



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 10:55 AM EDT

PDB ID : 4X6A
Title : Crystal structure of yeast RNA polymerase II encountering oxidative Cyclopurine DNA lesions
Authors : Wang, L.; Chong, J.; Wang, D.
Deposited on : 2014-12-07
Resolution : 3.96 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

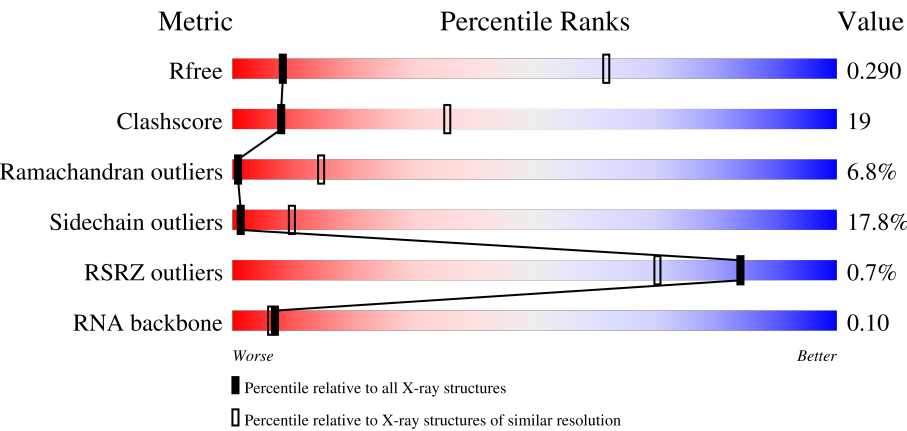
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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}	164625	1115 (4.20-3.72)
Clashscore	180529	1009 (4.16-3.76)
Ramachandran outliers	177936	1006 (4.18-3.74)
Sidechain outliers	177891	1117 (4.20-3.72)
RSRZ outliers	164620	1116 (4.20-3.72)
RNA backbone	3690	1136 (4.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1733	<div><div></div><div><div>44%</div><div>27%</div><div>8%</div><div>•</div><div>20%</div></div></div>
2	B	1224	<div><div></div><div><div>49%</div><div>34%</div><div>6%</div><div>•</div><div>10%</div></div></div>
3	C	318	<div><div></div><div><div>45%</div><div>30%</div><div>8%</div><div>•</div><div>16%</div></div></div>
4	E	215	<div><div></div><div><div>55%</div><div>34%</div><div>10%</div></div></div>

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

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28548 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	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8773	5555	1536	1627	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 polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA_9 mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	9	Total	C	N	O	P	0	0	0
			195	87	37	62	9			

- Molecule 12 is a DNA chain called Template DNA_29 mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	11	Total	C	N	O	P	0	0	0
			224	107	40	66	11			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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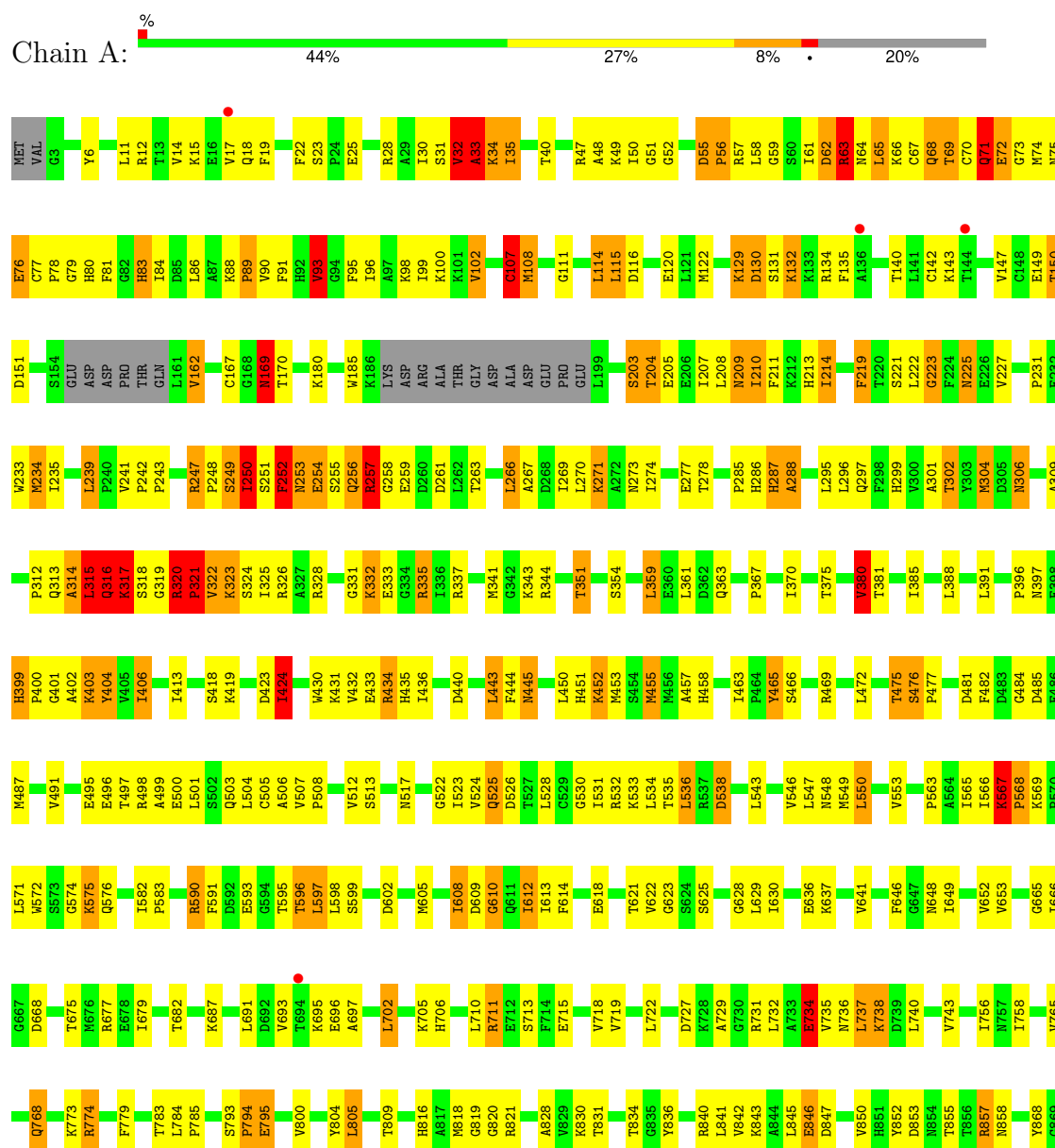
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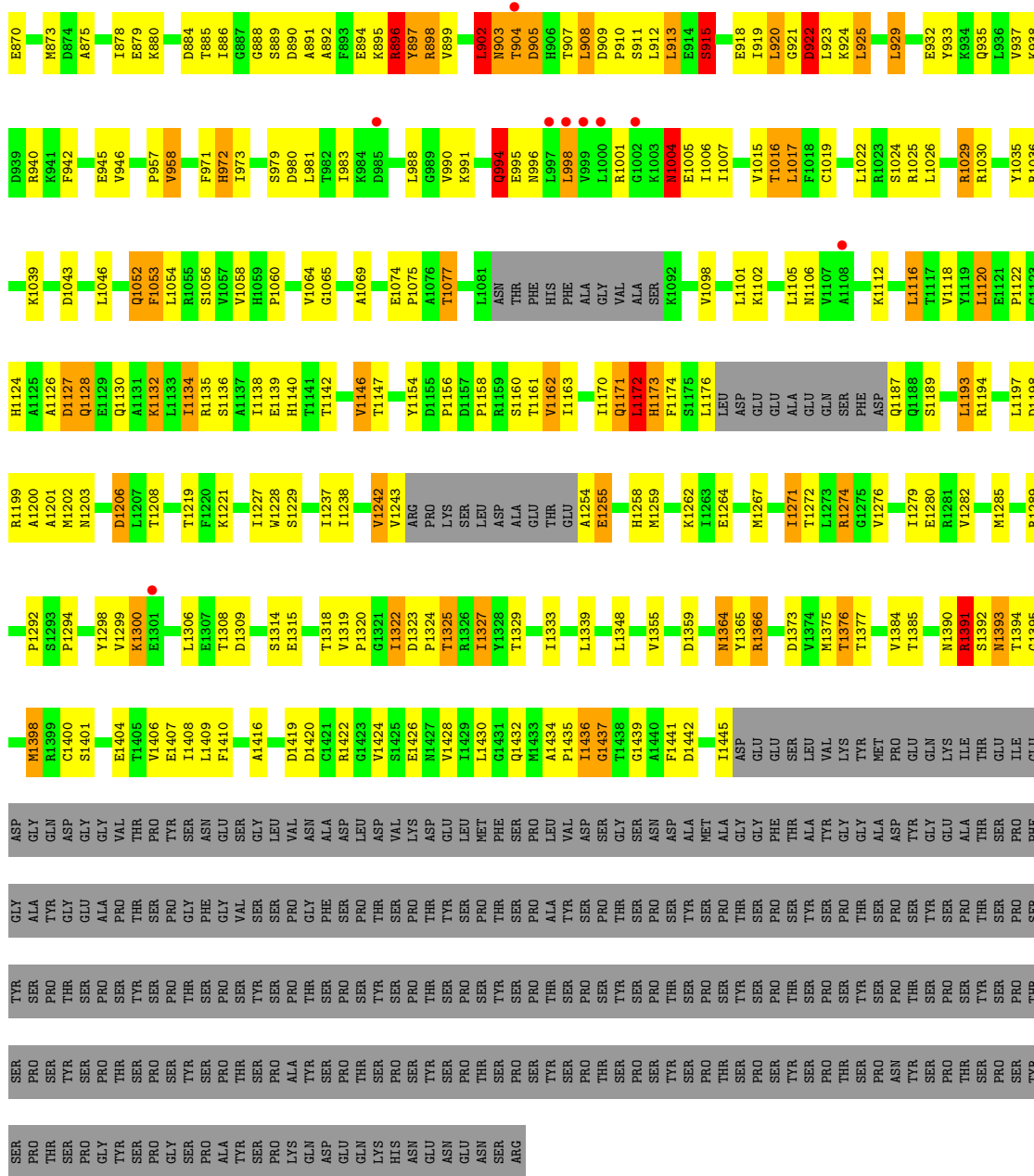
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

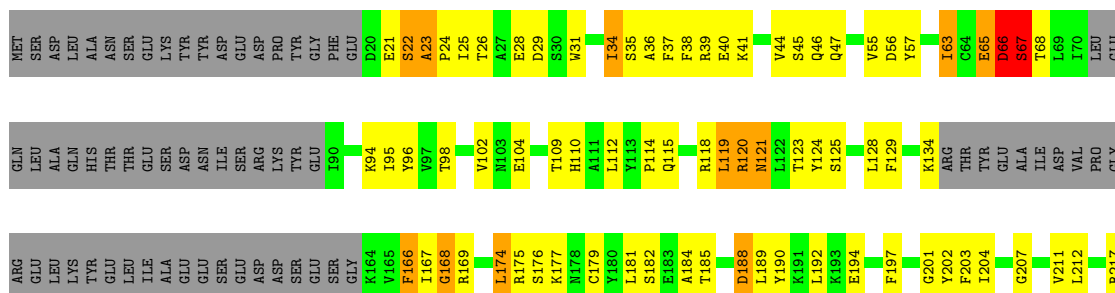
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

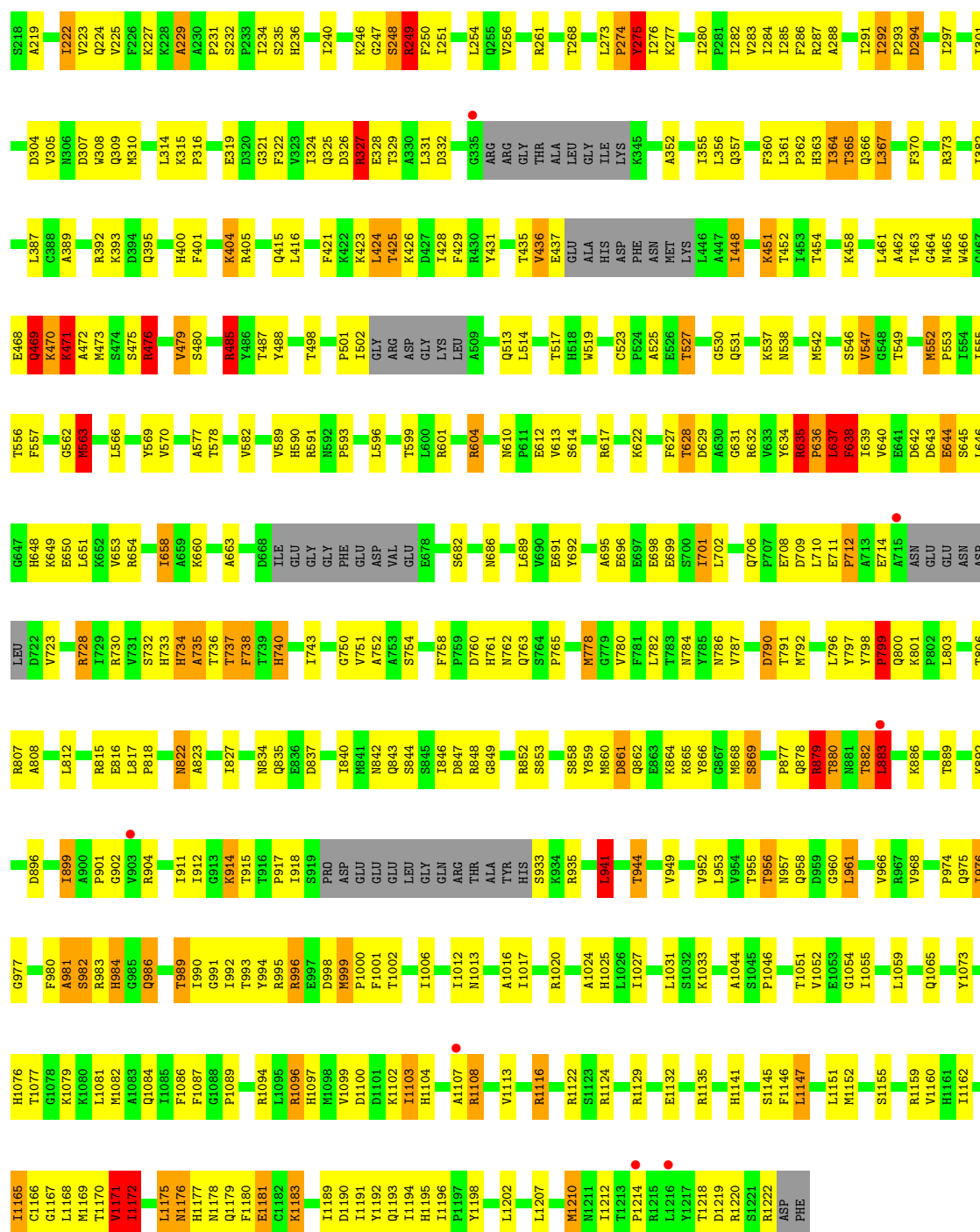




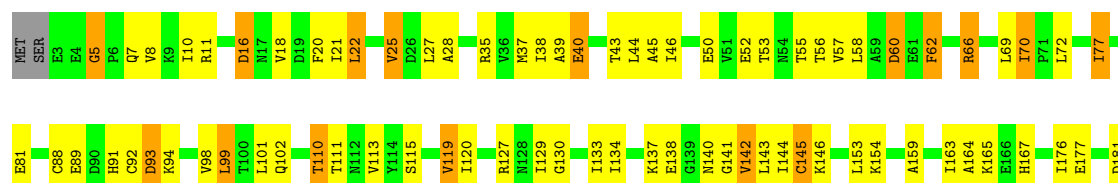
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

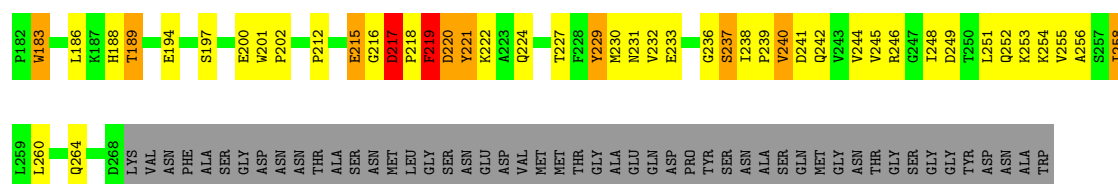
Chain B:  49% 34% 6% 10%



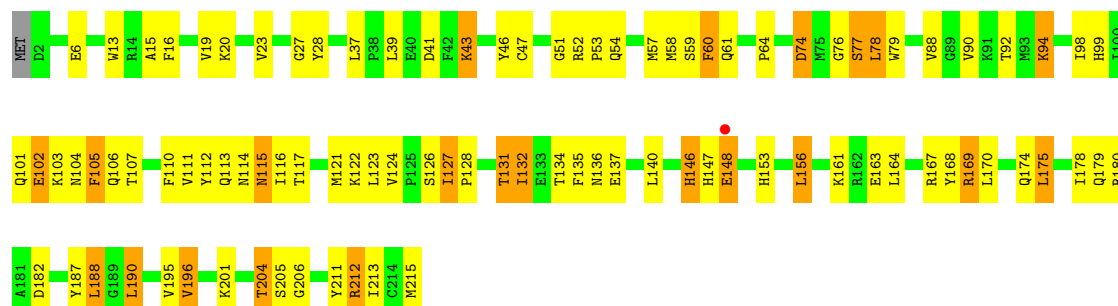


Chain C:

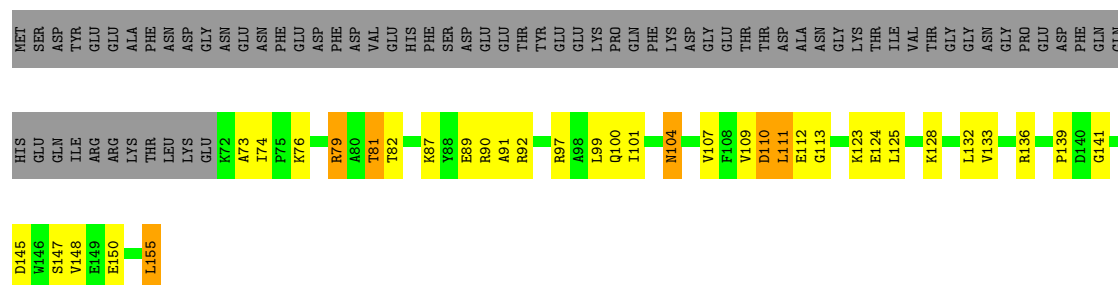
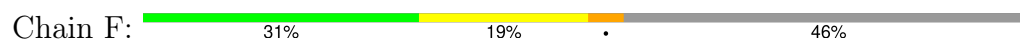




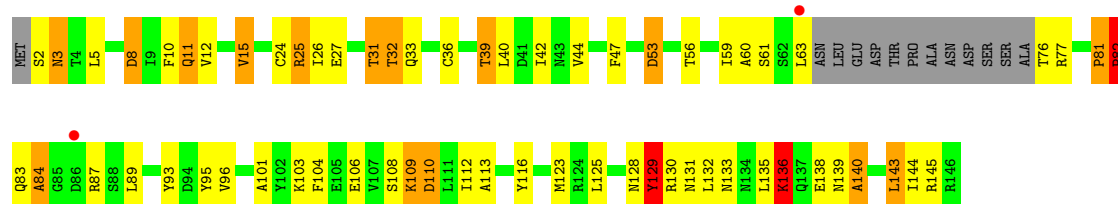
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



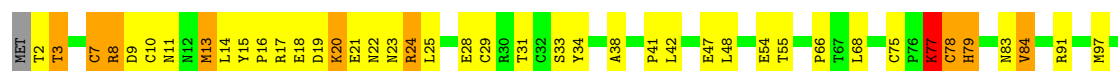
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



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





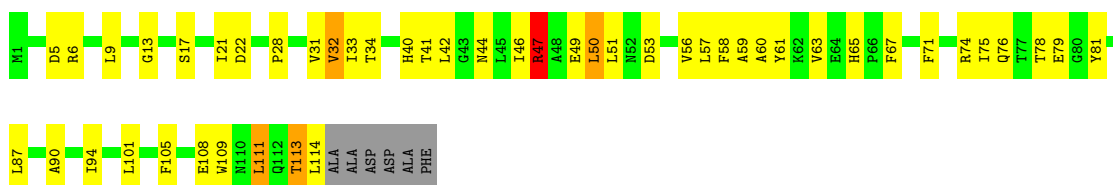
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 41% 40% 10% 7%



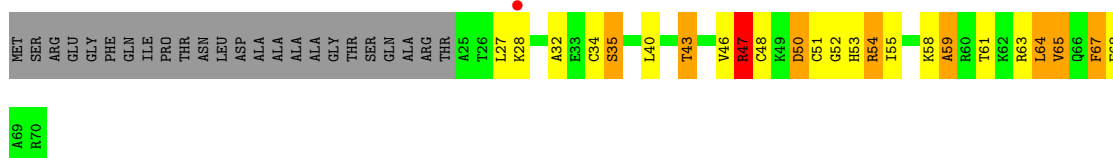
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 55% 36% 5%



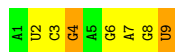
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 31% 21% 11% 34%



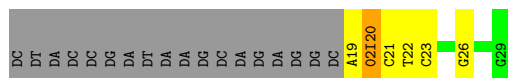
- Molecule 11: RNA_9 mer

Chain R: 22% 56% 22%



- Molecule 12: Template DNA _29 mer

Chain T: 17% 17% 62%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.55Å 220.33Å 191.56Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.96 50.00 – 3.96	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-3.96) 89.1 (50.00-3.96)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 4.00Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.249 , 0.296 0.243 , 0.290	Depositor DCC
R_{free} test set	2773 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	1.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28548	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 02I, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/11163	0.76	4/15091 (0.0%)
2	B	0.42	0/8943	0.74	5/12059 (0.0%)
3	C	0.40	0/2133	0.70	0/2891
4	E	0.40	0/1788	0.71	0/2406
5	F	0.41	0/691	0.71	0/933
6	H	0.43	0/1086	0.79	0/1470
7	I	0.44	0/989	0.75	1/1331 (0.1%)
8	J	0.42	0/541	0.75	0/727
9	K	0.40	0/937	0.71	1/1265 (0.1%)
10	L	0.48	0/365	0.93	0/485
11	R	0.31	0/218	0.60	0/338
12	T	0.32	0/225	0.56	0/342
All	All	0.42	0/29079	0.74	11/39338 (0.0%)

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	13
2	B	0	6
4	E	0	1
6	H	0	5
7	I	0	1
10	L	0	1
All	All	0	27

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	637	LEU	CA-CB-CG	9.57	137.31	115.30
7	I	77	LYS	CB-CA-C	-7.66	95.08	110.40
2	B	485	ARG	NE-CZ-NH1	6.82	123.71	120.30
9	K	47	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	315	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	239	LEU	CA-CB-CG	5.65	128.29	115.30
2	B	941	LEU	CA-CB-CG	5.59	128.16	115.30
2	B	638	PHE	CB-CA-C	-5.57	99.26	110.40
2	B	638	PHE	N-CA-CB	5.54	120.57	110.60
1	A	1391	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	590	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	CYS	Peptide
1	A	1172	LEU	Peptide
1	A	169	ASN	Peptide
1	A	203	SER	Peptide
1	A	209	ASN	Peptide
1	A	252	PHE	Peptide
1	A	257	ARG	Peptide
1	A	258	GLY	Peptide
1	A	316	GLN	Peptide
1	A	317	LYS	Peptide
1	A	321	PRO	Peptide
1	A	33	ALA	Peptide
1	A	820	GLY	Peptide
2	B	1171	VAL	Peptide
2	B	222	ILE	Peptide
2	B	635	ARG	Peptide
2	B	879	ARG	Peptide
2	B	883	LEU	Peptide
2	B	980	PHE	Peptide
4	E	131	THR	Peptide
6	H	129	TYR	Peptide
6	H	136	LYS	Peptide
6	H	61	SER	Peptide
6	H	82	PRO	Peptide
6	H	84	ALA	Peptide
7	I	20	LYS	Peptide
10	L	67	PHE	Peptide

5.2 Too-close contacts ⓘ

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	10969	0	11069	432	0
2	B	8773	0	8811	387	0
3	C	2095	0	2051	104	0
4	E	1752	0	1776	64	0
5	F	679	0	701	20	0
6	H	1068	0	1040	46	0
7	I	971	0	927	43	0
8	J	532	0	542	35	0
9	K	919	0	929	44	0
10	L	363	0	387	20	0
11	R	195	0	98	6	0
12	T	224	0	123	15	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28548	0	28454	1095	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 19.

All (1095) 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)
3:C:38:ILE:HD11	3:C:176:ILE:CD1	1.39	1.51
3:C:38:ILE:CD1	3:C:176:ILE:HD11	1.72	1.19
7:I:7:CYS:HB3	7:I:14:LEU:HD21	1.23	1.14
3:C:38:ILE:CD1	3:C:176:ILE:CD1	2.27	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.37	1.07
3:C:38:ILE:HD11	3:C:176:ILE:HD13	1.35	1.06
3:C:38:ILE:HD11	3:C:176:ILE:HD11	1.13	1.04
2:B:227:LYS:HG2	2:B:236:HIS:CE1	1.94	1.01
1:A:315:LEU:HB3	1:A:316:GLN:HA	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.46	0.98
1:A:315:LEU:CB	1:A:316:GLN:HA	1.98	0.93
7:I:77:LYS:O	7:I:78:CYS:SG	2.27	0.92
1:A:320:ARG:HB2	1:A:321:PRO:CA	2.02	0.89
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.55	0.89
2:B:882:THR:HG21	2:B:935:ARG:HA	1.55	0.87
1:A:332:LYS:HE2	12:T:21:DC:OP2	1.74	0.87
1:A:322:VAL:HB	1:A:323:LYS:HD3	1.57	0.87
1:A:1004:ASN:HD22	4:E:167:ARG:HD2	1.37	0.87
1:A:321:PRO:O	1:A:322:VAL:HG22	1.75	0.86
7:I:7:CYS:HB3	7:I:14:LEU:CD2	2.05	0.86
7:I:78:CYS:O	7:I:79:HIS:HB2	1.73	0.86
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.10	0.86
7:I:78:CYS:SG	7:I:79:HIS:N	2.48	0.86
2:B:274:PRO:O	2:B:276:ILE:HG13	1.76	0.86
7:I:29:CYS:SG	7:I:31:THR:HB	2.17	0.84
1:A:921:GLY:O	1:A:922:ASP:O	1.96	0.83
8:J:43:ARG:HB2	8:J:46:CYS:SG	2.18	0.82
3:C:133:ILE:HD11	3:C:237:SER:HA	1.62	0.82
3:C:70:ILE:HD12	3:C:144:ILE:HD11	1.62	0.82
2:B:248:SER:O	2:B:249:ARG:HB2	1.79	0.81
10:L:46:VAL:O	10:L:47:ARG:HB2	1.81	0.80
6:H:108:SER:O	6:H:109:LYS:HB2	1.80	0.80
3:C:215:GLU:HG3	3:C:216:GLY:H	1.46	0.79
1:A:320:ARG:HB2	1:A:321:PRO:HA	1.63	0.79
2:B:640:VAL:HG13	2:B:650:GLU:C	2.02	0.79
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.04	0.78
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.64	0.78
2:B:698:GLU:O	2:B:701:ILE:HD12	1.84	0.78
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.66	0.78
8:J:10:CYS:HB3	8:J:45:CYS:SG	2.22	0.78
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.67	0.77
2:B:128:LEU:HB3	2:B:167:ILE:O	1.85	0.77
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.14	0.76
3:C:38:ILE:HD13	3:C:176:ILE:HD11	1.68	0.76
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.17	0.75
1:A:649:ILE:O	1:A:653:VAL:HG23	1.87	0.75
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.69	0.75
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.70	0.74
2:B:470:LYS:O	2:B:471:LYS:HG3	1.87	0.74
2:B:859:TYR:OH	2:B:941:LEU:HD22	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:GLN:O	2:B:366:GLN:HA	1.86	0.74
1:A:314:ALA:HA	1:A:320:ARG:HA	1.70	0.74
1:A:71:GLN:O	1:A:73:GLY:N	2.22	0.73
2:B:129:PHE:CE1	2:B:166:PHE:HB2	2.24	0.73
2:B:25:ILE:HD12	2:B:651:LEU:HD12	1.71	0.73
2:B:1103:ILE:N	2:B:1103:ILE:HD13	2.03	0.73
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.68	0.73
1:A:888:GLY:O	1:A:940:ARG:NH2	2.21	0.73
2:B:227:LYS:HG2	2:B:236:HIS:ND1	2.03	0.73
2:B:834:ASN:O	2:B:1013:ASN:HB2	1.89	0.73
1:A:546:VAL:HG12	1:A:550:LEU:CD2	2.18	0.72
1:A:1391:ARG:HG2	1:A:1391:ARG:HH11	1.54	0.72
2:B:800:GLN:HG2	8:J:52:THR:HG21	1.70	0.72
12:T:20:O2I:H4'	12:T:21:DC:OP1	1.89	0.72
2:B:280:ILE:HG21	2:B:285:ILE:HG12	1.70	0.72
2:B:274:PRO:O	2:B:276:ILE:N	2.21	0.72
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.20	0.72
1:A:1140:HIS:HB3	1:A:1279:ILE:O	1.89	0.72
1:A:19:PHE:O	1:A:1416:ALA:HA	1.89	0.72
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.20	0.72
1:A:320:ARG:HG2	2:B:471:LYS:HE2	1.71	0.71
1:A:67:CYS:O	1:A:70:CYS:HB3	1.91	0.71
1:A:899:VAL:HG12	1:A:929:LEU:HD12	1.71	0.71
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.23	0.71
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.06	0.70
3:C:60:ASP:HB3	10:L:67:PHE:CE2	2.25	0.70
6:H:101:ALA:HB2	6:H:116:TYR:CE1	2.26	0.70
2:B:1099:VAL:CG1	2:B:1103:ILE:HD11	2.20	0.70
3:C:20:PHE:HE2	3:C:22:LEU:HD12	1.54	0.70
1:A:135:PHE:HB2	1:A:222:LEU:O	1.92	0.70
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.73	0.70
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.21	0.70
5:F:73:ALA:O	5:F:74:ILE:HG12	1.92	0.69
2:B:737:THR:HG21	7:I:66:PRO:O	1.91	0.69
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.74	0.69
2:B:1099:VAL:HG12	2:B:1103:ILE:CD1	2.22	0.69
1:A:55:ASP:O	1:A:57:ARG:N	2.26	0.69
2:B:211:VAL:O	2:B:480:SER:HA	1.93	0.69
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.74	0.69
2:B:479:VAL:O	2:B:480:SER:HB3	1.93	0.69
1:A:35:ILE:HG22	1:A:270:LEU:HD13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:107:VAL:HG11	5:F:111:LEU:HD11	1.75	0.68
1:A:908:LEU:HB3	1:A:912:LEU:HD12	1.74	0.68
4:E:168:TYR:C	4:E:169:ARG:HG2	2.14	0.68
1:A:278:THR:O	1:A:278:THR:HG22	1.93	0.68
8:J:10:CYS:SG	8:J:11:GLY:N	2.67	0.68
1:A:302:THR:OG1	1:A:313:GLN:NE2	2.27	0.68
3:C:221:TYR:CE1	3:C:222:LYS:HD2	2.29	0.68
7:I:7:CYS:CB	7:I:14:LEU:HD21	2.13	0.68
2:B:956:THR:HA	2:B:961:LEU:O	1.93	0.68
1:A:134:ARG:HD3	1:A:221:SER:O	1.95	0.67
3:C:57:VAL:CG1	8:J:60:PHE:HB2	2.23	0.67
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.75	0.67
7:I:78:CYS:O	7:I:79:HIS:CB	2.41	0.67
10:L:46:VAL:O	10:L:47:ARG:CB	2.43	0.67
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.77	0.67
2:B:1162:ILE:HD13	2:B:1168:LEU:C	2.15	0.67
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.77	0.67
2:B:120:ARG:HD2	2:B:955:THR:HG21	1.75	0.67
2:B:466:TRP:HB3	2:B:475:SER:HB3	1.76	0.67
9:K:53:ASP:O	9:K:56:VAL:HG23	1.95	0.66
3:C:56:THR:HG21	3:C:145:CYS:SG	2.34	0.66
6:H:2:SER:O	6:H:3:ASN:HB2	1.95	0.66
2:B:235:SER:O	2:B:236:HIS:ND1	2.28	0.66
1:A:590:ARG:HH21	1:A:621:THR:HA	1.60	0.66
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.77	0.66
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.79	0.65
3:C:88:CYS:SG	3:C:92:CYS:HB3	2.36	0.65
6:H:108:SER:O	6:H:109:LYS:CB	2.44	0.65
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.36	0.65
9:K:113:THR:C	9:K:114:LEU:HD12	2.17	0.65
1:A:261:ASP:HB3	1:A:323:LYS:HD2	1.77	0.65
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.78	0.65
1:A:913:LEU:HD11	1:A:981:LEU:O	1.97	0.65
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.78	0.65
11:R:8:G:O2'	11:R:9:U:H5'	1.97	0.65
11:R:8:G:H1	12:T:21:DC:H42	1.44	0.65
1:A:855:THR:HG21	1:A:857:ARG:HE	1.61	0.64
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.62	0.64
1:A:1198:ASP:O	1:A:1202:MET:HG2	1.97	0.64
2:B:470:LYS:O	2:B:471:LYS:CG	2.44	0.64
1:A:320:ARG:CB	1:A:321:PRO:HA	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:981:ALA:O	2:B:982:SER:O	2.14	0.64
1:A:648:ASN:O	1:A:652:VAL:HG23	1.96	0.64
8:J:2:ILE:O	8:J:53:HIS:NE2	2.30	0.64
10:L:58:LYS:O	10:L:59:ALA:HB3	1.98	0.64
5:F:81:THR:CG2	5:F:136:ARG:HD3	2.28	0.64
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.78	0.63
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.32	0.63
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.81	0.63
3:C:38:ILE:CD1	3:C:176:ILE:HD13	2.15	0.63
1:A:406:ILE:HD13	1:A:431:LYS:HB2	1.81	0.63
12:T:21:DC:C4	12:T:22:DT:C4	2.87	0.63
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.29	0.62
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.81	0.62
2:B:287:ARG:NH1	2:B:324:ILE:O	2.32	0.62
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.81	0.62
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.81	0.62
1:A:91:PHE:HD2	1:A:297:GLN:OE1	1.82	0.62
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.81	0.62
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.81	0.62
2:B:706:GLN:O	2:B:710:LEU:HB2	1.99	0.62
2:B:274:PRO:O	2:B:276:ILE:CG1	2.47	0.62
9:K:46:ILE:HG23	9:K:50:LEU:HD12	1.82	0.62
2:B:176:SER:O	2:B:182:SER:HB3	2.00	0.62
3:C:238:ILE:HG22	3:C:239:PRO:O	2.00	0.62
7:I:7:CYS:O	7:I:11:ASN:HA	2.00	0.62
1:A:273:ASN:O	1:A:277:GLU:HG3	2.00	0.61
1:A:566:ILE:O	1:A:567:LYS:O	2.17	0.61
2:B:34:ILE:HD12	2:B:542:MET:HE1	1.81	0.61
3:C:66:ARG:NH2	8:J:5:VAL:HG23	2.15	0.61
8:J:52:THR:O	8:J:53:HIS:C	2.37	0.61
5:F:109:VAL:CG2	5:F:124:GLU:HG2	2.30	0.61
1:A:88:LYS:O	1:A:89:PRO:O	2.18	0.61
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.82	0.61
4:E:94:LYS:O	4:E:98:ILE:HG12	2.00	0.61
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.15	0.61
10:L:48:CYS:HB3	10:L:51:CYS:O	2.00	0.61
2:B:977:GLY:CA	2:B:1099:VAL:HG21	2.31	0.61
2:B:902:GLY:O	10:L:65:VAL:HG11	2.00	0.61
2:B:523:CYS:SG	2:B:750:GLY:N	2.73	0.61
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.83	0.61
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:64:PRO:CG	4:E:76:GLY:HA2	2.31	0.61
3:C:217:ASP:H	3:C:218:PRO:HD3	1.65	0.61
6:H:47:PHE:HB3	6:H:95:TYR:HD2	1.66	0.61
2:B:476:ARG:O	2:B:476:ARG:HG3	2.01	0.60
4:E:23:VAL:HG13	4:E:28:TYR:HD2	1.66	0.60
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.83	0.60
2:B:167:ILE:HG23	2:B:424:LEU:HD13	1.82	0.60
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.49	0.60
4:E:15:ALA:O	4:E:19:VAL:HG23	2.02	0.60
6:H:76:THR:HG22	6:H:76:THR:O	2.00	0.60
1:A:1436:ILE:O	1:A:1437:GLY:C	2.38	0.60
1:A:322:VAL:CB	1:A:323:LYS:HD3	2.30	0.60
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.34	0.60
2:B:848:ARG:NH1	8:J:8:PHE:O	2.34	0.60
4:E:116:ILE:HG21	4:E:121:MET:HG2	1.84	0.60
2:B:640:VAL:CG2	2:B:651:LEU:CD2	2.80	0.60
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.83	0.60
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.82	0.60
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.67	0.60
2:B:882:THR:HG22	2:B:883:LEU:N	2.17	0.60
1:A:315:LEU:HB3	1:A:316:GLN:CA	2.25	0.59
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.83	0.59
8:J:51:LEU:HD12	8:J:51:LEU:O	2.02	0.59
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.01	0.59
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.37	0.59
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.02	0.59
2:B:635:ARG:HB2	2:B:636:PRO:HD3	1.84	0.59
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.83	0.59
1:A:99:ILE:HA	1:A:102:VAL:HG23	1.84	0.59
1:A:530:GLY:O	1:A:532:ARG:N	2.35	0.59
2:B:115:GLN:O	2:B:119:LEU:HD12	2.02	0.59
2:B:464:GLY:HA2	2:B:479:VAL:O	2.02	0.59
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.83	0.59
1:A:623:GLY:O	1:A:630:ILE:HD13	2.02	0.59
2:B:634:TYR:CE1	2:B:692:TYR:CD2	2.91	0.59
4:E:58:MET:O	4:E:60:PHE:N	2.31	0.59
2:B:562:GLY:O	2:B:563:MET:C	2.40	0.59
1:A:320:ARG:HD2	1:A:320:ARG:N	2.17	0.59
2:B:736:THR:O	2:B:737:THR:OG1	2.20	0.59
2:B:737:THR:HG23	7:I:66:PRO:CB	2.33	0.59
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:64:PRO:HG3	4:E:76:GLY:HA2	1.85	0.59
7:I:7:CYS:O	7:I:8:ARG:O	2.20	0.59
2:B:1081:LEU:O	3:C:189:THR:HG23	2.03	0.58
1:A:61:ILE:O	1:A:63:ARG:N	2.35	0.58
1:A:547:LEU:HD22	9:K:58:PHE:HD2	1.68	0.58
2:B:976:ILE:O	2:B:990:ILE:HB	2.03	0.58
6:H:101:ALA:HB2	6:H:116:TYR:CD1	2.38	0.58
1:A:547:LEU:HD22	9:K:58:PHE:CD2	2.38	0.58
1:A:320:ARG:NH2	2:B:471:LYS:HB3	2.18	0.58
1:A:534:LEU:O	1:A:574:GLY:HA3	2.03	0.58
1:A:1228:TRP:HB3	1:A:1238:ILE:HD13	1.85	0.58
2:B:801:LYS:HG2	8:J:52:THR:HG23	1.85	0.58
2:B:635:ARG:CG	2:B:636:PRO:HD3	2.34	0.58
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.84	0.58
2:B:34:ILE:HD13	2:B:34:ILE:N	2.18	0.58
2:B:284:ILE:HD12	2:B:324:ILE:HD12	1.85	0.58
2:B:1116:ARG:HG3	2:B:1198:TYR:CD1	2.39	0.58
2:B:698:GLU:O	2:B:701:ILE:CD1	2.52	0.58
1:A:853:ASP:OD1	1:A:855:THR:HB	2.04	0.58
1:A:1292:PRO:HD3	1:A:1298:TYR:CE1	2.38	0.58
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.72	0.57
4:E:170:LEU:HD13	4:E:175:LEU:CD2	2.34	0.57
1:A:76:GLU:O	1:A:78:PRO:HD3	2.03	0.57
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.84	0.57
7:I:7:CYS:C	7:I:8:ARG:O	2.41	0.57
2:B:363:HIS:O	2:B:364:ILE:HB	2.04	0.57
2:B:638:PHE:O	2:B:740:HIS:HB2	2.04	0.57
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	2.18	0.57
6:H:128:ASN:OD1	6:H:131:ASN:ND2	2.37	0.57
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.39	0.57
2:B:190:TYR:CE2	8:J:62:ARG:HG2	2.40	0.57
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.86	0.57
1:A:805:LEU:C	1:A:805:LEU:HD12	2.25	0.57
1:A:1004:ASN:HD21	1:A:1007:ILE:HG12	1.68	0.57
11:R:8:G:H1	12:T:21:DC:N4	2.02	0.57
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.34	0.57
1:A:530:GLY:C	1:A:532:ARG:N	2.58	0.57
1:A:718:VAL:O	1:A:722:LEU:HD12	2.05	0.57
1:A:58:LEU:HD22	1:A:243:PRO:HB3	1.87	0.57
2:B:635:ARG:CD	2:B:636:PRO:HD3	2.35	0.57
1:A:1434:ALA:HB1	1:A:1436:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:CG	2:B:66:ASP:N	2.68	0.57
1:A:380:VAL:CG2	1:A:430:TRP:H	2.18	0.56
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.70	0.56
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.87	0.56
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.87	0.56
3:C:66:ARG:NH2	8:J:3:VAL:O	2.37	0.56
9:K:32:VAL:HG23	9:K:74:ARG:HG3	1.86	0.56
1:A:482:PHE:O	2:B:989:THR:HG23	2.05	0.56
2:B:955:THR:HG23	10:L:54:ARG:O	2.05	0.56
1:A:675:THR:HG21	1:A:736:ASN:HD21	1.71	0.56
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.69	0.56
1:A:873:MET:HG2	1:A:957:PRO:CG	2.36	0.56
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.59	0.56
8:J:7:CYS:HA	8:J:49:MET:HE3	1.88	0.56
1:A:80:HIS:O	1:A:243:PRO:HG3	2.06	0.56
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.87	0.56
2:B:1076:HIS:CG	9:K:40:HIS:CD2	2.94	0.56
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.05	0.56
4:E:57:MET:O	4:E:57:MET:HG2	2.06	0.56
1:A:68:GLN:NE2	1:A:80:HIS:CE1	2.74	0.56
3:C:37:MET:SD	3:C:232:VAL:HG21	2.46	0.56
3:C:98:VAL:C	3:C:99:LEU:HD23	2.26	0.56
9:K:113:THR:O	9:K:114:LEU:HD12	2.06	0.56
1:A:320:ARG:HB2	1:A:321:PRO:CB	2.36	0.55
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.88	0.55
2:B:525:ALA:O	2:B:527:THR:HG22	2.05	0.55
1:A:203:SER:O	1:A:205:GLU:N	2.39	0.55
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.37	0.55
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.88	0.55
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.35	0.55
6:H:139:ASN:O	6:H:140:ALA:HB2	2.07	0.55
1:A:946:VAL:HG22	4:E:201:LYS:HB3	1.87	0.55
1:A:1006:ILE:HD11	4:E:163:GLU:HG2	1.89	0.55
2:B:882:THR:CG2	2:B:935:ARG:HA	2.33	0.55
8:J:2:ILE:C	8:J:53:HIS:NE2	2.59	0.55
2:B:65:GLU:HG2	2:B:66:ASP:N	2.22	0.55
3:C:221:TYR:CD1	3:C:222:LYS:HD2	2.41	0.55
1:A:919:ILE:CG2	1:A:925:LEU:HD12	2.36	0.55
2:B:56:ASP:C	2:B:57:TYR:HD1	2.09	0.55
2:B:640:VAL:CG2	2:B:651:LEU:HD22	2.37	0.55
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:TYR:CE2	4:E:78:LEU:HD13	2.42	0.55
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.87	0.55
1:A:1004:ASN:OD1	1:A:1005:GLU:N	2.40	0.55
1:A:734:GLU:O	1:A:734:GLU:HG3	2.07	0.55
2:B:203:PHE:HE2	2:B:212:LEU:HD12	1.72	0.55
2:B:701:ILE:HG13	2:B:740:HIS:HE1	1.71	0.55
3:C:145:CYS:HA	8:J:2:ILE:HD11	1.88	0.55
10:L:34:CYS:O	10:L:35:SER:CB	2.54	0.55
1:A:1154:TYR:CE1	7:I:18:GLU:HG3	2.42	0.55
1:A:469:ARG:NH2	2:B:991:GLY:O	2.37	0.55
2:B:326:ASP:O	2:B:328:GLU:N	2.40	0.55
2:B:1031:LEU:HD13	2:B:1055:ILE:HD12	1.89	0.55
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.89	0.55
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.47	0.54
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.89	0.54
8:J:9:SER:OG	8:J:45:CYS:HB2	2.07	0.54
9:K:63:VAL:HG23	9:K:63:VAL:O	2.06	0.54
1:A:35:ILE:HG22	1:A:270:LEU:CD1	2.37	0.54
1:A:530:GLY:C	1:A:532:ARG:H	2.08	0.54
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.37	0.54
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.90	0.54
1:A:253:ASN:CG	1:A:254:GLU:N	2.61	0.54
3:C:99:LEU:HD23	3:C:99:LEU:N	2.23	0.54
2:B:636:PRO:CB	2:B:637:LEU:HB3	2.37	0.54
1:A:546:VAL:HG12	1:A:550:LEU:HD23	1.89	0.54
2:B:34:ILE:HD12	2:B:542:MET:CE	2.38	0.54
6:H:113:ALA:HA	6:H:125:LEU:O	2.07	0.54
9:K:47:ARG:HH11	9:K:47:ARG:HG2	1.72	0.54
1:A:765:VAL:HG23	1:A:800:VAL:HB	1.89	0.54
2:B:955:THR:HG22	2:B:956:THR:N	2.22	0.54
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.90	0.54
2:B:1076:HIS:CG	9:K:40:HIS:HD2	2.26	0.54
6:H:31:THR:O	6:H:32:THR:CB	2.56	0.54
1:A:95:PHE:CD2	1:A:234:MET:HG2	2.43	0.54
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.38	0.54
2:B:469:GLN:O	2:B:470:LYS:C	2.46	0.54
2:B:701:ILE:CB	2:B:740:HIS:HE1	2.20	0.54
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	2.06	0.54
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.42	0.54
9:K:49:GLU:HG3	9:K:94:ILE:HD11	1.89	0.54
9:K:49:GLU:CB	9:K:94:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.36	0.53
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.89	0.53
4:E:43:LYS:O	4:E:47:CYS:HB2	2.07	0.53
1:A:249:SER:O	1:A:250:ILE:HG12	2.09	0.53
1:A:361:LEU:HD22	1:A:646:PHE:CD2	2.44	0.53
7:I:11:ASN:ND2	7:I:11:ASN:O	2.41	0.53
1:A:399:HIS:O	1:A:435:HIS:CD2	2.62	0.53
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.39	0.53
3:C:145:CYS:SG	3:C:146:LYS:N	2.81	0.53
1:A:313:GLN:O	1:A:314:ALA:HB2	2.09	0.53
1:A:1127:ASP:HB2	1:A:1130:GLN:HB3	1.90	0.53
2:B:635:ARG:CB	2:B:636:PRO:HD3	2.38	0.53
3:C:62:PHE:CE1	3:C:66:ARG:HD2	2.43	0.53
3:C:221:TYR:HE1	3:C:222:LYS:HD2	1.72	0.53
6:H:11:GLN:HA	6:H:53:ASP:O	2.09	0.53
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.90	0.53
1:A:30:ILE:HA	2:B:1183:LYS:HE3	1.90	0.53
1:A:1004:ASN:OD1	1:A:1004:ASN:C	2.47	0.53
2:B:638:PHE:O	2:B:740:HIS:CB	2.56	0.53
2:B:701:ILE:HG12	2:B:702:LEU:N	2.24	0.53
1:A:249:SER:HB3	1:A:259:GLU:HG3	1.91	0.53
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.91	0.53
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.73	0.53
1:A:99:ILE:HA	1:A:102:VAL:CG2	2.39	0.52
1:A:528:LEU:HD12	1:A:528:LEU:O	2.09	0.52
1:A:971:PHE:O	1:A:972:HIS:C	2.47	0.52
1:A:1219:THR:CG2	1:A:1271:ILE:HD11	2.39	0.52
2:B:435:THR:O	2:B:437:GLU:N	2.42	0.52
8:J:45:CYS:SG	8:J:46:CYS:N	2.82	0.52
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.91	0.52
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.91	0.52
2:B:129:PHE:CD1	2:B:166:PHE:HB2	2.43	0.52
2:B:823:ALA:O	2:B:1089:PRO:HA	2.10	0.52
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.15	0.52
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.90	0.52
6:H:106:GLU:C	6:H:108:SER:H	2.12	0.52
1:A:261:ASP:HB3	1:A:323:LYS:CG	2.39	0.52
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.90	0.52
8:J:57:ILE:HA	8:J:60:PHE:HD1	1.75	0.52
1:A:247:ARG:CG	1:A:247:ARG:O	2.58	0.52
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.92	0.52
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.09	0.52
7:I:77:LYS:O	7:I:78:CYS:CB	2.55	0.52
9:K:59:ALA:HA	9:K:74:ARG:O	2.09	0.52
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.40	0.52
2:B:892:LYS:HE2	2:B:904:ARG:O	2.10	0.52
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.92	0.52
1:A:899:VAL:HG21	1:A:908:LEU:CD2	2.40	0.52
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.92	0.52
2:B:728:ARG:NH2	2:B:760:ASP:OD2	2.41	0.52
1:A:51:GLY:HA2	1:A:56:PRO:HG3	1.92	0.52
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.92	0.52
2:B:800:GLN:CG	8:J:52:THR:HG21	2.37	0.52
3:C:134:ILE:CD1	3:C:141:GLY:HA3	2.40	0.52
6:H:129:TYR:C	6:H:131:ASN:H	2.13	0.52
1:A:567:LYS:HB3	6:H:96:VAL:H	1.75	0.52
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.90	0.52
2:B:984:HIS:CD2	2:B:1024:ALA:HB3	2.45	0.52
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.92	0.52
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.44	0.52
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.44	0.52
2:B:287:ARG:NH1	2:B:321:GLY:O	2.43	0.52
2:B:640:VAL:CG2	2:B:651:LEU:HD23	2.39	0.52
9:K:78:THR:HG22	9:K:79:GLU:N	2.25	0.52
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.43	0.51
3:C:217:ASP:N	3:C:218:PRO:HD3	2.25	0.51
4:E:78:LEU:HG	4:E:79:TRP:N	2.25	0.51
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.92	0.51
1:A:582:ILE:HG22	1:A:610:GLY:HA2	1.91	0.51
1:A:630:ILE:HD12	1:A:630:ILE:H	1.74	0.51
1:A:705:LYS:HG3	1:A:713:SER:HB3	1.92	0.51
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.10	0.51
1:A:1410:PHE:CD1	2:B:1212:ILE:HD11	2.46	0.51
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.10	0.51
9:K:65:HIS:HD2	9:K:67:PHE:H	1.58	0.51
1:A:935:GLN:HA	1:A:938:LYS:HG3	1.92	0.51
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.09	0.51
1:A:1391:ARG:HG2	1:A:1391:ARG:NH1	2.23	0.51
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.40	0.51
4:E:16:PHE:CZ	4:E:20:LYS:HE3	2.45	0.51
6:H:104:PHE:CZ	6:H:136:LYS:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:HD11	2:B:835:GLN:HE22	1.74	0.51
1:A:622:VAL:HG22	1:A:622:VAL:O	2.11	0.51
2:B:806:THR:HG22	2:B:808:ALA:H	1.75	0.51
7:I:119:THR:HG22	7:I:119:THR:O	2.11	0.51
1:A:401:GLY:C	1:A:435:HIS:CD2	2.84	0.51
1:A:1434:ALA:CB	1:A:1436:ILE:HD12	2.40	0.51
2:B:531:GLN:HG2	12:T:20:O2I:C2	2.40	0.51
5:F:79:ARG:NH2	5:F:145:ASP:O	2.44	0.51
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.44	0.51
2:B:469:GLN:O	2:B:471:LYS:N	2.44	0.51
1:A:30:ILE:O	2:B:1183:LYS:NZ	2.43	0.51
1:A:169:ASN:N	1:A:169:ASN:HD22	2.07	0.51
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.91	0.51
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.93	0.51
10:L:43:THR:HG22	10:L:43:THR:O	2.10	0.51
1:A:33:ALA:O	1:A:34:LYS:HG3	2.10	0.51
2:B:307:ASP:O	2:B:309:GLN:N	2.44	0.51
2:B:485:ARG:HH11	2:B:485:ARG:CG	2.23	0.51
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.40	0.51
2:B:844:SER:HG	2:B:996:ARG:H	1.59	0.51
1:A:129:LYS:O	1:A:130:ASP:HB2	2.11	0.51
1:A:274:ILE:O	1:A:274:ILE:HG22	2.11	0.51
2:B:868:MET:O	2:B:869:SER:CB	2.58	0.51
3:C:227:THR:HG22	3:C:229:TYR:CE1	2.46	0.51
2:B:701:ILE:CG1	2:B:740:HIS:HE1	2.24	0.51
2:B:733:HIS:O	2:B:735:ALA:N	2.44	0.51
11:R:6:G:H2'	11:R:7:A:H5'	1.92	0.51
1:A:894:GLU:HG3	1:A:898:ARG:HB3	1.93	0.50
1:A:304:MET:HG3	2:B:1210:MET:HG3	1.94	0.50
2:B:248:SER:O	2:B:249:ARG:CB	2.57	0.50
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.93	0.50
3:C:93:ASP:O	3:C:127:ARG:NH2	2.44	0.50
4:E:156:LEU:HG	4:E:195:VAL:O	2.11	0.50
2:B:167:ILE:HD12	2:B:424:LEU:HD11	1.92	0.50
2:B:286:PHE:HB3	2:B:297:ILE:CD1	2.41	0.50
3:C:44:LEU:HD22	3:C:129:ILE:HG13	1.92	0.50
4:E:204:THR:CG2	4:E:205:SER:N	2.74	0.50
10:L:58:LYS:O	10:L:59:ALA:CB	2.59	0.50
1:A:91:PHE:CD2	1:A:297:GLN:OE1	2.63	0.50
1:A:495:GLU:HA	1:A:498:ARG:HG3	1.94	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.93	0.50
4:E:77:SER:HB3	4:E:105:PHE:HD1	1.75	0.50
1:A:402:ALA:HB1	1:A:433:GLU:O	2.11	0.50
2:B:636:PRO:HD2	2:B:637:LEU:HB3	1.94	0.50
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.77	0.50
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.47	0.50
2:B:701:ILE:HB	2:B:740:HIS:HE1	1.76	0.50
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.94	0.50
3:C:251:LEU:O	3:C:255:VAL:HG23	2.10	0.50
7:I:7:CYS:SG	7:I:8:ARG:O	2.70	0.50
1:A:225:ASN:O	1:A:227:VAL:N	2.42	0.50
1:A:367:PRO:HB3	1:A:465:TYR:O	2.11	0.50
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.27	0.50
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.40	0.50
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.11	0.50
2:B:1006:ILE:HG21	2:B:1087:PHE:HE2	1.76	0.50
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.14	0.50
2:B:639:ILE:HA	2:B:740:HIS:HB3	1.94	0.50
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.47	0.49
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.94	0.49
2:B:798:TYR:N	2:B:799:PRO:CD	2.74	0.49
7:I:8:ARG:O	7:I:10:CYS:N	2.44	0.49
1:A:472:LEU:O	1:A:475:THR:HB	2.13	0.49
1:A:1116:LEU:H	1:A:1308:THR:HB	1.75	0.49
1:A:129:LYS:O	1:A:130:ASP:CB	2.60	0.49
1:A:406:ILE:HD12	1:A:406:ILE:N	2.27	0.49
1:A:320:ARG:HG2	2:B:471:LYS:CE	2.41	0.49
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.47	0.49
2:B:274:PRO:O	2:B:275:TYR:C	2.51	0.49
3:C:244:VAL:HG21	9:K:105:PHE:CZ	2.47	0.49
6:H:81:PRO:CB	6:H:82:PRO:HD2	2.43	0.49
1:A:903:ASN:O	1:A:905:ASP:N	2.46	0.49
1:A:1171:GLN:HB2	1:A:1172:LEU:HD23	1.93	0.49
2:B:236:HIS:HD2	2:B:389:ALA:HB2	1.77	0.49
4:E:187:TYR:HD1	4:E:188:LEU:HD23	1.76	0.49
1:A:249:SER:C	1:A:250:ILE:HG23	2.33	0.49
1:A:315:LEU:CB	1:A:316:GLN:CA	2.82	0.49
1:A:320:ARG:HG3	1:A:320:ARG:HH11	1.77	0.49
1:A:507:VAL:N	1:A:508:PRO:CD	2.75	0.49
1:A:567:LYS:O	1:A:569:LYS:N	2.45	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:TRP:HA	2:B:34:ILE:HG12	1.93	0.49
2:B:470:LYS:O	2:B:471:LYS:CB	2.61	0.49
2:B:635:ARG:HD2	2:B:636:PRO:HD3	1.95	0.49
2:B:701:ILE:HG13	2:B:740:HIS:CE1	2.48	0.49
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.93	0.49
2:B:96:TYR:N	2:B:129:PHE:O	2.42	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.93	0.49
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.78	0.49
1:A:630:ILE:HD12	1:A:630:ILE:N	2.28	0.49
2:B:458:LYS:O	2:B:462:ALA:N	2.45	0.49
2:B:787:VAL:HG12	2:B:787:VAL:O	2.12	0.49
9:K:47:ARG:HH11	9:K:47:ARG:CG	2.25	0.49
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.48	0.49
2:B:737:THR:CG2	7:I:66:PRO:CB	2.91	0.49
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.48	0.49
3:C:215:GLU:HG3	3:C:216:GLY:N	2.23	0.49
6:H:59:ILE:O	6:H:60:ALA:HB3	2.13	0.49
1:A:304:MET:CG	2:B:1210:MET:HG3	2.43	0.49
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.94	0.49
1:A:1422:ARG:HH21	2:B:1220:ARG:HD3	1.78	0.49
2:B:737:THR:CG2	7:I:66:PRO:HB2	2.43	0.49
2:B:956:THR:OG1	2:B:960:GLY:O	2.31	0.49
2:B:957:ASN:HB3	2:B:961:LEU:HD12	1.95	0.49
2:B:1180:PHE:O	2:B:1181:GLU:O	2.31	0.49
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.95	0.49
5:F:147:SER:OG	5:F:150:GLU:HG3	2.12	0.49
7:I:17:ARG:HG2	7:I:18:GLU:H	1.77	0.49
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.48	0.49
1:A:403:LYS:O	1:A:404:TYR:O	2.30	0.48
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.94	0.48
1:A:531:ILE:O	1:A:535:THR:HG23	2.12	0.48
1:A:1101:LEU:O	1:A:1105:LEU:HD12	2.13	0.48
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.43	0.48
1:A:251:SER:HB2	1:A:253:ASN:HB3	1.94	0.48
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.94	0.48
2:B:555:ILE:HD11	2:B:582:VAL:HG11	1.95	0.48
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.42	0.48
2:B:1102:LYS:O	2:B:1104:HIS:N	2.43	0.48
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.12	0.48
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.95	0.48
7:I:17:ARG:HG2	7:I:18:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ALA:CA	1:A:320:ARG:HA	2.39	0.48
1:A:359:LEU:HD22	1:A:363:GLN:HB2	1.94	0.48
2:B:65:GLU:CG	2:B:66:ASP:H	2.27	0.48
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.43	0.48
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.95	0.48
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.49	0.48
1:A:89:PRO:O	1:A:204:THR:CG2	2.61	0.48
1:A:278:THR:O	1:A:278:THR:CG2	2.60	0.48
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.13	0.48
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.42	0.48
2:B:642:ASP:O	2:B:644:GLU:N	2.46	0.48
2:B:817:LEU:N	2:B:818:PRO:HD3	2.29	0.48
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.96	0.48
1:A:804:TYR:CE1	2:B:763:GLN:HA	2.48	0.48
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.43	0.48
2:B:711:GLU:N	2:B:712:PRO:HD3	2.29	0.48
4:E:164:LEU:HD13	4:E:211:TYR:CE2	2.49	0.48
4:E:204:THR:HG22	4:E:205:SER:N	2.28	0.48
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.43	0.48
6:H:93:TYR:HD1	6:H:145:ARG:HB3	1.79	0.48
1:A:705:LYS:HE3	1:A:713:SER:HB2	1.96	0.48
1:A:842:VAL:O	1:A:846:GLU:HB2	2.14	0.48
2:B:531:GLN:HG2	12:T:20:O2I:H2	1.96	0.48
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.47	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.13	0.48
10:L:53:HIS:O	10:L:55:ILE:N	2.47	0.48
1:A:55:ASP:O	1:A:58:LEU:N	2.33	0.48
1:A:325:ILE:O	1:A:328:ARG:HB2	2.14	0.48
1:A:845:LEU:O	1:A:847:ASP:N	2.47	0.48
2:B:519:TRP:CD1	2:B:519:TRP:C	2.87	0.48
2:B:858:SER:HA	2:B:966:VAL:O	2.12	0.48
2:B:35:SER:O	2:B:39:ARG:HG3	2.14	0.47
2:B:792:MET:CE	12:T:26:DG:OP1	2.62	0.47
1:A:98:LYS:O	1:A:102:VAL:HG22	2.14	0.47
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.96	0.47
2:B:249:ARG:O	2:B:250:PHE:C	2.53	0.47
3:C:141:GLY:O	3:C:142:VAL:O	2.32	0.47
8:J:7:CYS:CA	8:J:49:MET:HE3	2.44	0.47
10:L:47:ARG:HG3	10:L:48:CYS:H	1.78	0.47
1:A:343:LYS:HE3	2:B:1151:LEU:HG	1.95	0.47
1:A:1242:VAL:HG11	1:A:1259:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.96	0.47
2:B:276:ILE:HG22	2:B:277:LYS:N	2.29	0.47
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.96	0.47
1:A:898:ARG:HD2	1:A:899:VAL:N	2.29	0.47
1:A:919:ILE:HG21	1:A:925:LEU:HD12	1.96	0.47
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.50	0.47
2:B:363:HIS:O	2:B:364:ILE:CB	2.62	0.47
2:B:761:HIS:N	2:B:761:HIS:CD2	2.83	0.47
2:B:977:GLY:C	2:B:1099:VAL:CG2	2.83	0.47
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.95	0.47
1:A:1015:VAL:O	1:A:1016:THR:C	2.53	0.47
4:E:116:ILE:HG21	4:E:121:MET:CG	2.43	0.47
4:E:135:PHE:CB	4:E:140:LEU:HD11	2.45	0.47
1:A:818:MET:HG3	2:B:514:LEU:HD23	1.96	0.47
2:B:451:LYS:O	2:B:452:THR:C	2.53	0.47
4:E:52:ARG:HB3	4:E:53:PRO:HD2	1.97	0.47
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.25	0.47
1:A:715:GLU:O	1:A:719:VAL:HG23	2.14	0.47
1:A:908:LEU:HA	1:A:1029:ARG:HH21	1.79	0.47
1:A:990:VAL:HG21	1:A:1026:LEU:O	2.15	0.47
2:B:22:SER:O	2:B:654:ARG:HD2	2.15	0.47
2:B:63:ILE:CD1	2:B:95:ILE:HD12	2.44	0.47
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.49	0.47
2:B:546:SER:OG	2:B:631:GLY:N	2.39	0.47
2:B:638:PHE:CE2	2:B:743:ILE:HA	2.50	0.47
2:B:901:PRO:O	2:B:949:VAL:O	2.33	0.47
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.96	0.47
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.95	0.47
1:A:1053:PHE:O	1:A:1056:SER:N	2.41	0.47
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.54	0.47
2:B:352:ALA:O	2:B:356:LEU:HG	2.14	0.47
4:E:114:ASN:O	4:E:115:ASN:CB	2.63	0.47
1:A:902:LEU:HD21	1:A:923:LEU:HD23	1.97	0.47
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.14	0.47
3:C:16:ASP:HA	3:C:240:VAL:HG22	1.96	0.47
3:C:218:PRO:O	3:C:219:PHE:CB	2.63	0.47
6:H:5:LEU:HD22	6:H:133:ASN:O	2.15	0.47
11:R:4:G:N3	11:R:4:G:H2'	2.30	0.47
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.97	0.47
1:A:320:ARG:HB2	1:A:321:PRO:HB3	1.97	0.47
2:B:1129:ARG:HD3	12:T:22:DT:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:VAL:HG12	3:C:119:VAL:O	2.14	0.47
3:C:219:PHE:CD1	3:C:219:PHE:C	2.89	0.47
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.88	0.46
1:A:805:LEU:C	1:A:805:LEU:CD1	2.83	0.46
1:A:1392:SER:O	1:A:1394:THR:N	2.48	0.46
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.44	0.46
6:H:40:LEU:CD2	6:H:42:ILE:HD11	2.45	0.46
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.97	0.46
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.63	0.46
1:A:31:SER:HB2	1:A:83:HIS:HB3	1.95	0.46
1:A:563:PRO:HB2	1:A:565:ILE:O	2.15	0.46
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.97	0.46
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.56	0.46
2:B:461:LEU:HD12	2:B:466:TRP:CZ3	2.50	0.46
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.15	0.46
5:F:109:VAL:HG12	5:F:110:ASP:H	1.80	0.46
6:H:56:THR:O	6:H:144:ILE:HA	2.15	0.46
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.30	0.46
1:A:1146:VAL:HG12	1:A:1201:ALA:HB3	1.98	0.46
2:B:696:GLU:O	2:B:699:GLU:HB2	2.15	0.46
1:A:484:GLY:O	1:A:485:ASP:C	2.53	0.46
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.80	0.46
2:B:188:ASP:O	2:B:192:LEU:HG	2.16	0.46
1:A:73:GLY:O	1:A:75:ASN:N	2.44	0.46
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.45	0.46
1:A:910:PRO:C	1:A:912:LEU:H	2.19	0.46
2:B:46:GLN:HG3	2:B:47:GLN:H	1.81	0.46
2:B:227:LYS:HB2	2:B:395:GLN:CD	2.36	0.46
6:H:24:CYS:HB2	6:H:44:VAL:HG21	1.98	0.46
1:A:913:LEU:HD12	1:A:915:SER:H	1.81	0.46
2:B:174:LEU:HD23	2:B:202:TYR:CE2	2.50	0.46
2:B:780:VAL:HG21	8:J:56:LEU:HD11	1.96	0.46
2:B:1166:CYS:O	2:B:1168:LEU:N	2.48	0.46
3:C:102:GLN:HG2	3:C:154:LYS:HD2	1.97	0.46
6:H:106:GLU:C	6:H:108:SER:N	2.69	0.46
1:A:315:LEU:HD12	1:A:319:GLY:HA2	1.96	0.46
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.97	0.46
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.98	0.46
2:B:1024:ALA:O	2:B:1027:ILE:N	2.48	0.46
1:A:31:SER:CB	1:A:83:HIS:HB3	2.45	0.46
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:O	2:B:39:ARG:CG	2.64	0.46
2:B:44:VAL:O	2:B:45:SER:C	2.54	0.46
2:B:361:LEU:O	2:B:363:HIS:O	2.33	0.46
2:B:547:VAL:N	2:B:612:GLU:OE2	2.47	0.46
2:B:977:GLY:CA	2:B:1099:VAL:CG2	2.94	0.46
1:A:316:GLN:O	1:A:317:LYS:HB2	2.16	0.46
1:A:894:GLU:HG3	1:A:898:ARG:CB	2.46	0.46
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.98	0.46
2:B:431:TYR:O	2:B:435:THR:OG1	2.25	0.46
2:B:737:THR:HG23	7:I:66:PRO:HB3	1.97	0.46
2:B:955:THR:OG1	10:L:55:ILE:HA	2.16	0.46
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.50	0.46
6:H:93:TYR:CD2	6:H:143:LEU:HB3	2.50	0.46
1:A:89:PRO:O	1:A:204:THR:HG21	2.16	0.46
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.98	0.46
1:A:548:ASN:HD21	9:K:47:ARG:HE	1.64	0.46
1:A:622:VAL:HA	1:A:630:ILE:HD11	1.98	0.46
1:A:711:ARG:HG3	7:I:97:MET:HE2	1.98	0.46
1:A:1006:ILE:HD11	4:E:163:GLU:CG	2.46	0.46
1:A:1319:VAL:HB	1:A:1322:ILE:HD12	1.98	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.46	0.46
2:B:501:PRO:O	2:B:502:ILE:HB	2.16	0.46
2:B:868:MET:O	2:B:869:SER:HB3	2.15	0.46
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.47	0.46
7:I:25:LEU:HB3	7:I:38:ALA:HB2	1.97	0.46
1:A:451:HIS:HB3	1:A:453:MET:N	2.31	0.45
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.51	0.45
1:A:531:ILE:N	1:A:653:VAL:HG11	2.31	0.45
1:A:1120:LEU:HB3	1:A:1124:HIS:O	2.16	0.45
2:B:227:LYS:CG	2:B:236:HIS:CE1	2.82	0.45
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.46	0.45
3:C:133:ILE:HD13	3:C:236:GLY:C	2.37	0.45
2:B:38:PHE:O	2:B:39:ARG:C	2.54	0.45
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.15	0.45
3:C:5:GLY:O	3:C:7:GLN:HG2	2.16	0.45
7:I:19:ASP:CB	7:I:24:ARG:HG3	2.46	0.45
1:A:834:THR:HG21	1:A:1077:THR:CA	2.46	0.45
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.32	0.45
1:A:1406:VAL:HG12	1:A:1407:GLU:N	2.32	0.45
2:B:660:LYS:O	2:B:663:ALA:HB3	2.17	0.45
2:B:701:ILE:HB	2:B:740:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.52	0.45
4:E:46:TYR:CE2	4:E:58:MET:HA	2.52	0.45
4:E:127:ILE:O	4:E:127:ILE:HG12	2.15	0.45
9:K:57:LEU:HD12	9:K:76:GLN:CG	2.45	0.45
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.98	0.45
1:A:809:THR:CG2	2:B:730:ARG:HG3	2.47	0.45
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.98	0.45
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.31	0.45
2:B:288:ALA:O	2:B:327:ARG:NH2	2.50	0.45
2:B:760:ASP:OD1	2:B:760:ASP:N	2.49	0.45
7:I:10:CYS:SG	7:I:31:THR:HB	2.57	0.45
1:A:913:LEU:CD1	1:A:981:LEU:O	2.64	0.45
1:A:919:ILE:O	1:A:920:LEU:C	2.53	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.99	0.45
1:A:11:LEU:HA	2:B:1193:GLN:O	2.17	0.45
1:A:583:PRO:O	1:A:610:GLY:HA3	2.16	0.45
1:A:891:ALA:O	1:A:895:LYS:N	2.48	0.45
1:A:1172:LEU:HD23	1:A:1172:LEU:N	2.32	0.45
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.51	0.45
3:C:46:ILE:HD11	3:C:72:LEU:HD11	1.99	0.45
3:C:249:ASP:O	3:C:252:GLN:HB3	2.17	0.45
4:E:114:ASN:O	4:E:115:ASN:HB3	2.17	0.45
1:A:62:ASP:O	1:A:63:ARG:C	2.54	0.45
1:A:1376:THR:HG23	1:A:1376:THR:O	2.16	0.45
4:E:20:LYS:HE2	4:E:60:PHE:CZ	2.52	0.45
1:A:590:ARG:HB3	1:A:605:MET:N	2.32	0.45
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.32	0.45
2:B:640:VAL:HG13	2:B:650:GLU:O	2.17	0.45
7:I:19:ASP:HB3	7:I:24:ARG:HG3	1.99	0.45
2:B:197:PHE:CG	2:B:817:LEU:HD11	2.52	0.45
2:B:236:HIS:NE2	2:B:389:ALA:HA	2.32	0.45
2:B:552:MET:N	2:B:553:PRO:HD2	2.32	0.45
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.98	0.45
2:B:682:SER:O	2:B:686:ASN:ND2	2.50	0.45
4:E:112:TYR:CZ	4:E:136:ASN:HB2	2.52	0.45
4:E:136:ASN:OD1	4:E:136:ASN:C	2.55	0.45
7:I:29:CYS:SG	7:I:31:THR:CB	2.99	0.45
1:A:134:ARG:CD	1:A:221:SER:O	2.65	0.45
1:A:321:PRO:CD	1:A:322:VAL:N	2.80	0.45
2:B:110:HIS:NE2	10:L:53:HIS:HE1	2.14	0.45
2:B:1135:ARG:HG3	2:B:1147:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:TYR:HE2	4:E:78:LEU:HD13	1.80	0.45
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.99	0.45
1:A:321:PRO:C	1:A:322:VAL:HG13	2.37	0.44
1:A:705:LYS:O	1:A:706:HIS:C	2.55	0.44
2:B:34:ILE:HD12	2:B:743:ILE:HG21	1.98	0.44
3:C:229:TYR:CD1	3:C:229:TYR:N	2.85	0.44
7:I:10:CYS:SG	7:I:31:THR:CG2	3.05	0.44
12:T:21:DC:C5	12:T:22:DT:C4	3.05	0.44
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.50	0.44
1:A:933:TYR:O	1:A:937:VAL:HG23	2.17	0.44
2:B:65:GLU:C	2:B:67:SER:N	2.69	0.44
2:B:778:MET:CE	2:B:853:SER:HB3	2.47	0.44
2:B:1031:LEU:HD13	2:B:1055:ILE:CD1	2.48	0.44
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.14	0.44
3:C:134:ILE:HD12	3:C:141:GLY:N	2.32	0.44
4:E:112:TYR:CE1	4:E:136:ASN:HB2	2.52	0.44
7:I:119:THR:C	7:I:120:GLN:CG	2.86	0.44
1:A:72:GLU:HB3	1:A:76:GLU:HG2	2.00	0.44
1:A:380:VAL:HG23	1:A:430:TRP:H	1.81	0.44
1:A:525:GLN:O	1:A:526:ASP:C	2.55	0.44
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.31	0.44
1:A:1436:ILE:O	1:A:1439:GLY:N	2.50	0.44
2:B:596:LEU:O	2:B:599:THR:HB	2.16	0.44
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.51	0.44
1:A:320:ARG:HG3	1:A:320:ARG:NH1	2.32	0.44
1:A:569:LYS:O	1:A:571:LEU:HD13	2.18	0.44
1:A:1154:TYR:HE1	7:I:18:GLU:HG3	1.81	0.44
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.66	0.44
2:B:862:GLN:O	2:B:914:LYS:NZ	2.51	0.44
6:H:93:TYR:CD2	6:H:143:LEU:CB	3.00	0.44
8:J:2:ILE:C	8:J:53:HIS:CE1	2.91	0.44
9:K:49:GLU:HB2	9:K:94:ILE:HD11	1.99	0.44
1:A:1325:THR:O	4:E:148:GLU:HB2	2.18	0.44
2:B:640:VAL:HG22	2:B:651:LEU:HA	1.99	0.44
5:F:97:ARG:HA	5:F:100:GLN:OE1	2.18	0.44
9:K:6:ARG:O	9:K:9:LEU:HG	2.18	0.44
1:A:65:LEU:O	1:A:67:CYS:N	2.44	0.44
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.98	0.44
2:B:792:MET:HE3	12:T:26:DG:OP1	2.16	0.44
2:B:896:ASP:OD2	10:L:58:LYS:HE3	2.17	0.44
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:VAL:O	1:A:433:GLU:C	2.56	0.44
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.17	0.44
2:B:816:GLU:N	2:B:816:GLU:OE1	2.51	0.44
3:C:244:VAL:HG21	9:K:105:PHE:CE2	2.52	0.44
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.99	0.44
5:F:155:LEU:HD23	5:F:155:LEU:N	2.33	0.44
7:I:17:ARG:O	7:I:25:LEU:HD12	2.17	0.44
9:K:21:ILE:HG12	9:K:33:ILE:HG12	2.00	0.44
1:A:693:VAL:O	1:A:696:GLU:HB3	2.17	0.44
1:A:1271:ILE:HD13	1:A:1271:ILE:HA	1.73	0.44
1:A:1325:THR:OG1	4:E:146:HIS:O	2.35	0.44
2:B:292:ILE:HB	2:B:293:PRO:HD3	2.00	0.44
2:B:1033:LYS:HD3	2:B:1059:LEU:HD11	1.99	0.44
1:A:273:ASN:HB2	1:A:296:LEU:HD11	1.99	0.44
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.48	0.44
1:A:892:ALA:HA	1:A:895:LYS:HD3	2.00	0.44
2:B:247:GLY:O	2:B:248:SER:CB	2.66	0.44
2:B:628:THR:O	2:B:628:THR:CG2	2.66	0.44
3:C:60:ASP:HB3	10:L:67:PHE:CZ	2.53	0.44
8:J:57:ILE:HA	8:J:60:PHE:CD1	2.53	0.44
2:B:273:LEU:HD11	2:B:285:ILE:HD11	2.00	0.43
2:B:843:GLN:HA	2:B:846:ILE:HD12	2.00	0.43
3:C:52:GLU:HA	10:L:64:LEU:HD22	2.00	0.43
3:C:133:ILE:CD1	3:C:237:SER:HA	2.41	0.43
4:E:15:ALA:HA	4:E:140:LEU:O	2.18	0.43
1:A:320:ARG:HH11	1:A:320:ARG:H	1.66	0.43
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.32	0.43
2:B:636:PRO:CD	2:B:637:LEU:HB3	2.49	0.43
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.52	0.43
6:H:82:PRO:O	6:H:83:GLN:HB2	2.18	0.43
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.83	0.43
1:A:599:SER:O	1:A:602:ASP:N	2.49	0.43
2:B:219:ALA:HB2	2:B:405:ARG:HG2	2.00	0.43
2:B:329:THR:HA	2:B:332:ASP:HB2	1.99	0.43
2:B:485:ARG:HH11	2:B:485:ARG:HG3	1.83	0.43
5:F:73:ALA:O	5:F:74:ILE:CG1	2.64	0.43
1:A:107:CYS:N	1:A:114:LEU:HD21	2.33	0.43
1:A:404:TYR:HB2	1:A:433:GLU:HG3	1.99	0.43
1:A:590:ARG:O	1:A:591:PHE:HB2	2.18	0.43
1:A:840:ARG:O	1:A:841:LEU:C	2.57	0.43
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:HD11	2:B:355:ILE:HG21	2.00	0.43
2:B:627:PHE:O	2:B:632:ARG:NH1	2.52	0.43
2:B:778:MET:HE3	2:B:853:SER:HB3	2.00	0.43
3:C:181:ASP:OD1	3:C:183:TRP:O	2.36	0.43
1:A:287:HIS:O	1:A:288:ALA:HB2	2.18	0.43
1:A:608:ILE:HG12	1:A:613:ILE:CG1	2.48	0.43
1:A:665:GLY:HA2	2:B:1086:PHE:CD1	2.54	0.43
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.00	0.43
3:C:194:GLU:N	3:C:200:GLU:OE1	2.44	0.43
4:E:195:VAL:CG2	4:E:213:ILE:HD13	2.48	0.43
9:K:47:ARG:CD	9:K:60:ALA:HA	2.48	0.43
1:A:32:VAL:HB	1:A:57:ARG:HB2	2.00	0.43
1:A:68:GLN:O	1:A:70:CYS:N	2.52	0.43
1:A:70:CYS:C	1:A:71:GLN:HG3	2.38	0.43
1:A:320:ARG:CB	1:A:321:PRO:CA	2.79	0.43
1:A:596:THR:C	1:A:598:LEU:H	2.21	0.43
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.48	0.43
2:B:37:PHE:O	2:B:38:PHE:HB2	2.19	0.43
3:C:221:TYR:HD1	3:C:222:LYS:HG3	1.82	0.43
3:C:242:GLN:O	3:C:246:ARG:HG3	2.17	0.43
4:E:102:GLU:C	4:E:104:ASN:H	2.22	0.43
1:A:549:MET:O	1:A:550:LEU:C	2.57	0.43
1:A:942:PHE:CD1	1:A:942:PHE:C	2.92	0.43
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.84	0.43
1:A:1394:THR:CG2	1:A:1398:MET:HE3	2.49	0.43
1:A:1404:GLU:O	1:A:1408:ILE:HG12	2.18	0.43
4:E:126:SER:O	4:E:128:PRO:HD3	2.19	0.43
6:H:39:THR:O	6:H:123:MET:HA	2.18	0.43
11:R:7:A:C2	12:T:23:DC:C2	3.07	0.43
1:A:805:LEU:O	2:B:761:HIS:ND1	2.52	0.43
1:A:902:LEU:O	1:A:903:ASN:CB	2.66	0.43
1:A:1126:ALA:O	1:A:1128:GLN:N	2.51	0.43
2:B:249:ARG:CG	2:B:249:ARG:HH21	2.31	0.43
5:F:97:ARG:HG3	5:F:101:ILE:HD11	1.99	0.43
1:A:1194:ARG:NH2	1:A:1237:ILE:CD1	2.82	0.43
2:B:784:ASN:HB3	8:J:63:TYR:CZ	2.53	0.43
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	2.15	0.43
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.19	0.43
5:F:132:LEU:O	5:F:148:VAL:HG23	2.19	0.43
10:L:46:VAL:HG12	10:L:47:ARG:H	1.84	0.43
1:A:219:PHE:CE1	1:A:231:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:SER:HA	1:A:482:PHE:CD1	2.54	0.43
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.48	0.43
2:B:1104:HIS:HB2	2:B:1122:ARG:HB2	2.01	0.43
2:B:1129:ARG:HB2	12:T:23:DC:OP2	2.18	0.43
3:C:70:ILE:HD11	3:C:115:SER:HB3	2.00	0.43
7:I:7:CYS:HB2	7:I:34:TYR:CD1	2.54	0.43
1:A:351:THR:HG23	2:B:1103:ILE:HG23	2.01	0.42
1:A:367:PRO:HA	1:A:463:ILE:HD12	2.00	0.42
2:B:365:THR:HG22	2:B:370:PHE:HB2	2.01	0.42
2:B:428:ILE:HG13	2:B:448:ILE:HD13	2.01	0.42
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.54	0.42
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.01	0.42
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.19	0.42
3:C:177:GLU:O	3:C:230:MET:HA	2.19	0.42
4:E:88:VAL:HG21	4:E:112:TYR:HB2	2.01	0.42
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.34	0.42
1:A:326:ARG:CG	1:A:1406:VAL:HG21	2.49	0.42
1:A:991:LYS:O	1:A:994:GLN:HB3	2.19	0.42
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.19	0.42
2:B:329:THR:O	2:B:332:ASP:HB3	2.19	0.42
2:B:557:PHE:C	2:B:557:PHE:CD1	2.91	0.42
3:C:110:THR:HG22	3:C:110:THR:O	2.19	0.42
7:I:2:THR:O	7:I:3:THR:C	2.56	0.42
1:A:78:PRO:O	1:A:79:GLY:C	2.58	0.42
1:A:207:ILE:HG22	1:A:211:PHE:CE2	2.54	0.42
1:A:499:ALA:O	1:A:503:GLN:HG2	2.19	0.42
1:A:737:LEU:HD11	1:A:758:ILE:HG21	2.01	0.42
1:A:885:THR:OG1	1:A:1024:SER:HB3	2.19	0.42
1:A:892:ALA:HA	1:A:895:LYS:HB2	2.01	0.42
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	2.01	0.42
2:B:1170:THR:CG2	2:B:1183:LYS:HZ1	2.33	0.42
4:E:23:VAL:HG13	4:E:28:TYR:CD2	2.50	0.42
6:H:33:GLN:OE1	6:H:129:TYR:CZ	2.73	0.42
1:A:57:ARG:HB3	1:A:68:GLN:HG2	2.01	0.42
1:A:351:THR:CG2	2:B:1103:ILE:HD12	2.44	0.42
1:A:452:LYS:HB2	2:B:1141:HIS:HE1	1.83	0.42
3:C:16:ASP:O	3:C:233:GLU:HA	2.20	0.42
3:C:120:ILE:HD11	3:C:130:GLY:O	2.19	0.42
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.85	0.42
6:H:84:ALA:CA	6:H:87:ARG:HB2	2.49	0.42
1:A:93:VAL:HG22	1:A:301:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:TYR:HA	1:A:413:ILE:O	2.18	0.42
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.54	0.42
2:B:276:ILE:HG22	2:B:277:LYS:H	1.85	0.42
2:B:316:PRO:HA	2:B:319:GLU:HG3	2.01	0.42
2:B:1102:LYS:HB2	2:B:1103:ILE:HD13	2.01	0.42
1:A:242:PRO:O	1:A:247:ARG:NH2	2.48	0.42
1:A:475:THR:HG22	1:A:476:SER:N	2.35	0.42
1:A:505:CYS:SG	2:B:1141:HIS:HD2	2.42	0.42
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.33	0.42
1:A:1327:ILE:HG23	1:A:1327:ILE:O	2.20	0.42
1:A:1426:GLU:O	1:A:1430:LEU:HG	2.20	0.42
2:B:211:VAL:HG12	2:B:212:LEU:N	2.35	0.42
2:B:361:LEU:N	2:B:362:PRO:CD	2.83	0.42
3:C:144:ILE:HD13	3:C:144:ILE:HA	1.90	0.42
1:A:120:GLU:CG	1:A:120:GLU:O	2.66	0.42
1:A:241:VAL:HG13	1:A:266:LEU:HD12	2.01	0.42
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.55	0.42
1:A:574:GLY:O	1:A:575:LYS:C	2.57	0.42
1:A:1200:ALA:O	1:A:1203:ASN:HB2	2.19	0.42
2:B:118:ARG:HA	2:B:207:GLY:HA2	2.02	0.42
1:A:150:THR:O	1:A:151:ASP:CG	2.58	0.42
1:A:269:ILE:HG13	1:A:299:HIS:HB3	2.00	0.42
1:A:535:THR:O	1:A:536:LEU:C	2.57	0.42
1:A:567:LYS:HB3	6:H:96:VAL:N	2.33	0.42
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.54	0.42
3:C:10:ILE:HD13	3:C:20:PHE:HB3	2.01	0.42
3:C:101:LEU:HD21	3:C:113:VAL:HG11	2.01	0.42
4:E:113:GLN:O	4:E:114:ASN:ND2	2.52	0.42
1:A:115:LEU:HD12	1:A:122:MET:HE2	2.02	0.42
1:A:314:ALA:O	1:A:315:LEU:O	2.38	0.42
2:B:604:ARG:NH2	2:B:614:SER:HA	2.35	0.42
2:B:849:GLY:HA2	2:B:852:ARG:HD2	2.02	0.42
2:B:994:TYR:HB2	2:B:999:MET:CE	2.50	0.42
9:K:50:LEU:HD21	9:K:75:ILE:HD13	2.02	0.42
1:A:207:ILE:HA	1:A:210:ILE:HG13	2.02	0.42
3:C:46:ILE:HD13	3:C:159:ALA:HB2	2.02	0.42
4:E:54:GLN:O	4:E:57:MET:HB3	2.18	0.42
1:A:423:ASP:C	1:A:424:ILE:HG13	2.40	0.41
1:A:768:GLN:CG	1:A:816:HIS:HA	2.49	0.41
2:B:25:ILE:HG22	2:B:26:THR:N	2.35	0.41
2:B:236:HIS:CD2	2:B:389:ALA:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:ARG:NH2	3:C:38:ILE:HD12	2.35	0.41
6:H:32:THR:HG22	6:H:33:GLN:HG2	2.02	0.41
1:A:108:MET:SD	1:A:108:MET:N	2.92	0.41
1:A:213:HIS:O	1:A:214:ILE:O	2.37	0.41
1:A:253:ASN:CG	1:A:254:GLU:H	2.22	0.41
1:A:899:VAL:HG23	1:A:1029:ARG:HG2	2.01	0.41
2:B:322:PHE:O	2:B:322:PHE:CD1	2.73	0.41
2:B:877:PRO:HB3	2:B:915:THR:CG2	2.50	0.41
4:E:98:ILE:O	4:E:99:HIS:C	2.57	0.41
4:E:127:ILE:O	4:E:127:ILE:CG1	2.68	0.41
5:F:76:LYS:O	5:F:79:ARG:HD3	2.20	0.41
9:K:78:THR:CG2	9:K:79:GLU:N	2.83	0.41
1:A:476:SER:N	1:A:477:PRO:HD2	2.35	0.41
1:A:736:ASN:O	1:A:737:LEU:C	2.58	0.41
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.54	0.41
2:B:57:TYR:N	2:B:57:TYR:CD1	2.88	0.41
2:B:123:THR:HG22	2:B:125:SER:HB3	2.01	0.41
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.69	0.41
6:H:56:THR:HB	6:H:145:ARG:HG2	2.01	0.41
1:A:267:ALA:O	1:A:271:LYS:N	2.40	0.41
1:A:1434:ALA:O	1:A:1436:ILE:N	2.53	0.41
2:B:41:LYS:HB3	2:B:45:SER:HB3	2.02	0.41
2:B:315:LYS:HG2	7:I:13:MET:HE1	2.02	0.41
2:B:790:ASP:OD1	2:B:790:ASP:N	2.54	0.41
3:C:8:VAL:HA	3:C:21:ILE:O	2.20	0.41
3:C:43:THR:CG2	3:C:44:LEU:N	2.83	0.41
3:C:145:CYS:HA	8:J:2:ILE:CD1	2.51	0.41
4:E:136:ASN:OD1	4:E:137:GLU:N	2.54	0.41
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.55	0.41
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.51	0.41
9:K:47:ARG:HD2	9:K:60:ALA:HA	2.01	0.41
12:T:19:DA:H2'	12:T:20:O2I:N7	2.35	0.41
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.55	0.41
1:A:254:GLU:O	2:B:918:ILE:HG13	2.21	0.41
1:A:783:THR:O	1:A:784:LEU:HD23	2.20	0.41
1:A:1160:SER:HA	1:A:1170:ILE:HG21	2.03	0.41
2:B:1051:THR:HB	2:B:1054:GLY:H	1.85	0.41
2:B:1160:VAL:HG11	2:B:1169:MET:HG2	2.02	0.41
3:C:134:ILE:HD12	3:C:141:GLY:HA3	2.03	0.41
7:I:111:THR:HG22	7:I:113:ASP:H	1.84	0.41
1:A:15:LYS:HB3	2:B:1220:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.55	0.41
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.02	0.41
2:B:355:ILE:HG22	2:B:356:LEU:HD23	2.02	0.41
2:B:917:PRO:O	2:B:918:ILE:HD13	2.21	0.41
2:B:1171:VAL:HG12	2:B:1172:ILE:H	1.85	0.41
3:C:134:ILE:HD12	3:C:141:GLY:CA	2.51	0.41
3:C:165:LYS:O	9:K:6:ARG:NH1	2.54	0.41
3:C:245:VAL:HA	3:C:248:ILE:HD12	2.02	0.41
6:H:76:THR:O	6:H:76:THR:CG2	2.68	0.41
6:H:139:ASN:O	6:H:140:ALA:CB	2.68	0.41
1:A:322:VAL:HB	1:A:323:LYS:CD	2.37	0.41
1:A:929:LEU:HD21	1:A:983:ILE:HG21	2.00	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.51	0.41
2:B:307:ASP:OD2	2:B:392:ARG:NH1	2.53	0.41
2:B:421:PHE:O	2:B:425:THR:HB	2.21	0.41
2:B:844:SER:HG	2:B:996:ARG:N	2.16	0.41
3:C:92:CYS:SG	3:C:94:LYS:CB	3.09	0.41
5:F:111:LEU:N	5:F:111:LEU:CD1	2.84	0.41
1:A:261:ASP:HB3	1:A:323:LYS:HE3	2.03	0.41
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.85	0.41
1:A:614:PHE:CD1	1:A:614:PHE:C	2.93	0.41
1:A:870:GLU:HB2	4:E:204:THR:CG2	2.46	0.41
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.02	0.41
2:B:256:VAL:HG11	2:B:382:ILE:CD1	2.50	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.36	0.41
2:B:531:GLN:CG	12:T:20:O2I:H2	2.50	0.41
2:B:896:ASP:N	2:B:896:ASP:OD1	2.54	0.41
2:B:1177:HIS:O	2:B:1179:GLN:N	2.54	0.41
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.50	0.41
5:F:109:VAL:CG2	5:F:124:GLU:CG	2.97	0.41
6:H:40:LEU:HD13	6:H:123:MET:HE3	2.03	0.41
1:A:306:ASN:OD1	1:A:313:GLN:NE2	2.53	0.41
1:A:857:ARG:CZ	5:F:139:PRO:HG2	2.51	0.41
1:A:1154:TYR:OH	7:I:18:GLU:HG2	2.20	0.41
1:A:1319:VAL:HG12	1:A:1320:PRO:N	2.36	0.41
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.02	0.41
2:B:307:ASP:O	2:B:310:MET:N	2.54	0.41
2:B:463:THR:HG21	2:B:465:ASN:ND2	2.36	0.41
2:B:635:ARG:CB	2:B:636:PRO:CD	2.98	0.41
2:B:737:THR:O	2:B:738:PHE:C	2.59	0.41
2:B:778:MET:HE2	2:B:1094:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:860:MET:HG2	2:B:861:ASP:N	2.36	0.41
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.43	0.41
3:C:52:GLU:HB3	3:C:154:LYS:HB3	2.02	0.41
3:C:70:ILE:HD11	3:C:115:SER:CB	2.51	0.41
3:C:92:CYS:C	3:C:94:LYS:H	2.23	0.41
4:E:111:VAL:HG12	4:E:111:VAL:O	2.21	0.41
9:K:49:GLU:CG	9:K:94:ILE:HD11	2.50	0.41
10:L:51:CYS:O	10:L:51:CYS:SG	2.79	0.41
1:A:225:ASN:O	1:A:225:ASN:ND2	2.53	0.41
1:A:254:GLU:HA	1:A:255:SER:HA	1.86	0.41
1:A:979:SER:OG	1:A:980:ASP:N	2.54	0.41
1:A:1064:VAL:O	1:A:1065:GLY:C	2.58	0.41
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.21	0.41
2:B:798:TYR:N	2:B:799:PRO:HD2	2.35	0.41
2:B:803:LEU:N	2:B:822:ASN:HD21	2.19	0.41
3:C:253:LYS:O	3:C:256:ALA:HB3	2.21	0.41
9:K:108:GLU:HA	9:K:111:LEU:HG	2.03	0.41
1:A:401:GLY:C	1:A:435:HIS:HD2	2.24	0.40
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.02	0.40
2:B:734:HIS:O	2:B:735:ALA:HB2	2.21	0.40
2:B:751:VAL:HG12	2:B:752:ALA:N	2.37	0.40
2:B:1024:ALA:O	2:B:1025:HIS:C	2.60	0.40
3:C:220:ASP:O	3:C:221:TYR:HB3	2.21	0.40
1:A:72:GLU:CB	1:A:76:GLU:HG2	2.51	0.40
1:A:320:ARG:HG2	2:B:471:LYS:HG2	2.02	0.40
1:A:1289:ARG:O	1:A:1300:LYS:HA	2.22	0.40
2:B:34:ILE:HD13	2:B:34:ILE:H	1.85	0.40
2:B:46:GLN:HG3	2:B:47:GLN:N	2.36	0.40
2:B:121:ASN:N	2:B:121:ASN:HD22	2.18	0.40
2:B:314:LEU:O	2:B:315:LYS:C	2.60	0.40
2:B:326:ASP:CG	2:B:329:THR:HG1	2.24	0.40
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.36	0.40
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.40
2:B:911:ILE:CD1	2:B:941:LEU:HD23	2.51	0.40
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.56	0.40
4:E:124:VAL:HG13	4:E:132:ILE:HG22	2.03	0.40
6:H:129:TYR:C	6:H:131:ASN:N	2.74	0.40
7:I:109:ILE:N	7:I:109:ILE:HD12	2.36	0.40
2:B:36:ALA:C	2:B:37:PHE:O	2.57	0.40
2:B:487:THR:CG2	2:B:488:TYR:N	2.83	0.40
1:A:68:GLN:HE21	1:A:80:HIS:CE1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:O	1:A:314:ALA:CB	2.69	0.40
1:A:522:GLY:C	1:A:523:ILE:HD12	2.42	0.40
1:A:971:PHE:HB2	1:A:973:ILE:HD13	2.02	0.40
2:B:179:CYS:SG	2:B:181:LEU:HD12	2.62	0.40
2:B:181:LEU:HD22	2:B:189:LEU:HD21	2.03	0.40
4:E:179:GLN:HB2	4:E:182:ASP:HB2	2.03	0.40
6:H:15:VAL:CG2	6:H:26:ILE:HD11	2.51	0.40
1:A:12:ARG:HD3	2:B:1192:TYR:CE1	2.56	0.40
1:A:531:ILE:HD12	1:A:649:ILE:CG2	2.52	0.40
1:A:553:VAL:HG22	1:A:652:VAL:HG22	2.04	0.40
1:A:591:PHE:HA	1:A:595:THR:HG21	2.04	0.40
1:A:668:ASP:HB3	1:A:743:VAL:HG23	2.04	0.40
1:A:697:ALA:HB2	1:A:702:LEU:HG	2.03	0.40
2:B:23:ALA:O	2:B:654:ARG:HB3	2.22	0.40
2:B:34:ILE:N	2:B:34:ILE:CD1	2.84	0.40
2:B:640:VAL:O	2:B:640:VAL:HG12	2.22	0.40
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.04	0.40
4:E:74:ASP:O	4:E:106:GLN:NE2	2.55	0.40
4:E:190:LEU:HD11	4:E:196:VAL:HG13	2.03	0.40
7:I:119:THR:O	7:I:119:THR:CG2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1057 (76%)	217 (16%)	109 (8%)	1	12
2	B	1086/1224 (89%)	858 (79%)	162 (15%)	66 (6%)	1	16
3	C	264/318 (83%)	206 (78%)	45 (17%)	13 (5%)	2	19
4	E	212/215 (99%)	174 (82%)	29 (14%)	9 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1	16
6	H	129/146 (88%)	97 (75%)	23 (18%)	9 (7%)	1	14
7	I	117/122 (96%)	85 (73%)	20 (17%)	12 (10%)	0	7
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	16
9	K	112/120 (93%)	95 (85%)	14 (12%)	3 (3%)	4	28
10	L	44/70 (63%)	26 (59%)	10 (23%)	8 (18%)	0	2
All	All	3492/4173 (84%)	2708 (78%)	546 (16%)	238 (7%)	1	15

All (238) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	55	ASP
1	A	62	ASP
1	A	63	ARG
1	A	68	GLN
1	A	69	THR
1	A	72	GLU
1	A	76	GLU
1	A	89	PRO
1	A	93	VAL
1	A	108	MET
1	A	130	ASP
1	A	167	CYS
1	A	204	THR
1	A	209	ASN
1	A	210	ILE
1	A	214	ILE
1	A	285	PRO
1	A	286	HIS
1	A	288	ALA
1	A	314	ALA
1	A	315	LEU
1	A	321	PRO
1	A	322	VAL
1	A	331	GLY
1	A	335	ARG
1	A	404	TYR
1	A	465	TYR
1	A	517	ASN

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Mol	Chain	Res	Type
1	A	567	LYS
1	A	568	PRO
1	A	575	LYS
1	A	593	GLU
1	A	628	GLY
1	A	795	GLU
1	A	846	GLU
1	A	889	SER
1	A	903	ASN
1	A	904	THR
1	A	922	ASP
1	A	972	HIS
1	A	1016	THR
1	A	1255	GLU
1	A	1327	ILE
1	A	1393	ASN
2	B	23	ALA
2	B	66	ASP
2	B	168	GLY
2	B	223	VAL
2	B	229	ALA
2	B	248	SER
2	B	249	ARG
2	B	274	PRO
2	B	275	TYR
2	B	327	ARG
2	B	367	LEU
2	B	436	VAL
2	B	451	LYS
2	B	470	LYS
2	B	635	ARG
2	B	643	ASP
2	B	645	SER
2	B	695	ALA
2	B	708	GLU
2	B	709	ASP
2	B	734	HIS
2	B	737	THR
2	B	869	SER
2	B	958	GLN
2	B	961	LEU
2	B	981	ALA

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Mol	Chain	Res	Type
2	B	982	SER
2	B	1167	GLY
2	B	1176	ASN
2	B	1178	ASN
3	C	60	ASP
3	C	142	VAL
3	C	219	PHE
3	C	220	ASP
4	E	59	SER
4	E	115	ASN
5	F	81	THR
5	F	104	ASN
5	F	128	LYS
6	H	32	THR
6	H	81	PRO
6	H	82	PRO
6	H	130	ARG
6	H	135	LEU
6	H	140	ALA
7	I	3	THR
7	I	8	ARG
7	I	16	PRO
7	I	20	LYS
7	I	21	GLU
7	I	78	CYS
7	I	79	HIS
8	J	2	ILE
10	L	35	SER
10	L	47	ARG
10	L	54	ARG
10	L	59	ALA
10	L	64	LEU
1	A	34	LYS
1	A	129	LYS
1	A	149	GLU
1	A	250	ILE
1	A	309	ALA
1	A	312	PRO
1	A	320	ARG
1	A	880	LYS
1	A	896	ARG
1	A	902	LEU

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Mol	Chain	Res	Type
1	A	915	SER
1	A	998	LEU
1	A	1036	ARG
1	A	1054	LEU
1	A	1127	ASP
1	A	1139	GLU
1	A	1221	LYS
1	A	1437	GLY
2	B	67	SER
2	B	94	LYS
2	B	184	ALA
2	B	294	ASP
2	B	308	TRP
2	B	364	ILE
2	B	448	ILE
2	B	476	ARG
2	B	636	PRO
2	B	842	ASN
2	B	880	THR
2	B	1132	GLU
2	B	1181	GLU
3	C	5	GLY
3	C	28	ALA
3	C	110	THR
3	C	221	TYR
5	F	113	GLY
6	H	3	ASN
6	H	77	ARG
6	H	109	LYS
7	I	9	ASP
7	I	23	ASN
7	I	54	GLU
8	J	6	ARG
9	K	13	GLY
9	K	28	PRO
1	A	33	ALA
1	A	48	ALA
1	A	52	GLY
1	A	56	PRO
1	A	71	GLN
1	A	111	GLY
1	A	219	PHE

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Mol	Chain	Res	Type
1	A	248	PRO
1	A	317	LYS
1	A	385	ILE
1	A	536	LEU
1	A	538	ASP
1	A	543	LEU
1	A	794	PRO
1	A	911	SER
1	A	958	VAL
1	A	1365	TYR
1	A	1401	SER
2	B	65	GLU
2	B	201	GLY
2	B	469	GLN
2	B	472	ALA
2	B	563	MET
2	B	738	PHE
2	B	799	PRO
2	B	1046	PRO
2	B	1155	SER
3	C	197	SER
3	C	202	PRO
3	C	215	GLU
4	E	77	SER
4	E	103	LYS
7	I	47	GLU
10	L	43	THR
10	L	50	ASP
1	A	77	CYS
1	A	86	LEU
1	A	252	PHE
1	A	332	LYS
1	A	994	GLN
1	A	1004	ASN
2	B	55	VAL
2	B	471	LYS
2	B	735	ALA
2	B	879	ARG
2	B	1017	ILE
3	C	217	ASP
5	F	141	GLY
7	I	15	TYR

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Mol	Chain	Res	Type
9	K	90	ALA
1	A	66	LYS
1	A	132	LYS
1	A	324	SER
1	A	418	SER
1	A	424	ILE
1	A	597	LEU
1	A	609	ASP
1	A	734	GLU
1	A	819	GLY
1	A	1053	PHE
1	A	1122	PRO
2	B	292	ILE
2	B	468	GLU
4	E	102	GLU
4	E	174	GLN
8	J	64	ASN
1	A	74	MET
1	A	223	GLY
1	A	610	GLY
2	B	712	PRO
1	A	1098	VAL
1	A	1294	PRO
1	A	1435	PRO
2	B	1172	ILE
2	B	1103	ILE
4	E	51	GLY
4	E	90	VAL
10	L	52	GLY
1	A	380	VAL
1	A	396	PRO
2	B	301	ILE
4	E	27	GLY
1	A	35	ILE
1	A	162	VAL
1	A	399	HIS
2	B	1165	ILE
2	B	24	PRO
2	B	240	ILE
3	C	212	PRO
8	J	14	VAL

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	1218/1520 (80%)	984 (81%)	234 (19%)	1	8
2	B	958/1061 (90%)	802 (84%)	156 (16%)	2	12
3	C	234/274 (85%)	194 (83%)	40 (17%)	1	11
4	E	196/197 (100%)	162 (83%)	34 (17%)	1	10
5	F	74/137 (54%)	61 (82%)	13 (18%)	1	10
6	H	117/128 (91%)	98 (84%)	19 (16%)	2	12
7	I	113/116 (97%)	95 (84%)	18 (16%)	2	13
8	J	60/65 (92%)	44 (73%)	16 (27%)	0	3
9	K	99/102 (97%)	86 (87%)	13 (13%)	3	17
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	5
All	All	3109/3657 (85%)	2557 (82%)	552 (18%)	1	10

All (552) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	18	GLN
1	A	22	PHE
1	A	25	GLU
1	A	28	ARG
1	A	32	VAL
1	A	40	THR
1	A	47	ARG
1	A	49	LYS
1	A	50	ILE
1	A	63	ARG
1	A	64	ASN
1	A	65	LEU
1	A	69	THR
1	A	71	GLN
1	A	81	PHE

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Mol	Chain	Res	Type
1	A	83	HIS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	100	LYS
1	A	102	VAL
1	A	107	CYS
1	A	114	LEU
1	A	115	LEU
1	A	116	ASP
1	A	132	LYS
1	A	140	THR
1	A	142	CYS
1	A	143	LYS
1	A	147	VAL
1	A	150	THR
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	180	LYS
1	A	185	TRP
1	A	208	LEU
1	A	225	ASN
1	A	234	MET
1	A	235	ILE
1	A	239	LEU
1	A	247	ARG
1	A	249	SER
1	A	250	ILE
1	A	252	PHE
1	A	253	ASN
1	A	254	GLU
1	A	256	GLN
1	A	257	ARG
1	A	263	THR
1	A	266	LEU
1	A	271	LYS
1	A	287	HIS
1	A	295	LEU
1	A	302	THR
1	A	304	MET
1	A	306	ASN

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	316	GLN
1	A	317	LYS
1	A	318	SER
1	A	320	ARG
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	351	THR
1	A	359	LEU
1	A	375	THR
1	A	380	VAL
1	A	381	THR
1	A	388	LEU
1	A	391	LEU
1	A	397	ASN
1	A	403	LYS
1	A	406	ILE
1	A	419	LYS
1	A	424	ILE
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	455	MET
1	A	466	SER
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	487	MET
1	A	496	GLU
1	A	500	GLU
1	A	501	LEU
1	A	512	VAL
1	A	513	SER
1	A	524	VAL
1	A	525	GLN
1	A	533	LYS
1	A	538	ASP
1	A	550	LEU

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Mol	Chain	Res	Type
1	A	567	LYS
1	A	576	GLN
1	A	596	THR
1	A	597	LEU
1	A	608	ILE
1	A	612	ILE
1	A	618	GLU
1	A	625	SER
1	A	629	LEU
1	A	636	GLU
1	A	666	ILE
1	A	677	ARG
1	A	682	THR
1	A	687	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU
1	A	710	LEU
1	A	711	ARG
1	A	727	ASP
1	A	731	ARG
1	A	732	LEU
1	A	734	GLU
1	A	735	VAL
1	A	737	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	768	GLN
1	A	773	LYS
1	A	774	ARG
1	A	795	GLU
1	A	805	LEU
1	A	821	ARG
1	A	830	LYS
1	A	831	THR
1	A	857	ARG
1	A	858	ASN
1	A	879	GLU
1	A	884	ASP
1	A	886	ILE
1	A	890	ASP

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Mol	Chain	Res	Type
1	A	896	ARG
1	A	897	TYR
1	A	898	ARG
1	A	902	LEU
1	A	904	THR
1	A	905	ASP
1	A	907	THR
1	A	908	LEU
1	A	909	ASP
1	A	913	LEU
1	A	915	SER
1	A	918	GLU
1	A	920	LEU
1	A	922	ASP
1	A	924	LYS
1	A	925	LEU
1	A	929	LEU
1	A	932	GLU
1	A	945	GLU
1	A	988	LEU
1	A	994	GLN
1	A	995	GLU
1	A	996	ASN
1	A	998	LEU
1	A	1001	ARG
1	A	1004	ASN
1	A	1017	LEU
1	A	1022	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1030	ARG
1	A	1035	TYR
1	A	1043	ASP
1	A	1046	LEU
1	A	1052	GLN
1	A	1077	THR
1	A	1112	LYS
1	A	1116	LEU
1	A	1120	LEU
1	A	1128	GLN
1	A	1132	LYS
1	A	1134	ILE

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Mol	Chain	Res	Type
1	A	1136	SER
1	A	1142	THR
1	A	1146	VAL
1	A	1162	VAL
1	A	1171	GLN
1	A	1172	LEU
1	A	1173	HIS
1	A	1174	PHE
1	A	1176	LEU
1	A	1187	GLN
1	A	1189	SER
1	A	1193	LEU
1	A	1199	ARG
1	A	1206	ASP
1	A	1208	THR
1	A	1229	SER
1	A	1242	VAL
1	A	1258	HIS
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1271	ILE
1	A	1272	THR
1	A	1274	ARG
1	A	1280	GLU
1	A	1282	VAL
1	A	1285	MET
1	A	1299	VAL
1	A	1300	LYS
1	A	1314	SER
1	A	1315	GLU
1	A	1318	THR
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1384	VAL
1	A	1385	THR

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Mol	Chain	Res	Type
1	A	1390	ASN
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1420	ASP
1	A	1436	ILE
1	A	1442	ASP
1	A	1445	ILE
2	B	21	GLU
2	B	22	SER
2	B	28	GLU
2	B	34	ILE
2	B	40	GLU
2	B	63	ILE
2	B	66	ASP
2	B	67	SER
2	B	68	THR
2	B	98	THR
2	B	104	GLU
2	B	109	THR
2	B	119	LEU
2	B	120	ARG
2	B	121	ASN
2	B	134	LYS
2	B	166	PHE
2	B	174	LEU
2	B	175	ARG
2	B	177	LYS
2	B	185	THR
2	B	188	ASP
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	224	GLN
2	B	225	VAL
2	B	232	SER
2	B	234	ILE
2	B	246	LYS
2	B	249	ARG
2	B	251	ILE
2	B	261	ARG
2	B	268	THR

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Mol	Chain	Res	Type
2	B	275	TYR
2	B	283	VAL
2	B	304	ASP
2	B	305	VAL
2	B	325	GLN
2	B	327	ARG
2	B	331	LEU
2	B	365	THR
2	B	367	LEU
2	B	387	LEU
2	B	393	LYS
2	B	404	LYS
2	B	415	GLN
2	B	416	LEU
2	B	423	LYS
2	B	424	LEU
2	B	425	THR
2	B	426	LYS
2	B	429	PHE
2	B	436	VAL
2	B	469	GLN
2	B	471	LYS
2	B	473	MET
2	B	476	ARG
2	B	479	VAL
2	B	485	ARG
2	B	498	THR
2	B	513	GLN
2	B	527	THR
2	B	537	LYS
2	B	538	ASN
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	556	THR
2	B	563	MET
2	B	570	VAL
2	B	591	ARG
2	B	601	ARG
2	B	604	ARG
2	B	622	LYS
2	B	628	THR

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Mol	Chain	Res	Type
2	B	629	ASP
2	B	637	LEU
2	B	638	PHE
2	B	644	GLU
2	B	646	LEU
2	B	648	HIS
2	B	658	ILE
2	B	701	ILE
2	B	714	GLU
2	B	723	VAL
2	B	728	ARG
2	B	732	SER
2	B	740	HIS
2	B	754	SER
2	B	762	ASN
2	B	778	MET
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	799	PRO
2	B	807	ARG
2	B	812	LEU
2	B	815	ARG
2	B	822	ASN
2	B	837	ASP
2	B	861	ASP
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	889	THR
2	B	899	ILE
2	B	914	LYS
2	B	933	SER
2	B	941	LEU
2	B	944	THR
2	B	953	LEU

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Mol	Chain	Res	Type
2	B	956	THR
2	B	968	VAL
2	B	976	ILE
2	B	983	ARG
2	B	984	HIS
2	B	986	GLN
2	B	989	THR
2	B	993	THR
2	B	995	ARG
2	B	996	ARG
2	B	999	MET
2	B	1020	ARG
2	B	1052	VAL
2	B	1065	GLN
2	B	1082	MET
2	B	1096	ARG
2	B	1108	ARG
2	B	1113	VAL
2	B	1116	ARG
2	B	1124	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1152	MET
2	B	1171	VAL
2	B	1172	ILE
2	B	1175	LEU
2	B	1183	LYS
2	B	1189	ILE
2	B	1190	ASP
2	B	1191	ILE
2	B	1194	ILE
2	B	1195	HIS
2	B	1196	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1218	THR
2	B	1219	ASP
2	B	1222	ARG
3	C	11	ARG
3	C	16	ASP
3	C	22	LEU
3	C	25	VAL

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Mol	Chain	Res	Type
3	C	27	LEU
3	C	40	GLU
3	C	50	GLU
3	C	53	THR
3	C	55	THR
3	C	62	PHE
3	C	66	ARG
3	C	69	LEU
3	C	70	ILE
3	C	77	ILE
3	C	81	GLU
3	C	89	GLU
3	C	91	HIS
3	C	93	ASP
3	C	99	LEU
3	C	111	THR
3	C	119	VAL
3	C	137	LYS
3	C	138	GLU
3	C	140	ASN
3	C	143	LEU
3	C	145	CYS
3	C	153	LEU
3	C	163	ILE
3	C	183	TRP
3	C	189	THR
3	C	217	ASP
3	C	219	PHE
3	C	224	GLN
3	C	229	TYR
3	C	231	ASN
3	C	237	SER
3	C	240	VAL
3	C	258	ILE
3	C	260	LEU
3	C	264	GLN
4	E	6	GLU
4	E	37	LEU
4	E	41	ASP
4	E	43	LYS
4	E	60	PHE
4	E	61	GLN

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Mol	Chain	Res	Type
4	E	74	ASP
4	E	78	LEU
4	E	92	THR
4	E	94	LYS
4	E	101	GLN
4	E	105	PHE
4	E	107	THR
4	E	110	PHE
4	E	117	THR
4	E	122	LYS
4	E	123	LEU
4	E	127	ILE
4	E	131	THR
4	E	132	ILE
4	E	134	THR
4	E	146	HIS
4	E	148	GLU
4	E	153	HIS
4	E	156	LEU
4	E	169	ARG
4	E	175	LEU
4	E	180	ARG
4	E	188	LEU
4	E	190	LEU
4	E	196	VAL
4	E	204	THR
4	E	212	ARG
4	E	215	MET
5	F	79	ARG
5	F	82	THR
5	F	87	LYS
5	F	90	ARG
5	F	92	ARG
5	F	99	LEU
5	F	104	ASN
5	F	110	ASP
5	F	111	LEU
5	F	112	GLU
5	F	125	LEU
5	F	133	VAL
5	F	155	LEU
6	H	8	ASP

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Mol	Chain	Res	Type
6	H	11	GLN
6	H	15	VAL
6	H	25	ARG
6	H	27	GLU
6	H	31	THR
6	H	36	CYS
6	H	39	THR
6	H	53	ASP
6	H	63	LEU
6	H	89	LEU
6	H	103	LYS
6	H	110	ASP
6	H	112	ILE
6	H	129	TYR
6	H	132	LEU
6	H	136	LYS
6	H	138	GLU
6	H	143	LEU
7	I	7	CYS
7	I	13	MET
7	I	22	ASN
7	I	24	ARG
7	I	28	GLU
7	I	33	SER
7	I	42	LEU
7	I	48	LEU
7	I	55	THR
7	I	75	CYS
7	I	77	LYS
7	I	83	ASN
7	I	84	VAL
7	I	91	ARG
7	I	107	SER
7	I	111	THR
7	I	118	ARG
7	I	120	GLN
8	J	1	MET
8	J	2	ILE
8	J	7	CYS
8	J	9	SER
8	J	10	CYS
8	J	13	VAL

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Mol	Chain	Res	Type
8	J	14	VAL
8	J	28	ASP
8	J	31	ASP
8	J	36	LEU
8	J	46	CYS
8	J	48	ARG
8	J	54	VAL
8	J	55	ASP
8	J	60	PHE
8	J	62	ARG
9	K	5	ASP
9	K	17	SER
9	K	22	ASP
9	K	31	VAL
9	K	32	VAL
9	K	34	THR
9	K	47	ARG
9	K	50	LEU
9	K	71	PHE
9	K	81	TYR
9	K	101	LEU
9	K	111	LEU
9	K	113	THR
10	L	27	LEU
10	L	28	LYS
10	L	40	LEU
10	L	47	ARG
10	L	50	ASP
10	L	61	THR
10	L	63	ARG
10	L	65	VAL
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	80	HIS
1	A	92	HIS
1	A	169	ASN
1	A	306	ASN
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	435	HIS
1	A	451	HIS
1	A	493	GLN
1	A	517	ASN
1	A	587	HIS
1	A	706	HIS
1	A	736	ASN
1	A	757	ASN
1	A	851	HIS
1	A	858	ASN
1	A	926	GLN
1	A	965	GLN
1	A	1171	GLN
1	A	1173	HIS
1	A	1364	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	121	ASN
2	B	325	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	590	HIS
2	B	686	ASN
2	B	734	HIS
2	B	740	HIS
2	B	744	HIS
2	B	822	ASN
2	B	878	GLN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	188	HIS
3	C	242	GLN
4	E	114	ASN

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Mol	Chain	Res	Type
6	H	11	GLN
7	I	11	ASN
7	I	12	ASN
9	K	40	HIS
9	K	65	HIS
10	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	8/9 (88%)	4 (50%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	2	U
11	R	3	C
11	R	4	G
11	R	9	U

There are no RNA pucker outliers to report.

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

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	$\# Z > 2$
12	02I	T	20	12	15,24,25	3.45	6 (40%)	15,37,40	4.17	6 (40%)

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
12	02I	T	20	12	-	0/0/28/29	0/3/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	20	02I	O4'-C1'	-7.69	1.25	1.42
12	T	20	02I	O4'-C4'	-7.47	1.33	1.44
12	T	20	02I	C2-N3	4.10	1.38	1.32
12	T	20	02I	C4'-C5'	-4.08	1.45	1.52
12	T	20	02I	O3'-C3'	-3.75	1.35	1.43
12	T	20	02I	C2-N1	2.39	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	20	02I	C5-C6-N6	11.29	137.50	120.31
12	T	20	02I	N6-C6-N1	-7.44	102.44	118.33
12	T	20	02I	N3-C2-N1	-6.33	120.08	128.67
12	T	20	02I	O4'-C1'-C2'	-4.47	97.89	106.24
12	T	20	02I	C2'-C1'-N9	-2.53	105.65	110.52
12	T	20	02I	C4'-O4'-C1'	2.31	115.11	108.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	20	02I	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	1395/1733 (80%)	-0.25	13 (0%) 81 66	84, 144, 236, 306	0
2	B	1104/1224 (90%)	-0.30	7 (0%) 85 72	76, 131, 209, 281	0
3	C	266/318 (83%)	-0.41	0 100 100	89, 133, 192, 229	0
4	E	214/215 (99%)	-0.36	1 (0%) 87 75	99, 166, 231, 267	0
5	F	84/155 (54%)	-0.51	0 100 100	102, 142, 185, 209	0
6	H	133/146 (91%)	-0.23	2 (1%) 71 55	119, 168, 238, 262	0
7	I	119/122 (97%)	-0.41	0 100 100	96, 151, 190, 216	0
8	J	65/70 (92%)	-0.43	0 100 100	98, 128, 168, 192	0
9	K	114/120 (95%)	-0.51	0 100 100	94, 137, 177, 200	0
10	L	46/70 (65%)	-0.01	1 (2%) 62 46	119, 180, 250, 264	0
11	R	9/9 (100%)	-0.47	0 100 100	102, 124, 217, 261	0
12	T	10/29 (34%)	-0.23	0 100 100	108, 136, 243, 256	0
All	All	3559/4211 (84%)	-0.31	24 (0%) 84 70	76, 141, 224, 306	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	997	LEU	6.4
1	A	1108	ALA	4.1
1	A	1002	GLY	3.1
1	A	144	THR	3.0
2	B	335	GLY	2.9
1	A	998	LEU	2.8
1	A	1000	LEU	2.7
2	B	903	VAL	2.7
6	H	63	LEU	2.7
2	B	883	LEU	2.6
2	B	715	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	985	ASP	2.5
1	A	1301	GLU	2.4
1	A	904	THR	2.3
4	E	148	GLU	2.3
6	H	86	ASP	2.2
2	B	1216	LEU	2.2
1	A	694	THR	2.1
1	A	17	VAL	2.1
10	L	28	LYS	2.1
1	A	136	ALA	2.1
2	B	1214	PRO	2.1
2	B	1107	ALA	2.0
1	A	999	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
12	02I	T	20	21/22	0.55	0.13	204,227,305,321	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
13	ZN	A	1801	1/1	0.89	0.07	244,244,244,244	0
13	ZN	J	101	1/1	0.98	0.04	124,124,124,124	0
13	ZN	B	1301	1/1	0.99	0.03	202,202,202,202	0
13	ZN	I	201	1/1	0.99	0.03	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	ZN	A	1802	1/1	0.99	0.02	170,170,170,170	0
13	ZN	L	101	1/1	0.99	0.03	175,175,175,175	0
13	ZN	C	401	1/1	1.00	0.02	135,135,135,135	0
13	ZN	I	202	1/1	1.00	0.02	128,128,128,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.