Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 12:21 PM EST

PDB ID	:	3S1Q
Title	:	RNA Polymerase II Initiation Complex with a 5-nt 3'-deoxy RNA soaked with ATP
Authors	:	Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on	:	2011-05-16
Resolution	:	3.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

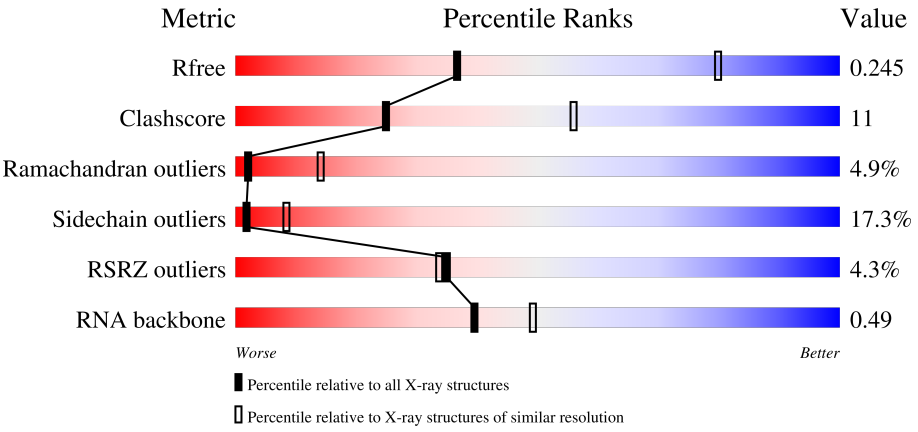
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1733	5% 50% 25% 5% • 19%
2	B	1224	4% 57% 28% 5% • 9%
3	C	318	52% 25% 6% • 16%
4	E	215	2% 69% 28% •

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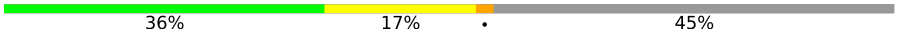
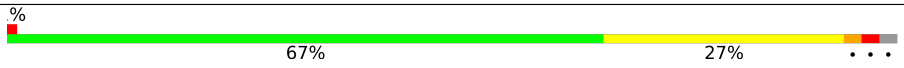
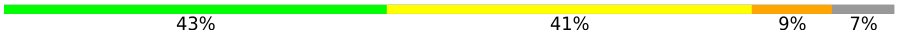
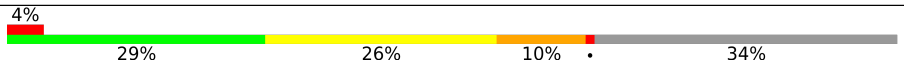
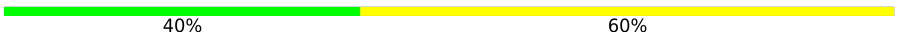
Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	5	
12	T	29	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 28703 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
			Total	C	N	O	S			
1	A	1405	11043	6965	1936	2081	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1114	8861	5610	1549	1647	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	85	688	439	116	130	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			109	50	25	30	4			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP *GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

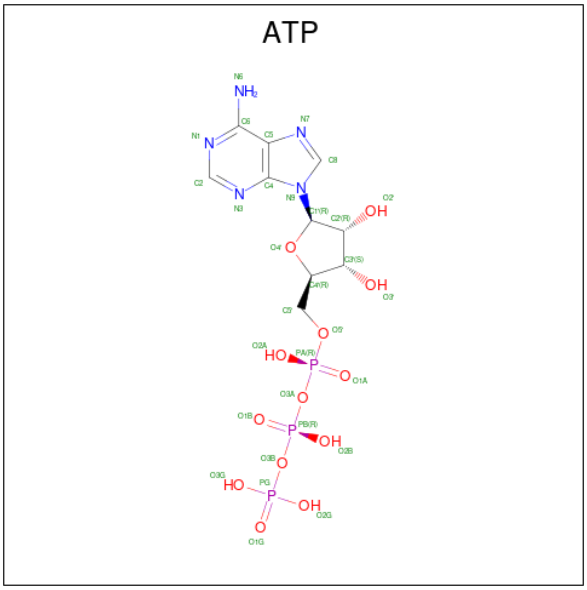
- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Mg	0	0
			2	2		

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



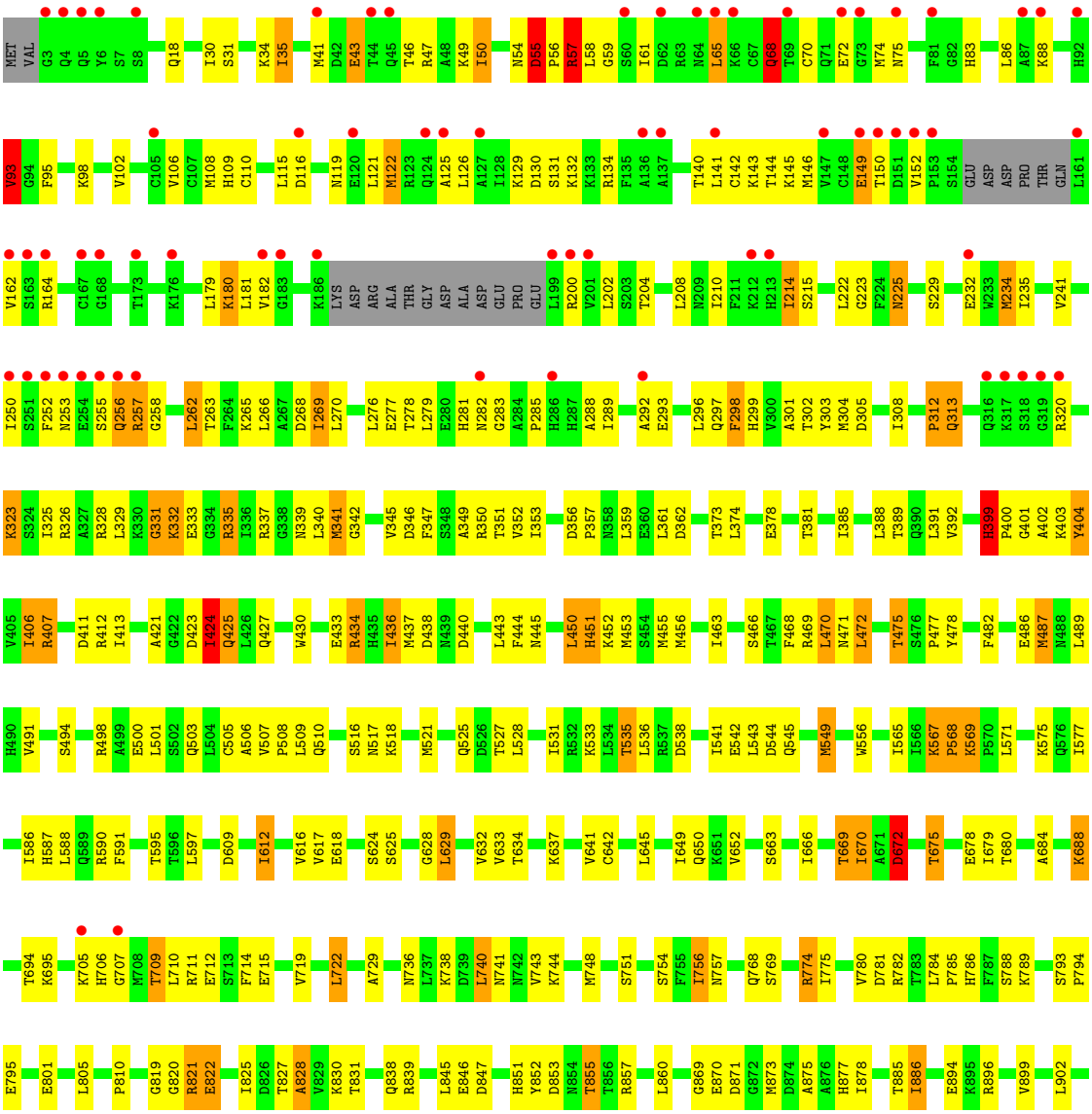
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C N O P 31 10 5 13 3	0	0

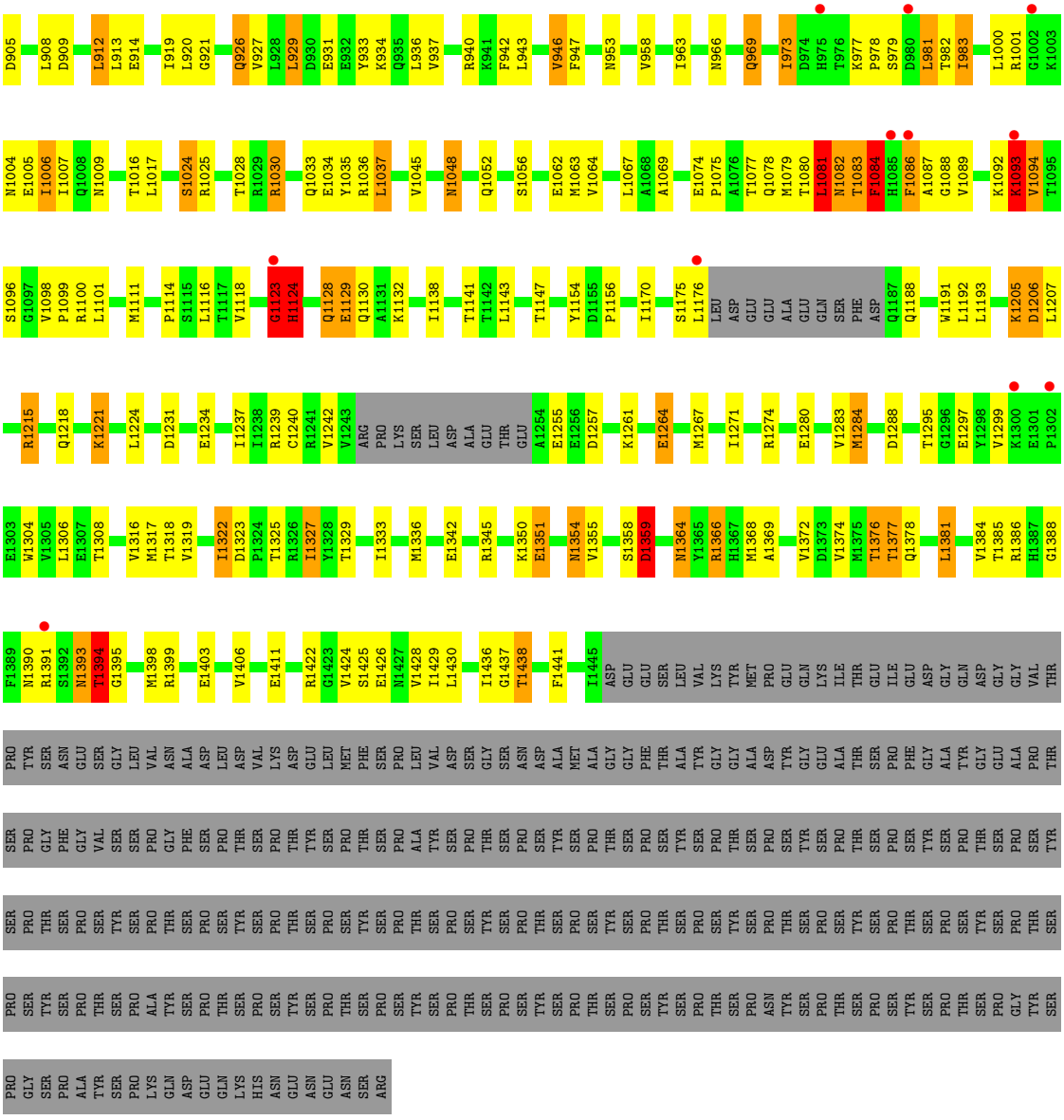
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

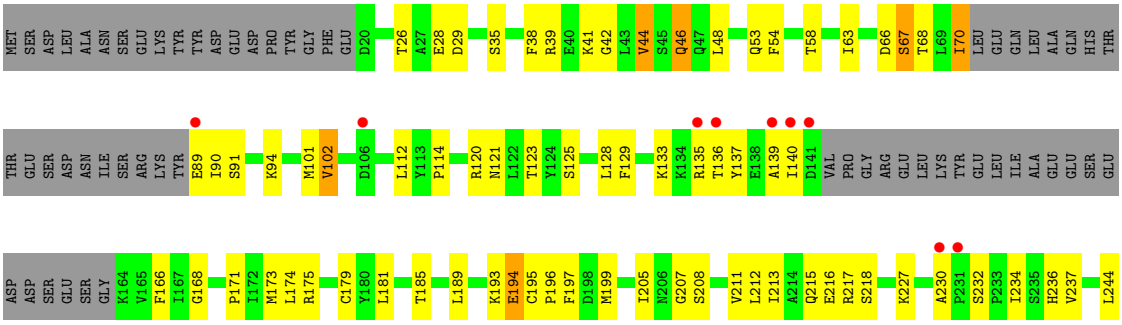
Chain A:

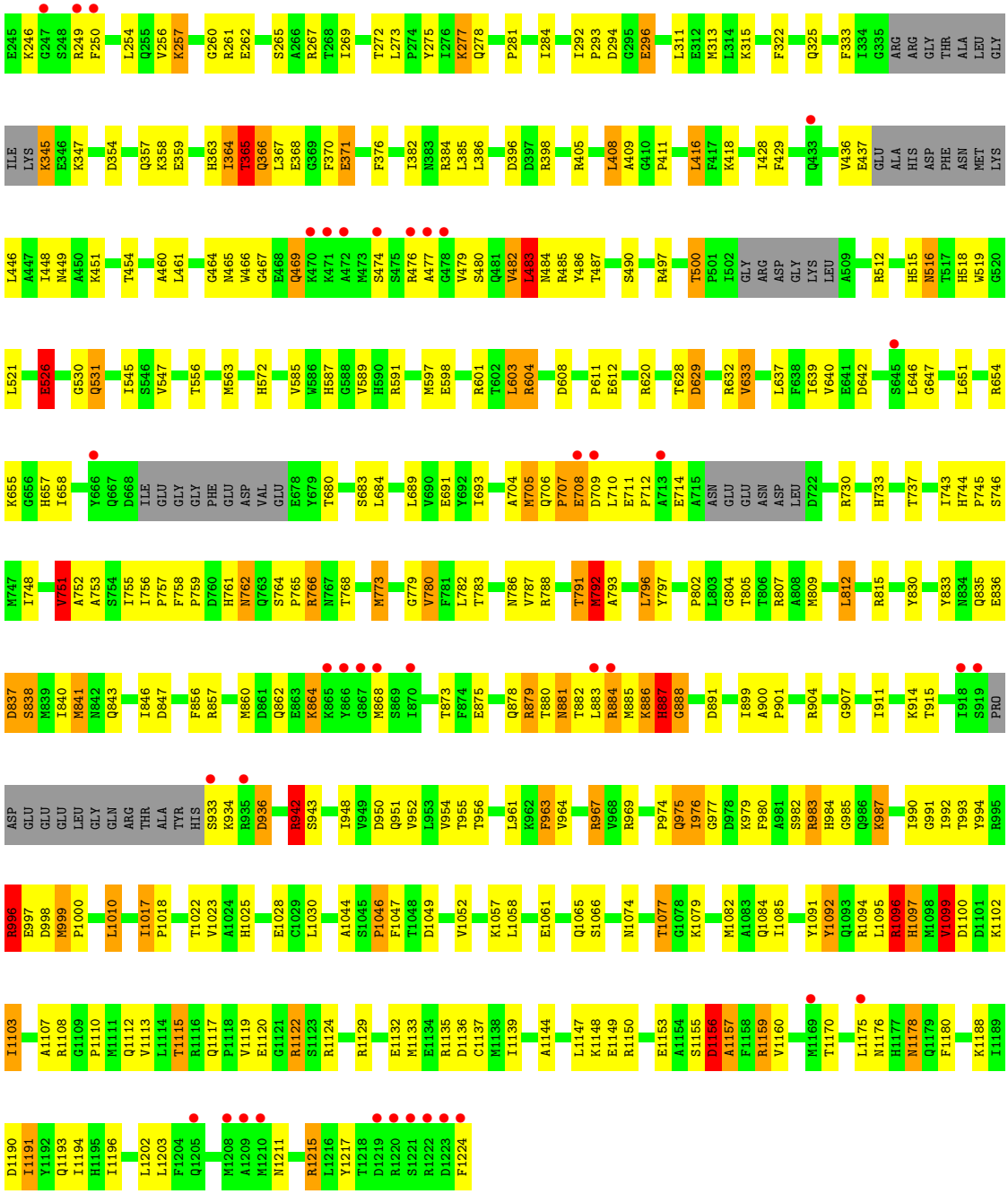




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

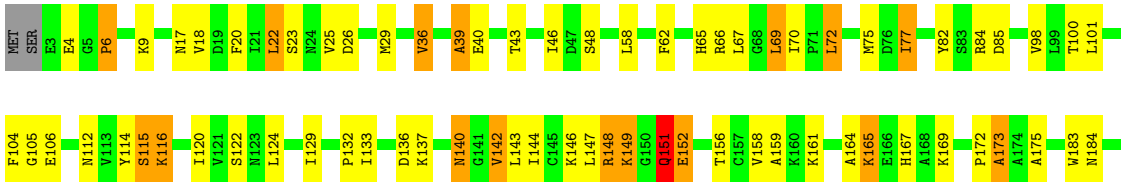
Chain B:

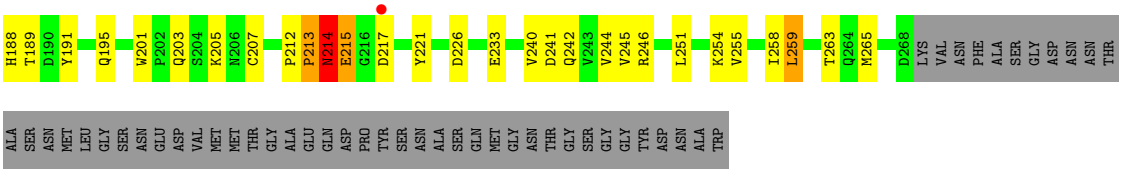




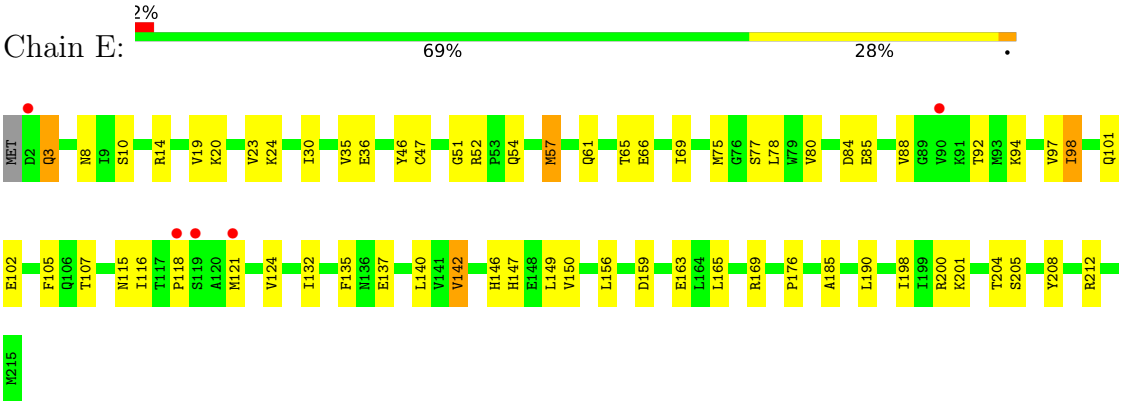
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

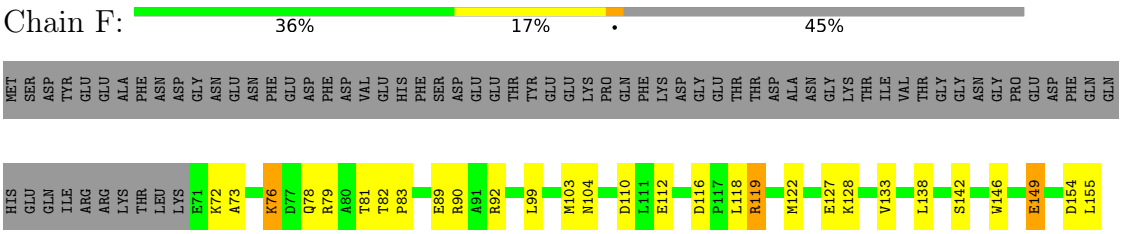




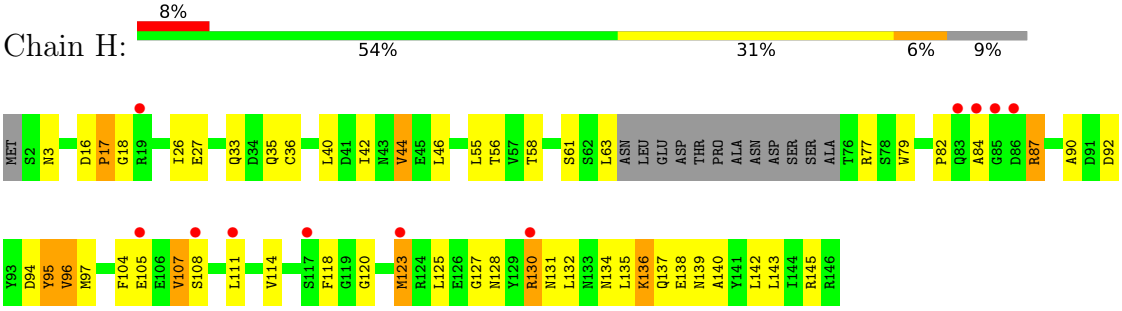
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



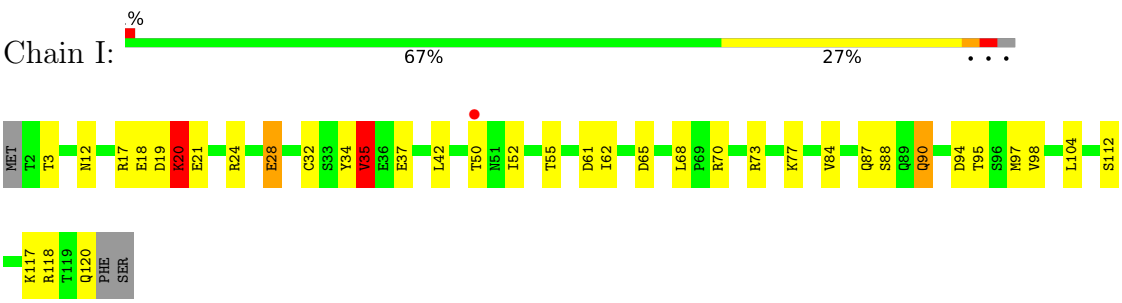
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

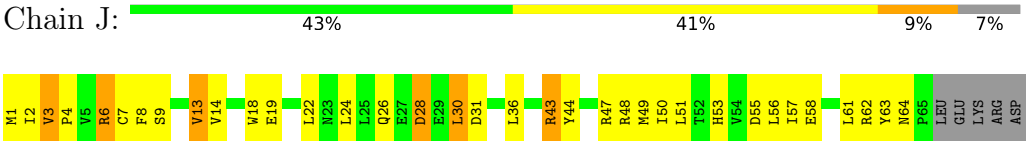


• Molecule 7: DNA-directed RNA polymerase II subunit RPB9



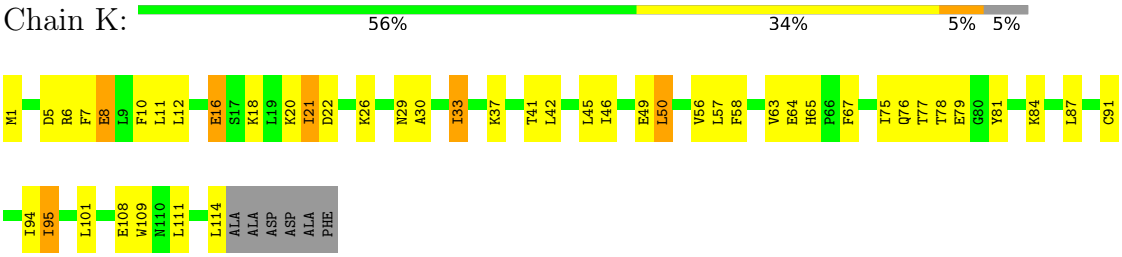
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



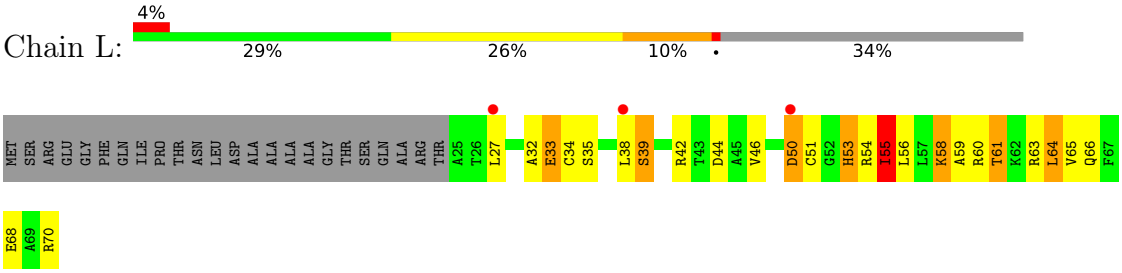
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:



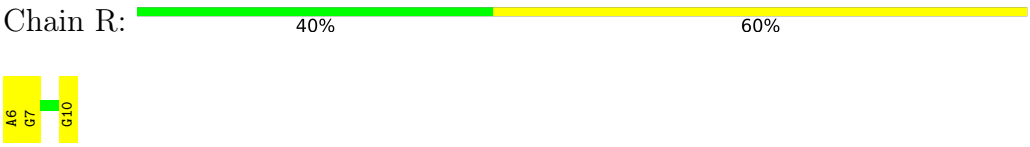
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



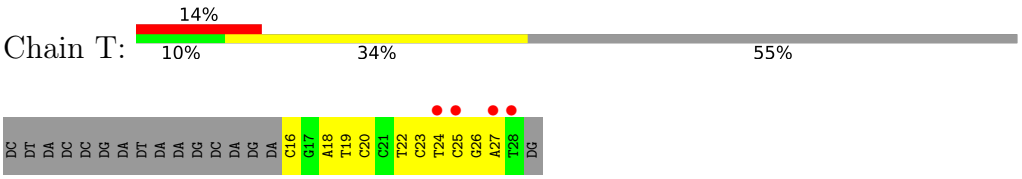
• Molecule 11: RNA (5'-R(*AP*GP*AP*GP*G)-3')

Chain R:



• Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*C P*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.94Å 220.53Å 193.72Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	29.67 – 3.30 29.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.67-3.30) 99.3 (29.67-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.31Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.176 , 0.229 0.194 , 0.245	Depositor DCC
R_{free} test set	4995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	97.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 111.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28703	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, ATP, ZN

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	0.51	0/11241	0.83	6/15199 (0.0%)
2	B	0.54	0/9033	0.83	3/12181 (0.0%)
3	C	0.49	0/2133	0.84	1/2891 (0.0%)
4	E	0.46	0/1788	0.72	0/2406
5	F	0.49	0/700	0.74	0/945
6	H	0.49	0/1086	0.82	0/1470
7	I	0.50	0/989	0.81	0/1331
8	J	0.59	0/541	0.93	0/727
9	K	0.46	0/937	0.74	0/1265
10	L	0.58	0/365	1.05	0/485
11	R	0.93	0/123	1.42	0/191
12	T	1.14	0/290	2.13	17/444 (3.8%)
All	All	0.53	0/29226	0.85	27/39535 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	16	DC	P-O3'-C3'	10.52	132.32	119.70
12	T	25	DC	O4'-C1'-N1	9.54	114.68	108.00
12	T	23	DC	O4'-C1'-N1	8.20	113.74	108.00
12	T	22	DT	C4'-C3'-C2'	-8.13	95.78	103.10
12	T	24	DT	O4'-C1'-N1	8.12	113.69	108.00
12	T	18	DA	O4'-C4'-C3'	-7.73	101.36	106.00
12	T	26	DG	O4'-C1'-N9	7.11	112.97	108.00
3	C	172	PRO	C-N-CA	6.83	138.77	121.70
12	T	20	DC	O4'-C1'-N1	6.58	112.60	108.00
12	T	27	DA	P-O3'-C3'	6.43	127.41	119.70
2	B	628	THR	C-N-CA	6.19	137.17	121.70
1	A	451	HIS	N-CA-CB	-5.75	100.24	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	22	DT	C4-C5-C7	5.66	122.39	119.00
1	A	1123	GLY	C-N-CA	5.63	135.78	121.70
1	A	399	HIS	N-CA-CB	5.58	120.65	110.60
12	T	19	DT	O4'-C4'-C3'	-5.40	102.34	104.50
1	A	1082	ASN	C-N-CA	5.35	135.07	121.70
2	B	140	ILE	C-N-CA	5.31	134.97	121.70
12	T	24	DT	C6-C5-C7	-5.20	119.78	122.90
1	A	1093	LYS	C-N-CA	5.19	134.67	121.70
2	B	887	HIS	C-N-CA	5.17	133.16	122.30
12	T	22	DT	C6-C5-C7	-5.12	119.83	122.90
12	T	25	DC	P-O3'-C3'	5.11	125.83	119.70
12	T	22	DT	P-O3'-C3'	5.07	125.78	119.70
12	T	26	DG	C4'-C3'-C2'	5.07	107.66	103.10
1	A	1083	THR	C-N-CA	5.06	134.35	121.70
12	T	24	DT	C4-C5-C7	5.02	122.01	119.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	280	0
2	B	8861	0	8884	215	0
3	C	2095	0	2051	56	0
4	E	1752	0	1776	36	0
5	F	688	0	707	9	0
6	H	1068	0	1040	20	0
7	I	971	0	927	11	0
8	J	532	0	542	23	0
9	K	919	0	929	27	0
10	L	363	0	386	14	0
11	R	109	0	55	2	0
12	T	261	0	148	0	0
13	A	2	0	0	0	0
14	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	31	0	12	5	0
All	All	28703	0	28590	619	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 11.

All (619) 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)
15:A:1736:ATP:H5'1	15:A:1736:ATP:H8	1.25	1.01
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.45	0.99
1:A:855:THR:HG21	1:A:857:ARG:HE	1.37	0.88
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.55	0.87
1:A:525:GLN:HB2	2:B:835:GLN:HE21	1.43	0.84
15:A:1736:ATP:H5'1	15:A:1736:ATP:C8	2.13	0.83
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.41	0.83
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.58	0.83
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.62	0.81
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.60	0.81
1:A:869:GLY:O	4:E:204:THR:HG21	1.83	0.80
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.64	0.79
1:A:741:ASN:HD22	1:A:744:LYS:H	1.32	0.78
1:A:421:ALA:HA	1:A:424:ILE:HD11	1.68	0.75
2:B:797:TYR:O	8:J:1:MET:HG2	1.87	0.75
10:L:32:ALA:HB3	10:L:55:ILE:HG13	1.67	0.75
1:A:1004:ASN:HD21	1:A:1007:ILE:HD12	1.52	0.74
2:B:232:SER:HB3	2:B:261:ARG:HH22	1.52	0.73
2:B:744:HIS:CD2	2:B:746:SER:OG	2.41	0.73
1:A:756:ILE:HD12	1:A:756:ILE:H	1.53	0.73
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.69	0.73
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.19	0.72
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.72	0.71
2:B:244:LEU:HD12	2:B:250:PHE:HB2	1.73	0.71
2:B:516:ASN:H	2:B:516:ASN:HD22	1.39	0.70
2:B:54:PHE:HA	2:B:58:THR:HB	1.72	0.70
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG11	1:A:214:ILE:HD12	1.73	0.70
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.72	0.70
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.73	0.69
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.73	0.69
3:C:214:ASN:HB3	3:C:217:ASP:HB2	1.73	0.69
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.68
2:B:38:PHE:HA	2:B:42:GLY:H	1.59	0.67
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.74	0.67
7:I:28:GLU:HB3	7:I:35:VAL:HG13	1.76	0.67
2:B:38:PHE:H	2:B:41:LYS:HB2	1.60	0.67
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.60	0.67
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.10	0.66
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.76	0.66
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.77	0.66
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.43	0.65
2:B:887:HIS:HA	2:B:888:GLY:O	1.96	0.65
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.78	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.65
1:A:709:THR:HB	1:A:712:GLU:H	1.61	0.65
2:B:63:ILE:O	2:B:67:SER:HB3	1.97	0.65
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.78	0.65
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.77	0.65
2:B:363:HIS:O	2:B:364:ILE:HB	1.96	0.65
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.64
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.78	0.64
1:A:466:SER:HB3	2:B:1103:ILE:HD13	1.79	0.64
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.79	0.64
2:B:1180:PHE:HB3	2:B:1191:ILE:HG21	1.79	0.64
1:A:57:ARG:HB3	1:A:68:GLN:H	1.63	0.64
2:B:843:GLN:HB2	2:B:993:THR:HB	1.79	0.64
1:A:378:GLU:OE2	1:A:434:ARG:HD3	1.97	0.63
8:J:28:ASP:HB3	8:J:30:LEU:HD12	1.79	0.63
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.80	0.63
1:A:827:THR:OG1	1:A:1083:THR:HG21	1.99	0.63
2:B:762:ASN:HD21	2:B:1022:THR:HA	1.62	0.63
1:A:140:THR:HA	1:A:143:LYS:HE3	1.80	0.63
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.81	0.63
1:A:855:THR:CG2	1:A:857:ARG:HE	2.10	0.63
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.13	0.63
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.81	0.63
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:HB2	1:A:675:THR:HB	1.81	0.62
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.82	0.62
2:B:744:HIS:HD2	2:B:746:SER:H	1.47	0.62
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.81	0.62
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.80	0.62
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.80	0.62
1:A:853:ASP:OD2	1:A:855:THR:HG22	2.00	0.62
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.82	0.62
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.34	0.62
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.64	0.62
1:A:1083:THR:N	1:A:1084:PHE:O	2.33	0.61
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.65	0.61
1:A:349:ALA:HB3	1:A:489:LEU:HB3	1.82	0.61
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.41	0.61
1:A:567:LYS:HB3	6:H:96:VAL:H	1.64	0.61
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.83	0.60
1:A:1083:THR:HG23	1:A:1084:PHE:HB3	1.82	0.60
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.36	0.60
2:B:976:ILE:O	2:B:990:ILE:HB	2.00	0.60
2:B:887:HIS:HA	2:B:888:GLY:C	2.21	0.60
1:A:278:THR:O	1:A:282:ASN:HB3	2.00	0.60
1:A:885:THR:O	1:A:940:ARG:HD3	2.01	0.60
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.84	0.60
2:B:873:THR:O	2:B:914:LYS:HA	2.01	0.60
2:B:976:ILE:HG23	2:B:977:GLY:H	1.67	0.60
5:F:90:ARG:HD2	5:F:155:LEU:HD13	1.84	0.60
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.84	0.60
2:B:486:TYR:CZ	2:B:1096:ARG:HG2	2.36	0.59
1:A:304:MET:HG2	1:A:325:ILE:HD12	1.83	0.59
1:A:388:LEU:O	1:A:392:VAL:HG23	2.02	0.59
9:K:21:ILE:HG23	9:K:33:ILE:HG12	1.84	0.59
2:B:654:ARG:H	2:B:657:HIS:HD2	1.48	0.59
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.67	0.59
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.85	0.59
1:A:331:GLY:HA2	1:A:337:ARG:HG3	1.84	0.59
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.50	0.59
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.85	0.59
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.84	0.59
3:C:115:SER:HB3	3:C:142:VAL:H	1.67	0.59
3:C:36:VAL:HG23	9:K:41:THR:HG21	1.85	0.59
2:B:975:GLN:O	2:B:990:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:TYR:HB3	3:C:84:ARG:HG2	1.85	0.58
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.85	0.58
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.33	0.58
1:A:709:THR:HG23	7:I:94:ASP:HA	1.84	0.58
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.84	0.58
1:A:587:HIS:HD2	1:A:966:ASN:HA	1.69	0.58
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.85	0.58
1:A:119:ASN:HB2	1:A:122:MET:HB2	1.83	0.58
1:A:830:LYS:HD3	1:A:1080:THR:HB	1.85	0.58
1:A:1325:THR:HA	4:E:147:HIS:HA	1.86	0.58
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.86	0.58
1:A:913:LEU:HD11	1:A:981:LEU:O	2.04	0.58
1:A:1080:THR:C	1:A:1082:ASN:H	2.06	0.58
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.85	0.58
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.34	0.58
1:A:628:GLY:O	1:A:632:VAL:HG23	2.04	0.57
3:C:147:LEU:HD23	3:C:151:GLN:HB2	1.85	0.57
2:B:345:LYS:HA	2:B:347:LYS:H	1.69	0.57
1:A:152:VAL:HG23	1:A:162:VAL:HG23	1.85	0.57
2:B:885:MET:HA	2:B:936:ASP:HB2	1.87	0.57
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.69	0.57
2:B:516:ASN:H	2:B:516:ASN:ND2	2.02	0.57
1:A:179:LEU:HB3	1:A:297:GLN:HG2	1.87	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.69	0.57
10:L:53:HIS:HB3	10:L:55:ILE:CD1	2.35	0.57
1:A:1354:ASN:O	1:A:1358:SER:HB2	2.05	0.57
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.86	0.57
1:A:567:LYS:HE3	6:H:46:LEU:HB2	1.87	0.56
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.87	0.56
3:C:167:HIS:HD2	3:C:169:LYS:H	1.51	0.56
1:A:885:THR:HG23	1:A:1024:SER:HB2	1.86	0.56
15:A:1736:ATP:H5'2	11:R:10:G:H2'	1.87	0.56
2:B:950:ASP:HB3	2:B:967:ARG:HG3	1.87	0.56
1:A:1081:LEU:HD11	15:A:1736:ATP:C5	2.41	0.56
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.87	0.56
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.56
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.41	0.56
2:B:862:GLN:HB3	2:B:963:PHE:HB2	1.88	0.56
1:A:323:LYS:HE2	1:A:328:ARG:HE	1.70	0.56
3:C:251:LEU:O	3:C:255:VAL:HG23	2.06	0.56
2:B:955:THR:HG22	2:B:956:THR:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.88	0.56
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.38	0.56
4:E:19:VAL:O	4:E:23:VAL:HG23	2.04	0.56
10:L:55:ILE:HD13	10:L:55:ILE:H	1.69	0.56
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.87	0.55
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.10	0.55
2:B:915:THR:HA	2:B:936:ASP:O	2.06	0.55
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.86	0.55
1:A:1264:GLU:HA	1:A:1267:MET:HE2	1.87	0.55
2:B:879:ARG:NH1	2:B:879:ARG:HA	2.21	0.55
2:B:654:ARG:H	2:B:657:HIS:CD2	2.24	0.55
1:A:256:GLN:HG2	1:A:257:ARG:HD2	1.89	0.55
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.21	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.88	0.55
5:F:72:LYS:HB3	5:F:142:SER:HA	1.89	0.55
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.89	0.55
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.39	0.55
1:A:831:THR:HG21	1:A:1081:LEU:HD13	1.87	0.55
4:E:10:SER:O	4:E:14:ARG:HG3	2.06	0.55
3:C:148:ARG:H	3:C:151:GLN:HG3	1.72	0.55
3:C:98:VAL:H	3:C:122:SER:HB2	1.71	0.54
1:A:1092:LYS:HB2	1:A:1096:SER:HB3	1.89	0.54
3:C:105:GLY:O	3:C:149:LYS:O	2.26	0.54
1:A:55:ASP:O	1:A:57:ARG:N	2.32	0.54
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.07	0.54
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.89	0.54
2:B:791:THR:HG22	2:B:792:MET:HE3	1.89	0.54
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.88	0.54
2:B:706:GLN:H	2:B:710:LEU:HG	1.72	0.54
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.88	0.54
2:B:787:VAL:HG12	2:B:787:VAL:O	2.08	0.54
1:A:756:ILE:H	1:A:756:ILE:CD1	2.21	0.53
2:B:904:ARG:HG2	2:B:948:ILE:HG12	1.90	0.53
2:B:1097:HIS:HB2	2:B:1102:LYS:HE3	1.90	0.53
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.89	0.53
2:B:755:ILE:HD13	2:B:809:MET:HG2	1.90	0.53
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.38	0.53
1:A:332:LYS:O	1:A:333:GLU:HG2	2.08	0.53
1:A:743:VAL:HG13	2:B:1018:PRO:HB3	1.91	0.53
2:B:237:VAL:HG22	2:B:257:LYS:HB3	1.90	0.53
1:A:86:LEU:HD12	1:A:296:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.53
5:F:76:LYS:HA	5:F:79:ARG:HH11	1.74	0.53
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.90	0.53
1:A:587:HIS:CD2	1:A:966:ASN:HA	2.43	0.52
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.91	0.52
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.91	0.52
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.91	0.52
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.91	0.52
1:A:31:SER:HB2	1:A:83:HIS:HD2	1.73	0.52
1:A:95:PHE:HB3	1:A:234:MET:HE3	1.92	0.52
1:A:518:LYS:HD2	1:A:624:SER:O	2.08	0.52
4:E:94:LYS:HA	4:E:97:VAL:HG22	1.92	0.52
1:A:351:THR:O	1:A:486:GLU:O	2.28	0.52
1:A:549:MET:HB3	1:A:577:ILE:HD13	1.91	0.52
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.90	0.52
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.92	0.52
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.92	0.52
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.74	0.52
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.91	0.52
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.90	0.52
1:A:886:ILE:HG13	1:A:943:LEU:HB3	1.90	0.52
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.92	0.52
2:B:597:MET:HG3	2:B:601:ARG:HH12	1.75	0.52
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.45	0.52
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.40	0.52
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.58	0.52
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.44	0.52
1:A:1075:PRO:O	1:A:1079:MET:HG2	2.10	0.52
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.31	0.52
2:B:70:ILE:H	2:B:429:PHE:HE1	1.57	0.51
2:B:1115:THR:HG23	2:B:1117:GLN:HB2	1.92	0.51
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.25	0.51
3:C:175:ALA:HB3	8:J:43:ARG:HE	1.75	0.51
1:A:1016:THR:HB	4:E:205:SER:O	2.11	0.51
2:B:792:MET:HE2	2:B:857:ARG:HG3	1.91	0.51
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.92	0.51
1:A:341:MET:HB3	2:B:1132:GLU:HG2	1.93	0.51
2:B:563:MET:HA	2:B:589:VAL:O	2.10	0.51
6:H:104:PHE:CE1	6:H:136:LYS:HA	2.45	0.51
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.93	0.51
2:B:766:ARG:HG2	2:B:1022:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:804:GLY:O	2:B:983:ARG:NH2	2.43	0.51
1:A:225:ASN:HB3	1:A:229:SER:H	1.75	0.51
2:B:1215:ARG:HB2	2:B:1217:TYR:CE1	2.46	0.51
2:B:857:ARG:NH2	2:B:942:ARG:HE	2.09	0.51
2:B:955:THR:HG23	10:L:54:ARG:O	2.10	0.51
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.76	0.51
1:A:820:GLY:HA3	2:B:764:SER:OG	2.11	0.51
1:A:1035:TYR:CB	1:A:1037:LEU:HD23	2.41	0.51
1:A:179:LEU:HB2	1:A:180:LYS:HE2	1.92	0.51
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.75	0.51
1:A:406:ILE:HD11	1:A:433:GLU:HG3	1.92	0.51
6:H:58:THR:HB	6:H:143:LEU:HB2	1.93	0.51
1:A:528:LEU:HD23	1:A:751:SER:HA	1.93	0.50
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.46	0.50
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.94	0.50
5:F:128:LYS:HD3	5:F:149:GLU:HA	1.93	0.50
1:A:402:ALA:CB	1:A:434:ARG:HA	2.42	0.50
3:C:39:ALA:HB1	3:C:165:LYS:HB2	1.92	0.50
1:A:1284:MET:HG3	1:A:1306:LEU:CD2	2.41	0.50
4:E:66:GLU:HA	4:E:69:ILE:HD12	1.93	0.50
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.46	0.50
1:A:830:LYS:HE3	1:A:1098:VAL:HB	1.94	0.50
1:A:423:ASP:CG	1:A:424:ILE:H	2.14	0.50
3:C:98:VAL:H	3:C:122:SER:CB	2.25	0.50
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.94	0.50
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.94	0.50
8:J:8:PHE:H	8:J:49:MET:HE3	1.77	0.50
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.93	0.49
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.94	0.49
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.93	0.49
8:J:36:LEU:HD11	8:J:51:LEU:HD13	1.94	0.49
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.77	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.93	0.49
2:B:1112:GLN:HB3	2:B:1115:THR:HG22	1.94	0.49
3:C:242:GLN:HG3	3:C:246:ARG:HH21	1.77	0.49
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.94	0.49
2:B:357:GLN:HG3	2:B:368:GLU:HA	1.95	0.49
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.27	0.49
1:A:981:LEU:HD12	1:A:981:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:N	3:C:151:GLN:HG3	2.27	0.49
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.94	0.49
1:A:252:PHE:HD1	1:A:253:ASN:H	1.60	0.49
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.42	0.49
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.95	0.49
3:C:184:ASN:ND2	3:C:189:THR:O	2.45	0.49
9:K:63:VAL:HG23	9:K:63:VAL:O	2.13	0.49
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.94	0.49
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	1.95	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.49
6:H:33:GLN:HB2	6:H:36:CYS:HB3	1.95	0.49
1:A:781:ASP:HB2	1:A:789:LYS:HD3	1.95	0.49
3:C:18:VAL:CG2	9:K:109:TRP:HZ3	2.26	0.49
1:A:456:MET:HE2	1:A:510:GLN:HB2	1.95	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.95	0.48
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.46	0.48
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.95	0.48
1:A:810:PRO:HB2	2:B:519:TRP:HH2	1.78	0.48
2:B:840:ILE:O	2:B:1010:LEU:HA	2.14	0.48
2:B:847:ASP:O	3:C:65:HIS:HE1	1.96	0.48
3:C:66:ARG:NH2	8:J:3:VAL:O	2.43	0.48
9:K:5:ASP:HB2	9:K:8:GLU:OE2	2.12	0.48
11:R:6:A:H2'	11:R:7:G:H8	1.78	0.48
1:A:684:ALA:O	1:A:688:LYS:HG2	2.13	0.48
1:A:942:PHE:O	1:A:946:VAL:HG12	2.13	0.48
1:A:567:LYS:CE	6:H:46:LEU:HB2	2.43	0.48
1:A:586:ILE:N	1:A:609:ASP:O	2.47	0.48
2:B:515:HIS:H	2:B:518:HIS:CD2	2.31	0.48
2:B:707:PRO:HG2	2:B:708:GLU:HG3	1.95	0.48
1:A:297:GLN:C	1:A:299:HIS:H	2.17	0.48
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.94	0.48
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.96	0.48
2:B:879:ARG:HA	2:B:879:ARG:CZ	2.43	0.48
2:B:884:ARG:O	2:B:936:ASP:HB2	2.13	0.48
1:A:825:ILE:CD1	2:B:512:ARG:HB3	2.44	0.48
10:L:61:THR:HB	10:L:63:ARG:H	1.78	0.48
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.95	0.48
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.28	0.48
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.48	0.48
1:A:276:LEU:HD11	1:A:292:ALA:HB1	1.96	0.48
2:B:35:SER:O	2:B:39:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:THR:HG23	2:B:490:SER:H	1.78	0.48
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.96	0.48
2:B:1110:PRO:HG2	2:B:1124:ARG:O	2.14	0.48
4:E:118:PRO:HA	4:E:121:MET:HB2	1.96	0.47
1:A:715:GLU:O	1:A:719:VAL:HG23	2.14	0.47
3:C:213:PRO:O	3:C:214:ASN:HB2	2.14	0.47
1:A:709:THR:CG2	7:I:94:ASP:HA	2.43	0.47
2:B:68:THR:HA	2:B:90:ILE:O	2.14	0.47
8:J:1:MET:HB2	8:J:56:LEU:HD12	1.96	0.47
1:A:1088:GLY:HA2	1:A:1089:VAL:HA	1.71	0.47
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.31	0.47
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.54	0.47
2:B:358:LYS:HA	2:B:366:GLN:HG2	1.97	0.47
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.96	0.47
2:B:994:TYR:HD1	2:B:999:MET:HE3	1.80	0.47
3:C:191:TYR:HD2	3:C:201:TRP:CE2	2.32	0.47
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.96	0.47
2:B:881:ASN:HB3	2:B:933:SER:OG	2.15	0.47
6:H:130:ARG:HB3	6:H:134:ASN:HD21	1.80	0.47
8:J:36:LEU:HD13	8:J:47:ARG:HD2	1.95	0.47
9:K:65:HIS:CD2	9:K:67:PHE:H	2.32	0.47
1:A:642:CYS:O	1:A:645:LEU:HB3	2.15	0.47
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.97	0.47
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.50	0.47
1:A:494:SER:O	1:A:498:ARG:HG3	2.14	0.47
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.44	0.47
2:B:545:ILE:HG13	2:B:633:VAL:HG13	1.96	0.47
7:I:73:ARG:HH12	7:I:112:SER:HA	1.80	0.47
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.80	0.47
1:A:262:LEU:HD11	1:A:325:ILE:HG12	1.97	0.46
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.97	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.56	0.46
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.96	0.46
1:A:1368:MET:O	1:A:1372:VAL:HG23	2.15	0.46
6:H:137:GLN:C	6:H:139:ASN:H	2.19	0.46
1:A:116:ASP:HB3	1:A:164:ARG:HH12	1.80	0.46
1:A:830:LYS:HG3	1:A:1098:VAL:CG1	2.37	0.46
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.50	0.46
2:B:563:MET:HE1	2:B:587:HIS:CB	2.45	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.46
2:B:1110:PRO:HB2	2:B:1119:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:101:GLN:HG3	4:E:102:GLU:HG3	1.96	0.46
9:K:50:LEU:O	9:K:56:VAL:HG11	2.15	0.46
1:A:109:HIS:H	1:A:210:ILE:HD12	1.80	0.46
1:A:352:VAL:HB	2:B:1099:VAL:HG13	1.96	0.46
2:B:979:LYS:HD3	2:B:1095:LEU:HD12	1.97	0.46
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.81	0.46
1:A:780:VAL:HG12	1:A:789:LYS:HE2	1.97	0.46
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.98	0.46
2:B:408:LEU:H	2:B:411:PRO:HG2	1.79	0.46
1:A:181:LEU:O	1:A:202:LEU:HB3	2.16	0.46
1:A:353:ILE:HG22	1:A:468:PHE:CB	2.45	0.46
2:B:680:THR:O	2:B:683:SER:HB2	2.16	0.46
1:A:535:THR:HG22	1:A:575:LYS:HG2	1.98	0.46
1:A:695:LYS:HD2	1:A:695:LYS:HA	1.88	0.46
1:A:1205:LYS:O	1:A:1207:LEU:N	2.45	0.46
2:B:212:LEU:HD13	2:B:409:ALA:HA	1.98	0.46
2:B:955:THR:HG22	2:B:956:THR:N	2.31	0.46
2:B:1120:GLU:H	2:B:1124:ARG:HH21	1.64	0.46
4:E:94:LYS:O	4:E:98:ILE:HB	2.16	0.46
8:J:43:ARG:HG2	8:J:43:ARG:HH11	1.81	0.46
1:A:43:GLU:HG3	1:A:50:ILE:HG12	1.97	0.46
1:A:983:ILE:HD12	1:A:1028:THR:HG21	1.97	0.46
2:B:1058:LEU:O	2:B:1061:GLU:HB2	2.15	0.46
1:A:41:MET:HA	1:A:49:LYS:HA	1.97	0.46
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.29	0.45
1:A:1080:THR:O	1:A:1082:ASN:N	2.46	0.45
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.98	0.45
3:C:65:HIS:O	3:C:69:LEU:HD12	2.16	0.45
4:E:98:ILE:HA	4:E:101:GLN:HG2	1.97	0.45
9:K:12:LEU:HD21	9:K:18:LYS:HG2	1.98	0.45
1:A:694:THR:HA	1:A:714:PHE:HE1	1.80	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.52	0.45
3:C:173:ALA:O	3:C:233:GLU:O	2.34	0.45
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.97	0.45
1:A:1093:LYS:HG3	1:A:1359:ASP:HB2	1.98	0.45
6:H:118:PHE:HE1	6:H:123:MET:HB2	1.80	0.45
1:A:131:SER:HB3	1:A:223:GLY:CA	2.45	0.45
2:B:835:GLN:O	2:B:838:SER:HB2	2.17	0.45
3:C:151:GLN:H	3:C:151:GLN:HG2	1.25	0.45
8:J:4:PRO:O	8:J:14:VAL:HG23	2.15	0.45
1:A:947:PHE:HE2	1:A:1017:LEU:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:LEU:HG	15:A:1736:ATP:H2'	1.99	0.45
2:B:114:PRO:HB3	2:B:174:LEU:HD21	1.99	0.45
2:B:841:MET:HG2	2:B:1010:LEU:HD12	1.99	0.45
2:B:1099:VAL:O	2:B:1103:ILE:HG12	2.17	0.45
7:I:18:GLU:HG2	7:I:20:LYS:H	1.82	0.45
1:A:279:LEU:HD22	1:A:289:ILE:HA	1.98	0.45
3:C:6:PRO:HB2	9:K:101:LEU:HD13	1.99	0.45
10:L:34:CYS:SG	10:L:34:CYS:O	2.75	0.45
1:A:1317:MET:HG3	4:E:142:VAL:HG21	1.99	0.45
2:B:744:HIS:HD2	2:B:746:SER:OG	1.96	0.45
2:B:900:ALA:HA	10:L:58:LYS:HD3	1.98	0.45
3:C:255:VAL:O	3:C:258:ILE:HG22	2.16	0.45
1:A:744:LYS:O	1:A:748:MET:HG3	2.17	0.45
1:A:946:VAL:HB	4:E:201:LYS:HD2	1.98	0.45
8:J:6:ARG:HG3	8:J:13:VAL:HG13	1.99	0.45
2:B:44:VAL:HA	2:B:46:GLN:HE21	1.82	0.45
4:E:61:GLN:HG3	4:E:105:PHE:CE2	2.51	0.45
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.17	0.44
9:K:65:HIS:HD2	9:K:67:PHE:H	1.65	0.44
1:A:129:LYS:HA	1:A:134:ARG:HH21	1.82	0.44
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.99	0.44
1:A:1318:THR:HG22	4:E:142:VAL:HG22	1.99	0.44
2:B:125:SER:HB3	2:B:171:PRO:HA	1.98	0.44
2:B:751:VAL:HG22	2:B:812:LEU:HD22	1.98	0.44
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.99	0.44
3:C:259:LEU:HD13	9:K:91:CYS:HB2	1.99	0.44
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.82	0.44
8:J:24:LEU:HA	8:J:28:ASP:HB2	2.00	0.44
1:A:55:ASP:C	1:A:57:ARG:H	2.19	0.44
1:A:711:ARG:HA	7:I:97:MET:HE1	2.00	0.44
1:A:795:GLU:CD	1:A:795:GLU:H	2.21	0.44
3:C:165:LYS:O	9:K:6:ARG:NH1	2.51	0.44
8:J:53:HIS:CE1	8:J:55:ASP:HB2	2.53	0.44
10:L:61:THR:HB	10:L:63:ARG:HB2	2.00	0.44
1:A:115:LEU:HD21	1:A:145:LYS:HG3	1.99	0.44
2:B:765:PRO:O	2:B:768:THR:N	2.50	0.44
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.52	0.44
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.99	0.44
2:B:446:LEU:O	2:B:448:ILE:HD12	2.18	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.44
2:B:773:MET:SD	2:B:987:LYS:HG3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.53	0.44
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.44
2:B:213:ILE:O	2:B:215:GLN:HG2	2.18	0.44
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.99	0.44
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.92	0.44
1:A:98:LYS:O	1:A:102:VAL:HG23	2.18	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.99	0.43
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.99	0.43
2:B:597:MET:HG3	2:B:601:ARG:NH1	2.32	0.43
2:B:637:LEU:HD12	2:B:693:ILE:HG13	2.00	0.43
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.48	0.43
1:A:456:MET:HB2	1:A:478:TYR:OH	2.18	0.43
1:A:877:HIS:HB3	1:A:1056:SER:HA	2.00	0.43
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.18	0.43
2:B:211:VAL:CG2	2:B:483:LEU:HA	2.47	0.43
2:B:836:GLU:O	2:B:837:ASP:HB2	2.18	0.43
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	2.00	0.43
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.51	0.43
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.65	0.43
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.43
2:B:48:LEU:HD23	2:B:173:MET:SD	2.58	0.43
6:H:79:TRP:CH2	6:H:82:PRO:HD3	2.54	0.43
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.99	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.49	0.43
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.33	0.43
1:A:1376:THR:HG22	1:A:1377:THR:N	2.34	0.43
2:B:365:THR:HG21	2:B:370:PHE:HD1	1.83	0.43
9:K:30:ALA:HA	9:K:75:ILE:O	2.19	0.43
1:A:1316:VAL:O	1:A:1319:VAL:HB	2.18	0.43
4:E:20:LYS:HE3	4:E:35:VAL:HA	2.00	0.43
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.54	0.43
1:A:208:LEU:HG	1:A:235:ILE:HD11	2.01	0.43
1:A:587:HIS:CE1	1:A:969:GLN:HE21	2.37	0.43
1:A:852:TYR:O	5:F:81:THR:HG22	2.18	0.43
1:A:933:TYR:O	1:A:937:VAL:HG13	2.19	0.43
2:B:640:VAL:HG22	2:B:651:LEU:HG	2.01	0.43
4:E:176:PRO:O	4:E:212:ARG:HA	2.19	0.43
1:A:361:LEU:HD11	1:A:521:MET:HE2	2.00	0.43
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.53	0.43
1:A:830:LYS:HD2	1:A:1094:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG13	1:A:241:VAL:HG21	2.01	0.43
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	2.01	0.43
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.54	0.43
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.47	0.43
1:A:710:LEU:H	1:A:710:LEU:HD22	1.83	0.43
1:A:754:SER:H	1:A:757:ASN:HD22	1.67	0.43
1:A:851:HIS:HB2	1:A:855:THR:HG22	2.01	0.43
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	2.01	0.43
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.52	0.43
6:H:40:LEU:HD21	6:H:142:LEU:HD21	2.00	0.43
2:B:753:ALA:HA	2:B:756:ILE:HD12	2.01	0.42
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.54	0.42
7:I:19:ASP:HB3	7:I:24:ARG:H	1.84	0.42
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.01	0.42
9:K:79:GLU:CD	9:K:79:GLU:H	2.23	0.42
1:A:588:LEU:HD12	1:A:632:VAL:HG21	2.01	0.42
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.23	0.42
1:A:738:LYS:HD2	1:A:740:LEU:HD21	2.01	0.42
1:A:1390:ASN:O	1:A:1399:ARG:HD2	2.19	0.42
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	2.00	0.42
2:B:956:THR:HB	10:L:46:VAL:HG21	2.01	0.42
4:E:65:THR:O	4:E:69:ILE:HG13	2.20	0.42
8:J:1:MET:N	8:J:56:LEU:N	2.67	0.42
2:B:123:THR:HG23	2:B:205:ILE:HA	2.01	0.42
2:B:487:THR:HG22	2:B:490:SER:HB3	2.01	0.42
2:B:764:SER:HB3	2:B:765:PRO:HD3	2.01	0.42
3:C:148:ARG:HD3	8:J:61:LEU:O	2.18	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.55	0.42
4:E:97:VAL:HG23	4:E:98:ILE:HD12	2.01	0.42
1:A:353:ILE:HG21	1:A:487:MET:HB2	2.02	0.42
1:A:404:TYR:HA	1:A:413:ILE:O	2.19	0.42
1:A:774:ARG:HH21	1:A:794:PRO:HA	1.83	0.42
2:B:54:PHE:HA	2:B:58:THR:CB	2.45	0.42
2:B:91:SER:HB3	2:B:133:LYS:HB2	2.01	0.42
2:B:857:ARG:HH21	2:B:942:ARG:HE	1.66	0.42
1:A:516:SER:C	1:A:518:LYS:H	2.23	0.42
1:A:694:THR:HA	1:A:714:PHE:CE1	2.55	0.42
1:A:819:GLY:O	1:A:822:GLU:HB2	2.20	0.42
1:A:131:SER:CB	1:A:223:GLY:HA2	2.49	0.42
1:A:182:VAL:HG22	1:A:202:LEU:H	1.84	0.42
8:J:44:TYR:HA	8:J:47:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:H	1:A:56:PRO:HD3	1.85	0.42
1:A:121:LEU:HB3	1:A:141:LEU:HD22	2.00	0.42
1:A:506:ALA:HB3	1:A:509:LEU:HD12	2.01	0.42
1:A:670:ILE:HD12	2:B:1052:VAL:HG11	2.01	0.42
1:A:860:LEU:HD21	1:A:1394:THR:HA	2.02	0.42
1:A:877:HIS:CB	1:A:1056:SER:HA	2.50	0.42
1:A:1128:GLN:HG2	1:A:1304:TRP:NE1	2.35	0.42
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	2.00	0.42
2:B:428:ILE:HG12	2:B:448:ILE:HG13	2.01	0.42
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	2.02	0.42
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.02	0.42
1:A:1366:ARG:HA	1:A:1369:ALA:HB3	2.02	0.42
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.31	0.42
3:C:77:ILE:CD1	3:C:161:LYS:HG3	2.50	0.42
3:C:241:ASP:O	3:C:245:VAL:HG23	2.20	0.42
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.55	0.42
9:K:91:CYS:O	9:K:95:ILE:HG12	2.20	0.42
1:A:453:MET:HB3	1:A:477:PRO:HB2	2.02	0.42
7:I:32:CYS:SG	7:I:34:TYR:HB2	2.60	0.42
10:L:68:GLU:C	10:L:70:ARG:H	2.23	0.42
1:A:568:PRO:O	1:A:569:LYS:HB2	2.19	0.42
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.42
1:A:793:SER:HB2	1:A:795:GLU:OE2	2.19	0.41
2:B:293:PRO:HB2	2:B:296:GLU:HB2	2.02	0.41
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.84	0.41
1:A:342:GLY:HA3	2:B:1129:ARG:NH2	2.35	0.41
2:B:260:GLY:O	2:B:267:ARG:HD3	2.20	0.41
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.41
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.54	0.41
4:E:124:VAL:HA	4:E:132:ILE:HD11	2.01	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.41
4:E:47:CYS:HB3	4:E:51:GLY:HA2	2.03	0.41
6:H:87:ARG:HH11	6:H:87:ARG:HA	1.84	0.41
1:A:302:THR:HA	1:A:305:ASP:O	2.21	0.41
1:A:456:MET:CE	1:A:510:GLN:HB2	2.50	0.41
2:B:29:ASP:HB3	2:B:658:ILE:HG13	2.03	0.41
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.65	0.41
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.85	0.41
10:L:55:ILE:HG12	10:L:56:LEU:H	1.85	0.41
1:A:870:GLU:HG2	4:E:208:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:HD13	2:B:585:VAL:HG13	2.02	0.41
2:B:791:THR:HG22	2:B:792:MET:CE	2.50	0.41
2:B:899:ILE:HD11	2:B:911:ILE:HA	2.02	0.41
3:C:58:LEU:HD21	8:J:57:ILE:HD12	2.02	0.41
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.99	0.41
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.85	0.41
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.02	0.41
2:B:193:LYS:HB3	2:B:787:VAL:HG11	2.02	0.41
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.02	0.41
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.50	0.41
3:C:29:MET:HE2	9:K:45:LEU:HD11	2.02	0.41
1:A:345:VAL:HA	2:B:1155:SER:HB2	2.02	0.41
1:A:407:ARG:HD2	1:A:413:ILE:HD11	2.03	0.41
2:B:189:LEU:HB3	2:B:194:GLU:O	2.21	0.41
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.41
9:K:16:GLU:OE2	9:K:37:LYS:NZ	2.53	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.73	0.41
2:B:46:GLN:H	2:B:46:GLN:HG3	1.71	0.41
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.56	0.41
6:H:56:THR:HB	6:H:145:ARG:HB3	2.02	0.41
1:A:41:MET:HB3	1:A:49:LYS:HE3	2.03	0.41
1:A:456:MET:HE2	1:A:507:VAL:HA	2.03	0.41
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.01	0.41
1:A:912:LEU:HB3	1:A:1036:ARG:HH22	1.86	0.41
1:A:1086:PHE:HB2	1:A:1087:ALA:H	1.73	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.01	0.41
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.56	0.41
2:B:684:LEU:HA	2:B:689:LEU:HD12	2.01	0.41
2:B:843:GLN:HA	2:B:846:ILE:HD12	2.01	0.41
2:B:976:ILE:HG23	2:B:977:GLY:N	2.32	0.41
2:B:982:SER:HB3	2:B:1092:TYR:CZ	2.56	0.41
2:B:1100:ASP:OD1	2:B:1103:ILE:HD11	2.21	0.41
1:A:312:PRO:HB2	1:A:313:GLN:H	1.74	0.41
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.74	0.41
3:C:67:LEU:HA	3:C:70:ILE:HD12	2.02	0.41
3:C:72:LEU:HB3	3:C:132:PRO:HA	2.03	0.41
1:A:425:GLN:H	1:A:425:GLN:NE2	2.19	0.40
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.02	0.40
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.04	0.40
2:B:745:PRO:HB2	2:B:1047:PHE:CD1	2.56	0.40
2:B:780:VAL:HG11	8:J:56:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.22	0.40
3:C:62:PHE:O	3:C:66:ARG:HG3	2.21	0.40
9:K:42:LEU:HG	9:K:46:ILE:HD12	2.01	0.40
1:A:669:THR:HB	1:A:805:LEU:HD13	2.02	0.40
2:B:275:TYR:CD1	2:B:275:TYR:N	2.89	0.40
4:E:147:HIS:CD2	4:E:149:LEU:H	2.39	0.40
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.51	0.40
9:K:5:ASP:HB3	9:K:7:PHE:CE2	2.57	0.40
1:A:535:THR:HB	1:A:616:VAL:HG13	2.02	0.40
7:I:88:SER:C	7:I:90:GLN:H	2.25	0.40
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.02	0.40
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.03	0.40
2:B:1149:GLU:HG2	2:B:1153:GLU:HB2	2.04	0.40
9:K:33:ILE:HD13	9:K:87:LEU:HD22	2.04	0.40
1:A:31:SER:HB2	1:A:83:HIS:CD2	2.53	0.40
2:B:53:GLN:HG2	2:B:547:VAL:HB	2.04	0.40
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.86	0.40
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.02	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	1395/1733 (80%)	1177 (84%)	149 (11%)	69 (5%)	2 14
2	B	1096/1224 (90%)	927 (85%)	110 (10%)	59 (5%)	2 12
3	C	264/318 (83%)	235 (89%)	19 (7%)	10 (4%)	3 19
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	17 48
5	F	83/155 (54%)	73 (88%)	7 (8%)	3 (4%)	3 20
6	H	129/146 (88%)	93 (72%)	24 (19%)	12 (9%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	I	117/122 (96%)	103 (88%)	10 (8%)	4 (3%)	3 22
8	J	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	4 22
9	K	112/120 (93%)	101 (90%)	8 (7%)	3 (3%)	5 26
10	L	44/70 (63%)	28 (64%)	7 (16%)	9 (20%)	0 0
All	All	3515/4173 (84%)	2991 (85%)	351 (10%)	173 (5%)	2 14

All (173) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	215	SER
1	A	250	ILE
1	A	312	PRO
1	A	556	TRP
1	A	569	LYS
1	A	672	ASP
1	A	978	PRO
1	A	1206	ASP
1	A	1377	THR
1	A	1394	THR
2	B	67	SER
2	B	168	GLY
2	B	230	ALA
2	B	265	SER
2	B	451	LYS
2	B	474	SER
2	B	477	ALA
2	B	479	VAL
2	B	712	PRO
2	B	880	THR
2	B	883	LEU
2	B	888	GLY
2	B	936	ASP
2	B	976	ILE
2	B	1156	ASP
2	B	1178	ASN
3	C	4	GLU
3	C	40	GLU
3	C	173	ALA
3	C	213	PRO
3	C	214	ASN

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Mol	Chain	Res	Type
3	C	215	GLU
8	J	2	ILE
8	J	6	ARG
9	K	16	GLU
10	L	53	HIS
10	L	55	ILE
1	A	54	ASN
1	A	65	LEU
1	A	200	ARG
1	A	214	ILE
1	A	255	SER
1	A	331	GLY
1	A	385	ILE
1	A	399	HIS
1	A	411	ASP
1	A	487	MET
1	A	775	ILE
1	A	1005	GLU
1	A	1094	VAL
1	A	1123	GLY
1	A	1124	HIS
1	A	1221	LYS
1	A	1359	ASP
1	A	1378	GLN
1	A	1393	ASN
1	A	1437	GLY
2	B	137	TYR
2	B	277	LYS
2	B	371	GLU
2	B	449	ASN
2	B	629	ASP
2	B	647	GLY
2	B	707	PRO
2	B	751	VAL
2	B	864	LYS
2	B	881	ASN
2	B	884	ARG
2	B	887	HIS
2	B	907	GLY
2	B	943	SER
2	B	996	ARG
2	B	1099	VAL

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Mol	Chain	Res	Type
2	B	1176	ASN
5	F	73	ALA
6	H	61	SER
6	H	90	ALA
6	H	131	ASN
6	H	135	LEU
10	L	35	SER
10	L	39	SER
10	L	50	ASP
10	L	51	CYS
1	A	110	CYS
1	A	258	GLY
1	A	298	PHE
1	A	517	ASN
1	A	707	GLY
1	A	846	GLU
1	A	1064	VAL
1	A	1081	LEU
2	B	467	GLY
2	B	484	ASN
2	B	705	MET
2	B	792	MET
2	B	837	ASP
2	B	886	LYS
2	B	891	ASP
2	B	934	LYS
3	C	165	LYS
4	E	3	GLN
4	E	36	GLU
6	H	44	VAL
7	I	77	LYS
9	K	26	LYS
1	A	57	ARG
1	A	72	GLU
1	A	125	ALA
1	A	149	GLU
1	A	404	TYR
1	A	567	LYS
1	A	591	PHE
1	A	706	HIS
1	A	828	ALA
1	A	1084	PHE

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Mol	Chain	Res	Type
1	A	1175	SER
1	A	1376	THR
2	B	139	ALA
2	B	365	THR
2	B	469	GLN
2	B	483	LEU
2	B	531	GLN
2	B	974	PRO
2	B	1017	ILE
2	B	1046	PRO
2	B	1096	ARG
2	B	1097	HIS
2	B	1157	ALA
3	C	151	GLN
5	F	154	ASP
6	H	77	ARG
6	H	84	ALA
6	H	107	VAL
7	I	3	THR
7	I	20	LYS
10	L	64	LEU
1	A	35	ILE
1	A	55	ASP
1	A	130	ASP
1	A	132	LYS
1	A	283	GLY
1	A	350	ARG
1	A	424	ILE
1	A	958	VAL
1	A	973	ILE
1	A	1255	GLU
1	A	1388	GLY
2	B	526	GLU
2	B	704	ALA
2	B	942	ARG
3	C	39	ALA
5	F	78	GLN
6	H	17	PRO
6	H	18	GLY
6	H	140	ALA
7	I	35	VAL
9	K	64	GLU

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Mol	Chain	Res	Type
10	L	33	GLU
10	L	59	ALA
1	A	400	PRO
1	A	1093	LYS
1	A	1395	GLY
2	B	737	THR
6	H	128	ASN
2	B	482	VAL
1	A	93	VAL
1	A	568	PRO
1	A	1384	VAL
2	B	1023	VAL
1	A	59	GLY
2	B	364	ILE
3	C	6	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	1225/1520 (81%)	1008 (82%)	217 (18%)	2 8
2	B	967/1061 (91%)	811 (84%)	156 (16%)	2 10
3	C	234/274 (85%)	191 (82%)	43 (18%)	1 7
4	E	196/197 (100%)	173 (88%)	23 (12%)	5 21
5	F	75/137 (55%)	60 (80%)	15 (20%)	1 5
6	H	117/128 (91%)	96 (82%)	21 (18%)	2 8
7	I	113/116 (97%)	91 (80%)	22 (20%)	1 5
8	J	60/65 (92%)	46 (77%)	14 (23%)	1 3
9	K	99/102 (97%)	83 (84%)	16 (16%)	2 10
10	L	40/57 (70%)	26 (65%)	14 (35%)	0 1
All	All	3126/3657 (86%)	2585 (83%)	541 (17%)	2 8

All (541) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	30	ILE
1	A	34	LYS
1	A	43	GLU
1	A	46	THR
1	A	47	ARG
1	A	50	ILE
1	A	55	ASP
1	A	57	ARG
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	74	MET
1	A	75	ASN
1	A	88	LYS
1	A	93	VAL
1	A	108	MET
1	A	122	MET
1	A	126	LEU
1	A	142	CYS
1	A	144	THR
1	A	146	MET
1	A	149	GLU
1	A	150	THR
1	A	180	LYS
1	A	204	THR
1	A	222	LEU
1	A	225	ASN
1	A	232	GLU
1	A	234	MET
1	A	256	GLN
1	A	257	ARG
1	A	262	LEU
1	A	263	THR
1	A	265	LYS
1	A	266	LEU
1	A	268	ASP
1	A	269	ILE
1	A	270	LEU
1	A	277	GLU
1	A	281	HIS

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Mol	Chain	Res	Type
1	A	293	GLU
1	A	298	PHE
1	A	303	TYR
1	A	308	ILE
1	A	313	GLN
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	332	LYS
1	A	335	ARG
1	A	341	MET
1	A	373	THR
1	A	381	THR
1	A	389	THR
1	A	391	LEU
1	A	403	LYS
1	A	406	ILE
1	A	407	ARG
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	437	MET
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	455	MET
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	500	GLU
1	A	501	LEU
1	A	505	CYS
1	A	527	THR
1	A	533	LYS
1	A	535	THR
1	A	536	LEU
1	A	538	ASP

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Mol	Chain	Res	Type
1	A	541	ILE
1	A	542	GLU
1	A	543	LEU
1	A	544	ASP
1	A	545	GLN
1	A	549	MET
1	A	571	LEU
1	A	590	ARG
1	A	595	THR
1	A	597	LEU
1	A	612	ILE
1	A	618	GLU
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	652	VAL
1	A	669	THR
1	A	670	ILE
1	A	672	ASP
1	A	675	THR
1	A	678	GLU
1	A	680	THR
1	A	688	LYS
1	A	705	LYS
1	A	709	THR
1	A	722	LEU
1	A	740	LEU
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	788	SER
1	A	801	GLU
1	A	821	ARG
1	A	822	GLU
1	A	838	GLN
1	A	839	ARG
1	A	847	ASP
1	A	855	THR
1	A	886	ILE
1	A	894	GLU
1	A	896	ARG

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Mol	Chain	Res	Type
1	A	905	ASP
1	A	908	LEU
1	A	909	ASP
1	A	912	LEU
1	A	914	GLU
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	927	VAL
1	A	929	LEU
1	A	931	GLU
1	A	934	LYS
1	A	936	LEU
1	A	946	VAL
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE
1	A	977	LYS
1	A	979	SER
1	A	981	LEU
1	A	982	THR
1	A	983	ILE
1	A	1000	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1009	ASN
1	A	1024	SER
1	A	1025	ARG
1	A	1030	ARG
1	A	1033	GLN
1	A	1037	LEU
1	A	1048	ASN
1	A	1052	GLN
1	A	1062	GLU
1	A	1067	LEU
1	A	1077	THR
1	A	1078	GLN
1	A	1081	LEU
1	A	1084	PHE
1	A	1086	PHE
1	A	1093	LYS
1	A	1124	HIS

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Mol	Chain	Res	Type
1	A	1128	GLN
1	A	1129	GLU
1	A	1130	GLN
1	A	1143	LEU
1	A	1147	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1188	GLN
1	A	1205	LYS
1	A	1215	ARG
1	A	1221	LYS
1	A	1224	LEU
1	A	1231	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1257	ASP
1	A	1261	LYS
1	A	1264	GLU
1	A	1271	ILE
1	A	1280	GLU
1	A	1283	VAL
1	A	1284	MET
1	A	1288	ASP
1	A	1299	VAL
1	A	1308	THR
1	A	1322	ILE
1	A	1327	ILE
1	A	1333	ILE
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1381	LEU
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET

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Mol	Chain	Res	Type
1	A	1403	GLU
1	A	1406	VAL
1	A	1411	GLU
1	A	1422	ARG
1	A	1425	SER
1	A	1438	THR
2	B	26	THR
2	B	28	GLU
2	B	44	VAL
2	B	46	GLN
2	B	66	ASP
2	B	70	ILE
2	B	89	GLU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	128	LEU
2	B	135	ARG
2	B	136	THR
2	B	175	ARG
2	B	185	THR
2	B	194	GLU
2	B	199	MET
2	B	208	SER
2	B	217	ARG
2	B	218	SER
2	B	234	ILE
2	B	246	LYS
2	B	249	ARG
2	B	254	LEU
2	B	257	LYS
2	B	262	GLU
2	B	272	THR
2	B	273	LEU
2	B	277	LYS
2	B	278	GLN
2	B	292	ILE
2	B	296	GLU
2	B	311	LEU
2	B	315	LYS
2	B	322	PHE
2	B	325	GLN

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Mol	Chain	Res	Type
2	B	333	PHE
2	B	345	LYS
2	B	354	ASP
2	B	359	GLU
2	B	365	THR
2	B	366	GLN
2	B	367	LEU
2	B	371	GLU
2	B	376	PHE
2	B	382	ILE
2	B	384	ARG
2	B	396	ASP
2	B	398	ARG
2	B	405	ARG
2	B	408	LEU
2	B	416	LEU
2	B	418	LYS
2	B	436	VAL
2	B	437	GLU
2	B	454	THR
2	B	465	ASN
2	B	469	GLN
2	B	476	ARG
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	500	THR
2	B	516	ASN
2	B	521	LEU
2	B	526	GLU
2	B	531	GLN
2	B	556	THR
2	B	572	HIS
2	B	591	ARG
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	612	GLU
2	B	620	ARG
2	B	633	VAL
2	B	642	ASP
2	B	646	LEU

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Mol	Chain	Res	Type
2	B	655	LYS
2	B	708	GLU
2	B	709	ASP
2	B	711	GLU
2	B	714	GLU
2	B	730	ARG
2	B	733	HIS
2	B	743	ILE
2	B	751	VAL
2	B	762	ASN
2	B	766	ARG
2	B	773	MET
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	791	THR
2	B	792	MET
2	B	796	LEU
2	B	807	ARG
2	B	812	LEU
2	B	815	ARG
2	B	838	SER
2	B	841	MET
2	B	860	MET
2	B	864	LYS
2	B	868	MET
2	B	875	GLU
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	886	LYS
2	B	942	ARG
2	B	951	GLN
2	B	954	VAL
2	B	961	LEU
2	B	963	PHE
2	B	964	VAL
2	B	967	ARG
2	B	975	GLN
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG

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Mol	Chain	Res	Type
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1010	LEU
2	B	1028	GLU
2	B	1049	ASP
2	B	1057	LYS
2	B	1065	GLN
2	B	1066	SER
2	B	1077	THR
2	B	1092	TYR
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1122	ARG
2	B	1133	MET
2	B	1137	CYS
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1175	LEU
2	B	1178	ASN
2	B	1188	LYS
2	B	1190	ASP
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1215	ARG
2	B	1224	PHE
3	C	9	LYS
3	C	17	ASN
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP

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Mol	Chain	Res	Type
3	C	36	VAL
3	C	43	THR
3	C	48	SER
3	C	69	LEU
3	C	72	LEU
3	C	75	MET
3	C	77	ILE
3	C	85	ASP
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	115	SER
3	C	116	LYS
3	C	129	ILE
3	C	133	ILE
3	C	136	ASP
3	C	137	LYS
3	C	140	ASN
3	C	142	VAL
3	C	148	ARG
3	C	149	LYS
3	C	151	GLN
3	C	152	GLU
3	C	156	THR
3	C	188	HIS
3	C	195	GLN
3	C	203	GLN
3	C	205	LYS
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	263	THR
3	C	265	MET
4	E	3	GLN
4	E	8	ASN
4	E	52	ARG
4	E	54	GLN
4	E	57	MET

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Mol	Chain	Res	Type
4	E	75	MET
4	E	77	SER
4	E	78	LEU
4	E	80	VAL
4	E	84	ASP
4	E	85	GLU
4	E	92	THR
4	E	98	ILE
4	E	107	THR
4	E	115	ASN
4	E	137	GLU
4	E	142	VAL
4	E	146	HIS
4	E	156	LEU
4	E	159	ASP
4	E	165	LEU
4	E	169	ARG
4	E	200	ARG
5	F	76	LYS
5	F	82	THR
5	F	92	ARG
5	F	99	LEU
5	F	103	MET
5	F	104	ASN
5	F	110	ASP
5	F	112	GLU
5	F	118	LEU
5	F	119	ARG
5	F	122	MET
5	F	127	GLU
5	F	133	VAL
5	F	138	LEU
5	F	149	GLU
6	H	3	ASN
6	H	26	ILE
6	H	27	GLU
6	H	35	GLN
6	H	44	VAL
6	H	55	LEU
6	H	63	LEU
6	H	87	ARG
6	H	92	ASP

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Mol	Chain	Res	Type
6	H	94	ASP
6	H	95	TYR
6	H	96	VAL
6	H	105	GLU
6	H	107	VAL
6	H	108	SER
6	H	111	LEU
6	H	123	MET
6	H	130	ARG
6	H	132	LEU
6	H	136	LYS
6	H	138	GLU
7	I	17	ARG
7	I	20	LYS
7	I	21	GLU
7	I	28	GLU
7	I	35	VAL
7	I	37	GLU
7	I	42	LEU
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	61	ASP
7	I	62	ILE
7	I	70	ARG
7	I	84	VAL
7	I	87	GLN
7	I	90	GLN
7	I	95	THR
7	I	98	VAL
7	I	104	LEU
7	I	117	LYS
7	I	118	ARG
7	I	120	GLN
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	26	GLN
8	J	28	ASP

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Mol	Chain	Res	Type
8	J	30	LEU
8	J	31	ASP
8	J	43	ARG
8	J	48	ARG
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	8	GLU
9	K	20	LYS
9	K	21	ILE
9	K	22	ASP
9	K	29	ASN
9	K	33	ILE
9	K	50	LEU
9	K	77	THR
9	K	78	THR
9	K	81	TYR
9	K	84	LYS
9	K	95	ILE
9	K	108	GLU
9	K	111	LEU
9	K	114	LEU
10	L	27	LEU
10	L	33	GLU
10	L	38	LEU
10	L	39	SER
10	L	42	ARG
10	L	44	ASP
10	L	50	ASP
10	L	55	ILE
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	64	LEU
10	L	65	VAL
10	L	66	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN

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Mol	Chain	Res	Type
1	A	18	GLN
1	A	83	HIS
1	A	225	ASN
1	A	297	GLN
1	A	339	ASN
1	A	425	GLN
1	A	451	HIS
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	587	HIS
1	A	626	ASN
1	A	631	HIS
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	877	HIS
1	A	906	HIS
1	A	965	GLN
1	A	969	GLN
1	A	1004	ASN
1	A	1009	ASN
1	A	1033	GLN
1	A	1140	HIS
1	A	1203	ASN
1	A	1265	ASN
1	A	1364	ASN
2	B	46	GLN
2	B	53	GLN
2	B	103	ASN
2	B	366	GLN
2	B	383	ASN
2	B	499	ASN
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN

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Mol	Chain	Res	Type
2	B	763	GLN
2	B	776	GLN
2	B	835	GLN
2	B	887	HIS
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1097	HIS
2	B	1161	HIS
2	B	1195	HIS
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
4	E	147	HIS
6	H	11	GLN
6	H	83	GLN
6	H	133	ASN
6	H	134	ASN
7	I	60	GLN
7	I	108	HIS
8	J	23	ASN
9	K	65	HIS
9	K	76	GLN
9	K	89	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
15	ATP	A	1736	13	26,33,33	1.25	3 (11%)	31,52,52	1.50	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
15	ATP	A	1736	13	-	7/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1736	ATP	C2-N3	3.49	1.37	1.32
15	A	1736	ATP	C2-N1	2.33	1.38	1.33
15	A	1736	ATP	PB-O1B	2.30	1.59	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1736	ATP	O3'-C3'-C2'	3.28	122.43	111.82
15	A	1736	ATP	O4'-C1'-C2'	-3.25	102.18	106.93
15	A	1736	ATP	O3'-C3'-C4'	2.47	118.19	111.05
15	A	1736	ATP	O3G-PG-O3B	2.43	112.78	104.64
15	A	1736	ATP	C4-C5-N7	2.38	111.88	109.40
15	A	1736	ATP	C1'-N9-C4	-2.06	123.01	126.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	1736	ATP	PB-O3B-PG-O3G
15	A	1736	ATP	PB-O3B-PG-O2G
15	A	1736	ATP	C5'-O5'-PA-O3A
15	A	1736	ATP	C4'-C5'-O5'-PA
15	A	1736	ATP	C5'-O5'-PA-O1A
15	A	1736	ATP	PB-O3B-PG-O1G
15	A	1736	ATP	O4'-C4'-C5'-O5'

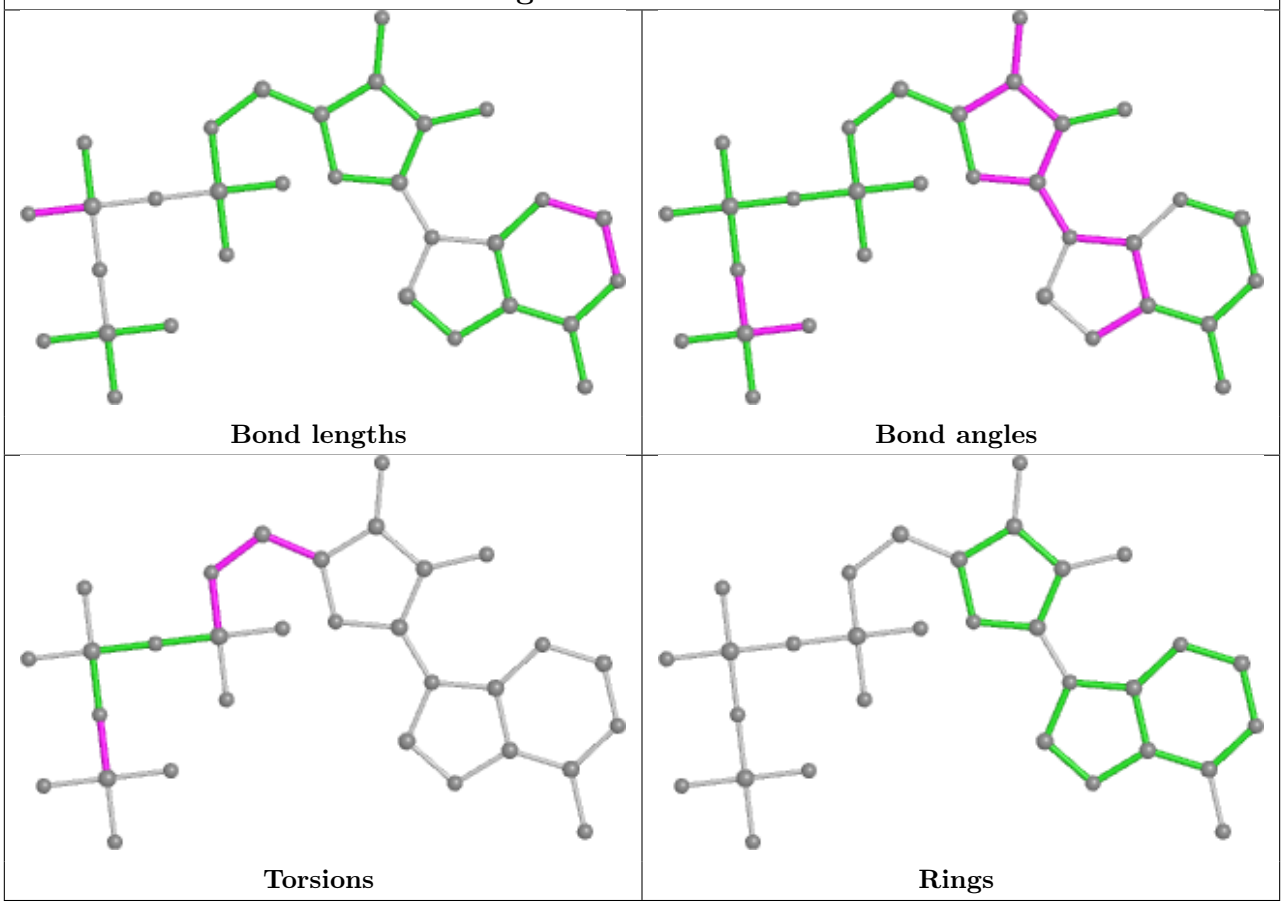
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1736	ATP	5	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 ATP A 1736



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	1405/1733 (81%)	0.06	82 (5%) 23 22	78, 133, 223, 254	0
2	B	1114/1224 (91%)	-0.05	48 (4%) 35 34	71, 115, 183, 241	0
3	C	266/318 (83%)	-0.23	1 (0%) 92 93	87, 113, 153, 215	0
4	E	214/215 (99%)	-0.06	5 (2%) 60 59	102, 159, 206, 216	0
5	F	85/155 (54%)	-0.15	0 100 100	109, 139, 178, 196	0
6	H	133/146 (91%)	0.35	11 (8%) 11 11	131, 172, 202, 222	0
7	I	119/122 (97%)	-0.16	1 (0%) 86 86	93, 138, 185, 200	0
8	J	65/70 (92%)	-0.18	0 100 100	81, 104, 136, 151	0
9	K	114/120 (95%)	-0.23	0 100 100	87, 123, 150, 175	0
10	L	46/70 (65%)	0.25	3 (6%) 18 18	99, 155, 188, 214	0
11	R	5/5 (100%)	0.27	0 100 100	148, 153, 180, 183	0
12	T	13/29 (44%)	1.33	4 (30%) 0 0	150, 170, 237, 245	0
All	All	3579/4207 (85%)	-0.01	155 (4%) 35 34	71, 128, 208, 254	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	8.7
2	B	1222	ARG	7.0
2	B	1224	PHE	6.8
1	A	1176	LEU	6.5
1	A	66	LYS	6.3
1	A	72	GLU	5.7
2	B	1221	SER	5.3
1	A	45	GLN	5.3
6	H	84	ALA	5.2
12	T	28	DT	4.8
2	B	866	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	4.7
2	B	1223	ASP	4.6
6	H	83	GLN	4.6
2	B	477	ALA	4.6
1	A	44	THR	4.5
1	A	319	GLY	4.3
2	B	919	SER	4.3
2	B	231	PRO	4.3
1	A	253	ASN	4.2
1	A	251	SER	4.2
1	A	318	SER	4.2
1	A	182	VAL	4.1
1	A	87	ALA	4.1
1	A	256	GLN	4.1
1	A	250	ILE	4.1
1	A	124	GLN	4.0
2	B	250	PHE	4.0
2	B	470	LYS	4.0
6	H	86	ASP	4.0
2	B	884	ARG	4.0
1	A	65	LEU	3.9
2	B	935	ARG	3.9
1	A	73	GLY	3.9
1	A	152	VAL	3.8
1	A	255	SER	3.8
2	B	471	LYS	3.8
1	A	252	PHE	3.8
2	B	135	ARG	3.8
10	L	50	ASP	3.7
2	B	1169	MET	3.7
2	B	1205	GLN	3.7
1	A	316	GLN	3.6
6	H	85	GLY	3.6
1	A	151	ASP	3.6
1	A	141	LEU	3.5
4	E	119	SER	3.5
1	A	1302	PRO	3.4
1	A	125	ALA	3.4
1	A	161	LEU	3.4
2	B	136	THR	3.4
2	B	645	SER	3.4
10	L	27	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	317	LYS	3.4
1	A	1085	HIS	3.3
12	T	25	DC	3.3
2	B	883	LEU	3.3
1	A	232	GLU	3.3
2	B	867	GLY	3.3
1	A	168	GLY	3.3
1	A	137	ALA	3.2
1	A	88	LYS	3.2
1	A	1093	LYS	3.2
1	A	6	TYR	3.1
1	A	149	GLU	3.1
2	B	1209	ALA	3.1
1	A	1002	GLY	3.0
1	A	282	ASN	3.0
1	A	176	LYS	2.9
4	E	90	VAL	2.9
1	A	257	ARG	2.9
2	B	474	SER	2.9
2	B	230	ALA	2.9
2	B	140	ILE	2.9
12	T	27	DA	2.8
2	B	472	ALA	2.8
2	B	1208	MET	2.8
1	A	199	LEU	2.8
2	B	708	GLU	2.8
2	B	865	LYS	2.8
1	A	254	GLU	2.7
10	L	38	LEU	2.7
1	A	1391	ARG	2.7
2	B	868	MET	2.7
1	A	183	GLY	2.7
1	A	41	MET	2.7
12	T	24	DT	2.7
2	B	478	GLY	2.7
6	H	130	ARG	2.6
4	E	2	ASP	2.6
1	A	136	ALA	2.6
1	A	320	ARG	2.6
1	A	8	SER	2.6
2	B	918	ILE	2.6
2	B	933	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	1219	ASP	2.6
2	B	1220	ARG	2.5
3	C	217	ASP	2.5
6	H	108	SER	2.5
2	B	141	ASP	2.5
1	A	3	GLY	2.5
1	A	116	ASP	2.5
2	B	249	ARG	2.5
1	A	62	ASP	2.5
2	B	476	ARG	2.5
4	E	118	PRO	2.5
1	A	1300	LYS	2.5
1	A	60	SER	2.5
2	B	709	ASP	2.5
1	A	286	HIS	2.5
1	A	201	VAL	2.4
6	H	117	SER	2.4
2	B	870	ILE	2.4
6	H	105	GLU	2.4
2	B	1175	LEU	2.4
6	H	111	LEU	2.4
1	A	147	VAL	2.4
1	A	163	SER	2.4
1	A	975	HIS	2.4
1	A	120	GLU	2.3
1	A	81	PHE	2.3
1	A	980	ASP	2.3
2	B	89	GLU	2.3
1	A	167	CYS	2.3
1	A	212	LYS	2.3
1	A	5	GLN	2.3
1	A	150	THR	2.3
1	A	153	PRO	2.3
1	A	1123	GLY	2.3
2	B	1210	MET	2.3
2	B	666	TYR	2.3
2	B	247	GLY	2.2
1	A	200	ARG	2.2
1	A	173	THR	2.2
2	B	139	ALA	2.2
1	A	64	ASN	2.2
1	A	164	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	433	GLN	2.2
1	A	705	LYS	2.2
1	A	162	VAL	2.2
1	A	75	ASN	2.2
1	A	186	LYS	2.2
1	A	127	ALA	2.1
2	B	713	ALA	2.1
6	H	19	ARG	2.1
1	A	292	ALA	2.1
1	A	92	HIS	2.1
1	A	4	GLN	2.1
4	E	121	MET	2.0
1	A	707	GLY	2.0
6	H	123	MET	2.0
7	I	50	THR	2.0
1	A	213	HIS	2.0
1	A	105	CYS	2.0
2	B	106	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ZN	A	1734	1/1	0.24	0.15	300,300,300,300	0
14	ZN	B	1307	1/1	0.82	0.10	221,221,221,221	0
15	ATP	A	1736	31/31	0.88	0.23	162,165,195,197	0
13	MG	A	2002	1/1	0.91	0.14	131,131,131,131	0
13	MG	A	2001	1/1	0.92	0.04	102,102,102,102	0

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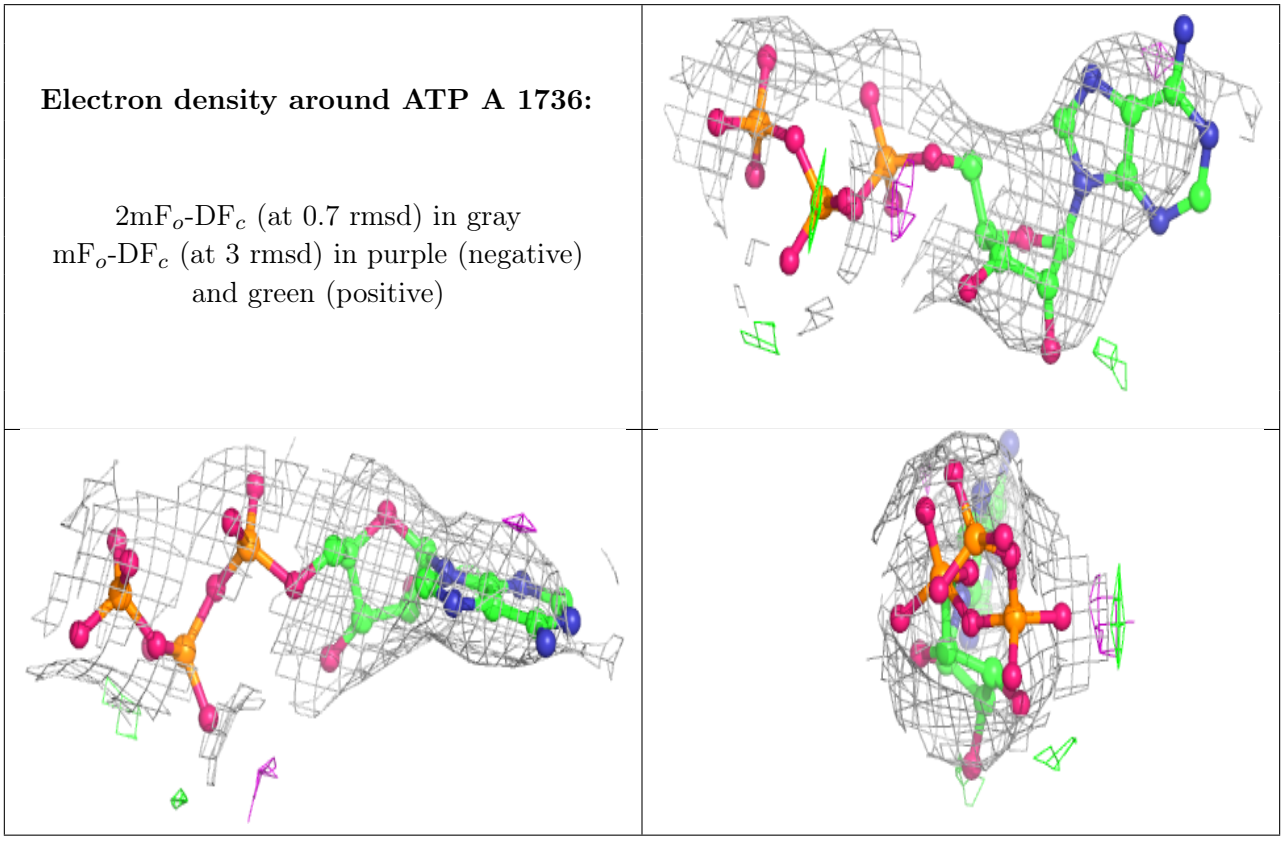
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ZN	A	1735	1/1	0.94	0.15	198,198,198,198	0
14	ZN	L	105	1/1	0.97	0.03	142,142,142,142	0
14	ZN	I	203	1/1	0.98	0.08	134,134,134,134	0
14	ZN	J	101	1/1	0.98	0.20	102,102,102,102	0
14	ZN	I	204	1/1	0.99	0.07	112,112,112,112	0
14	ZN	C	319	1/1	0.99	0.09	113,113,113,113	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 ATP A 1736:

$2mF_o$-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.