wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:06 PM BST

PDB ID	:	4V1M
EMDB ID:	:	EMD-2784
Title	:	Architecture of the RNA polymerase II-Mediator core transcription initiation complex
Authors	:	Plaschka, C.; Lariviere, L.; Wenzeck, L.; Hemann, M.; Tegunov, D.; Petrotchenko, E.V.; Borchers, C.H.; Baumeister, W.; Herzog, F.; Villa, E.; Cramer, P.
Deposited on	:	2014-09-29
Resolution	:	6.60 Å(reported)
Based on PDB ID	:	4A3D

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

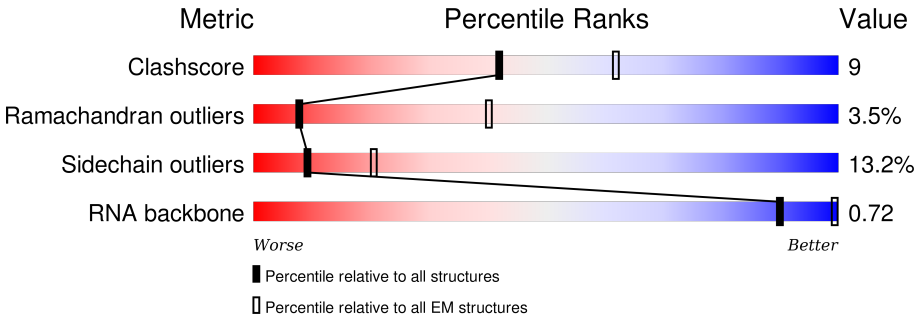
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1733	58% 20% • • 18%
2	B	1224	63% 28% • 6%
3	C	318	61% 19% • 16%
4	E	215	74% 23% •
5	F	155	37% 15% • 46%
6	H	146	55% 30% 5% • 9%
7	I	122	74% 21% • •
8	J	70	54% 29% 10% 7%

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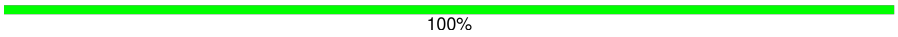
Mol	Chain	Length	Quality of chain
9	K	120	
10	L	70	
11	N	10	
12	P	6	
13	T	20	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29447 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
			Total	C	N	O	S		
1	A	1422	11174	7037	1954	2121	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1156	9143	5784	1606	1697	56	0	0

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

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	84	679	434	115	127	3	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

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

- Molecule 11 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	10	Total	C	N	O	P	0	0
			207	99	39	59	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	6	Total	C	N	O	P	0	0
			130	58	26	40	6		

- Molecule 13 is a DNA chain called 5'-D(*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TP*CP *CP*BRUP*GP*GP*TP*C)-3'.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	T	20	Total	Br	C	N	O	P	0	0
			404	1	194	63	126	20		

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

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

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

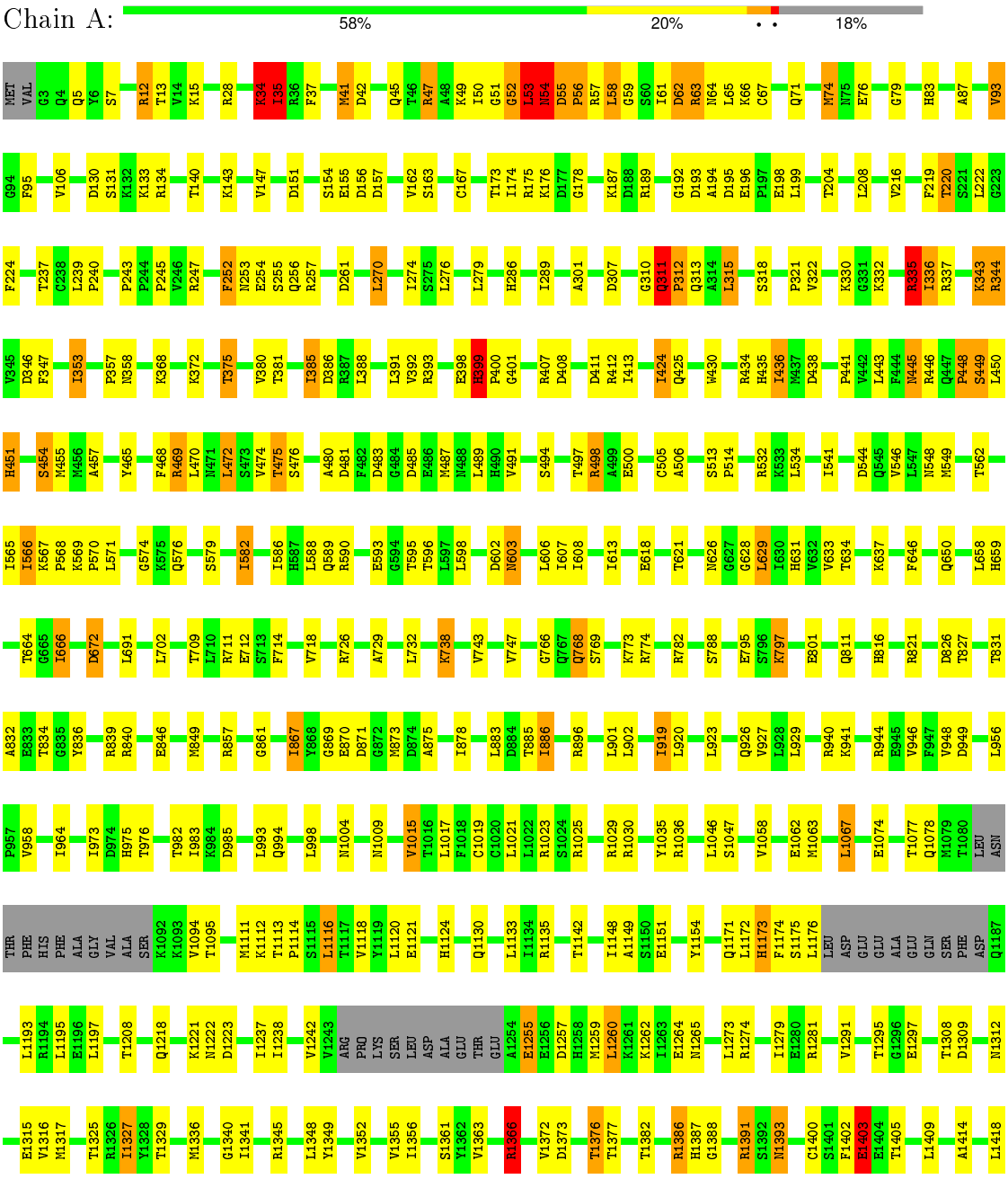
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

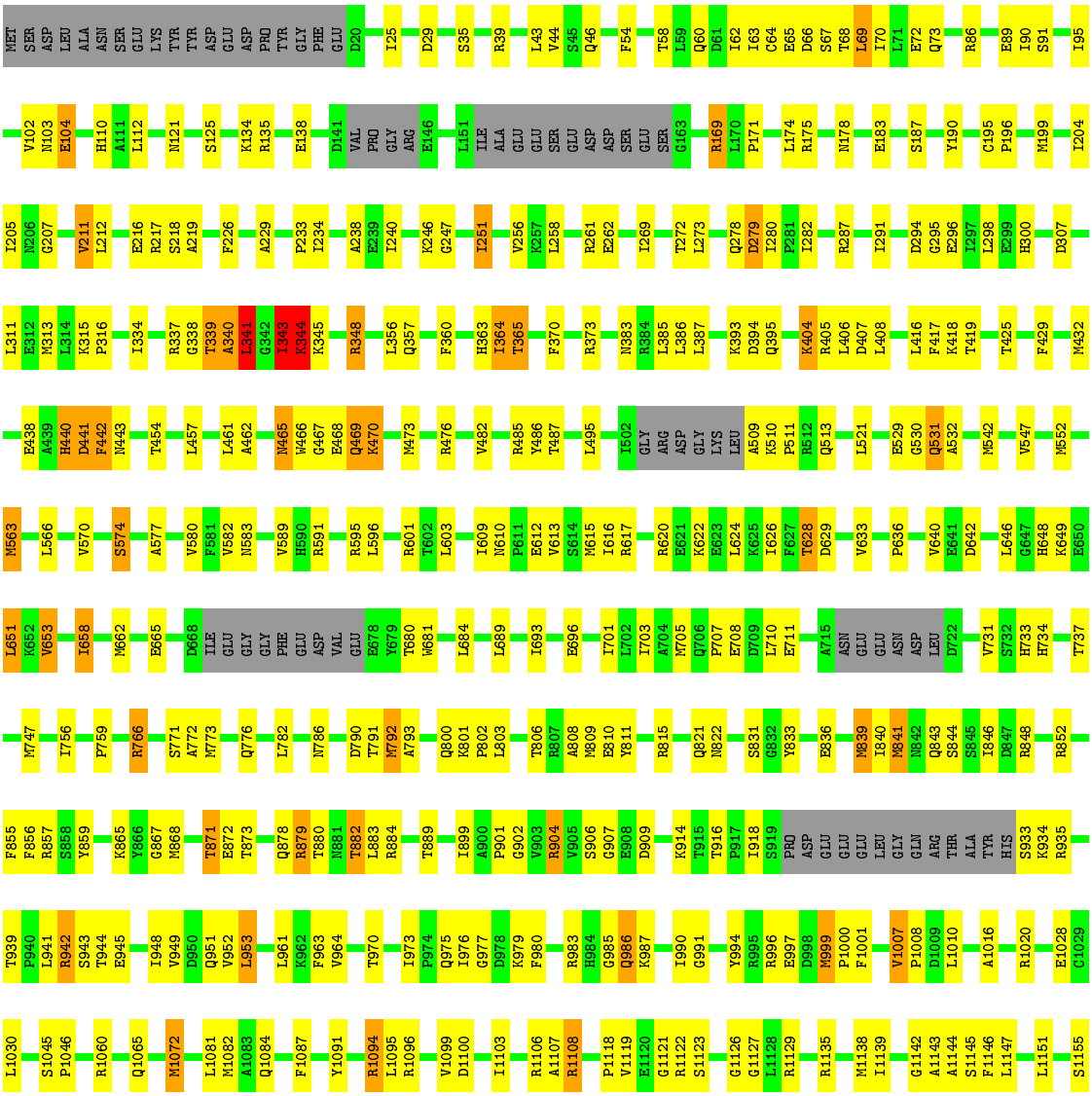
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

Chain A:



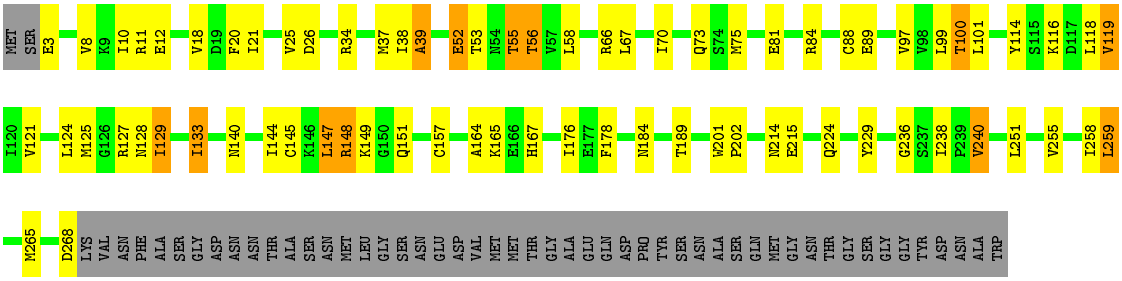
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B:



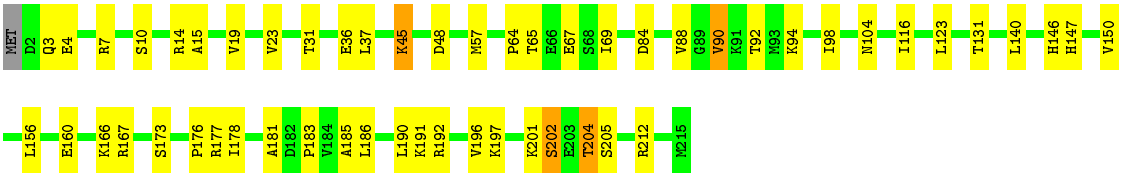
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



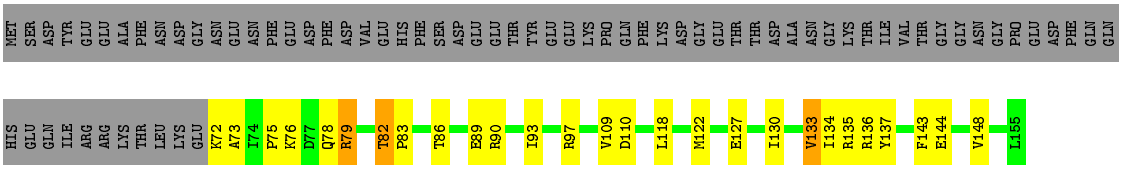
• Molecule 4: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



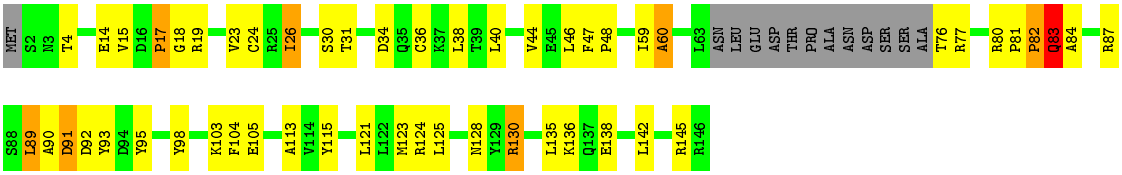
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:

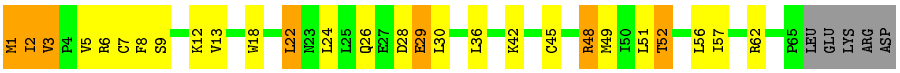


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:

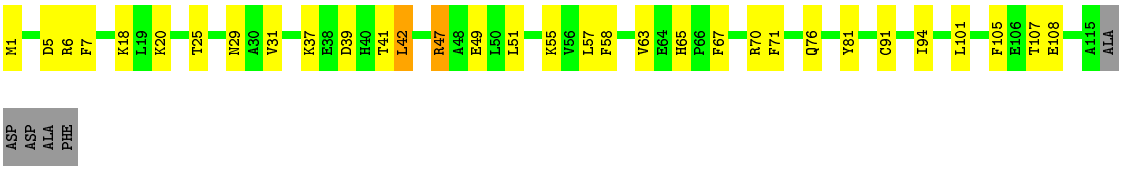
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



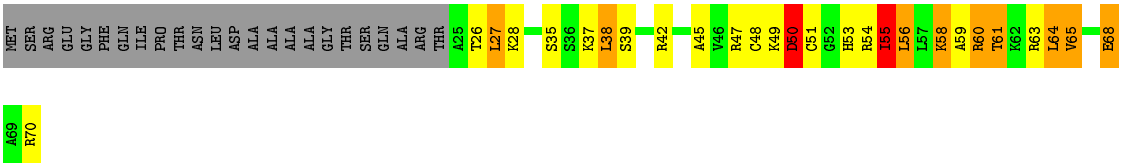
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



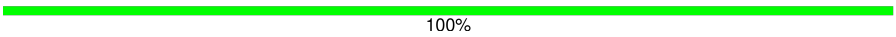
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:



• Molecule 11: 5'-D(*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'

Chain N:



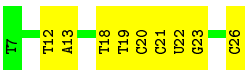
There are no outlier residues recorded for this chain.

• Molecule 12: 5'-D(*CP*CP*AP*GP*GP*AP)-3'

Chain P:

• Molecule 13: 5'-D(*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TP*TP*CP *CP*BRUP* GP*GP*TP*C)-3'

Chain T:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37000	Depositor
Image detector	GATAN K2 (4K X 4K)	Depositor

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, BRU

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.54	0/11374	0.85	10/15383 (0.1%)
10	L	0.54	0/365	0.95	0/485
11	N	1.07	0/232	1.06	0/356
12	P	1.21	0/145	0.79	0/224
13	T	1.26	1/426 (0.2%)	1.08	0/652
2	B	0.49	0/9318	0.79	10/12565 (0.1%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	E	0.48	0/1788	0.71	0/2406
5	F	0.62	0/691	0.81	0/933
6	H	0.51	0/1086	0.80	0/1470
7	I	0.47	0/989	0.78	0/1331
8	J	0.54	0/541	0.88	1/727 (0.1%)
9	K	0.47	0/938	0.71	0/1267
All	All	0.55	1/30026 (0.0%)	0.82	23/40690 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	26	DC	C1'-N1	5.58	1.56	1.49

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	465	ASN	O-C-N	15.46	147.44	122.70
2	B	465	ASN	CA-C-N	-12.77	89.11	117.20
2	B	465	ASN	C-N-CA	-9.63	97.63	121.70
2	B	218	SER	O-C-N	7.31	134.39	122.70
1	A	399	HIS	N-CA-CB	7.26	123.67	110.60
1	A	34	LYS	C-N-CA	7.21	139.72	121.70
2	B	218	SER	C-N-CA	-7.08	104.00	121.70
2	B	218	SER	CA-C-N	-6.17	103.61	117.20
1	A	56	PRO	C-N-CA	6.01	136.72	121.70
1	A	35	ILE	N-CA-CB	5.96	124.50	110.80
2	B	340	ALA	C-N-CA	5.68	135.91	121.70
1	A	194	ALA	C-N-CA	5.66	135.84	121.70
1	A	311	GLN	N-CA-C	5.55	125.99	111.00
1	A	54	ASN	C-N-CA	5.44	135.30	121.70
3	C	39	ALA	N-CA-C	5.44	125.69	111.00
2	B	628	THR	C-N-CA	5.44	135.29	121.70
3	C	89	GLU	N-CA-C	-5.30	96.69	111.00
1	A	53	LEU	N-CA-CB	5.28	120.97	110.40
1	A	310	GLY	C-N-CA	5.17	134.64	121.70
2	B	1181	GLU	N-CA-C	5.14	124.87	111.00
1	A	1403	GLU	N-CA-C	5.11	124.79	111.00
8	J	5	VAL	N-CA-C	-5.04	97.40	111.00
2	B	1156	ASP	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide
2	B	404	LYS	Mainchain
2	B	43	LEU	Mainchain

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	11174	0	11233	204	0
2	B	9143	0	9122	204	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2095	0	2051	42	0
4	E	1752	0	1776	26	0
5	F	679	0	701	19	0
6	H	1068	0	1040	24	0
7	I	971	0	927	15	0
8	J	532	0	542	15	0
9	K	920	0	929	20	0
10	L	363	0	386	20	0
11	N	207	0	114	0	0
12	P	130	0	66	1	0
13	T	404	0	227	6	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	29447	0	29114	514	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 9.

All (514) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.83	1.51
2:B:104:GLU:OE2	10:L:54:ARG:HD3	1.50	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	1.03	1.10
2:B:121:ASN:ND2	2:B:963:PHE:CZ	2.25	1.04
2:B:104:GLU:OE2	10:L:54:ARG:CD	2.10	1.00
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.27	0.98
2:B:121:ASN:ND2	2:B:963:PHE:HZ	1.62	0.92
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.52	0.91
1:A:53:LEU:HD23	1:A:54:ASN:N	1.87	0.90
8:J:48:ARG:HE	8:J:49:MET:HE2	1.37	0.89
5:F:76:LYS:HA	5:F:79:ARG:HD3	1.56	0.88
3:C:148:ARG:H	3:C:151:GLN:HG3	1.43	0.82
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.59	0.82
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.61	0.82
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:CD2	1:A:54:ASN:H	1.91	0.81
2:B:465:ASN:O	2:B:467:GLY:N	2.13	0.81
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.64	0.78
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.66	0.78
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.67	0.77
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.17	0.77
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.77
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.75
1:A:1444:MET:HE1	5:F:135:ARG:HB2	1.67	0.74
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.52	0.73
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.71	0.72
5:F:75:PRO:HG2	5:F:78:GLN:HB2	1.72	0.72
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.71	0.72
2:B:1198:TYR:CE2	2:B:1201:LYS:HE3	2.25	0.71
2:B:104:GLU:OE2	10:L:54:ARG:NE	2.24	0.71
2:B:246:LYS:HG2	2:B:418:LYS:CE	2.21	0.71
3:C:66:ARG:NH2	8:J:3:VAL:O	2.23	0.71
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.74	0.70
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.72	0.70
2:B:104:GLU:OE1	10:L:47:ARG:NH2	2.25	0.69
2:B:405:ARG:NH2	2:B:629:ASP:OD2	2.25	0.69
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.74	0.69
1:A:61:ILE:HG22	1:A:62:ASP:H	1.57	0.69
2:B:563:MET:HE2	2:B:580:VAL:HB	1.72	0.69
2:B:429:PHE:HA	2:B:432:MET:HE2	1.73	0.69
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.74	0.69
2:B:246:LYS:HG2	2:B:418:LYS:HE2	1.75	0.69
3:C:259:LEU:HD22	9:K:91:CYS:HB3	1.75	0.68
1:A:140:THR:HA	1:A:143:LYS:HE2	1.75	0.68
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.60	0.67
4:E:4:GLU:HB3	4:E:7:ARG:HE	1.59	0.67
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.76	0.67
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.30	0.67
2:B:121:ASN:HD21	2:B:963:PHE:HZ	1.37	0.67
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.76	0.66
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.75	0.66
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.76	0.66
10:L:61:THR:CG2	10:L:63:ARG:HG2	2.26	0.66
1:A:1442:ASP:HB2	5:F:137:TYR:HE1	1.61	0.66
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.65
2:B:104:GLU:CD	10:L:54:ARG:NE	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.65
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.32	0.64
2:B:806:THR:HG22	2:B:808:ALA:H	1.63	0.64
2:B:68:THR:HG22	2:B:91:SER:HA	1.80	0.64
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.64
10:L:28:LYS:HB2	10:L:39:SER:HA	1.80	0.64
3:C:56:THR:HG21	3:C:145:CYS:SG	2.37	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.64
1:A:1402:PHE:CE1	1:A:1403:GLU:HG2	2.33	0.63
3:C:10:ILE:HD12	9:K:108:GLU:HB3	1.81	0.63
2:B:918:ILE:HD13	2:B:935:ARG:HH22	1.65	0.62
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.81	0.62
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.81	0.62
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.62
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.62
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.82	0.62
1:A:343:LYS:HD3	2:B:1156:ASP:HB2	1.82	0.61
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.61
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.61
1:A:448:PRO:O	1:A:449:SER:HB2	2.01	0.61
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.41	0.61
4:E:4:GLU:HB3	4:E:7:ARG:NE	2.16	0.61
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.61
4:E:202:SER:HB3	4:E:205:SER:H	1.66	0.61
2:B:486:TYR:HB3	2:B:1096:ARG:CZ	2.31	0.61
2:B:205:ILE:HD11	2:B:461:LEU:HD13	1.82	0.61
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.83	0.60
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.60
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.02	0.60
2:B:246:LYS:HG3	2:B:418:LYS:HZ1	1.67	0.60
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.60
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.36	0.60
3:C:184:ASN:HD21	3:C:189:THR:H	1.50	0.60
2:B:216:GLU:OE2	2:B:404:LYS:HD2	2.02	0.60
2:B:104:GLU:CD	10:L:54:ARG:HE	2.06	0.59
1:A:483:ASP:HB2	2:B:987:LYS:HE3	1.84	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.59
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.84	0.59
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.59
6:H:82:PRO:C	6:H:84:ALA:H	2.05	0.59
10:L:61:THR:HG21	10:L:63:ARG:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.02	0.59
1:A:566:ILE:HD11	6:H:98:TYR:HB2	1.85	0.59
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.59
2:B:976:ILE:O	2:B:990:ILE:HB	2.02	0.58
6:H:47:PHE:HB3	6:H:95:TYR:CD2	2.38	0.58
1:A:315:LEU:HA	1:A:321:PRO:HA	1.86	0.58
10:L:47:ARG:HH21	10:L:54:ARG:HH21	1.50	0.58
2:B:405:ARG:CZ	2:B:629:ASP:OD2	2.52	0.58
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.86	0.58
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.85	0.58
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.85	0.58
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.84	0.58
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.58
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.57
2:B:792:MET:HA	2:B:856:PHE:O	2.04	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.69	0.57
2:B:465:ASN:C	2:B:467:GLY:N	2.58	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.56
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.86	0.56
2:B:405:ARG:HE	2:B:629:ASP:CG	2.09	0.56
5:F:79:ARG:HG2	5:F:144:GLU:HB3	1.88	0.56
2:B:406:LEU:HD12	2:B:633:VAL:HG22	1.87	0.56
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.56
5:F:118:LEU:O	5:F:122:MET:HG3	2.06	0.56
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.88	0.55
2:B:882:THR:HG1	2:B:935:ARG:N	2.03	0.55
5:F:89:GLU:O	5:F:93:ILE:HD12	2.06	0.55
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.39	0.55
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.87	0.55
2:B:246:LYS:CG	2:B:418:LYS:NZ	2.70	0.55
2:B:246:LYS:HG2	2:B:418:LYS:NZ	2.21	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.88	0.55
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.47	0.55
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.40	0.55
1:A:35:ILE:HA	1:A:52:GLY:O	2.07	0.54
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.88	0.54
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.89	0.54
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.54
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.88	0.54
2:B:343:ILE:O	2:B:344:LYS:HB2	2.07	0.54
2:B:216:GLU:OE2	2:B:404:LYS:CD	2.56	0.54
8:J:24:LEU:O	8:J:30:LEU:HB2	2.08	0.54
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.22	0.54
5:F:109:VAL:HG23	5:F:127:GLU:OE1	2.07	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.54
2:B:1100:ASP:OD2	9:K:1:MET:HB3	2.07	0.54
8:J:1:MET:HB2	8:J:56:LEU:HB2	1.89	0.54
1:A:832:ALA:HB1	13:T:18:DT:H2"	1.89	0.54
4:E:94:LYS:HE2	4:E:98:ILE:HD11	1.90	0.54
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.89	0.54
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.90	0.54
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.54
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.54
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.54
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.89	0.53
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.89	0.53
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.91	0.53
1:A:982:THR:HB	1:A:985:ASP:H	1.73	0.53
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.91	0.53
2:B:815:ARG:HH11	2:B:815:ARG:HG3	1.72	0.53
2:B:338:GLY:CA	2:B:339:THR:HB	2.38	0.53
4:E:19:VAL:O	4:E:23:VAL:HG23	2.08	0.53
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.53
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.91	0.53
3:C:164:ALA:HA	3:C:167:HIS:O	2.09	0.53
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.08	0.53
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.91	0.53
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.52
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.72	0.52
1:A:646:PHE:O	1:A:650:GLN:HG2	2.10	0.52
2:B:291:ILE:HD12	2:B:291:ILE:H	1.74	0.52
1:A:63:ARG:HA	1:A:74:MET:HG3	1.91	0.52
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.91	0.52
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.91	0.52
2:B:873:THR:O	2:B:914:LYS:HA	2.10	0.52
2:B:90:ILE:HD11	2:B:134:LYS:HE2	1.91	0.52
9:K:55:LYS:HB3	9:K:81:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:5:ASP:HB3	9:K:7:PHE:CE2	2.45	0.52
1:A:1149:ALA:HB2	7:I:47:GLU:HA	1.92	0.52
4:E:156:LEU:HD11	4:E:197:LYS:HB2	1.90	0.52
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.23	0.52
2:B:246:LYS:CG	2:B:418:LYS:HZ1	2.22	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.51
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.51
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.92	0.51
1:A:940:ARG:HB3	1:A:941:LYS:HE2	1.92	0.51
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.23	0.51
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.92	0.51
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.76	0.51
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.51
6:H:89:LEU:C	6:H:91:ASP:H	2.14	0.51
1:A:55:ASP:H	1:A:56:PRO:HD3	1.75	0.51
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.44	0.51
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.40	0.51
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.93	0.51
1:A:494:SER:HB3	1:A:497:THR:OG1	2.10	0.51
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.11	0.51
1:A:79:GLY:HA3	1:A:243:PRO:HB2	1.92	0.50
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.45	0.50
4:E:64:PRO:HB2	4:E:69:ILE:HD11	1.93	0.50
2:B:806:THR:HB	2:B:809:MET:HG3	1.94	0.50
4:E:15:ALA:O	4:E:19:VAL:HG23	2.10	0.50
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.46	0.50
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.94	0.50
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.93	0.50
1:A:52:GLY:N	1:A:56:PRO:HB3	2.26	0.50
2:B:1122:ARG:HB3	13:T:23:DG:OP1	2.12	0.50
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.93	0.50
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.77	0.50
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.92	0.50
2:B:773:MET:CE	2:B:985:GLY:HA2	2.40	0.50
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.50
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.94	0.50
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.50
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.93	0.50
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.11	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:574:SER:HB3	2:B:591:ARG:HE	1.77	0.50
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.93	0.50
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.12	0.50
2:B:916:THR:O	2:B:935:ARG:HG2	2.12	0.49
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.42	0.49
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.49
2:B:902:GLY:O	10:L:65:VAL:HG11	2.11	0.49
1:A:315:LEU:HD12	1:A:315:LEU:H	1.76	0.49
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.94	0.49
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.47	0.49
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.49
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.49
1:A:252:PHE:HD1	1:A:256:GLN:HB3	1.78	0.49
2:B:693:ILE:HG21	2:B:701:ILE:HD13	1.95	0.49
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.49
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.49
1:A:216:VAL:O	1:A:220:THR:HB	2.12	0.49
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.95	0.49
1:A:448:PRO:HG3	13:T:19:DT:O2	2.13	0.49
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.49
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.94	0.49
1:A:497:THR:HG22	2:B:1146:PHE:CD1	2.41	0.49
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.95	0.49
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.52	0.49
1:A:58:LEU:HB3	1:A:59:GLY:H	1.45	0.48
2:B:933:SER:O	2:B:935:ARG:N	2.45	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:NE	2.29	0.48
2:B:338:GLY:HA2	2:B:339:THR:HB	1.94	0.48
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.78	0.48
2:B:441:ASP:O	2:B:443:ASN:N	2.46	0.48
1:A:1004:ASN:CG	4:E:167:ARG:HD2	2.33	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.95	0.48
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.77	0.48
1:A:55:ASP:N	1:A:56:PRO:HD3	2.28	0.48
10:L:68:GLU:HB2	10:L:70:ARG:HD2	1.96	0.48
6:H:23:VAL:HG11	6:H:121:LEU:HD22	1.95	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.48
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.48
1:A:66:LYS:HB3	1:A:71:GLN:O	2.13	0.48
2:B:187:SER:HB3	8:J:62:ARG:HH22	1.77	0.48
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:HB2	4:E:204:THR:CG2	2.40	0.48
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.96	0.48
2:B:705:MET:H	2:B:710:LEU:HD12	1.78	0.48
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.48
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.96	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.48
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.73	0.48
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.79	0.48
6:H:115:TYR:CE1	6:H:124:ARG:HG3	2.49	0.48
1:A:64:ASN:O	1:A:65:LEU:HB3	2.12	0.47
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.96	0.47
1:A:738:LYS:HA	6:H:19:ARG:HH12	1.79	0.47
2:B:542:MET:HG3	2:B:747:MET:HB3	1.95	0.47
1:A:12:ARG:HB3	2:B:1218:THR:HB	1.96	0.47
3:C:165:LYS:O	9:K:6:ARG:NH1	2.46	0.47
1:A:568:PRO:HG2	6:H:46:LEU:HD12	1.95	0.47
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.47
8:J:9:SER:HB2	8:J:45:CYS:HB2	1.95	0.47
1:A:448:PRO:O	1:A:449:SER:CB	2.63	0.47
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.47
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.47
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.95	0.47
1:A:253:ASN:HB3	2:B:935:ARG:NE	2.29	0.47
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.95	0.47
3:C:58:LEU:HD21	8:J:57:ILE:HD12	1.97	0.47
1:A:1444:MET:CE	5:F:135:ARG:HB2	2.39	0.47
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.14	0.47
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.55	0.47
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.47
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.95	0.47
9:K:63:VAL:HG12	9:K:71:PHE:HB3	1.96	0.47
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.47
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.80	0.47
8:J:48:ARG:HE	8:J:49:MET:CE	2.19	0.47
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.95	0.47
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.50	0.47
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.46
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.95	0.46
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.15	0.46
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.98	0.46
2:B:882:THR:HG21	2:B:935:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:176:PRO:O	4:E:212:ARG:HA	2.14	0.46
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.97	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.16	0.46
4:E:65:THR:O	4:E:69:ILE:HD12	2.16	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
3:C:34:ARG:HA	3:C:37:MET:HE2	1.98	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.46
2:B:803:LEU:HG	8:J:52:THR:HG21	1.98	0.46
2:B:64:CYS:HA	2:B:67:SER:HB3	1.98	0.46
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.81	0.46
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.97	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.46
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.46
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.46
2:B:365:THR:HG21	2:B:370:PHE:CG	2.51	0.46
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.46
2:B:882:THR:C	2:B:884:ARG:H	2.19	0.46
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.97	0.46
2:B:211:VAL:CG1	2:B:495:LEU:HD23	2.45	0.46
2:B:406:LEU:HD12	2:B:633:VAL:CG2	2.46	0.46
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.46
7:I:83:ASN:HA	7:I:104:LEU:HG	1.98	0.46
2:B:291:ILE:HD12	2:B:291:ILE:N	2.30	0.45
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.99	0.45
1:A:7:SER:HG	2:B:1161:HIS:HE2	1.63	0.45
1:A:743:VAL:O	1:A:747:VAL:HG23	2.16	0.45
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.97	0.45
4:E:90:VAL:HG23	4:E:123:LEU:HD11	1.98	0.45
6:H:30:SER:HB3	6:H:36:CYS:HB3	1.98	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.98	0.45
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.81	0.45
2:B:852:ARG:HH22	10:L:70:ARG:C	2.19	0.45
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.99	0.45
1:A:270:LEU:HD12	1:A:274:ILE:HD11	1.98	0.45
2:B:901:PRO:O	10:L:60:ARG:HA	2.17	0.45
2:B:468:GLU:HG2	2:B:469:GLN:HB2	1.99	0.45
7:I:50:THR:HG22	7:I:52:ILE:H	1.81	0.45
3:C:55:THR:HB	3:C:151:GLN:HA	1.99	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.99	0.45
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.45
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.45
9:K:65:HIS:HE1	9:K:67:PHE:CG	2.35	0.45
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.97	0.45
12:P:8:G:H2'	12:P:9:G:H8	1.81	0.45
1:A:254:GLU:H	2:B:935:ARG:HH21	1.64	0.45
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.99	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.45
2:B:662:MET:HA	2:B:665:GLU:HB2	1.97	0.45
1:A:35:ILE:HG13	1:A:56:PRO:HG2	1.99	0.44
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.99	0.44
1:A:548:ASN:HD21	9:K:47:ARG:HH21	1.65	0.44
13:T:12:DT:H2'	13:T:13:DA:C8	2.52	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.99	0.44
2:B:394:ASP:OD2	7:I:91:ARG:HD2	2.17	0.44
7:I:72:ASP:O	7:I:81:ARG:HG2	2.16	0.44
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44
1:A:1154:TYR:CE1	7:I:18:GLU:HG3	2.53	0.44
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.99	0.44
1:A:1444:MET:HE1	5:F:135:ARG:NE	2.32	0.44
1:A:1151:GLU:HG2	7:I:45:ARG:HG3	1.99	0.44
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.15	0.44
1:A:1148:ILE:HA	7:I:49:ILE:HD12	2.00	0.44
1:A:869:GLY:O	4:E:204:THR:HG21	2.18	0.44
1:A:41:MET:HB3	1:A:49:LYS:HA	2.00	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	1.99	0.44
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.00	0.44
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.48	0.44
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.44
6:H:123:MET:HE1	6:H:142:LEU:HD11	2.00	0.44
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.44
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.44
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.44
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.44
6:H:4:THR:HA	6:H:60:ALA:HB2	2.00	0.44
1:A:62:ASP:HB2	1:A:65:LEU:HD22	1.99	0.43
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.53	0.43
13:T:19:DT:H2'	13:T:20:DC:C6	2.54	0.43
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:GLU:HB2	2:B:135:ARG:HB2	1.99	0.43
13:T:21:DC:H2'	13:T:22:BRU:H6	2.01	0.43
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.83	0.43
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.99	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.43
1:A:347:PHE:H	2:B:1107:ALA:HA	1.82	0.43
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.83	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.43
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.43
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.83	0.43
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.65	0.43
2:B:383:ASN:O	2:B:387:LEU:HB2	2.19	0.43
1:A:598:LEU:HA	1:A:598:LEU:HD23	1.83	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.01	0.43
2:B:542:MET:HE3	2:B:636:PRO:HG2	1.99	0.43
6:H:105:GLU:HB3	6:H:113:ALA:HB3	2.00	0.43
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.00	0.43
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.01	0.43
1:A:1438:THR:HB	2:B:1142:GLY:O	2.19	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.43
1:A:239:LEU:HD12	1:A:240:PRO:HD2	2.01	0.43
10:L:49:LYS:O	10:L:50:ASP:HB2	2.19	0.43
5:F:130:ILE:HB	5:F:148:VAL:HG21	1.99	0.43
5:F:82:THR:HG22	5:F:83:PRO:HD2	2.01	0.43
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	2.01	0.43
2:B:199:MET:SD	2:B:199:MET:N	2.90	0.43
1:A:344:ARG:HG2	2:B:1127:GLY:O	2.18	0.42
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.84	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.42
2:B:125:SER:HA	2:B:171:PRO:HA	2.00	0.42
6:H:15:VAL:HG22	6:H:26:ILE:HG13	2.00	0.42
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.02	0.42
1:A:449:SER:HA	1:A:454:SER:CB	2.49	0.42
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.42
2:B:65:GLU:HG3	2:B:66:ASP:H	1.85	0.42
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.42
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.19	0.42
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.49	0.42
8:J:48:ARG:NE	8:J:49:MET:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.42
1:A:358:ASN:HB2	9:K:65:HIS:HD2	1.83	0.42
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.54	0.42
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.42
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.52	0.42
1:A:1025:ARG:O	1:A:1035:TYR:HE2	2.01	0.42
3:C:148:ARG:HG3	3:C:151:GLN:HG3	2.01	0.42
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.42
7:I:76:PRO:HD2	7:I:108:HIS:HD2	1.84	0.42
8:J:22:LEU:O	8:J:26:GLN:HG2	2.20	0.42
4:E:10:SER:O	4:E:14:ARG:HG3	2.19	0.42
6:H:38:LEU:HD13	6:H:125:LEU:HD13	2.02	0.42
3:C:99:LEU:HB3	3:C:118:LEU:HD22	2.02	0.42
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.85	0.42
2:B:952:VAL:HB	10:L:58:LYS:HB2	2.01	0.42
4:E:181:ALA:HA	4:E:186:LEU:HD21	2.01	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.52	0.42
2:B:848:ARG:HD2	8:J:8:PHE:O	2.20	0.42
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.01	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.41
1:A:1094:VAL:HG22	1:A:1113:THR:HB	2.02	0.41
6:H:125:LEU:HG	6:H:130:ARG:HH22	1.85	0.41
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.41
1:A:336:ILE:H	1:A:336:ILE:HG12	1.68	0.41
2:B:311:LEU:HB3	7:I:4:PHE:HE2	1.85	0.41
2:B:190:TYR:CE2	2:B:196:PRO:HG3	2.55	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.01	0.41
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.41
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.20	0.41
10:L:38:LEU:HD21	10:L:48:CYS:HA	2.02	0.41
2:B:865:LYS:HB2	2:B:961:LEU:HD21	2.00	0.41
2:B:226:PHE:HA	2:B:395:GLN:CG	2.49	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
2:B:953:LEU:HD11	10:L:55:ILE:HG22	2.03	0.41
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.41
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.41
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.03	0.41
2:B:341:LEU:HD11	2:B:343:ILE:HB	2.02	0.41
3:C:148:ARG:N	3:C:151:GLN:HG3	2.22	0.41
2:B:792:MET:HG2	2:B:855:PHE:CZ	2.55	0.41
1:A:541:ILE:HG21	1:A:549:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:O	1:A:53:LEU:HB2	2.21	0.41
6:H:82:PRO:O	6:H:84:ALA:N	2.52	0.41
2:B:841:MET:HG2	2:B:1010:LEU:HD12	2.01	0.41
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.41
2:B:792:MET:H	2:B:857:ARG:HA	1.86	0.41
8:J:28:ASP:C	8:J:30:LEU:H	2.24	0.41
4:E:156:LEU:HD23	4:E:160:GLU:HB3	2.03	0.41
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.86	0.41
2:B:899:ILE:HG21	2:B:949:VAL:HG21	2.03	0.41
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.86	0.41
1:A:311:GLN:O	1:A:312:PRO:C	2.59	0.41
9:K:39:ASP:OD1	9:K:41:THR:HB	2.21	0.41
2:B:1082:MET:HA	3:C:189:THR:HA	2.03	0.41
3:C:258:ILE:HG13	9:K:42:LEU:HD21	2.03	0.41
5:F:97:ARG:HD2	5:F:97:ARG:HA	1.82	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
6:H:82:PRO:HB2	6:H:83:GLN:H	1.65	0.40
3:C:255:VAL:HG21	9:K:94:ILE:HG21	2.03	0.40
1:A:93:VAL:HG22	1:A:301:ALA:HA	2.03	0.40
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.03	0.40
2:B:509:ALA:O	2:B:511:PRO:HD3	2.20	0.40
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.52	0.40
7:I:111:THR:HG21	7:I:118:ARG:HD2	2.03	0.40
1:A:1418:LEU:HD23	2:B:1222:ARG:HD3	2.03	0.40
1:A:133:LYS:HE3	1:A:1391:ARG:HH12	1.85	0.40
1:A:626:ASN:O	1:A:631:HIS:ND1	2.53	0.40
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.03	0.40
1:A:1221:LYS:HB3	1:A:1222:ASN:H	1.72	0.40
2:B:979:LYS:HD3	2:B:1095:LEU:HD13	2.04	0.40
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.03	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
2:B:622:LYS:HE3	7:I:59:VAL:HG22	2.02	0.40
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.02	0.40
3:C:99:LEU:HD12	3:C:118:LEU:HB3	2.02	0.40
4:E:167:ARG:HA	4:E:167:ARG:HD3	1.78	0.40
2:B:469:GLN:HB3	2:B:470:LYS:H	1.72	0.40
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.04	0.40
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	2.04	0.40
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.97	0.40
6:H:104:PHE:CE1	6:H:136:LYS:HG3	2.57	0.40
5:F:89:GLU:C	5:F:93:ILE:HD12	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:SER:HG	2:B:994:TYR:HE2	1.66	0.40
9:K:65:HIS:CE1	9:K:67:PHE:CG	3.10	0.40
1:A:1356:ILE:HG23	1:A:1361:SER:HB2	2.03	0.40
2:B:65:GLU:OE1	2:B:247:GLY:HA2	2.20	0.40
2:B:871:THR:HG22	2:B:872:GLU:H	1.86	0.40
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.04	0.40
1:A:886:ILE:HD13	1:A:944:ARG:HG2	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 PDB entries followed by that with respect to all EM entries.

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	1414/1733 (82%)	1236 (87%)	126 (9%)	52 (4%)	4 37
2	B	1138/1224 (93%)	1008 (89%)	86 (8%)	44 (4%)	4 36
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	24 69
4	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	10 52
5	F	82/155 (53%)	76 (93%)	6 (7%)	0	100 100
6	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1 22
7	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	7 45
8	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	3 32
9	K	113/120 (94%)	109 (96%)	4 (4%)	0	100 100
10	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0 4
All	All	3576/4173 (86%)	3148 (88%)	303 (8%)	125 (4%)	8 39

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	189	ARG
1	A	195	ASP
1	A	257	ARG
1	A	318	SER
1	A	399	HIS
1	A	449	SER
1	A	628	GLY
1	A	1377	THR
1	A	1403	GLU
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	442	PHE
2	B	466	TRP
2	B	473	MET
2	B	531	GLN
2	B	772	ALA
2	B	867	GLY
2	B	943	SER
2	B	1046	PRO
2	B	1181	GLU
7	I	9	ASP
7	I	95	THR
10	L	50	ASP
10	L	53	HIS
1	A	47	ARG
1	A	54	ASN
1	A	167	CYS
1	A	178	GLY
1	A	193	ASP
1	A	224	PHE
1	A	286	HIS
1	A	332	LYS
1	A	672	ASP
1	A	1175	SER
1	A	1281	ARG
2	B	262	GLU
2	B	282	ILE
2	B	339	THR

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Mol	Chain	Res	Type
2	B	341	LEU
2	B	707	PRO
2	B	731	VAL
2	B	792	MET
2	B	879	ARG
2	B	1175	LEU
2	B	1176	ASN
4	E	36	GLU
6	H	17	PRO
6	H	81	PRO
6	H	82	PRO
6	H	83	GLN
6	H	90	ALA
8	J	6	ARG
10	L	45	ALA
10	L	56	LEU
1	A	335	ARG
1	A	975	HIS
1	A	1173	HIS
2	B	340	ALA
2	B	343	ILE
2	B	711	GLU
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
4	E	45	LYS
4	E	48	ASP
6	H	18	GLY
10	L	59	ALA
1	A	42	ASP
1	A	52	GLY
1	A	74	MET
1	A	465	TYR
1	A	569	LYS
1	A	846	GLU
1	A	958	VAL
1	A	1255	GLU
1	A	1437	GLY
1	A	1438	THR
2	B	441	ASP
2	B	648	HIS
2	B	883	LEU

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Mol	Chain	Res	Type
2	B	942	ARG
2	B	1108	ARG
2	B	1155	SER
3	C	88	CYS
7	I	91	ARG
8	J	29	GLU
10	L	26	THR
10	L	55	ILE
10	L	64	LEU
1	A	156	ASP
1	A	311	GLN
1	A	336	ILE
1	A	567	LYS
1	A	1171	GLN
1	A	1366	ARG
2	B	251	ILE
2	B	462	ALA
2	B	469	GLN
2	B	880	THR
2	B	907	GLY
2	B	1223	ASP
6	H	60	ALA
6	H	128	ASN
8	J	2	ILE
1	A	35	ILE
1	A	55	ASP
1	A	155	GLU
1	A	885	THR
3	C	214	ASN
1	A	196	GLU
1	A	1388	GLY
4	E	90	VAL
2	B	44	VAL
2	B	364	ILE
1	A	192	GLY
1	A	312	PRO
2	B	1121	GLY
1	A	448	PRO
2	B	1214	PRO
6	H	59	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 PDB entries followed by that with respect to all EM entries.

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	1240/1520 (82%)	1062 (86%)	178 (14%)	4 25
2	B	986/1061 (93%)	861 (87%)	125 (13%)	5 29
3	C	234/274 (85%)	206 (88%)	28 (12%)	6 31
4	E	196/197 (100%)	175 (89%)	21 (11%)	8 36
5	F	74/137 (54%)	67 (90%)	7 (10%)	11 41
6	H	117/128 (91%)	103 (88%)	14 (12%)	6 31
7	I	113/116 (97%)	106 (94%)	7 (6%)	23 60
8	J	60/65 (92%)	49 (82%)	11 (18%)	2 14
9	K	99/102 (97%)	87 (88%)	12 (12%)	6 31
10	L	40/57 (70%)	27 (68%)	13 (32%)	0 2
All	All	3159/3657 (86%)	2743 (87%)	416 (13%)	9 28

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	15	LYS
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	45	GLN
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	93	VAL
1	A	106	VAL
1	A	131	SER

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Mol	Chain	Res	Type
1	A	134	ARG
1	A	147	VAL
1	A	157	ASP
1	A	173	THR
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	237	THR
1	A	252	PHE
1	A	255	SER
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	289	ILE
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU
1	A	322	VAL
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	411	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG

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Mol	Chain	Res	Type
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	532	ARG
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	596	THR
1	A	602	ASP
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	738	LYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	795	GLU

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Mol	Chain	Res	Type
1	A	797	LYS
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	849	MET
1	A	867	ILE
1	A	886	ILE
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	949	ASP
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	998	LEU
1	A	1009	ASN
1	A	1015	VAL
1	A	1029	ARG
1	A	1030	ARG
1	A	1047	SER
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN

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Mol	Chain	Res	Type
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1273	LEU
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU
2	B	73	GLN

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Mol	Chain	Res	Type
2	B	103	ASN
2	B	104	GLU
2	B	110	HIS
2	B	169	ARG
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	211	VAL
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN
2	B	365	THR
2	B	393	LYS
2	B	408	LEU
2	B	419	THR
2	B	440	HIS
2	B	442	PHE
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	529	GLU
2	B	531	GLN
2	B	547	VAL
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG

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Mol	Chain	Res	Type
2	B	596	LEU
2	B	601	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	646	LEU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	696	GLU
2	B	708	GLU
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	771	SER
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	801	LYS
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	906	SER
2	B	909	ASP
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	951	GLN
2	B	953	LEU

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Mol	Chain	Res	Type
2	B	964	VAL
2	B	970	THR
2	B	973	ILE
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1094	ARG
2	B	1106	ARG
2	B	1123	SER
2	B	1129	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1193	GLN
2	B	1201	LYS
2	B	1202	LEU
2	B	1210	MET
2	B	1220	ARG
2	B	1223	ASP
3	C	3	GLU
3	C	12	GLU
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	53	THR
3	C	55	THR

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Mol	Chain	Res	Type
3	C	56	THR
3	C	81	GLU
3	C	84	ARG
3	C	100	THR
3	C	101	LEU
3	C	119	VAL
3	C	121	VAL
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	147	LEU
3	C	148	ARG
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP
4	E	3	GLN
4	E	31	THR
4	E	37	LEU
4	E	45	LYS
4	E	57	MET
4	E	67	GLU
4	E	84	ASP
4	E	92	THR
4	E	104	ASN
4	E	131	THR
4	E	140	LEU
4	E	146	HIS
4	E	166	LYS
4	E	173	SER
4	E	177	ARG
4	E	178	ILE
4	E	191	LYS
4	E	192	ARG
4	E	196	VAL
4	E	202	SER
4	E	204	THR

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Mol	Chain	Res	Type
5	F	72	LYS
5	F	79	ARG
5	F	82	THR
5	F	86	THR
5	F	90	ARG
5	F	110	ASP
5	F	133	VAL
6	H	14	GLU
6	H	26	ILE
6	H	31	THR
6	H	34	ASP
6	H	76	THR
6	H	77	ARG
6	H	83	GLN
6	H	89	LEU
6	H	91	ASP
6	H	92	ASP
6	H	103	LYS
6	H	130	ARG
6	H	135	LEU
6	H	138	GLU
7	I	8	ARG
7	I	31	THR
7	I	35	VAL
7	I	74	GLU
7	I	94	ASP
7	I	106	CYS
7	I	111	THR
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	12	LYS
8	J	13	VAL
8	J	22	LEU
8	J	29	GLU
8	J	42	LYS
8	J	48	ARG
8	J	52	THR
9	K	18	LYS
9	K	20	LYS
9	K	25	THR

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Mol	Chain	Res	Type
9	K	29	ASN
9	K	31	VAL
9	K	37	LYS
9	K	42	LEU
9	K	47	ARG
9	K	51	LEU
9	K	70	ARG
9	K	101	LEU
9	K	107	THR
10	L	27	LEU
10	L	35	SER
10	L	38	LEU
10	L	42	ARG
10	L	50	ASP
10	L	51	CYS
10	L	55	ILE
10	L	56	LEU
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	65	VAL
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	253	ASN
1	A	399	HIS
1	A	425	GLN
1	A	545	GLN
1	A	548	ASN
1	A	603	ASN
1	A	994	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1173	HIS
1	A	1270	ASN
1	A	1393	ASN
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN

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Mol	Chain	Res	Type
2	B	842	ASN
2	B	975	GLN
2	B	1025	HIS
2	B	1117	GLN
3	C	184	ASN
4	E	3	GLN
6	H	35	GLN
6	H	83	GLN
7	I	83	ASN
7	I	89	GLN
7	I	108	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	P	5/6 (83%)	1 (20%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	P	8	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	BRU	T	22	13,12	12,21,22	1.09	1 (8%)	16,30,33	3.82	4 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BRU	T	22	13,12	-	0/3/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	22	BRU	C4-C5	2.85	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	22	BRU	C5-C4-N3	-8.59	114.83	124.00
13	T	22	BRU	C2'-C1'-N1	-2.39	108.25	114.14
13	T	22	BRU	O4'-C1'-N1	4.35	115.31	107.71
13	T	22	BRU	C4-N3-C2	11.56	124.81	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	22	BRU	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.