Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:44 am BST

PDB ID	:	4BBS
Title	:	Structure of an initially transcribing RNA polymerase II-TFIIB complex
Authors	:	Sainsbury, S.; Niesser, J.; Cramer, P.
Deposited on	:	2012-09-27
Resolution	:	3.60 Å(reported)

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

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

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

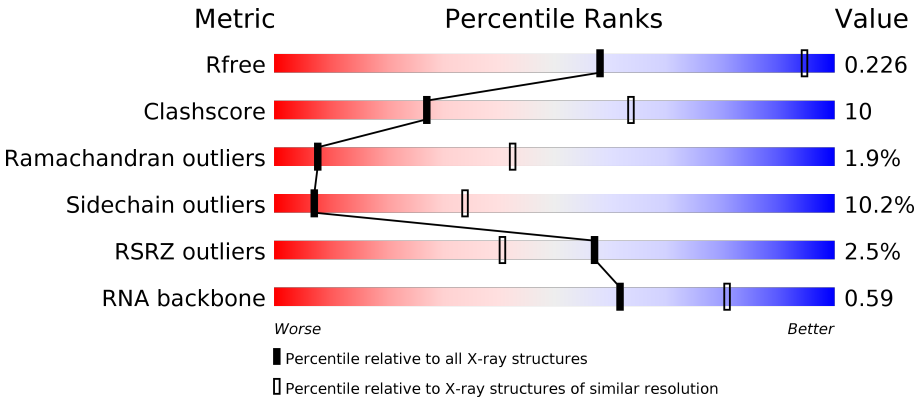
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	% 57% 21% • 18%
2	B	1224	2% 65% 26% • 6%
3	C	318	57% 24% • 16%
4	D	221	% 52% 22% 6% 19%

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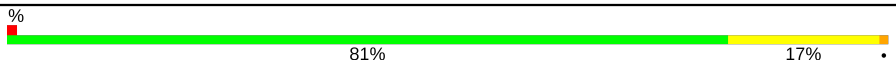
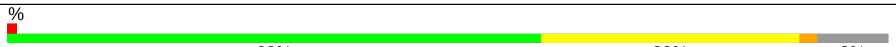
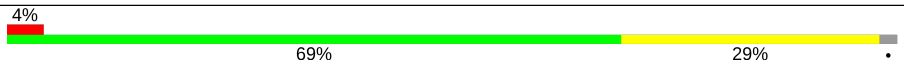
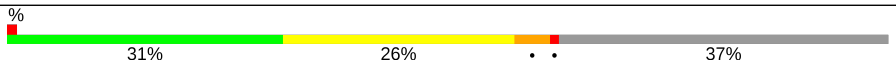
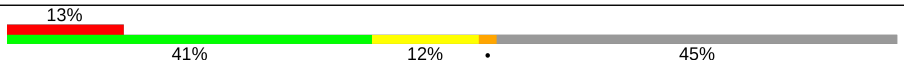
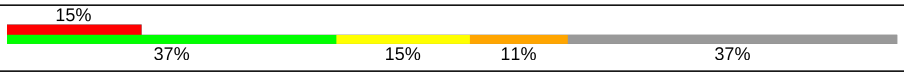
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	14	
15	P	6	
16	T	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	MG	A	2459	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 33420 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11170	7039	1953	2116	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9095	5751	1598	1690	56			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

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

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	189	Total	C	N	O	S	0	0	0
			1357	838	240	267	12			

- Molecule 14 is a DNA chain called 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

- Molecule 15 is a RNA chain called 5'-R(*AP*UP*AP*UP*CP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

- Molecule 16 is a DNA chain called 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP*CP*TP *AP*TP*GP*AP*TP*AP*TP*TP*TP*TP*TP*AP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	17	Total	C	N	O	P	0	0	0
			350	169	56	108	17			

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

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

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

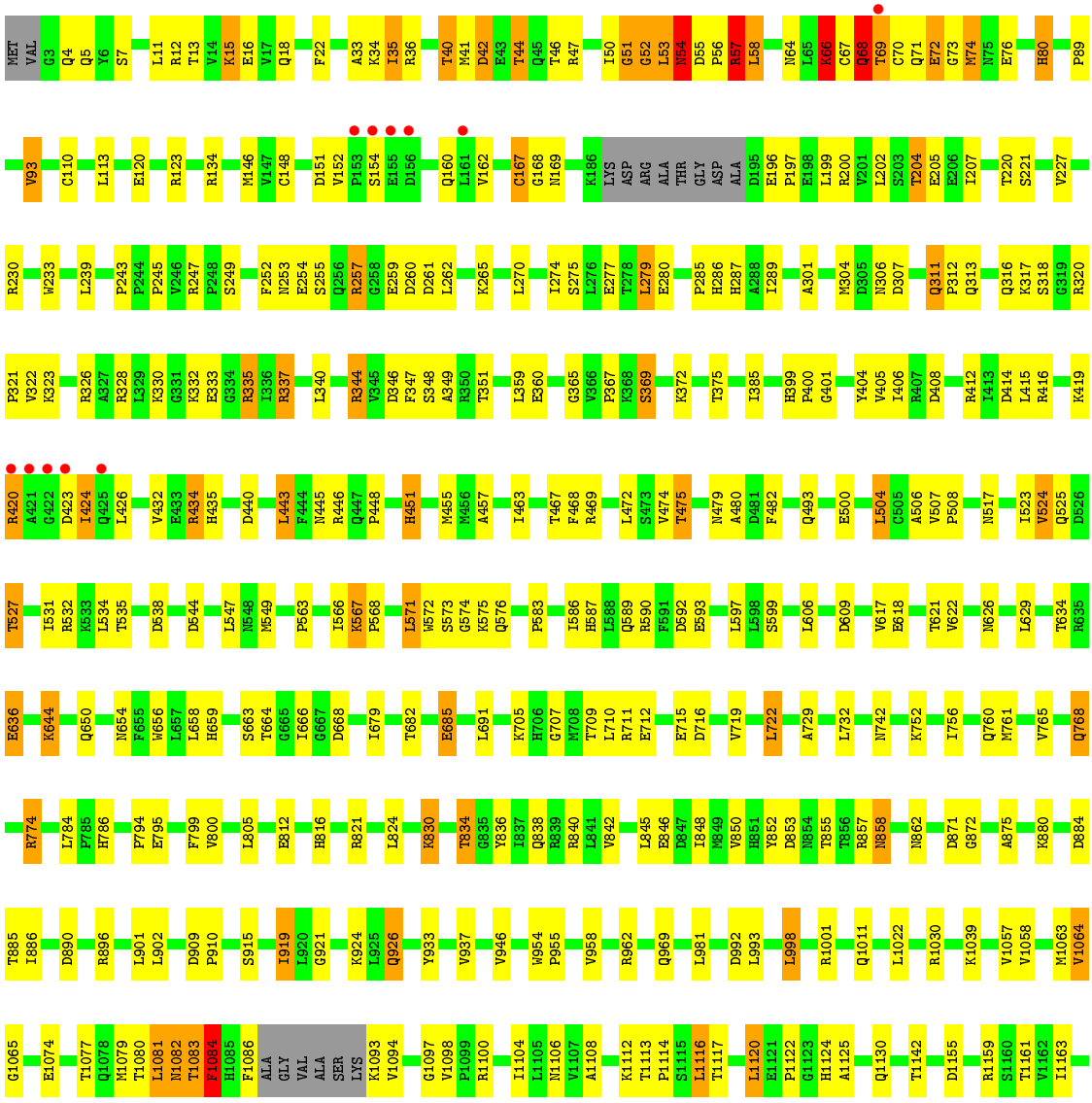
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	2	Total Mg 2 2	0	0

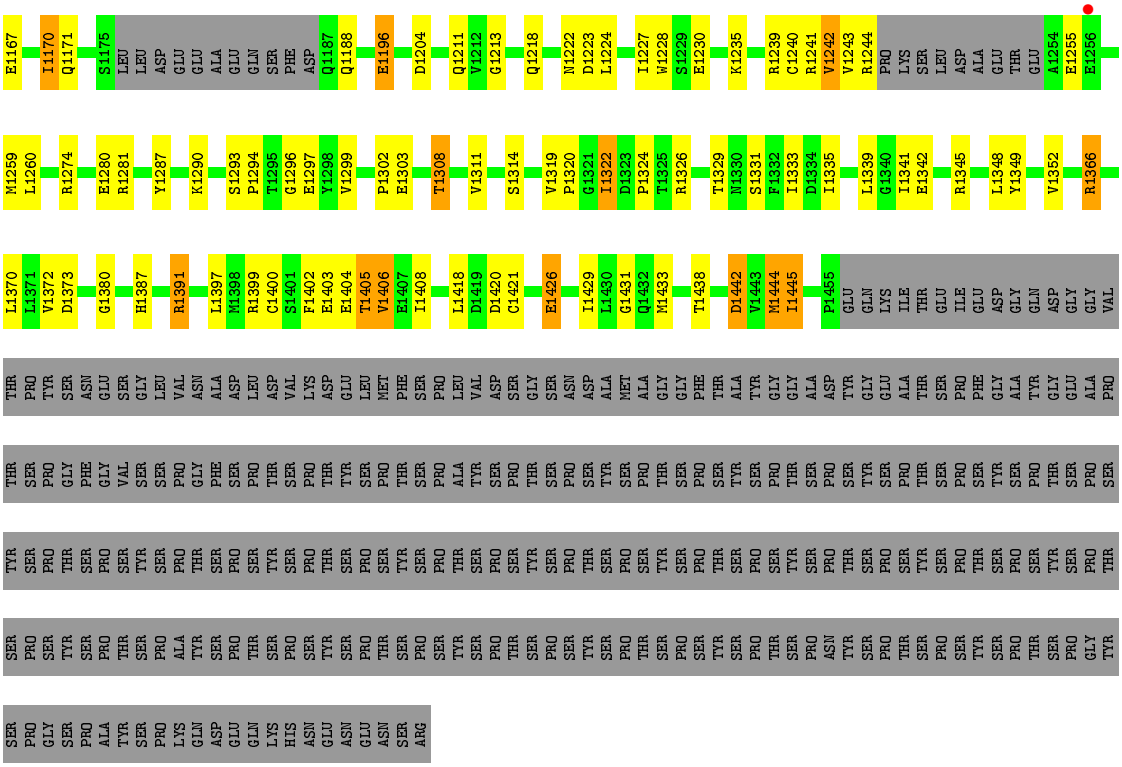
3 Residue-property plots (i)

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

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

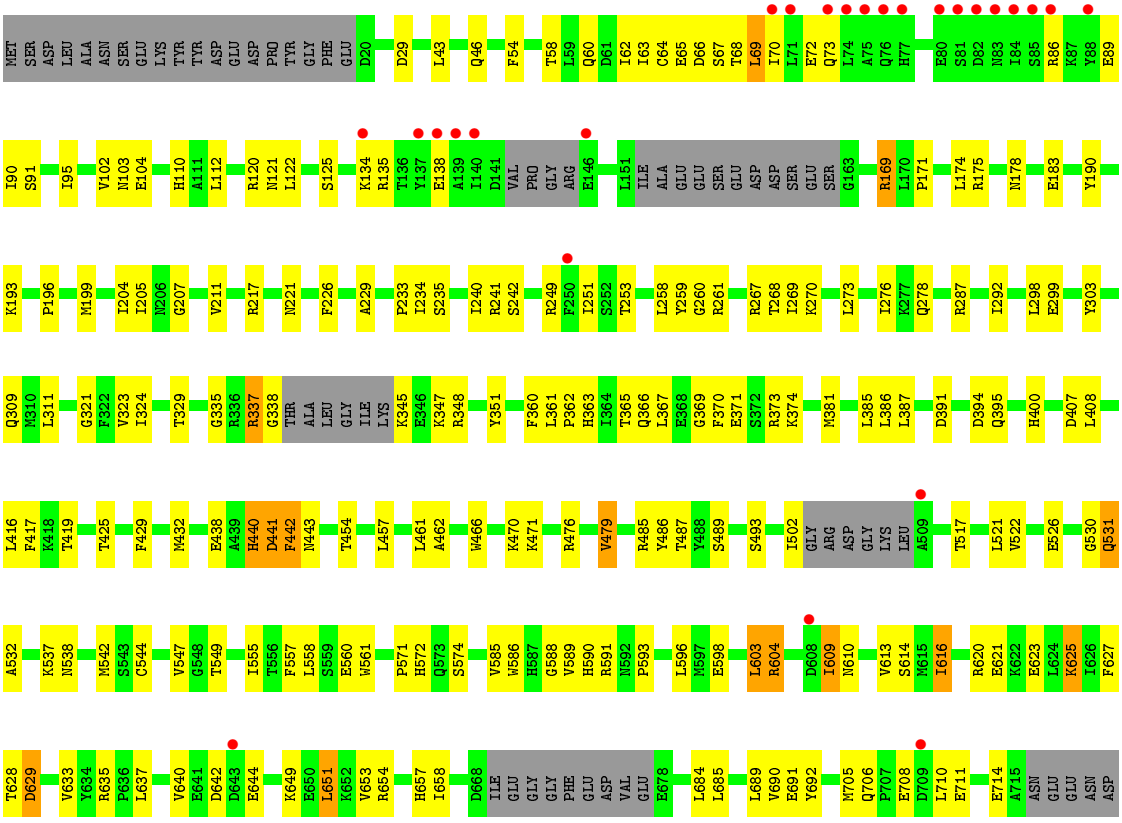
Chain A:

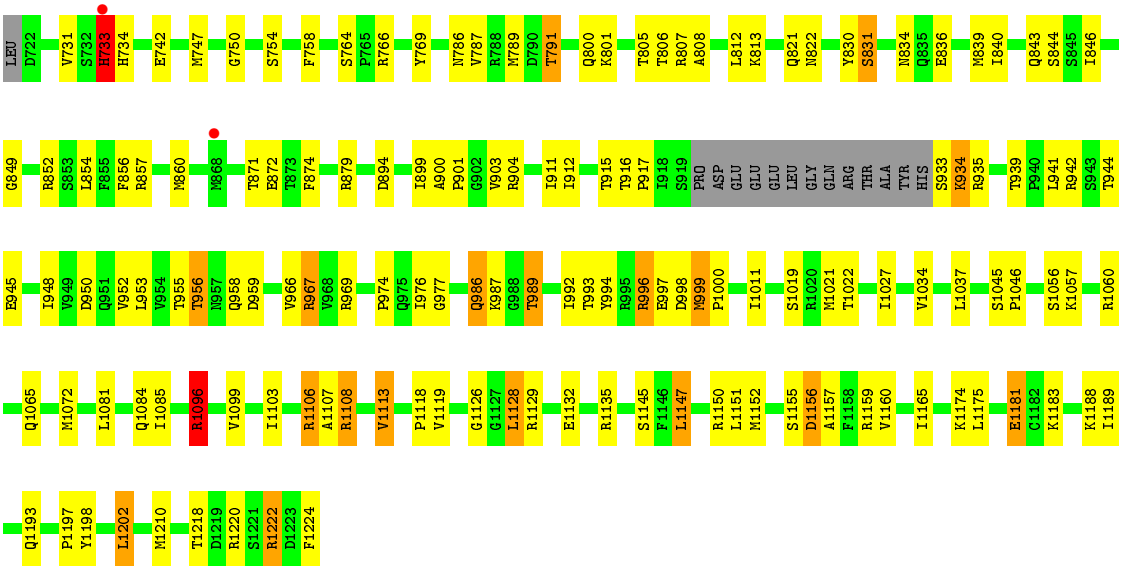




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

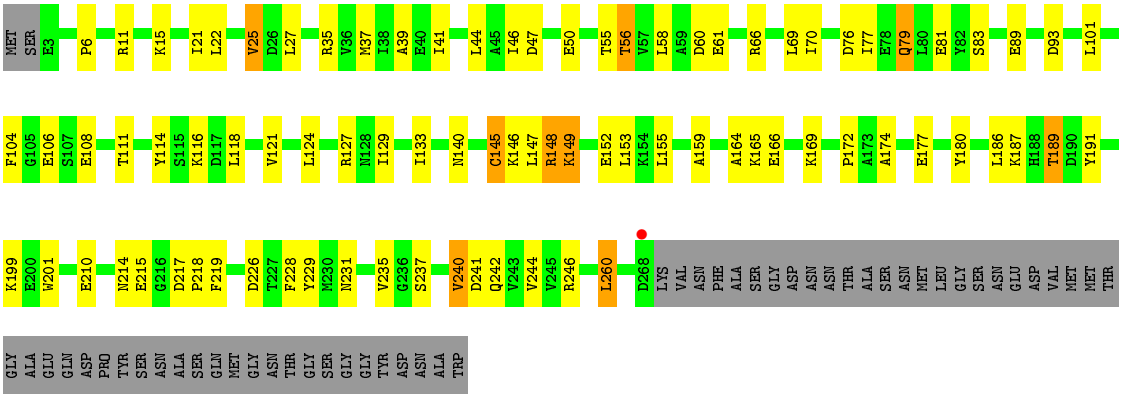
Chain B:





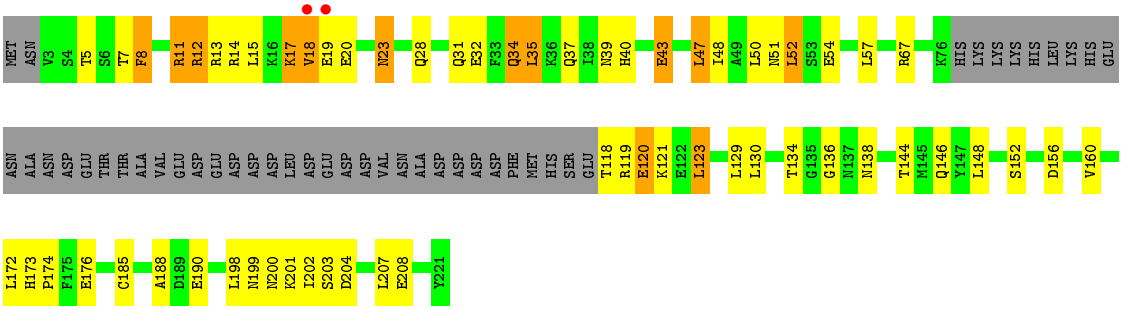
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



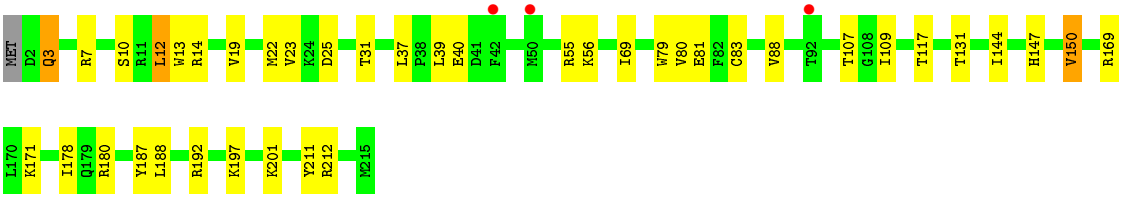
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



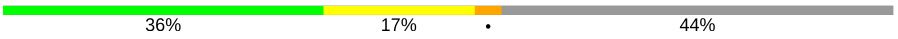
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

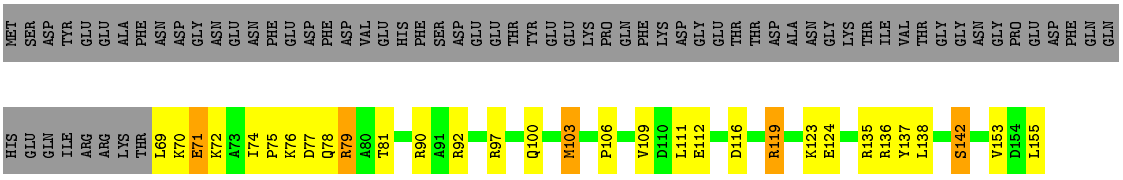
Chain E:



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

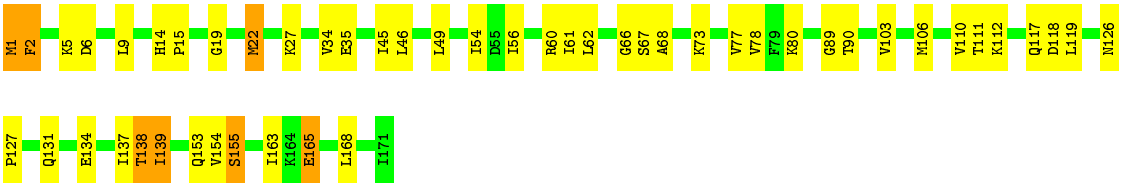
Chain F:





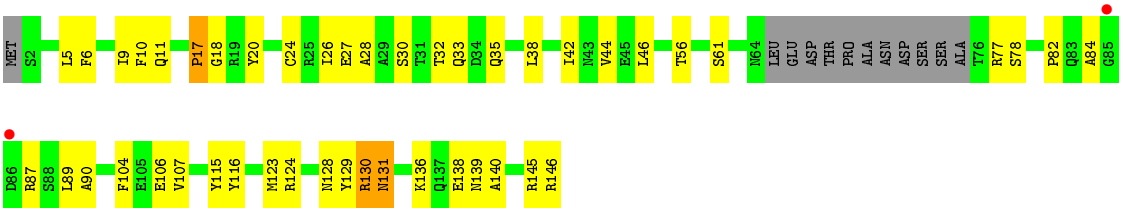
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



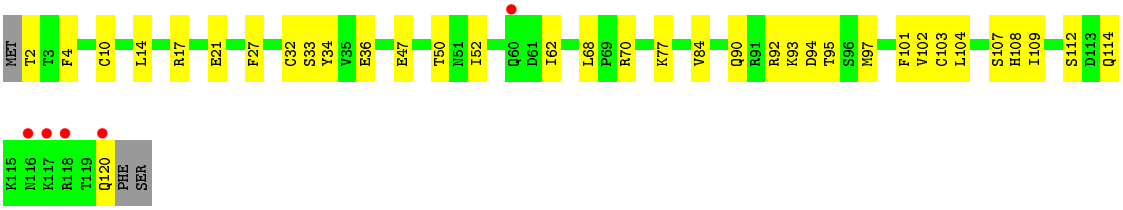
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



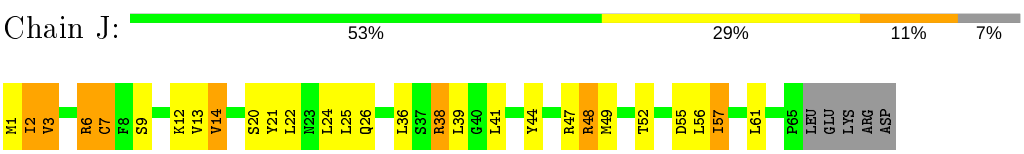
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



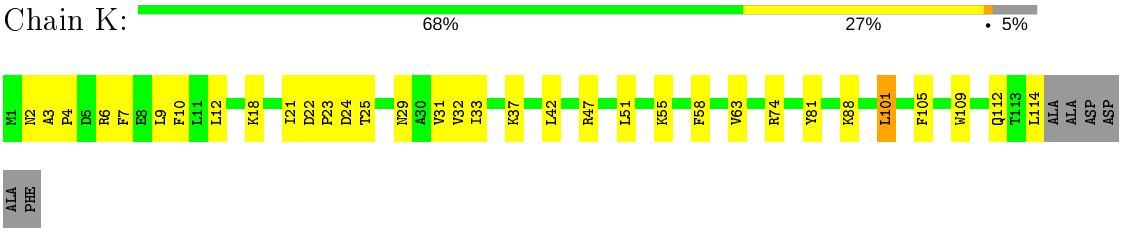
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



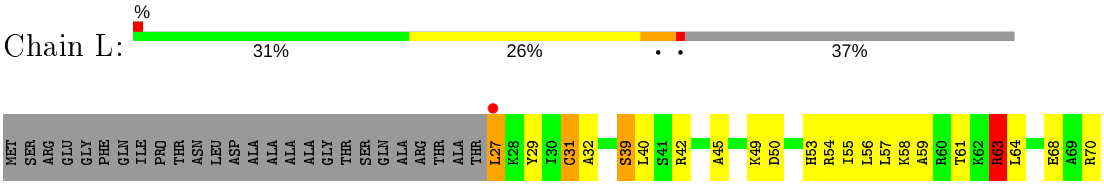
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



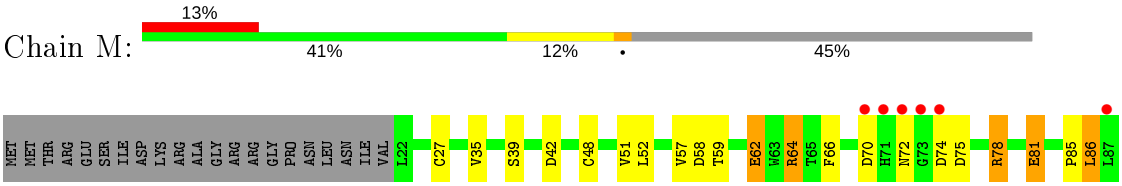
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:



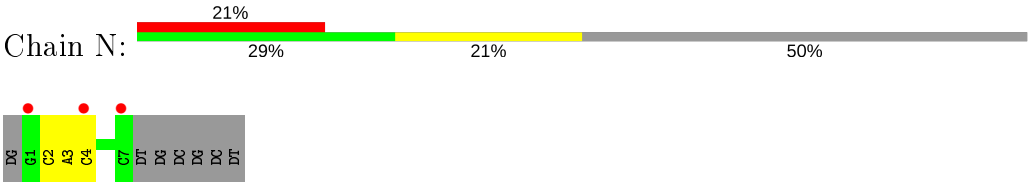
• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

Chain M:



• Molecule 14: 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*CP*TP)-3'

Chain N:

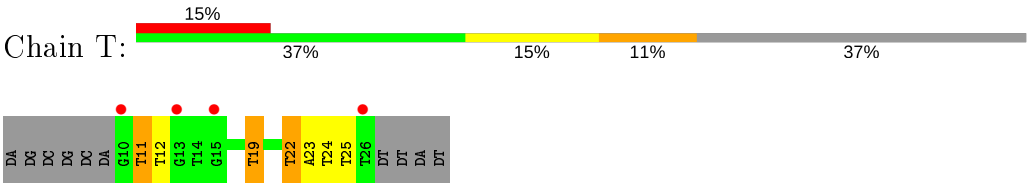


• Molecule 15: 5'-R(*AP*UP*AP*UP*CP*AP)-3'

Chain P:

• Molecule 16: 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP*CP*TP *AP*TP*GP*AP*TP*AP*TP*TP*TP*TP*TP*AP*TP)-3'

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.17Å 386.01Å 254.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 3.60 49.33 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-3.60) 100.0 (49.33-3.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.225 0.182 , 0.226	Depositor DCC
R_{free} test set	2520 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	87.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 99.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	33420	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: 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	0.38	0/11372	0.59	1/15380 (0.0%)
2	B	0.36	0/9271	0.56	0/12505
3	C	0.42	0/2133	0.58	0/2891
4	D	0.38	0/1444	0.59	0/1935
5	E	0.32	0/1788	0.51	0/2406
6	F	0.41	0/717	0.63	0/967
7	G	0.43	0/1368	0.61	0/1844
8	H	0.35	0/1094	0.55	0/1481
9	I	0.32	0/989	0.50	0/1331
10	J	0.45	0/541	0.70	1/727 (0.1%)
11	K	0.40	0/937	0.53	0/1265
12	L	0.41	0/353	0.58	0/468
13	M	0.29	0/1373	0.47	0/1863
14	N	0.63	0/156	1.06	0/238
15	P	0.32	0/137	0.81	0/211
16	T	0.62	0/390	1.37	3/601 (0.5%)
All	All	0.38	0/34063	0.59	5/46113 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	19	DT	O4'-C4'-C3'	-7.33	101.57	104.50
1	A	58	LEU	CA-CB-CG	5.74	128.51	115.30
16	T	22	DT	O4'-C1'-N1	5.73	112.01	108.00
10	J	3	VAL	CB-CA-C	-5.61	100.74	111.40
16	T	11	DT	N3-C4-O4	5.18	123.01	119.90

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	11170	0	11222	271	0
2	B	9095	0	9055	196	0
3	C	2095	0	2051	54	0
4	D	1434	0	1460	38	0
5	E	1752	0	1776	21	0
6	F	705	0	731	20	0
7	G	1340	0	1357	35	0
8	H	1076	0	1046	25	0
9	I	971	0	927	15	0
10	J	532	0	542	23	0
11	K	919	0	929	19	0
12	L	351	0	374	17	0
13	M	1357	0	1263	27	0
14	N	139	0	79	2	0
15	P	123	0	66	1	0
16	T	350	0	197	6	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	M	1	0	0	0	0
18	A	2	0	0	0	0
All	All	33420	0	33075	674	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 (674) 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)
7:G:1:MET:HE3	7:G:80:LYS:H	1.15	1.04
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.30	0.95
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.36	0.90
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.59	0.84
2:B:470:LYS:HB2	2:B:471:LYS:HB2	1.58	0.84
1:A:53:LEU:HD23	1:A:54:ASN:H	1.44	0.83
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.43	0.83
13:M:66:PHE:O	13:M:78:ARG:NH2	2.12	0.83
1:A:1329:THR:HG22	1:A:1331:SER:H	1.41	0.83
1:A:68:GLN:O	1:A:68:GLN:NE2	2.11	0.83
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.61	0.81
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.63	0.81
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.62	0.80
3:C:66:ARG:NH2	10:J:3:VAL:O	2.15	0.78
2:B:843:GLN:HB2	2:B:993:THR:HB	1.66	0.75
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.51	0.75
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.20	0.75
1:A:412:ARG:NH1	13:M:42:ASP:OD2	2.19	0.75
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.66	0.75
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.16	0.74
7:G:1:MET:HE3	7:G:80:LYS:N	1.98	0.74
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.68	0.74
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.20	0.73
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.73
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.70	0.73
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.71	0.72
1:A:50:ILE:O	1:A:52:GLY:N	2.22	0.72
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.23	0.72
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.72	0.71
4:D:134:THR:HG23	4:D:136:GLY:H	1.56	0.71
2:B:429:PHE:HA	2:B:432:MET:HE2	1.73	0.71
4:D:123:LEU:HD11	4:D:146:GLN:HG2	1.72	0.71
4:D:12:ARG:HD3	4:D:14:ARG:HG2	1.74	0.69
2:B:530:GLY:O	2:B:532:ALA:N	2.23	0.69
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.72	0.69
7:G:1:MET:CE	7:G:80:LYS:H	2.02	0.69
1:A:320:ARG:NH2	13:M:81:GLU:HG3	2.08	0.68
1:A:53:LEU:CD2	1:A:54:ASN:H	2.06	0.68
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.75	0.68
1:A:1063:MET:O	1:A:1065:GLY:N	2.27	0.68
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.28	0.68
13:M:70:ASP:HB3	13:M:78:ARG:HD2	1.75	0.68
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.76	0.67
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.26	0.67
3:C:93:ASP:O	3:C:127:ARG:NH2	2.28	0.66
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.78	0.66
1:A:69:THR:HG22	2:B:1174:LYS:HD3	1.76	0.66
1:A:311:GLN:HG3	1:A:312:PRO:HD2	1.77	0.66
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.78	0.66
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.76	0.66
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.76	0.66
1:A:46:THR:HG22	1:A:47:ARG:H	1.61	0.65
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.77	0.65
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.61	0.65
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.77	0.65
1:A:57:ARG:O	1:A:68:GLN:HG2	1.96	0.65
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.79	0.65
1:A:316:GLN:O	1:A:318:SER:N	2.30	0.65
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.79	0.64
4:D:51:ASN:ND2	4:D:54:GLU:OE1	2.30	0.64
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.29	0.64
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.80	0.64
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.31	0.64
8:H:128:ASN:O	8:H:131:ASN:ND2	2.30	0.64
2:B:68:THR:HG22	2:B:91:SER:HA	1.80	0.64
1:A:711:ARG:HE	9:I:97:MET:HG3	1.63	0.64
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.31	0.64
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.78	0.64
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.80	0.63
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.79	0.63
2:B:806:THR:HG22	2:B:808:ALA:H	1.64	0.63
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.32	0.63
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.80	0.63
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.79	0.63
2:B:614:SER:HB3	2:B:627:PHE:HB2	1.81	0.63
1:A:709:THR:HG23	9:I:94:ASP:HA	1.79	0.63
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.81	0.62
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.81	0.62
2:B:917:PRO:HA	2:B:934:LYS:HB3	1.80	0.62
2:B:486:TYR:HB3	2:B:1096:ARG:HH12	1.63	0.62
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.82	0.62
8:H:130:ARG:H	8:H:130:ARG:HD3	1.64	0.62
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:OE1	1:A:816:HIS:ND1	2.26	0.62
8:H:6:PHE:HD1	8:H:130:ARG:HG2	1.65	0.62
10:J:1:MET:H2	10:J:56:LEU:H	1.48	0.62
16:T:24:DT:H2"	16:T:25:DT:H5'	1.80	0.61
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.66	0.61
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.82	0.61
1:A:707:GLY:O	1:A:1281:ARG:NH1	2.33	0.61
5:E:12:LEU:HD21	5:E:55:ARG:HH21	1.64	0.61
2:B:894:ASP:OD2	12:L:58:LYS:NZ	2.34	0.61
1:A:66:LYS:HE2	1:A:68:GLN:H	1.64	0.61
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.82	0.61
1:A:68:GLN:O	1:A:70:CYS:N	2.31	0.61
4:D:52:LEU:O	4:D:54:GLU:N	2.34	0.61
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.84	0.60
4:D:148:LEU:O	4:D:152:SER:OG	2.17	0.60
1:A:534:LEU:O	1:A:574:GLY:HA3	2.02	0.60
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.83	0.60
4:D:12:ARG:NH2	4:D:13:ARG:O	2.34	0.60
3:C:56:THR:HB	3:C:58:LEU:H	1.66	0.60
1:A:230:ARG:HD2	1:A:233:TRP:CZ2	2.36	0.60
2:B:205:ILE:HD11	2:B:461:LEU:HD13	1.82	0.60
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.84	0.60
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.83	0.59
2:B:651:LEU:H	2:B:651:LEU:HD23	1.67	0.59
13:M:197:HIS:H	13:M:198:VAL:HA	1.67	0.59
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.84	0.59
2:B:654:ARG:H	2:B:657:HIS:HD2	1.47	0.59
1:A:567:LYS:HG3	1:A:568:PRO:HA	1.84	0.59
1:A:523:ILE:HG13	1:A:622:VAL:HG22	1.84	0.59
1:A:53:LEU:HD23	1:A:54:ASN:N	2.15	0.59
1:A:845:LEU:HA	1:A:848:ILE:HD13	1.85	0.59
2:B:874:PHE:O	12:L:42:ARG:NH2	2.31	0.59
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.85	0.59
9:I:50:THR:H	9:I:92:ARG:HH22	1.51	0.59
2:B:486:TYR:HA	2:B:1096:ARG:HH22	1.69	0.58
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.36	0.58
10:J:1:MET:N	10:J:56:LEU:H	2.01	0.58
1:A:304:MET:HG2	2:B:1210:MET:HG2	1.86	0.58
1:A:1329:THR:HG22	1:A:1331:SER:N	2.15	0.58
2:B:311:LEU:HB3	9:I:4:PHE:CZ	2.38	0.58
1:A:1387:HIS:HA	1:A:1391:ARG:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.39	0.58
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.86	0.57
4:D:52:LEU:HB3	4:D:148:LEU:HD23	1.85	0.57
4:D:23:ASN:N	4:D:23:ASN:OD1	2.36	0.57
1:A:1188:GLN:HG2	1:A:1243:VAL:HG12	1.87	0.57
1:A:535:THR:HG21	1:A:617:VAL:H	1.70	0.57
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.85	0.57
1:A:1303:GLU:OE2	1:A:1326:ARG:NH2	2.31	0.57
4:D:67:ARG:HH21	4:D:129:LEU:HD13	1.68	0.57
14:N:2:DC:H2'	14:N:3:DA:C8	2.40	0.57
2:B:834:ASN:HB2	2:B:839:MET:HA	1.86	0.56
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.86	0.56
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.87	0.56
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.39	0.56
7:G:1:MET:SD	7:G:2:PHE:N	2.62	0.56
2:B:996:ARG:NH2	3:C:174:ALA:O	2.38	0.56
1:A:709:THR:HB	1:A:712:GLU:H	1.69	0.56
1:A:253:ASN:O	1:A:255:SER:N	2.38	0.56
2:B:1037:LEU:O	10:J:47:ARG:NH1	2.39	0.56
1:A:715:GLU:O	1:A:719:VAL:HG23	2.06	0.56
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.56
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.87	0.56
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.56
2:B:685:LEU:HD12	2:B:690:VAL:HG23	1.88	0.55
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.71	0.55
1:A:197:PRO:HG2	1:A:199:LEU:HD11	1.87	0.55
1:A:275:SER:OG	13:M:117:ASN:OD1	2.24	0.55
2:B:1113:VAL:HG23	13:M:57:VAL:HG11	1.88	0.55
1:A:257:ARG:HH11	1:A:257:ARG:HB2	1.71	0.55
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.87	0.55
1:A:858:ASN:ND2	1:A:862:ASN:HB2	2.22	0.55
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.87	0.55
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.88	0.55
8:H:9:ILE:HG13	8:H:56:THR:HG23	1.88	0.55
1:A:858:ASN:H	1:A:858:ASN:HD22	1.54	0.55
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.89	0.55
1:A:915:SER:O	1:A:919:ILE:HB	2.07	0.55
2:B:287:ARG:NH1	2:B:321:GLY:O	2.40	0.54
2:B:731:VAL:O	2:B:734:HIS:NE2	2.40	0.54
2:B:900:ALA:HB3	12:L:61:THR:HG22	1.87	0.54
2:B:831:SER:HG	2:B:994:TYR:HE2	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HG2	1:A:321:PRO:HD2	1.89	0.54
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.07	0.54
13:M:75:ASP:HB3	13:M:78:ARG:HB3	1.89	0.54
1:A:33:ALA:HA	1:A:57:ARG:HD3	1.89	0.54
9:I:102:VAL:HG22	9:I:109:ILE:HG13	1.90	0.54
1:A:34:LYS:H	1:A:57:ARG:HH11	1.55	0.54
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.06	0.54
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.40	0.54
10:J:44:TYR:HA	10:J:47:ARG:HG3	1.89	0.54
13:M:58:ASP:O	13:M:62:GLU:HB2	2.08	0.54
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.89	0.54
2:B:235:SER:HA	2:B:261:ARG:HH21	1.72	0.54
2:B:642:ASP:HA	2:B:649:LYS:HA	1.89	0.54
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.90	0.53
1:A:42:ASP:OD1	1:A:46:THR:N	2.41	0.53
2:B:586:TRP:NE1	2:B:588:GLY:O	2.39	0.53
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.90	0.53
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.90	0.53
1:A:709:THR:HG22	1:A:711:ARG:H	1.72	0.53
2:B:487:THR:HG22	2:B:489:SER:H	1.72	0.53
1:A:1397:LEU:HB3	1:A:1429:ILE:HD12	1.90	0.53
2:B:603:LEU:HB3	2:B:609:ILE:HG23	1.89	0.53
1:A:589:GLN:HG3	1:A:606:LEU:HD13	1.90	0.53
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.90	0.53
3:C:145:CYS:SG	3:C:146:LYS:N	2.81	0.53
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.91	0.53
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.90	0.53
7:G:153:GLN:O	7:G:155:SER:N	2.41	0.53
1:A:568:PRO:HG2	8:H:46:LEU:HD22	1.91	0.53
2:B:278:GLN:OE1	2:B:337:ARG:NH1	2.41	0.53
2:B:953:LEU:HB3	12:L:57:LEU:HD23	1.91	0.53
2:B:241:ARG:HA	2:B:253:THR:HG22	1.91	0.53
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.39	0.53
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.74	0.53
1:A:705:LYS:NZ	1:A:716:ASP:OD2	2.42	0.53
3:C:76:ASP:HB3	3:C:79:GLN:HG3	1.90	0.52
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.42	0.52
1:A:998:LEU:HA	1:A:1011:GLN:HE22	1.75	0.52
1:A:320:ARG:HH22	13:M:81:GLU:HG3	1.74	0.52
1:A:830:LYS:O	1:A:834:THR:HB	2.10	0.52
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.73	0.52
1:A:33:ALA:HB2	1:A:57:ARG:HB2	1.90	0.52
2:B:493:SER:OG	2:B:526:GLU:OE2	2.22	0.52
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.92	0.52
1:A:722:LEU:HG	1:A:799:PHE:CD1	2.45	0.52
2:B:260:GLY:O	2:B:267:ARG:NH1	2.42	0.52
2:B:750:GLY:O	2:B:754:SER:OG	2.19	0.52
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.91	0.52
5:E:80:VAL:HG22	5:E:109:ILE:HB	1.92	0.52
2:B:90:ILE:HD11	2:B:134:LYS:HE2	1.91	0.52
2:B:591:ARG:O	2:B:593:PRO:HD3	2.09	0.52
13:M:157:CYS:HB3	13:M:210:MET:HE2	1.92	0.52
1:A:800:VAL:HG22	1:A:812:GLU:HG2	1.92	0.51
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.92	0.51
13:M:196:ILE:HG13	13:M:197:HIS:HB3	1.92	0.51
1:A:1080:THR:HB	1:A:1082:ASN:HB2	1.93	0.51
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.91	0.51
16:T:22:DT:H2'	16:T:23:DA:C8	2.45	0.51
1:A:830:LYS:HE2	1:A:1098:VAL:HB	1.91	0.51
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.75	0.51
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.51
3:C:55:THR:HG1	3:C:152:GLU:H	1.54	0.51
5:E:10:SER:O	5:E:14:ARG:HG2	2.10	0.51
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.91	0.51
1:A:1081:LEU:HA	1:A:1082:ASN:C	2.30	0.51
1:A:344:ARG:HD2	2:B:1118:PRO:O	2.09	0.51
6:F:100:GLN:HE22	7:G:61:ILE:HD13	1.75	0.51
5:E:169:ARG:HH12	6:F:74:ILE:HD11	1.76	0.51
8:H:84:ALA:HA	8:H:87:ARG:HG2	1.91	0.51
1:A:443:LEU:HD11	1:A:455:MET:HB3	1.92	0.51
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.92	0.51
4:D:198:LEU:O	4:D:200:ASN:N	2.43	0.51
1:A:120:GLU:HG3	1:A:123:ARG:HH12	1.76	0.51
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.93	0.51
7:G:15:PRO:HD3	7:G:67:SER:HA	1.92	0.51
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.93	0.51
3:C:148:ARG:HG2	3:C:149:LYS:H	1.76	0.51
6:F:77:ASP:O	6:F:78:GLN:HB2	2.11	0.51
2:B:338:GLY:HA3	2:B:351:TYR:HE2	1.76	0.51
1:A:524:VAL:HG12	1:A:525:GLN:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:574:SER:OG	2:B:591:ARG:NH1	2.44	0.50
1:A:369:SER:HB3	11:K:2:ASN:ND2	2.21	0.50
10:J:1:MET:H2	10:J:56:LEU:N	2.08	0.50
1:A:67:CYS:O	1:A:70:CYS:HB3	2.11	0.50
2:B:557:PHE:O	2:B:561:TRP:HD1	1.93	0.50
1:A:858:ASN:HD21	1:A:862:ASN:HB2	1.77	0.50
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.47	0.50
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.76	0.50
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.27	0.50
1:A:55:ASP:HA	1:A:58:LEU:H	1.76	0.50
1:A:933:TYR:O	1:A:937:VAL:HG13	2.11	0.50
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.47	0.50
3:C:104:PHE:CD2	3:C:106:GLU:HG3	2.47	0.50
12:L:27:LEU:HA	12:L:39:SER:HB2	1.94	0.50
1:A:7:SER:HB2	2:B:1175:LEU:HD22	1.94	0.50
2:B:901:PRO:O	12:L:61:THR:HG23	2.13	0.49
4:D:173:HIS:CG	4:D:174:PRO:HD2	2.47	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.93	0.49
1:A:1112:LYS:O	1:A:1114:PRO:HD3	2.12	0.49
1:A:846:GLU:OE2	2:B:1135:ARG:NH2	2.45	0.49
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.76	0.49
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.94	0.49
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.94	0.49
4:D:118:THR:HG21	4:D:121:LYS:HE3	1.94	0.49
7:G:118:ASP:N	7:G:118:ASP:OD1	2.42	0.49
4:D:130:LEU:O	4:D:134:THR:HG22	2.13	0.49
1:A:1244:ARG:HD2	1:A:1244:ARG:O	2.12	0.49
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.12	0.49
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.47	0.49
2:B:801:LYS:O	10:J:52:THR:HG23	2.11	0.49
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.12	0.49
2:B:299:GLU:OE2	2:B:572:HIS:ND1	2.38	0.49
2:B:324:ILE:HG13	2:B:329:THR:HG22	1.93	0.49
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.93	0.49
1:A:406:ILE:HG12	1:A:412:ARG:HG3	1.94	0.49
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.48	0.49
2:B:705:MET:H	2:B:710:LEU:HG	1.78	0.49
1:A:412:ARG:O	13:M:51:VAL:HG12	2.13	0.49
3:C:104:PHE:HD2	3:C:106:GLU:HG3	1.78	0.49
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.48	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:129:TYR:CD2	8:H:130:ARG:HG3	2.48	0.48
2:B:120:ARG:HH12	12:L:54:ARG:HH11	1.61	0.48
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.78	0.48
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.45	0.48
2:B:303:TYR:CD1	2:B:571:PRO:HB3	2.35	0.48
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.95	0.48
9:I:103:CYS:O	9:I:107:SER:HA	2.12	0.48
1:A:280:GLU:HG2	1:A:289:ILE:HD13	1.96	0.48
2:B:441:ASP:O	2:B:443:ASN:N	2.46	0.48
4:D:118:THR:O	4:D:120:GLU:N	2.42	0.48
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.48	0.48
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.96	0.48
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.95	0.48
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.12	0.48
1:A:535:THR:HG21	1:A:617:VAL:N	2.28	0.48
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.48
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.12	0.48
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.96	0.48
1:A:285:PRO:O	1:A:287:HIS:N	2.46	0.48
2:B:242:SER:OG	2:B:362:PRO:HD2	2.12	0.48
2:B:345:LYS:O	2:B:347:LYS:HG2	2.14	0.48
3:C:58:LEU:HD12	3:C:145:CYS:HB2	1.95	0.48
6:F:76:LYS:O	6:F:79:ARG:HD3	2.13	0.48
15:P:7:A:H2'	15:P:8:U:O4'	2.14	0.48
1:A:1083:THR:OG1	1:A:1084:PHE:N	2.43	0.48
1:A:405:VAL:HG22	1:A:432:VAL:HG22	1.95	0.48
1:A:71:GLN:O	1:A:73:GLY:N	2.47	0.48
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.47	0.48
3:C:69:LEU:O	10:J:6:ARG:NH1	2.43	0.47
13:M:196:ILE:HA	13:M:197:HIS:HA	1.65	0.47
1:A:1120:LEU:HD13	1:A:1125:ALA:HA	1.96	0.47
1:A:275:SER:O	1:A:279:LEU:HD12	2.14	0.47
13:M:136:LEU:HD21	13:M:196:ILE:HG22	1.96	0.47
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.96	0.47
2:B:640:VAL:HG22	2:B:651:LEU:HB3	1.95	0.47
3:C:180:TYR:HB3	3:C:228:PHE:CD1	2.49	0.47
1:A:257:ARG:HB2	1:A:257:ARG:NH1	2.29	0.47
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.95	0.47
7:G:127:PRO:HD2	7:G:138:THR:HG21	1.96	0.47
7:G:1:MET:CE	7:G:2:PHE:H	2.27	0.47
8:H:77:ARG:HG2	8:H:78:SER:H	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.27	0.47
1:A:110:CYS:SG	1:A:167:CYS:HB3	2.54	0.47
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.49	0.47
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.96	0.47
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.30	0.47
1:A:1211:GLN:NE2	1:A:1274:ARG:HD2	2.29	0.47
1:A:420:ARG:HB2	1:A:423:ASP:HB3	1.96	0.47
1:A:67:CYS:C	1:A:68:GLN:HG3	2.35	0.47
1:A:852:TYR:CZ	6:F:136:ARG:HG2	2.50	0.47
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.50	0.47
2:B:1165:ILE:HD13	4:D:17:LYS:HB3	1.97	0.47
16:T:22:DT:H2'	16:T:23:DA:H8	1.80	0.47
1:A:836:TYR:OH	1:A:1403:GLU:OE2	2.12	0.47
3:C:148:ARG:HG2	3:C:149:LYS:N	2.30	0.47
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.55	0.47
8:H:5:LEU:HD11	8:H:61:SER:HB3	1.96	0.47
1:A:482:PHE:O	2:B:989:THR:HG23	2.15	0.47
8:H:26:ILE:HD13	8:H:42:ILE:HD12	1.96	0.47
1:A:260:ASP:OD1	1:A:328:ARG:NH2	2.42	0.46
1:A:448:PRO:HB3	16:T:19:DT:H1'	1.97	0.46
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.46
2:B:654:ARG:H	2:B:657:HIS:CD2	2.31	0.46
3:C:127:ARG:O	3:C:129:ILE:HG22	2.15	0.46
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.98	0.46
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.97	0.46
1:A:852:TYR:O	6:F:81:THR:HG22	2.15	0.46
1:A:1420:ASP:HB3	2:B:1222:ARG:HH11	1.80	0.46
7:G:138:THR:HG22	7:G:139:ILE:H	1.80	0.46
13:M:193:GLN:HG2	13:M:198:VAL:HG12	1.97	0.46
13:M:72:ASN:ND2	13:M:74:ASP:OD2	2.47	0.46
1:A:89:PRO:HG2	1:A:204:THR:HB	1.97	0.46
2:B:242:SER:HB2	2:B:363:HIS:HB3	1.97	0.46
2:B:791:THR:OG1	2:B:791:THR:O	2.26	0.46
6:F:97:ARG:NH2	6:F:106:PRO:O	2.48	0.46
1:A:573:SER:OG	1:A:576:GLN:HB2	2.15	0.46
1:A:34:LYS:N	1:A:57:ARG:HH11	2.13	0.46
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.97	0.46
2:B:555:ILE:HA	2:B:558:LEU:HD12	1.97	0.46
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.97	0.46
10:J:7:CYS:HA	10:J:49:MET:HG2	1.96	0.46
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:THR:O	1:A:685:GLU:HG3	2.15	0.46
3:C:15:LYS:O	3:C:240:VAL:HG22	2.15	0.46
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.51	0.46
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.16	0.46
2:B:903:VAL:HG23	12:L:61:THR:HG21	1.97	0.46
1:A:347:PHE:CE1	2:B:1107:ALA:HB1	2.51	0.46
12:L:53:HIS:CD2	12:L:54:ARG:H	2.34	0.46
13:M:85:PRO:HA	13:M:89:GLY:O	2.15	0.46
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.15	0.46
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.43	0.46
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.16	0.46
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.98	0.46
2:B:122:LEU:HD22	2:B:958:GLN:HG2	1.97	0.46
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.97	0.46
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.64	0.46
7:G:119:LEU:HD21	7:G:137:ILE:HD12	1.97	0.46
1:A:472:LEU:O	1:A:475:THR:HB	2.16	0.45
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.20	0.45
1:A:348:SER:OG	2:B:1128:LEU:HG	2.17	0.45
3:C:148:ARG:HH11	3:C:149:LYS:HE3	1.81	0.45
1:A:58:LEU:HD22	1:A:80:HIS:O	2.16	0.45
1:A:587:HIS:HB2	1:A:969:GLN:NE2	2.31	0.45
2:B:1081:LEU:O	3:C:189:THR:HG23	2.16	0.45
4:D:39:ASN:ND2	4:D:43:GLU:OE2	2.49	0.45
2:B:311:LEU:HB3	9:I:4:PHE:HZ	1.79	0.45
10:J:48:ARG:HD3	10:J:49:MET:HE2	1.97	0.45
1:A:500:GLU:O	1:A:504:LEU:HB2	2.16	0.45
1:A:872:GLY:O	1:A:1057:VAL:HG13	2.16	0.45
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.49	0.45
6:F:103:MET:HE1	7:G:66:GLY:H	1.80	0.45
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.77	0.45
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.98	0.45
2:B:64:CYS:HA	2:B:67:SER:HB3	1.98	0.45
5:E:88:VAL:O	5:E:117:THR:OG1	2.32	0.45
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.98	0.45
13:M:64:ARG:NH2	16:T:25:DT:O4	2.49	0.45
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.17	0.45
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.81	0.45
2:B:278:GLN:HG2	2:B:337:ARG:HG2	1.98	0.45
2:B:840:ILE:HG21	2:B:999:MET:HE1	1.97	0.45
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:72:LYS:HB2	6:F:142:SER:HA	1.97	0.45
8:H:6:PHE:CD1	8:H:130:ARG:HG2	2.50	0.45
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.97	0.45
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.82	0.45
1:A:527:THR:HG21	1:A:650:GLN:HA	1.98	0.45
1:A:56:PRO:O	1:A:57:ARG:HG3	2.16	0.45
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.57	0.45
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.50	0.45
4:D:7:THR:OG1	4:D:8:PHE:N	2.48	0.45
10:J:20:SER:O	10:J:24:LEU:HG	2.17	0.45
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.99	0.45
2:B:486:TYR:HD2	2:B:1096:ARG:CZ	2.30	0.45
2:B:335:GLY:HA3	2:B:348:ARG:HB2	1.98	0.45
2:B:1224:PHE:HE1	5:E:171:LYS:HE3	1.82	0.45
1:A:351:THR:HB	2:B:1103:ILE:HG13	1.99	0.45
2:B:1224:PHE:CE1	5:E:171:LYS:HE3	2.52	0.45
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.52	0.45
8:H:130:ARG:CD	8:H:130:ARG:H	2.27	0.45
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.17	0.45
1:A:11:LEU:HD12	2:B:1193:GLN:O	2.17	0.45
1:A:70:CYS:O	1:A:72:GLU:HG2	2.17	0.45
3:C:148:ARG:NH1	3:C:149:LYS:HE3	2.32	0.44
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.52	0.44
1:A:1124:HIS:HB3	1:A:1130:GLN:CG	2.47	0.44
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.52	0.44
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.99	0.44
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.52	0.44
2:B:89:GLU:HB2	2:B:135:ARG:HB2	1.99	0.44
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.99	0.44
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.32	0.44
1:A:399:HIS:O	1:A:401:GLY:N	2.50	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44
2:B:273:LEU:HB3	2:B:276:ILE:HD12	2.00	0.44
2:B:684:LEU:CD2	2:B:689:LEU:HD12	2.47	0.44
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.33	0.44
7:G:1:MET:HE1	7:G:2:PHE:N	2.33	0.44
9:I:77:LYS:HD2	9:I:108:HIS:HB2	1.99	0.44
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.18	0.44
1:A:1163:ILE:HG13	1:A:1163:ILE:H	1.53	0.44
8:H:104:PHE:CE1	8:H:136:LYS:HA	2.53	0.44
13:M:193:GLN:HG2	13:M:198:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:GLN:O	1:A:842:VAL:HG23	2.18	0.44
4:D:34:GLN:HG3	4:D:34:GLN:H	1.58	0.44
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.00	0.44
6:F:138:LEU:HD23	6:F:138:LEU:HA	1.81	0.44
1:A:1213:GLY:HA3	1:A:1228:TRP:CE3	2.53	0.44
1:A:66:LYS:CE	1:A:68:GLN:H	2.31	0.44
2:B:249:ARG:HB2	2:B:249:ARG:NH1	2.33	0.44
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.52	0.44
4:D:11:ARG:HD3	4:D:12:ARG:N	2.33	0.44
7:G:165:GLU:HG2	7:G:168:LEU:HD12	1.99	0.44
7:G:89:GLY:HA3	7:G:103:VAL:HG22	1.99	0.44
16:T:11:DT:H2'	16:T:12:DT:C6	2.53	0.44
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.99	0.44
6:F:109:VAL:HG21	6:F:124:GLU:HA	2.00	0.44
13:M:189:PHE:O	13:M:193:GLN:HG3	2.18	0.44
1:A:1167:GLU:O	1:A:1170:ILE:HG13	2.18	0.43
1:A:1196:GLU:OE2	1:A:1235:LYS:HE2	2.17	0.43
1:A:535:THR:O	1:A:575:LYS:HE2	2.18	0.43
2:B:714:GLU:HB2	2:B:733:HIS:CE1	2.53	0.43
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43
1:A:33:ALA:HB1	1:A:56:PRO:HB2	2.00	0.43
2:B:1181:GLU:HA	2:B:1188:LYS:HA	2.00	0.43
2:B:915:THR:O	2:B:917:PRO:HD3	2.19	0.43
2:B:935:ARG:H	2:B:935:ARG:HD2	1.84	0.43
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.39	0.43
1:A:525:GLN:HG3	2:B:836:GLU:HG2	2.00	0.43
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.00	0.43
11:K:22:ASP:HA	11:K:23:PRO:HD3	1.88	0.43
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.54	0.43
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.00	0.43
1:A:507:VAL:N	1:A:508:PRO:HD2	2.33	0.43
4:D:172:LEU:HB3	4:D:176:GLU:OE1	2.18	0.43
9:I:34:TYR:CE2	9:I:36:GLU:HG2	2.54	0.43
2:B:542:MET:HG2	2:B:747:MET:HB3	2.00	0.43
2:B:955:THR:HG22	2:B:956:THR:N	2.34	0.43
7:G:126:ASN:HA	7:G:127:PRO:HA	1.91	0.43
13:M:27:CYS:SG	13:M:48:CYS:HB3	2.57	0.43
1:A:909:ASP:OD1	1:A:910:PRO:HD2	2.19	0.43
1:A:752:LYS:HD2	2:B:1019:SER:HB3	2.00	0.43
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	2.01	0.43
2:B:199:MET:N	2:B:199:MET:SD	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:CYS:HA	12:L:56:LEU:HD23	2.00	0.43
1:A:306:ASN:O	1:A:313:GLN:HG2	2.19	0.43
1:A:367:PRO:HD3	1:A:467:THR:O	2.17	0.43
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.19	0.43
3:C:56:THR:HG21	3:C:145:CYS:SG	2.59	0.43
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.83	0.43
4:D:12:ARG:CZ	4:D:14:ARG:HA	2.48	0.43
10:J:6:ARG:H	10:J:14:VAL:H	1.66	0.43
1:A:332:LYS:HA	1:A:337:ARG:HB2	2.00	0.43
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.01	0.43
2:B:684:LEU:HD23	2:B:689:LEU:HD12	2.01	0.43
3:C:47:ASP:HA	3:C:169:LYS:HZ2	1.83	0.43
1:A:1080:THR:C	1:A:1082:ASN:HB2	2.39	0.43
1:A:1116:LEU:HD22	1:A:1311:VAL:HG13	2.01	0.43
3:C:242:GLN:NE2	3:C:246:ARG:HH21	2.17	0.43
11:K:88:LYS:HE3	11:K:88:LYS:HB2	1.84	0.43
1:A:134:ARG:HD2	1:A:221:SER:O	2.19	0.42
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.86	0.42
2:B:125:SER:HA	2:B:171:PRO:HA	2.00	0.42
7:G:34:VAL:HG13	7:G:45:ILE:HG21	2.00	0.42
6:F:103:MET:CE	7:G:66:GLY:H	2.32	0.42
10:J:21:TYR:HB2	10:J:39:LEU:HD11	2.01	0.42
12:L:40:LEU:HD11	12:L:49:LYS:NZ	2.34	0.42
1:A:253:ASN:C	1:A:255:SER:H	2.22	0.42
2:B:470:LYS:CB	2:B:471:LYS:HB2	2.40	0.42
2:B:65:GLU:HG3	2:B:66:ASP:H	1.85	0.42
3:C:37:MET:HB2	3:C:37:MET:HE3	1.82	0.42
4:D:202:ILE:HD13	4:D:207:LEU:HB2	2.01	0.42
8:H:138:GLU:O	8:H:140:ALA:N	2.52	0.42
1:A:1108:ALA:HA	14:N:4:DC:OP1	2.19	0.42
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.00	0.42
1:A:152:VAL:O	1:A:162:VAL:N	2.50	0.42
1:A:663:SER:OG	1:A:664:THR:N	2.52	0.42
2:B:268:THR:HG21	2:B:270:LYS:HE2	2.01	0.42
2:B:370:PHE:HB3	2:B:373:ARG:HB2	2.02	0.42
2:B:43:LEU:HD11	2:B:812:LEU:HD23	2.02	0.42
7:G:110:VAL:HG11	7:G:163:ILE:HG23	2.01	0.42
1:A:42:ASP:O	1:A:44:THR:N	2.51	0.42
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.42
3:C:56:THR:HG23	3:C:147:LEU:HD23	2.00	0.42
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	2.01	0.42
1:A:332:LYS:HA	1:A:337:ARG:CB	2.49	0.42
1:A:4:GLN:NE2	1:A:76:GLU:OE2	2.51	0.42
1:A:774:ARG:H	1:A:774:ARG:HG2	1.62	0.42
1:A:884:ASP:O	1:A:886:ILE:N	2.53	0.42
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.53	0.42
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.00	0.42
10:J:57:ILE:O	10:J:61:LEU:HG	2.20	0.42
13:M:123:ASP:HA	13:M:126:VAL:HG23	2.02	0.42
1:A:230:ARG:HD2	1:A:233:TRP:CH2	2.53	0.42
2:B:361:LEU:HD11	2:B:381:MET:HE1	2.00	0.42
6:F:155:LEU:H	6:F:155:LEU:HD12	1.83	0.42
6:F:74:ILE:HA	6:F:75:PRO:HD2	1.78	0.42
4:D:32:GLU:O	7:G:5:LYS:NZ	2.53	0.42
12:L:29:TYR:CE2	12:L:58:LYS:HG2	2.54	0.42
1:A:1120:LEU:HA	1:A:1322:ILE:HA	2.00	0.42
1:A:167:CYS:SG	1:A:169:ASN:ND2	2.91	0.42
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.54	0.42
11:K:7:PHE:C	11:K:9:LEU:H	2.22	0.42
1:A:202:LEU:HB3	1:A:207:ILE:HD11	2.01	0.42
5:E:197:LYS:HG3	5:E:211:TYR:CE1	2.54	0.42
7:G:46:LEU:HA	7:G:46:LEU:HD23	1.87	0.42
10:J:38:ARG:HB2	10:J:38:ARG:NH1	2.35	0.42
12:L:61:THR:HB	12:L:63:ARG:HG3	2.02	0.42
1:A:332:LYS:O	1:A:333:GLU:HB2	2.19	0.42
1:A:365:GLY:O	1:A:468:PHE:HA	2.20	0.42
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.02	0.42
3:C:21:ILE:HD13	3:C:229:TYR:HE1	1.84	0.42
3:C:244:VAL:HG11	11:K:105:PHE:CE2	2.55	0.42
3:C:66:ARG:O	3:C:70:ILE:HG13	2.20	0.42
4:D:17:LYS:HD2	4:D:18:VAL:HG13	2.02	0.42
8:H:145:ARG:HE	8:H:146:ARG:NH1	2.17	0.42
1:A:954:TRP:HA	1:A:955:PRO:HD3	1.87	0.41
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.35	0.41
9:I:32:CYS:SG	9:I:33:SER:N	2.93	0.41
2:B:1202:LEU:HA	2:B:1202:LEU:HD22	1.73	0.41
2:B:637:LEU:HD23	2:B:742:GLU:HA	2.01	0.41
2:B:789:MET:HG3	2:B:953:LEU:HD21	2.02	0.41
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.41
8:H:18:GLY:O	8:H:20:TYR:N	2.44	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CZ2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:3:ALA:HA	11:K:4:PRO:HD3	1.87	0.41
1:A:34:LYS:H	1:A:57:ARG:NH1	2.17	0.41
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.55	0.41
4:D:185:CYS:SG	4:D:190:GLU:HG2	2.60	0.41
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.55	0.41
9:I:14:LEU:HB3	9:I:27:PHE:HB3	2.01	0.41
1:A:761:MET:HG3	2:B:1021:MET:HG2	2.01	0.41
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.50	0.41
2:B:522:VAL:HG11	2:B:537:LYS:HB3	2.02	0.41
3:C:210:GLU:HG3	3:C:229:TYR:OH	2.20	0.41
1:A:1339:LEU:HD23	5:E:144:ILE:HB	2.03	0.41
5:E:69:ILE:HG13	5:E:69:ILE:H	1.61	0.41
9:I:68:LEU:HD23	9:I:68:LEU:HA	1.92	0.41
1:A:270:LEU:O	1:A:274:ILE:HG13	2.19	0.41
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.47	0.41
11:K:63:VAL:HG23	11:K:63:VAL:O	2.21	0.41
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	2.02	0.41
1:A:262:LEU:HG	1:A:328:ARG:NH2	2.35	0.41
2:B:871:THR:HG22	2:B:872:GLU:O	2.20	0.41
2:B:955:THR:HG22	2:B:956:THR:H	1.85	0.41
3:C:50:GLU:OE1	12:L:64:LEU:HD13	2.21	0.41
11:K:112:GLN:H	11:K:112:GLN:HG2	1.67	0.41
1:A:404:TYR:CD1	1:A:414:ASP:HA	2.56	0.41
2:B:486:TYR:CA	2:B:1096:ARG:HH22	2.33	0.41
2:B:259:TYR:CE2	2:B:270:LYS:HD2	2.56	0.41
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.41
2:B:623:GLU:OE1	2:B:625:LYS:NZ	2.54	0.41
1:A:824:LEU:HD21	2:B:769:TYR:HE1	1.86	0.41
6:F:69:LEU:HB3	6:F:71:GLU:OE2	2.21	0.41
2:B:900:ALA:CB	12:L:61:THR:HG22	2.50	0.41
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.86	0.41
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.01	0.41
2:B:43:LEU:HA	2:B:43:LEU:HD23	1.91	0.41
3:C:165:LYS:O	11:K:6:ARG:NH1	2.54	0.41
10:J:38:ARG:HH11	10:J:38:ARG:HB2	1.85	0.41
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.86	0.41
1:A:401:GLY:H	1:A:435:HIS:HD2	1.68	0.41
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.51	0.41
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.02	0.41
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.56	0.41
5:E:56:LYS:NZ	5:E:83:CYS:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10:PHE:HA	11:K:37:LYS:HB3	2.03	0.41
1:A:227:VAL:HG12	4:D:15:LEU:HD23	2.03	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
1:A:401:GLY:C	1:A:435:HIS:CD2	2.94	0.41
2:B:1106:ARG:NH1	2:B:1126:GLY:HA2	2.36	0.41
2:B:190:TYR:CE2	2:B:196:PRO:HG3	2.55	0.41
2:B:221:ASN:OD1	2:B:242:SER:HA	2.21	0.41
10:J:6:ARG:HA	10:J:12:LYS:O	2.21	0.41
1:A:1120:LEU:CD1	1:A:1125:ALA:HA	2.50	0.41
1:A:1224:LEU:HD12	1:A:1242:VAL:H	1.85	0.41
1:A:148:CYS:O	1:A:168:GLY:HA2	2.21	0.41
1:A:34:LYS:HG2	1:A:36:ARG:NH1	2.36	0.41
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.86	0.41
3:C:124:LEU:O	3:C:127:ARG:HG2	2.20	0.41
3:C:235:VAL:HG11	10:J:6:ARG:HH21	1.86	0.41
5:E:19:VAL:O	5:E:23:VAL:HG23	2.21	0.41
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.56	0.41
9:I:50:THR:H	9:I:92:ARG:NH2	2.18	0.41
2:B:852:ARG:NH2	12:L:70:ARG:O	2.53	0.41
13:M:182:ARG:HE	13:M:182:ARG:HB2	1.77	0.41
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.03	0.40
1:A:255:SER:HB3	13:M:86:LEU:HD12	2.03	0.40
2:B:400:HIS:CD2	2:B:517:THR:HG21	2.56	0.40
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.02	0.40
2:B:685:LEU:HD21	2:B:692:TYR:CE2	2.57	0.40
3:C:260:LEU:O	3:C:260:LEU:HG	2.21	0.40
9:I:62:ILE:HG21	9:I:102:VAL:HG11	2.03	0.40
10:J:36:LEU:HD22	10:J:41:LEU:HD12	2.03	0.40
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	2.03	0.40
1:A:650:GLN:O	1:A:654:ASN:HB2	2.20	0.40
2:B:360:PHE:O	2:B:374:LYS:HD3	2.21	0.40
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.55	0.40
1:A:1120:LEU:HD12	1:A:1120:LEU:H	1.86	0.40
1:A:1319:VAL:HA	1:A:1320:PRO:HD3	1.91	0.40
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	2.03	0.40
1:A:1404:GLU:HB3	1:A:1408:ILE:HG13	2.02	0.40
1:A:360:GLU:OE2	1:A:644:LYS:NZ	2.50	0.40
1:A:420:ARG:NH1	1:A:424:ILE:HG12	2.36	0.40
1:A:426:LEU:HA	1:A:426:LEU:HD23	1.94	0.40
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.22	0.40
2:B:616:ILE:HD12	2:B:625:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:19:GLY:O	7:G:22:MET:HB2	2.21	0.40
8:H:30:SER:HB3	8:H:33:GLN:O	2.22	0.40
1:A:15:LYS:NZ	2:B:1220:ARG:HH21	2.19	0.40
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.82	0.40
1:A:590:ARG:NH1	1:A:592:ASP:OD1	2.55	0.40
1:A:853:ASP:N	1:A:853:ASP:OD1	2.41	0.40
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.03	0.40
4:D:57:LEU:HD12	4:D:160:VAL:HG21	2.03	0.40
13:M:199:LYS:O	13:M:201:LYS:N	2.54	0.40
1:A:1082:ASN:N	1:A:1082:ASN:OD1	2.54	0.40
1:A:205:GLU:CD	1:A:205:GLU:H	2.24	0.40
1:A:549:MET:CE	1:A:656:TRP:HD1	2.33	0.40
5:E:188:LEU:HD23	5:E:188:LEU:HA	1.92	0.40
10:J:1:MET:H1	10:J:56:LEU:HB2	1.86	0.40
13:M:137:CYS:SG	13:M:147:LYS:HG2	2.62	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	1409/1733 (81%)	1273 (90%)	104 (7%)	32 (2%)	6 38
2	B	1134/1224 (93%)	1016 (90%)	97 (9%)	21 (2%)	8 42
3	C	264/318 (83%)	245 (93%)	17 (6%)	2 (1%)	19 59
4	D	174/221 (79%)	157 (90%)	12 (7%)	5 (3%)	4 33
5	E	212/215 (99%)	200 (94%)	11 (5%)	1 (0%)	29 68
6	F	85/155 (55%)	81 (95%)	4 (5%)	0	100 100
7	G	169/171 (99%)	152 (90%)	15 (9%)	2 (1%)	13 51
8	H	130/146 (89%)	111 (85%)	15 (12%)	4 (3%)	4 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	9 45
10	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4 31
11	K	112/120 (93%)	107 (96%)	5 (4%)	0	100 100
12	L	42/70 (60%)	29 (69%)	8 (19%)	5 (12%)	0 5
13	M	185/345 (54%)	164 (89%)	19 (10%)	2 (1%)	14 53
All	All	4096/4910 (83%)	3691 (90%)	327 (8%)	78 (2%)	8 42

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	286	HIS
1	A	317	LYS
1	A	593	GLU
1	A	885	THR
1	A	1064	VAL
1	A	1083	THR
1	A	1084	PHE
1	A	1405	THR
2	B	442	PHE
2	B	531	GLN
2	B	708	GLU
2	B	1046	PRO
2	B	1108	ARG
4	D	5	THR
7	G	154	VAL
7	G	155	SER
8	H	139	ASN
13	M	200	THR
1	A	40	THR
1	A	44	THR
1	A	51	GLY
1	A	52	GLY
1	A	57	ARG
1	A	66	LYS
1	A	68	GLN
1	A	167	CYS
1	A	252	PHE
1	A	254	GLU
1	A	330	LYS

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Mol	Chain	Res	Type
1	A	424	ILE
1	A	1242	VAL
2	B	369	GLY
2	B	629	ASP
2	B	1096	ARG
2	B	1155	SER
4	D	199	ASN
8	H	17	PRO
8	H	82	PRO
10	J	2	ILE
12	L	45	ALA
1	A	54	ASN
1	A	1122	PRO
2	B	229	ALA
2	B	711	GLU
2	B	733	HIS
2	B	1222	ARG
3	C	214	ASN
4	D	52	LEU
8	H	90	ALA
10	J	6	ARG
12	L	63	ARG
1	A	69	THR
1	A	72	GLU
1	A	196	GLU
1	A	958	VAL
1	A	1255	GLU
2	B	441	ASP
2	B	1156	ASP
5	E	3	GLN
9	I	47	GLU
9	I	90	GLN
12	L	39	SER
12	L	59	ALA
1	A	1204	ASP
2	B	462	ALA
2	B	1181	GLU
3	C	11	ARG
4	D	119	ARG
12	L	50	ASP
1	A	35	ILE
2	B	251	ILE

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Mol	Chain	Res	Type
2	B	644	GLU
13	M	164	LYS
1	A	599	SER
2	B	292	ILE
2	B	992	ILE
4	D	18	VAL

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	1241/1520 (82%)	1112 (90%)	129 (10%)	7 33
2	B	980/1061 (92%)	886 (90%)	94 (10%)	8 37
3	C	234/274 (85%)	211 (90%)	23 (10%)	8 36
4	D	160/200 (80%)	140 (88%)	20 (12%)	4 25
5	E	196/197 (100%)	186 (95%)	10 (5%)	24 58
6	F	77/137 (56%)	67 (87%)	10 (13%)	4 24
7	G	152/152 (100%)	136 (90%)	16 (10%)	7 33
8	H	118/128 (92%)	109 (92%)	9 (8%)	13 45
9	I	113/116 (97%)	101 (89%)	12 (11%)	6 32
10	J	60/65 (92%)	49 (82%)	11 (18%)	1 10
11	K	99/102 (97%)	89 (90%)	10 (10%)	7 34
12	L	39/57 (68%)	35 (90%)	4 (10%)	7 34
13	M	136/299 (46%)	118 (87%)	18 (13%)	4 23
All	All	3605/4308 (84%)	3239 (90%)	366 (10%)	7 34

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	15	LYS

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Mol	Chain	Res	Type
1	A	22	PHE
1	A	41	MET
1	A	42	ASP
1	A	53	LEU
1	A	54	ASN
1	A	57	ARG
1	A	64	ASN
1	A	66	LYS
1	A	68	GLN
1	A	74	MET
1	A	80	HIS
1	A	93	VAL
1	A	113	LEU
1	A	146	MET
1	A	151	ASP
1	A	160	GLN
1	A	200	ARG
1	A	204	THR
1	A	220	THR
1	A	249	SER
1	A	257	ARG
1	A	265	LYS
1	A	277	GLU
1	A	279	LEU
1	A	307	ASP
1	A	311	GLN
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	369	SER
1	A	375	THR
1	A	385	ILE
1	A	408	ASP
1	A	419	LYS
1	A	420	ARG
1	A	434	ARG
1	A	443	LEU
1	A	451	HIS
1	A	463	ILE
1	A	474	VAL
1	A	475	THR

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Mol	Chain	Res	Type
1	A	479	ASN
1	A	493	GLN
1	A	504	LEU
1	A	517	ASN
1	A	524	VAL
1	A	527	THR
1	A	532	ARG
1	A	538	ASP
1	A	544	ASP
1	A	566	ILE
1	A	567	LYS
1	A	571	LEU
1	A	597	LEU
1	A	609	ASP
1	A	618	GLU
1	A	621	THR
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	636	GLU
1	A	644	LYS
1	A	666	ILE
1	A	685	GLU
1	A	691	LEU
1	A	710	LEU
1	A	722	LEU
1	A	732	LEU
1	A	756	ILE
1	A	768	GLN
1	A	774	ARG
1	A	795	GLU
1	A	805	LEU
1	A	821	ARG
1	A	830	LYS
1	A	834	THR
1	A	858	ASN
1	A	880	LYS
1	A	896	ARG
1	A	919	ILE
1	A	924	LYS
1	A	926	GLN
1	A	992	ASP

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Mol	Chain	Res	Type
1	A	998	LEU
1	A	1001	ARG
1	A	1030	ARG
1	A	1058	VAL
1	A	1079	MET
1	A	1081	LEU
1	A	1082	ASN
1	A	1084	PHE
1	A	1086	PHE
1	A	1093	LYS
1	A	1116	LEU
1	A	1117	THR
1	A	1120	LEU
1	A	1142	THR
1	A	1159	ARG
1	A	1170	ILE
1	A	1171	GLN
1	A	1196	GLU
1	A	1218	GLN
1	A	1222	ASN
1	A	1223	ASP
1	A	1227	ILE
1	A	1230	GLU
1	A	1259	MET
1	A	1260	LEU
1	A	1280	GLU
1	A	1290	LYS
1	A	1297	GLU
1	A	1299	VAL
1	A	1308	THR
1	A	1314	SER
1	A	1322	ILE
1	A	1333	ILE
1	A	1366	ARG
1	A	1391	ARG
1	A	1400	CYS
1	A	1405	THR
1	A	1406	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1442	ASP
1	A	1444	MET

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Mol	Chain	Res	Type
1	A	1445	ILE
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU
2	B	73	GLN
2	B	103	ASN
2	B	104	GLU
2	B	110	HIS
2	B	169	ARG
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	211	VAL
2	B	240	ILE
2	B	298	LEU
2	B	309	GLN
2	B	323	VAL
2	B	337	ARG
2	B	366	GLN
2	B	367	LEU
2	B	371	GLU
2	B	387	LEU
2	B	391	ASP
2	B	394	ASP
2	B	408	LEU
2	B	419	THR
2	B	440	HIS
2	B	442	PHE
2	B	476	ARG
2	B	479	VAL
2	B	485	ARG
2	B	502	ILE
2	B	531	GLN
2	B	544	CYS
2	B	547	VAL
2	B	549	THR
2	B	560	GLU
2	B	589	VAL
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG

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Mol	Chain	Res	Type
2	B	609	ILE
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	625	LYS
2	B	628	THR
2	B	629	ASP
2	B	651	LEU
2	B	706	GLN
2	B	733	HIS
2	B	764	SER
2	B	766	ARG
2	B	786	ASN
2	B	791	THR
2	B	805	THR
2	B	813	LYS
2	B	831	SER
2	B	844	SER
2	B	860	MET
2	B	879	ARG
2	B	933	SER
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	956	THR
2	B	959	ASP
2	B	967	ARG
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	989	THR
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1034	VAL
2	B	1056	SER
2	B	1057	LYS
2	B	1060	ARG
2	B	1065	GLN
2	B	1096	ARG
2	B	1106	ARG

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Mol	Chain	Res	Type
2	B	1108	ARG
2	B	1113	VAL
2	B	1119	VAL
2	B	1128	LEU
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1160	VAL
2	B	1183	LYS
2	B	1189	ILE
2	B	1202	LEU
3	C	25	VAL
3	C	56	THR
3	C	60	ASP
3	C	79	GLN
3	C	81	GLU
3	C	83	SER
3	C	89	GLU
3	C	108	GLU
3	C	111	THR
3	C	121	VAL
3	C	133	ILE
3	C	145	CYS
3	C	148	ARG
3	C	149	LYS
3	C	166	GLU
3	C	186	LEU
3	C	189	THR
3	C	199	LYS
3	C	215	GLU
3	C	226	ASP
3	C	237	SER
3	C	240	VAL
3	C	260	LEU
4	D	8	PHE
4	D	11	ARG
4	D	12	ARG
4	D	17	LYS
4	D	19	GLU
4	D	20	GLU
4	D	23	ASN
4	D	31	GLN

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Mol	Chain	Res	Type
4	D	34	GLN
4	D	35	LEU
4	D	43	GLU
4	D	47	LEU
4	D	48	ILE
4	D	50	LEU
4	D	120	GLU
4	D	123	LEU
4	D	156	ASP
4	D	201	LYS
4	D	203	SER
4	D	204	ASP
5	E	3	GLN
5	E	7	ARG
5	E	12	LEU
5	E	25	ASP
5	E	31	THR
5	E	37	LEU
5	E	40	GLU
5	E	107	THR
5	E	131	THR
5	E	150	VAL
6	F	70	LYS
6	F	71	GLU
6	F	79	ARG
6	F	90	ARG
6	F	103	MET
6	F	111	LEU
6	F	112	GLU
6	F	119	ARG
6	F	142	SER
6	F	153	VAL
7	G	1	MET
7	G	2	PHE
7	G	22	MET
7	G	56	ILE
7	G	60	ARG
7	G	62	LEU
7	G	90	THR
7	G	106	MET
7	G	111	THR
7	G	112	LYS

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Mol	Chain	Res	Type
7	G	117	GLN
7	G	131	GLN
7	G	134	GLU
7	G	138	THR
7	G	139	ILE
7	G	165	GLU
8	H	11	GLN
8	H	27	GLU
8	H	32	THR
8	H	35	GLN
8	H	89	LEU
8	H	106	GLU
8	H	107	VAL
8	H	130	ARG
8	H	131	ASN
9	I	2	THR
9	I	10	CYS
9	I	17	ARG
9	I	21	GLU
9	I	52	ILE
9	I	70	ARG
9	I	84	VAL
9	I	93	LYS
9	I	95	THR
9	I	104	LEU
9	I	114	GLN
9	I	120	GLN
10	J	2	ILE
10	J	7	CYS
10	J	9	SER
10	J	13	VAL
10	J	14	VAL
10	J	22	LEU
10	J	26	GLN
10	J	38	ARG
10	J	48	ARG
10	J	55	ASP
10	J	57	ILE
11	K	12	LEU
11	K	18	LYS
11	K	25	THR
11	K	29	ASN

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Mol	Chain	Res	Type
11	K	31	VAL
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	101	LEU
11	K	114	LEU
12	L	27	LEU
12	L	31	CYS
12	L	63	ARG
12	L	68	GLU
13	M	35	VAL
13	M	39	SER
13	M	52	LEU
13	M	59	THR
13	M	62	GLU
13	M	64	ARG
13	M	78	ARG
13	M	81	GLU
13	M	86	LEU
13	M	101	THR
13	M	114	GLN
13	M	142	LEU
13	M	145	ILE
13	M	168	MET
13	M	171	ILE
13	M	182	ARG
13	M	198	VAL
13	M	209	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	HIS
1	A	584	ASN
1	A	659	HIS
1	A	786	HIS
1	A	858	ASN
1	A	969	GLN
2	B	236	HIS
2	B	325	GLN
2	B	975	GLN
3	C	112	ASN

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Mol	Chain	Res	Type
4	D	51	ASN
5	E	153	HIS
11	K	2	ASN
12	L	53	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	5/6 (83%)	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	1419/1733 (81%)	-0.26	12 (0%) 86 75	47, 92, 160, 278	0
2	B	1150/1224 (93%)	-0.27	28 (2%) 59 42	49, 99, 176, 251	0
3	C	266/318 (83%)	-0.28	1 (0%) 92 86	49, 77, 123, 208	0
4	D	178/221 (80%)	-0.17	2 (1%) 80 68	63, 102, 166, 211	0
5	E	214/215 (99%)	0.07	3 (1%) 75 61	73, 130, 188, 213	0
6	F	87/155 (56%)	-0.42	0 100 100	58, 80, 123, 140	0
7	G	171/171 (100%)	-0.34	0 100 100	58, 81, 123, 136	0
8	H	134/146 (91%)	-0.03	2 (1%) 73 60	76, 120, 176, 222	0
9	I	119/122 (97%)	0.03	5 (4%) 36 23	90, 126, 199, 218	0
10	J	65/70 (92%)	-0.48	0 100 100	58, 79, 119, 152	0
11	K	114/120 (95%)	-0.25	0 100 100	57, 80, 129, 153	0
12	L	44/70 (62%)	-0.24	1 (2%) 60 44	80, 128, 181, 210	0
13	M	189/345 (54%)	1.03	44 (23%) 0 0	81, 170, 229, 272	0
14	N	7/14 (50%)	2.04	3 (42%) 0 0	200, 213, 233, 239	0
15	P	6/6 (100%)	1.01	0 100 100	169, 184, 220, 237	0
16	T	17/27 (62%)	1.28	4 (23%) 0 0	163, 197, 261, 274	0
All	All	4180/4957 (84%)	-0.17	105 (2%) 57 41	47, 97, 183, 278	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	73	GLY	5.6
13	M	72	ASN	5.5
1	A	422	GLY	5.2
1	A	69	THR	5.0
2	B	81	SER	4.7

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Mol	Chain	Res	Type	RSRZ
13	M	71	HIS	4.6
13	M	74	ASP	4.5
9	I	116	ASN	4.4
12	L	27	LEU	4.3
13	M	196	ILE	4.3
2	B	643	ASP	4.1
13	M	159	ASP	4.0
14	N	7	DC	3.9
2	B	77	HIS	3.8
1	A	421	ALA	3.8
13	M	172	MET	3.6
2	B	84	ILE	3.5
13	M	198	VAL	3.5
2	B	76	GLN	3.4
2	B	75	ALA	3.3
13	M	178	ILE	3.3
13	M	174	ALA	3.3
13	M	157	CYS	3.3
2	B	71	LEU	3.2
13	M	197	HIS	3.2
13	M	154	TYR	3.1
3	C	268	ASP	3.1
2	B	139	ALA	3.1
13	M	203	PHE	3.0
2	B	509	ALA	3.0
13	M	123	ASP	3.0
13	M	169	GLU	3.0
2	B	85	SER	3.0
9	I	120	GLN	2.9
13	M	177	LEU	2.9
1	A	1256	GLU	2.8
2	B	74	LEU	2.8
9	I	60	GLN	2.8
5	E	42	PHE	2.8
2	B	250	PHE	2.7
13	M	153	ALA	2.7
14	N	1	DG	2.7
13	M	162	THR	2.7
13	M	200	THR	2.7
1	A	154	SER	2.7
2	B	73	GLN	2.7
13	M	204	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	88	TYR	2.7
13	M	210	MET	2.6
13	M	167	SER	2.6
2	B	138	GLU	2.6
2	B	140	ILE	2.6
2	B	146	GLU	2.6
13	M	70	ASP	2.6
4	D	19	GLU	2.6
13	M	149	CYS	2.6
13	M	115	GLY	2.5
13	M	175	SER	2.5
13	M	158	HIS	2.5
1	A	155	GLU	2.5
2	B	83	ASN	2.5
13	M	171	ILE	2.5
2	B	137	TYR	2.4
1	A	161	LEU	2.4
2	B	608	ASP	2.4
8	H	86	ASP	2.4
13	M	165	GLY	2.4
2	B	134	LYS	2.4
14	N	4	DC	2.4
13	M	160	GLU	2.3
16	T	10	DG	2.3
2	B	82	ASP	2.3
16	T	26	DT	2.3
13	M	194	SER	2.3
1	A	423	ASP	2.3
13	M	148	ASP	2.3
2	B	86	ARG	2.3
9	I	118	ARG	2.3
2	B	80	GLU	2.3
13	M	116	LYS	2.3
1	A	156	ASP	2.3
2	B	868	MET	2.3
16	T	15	DG	2.3
13	M	88	ASP	2.3
13	M	183	ALA	2.2
2	B	709	ASP	2.2
9	I	117	LYS	2.2
16	T	13	DG	2.2
13	M	87	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
13	M	173	ALA	2.1
2	B	733	HIS	2.1
1	A	425	GLN	2.1
8	H	85	GLY	2.1
1	A	153	PRO	2.1
1	A	420	ARG	2.1
13	M	184	GLU	2.1
13	M	117	ASN	2.1
13	M	209	ILE	2.1
13	M	168	MET	2.1
4	D	18	VAL	2.0
13	M	152	GLU	2.0
5	E	92	THR	2.0
5	E	50	MET	2.0
2	B	70	ILE	2.0
13	M	206	THR	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. 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
18	MG	A	2458	1/1	0.78	0.25	109,109,109,109	0
18	MG	A	2459	1/1	0.80	0.74	104,104,104,104	0
17	ZN	M	1216	1/1	0.98	0.06	111,111,111,111	0
17	ZN	L	1071	1/1	0.98	0.07	162,162,162,162	0
17	ZN	J	1066	1/1	0.99	0.17	69,69,69,69	0
17	ZN	I	1122	1/1	0.99	0.04	145,145,145,145	0
17	ZN	A	2457	1/1	0.99	0.12	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	ZN	A	2456	1/1	1.00	0.05	118,118,118,118	0
17	ZN	B	2225	1/1	1.00	0.16	71,71,71,71	0
17	ZN	I	1121	1/1	1.00	0.09	109,109,109,109	0
17	ZN	C	1269	1/1	1.00	0.07	86,86,86,86	0

6.5 Other polymers

There are no such residues in this entry.