:PHE:CG	2.55	0.42
3:C:38:ILE:HG13	3:C:176:ILE:HD12	2.01	0.42
8:H:89:LEU:C	8:H:91:ASP:N	2.71	0.42
1:A:701:LEU:H	1:A:701:LEU:HG	1.56	0.42
2:B:453:ILE:HD12	2:B:453:ILE:H	1.84	0.42
2:B:976:ILE:HG12	2:B:991:GLY:O	2.19	0.42
7:G:62:LEU:HA	7:G:63:PRO:HD2	1.82	0.42
8:H:24:CYS:HB2	8:H:44:VAL:HG21	2.01	0.42
2:B:294:ASP:HB2	9:I:13:MET:H	1.84	0.42
1:A:1111:MET:H	1:A:1111:MET:HG2	1.66	0.42
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.54	0.42
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.83	0.42
2:B:1202:LEU:HA	2:B:1202:LEU:HD23	1.86	0.42
2:B:420:LEU:HD21	2:B:456:GLY:HA3	2.01	0.42
1:A:662:PHE:HB3	2:B:829:CYS:HB2	2.00	0.42
2:B:797:TYR:HB2	2:B:852:ARG:O	2.20	0.42
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.85	0.42
6:F:76:LYS:O	6:F:79:ARG:NH1	2.48	0.42
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.77	0.42
1:A:50:ILE:C	1:A:52:GLY:H	2.22	0.42
3:C:101:LEU:HD22	3:C:155:LEU:HD12	2.01	0.42
1:A:1006:ILE:HB	5:E:167:ARG:HG3	2.00	0.42
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.85	0.42
8:H:15:VAL:HG22	8:H:26:ILE:HD11	2.02	0.42
12:L:47:ARG:HH21	12:L:54:ARG:HE	1.67	0.42
15:T:16:DT:C2'	15:T:17:DT:C5'	2.97	0.42
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.85	0.42
3:C:50:GLU:HG3	12:L:66:GLN:HG3	2.00	0.42
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.20	0.42
1:A:646:PHE:O	1:A:650:GLN:HG2	2.20	0.42
2:B:825:VAL:HG22	2:B:1010:LEU:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD11	2:B:1195:HIS:HD2	1.85	0.42
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.54	0.42
1:A:926:GLN:O	1:A:930:ASP:HB2	2.20	0.42
8:H:84:ALA:HA	8:H:87:ARG:HD2	2.00	0.42
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.68	0.42
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.34	0.42
1:A:354:SER:O	1:A:469:ARG:HA	2.20	0.42
1:A:913:LEU:HD12	1:A:915:SER:OG	2.19	0.42
2:B:1001:PHE:HB3	2:B:1007:VAL:HG23	2.02	0.42
2:B:604:ARG:HG2	2:B:611:PRO:HA	2.02	0.42
7:G:153:GLN:HB3	7:G:156:SER:O	2.20	0.42
1:A:830:LYS:HD3	1:A:1098:VAL:HG21	2.02	0.41
2:B:522:VAL:HG12	2:B:539:LEU:HA	2.01	0.41
2:B:713:ALA:HA	2:B:733:HIS:NE2	2.35	0.41
2:B:193:LYS:HB3	2:B:787:VAL:HG21	2.02	0.41
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.49	0.41
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.36	0.41
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.03	0.41
2:B:102:VAL:HG22	2:B:112:LEU:HB2	2.02	0.41
2:B:184:ALA:HB1	2:B:188:ASP:HB2	2.02	0.41
2:B:314:LEU:HD21	2:B:386:LEU:HD11	2.03	0.41
2:B:705:MET:HA	2:B:705:MET:HE3	2.02	0.41
1:A:601:LYS:HD3	1:A:603:ASN:HD21	1.85	0.41
3:C:83:SER:HA	3:C:95:CYS:HB2	2.01	0.41
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.35	0.41
3:C:56:THR:HG23	3:C:147:LEU:HD23	2.02	0.41
1:A:185:TRP:CZ3	1:A:200:ARG:HG3	2.56	0.41
1:A:523:ILE:HG23	1:A:527:THR:HB	2.03	0.41
2:B:661:LEU:HD21	2:B:684:LEU:HD11	2.03	0.41
2:B:756:ILE:O	2:B:759:PRO:HD3	2.21	0.41
5:E:69:ILE:H	5:E:69:ILE:HG13	1.64	0.41
14:P:9:G:H1	15:T:20:DC:H42	1.68	0.41
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.02	0.41
1:A:1340:GLY:O	1:A:1342:GLU:N	2.54	0.41
1:A:606:LEU:HG	1:A:613:ILE:HD13	2.03	0.41
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.86	0.41
2:B:662:MET:HA	2:B:665:GLU:HB2	2.02	0.41
4:D:164:ILE:HG23	4:D:168:LYS:HD2	2.03	0.41
3:C:142:VAL:HG21	10:J:5:VAL:HG13	2.03	0.41
2:B:521:LEU:HA	2:B:543:SER:OG	2.21	0.41
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:LEU:O	1:A:1147:THR:OG1	2.38	0.41
1:A:35:ILE:HA	1:A:52:GLY:O	2.21	0.41
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.03	0.41
6:F:109:VAL:HG22	6:F:110:ASP:N	2.36	0.41
8:H:82:PRO:O	8:H:84:ALA:N	2.54	0.41
1:A:708:MET:HG2	1:A:712:GLU:HB3	2.03	0.41
2:B:102:VAL:HG23	2:B:110:HIS:HB3	2.03	0.41
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.55	0.41
3:C:239:PRO:HG2	3:C:242:GLN:HB2	2.03	0.41
1:A:511:ILE:O	1:A:519:PRO:HA	2.21	0.40
1:A:565:ILE:O	1:A:570:PRO:HA	2.21	0.40
1:A:763:ALA:O	1:A:803:SER:HB3	2.21	0.40
2:B:641:GLU:HB3	2:B:643:ASP:CG	2.42	0.40
3:C:98:VAL:H	3:C:122:SER:HB3	1.84	0.40
7:G:145:VAL:HG22	7:G:163:ILE:CG2	2.51	0.40
1:A:1148:ILE:HG23	9:I:49:ILE:HB	2.03	0.40
2:B:603:LEU:HD12	2:B:609:ILE:HG13	2.02	0.40
4:D:187:THR:C	4:D:189:ASP:N	2.74	0.40
10:J:58:GLU:HA	10:J:61:LEU:HD12	2.03	0.40
1:A:1009:ASN:HA	1:A:1012:ARG:HD2	2.03	0.40
4:D:70:PHE:O	4:D:74:GLN:HB2	2.21	0.40
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.77	0.40
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.02	0.40
11:K:35:PHE:O	11:K:70:ARG:HA	2.21	0.40
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.03	0.40
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.04	0.40
2:B:1048:THR:HB	2:B:1049:ASP:H	1.76	0.40
2:B:276:ILE:HG21	2:B:280:ILE:HD11	2.03	0.40
2:B:806:THR:HB	2:B:809:MET:HG3	2.04	0.40
2:B:908:GLU:O	2:B:940:PRO:HB2	2.21	0.40
11:K:7:PHE:HB2	11:K:11:LEU:HD22	2.03	0.40
1:A:30:ILE:HA	2:B:1183:LYS:HE3	2.03	0.40
7:G:111:THR:HB	7:G:114:LEU:HD23	2.03	0.40
8:H:38:LEU:HD13	8:H:125:LEU:HD13	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	1417/1732 (82%)	1198 (84%)	145 (10%)	74 (5%)	2 23
2	B	1095/1224 (90%)	916 (84%)	127 (12%)	52 (5%)	2 24
3	C	264/318 (83%)	236 (89%)	20 (8%)	8 (3%)	4 33
4	D	174/221 (79%)	146 (84%)	19 (11%)	9 (5%)	2 23
5	E	212/215 (99%)	192 (91%)	15 (7%)	5 (2%)	6 37
6	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	13 49
7	G	169/171 (99%)	152 (90%)	14 (8%)	3 (2%)	8 42
8	H	129/146 (88%)	99 (77%)	19 (15%)	11 (8%)	1 13
9	I	117/122 (96%)	94 (80%)	20 (17%)	3 (3%)	5 35
10	J	63/70 (90%)	52 (82%)	5 (8%)	6 (10%)	0 11
11	K	113/120 (94%)	106 (94%)	7 (6%)	0	100 100
12	L	44/70 (63%)	21 (48%)	13 (30%)	10 (23%)	0 1
All	All	3879/4564 (85%)	3286 (85%)	411 (11%)	182 (5%)	2 24

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	69	THR
1	A	78	PRO
1	A	169	ASN
1	A	193	ASP
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	331	GLY
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	384	ASN
1	A	775	ILE
1	A	1206	ASP
1	A	1341	ILE
1	A	1405	THR
2	B	108	VAL
2	B	208	SER
2	B	229	ALA
2	B	282	ILE
2	B	340	ALA
2	B	344	LYS
2	B	368	GLU
2	B	473	MET
2	B	629	ASP
2	B	643	ASP
2	B	707	PRO
2	B	711	GLU
2	B	731	VAL
2	B	751	VAL
2	B	879	ARG
2	B	880	THR
2	B	883	LEU
2	B	1046	PRO
2	B	1107	ALA
4	D	16	LYS
4	D	18	VAL
6	F	73	ALA
7	G	2	PHE
7	G	63	PRO
7	G	154	VAL
8	H	90	ALA
9	I	9	ASP
10	J	6	ARG
12	L	28	LYS
12	L	45	ALA
12	L	50	ASP
1	A	41	MET
1	A	43	GLU
1	A	167	CYS
1	A	189	ARG
1	A	224	PHE
1	A	257	ARG

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Mol	Chain	Res	Type
1	A	409	SER
1	A	419	LYS
1	A	449	SER
1	A	569	LYS
1	A	639	PRO
1	A	922	ASP
1	A	1124	HIS
1	A	1175	SER
1	A	1242	VAL
1	A	1255	GLU
1	A	1365	TYR
1	A	1366	ARG
1	A	1394	THR
1	A	1401	SER
2	B	322	PHE
2	B	338	GLY
2	B	341	LEU
2	B	343	ILE
2	B	371	GLU
2	B	526	GLU
2	B	772	ALA
2	B	867	GLY
2	B	1096	ARG
2	B	1157	ALA
3	C	215	GLU
3	C	237	SER
4	D	27	LEU
4	D	53	SER
8	H	17	PRO
8	H	81	PRO
8	H	83	GLN
9	I	95	THR
10	J	13	VAL
10	J	57	ILE
12	L	39	SER
12	L	55	ILE
12	L	56	LEU
1	A	73	GLY
1	A	76	GLU
1	A	155	GLU
1	A	195	ASP
1	A	197	PRO

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Mol	Chain	Res	Type
1	A	312	PRO
1	A	332	LYS
1	A	418	SER
1	A	421	ALA
1	A	465	TYR
1	A	916	GLY
1	A	1002	GLY
1	A	1403	GLU
2	B	531	GLN
2	B	648	HIS
2	B	655	LYS
2	B	667	GLN
2	B	734	HIS
2	B	792	MET
2	B	831	SER
2	B	1155	SER
2	B	1156	ASP
2	B	1188	LYS
3	C	90	ASP
3	C	184	ASN
3	C	214	ASN
4	D	119	ARG
4	D	198	LEU
4	D	199	ASN
5	E	48	ASP
8	H	32	THR
8	H	78	SER
8	H	82	PRO
8	H	128	ASN
10	J	3	VAL
12	L	26	THR
12	L	59	ALA
1	A	187	LYS
1	A	448	PRO
1	A	466	SER
1	A	870	GLU
2	B	476	ARG
3	C	117	ASP
3	C	150	GLY
4	D	15	LEU
5	E	36	GLU
5	E	50	MET

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Mol	Chain	Res	Type
8	H	19	ARG
8	H	60	ALA
8	H	89	LEU
10	J	64	ASN
12	L	53	HIS
1	A	35	ILE
1	A	62	ASP
1	A	196	GLU
1	A	567	LYS
1	A	599	SER
1	A	629	LEU
1	A	958	VAL
2	B	764	SER
2	B	1143	ALA
2	B	1221	SER
5	E	145	THR
5	E	174	GLN
9	I	47	GLU
10	J	2	ILE
12	L	38	LEU
1	A	117	GLU
1	A	479	ASN
1	A	672	ASP
1	A	1122	PRO
2	B	305	VAL
2	B	395	GLN
2	B	466	TRP
2	B	870	ILE
2	B	1181	GLU
4	D	218	GLU
1	A	178	GLY
1	A	283	GLY
2	B	907	GLY
1	A	61	ILE
2	B	436	VAL
2	B	743	ILE
3	C	38	ILE
1	A	51	GLY
1	A	244	PRO
1	A	310	GLY
2	B	364	ILE
1	A	385	ILE

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Mol	Chain	Res	Type
1	A	1388	GLY
1	A	910	PRO

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%)	1020 (82%)	223 (18%)	2 12
2	B	966/1061 (91%)	803 (83%)	163 (17%)	2 14
3	C	234/274 (85%)	194 (83%)	40 (17%)	2 14
4	D	160/200 (80%)	131 (82%)	29 (18%)	1 12
5	E	196/197 (100%)	170 (87%)	26 (13%)	4 22
6	F	74/137 (54%)	62 (84%)	12 (16%)	2 16
7	G	152/152 (100%)	128 (84%)	24 (16%)	2 17
8	H	117/128 (91%)	98 (84%)	19 (16%)	2 16
9	I	113/116 (97%)	99 (88%)	14 (12%)	4 24
10	J	60/65 (92%)	45 (75%)	15 (25%)	0 4
11	K	99/102 (97%)	82 (83%)	17 (17%)	2 14
12	L	40/57 (70%)	28 (70%)	12 (30%)	0 2
All	All	3454/4008 (86%)	2860 (83%)	594 (17%)	2 14

All (594) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	22	PHE
1	A	23	SER
1	A	28	ARG
1	A	34	LYS
1	A	39	GLU
1	A	41	MET
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	43	GLU
1	A	53	LEU
1	A	58	LEU
1	A	61	ILE
1	A	63	ARG
1	A	65	LEU
1	A	67	CYS
1	A	81	PHE
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	117	GLU
1	A	126	LEU
1	A	132	LYS
1	A	143	LYS
1	A	144	THR
1	A	147	VAL
1	A	157	ASP
1	A	159	THR
1	A	164	ARG
1	A	174	ILE
1	A	175	ARG
1	A	188	ASP
1	A	195	ASP
1	A	204	THR
1	A	208	LEU
1	A	220	THR
1	A	227	VAL
1	A	236	LEU
1	A	237	THR
1	A	238	CYS
1	A	250	ILE
1	A	252	PHE
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	290	GLU
1	A	293	GLU
1	A	295	LEU
1	A	307	ASP
1	A	308	ILE
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	343	LYS
1	A	344	ARG
1	A	369	SER
1	A	375	THR
1	A	383	TYR
1	A	385	ILE
1	A	386	ASP
1	A	391	LEU
1	A	393	ARG
1	A	398	GLU
1	A	403	LYS
1	A	408	ASP
1	A	412	ARG
1	A	423	ASP
1	A	425	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	437	MET
1	A	438	ASP
1	A	443	LEU
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	455	MET
1	A	461	LYS
1	A	463	ILE
1	A	466	SER
1	A	472	LEU
1	A	476	SER
1	A	481	ASP
1	A	485	ASP
1	A	493	GLN
1	A	498	ARG
1	A	500	GLU
1	A	504	LEU
1	A	518	LYS
1	A	526	ASP
1	A	527	THR
1	A	536	LEU
1	A	538	ASP
1	A	544	ASP

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Mol	Chain	Res	Type
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	584	ASN
1	A	588	LEU
1	A	597	LEU
1	A	598	LEU
1	A	603	ASN
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	645	LEU
1	A	646	PHE
1	A	657	LEU
1	A	670	ILE
1	A	680	THR
1	A	685	GLU
1	A	691	LEU
1	A	701	LEU
1	A	711	ARG
1	A	719	VAL
1	A	734	GLU
1	A	738	LYS
1	A	754	SER
1	A	756	ILE
1	A	758	ILE
1	A	768	GLN
1	A	770	VAL
1	A	773	LYS
1	A	774	ARG
1	A	782	ARG
1	A	783	THR
1	A	788	SER
1	A	791	ASP
1	A	795	GLU
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	827	THR

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Mol	Chain	Res	Type
1	A	831	THR
1	A	839	ARG
1	A	842	VAL
1	A	871	ASP
1	A	886	ILE
1	A	890	ASP
1	A	896	ARG
1	A	898	ARG
1	A	905	ASP
1	A	908	LEU
1	A	915	SER
1	A	919	ILE
1	A	930	ASP
1	A	948	VAL
1	A	980	ASP
1	A	982	THR
1	A	993	LEU
1	A	998	LEU
1	A	1001	ARG
1	A	1005	GLU
1	A	1009	ASN
1	A	1024	SER
1	A	1030	ARG
1	A	1036	ARG
1	A	1038	THR
1	A	1040	GLN
1	A	1058	VAL
1	A	1064	VAL
1	A	1067	LEU
1	A	1080	THR
1	A	1098	VAL
1	A	1111	MET
1	A	1113	THR
1	A	1116	LEU
1	A	1124	HIS
1	A	1134	ILE
1	A	1135	ARG
1	A	1142	THR
1	A	1145	SER
1	A	1146	VAL
1	A	1147	THR
1	A	1170	ILE

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Mol	Chain	Res	Type
1	A	1173	HIS
1	A	1176	LEU
1	A	1188	GLN
1	A	1193	LEU
1	A	1195	LEU
1	A	1197	LEU
1	A	1207	LEU
1	A	1218	GLN
1	A	1223	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1255	GLU
1	A	1260	LEU
1	A	1264	GLU
1	A	1274	ARG
1	A	1289	ARG
1	A	1290	LYS
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1309	ASP
1	A	1314	SER
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1341	ILE
1	A	1366	ARG
1	A	1387	HIS
1	A	1391	ARG
1	A	1400	CYS
1	A	1403	GLU
1	A	1405	THR
1	A	1419	ASP
1	A	1420	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1432	GLN
1	A	1436	ILE
1	A	1442	ASP
1	A	1443	VAL

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Mol	Chain	Res	Type
1	A	1444	MET
1	A	1445	ILE
1	A	1447	GLU
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	35	SER
2	B	44	VAL
2	B	46	GLN
2	B	56	ASP
2	B	64	CYS
2	B	91	SER
2	B	97	VAL
2	B	102	VAL
2	B	108	VAL
2	B	118	ARG
2	B	126	SER
2	B	167	ILE
2	B	169	ARG
2	B	170	LEU
2	B	188	ASP
2	B	199	MET
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	241	ARG
2	B	261	ARG
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	305	VAL
2	B	309	GLN
2	B	324	ILE
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	365	THR

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Mol	Chain	Res	Type
2	B	368	GLU
2	B	370	PHE
2	B	387	LEU
2	B	393	LYS
2	B	395	GLN
2	B	398	ARG
2	B	401	PHE
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	418	LYS
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	454	THR
2	B	469	GLN
2	B	470	LYS
2	B	481	GLN
2	B	482	VAL
2	B	485	ARG
2	B	489	SER
2	B	502	ILE
2	B	527	THR
2	B	529	GLU
2	B	531	GLN
2	B	544	CYS
2	B	547	VAL
2	B	552	MET
2	B	554	ILE
2	B	567	GLU
2	B	570	VAL
2	B	574	SER
2	B	576	ASP
2	B	595	ARG
2	B	602	THR
2	B	603	LEU
2	B	604	ARG
2	B	615	MET
2	B	619	ILE
2	B	620	ARG
2	B	628	THR
2	B	653	VAL

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Mol	Chain	Res	Type
2	B	657	HIS
2	B	658	ILE
2	B	680	THR
2	B	708	GLU
2	B	731	VAL
2	B	736	THR
2	B	743	ILE
2	B	754	SER
2	B	766	ARG
2	B	775	LYS
2	B	776	GLN
2	B	786	ASN
2	B	787	VAL
2	B	790	ASP
2	B	792	MET
2	B	815	ARG
2	B	816	GLU
2	B	839	MET
2	B	844	SER
2	B	854	LEU
2	B	871	THR
2	B	875	GLU
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	885	MET
2	B	889	THR
2	B	891	ASP
2	B	894	ASP
2	B	895	ASP
2	B	899	ILE
2	B	904	ARG
2	B	906	SER
2	B	908	GLU
2	B	909	ASP
2	B	934	LYS
2	B	935	ARG
2	B	944	THR
2	B	945	GLU
2	B	946	ASN
2	B	953	LEU
2	B	954	VAL

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Mol	Chain	Res	Type
2	B	956	THR
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1017	ILE
2	B	1026	LEU
2	B	1045	SER
2	B	1049	ASP
2	B	1050	ILE
2	B	1060	ARG
2	B	1065	GLN
2	B	1071	VAL
2	B	1072	MET
2	B	1084	GLN
2	B	1098	MET
2	B	1112	GLN
2	B	1122	ARG
2	B	1123	SER
2	B	1133	MET
2	B	1135	ARG
2	B	1137	CYS
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1148	LYS
2	B	1149	GLU
2	B	1155	SER
2	B	1159	ARG
2	B	1170	THR
2	B	1182	CYS
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
2	B	1189	ILE
2	B	1212	ILE

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Mol	Chain	Res	Type
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	43	THR
3	C	46	ILE
3	C	52	GLU
3	C	53	THR
3	C	56	THR
3	C	58	LEU
3	C	60	ASP
3	C	62	PHE
3	C	76	ASP
3	C	78	GLU
3	C	81	GLU
3	C	84	ARG
3	C	89	GLU
3	C	108	GLU
3	C	111	THR
3	C	121	VAL
3	C	122	SER
3	C	125	MET
3	C	133	ILE
3	C	142	VAL
3	C	145	CYS
3	C	148	ARG
3	C	158	VAL
3	C	163	ILE
3	C	186	LEU
3	C	197	SER
3	C	215	GLU
3	C	226	ASP
3	C	238	ILE
3	C	240	VAL
3	C	260	LEU
3	C	262	LEU
3	C	263	THR
3	C	264	GLN
3	C	265	MET
4	D	5	THR
4	D	7	THR

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Mol	Chain	Res	Type
4	D	9	GLN
4	D	10	THR
4	D	11	ARG
4	D	13	ARG
4	D	18	VAL
4	D	19	GLU
4	D	23	ASN
4	D	27	LEU
4	D	37	GLN
4	D	38	ILE
4	D	43	GLU
4	D	47	LEU
4	D	67	ARG
4	D	123	LEU
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	156	ASP
4	D	159	THR
4	D	173	HIS
4	D	183	LEU
4	D	187	THR
4	D	197	SER
4	D	200	ASN
4	D	208	GLU
4	D	221	TYR
5	E	3	GLN
5	E	31	THR
5	E	40	GLU
5	E	41	ASP
5	E	46	TYR
5	E	56	LYS
5	E	60	PHE
5	E	65	THR
5	E	67	GLU
5	E	69	ILE
5	E	75	MET
5	E	84	ASP
5	E	92	THR
5	E	94	LYS
5	E	95	THR

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Mol	Chain	Res	Type
5	E	126	SER
5	E	144	ILE
5	E	150	VAL
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	72	LYS
6	F	77	ASP
6	F	97	ARG
6	F	110	ASP
6	F	111	LEU
6	F	118	LEU
6	F	119	ARG
6	F	129	LYS
6	F	152	ILE
6	F	153	VAL
6	F	154	ASP
6	F	155	LEU
7	G	13	LEU
7	G	21	ARG
7	G	26	LEU
7	G	31	LEU
7	G	37	SER
7	G	39	THR
7	G	55	ASP
7	G	64	THR
7	G	65	ASP
7	G	75	ARG
7	G	80	LYS
7	G	96	GLN
7	G	106	MET
7	G	110	VAL
7	G	112	LYS
7	G	118	ASP
7	G	120	THR
7	G	134	GLU
7	G	138	THR

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Mol	Chain	Res	Type
7	G	141	SER
7	G	143	ILE
7	G	152	SER
7	G	155	SER
7	G	160	ILE
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	39	THR
8	H	49	VAL
8	H	54	SER
8	H	56	THR
8	H	76	THR
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	92	ASP
8	H	103	LYS
8	H	107	VAL
8	H	109	LYS
8	H	112	ILE
8	H	123	MET
8	H	124	ARG
8	H	130	ARG
9	I	4	PHE
9	I	8	ARG
9	I	26	LEU
9	I	31	THR
9	I	42	LEU
9	I	43	VAL
9	I	50	THR
9	I	51	ASN
9	I	52	ILE
9	I	94	ASP
9	I	104	LEU
9	I	109	ILE
9	I	114	GLN
9	I	118	ARG
10	J	3	VAL
10	J	13	VAL
10	J	14	VAL
10	J	17	LYS

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Mol	Chain	Res	Type
10	J	19	GLU
10	J	24	LEU
10	J	26	GLN
10	J	41	LEU
10	J	42	LYS
10	J	48	ARG
10	J	51	LEU
10	J	55	ASP
10	J	56	LEU
10	J	57	ILE
10	J	62	ARG
11	K	1	MET
11	K	5	ASP
11	K	20	LYS
11	K	21	ILE
11	K	25	THR
11	K	33	ILE
11	K	35	PHE
11	K	47	ARG
11	K	51	LEU
11	K	79	GLU
11	K	91	CYS
11	K	95	ILE
11	K	101	LEU
11	K	102	LYS
11	K	103	THR
11	K	108	GLU
11	K	114	LEU
12	L	27	LEU
12	L	28	LYS
12	L	38	LEU
12	L	44	ASP
12	L	54	ARG
12	L	55	ILE
12	L	56	LEU
12	L	61	THR
12	L	63	ARG
12	L	64	LEU
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	169	ASN
1	A	253	ASN
1	A	363	GLN
1	A	390	GLN
1	A	394	ASN
1	A	760	GLN
1	A	851	HIS
1	A	1106	ASN
1	A	1387	HIS
1	A	1390	ASN
2	B	46	GLN
2	B	47	GLN
2	B	357	GLN
2	B	363	HIS
2	B	449	ASN
2	B	975	GLN
2	B	986	GLN
2	B	1065	GLN
2	B	1093	GLN
2	B	1117	GLN
2	B	1195	HIS
3	C	140	ASN
4	D	143	ASN
4	D	150	ASN
5	E	3	GLN
5	E	8	ASN
5	E	32	GLN
5	E	179	GLN
8	H	35	GLN
8	H	137	GLN
9	I	46	HIS
9	I	51	ASN
9	I	60	GLN
11	K	29	ASN
11	K	76	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/4 (75%)	2 (66%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	G
14	P	10	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	BRU	T	22	15,14	15,21,22	1.24	2 (13%)	17,30,33	2.29	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	15,14	-	2/4/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	3.08	1.42	1.38
15	T	22	BRU	C4-N3	2.15	1.36	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	22	BRU	C4-N3-C2	8.12	122.00	115.14
15	T	22	BRU	C5-C4-N3	-3.61	119.32	123.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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 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	$\#\|Z\| > 2$
16	APC	A	2455	-	27,33,33	2.40	9 (33%)	31,52,52	1.64	6 (19%)

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
16	APC	A	2455	-	-	2/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2455	APC	PA-O5'	5.42	1.65	1.57
16	A	2455	APC	PB-O3B	4.92	1.63	1.58
16	A	2455	APC	O4'-C1'	4.36	1.47	1.41
16	A	2455	APC	PA-O1A	3.86	1.60	1.51
16	A	2455	APC	PA-O2A	-3.73	1.47	1.56
16	A	2455	APC	PG-O1G	3.68	1.62	1.50
16	A	2455	APC	C8-N7	-2.64	1.30	1.34
16	A	2455	APC	PB-O2B	2.36	1.61	1.56
16	A	2455	APC	C5'-C4'	2.08	1.58	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	2455	APC	PG-O3B-PB	-5.23	114.20	132.62
16	A	2455	APC	C4-C5-N7	-2.98	106.29	109.40
16	A	2455	APC	C3'-C2'-C1'	2.75	105.12	100.98
16	A	2455	APC	N3-C2-N1	-2.42	124.89	128.68
16	A	2455	APC	O5'-C5'-C4'	2.20	116.55	108.99
16	A	2455	APC	O2G-PG-O3B	2.07	111.57	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	2455	APC	C5'-O5'-PA-O1A
16	A	2455	APC	PB-O3B-PG-O1G

There are no ring outliers.

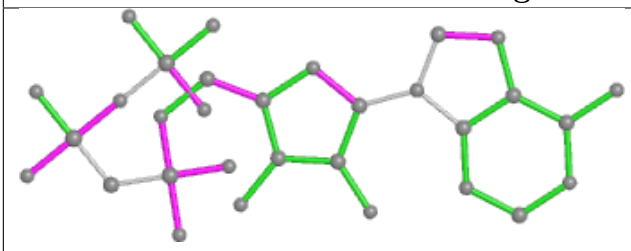
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2455	APC	2	0

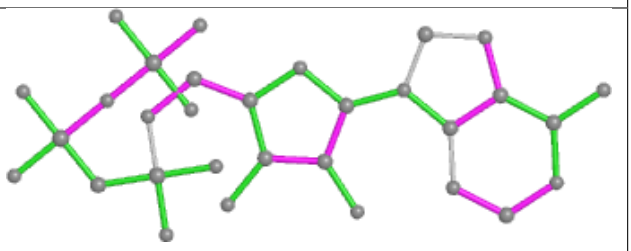
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

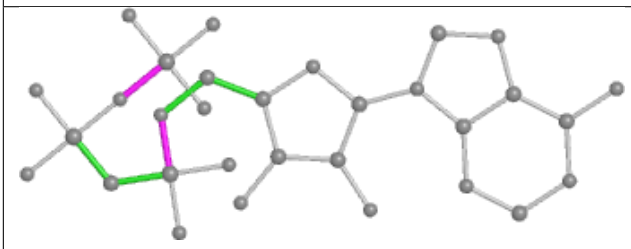
Ligand APC A 2455



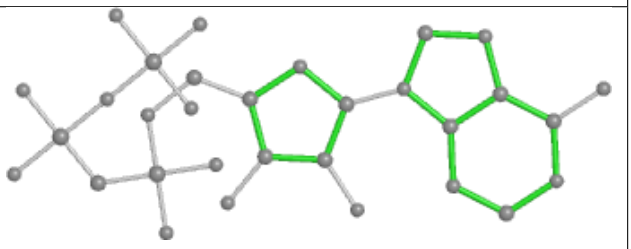
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.72
1	B	351:TYR	C	352:ALA	N	3.12

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%)	0.07	29 (2%) 65 55	84, 142, 199, 264	0
2	B	1115/1224 (91%)	0.13	26 (2%) 60 50	87, 157, 218, 237	0
3	C	266/318 (83%)	-0.09	1 (0%) 92 87	107, 144, 187, 216	0
4	D	178/221 (80%)	0.13	3 (1%) 70 60	115, 159, 205, 225	0
5	E	214/215 (99%)	0.13	5 (2%) 60 50	116, 177, 224, 237	0
6	F	84/155 (54%)	-0.12	0 100 100	85, 121, 151, 168	0
7	G	171/171 (100%)	0.14	1 (0%) 89 84	111, 139, 176, 198	0
8	H	133/146 (91%)	0.57	12 (9%) 9 7	151, 186, 222, 233	0
9	I	119/122 (97%)	0.18	1 (0%) 86 79	144, 192, 223, 236	0
10	J	65/70 (92%)	0.01	0 100 100	119, 137, 182, 189	0
11	K	115/120 (95%)	-0.13	1 (0%) 84 77	112, 138, 180, 193	0
12	L	46/70 (65%)	0.87	8 (17%) 1 1	143, 208, 222, 231	0
13	N	9/14 (64%)	0.63	2 (22%) 0 0	271, 282, 299, 300	0
14	P	4/4 (100%)	1.25	0 100 100	208, 215, 222, 235	0
15	T	16/26 (61%)	0.03	1 (6%) 20 14	200, 241, 295, 296	0
All	All	3960/4608 (85%)	0.10	90 (2%) 60 50	84, 151, 215, 300	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1082	ASN	5.4
1	A	1083	THR	5.1
5	E	110	PHE	4.4
1	A	1176	LEU	4.1
2	B	715	ALA	3.5
2	B	263	GLY	3.4
12	L	53	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
8	H	125	LEU	3.2
12	L	27	LEU	3.2
1	A	114	LEU	3.2
1	A	1257	ASP	3.1
5	E	82	PHE	3.1
12	L	46	VAL	3.1
2	B	566	LEU	3.1
1	A	257	ARG	3.0
12	L	32	ALA	3.0
1	A	145	LYS	3.0
1	A	155	GLU	2.9
2	B	364	ILE	2.9
11	K	115	ALA	2.9
1	A	1080	THR	2.8
8	H	134	ASN	2.8
12	L	29	TYR	2.8
1	A	3	GLY	2.8
1	A	194	ALA	2.7
1	A	174	ILE	2.7
8	H	139	ASN	2.7
1	A	1317	MET	2.7
2	B	25	ILE	2.7
1	A	1150	SER	2.7
2	B	865	LYS	2.7
1	A	108	MET	2.7
1	A	115	LEU	2.6
2	B	864	LYS	2.6
2	B	722	ASP	2.6
2	B	340	ALA	2.6
13	N	9	DT	2.6
5	E	109	ILE	2.6
9	I	84	VAL	2.6
12	L	54	ARG	2.6
2	B	92	PHE	2.5
1	A	1455	PRO	2.5
1	A	1092	LYS	2.5
12	L	26	THR	2.5
2	B	431	TYR	2.5
1	A	183	GLY	2.4
1	A	1321	GLY	2.4
2	B	250	PHE	2.4
7	G	51	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
15	T	24	DG	2.4
13	N	8	DT	2.4
5	E	53	PRO	2.4
8	H	126	GLU	2.3
1	A	164	ARG	2.3
2	B	708	GLU	2.3
1	A	147	VAL	2.3
8	H	56	THR	2.3
8	H	142	LEU	2.3
1	A	256	GLN	2.3
4	D	138	ASN	2.3
2	B	866	TYR	2.3
2	B	339	THR	2.3
2	B	132	VAL	2.3
8	H	140	ALA	2.2
2	B	301	ILE	2.2
1	A	199	LEU	2.2
2	B	956	THR	2.2
1	A	908	LEU	2.2
5	E	81	GLU	2.2
8	H	146	ARG	2.2
2	B	259	TYR	2.2
12	L	28	LYS	2.1
2	B	837	ASP	2.1
1	A	152	VAL	2.1
1	A	38	PRO	2.1
2	B	366	GLN	2.1
3	C	213	PRO	2.1
1	A	106	VAL	2.1
4	D	76	LYS	2.1
2	B	165	VAL	2.1
8	H	113	ALA	2.1
2	B	962	LYS	2.1
4	D	9	GLN	2.1
2	B	679	TYR	2.0
2	B	713	ALA	2.0
8	H	59	ILE	2.0
8	H	55	LEU	2.0
2	B	373	ARG	2.0
8	H	112	ILE	2.0
1	A	172	PRO	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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	BRU	T	22	20/21	0.93	0.12	222,232,237,237	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

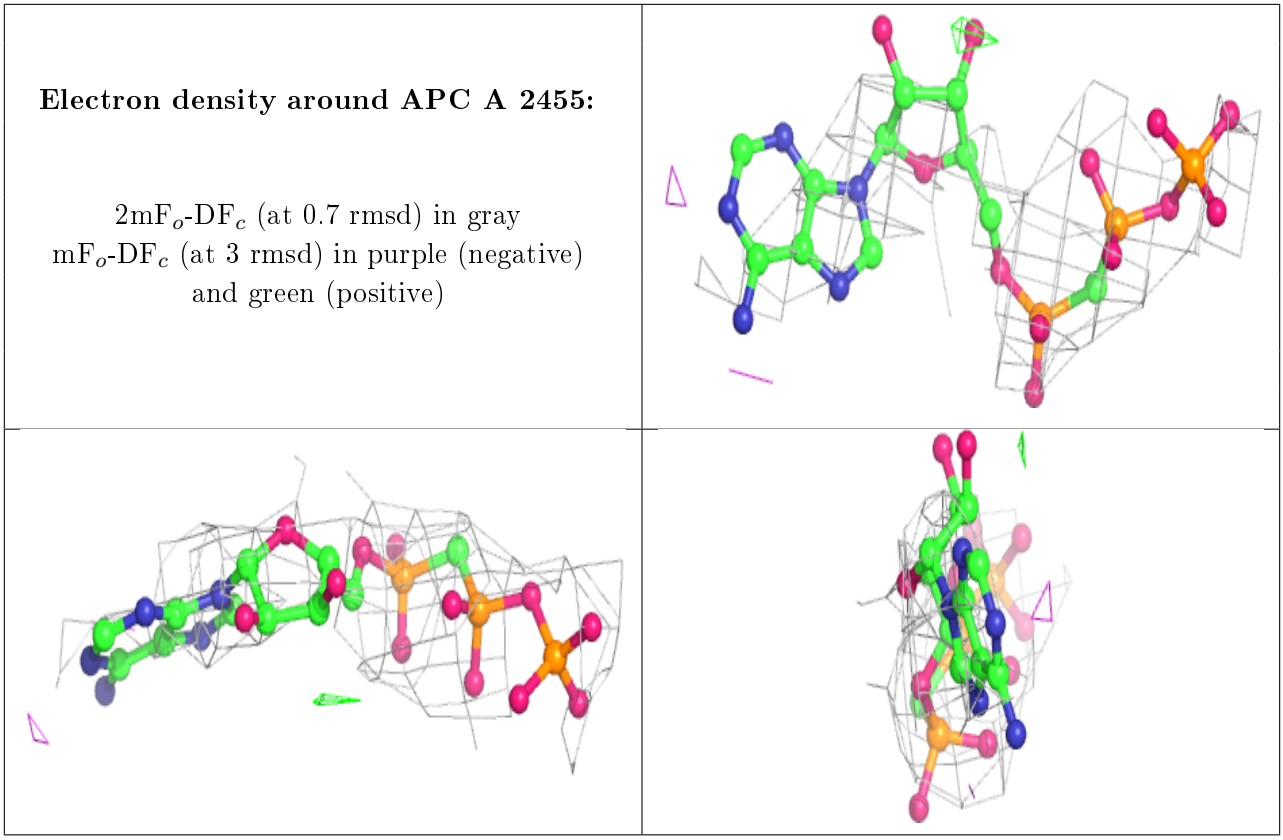
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	APC	A	2455	31/31	0.59	0.49	265,268,278,278	0
18	MG	A	2458	1/1	0.94	0.15	230,230,230,230	0
17	ZN	L	1071	1/1	0.98	0.07	235,235,235,235	0
17	ZN	A	2456	1/1	0.98	0.04	177,177,177,177	0
17	ZN	I	1122	1/1	0.98	0.05	248,248,248,248	0
17	ZN	B	2225	1/1	0.99	0.22	112,112,112,112	0
17	ZN	I	1121	1/1	0.99	0.13	155,155,155,155	0
17	ZN	A	2457	1/1	1.00	0.17	101,101,101,101	0
17	ZN	J	1066	1/1	1.00	0.26	124,124,124,124	0
17	ZN	C	1269	1/1	1.00	0.17	129,129,129,129	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around APC A 2455:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.