Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 09:49 PM EDT

PDB ID	:	5IP7
Title	:	Structure of RNA Polymerase II-Tfg1 peptide complex
Authors	:	Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on	:	2016-03-09
Resolution	:	3.52 Å(reported)

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

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

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

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

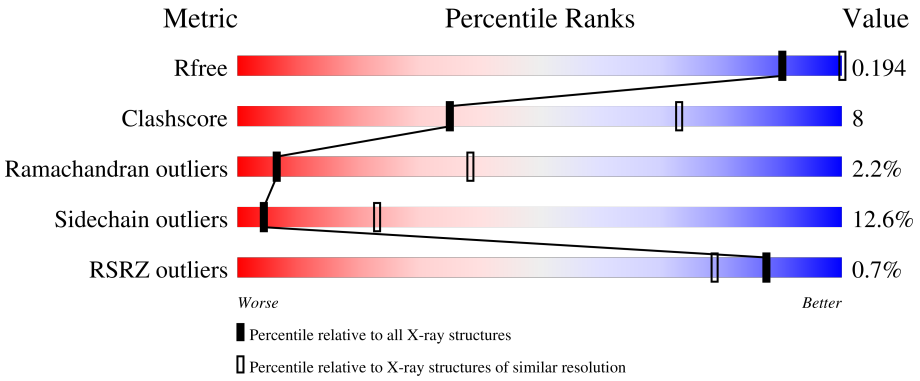
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.52 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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

Mol	Chain	Length	Quality of chain
1	A	1732	58% 20% 18%
2	B	1223	66% 22% 9%
3	C	266	70% 23% 6%
4	D	221	60% 18% 19%
5	E	214	82% 17%

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Mol	Chain	Length	Quality of chain
6	F	87	71% 24% 5%
7	G	171	68% 27% 5%
8	H	145	% 64% 24% 8%
9	I	119	3% 60% 34% 6%
10	J	65	62% 32% 6%
11	K	115	% 74% 23%
12	L	46	48% 39% 13%
13	Q	15	93% 7%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 31339 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	1421	11190	7052	1957	2119	62	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	1118	8876	5620	1557	1644	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 polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	180	1440	890	256	291	3	0	0	0

- Molecule 5 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			
5	E	214	1752	1111	309	321	11	0	0	0

- Molecule 6 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			
6	F	87	705	451	119	132	3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a protein called PHE-ILE-LYS-ARG-ASP-ARG-MET-ARG-ARG-ASN-PHE-LEU-ARG-MET-ARG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	15	Total	C	N	O	S	0	0	0
			78	47	15	15	1			

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

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

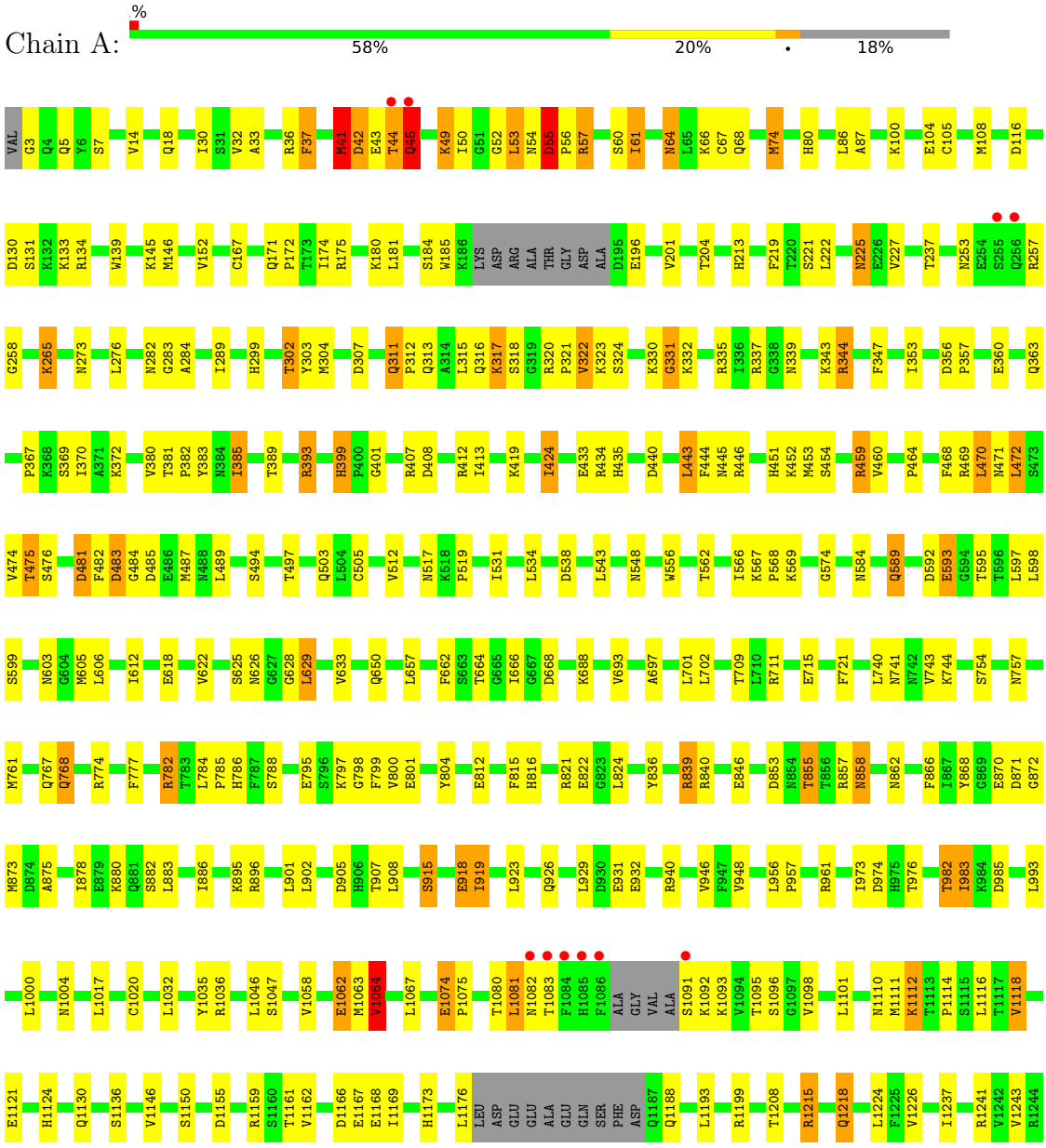
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0

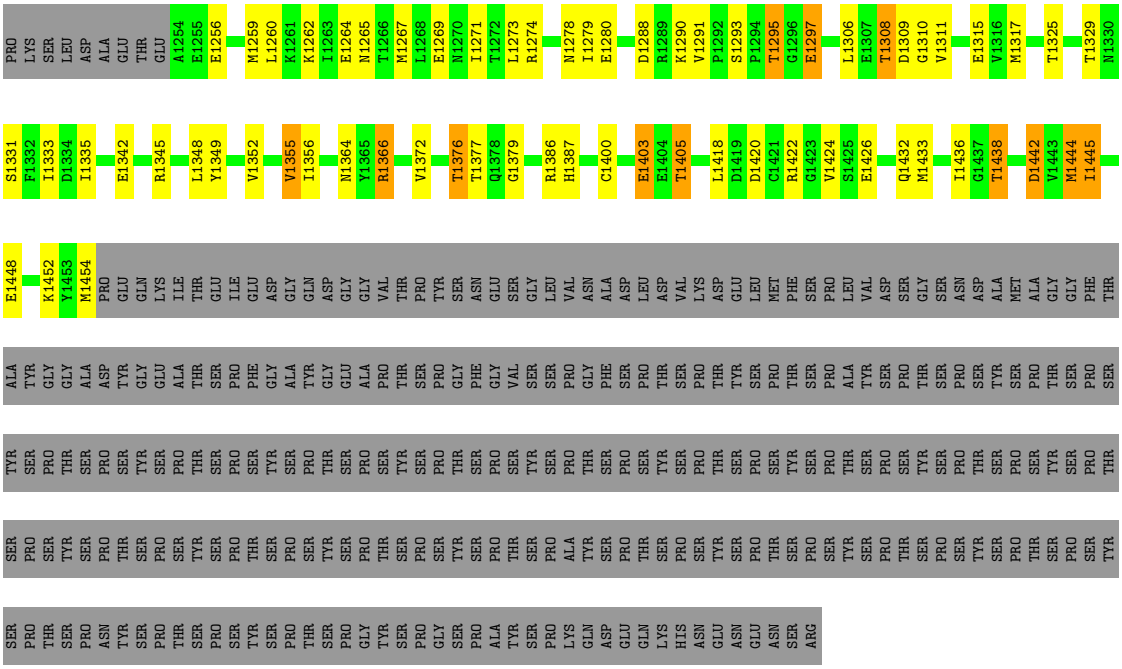
3 Residue-property plots (i)

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

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

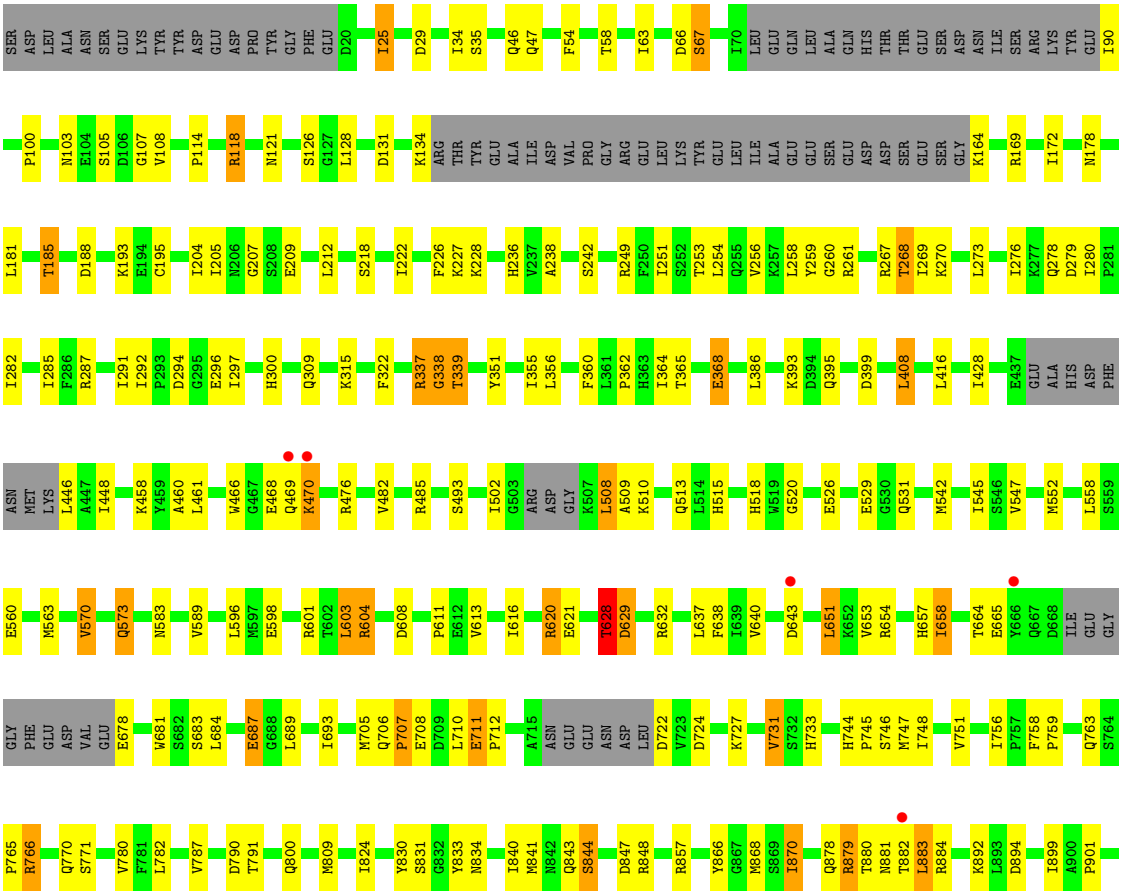
Chain A:

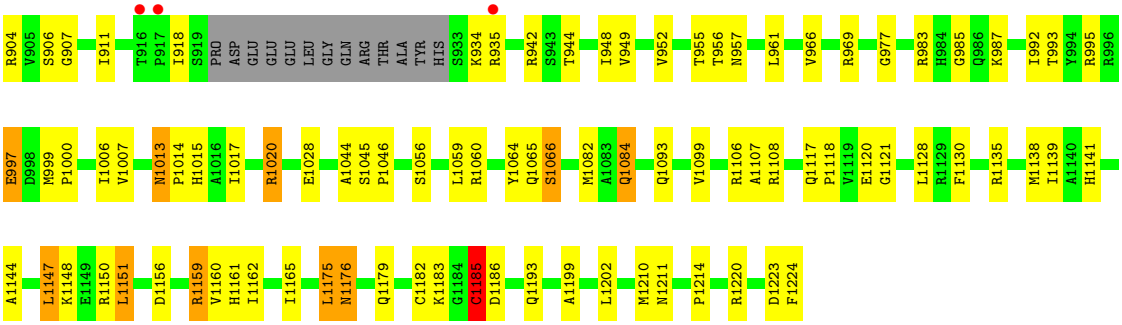




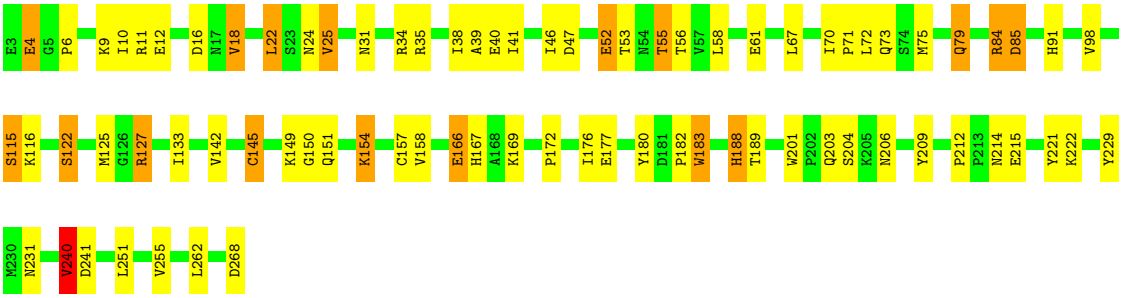
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

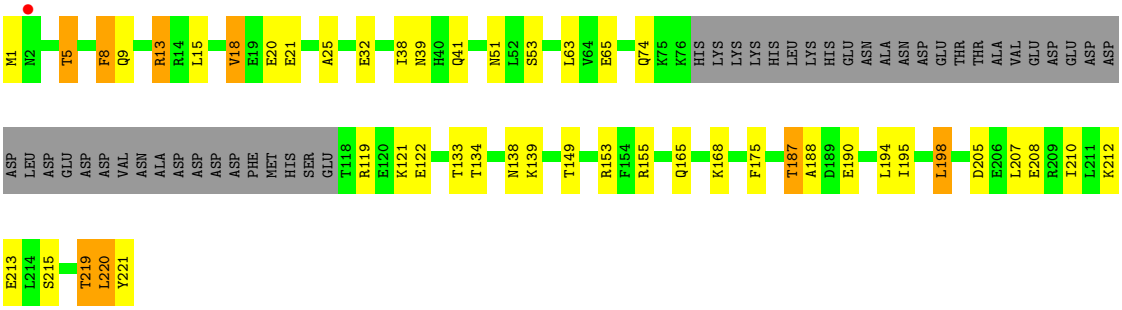




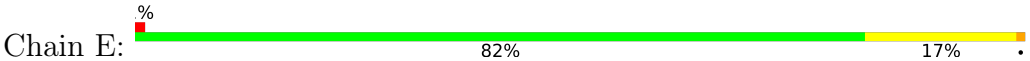
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

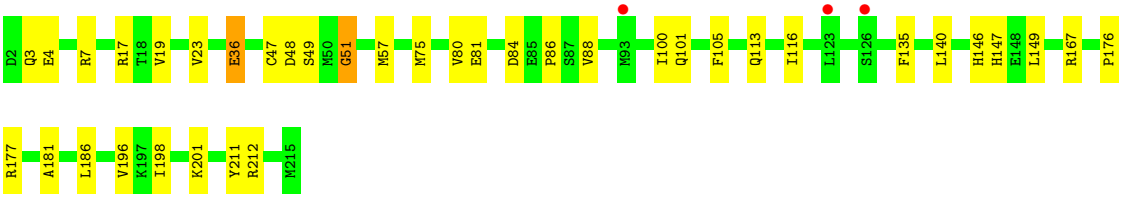


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



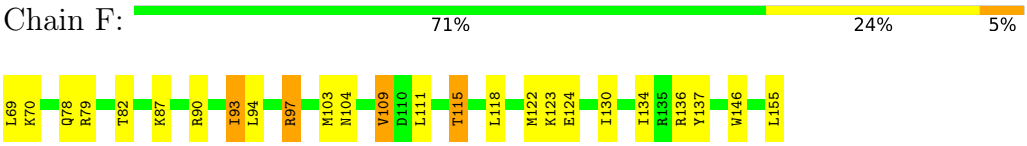
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1





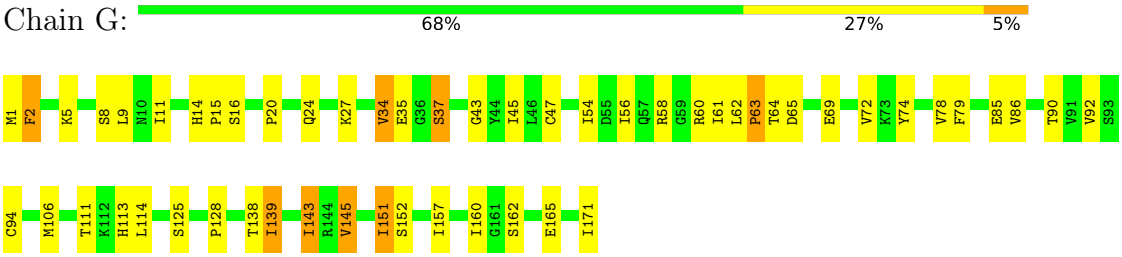
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



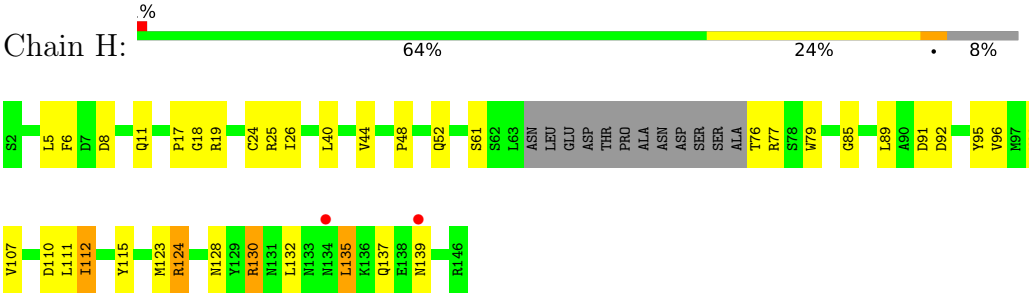
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



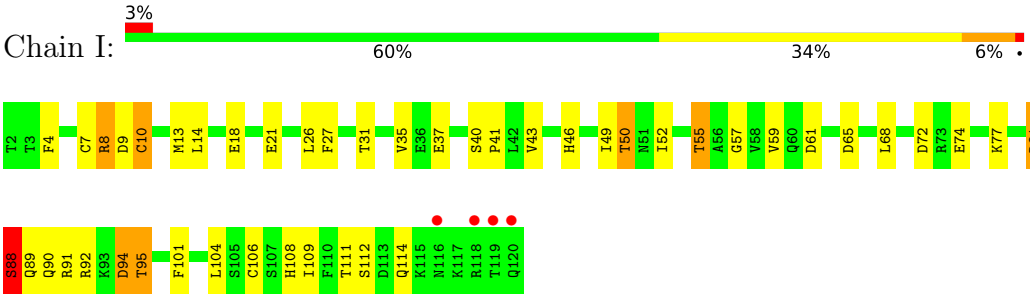
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



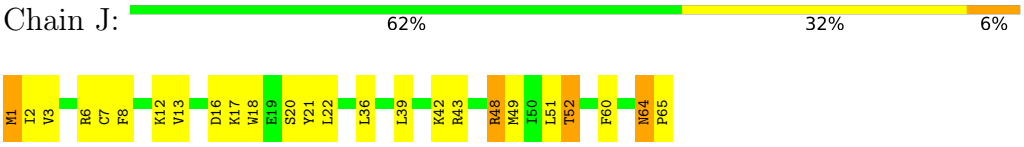
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



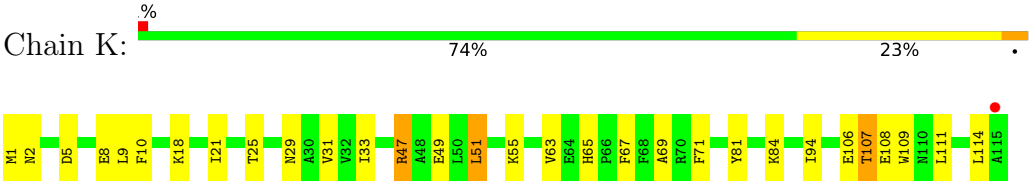
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



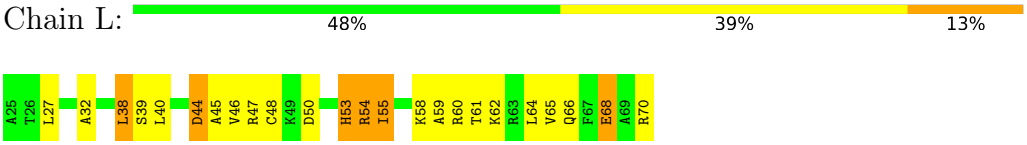
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



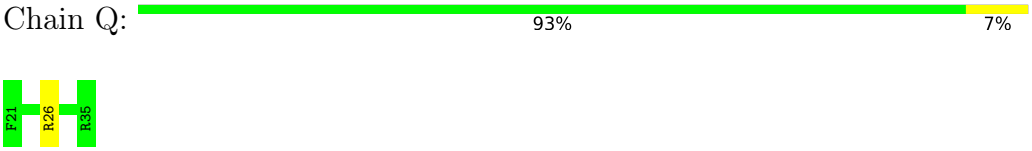
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



• Molecule 13: PHE-ILE-LYS-ARG-ASP-ARG-MET-ARG-ARG-ASN-PHE-LEU-ARG-MET-ARG

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	221.22Å 392.73Å 282.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 3.52 48.70 – 3.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.93-3.52) 100.0 (48.70-3.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.48Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.154 , 0.180 0.172 , 0.194	Depositor DCC
R_{free} test set	2983 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	111.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 101.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.007 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.008 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31339	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.55	4/11391 (0.0%)	0.81	10/15402 (0.1%)
2	B	0.50	0/9048	0.76	3/12200 (0.0%)
3	C	0.49	0/2133	0.78	1/2891 (0.0%)
4	D	0.52	0/1450	0.82	2/1945 (0.1%)
5	E	0.45	0/1788	0.71	0/2406
6	F	0.60	0/717	0.87	0/967
7	G	0.50	0/1368	0.76	0/1844
8	H	0.48	0/1086	0.75	0/1470
9	I	0.45	0/989	0.78	1/1331 (0.1%)
10	J	0.55	0/541	0.86	0/727
11	K	0.47	0/938	0.68	0/1267
12	L	0.51	0/365	0.87	0/485
13	Q	0.70	0/77	0.71	0/105
All	All	0.52	4/31891 (0.0%)	0.78	17/43040 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-CB	5.50	1.66	1.53
1	A	57	ARG	CA-C	5.27	1.66	1.52
1	A	57	ARG	CG-CD	5.27	1.65	1.51
1	A	57	ARG	CB-CG	5.09	1.66	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	25	ALA	C-N-CA	7.60	140.70	121.70
1	A	41	MET	C-N-CA	7.17	139.63	121.70
1	A	399	HIS	N-CA-CB	7.15	123.47	110.60
1	A	57	ARG	CA-CB-CG	7.14	129.12	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	628	THR	C-N-CA	6.08	136.89	121.70
1	A	483	ASP	CA-CB-CG	5.97	126.54	113.40
1	A	3	GLY	C-N-CA	5.62	135.76	121.70
1	A	957	PRO	C-N-CA	-5.62	107.66	121.70
1	A	331	GLY	N-CA-C	5.56	127.00	113.10
1	A	44	THR	C-N-CA	5.52	135.51	121.70
3	C	183	TRP	N-CA-C	-5.43	96.33	111.00
2	B	338	GLY	C-N-CA	5.38	135.14	121.70
1	A	57	ARG	CG-CD-NE	5.35	123.04	111.80
4	D	220	LEU	C-N-CA	5.35	135.08	121.70
2	B	1175	LEU	CA-CB-CG	5.31	127.52	115.30
9	I	88	SER	C-N-CA	5.14	134.55	121.70
1	A	1064	VAL	N-CA-CB	-5.09	100.30	111.50

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	11190	0	11255	220	0
2	B	8876	0	8919	145	0
3	C	2095	0	2051	49	0
4	D	1440	0	1456	16	0
5	E	1752	0	1776	19	0
6	F	705	0	731	17	0
7	G	1340	0	1357	32	0
8	H	1068	0	1040	19	0
9	I	971	0	927	23	0
10	J	532	0	542	19	0
11	K	920	0	929	25	0
12	L	363	0	386	10	0
13	Q	78	0	36	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31339	0	31405	517	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (517) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:CD1	1:A:30:ILE:CG1	1.75	1.56
1:A:56:PRO:HB2	1:A:68:GLN:HG3	1.37	1.06
1:A:1081:LEU:HB3	1:A:1082:ASN:HA	1.45	0.98
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.48	0.92
1:A:855:THR:HG21	1:A:857:ARG:HE	1.34	0.92
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.53	0.89
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.20	0.87
4:D:13:ARG:HH22	4:D:18:VAL:HA	1.44	0.82
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.60	0.82
1:A:369:SER:H	11:K:2:ASN:HD21	1.28	0.81
3:C:98:VAL:H	3:C:122:SER:HB3	1.46	0.80
1:A:56:PRO:HB2	1:A:68:GLN:CG	2.11	0.80
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.80
4:D:155:ARG:HB2	4:D:219:THR:HG21	1.63	0.80
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.63	0.79
2:B:918:ILE:HD11	2:B:935:ARG:HD2	1.62	0.79
7:G:138:THR:HG22	7:G:139:ILE:H	1.49	0.78
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.66	0.78
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.65	0.77
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.69	0.74
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.71	0.73
7:G:151:ILE:HD11	7:G:160:ILE:CD1	2.19	0.72
1:A:741:ASN:HD22	1:A:744:LYS:H	1.37	0.72
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.71	0.72
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.38	0.71
7:G:34:VAL:O	7:G:37:SER:HB3	1.90	0.71
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.72	0.71
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.09	0.71
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.07	0.70
1:A:471:ASN:HD21	1:A:650:GLN:NE2	1.89	0.70
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.71	0.70
3:C:79:GLN:HB3	3:C:127:ARG:HD2	1.73	0.70
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.73	0.69
1:A:1445:ILE:HG12	7:G:61:ILE:HD11	1.75	0.69
9:I:50:THR:HG22	9:I:52:ILE:H	1.58	0.69
2:B:1013:ASN:HD22	2:B:1015:HIS:H	1.39	0.68
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.74	0.68
2:B:744:HIS:HD2	2:B:746:SER:H	1.42	0.68
1:A:54:ASN:HD22	1:A:61:ILE:HD11	1.59	0.68
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.59	0.68
7:G:62:LEU:HD21	7:G:69:GLU:HB2	1.75	0.67
2:B:34:ILE:HG12	2:B:542:MET:CE	2.24	0.67
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.77	0.67
1:A:709:THR:HG23	9:I:94:ASP:HA	1.75	0.66
2:B:683:SER:O	2:B:687:GLU:HB2	1.95	0.66
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.78	0.66
10:J:8:PHE:H	10:J:49:MET:HE3	1.61	0.65
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.97	0.65
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.36	0.65
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.59	0.65
7:G:111:THR:HG22	7:G:113:HIS:H	1.62	0.65
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.78	0.65
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.78	0.65
3:C:206:ASN:HA	3:C:209:TYR:HD1	1.61	0.64
1:A:1329:THR:HG22	1:A:1331:SER:H	1.63	0.64
2:B:706:GLN:H	2:B:710:LEU:HD13	1.62	0.64
1:A:512:VAL:HA	1:A:519:PRO:HA	1.79	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.64
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.79	0.64
1:A:1081:LEU:CB	1:A:1082:ASN:HA	2.26	0.64
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.80	0.64
7:G:151:ILE:HD11	7:G:160:ILE:HD12	1.79	0.63
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.80	0.63
11:K:65:HIS:CD2	11:K:67:PHE:H	2.17	0.62
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.64	0.62
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.81	0.62
1:A:907:THR:HG22	1:A:908:LEU:H	1.63	0.62
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.39	0.62
1:A:754:SER:H	1:A:757:ASN:HD22	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:C	1:A:435:HIS:HD2	2.03	0.62
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.83	0.61
9:I:74:GLU:HB3	9:I:81:ARG:HD3	1.82	0.61
1:A:18:GLN:HG2	1:A:1418:LEU:HD12	1.82	0.61
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.82	0.61
12:L:68:GLU:CD	12:L:68:GLU:H	2.04	0.61
8:H:135:LEU:C	8:H:137:GLN:H	2.04	0.60
1:A:471:ASN:ND2	1:A:650:GLN:HE22	1.96	0.60
1:A:1424:VAL:HG11	2:B:1139:ILE:HG12	1.84	0.60
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.84	0.60
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.66	0.60
1:A:311:GLN:HE21	1:A:312:PRO:HD2	1.66	0.60
4:D:187:THR:HB	4:D:190:GLU:H	1.65	0.60
2:B:883:LEU:HD23	2:B:934:LYS:HB2	1.83	0.60
5:E:176:PRO:O	5:E:212:ARG:HA	2.02	0.60
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.83	0.60
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.37	0.60
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.83	0.59
6:F:118:LEU:O	6:F:122:MET:HG3	2.02	0.59
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.37	0.59
3:C:149:LYS:HG3	3:C:150:GLY:H	1.68	0.59
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.68	0.59
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.84	0.59
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.85	0.59
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.03	0.59
1:A:369:SER:H	11:K:2:ASN:ND2	1.97	0.59
11:K:107:THR:O	11:K:111:LEU:HG	2.02	0.59
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.85	0.58
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.28	0.58
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.85	0.58
1:A:481:ASP:OD1	1:A:483:ASP:OD1	2.21	0.58
2:B:315:LYS:HG2	9:I:13:MET:HE2	1.85	0.58
2:B:34:ILE:HG12	2:B:542:MET:HE2	1.85	0.58
1:A:316:GLN:HG3	1:A:317:LYS:H	1.68	0.58
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.85	0.57
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.85	0.57
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.87	0.57
1:A:451:HIS:CE1	1:A:1074:GLU:HG2	2.40	0.57
1:A:1386:ARG:HB2	1:A:1403:GLU:OE1	2.05	0.57
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.87	0.56
4:D:165:GLN:HA	4:D:168:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.87	0.56
1:A:225:ASN:HD22	1:A:227:VAL:H	1.52	0.56
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.35	0.56
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.87	0.56
10:J:48:ARG:HE	10:J:49:MET:HE2	1.69	0.56
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.70	0.56
2:B:126:SER:OG	2:B:172:ILE:HD11	2.06	0.56
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.88	0.56
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.88	0.55
2:B:515:HIS:H	2:B:518:HIS:CD2	2.24	0.55
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.86	0.55
12:L:32:ALA:HB3	12:L:55:ILE:HG23	1.88	0.55
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.88	0.55
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.71	0.55
1:A:1074:GLU:HG3	1:A:1075:PRO:HD3	1.88	0.55
2:B:338:GLY:HA3	2:B:351:TYR:HE2	1.71	0.55
1:A:1329:THR:HG22	1:A:1331:SER:N	2.21	0.55
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.89	0.55
2:B:848:ARG:HD2	10:J:8:PHE:O	2.06	0.55
2:B:1165:ILE:HG12	4:D:13:ARG:HE	1.71	0.55
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.88	0.55
2:B:212:LEU:HD21	2:B:461:LEU:HD23	1.89	0.55
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.88	0.54
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.42	0.54
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.89	0.54
1:A:53:LEU:HD23	1:A:54:ASN:H	1.73	0.54
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.89	0.54
6:F:109:VAL:CG1	6:F:123:LYS:HD3	2.37	0.54
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.90	0.54
2:B:542:MET:HG2	2:B:747:MET:HE3	1.90	0.54
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.72	0.54
11:K:65:HIS:HD2	11:K:67:PHE:H	1.53	0.54
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.43	0.54
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.90	0.54
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.73	0.53
1:A:353:ILE:HD13	1:A:487:MET:CE	2.38	0.53
1:A:503:GLN:HE21	6:F:90:ARG:HH12	1.55	0.53
1:A:32:VAL:HG21	1:A:80:HIS:HB2	1.91	0.53
1:A:382:PRO:HD3	6:F:104:ASN:HD21	1.73	0.53
2:B:955:THR:HG22	12:L:55:ILE:HA	1.89	0.53
1:A:316:GLN:HG3	1:A:317:LYS:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.91	0.53
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.90	0.53
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.91	0.53
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.37	0.53
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.91	0.53
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.91	0.53
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.90	0.53
9:I:49:ILE:HA	9:I:92:ARG:HH12	1.73	0.52
1:A:472:LEU:O	1:A:475:THR:HB	2.09	0.52
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.44	0.52
2:B:901:PRO:O	2:B:949:VAL:O	2.28	0.52
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.90	0.52
2:B:399:ASP:O	2:B:515:HIS:HD2	1.91	0.52
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.91	0.52
1:A:567:LYS:HE3	8:H:91:ASP:HB2	1.92	0.52
5:E:17:ARG:HH22	5:E:36:GLU:HG3	1.74	0.52
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.24	0.52
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.74	0.52
2:B:570:VAL:HB	2:B:573:GLN:HB2	1.92	0.52
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.91	0.52
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.91	0.52
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.91	0.52
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.92	0.52
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.48	0.51
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.91	0.51
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.75	0.51
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.90	0.51
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.10	0.51
2:B:654:ARG:H	2:B:657:HIS:CD2	2.18	0.51
2:B:705:MET:H	2:B:710:LEU:HD22	1.76	0.51
7:G:1:MET:SD	7:G:2:PHE:N	2.82	0.51
1:A:50:ILE:O	1:A:55:ASP:HB2	2.10	0.51
1:A:858:ASN:ND2	1:A:862:ASN:H	2.08	0.51
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.91	0.51
2:B:47:GLN:NE2	2:B:408:LEU:HD12	2.25	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
9:I:88:SER:HB3	9:I:91:ARG:HE	1.76	0.51
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.92	0.51
1:A:49:LYS:HZ2	1:A:61:ILE:H	1.59	0.51
1:A:709:THR:HG22	1:A:711:ARG:H	1.76	0.51
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:O	1:A:574:GLY:HA3	2.11	0.51
3:C:115:SER:HB2	3:C:142:VAL:H	1.76	0.51
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.92	0.51
2:B:105:SER:C	2:B:107:GLY:H	2.14	0.51
1:A:146:MET:HA	1:A:171:GLN:HB2	1.93	0.50
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.58	0.50
1:A:568:PRO:HG2	8:H:95:TYR:HD1	1.76	0.50
2:B:1082:MET:HA	3:C:189:THR:HA	1.92	0.50
3:C:55:THR:HB	3:C:151:GLN:HA	1.94	0.50
7:G:14:HIS:CD2	7:G:16:SER:H	2.29	0.50
1:A:1215:ARG:HH21	1:A:1218:GLN:HG3	1.77	0.50
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.93	0.50
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.94	0.50
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.94	0.50
1:A:929:LEU:HD21	1:A:983:ILE:HG12	1.93	0.50
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	1.92	0.50
1:A:605:MET:HE2	1:A:612:ILE:HG12	1.93	0.50
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.12	0.50
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.11	0.50
2:B:744:HIS:CD2	2:B:746:SER:OG	2.64	0.50
2:B:515:HIS:H	2:B:518:HIS:HD2	1.60	0.50
2:B:957:ASN:HD22	2:B:961:LEU:HD11	1.77	0.50
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.93	0.50
2:B:47:GLN:HE21	2:B:408:LEU:HD12	1.76	0.50
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.94	0.50
3:C:180:TYR:OH	3:C:188:HIS:HD2	1.95	0.49
1:A:36:ARG:NH2	1:A:57:ARG:HH12	2.10	0.49
2:B:291:ILE:HD12	2:B:291:ILE:N	2.27	0.49
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.93	0.49
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.93	0.49
1:A:754:SER:N	1:A:757:ASN:HD22	2.10	0.49
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.94	0.49
3:C:73:GLN:HE21	3:C:75:MET:H	1.61	0.49
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.53	0.49
2:B:756:ILE:O	2:B:759:PRO:HD3	2.12	0.49
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.95	0.49
3:C:71:PRO:HB2	3:C:133:ILE:HB	1.95	0.49
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.95	0.49
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.94	0.49
2:B:63:ILE:O	2:B:67:SER:HB3	2.13	0.48
2:B:664:THR:HG1	2:B:678:GLU:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:ARG:NH2	4:D:18:VAL:HA	2.21	0.48
10:J:48:ARG:O	10:J:52:THR:HG22	2.13	0.48
1:A:503:GLN:NE2	6:F:90:ARG:HH22	2.11	0.48
1:A:853:ASP:OD1	1:A:855:THR:HB	2.14	0.48
1:A:901:LEU:HA	1:A:907:THR:HG23	1.95	0.48
1:A:175:ARG:HH22	1:A:184:SER:HB2	1.78	0.48
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.48	0.48
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.43	0.48
10:J:48:ARG:HE	10:J:49:MET:CE	2.26	0.48
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.95	0.48
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.28	0.48
3:C:251:LEU:O	3:C:255:VAL:HG23	2.13	0.48
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.96	0.48
9:I:84:VAL:HG23	9:I:104:LEU:HD11	1.95	0.48
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.95	0.48
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.48	0.48
1:A:471:ASN:O	1:A:474:VAL:HG12	2.13	0.48
1:A:567:LYS:HB2	8:H:96:VAL:HB	1.94	0.48
9:I:59:VAL:HG12	9:I:61:ASP:H	1.79	0.48
1:A:134:ARG:HD2	1:A:221:SER:O	2.13	0.48
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.94	0.48
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.49	0.48
2:B:1120:GLU:HG3	2:B:1121:GLY:N	2.28	0.48
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.44	0.48
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.95	0.47
1:A:49:LYS:HD3	1:A:61:ILE:HG13	1.96	0.47
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.49	0.47
2:B:901:PRO:HA	2:B:949:VAL:HG12	1.97	0.47
1:A:883:LEU:O	1:A:886:ILE:HG22	2.14	0.47
6:F:87:LYS:HA	6:F:155:LEU:HD21	1.95	0.47
7:G:43:GLY:HA2	7:G:157:ILE:HD11	1.96	0.47
9:I:72:ASP:O	9:I:81:ARG:HD2	2.15	0.47
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.14	0.47
2:B:603:LEU:HD22	2:B:608:ASP:HB2	1.96	0.47
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.50	0.47
1:A:901:LEU:H	1:A:926:GLN:NE2	2.12	0.47
5:E:147:HIS:CD2	5:E:149:LEU:H	2.32	0.47
1:A:299:HIS:HA	1:A:302:THR:HG22	1.96	0.47
2:B:745:PRO:O	2:B:748:ILE:HG12	2.15	0.47
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.97	0.47
7:G:138:THR:CG2	7:G:139:ILE:H	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.95	0.47
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.15	0.47
1:A:482:PHE:C	1:A:484:GLY:H	2.17	0.47
1:A:657:LEU:HD11	1:A:662:PHE:HB2	1.97	0.47
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.50	0.47
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.45	0.47
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.79	0.47
3:C:11:ARG:HH21	3:C:229:TYR:HD1	1.62	0.47
1:A:907:THR:HG22	1:A:908:LEU:N	2.29	0.47
2:B:273:LEU:HD12	2:B:280:ILE:HD13	1.97	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.97	0.47
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.95	0.46
1:A:335:ARG:HH11	1:A:339:ASN:ND2	2.14	0.46
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.96	0.46
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.50	0.46
3:C:31:ASN:O	3:C:34:ARG:HB3	2.15	0.46
4:D:155:ARG:CB	4:D:219:THR:HG21	2.40	0.46
12:L:40:LEU:HD22	12:L:44:ASP:HB3	1.97	0.46
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.39	0.46
3:C:58:LEU:HD22	3:C:145:CYS:HB2	1.96	0.46
1:A:597:LEU:HD13	8:H:103:LYS:HG3	1.98	0.46
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.97	0.46
2:B:428:ILE:HG12	2:B:448:ILE:HG12	1.96	0.46
4:D:5:THR:HG21	7:G:74:TYR:OH	2.15	0.46
7:G:1:MET:HB3	7:G:1:MET:HE3	1.66	0.46
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.96	0.46
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.51	0.46
1:A:369:SER:N	11:K:2:ASN:HD21	2.05	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.97	0.46
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.97	0.46
1:A:401:GLY:C	1:A:435:HIS:CD2	2.87	0.46
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.97	0.46
6:F:90:ARG:HD3	6:F:155:LEU:HD22	1.97	0.46
9:I:7:CYS:SG	9:I:8:ARG:O	2.74	0.46
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.46	0.46
9:I:55:THR:HG21	9:I:109:ILE:HG21	1.97	0.46
1:A:1081:LEU:HD21	1:A:1098:VAL:H	1.81	0.46
2:B:270:LYS:HB3	2:B:279:ASP:HB3	1.97	0.46
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.81	0.46
1:A:344:ARG:HB2	2:B:1118:PRO:HB2	1.98	0.45
2:B:508:LEU:HD13	2:B:508:LEU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:60:ARG:NH2	7:G:63:PRO:HD3	2.30	0.45
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.97	0.45
1:A:105:CYS:SG	1:A:139:TRP:HA	2.56	0.45
1:A:304:MET:HG2	2:B:1210:MET:HG2	1.99	0.45
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.99	0.45
2:B:296:GLU:O	2:B:300:HIS:HD2	1.99	0.45
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.98	0.45
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.98	0.45
1:A:1121:GLU:HB3	1:A:1124:HIS:HD2	1.82	0.45
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.98	0.45
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.98	0.45
4:D:63:LEU:O	4:D:133:THR:HG21	2.16	0.45
1:A:49:LYS:HZ1	1:A:60:SER:HA	1.82	0.45
1:A:1062:GLU:HB3	1:A:1064:VAL:HG23	1.99	0.45
10:J:7:CYS:HA	10:J:49:MET:HG2	1.99	0.45
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.64	0.45
2:B:620:ARG:HG3	9:I:57:GLY:HA3	1.99	0.45
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.99	0.45
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.99	0.45
3:C:125:MET:HB2	3:C:127:ARG:NE	2.32	0.45
8:H:106:GLU:HA	8:H:112:ILE:HG13	1.98	0.45
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.46	0.45
1:A:332:LYS:H	1:A:337:ARG:CB	2.30	0.45
2:B:242:SER:OG	2:B:362:PRO:HD2	2.17	0.45
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.64	0.45
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.17	0.45
7:G:125:SER:OG	7:G:128:PRO:HA	2.17	0.45
1:A:629:LEU:O	1:A:633:VAL:HG23	2.16	0.45
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.51	0.45
11:K:51:LEU:HD12	11:K:51:LEU:HA	1.88	0.45
1:A:866:PHE:CZ	5:E:211:TYR:HD2	2.35	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.99	0.45
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.57	0.45
1:A:344:ARG:HB3	1:A:344:ARG:NH1	2.31	0.44
1:A:413:ILE:HG21	1:A:424:ILE:HD11	1.99	0.44
4:D:8:PHE:HB3	4:D:38:ILE:O	2.17	0.44
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.32	0.44
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.82	0.44
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.97	0.44
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.98	0.44
1:A:440:ASP:O	1:A:460:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.99	0.44
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.99	0.44
1:A:873:MET:C	1:A:1058:VAL:HG22	2.38	0.44
1:A:1150:SER:HB3	9:I:46:HIS:HB2	1.98	0.44
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.17	0.44
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.84	0.44
1:A:284:ALA:HA	1:A:289:ILE:HD11	2.00	0.44
3:C:73:GLN:HE21	3:C:75:MET:N	2.15	0.44
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.99	0.44
1:A:64:ASN:HD22	1:A:66:LYS:HB2	1.83	0.44
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.98	0.44
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.48	0.44
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.99	0.44
2:B:613:VAL:HG22	2:B:628:THR:HA	2.00	0.44
8:H:89:LEU:HB2	8:H:91:ASP:HB3	2.00	0.44
1:A:67:CYS:SG	1:A:67:CYS:O	2.76	0.43
2:B:291:ILE:HD12	2:B:291:ILE:H	1.83	0.43
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.43
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.00	0.43
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.18	0.43
8:H:6:PHE:HD2	8:H:130:ARG:HG2	1.82	0.43
11:K:1:MET:O	11:K:1:MET:HG2	2.18	0.43
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.82	0.43
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.33	0.43
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.99	0.43
1:A:800:VAL:HA	1:A:812:GLU:HG2	2.00	0.43
1:A:1193:LEU:HB2	1:A:1260:LEU:HD23	2.00	0.43
2:B:25:ILE:CD1	2:B:658:ILE:HD13	2.47	0.43
3:C:84:ARG:HG3	3:C:85:ASP:N	2.33	0.43
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.99	0.43
1:A:668:ASP:HB3	1:A:743:VAL:HG23	2.00	0.43
12:L:32:ALA:HB3	12:L:55:ILE:CG2	2.47	0.43
2:B:520:GLY:HA2	2:B:748:ILE:HA	2.00	0.43
3:C:241:ASP:HB3	11:K:109:TRP:CD2	2.53	0.43
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.52	0.43
1:A:49:LYS:NZ	1:A:61:ILE:H	2.17	0.43
1:A:363:GLN:HG2	1:A:459:ARG:NH1	2.34	0.43
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.82	0.43
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.83	0.43
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.32	0.43
2:B:1013:ASN:ND2	2:B:1014:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:114:LEU:HD23	7:G:162:SER:HB3	2.01	0.43
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.00	0.43
2:B:841:MET:O	2:B:993:THR:HA	2.18	0.43
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.19	0.43
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.54	0.43
1:A:701:LEU:HD21	9:I:114:GLN:HB3	2.01	0.43
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.19	0.43
1:A:1116:LEU:HD12	1:A:1311:VAL:HG22	2.00	0.43
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.83	0.43
3:C:47:ASP:HA	3:C:169:LYS:HZ2	1.84	0.43
1:A:100:LYS:HG3	1:A:181:LEU:HD22	2.01	0.42
2:B:770:GLN:HB2	2:B:985:GLY:H	1.84	0.42
1:A:858:ASN:HD21	1:A:862:ASN:H	1.67	0.42
2:B:309:GLN:HB2	9:I:52:ILE:HD11	2.01	0.42
2:B:892:LYS:HB3	2:B:899:ILE:HD13	2.01	0.42
2:B:899:ILE:HG13	2:B:911:ILE:HA	2.01	0.42
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.01	0.42
3:C:91:HIS:CD2	3:C:158:VAL:HG11	2.54	0.42
1:A:360:GLU:HB2	1:A:363:GLN:HG3	2.00	0.42
1:A:982:THR:HG23	1:A:985:ASP:OD2	2.19	0.42
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.02	0.42
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.42
2:B:866:TYR:O	2:B:870:ILE:HB	2.19	0.42
1:A:393:ARG:HE	1:A:393:ARG:HA	1.84	0.42
1:A:494:SER:HB3	1:A:497:THR:H	1.83	0.42
1:A:1259:MET:HA	1:A:1262:LYS:HD2	2.00	0.42
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.85	0.42
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.54	0.42
3:C:182:PRO:HB3	3:C:204:SER:HB3	2.01	0.42
1:A:543:LEU:HD13	8:H:79:TRP:CZ3	2.55	0.42
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.01	0.42
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.83	0.42
2:B:338:GLY:O	2:B:339:THR:HG22	2.20	0.42
2:B:468:GLU:HG2	2:B:469:GLN:HB2	2.01	0.42
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.85	0.42
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.55	0.42
1:A:1136:SER:O	1:A:1274:ARG:HD3	2.19	0.42
2:B:707:PRO:O	2:B:711:GLU:HG2	2.20	0.42
2:B:1059:LEU:HG	2:B:1064:TYR:HB2	2.00	0.42
8:H:76:THR:HG22	8:H:77:ARG:HD2	2.01	0.42
1:A:761:MET:HA	1:A:804:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:O	5:E:23:VAL:HG23	2.20	0.42
7:G:1:MET:HE1	7:G:79:PHE:CD2	2.55	0.42
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.01	0.42
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.20	0.42
5:E:47:CYS:HB3	5:E:51:GLY:HA2	2.01	0.42
12:L:47:ARG:HH21	12:L:54:ARG:HE	1.68	0.42
1:A:180:LYS:HD3	1:A:201:VAL:HG21	2.02	0.42
2:B:558:LEU:HD23	2:B:596:LEU:HD11	2.01	0.42
3:C:145:CYS:HA	10:J:2:ILE:HD13	2.02	0.42
7:G:151:ILE:HD11	7:G:160:ILE:HD11	1.97	0.42
8:H:107:VAL:CG2	8:H:111:LEU:HB3	2.50	0.41
1:A:1224:LEU:HD23	1:A:1226:VAL:HG22	2.02	0.41
2:B:209:GLU:O	2:B:482:VAL:HA	2.19	0.41
3:C:206:ASN:HA	3:C:209:TYR:CD1	2.49	0.41
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.03	0.41
2:B:54:PHE:HA	2:B:58:THR:HB	2.02	0.41
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.84	0.41
3:C:31:ASN:O	3:C:35:ARG:HG3	2.20	0.41
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.85	0.41
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.85	0.41
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.68	0.41
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.51	0.41
1:A:568:PRO:HD3	8:H:95:TYR:HA	2.03	0.41
12:L:53:HIS:ND1	12:L:55:ILE:HG22	2.36	0.41
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.47	0.41
1:A:1444:MET:HG2	7:G:58:ARG:HB3	2.02	0.41
2:B:131:ASP:HA	2:B:164:LYS:HB3	2.03	0.41
2:B:640:VAL:HG22	2:B:651:LEU:HG	2.03	0.41
5:E:19:VAL:HG11	5:E:80:VAL:HG11	2.01	0.41
2:B:260:GLY:O	2:B:267:ARG:HD3	2.20	0.41
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.03	0.41
3:C:4:GLU:H	3:C:4:GLU:HG2	1.68	0.41
7:G:14:HIS:HD2	7:G:16:SER:OG	2.04	0.41
11:K:9:LEU:HD23	11:K:69:ALA:HB2	2.02	0.41
1:A:598:LEU:HD13	8:H:124:ARG:HB2	2.03	0.41
1:A:598:LEU:HG	8:H:25:ARG:NH1	2.36	0.41
1:A:872:GLY:O	1:A:1058:VAL:HG23	2.20	0.41
2:B:315:LYS:HA	9:I:13:MET:HE1	2.01	0.41
3:C:115:SER:HB2	3:C:142:VAL:N	2.35	0.41
1:A:7:SER:OG	2:B:1161:HIS:HE1	2.04	0.41
2:B:416:LEU:HD11	2:B:460:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:GLN:O	2:B:710:LEU:HB2	2.21	0.41
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.56	0.41
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.02	0.41
10:J:21:TYR:HA	10:J:39:LEU:HD11	2.02	0.41
11:K:5:ASP:O	11:K:8:GLU:HB2	2.20	0.41
1:A:33:ALA:CB	1:A:57:ARG:HD3	2.51	0.41
1:A:777:PHE:HD2	1:A:782:ARG:HA	1.86	0.41
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.55	0.41
2:B:724:ASP:HB3	2:B:727:LYS:HD2	2.03	0.41
6:F:124:GLU:HB3	6:F:130:ILE:HG13	2.03	0.41
2:B:955:THR:CG2	12:L:55:ILE:HG13	2.51	0.40
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.04	0.40
1:A:43:GLU:C	1:A:45:GLN:H	2.24	0.40
1:A:347:PHE:H	2:B:1107:ALA:HA	1.85	0.40
1:A:446:ARG:HB2	1:A:487:MET:SD	2.61	0.40
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.40
2:B:121:ASN:ND2	2:B:207:GLY:HA3	2.36	0.40
2:B:844:SER:O	2:B:847:ASP:HB2	2.21	0.40
2:B:880:THR:O	2:B:883:LEU:HG	2.22	0.40
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.56	0.40
6:F:103:MET:HG3	7:G:15:PRO:HG2	2.02	0.40
1:A:104:GLU:HG3	1:A:174:ILE:HD12	2.03	0.40
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.03	0.40
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.02	0.40
1:A:1454:MET:HB2	7:G:20:PRO:HG3	2.02	0.40
3:C:167:HIS:ND1	3:C:169:LYS:HB3	2.37	0.40
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.86	0.40
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.57	0.40
7:G:11:ILE:HD12	7:G:72:VAL:HG21	2.04	0.40
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.86	0.40
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.56	0.40
1:A:86:LEU:HA	1:A:273:ASN:OD1	2.22	0.40
1:A:321:PRO:O	1:A:322:VAL:HB	2.21	0.40
1:A:915:SER:O	1:A:918:GLU:HG3	2.21	0.40
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	2.02	0.40
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.90	0.40
3:C:53:THR:HG22	3:C:154:LYS:HB2	2.04	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	1411/1732 (82%)	1269 (90%)	116 (8%)	26 (2%)	8 42
2	B	1102/1223 (90%)	996 (90%)	79 (7%)	27 (2%)	5 35
3	C	264/266 (99%)	243 (92%)	18 (7%)	3 (1%)	14 53
4	D	176/221 (80%)	155 (88%)	17 (10%)	4 (2%)	6 37
5	E	212/214 (99%)	198 (93%)	10 (5%)	4 (2%)	8 41
6	F	85/87 (98%)	79 (93%)	6 (7%)	0	100 100
7	G	169/171 (99%)	162 (96%)	5 (3%)	2 (1%)	13 51
8	H	129/145 (89%)	105 (81%)	17 (13%)	7 (5%)	2 19
9	I	117/119 (98%)	98 (84%)	17 (14%)	2 (2%)	9 44
10	J	63/65 (97%)	56 (89%)	4 (6%)	3 (5%)	2 21
11	K	113/115 (98%)	109 (96%)	4 (4%)	0	100 100
12	L	44/46 (96%)	33 (75%)	6 (14%)	5 (11%)	0 6
13	Q	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1 11
All	All	3898/4419 (88%)	3514 (90%)	300 (8%)	84 (2%)	6 38

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	45	GLN
1	A	74	MET
1	A	593	GLU
1	A	1403	GLU
1	A	1405	THR
2	B	67	SER
2	B	339	THR
2	B	629	ASP
2	B	731	VAL

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Mol	Chain	Res	Type
2	B	751	VAL
2	B	879	ARG
2	B	1066	SER
2	B	1185	CYS
4	D	13	ARG
4	D	119	ARG
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	331	GLY
1	A	846	GLU
1	A	1379	GLY
2	B	368	GLU
2	B	1046	PRO
2	B	1176	ASN
8	H	17	PRO
8	H	85	GLY
8	H	128	ASN
9	I	89	GLN
10	J	17	LYS
1	A	41	MET
1	A	556	TRP
2	B	364	ILE
2	B	509	ALA
2	B	643	ASP
2	B	707	PRO
2	B	881	ASN
4	D	198	LEU
5	E	36	GLU
5	E	48	ASP
5	E	49	SER
8	H	18	GLY
8	H	52	GLN
12	L	39	SER
1	A	167	CYS
1	A	322	VAL
1	A	599	SER
1	A	870	GLU
2	B	249	ARG
2	B	322	PHE
2	B	470	LYS
2	B	711	GLU

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Mol	Chain	Res	Type
3	C	214	ASN
7	G	63	PRO
10	J	6	ARG
13	Q	26	ARG
1	A	49	LYS
1	A	108	MET
1	A	282	ASN
1	A	399	HIS
1	A	628	GLY
2	B	712	PRO
2	B	907	GLY
2	B	1017	ILE
2	B	1108	ARG
2	B	1223	ASP
4	D	18	VAL
7	G	139	ILE
8	H	132	LEU
8	H	139	ASN
9	I	95	THR
10	J	64	ASN
1	A	55	ASP
1	A	1173	HIS
2	B	108	VAL
12	L	45	ALA
1	A	283	GLY
1	A	1064	VAL
2	B	1214	PRO
1	A	258	GLY
3	C	240	VAL
5	E	51	GLY
1	A	196	GLU
3	C	38	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	1244/1519 (82%)	1084 (87%)	160 (13%)	4 22
2	B	967/1060 (91%)	853 (88%)	114 (12%)	5 26
3	C	234/234 (100%)	205 (88%)	29 (12%)	4 24
4	D	160/200 (80%)	132 (82%)	28 (18%)	2 11
5	E	196/196 (100%)	187 (95%)	9 (5%)	27 61
6	F	77/77 (100%)	67 (87%)	10 (13%)	4 22
7	G	152/152 (100%)	132 (87%)	20 (13%)	4 22
8	H	117/127 (92%)	104 (89%)	13 (11%)	6 29
9	I	113/113 (100%)	93 (82%)	20 (18%)	2 11
10	J	60/60 (100%)	50 (83%)	10 (17%)	2 13
11	K	99/99 (100%)	89 (90%)	10 (10%)	7 33
12	L	40/40 (100%)	26 (65%)	14 (35%)	0 1
13	Q	1/15 (7%)	1 (100%)	0	100 100
All	All	3460/3892 (89%)	3023 (87%)	437 (13%)	4 23

All (437) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	41	MET
1	A	42	ASP
1	A	44	THR
1	A	45	GLN
1	A	53	LEU
1	A	55	ASP
1	A	61	ILE
1	A	64	ASN
1	A	74	MET
1	A	116	ASP
1	A	131	SER
1	A	145	LYS
1	A	152	VAL
1	A	204	THR
1	A	213	HIS
1	A	225	ASN
1	A	237	THR
1	A	253	ASN
1	A	257	ARG

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	313	GLN
1	A	315	LEU
1	A	317	LYS
1	A	318	SER
1	A	320	ARG
1	A	323	LYS
1	A	324	SER
1	A	330	LYS
1	A	344	ARG
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	393	ARG
1	A	408	ASP
1	A	412	ARG
1	A	419	LYS
1	A	424	ILE
1	A	433	GLU
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	453	MET
1	A	454	SER
1	A	459	ARG
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	489	LEU
1	A	505	CYS
1	A	538	ASP
1	A	562	THR
1	A	584	ASN
1	A	589	GLN
1	A	618	GLU
1	A	625	SER

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Mol	Chain	Res	Type
1	A	626	ASN
1	A	629	LEU
1	A	664	THR
1	A	666	ILE
1	A	688	LYS
1	A	740	LEU
1	A	768	GLN
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	801	GLU
1	A	821	ARG
1	A	824	LEU
1	A	839	ARG
1	A	855	THR
1	A	858	ASN
1	A	880	LYS
1	A	882	SER
1	A	895	LYS
1	A	896	ARG
1	A	905	ASP
1	A	915	SER
1	A	918	GLU
1	A	919	ILE
1	A	923	LEU
1	A	931	GLU
1	A	932	GLU
1	A	940	ARG
1	A	948	VAL
1	A	961	ARG
1	A	973	ILE
1	A	974	ASP
1	A	976	THR
1	A	982	THR
1	A	983	ILE
1	A	1000	LEU
1	A	1035	TYR
1	A	1047	SER
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1074	GLU

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Mol	Chain	Res	Type
1	A	1080	THR
1	A	1081	LEU
1	A	1083	THR
1	A	1091	SER
1	A	1092	LYS
1	A	1093	LYS
1	A	1096	SER
1	A	1110	ASN
1	A	1112	LYS
1	A	1118	VAL
1	A	1146	VAL
1	A	1159	ARG
1	A	1167	GLU
1	A	1168	GLU
1	A	1176	LEU
1	A	1188	GLN
1	A	1199	ARG
1	A	1208	THR
1	A	1215	ARG
1	A	1218	GLN
1	A	1237	ILE
1	A	1243	VAL
1	A	1256	GLU
1	A	1264	GLU
1	A	1265	ASN
1	A	1269	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1290	LYS
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1333	ILE
1	A	1335	ILE
1	A	1355	VAL
1	A	1356	ILE
1	A	1366	ARG

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Mol	Chain	Res	Type
1	A	1376	THR
1	A	1387	HIS
1	A	1400	CYS
1	A	1405	THR
1	A	1420	ASP
1	A	1422	ARG
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1448	GLU
1	A	1452	LYS
2	B	25	ILE
2	B	35	SER
2	B	46	GLN
2	B	66	ASP
2	B	90	ILE
2	B	103	ASN
2	B	118	ARG
2	B	128	LEU
2	B	134	LYS
2	B	169	ARG
2	B	185	THR
2	B	205	ILE
2	B	218	SER
2	B	222	ILE
2	B	228	LYS
2	B	251	ILE
2	B	253	THR
2	B	254	LEU
2	B	258	LEU
2	B	261	ARG
2	B	268	THR
2	B	294	ASP
2	B	337	ARG
2	B	365	THR
2	B	368	GLU
2	B	393	LYS
2	B	408	LEU
2	B	446	LEU

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Mol	Chain	Res	Type
2	B	458	LYS
2	B	466	TRP
2	B	470	LYS
2	B	476	ARG
2	B	485	ARG
2	B	493	SER
2	B	502	ILE
2	B	508	LEU
2	B	510	LYS
2	B	529	GLU
2	B	531	GLN
2	B	547	VAL
2	B	552	MET
2	B	560	GLU
2	B	563	MET
2	B	570	VAL
2	B	573	GLN
2	B	589	VAL
2	B	598	GLU
2	B	601	ARG
2	B	603	LEU
2	B	604	ARG
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	628	THR
2	B	651	LEU
2	B	658	ILE
2	B	665	GLU
2	B	687	GLU
2	B	708	GLU
2	B	722	ASP
2	B	731	VAL
2	B	766	ARG
2	B	780	VAL
2	B	790	ASP
2	B	791	THR
2	B	809	MET
2	B	831	SER
2	B	843	GLN
2	B	844	SER
2	B	857	ARG

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Mol	Chain	Res	Type
2	B	868	MET
2	B	870	ILE
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	894	ASP
2	B	906	SER
2	B	942	ARG
2	B	944	THR
2	B	956	THR
2	B	987	LYS
2	B	992	ILE
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1013	ASN
2	B	1020	ARG
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1084	GLN
2	B	1106	ARG
2	B	1128	LEU
2	B	1135	ARG
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1162	ILE
2	B	1175	LEU
2	B	1176	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1185	CYS
2	B	1186	ASP
2	B	1202	LEU
2	B	1211	ASN

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Mol	Chain	Res	Type
2	B	1220	ARG
2	B	1224	PHE
3	C	4	GLU
3	C	9	LYS
3	C	12	GLU
3	C	16	ASP
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	40	GLU
3	C	52	GLU
3	C	55	THR
3	C	56	THR
3	C	79	GLN
3	C	84	ARG
3	C	85	ASP
3	C	115	SER
3	C	116	LYS
3	C	122	SER
3	C	127	ARG
3	C	145	CYS
3	C	154	LYS
3	C	166	GLU
3	C	176	ILE
3	C	188	HIS
3	C	203	GLN
3	C	215	GLU
3	C	222	LYS
3	C	240	VAL
3	C	262	LEU
3	C	268	ASP
4	D	1	MET
4	D	5	THR
4	D	8	PHE
4	D	9	GLN
4	D	15	LEU
4	D	20	GLU
4	D	21	GLU
4	D	32	GLU
4	D	39	ASN
4	D	41	GLN
4	D	51	ASN

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Mol	Chain	Res	Type
4	D	53	SER
4	D	65	GLU
4	D	74	GLN
4	D	121	LYS
4	D	122	GLU
4	D	134	THR
4	D	139	LYS
4	D	149	THR
4	D	153	ARG
4	D	187	THR
4	D	205	ASP
4	D	212	LYS
4	D	213	GLU
4	D	215	SER
4	D	219	THR
4	D	220	LEU
4	D	221	TYR
5	E	3	GLN
5	E	57	MET
5	E	75	MET
5	E	81	GLU
5	E	84	ASP
5	E	101	GLN
5	E	146	HIS
5	E	177	ARG
5	E	196	VAL
6	F	69	LEU
6	F	70	LYS
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	93	ILE
6	F	97	ARG
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
7	G	2	PHE
7	G	5	LYS
7	G	8	SER
7	G	24	GLN
7	G	34	VAL
7	G	37	SER

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Mol	Chain	Res	Type
7	G	47	CYS
7	G	56	ILE
7	G	64	THR
7	G	65	ASP
7	G	90	THR
7	G	92	VAL
7	G	94	CYS
7	G	106	MET
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	152	SER
7	G	165	GLU
7	G	171	ILE
8	H	5	LEU
8	H	8	ASP
8	H	11	GLN
8	H	19	ARG
8	H	26	ILE
8	H	61	SER
8	H	92	ASP
8	H	103	LYS
8	H	110	ASP
8	H	112	ILE
8	H	124	ARG
8	H	130	ARG
8	H	135	LEU
9	I	4	PHE
9	I	8	ARG
9	I	9	ASP
9	I	10	CYS
9	I	18	GLU
9	I	21	GLU
9	I	31	THR
9	I	35	VAL
9	I	40	SER
9	I	43	VAL
9	I	50	THR
9	I	55	THR
9	I	77	LYS
9	I	81	ARG
9	I	87	GLN

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Mol	Chain	Res	Type
9	I	88	SER
9	I	90	GLN
9	I	94	ASP
9	I	95	THR
9	I	111	THR
10	J	1	MET
10	J	12	LYS
10	J	13	VAL
10	J	16	ASP
10	J	20	SER
10	J	22	LEU
10	J	42	LYS
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
11	K	18	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	47	ARG
11	K	51	LEU
11	K	84	LYS
11	K	106	GLU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	44	ASP
12	L	46	VAL
12	L	53	HIS
12	L	54	ARG
12	L	55	ILE
12	L	61	THR
12	L	62	LYS
12	L	64	LEU
12	L	65	VAL
12	L	66	GLN
12	L	68	GLU
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	118	HIS
1	A	225	ASN
1	A	299	HIS
1	A	311	GLN
1	A	339	ASN
1	A	399	HIS
1	A	435	HIS
1	A	451	HIS
1	A	503	GLN
1	A	517	ASN
1	A	650	GLN
1	A	700	ASN
1	A	741	ASN
1	A	757	ASN
1	A	760	GLN
1	A	768	GLN
1	A	858	ASN
1	A	926	GLN
1	A	1124	HIS
1	A	1128	GLN
1	A	1211	GLN
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	178	ASN
2	B	278	GLN
2	B	300	HIS
2	B	309	GLN
2	B	518	HIS
2	B	590	HIS
2	B	648	HIS
2	B	657	HIS
2	B	744	HIS
2	B	842	ASN
2	B	843	GLN
2	B	862	GLN
2	B	957	ASN
2	B	986	GLN
2	B	1013	ASN
2	B	1015	HIS
2	B	1040	ASN
2	B	1093	GLN

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Mol	Chain	Res	Type
2	B	1097	HIS
2	B	1117	GLN
2	B	1161	HIS
3	C	7	GLN
3	C	73	GLN
3	C	112	ASN
3	C	188	HIS
4	D	37	GLN
4	D	143	ASN
4	D	179	GLN
5	E	5	ASN
5	E	147	HIS
6	F	104	ASN
7	G	14	HIS
7	G	122	ASN
7	G	126	ASN
8	H	21	ASN
8	H	134	ASN
8	H	137	GLN
9	I	12	ASN
9	I	23	ASN
9	I	116	ASN
11	K	2	ASN
11	K	65	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1421/1732 (82%)	-0.28	10 (0%) 87 79	64, 112, 182, 240	0
2	B	1118/1223 (91%)	-0.19	8 (0%) 87 79	68, 126, 195, 228	0
3	C	266/266 (100%)	-0.26	0 100 100	80, 116, 160, 192	0
4	D	180/221 (81%)	-0.24	1 (0%) 89 81	97, 131, 188, 211	0
5	E	214/214 (100%)	-0.19	3 (1%) 75 62	91, 157, 206, 216	0
6	F	87/87 (100%)	-0.51	0 100 100	69, 92, 124, 138	0
7	G	171/171 (100%)	-0.25	0 100 100	83, 112, 149, 185	0
8	H	133/145 (91%)	0.07	2 (1%) 73 61	118, 160, 196, 204	0
9	I	119/119 (100%)	-0.16	4 (3%) 45 34	123, 153, 195, 219	0
10	J	65/65 (100%)	-0.35	0 100 100	89, 113, 155, 173	0
11	K	115/115 (100%)	-0.26	1 (0%) 84 73	79, 112, 160, 181	0
12	L	46/46 (100%)	-0.12	0 100 100	97, 155, 190, 204	0
13	Q	15/15 (100%)	0.38	0 100 100	132, 200, 214, 222	0
All	All	3950/4419 (89%)	-0.23	29 (0%) 87 79	64, 122, 191, 240	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	7.3
1	A	1085	HIS	5.3
1	A	1082	ASN	5.0
1	A	44	THR	4.1
11	K	115	ALA	3.8
9	I	119	THR	3.7
1	A	1083	THR	3.3
9	I	120	GLN	3.2
1	A	1086	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	469	GLN	3.2
1	A	255	SER	3.1
4	D	2	ASN	3.0
5	E	123	LEU	3.0
8	H	139	ASN	2.8
1	A	1084	PHE	2.7
2	B	470	LYS	2.7
1	A	1091	SER	2.5
2	B	643	ASP	2.5
8	H	134	ASN	2.5
2	B	666	TYR	2.4
9	I	118	ARG	2.4
5	E	93	MET	2.4
1	A	45	GLN	2.3
2	B	935	ARG	2.3
5	E	126	SER	2.2
2	B	917	PRO	2.2
2	B	916	THR	2.2
1	A	256	GLN	2.2
9	I	116	ASN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	A	1803	1/1	0.96	0.44	62,62,62,62	0
14	ZN	I	202	1/1	0.98	0.04	209,209,209,209	0
14	ZN	L	101	1/1	0.98	0.09	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ZN	A	1801	1/1	0.98	0.06	164,164,164,164	0
14	ZN	I	201	1/1	0.99	0.12	125,125,125,125	0
14	ZN	J	101	1/1	0.99	0.26	110,110,110,110	0
14	ZN	C	301	1/1	1.00	0.10	94,94,94,94	0
14	ZN	A	1802	1/1	1.00	0.15	97,97,97,97	0
14	ZN	B	1301	1/1	1.00	0.22	115,115,115,115	0

6.5 Other polymers (i)

There are no such residues in this entry.