



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:43 PM UTC

PDB ID : 4X6A / pdb_00004x6a
Title : Crystal structure of yeast RNA polymerase II encountering oxidative Cyclop-
urine 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

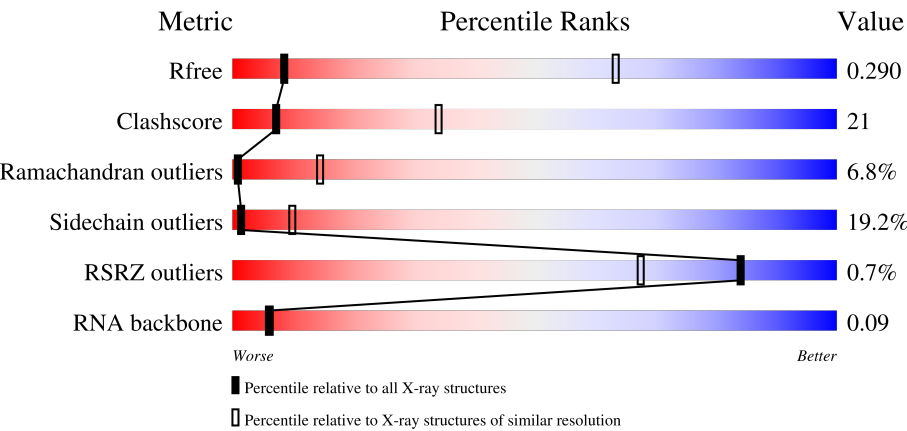
1 Overall quality at a glance i

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}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)
RNA backbone	3983	1016 (4.80-3.10)

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	41% 29% 9% • 20%
2	B	1224	45% 36% 7% • 10%
3	C	318	44% 30% 8% • 16%
4	E	215	53% 38% 9%

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Mol	Chain	Length	Quality of chain
5	F	155	32%15%8%46%
6	H	146	% 43%32%12%9%
7	I	122	56%34%7%..
8	J	70	43%39%10%7%
9	K	120	55%32%8%5%
10	L	70	% 30%21%14%34%
11	R	9	22%56%22%
12	T	29	17%17%.62%

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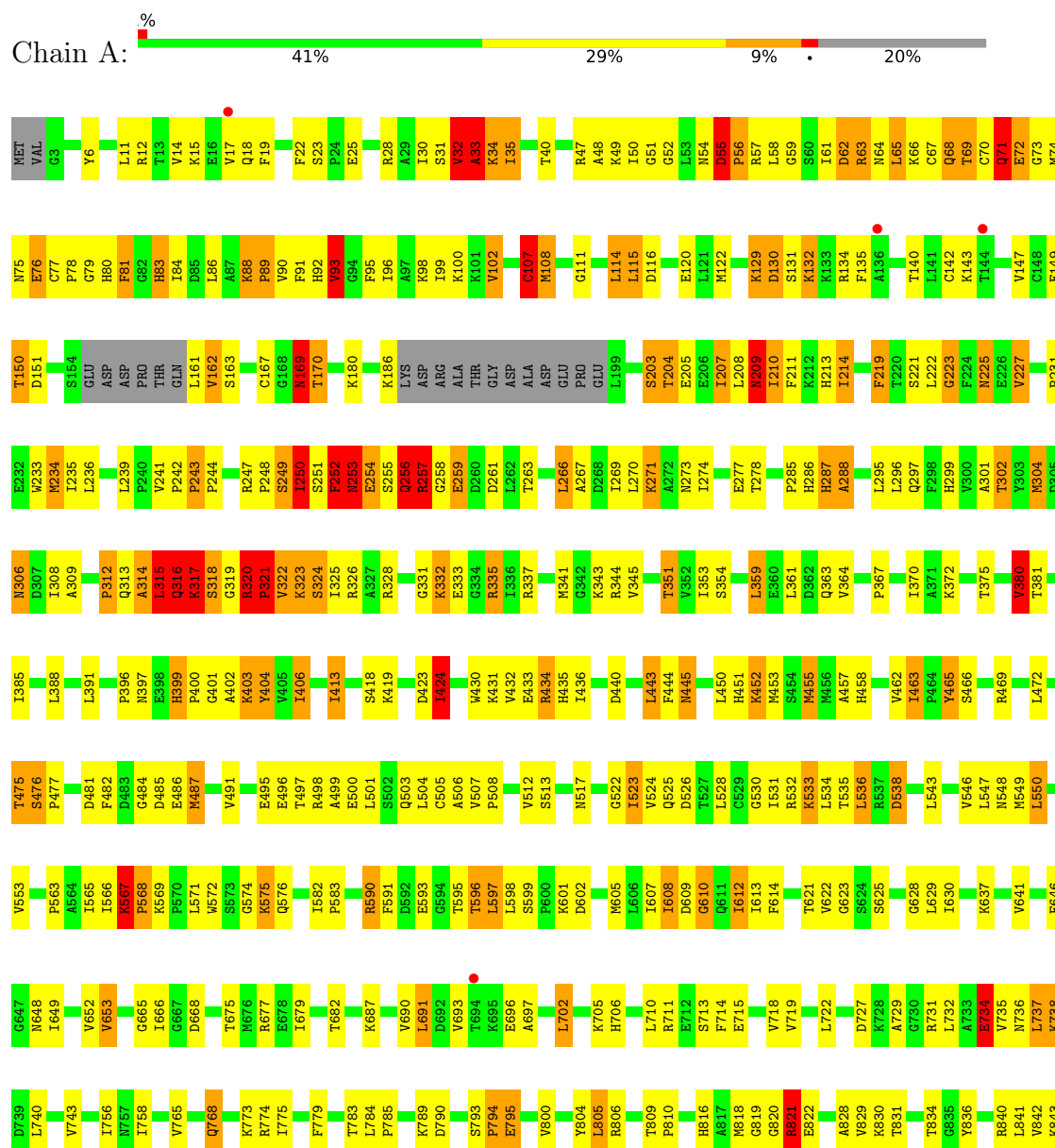
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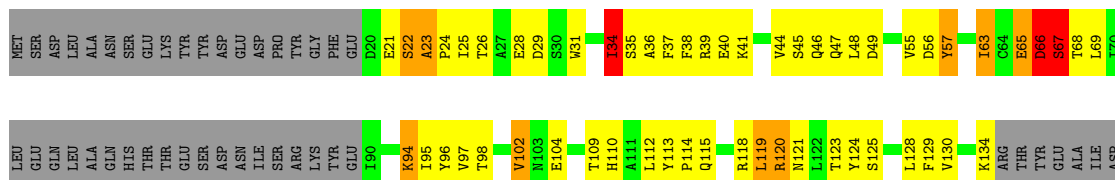
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

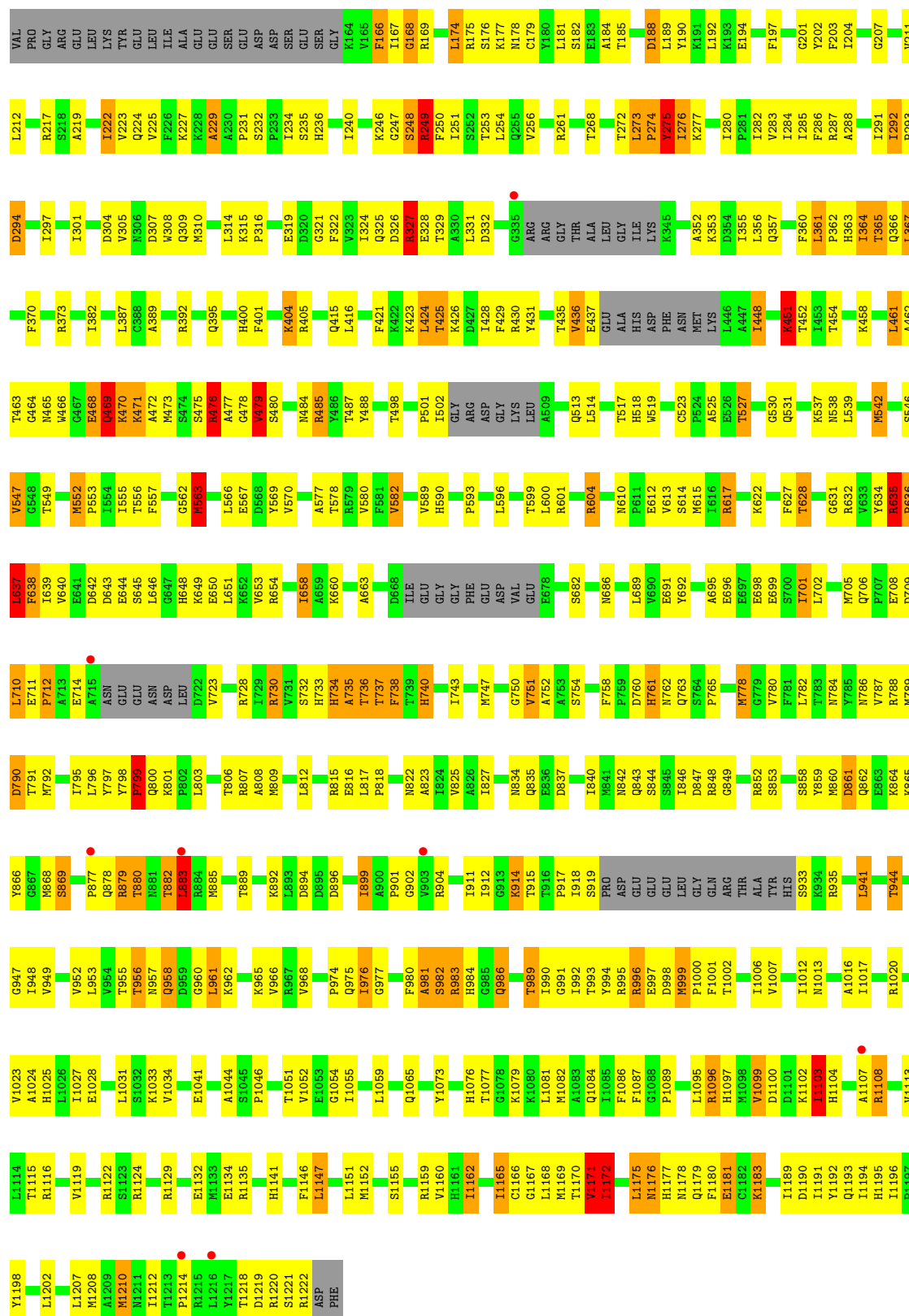
3 Residue-property plots

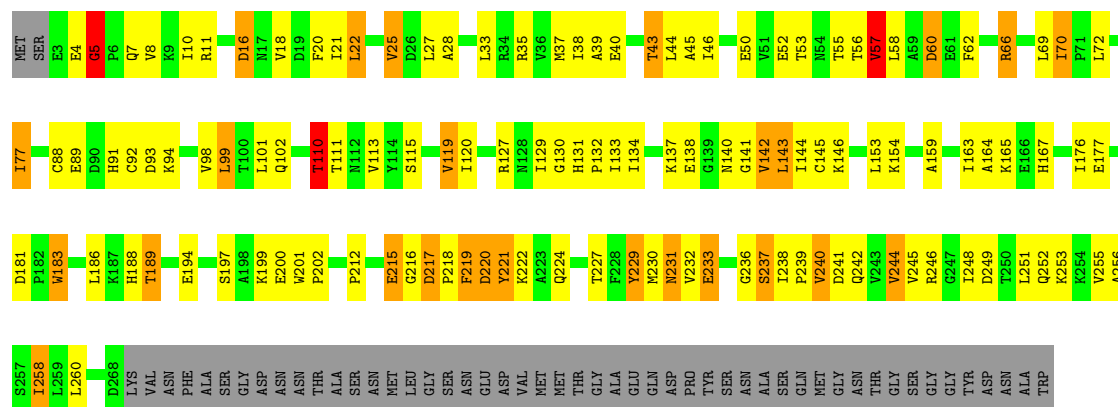
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

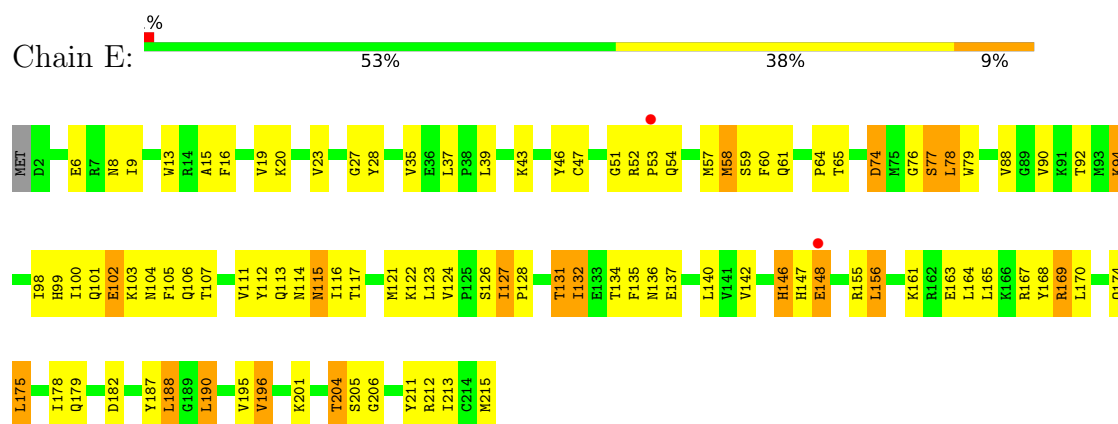




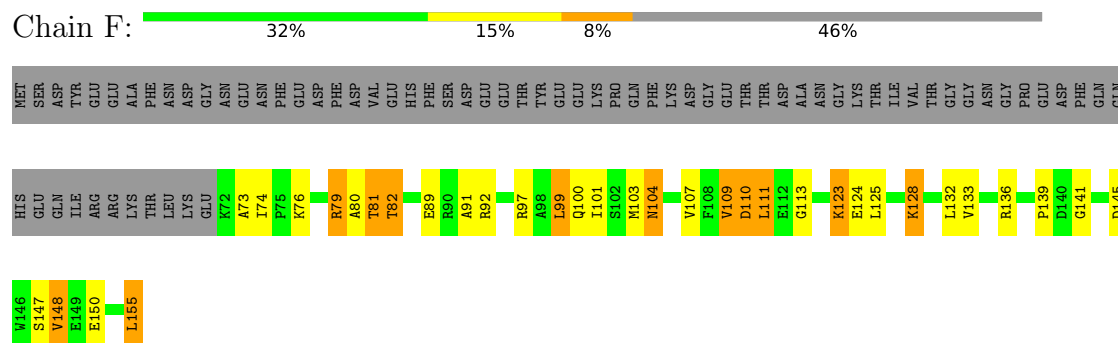




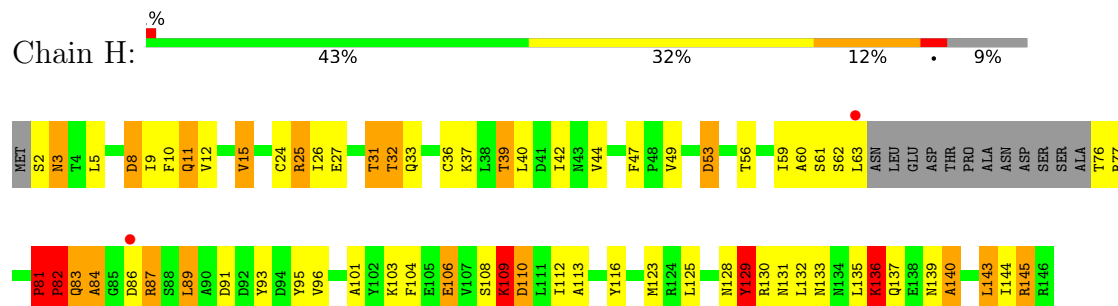
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



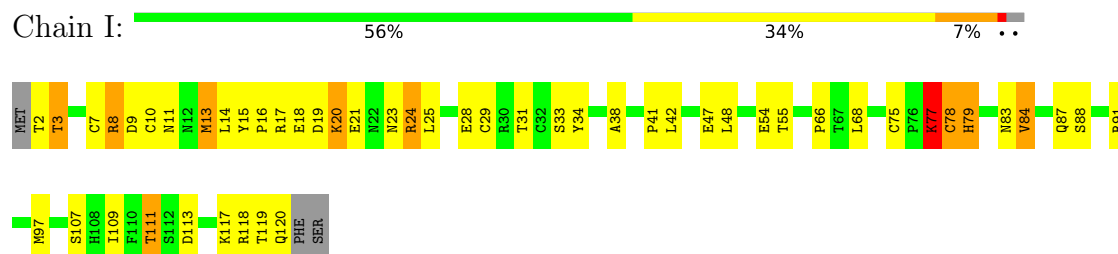
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



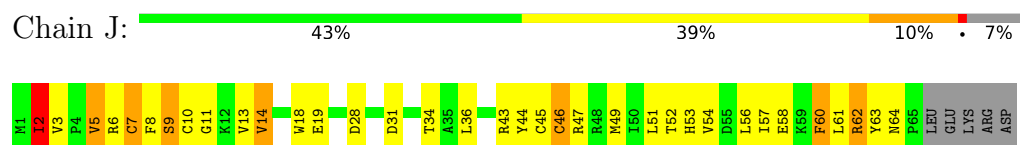
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



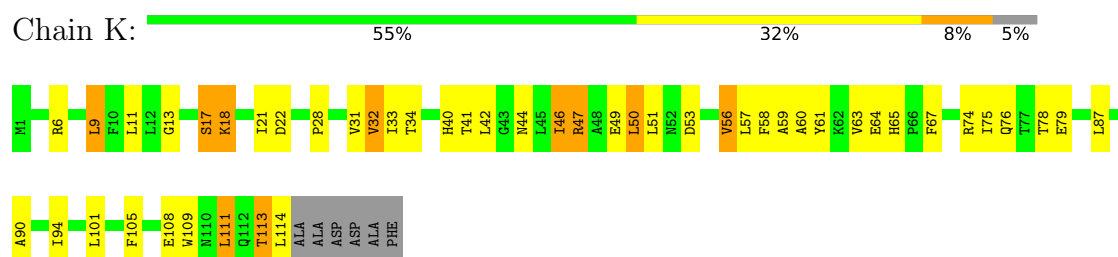
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



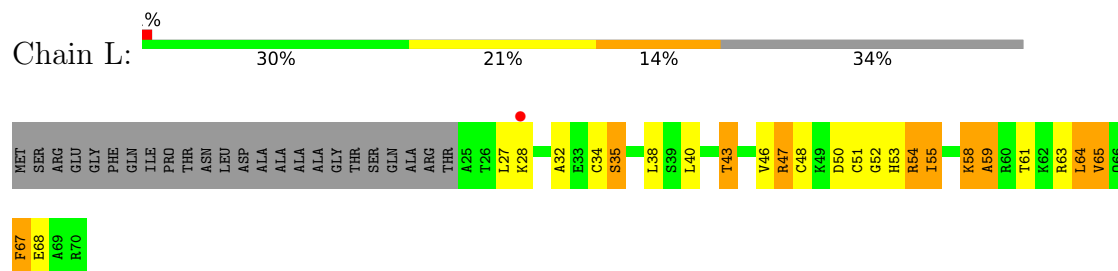
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



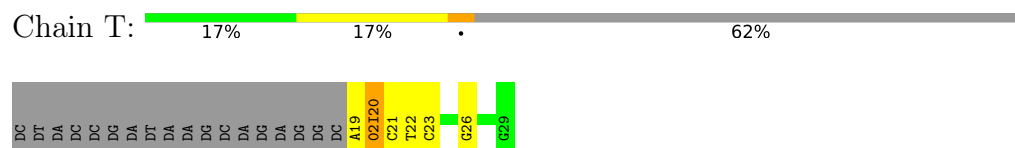
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: RNA_9 mer



- Molecule 12: Template DNA _29 mer



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 (4.94%)	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 , 100.1	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: ZN, 02I

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	0.62	0/11163	1.01	30/15091 (0.2%)
2	B	0.60	0/8943	0.95	15/12059 (0.1%)
3	C	0.56	0/2133	0.94	3/2891 (0.1%)
4	E	0.57	0/1788	0.96	1/2406 (0.0%)
5	F	0.59	0/691	0.92	0/933
6	H	0.62	0/1086	1.08	10/1470 (0.7%)
7	I	0.62	0/989	0.94	2/1331 (0.2%)
8	J	0.61	0/541	1.04	1/727 (0.1%)
9	K	0.56	0/937	0.88	0/1265
10	L	0.66	0/365	1.08	0/485
11	R	0.43	0/218	0.83	0/338
12	T	0.31	0/225	0.58	0/342
All	All	0.60	0/29079	0.98	62/39338 (0.2%)

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 (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	77	LYS	CB-CA-C	-10.12	95.08	110.26
1	A	259	GLU	N-CA-C	8.30	122.03	109.41
1	A	170	THR	N-CA-C	7.81	121.91	110.59
2	B	479	VAL	N-CA-C	-7.81	98.39	109.63
1	A	821	ARG	N-CA-C	-7.21	102.25	112.13
2	B	638	PHE	N-CA-CB	7.21	120.57	110.26
1	A	243	PRO	CA-C-N	6.81	127.39	120.38
1	A	243	PRO	C-N-CA	6.81	127.39	120.38
1	A	1207	LEU	N-CA-C	6.71	119.52	108.99
2	B	69	LEU	N-CA-C	6.69	119.58	109.41
6	H	62	SER	N-CA-C	6.59	116.75	108.45
1	A	857	ARG	N-CA-C	6.57	119.30	108.99
1	A	244	PRO	N-CA-C	6.54	118.68	110.70
1	A	55	ASP	N-CA-C	6.24	123.59	109.81
1	A	1256	GLU	N-CA-C	6.18	120.89	112.68
2	B	273	LEU	CA-C-N	6.13	127.50	119.84
2	B	273	LEU	C-N-CA	6.13	127.50	119.84
1	A	163	SER	N-CA-C	6.05	118.61	109.23
2	B	1221	SER	N-CA-C	6.05	119.38	109.76
2	B	637	LEU	CA-CB-CG	6.00	137.31	116.30
1	A	345	VAL	N-CA-C	6.00	116.99	108.42
6	H	83	GLN	N-CA-C	-5.91	106.02	113.23
2	B	1115	THR	N-CA-C	5.90	117.71	111.28
1	A	533	LYS	N-CA-CB	5.88	118.53	110.01
1	A	54	ASN	N-CA-C	5.85	119.42	111.17
1	A	1311	VAL	N-CA-C	5.78	116.33	107.77
3	C	57	VAL	CB-CA-C	-5.71	104.58	111.88
2	B	430	ARG	N-CA-C	5.69	120.35	113.41
6	H	87	ARG	N-CA-C	5.63	116.83	108.60
6	H	109	LYS	CA-C-N	5.56	131.72	121.70
6	H	109	LYS	C-N-CA	5.56	131.72	121.70
1	A	1226	VAL	N-CA-C	5.56	116.74	108.46
6	H	81	PRO	CA-C-N	5.54	126.77	119.84
6	H	81	PRO	C-N-CA	5.54	126.77	119.84
1	A	324	SER	N-CA-C	5.54	122.60	110.80
2	B	736	THR	CB-CA-C	-5.52	104.19	111.42
4	E	65	THR	N-CA-C	-5.50	102.75	110.50
6	H	129	TYR	N-CA-C	-5.48	107.24	114.04
2	B	883	LEU	N-CA-C	5.46	118.97	111.54
1	A	1228	TRP	N-CA-C	5.38	117.02	108.79
1	A	88	LYS	CA-C-N	5.38	126.56	119.84
1	A	88	LYS	C-N-CA	5.38	126.56	119.84
6	H	137	GLN	N-CA-C	5.35	117.82	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1006	ILE	CB-CA-C	-5.32	104.88	112.22
7	I	118	ARG	N-CA-C	5.31	117.47	109.23
8	J	5	VAL	N-CA-C	-5.31	102.67	109.30
1	A	993	LEU	N-CA-C	-5.30	105.40	111.07
1	A	954	TRP	N-CA-C	5.28	116.79	108.23
2	B	34	ILE	N-CA-C	-5.23	105.61	110.53
1	A	236	LEU	N-CA-C	5.21	116.80	108.41
2	B	484	ASN	N-CA-C	-5.20	101.86	109.81
1	A	380	VAL	CB-CA-C	-5.19	102.77	111.29
1	A	344	ARG	N-CA-C	-5.14	102.86	110.48
1	A	253	ASN	N-CA-C	5.14	121.74	110.80
3	C	5	GLY	CA-C-N	5.13	126.25	119.84
3	C	5	GLY	C-N-CA	5.13	126.25	119.84
6	H	145	ARG	N-CA-C	5.10	117.72	109.40
1	A	93	VAL	N-CA-C	5.10	119.95	109.34
1	A	318	SER	N-CA-C	-5.10	99.94	110.80
2	B	1099	VAL	N-CA-C	-5.05	106.15	110.74
1	A	256	GLN	N-CA-C	5.03	115.75	107.20
2	B	638	PHE	CB-CA-C	-5.02	99.26	109.65

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

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Mol	Chain	Res	Type	Group
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 [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	10969	0	11069	473	0
2	B	8773	0	8811	413	0
3	C	2095	0	2051	108	0
4	E	1752	0	1776	65	0
5	F	679	0	701	23	0
6	H	1068	0	1040	52	0
7	I	971	0	927	48	0
8	J	532	0	542	35	0
9	K	919	0	929	45	0
10	L	363	0	387	21	0
11	R	195	0	98	7	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	1178	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 21.

All (1178) 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
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
2:B:274:PRO:O	2:B:276:ILE:HG13	1.76	0.86
7:I:78:CYS:SG	7:I:79:HIS:N	2.48	0.85
7:I:29:CYS:SG	7:I:31:THR:HB	2.17	0.84
2:B:640:VAL:HG13	2:B:650:GLU:C	2.02	0.84
1:A:921:GLY:O	1:A:922:ASP:O	1.96	0.83
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.04	0.82
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
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
6:H:40:LEU:HD13	6:H:123:MET:HE3	1.66	0.77
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:E:168:TYR:C	4:E:169:ARG:HG2	2.14	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
2:B:1162:ILE:HD13	2:B:1168:LEU:C	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:K:113:THR:C	9:K:114:LEU:HD12	2.17	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
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
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
2:B:34:ILE:HD12	2:B:542:MET:HE1	1.76	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
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
8:J:52:THR:O	8:J:53:HIS:C	2.37	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
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.78	0.66
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1436:ILE:O	1:A:1437:GLY:C	2.38	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
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
2:B:562:GLY:O	2:B:563:MET:C	2.40	0.63
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:563:MET:HE1	2:B:580:VAL:HB	1.80	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
7:I:7:CYS:C	7:I:8:ARG:O	2.41	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
1:A:805:LEU:C	1:A:805:LEU:HD12	2.25	0.62
2:B:274:PRO:O	2:B:276:ILE:CG1	2.47	0.62
2:B:778:MET:HE3	2:B:853:SER:HB3	1.82	0.62
9:K:46:ILE:HG23	9:K:50:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:66:ARG:NH2	8:J:5:VAL:HG23	2.15	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
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
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
3:C:98:VAL:C	3:C:99:LEU:HD23	2.26	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
1:A:530:GLY:C	1:A:532:ARG:N	2.58	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
8:J:2:ILE:C	8:J:53:HIS:NE2	2.59	0.60
2:B:56:ASP:C	2:B:57:TYR:HD1	2.09	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
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.59	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:253:ASN:CG	1:A:254:GLU:N	2.61	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
1:A:320:ARG:HD2	1:A:320:ARG:N	2.17	0.59
1:A:530:GLY:C	1:A:532:ARG:H	2.08	0.59
1:A:1242:VAL:HG11	1:A:1259:MET:HE3	1.85	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:860:MET:HE2	2:B:965:LYS:HE2	1.85	0.59
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.67	0.59
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:542:MET:HE1	2:B:743:ILE:HG21	1.84	0.58
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
2:B:469:GLN:O	2:B:470:LYS:C	2.46	0.58
2:B:519:TRP:CZ2	2:B:705:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1004:ASN:C	1:A:1004:ASN:OD1	2.47	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
1:A:605:MET:HE3	1:A:605:MET:HA	1.86	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:971:PHE:O	1:A:972:HIS:C	2.47	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: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:81:PHE:CE1	2:B:1208:MET:HE2	2.39	0.57
1:A:1434:ALA:HB1	1:A:1436:ILE:HD12	1.86	0.57
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
6:H:129:TYR:C	6:H:131:ASN:H	2.13	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
2:B:542:MET:HE3	2:B:747:MET:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:HE3	2:B:853:SER:CB	2.36	0.56
1:A:401:GLY:C	1:A:435:HIS:CD2	2.84	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
6:H:106:GLU:C	6:H:108:SER:H	2.12	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
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:640:VAL:CG2	2:B:651:LEU:HD22	2.37	0.55
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:445:ASN:HB3	1:A:455:MET:HE2	1.89	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:99:LEU:HD11	5:F:103:MET:HE3	1.88	0.55
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1364:ASN:C	1:A:1364:ASN:HD22	2.14	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
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.90	0.54
3:C:99:LEU:HD23	3:C:99:LEU:N	2.23	0.54
8:J:7:CYS:HA	8:J:49:MET:HE3	1.89	0.54
2:B:274:PRO:O	2:B:275:TYR:C	2.51	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:249:SER:C	1:A:250:ILE:HG23	2.33	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
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.22	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
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:1336:MET:HE3	1:A:1381:LEU:HG	1.90	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: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
2:B:519:TRP:CD1	2:B:519:TRP:C	2.87	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
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
2:B:249:ARG:O	2:B:250:PHE:C	2.53	0.52
8:J:57:ILE:HA	8:J:60:PHE:HD1	1.75	0.52
1:A:92:HIS:CD2	1:A:304:MET:HE3	2.45	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
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
2:B:977:GLY:C	2:B:1099:VAL:CG2	2.83	0.52
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HG21	1:A:908:LEU:CD2	2.40	0.52
1:A:1015:VAL:O	1:A:1016:THR:C	2.53	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:451:LYS:O	2:B:452:THR:C	2.53	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
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:115:LEU:HB2	1:A:122:MET:HE3	1.92	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
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:219:PHE:CD1	3:C:219:PHE:C	2.89	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
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
1:A:805:LEU:C	1:A:805:LEU:CD1	2.83	0.51
2:B:34:ILE:HG23	2:B:542:MET:HE2	1.92	0.51
2:B:806:THR:HG22	2:B:808:ALA:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:119:THR:HG22	7:I:119:THR:O	2.11	0.51
1:A:1434:ALA:CB	1:A:1436:ILE:HD12	2.40	0.51
2:B:531:GLN:HG2	12:T:20:02I:C2	2.40	0.51
4:E:78:LEU:HG	4:E:79:TRP:N	2.25	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
1:A:484:GLY:O	1:A:485:ASP:C	2.53	0.51
1:A:910:PRO:C	1:A:912:LEU:H	2.19	0.51
2:B:227:LYS:HB2	2:B:395:GLN:CD	2.36	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
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
6:H:106:GLU:C	6:H:108:SER:N	2.69	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
2:B:44:VAL:O	2:B:45:SER:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
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:38:PHE:O	2:B:39:ARG:C	2.54	0.50
2:B:636:PRO:HD2	2:B:637:LEU:HB3	1.94	0.50
3:C:133:ILE:HD13	3:C:236:GLY:C	2.37	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:919:ILE:O	1:A:920:LEU:C	2.53	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
2:B:639:ILE:HA	2:B:740:HIS:HB3	1.94	0.50
1:A:62:ASP:O	1:A:63:ARG:C	2.54	0.49
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
4:E:136:ASN:OD1	4:E:136:ASN:C	2.55	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
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:321:PRO:C	1:A:322:VAL:HG13	2.37	0.49
1:A:705:LYS:O	1:A:706:HIS:C	2.55	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:65:GLU:C	2:B:67:SER:N	2.69	0.49
2:B:236:HIS:HD2	2:B:389:ALA:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:187:TYR:HD1	4:E:188:LEU:HD23	1.76	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
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:525:GLN:O	1:A:526:ASP:C	2.55	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
8:J:2:ILE:C	8:J:53:HIS:CE1	2.91	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:432:VAL:O	1:A:433:GLU:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:596:THR:C	1:A:598:LEU:H	2.21	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
7:I:119:THR:C	7:I:120:GLN:CG	2.86	0.48
1:A:840:ARG:O	1:A:841:LEU:C	2.57	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
4:E:102:GLU:C	4:E:104:ASN:H	2.22	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:70:CYS:C	1:A:71:GLN:HG3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:O	1:A:328:ARG:HB2	2.14	0.48
1:A:549:MET:O	1:A:550:LEU:C	2.57	0.48
1:A:845:LEU:O	1:A:847:ASP:N	2.47	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
3:C:141:GLY:O	3:C:142:VAL:O	2.32	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:942:PHE:CD1	1:A:942:PHE:C	2.92	0.47
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
1:A:1336:MET:HE2	1:A:1341:ILE:CD1	2.45	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
7:I:2:THR:O	7:I:3:THR:C	2.56	0.47
1:A:78:PRO:O	1:A:79:GLY:C	2.58	0.47
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.95	0.47
2:B:557:PHE:C	2:B:557:PHE:CD1	2.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:574:GLY:O	1:A:575:LYS:C	2.57	0.47
1:A:902:LEU:HD21	1:A:923:LEU:HD23	1.97	0.47
1:A:1242:VAL:HG11	1:A:1259:MET:CE	2.45	0.47
2:B:705:MET:HE3	2:B:705:MET:HA	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:253:ASN:CG	1:A:254:GLU:H	2.22	0.47
1:A:320:ARG:HB2	1:A:321:PRO:HB3	1.97	0.47
1:A:535:THR:O	1:A:536:LEU:C	2.57	0.47
2:B:1129:ARG:HD3	12:T:22:DT:H5'	1.97	0.47
3:C:119:VAL:HG12	3:C:119:VAL:O	2.14	0.47
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.88	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
3:C:92:CYS:C	3:C:94:LYS:H	2.23	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:150:THR:O	1:A:151:ASP:CG	2.58	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
8:J:7:CYS:CA	8:J:49:MET:HE3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:98:ILE:O	4:E:99:HIS:C	2.57	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:736:ASN:O	1:A:737:LEU:C	2.58	0.46
2:B:46:GLN:HG3	2:B:47:GLN:H	1.81	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
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:36:ALA:C	2:B:37:PHE:O	2.57	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
2:B:35:SER:O	2:B:39:ARG:CG	2.64	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:423:ASP:C	1:A:424:ILE:HG13	2.40	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:614:PHE:CD1	1:A:614:PHE:C	2.93	0.46
1:A:622:VAL:HA	1:A:630:ILE:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:737:THR:O	2:B:738:PHE:C	2.59	0.45
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.46	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:1064:VAL:O	1:A:1065:GLY:C	2.58	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
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:316:GLN:O	1:A:317:LYS:HB2	2.16	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
2:B:1024:ALA:O	2:B:1025:HIS:C	2.60	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
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.99	0.45
2:B:314:LEU:O	2:B:315:LYS:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:129:TYR:C	6:H:131:ASN:N	2.74	0.45
1:A:522:GLY:C	1:A:523:ILE:HD12	2.42	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:445:ASN:CB	1:A:455:MET:HE2	2.47	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
1:A:1203:ASN:O	1:A:1204:ASP:C	2.60	0.45
2:B:477:ALA:O	2:B:478:GLY:C	2.59	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
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
1:A:789:LYS:O	1:A:790:ASP:C	2.60	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
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
2:B:34:ILE:HD12	2:B:743:ILE:HG21	1.98	0.44
2:B:797:TYR:C	2:B:799:PRO:HD2	2.42	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
1:A:1256:GLU:O	1:A:1257:ASP:C	2.60	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
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:401:GLY:C	1:A:435:HIS:HD2	2.24	0.44
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:113:TYR:O	2:B:114:PRO:C	2.61	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
1:A:455:MET:HE3	2:B:1134:GLU:CG	2.47	0.44
1:A:485:ASP:CG	11:R:8:G:HO2'	2.25	0.44
1:A:714:PHE:CD2	7:I:97:MET:HE1	2.53	0.44
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.98	0.44
2:B:896:ASP:OD2	10:L:58:LYS:HE3	2.17	0.44
2:B:1084:GLN:CD	2:B:1084:GLN:N	2.76	0.44
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.00	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
7:I:87:GLN:O	7:I:88:SER:C	2.60	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:1027:ILE:O	2:B:1028:GLU:C	2.61	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
1:A:1171:GLN:C	1:A:1172:LEU:HD23	2.43	0.44
2:B:247:GLY:O	2:B:248:SER:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:67:CYS:O	1:A:68:GLN:C	2.61	0.43
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
2:B:1095:LEU:C	2:B:1096:ARG:O	2.59	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
1:A:1030:ARG:O	1:A:1031:VAL:C	2.61	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:852:TYR:CE1	1:A:1060:PRO:HB2	2.54	0.43
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
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:774:ARG:O	1:A:775:ILE:C	2.60	0.43
1:A:962:ARG:O	1:A:963:ILE:C	2.61	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:320:ARG:CB	1:A:321:PRO:CA	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:PHE:CG	7:I:97:MET:HE1	2.53	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
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.84	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:886:ILE:HD11	1:A:943:LEU:C	2.43	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
6:H:5:LEU:HD22	6:H:133:ASN:C	2.44	0.43
6:H:40:LEU:CD1	6:H:123:MET:HE3	2.44	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
1:A:354:SER:HA	1:A:482:PHE:CD1	2.54	0.43
2:B:178:ASN:O	2:B:179:CYS:C	2.62	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
3:C:231:ASN:HD22	3:C:231:ASN:C	2.26	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:48:LEU:O	2:B:49:ASP:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:110:THR:O	3:C:110:THR:HG22	2.19	0.42
6:H:84:ALA:C	6:H:86:ASP:N	2.75	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:947:GLY:C	2:B:948:ILE:HG13	2.45	0.42
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	2.01	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:209:ASN:O	1:A:210:ILE:C	2.61	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
1:A:953:ASN:C	1:A:954:TRP:CD1	2.98	0.42
1:A:1204:ASP:C	1:A:1204:ASP:OD1	2.63	0.42
2:B:634:TYR:CD1	2:B:634:TYR:C	2.98	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
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
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.66	0.42
2:B:276:ILE:HG22	2:B:277:LYS:H	1.85	0.42
2:B:315:LYS:HG2	7:I:13:MET:HE1	2.02	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:648:ASN:O	1:A:649:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:HIS:O	3:C:132:PRO:C	2.62	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: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:269:ILE:HG13	1:A:299:HIS:HB3	2.00	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:68:GLN:C	1:A:70:CYS:H	2.28	0.42
1:A:314:ALA:O	1:A:315:LEU:O	2.38	0.42
1:A:718:VAL:O	1:A:719:VAL:C	2.62	0.42
1:A:1017:LEU:O	1:A:1018:PHE:C	2.63	0.42
2:B:604:ARG:NH2	2:B:614:SER:HA	2.35	0.42
2:B:778:MET:CE	2:B:853:SER:HB3	2.47	0.42
2:B:849:GLY:HA2	2:B:852:ARG:HD2	2.02	0.42
5:F:81:THR:O	5:F:82:THR:C	2.63	0.42
9:K:17:SER:O	9:K:18:LYS:C	2.62	0.42
9:K:50:LEU:HD21	9:K:75:ILE:HD13	2.02	0.42
1:A:55:ASP:O	1:A:56:PRO:C	2.63	0.42
1:A:207:ILE:HA	1:A:210:ILE:HG13	2.02	0.42
1:A:312:PRO:C	1:A:313:GLN:HG3	2.45	0.42
2:B:518:HIS:O	2:B:519:TRP:C	2.62	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:714:PHE:CB	7:I:97:MET:HE1	2.50	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
2:B:314:LEU:C	2:B:316:PRO:HD2	2.45	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:792:MET:HE1	12:T:26:DG:OP1	2.20	0.41
2:B:877:PRO:HB3	2:B:915:THR:CG2	2.50	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
1:A:321:PRO:C	1:A:322:VAL:HG22	2.43	0.41
1:A:476:SER:N	1:A:477:PRO:HD2	2.35	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
5:F:80:ALA:O	5:F:81:THR:C	2.64	0.41
6:H:56:THR:HB	6:H:145:ARG:HG2	2.01	0.41
6:H:89:LEU:C	6:H:91:ASP:H	2.28	0.41
1:A:267:ALA:O	1:A:271:LYS:N	2.40	0.41
1:A:809:THR:O	1:A:810:PRO:C	2.63	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:790:ASP:OD1	2:B:790:ASP:N	2.54	0.41
2:B:994:TYR:HB2	2:B:999:MET:CE	2.50	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
6:H:109:LYS:HB3	6:H:110:ASP:C	2.45	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
10:L:53:HIS:C	10:L:55:ILE:H	2.28	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:341:MET:HE1	1:A:843:LYS:HZ3	1.84	0.41
1:A:690:VAL:O	1:A:691:LEU:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:HG	3:C:37:MET:HE2	2.01	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
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:25:ARG:C	6:H:26:ILE:HD12	2.46	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
7:I:119:THR:C	7:I:120:GLN:HG2	2.45	0.41
1:A:322:VAL:HB	1:A:323:LYS:CD	2.37	0.41
1:A:714:PHE:HB3	7:I:97:MET:HE1	2.03	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
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: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:600:LEU:C	2:B:615:MET:HE1	2.46	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
1:A:306:ASN:OD1	1:A:313:GLN:NE2	2.53	0.41
1:A:530:GLY:O	1:A:531:ILE:C	2.63	0.41
1:A:857:ARG:CZ	5:F:139:PRO:HG2	2.51	0.41
1:A:1134:ILE:O	1:A:1135:ARG:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:THR:CG2	1:A:1398:MET:HE3	2.50	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:635:ARG:O	2:B:636:PRO:C	2.63	0.41
2:B:860:MET:HG2	2:B:861:ASP:N	2.36	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
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: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:78:THR:CG2	9:K:79:GLU:N	2.83	0.41
9:K:108:GLU:HA	9:K:111:LEU:HG	2.03	0.41
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.02	0.40
2:B:326:ASP:O	2:B:327:ARG:C	2.64	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:760:ASP:CG	2:B:761:HIS:HD2	2.29	0.40
2:B:1023:VAL:O	2:B:1024:ALA:C	2.62	0.40
3:C:220:ASP:O	3:C:221:TYR:HB3	2.21	0.40
1:A:55:ASP:O	1:A:55:ASP:CG	2.63	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: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:784:ASN:CG	2:B:788:ARG:HD2	2.46	0.40
2:B:809:MET:HE1	2:B:983:ARG:NH2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:76:GLY:O	4:E:77:SER:C	2.63	0.40
4:E:124:VAL:HG13	4:E:132:ILE:HG22	2.03	0.40
7:I:109:ILE:N	7:I:109:ILE:HD12	2.36	0.40
1:A:805:LEU:O	1:A:806:ARG:C	2.64	0.40
2:B:487:THR:CG2	2:B:488:TYR:N	2.83	0.40
2:B:1168:LEU:C	2:B:1170:THR:H	2.30	0.40
1:A:68:GLN:HE21	1:A:80:HIS:CE1	2.38	0.40
1:A:313:GLN:O	1:A:314:ALA:CB	2.69	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
1:A:821:ARG:O	1:A:822:GLU:C	2.65	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
3:C:143:LEU:HD12	3:C:143:LEU:C	2.47	0.40
3:C:231:ASN:C	3:C:231:ASN:ND2	2.80	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1057 (76%)	217 (16%)	109 (8%)	1	12
2	B	1086/1224 (89%)	858 (79%)	162 (15%)	66 (6%)	1	15
3	C	264/318 (83%)	206 (78%)	45 (17%)	13 (5%)	1	19
4	E	212/215 (99%)	174 (82%)	29 (14%)	9 (4%)	2	20
5	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1	15
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	15
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	14

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

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Mol	Chain	Res	Type
1	A	331	GLY
1	A	335	ARG
1	A	404	TYR
1	A	465	TYR
1	A	517	ASN
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

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Mol	Chain	Res	Type
2	B	737	THR
2	B	869	SER
2	B	958	GLN
2	B	961	LEU
2	B	981	ALA
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

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Mol	Chain	Res	Type
1	A	312	PRO
1	A	320	ARG
1	A	880	LYS
1	A	896	ARG
1	A	902	LEU
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

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Mol	Chain	Res	Type
1	A	52	GLY
1	A	56	PRO
1	A	71	GLN
1	A	111	GLY
1	A	219	PHE
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

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Mol	Chain	Res	Type
2	B	879	ARG
2	B	1017	ILE
3	C	217	ASP
5	F	141	GLY
7	I	15	TYR
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

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Mol	Chain	Res	Type
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%)	965 (79%)	253 (21%)	1	7
2	B	958/1061 (90%)	778 (81%)	180 (19%)	1	10
3	C	234/274 (85%)	194 (83%)	40 (17%)	2	13
4	E	196/197 (100%)	162 (83%)	34 (17%)	2	12
5	F	74/137 (54%)	60 (81%)	14 (19%)	1	10
6	H	117/128 (91%)	95 (81%)	22 (19%)	1	10
7	I	113/116 (97%)	98 (87%)	15 (13%)	4	18
8	J	60/65 (92%)	46 (77%)	14 (23%)	1	5
9	K	99/102 (97%)	83 (84%)	16 (16%)	2	14
10	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3109/3657 (85%)	2511 (81%)	598 (19%)	1	10

All (598) 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

Continued on next page...

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Mol	Chain	Res	Type
1	A	50	ILE
1	A	64	ASN
1	A	65	LEU
1	A	69	THR
1	A	71	GLN
1	A	81	PHE
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	161	LEU
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	180	LYS
1	A	186	LYS
1	A	207	ILE
1	A	208	LEU
1	A	225	ASN
1	A	227	VAL
1	A	234	MET
1	A	235	ILE
1	A	239	LEU
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

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Mol	Chain	Res	Type
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
1	A	308	ILE
1	A	315	LEU
1	A	316	GLN
1	A	318	SER
1	A	320	ARG
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	351	THR
1	A	359	LEU
1	A	364	VAL
1	A	372	LYS
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	413	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	462	VAL
1	A	463	ILE
1	A	466	SER
1	A	475	THR
1	A	476	SER

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Mol	Chain	Res	Type
1	A	481	ASP
1	A	486	GLU
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	523	ILE
1	A	524	VAL
1	A	533	LYS
1	A	538	ASP
1	A	550	LEU
1	A	567	LYS
1	A	576	GLN
1	A	590	ARG
1	A	596	THR
1	A	597	LEU
1	A	601	LYS
1	A	607	ILE
1	A	608	ILE
1	A	612	ILE
1	A	625	SER
1	A	629	LEU
1	A	653	VAL
1	A	666	ILE
1	A	677	ARG
1	A	682	THR
1	A	687	LYS
1	A	691	LEU
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

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Mol	Chain	Res	Type
1	A	768	GLN
1	A	773	LYS
1	A	795	GLU
1	A	805	LEU
1	A	821	ARG
1	A	829	VAL
1	A	830	LYS
1	A	831	THR
1	A	854	ASN
1	A	858	ASN
1	A	867	ILE
1	A	879	GLU
1	A	884	ASP
1	A	886	ILE
1	A	890	ASP
1	A	896	ARG
1	A	899	VAL
1	A	902	LEU
1	A	904	THR
1	A	905	ASP
1	A	907	THR
1	A	908	LEU
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	927	VAL
1	A	929	LEU
1	A	932	GLU
1	A	934	LYS
1	A	945	GLU
1	A	964	ILE
1	A	973	ILE
1	A	988	LEU
1	A	990	VAL
1	A	991	LYS
1	A	994	GLN
1	A	995	GLU
1	A	996	ASN

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Mol	Chain	Res	Type
1	A	997	LEU
1	A	998	LEU
1	A	1001	ARG
1	A	1004	ASN
1	A	1006	ILE
1	A	1009	ASN
1	A	1017	LEU
1	A	1022	LEU
1	A	1029	ARG
1	A	1043	ASP
1	A	1046	LEU
1	A	1052	GLN
1	A	1077	THR
1	A	1081	LEU
1	A	1107	VAL
1	A	1112	LYS
1	A	1116	LEU
1	A	1120	LEU
1	A	1128	GLN
1	A	1132	LYS
1	A	1133	LEU
1	A	1134	ILE
1	A	1136	SER
1	A	1142	THR
1	A	1146	VAL
1	A	1162	VAL
1	A	1167	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1173	HIS
1	A	1176	LEU
1	A	1187	GLN
1	A	1189	SER
1	A	1193	LEU
1	A	1199	ARG
1	A	1208	THR
1	A	1218	GLN
1	A	1229	SER
1	A	1242	VAL
1	A	1243	VAL
1	A	1258	HIS
1	A	1262	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	A	1264	GLU
1	A	1267	MET
1	A	1271	ILE
1	A	1272	THR
1	A	1274	ARG
1	A	1276	VAL
1	A	1280	GLU
1	A	1282	VAL
1	A	1299	VAL
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	1355	VAL
1	A	1364	ASN
1	A	1376	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1387	HIS
1	A	1390	ASN
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1406	VAL
1	A	1407	GLU
1	A	1420	ASP
1	A	1428	VAL
1	A	1433	MET
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	57	TYR
2	B	63	ILE
2	B	66	ASP

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Mol	Chain	Res	Type
2	B	67	SER
2	B	68	THR
2	B	94	LYS
2	B	97	VAL
2	B	98	THR
2	B	102	VAL
2	B	104	GLU
2	B	109	THR
2	B	119	LEU
2	B	120	ARG
2	B	130	VAL
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	253	THR
2	B	261	ARG
2	B	268	THR
2	B	272	THR
2	B	275	TYR
2	B	276	ILE
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	353	LYS
2	B	361	LEU

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Mol	Chain	Res	Type
2	B	365	THR
2	B	367	LEU
2	B	387	LEU
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	451	LYS
2	B	461	LEU
2	B	468	GLU
2	B	469	GLN
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	539	LEU
2	B	542	MET
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	556	THR
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	582	VAL
2	B	601	ARG
2	B	604	ARG
2	B	617	ARG
2	B	622	LYS
2	B	628	THR
2	B	637	LEU
2	B	646	LEU

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Mol	Chain	Res	Type
2	B	648	HIS
2	B	658	ILE
2	B	701	ILE
2	B	710	LEU
2	B	714	GLU
2	B	723	VAL
2	B	730	ARG
2	B	732	SER
2	B	740	HIS
2	B	751	VAL
2	B	754	SER
2	B	761	HIS
2	B	762	ASN
2	B	778	MET
2	B	786	ASN
2	B	789	MET
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	799	PRO
2	B	807	ARG
2	B	812	LEU
2	B	815	ARG
2	B	825	VAL
2	B	837	ASP
2	B	844	SER
2	B	861	ASP
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	878	GLN
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	885	MET
2	B	889	THR
2	B	894	ASP
2	B	899	ILE
2	B	914	LYS
2	B	919	SER
2	B	933	SER
2	B	941	LEU

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Mol	Chain	Res	Type
2	B	944	THR
2	B	953	LEU
2	B	956	THR
2	B	958	GLN
2	B	962	LYS
2	B	968	VAL
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	989	THR
2	B	993	THR
2	B	995	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1020	ARG
2	B	1034	VAL
2	B	1041	GLU
2	B	1052	VAL
2	B	1065	GLN
2	B	1082	MET
2	B	1096	ARG
2	B	1103	ILE
2	B	1108	ARG
2	B	1113	VAL
2	B	1119	VAL
2	B	1124	ARG
2	B	1147	LEU
2	B	1152	MET
2	B	1162	ILE
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

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Mol	Chain	Res	Type
2	B	1210	MET
2	B	1218	THR
2	B	1219	ASP
2	B	1222	ARG
3	C	4	GLU
3	C	11	ARG
3	C	16	ASP
3	C	22	LEU
3	C	25	VAL
3	C	27	LEU
3	C	40	GLU
3	C	43	THR
3	C	50	GLU
3	C	53	THR
3	C	55	THR
3	C	57	VAL
3	C	66	ARG
3	C	69	LEU
3	C	70	ILE
3	C	77	ILE
3	C	89	GLU
3	C	91	HIS
3	C	99	LEU
3	C	110	THR
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	153	LEU
3	C	163	ILE
3	C	183	TRP
3	C	189	THR
3	C	199	LYS
3	C	224	GLN
3	C	229	TYR
3	C	231	ASN
3	C	233	GLU
3	C	237	SER
3	C	240	VAL
3	C	244	VAL

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Mol	Chain	Res	Type
3	C	258	ILE
3	C	260	LEU
4	E	6	GLU
4	E	8	ASN
4	E	9	ILE
4	E	35	VAL
4	E	37	LEU
4	E	58	MET
4	E	61	GLN
4	E	74	ASP
4	E	78	LEU
4	E	92	THR
4	E	94	LYS
4	E	100	ILE
4	E	101	GLN
4	E	107	THR
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	142	VAL
4	E	146	HIS
4	E	148	GLU
4	E	155	ARG
4	E	156	LEU
4	E	165	LEU
4	E	169	ARG
4	E	175	LEU
4	E	188	LEU
4	E	190	LEU
4	E	196	VAL
4	E	204	THR
4	E	215	MET
5	F	79	ARG
5	F	82	THR
5	F	92	ARG
5	F	99	LEU
5	F	104	ASN
5	F	109	VAL

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Mol	Chain	Res	Type
5	F	110	ASP
5	F	111	LEU
5	F	123	LYS
5	F	125	LEU
5	F	128	LYS
5	F	133	VAL
5	F	148	VAL
5	F	155	LEU
6	H	8	ASP
6	H	9	ILE
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	37	LYS
6	H	39	THR
6	H	49	VAL
6	H	53	ASP
6	H	63	LEU
6	H	89	LEU
6	H	103	LYS
6	H	106	GLU
6	H	110	ASP
6	H	112	ILE
6	H	129	TYR
6	H	132	LEU
6	H	136	LYS
6	H	143	LEU
7	I	13	MET
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

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Mol	Chain	Res	Type
7	I	107	SER
7	I	111	THR
7	I	117	LYS
8	J	2	ILE
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	14	VAL
8	J	19	GLU
8	J	28	ASP
8	J	31	ASP
8	J	34	THR
8	J	36	LEU
8	J	46	CYS
8	J	54	VAL
8	J	60	PHE
8	J	62	ARG
9	K	9	LEU
9	K	11	LEU
9	K	17	SER
9	K	18	LYS
9	K	22	ASP
9	K	31	VAL
9	K	32	VAL
9	K	34	THR
9	K	46	ILE
9	K	47	ARG
9	K	50	LEU
9	K	56	VAL
9	K	64	GLU
9	K	101	LEU
9	K	111	LEU
9	K	113	THR
10	L	27	LEU
10	L	28	LYS
10	L	38	LEU
10	L	40	LEU
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	63	ARG
10	L	65	VAL

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Mol	Chain	Res	Type
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	80	HIS
1	A	92	HIS
1	A	169	ASN
1	A	313	GLN
1	A	435	HIS
1	A	587	HIS
1	A	706	HIS
1	A	736	ASN
1	A	851	HIS
1	A	906	HIS
1	A	926	GLN
1	A	965	GLN
1	A	1171	GLN
1	A	1173	HIS
1	A	1211	GLN
1	A	1432	GLN
2	B	46	GLN
2	B	121	ASN
2	B	215	GLN
2	B	309	GLN
2	B	325	GLN
2	B	357	GLN
2	B	366	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	538	ASN
2	B	590	HIS
2	B	592	ASN
2	B	686	ASN
2	B	734	HIS
2	B	740	HIS
2	B	744	HIS
2	B	786	ASN
2	B	957	ASN

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1097	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1193	GLN
3	C	65	HIS
3	C	135	GLN
3	C	140	ASN
3	C	167	HIS
3	C	188	HIS
3	C	203	GLN
3	C	242	GLN
4	E	114	ASN
4	E	146	HIS
6	H	11	GLN
7	I	11	ASN
7	I	12	ASN
7	I	79	HIS
7	I	114	GLN
9	K	40	HIS
9	K	65	HIS
10	L	53	HIS

5.3.3 RNA [i](#)

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	18,24,25	3.22	8 (44%)	22,37,40	3.65	14 (63%)

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	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	20	02I	O4'-C1'	-7.70	1.25	1.42
12	T	20	02I	O4'-C4'	-7.47	1.33	1.44
12	T	20	02I	C4'-C5'	-4.33	1.45	1.52
12	T	20	02I	O3'-C3'	-3.75	1.35	1.43
12	T	20	02I	C8-N7	3.29	1.36	1.32
12	T	20	02I	C2-N3	2.54	1.38	1.33
12	T	20	02I	C6-N6	2.51	1.40	1.34
12	T	20	02I	C2-N1	2.39	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	20	02I	N6-C6-N1	-7.16	102.44	118.38
12	T	20	02I	N9-C8-N7	-6.75	107.89	113.13
12	T	20	02I	C5-C6-N6	5.74	137.50	123.29
12	T	20	02I	N3-C2-N1	-5.62	120.08	128.58
12	T	20	02I	C5-C4-N3	-5.01	119.82	126.72
12	T	20	02I	O4'-C1'-C2'	-4.47	97.89	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	20	02I	C4-N9-C1'	4.36	135.29	126.73
12	T	20	02I	C5-C4-N9	4.31	108.34	105.63
12	T	20	02I	C2-N3-C4	3.38	120.09	111.83
12	T	20	02I	N3-C4-N9	3.13	131.84	127.33
12	T	20	02I	C4-C5-N7	-2.78	108.07	110.91
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
12	T	20	02I	C6-C5-C4	2.04	119.96	117.18

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

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%)	-0.09	13 (0%) 81 62	84, 144, 236, 306	0
2	B	1104/1224 (90%)	-0.14	8 (0%) 84 67	76, 131, 209, 281	0
3	C	266/318 (83%)	-0.24	0 100 100	89, 133, 192, 229	0
4	E	214/215 (99%)	-0.19	2 (0%) 81 62	99, 166, 231, 267	0
5	F	84/155 (54%)	-0.33	0 100 100	102, 142, 185, 209	0
6	H	133/146 (91%)	-0.07	2 (1%) 72 51	119, 168, 238, 262	0
7	I	119/122 (97%)	-0.24	0 100 100	96, 151, 190, 216	0
8	J	65/70 (92%)	-0.26	0 100 100	98, 128, 168, 192	0
9	K	114/120 (95%)	-0.34	0 100 100	94, 137, 177, 200	0
10	L	46/70 (65%)	0.15	1 (2%) 62 44	119, 180, 250, 264	0
11	R	9/9 (100%)	-0.33	0 100 100	102, 124, 217, 261	0
12	T	10/29 (34%)	-0.05	0 100 100	108, 136, 243, 256	0
All	All	3559/4211 (84%)	-0.14	26 (0%) 84 67	76, 141, 224, 306	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	997	LEU	6.4
1	A	1108	ALA	4.3
1	A	1002	GLY	3.3
2	B	335	GLY	3.1
1	A	144	THR	3.0
2	B	903	VAL	2.9
2	B	715	ALA	2.9
1	A	998	LEU	2.9
1	A	1000	LEU	2.8
1	A	985	ASP	2.8
6	H	63	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	2.7
4	E	148	GLU	2.6
1	A	1301	GLU	2.5
1	A	904	THR	2.5
1	A	17	VAL	2.4
6	H	86	ASP	2.3
2	B	1216	LEU	2.3
2	B	1214	PRO	2.3
1	A	136	ALA	2.2
10	L	28	LYS	2.2
2	B	1107	ALA	2.2
1	A	999	VAL	2.1
1	A	694	THR	2.1
4	E	53	PRO	2.0
2	B	877	PRO	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	0.56	0.13	204,227,305,321	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	0.03	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
13	ZN	I	202	1/1	0.99	0.02	128,128,128,128	0
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

6.5 Other polymers [i](#)

There are no such residues in this entry.