



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:12 am GMT

PDB ID : 5IP9
Title : Structure of RNA Polymerase II-TFIIF complex
Authors : Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-03-09
Resolution : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

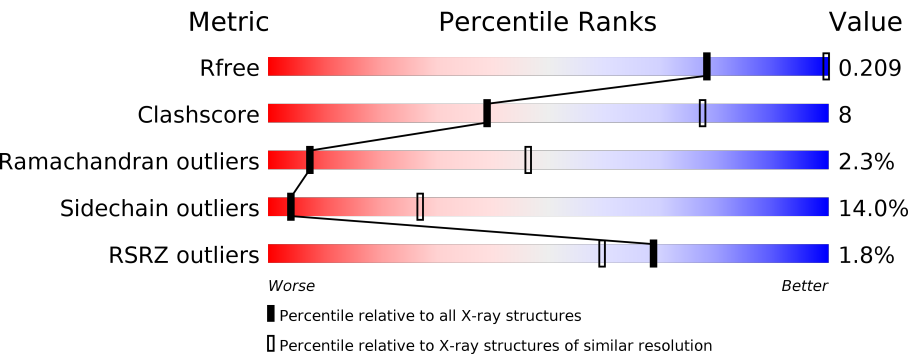
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>56%22%•18%</div></div>
2	B	1223	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>64%25%•9%</div></div>
3	C	266	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>71%25%•</div></div>
4	D	221	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>61%18%•19%</div></div>
5	E	214	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>78%21%•</div></div>
6	F	87	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%26%•</div></div>

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Mol	Chain	Length	Quality of chain
7	G	171	<div><div>%</div><div><div></div><div>69%</div><div>26%</div><div>5%</div></div></div>
8	H	145	<div><div>3%</div><div><div></div><div>59%</div><div>29%</div><div>8%</div></div></div>
9	I	119	<div><div>3%</div><div><div></div><div>69%</div><div>26%</div><div>5%</div></div></div>
10	J	65	<div><div></div><div><div></div><div>60%</div><div>31%</div><div>9%</div></div></div>
11	K	115	<div><div></div><div><div></div><div>75%</div><div>23%</div><div></div></div></div>
12	L	46	<div><div>2%</div><div><div></div><div>50%</div><div>41%</div><div>9%</div></div></div>
13	Q	15	<div><div>7%</div><div><div></div><div>80%</div><div>13%</div><div>7%</div></div></div>

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
1	A	1421	Total	C	N	O	S	0	0	0
			11190	7052	1957	2119	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1118	Total	C	N	O	S	0	0	0
			8876	5620	1557	1644	55			

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

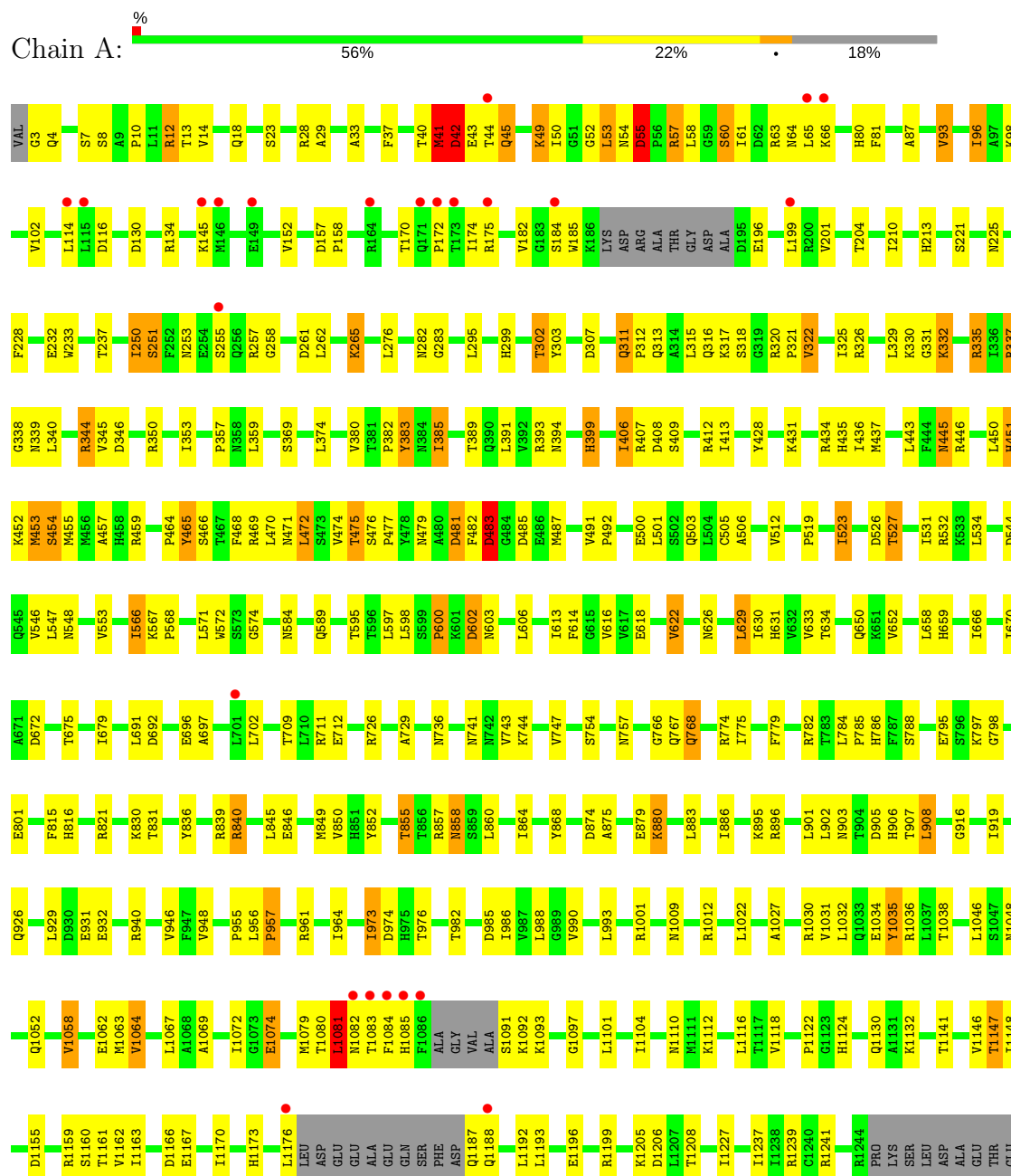
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

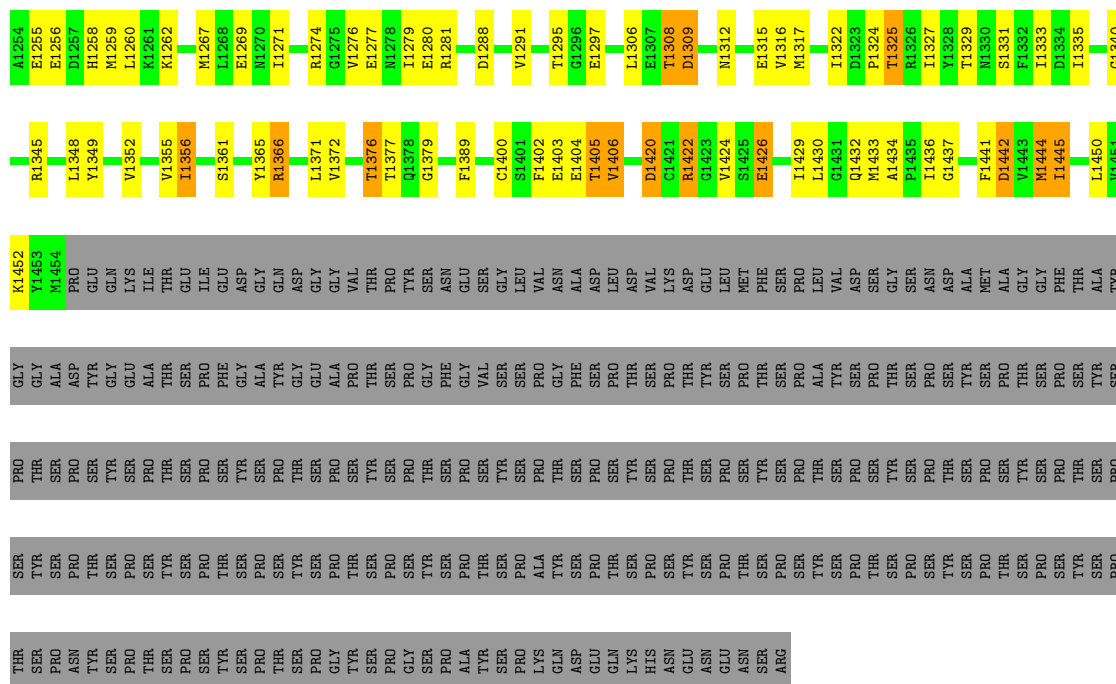
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

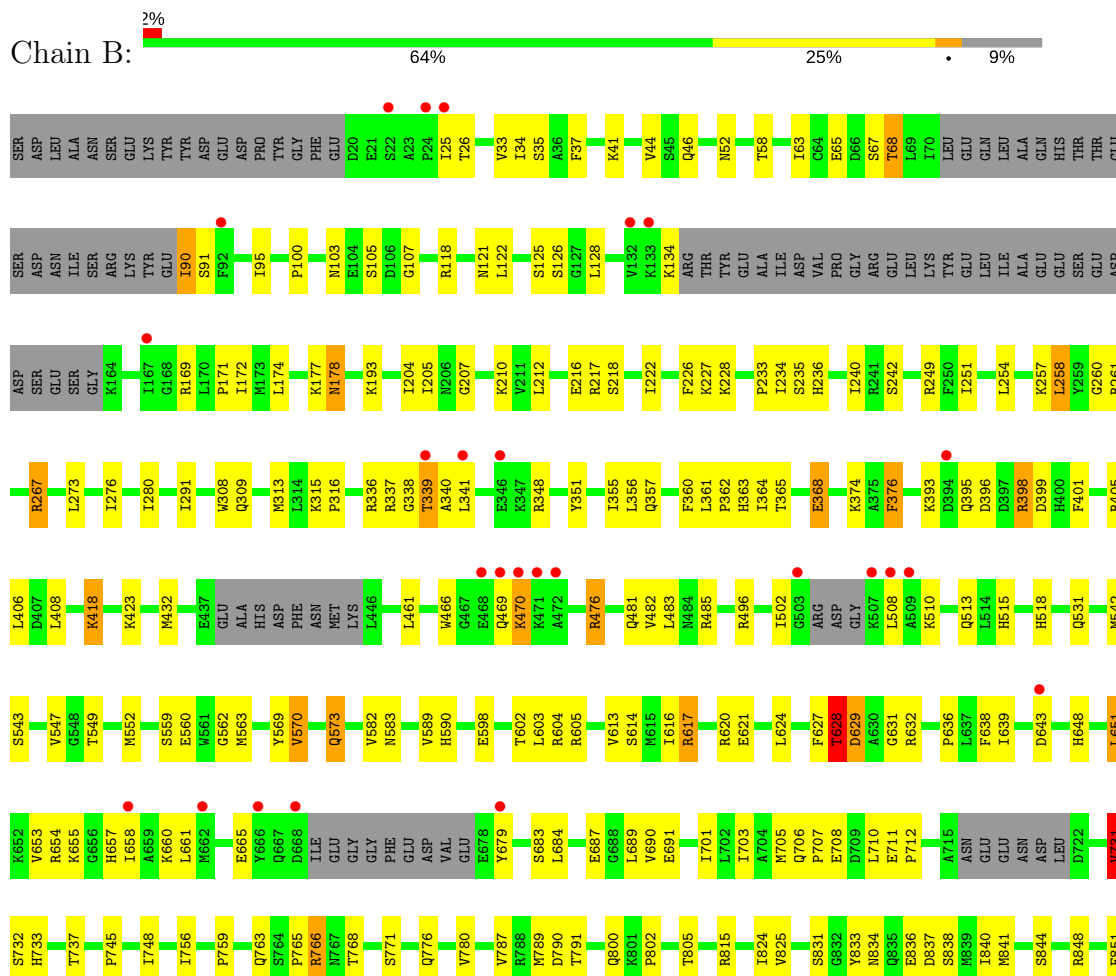
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

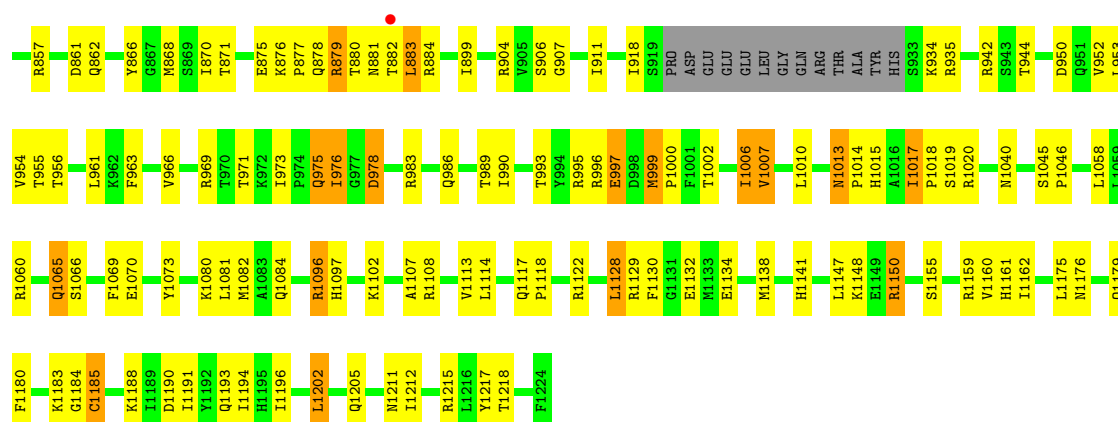
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



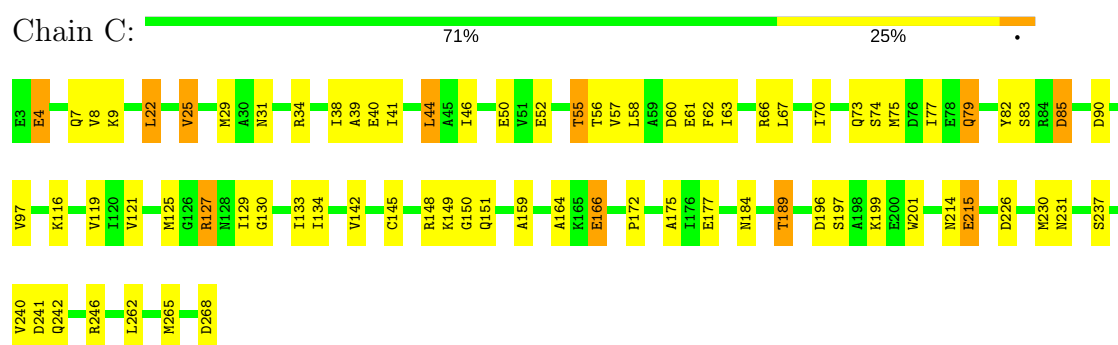


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

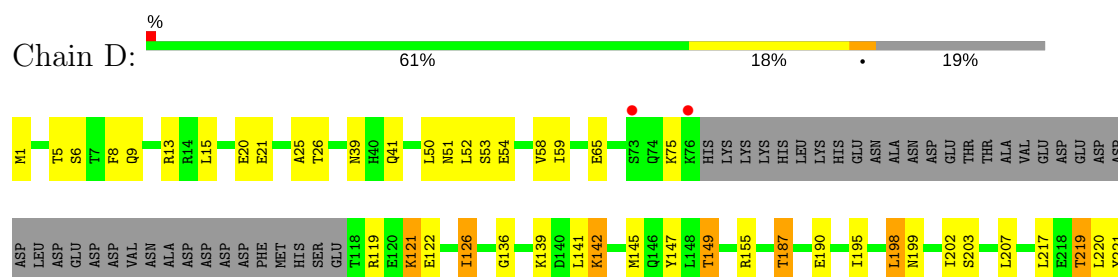




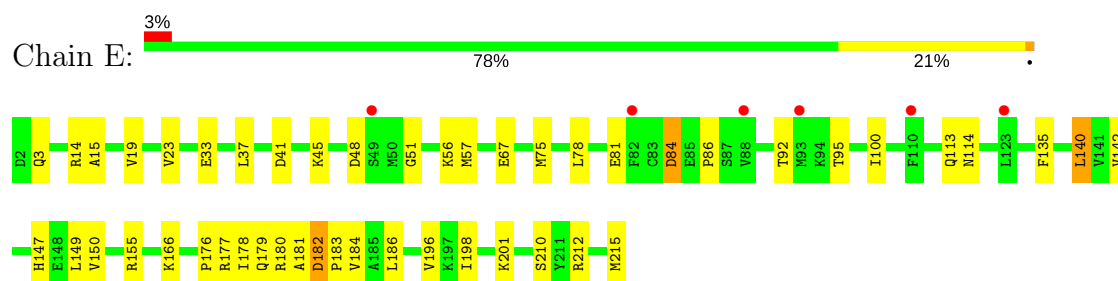
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



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

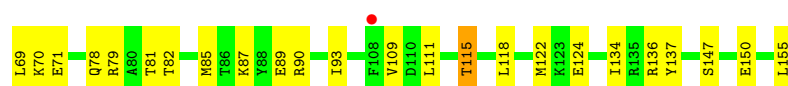


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

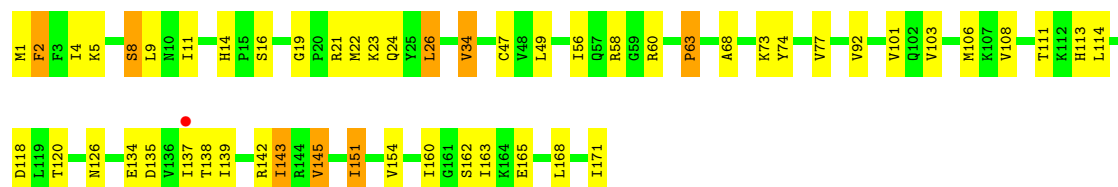


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

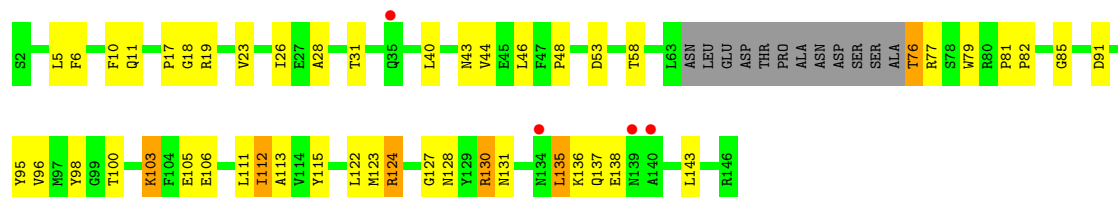




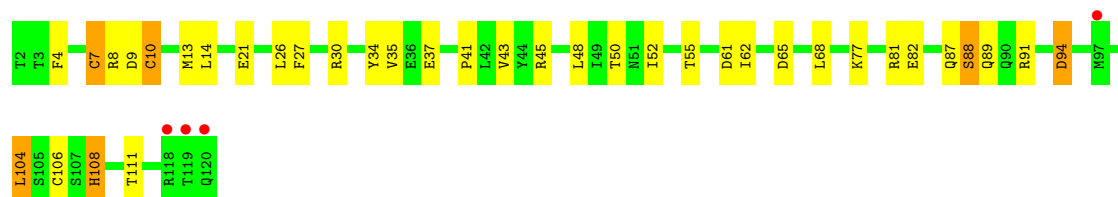
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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



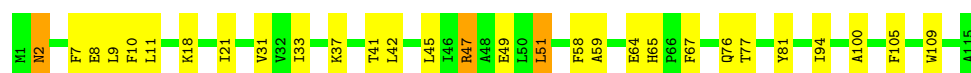
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



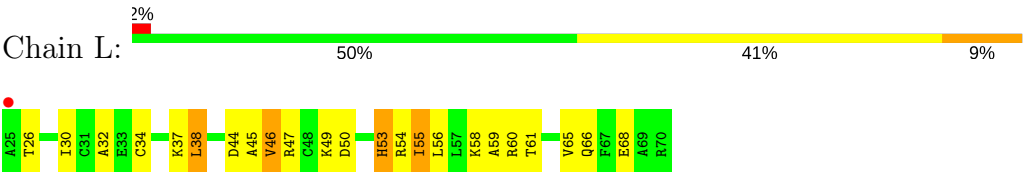
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



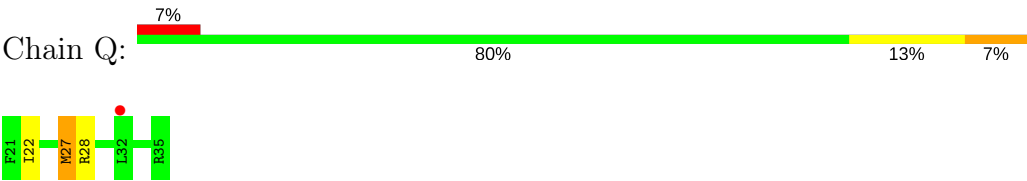
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.82Å 392.73Å 283.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 3.90 48.93 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.93-3.90) 100.0 (48.93-3.90)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.88Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.162 , 0.194 0.180 , 0.209	Depositor DCC
R_{free} test set	2265 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	129.8	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 138.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 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	31339	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.53	1/11391 (0.0%)	0.79	5/15402 (0.0%)
2	B	0.49	0/9048	0.75	1/12200 (0.0%)
3	C	0.46	0/2133	0.72	0/2891
4	D	0.50	0/1450	0.79	3/1945 (0.2%)
5	E	0.44	0/1788	0.70	0/2406
6	F	0.54	0/717	0.81	0/967
7	G	0.48	0/1368	0.74	0/1844
8	H	0.44	0/1086	0.73	0/1470
9	I	0.47	0/989	0.77	0/1331
10	J	0.51	0/541	0.77	0/727
11	K	0.45	0/938	0.68	0/1267
12	L	0.46	0/365	0.83	0/485
13	Q	1.91	2/77 (2.6%)	1.03	1/105 (1.0%)
All	All	0.51	3/31891 (0.0%)	0.76	10/43040 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q	27	MET	SD-CE	12.89	2.50	1.77
13	Q	27	MET	CG-SD	7.85	2.01	1.81
1	A	57	ARG	CA-C	5.39	1.67	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	CA-CB-CG	6.97	128.73	113.40
1	A	483	ASP	CA-CB-CG	6.48	127.65	113.40
1	A	399	HIS	N-CA-CB	6.47	122.24	110.60
1	A	41	MET	C-N-CA	5.76	136.11	121.70
13	Q	28	ARG	N-CA-C	-5.68	95.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	957	PRO	C-N-CA	-5.55	107.83	121.70
4	D	26	THR	C-N-CA	5.28	134.90	121.70
4	D	25	ALA	C-N-CA	5.20	134.71	121.70
2	B	628	THR	C-N-CA	5.11	134.49	121.70
4	D	26	THR	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11190	0	11255	242	0
2	B	8876	0	8919	157	0
3	C	2095	0	2051	42	0
4	D	1440	0	1456	16	0
5	E	1752	0	1776	22	0
6	F	705	0	731	16	0
7	G	1340	0	1357	25	0
8	H	1068	0	1040	24	0
9	I	971	0	927	17	0
10	J	532	0	542	18	0
11	K	920	0	929	22	0
12	L	363	0	386	10	0
13	Q	78	0	36	3	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31339	0	31405	530	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 (530) 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)
13:Q:27:MET:SD	13:Q:27:MET:CG	2.01	1.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.85	1.10
1:A:1081:LEU:HB3	1:A:1082:ASN:HA	1.40	1.04
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.24	1.02
13:Q:27:MET:CE	13:Q:27:MET:SD	2.50	0.99
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.53	0.91
11:K:65:HIS:HD2	11:K:67:PHE:H	1.19	0.90
10:J:8:PHE:H	10:J:49:MET:HE3	1.36	0.89
1:A:369:SER:H	11:K:2:ASN:HD21	1.21	0.88
1:A:631:HIS:HE1	1:A:879:GLU:HG2	1.40	0.87
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.19	0.87
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.56	0.87
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.54	0.87
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.57	0.86
1:A:225:ASN:HD22	1:A:228:PHE:H	1.22	0.85
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.23	0.84
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.61	0.83
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.60	0.82
2:B:654:ARG:H	2:B:657:HIS:HD2	1.26	0.81
3:C:125:MET:HB2	3:C:127:ARG:HE	1.44	0.81
1:A:451:HIS:CE1	1:A:1074:GLU:HG2	2.18	0.79
1:A:1329:THR:HG22	1:A:1331:SER:H	1.48	0.79
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.51	0.76
1:A:1450:LEU:HD21	7:G:19:GLY:O	1.86	0.76
2:B:986:GLN:HE22	2:B:1020:ARG:HD2	1.51	0.76
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.68	0.75
7:G:138:THR:HG22	7:G:139:ILE:H	1.51	0.75
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.67	0.75
2:B:995:ARG:HB3	2:B:997:GLU:OE2	1.87	0.74
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.51	0.74
10:J:48:ARG:O	10:J:52:THR:HG22	1.88	0.74
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.50	0.74
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.53	0.73
2:B:338:GLY:HA3	2:B:351:TYR:HE2	1.54	0.73
1:A:855:THR:HG21	1:A:857:ARG:HE	1.53	0.72
1:A:741:ASN:HD22	1:A:744:LYS:H	1.37	0.72
1:A:53:LEU:HD23	1:A:54:ASN:H	1.55	0.71
1:A:399:HIS:O	1:A:435:HIS:HD2	1.73	0.71
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.71	0.71
1:A:225:ASN:ND2	1:A:228:PHE:H	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.70	0.70
1:A:1079:MET:HB3	1:A:1081:LEU:CD2	2.22	0.70
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.57	0.69
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.21	0.69
1:A:503:GLN:HE21	6:F:90:ARG:HH12	1.39	0.69
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.73	0.69
3:C:79:GLN:HB3	3:C:127:ARG:HD2	1.75	0.69
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.75	0.68
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.74	0.68
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.76	0.68
1:A:567:LYS:HB2	8:H:96:VAL:HB	1.76	0.68
12:L:38:LEU:HD11	12:L:49:LYS:H	1.59	0.67
2:B:955:THR:HG22	12:L:55:ILE:HA	1.77	0.67
3:C:148:ARG:HB2	3:C:151:GLN:NE2	2.10	0.67
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.66
3:C:149:LYS:HG3	3:C:150:GLY:H	1.60	0.66
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.66
1:A:1032:LEU:O	1:A:1036:ARG:HD2	1.96	0.65
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.78	0.65
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.78	0.65
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.79	0.65
1:A:1081:LEU:HB3	1:A:1082:ASN:CA	2.23	0.65
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.61	0.65
1:A:64:ASN:HD22	1:A:66:LYS:HB2	1.61	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	2.10	0.65
4:D:155:ARG:CB	4:D:219:THR:HG21	2.28	0.64
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.78	0.64
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.80	0.64
2:B:654:ARG:H	2:B:657:HIS:CD2	2.14	0.63
7:G:26:LEU:HB3	7:G:56:ILE:HD11	1.80	0.63
1:A:631:HIS:CE1	1:A:879:GLU:HG2	2.28	0.63
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.79	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.62
1:A:134:ARG:HD2	1:A:221:SER:O	1.99	0.62
2:B:315:LYS:HG2	9:I:13:MET:HE2	1.80	0.62
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.80	0.62
3:C:55:THR:HB	3:C:151:GLN:HA	1.80	0.62
2:B:1013:ASN:ND2	2:B:1014:PRO:HD2	2.15	0.62
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.81	0.62
2:B:956:THR:HB	12:L:46:VAL:HG21	1.81	0.61
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:918:ILE:HD11	2:B:935:ARG:HD2	1.82	0.61
7:G:151:ILE:HD11	7:G:160:ILE:HD12	1.82	0.61
1:A:353:ILE:HD13	1:A:487:MET:CE	2.31	0.61
2:B:880:THR:H	2:B:883:LEU:HD11	1.65	0.60
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.82	0.60
1:A:53:LEU:HD23	1:A:54:ASN:N	2.16	0.60
2:B:683:SER:O	2:B:687:GLU:HB2	2.01	0.60
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.41	0.60
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.83	0.60
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.83	0.59
2:B:862:GLN:HE21	2:B:961:LEU:HD11	1.67	0.59
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	1.83	0.59
6:F:85:MET:O	6:F:155:LEU:HD11	2.03	0.59
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.83	0.59
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.66	0.59
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.83	0.59
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.84	0.58
2:B:291:ILE:HD12	2:B:291:ILE:H	1.68	0.58
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.85	0.58
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.39	0.58
2:B:174:LEU:HD11	2:B:204:ILE:HD12	1.86	0.58
1:A:1030:ARG:HA	1:A:1034:GLU:HG3	1.86	0.58
1:A:481:ASP:OD1	1:A:483:ASP:OD1	2.22	0.58
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.86	0.57
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.85	0.57
1:A:598:LEU:HD13	8:H:124:ARG:HB2	1.85	0.57
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.85	0.57
11:K:8:GLU:O	11:K:37:LYS:HD2	2.04	0.57
1:A:1009:ASN:HA	1:A:1012:ARG:HD2	1.87	0.57
1:A:299:HIS:HA	1:A:302:THR:HG22	1.87	0.57
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.87	0.57
3:C:148:ARG:H	3:C:151:GLN:HB2	1.70	0.57
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.87	0.57
7:G:151:ILE:HD11	7:G:160:ILE:CD1	2.35	0.56
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.40	0.56
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.39	0.56
6:F:87:LYS:HA	6:F:155:LEU:HD21	1.87	0.56
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.87	0.56
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.87	0.56
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.41	0.56
3:C:145:CYS:HA	10:J:2:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:HIS:CD2	11:K:67:PHE:H	2.11	0.56
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.88	0.56
4:D:155:ARG:HB3	4:D:219:THR:HG21	1.87	0.56
3:C:46:ILE:HD12	3:C:67:LEU:O	2.05	0.56
2:B:260:GLY:O	2:B:267:ARG:HD3	2.06	0.56
2:B:121:ASN:ND2	2:B:207:GLY:HA3	2.08	0.56
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.88	0.56
1:A:629:LEU:O	1:A:633:VAL:HG23	2.06	0.55
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.88	0.55
2:B:1215:ARG:HB3	2:B:1217:TYR:CE2	2.41	0.55
1:A:566:ILE:HD12	8:H:96:VAL:HG12	1.88	0.55
2:B:617:ARG:HG3	2:B:624:LEU:HD12	1.87	0.55
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.87	0.55
4:D:187:THR:HB	4:D:190:GLU:H	1.72	0.55
1:A:58:LEU:HD22	1:A:80:HIS:O	2.06	0.55
2:B:706:GLN:H	2:B:710:LEU:HD13	1.72	0.55
3:C:148:ARG:HB2	3:C:151:GLN:HE21	1.71	0.55
5:E:19:VAL:HG22	5:E:140:LEU:HD22	1.89	0.55
8:H:135:LEU:C	8:H:137:GLN:H	2.10	0.55
1:A:883:LEU:O	1:A:886:ILE:HG22	2.07	0.55
2:B:1013:ASN:HD22	2:B:1015:HIS:H	1.55	0.55
3:C:184:ASN:HD21	3:C:189:THR:H	1.55	0.54
10:J:8:PHE:N	10:J:49:MET:HE3	2.16	0.54
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.89	0.54
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.89	0.54
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.89	0.54
2:B:986:GLN:NE2	2:B:1020:ARG:HD2	2.20	0.54
1:A:335:ARG:NE	2:B:1202:LEU:HD13	2.23	0.54
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.89	0.54
1:A:1281:ARG:H	1:A:1309:ASP:HB2	1.72	0.54
2:B:570:VAL:HB	2:B:573:GLN:HB2	1.89	0.54
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.54
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.72	0.53
1:A:709:THR:HG23	9:I:94:ASP:HA	1.90	0.53
1:A:743:VAL:O	1:A:747:VAL:HG23	2.08	0.53
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.89	0.53
3:C:73:GLN:HE21	3:C:74:SER:H	1.57	0.53
1:A:1193:LEU:HB2	1:A:1260:LEU:HD23	1.91	0.53
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.53
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.27	0.53
1:A:1442:ASP:HB2	6:F:137:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HH22	1:A:184:SER:HB2	1.73	0.53
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.90	0.53
8:H:106:GLU:HA	8:H:112:ILE:HG13	1.91	0.53
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.91	0.53
8:H:103:LYS:HB3	8:H:115:TYR:HD1	1.74	0.53
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.90	0.53
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.74	0.53
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.89	0.52
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.91	0.52
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.24	0.52
2:B:776:GLN:HA	2:B:1096:ARG:HH11	1.74	0.52
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.92	0.52
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.09	0.52
8:H:6:PHE:HD2	8:H:130:ARG:HG2	1.74	0.52
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.75	0.52
1:A:741:ASN:ND2	1:A:744:LYS:H	2.06	0.52
1:A:523:ILE:HG23	1:A:527:THR:HB	1.91	0.52
2:B:1097:HIS:HB3	2:B:1102:LYS:HE3	1.91	0.52
2:B:660:LYS:HB3	2:B:679:TYR:CD2	2.44	0.52
2:B:710:LEU:HA	2:B:733:HIS:CB	2.34	0.52
1:A:567:LYS:HE3	8:H:91:ASP:HB2	1.92	0.52
1:A:49:LYS:HD3	1:A:61:ILE:HG13	1.91	0.52
1:A:29:ALA:HB1	2:B:1184:GLY:HA3	1.91	0.52
1:A:374:LEU:HB2	1:A:436:ILE:CD1	2.40	0.52
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.92	0.52
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.92	0.52
1:A:399:HIS:O	1:A:435:HIS:CD2	2.60	0.52
12:L:26:THR:O	12:L:37:LYS:HD3	2.09	0.52
5:E:176:PRO:O	5:E:212:ARG:HA	2.09	0.52
2:B:515:HIS:H	2:B:518:HIS:CD2	2.27	0.51
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.92	0.51
4:D:155:ARG:HB2	4:D:219:THR:HG21	1.90	0.51
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.92	0.51
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.92	0.51
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.40	0.51
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.73	0.51
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.92	0.51
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.91	0.51
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.91	0.51
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.11	0.51
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.45	0.51
2:B:613:VAL:HG22	2:B:628:THR:HA	1.93	0.51
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.59	0.51
1:A:1079:MET:HB3	1:A:1081:LEU:HD22	1.92	0.51
1:A:986:ILE:O	1:A:990:VAL:HG23	2.11	0.51
8:H:100:THR:HG23	8:H:138:GLU:HA	1.91	0.51
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.93	0.51
1:A:316:GLN:HB2	1:A:322:VAL:HG23	1.93	0.51
1:A:451:HIS:HB3	1:A:454:SER:H	1.75	0.51
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	1.93	0.51
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.95	0.50
3:C:31:ASN:O	3:C:34:ARG:HB3	2.11	0.50
3:C:73:GLN:HE21	3:C:75:MET:H	1.59	0.50
1:A:1081:LEU:HG	1:A:1097:GLY:HA3	1.92	0.50
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.93	0.50
10:J:48:ARG:HE	10:J:49:MET:HE2	1.75	0.50
7:G:111:THR:HG22	7:G:113:HIS:H	1.77	0.50
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.41	0.50
1:A:374:LEU:HB2	1:A:436:ILE:HD12	1.94	0.50
1:A:907:THR:HG22	1:A:908:LEU:N	2.27	0.50
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.47	0.50
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.46	0.50
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.93	0.50
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.26	0.50
1:A:709:THR:HB	1:A:712:GLU:H	1.76	0.50
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.94	0.50
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.50
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.77	0.50
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.93	0.49
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.93	0.49
1:A:335:ARG:HE	2:B:1202:LEU:HD13	1.77	0.49
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.94	0.49
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.51	0.49
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.94	0.49
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.94	0.49
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.95	0.49
9:I:8:ARG:HG2	9:I:34:TYR:CE1	2.47	0.49
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.42	0.49
2:B:308:TRP:CZ3	9:I:45:ARG:HB3	2.47	0.49
1:A:852:TYR:HB3	6:F:81:THR:HG22	1.95	0.49
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:TRP:HZ3	9:I:45:ARG:HB3	1.78	0.49
10:J:36:LEU:HD22	10:J:41:LEU:HD12	1.94	0.49
2:B:309:GLN:HB2	9:I:52:ILE:HD11	1.94	0.49
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.95	0.49
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.94	0.49
1:A:1389:PHE:CZ	1:A:1402:PHE:CE2	3.01	0.49
1:A:344:ARG:HB2	2:B:1118:PRO:HB2	1.94	0.49
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.94	0.49
2:B:315:LYS:N	2:B:316:PRO:HD2	2.27	0.49
2:B:52:ASN:OD1	2:B:177:LYS:HB2	2.13	0.49
7:G:137:ILE:HG12	7:G:143:ILE:HD11	1.95	0.49
2:B:745:PRO:O	2:B:748:ILE:HG12	2.13	0.49
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.12	0.49
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.94	0.49
7:G:145:VAL:HG13	7:G:163:ILE:HG23	1.94	0.49
2:B:34:ILE:HG12	2:B:542:MET:CE	2.43	0.48
3:C:125:MET:HB2	3:C:127:ARG:NE	2.21	0.48
2:B:944:THR:HB	2:B:1122:ARG:NH2	2.28	0.48
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.95	0.48
6:F:90:ARG:HD3	6:F:155:LEU:HD22	1.95	0.48
12:L:32:ALA:HB3	12:L:55:ILE:HG23	1.95	0.48
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.95	0.48
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.95	0.48
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.95	0.48
2:B:883:LEU:HD23	2:B:934:LYS:HB2	1.96	0.48
5:E:23:VAL:HG13	5:E:78:LEU:HD23	1.96	0.48
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.48	0.48
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.79	0.47
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.94	0.47
1:A:571:LEU:HD12	8:H:46:LEU:HD11	1.96	0.47
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.96	0.47
4:D:52:LEU:HD22	4:D:147:TYR:HE2	1.77	0.47
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.96	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.94	0.47
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.49	0.47
6:F:89:GLU:O	6:F:93:ILE:HD12	2.14	0.47
3:C:82:TYR:HB2	3:C:85:ASP:OD2	2.15	0.47
7:G:8:SER:HB3	7:G:73:LYS:HA	1.97	0.47
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.47
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.97	0.47
1:A:98:LYS:O	1:A:102:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASN:O	1:A:474:VAL:HG12	2.14	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
1:A:332:LYS:H	1:A:337:ARG:CB	2.28	0.47
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.79	0.47
2:B:841:MET:O	2:B:993:THR:HA	2.15	0.47
10:J:6:ARG:HG3	10:J:13:VAL:HG13	1.96	0.47
1:A:81:PHE:HE1	2:B:1205:GLN:HG2	1.80	0.47
2:B:1215:ARG:HB3	2:B:1217:TYR:HE2	1.78	0.47
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.80	0.47
2:B:766:ARG:HH11	2:B:766:ARG:HG3	1.79	0.47
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.79	0.47
4:D:202:ILE:HG21	4:D:207:LEU:HB2	1.96	0.47
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.80	0.47
2:B:705:MET:H	2:B:710:LEU:HD22	1.79	0.47
4:D:145:MET:O	4:D:149:THR:HB	2.15	0.47
3:C:175:ALA:HB3	10:J:43:ARG:HE	1.80	0.47
1:A:345:VAL:HG12	2:B:1155:SER:HB3	1.96	0.47
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.53	0.47
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.97	0.47
1:A:406:ILE:HD12	1:A:431:LYS:HB2	1.97	0.46
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.15	0.46
5:E:19:VAL:O	5:E:23:VAL:HG23	2.15	0.46
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.96	0.46
2:B:95:ILE:HD11	2:B:128:LEU:HG	1.98	0.46
3:C:46:ILE:HA	3:C:159:ALA:HA	1.97	0.46
6:F:147:SER:H	6:F:150:GLU:HG2	1.81	0.46
1:A:49:LYS:NZ	1:A:61:ILE:H	2.13	0.46
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.97	0.46
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.34	0.46
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.97	0.46
1:A:311:GLN:HE21	1:A:312:PRO:HD2	1.80	0.46
2:B:336:ARG:HD3	2:B:348:ARG:HD3	1.96	0.46
2:B:68:THR:HG23	2:B:91:SER:HB3	1.98	0.46
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.98	0.46
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.16	0.46
1:A:672:ASP:HB3	1:A:736:ASN:HD21	1.80	0.46
2:B:1006:ILE:H	2:B:1006:ILE:HG13	1.56	0.46
2:B:105:SER:C	2:B:107:GLY:H	2.19	0.46
3:C:77:ILE:HD12	3:C:129:ILE:HD11	1.96	0.46
1:A:313:GLN:HG2	1:A:321:PRO:HB3	1.97	0.46
1:A:880:LYS:HA	1:A:955:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:ARG:HH12	5:E:142:VAL:HG22	1.81	0.46
1:A:874:ASP:HA	1:A:1058:VAL:HG13	1.98	0.46
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.97	0.46
1:A:786:HIS:H	1:A:786:HIS:CD2	2.34	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46
1:A:344:ARG:HA	2:B:1128:LEU:O	2.16	0.46
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.97	0.45
1:A:1329:THR:HG22	1:A:1331:SER:N	2.26	0.45
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.27	0.45
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.50	0.45
10:J:25:LEU:HD21	10:J:32:GLU:HA	1.98	0.45
1:A:606:LEU:HG	1:A:613:ILE:HD13	1.98	0.45
6:F:118:LEU:O	6:F:122:MET:HG3	2.16	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.15	0.45
1:A:1147:THR:HB	9:I:48:LEU:HD13	1.98	0.45
1:A:1031:VAL:HA	1:A:1035:TYR:CD2	2.52	0.45
1:A:446:ARG:NH1	1:A:479:ASN:HB3	2.32	0.45
2:B:1040:ASN:HB3	13:Q:22:ILE:CB	2.47	0.45
2:B:975:GLN:O	2:B:990:ILE:HD12	2.17	0.45
4:D:54:GLU:O	4:D:58:VAL:HG23	2.17	0.45
1:A:130:ASP:O	1:A:134:ARG:HB2	2.17	0.45
1:A:33:ALA:HB2	1:A:57:ARG:HB3	1.99	0.45
2:B:954:VAL:O	12:L:56:LEU:HB2	2.16	0.45
1:A:1084:PHE:CG	1:A:1085:HIS:N	2.83	0.45
4:D:59:ILE:HG21	4:D:141:LEU:HD11	1.98	0.45
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.99	0.45
1:A:265:LYS:HG2	1:A:303:TYR:HA	1.98	0.45
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.99	0.45
1:A:43:GLU:CD	1:A:50:ILE:HG13	2.38	0.45
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.98	0.45
1:A:903:ASN:HB3	1:A:906:HIS:HB2	1.99	0.45
2:B:766:ARG:NH1	2:B:766:ARG:HG3	2.32	0.45
8:H:105:GLU:HB3	8:H:113:ALA:HB3	1.99	0.45
1:A:858:ASN:ND2	1:A:860:LEU:H	2.16	0.44
1:A:864:ILE:HA	1:A:1377:THR:HG21	1.98	0.44
2:B:756:ILE:O	2:B:759:PRO:HD3	2.17	0.44
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.52	0.44
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.99	0.44
1:A:754:SER:H	1:A:757:ASN:HD22	1.65	0.44
2:B:1180:PHE:HD1	4:D:1:MET:HG3	1.82	0.44
2:B:361:LEU:N	2:B:362:PRO:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ARG:HH12	2:B:418:LYS:HB3	1.81	0.44
2:B:848:ARG:HH12	2:B:996:ARG:HD2	1.82	0.44
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.52	0.44
6:F:134:ILE:HG22	6:F:136:ARG:HG3	2.00	0.44
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.98	0.44
1:A:852:TYR:HB3	6:F:81:THR:CG2	2.47	0.44
8:H:76:THR:HG22	8:H:77:ARG:HD2	1.98	0.44
2:B:376:PHE:CE1	2:B:569:TYR:HD2	2.36	0.44
2:B:515:HIS:H	2:B:518:HIS:HD2	1.66	0.44
5:E:179:GLN:O	5:E:182:ASP:HB2	2.18	0.44
2:B:273:LEU:HD12	2:B:280:ILE:HD13	2.00	0.44
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.98	0.44
11:K:77:THR:HB	11:K:81:TYR:HD2	1.82	0.44
2:B:731:VAL:HB	2:B:732:SER:H	1.72	0.44
1:A:711:ARG:HH22	9:I:88:SER:HB2	1.82	0.44
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.00	0.44
1:A:1276:VAL:HG21	1:A:1316:VAL:HG22	1.99	0.44
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.00	0.44
1:A:1325:THR:HA	5:E:147:HIS:HA	2.00	0.44
1:A:907:THR:HG22	1:A:908:LEU:H	1.82	0.43
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.53	0.43
3:C:58:LEU:HB3	3:C:63:ILE:HD11	1.99	0.43
7:G:60:ARG:HH22	7:G:63:PRO:HG3	1.82	0.43
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.43
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.83	0.43
3:C:29:MET:HA	11:K:45:LEU:HD13	2.01	0.43
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.99	0.43
2:B:1162:ILE:HG12	2:B:1194:ILE:HG12	2.01	0.43
9:I:82:GLU:HG2	9:I:104:LEU:HD13	1.99	0.43
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.00	0.43
1:A:768:GLN:CG	1:A:816:HIS:HA	2.37	0.43
1:A:982:THR:H	1:A:985:ASP:HB2	1.82	0.43
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.53	0.43
7:G:1:MET:HB3	7:G:1:MET:HE3	1.84	0.43
8:H:79:TRP:CH2	8:H:81:PRO:HA	2.54	0.43
1:A:1433:MET:HE3	7:G:63:PRO:HB3	2.01	0.43
1:A:774:ARG:H	1:A:774:ARG:HG3	1.67	0.43
2:B:866:TYR:O	2:B:870:ILE:HB	2.19	0.43
3:C:148:ARG:HB3	3:C:149:LYS:H	1.65	0.43
8:H:58:THR:HB	8:H:143:LEU:HB2	2.01	0.43
11:K:45:LEU:HG	11:K:94:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PRO:HD2	2:B:1191:ILE:O	2.18	0.43
2:B:242:SER:OG	2:B:362:PRO:HD2	2.19	0.43
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	2.01	0.43
7:G:134:GLU:HG2	7:G:135:ASP:H	1.83	0.43
1:A:262:LEU:HD11	1:A:325:ILE:HG12	2.00	0.43
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.88	0.43
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.00	0.43
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.83	0.43
2:B:875:GLU:O	2:B:877:PRO:HD3	2.19	0.43
5:E:147:HIS:CD2	5:E:149:LEU:H	2.37	0.43
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.54	0.43
1:A:382:PRO:HA	1:A:428:TYR:HE1	1.84	0.43
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	2.00	0.43
2:B:476:ARG:HH21	2:B:476:ARG:HB2	1.84	0.43
2:B:768:THR:O	2:B:771:SER:HB2	2.19	0.43
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.52	0.42
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.01	0.42
2:B:398:ARG:HB2	2:B:398:ARG:HH11	1.83	0.42
12:L:32:ALA:HB3	12:L:55:ILE:CG2	2.49	0.42
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.34	0.42
2:B:825:VAL:HG22	2:B:1010:LEU:HB2	2.01	0.42
3:C:125:MET:HG2	3:C:127:ARG:HH21	1.84	0.42
5:E:56:LYS:HE3	5:E:84:ASP:HB2	2.01	0.42
7:G:14:HIS:HD2	7:G:16:SER:OG	2.02	0.42
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.00	0.42
1:A:901:LEU:H	1:A:926:GLN:NE2	2.17	0.42
2:B:1002:THR:HG21	2:B:1070:GLU:OE2	2.20	0.42
2:B:1130:PHE:CG	2:B:1150:ARG:HG3	2.55	0.42
2:B:125:SER:HA	2:B:171:PRO:HA	2.01	0.42
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.01	0.42
8:H:10:PHE:HB3	8:H:28:ALA:HB1	2.02	0.42
9:I:7:CYS:SG	9:I:8:ARG:O	2.78	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.59	0.42
1:A:453:MET:HB3	1:A:477:PRO:HB2	1.99	0.42
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.00	0.42
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.42
5:E:15:ALA:O	5:E:19:VAL:HG23	2.18	0.42
10:J:14:VAL:HB	10:J:50:ILE:HD11	2.01	0.42
12:L:53:HIS:ND1	12:L:55:ILE:HG22	2.33	0.42
5:E:178:ILE:HB	5:E:212:ARG:HB3	2.01	0.42
8:H:81:PRO:HA	8:H:82:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.85	0.42
2:B:614:SER:HB3	2:B:627:PHE:HB2	2.01	0.42
1:A:1173:HIS:CB	1:A:1227:ILE:HG23	2.50	0.42
1:A:33:ALA:HB2	1:A:57:ARG:CB	2.50	0.42
1:A:182:VAL:HG22	1:A:201:VAL:HA	2.02	0.42
1:A:692:ASP:O	1:A:696:GLU:HB2	2.20	0.42
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.02	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.42
2:B:121:ASN:HA	2:B:207:GLY:CA	2.50	0.42
2:B:90:ILE:HG21	2:B:432:MET:SD	2.60	0.42
10:J:7:CYS:HA	10:J:49:MET:HG2	2.02	0.42
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.54	0.41
1:A:568:PRO:HG2	8:H:95:TYR:CD1	2.55	0.41
1:A:1079:MET:HB3	1:A:1081:LEU:HD21	2.00	0.41
1:A:1255:GLU:OE2	1:A:1258:HIS:HB3	2.20	0.41
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.20	0.41
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.55	0.41
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.50	0.41
1:A:41:MET:HB2	1:A:42:ASP:H	1.58	0.41
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.54	0.41
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.34	0.41
1:A:49:LYS:HZ1	1:A:60:SER:HA	1.85	0.41
1:A:956:LEU:HB3	1:A:957:PRO:HD2	2.02	0.41
4:D:126:ILE:HG21	4:D:145:MET:HB3	2.02	0.41
1:A:1031:VAL:HA	1:A:1035:TYR:HD2	1.84	0.41
1:A:1081:LEU:CG	1:A:1097:GLY:HA3	2.51	0.41
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.50	0.41
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.55	0.41
3:C:242:GLN:O	3:C:246:ARG:HB2	2.20	0.41
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.02	0.41
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.56	0.41
2:B:309:GLN:HE22	9:I:50:THR:HG23	1.85	0.41
12:L:38:LEU:HD22	12:L:56:LEU:HD21	2.03	0.41
1:A:986:ILE:HD13	1:A:1031:VAL:HB	2.02	0.41
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.61	0.41
1:A:55:ASP:OD1	1:A:57:ARG:HB2	2.20	0.41
2:B:126:SER:CB	2:B:172:ILE:HD11	2.50	0.41
2:B:235:SER:HB3	2:B:258:LEU:HD13	2.01	0.41
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.02	0.41
2:B:602:THR:HA	2:B:605:ARG:HB2	2.03	0.41
10:J:45:CYS:O	10:J:48:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	2.03	0.41
1:A:849:MET:HG2	1:A:850:VAL:N	2.35	0.41
1:A:973:ILE:HD11	1:A:1038:THR:HG23	2.02	0.41
2:B:997:GLU:CD	2:B:997:GLU:H	2.21	0.41
3:C:22:LEU:HD22	3:C:230:MET:HE2	2.02	0.41
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.21	0.41
1:A:675:THR:HG21	1:A:736:ASN:HB2	2.03	0.41
2:B:228:LYS:HD2	2:B:228:LYS:HA	1.91	0.41
2:B:361:LEU:O	2:B:374:LYS:HE2	2.21	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
2:B:978:ASP:O	2:B:989:THR:HA	2.21	0.41
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.03	0.41
1:A:548:ASN:ND2	11:K:47:ARG:HE	2.19	0.41
11:K:37:LYS:HD3	11:K:37:LYS:HA	1.94	0.41
1:A:622:VAL:HG23	1:A:629:LEU:HD12	2.02	0.41
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	2.03	0.41
7:G:101:VAL:HG12	7:G:103:VAL:HG23	2.03	0.41
8:H:111:LEU:HA	8:H:127:GLY:O	2.21	0.41
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	2.03	0.40
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.99	0.40
2:B:210:LYS:HD3	2:B:482:VAL:HG22	2.02	0.40
2:B:212:LEU:HD21	2:B:461:LEU:HD23	2.02	0.40
2:B:862:GLN:HG3	2:B:963:PHE:HD1	1.86	0.40
4:D:5:THR:HG21	7:G:74:TYR:OH	2.20	0.40
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	2.03	0.40
7:G:1:MET:SD	7:G:2:PHE:N	2.87	0.40
1:A:472:LEU:HD21	2:B:836:GLU:HG3	2.04	0.40
2:B:234:ILE:HG12	2:B:257:LYS:HB3	2.03	0.40
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.03	0.40
3:C:4:GLU:O	11:K:100:ALA:HB1	2.22	0.40
5:E:182:ASP:O	5:E:186:LEU:HG	2.20	0.40
5:E:37:LEU:HD11	5:E:45:LYS:HZ2	1.86	0.40
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.02	0.40
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.57	0.40
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.88	0.40
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.04	0.40
1:A:3:GLY:HA3	2:B:1159:ARG:HB3	2.04	0.40
4:D:121:LYS:H	4:D:121:LYS:HE3	1.86	0.40
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	1237 (88%)	140 (10%)	34 (2%)	7	45
2	B	1102/1223 (90%)	961 (87%)	114 (10%)	27 (2%)	6	44
3	C	264/266 (99%)	240 (91%)	20 (8%)	4 (2%)	12	54
4	D	176/221 (80%)	156 (89%)	15 (8%)	5 (3%)	6	43
5	E	212/214 (99%)	196 (92%)	14 (7%)	2 (1%)	20	63
6	F	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	15	58
8	H	129/145 (89%)	110 (85%)	14 (11%)	5 (4%)	3	35
9	I	117/119 (98%)	100 (86%)	15 (13%)	2 (2%)	11	52
10	J	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2	30
11	K	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	20	63
12	L	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	1	15
13	Q	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	3898/4419 (88%)	3441 (88%)	368 (9%)	89 (2%)	7	46

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	335	ARG
1	A	775	ILE
2	B	67	SER
2	B	339	THR
2	B	368	GLU
2	B	629	ASP
2	B	731	VAL
2	B	879	ARG
2	B	1046	PRO

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Mol	Chain	Res	Type
4	D	13	ARG
4	D	119	ARG
8	H	17	PRO
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	45	GLN
1	A	65	LEU
1	A	251	SER
1	A	331	GLY
1	A	466	SER
1	A	846	GLU
1	A	1379	GLY
2	B	65	GLU
2	B	364	ILE
2	B	643	ASP
2	B	712	PRO
2	B	907	GLY
2	B	1066	SER
2	B	1096	ARG
2	B	1176	ASN
2	B	1185	CYS
4	D	199	ASN
7	G	2	PHE
8	H	18	GLY
8	H	85	GLY
8	H	128	ASN
10	J	6	ARG
10	J	17	LYS
1	A	41	MET
1	A	114	LEU
1	A	483	ASP
1	A	1403	GLU
2	B	711	GLU
2	B	851	PHE
2	B	881	ASN
3	C	38	ILE
3	C	215	GLU
4	D	75	LYS
4	D	198	LEU
5	E	48	ASP
1	A	49	LYS

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	322	VAL
1	A	1327	ILE
2	B	363	HIS
2	B	470	LYS
2	B	655	LYS
2	B	1017	ILE
3	C	90	ASP
10	J	56	LEU
1	A	196	GLU
1	A	409	SER
1	A	465	TYR
1	A	600	PRO
1	A	1122	PRO
1	A	1365	TYR
1	A	1405	THR
2	B	340	ALA
2	B	648	HIS
2	B	707	PRO
3	C	214	ASN
7	G	63	PRO
8	H	136	LYS
9	I	89	GLN
9	I	91	ARG
11	K	64	GLU
12	L	45	ALA
1	A	55	ASP
1	A	250	ILE
1	A	283	GLY
1	A	332	LYS
1	A	1081	LEU
2	B	58	THR
5	E	51	GLY
1	A	258	GLY
1	A	916	GLY
1	A	93	VAL
1	A	1437	GLY

5.3.2 Protein sidechains

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%)	1064 (86%)	180 (14%)	4	25
2	B	967/1060 (91%)	832 (86%)	135 (14%)	4	27
3	C	234/234 (100%)	201 (86%)	33 (14%)	4	27
4	D	160/200 (80%)	137 (86%)	23 (14%)	4	26
5	E	196/196 (100%)	175 (89%)	21 (11%)	8	36
6	F	77/77 (100%)	69 (90%)	8 (10%)	8	37
7	G	152/152 (100%)	130 (86%)	22 (14%)	4	25
8	H	117/127 (92%)	104 (89%)	13 (11%)	7	35
9	I	113/113 (100%)	94 (83%)	19 (17%)	2	19
10	J	60/60 (100%)	52 (87%)	8 (13%)	4	28
11	K	99/99 (100%)	91 (92%)	8 (8%)	14	49
12	L	40/40 (100%)	27 (68%)	13 (32%)	0	2
13	Q	1/15 (7%)	1 (100%)	0	100	100
All	All	3460/3892 (89%)	2977 (86%)	483 (14%)	4	27

All (483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	28	ARG
1	A	42	ASP
1	A	44	THR
1	A	45	GLN
1	A	53	LEU
1	A	55	ASP
1	A	60	SER
1	A	63	ARG
1	A	96	ILE
1	A	116	ASP
1	A	145	LYS

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Mol	Chain	Res	Type
1	A	152	VAL
1	A	170	THR
1	A	174	ILE
1	A	199	LEU
1	A	204	THR
1	A	210	ILE
1	A	213	HIS
1	A	232	GLU
1	A	237	THR
1	A	250	ILE
1	A	251	SER
1	A	253	ASN
1	A	255	SER
1	A	257	ARG
1	A	261	ASP
1	A	265	LYS
1	A	295	LEU
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	315	LEU
1	A	317	LYS
1	A	318	SER
1	A	320	ARG
1	A	329	LEU
1	A	330	LYS
1	A	337	ARG
1	A	344	ARG
1	A	383	TYR
1	A	385	ILE
1	A	389	THR
1	A	391	LEU
1	A	393	ARG
1	A	394	ASN
1	A	406	ILE
1	A	408	ASP
1	A	412	ARG
1	A	434	ARG
1	A	437	MET
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU

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Mol	Chain	Res	Type
1	A	451	HIS
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	500	GLU
1	A	505	CYS
1	A	523	ILE
1	A	526	ASP
1	A	527	THR
1	A	532	ARG
1	A	544	ASP
1	A	566	ILE
1	A	584	ASN
1	A	597	LEU
1	A	600	PRO
1	A	602	ASP
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	666	ILE
1	A	670	ILE
1	A	691	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	830	LYS
1	A	831	THR
1	A	839	ARG
1	A	840	ARG
1	A	855	THR

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Mol	Chain	Res	Type
1	A	858	ASN
1	A	880	LYS
1	A	895	LYS
1	A	896	ARG
1	A	905	ASP
1	A	908	LEU
1	A	919	ILE
1	A	929	LEU
1	A	931	GLU
1	A	932	GLU
1	A	940	ARG
1	A	948	VAL
1	A	961	ARG
1	A	964	ILE
1	A	973	ILE
1	A	974	ASP
1	A	976	THR
1	A	988	LEU
1	A	1001	ARG
1	A	1035	TYR
1	A	1058	VAL
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1074	GLU
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	1110	ASN
1	A	1112	LYS
1	A	1116	LEU
1	A	1132	LYS
1	A	1146	VAL
1	A	1147	THR
1	A	1159	ARG
1	A	1160	SER
1	A	1167	GLU
1	A	1170	ILE
1	A	1176	LEU

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Mol	Chain	Res	Type
1	A	1187	GLN
1	A	1188	GLN
1	A	1199	ARG
1	A	1206	ASP
1	A	1208	THR
1	A	1237	ILE
1	A	1256	GLU
1	A	1269	GLU
1	A	1274	ARG
1	A	1277	GLU
1	A	1280	GLU
1	A	1288	ASP
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	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1356	ILE
1	A	1361	SER
1	A	1366	ARG
1	A	1371	LEU
1	A	1376	THR
1	A	1400	CYS
1	A	1404	GLU
1	A	1405	THR
1	A	1406	VAL
1	A	1420	ASP
1	A	1422	ARG
1	A	1426	GLU
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1452	LYS
2	B	25	ILE
2	B	26	THR
2	B	35	SER
2	B	44	VAL

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Mol	Chain	Res	Type
2	B	46	GLN
2	B	63	ILE
2	B	68	THR
2	B	90	ILE
2	B	103	ASN
2	B	122	LEU
2	B	134	LYS
2	B	169	ARG
2	B	178	ASN
2	B	205	ILE
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	240	ILE
2	B	251	ILE
2	B	254	LEU
2	B	258	LEU
2	B	261	ARG
2	B	267	ARG
2	B	313	MET
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	357	GLN
2	B	365	THR
2	B	368	GLU
2	B	376	PHE
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	399	ASP
2	B	401	PHE
2	B	408	LEU
2	B	418	LYS
2	B	423	LYS
2	B	466	TRP
2	B	469	GLN
2	B	470	LYS
2	B	476	ARG
2	B	481	GLN
2	B	483	LEU
2	B	485	ARG

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Mol	Chain	Res	Type
2	B	496	ARG
2	B	502	ILE
2	B	508	LEU
2	B	510	LYS
2	B	513	GLN
2	B	531	GLN
2	B	543	SER
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	559	SER
2	B	560	GLU
2	B	563	MET
2	B	570	VAL
2	B	573	GLN
2	B	582	VAL
2	B	589	VAL
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	616	ILE
2	B	617	ARG
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	690	VAL
2	B	708	GLU
2	B	731	VAL
2	B	737	THR
2	B	766	ARG
2	B	780	VAL
2	B	789	MET
2	B	790	ASP
2	B	791	THR
2	B	815	ARG
2	B	831	SER
2	B	837	ASP
2	B	844	SER
2	B	857	ARG

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Mol	Chain	Res	Type
2	B	861	ASP
2	B	868	MET
2	B	871	THR
2	B	876	LYS
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	904	ARG
2	B	906	SER
2	B	942	ARG
2	B	953	LEU
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	978	ASP
2	B	983	ARG
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1013	ASN
2	B	1019	SER
2	B	1045	SER
2	B	1058	LEU
2	B	1060	ARG
2	B	1065	GLN
2	B	1081	LEU
2	B	1113	VAL
2	B	1128	LEU
2	B	1134	GLU
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1185	CYS

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Mol	Chain	Res	Type
2	B	1188	LYS
2	B	1190	ASP
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
3	C	4	GLU
3	C	7	GLN
3	C	9	LYS
3	C	22	LEU
3	C	25	VAL
3	C	40	GLU
3	C	44	LEU
3	C	50	GLU
3	C	52	GLU
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	60	ASP
3	C	79	GLN
3	C	83	SER
3	C	85	ASP
3	C	116	LYS
3	C	119	VAL
3	C	121	VAL
3	C	127	ARG
3	C	133	ILE
3	C	134	ILE
3	C	142	VAL
3	C	166	GLU
3	C	189	THR
3	C	197	SER
3	C	215	GLU
3	C	226	ASP
3	C	237	SER
3	C	240	VAL
3	C	262	LEU
3	C	265	MET
3	C	268	ASP
4	D	6	SER
4	D	8	PHE
4	D	9	GLN
4	D	15	LEU

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Mol	Chain	Res	Type
4	D	20	GLU
4	D	21	GLU
4	D	39	ASN
4	D	41	GLN
4	D	51	ASN
4	D	53	SER
4	D	65	GLU
4	D	121	LYS
4	D	122	GLU
4	D	126	ILE
4	D	139	LYS
4	D	142	LYS
4	D	149	THR
4	D	187	THR
4	D	203	SER
4	D	217	LEU
4	D	219	THR
4	D	220	LEU
4	D	221	TYR
5	E	3	GLN
5	E	33	GLU
5	E	41	ASP
5	E	57	MET
5	E	67	GLU
5	E	75	MET
5	E	81	GLU
5	E	84	ASP
5	E	92	THR
5	E	95	THR
5	E	100	ILE
5	E	114	ASN
5	E	140	LEU
5	E	155	ARG
5	E	166	LYS
5	E	177	ARG
5	E	182	ASP
5	E	184	VAL
5	E	196	VAL
5	E	198	ILE
5	E	210	SER
6	F	69	LEU
6	F	70	LYS

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Mol	Chain	Res	Type
6	F	71	GLU
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	111	LEU
6	F	115	THR
7	G	5	LYS
7	G	8	SER
7	G	11	ILE
7	G	21	ARG
7	G	22	MET
7	G	23	LYS
7	G	24	GLN
7	G	26	LEU
7	G	34	VAL
7	G	47	CYS
7	G	92	VAL
7	G	106	MET
7	G	108	VAL
7	G	118	ASP
7	G	120	THR
7	G	126	ASN
7	G	142	ARG
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	154	VAL
7	G	171	ILE
8	H	5	LEU
8	H	11	GLN
8	H	19	ARG
8	H	26	ILE
8	H	31	THR
8	H	53	ASP
8	H	76	THR
8	H	103	LYS
8	H	112	ILE
8	H	124	ARG
8	H	130	ARG
8	H	131	ASN
8	H	135	LEU
9	I	4	PHE

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Mol	Chain	Res	Type
9	I	7	CYS
9	I	9	ASP
9	I	10	CYS
9	I	21	GLU
9	I	30	ARG
9	I	35	VAL
9	I	43	VAL
9	I	55	THR
9	I	61	ASP
9	I	62	ILE
9	I	77	LYS
9	I	81	ARG
9	I	87	GLN
9	I	88	SER
9	I	94	ASP
9	I	104	LEU
9	I	108	HIS
9	I	111	THR
10	J	1	MET
10	J	3	VAL
10	J	13	VAL
10	J	20	SER
10	J	42	LYS
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
11	K	2	ASN
11	K	9	LEU
11	K	18	LYS
11	K	31	VAL
11	K	41	THR
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
12	L	30	ILE
12	L	34	CYS
12	L	38	LEU
12	L	44	ASP
12	L	46	VAL
12	L	47	ARG
12	L	53	HIS
12	L	54	ARG

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Mol	Chain	Res	Type
12	L	55	ILE
12	L	61	THR
12	L	65	VAL
12	L	66	GLN
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	299	HIS
1	A	311	GLN
1	A	339	ASN
1	A	358	ASN
1	A	435	HIS
1	A	451	HIS
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	603	ASN
1	A	631	HIS
1	A	650	GLN
1	A	660	ASN
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	757	ASN
1	A	760	GLN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1124	HIS
1	A	1128	GLN
1	A	1130	GLN
1	A	1211	GLN
1	A	1390	ASN

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Mol	Chain	Res	Type
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	278	GLN
2	B	300	HIS
2	B	309	GLN
2	B	325	GLN
2	B	484	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS
2	B	744	HIS
2	B	842	ASN
2	B	862	GLN
2	B	986	GLN
2	B	1013	ASN
2	B	1015	HIS
2	B	1097	HIS
2	B	1117	GLN
2	B	1161	HIS
2	B	1195	HIS
2	B	1211	ASN
3	C	73	GLN
3	C	112	ASN
3	C	128	ASN
3	C	151	GLN
3	C	184	ASN
3	C	188	HIS
4	D	28	GLN
4	D	143	ASN
5	E	147	HIS
6	F	104	ASN
7	G	14	HIS
7	G	57	GLN
7	G	122	ASN
7	G	126	ASN
8	H	21	ASN
8	H	134	ASN
8	H	137	GLN
9	I	116	ASN
11	K	2	ASN
11	K	65	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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, 95th 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%)	-0.08	24 (1%) 70 61	55, 112, 198, 278	0
2	B	1118/1223 (91%)	0.02	27 (2%) 59 49	59, 127, 216, 300	0
3	C	266/266 (100%)	-0.07	0 100 100	76, 117, 173, 219	0
4	D	180/221 (81%)	-0.09	2 (1%) 80 72	92, 131, 203, 241	0
5	E	214/214 (100%)	0.04	6 (2%) 53 43	86, 162, 233, 254	0
6	F	87/87 (100%)	-0.28	1 (1%) 80 72	59, 89, 131, 142	0
7	G	171/171 (100%)	-0.09	1 (0%) 89 84	79, 111, 158, 224	0
8	H	133/145 (91%)	0.30	4 (3%) 51 40	104, 166, 223, 237	0
9	I	119/119 (100%)	0.23	4 (3%) 46 36	128, 157, 227, 246	0
10	J	65/65 (100%)	-0.22	0 100 100	85, 111, 162, 184	0
11	K	115/115 (100%)	-0.06	0 100 100	66, 113, 165, 200	0
12	L	46/46 (100%)	0.28	1 (2%) 62 53	98, 169, 211, 238	0
13	Q	15/15 (100%)	0.84	1 (6%) 19 14	108, 188, 212, 222	0
All	All	3950/4419 (89%)	-0.02	71 (1%) 69 59	55, 122, 210, 300	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	4.3
1	A	1086	PHE	4.2
2	B	469	GLN	4.2
9	I	118	ARG	3.8
9	I	120	GLN	3.6
1	A	1085	HIS	3.6
2	B	470	LYS	3.5
2	B	507	LYS	3.5
9	I	119	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	145	LYS	3.3
2	B	92	PHE	3.3
1	A	1176	LEU	3.2
5	E	93	MET	3.2
2	B	394	ASP	3.2
2	B	508	LEU	3.2
1	A	255	SER	3.1
1	A	115	LEU	3.1
5	E	88	VAL	3.0
2	B	132	VAL	3.0
1	A	1082	ASN	2.9
2	B	668	ASP	2.9
2	B	643	ASP	2.9
1	A	199	LEU	2.8
8	H	35	GLN	2.8
2	B	468	GLU	2.8
2	B	25	ILE	2.8
8	H	134	ASN	2.8
1	A	44	THR	2.7
1	A	184	SER	2.7
1	A	114	LEU	2.7
8	H	140	ALA	2.7
5	E	110	PHE	2.7
8	H	139	ASN	2.6
2	B	24	PRO	2.6
2	B	658	ILE	2.5
5	E	82	PHE	2.5
1	A	1084	PHE	2.5
1	A	1083	THR	2.5
1	A	164	ARG	2.5
1	A	171	GLN	2.5
1	A	173	THR	2.4
9	I	97	MET	2.4
2	B	666	TYR	2.4
2	B	339	THR	2.3
2	B	679	TYR	2.3
6	F	108	PHE	2.3
1	A	172	PRO	2.3
1	A	1188	GLN	2.3
2	B	167	ILE	2.2
12	L	25	ALA	2.2
1	A	65	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	146	MET	2.2
1	A	149	GLU	2.2
1	A	66	LYS	2.2
2	B	133	LYS	2.2
4	D	76	LYS	2.2
13	Q	32	LEU	2.1
2	B	341	LEU	2.1
2	B	503	GLY	2.1
5	E	49	SER	2.1
2	B	471	LYS	2.1
1	A	175	ARG	2.1
4	D	73	SER	2.1
1	A	701	LEU	2.1
7	G	137	ILE	2.0
2	B	662	MET	2.0
2	B	22	SER	2.0
5	E	123	LEU	2.0
2	B	509	ALA	2.0
2	B	472	ALA	2.0
2	B	346	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	ZN	B	1301	1/1	0.99	0.23	0.49	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	ZN	J	101	1/1	0.99	0.28	-0.23	111,111,111,111	0
14	ZN	I	201	1/1	0.99	0.12	-0.63	127,127,127,127	0
14	ZN	C	301	1/1	1.00	0.10	-1.25	94,94,94,94	0
14	ZN	A	1802	1/1	1.00	0.15	-1.48	97,97,97,97	0
14	ZN	I	202	1/1	0.99	0.07	-1.95	211,211,211,211	0
14	ZN	A	1801	1/1	0.98	0.05	-1.98	163,163,163,163	0
14	ZN	L	101	1/1	0.95	0.05	-2.60	149,149,149,149	0
15	MG	A	1803	1/1	0.92	0.64	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.