Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 PM GMT

PDB ID	:	3S15
Title	:	RNA Polymerase II Initiation Complex with a 7-nt RNA
Authors	:	Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on	:	2011-05-14
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
http://wwpdb.org/validation/2016/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:

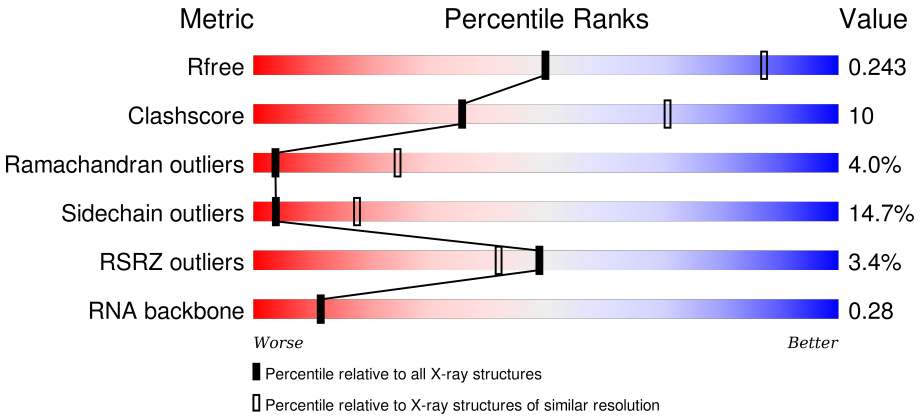
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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

Mol	Chain	Length	Quality of chain
1	A	1733	4% 54% 23% 19%
2	B	1224	3% 59% 26% 5% 9%
3	C	318	56% 25% 16%
4	E	215	9% 70% 26%

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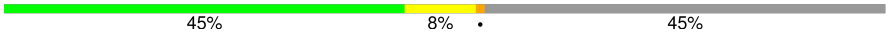
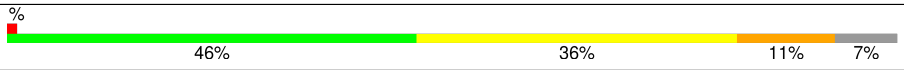
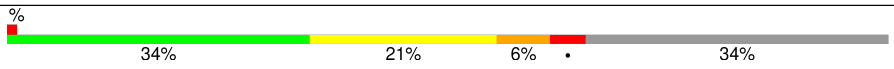
Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	7	
12	T	29	

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
14	MG	B	2002[B]	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28717 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(*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	7	Total	C	N	O	P	0	0	0
			153	69	33	45	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

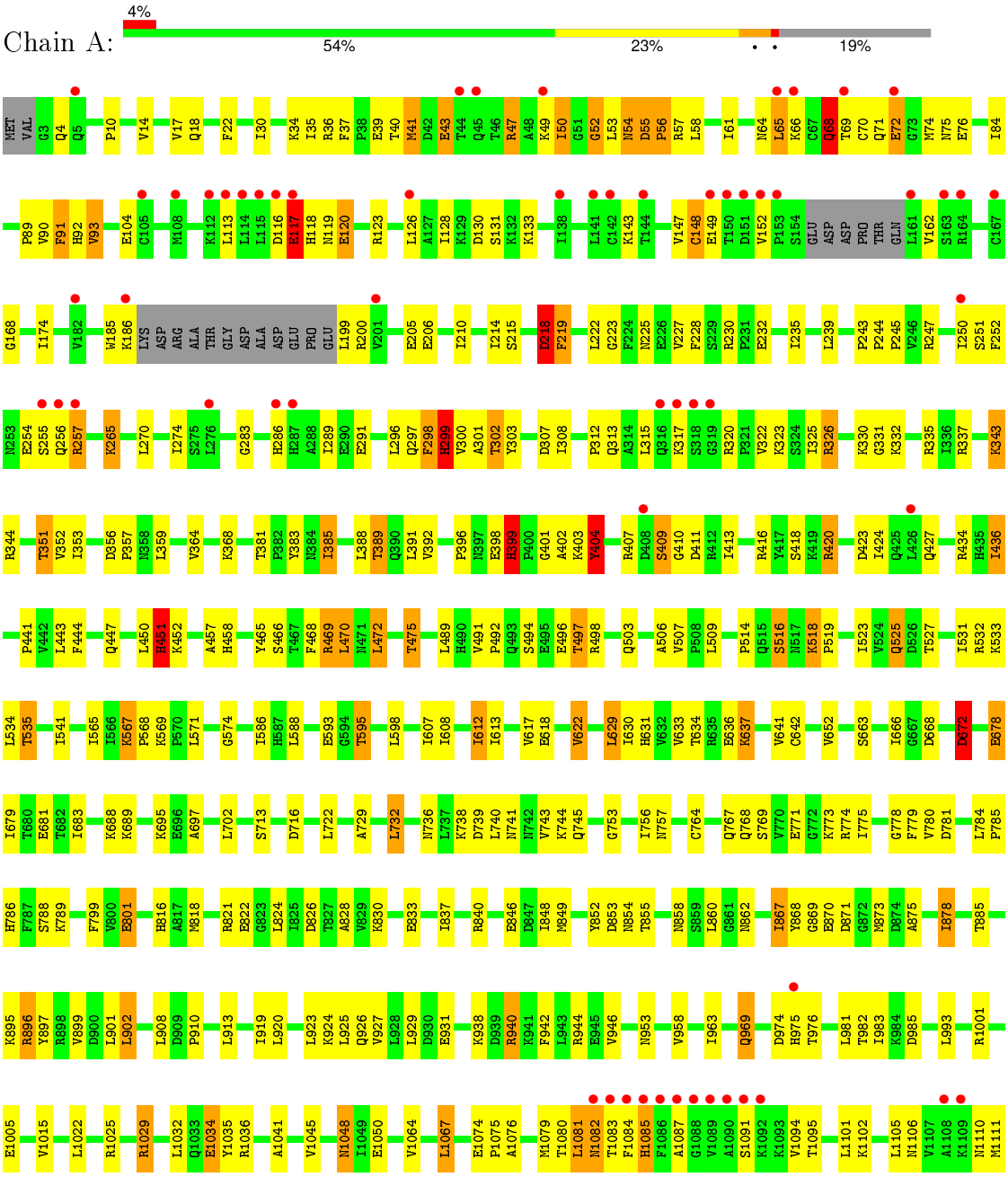
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total Mg 2 2	0	1
14	A	1	Total Mg 1 1	0	0

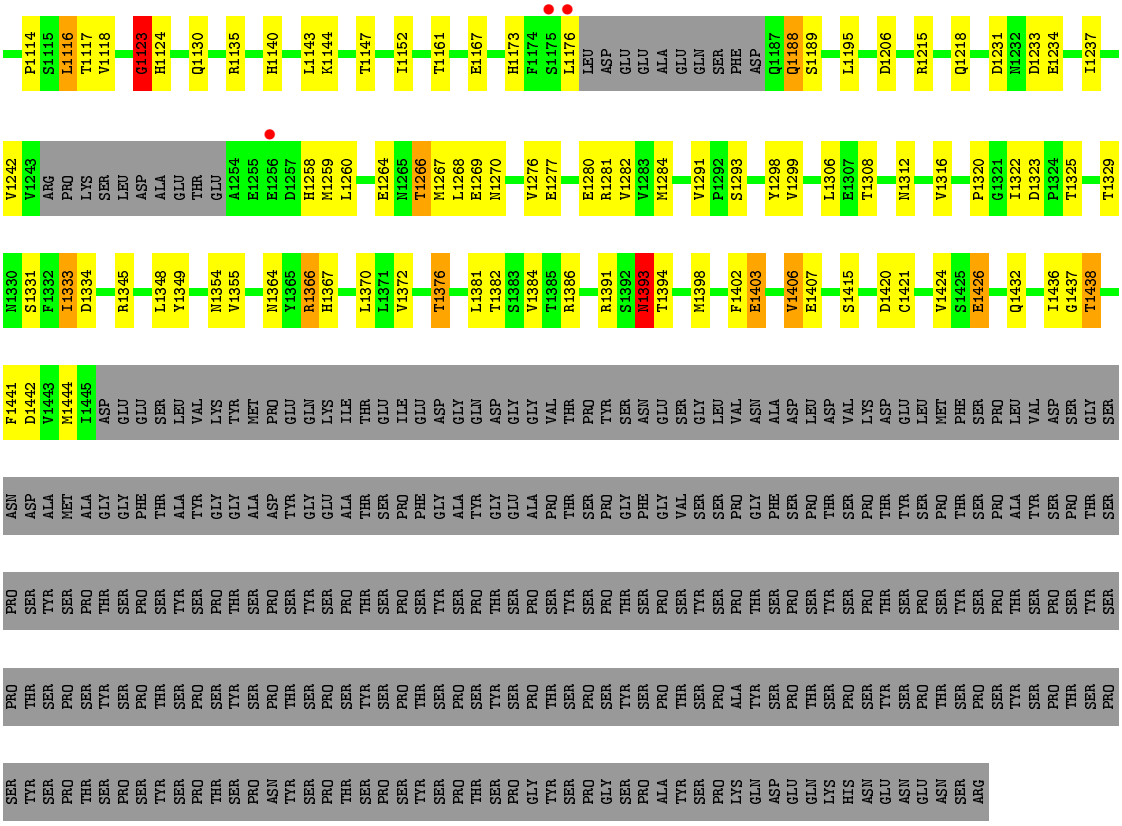
3 Residue-property plots (i)

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

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

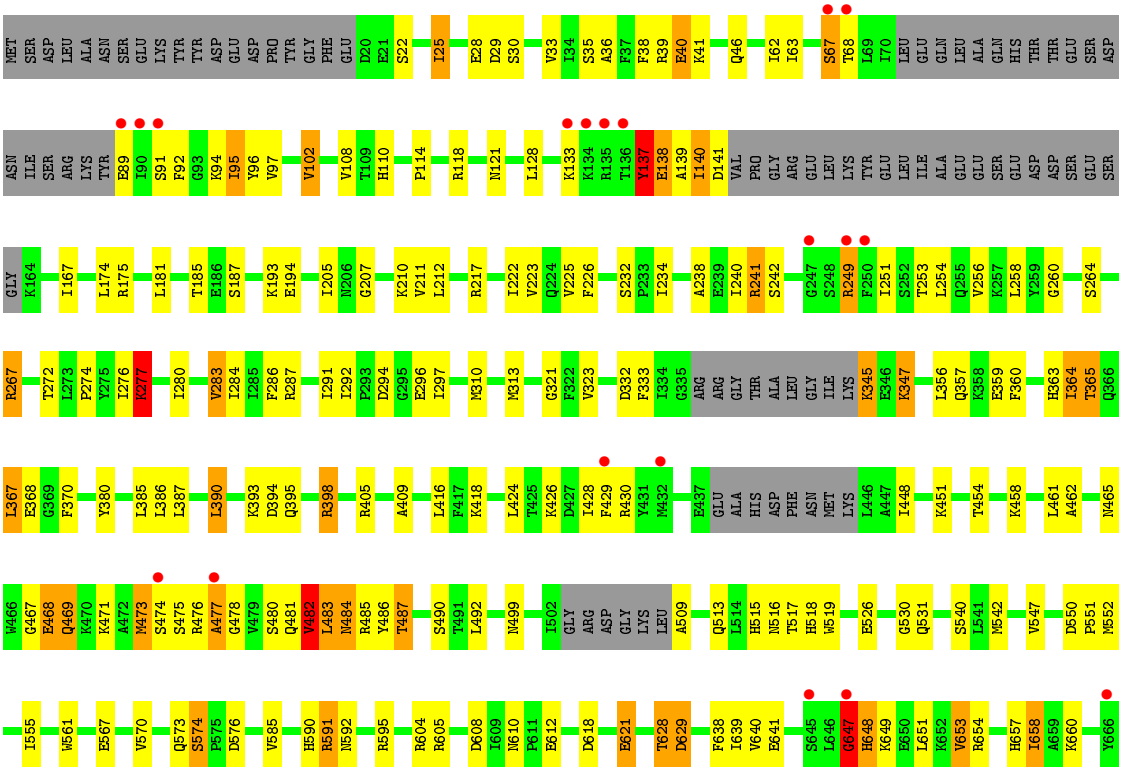
Chain A:

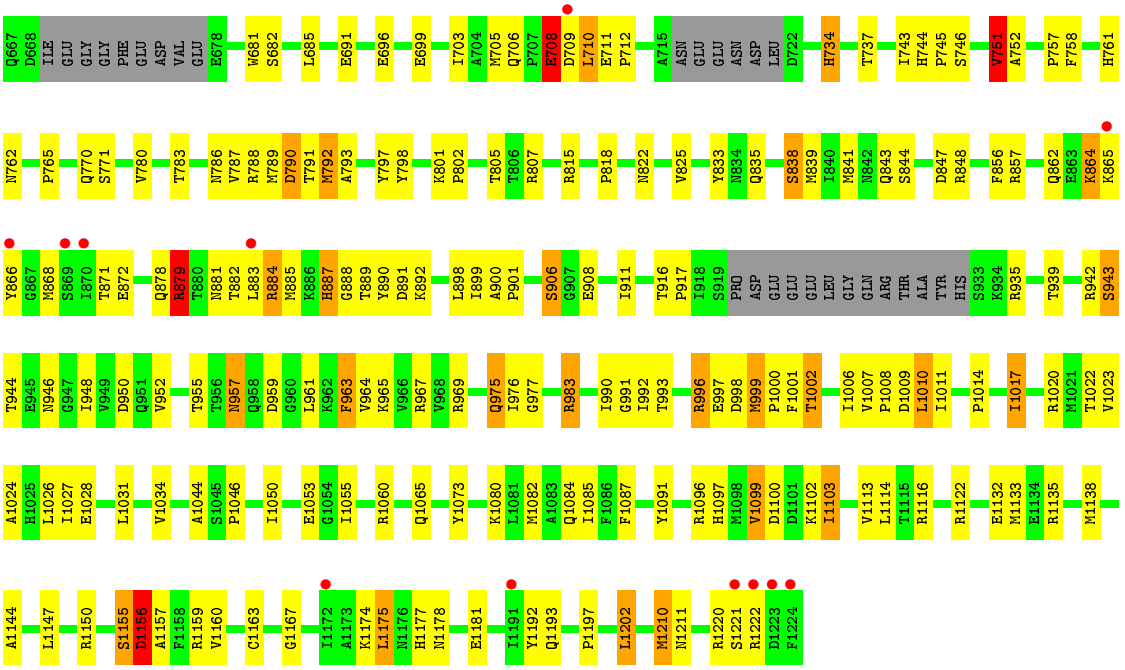




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

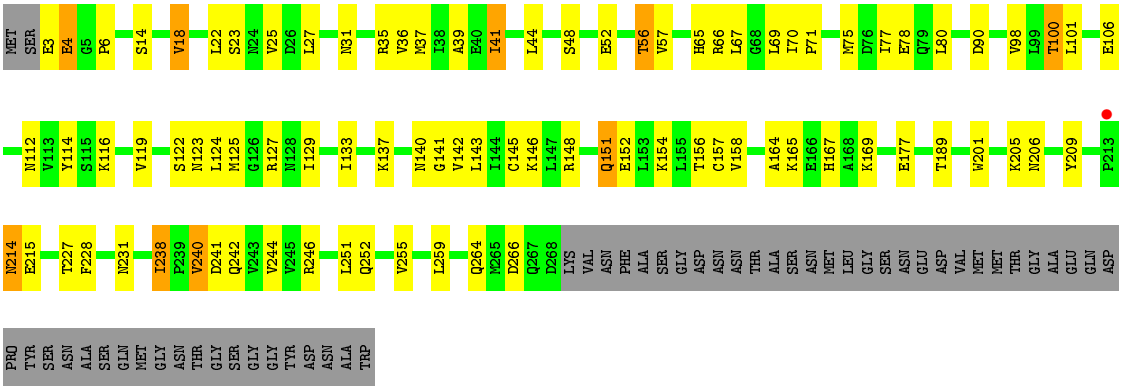
Chain B:





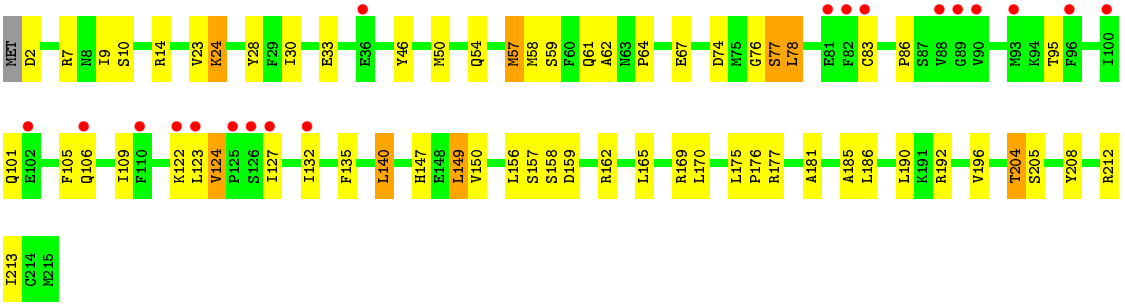
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



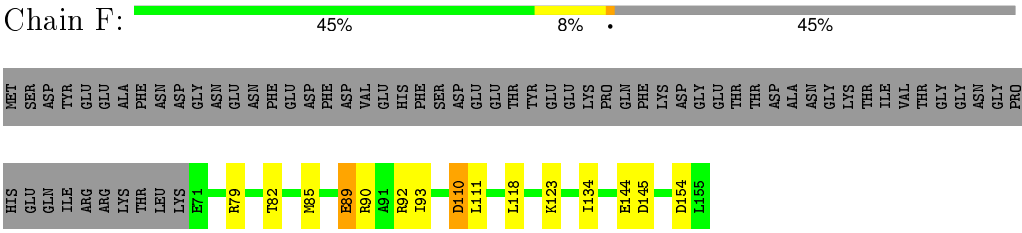
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



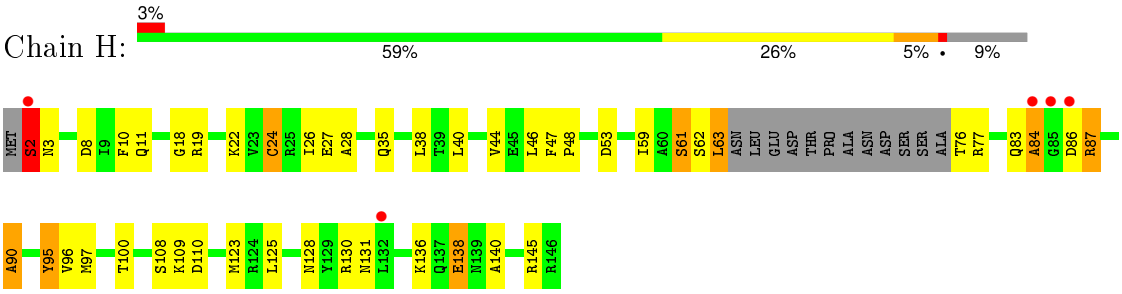
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



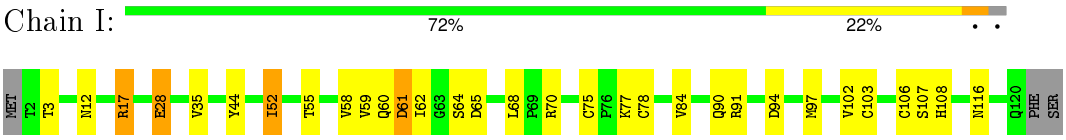
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



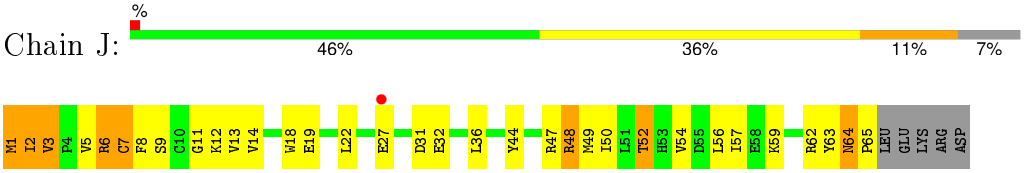
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



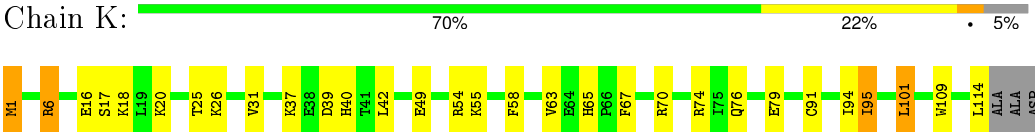
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



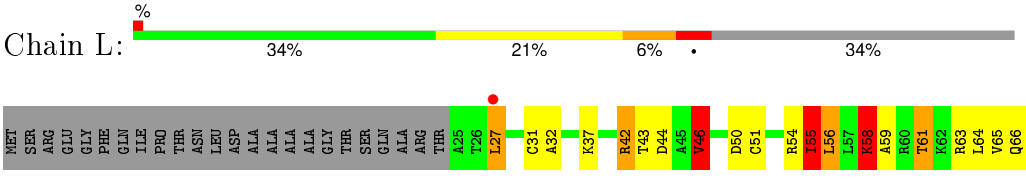
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:



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

Chain L:



• Molecule 11: RNA (5'-R(*CP*GP*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	167.93Å 220.89Å 194.62Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	44.11 – 3.30 44.11 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.11-3.30) 99.8 (44.11-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.174 , 0.228 0.191 , 0.243	Depositor DCC
R_{free} test set	5222 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 104.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 104927 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28717	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.82	6/15199 (0.0%)
2	B	0.54	0/9033	0.84	7/12181 (0.1%)
3	C	0.48	0/2133	0.81	0/2891
4	E	0.45	0/1788	0.71	0/2406
5	F	0.50	0/700	0.70	0/945
6	H	0.47	0/1086	0.83	2/1470 (0.1%)
7	I	0.50	0/989	0.84	0/1331
8	J	0.56	0/541	0.90	1/727 (0.1%)
9	K	0.45	0/937	0.71	0/1265
10	L	0.56	0/365	1.03	1/485 (0.2%)
11	R	0.88	0/172	1.62	3/268 (1.1%)
12	T	1.20	0/290	2.48	30/444 (6.8%)
All	All	0.53	0/29275	0.86	50/39612 (0.1%)

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
2	B	0	1

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	16	DC	P-O3'-C3'	11.73	133.77	119.70
12	T	21	DC	O4'-C4'-C3'	-9.95	100.03	106.00
12	T	26	DG	P-O3'-C3'	9.52	131.12	119.70
12	T	20	DC	O4'-C4'-C3'	-8.84	100.69	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	19	DT	O4'-C4'-C3'	-8.80	100.72	106.00
2	B	647	GLY	C-N-CA	8.78	143.64	121.70
12	T	21	DC	C4'-C3'-C2'	-8.74	95.23	103.10
12	T	22	DT	O4'-C4'-C3'	-8.38	100.97	106.00
12	T	19	DT	C4'-C3'-C2'	-7.72	96.15	103.10
12	T	20	DC	O4'-C1'-N1	7.60	113.32	108.00
12	T	22	DT	C4'-C3'-C2'	-7.38	96.46	103.10
1	A	218	ASP	C-N-CA	7.35	140.07	121.70
12	T	27	DA	C1'-O4'-C4'	-7.28	102.82	110.10
2	B	648	HIS	N-CA-CB	7.00	123.20	110.60
12	T	23	DC	O4'-C4'-C3'	-6.96	101.72	104.50
12	T	20	DC	C4'-C3'-C2'	-6.86	96.92	103.10
12	T	19	DT	C4-C5-C7	6.82	123.09	119.00
12	T	16	DC	N1-C2-O2	6.71	122.92	118.90
12	T	16	DC	C2-N1-C1'	6.65	126.11	118.80
12	T	22	DT	C4-C5-C7	6.60	122.96	119.00
12	T	27	DA	O4'-C1'-N9	6.58	112.61	108.00
12	T	24	DT	O4'-C1'-N1	6.54	112.58	108.00
12	T	21	DC	O4'-C1'-N1	6.32	112.42	108.00
12	T	22	DT	C6-C5-C7	-6.23	119.16	122.90
1	A	298	PHE	C-N-CA	6.03	136.78	121.70
6	H	2	SER	C-N-CA	5.99	136.66	121.70
2	B	628	THR	C-N-CA	5.98	136.65	121.70
12	T	23	DC	O4'-C1'-N1	5.88	112.11	108.00
2	B	1156	ASP	N-CA-C	5.85	126.80	111.00
12	T	24	DT	C6-C5-C7	-5.77	119.44	122.90
1	A	117	GLU	C-N-CA	5.72	136.00	121.70
12	T	24	DT	C4-C5-C7	5.68	122.41	119.00
11	R	4	C	O4'-C1'-N1	5.67	112.74	108.20
1	A	451	HIS	CB-CA-C	-5.67	99.07	110.40
10	L	58	LYS	N-CA-C	5.62	126.18	111.00
2	B	1155	SER	C-N-CA	5.55	135.57	121.70
1	A	399	HIS	N-CA-CB	5.53	120.55	110.60
11	R	10	G	O4'-C1'-N9	5.53	112.62	108.20
11	R	9	G	P-O3'-C3'	-5.52	113.07	119.70
2	B	345	LYS	C-N-CA	5.51	135.47	121.70
6	H	61	SER	C-N-CA	5.43	135.28	121.70
12	T	20	DC	P-O3'-C3'	5.41	126.20	119.70
12	T	16	DC	C5-C6-N1	5.39	123.69	121.00
12	T	19	DT	C6-C5-C7	-5.33	119.70	122.90
2	B	140	ILE	C-N-CA	5.32	134.99	121.70
12	T	23	DC	N1-C2-O2	5.25	122.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	16	DC	C6-N1-C2	-5.23	118.21	120.30
1	A	1123	GLY	C-N-CA	5.11	134.47	121.70
12	T	27	DA	P-O3'-C3'	5.09	125.81	119.70
8	J	5	VAL	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	647	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	237	0
2	B	8861	0	8884	214	0
3	C	2095	0	2051	48	0
4	E	1752	0	1776	27	0
5	F	688	0	707	8	0
6	H	1068	0	1040	27	0
7	I	971	0	927	10	0
8	J	532	0	542	26	0
9	K	919	0	929	17	0
10	L	363	0	386	13	0
11	R	153	0	78	0	0
12	T	261	0	148	5	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
All	All	28717	0	28601	554	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 10.

All (554) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.77	1.60
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.42	1.01
1:A:494:SER:HB3	1:A:497:THR:HB	1.45	0.98
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.97	0.97
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.46	0.94
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.15	0.93
1:A:535:THR:HG21	1:A:617:VAL:H	1.32	0.92
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.54	0.88
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.03	0.86
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.58	0.86
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.59	0.84
2:B:706:GLN:O	2:B:710:LEU:HB2	1.78	0.84
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.60	0.84
2:B:654:ARG:H	2:B:657:HIS:HD2	1.25	0.83
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.61	0.82
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.61	0.81
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.46	0.80
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.64	0.79
3:C:167:HIS:HD2	3:C:169:LYS:H	1.28	0.79
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.47	0.78
1:A:869:GLY:O	4:E:204:THR:HG21	1.84	0.77
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.68	0.76
1:A:1329:THR:HG22	1:A:1331:SER:H	1.49	0.75
2:B:1050:ILE:HG23	2:B:1055:ILE:HD11	1.67	0.75
4:E:77:SER:HB3	4:E:105:PHE:HA	1.68	0.75
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.67	0.74
8:J:1:MET:N	8:J:57:ILE:H	1.85	0.74
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.52	0.74
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.53	0.74
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.17	0.74
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.69	0.73
1:A:535:THR:HG21	1:A:617:VAL:N	2.04	0.73
2:B:906:SER:HA	2:B:946:ASN:HB3	1.70	0.73
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.71	0.73
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.69	0.72
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.72	0.72
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.23	0.71
1:A:535:THR:CG2	1:A:617:VAL:H	2.03	0.71
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.73	0.71
1:A:565:ILE:CG2	1:A:567:LYS:HE3	2.20	0.71
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.19	0.70
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.56	0.70
2:B:744:HIS:HD2	2:B:746:SER:H	1.40	0.70
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.57	0.69
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.73	0.69
1:A:43:GLU:HG3	1:A:50:ILE:HG12	1.75	0.69
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.73	0.69
1:A:924:LYS:O	1:A:927:VAL:HG12	1.93	0.68
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.24	0.68
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.76	0.67
2:B:428:ILE:HD11	2:B:448:ILE:HA	1.76	0.67
3:C:56:THR:HG21	3:C:145:CYS:SG	2.34	0.66
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.23	0.66
2:B:843:GLN:HB2	2:B:993:THR:HB	1.78	0.65
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.77	0.65
1:A:1091:SER:HB2	1:A:1281:ARG:HH12	1.61	0.65
1:A:567:LYS:HB3	6:H:96:VAL:H	1.60	0.65
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.10	0.64
3:C:167:HIS:CD2	3:C:169:LYS:H	2.14	0.64
2:B:345:LYS:HA	2:B:347:LYS:H	1.62	0.64
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.30	0.64
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.80	0.64
2:B:91:SER:HB3	2:B:133:LYS:HB2	1.80	0.64
1:A:741:ASN:HD22	1:A:744:LYS:H	1.44	0.64
6:H:2:SER:N	6:H:61:SER:HG	1.96	0.63
1:A:219:PHE:HZ	1:A:230:ARG:HG2	1.63	0.63
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.28	0.63
2:B:864:LYS:HB3	2:B:872:GLU:H	1.62	0.63
2:B:900:ALA:HA	10:L:58:LYS:HD3	1.81	0.63
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.92	0.63
6:H:100:THR:HG23	6:H:138:GLU:HA	1.79	0.63
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.93	0.63
2:B:40:GLU:HG2	2:B:681:TRP:HB3	1.81	0.63
9:K:91:CYS:O	9:K:95:ILE:HG12	1.99	0.63
2:B:516:ASN:HD22	2:B:516:ASN:H	1.48	0.62
2:B:618:ASP:OD2	2:B:621:GLU:HB2	1.99	0.62
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:ARG:O	2:B:478:GLY:N	2.31	0.62
6:H:24:CYS:HB2	6:H:44:VAL:HG21	1.80	0.62
2:B:137:TYR:H	2:B:137:TYR:HD2	1.47	0.62
3:C:100:THR:HG22	3:C:119:VAL:HG13	1.81	0.62
2:B:906:SER:HA	2:B:946:ASN:CB	2.29	0.61
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.33	0.61
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.82	0.61
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.00	0.61
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.83	0.61
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.83	0.60
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.82	0.60
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.82	0.60
3:C:98:VAL:H	3:C:122:SER:HB2	1.65	0.60
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.82	0.60
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.83	0.60
1:A:41:MET:HB2	1:A:49:LYS:HA	1.82	0.60
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.61	0.60
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.83	0.60
2:B:801:LYS:O	8:J:52:THR:CG2	2.49	0.60
1:A:518:LYS:HA	1:A:631:HIS:CD2	2.36	0.60
8:J:1:MET:H2	8:J:57:ILE:H	1.47	0.60
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.84	0.60
3:C:165:LYS:O	9:K:6:ARG:NH1	2.34	0.60
2:B:241:ARG:HG3	2:B:253:THR:HG22	1.82	0.60
1:A:364:VAL:HG12	1:A:458:HIS:HB3	1.83	0.60
1:A:152:VAL:HG23	1:A:162:VAL:HB	1.84	0.60
2:B:542:MET:HE1	2:B:743:ILE:HG13	1.84	0.59
2:B:249:ARG:HH11	2:B:251:ILE:HD11	1.66	0.59
1:A:117:GLU:H	1:A:118:HIS:CB	2.15	0.59
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.66	0.59
1:A:666:ILE:HD13	2:B:1026:LEU:HB2	1.84	0.59
1:A:913:LEU:HD11	1:A:981:LEU:O	2.02	0.59
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.68	0.59
1:A:34:LYS:HD3	1:A:36:ARG:HH21	1.67	0.59
1:A:225:ASN:HD22	1:A:228:PHE:H	1.49	0.59
2:B:515:HIS:HD2	2:B:517:THR:H	1.51	0.58
1:A:860:LEU:HD21	1:A:1394:THR:HA	1.85	0.58
2:B:879:ARG:O	2:B:882:THR:HG22	2.03	0.58
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.84	0.58
1:A:55:ASP:O	1:A:57:ARG:N	2.37	0.58
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:CD2	2:B:517:THR:H	2.22	0.58
1:A:351:THR:HG21	1:A:466:SER:O	2.03	0.58
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.85	0.58
2:B:835:GLN:O	2:B:838:SER:HB2	2.04	0.58
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.69	0.58
1:A:218:ASP:H	1:A:219:PHE:HB3	1.69	0.57
2:B:482:VAL:HG11	12:T:26:DG:H5"	1.86	0.57
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.85	0.57
1:A:567:LYS:HB3	6:H:96:VAL:N	2.19	0.57
1:A:299:HIS:O	1:A:301:ALA:N	2.37	0.57
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.70	0.57
2:B:38:PHE:H	2:B:41:LYS:HB2	1.69	0.57
3:C:123:ASN:ND2	3:C:125:MET:HG3	2.19	0.57
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.86	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.56
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.87	0.56
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.40	0.56
7:I:17:ARG:HB2	7:I:28:GLU:HG2	1.86	0.56
2:B:211:VAL:O	2:B:480:SER:HA	2.04	0.56
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.87	0.56
1:A:982:THR:HB	1:A:985:ASP:H	1.70	0.56
3:C:71:PRO:HB2	3:C:133:ILE:HB	1.85	0.56
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.37	0.56
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.88	0.56
1:A:75:ASN:HA	2:B:1116:ARG:NH1	2.21	0.56
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.69	0.56
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.88	0.55
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.36	0.55
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.86	0.55
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.53	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.35	0.55
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.89	0.55
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.88	0.55
10:L:31:CYS:HA	10:L:56:LEU:HD23	1.88	0.55
2:B:102:VAL:HG23	2:B:110:HIS:HB3	1.87	0.55
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.87	0.55
3:C:37:MET:HA	3:C:41:ILE:HD11	1.89	0.55
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.87	0.55
2:B:35:SER:O	2:B:39:ARG:HB2	2.07	0.55
1:A:567:LYS:CB	1:A:568:PRO:CD	2.82	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:GLN:H	2:B:710:LEU:HG	1.72	0.55
4:E:64:PRO:HD3	4:E:76:GLY:HA2	1.89	0.55
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	1.89	0.54
2:B:140:ILE:HB	2:B:141:ASP:HB2	1.89	0.54
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.41	0.54
3:C:167:HIS:HD2	3:C:169:LYS:N	2.03	0.54
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.07	0.54
1:A:516:SER:HB3	1:A:518:LYS:HG2	1.89	0.54
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.42	0.54
1:A:523:ILE:HG23	1:A:527:THR:HG22	1.90	0.54
2:B:879:ARG:CZ	2:B:879:ARG:HA	2.38	0.54
1:A:57:ARG:HB3	1:A:68:GLN:HG2	1.89	0.54
3:C:14:SER:HA	9:K:114:LEU:HD23	1.89	0.54
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.89	0.54
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.89	0.54
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.73	0.54
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.89	0.54
1:A:519:PRO:HD3	1:A:631:HIS:HD2	1.72	0.54
2:B:94:LYS:HG2	2:B:96:TYR:CZ	2.43	0.53
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.90	0.53
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.90	0.53
4:E:165:LEU:HD13	4:E:170:LEU:HB2	1.91	0.53
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.09	0.53
1:A:982:THR:H	1:A:985:ASP:HB2	1.73	0.53
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.91	0.53
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.90	0.53
5:F:85:MET:HG3	5:F:89:GLU:HB3	1.91	0.53
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.42	0.53
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.43	0.53
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.38	0.52
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.91	0.52
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.90	0.52
4:E:124:VAL:HG13	4:E:132:ILE:HG13	1.91	0.52
1:A:567:LYS:CB	6:H:96:VAL:H	2.23	0.52
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.25	0.52
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.92	0.52
1:A:117:GLU:H	1:A:118:HIS:HB2	1.75	0.52
2:B:97:VAL:HG22	2:B:128:LEU:HD23	1.91	0.52
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.91	0.52
1:A:567:LYS:HG2	6:H:96:VAL:H	1.74	0.51
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.91	0.51
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.57	0.51
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.93	0.51
1:A:1393:ASN:HD22	1:A:1393:ASN:H	1.58	0.51
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.26	0.51
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.91	0.51
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.92	0.51
2:B:975:GLN:O	2:B:990:ILE:HD12	2.11	0.51
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.50	0.51
1:A:534:LEU:O	1:A:574:GLY:HA3	2.11	0.51
1:A:781:ASP:HB2	1:A:789:LYS:HD3	1.92	0.51
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.92	0.51
8:J:1:MET:H1	8:J:57:ILE:H	1.58	0.51
2:B:957:ASN:HD21	2:B:959:ASP:HB2	1.75	0.51
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.40	0.51
3:C:31:ASN:O	3:C:35:ARG:HG3	2.09	0.51
3:C:57:VAL:HG11	8:J:57:ILE:HD12	1.93	0.51
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.93	0.51
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.93	0.51
1:A:678:GLU:HA	1:A:681:GLU:HG2	1.93	0.51
2:B:605:ARG:HH21	2:B:639:ILE:HG12	1.76	0.51
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.76	0.51
2:B:451:LYS:HA	2:B:454:THR:HB	1.92	0.50
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.44	0.50
2:B:610:ASN:OD1	2:B:612:GLU:HG2	2.11	0.50
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.94	0.50
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.58	0.50
2:B:286:PHE:HB3	2:B:297:ILE:HG12	1.92	0.50
2:B:744:HIS:CD2	2:B:746:SER:OG	2.65	0.50
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.94	0.50
2:B:574:SER:HB3	2:B:591:ARG:HH22	1.77	0.50
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.94	0.50
2:B:310:MET:O	2:B:313:MET:HB2	2.11	0.50
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.41	0.50
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.50
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.42	0.50
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.93	0.50
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.94	0.50
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.77	0.49
2:B:211:VAL:CG2	2:B:483:LEU:HA	2.42	0.49
1:A:469:ARG:NH2	2:B:991:GLY:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.94	0.49
1:A:531:ILE:O	1:A:535:THR:HB	2.12	0.49
1:A:47:ARG:HA	1:A:47:ARG:NH1	2.26	0.49
1:A:1215:ARG:HH21	1:A:1218:GLN:HG3	1.76	0.49
1:A:833:GLU:O	1:A:837:ILE:HG12	2.13	0.49
1:A:567:LYS:CG	6:H:96:VAL:H	2.25	0.49
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.49
1:A:402:ALA:CB	1:A:434:ARG:HA	2.42	0.49
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.53	0.49
2:B:167:ILE:HD12	2:B:424:LEU:HD21	1.94	0.49
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.94	0.49
2:B:889:THR:HG22	2:B:891:ASP:HB2	1.94	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.94	0.49
8:J:32:GLU:H	8:J:32:GLU:CD	2.14	0.49
2:B:818:PRO:HG3	8:J:54:VAL:HG21	1.93	0.49
2:B:862:GLN:HG2	2:B:963:PHE:HB2	1.93	0.49
8:J:1:MET:HB2	8:J:56:LEU:HB2	1.95	0.49
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.95	0.49
1:A:10:PRO:HD2	2:B:1192:TYR:HA	1.95	0.49
1:A:120:GLU:HA	1:A:123:ARG:HD3	1.94	0.49
2:B:398:ARG:HD2	2:B:509:ALA:HB2	1.95	0.49
2:B:550:ASP:OD1	2:B:552:MET:HB2	2.13	0.49
5:F:110:ASP:O	5:F:123:LYS:HE2	2.13	0.49
2:B:696:GLU:O	2:B:699:GLU:HB2	2.13	0.48
2:B:210:LYS:HE2	2:B:462:ALA:O	2.13	0.48
1:A:399:HIS:O	1:A:401:GLY:N	2.45	0.48
3:C:206:ASN:HA	3:C:209:TYR:HD1	1.78	0.48
2:B:848:ARG:HD3	8:J:11:GLY:HA2	1.95	0.48
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.29	0.48
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.96	0.48
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.95	0.48
7:I:103:CYS:O	7:I:107:SER:HA	2.13	0.48
8:J:6:ARG:HA	8:J:12:LYS:O	2.12	0.48
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.78	0.48
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.79	0.48
1:A:34:LYS:HD2	1:A:57:ARG:HH22	1.78	0.48
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.96	0.48
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.96	0.48
1:A:91:PHE:H	1:A:297:GLN:HE22	1.61	0.48
8:J:64:ASN:N	8:J:65:PRO:HD2	2.29	0.48
5:F:79:ARG:NH1	5:F:145:ASP:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.95	0.47
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.95	0.47
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.96	0.47
1:A:206:GLU:O	1:A:210:ILE:HG12	2.13	0.47
2:B:892:LYS:HA	10:L:63:ARG:HH22	1.80	0.47
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.95	0.47
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.29	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.68	0.47
9:K:65:HIS:CD2	9:K:67:PHE:H	2.32	0.47
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.78	0.47
2:B:879:ARG:O	2:B:882:THR:CG2	2.63	0.47
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.12	0.47
3:C:251:LEU:O	3:C:255:VAL:HG23	2.15	0.47
6:H:130:ARG:H	6:H:130:ARG:HD2	1.79	0.47
1:A:1144:LYS:HG3	1:A:1268:LEU:HB3	1.95	0.47
10:L:61:THR:HB	10:L:63:ARG:H	1.80	0.47
3:C:22:LEU:CD2	9:K:101:LEU:HD21	2.44	0.47
4:E:78:LEU:HD21	4:E:109:ILE:HG12	1.97	0.47
1:A:447:GLN:NE2	12:T:21:DC:H4'	2.30	0.47
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.50	0.47
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.79	0.47
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.96	0.47
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.96	0.47
1:A:739:ASP:OD2	6:H:19:ARG:HD3	2.15	0.47
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.97	0.47
2:B:857:ARG:NH2	12:T:25:DC:OP1	2.48	0.47
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.50	0.47
8:J:7:CYS:HA	8:J:49:MET:HG2	1.97	0.47
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.50	0.46
1:A:775:ILE:HD12	1:A:818:MET:HE2	1.97	0.46
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.50	0.46
1:A:104:GLU:HG3	1:A:174:ILE:HD12	1.95	0.46
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.96	0.46
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.96	0.46
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.51	0.46
1:A:826:ASP:HB2	1:A:1082:ASN:CB	2.45	0.46
8:J:36:LEU:HD13	8:J:47:ARG:HB3	1.97	0.46
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.97	0.46
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.55	0.46
2:B:639:ILE:CD1	2:B:691:GLU:HB2	2.42	0.46
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.96	0.46
7:I:75:CYS:O	7:I:78:CYS:O	2.33	0.46
1:A:420:ARG:HB3	1:A:420:ARG:HE	1.53	0.46
1:A:299:HIS:HA	1:A:302:THR:HB	1.96	0.46
4:E:147:HIS:CD2	4:E:149:LEU:H	2.33	0.46
1:A:826:ASP:HB2	1:A:1082:ASN:HB3	1.96	0.46
2:B:363:HIS:O	2:B:364:ILE:HB	2.15	0.46
2:B:705:MET:CE	2:B:745:PRO:HB3	2.44	0.46
1:A:58:LEU:HD12	1:A:243:PRO:HA	1.98	0.46
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.98	0.46
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.97	0.46
1:A:533:LYS:HE2	1:A:745:GLN:HE22	1.81	0.46
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.98	0.46
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.46	0.46
1:A:858:ASN:HD21	1:A:862:ASN:HB2	1.80	0.46
3:C:164:ALA:HA	3:C:167:HIS:O	2.17	0.45
1:A:1323:ASP:OD1	1:A:1325:THR:CG2	2.64	0.45
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.82	0.45
2:B:1156:ASP:HB3	2:B:1197:PRO:CB	2.46	0.45
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.45
4:E:159:ASP:HA	4:E:162:ARG:HH11	1.81	0.45
1:A:942:PHE:O	1:A:946:VAL:HG23	2.16	0.45
3:C:148:ARG:H	3:C:151:GLN:HG3	1.80	0.45
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.37	0.45
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.82	0.45
6:H:95:TYR:HE2	6:H:97:MET:CG	2.25	0.45
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.99	0.45
2:B:792:MET:CE	12:T:25:DC:H5'	2.47	0.45
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.52	0.45
2:B:473:MET:C	2:B:475:SER:H	2.19	0.45
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.39	0.45
1:A:1067:LEU:HD22	1:A:1367:HIS:CE1	2.52	0.45
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.45
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.98	0.45
1:A:148:CYS:HB3	1:A:168:GLY:H	1.82	0.45
2:B:847:ASP:O	3:C:65:HIS:HE1	2.00	0.45
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.97	0.45
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.52	0.45
1:A:1080:THR:HG23	1:A:1085:HIS:HE1	1.81	0.45
1:A:436:ILE:CD1	1:A:491:VAL:HG11	2.38	0.45
2:B:976:ILE:O	2:B:990:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:LEU:O	8:J:6:ARG:NH1	2.50	0.45
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.98	0.45
3:C:6:PRO:HB2	9:K:101:LEU:HG	1.98	0.45
2:B:30:SER:HB2	2:B:743:ILE:O	2.17	0.45
1:A:56:PRO:HB2	1:A:57:ARG:HH21	1.82	0.45
2:B:801:LYS:O	8:J:52:THR:HG22	2.15	0.45
3:C:124:LEU:O	3:C:127:ARG:HG2	2.17	0.45
2:B:887:HIS:HA	2:B:888:GLY:O	2.17	0.45
1:A:1032:LEU:O	1:A:1036:ARG:HG2	2.17	0.45
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.51	0.45
1:A:265:LYS:HE3	1:A:299:HIS:HB3	1.99	0.45
2:B:592:ASN:HD21	2:B:595:ARG:HD3	1.81	0.45
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.82	0.44
1:A:974:ASP:C	1:A:976:THR:H	2.21	0.44
1:A:525:GLN:HE21	2:B:835:GLN:HG2	1.82	0.44
6:H:28:ALA:HB3	6:H:38:LEU:HB3	1.99	0.44
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.47	0.44
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.99	0.44
2:B:654:ARG:H	2:B:657:HIS:CD2	2.17	0.44
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.44
1:A:343:LYS:CE	2:B:1156:ASP:HB2	2.48	0.44
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.83	0.44
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.47	0.44
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.45	0.44
1:A:518:LYS:HA	1:A:631:HIS:HD2	1.81	0.44
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.98	0.44
2:B:1175:LEU:C	2:B:1177:HIS:H	2.21	0.44
1:A:944:ARG:HG2	1:A:1298:TYR:OH	2.17	0.44
1:A:404:TYR:HA	1:A:413:ILE:O	2.18	0.44
1:A:1188:GLN:HB3	1:A:1189:SER:H	1.60	0.44
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	1.98	0.44
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.99	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.99	0.44
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.37	0.44
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.48	0.44
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.99	0.44
2:B:223:VAL:HG11	2:B:380:TYR:HE2	1.83	0.44
4:E:176:PRO:O	4:E:212:ARG:HA	2.18	0.44
9:K:95:ILE:H	9:K:95:ILE:HG12	1.60	0.44
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.98	0.44
1:A:265:LYS:HD2	1:A:322:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:H	2:B:1116:ARG:HH22	1.65	0.44
2:B:68:THR:HG22	2:B:91:SER:HA	2.00	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	2.00	0.44
1:A:351:THR:HG22	1:A:352:VAL:H	1.83	0.43
2:B:62:ILE:HG23	2:B:418:LYS:HG2	2.00	0.43
1:A:388:LEU:O	1:A:392:VAL:HG23	2.18	0.43
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.53	0.43
1:A:919:ILE:HD11	1:A:925:LEU:HG	2.00	0.43
1:A:1152:ILE:HB	7:I:44:TYR:HB3	2.00	0.43
4:E:204:THR:HG22	4:E:205:SER:N	2.33	0.43
1:A:853:ASP:OD1	1:A:855:THR:HB	2.19	0.43
4:E:77:SER:HB2	4:E:106:GLN:H	1.83	0.43
2:B:516:ASN:ND2	2:B:516:ASN:H	2.14	0.43
1:A:503:GLN:HE21	5:F:90:ARG:NH1	2.16	0.43
10:L:46:VAL:HG12	10:L:56:LEU:HD12	1.99	0.43
2:B:473:MET:HG3	2:B:473:MET:H	1.48	0.43
2:B:1100:ASP:OD2	9:K:1:MET:HB3	2.18	0.43
2:B:770:GLN:HG2	2:B:983:ARG:O	2.18	0.43
2:B:762:ASN:ND2	2:B:1024:ALA:HB3	2.33	0.43
1:A:729:ALA:O	1:A:732:LEU:HB2	2.19	0.43
1:A:64:ASN:HB3	1:A:66:LYS:HZ3	1.82	0.43
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.99	0.43
1:A:92:HIS:HE1	2:B:1210:MET:O	2.01	0.43
2:B:212:LEU:HD13	2:B:409:ALA:HA	2.01	0.43
1:A:568:PRO:HG2	6:H:46:LEU:HB3	2.00	0.43
10:L:42:ARG:HD2	10:L:43:THR:H	1.84	0.43
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	2.01	0.43
4:E:24:LYS:HB2	4:E:30:ILE:HB	2.00	0.43
1:A:117:GLU:N	1:A:118:HIS:HB2	2.33	0.43
1:A:767:GLN:HA	1:A:799:PHE:HA	2.00	0.43
2:B:277:LYS:H	2:B:277:LYS:HG3	1.37	0.43
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.01	0.43
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.01	0.43
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.43
1:A:663:SER:HA	2:B:1014:PRO:HG3	2.00	0.43
2:B:526:GLU:HG3	2:B:771:SER:HB3	2.01	0.43
2:B:887:HIS:H	2:B:890:TYR:HE1	1.67	0.43
1:A:629:LEU:O	1:A:633:VAL:HG23	2.19	0.43
2:B:561:TRP:O	2:B:590:HIS:HE1	2.01	0.43
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.18	0.43
2:B:260:GLY:O	2:B:267:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:908:GLU:HG2	2:B:943:SER:HA	2.01	0.43
2:B:1097:HIS:HB3	2:B:1102:LYS:HE3	2.00	0.43
2:B:942:ARG:HH22	12:T:25:DC:P	2.42	0.42
2:B:574:SER:HB3	2:B:591:ARG:HH12	1.84	0.42
2:B:848:ARG:HD2	8:J:8:PHE:O	2.18	0.42
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.01	0.42
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	2.01	0.42
2:B:976:ILE:HG23	2:B:977:GLY:N	2.34	0.42
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	2.01	0.42
10:L:27:LEU:HB3	10:L:37:LYS:HE2	2.01	0.42
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.01	0.42
2:B:1017:ILE:HD12	2:B:1026:LEU:HD21	2.02	0.42
1:A:57:ARG:CB	1:A:68:GLN:HG2	2.49	0.42
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.00	0.42
1:A:785:PRO:HG2	2:B:703:ILE:HD12	2.01	0.42
2:B:365:THR:HG21	2:B:370:PHE:CG	2.54	0.42
1:A:1320:PRO:HG3	4:E:7:ARG:HH12	1.84	0.42
2:B:483:LEU:O	2:B:484:ASN:HB2	2.19	0.42
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.42
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.01	0.42
2:B:33:VAL:O	2:B:36:ALA:HB3	2.20	0.42
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.01	0.42
1:A:70:CYS:O	1:A:72:GLU:HG2	2.20	0.42
2:B:95:ILE:HD11	2:B:128:LEU:HB3	2.02	0.42
1:A:780:VAL:HG13	1:A:789:LYS:HE2	2.01	0.42
1:A:68:GLN:O	1:A:70:CYS:N	2.34	0.42
2:B:121:ASN:HA	2:B:207:GLY:CA	2.50	0.42
2:B:405:ARG:NE	2:B:629:ASP:OD1	2.45	0.42
4:E:10:SER:O	4:E:14:ARG:HG3	2.20	0.42
1:A:1116:LEU:H	1:A:1308:THR:HB	1.84	0.42
9:K:79:GLU:CD	9:K:79:GLU:H	2.23	0.42
3:C:3:GLU:HG3	3:C:4:GLU:HG3	2.01	0.42
1:A:55:ASP:N	1:A:56:PRO:HD2	2.35	0.42
1:A:230:ARG:HB3	1:A:232:GLU:HG2	2.02	0.42
1:A:298:PHE:HA	1:A:299:HIS:O	2.20	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.37	0.42
1:A:385:ILE:O	1:A:389:THR:OG1	2.38	0.42
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.44	0.42
3:C:167:HIS:HE1	10:L:70:ARG:O	2.03	0.42
1:A:822:GLU:HG3	2:B:513:GLN:NE2	2.34	0.42
1:A:47:ARG:HA	1:A:47:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:46:TYR:CE2	4:E:58:MET:HA	2.55	0.42
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.54	0.42
1:A:396:PRO:HG2	1:A:416:ARG:HB3	2.02	0.42
1:A:457:ALA:O	1:A:507:VAL:HG23	2.20	0.42
2:B:899:ILE:HD12	2:B:911:ILE:HA	2.02	0.41
6:H:10:PHE:HB3	6:H:28:ALA:HB1	2.02	0.41
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.84	0.41
1:A:472:LEU:O	1:A:475:THR:HB	2.20	0.41
4:E:64:PRO:CD	4:E:76:GLY:HA2	2.49	0.41
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.84	0.41
1:A:885:THR:O	1:A:940:ARG:HD2	2.20	0.41
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.02	0.41
1:A:58:LEU:HD12	1:A:244:PRO:HD3	2.02	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.55	0.41
2:B:487:THR:HG22	2:B:490:SER:H	1.84	0.41
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.01	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.41
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.19	0.41
5:F:79:ARG:HG2	5:F:144:GLU:HG2	2.03	0.41
1:A:409:SER:O	1:A:411:ASP:N	2.54	0.41
2:B:492:LEU:HB3	2:B:751:VAL:HG21	2.02	0.41
1:A:523:ILE:CG2	1:A:527:THR:HG22	2.49	0.41
2:B:708:GLU:O	2:B:710:LEU:N	2.54	0.41
2:B:364:ILE:HD13	2:B:585:VAL:HG13	2.03	0.41
1:A:929:LEU:HD11	1:A:983:ILE:HD12	2.03	0.41
9:K:39:ASP:HB2	9:K:40:HIS:H	1.74	0.41
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.01	0.41
2:B:807:ARG:HA	2:B:807:ARG:HD2	1.93	0.41
2:B:477:ALA:HB1	2:B:499:ASN:HD21	1.85	0.41
3:C:52:GLU:HB3	3:C:154:LYS:HB3	2.02	0.41
7:I:62:ILE:HG21	7:I:102:VAL:HG11	2.02	0.41
2:B:789:MET:HE2	2:B:965:LYS:HB3	2.02	0.41
2:B:95:ILE:HG13	2:B:96:TYR:N	2.36	0.41
4:E:175:LEU:HD23	4:E:213:ILE:HB	2.03	0.41
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	2.03	0.41
1:A:326:ARG:HA	1:A:1406:VAL:HG21	2.03	0.41
1:A:265:LYS:HE3	1:A:299:HIS:CD2	2.56	0.41
2:B:797:TYR:O	8:J:1:MET:HG3	2.20	0.41
1:A:55:ASP:H	1:A:56:PRO:HD2	1.86	0.41
2:B:426:LYS:HE2	2:B:430:ARG:HH22	1.85	0.41
1:A:313:GLN:HB3	1:A:322:VAL:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.56	0.40
2:B:705:MET:HE3	2:B:745:PRO:HB3	2.03	0.40
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.86	0.40
1:A:1333:ILE:HG12	1:A:1381:LEU:HD12	2.02	0.40
7:I:61:ASP:OD2	7:I:61:ASP:N	2.53	0.40
2:B:864:LYS:N	2:B:872:GLU:HB2	2.36	0.40
3:C:18:VAL:O	3:C:231:ASN:HA	2.21	0.40
2:B:283:VAL:HG22	2:B:321:GLY:HA3	2.03	0.40
2:B:1163:CYS:O	2:B:1167:GLY:HA2	2.21	0.40
2:B:367:LEU:HB3	2:B:368:GLU:H	1.73	0.40
1:A:1135:ARG:HG2	1:A:1282:VAL:HB	2.03	0.40
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.40
2:B:898:LEU:HD11	2:B:964:VAL:HG11	2.03	0.40
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.85	0.40
1:A:117:GLU:H	1:A:118:HIS:CG	2.38	0.40
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.55	0.40
2:B:274:PRO:HG3	2:B:359:GLU:O	2.22	0.40
2:B:386:LEU:O	2:B:390:LEU:HD12	2.22	0.40
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	2.02	0.40
2:B:551:PRO:HA	2:B:628:THR:HG21	2.04	0.40
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.02	0.40
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.36	0.40
1:A:325:ILE:HB	2:B:1210:MET:SD	2.62	0.40
2:B:225:VAL:HG11	2:B:385:LEU:HA	2.04	0.40
1:A:89:PRO:HG2	1:A:205:GLU:HA	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	1395/1733 (80%)	1210 (87%)	126 (9%)	59 (4%)	3 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	1096/1224 (90%)	948 (86%)	102 (9%)	46 (4%)	3 23
3	C	264/318 (83%)	237 (90%)	21 (8%)	6 (2%)	8 39
4	E	212/215 (99%)	197 (93%)	11 (5%)	4 (2%)	10 45
5	F	83/155 (54%)	76 (92%)	6 (7%)	1 (1%)	16 54
6	H	129/146 (88%)	109 (84%)	9 (7%)	11 (8%)	1 7
7	I	117/122 (96%)	95 (81%)	18 (15%)	4 (3%)	5 29
8	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	5 31
9	K	112/120 (93%)	104 (93%)	6 (5%)	2 (2%)	11 46
10	L	44/70 (63%)	29 (66%)	9 (20%)	6 (14%)	0 2
All	All	3515/4173 (84%)	3061 (87%)	313 (9%)	141 (4%)	4 24

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	56	PRO
1	A	69	THR
1	A	72	GLU
1	A	117	GLU
1	A	215	SER
1	A	219	PHE
1	A	257	ARG
1	A	299	HIS
1	A	315	LEU
1	A	404	TYR
1	A	410	GLY
1	A	424	ILE
1	A	567	LYS
1	A	672	ASP
1	A	923	LEU
1	A	1087	ALA
1	A	1123	GLY
1	A	1167	GLU
2	B	67	SER
2	B	137	TYR
2	B	138	GLU
2	B	465	ASN
2	B	477	ALA

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Mol	Chain	Res	Type
2	B	482	VAL
2	B	484	ASN
2	B	709	ASP
2	B	734	HIS
2	B	737	THR
2	B	751	VAL
2	B	883	LEU
2	B	1156	ASP
2	B	1221	SER
3	C	227	THR
4	E	86	PRO
6	H	62	SER
6	H	131	ASN
6	H	140	ALA
8	J	2	ILE
10	L	51	CYS
1	A	76	GLU
1	A	250	ILE
1	A	283	GLY
1	A	300	VAL
1	A	312	PRO
1	A	399	HIS
1	A	418	SER
1	A	423	ASP
1	A	969	GLN
1	A	975	HIS
1	A	1437	GLY
2	B	277	LYS
2	B	364	ILE
2	B	468	GLU
2	B	469	GLN
2	B	474	SER
2	B	483	LEU
2	B	531	GLN
2	B	648	HIS
2	B	708	GLU
2	B	712	PRO
2	B	792	MET
2	B	879	ARG
2	B	1046	PRO
2	B	1155	SER
3	C	48	SER

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Mol	Chain	Res	Type
3	C	141	GLY
4	E	77	SER
6	H	18	GLY
6	H	90	ALA
6	H	108	SER
6	H	110	ASP
7	I	52	ILE
7	I	60	GLN
8	J	6	ARG
9	K	16	GLU
10	L	46	VAL
10	L	55	ILE
10	L	59	ALA
1	A	65	LEU
1	A	68	GLN
1	A	71	GLN
1	A	91	PHE
1	A	130	ASP
1	A	317	LYS
1	A	331	GLY
1	A	595	THR
1	A	1081	LEU
1	A	1083	THR
1	A	1393	ASN
2	B	139	ALA
2	B	629	ASP
2	B	943	SER
2	B	1017	ILE
2	B	1157	ALA
3	C	214	ASN
4	E	59	SER
5	F	154	ASP
10	L	56	LEU
10	L	64	LEU
1	A	214	ILE
1	A	254	GLU
1	A	569	LYS
1	A	852	TYR
1	A	1034	GLU
2	B	467	GLY
2	B	881	ASN
2	B	884	ARG

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Mol	Chain	Res	Type
2	B	887	HIS
2	B	1181	GLU
2	B	1211	ASN
3	C	90	ASP
3	C	142	VAL
6	H	84	ALA
6	H	128	ASN
7	I	3	THR
1	A	35	ILE
1	A	52	GLY
1	A	119	ASN
1	A	251	SER
1	A	255	SER
1	A	910	PRO
1	A	958	VAL
2	B	367	LEU
2	B	608	ASP
2	B	711	GLU
2	B	864	LYS
4	E	124	VAL
6	H	3	ASN
6	H	109	LYS
7	I	77	LYS
9	K	37	LYS
1	A	149	GLU
1	A	286	HIS
1	A	409	SER
1	A	593	GLU
2	B	647	GLY
2	B	108	VAL
2	B	1099	VAL
1	A	385	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1225/1520 (81%)	1033 (84%)	192 (16%)	3 15
2	B	967/1061 (91%)	838 (87%)	129 (13%)	5 21
3	C	234/274 (85%)	205 (88%)	29 (12%)	6 25
4	E	196/197 (100%)	169 (86%)	27 (14%)	4 20
5	F	75/137 (55%)	69 (92%)	6 (8%)	15 49
6	H	117/128 (91%)	97 (83%)	20 (17%)	2 12
7	I	113/116 (97%)	99 (88%)	14 (12%)	6 25
8	J	60/65 (92%)	45 (75%)	15 (25%)	1 3
9	K	99/102 (97%)	84 (85%)	15 (15%)	3 16
10	L	40/57 (70%)	28 (70%)	12 (30%)	0 1
All	All	3126/3657 (86%)	2667 (85%)	459 (15%)	4 18

All (459) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	39	GLU
1	A	41	MET
1	A	43	GLU
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	54	ASN
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	74	MET
1	A	90	VAL
1	A	93	VAL
1	A	113	LEU
1	A	116	ASP
1	A	117	GLU
1	A	120	GLU
1	A	126	LEU
1	A	128	ILE
1	A	133	LYS
1	A	143	LYS

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Mol	Chain	Res	Type
1	A	147	VAL
1	A	148	CYS
1	A	186	LYS
1	A	199	LEU
1	A	218	ASP
1	A	222	LEU
1	A	227	VAL
1	A	235	ILE
1	A	252	PHE
1	A	256	GLN
1	A	257	ARG
1	A	265	LYS
1	A	270	LEU
1	A	274	ILE
1	A	289	ILE
1	A	291	GLU
1	A	296	LEU
1	A	299	HIS
1	A	302	THR
1	A	307	ASP
1	A	308	ILE
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	330	LYS
1	A	332	LYS
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	344	ARG
1	A	351	THR
1	A	368	LYS
1	A	381	THR
1	A	383	TYR
1	A	389	THR
1	A	391	LEU
1	A	398	GLU
1	A	403	LYS
1	A	404	TYR
1	A	407	ARG
1	A	420	ARG
1	A	427	GLN

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Mol	Chain	Res	Type
1	A	436	ILE
1	A	443	LEU
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	489	LEU
1	A	496	GLU
1	A	497	THR
1	A	516	SER
1	A	518	LYS
1	A	525	GLN
1	A	532	ARG
1	A	535	THR
1	A	541	ILE
1	A	571	LEU
1	A	588	LEU
1	A	595	THR
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	636	GLU
1	A	637	LYS
1	A	652	VAL
1	A	672	ASP
1	A	678	GLU
1	A	688	LYS
1	A	689	LYS
1	A	695	LYS
1	A	713	SER
1	A	716	ASP
1	A	722	LEU
1	A	732	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE

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Mol	Chain	Res	Type
1	A	764	CYS
1	A	769	SER
1	A	771	GLU
1	A	773	LYS
1	A	774	ARG
1	A	788	SER
1	A	801	GLU
1	A	821	ARG
1	A	830	LYS
1	A	846	GLU
1	A	849	MET
1	A	854	ASN
1	A	867	ILE
1	A	878	ILE
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	908	LEU
1	A	920	LEU
1	A	931	GLU
1	A	938	LYS
1	A	940	ARG
1	A	953	ASN
1	A	969	GLN
1	A	1001	ARG
1	A	1005	GLU
1	A	1015	VAL
1	A	1025	ARG
1	A	1029	ARG
1	A	1034	GLU
1	A	1035	TYR
1	A	1048	ASN
1	A	1050	GLU
1	A	1067	LEU
1	A	1081	LEU
1	A	1082	ASN
1	A	1084	PHE
1	A	1085	HIS
1	A	1094	VAL
1	A	1095	THR
1	A	1110	ASN
1	A	1116	LEU

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Mol	Chain	Res	Type
1	A	1117	THR
1	A	1130	GLN
1	A	1147	THR
1	A	1161	THR
1	A	1173	HIS
1	A	1176	LEU
1	A	1188	GLN
1	A	1206	ASP
1	A	1231	ASP
1	A	1233	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1258	HIS
1	A	1259	MET
1	A	1264	GLU
1	A	1266	THR
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1284	MET
1	A	1291	VAL
1	A	1322	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1354	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1403	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1415	SER
1	A	1420	ASP
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET

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Mol	Chain	Res	Type
2	B	22	SER
2	B	25	ILE
2	B	28	GLU
2	B	40	GLU
2	B	46	GLN
2	B	63	ILE
2	B	89	GLU
2	B	95	ILE
2	B	102	VAL
2	B	137	TYR
2	B	138	GLU
2	B	174	LEU
2	B	175	ARG
2	B	185	THR
2	B	187	SER
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	232	SER
2	B	234	ILE
2	B	240	ILE
2	B	241	ARG
2	B	242	SER
2	B	249	ARG
2	B	254	LEU
2	B	264	SER
2	B	267	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	280	ILE
2	B	283	VAL
2	B	296	GLU
2	B	323	VAL
2	B	332	ASP
2	B	347	LYS
2	B	357	GLN
2	B	365	THR
2	B	387	LEU
2	B	390	LEU
2	B	393	LYS
2	B	394	ASP

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Mol	Chain	Res	Type
2	B	398	ARG
2	B	416	LEU
2	B	429	PHE
2	B	458	LYS
2	B	468	GLU
2	B	469	GLN
2	B	471	LYS
2	B	473	MET
2	B	481	GLN
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	540	SER
2	B	547	VAL
2	B	555	ILE
2	B	567	GLU
2	B	574	SER
2	B	576	ASP
2	B	591	ARG
2	B	604	ARG
2	B	621	GLU
2	B	641	GLU
2	B	649	LYS
2	B	653	VAL
2	B	658	ILE
2	B	660	LYS
2	B	682	SER
2	B	685	LEU
2	B	708	GLU
2	B	710	LEU
2	B	734	HIS
2	B	751	VAL
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	815	ARG
2	B	838	SER
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	865	LYS

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Mol	Chain	Res	Type
2	B	866	TYR
2	B	868	MET
2	B	878	GLN
2	B	879	ARG
2	B	884	ARG
2	B	885	MET
2	B	906	SER
2	B	917	PRO
2	B	939	THR
2	B	944	THR
2	B	948	ILE
2	B	955	THR
2	B	957	ASN
2	B	963	PHE
2	B	975	GLN
2	B	983	ARG
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1028	GLU
2	B	1034	VAL
2	B	1053	GLU
2	B	1060	ARG
2	B	1065	GLN
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1150	ARG
2	B	1156	ASP
2	B	1160	VAL
2	B	1174	LYS
2	B	1175	LEU
2	B	1178	ASN
2	B	1202	LEU

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Mol	Chain	Res	Type
2	B	1210	MET
2	B	1220	ARG
2	B	1222	ARG
3	C	4	GLU
3	C	18	VAL
3	C	23	SER
3	C	25	VAL
3	C	36	VAL
3	C	41	ILE
3	C	56	THR
3	C	75	MET
3	C	78	GLU
3	C	80	LEU
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	129	ILE
3	C	137	LYS
3	C	151	GLN
3	C	152	GLU
3	C	156	THR
3	C	157	CYS
3	C	205	LYS
3	C	214	ASN
3	C	215	GLU
3	C	238	ILE
3	C	240	VAL
3	C	244	VAL
3	C	252	GLN
3	C	259	LEU
3	C	264	GLN
3	C	266	ASP
4	E	2	ASP
4	E	9	ILE
4	E	24	LYS
4	E	33	GLU
4	E	50	MET
4	E	54	GLN
4	E	57	MET
4	E	61	GLN
4	E	67	GLU
4	E	74	ASP

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Mol	Chain	Res	Type
4	E	78	LEU
4	E	83	CYS
4	E	95	THR
4	E	101	GLN
4	E	122	LYS
4	E	123	LEU
4	E	127	ILE
4	E	140	LEU
4	E	149	LEU
4	E	156	LEU
4	E	157	SER
4	E	158	SER
4	E	169	ARG
4	E	177	ARG
4	E	192	ARG
4	E	196	VAL
4	E	204	THR
5	F	82	THR
5	F	89	GLU
5	F	92	ARG
5	F	110	ASP
5	F	111	LEU
5	F	118	LEU
6	H	2	SER
6	H	8	ASP
6	H	11	GLN
6	H	22	LYS
6	H	24	CYS
6	H	26	ILE
6	H	27	GLU
6	H	35	GLN
6	H	53	ASP
6	H	59	ILE
6	H	63	LEU
6	H	76	THR
6	H	77	ARG
6	H	83	GLN
6	H	86	ASP
6	H	87	ARG
6	H	95	TYR
6	H	136	LYS
6	H	138	GLU

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Mol	Chain	Res	Type
6	H	145	ARG
7	I	17	ARG
7	I	28	GLU
7	I	35	VAL
7	I	52	ILE
7	I	59	VAL
7	I	61	ASP
7	I	64	SER
7	I	70	ARG
7	I	84	VAL
7	I	90	GLN
7	I	91	ARG
7	I	94	ASP
7	I	97	MET
7	I	116	ASN
8	J	1	MET
8	J	2	ILE
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	27	GLU
8	J	31	ASP
8	J	48	ARG
8	J	52	THR
8	J	59	LYS
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	6	ARG
9	K	17	SER
9	K	18	LYS
9	K	20	LYS
9	K	25	THR
9	K	26	LYS
9	K	31	VAL
9	K	42	LEU
9	K	54	ARG
9	K	55	LYS
9	K	63	VAL

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Mol	Chain	Res	Type
9	K	70	ARG
9	K	95	ILE
9	K	101	LEU
10	L	27	LEU
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	50	ASP
10	L	54	ARG
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	18	GLN
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	118	HIS
1	A	225	ASN
1	A	297	GLN
1	A	306	ASN
1	A	313	GLN
1	A	339	ASN
1	A	503	GLN
1	A	525	GLN
1	A	584	ASN
1	A	631	HIS
1	A	700	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN

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Mol	Chain	Res	Type
1	A	786	HIS
1	A	854	ASN
1	A	877	HIS
1	A	935	GLN
1	A	968	GLN
1	A	1085	HIS
1	A	1130	GLN
1	A	1270	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	255	GLN
2	B	325	GLN
2	B	357	GLN
2	B	383	ASN
2	B	481	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	590	HIS
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	763	GLN
2	B	822	ASN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
2	B	1178	ASN
3	C	65	HIS
3	C	73	GLN
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	214	ASN
3	C	242	GLN
6	H	133	ASN

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Mol	Chain	Res	Type
7	I	12	ASN
7	I	46	HIS
7	I	90	GLN
7	I	116	ASN
9	K	52	ASN
9	K	65	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	6/7 (85%)	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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1405/1733 (81%)	0.07	63 (4%) 37 30	48, 92, 168, 202	0
2	B	1114/1224 (91%)	-0.08	31 (2%) 56 50	43, 79, 139, 202	0
3	C	266/318 (83%)	-0.27	1 (0%) 93 92	52, 80, 117, 169	0
4	E	214/215 (99%)	0.30	19 (8%) 12 10	69, 130, 190, 204	0
5	F	85/155 (54%)	-0.08	0 100 100	66, 97, 133, 162	0
6	H	133/146 (91%)	0.26	5 (3%) 44 37	86, 127, 158, 170	0
7	I	119/122 (97%)	-0.27	0 100 100	59, 97, 131, 150	0
8	J	65/70 (92%)	-0.28	1 (1%) 76 71	47, 70, 100, 127	0
9	K	114/120 (95%)	-0.25	0 100 100	60, 87, 112, 127	0
10	L	46/70 (65%)	-0.09	1 (2%) 65 59	65, 109, 149, 161	0
11	R	7/7 (100%)	-0.59	0 100 100	89, 97, 131, 139	0
12	T	13/29 (44%)	-0.25	0 100 100	110, 124, 160, 169	0
All	All	3581/4209 (85%)	-0.02	121 (3%) 49 42	43, 90, 161, 204	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1082	ASN	10.5
1	A	1176	LEU	10.2
1	A	318	SER	8.4
1	A	1087	ALA	8.2
1	A	1086	PHE	7.4
1	A	1090	ALA	6.6
1	A	1083	THR	6.4
1	A	1088	GLY	6.2
1	A	44	THR	6.2
1	A	1089	VAL	6.1
1	A	1085	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
2	B	1223	ASP	5.8
6	H	2	SER	5.2
1	A	69	THR	5.2
1	A	316	GLN	5.2
1	A	1091	SER	4.8
1	A	317	LYS	4.5
2	B	1222	ARG	4.5
4	E	126	SER	4.3
1	A	115	LEU	4.2
1	A	149	GLU	4.1
6	H	132	LEU	4.0
4	E	122	LYS	4.0
2	B	870	ILE	3.9
2	B	1224	PHE	3.9
1	A	161	LEU	3.9
1	A	113	LEU	3.8
1	A	116	ASP	3.8
2	B	250	PHE	3.8
1	A	105	CYS	3.8
1	A	257	ARG	3.8
2	B	869	SER	3.7
2	B	136	THR	3.7
4	E	96	PHE	3.7
2	B	432	MET	3.6
2	B	133	LYS	3.5
1	A	164	ARG	3.5
10	L	27	LEU	3.4
4	E	88	VAL	3.3
6	H	86	ASP	3.3
4	E	123	LEU	3.3
1	A	152	VAL	3.2
1	A	1256	GLU	3.2
2	B	89	GLU	3.2
1	A	114	LEU	3.2
2	B	866	TYR	3.2
1	A	319	GLY	3.1
1	A	45	GLN	3.1
2	B	474	SER	3.1
1	A	1175	SER	3.1
6	H	85	GLY	3.1
1	A	49	LYS	3.0
4	E	83	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	90	ILE	3.0
1	A	108	MET	2.9
1	A	141	LEU	2.9
4	E	89	GLY	2.9
2	B	135	ARG	2.9
1	A	186	LYS	2.8
1	A	65	LEU	2.8
1	A	153	PRO	2.8
4	E	110	PHE	2.8
1	A	182	VAL	2.8
1	A	167	CYS	2.8
1	A	1084	PHE	2.8
1	A	117	GLU	2.8
2	B	1221	SER	2.7
1	A	5	GLN	2.7
1	A	256	GLN	2.7
1	A	1108	ALA	2.7
2	B	883	LEU	2.7
1	A	66	LYS	2.6
1	A	138	ILE	2.5
1	A	1092	LYS	2.5
1	A	144	THR	2.5
4	E	125	PRO	2.5
1	A	255	SER	2.5
4	E	106	GLN	2.5
2	B	134	LYS	2.4
2	B	477	ALA	2.4
1	A	151	ASP	2.4
4	E	93	MET	2.4
1	A	163	SER	2.4
2	B	1172	ILE	2.4
2	B	91	SER	2.4
1	A	126	LEU	2.3
1	A	276	LEU	2.3
2	B	666	TYR	2.3
1	A	426	LEU	2.3
6	H	84	ALA	2.3
2	B	429	PHE	2.3
1	A	975	HIS	2.3
2	B	645	SER	2.3
2	B	67	SER	2.3
3	C	213	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
4	E	127	ILE	2.2
2	B	647	GLY	2.2
1	A	286	HIS	2.2
4	E	36	GLU	2.2
1	A	72	GLU	2.2
1	A	112	LYS	2.2
1	A	142	CYS	2.2
1	A	150	THR	2.2
1	A	250	ILE	2.2
1	A	1109	LYS	2.2
4	E	100	ILE	2.2
4	E	102	GLU	2.2
2	B	709	ASP	2.2
4	E	81	GLU	2.1
2	B	249	ARG	2.1
1	A	201	VAL	2.1
2	B	1191	ILE	2.1
2	B	865	LYS	2.1
1	A	287	HIS	2.1
1	A	408	ASP	2.1
4	E	132	ILE	2.1
4	E	82	PHE	2.1
2	B	68	THR	2.1
8	J	27	GLU	2.1
2	B	247	GLY	2.0
4	E	90	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
14	MG	B	2002[B]	1/1	0.56	0.69	33.14	3,3,3,3	1
13	ZN	I	203	1/1	0.99	0.14	0.22	98,98,98,98	0
13	ZN	J	101	1/1	0.99	0.20	-0.66	75,75,75,75	0
13	ZN	B	1307	1/1	0.98	0.13	-0.83	147,147,147,147	0
13	ZN	L	105	1/1	0.99	0.08	-0.85	112,112,112,112	0
13	ZN	C	319	1/1	1.00	0.09	-0.88	78,78,78,78	0
13	ZN	I	204	1/1	0.99	0.10	-1.05	74,74,74,74	0
13	ZN	A	1735	1/1	0.96	0.11	-1.42	112,112,112,112	0
13	ZN	A	1734	1/1	0.88	0.06	-2.92	236,236,236,236	0
14	MG	A	2001	1/1	0.98	0.08	-	68,68,68,68	0
14	MG	B	2002[A]	1/1	0.56	0.69	-	41,41,41,41	1

6.5 Other polymers

There are no such residues in this entry.