



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:48 PM UTC

PDB ID : 4X67 / pdb_00004x67
Title : Crystal structure of elongating yeast RNA polymerase II stalled at oxidative
Cyclopurine DNA lesions.
Authors : Wang, L.; Chong, J.; Wang, D.
Deposited on : 2014-12-07
Resolution : 4.10 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:

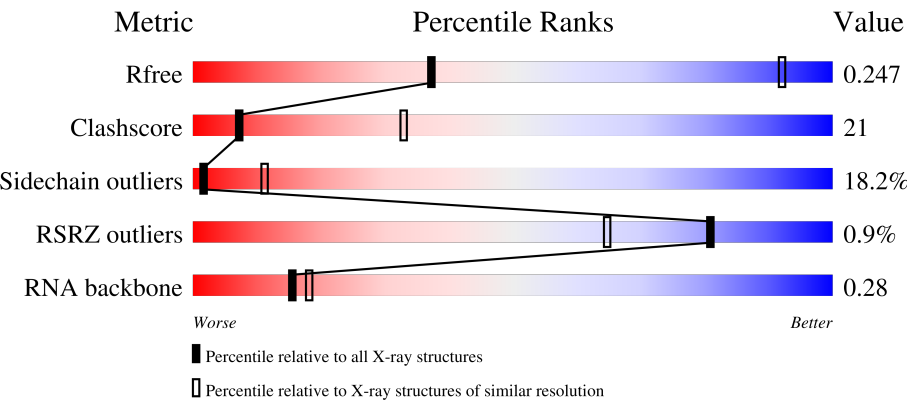
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)
RNA backbone	3983	1026 (5.04-3.10)

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	44%30%6%20%
2	B	1224	48%34%7%10%
3	C	318	50%28%5%16%
4	E	215	2%60%34%6%
5	F	155	32%19%46%

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Mol	Chain	Length	Quality of chain
6	H	146	% 42%40%8%9%
7	I	122	62%31%. .
8	J	70	43%43%7%7%
9	K	120	% 57%32%6%5%
10	L	70	26%37%.34%
11	R	9	22%67%11%
12	T	29	14%17%.66%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28521 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	1394	Total	C	N	O	S	0	0	0
			10961	6911	1922	2067	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	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
			176	77	32	58	9			

- Molecule 12 is a DNA chain called Template DNA _29 mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	10	Total	C	N	O	P	0	0	0
			205	98	37	60	10			

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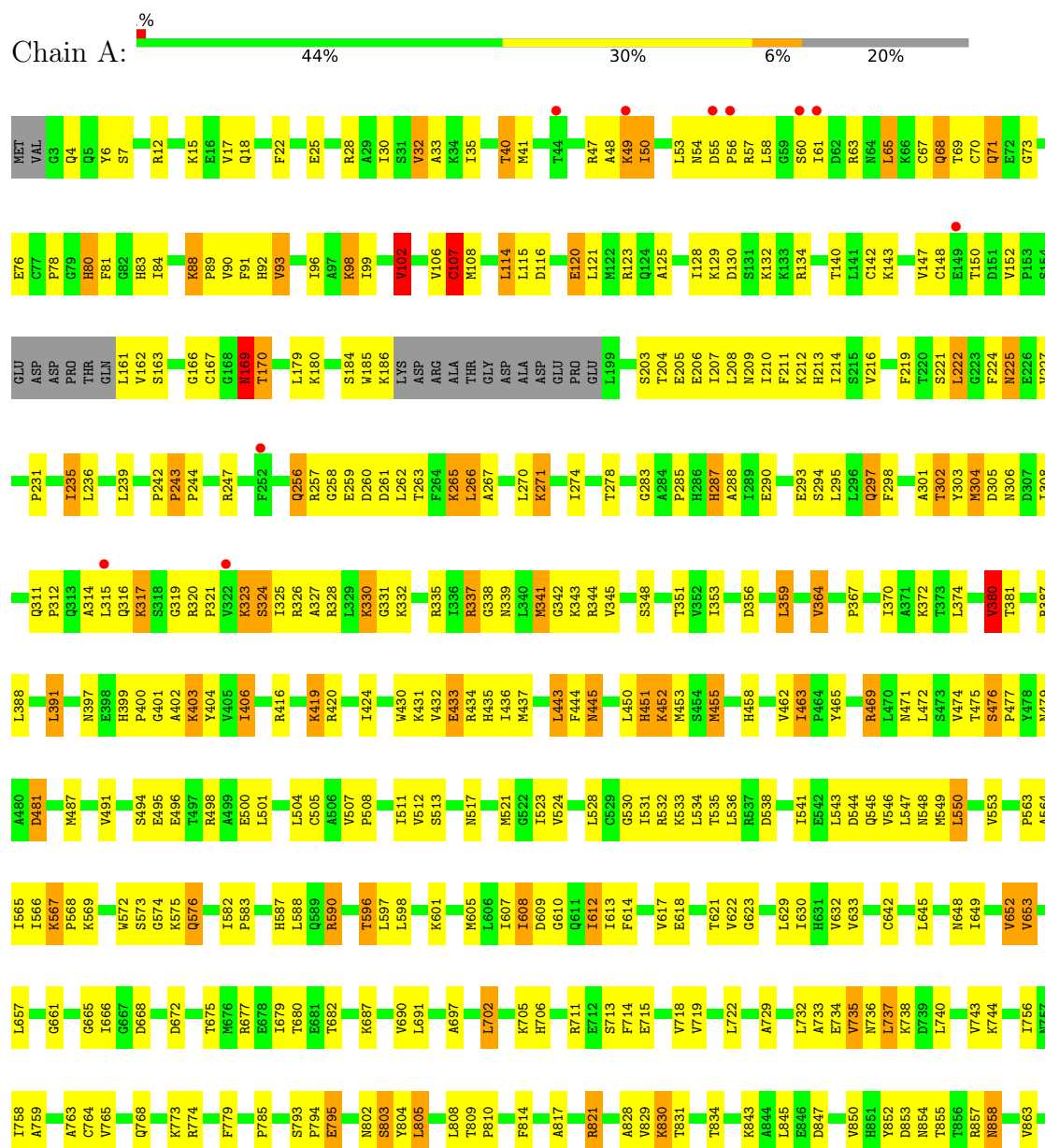
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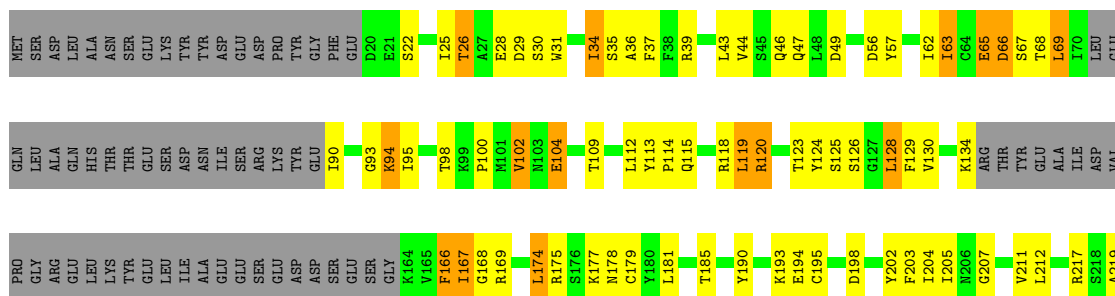
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

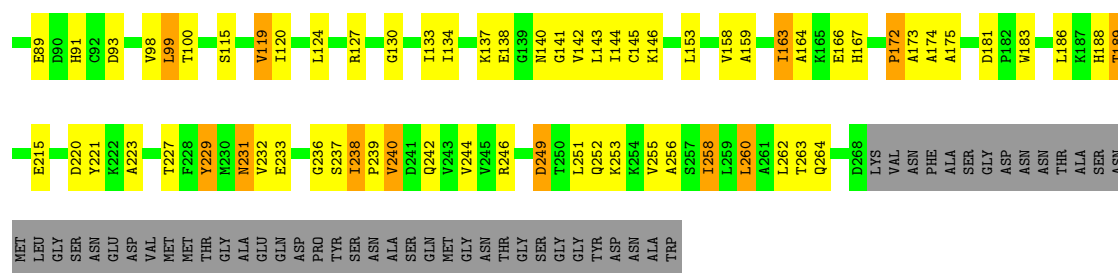
3 Residue-property plots

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.

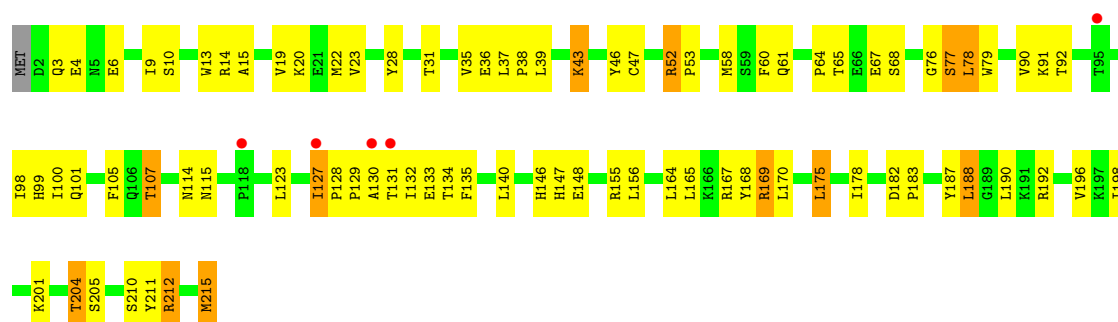
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



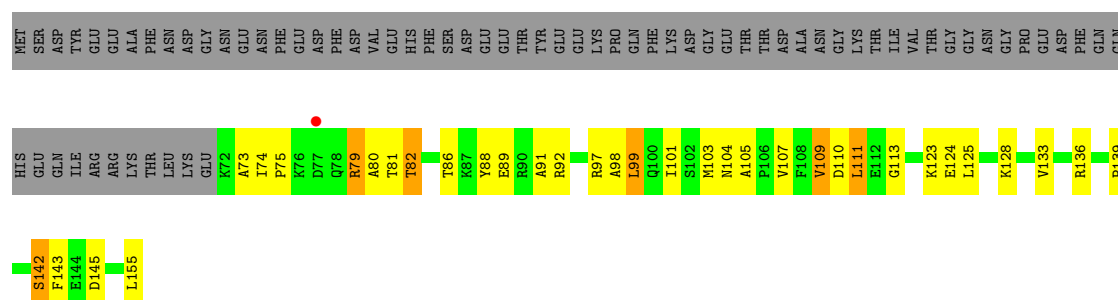
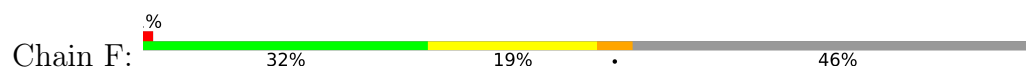




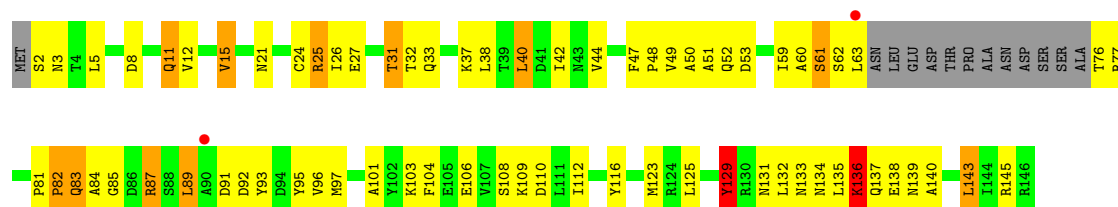
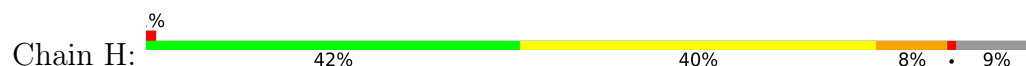
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

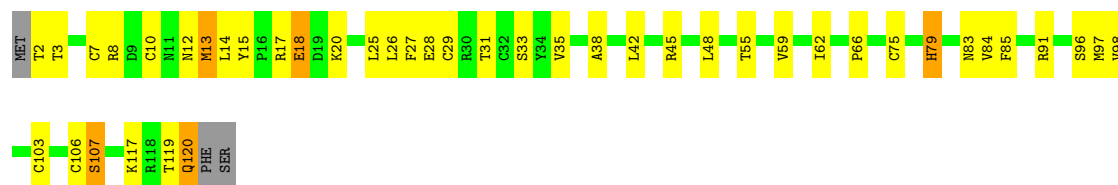


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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

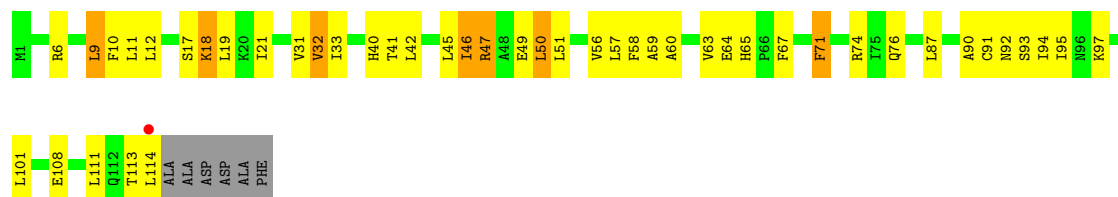




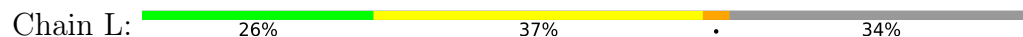
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



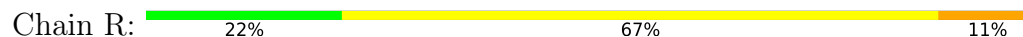
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



- 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	167.15Å 220.80Å 193.92Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	50.00 – 4.10 50.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	75.9 (50.00-4.10) 76.0 (50.00-4.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 4.14Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.289 (Not available) , 0.247	Depositor DCC
R_{free} test set	2105 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28521	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.60	0/11155	0.99	30/15080 (0.2%)
2	B	0.61	0/8963	0.97	21/12086 (0.2%)
3	C	0.57	0/2133	0.96	8/2891 (0.3%)
4	E	0.61	0/1788	1.00	2/2406 (0.1%)
5	F	0.57	0/691	0.91	0/933
6	H	0.62	0/1086	0.99	9/1470 (0.6%)
7	I	0.65	0/989	0.94	1/1331 (0.1%)
8	J	0.59	0/541	1.00	0/727
9	K	0.56	0/937	0.91	0/1265
10	L	0.61	0/365	0.89	0/485
11	R	0.41	0/196	0.75	0/304
12	T	0.29	0/204	0.51	0/310
All	All	0.60	0/29048	0.97	71/39288 (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	6
2	B	0	9
3	C	0	1
6	H	0	3
7	I	0	1
All	All	0	20

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	69	LEU	N-CA-C	7.99	121.55	109.41
1	A	1403	GLU	N-CA-C	7.51	119.10	111.07
2	B	430	ARG	N-CA-C	7.22	122.39	113.50
1	A	170	THR	N-CA-C	7.08	120.94	110.46
1	A	244	PRO	N-CA-C	7.08	119.33	110.70
2	B	479	VAL	N-CA-C	-6.96	99.53	108.93
1	A	1207	LEU	N-CA-C	6.67	120.04	109.50
1	A	243	PRO	CA-C-N	6.63	127.21	120.38
1	A	243	PRO	C-N-CA	6.63	127.21	120.38
3	C	57	VAL	CB-CA-C	-6.61	103.22	112.14
6	H	83	GLN	N-CA-C	-6.38	105.45	113.23
2	B	638	PHE	N-CA-CB	6.37	118.95	110.29
2	B	296	GLU	N-CA-C	-6.31	104.50	111.82
2	B	640	VAL	N-CA-C	6.30	119.25	113.20
2	B	479	VAL	N-CA-CB	6.25	117.68	110.49
3	C	238	ILE	CA-C-N	-6.22	113.88	120.03
3	C	238	ILE	C-N-CA	-6.22	113.88	120.03
1	A	821	ARG	N-CA-C	-6.17	103.26	111.96
6	H	3	ASN	N-CA-C	6.17	116.58	107.88
1	A	102	VAL	CB-CA-C	-6.13	103.76	112.22
7	I	79	HIS	N-CA-CB	6.10	120.79	110.49
2	B	637	LEU	CA-CB-CG	6.09	137.63	116.30
1	A	993	LEU	N-CA-C	-6.05	104.60	111.07
1	A	163	SER	N-CA-C	5.95	119.17	109.06
2	B	883	LEU	N-CA-C	5.91	119.33	111.30
1	A	886	ILE	N-CA-C	5.85	116.03	110.53
2	B	900	ALA	CA-C-N	5.79	125.26	119.24
2	B	900	ALA	C-N-CA	5.79	125.26	119.24
6	H	85	GLY	N-CA-C	-5.75	106.63	113.99
1	A	954	TRP	N-CA-C	5.75	117.54	108.23
1	A	152	VAL	CA-C-N	5.71	126.98	119.84
1	A	152	VAL	C-N-CA	5.71	126.98	119.84
1	A	259	GLU	N-CA-C	5.71	118.98	110.14
6	H	50	ALA	N-CA-C	5.68	115.61	108.45
1	A	50	ILE	N-CA-C	5.64	118.26	108.90
1	A	1226	VAL	N-CA-C	5.63	115.98	108.27
2	B	640	VAL	CB-CA-C	-5.60	105.15	110.70
2	B	273	LEU	CA-C-N	5.60	126.84	119.84
2	B	273	LEU	C-N-CA	5.60	126.84	119.84
6	H	129	TYR	N-CA-C	-5.60	108.24	114.62
3	C	7	GLN	N-CA-C	5.58	118.54	109.06
2	B	277	LYS	N-CA-C	5.55	118.26	111.82
6	H	137	GLN	N-CA-C	5.55	118.61	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	478	GLY	N-CA-C	-5.52	105.32	114.48
1	A	1228	TRP	N-CA-C	5.50	117.45	108.76
1	A	107	CYS	N-CA-C	5.38	117.82	107.44
6	H	87	ARG	N-CA-C	5.34	116.39	108.60
6	H	40	LEU	N-CA-C	5.32	116.86	107.61
3	C	5	GLY	CA-C-N	5.31	126.47	119.84
3	C	5	GLY	C-N-CA	5.31	126.47	119.84
1	A	1311	VAL	N-CA-C	5.27	115.57	107.77
1	A	236	LEU	N-CA-C	5.26	117.53	107.75
1	A	121	LEU	N-CA-C	-5.21	106.60	113.17
1	A	345	VAL	N-CA-C	5.20	115.86	108.42
1	A	1237	ILE	N-CA-C	5.20	116.14	108.45
2	B	167	ILE	CB-CA-C	-5.20	104.23	110.99
4	E	52	ARG	CA-C-N	5.19	126.33	119.84
4	E	52	ARG	C-N-CA	5.19	126.33	119.84
1	A	1256	GLU	N-CA-C	5.14	119.44	112.04
2	B	706	GLN	N-CA-C	-5.14	103.71	110.39
6	H	92	ASP	N-CA-C	-5.13	107.08	113.19
1	A	380	VAL	CB-CA-C	-5.13	102.88	111.29
2	B	1192	TYR	N-CA-C	5.12	116.76	108.26
1	A	166	GLY	N-CA-C	5.08	118.56	111.19
1	A	596	THR	N-CA-C	5.06	120.29	113.21
3	C	158	VAL	CB-CA-C	-5.04	106.14	111.23
2	B	699	GLU	N-CA-C	5.04	117.51	111.71
2	B	756	ILE	N-CA-C	5.04	112.97	108.63
1	A	88	LYS	CA-C-N	5.00	126.10	119.84
1	A	88	LYS	C-N-CA	5.00	126.10	119.84
3	C	183	TRP	N-CA-C	-5.00	103.45	110.50

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	CYS	Peptide
1	A	120	GLU	Peptide
1	A	169	ASN	Peptide
1	A	324	SER	Peptide
1	A	451	HIS	Peptide
1	A	997	LEU	Peptide
2	B	1221	SER	Peptide
2	B	222	ILE	Peptide
2	B	474	SER	Peptide

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Mol	Chain	Res	Type	Group
2	B	635	ARG	Peptide
2	B	636	PRO	Peptide
2	B	730	ARG	Peptide
2	B	879	ARG	Peptide
2	B	883	LEU	Peptide
2	B	980	PHE	Peptide
3	C	172	PRO	Peptide
6	H	129	TYR	Peptide
6	H	136	LYS	Peptide
6	H	82	PRO	Peptide
7	I	20	LYS	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	10961	0	11059	487	0
2	B	8792	0	8823	413	0
3	C	2095	0	2051	84	0
4	E	1752	0	1776	61	0
5	F	679	0	701	23	0
6	H	1068	0	1040	66	0
7	I	971	0	927	33	0
8	J	532	0	542	46	0
9	K	919	0	929	46	0
10	L	363	0	386	23	0
11	R	176	0	86	7	0
12	T	205	0	112	8	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	28521	0	28432	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)
6:H:109:LYS:HB3	6:H:110:ASP:CB	1.71	1.21
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.28	1.14
6:H:109:LYS:HB3	6:H:110:ASP:HB2	1.32	1.12
6:H:109:LYS:CB	6:H:110:ASP:HB2	1.80	1.11
2:B:806:THR:HG23	2:B:809:MET:HE3	1.27	1.09
2:B:472:ALA:HB3	2:B:473:MET:HB2	1.43	0.97
2:B:882:THR:HG21	2:B:935:ARG:HA	1.42	0.97
1:A:1173:HIS:CD2	1:A:1227:ILE:HG12	2.02	0.95
1:A:804:TYR:O	2:B:761:HIS:HB3	1.67	0.94
6:H:109:LYS:CA	6:H:110:ASP:HB2	1.98	0.93
1:A:327:ALA:HA	1:A:330:LYS:HB2	1.51	0.92
2:B:806:THR:CG2	2:B:809:MET:HE3	1.99	0.92
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.10	0.91
1:A:128:ILE:HG22	1:A:134:ARG:HG3	1.50	0.90
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.08	0.89
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.56	0.87
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.14	0.87
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.57	0.86
6:H:108:SER:O	6:H:109:LYS:HB2	1.73	0.86
4:E:46:TYR:CD2	4:E:58:MET:HG3	2.11	0.84
4:E:132:ILE:HG22	4:E:133:GLU:H	1.41	0.84
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.44	0.83
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.08	0.82
2:B:280:ILE:HG21	2:B:285:ILE:HG12	1.62	0.82
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.09	0.81
4:E:132:ILE:HG22	4:E:133:GLU:N	1.93	0.81
1:A:257:ARG:HB2	1:A:258:GLY:CA	2.10	0.81
1:A:855:THR:HG21	1:A:857:ARG:HE	1.46	0.81
1:A:107:CYS:SG	1:A:114:LEU:HD22	2.22	0.80
2:B:1175:LEU:O	2:B:1176:ASN:HB2	1.79	0.80
1:A:649:ILE:O	1:A:653:VAL:HG23	1.82	0.79
4:E:46:TYR:CE2	4:E:58:MET:HG3	2.17	0.79
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.64	0.79
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.13	0.78
4:E:130:ALA:HB1	4:E:131:THR:HB	1.66	0.78
5:F:107:VAL:HG11	5:F:111:LEU:HD11	1.66	0.78
3:C:56:THR:HG21	3:C:145:CYS:SG	2.24	0.78
1:A:56:PRO:HD2	1:A:58:LEU:HD13	1.64	0.78
2:B:129:PHE:CE1	2:B:166:PHE:HB2	2.20	0.77
6:H:109:LYS:HB3	6:H:110:ASP:C	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:HA	1:A:257:ARG:O	1.83	0.77
2:B:800:GLN:HG2	8:J:52:THR:HG21	1.67	0.77
2:B:115:GLN:O	2:B:119:LEU:HD12	1.85	0.77
11:R:3:C:H2'	11:R:4:G:C8	2.20	0.76
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.66	0.76
1:A:67:CYS:SG	1:A:70:CYS:HB3	2.25	0.76
10:L:48:CYS:SG	10:L:49:LYS:N	2.57	0.76
2:B:834:ASN:O	2:B:1013:ASN:HB2	1.85	0.76
1:A:76:GLU:O	1:A:78:PRO:HD3	1.87	0.75
10:L:53:HIS:O	10:L:55:ILE:HG12	1.86	0.75
3:C:66:ARG:NH2	8:J:5:VAL:HG23	2.02	0.75
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.53	0.74
2:B:120:ARG:HD2	2:B:955:THR:HG21	1.68	0.74
1:A:1076:ALA:HA	1:A:1079:MET:HE3	1.69	0.74
4:E:168:TYR:C	4:E:169:ARG:HG2	2.12	0.74
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.69	0.74
1:A:451:HIS:O	2:B:1137:CYS:SG	2.43	0.74
2:B:754:SER:O	2:B:806:THR:HG21	1.87	0.74
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.69	0.73
6:H:109:LYS:HA	6:H:110:ASP:HB2	1.68	0.73
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.70	0.73
1:A:261:ASP:HB3	1:A:323:LYS:CE	2.18	0.73
2:B:1129:ARG:HH21	2:B:1131:GLY:HA2	1.53	0.73
3:C:41:ILE:HG12	3:C:172:PRO:HG3	1.70	0.73
11:R:7:A:H2'	11:R:8:U:O4'	1.88	0.73
2:B:806:THR:HG23	2:B:809:MET:CE	2.15	0.73
2:B:287:ARG:HG2	2:B:292:ILE:HD13	1.70	0.72
2:B:733:HIS:O	2:B:735:ALA:N	2.23	0.71
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.21	0.71
4:E:130:ALA:CB	4:E:131:THR:HB	2.20	0.71
1:A:901:LEU:HA	1:A:907:THR:HG23	1.71	0.71
6:H:129:TYR:C	6:H:131:ASN:H	1.99	0.71
2:B:475:SER:O	2:B:477:ALA:N	2.23	0.70
4:E:132:ILE:CG2	4:E:133:GLU:H	2.03	0.70
2:B:477:ALA:HB3	2:B:479:VAL:HG22	1.73	0.70
3:C:70:ILE:HD12	3:C:144:ILE:HD11	1.74	0.70
6:H:134:ASN:O	6:H:135:LEU:O	2.09	0.70
10:L:48:CYS:HB3	10:L:52:GLY:HA2	1.74	0.70
1:A:129:LYS:O	1:A:130:ASP:HB2	1.90	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.17	0.70
1:A:1436:ILE:O	1:A:1437:GLY:C	2.33	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:7:CYS:HB3	7:I:14:LEU:HD21	1.73	0.70
2:B:1103:ILE:N	2:B:1103:ILE:HD13	2.07	0.69
1:A:893:PHE:CE2	1:A:940:ARG:HG3	2.27	0.69
6:H:40:LEU:HD13	6:H:123:MET:HE3	1.74	0.69
1:A:546:VAL:HG12	1:A:550:LEU:CD2	2.22	0.69
2:B:34:ILE:HD12	2:B:542:MET:HE1	1.74	0.69
2:B:1099:VAL:CG1	2:B:1103:ILE:HD11	2.22	0.69
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.74	0.69
1:A:1173:HIS:NE2	1:A:1227:ILE:HG12	2.07	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.69
4:E:170:LEU:HD13	4:E:175:LEU:CD2	2.23	0.69
1:A:54:ASN:O	1:A:55:ASP:HB2	1.93	0.68
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.57	0.68
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.76	0.68
4:E:20:LYS:HE2	4:E:60:PHE:CZ	2.29	0.68
1:A:590:ARG:HH21	1:A:621:THR:HA	1.59	0.68
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.07	0.68
2:B:977:GLY:CA	2:B:1099:VAL:HG21	2.24	0.68
5:F:109:VAL:CG2	5:F:124:GLU:HG2	2.24	0.68
7:I:10:CYS:SG	7:I:31:THR:HB	2.34	0.68
1:A:913:LEU:HD11	1:A:981:LEU:O	1.94	0.67
2:B:329:THR:HA	2:B:332:ASP:HB2	1.76	0.67
1:A:323:LYS:HB2	1:A:324:SER:CA	2.24	0.67
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.09	0.67
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.76	0.67
3:C:36:VAL:HG23	9:K:41:THR:HG21	1.76	0.67
8:J:43:ARG:CG	8:J:46:CYS:SG	2.83	0.67
1:A:605:MET:HE3	1:A:605:MET:HA	1.76	0.67
6:H:108:SER:O	6:H:109:LYS:CB	2.43	0.67
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.82	0.66
2:B:316:PRO:HA	2:B:319:GLU:HG3	1.76	0.66
2:B:617:ARG:HG2	2:B:617:ARG:HH11	1.59	0.66
2:B:737:THR:HG21	7:I:66:PRO:O	1.95	0.66
6:H:61:SER:O	6:H:62:SER:HB2	1.94	0.66
12:T:21:02I:H12'	12:T:22:DT:C6	2.30	0.66
1:A:257:ARG:CB	1:A:258:GLY:HA2	2.24	0.66
1:A:257:ARG:CB	1:A:258:GLY:CA	2.73	0.66
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.29	0.66
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.77	0.66
6:H:47:PHE:HB3	6:H:95:TYR:HD2	1.60	0.66
2:B:638:PHE:O	2:B:740:HIS:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.11	0.66
8:J:52:THR:O	8:J:53:HIS:C	2.38	0.66
1:A:35:ILE:HG22	1:A:270:LEU:HD13	1.78	0.65
2:B:43:LEU:HD11	2:B:811:TYR:O	1.95	0.65
4:E:132:ILE:O	4:E:133:GLU:HG3	1.94	0.65
10:L:58:LYS:O	10:L:59:ALA:HB3	1.95	0.65
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.30	0.65
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.26	0.65
2:B:976:ILE:O	2:B:990:ILE:HB	1.97	0.65
2:B:981:ALA:O	2:B:982:SER:O	2.13	0.65
10:L:33:GLU:HG3	10:L:53:HIS:CB	2.27	0.65
2:B:981:ALA:HB3	2:B:987:LYS:HA	1.79	0.65
1:A:278:THR:O	1:A:278:THR:HG22	1.96	0.65
2:B:635:ARG:CG	2:B:636:PRO:HD3	2.27	0.65
6:H:109:LYS:CB	6:H:110:ASP:CB	2.49	0.65
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.79	0.65
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.62	0.65
10:L:46:VAL:O	10:L:47:ARG:CB	2.45	0.65
2:B:1155:SER:OG	2:B:1156:ASP:N	2.28	0.65
9:K:65:HIS:HD2	9:K:67:PHE:H	1.45	0.65
1:A:203:SER:O	1:A:205:GLU:N	2.29	0.64
4:E:132:ILE:CG2	4:E:133:GLU:N	2.60	0.64
2:B:701:ILE:HG13	2:B:740:HIS:HE1	1.62	0.64
1:A:54:ASN:O	1:A:55:ASP:CB	2.44	0.64
2:B:737:THR:HG23	7:I:66:PRO:CB	2.27	0.64
1:A:805:LEU:C	1:A:805:LEU:HD12	2.23	0.64
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.78	0.64
3:C:133:ILE:HD11	3:C:237:SER:HA	1.77	0.64
2:B:546:SER:OG	2:B:631:GLY:N	2.31	0.64
2:B:555:ILE:HD11	2:B:582:VAL:HG11	1.80	0.64
1:A:344:ARG:CZ	2:B:1129:ARG:HG3	2.27	0.63
2:B:357:GLN:O	2:B:366:GLN:HA	1.98	0.63
1:A:532:ARG:O	1:A:535:THR:N	2.30	0.63
2:B:65:GLU:HG2	2:B:66:ASP:N	2.14	0.63
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.28	0.63
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.79	0.63
1:A:1004:ASN:CG	1:A:1005:GLU:H	2.07	0.63
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.81	0.63
4:E:15:ALA:O	4:E:19:VAL:HG23	1.98	0.63
1:A:675:THR:HG21	1:A:736:ASN:HD21	1.63	0.62
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:OE1	1:A:80:HIS:CE1	2.53	0.62
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.81	0.62
2:B:801:LYS:HG2	8:J:52:THR:HG23	1.81	0.62
4:E:64:PRO:CG	4:E:76:GLY:HA2	2.30	0.62
2:B:778:MET:HE3	2:B:853:SER:HB3	1.80	0.62
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.34	0.62
1:A:1434:ALA:HB1	1:A:1436:ILE:HD12	1.82	0.62
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.81	0.62
7:I:17:ARG:HG2	7:I:18:GLU:H	1.65	0.62
1:A:648:ASN:O	1:A:652:VAL:HG23	2.00	0.62
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.81	0.62
2:B:635:ARG:HB2	2:B:636:PRO:HD3	1.82	0.62
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.35	0.61
3:C:98:VAL:C	3:C:99:LEU:HD23	2.25	0.61
1:A:316:GLN:O	1:A:317:LYS:O	2.18	0.61
1:A:89:PRO:O	1:A:204:THR:HG21	2.01	0.61
1:A:320:ARG:HB2	1:A:321:PRO:HA	1.82	0.61
1:A:341:MET:HE1	1:A:843:LYS:HZ3	1.65	0.61
1:A:1172:LEU:O	1:A:1173:HIS:HB2	1.99	0.61
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.35	0.61
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.83	0.61
1:A:257:ARG:HB2	1:A:258:GLY:HA3	1.82	0.61
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.36	0.60
1:A:261:ASP:HB3	1:A:323:LYS:HD3	1.83	0.60
1:A:566:ILE:O	1:A:567:LYS:O	2.19	0.60
2:B:640:VAL:HG23	2:B:740:HIS:CA	2.29	0.60
2:B:25:ILE:HD12	2:B:651:LEU:HD12	1.83	0.60
2:B:322:PHE:O	2:B:322:PHE:CD1	2.55	0.60
2:B:65:GLU:CG	2:B:66:ASP:N	2.65	0.60
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.83	0.60
2:B:129:PHE:CD1	2:B:166:PHE:HB2	2.37	0.60
2:B:1081:LEU:O	3:C:189:THR:HG23	2.02	0.60
1:A:71:GLN:O	1:A:73:GLY:N	2.35	0.60
1:A:530:GLY:C	1:A:532:ARG:N	2.58	0.60
10:L:33:GLU:HG3	10:L:53:HIS:CG	2.36	0.60
10:L:33:GLU:HG3	10:L:53:HIS:HB2	1.82	0.59
1:A:302:THR:HA	1:A:305:ASP:O	2.02	0.59
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.85	0.59
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.83	0.59
2:B:471:LYS:N	2:B:472:ALA:HA	2.17	0.59
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.32	0.59
6:H:109:LYS:CB	6:H:110:ASP:C	2.75	0.59
2:B:882:THR:HG22	2:B:883:LEU:N	2.18	0.59
6:H:44:VAL:HG12	6:H:44:VAL:O	2.03	0.59
6:H:106:GLU:C	6:H:108:SER:H	2.10	0.59
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.84	0.59
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.49	0.59
9:K:63:VAL:HG23	9:K:63:VAL:O	2.02	0.59
2:B:640:VAL:O	2:B:641:GLU:C	2.45	0.59
1:A:125:ALA:O	1:A:134:ARG:CG	2.51	0.58
2:B:167:ILE:HG23	2:B:424:LEU:HD13	1.84	0.58
2:B:273:LEU:O	2:B:274:PRO:O	2.21	0.58
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.86	0.58
2:B:635:ARG:CB	2:B:636:PRO:HD3	2.33	0.58
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.69	0.58
4:E:130:ALA:CA	4:E:131:THR:HB	2.34	0.58
4:E:192:ARG:O	4:E:192:ARG:HG3	2.03	0.58
1:A:262:LEU:O	1:A:266:LEU:HB2	2.03	0.58
2:B:617:ARG:NH1	2:B:619:ILE:HD13	2.18	0.58
3:C:3:GLU:HG3	3:C:4:GLU:H	1.68	0.58
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.38	0.58
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.69	0.58
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.17	0.58
2:B:1187:ASN:HD21	2:B:1190:ASP:CB	2.16	0.58
4:E:187:TYR:HD1	4:E:188:LEU:HD23	1.68	0.58
8:J:51:LEU:HD12	8:J:51:LEU:O	2.04	0.58
1:A:402:ALA:HB1	1:A:433:GLU:O	2.04	0.57
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.39	0.57
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.57
1:A:134:ARG:HD2	1:A:221:SER:O	2.04	0.57
3:C:57:VAL:CG1	8:J:60:PHE:HB2	2.32	0.57
1:A:391:LEU:HD13	1:A:400:PRO:O	2.04	0.57
2:B:31:TRP:HA	2:B:34:ILE:HG12	1.87	0.57
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.04	0.57
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.86	0.57
2:B:996:ARG:NH2	3:C:38:ILE:HD12	2.20	0.57
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.18	0.57
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.87	0.57
2:B:701:ILE:HG12	2:B:702:LEU:N	2.19	0.57
4:E:28:TYR:HE2	4:E:78:LEU:HD13	1.70	0.57
1:A:452:LYS:HB2	2:B:1141:HIS:HE1	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ARG:CD	2:B:636:PRO:HD3	2.34	0.57
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.86	0.57
2:B:274:PRO:O	2:B:276:ILE:N	2.38	0.57
2:B:638:PHE:O	2:B:740:HIS:CB	2.53	0.57
2:B:917:PRO:HA	2:B:933:SER:O	2.04	0.57
8:J:57:ILE:HA	8:J:60:PHE:HD1	1.70	0.57
10:L:58:LYS:O	10:L:59:ALA:CB	2.53	0.57
1:A:323:LYS:HB2	1:A:324:SER:O	2.05	0.57
3:C:141:GLY:O	3:C:142:VAL:O	2.23	0.57
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.70	0.57
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.35	0.57
1:A:128:ILE:CG2	1:A:134:ARG:HG3	2.31	0.56
1:A:528:LEU:HD12	1:A:528:LEU:O	2.05	0.56
3:C:251:LEU:O	3:C:255:VAL:HG23	2.05	0.56
1:A:267:ALA:O	1:A:271:LYS:N	2.38	0.56
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.87	0.56
2:B:428:ILE:HG13	2:B:448:ILE:HD13	1.88	0.56
2:B:563:MET:HG3	2:B:563:MET:O	2.04	0.56
2:B:798:TYR:CD2	8:J:4:PRO:HB3	2.41	0.56
2:B:822:ASN:O	8:J:48:ARG:NH1	2.39	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.87	0.56
2:B:977:GLY:C	2:B:1099:VAL:CG2	2.78	0.56
2:B:1099:VAL:HG12	2:B:1103:ILE:CD1	2.30	0.56
4:E:130:ALA:HB1	4:E:131:THR:CB	2.33	0.56
7:I:17:ARG:HG2	7:I:18:GLU:N	2.21	0.56
1:A:583:PRO:O	1:A:610:GLY:HA3	2.06	0.56
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.87	0.56
8:J:3:VAL:HG12	8:J:4:PRO:HD2	1.88	0.56
1:A:89:PRO:O	1:A:204:THR:CG2	2.54	0.56
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.87	0.56
7:I:25:LEU:HB3	7:I:38:ALA:HB2	1.88	0.56
1:A:81:PHE:CE1	2:B:1208:MET:HE2	2.41	0.56
1:A:568:PRO:HB3	3:C:221:TYR:CE2	2.40	0.56
2:B:636:PRO:HD2	2:B:637:LEU:HB3	1.87	0.56
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.88	0.56
1:A:225:ASN:O	1:A:227:VAL:N	2.37	0.55
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	2.22	0.55
2:B:479:VAL:O	2:B:480:SER:HB3	2.05	0.55
4:E:23:VAL:HG13	4:E:28:TYR:HD2	1.71	0.55
6:H:59:ILE:O	6:H:60:ALA:HB3	2.07	0.55
1:A:834:THR:HG21	1:A:1077:THR:CA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:GLN:CD	1:A:1188:GLN:H	2.14	0.55
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.88	0.55
2:B:901:PRO:O	2:B:949:VAL:O	2.24	0.55
4:E:129:PRO:O	4:E:130:ALA:HB3	2.06	0.55
2:B:128:LEU:HB3	2:B:167:ILE:O	2.06	0.55
7:I:7:CYS:C	7:I:8:ARG:O	2.49	0.55
1:A:530:GLY:C	1:A:532:ARG:H	2.12	0.55
1:A:1021:LEU:HD11	1:A:1025:ARG:NH1	2.22	0.55
2:B:957:ASN:O	2:B:959:ASP:N	2.39	0.55
1:A:432:VAL:O	1:A:433:GLU:C	2.49	0.55
2:B:634:TYR:CE1	2:B:692:TYR:CD2	2.94	0.55
2:B:857:ARG:NH2	12:T:26:DG:OP2	2.39	0.55
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.88	0.55
1:A:265:LYS:CE	1:A:323:LYS:HE2	2.36	0.55
2:B:363:HIS:O	2:B:364:ILE:HB	2.07	0.55
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.39	0.55
1:A:203:SER:O	1:A:206:GLU:N	2.39	0.55
2:B:698:GLU:O	2:B:701:ILE:HD12	2.07	0.55
2:B:1006:ILE:HD13	8:J:45:CYS:SG	2.47	0.55
4:E:64:PRO:HG3	4:E:76:GLY:HA2	1.89	0.55
2:B:284:ILE:HD12	2:B:324:ILE:HD12	1.88	0.55
2:B:378:LEU:O	2:B:382:ILE:HG12	2.07	0.55
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.87	0.55
3:C:173:ALA:O	3:C:233:GLU:O	2.25	0.55
4:E:28:TYR:CE2	4:E:78:LEU:HD13	2.42	0.55
6:H:89:LEU:C	6:H:91:ASP:H	2.14	0.55
1:A:120:GLU:O	1:A:120:GLU:HG2	2.07	0.55
1:A:323:LYS:HB2	1:A:324:SER:HA	1.88	0.55
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.88	0.55
1:A:469:ARG:NH2	2:B:991:GLY:O	2.40	0.55
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.89	0.55
2:B:1162:ILE:HD13	2:B:1168:LEU:C	2.32	0.55
9:K:49:GLU:HG3	9:K:94:ILE:HD11	1.88	0.55
1:A:1319:VAL:HB	1:A:1322:ILE:HD12	1.89	0.54
1:A:1436:ILE:O	1:A:1439:GLY:N	2.40	0.54
2:B:471:LYS:CB	2:B:472:ALA:HA	2.38	0.54
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.05	0.54
6:H:93:TYR:CD2	6:H:143:LEU:HB3	2.42	0.54
12:T:24:DT:H2'	12:T:24:DT:O2	2.07	0.54
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.88	0.54
2:B:461:LEU:O	2:B:480:SER:OG	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:28:DT:H4'	12:T:28:DT:OP1	2.06	0.54
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.88	0.54
1:A:531:ILE:N	1:A:653:VAL:HG11	2.21	0.54
1:A:548:ASN:HD21	9:K:47:ARG:HE	1.56	0.54
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.54
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.89	0.54
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.54
2:B:211:VAL:O	2:B:480:SER:HA	2.08	0.54
2:B:562:GLY:O	2:B:563:MET:C	2.51	0.54
2:B:638:PHE:CE2	2:B:743:ILE:HA	2.42	0.54
1:A:406:ILE:HD13	1:A:431:LYS:HB2	1.89	0.54
1:A:1021:LEU:CD1	1:A:1025:ARG:NH1	2.71	0.54
2:B:701:ILE:HG13	2:B:740:HIS:CE1	2.41	0.54
3:C:60:ASP:HB3	10:L:67:PHE:CE2	2.42	0.54
3:C:145:CYS:HA	8:J:2:ILE:HD11	1.89	0.54
9:K:32:VAL:HG23	9:K:74:ARG:HG3	1.88	0.54
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.88	0.54
2:B:273:LEU:HB3	2:B:274:PRO:HD2	1.89	0.54
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.37	0.54
3:C:37:MET:SD	3:C:232:VAL:HG21	2.48	0.54
1:A:481:ASP:N	1:A:481:ASP:OD1	2.41	0.54
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.74	0.54
2:B:863:GLU:O	2:B:864:LYS:HG3	2.08	0.54
3:C:120:ILE:HD11	3:C:130:GLY:O	2.07	0.54
1:A:331:GLY:O	1:A:332:LYS:HB3	2.08	0.53
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.08	0.53
2:B:315:LYS:HG2	7:I:13:MET:HE1	1.89	0.53
9:K:49:GLU:CB	9:K:94:ILE:HD11	2.37	0.53
10:L:53:HIS:O	10:L:55:ILE:N	2.40	0.53
1:A:903:ASN:O	1:A:905:ASP:N	2.42	0.53
2:B:35:SER:O	2:B:39:ARG:HG3	2.08	0.53
1:A:511:ILE:HG12	1:A:521:MET:HE3	1.90	0.53
1:A:544:ASP:OD1	1:A:545:GLN:N	2.41	0.53
1:A:737:LEU:HD11	1:A:758:ILE:HG21	1.91	0.53
6:H:32:THR:HG22	6:H:33:GLN:HG2	1.89	0.53
6:H:109:LYS:CB	6:H:110:ASP:CA	2.81	0.53
9:K:6:ARG:O	9:K:9:LEU:HG	2.07	0.53
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.44	0.53
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.90	0.53
1:A:216:VAL:O	1:A:219:PHE:HB2	2.09	0.53
1:A:1364:ASN:HD22	1:A:1366:ARG:CG	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:31:THR:O	6:H:32:THR:CB	2.56	0.53
11:R:2:U:H6	11:R:2:U:O5'	1.92	0.53
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.44	0.53
4:E:52:ARG:HB3	4:E:53:PRO:HD2	1.91	0.53
5:F:80:ALA:O	5:F:81:THR:C	2.51	0.53
5:F:142:SER:O	5:F:143:PHE:HB3	2.08	0.53
7:I:7:CYS:SG	7:I:10:CYS:HB2	2.48	0.53
1:A:714:PHE:CG	7:I:97:MET:HE1	2.44	0.53
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.74	0.53
2:B:254:LEU:HD12	2:B:272:THR:O	2.08	0.53
2:B:778:MET:HE3	2:B:853:SER:CB	2.38	0.53
2:B:882:THR:CG2	2:B:935:ARG:HA	2.29	0.53
3:C:16:ASP:HA	3:C:240:VAL:HG22	1.91	0.53
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.38	0.53
2:B:863:GLU:HG3	2:B:962:LYS:HB3	1.91	0.53
4:E:10:SER:O	4:E:14:ARG:HG3	2.08	0.53
1:A:67:CYS:O	1:A:68:GLN:OE1	2.27	0.52
1:A:630:ILE:HD12	1:A:630:ILE:H	1.74	0.52
2:B:114:PRO:CG	2:B:181:LEU:HD11	2.38	0.52
12:T:23:DC:H2'	12:T:23:DC:O2	2.08	0.52
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.89	0.52
6:H:104:PHE:CZ	6:H:136:LYS:HA	2.44	0.52
1:A:30:ILE:O	2:B:1183:LYS:NZ	2.43	0.52
1:A:1101:LEU:HG	1:A:1105:LEU:HD12	1.92	0.52
2:B:800:GLN:CG	8:J:52:THR:HG21	2.38	0.52
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.43	0.52
1:A:332:LYS:H	1:A:337:ARG:CB	2.23	0.52
3:C:99:LEU:HD23	3:C:99:LEU:N	2.24	0.52
9:K:92:ASN:O	9:K:93:SER:C	2.52	0.52
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.90	0.52
1:A:265:LYS:HZ2	1:A:302:THR:HG23	1.74	0.52
1:A:852:TYR:HH	1:A:1441:PHE:HD2	1.56	0.52
2:B:797:TYR:C	2:B:799:PRO:HD2	2.34	0.52
1:A:1188:GLN:H	1:A:1188:GLN:NE2	2.07	0.52
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.92	0.52
7:I:8:ARG:O	7:I:10:CYS:N	2.43	0.52
10:L:34:CYS:SG	10:L:35:SER:N	2.80	0.52
1:A:219:PHE:O	1:A:222:LEU:O	2.27	0.52
2:B:119:LEU:HD23	2:B:953:LEU:HD13	1.92	0.52
2:B:701:ILE:CG1	2:B:740:HIS:HE1	2.23	0.52
4:E:78:LEU:HA	4:E:107:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.92	0.52
11:R:1:A:O5'	11:R:1:A:H8	1.92	0.52
1:A:80:HIS:O	1:A:243:PRO:HG3	2.09	0.52
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.92	0.52
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.92	0.52
1:A:622:VAL:HG22	1:A:622:VAL:O	2.10	0.52
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.10	0.52
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.39	0.52
2:B:701:ILE:CB	2:B:740:HIS:HE1	2.23	0.52
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.92	0.51
1:A:1171:GLN:HB2	1:A:1172:LEU:HD23	1.91	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.92	0.51
2:B:862:GLN:O	2:B:914:LYS:NZ	2.42	0.51
5:F:73:ALA:O	5:F:74:ILE:HG12	2.10	0.51
8:J:2:ILE:C	8:J:53:HIS:NE2	2.68	0.51
1:A:125:ALA:O	1:A:134:ARG:HG3	2.11	0.51
1:A:387:ARG:O	1:A:391:LEU:HD23	2.10	0.51
1:A:853:ASP:OD2	1:A:855:THR:CG2	2.58	0.51
1:A:1134:ILE:O	1:A:1135:ARG:C	2.54	0.51
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.51	0.51
2:B:868:MET:O	2:B:869:SER:CB	2.58	0.51
1:A:919:ILE:HG21	1:A:925:LEU:HD12	1.91	0.51
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.51
2:B:957:ASN:HB3	2:B:961:LEU:HD12	1.90	0.51
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.91	0.51
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.91	0.51
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.51
2:B:34:ILE:HD11	2:B:743:ILE:HG22	1.92	0.51
2:B:123:THR:HG23	2:B:205:ILE:HD13	1.92	0.51
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.75	0.51
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.25	0.51
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.92	0.51
1:A:1022:LEU:CD1	1:A:1026:LEU:HD12	2.40	0.51
2:B:682:SER:O	2:B:686:ASN:ND2	2.44	0.51
8:J:10:CYS:SG	8:J:11:GLY:N	2.83	0.51
1:A:567:LYS:HB3	6:H:96:VAL:N	2.25	0.51
1:A:852:TYR:CD1	1:A:1060:PRO:HB2	2.45	0.51
1:A:942:PHE:CD1	1:A:942:PHE:C	2.89	0.51
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.50	0.51
2:B:34:ILE:HD13	2:B:34:ILE:N	2.24	0.51
2:B:475:SER:C	2:B:477:ALA:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:47:ARG:HH11	9:K:47:ARG:HG2	1.75	0.51
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.93	0.51
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.92	0.51
1:A:919:ILE:O	1:A:920:LEU:C	2.54	0.51
1:A:1022:LEU:O	1:A:1026:LEU:HB2	2.11	0.51
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.45	0.51
2:B:1006:ILE:CD1	8:J:45:CYS:SG	2.98	0.51
3:C:134:ILE:CD1	3:C:141:GLY:HA3	2.41	0.51
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.93	0.51
2:B:660:LYS:O	2:B:663:ALA:HB3	2.10	0.51
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.93	0.51
4:E:36:GLU:O	4:E:38:PRO:HD3	2.11	0.51
1:A:167:CYS:SG	1:A:167:CYS:O	2.69	0.51
4:E:130:ALA:HB1	4:E:131:THR:CG2	2.40	0.51
1:A:32:VAL:HB	1:A:57:ARG:HB2	1.93	0.51
1:A:857:ARG:CZ	5:F:139:PRO:HG2	2.41	0.51
2:B:65:GLU:CG	2:B:66:ASP:H	2.24	0.51
3:C:41:ILE:CG1	3:C:172:PRO:HG3	2.40	0.51
5:F:81:THR:CG2	5:F:136:ARG:HD3	2.41	0.51
8:J:28:ASP:N	8:J:28:ASP:OD1	2.44	0.51
1:A:547:LEU:HD22	9:K:58:PHE:HD1	1.77	0.50
1:A:1053:PHE:O	1:A:1056:SER:N	2.36	0.50
2:B:463:THR:HG21	2:B:465:ASN:ND2	2.27	0.50
2:B:745:PRO:C	2:B:747:MET:H	2.19	0.50
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.41	0.50
4:E:43:LYS:O	4:E:47:CYS:HB2	2.12	0.50
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.42	0.50
1:A:567:LYS:HB3	6:H:96:VAL:H	1.75	0.50
1:A:892:ALA:HA	1:A:895:LYS:HD3	1.93	0.50
2:B:841:MET:SD	2:B:990:ILE:HD11	2.51	0.50
2:B:1024:ALA:O	2:B:1025:HIS:C	2.54	0.50
3:C:260:LEU:O	3:C:264:GLN:HG3	2.12	0.50
6:H:76:THR:HG22	6:H:76:THR:O	2.12	0.50
7:I:119:THR:C	7:I:120:GLN:CG	2.84	0.50
4:E:204:THR:HG22	4:E:205:SER:N	2.27	0.50
1:A:705:LYS:HG3	1:A:713:SER:HB3	1.93	0.50
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.50
1:A:785:PRO:HB2	2:B:701:ILE:HD11	1.94	0.50
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.43	0.50
2:B:274:PRO:HG2	2:B:359:GLU:HB2	1.94	0.50
2:B:760:ASP:OD1	2:B:760:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.50
10:L:43:THR:HG22	10:L:43:THR:O	2.12	0.50
2:B:104:GLU:HG3	10:L:54:ARG:NH2	2.27	0.50
2:B:1170:THR:HG22	2:B:1170:THR:O	2.10	0.50
3:C:145:CYS:HA	8:J:2:ILE:CD1	2.41	0.50
4:E:130:ALA:HA	4:E:131:THR:HB	1.92	0.50
6:H:93:TYR:CD2	6:H:143:LEU:CB	2.94	0.50
1:A:265:LYS:HE3	1:A:323:LYS:HE2	1.93	0.50
1:A:472:LEU:HD11	2:B:835:GLN:HE22	1.76	0.50
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.75	0.50
1:A:1166:ASP:O	1:A:1170:ILE:HG12	2.11	0.50
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.93	0.50
5:F:103:MET:O	5:F:105:ALA:N	2.45	0.50
1:A:61:ILE:O	1:A:63:ARG:N	2.44	0.50
1:A:404:TYR:HB2	1:A:433:GLU:HG3	1.93	0.50
1:A:1292:PRO:HD3	1:A:1298:TYR:CE2	2.47	0.50
1:A:1434:ALA:CB	1:A:1436:ILE:HD12	2.40	0.50
2:B:472:ALA:CB	2:B:473:MET:HB2	2.29	0.50
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.79	0.50
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.12	0.50
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.94	0.50
10:L:46:VAL:O	10:L:47:ARG:HB2	2.11	0.50
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.47	0.49
1:A:902:LEU:O	1:A:903:ASN:CB	2.60	0.49
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.77	0.49
2:B:1076:HIS:CG	9:K:40:HIS:CD2	2.99	0.49
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.12	0.49
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.94	0.49
7:I:119:THR:HG22	7:I:119:THR:O	2.12	0.49
1:A:56:PRO:CD	1:A:57:ARG:H	2.25	0.49
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.47	0.49
1:A:257:ARG:HB2	1:A:258:GLY:HA2	1.83	0.49
1:A:403:LYS:O	1:A:404:TYR:O	2.30	0.49
1:A:881:GLN:NE2	1:A:958:VAL:O	2.45	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.94	0.49
4:E:65:THR:C	4:E:67:GLU:H	2.20	0.49
1:A:1101:LEU:HG	1:A:1105:LEU:CD1	2.42	0.49
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.42	0.49
1:A:107:CYS:SG	1:A:107:CYS:O	2.71	0.49
1:A:590:ARG:HB3	1:A:605:MET:N	2.27	0.49
1:A:805:LEU:C	1:A:805:LEU:CD1	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.95	0.49
1:A:1004:ASN:CG	1:A:1005:GLU:N	2.70	0.49
1:A:1004:ASN:HD22	4:E:167:ARG:HD2	1.76	0.49
4:E:128:PRO:HA	4:E:130:ALA:H	1.78	0.49
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.41	0.49
1:A:946:VAL:HG22	4:E:201:LYS:HB3	1.94	0.49
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.42	0.49
2:B:63:ILE:CD1	2:B:95:ILE:HD12	2.43	0.49
1:A:323:LYS:HB2	1:A:324:SER:C	2.37	0.49
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.94	0.49
2:B:30:SER:O	2:B:34:ILE:HD13	2.12	0.49
2:B:430:ARG:HA	2:B:433:GLN:HB2	1.95	0.49
2:B:788:ARG:NH1	2:B:790:ASP:OD2	2.41	0.49
1:A:209:ASN:O	1:A:210:ILE:C	2.54	0.49
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.48	0.49
6:H:109:LYS:CA	6:H:110:ASP:CB	2.77	0.49
9:K:47:ARG:HH11	9:K:47:ARG:CG	2.26	0.49
2:B:36:ALA:C	2:B:37:PHE:O	2.53	0.49
2:B:100:PRO:HA	2:B:126:SER:HA	1.94	0.49
1:A:971:PHE:O	1:A:972:HIS:C	2.55	0.49
1:A:1015:VAL:HG12	1:A:1019:CYS:HG	1.78	0.49
2:B:361:LEU:O	2:B:363:HIS:O	2.31	0.49
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.95	0.49
2:B:785:TYR:CD1	2:B:785:TYR:C	2.90	0.49
7:I:2:THR:O	7:I:3:THR:C	2.56	0.49
1:A:213:HIS:O	1:A:214:ILE:O	2.30	0.49
1:A:380:VAL:CG2	1:A:430:TRP:H	2.25	0.49
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.95	0.49
5:F:111:LEU:C	5:F:113:GLY:N	2.71	0.49
1:A:257:ARG:HB3	1:A:258:GLY:HA2	1.94	0.48
1:A:265:LYS:C	1:A:267:ALA:H	2.21	0.48
1:A:1266:THR:O	1:A:1271:ILE:HG12	2.13	0.48
2:B:868:MET:O	2:B:869:SER:HB3	2.13	0.48
3:C:175:ALA:HB3	8:J:43:ARG:NH2	2.27	0.48
1:A:530:GLY:O	1:A:532:ARG:N	2.46	0.48
1:A:633:VAL:HG11	1:A:645:LEU:HD22	1.95	0.48
1:A:1437:GLY:HA3	5:F:88:TYR:CD1	2.48	0.48
2:B:34:ILE:HD12	2:B:542:MET:CE	2.41	0.48
2:B:313:MET:O	2:B:316:PRO:HD2	2.13	0.48
2:B:314:LEU:C	2:B:316:PRO:HD2	2.38	0.48
5:F:79:ARG:NH2	5:F:145:ASP:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:3:VAL:HG12	8:J:4:PRO:CD	2.43	0.48
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.95	0.48
1:A:56:PRO:CD	1:A:58:LEU:HD13	2.37	0.48
1:A:623:GLY:O	1:A:630:ILE:HD13	2.13	0.48
1:A:1404:GLU:O	1:A:1408:ILE:HG12	2.13	0.48
2:B:34:ILE:HD12	2:B:743:ILE:HG21	1.95	0.48
2:B:639:ILE:HA	2:B:740:HIS:HB3	1.96	0.48
2:B:1104:HIS:HB2	2:B:1122:ARG:HB2	1.95	0.48
9:K:46:ILE:HG23	9:K:50:LEU:HD12	1.94	0.48
2:B:366:GLN:O	2:B:367:LEU:O	2.31	0.48
2:B:473:MET:C	2:B:475:SER:H	2.21	0.48
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.79	0.48
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.28	0.48
1:A:445:ASN:HB3	1:A:455:MET:HE2	1.95	0.48
1:A:990:VAL:CG2	1:A:1026:LEU:HB3	2.44	0.48
1:A:1015:VAL:O	1:A:1016:THR:C	2.56	0.48
2:B:46:GLN:HG3	2:B:47:GLN:H	1.79	0.48
2:B:479:VAL:O	2:B:480:SER:CB	2.61	0.48
2:B:485:ARG:HG3	2:B:485:ARG:HH11	1.77	0.48
6:H:129:TYR:C	6:H:131:ASN:N	2.66	0.48
1:A:91:PHE:HD2	1:A:297:GLN:OE1	1.97	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.48
2:B:637:LEU:HA	2:B:743:ILE:HG12	1.96	0.48
2:B:933:SER:OG	2:B:934:LYS:N	2.41	0.48
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.44	0.48
1:A:919:ILE:CG2	1:A:925:LEU:HD12	2.43	0.48
1:A:1172:LEU:HD23	1:A:1172:LEU:N	2.29	0.48
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.54	0.48
4:E:204:THR:CG2	4:E:205:SER:N	2.76	0.48
1:A:265:LYS:NZ	1:A:302:THR:CG2	2.76	0.48
1:A:290:GLU:HA	1:A:293:GLU:HG3	1.96	0.48
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.48	0.48
2:B:956:THR:HA	2:B:961:LEU:O	2.14	0.48
4:E:164:LEU:HD13	4:E:211:TYR:CE2	2.49	0.48
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.95	0.48
8:J:57:ILE:HA	8:J:60:PHE:CD1	2.49	0.48
1:A:319:GLY:O	1:A:320:ARG:HG3	2.14	0.48
1:A:351:THR:CG2	2:B:1103:ILE:HD12	2.42	0.48
2:B:552:MET:N	2:B:553:PRO:HD2	2.29	0.48
2:B:976:ILE:HG22	2:B:977:GLY:N	2.29	0.48
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.96	0.48
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.95	0.48
2:B:471:LYS:HB2	2:B:472:ALA:HA	1.96	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.96	0.48
4:E:127:ILE:O	4:E:127:ILE:HG12	2.13	0.48
1:A:67:CYS:O	1:A:70:CYS:HB3	2.13	0.47
1:A:274:ILE:O	1:A:274:ILE:HG22	2.13	0.47
2:B:451:LYS:O	2:B:452:THR:C	2.56	0.47
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.96	0.47
7:I:26:LEU:HD22	7:I:35:VAL:CG1	2.44	0.47
1:A:1021:LEU:CD1	1:A:1025:ARG:HH11	2.27	0.47
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.44	0.47
2:B:863:GLU:HG3	2:B:962:LYS:CB	2.43	0.47
2:B:473:MET:C	2:B:475:SER:N	2.71	0.47
2:B:778:MET:CE	2:B:853:SER:HB3	2.45	0.47
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.96	0.47
4:E:98:ILE:O	4:E:99:HIS:C	2.57	0.47
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.96	0.47
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.47
1:A:1120:LEU:HB3	1:A:1124:HIS:O	2.13	0.47
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.96	0.47
2:B:363:HIS:O	2:B:364:ILE:CB	2.62	0.47
2:B:435:THR:O	2:B:437:GLU:N	2.47	0.47
1:A:40:THR:HG22	1:A:41:MET:SD	2.55	0.47
1:A:469:ARG:HE	9:K:67:PHE:HZ	1.63	0.47
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	1.96	0.47
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.39	0.47
2:B:761:HIS:N	2:B:761:HIS:CD2	2.82	0.47
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.49	0.47
2:B:167:ILE:HD12	2:B:424:LEU:HD11	1.95	0.47
2:B:994:TYR:HB2	2:B:999:MET:CE	2.45	0.47
8:J:37:SER:OG	8:J:47:ARG:NH2	2.48	0.47
9:K:49:GLU:HB2	9:K:94:ILE:HD11	1.96	0.47
1:A:179:LEU:HD13	1:A:297:GLN:HG3	1.95	0.47
1:A:265:LYS:HZ3	1:A:302:THR:HG23	1.79	0.47
1:A:278:THR:O	1:A:278:THR:CG2	2.61	0.47
1:A:314:ALA:O	1:A:321:PRO:O	2.32	0.47
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.49	0.47
1:A:990:VAL:CG2	1:A:1026:LEU:HD13	2.45	0.47
1:A:1042:PHE:CE2	1:A:1046:LEU:HD12	2.50	0.47
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:PRO:HG3	2:B:181:LEU:CD1	2.44	0.47
2:B:977:GLY:CA	2:B:1099:VAL:CG2	2.92	0.47
2:B:446:LEU:O	2:B:447:ALA:HB3	2.14	0.47
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.97	0.47
2:B:1076:HIS:CG	9:K:40:HIS:HD2	2.32	0.47
1:A:261:ASP:HB3	1:A:323:LYS:HE3	1.96	0.47
1:A:535:THR:HG21	1:A:617:VAL:H	1.80	0.47
2:B:263:GLY:O	2:B:264:SER:C	2.58	0.47
2:B:809:MET:HE1	2:B:983:ARG:NH2	2.30	0.47
7:I:106:CYS:O	7:I:107:SER:C	2.58	0.47
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.97	0.47
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.45	0.46
1:A:1393:ASN:O	1:A:1394:THR:O	2.33	0.46
2:B:34:ILE:CD1	2:B:743:ILE:CG2	2.93	0.46
6:H:42:ILE:HD12	6:H:95:TYR:CE1	2.49	0.46
1:A:548:ASN:HA	9:K:60:ALA:HB1	1.96	0.46
1:A:1116:LEU:H	1:A:1308:THR:HB	1.80	0.46
1:A:341:MET:HB3	1:A:341:MET:HE3	1.65	0.46
1:A:737:LEU:HB2	1:A:744:LYS:HD2	1.97	0.46
2:B:617:ARG:HG2	2:B:617:ARG:NH1	2.27	0.46
3:C:163:ILE:CD1	9:K:10:PHE:CZ	2.98	0.46
3:C:163:ILE:HD11	9:K:10:PHE:CZ	2.50	0.46
1:A:169:ASN:N	1:A:169:ASN:HD22	2.13	0.46
1:A:323:LYS:CB	1:A:324:SER:HA	2.45	0.46
1:A:858:ASN:C	1:A:858:ASN:HD22	2.23	0.46
1:A:873:MET:HE3	1:A:957:PRO:HG2	1.98	0.46
1:A:1327:ILE:HG23	1:A:1327:ILE:O	2.16	0.46
4:E:114:ASN:O	4:E:115:ASN:CB	2.64	0.46
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.98	0.46
7:I:7:CYS:SG	7:I:8:ARG:O	2.74	0.46
1:A:108:MET:SD	1:A:108:MET:N	2.89	0.46
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.97	0.46
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.15	0.46
2:B:25:ILE:HG22	2:B:26:THR:N	2.30	0.46
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.46	0.46
3:C:262:LEU:HD21	9:K:19:LEU:HD12	1.97	0.46
1:A:495:GLU:HA	1:A:498:ARG:HG3	1.98	0.46
1:A:706:HIS:CG	1:A:1135:ARG:HH21	2.33	0.46
1:A:893:PHE:CD1	1:A:893:PHE:C	2.93	0.46
1:A:990:VAL:HG22	1:A:1026:LEU:CD1	2.45	0.46
1:A:1021:LEU:HD11	1:A:1025:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	2.14	0.46
4:E:77:SER:HB3	4:E:105:PHE:HD1	1.81	0.46
6:H:129:TYR:O	6:H:131:ASN:N	2.45	0.46
6:H:139:ASN:O	6:H:140:ALA:HB2	2.16	0.46
9:K:17:SER:O	9:K:18:LYS:C	2.57	0.46
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.97	0.46
1:A:65:LEU:O	1:A:67:CYS:N	2.44	0.46
1:A:351:THR:HG23	2:B:1103:ILE:HG23	1.97	0.46
1:A:531:ILE:HD13	1:A:649:ILE:CG2	2.46	0.46
2:B:1146:PHE:CZ	2:B:1150:ARG:HG3	2.51	0.46
6:H:109:LYS:HB3	6:H:110:ASP:HB3	1.81	0.46
7:I:15:TYR:O	7:I:27:PHE:HA	2.16	0.46
1:A:304:MET:CG	2:B:1210:MET:HG3	2.45	0.46
1:A:765:VAL:HG23	1:A:802:ASN:O	2.16	0.46
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.16	0.46
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.30	0.46
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.15	0.46
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.16	0.46
3:C:29:MET:HB2	9:K:45:LEU:CD1	2.46	0.46
1:A:367:PRO:HA	1:A:463:ILE:HD12	1.98	0.46
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.97	0.46
1:A:517:ASN:ND2	1:A:1364:ASN:OD1	2.48	0.46
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.16	0.46
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.16	0.46
1:A:1146:VAL:HG12	1:A:1201:ALA:HB3	1.98	0.46
2:B:104:GLU:CD	10:L:54:ARG:NH2	2.74	0.46
2:B:354:ASP:O	2:B:357:GLN:N	2.49	0.46
2:B:752:ALA:O	2:B:755:ILE:HB	2.15	0.46
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.98	0.46
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.98	0.46
1:A:763:ALA:O	1:A:803:SER:HB3	2.15	0.46
1:A:975:HIS:HA	1:A:1036:ARG:HD2	1.98	0.46
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.51	0.46
2:B:219:ALA:HB3	2:B:222:ILE:HD11	1.98	0.46
2:B:1060:ARG:C	2:B:1062:HIS:N	2.73	0.46
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.98	0.45
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.97	0.45
2:B:860:MET:HE2	2:B:965:LYS:HE2	1.98	0.45
1:A:134:ARG:NH1	1:A:221:SER:HA	2.30	0.45
1:A:247:ARG:CG	1:A:247:ARG:O	2.64	0.45
1:A:265:LYS:HZ3	1:A:302:THR:CG2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:ALA:HA	1:A:895:LYS:HB2	1.97	0.45
1:A:933:TYR:O	1:A:937:VAL:HG23	2.16	0.45
2:B:288:ALA:O	2:B:327:ARG:NH2	2.48	0.45
2:B:698:GLU:O	2:B:701:ILE:CD1	2.63	0.45
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.51	0.45
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.45
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.98	0.45
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.46	0.45
5:F:111:LEU:N	5:F:111:LEU:CD1	2.79	0.45
6:H:47:PHE:HB3	6:H:95:TYR:CD2	2.45	0.45
12:T:21:O2I:C8	12:T:22:DT:H72	2.45	0.45
1:A:294:SER:O	1:A:298:PHE:HB3	2.16	0.45
1:A:549:MET:O	1:A:550:LEU:C	2.60	0.45
1:A:808:LEU:O	2:B:728:ARG:NH1	2.49	0.45
1:A:997:LEU:O	1:A:1053:PHE:CE1	2.70	0.45
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.98	0.45
2:B:800:GLN:HG2	8:J:52:THR:CG2	2.43	0.45
5:F:98:ALA:HA	5:F:101:ILE:HD12	1.99	0.45
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.98	0.45
1:A:718:VAL:O	1:A:722:LEU:HD12	2.17	0.45
1:A:913:LEU:HD12	1:A:915:SER:H	1.80	0.45
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.99	0.45
8:J:45:CYS:SG	8:J:46:CYS:N	2.90	0.45
1:A:56:PRO:HD2	1:A:57:ARG:H	1.81	0.45
1:A:605:MET:SD	1:A:621:THR:HG21	2.57	0.45
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.56	0.45
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.98	0.45
1:A:990:VAL:HG21	1:A:1026:LEU:HB3	1.99	0.45
2:B:128:LEU:HD12	2:B:128:LEU:HA	1.84	0.45
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.97	0.45
2:B:530:GLY:O	2:B:531:GLN:C	2.59	0.45
2:B:832:GLY:O	2:B:835:GLN:NE2	2.49	0.45
6:H:5:LEU:HD22	6:H:133:ASN:O	2.17	0.45
9:K:57:LEU:HD12	9:K:76:GLN:CG	2.46	0.45
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.28	0.45
2:B:287:ARG:HG2	2:B:292:ILE:CD1	2.44	0.45
2:B:635:ARG:HD2	2:B:636:PRO:HD3	1.98	0.45
9:K:71:PHE:CD1	9:K:71:PHE:C	2.94	0.45
11:R:5:A:N1	12:T:24:DT:O4	2.50	0.45
1:A:338:GLY:O	1:A:342:GLY:O	2.34	0.45
1:A:870:GLU:CB	4:E:204:THR:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.98	0.45
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.98	0.45
2:B:364:ILE:O	2:B:365:THR:HB	2.17	0.45
2:B:421:PHE:O	2:B:425:THR:HB	2.15	0.45
2:B:737:THR:HG23	7:I:66:PRO:HB3	1.98	0.45
2:B:780:VAL:HA	2:B:795:ILE:HG23	1.98	0.45
2:B:1024:ALA:O	2:B:1027:ILE:N	2.50	0.45
7:I:75:CYS:HB3	7:I:103:CYS:HB2	1.99	0.45
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.97	0.45
3:C:124:LEU:O	3:C:127:ARG:HG2	2.17	0.45
3:C:231:ASN:HD22	3:C:231:ASN:C	2.25	0.45
4:E:78:LEU:HD12	4:E:107:THR:HG21	1.99	0.45
1:A:41:MET:HE2	1:A:61:ILE:CD1	2.46	0.45
1:A:98:LYS:O	1:A:102:VAL:HG22	2.17	0.45
1:A:401:GLY:C	1:A:435:HIS:ND1	2.75	0.45
1:A:1256:GLU:O	1:A:1257:ASP:C	2.60	0.45
2:B:475:SER:C	2:B:477:ALA:N	2.75	0.45
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.17	0.45
2:B:628:THR:O	2:B:628:THR:CG2	2.64	0.45
2:B:798:TYR:N	2:B:799:PRO:CD	2.80	0.45
10:L:31:CYS:SG	10:L:32:ALA:N	2.90	0.45
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.99	0.45
1:A:1347:ALA:O	1:A:1348:LEU:C	2.59	0.45
2:B:291:ILE:HG21	2:B:300:HIS:CD2	2.51	0.45
2:B:979:LYS:NZ	11:R:8:U:OP1	2.49	0.45
6:H:31:THR:O	6:H:32:THR:OG1	2.29	0.45
7:I:85:PHE:CD1	7:I:85:PHE:C	2.96	0.45
1:A:326:ARG:O	1:A:330:LYS:N	2.50	0.44
1:A:1349:TYR:O	1:A:1350:LYS:C	2.60	0.44
2:B:22:SER:O	2:B:654:ARG:HD2	2.17	0.44
3:C:17:ASN:OD1	3:C:233:GLU:HG3	2.17	0.44
3:C:134:ILE:HD12	3:C:141:GLY:N	2.32	0.44
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.98	0.44
2:B:104:GLU:HG3	10:L:54:ARG:HH21	1.82	0.44
2:B:636:PRO:CD	2:B:637:LEU:HB3	2.47	0.44
6:H:51:ALA:O	6:H:52:GLN:C	2.60	0.44
1:A:120:GLU:HG3	1:A:123:ARG:HD3	2.00	0.44
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.52	0.44
1:A:380:VAL:HG23	1:A:430:TRP:H	1.82	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.97	0.44
2:B:745:PRO:O	2:B:747:MET:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.50	0.44
6:H:106:GLU:C	6:H:108:SER:N	2.73	0.44
1:A:15:LYS:HB3	2:B:1220:ARG:HA	2.00	0.44
1:A:90:VAL:HG13	1:A:297:GLN:HB2	1.99	0.44
1:A:99:ILE:HA	1:A:102:VAL:CG2	2.47	0.44
1:A:543:LEU:O	1:A:547:LEU:HG	2.17	0.44
2:B:737:THR:HG23	7:I:66:PRO:HB2	1.99	0.44
2:B:1180:PHE:O	2:B:1181:GLU:O	2.35	0.44
4:E:114:ASN:O	4:E:115:ASN:HB3	2.18	0.44
1:A:1057:VAL:HG12	1:A:1058:VAL:O	2.18	0.44
1:A:1208:THR:O	1:A:1209:MET:C	2.60	0.44
2:B:295:GLY:HA2	2:B:298:LEU:HG	1.98	0.44
2:B:701:ILE:HB	2:B:740:HIS:CE1	2.52	0.44
2:B:849:GLY:HA2	2:B:852:ARG:HD2	2.00	0.44
2:B:955:THR:HG22	2:B:956:THR:N	2.32	0.44
3:C:46:ILE:HA	3:C:159:ALA:HA	1.98	0.44
1:A:546:VAL:HG12	1:A:550:LEU:HD23	1.97	0.44
1:A:1344:GLY:O	1:A:1345:ARG:C	2.60	0.44
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.66	0.44
6:H:40:LEU:CD2	6:H:42:ILE:HD11	2.48	0.44
1:A:476:SER:N	1:A:477:PRO:HD2	2.33	0.44
1:A:507:VAL:N	1:A:508:PRO:CD	2.80	0.44
1:A:733:ALA:O	1:A:735:VAL:N	2.51	0.44
2:B:174:LEU:HD23	2:B:202:TYR:CZ	2.53	0.44
2:B:634:TYR:HE1	2:B:692:TYR:CD2	2.34	0.44
2:B:635:ARG:CB	2:B:636:PRO:CD	2.95	0.44
5:F:81:THR:O	5:F:82:THR:C	2.61	0.44
7:I:17:ARG:CG	7:I:18:GLU:H	2.27	0.44
1:A:54:ASN:O	1:A:54:ASN:OD1	2.36	0.44
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.52	0.44
1:A:913:LEU:HD12	1:A:914:GLU:N	2.33	0.44
1:A:1158:PRO:HB3	1:A:1188:GLN:HG3	1.99	0.44
1:A:1365:TYR:O	1:A:1366:ARG:C	2.60	0.44
2:B:361:LEU:N	2:B:362:PRO:CD	2.80	0.44
2:B:485:ARG:HH11	2:B:485:ARG:CG	2.31	0.44
2:B:789:MET:HE1	2:B:965:LYS:O	2.18	0.44
2:B:1161:HIS:CD2	2:B:1173:ALA:HB2	2.53	0.44
3:C:6:PRO:HG2	9:K:97:LYS:HB3	2.00	0.44
5:F:99:LEU:HD13	5:F:99:LEU:C	2.43	0.44
6:H:82:PRO:O	6:H:83:GLN:HB2	2.17	0.44
1:A:129:LYS:O	1:A:130:ASP:CB	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PRO:O	1:A:247:ARG:NH2	2.44	0.44
1:A:532:ARG:HG2	1:A:533:LYS:N	2.33	0.44
1:A:894:GLU:C	1:A:896:ARG:H	2.25	0.44
2:B:247:GLY:O	2:B:248:SER:CB	2.66	0.44
2:B:642:ASP:O	2:B:644:GLU:N	2.51	0.44
3:C:39:ALA:HA	3:C:164:ALA:CB	2.47	0.44
3:C:166:GLU:O	9:K:6:ARG:NH1	2.50	0.44
6:H:42:ILE:HD12	6:H:95:TYR:CZ	2.53	0.44
6:H:91:ASP:C	6:H:93:TYR:H	2.26	0.44
1:A:314:ALA:HB1	1:A:321:PRO:HB2	2.00	0.43
1:A:325:ILE:O	1:A:328:ARG:HB2	2.18	0.43
1:A:834:THR:HG21	1:A:1077:THR:HA	2.00	0.43
1:A:1004:ASN:ND2	4:E:167:ARG:CD	2.80	0.43
1:A:1422:ARG:HH21	2:B:1220:ARG:HD3	1.83	0.43
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.00	0.43
2:B:640:VAL:O	2:B:640:VAL:HG12	2.17	0.43
4:E:135:PHE:CB	4:E:140:LEU:HD11	2.48	0.43
6:H:101:ALA:HB2	6:H:116:TYR:CE1	2.53	0.43
11:R:2:U:O5'	11:R:2:U:C6	2.71	0.43
1:A:209:ASN:O	1:A:212:LYS:N	2.51	0.43
1:A:582:ILE:CG2	1:A:610:GLY:HA2	2.49	0.43
2:B:557:PHE:CD1	2:B:557:PHE:C	2.96	0.43
2:B:1168:LEU:HD22	2:B:1208:MET:SD	2.58	0.43
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.28	0.43
1:A:148:CYS:HB3	1:A:167:CYS:O	2.17	0.43
1:A:553:VAL:HG22	1:A:652:VAL:HG22	2.00	0.43
1:A:1326:ARG:O	1:A:1327:ILE:C	2.60	0.43
2:B:113:TYR:O	2:B:114:PRO:C	2.62	0.43
2:B:634:TYR:CD1	2:B:634:TYR:C	2.96	0.43
3:C:144:ILE:HD13	3:C:144:ILE:HA	1.89	0.43
9:K:91:CYS:O	9:K:94:ILE:HB	2.19	0.43
10:L:34:CYS:O	10:L:35:SER:CB	2.66	0.43
1:A:1160:SER:HA	1:A:1170:ILE:HG21	2.00	0.43
2:B:203:PHE:HE2	2:B:212:LEU:HD12	1.84	0.43
2:B:333:PHE:CD1	2:B:333:PHE:O	2.71	0.43
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.53	0.43
2:B:596:LEU:O	2:B:599:THR:HB	2.18	0.43
2:B:728:ARG:NH2	2:B:760:ASP:OD2	2.49	0.43
2:B:790:ASP:OD1	2:B:790:ASP:N	2.51	0.43
2:B:1134:GLU:OE1	2:B:1134:GLU:N	2.51	0.43
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:22:DT:H5''	12:T:22:DT:H6	1.83	0.43
1:A:33:ALA:HA	1:A:56:PRO:CG	2.48	0.43
1:A:399:HIS:O	1:A:435:HIS:ND1	2.52	0.43
1:A:690:VAL:HG13	1:A:718:VAL:HG22	2.00	0.43
2:B:178:ASN:O	2:B:179:CYS:C	2.61	0.43
3:C:36:VAL:HG23	9:K:41:THR:CG2	2.45	0.43
8:J:43:ARG:O	8:J:47:ARG:HD2	2.19	0.43
1:A:92:HIS:CD2	1:A:304:MET:HE3	2.53	0.43
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.00	0.43
1:A:567:LYS:CB	1:A:568:PRO:CD	2.82	0.43
2:B:203:PHE:CE2	2:B:212:LEU:HD12	2.54	0.43
2:B:542:MET:HE3	2:B:747:MET:HG3	2.01	0.43
2:B:1039:GLY:HA2	8:J:51:LEU:CD2	2.49	0.43
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.43	0.43
3:C:62:PHE:O	3:C:65:HIS:HB3	2.18	0.43
6:H:101:ALA:HB2	6:H:116:TYR:CD1	2.53	0.43
1:A:884:ASP:OD1	1:A:884:ASP:N	2.46	0.43
1:A:924:LYS:HE3	1:A:924:LYS:HB2	1.91	0.43
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.19	0.43
2:B:124:TYR:OH	2:B:179:CYS:SG	2.74	0.43
2:B:315:LYS:N	2:B:316:PRO:CD	2.82	0.43
2:B:321:GLY:C	2:B:323:VAL:H	2.27	0.43
2:B:1043:ASP:OD1	2:B:1043:ASP:C	2.61	0.43
3:C:133:ILE:HD13	3:C:236:GLY:C	2.44	0.43
8:J:7:CYS:HA	8:J:49:MET:HE3	2.00	0.43
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.49	0.43
1:A:588:LEU:HD13	1:A:632:VAL:HG21	1.99	0.43
1:A:1173:HIS:CD2	1:A:1227:ILE:CG1	2.90	0.43
1:A:1386:ARG:HA	1:A:1390:ASN:HB2	2.01	0.43
2:B:461:LEU:HD12	2:B:466:TRP:CZ3	2.53	0.43
2:B:701:ILE:HB	2:B:740:HIS:HE1	1.84	0.43
2:B:711:GLU:N	2:B:712:PRO:HD3	2.33	0.43
3:C:238:ILE:HG22	3:C:239:PRO:O	2.18	0.43
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.18	0.43
10:L:42:ARG:O	10:L:43:THR:CB	2.67	0.43
1:A:359:LEU:O	1:A:471:ASN:ND2	2.51	0.43
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.51	0.43
1:A:1105:LEU:CD2	1:A:1384:VAL:HG21	2.49	0.43
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.33	0.43
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.34	0.43
2:B:549:THR:HG22	2:B:550:ASP:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:984:HIS:CD2	2:B:1024:ALA:HB3	2.54	0.43
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.18	0.43
3:C:220:ASP:CG	3:C:223:ALA:HB2	2.44	0.43
9:K:49:GLU:CG	9:K:94:ILE:HD11	2.48	0.43
10:L:46:VAL:O	10:L:47:ARG:HB3	2.18	0.43
1:A:90:VAL:O	1:A:235:ILE:HG22	2.19	0.43
1:A:675:THR:CG2	1:A:736:ASN:HD21	2.31	0.43
1:A:715:GLU:O	1:A:719:VAL:HG23	2.19	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.00	0.43
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.01	0.43
2:B:751:VAL:HG12	2:B:752:ALA:N	2.34	0.43
1:A:714:PHE:CD2	7:I:97:MET:HE1	2.54	0.42
1:A:902:LEU:O	1:A:903:ASN:HB2	2.18	0.42
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.49	0.42
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.34	0.42
1:A:451:HIS:HB3	1:A:453:MET:N	2.33	0.42
2:B:732:SER:CB	2:B:734:HIS:CD2	3.02	0.42
1:A:106:VAL:CG1	1:A:107:CYS:N	2.82	0.42
1:A:614:PHE:CD1	1:A:614:PHE:C	2.97	0.42
1:A:630:ILE:HD12	1:A:630:ILE:N	2.33	0.42
1:A:863:VAL:HG11	1:A:866:PHE:CE1	2.54	0.42
1:A:940:ARG:O	1:A:944:ARG:HG3	2.20	0.42
2:B:93:GLY:O	2:B:94:LYS:C	2.62	0.42
2:B:476:ARG:O	2:B:478:GLY:N	2.52	0.42
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.67	0.42
2:B:1084:GLN:CD	2:B:1084:GLN:N	2.77	0.42
1:A:314:ALA:HB1	1:A:321:PRO:CB	2.50	0.42
1:A:535:THR:O	1:A:536:LEU:C	2.62	0.42
1:A:573:SER:O	1:A:576:GLN:HB2	2.19	0.42
1:A:1242:VAL:O	1:A:1243:VAL:HG23	2.20	0.42
1:A:1397:LEU:O	1:A:1400:CYS:HB2	2.19	0.42
1:A:1406:VAL:HG12	1:A:1407:GLU:N	2.34	0.42
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.42
2:B:771:SER:O	2:B:775:LYS:HE3	2.20	0.42
3:C:18:VAL:HG23	3:C:240:VAL:HG11	2.01	0.42
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.84	0.42
4:E:19:VAL:HA	4:E:22:MET:HE2	2.00	0.42
6:H:125:LEU:HD12	6:H:125:LEU:HA	1.93	0.42
1:A:247:ARG:O	1:A:247:ARG:HG3	2.19	0.42
1:A:445:ASN:CB	1:A:455:MET:HE2	2.49	0.42
1:A:471:ASN:O	1:A:474:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:VAL:O	1:A:719:VAL:C	2.62	0.42
2:B:310:MET:O	2:B:313:MET:HB2	2.20	0.42
2:B:737:THR:O	2:B:738:PHE:C	2.63	0.42
1:A:211:PHE:CG	1:A:231:PRO:HB2	2.54	0.42
1:A:261:ASP:CB	1:A:323:LYS:HD3	2.48	0.42
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.55	0.42
1:A:845:LEU:O	1:A:847:ASP:N	2.52	0.42
2:B:286:PHE:HB3	2:B:297:ILE:CD1	2.48	0.42
5:F:97:ARG:HG3	5:F:101:ILE:HD11	2.01	0.42
5:F:99:LEU:HD11	5:F:103:MET:HE3	2.02	0.42
7:I:25:LEU:HD12	7:I:26:LEU:H	1.85	0.42
1:A:494:SER:N	2:B:1149:GLU:OE2	2.53	0.42
1:A:852:TYR:CD1	1:A:1060:PRO:CB	3.02	0.42
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	2.02	0.42
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.01	0.42
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.02	0.42
3:C:260:LEU:O	3:C:263:THR:HB	2.20	0.42
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.50	0.42
1:A:99:ILE:HA	1:A:102:VAL:HG23	2.01	0.42
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.55	0.42
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.50	0.42
1:A:1410:PHE:CD1	2:B:1212:ILE:HD11	2.54	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
2:B:816:GLU:C	2:B:818:PRO:HD3	2.45	0.42
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.97	0.42
1:A:12:ARG:HD3	2:B:1192:TYR:CE1	2.55	0.42
1:A:56:PRO:CD	1:A:57:ARG:N	2.83	0.42
1:A:283:GLY:O	1:A:285:PRO:HD3	2.20	0.42
1:A:338:GLY:C	1:A:339:ASN:HD22	2.28	0.42
1:A:733:ALA:C	1:A:735:VAL:N	2.77	0.42
1:A:794:PRO:O	1:A:795:GLU:C	2.63	0.42
2:B:488:TYR:CE2	2:B:492:LEU:HD11	2.55	0.42
2:B:636:PRO:CB	2:B:637:LEU:HB3	2.50	0.42
3:C:242:GLN:O	3:C:246:ARG:HG3	2.19	0.42
1:A:287:HIS:O	1:A:288:ALA:HB2	2.19	0.42
1:A:356:ASP:OD1	1:A:356:ASP:C	2.63	0.42
1:A:690:VAL:HG21	1:A:722:LEU:HD11	2.00	0.42
1:A:759:ALA:O	1:A:763:ALA:HB3	2.19	0.42
1:A:853:ASP:OD2	1:A:855:THR:HG22	2.20	0.42
1:A:929:LEU:HD13	1:A:929:LEU:HA	1.91	0.42
1:A:950:GLY:HA3	1:A:1298:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:LEU:CD1	1:A:1026:LEU:CD1	2.97	0.42
2:B:123:THR:HG22	2:B:125:SER:HB3	2.01	0.42
3:C:163:ILE:O	3:C:164:ALA:C	2.63	0.42
6:H:44:VAL:HG13	6:H:48:PRO:HA	2.02	0.42
7:I:75:CYS:CB	7:I:103:CYS:HB2	2.50	0.42
1:A:107:CYS:O	1:A:108:MET:O	2.37	0.41
1:A:1225:PHE:C	1:A:1226:VAL:HG23	2.45	0.41
2:B:34:ILE:CD1	2:B:743:ILE:HG21	2.50	0.41
2:B:461:LEU:HD12	2:B:466:TRP:CH2	2.55	0.41
2:B:585:VAL:HG12	2:B:587:HIS:CD2	2.55	0.41
3:C:70:ILE:HD11	3:C:115:SER:HB3	2.02	0.41
3:C:249:ASP:O	3:C:252:GLN:HB3	2.20	0.41
4:E:90:VAL:HG13	4:E:91:LYS:N	2.34	0.41
1:A:54:ASN:O	1:A:55:ASP:CG	2.64	0.41
1:A:857:ARG:HB3	1:A:863:VAL:HA	2.02	0.41
1:A:1140:HIS:HB3	1:A:1279:ILE:O	2.20	0.41
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.54	0.41
2:B:1022:THR:O	2:B:1022:THR:HG23	2.20	0.41
3:C:229:TYR:CD1	3:C:229:TYR:N	2.87	0.41
4:E:178:ILE:HB	4:E:212:ARG:HD3	2.01	0.41
1:A:511:ILE:CG1	1:A:521:MET:HE3	2.50	0.41
1:A:809:THR:HB	1:A:810:PRO:HD2	2.01	0.41
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.67	0.41
1:A:1433:MET:HE3	1:A:1439:GLY:HA2	2.01	0.41
2:B:56:ASP:C	2:B:57:TYR:HD1	2.28	0.41
2:B:816:GLU:O	8:J:56:LEU:HD21	2.20	0.41
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.55	0.41
7:I:59:VAL:O	7:I:62:ILE:HB	2.20	0.41
7:I:96:SER:HB2	7:I:98:VAL:HG23	2.02	0.41
1:A:332:LYS:H	1:A:337:ARG:HB2	1.84	0.41
1:A:505:CYS:SG	2:B:1141:HIS:HD2	2.43	0.41
1:A:1064:VAL:O	1:A:1065:GLY:C	2.63	0.41
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.20	0.41
2:B:167:ILE:HG23	2:B:424:LEU:CD1	2.50	0.41
2:B:957:ASN:O	2:B:958:GLN:C	2.63	0.41
3:C:14:SER:OG	3:C:17:ASN:N	2.53	0.41
1:A:33:ALA:HA	1:A:56:PRO:HG2	2.02	0.41
1:A:873:MET:HE1	1:A:1053:PHE:CZ	2.56	0.41
1:A:898:ARG:HB2	1:A:933:TYR:CE2	2.56	0.41
1:A:925:LEU:C	1:A:927:VAL:N	2.78	0.41
1:A:1025:ARG:O	1:A:1035:TYR:OH	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:PHE:C	1:A:1226:VAL:CG2	2.94	0.41
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.55	0.41
2:B:696:GLU:O	2:B:699:GLU:HB2	2.21	0.41
2:B:1171:VAL:HG12	2:B:1172:ILE:H	1.85	0.41
3:C:100:THR:O	3:C:119:VAL:HB	2.20	0.41
6:H:24:CYS:HB2	6:H:44:VAL:HG21	2.01	0.41
6:H:38:LEU:HD13	6:H:125:LEU:HD13	2.02	0.41
1:A:88:LYS:O	1:A:89:PRO:O	2.38	0.41
1:A:311:GLN:HB3	1:A:312:PRO:CD	2.50	0.41
1:A:795:GLU:OE1	2:B:731:VAL:HG11	2.21	0.41
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.55	0.41
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.61	0.41
1:A:1400:CYS:C	1:A:1402:PHE:H	2.29	0.41
1:A:1404:GLU:HB3	1:A:1407:GLU:HG3	2.03	0.41
2:B:1219:ASP:C	2:B:1221:SER:H	2.28	0.41
1:A:343:LYS:HE3	2:B:1151:LEU:HG	2.02	0.41
1:A:380:VAL:HG21	1:A:430:TRP:HB2	2.01	0.41
1:A:657:LEU:O	1:A:661:GLY:N	2.50	0.41
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.35	0.41
2:B:785:TYR:CD1	2:B:786:ASN:N	2.89	0.41
2:B:1060:ARG:C	2:B:1062:HIS:H	2.27	0.41
6:H:82:PRO:HA	6:H:84:ALA:HB3	2.01	0.41
9:K:90:ALA:O	9:K:91:CYS:C	2.63	0.41
1:A:120:GLU:O	1:A:120:GLU:CG	2.69	0.41
1:A:128:ILE:CG2	1:A:128:ILE:O	2.68	0.41
1:A:134:ARG:HH11	1:A:221:SER:C	2.26	0.41
1:A:901:LEU:O	1:A:902:LEU:C	2.63	0.41
2:B:69:LEU:HB2	2:B:90:ILE:HB	2.03	0.41
2:B:258:LEU:HD11	2:B:267:ARG:HB3	2.02	0.41
2:B:431:TYR:CG	2:B:447:ALA:HB1	2.56	0.41
2:B:912:ILE:O	2:B:938:SER:HB2	2.20	0.41
2:B:1146:PHE:CE2	2:B:1150:ARG:HG3	2.56	0.41
3:C:57:VAL:CG1	8:J:60:PHE:CB	2.98	0.41
3:C:166:GLU:O	9:K:6:ARG:HG3	2.20	0.41
4:E:127:ILE:O	4:E:127:ILE:CG1	2.69	0.41
8:J:59:LYS:O	8:J:62:ARG:HB2	2.21	0.41
1:A:317:LYS:HD2	1:A:317:LYS:N	2.36	0.41
1:A:370:ILE:HG22	1:A:374:LEU:HD12	2.01	0.41
1:A:455:MET:HE3	2:B:1134:GLU:CG	2.51	0.41
1:A:609:ASP:O	1:A:610:GLY:C	2.64	0.41
1:A:853:ASP:C	1:A:855:THR:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.20	0.41
2:B:431:TYR:CG	2:B:447:ALA:CB	3.04	0.41
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.36	0.41
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.36	0.41
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.41
2:B:1163:CYS:SG	2:B:1166:CYS:N	2.90	0.41
3:C:120:ILE:CD1	3:C:130:GLY:O	2.69	0.41
3:C:142:VAL:HG13	8:J:5:VAL:HG22	2.03	0.41
4:E:147:HIS:O	4:E:148:GLU:C	2.63	0.41
1:A:48:ALA:C	1:A:49:LYS:HG3	2.46	0.41
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.51	0.41
1:A:1444:MET:HB3	1:A:1445:ILE:H	1.72	0.41
2:B:34:ILE:HG23	2:B:542:MET:HE2	2.02	0.41
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.21	0.41
2:B:863:GLU:C	2:B:864:LYS:HG3	2.46	0.41
4:E:182:ASP:HA	4:E:183:PRO:HD2	1.88	0.41
7:I:17:ARG:O	7:I:25:LEU:HD12	2.19	0.41
7:I:119:THR:C	7:I:120:GLN:HG2	2.45	0.41
8:J:59:LYS:O	8:J:62:ARG:CB	2.69	0.41
10:L:32:ALA:HB3	10:L:55:ILE:O	2.20	0.41
1:A:665:GLY:HA2	2:B:1086:PHE:CD1	2.56	0.40
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.21	0.40
2:B:299:GLU:OE1	2:B:572:HIS:HB3	2.21	0.40
2:B:467:GLY:HA3	2:B:473:MET:SD	2.61	0.40
2:B:800:GLN:CG	8:J:52:THR:CG2	2.99	0.40
2:B:1095:LEU:C	2:B:1096:ARG:O	2.63	0.40
4:E:215:MET:HE3	4:E:215:MET:HB3	1.98	0.40
6:H:15:VAL:O	6:H:15:VAL:CG1	2.69	0.40
6:H:81:PRO:CB	6:H:82:PRO:HD2	2.51	0.40
1:A:364:VAL:HG12	1:A:458:HIS:HB3	2.03	0.40
1:A:541:ILE:CD1	1:A:574:GLY:HA2	2.51	0.40
1:A:648:ASN:O	1:A:649:ILE:C	2.65	0.40
1:A:1022:LEU:HD11	1:A:1026:LEU:HD12	2.03	0.40
1:A:1107:VAL:HG23	1:A:1383:SER:HA	2.02	0.40
2:B:190:TYR:CE2	8:J:62:ARG:HG2	2.56	0.40
2:B:737:THR:CG2	7:I:66:PRO:HB2	2.51	0.40
2:B:803:LEU:N	2:B:822:ASN:HD21	2.19	0.40
2:B:986:GLN:HE22	2:B:1016:ALA:HB1	1.86	0.40
2:B:1183:LYS:HE2	2:B:1183:LYS:O	2.21	0.40
4:E:198:ILE:N	4:E:210:SER:O	2.53	0.40
5:F:99:LEU:C	5:F:99:LEU:CD1	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:93:TYR:HD1	6:H:145:ARG:HB3	1.86	0.40
1:A:184:SER:O	1:A:185:TRP:CG	2.75	0.40
1:A:311:GLN:HB3	1:A:312:PRO:HD2	2.04	0.40
1:A:532:ARG:O	1:A:535:THR:HB	2.21	0.40
2:B:46:GLN:HG3	2:B:47:GLN:N	2.36	0.40
2:B:1129:ARG:HH21	2:B:1131:GLY:CA	2.27	0.40
3:C:175:ALA:HB3	8:J:43:ARG:HH22	1.86	0.40
4:E:76:GLY:O	4:E:77:SER:C	2.63	0.40
5:F:74:ILE:HG23	5:F:75:PRO:HD2	2.03	0.40
6:H:76:THR:O	6:H:77:ARG:O	2.39	0.40
9:K:49:GLU:HG3	9:K:94:ILE:CD1	2.52	0.40
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.86	0.40
1:A:734:GLU:O	1:A:734:GLU:HG3	2.20	0.40
1:A:814:PHE:O	1:A:817:ALA:HB3	2.22	0.40
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.57	0.40
3:C:253:LYS:O	3:C:256:ALA:HB3	2.21	0.40
6:H:11:GLN:HA	6:H:53:ASP:O	2.21	0.40
6:H:63:LEU:HD12	6:H:63:LEU:N	2.36	0.40
1:A:367:PRO:HB3	1:A:465:TYR:O	2.22	0.40
1:A:564:ALA:O	6:H:97:MET:HA	2.22	0.40
1:A:834:THR:HB	1:A:1077:THR:HG23	2.03	0.40
1:A:1364:ASN:O	1:A:1365:TYR:C	2.64	0.40
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.90	0.40
2:B:639:ILE:HD11	2:B:691:GLU:HG3	2.04	0.40
2:B:860:MET:HG2	2:B:861:ASP:N	2.36	0.40
2:B:979:LYS:C	2:B:980:PHE:CD1	2.99	0.40
3:C:141:GLY:C	3:C:142:VAL:O	2.64	0.40
3:C:174:ALA:O	8:J:10:CYS:O	2.39	0.40
4:E:78:LEU:HG	4:E:79:TRP:N	2.37	0.40
6:H:91:ASP:C	6:H:93:TYR:N	2.78	0.40
9:K:12:LEU:HD12	9:K:12:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	1217/1520 (80%)	984 (81%)	233 (19%)	1	9
2	B	960/1061 (90%)	782 (82%)	178 (18%)	1	10
3	C	234/274 (85%)	202 (86%)	32 (14%)	3	17
4	E	196/197 (100%)	165 (84%)	31 (16%)	2	14
5	F	74/137 (54%)	60 (81%)	14 (19%)	1	10
6	H	117/128 (91%)	98 (84%)	19 (16%)	2	13
7	I	113/116 (97%)	97 (86%)	16 (14%)	3	16
8	J	60/65 (92%)	45 (75%)	15 (25%)	0	4
9	K	99/102 (97%)	83 (84%)	16 (16%)	2	13
10	L	40/57 (70%)	28 (70%)	12 (30%)	0	3
All	All	3110/3657 (85%)	2544 (82%)	566 (18%)	2	11

All (566) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
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	53	LEU
1	A	60	SER
1	A	65	LEU
1	A	68	GLN
1	A	69	THR

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Mol	Chain	Res	Type
1	A	71	GLN
1	A	80	HIS
1	A	83	HIS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	98	LYS
1	A	102	VAL
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	222	LEU
1	A	225	ASN
1	A	235	ILE
1	A	239	LEU
1	A	256	GLN
1	A	260	ASP
1	A	263	THR
1	A	265	LYS
1	A	266	LEU
1	A	271	LYS
1	A	287	HIS
1	A	295	LEU
1	A	297	GLN
1	A	302	THR
1	A	304	MET
1	A	306	ASN
1	A	308	ILE

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	317	LYS
1	A	323	LYS
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	341	MET
1	A	348	SER
1	A	359	LEU
1	A	364	VAL
1	A	372	LYS
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	416	ARG
1	A	419	LYS
1	A	424	ILE
1	A	433	GLU
1	A	434	ARG
1	A	437	MET
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	469	ARG
1	A	475	THR
1	A	476	SER
1	A	479	ASN
1	A	481	ASP
1	A	496	GLU
1	A	500	GLU
1	A	501	LEU
1	A	512	VAL
1	A	513	SER
1	A	524	VAL

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Mol	Chain	Res	Type
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	618	GLU
1	A	629	LEU
1	A	652	VAL
1	A	653	VAL
1	A	666	ILE
1	A	677	ARG
1	A	680	THR
1	A	682	THR
1	A	687	LYS
1	A	691	LEU
1	A	702	LEU
1	A	711	ARG
1	A	732	LEU
1	A	735	VAL
1	A	737	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	773	LYS
1	A	795	GLU
1	A	803	SER
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

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Mol	Chain	Res	Type
1	A	879	GLU
1	A	882	SER
1	A	884	ASP
1	A	886	ILE
1	A	896	ARG
1	A	902	LEU
1	A	904	THR
1	A	905	ASP
1	A	907	THR
1	A	913	LEU
1	A	915	SER
1	A	918	GLU
1	A	920	LEU
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	940	ARG
1	A	945	GLU
1	A	961	ARG
1	A	964	ILE
1	A	973	ILE
1	A	982	THR
1	A	988	LEU
1	A	990	VAL
1	A	996	ASN
1	A	997	LEU
1	A	998	LEU
1	A	1001	ARG
1	A	1017	LEU
1	A	1022	LEU
1	A	1029	ARG
1	A	1037	LEU
1	A	1046	LEU
1	A	1052	GLN
1	A	1077	THR
1	A	1095	THR
1	A	1107	VAL
1	A	1112	LYS
1	A	1116	LEU

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Mol	Chain	Res	Type
1	A	1120	LEU
1	A	1128	GLN
1	A	1130	GLN
1	A	1132	LYS
1	A	1133	LEU
1	A	1134	ILE
1	A	1142	THR
1	A	1146	VAL
1	A	1162	VAL
1	A	1163	ILE
1	A	1171	GLN
1	A	1172	LEU
1	A	1193	LEU
1	A	1199	ARG
1	A	1208	THR
1	A	1229	SER
1	A	1230	GLU
1	A	1242	VAL
1	A	1243	VAL
1	A	1258	HIS
1	A	1262	LYS
1	A	1264	GLU
1	A	1272	THR
1	A	1280	GLU
1	A	1282	VAL
1	A	1295	THR
1	A	1299	VAL
1	A	1300	LYS
1	A	1312	ASN
1	A	1318	THR
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1355	VAL
1	A	1359	ASP
1	A	1376	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1390	ASN
1	A	1391	ARG

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Mol	Chain	Res	Type
1	A	1406	VAL
1	A	1407	GLU
1	A	1420	ASP
1	A	1428	VAL
1	A	1436	ILE
1	A	1442	ASP
1	A	1445	ILE
2	B	26	THR
2	B	28	GLU
2	B	34	ILE
2	B	49	ASP
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	67	SER
2	B	68	THR
2	B	94	LYS
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	128	LEU
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	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	225	VAL
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

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Mol	Chain	Res	Type
2	B	272	THR
2	B	275	TYR
2	B	276	ILE
2	B	283	VAL
2	B	305	VAL
2	B	319	GLU
2	B	322	PHE
2	B	327	ARG
2	B	331	LEU
2	B	345	LYS
2	B	346	GLU
2	B	347	LYS
2	B	350	GLN
2	B	353	LYS
2	B	361	LEU
2	B	365	THR
2	B	366	GLN
2	B	367	LEU
2	B	387	LEU
2	B	404	LYS
2	B	408	LEU
2	B	415	GLN
2	B	416	LEU
2	B	419	THR
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	461	LEU
2	B	468	GLU
2	B	469	GLN
2	B	471	LYS
2	B	475	SER
2	B	479	VAL
2	B	485	ARG
2	B	487	THR
2	B	498	THR
2	B	513	GLN
2	B	529	GLU
2	B	537	LYS

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Mol	Chain	Res	Type
2	B	542	MET
2	B	547	VAL
2	B	552	MET
2	B	556	THR
2	B	563	MET
2	B	570	VAL
2	B	573	GLN
2	B	582	VAL
2	B	591	ARG
2	B	604	ARG
2	B	613	VAL
2	B	617	ARG
2	B	622	LYS
2	B	628	THR
2	B	637	LEU
2	B	640	VAL
2	B	646	LEU
2	B	648	HIS
2	B	658	ILE
2	B	682	SER
2	B	701	ILE
2	B	710	LEU
2	B	714	GLU
2	B	722	ASP
2	B	723	VAL
2	B	728	ARG
2	B	730	ARG
2	B	732	SER
2	B	737	THR
2	B	740	HIS
2	B	751	VAL
2	B	761	HIS
2	B	762	ASN
2	B	786	ASN
2	B	789	MET
2	B	790	ASP
2	B	791	THR
2	B	792	MET
2	B	795	ILE
2	B	799	PRO
2	B	806	THR
2	B	807	ARG

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Mol	Chain	Res	Type
2	B	812	LEU
2	B	815	ARG
2	B	825	VAL
2	B	837	ASP
2	B	858	SER
2	B	866	TYR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	885	MET
2	B	889	THR
2	B	899	ILE
2	B	914	LYS
2	B	941	LEU
2	B	953	LEU
2	B	956	THR
2	B	958	GLN
2	B	968	VAL
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	989	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	1021	MET
2	B	1034	VAL
2	B	1052	VAL
2	B	1061	GLU
2	B	1065	GLN
2	B	1072	MET
2	B	1082	MET
2	B	1096	ARG
2	B	1103	ILE
2	B	1108	ARG
2	B	1113	VAL
2	B	1124	ARG

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Mol	Chain	Res	Type
2	B	1147	LEU
2	B	1152	MET
2	B	1155	SER
2	B	1162	ILE
2	B	1171	VAL
2	B	1172	ILE
2	B	1178	ASN
2	B	1183	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1195	HIS
2	B	1196	ILE
2	B	1202	LEU
2	B	1219	ASP
2	B	1222	ARG
2	B	1223	ASP
3	C	11	ARG
3	C	23	SER
3	C	25	VAL
3	C	27	LEU
3	C	34	ARG
3	C	41	ILE
3	C	50	GLU
3	C	53	THR
3	C	55	THR
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	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	189	THR
3	C	215	GLU
3	C	227	THR

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Mol	Chain	Res	Type
3	C	229	TYR
3	C	231	ASN
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	258	ILE
3	C	260	LEU
4	E	3	GLN
4	E	4	GLU
4	E	6	GLU
4	E	9	ILE
4	E	31	THR
4	E	35	VAL
4	E	37	LEU
4	E	43	LYS
4	E	61	GLN
4	E	68	SER
4	E	77	SER
4	E	78	LEU
4	E	92	THR
4	E	100	ILE
4	E	101	GLN
4	E	107	THR
4	E	123	LEU
4	E	127	ILE
4	E	134	THR
4	E	146	HIS
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	212	ARG
4	E	215	MET
5	F	79	ARG
5	F	82	THR
5	F	92	ARG
5	F	99	LEU

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Mol	Chain	Res	Type
5	F	104	ASN
5	F	109	VAL
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	142	SER
5	F	155	LEU
6	H	2	SER
6	H	8	ASP
6	H	11	GLN
6	H	15	VAL
6	H	21	ASN
6	H	25	ARG
6	H	27	GLU
6	H	31	THR
6	H	37	LYS
6	H	49	VAL
6	H	61	SER
6	H	89	LEU
6	H	103	LYS
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	12	ASN
7	I	13	MET
7	I	18	GLU
7	I	28	GLU
7	I	29	CYS
7	I	33	SER
7	I	42	LEU
7	I	48	LEU
7	I	55	THR
7	I	79	HIS
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	117	LYS
7	I	120	GLN
8	J	1	MET
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	27	GLU
8	J	28	ASP
8	J	31	ASP
8	J	36	LEU
8	J	43	ARG
8	J	54	VAL
8	J	55	ASP
8	J	62	ARG
9	K	9	LEU
9	K	11	LEU
9	K	18	LYS
9	K	31	VAL
9	K	32	VAL
9	K	46	ILE
9	K	47	ARG
9	K	50	LEU
9	K	56	VAL
9	K	64	GLU
9	K	71	PHE
9	K	101	LEU
9	K	108	GLU
9	K	111	LEU
9	K	113	THR
9	K	114	LEU
10	L	26	THR
10	L	27	LEU
10	L	28	LYS
10	L	35	SER
10	L	38	LEU
10	L	40	LEU
10	L	50	ASP
10	L	55	ILE

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Mol	Chain	Res	Type
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 (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	92	HIS
1	A	169	ASN
1	A	171	GLN
1	A	339	ASN
1	A	363	GLN
1	A	493	GLN
1	A	517	ASN
1	A	587	HIS
1	A	589	GLN
1	A	706	HIS
1	A	736	ASN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	906	HIS
1	A	1078	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1188	GLN
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	46	GLN
2	B	121	ASN
2	B	178	ASN
2	B	366	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	572	HIS
2	B	573	GLN

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Mol	Chain	Res	Type
2	B	592	ASN
2	B	706	GLN
2	B	734	HIS
2	B	740	HIS
2	B	763	GLN
2	B	786	ASN
2	B	842	ASN
2	B	843	GLN
2	B	951	GLN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1062	HIS
2	B	1141	HIS
2	B	1161	HIS
2	B	1187	ASN
2	B	1193	GLN
2	B	1211	ASN
3	C	135	GLN
3	C	231	ASN
3	C	242	GLN
4	E	63	ASN
4	E	104	ASN
4	E	113	GLN
4	E	179	GLN
6	H	11	GLN
6	H	33	GLN
6	H	52	GLN
6	H	128	ASN
6	H	137	GLN
7	I	11	ASN
9	K	40	HIS
9	K	65	HIS
9	K	76	GLN
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	7/9 (77%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	8	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	21	12	18,24,25	3.21	8 (44%)	22,37,40	3.67	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	21	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	21	02I	O4'-C1'	-7.67	1.25	1.42
12	T	21	02I	O4'-C4'	-7.43	1.33	1.44
12	T	21	02I	C4'-C5'	-4.36	1.45	1.52
12	T	21	02I	O3'-C3'	-3.76	1.35	1.43
12	T	21	02I	C8-N7	3.21	1.36	1.32
12	T	21	02I	C6-N6	2.54	1.40	1.34
12	T	21	02I	C2-N3	2.52	1.38	1.33
12	T	21	02I	C2-N1	2.40	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	21	02I	N6-C6-N1	-7.17	102.41	118.38
12	T	21	02I	N9-C8-N7	-6.78	107.87	113.13
12	T	21	02I	C5-C6-N6	5.75	137.52	123.29
12	T	21	02I	N3-C2-N1	-5.65	120.03	128.58
12	T	21	02I	C5-C4-N3	-5.06	119.74	126.72
12	T	21	02I	O4'-C1'-C2'	-4.52	97.79	106.25
12	T	21	02I	C4-N9-C1'	4.35	135.28	126.73
12	T	21	02I	C5-C4-N9	4.34	108.36	105.63
12	T	21	02I	C2-N3-C4	3.41	120.16	111.83
12	T	21	02I	N3-C4-N9	3.17	131.90	127.33
12	T	21	02I	C4-C5-N7	-2.86	107.98	110.91
12	T	21	02I	C2'-C1'-N9	-2.50	105.70	110.52
12	T	21	02I	C4'-O4'-C1'	2.29	115.06	108.67
12	T	21	02I	C6-C5-C4	2.06	119.99	117.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	21	02I	2	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

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	1394/1733 (80%)	-0.13	14 (1%) 79 62	35, 79, 170, 246	0
2	B	1106/1224 (90%)	-0.16	8 (0%) 84 69	37, 70, 142, 225	0
3	C	266/318 (83%)	-0.29	0 100 100	43, 70, 109, 146	0
4	E	214/215 (99%)	0.13	5 (2%) 61 46	55, 119, 208, 230	0
5	F	84/155 (54%)	-0.23	1 (1%) 76 60	52, 80, 114, 146	0
6	H	133/146 (91%)	-0.07	2 (1%) 72 54	64, 102, 154, 189	0
7	I	119/122 (97%)	-0.04	0 100 100	53, 93, 125, 166	0
8	J	65/70 (92%)	-0.27	0 100 100	40, 63, 90, 116	0
9	K	114/120 (95%)	-0.38	1 (0%) 81 65	43, 75, 104, 119	0
10	L	46/70 (65%)	0.35	0 100 100	57, 113, 169, 193	0
11	R	9/9 (100%)	-0.49	0 100 100	62, 81, 116, 136	0
12	T	9/29 (31%)	0.46	0 100 100	65, 83, 154, 163	0
All	All	3559/4211 (84%)	-0.14	31 (0%) 81 65	35, 78, 162, 246	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	LYS	4.3
1	A	322	VAL	3.3
2	B	709	ASP	3.1
4	E	118	PRO	3.0
1	A	55	ASP	2.9
1	A	1257	ASP	2.8
4	E	131	THR	2.8
1	A	44	THR	2.7
1	A	149	GLU	2.6
2	B	715	ALA	2.6
4	E	95	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1315	GLU	2.5
1	A	252	PHE	2.5
2	B	883	LEU	2.5
9	K	114	LEU	2.4
6	H	63	LEU	2.4
2	B	870	ILE	2.4
2	B	250	PHE	2.3
2	B	246	LYS	2.2
2	B	1167	GLY	2.2
4	E	130	ALA	2.2
2	B	468	GLU	2.2
5	F	77	ASP	2.2
1	A	56	PRO	2.2
1	A	1188	GLN	2.1
1	A	998	LEU	2.1
6	H	90	ALA	2.1
1	A	315	LEU	2.1
1	A	60	SER	2.1
1	A	61	ILE	2.0
4	E	127	ILE	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	21	21/22	0.92	0.10	87,93,115,121	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($\text{\AA}^2$)	Q<0.9
13	ZN	A	1801	1/1	0.95	0.06	199,199,199,199	0
13	ZN	L	101	1/1	0.97	0.05	111,111,111,111	0
13	ZN	I	201	1/1	0.98	0.04	118,118,118,118	0
13	ZN	B	1301	1/1	0.98	0.04	127,127,127,127	0
13	ZN	A	1802	1/1	0.99	0.03	120,120,120,120	0
13	ZN	I	202	1/1	0.99	0.03	74,74,74,74	0
13	ZN	J	101	1/1	0.99	0.03	61,61,61,61	0
13	ZN	C	401	1/1	0.99	0.04	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.