



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:04 am GMT

PDB ID : 2E2J
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with GMPCPP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

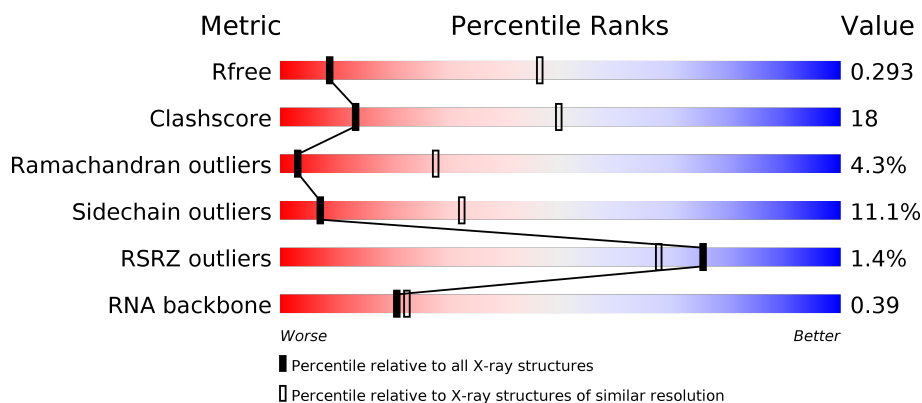
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	9	
2	T	27	
3	N	13	
4	A	1733	

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Mol	Chain	Length	Quality of chain
5	B	1224	<div><div>%</div><div><div></div><div>52%</div><div>32%</div><div>6%</div><div>10%</div></div></div>
6	C	318	<div><div></div><div>52%</div><div>28%</div><div></div><div>16%</div></div>
7	E	215	<div><div>3%</div><div><div></div><div>67%</div><div>28%</div><div></div></div></div>
8	F	155	<div><div></div><div>32%</div><div>19%</div><div></div><div>45%</div></div>
9	H	146	<div><div>%</div><div><div></div><div>51%</div><div>34%</div><div>5%</div><div>9%</div></div></div>
10	I	122	<div><div></div><div>62%</div><div>29%</div><div></div><div>7%</div></div>
11	J	70	<div><div></div><div>51%</div><div>31%</div><div>10%</div><div>7%</div></div>
12	K	120	<div><div></div><div>53%</div><div>38%</div><div></div><div>5%</div></div>
13	L	70	<div><div>%</div><div><div></div><div>34%</div><div>24%</div><div>6%</div><div></div><div>34%</div></div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29206 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 RNA chain called 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called 27-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	27	Total	C	N	O	P	0	0	0
			546	261	102	157	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			266	127	44	82	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1105	Total	C	N	O	S	0	0	0
			8782	5560	1537	1630	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			696	445	118	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

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

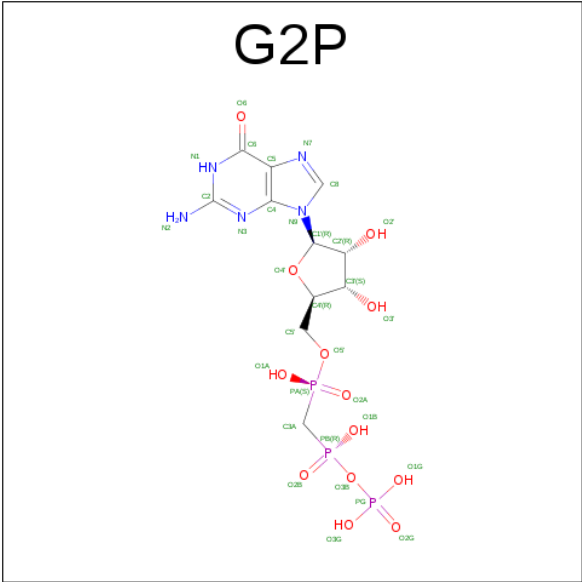
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	T	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

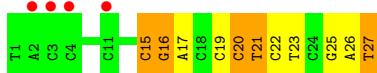
- Molecule 1: 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'

Chain R: 



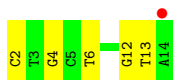
- Molecule 2: 27-MER DNA template strand

Chain T: 



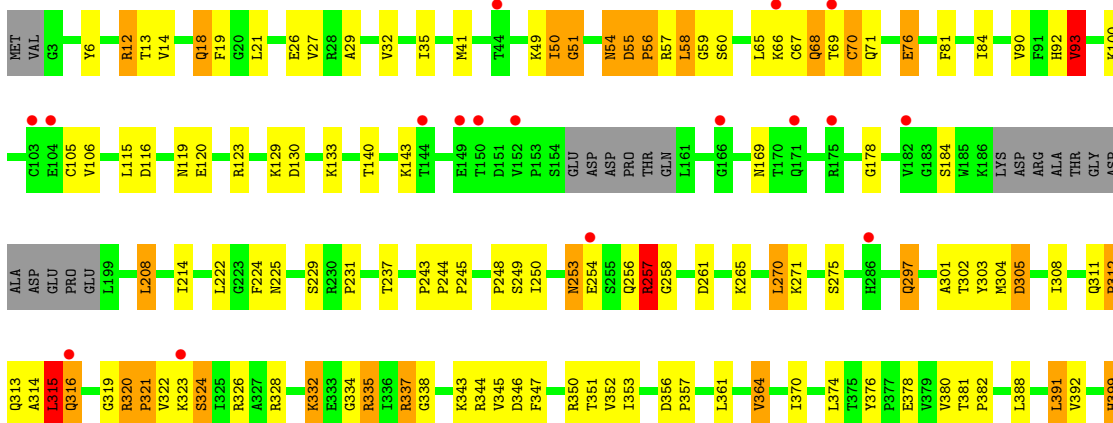
- Molecule 3: 5'-D(P*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*A)-3'

Chain N: 



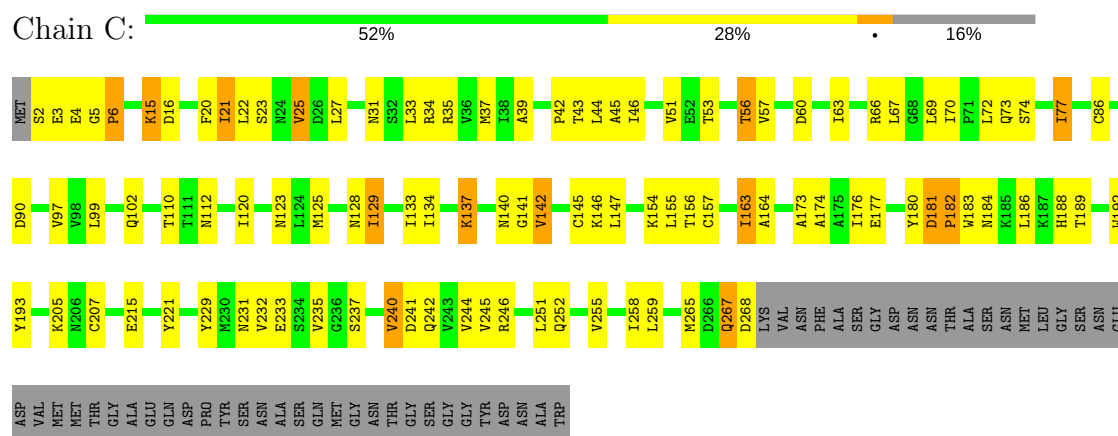
- Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A: 

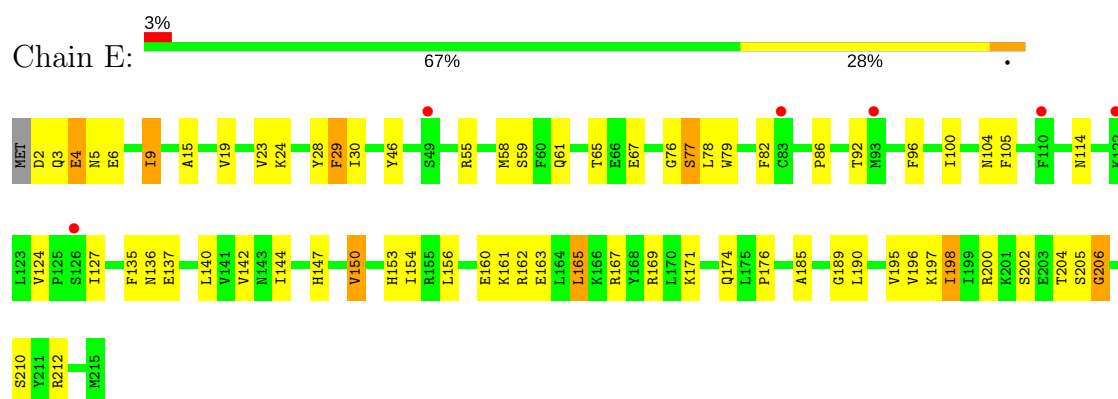




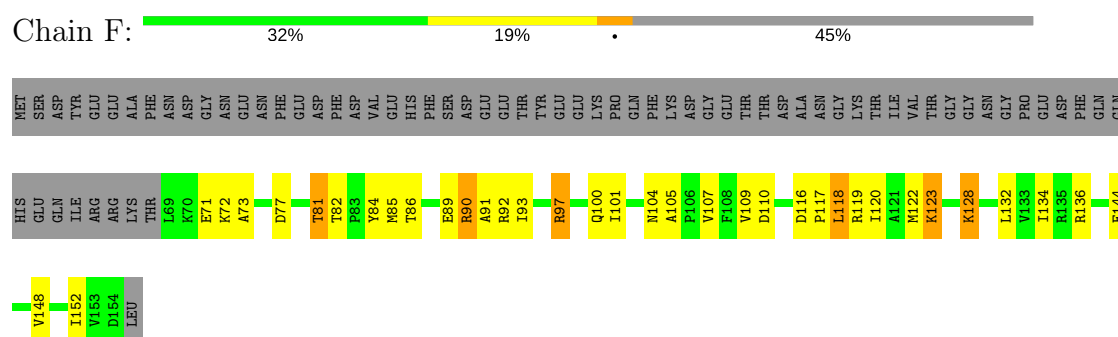




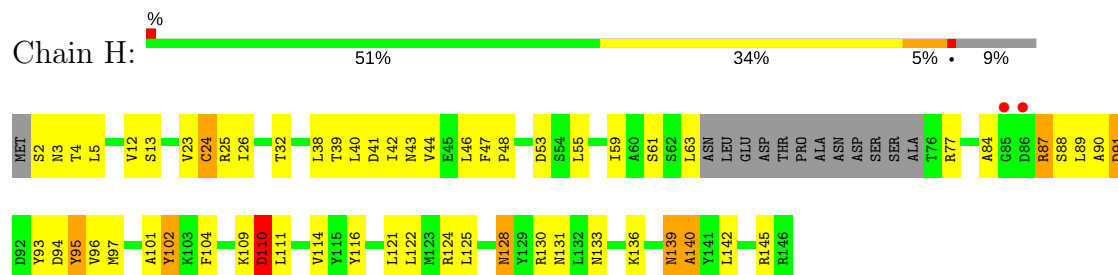
- Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



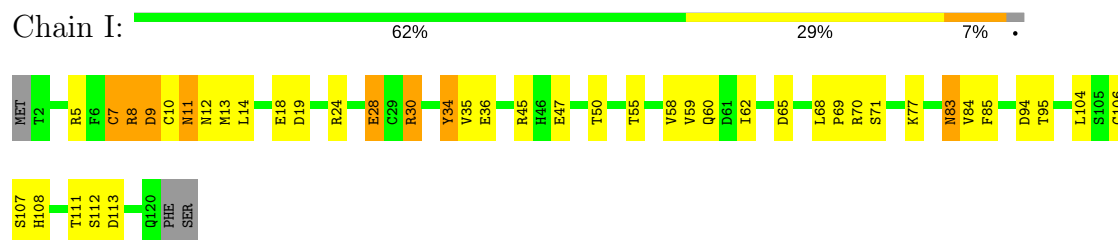
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



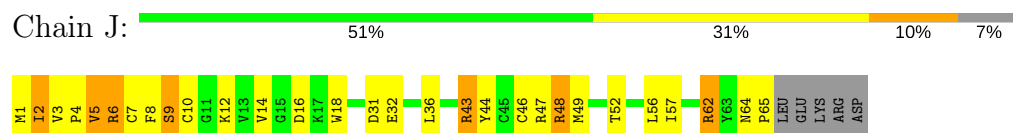
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



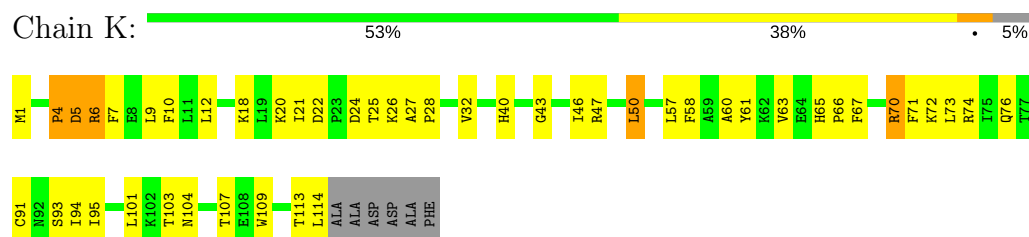
- Molecule 10: DNA-directed RNA polymerase II subunit 9



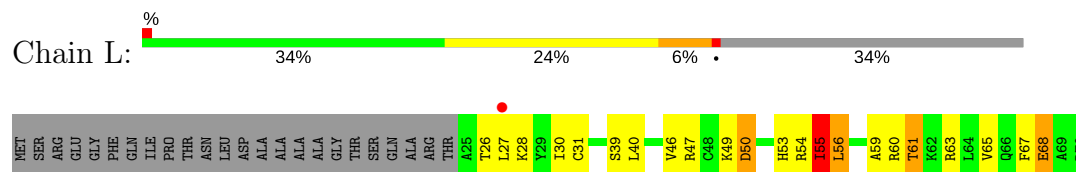
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.14Å 222.02Å 194.65Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.14 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-3.50) 94.6 (50.14-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.306 0.242 , 0.293	Depositor DCC
R_{free} test set	2511 reflections (3.08%)	DCC
Wilson B-factor (Å ²)	101.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29206	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, G2P

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	R	1.15	1/223 (0.4%)	1.88	8/345 (2.3%)
2	T	0.99	0/612	1.78	19/941 (2.0%)
3	N	1.15	2/296 (0.7%)	1.84	9/453 (2.0%)
4	A	0.61	0/11163	0.70	2/15091 (0.0%)
5	B	0.63	0/8952	0.72	1/12071 (0.0%)
6	C	0.61	0/2139	0.70	0/2899
7	E	0.56	0/1788	0.64	0/2406
8	F	0.57	0/708	0.66	0/956
9	H	0.53	0/1086	0.68	0/1470
10	I	0.62	0/989	0.68	0/1331
11	J	0.66	0/541	0.74	0/727
12	K	0.67	0/937	0.69	0/1265
13	L	0.60	0/365	0.78	0/485
All	All	0.64	3/29799 (0.0%)	0.78	39/40440 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	3
5	B	0	4
6	C	0	1
9	H	1	1
11	J	0	1
All	All	1	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	2	DC	OP3-P	-10.47	1.48	1.61
1	R	2	A	OP3-P	-9.50	1.49	1.61
3	N	13	DT	C5-C7	5.64	1.53	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	12	DG	O4'-C1'-N9	13.05	117.14	108.00
2	T	25	DG	O4'-C1'-N9	11.72	116.20	108.00
3	N	4	DG	O4'-C1'-N9	10.88	115.62	108.00
2	T	21	DT	O4'-C4'-C3'	-10.45	99.73	106.00
2	T	25	DG	C1'-O4'-C4'	-9.85	100.25	110.10
2	T	16	DG	O4'-C1'-N9	8.57	114.00	108.00
2	T	21	DT	C6-C5-C7	-8.30	117.92	122.90
5	B	635	ARG	C-N-CD	-8.09	102.81	120.60
2	T	20	DC	O4'-C1'-N1	7.99	113.59	108.00
1	R	9	G	O5'-P-OP2	-7.68	98.79	105.70
3	N	12	DG	C1'-O4'-C4'	-7.65	102.45	110.10
2	T	16	DG	C1'-O4'-C4'	-7.21	102.89	110.10
3	N	12	DG	C3'-C2'-C1'	-7.14	93.93	102.50
2	T	15	DC	O4'-C1'-N1	6.94	112.86	108.00
2	T	21	DT	O5'-P-OP2	-6.64	99.73	105.70
1	R	10	G	C5'-C4'-C3'	-6.61	105.42	116.00
3	N	12	DG	P-O3'-C3'	6.49	127.48	119.70
4	A	961	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	R	9	G	O5'-P-OP1	6.40	118.38	110.70
1	R	9	G	C5-C6-N1	6.29	114.64	111.50
2	T	27	DT	N3-C2-O2	-6.03	118.68	122.30
2	T	19	DC	O4'-C1'-N1	6.02	112.21	108.00
2	T	15	DC	P-O3'-C3'	6.01	126.92	119.70
2	T	21	DT	C4'-C3'-C2'	-5.95	97.75	103.10
2	T	16	DG	O4'-C4'-C3'	-5.87	102.15	104.50
3	N	12	DG	O4'-C1'-C2'	-5.76	101.29	105.90
2	T	23	DT	N3-C4-O4	5.71	123.33	119.90
1	R	9	G	C2-N3-C4	5.55	114.68	111.90
3	N	6	DT	O4'-C1'-N1	5.50	111.85	108.00
3	N	4	DG	C1'-O4'-C4'	-5.32	104.78	110.10
2	T	15	DC	O4'-C1'-C2'	-5.28	101.68	105.90
2	T	15	DC	N1-C2-O2	5.25	122.05	118.90
2	T	27	DT	C6-C5-C7	-5.24	119.75	122.90
2	T	22	DC	O4'-C1'-N1	5.16	111.61	108.00
4	A	455	MET	CB-CG-SD	-5.16	96.93	112.40
1	R	10	G	C5-C6-N1	5.16	114.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	7	G	C5-C6-O6	-5.05	125.57	128.60
1	R	10	G	O4'-C1'-N9	5.02	112.22	108.20
3	N	2	DC	P-O3'-C3'	5.01	125.71	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	H	110	ASP	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1392	SER	Peptide
4	A	257	ARG	Peptide
4	A	258	GLY	Peptide
5	B	1065	GLN	Peptide
5	B	293	PRO	Peptide
5	B	478	GLY	Peptide
5	B	828	ALA	Peptide
6	C	20	PHE	Peptide
9	H	110	ASP	Peptide
11	J	4	PRO	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	R	199	0	98	3	0
2	T	546	0	304	5	0
3	N	266	0	149	0	0
4	A	10969	0	11067	410	0
5	B	8782	0	8816	419	0
6	C	2101	0	2056	86	0
7	E	1752	0	1776	47	0
8	F	696	0	720	31	0
9	H	1068	0	1040	46	0
10	I	971	0	927	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	532	0	542	43	0
12	K	919	0	929	39	0
13	L	363	0	386	10	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	T	32	0	14	1	0
All	All	29206	0	28824	1043	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 18.

All (1043) 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)
9:H:109:LYS:HB3	9:H:110:ASP:CA	1.54	1.34
9:H:109:LYS:CB	9:H:110:ASP:HA	1.49	1.31
4:A:399:HIS:CB	4:A:400:PRO:HD3	1.65	1.27
5:B:635:ARG:CG	5:B:636:PRO:HD2	1.65	1.24
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.73	1.18
5:B:637:LEU:CD2	5:B:742:GLU:OE2	1.93	1.16
4:A:567:LYS:HB2	4:A:568:PRO:CD	1.74	1.15
7:E:3:GLN:HA	7:E:4:GLU:HB2	1.28	1.15
4:A:399:HIS:HB3	4:A:400:PRO:CD	1.76	1.14
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.31	1.11
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.29	1.11
4:A:315:LEU:HB2	4:A:316:GLN:CA	1.81	1.10
5:B:636:PRO:HB2	5:B:637:LEU:HB3	1.34	1.09
5:B:637:LEU:HD23	5:B:742:GLU:OE2	1.52	1.09
4:A:315:LEU:HB2	4:A:316:GLN:HA	1.08	1.08
4:A:399:HIS:CG	4:A:400:PRO:HD3	1.89	1.07
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.09	1.05
4:A:315:LEU:CB	4:A:316:GLN:HA	1.84	1.05
4:A:455:MET:SD	5:B:1137:CYS:HB2	1.97	1.05
5:B:864:LYS:HB2	5:B:865:LYS:HA	1.38	1.03
5:B:637:LEU:HD22	5:B:742:GLU:HA	1.42	1.00
5:B:636:PRO:CB	5:B:637:LEU:HB3	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.76	0.99
5:B:636:PRO:HB2	5:B:637:LEU:CB	1.93	0.97
5:B:635:ARG:HG3	5:B:636:PRO:HD2	1.44	0.97
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.47	0.95
5:B:292:ILE:H	5:B:293:PRO:HD2	1.29	0.95
4:A:315:LEU:CB	4:A:316:GLN:CA	2.41	0.95
5:B:205:ILE:HG22	5:B:206:ASN:ND2	1.82	0.94
5:B:635:ARG:CB	5:B:636:PRO:HD2	2.00	0.92
5:B:636:PRO:CB	5:B:637:LEU:CA	2.48	0.92
4:A:567:LYS:HB3	9:H:96:VAL:H	1.34	0.91
4:A:351:THR:HG22	4:A:352:VAL:N	1.86	0.90
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.52	0.90
5:B:636:PRO:HB3	5:B:637:LEU:HA	1.54	0.89
6:C:66:ARG:NH2	11:J:3:VAL:O	2.06	0.89
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.16	0.89
5:B:216:GLU:HB3	5:B:500:THR:HG23	1.54	0.86
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.40	0.86
5:B:636:PRO:CB	5:B:637:LEU:HA	2.05	0.85
5:B:848:ARG:HH22	5:B:996:ARG:NH1	1.72	0.85
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.14	0.85
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.57	0.85
4:A:633:VAL:HG11	4:A:645:LEU:HD22	1.58	0.85
4:A:455:MET:SD	5:B:1137:CYS:CB	2.65	0.84
4:A:1242:VAL:HG12	4:A:1243:VAL:H	1.41	0.84
8:F:72:LYS:HG3	8:F:73:ALA:H	1.41	0.84
5:B:549:THR:HG22	5:B:550:ASP:H	1.43	0.83
5:B:865:LYS:CG	5:B:866:TYR:HA	2.09	0.82
5:B:37:PHE:O	5:B:38:PHE:HB2	1.76	0.82
5:B:635:ARG:O	5:B:636:PRO:O	1.97	0.82
6:C:123:ASN:ND2	6:C:125:MET:HG2	1.95	0.82
4:A:573:SER:H	4:A:576:GLN:HG3	1.45	0.82
5:B:995:ARG:HB3	5:B:997:GLU:OE2	1.80	0.82
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.43	0.81
4:A:518:LYS:HB2	4:A:519:PRO:HD2	1.62	0.81
4:A:1338:VAL:HG12	4:A:1339:LEU:HD23	1.60	0.81
12:K:26:LYS:HA	12:K:27:ALA:HB3	1.60	0.81
10:I:111:THR:HG22	10:I:113:ASP:H	1.45	0.81
5:B:635:ARG:CB	5:B:636:PRO:CD	2.58	0.81
10:I:59:VAL:HG12	10:I:60:GLN:H	1.44	0.81
4:A:1370:LEU:O	4:A:1374:VAL:HG23	1.80	0.80
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:351:THR:CG2	4:A:352:VAL:N	2.42	0.80
5:B:636:PRO:CB	5:B:637:LEU:CB	2.55	0.80
7:E:198:ILE:HD11	7:E:212:ARG:HG3	1.64	0.80
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.64	0.80
5:B:635:ARG:HG2	5:B:636:PRO:HD2	1.62	0.79
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.64	0.79
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.64	0.79
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.64	0.79
5:B:865:LYS:CB	5:B:866:TYR:HA	2.14	0.78
4:A:567:LYS:HB2	4:A:568:PRO:HD2	0.84	0.78
5:B:857:ARG:HG3	5:B:857:ARG:HH11	1.49	0.77
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.66	0.77
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.65	0.77
7:E:3:GLN:HB3	7:E:5:ASN:H	1.50	0.76
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.48	0.76
5:B:325:GLN:HE22	10:I:12:ASN:ND2	1.84	0.76
12:K:6:ARG:HB3	12:K:6:ARG:HH11	1.51	0.76
4:A:467:THR:HG23	5:B:976:ILE:HG23	1.68	0.75
5:B:1147:LEU:HD22	5:B:1147:LEU:O	1.86	0.75
5:B:286:PHE:HB3	5:B:297:ILE:HD12	1.67	0.75
5:B:780:VAL:HG12	5:B:817:LEU:HD23	1.68	0.75
4:A:567:LYS:HZ1	9:H:43:ASN:HB3	1.51	0.75
8:F:109:VAL:HG11	8:F:123:LYS:HG2	1.68	0.75
5:B:1028:GLU:HG2	5:B:1090:THR:HG23	1.68	0.74
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.69	0.74
4:A:353:ILE:HD13	4:A:487:MET:CE	2.16	0.74
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.68	0.74
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.03	0.74
4:A:672:ASP:HB3	4:A:675:THR:OG1	1.88	0.73
6:C:2:SER:N	6:C:3:GLU:HB3	2.02	0.73
4:A:567:LYS:NZ	9:H:43:ASN:HB3	2.02	0.73
5:B:200:GLY:HA2	5:B:202:TYR:CE2	2.24	0.72
5:B:292:ILE:N	5:B:293:PRO:HD2	2.04	0.72
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.71	0.72
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.71	0.72
4:A:399:HIS:CG	4:A:400:PRO:CD	2.68	0.72
4:A:628:GLY:O	4:A:632:VAL:HG23	1.89	0.72
4:A:794:PRO:HD2	4:A:795:GLU:OE2	1.90	0.72
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.72	0.71
5:B:637:LEU:HD13	5:B:741:CYS:O	1.89	0.71
6:C:255:VAL:O	6:C:258:ILE:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.72	0.71
11:J:8:PHE:H	11:J:49:MET:HE3	1.53	0.71
5:B:636:PRO:HB3	5:B:637:LEU:CA	2.19	0.71
9:H:109:LYS:CB	9:H:110:ASP:CA	2.30	0.71
6:C:69:LEU:HD12	11:J:6:ARG:HD3	1.74	0.70
4:A:858:ASN:HD22	4:A:858:ASN:C	1.94	0.70
5:B:292:ILE:H	5:B:293:PRO:CD	2.04	0.70
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.73	0.70
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.71	0.70
4:A:208:LEU:O	4:A:208:LEU:HD22	1.91	0.70
13:L:55:ILE:O	13:L:56:LEU:HB2	1.90	0.70
4:A:666:ILE:HG23	5:B:1026:LEU:CB	2.22	0.70
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.74	0.70
11:J:10:CYS:SG	11:J:43:ARG:HD2	2.31	0.70
4:A:265:LYS:NZ	4:A:322:VAL:HB	2.07	0.69
4:A:21:LEU:HD12	4:A:229:SER:HB2	1.74	0.69
4:A:573:SER:O	4:A:576:GLN:HB2	1.92	0.69
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.28	0.68
5:B:654:ARG:H	5:B:657:HIS:HD2	1.39	0.68
5:B:859:TYR:OH	5:B:941:LEU:HD23	1.93	0.68
6:C:51:VAL:HG22	6:C:155:LEU:CD2	2.23	0.68
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	2.07	0.68
10:I:34:TYR:HE2	10:I:36:GLU:HG3	1.59	0.68
5:B:800:GLN:HG2	11:J:52:THR:HG22	1.76	0.68
5:B:1187:ASN:HD21	5:B:1190:ASP:H	1.42	0.68
4:A:1273:LEU:O	4:A:1274:ARG:HB3	1.93	0.67
5:B:1084:GLN:NE2	6:C:192:TRP:H	1.91	0.67
5:B:839:MET:CE	5:B:1010:LEU:HD21	2.24	0.67
6:C:67:LEU:HA	6:C:70:ILE:HD12	1.77	0.67
10:I:34:TYR:CE2	10:I:36:GLU:HG3	2.30	0.67
9:H:47:PHE:HB3	9:H:95:TYR:HD1	1.58	0.67
4:A:821:ARG:O	4:A:825:ILE:HG12	1.94	0.67
9:H:47:PHE:HB3	9:H:95:TYR:CD1	2.30	0.67
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.24	0.67
4:A:482:PHE:CD1	5:B:836:GLU:HB2	2.30	0.67
5:B:494:HIS:HD2	5:B:497:ARG:NH1	1.93	0.67
7:E:3:GLN:CA	7:E:4:GLU:HB2	2.17	0.67
5:B:1076:HIS:CD2	12:K:40:HIS:NE2	2.62	0.67
4:A:855:THR:CG2	4:A:857:ARG:HE	2.08	0.66
6:C:142:VAL:H	11:J:16:ASP:HB3	1.59	0.66
5:B:211:VAL:O	5:B:480:SER:HA	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:325:GLN:HE22	10:I:12:ASN:HD21	1.42	0.66
5:B:803:LEU:H	5:B:822:ASN:HD21	1.42	0.66
5:B:986:GLN:HE21	5:B:1022:THR:HG21	1.58	0.66
11:J:64:ASN:HB3	11:J:65:PRO:CD	2.17	0.66
4:A:1189:SER:OG	4:A:1190:PRO:HD2	1.94	0.66
4:A:446:ARG:HG2	4:A:447:GLN:N	2.09	0.66
5:B:911:ILE:HD11	5:B:941:LEU:HG	1.76	0.66
9:H:109:LYS:HD2	9:H:111:LEU:HG	1.77	0.66
5:B:464:GLY:HA2	5:B:479:VAL:O	1.95	0.66
5:B:287:ARG:NH1	5:B:324:ILE:O	2.29	0.65
5:B:955:THR:HG22	5:B:956:THR:N	2.09	0.65
4:A:457:ALA:O	4:A:507:VAL:HG23	1.96	0.65
4:A:901:LEU:H	4:A:926:GLN:NE2	1.94	0.65
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.77	0.65
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.10	0.65
5:B:839:MET:HE3	5:B:1010:LEU:HD21	1.77	0.65
4:A:424:ILE:O	4:A:424:ILE:HD12	1.97	0.65
5:B:20:ASP:O	5:B:22:SER:N	2.30	0.65
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.76	0.65
7:E:19:VAL:O	7:E:23:VAL:HG23	1.97	0.65
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.30	0.65
5:B:744:HIS:HD2	5:B:746:SER:OG	1.79	0.65
4:A:55:ASP:H	4:A:56:PRO:HD2	1.62	0.64
4:A:399:HIS:CD2	4:A:400:PRO:HD3	2.31	0.64
4:A:888:GLY:O	4:A:940:ARG:NH2	2.31	0.64
5:B:848:ARG:NH2	5:B:996:ARG:NH1	2.44	0.64
6:C:56:THR:HG21	6:C:145:CYS:SG	2.38	0.64
7:E:6:GLU:O	7:E:9:ILE:HG22	1.98	0.64
4:A:658:LEU:HD13	5:B:831:SER:HA	1.80	0.64
6:C:145:CYS:SG	6:C:146:LYS:N	2.71	0.64
11:J:52:THR:O	11:J:52:THR:HG22	1.98	0.64
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.31	0.64
4:A:672:ASP:H	4:A:736:ASN:HD21	1.46	0.64
4:A:645:LEU:O	4:A:649:ILE:HG13	1.98	0.64
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.80	0.63
5:B:744:HIS:CD2	5:B:746:SER:OG	2.51	0.63
5:B:999:MET:HG2	5:B:1007:VAL:HG13	1.78	0.63
6:C:133:ILE:HD11	6:C:237:SER:HA	1.78	0.63
5:B:393:LYS:HE3	5:B:393:LYS:HA	1.81	0.63
9:H:5:LEU:HD22	9:H:133:ASN:O	1.97	0.63
5:B:378:LEU:O	5:B:382:ILE:HG12	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:487:THR:CG2	5:B:488:TYR:N	2.61	0.63
5:B:402:GLY:HA2	5:B:695:ALA:HB3	1.81	0.63
5:B:711:GLU:O	5:B:711:GLU:HG3	1.99	0.63
6:C:57:VAL:HG23	11:J:57:ILE:HD11	1.80	0.63
4:A:470:LEU:HD21	4:A:487:MET:HE3	1.81	0.63
5:B:612:GLU:O	5:B:632:ARG:NH2	2.31	0.63
5:B:1002:THR:CG2	5:B:1006:ILE:HG12	2.29	0.63
5:B:635:ARG:O	5:B:636:PRO:C	2.37	0.63
5:B:957:ASN:O	5:B:959:ASP:N	2.31	0.63
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.63	0.63
11:J:8:PHE:N	11:J:49:MET:HE3	2.15	0.62
4:A:466:SER:O	5:B:1103:ILE:HD12	1.99	0.62
6:C:43:THR:HG22	6:C:44:LEU:N	2.14	0.62
5:B:1096:ARG:HG2	5:B:1096:ARG:HH11	1.64	0.62
12:K:26:LYS:CA	12:K:27:ALA:HB3	2.29	0.62
2:T:21:DT:OP1	4:A:344:ARG:NH1	2.27	0.62
1:R:10:G:O2'	4:A:446:ARG:NH2	2.33	0.62
5:B:708:GLU:O	5:B:709:ASP:HB2	2.00	0.62
5:B:1084:GLN:HE22	6:C:192:TRP:H	1.47	0.62
6:C:99:LEU:HD13	6:C:120:ILE:HA	1.81	0.62
10:I:8:ARG:O	10:I:9:ASP:HB2	1.98	0.62
5:B:428:ILE:HD11	5:B:448:ILE:HG12	1.82	0.62
5:B:796:LEU:O	5:B:799:PRO:HD3	1.99	0.62
4:A:504:LEU:HD11	8:F:91:ALA:CB	2.29	0.62
9:H:63:LEU:C	9:H:90:ALA:HB3	2.20	0.62
6:C:128:ASN:O	6:C:129:ILE:HD12	2.00	0.62
10:I:59:VAL:HG12	10:I:60:GLN:N	2.13	0.62
5:B:639:ILE:HA	5:B:740:HIS:HB3	1.81	0.62
5:B:865:LYS:HG2	5:B:866:TYR:HA	1.81	0.62
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.81	0.61
4:A:913:LEU:HD12	4:A:915:SER:H	1.65	0.61
4:A:565:ILE:HG23	4:A:567:LYS:HG2	1.82	0.61
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.82	0.61
4:A:793:SER:HB2	4:A:794:PRO:CD	2.30	0.61
5:B:636:PRO:HB3	5:B:637:LEU:HB3	1.78	0.61
6:C:46:ILE:HD12	6:C:157:CYS:HB3	1.83	0.61
5:B:114:PRO:HG3	5:B:181:LEU:HD21	1.80	0.61
4:A:1134:ILE:O	4:A:1138:ILE:HG12	2.00	0.61
4:A:315:LEU:CB	4:A:316:GLN:C	2.68	0.61
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.35	0.61
4:A:451:HIS:HB2	4:A:454:SER:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:784:ASN:OD1	5:B:788:ARG:HD2	2.01	0.61
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.35	0.61
8:F:118:LEU:HD12	8:F:118:LEU:O	2.01	0.61
4:A:12:ARG:HB3	5:B:1218:THR:HG22	1.82	0.61
4:A:910:PRO:HA	4:A:916:GLY:HA3	1.82	0.61
4:A:350:ARG:HB2	5:B:1128:LEU:HD11	1.83	0.61
5:B:864:LYS:CB	5:B:865:LYS:HA	2.14	0.60
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.36	0.60
5:B:999:MET:HG2	5:B:1008:PRO:HD2	1.84	0.60
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.34	0.60
12:K:63:VAL:HG23	12:K:63:VAL:O	2.01	0.60
12:K:6:ARG:HB3	12:K:6:ARG:NH1	2.16	0.60
4:A:853:ASP:OD1	4:A:855:THR:HG22	2.00	0.60
7:E:15:ALA:O	7:E:19:VAL:HG23	2.02	0.60
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.84	0.60
4:A:315:LEU:HB2	4:A:316:GLN:C	2.21	0.60
4:A:596:THR:O	4:A:598:LEU:N	2.35	0.60
4:A:92:HIS:HE1	5:B:1211:ASN:HB3	1.67	0.60
4:A:981:LEU:HD21	4:A:1039:LYS:HA	1.84	0.60
4:A:1341:ILE:HD13	4:A:1379:GLY:O	2.02	0.59
4:A:407:ARG:HD3	4:A:413:ILE:HD11	1.84	0.59
5:B:1002:THR:HG21	5:B:1006:ILE:HG12	1.83	0.59
5:B:310:MET:O	5:B:313:MET:HB2	2.02	0.59
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.37	0.59
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.17	0.59
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.36	0.59
5:B:637:LEU:HD22	5:B:742:GLU:CA	2.27	0.59
4:A:546:VAL:O	4:A:550:LEU:HD22	2.01	0.59
10:I:45:ARG:HE	10:I:47:GLU:HG3	1.66	0.59
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.84	0.59
4:A:765:VAL:HG13	4:A:802:ASN:O	2.01	0.59
5:B:25:ILE:HG23	5:B:29:ASP:HB2	1.83	0.59
5:B:992:ILE:CD1	12:K:67:PHE:HE2	2.16	0.59
7:E:3:GLN:HA	7:E:4:GLU:CB	2.19	0.59
5:B:976:ILE:O	5:B:990:ILE:HB	2.03	0.59
4:A:778:GLY:HA3	5:B:516:ASN:HB2	1.85	0.58
5:B:744:HIS:CD2	5:B:746:SER:H	2.20	0.58
4:A:896:ARG:HD2	4:A:897:TYR:CE1	2.38	0.58
5:B:635:ARG:HH11	5:B:635:ARG:HG3	1.68	0.58
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.84	0.58
5:B:322:PHE:CD1	5:B:322:PHE:O	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.85	0.58
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.83	0.58
4:A:58:LEU:HD21	4:A:243:PRO:HB3	1.86	0.58
6:C:67:LEU:HA	6:C:70:ILE:CD1	2.33	0.58
4:A:672:ASP:H	4:A:736:ASN:ND2	2.02	0.58
4:A:858:ASN:ND2	4:A:860:LEU:H	2.01	0.58
5:B:956:THR:HA	5:B:961:LEU:O	2.02	0.58
5:B:884:ARG:O	5:B:936:ASP:HB3	2.02	0.58
6:C:182:PRO:HB2	6:C:207:CYS:SG	2.44	0.58
4:A:407:ARG:HH11	4:A:413:ILE:HD11	1.69	0.58
4:A:754:SER:H	4:A:757:ASN:HD22	1.51	0.58
5:B:955:THR:CG2	5:B:956:THR:N	2.66	0.58
9:H:47:PHE:CB	9:H:95:TYR:HD1	2.17	0.58
9:H:95:TYR:HE2	9:H:97:MET:CG	2.15	0.58
4:A:1436:ILE:O	4:A:1438:THR:N	2.37	0.58
5:B:60:GLN:O	5:B:63:ILE:HG22	2.02	0.58
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.86	0.58
5:B:778:MET:CE	5:B:853:SER:HB3	2.34	0.58
5:B:269:ILE:CD1	5:B:386:LEU:HD21	2.32	0.58
5:B:635:ARG:HB2	5:B:636:PRO:CD	2.32	0.57
5:B:1117:GLN:HE21	5:B:1199:ALA:HB2	1.69	0.57
5:B:114:PRO:CG	5:B:181:LEU:HD21	2.34	0.57
6:C:134:ILE:HG23	6:C:141:GLY:H	1.68	0.57
4:A:477:PRO:HG3	4:A:521:MET:HE2	1.85	0.57
4:A:648:ASN:O	4:A:652:VAL:HG23	2.05	0.57
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.69	0.57
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.86	0.57
4:A:1400:CYS:SG	4:A:1409:LEU:HG	2.45	0.57
5:B:801:LYS:O	11:J:52:THR:HG23	2.04	0.57
5:B:778:MET:HE1	5:B:853:SER:HB3	1.87	0.57
7:E:202:SER:OG	7:E:204:THR:HG22	2.05	0.57
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.86	0.57
4:A:1161:THR:HG22	4:A:1162:VAL:N	2.20	0.57
4:A:265:LYS:HZ3	4:A:322:VAL:HB	1.69	0.57
5:B:479:VAL:O	5:B:480:SER:HB3	2.05	0.57
4:A:256:GLN:CA	4:A:257:ARG:HB3	2.35	0.57
4:A:741:ASN:HD22	4:A:744:LYS:H	1.52	0.57
6:C:242:GLN:O	6:C:246:ARG:HB2	2.05	0.57
6:C:133:ILE:CD1	6:C:237:SER:HA	2.35	0.56
4:A:1100:ARG:HH21	4:A:1351:GLU:HG3	1.71	0.56
5:B:227:LYS:N	5:B:395:GLN:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:19:ASP:HB3	10:I:24:ARG:H	1.71	0.56
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.54	0.56
4:A:596:THR:C	4:A:598:LEU:H	2.07	0.56
5:B:621:GLU:O	5:B:622:LYS:HG2	2.05	0.56
6:C:43:THR:CG2	6:C:44:LEU:N	2.68	0.56
4:A:896:ARG:HB3	4:A:897:TYR:HD1	1.70	0.56
4:A:497:THR:CG2	5:B:1146:PHE:HD1	2.18	0.56
5:B:287:ARG:HG2	5:B:292:ILE:HD13	1.87	0.56
5:B:654:ARG:H	5:B:657:HIS:CD2	2.22	0.56
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.87	0.56
4:A:14:VAL:H	4:A:1432:GLN:NE2	2.04	0.56
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.71	0.56
4:A:256:GLN:HA	4:A:257:ARG:CB	2.36	0.56
4:A:848:ILE:HD12	4:A:864:ILE:HG13	1.88	0.56
5:B:1115:THR:HB	5:B:1117:GLN:HG3	1.86	0.56
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.87	0.56
5:B:613:VAL:HG22	5:B:628:THR:HG23	1.87	0.56
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	1.87	0.56
8:F:72:LYS:HG3	8:F:73:ALA:N	2.16	0.56
4:A:924:LYS:O	4:A:927:VAL:HG12	2.05	0.56
5:B:803:LEU:N	5:B:822:ASN:HD21	2.04	0.56
6:C:181:ASP:OD2	6:C:186:LEU:HD13	2.05	0.56
4:A:106:VAL:HG11	4:A:214:ILE:HD11	1.87	0.56
4:A:590:ARG:HH21	4:A:621:THR:HA	1.71	0.56
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.06	0.56
10:I:30:ARG:HD2	10:I:30:ARG:N	2.20	0.56
5:B:216:GLU:HB3	5:B:500:THR:CG2	2.29	0.55
11:J:48:ARG:HH21	11:J:49:MET:CE	2.18	0.55
4:A:370:ILE:HG22	4:A:374:LEU:CD1	2.36	0.55
4:A:507:VAL:HB	4:A:508:PRO:HD3	1.87	0.55
5:B:477:ALA:O	5:B:479:VAL:N	2.38	0.55
7:E:2:ASP:O	7:E:3:GLN:HB2	2.06	0.55
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.88	0.55
9:H:91:ASP:HA	9:H:93:TYR:HD1	1.70	0.55
4:A:1015:VAL:CG1	4:A:1019:CYS:SG	2.91	0.55
4:A:407:ARG:HG2	4:A:430:TRP:CZ2	2.41	0.55
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.41	0.55
5:B:875:GLU:O	5:B:877:PRO:HD3	2.06	0.55
11:J:1:MET:H1	11:J:56:LEU:HB2	1.71	0.55
5:B:973:ILE:CG2	5:B:974:PRO:HD2	2.37	0.55
5:B:826:ALA:O	5:B:1011:ILE:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:64:ASN:CB	11:J:65:PRO:HD3	2.12	0.55
4:A:1282:VAL:HG22	4:A:1308:THR:HG23	1.89	0.55
4:A:364:VAL:O	4:A:364:VAL:HG13	2.06	0.55
6:C:56:THR:HG22	6:C:57:VAL:H	1.70	0.55
12:K:4:PRO:O	12:K:5:ASP:C	2.44	0.55
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.89	0.55
4:A:381:THR:OG1	4:A:382:PRO:HD2	2.07	0.55
5:B:778:MET:HE1	5:B:1094:ARG:HH11	1.72	0.55
5:B:205:ILE:HG22	5:B:206:ASN:HD21	1.68	0.55
5:B:620:ARG:HD2	10:I:68:LEU:HD11	1.87	0.55
4:A:14:VAL:HB	4:A:1432:GLN:HE22	1.72	0.54
4:A:507:VAL:O	4:A:510:GLN:HB2	2.07	0.54
4:A:840:ARG:HG2	4:A:1402:PHE:HZ	1.72	0.54
5:B:118:ARG:HA	5:B:207:GLY:HA2	1.88	0.54
4:A:1373:ASP:O	4:A:1377:THR:HG23	2.07	0.54
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.40	0.54
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.89	0.54
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.43	0.54
4:A:1105:LEU:HD23	4:A:1384:VAL:HG21	1.89	0.54
4:A:855:THR:HG21	4:A:857:ARG:HE	1.72	0.54
5:B:690:VAL:HG12	5:B:691:GLU:N	2.22	0.54
10:I:111:THR:HG22	10:I:112:SER:N	2.22	0.54
4:A:1059:HIS:HB3	8:F:86:THR:HB	1.88	0.54
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.20	0.54
12:K:57:LEU:HD12	12:K:76:GLN:HG2	1.90	0.54
4:A:302:THR:HA	4:A:305:ASP:O	2.06	0.54
4:A:981:LEU:CD2	4:A:1039:LYS:HA	2.38	0.54
5:B:174:LEU:HD21	5:B:204:ILE:HD11	1.89	0.54
5:B:230:ALA:H	5:B:231:PRO:HD2	1.73	0.54
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.91	0.54
5:B:642:ASP:C	5:B:644:GLU:H	2.10	0.54
5:B:638:PHE:O	5:B:740:HIS:HB2	2.08	0.54
5:B:861:ASP:OD1	5:B:914:LYS:HE2	2.08	0.54
5:B:980:PHE:CD1	5:B:980:PHE:N	2.75	0.54
6:C:33:LEU:O	6:C:37:MET:HB2	2.07	0.54
7:E:176:PRO:O	7:E:212:ARG:HA	2.06	0.54
7:E:144:ILE:O	7:E:150:VAL:HG21	2.08	0.54
9:H:101:ALA:HB2	9:H:116:TYR:CE2	2.43	0.54
13:L:28:LYS:HB2	13:L:39:SER:HA	1.89	0.54
4:A:573:SER:H	4:A:576:GLN:CG	2.18	0.54
4:A:759:ALA:O	4:A:763:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:814:PHE:O	4:A:817:ALA:HB3	2.08	0.54
13:L:60:ARG:HG3	13:L:61:THR:H	1.73	0.54
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.72	0.54
5:B:65:GLU:OE1	5:B:65:GLU:N	2.41	0.54
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.89	0.54
5:B:1076:HIS:ND1	5:B:1076:HIS:N	2.56	0.54
5:B:189:LEU:HA	5:B:192:LEU:HD12	1.90	0.54
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.43	0.54
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.17	0.53
4:A:1434:ALA:O	4:A:1436:ILE:N	2.41	0.53
4:A:351:THR:CG2	4:A:352:VAL:H	2.22	0.53
4:A:568:PRO:HD3	9:H:94:ASP:O	2.08	0.53
4:A:58:LEU:CD2	4:A:59:GLY:H	2.21	0.53
4:A:889:SER:HB2	4:A:892:ALA:H	1.73	0.53
5:B:487:THR:H	5:B:490:SER:HB3	1.73	0.53
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.90	0.53
6:C:51:VAL:HG22	6:C:155:LEU:HD22	1.90	0.53
4:A:449:SER:OG	5:B:1134:GLU:OE2	2.26	0.53
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.88	0.53
5:B:287:ARG:HA	5:B:291:ILE:O	2.09	0.53
10:I:55:THR:HG23	10:I:58:VAL:HG21	1.90	0.53
5:B:857:ARG:NH1	5:B:857:ARG:HG3	2.19	0.53
12:K:61:TYR:HA	12:K:72:LYS:O	2.08	0.53
4:A:855:THR:HG23	4:A:857:ARG:HE	1.74	0.53
5:B:731:VAL:O	5:B:732:SER:HB2	2.09	0.53
4:A:583:PRO:O	4:A:610:GLY:HA3	2.09	0.53
5:B:292:ILE:N	5:B:293:PRO:CD	2.67	0.53
5:B:784:ASN:CG	5:B:788:ARG:HD2	2.29	0.53
8:F:84:TYR:CE1	8:F:152:ILE:HD12	2.44	0.53
8:F:85:MET:CE	8:F:93:ILE:HG13	2.39	0.53
4:A:256:GLN:HA	4:A:257:ARG:HB3	1.90	0.53
4:A:315:LEU:HB3	4:A:316:GLN:C	2.29	0.53
4:A:58:LEU:HD22	4:A:59:GLY:H	1.74	0.53
5:B:120:ARG:HB3	5:B:955:THR:HG21	1.91	0.53
5:B:229:ALA:HB1	5:B:231:PRO:HD2	1.89	0.53
5:B:25:ILE:HG22	5:B:26:THR:N	2.23	0.53
5:B:321:GLY:O	5:B:323:VAL:N	2.42	0.53
4:A:1436:ILE:O	4:A:1437:GLY:C	2.46	0.53
5:B:176:SER:O	5:B:182:SER:CB	2.57	0.53
5:B:230:ALA:HA	5:B:261:ARG:NH1	2.23	0.53
4:A:467:THR:HG23	5:B:976:ILE:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:315:LYS:N	5:B:316:PRO:HD2	2.24	0.53
5:B:799:PRO:HB3	5:B:818:PRO:HG2	1.90	0.53
4:A:599:SER:C	4:A:601:LYS:H	2.13	0.53
4:A:896:ARG:HB3	4:A:897:TYR:CD1	2.43	0.53
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.74	0.53
4:A:1328:TYR:OH	4:A:1351:GLU:OE1	2.20	0.52
4:A:855:THR:HG21	4:A:857:ARG:HH21	1.73	0.52
5:B:286:PHE:CB	5:B:297:ILE:HD12	2.36	0.52
4:A:351:THR:HG23	5:B:1103:ILE:HD13	1.92	0.52
5:B:1076:HIS:CD2	12:K:40:HIS:CD2	2.98	0.52
4:A:265:LYS:HZ2	4:A:322:VAL:HB	1.75	0.52
4:A:528:LEU:HA	4:A:531:ILE:HG22	1.91	0.52
5:B:260:GLY:O	5:B:267:ARG:HD3	2.10	0.52
8:F:89:GLU:O	8:F:93:ILE:HG12	2.09	0.52
9:H:128:ASN:O	9:H:131:ASN:OD1	2.28	0.52
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.92	0.52
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.91	0.52
5:B:637:LEU:CD2	5:B:742:GLU:HA	2.29	0.52
4:A:477:PRO:HG3	4:A:521:MET:CE	2.39	0.52
4:A:897:TYR:HD2	4:A:936:LEU:HD13	1.74	0.52
5:B:1065:GLN:NE2	5:B:1069:PHE:H	2.08	0.52
6:C:2:SER:N	6:C:3:GLU:CB	2.71	0.52
9:H:109:LYS:HB2	9:H:111:LEU:HB2	1.92	0.52
4:A:642:CYS:O	4:A:645:LEU:HB3	2.09	0.52
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.43	0.52
4:A:434:ARG:HH21	4:A:437:MET:HG3	1.75	0.52
11:J:56:LEU:O	11:J:57:ILE:C	2.48	0.52
4:A:315:LEU:CD1	4:A:319:GLY:O	2.58	0.52
5:B:230:ALA:H	5:B:231:PRO:CD	2.22	0.52
4:A:140:THR:HA	4:A:143:LYS:HE3	1.92	0.52
5:B:168:GLY:H	5:B:450:ALA:HB1	1.75	0.52
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.10	0.51
4:A:208:LEU:HD22	4:A:208:LEU:C	2.30	0.51
5:B:470:LYS:O	5:B:471:LYS:HG3	2.10	0.51
4:A:69:THR:O	4:A:71:GLN:HG3	2.10	0.51
5:B:682:SER:O	5:B:686:ASN:ND2	2.42	0.51
5:B:1076:HIS:HD2	12:K:40:HIS:CE1	2.29	0.51
4:A:1206:ASP:HB2	4:A:1274:ARG:HH12	1.75	0.51
4:A:129:LYS:O	4:A:130:ASP:HB2	2.10	0.51
4:A:399:HIS:O	4:A:401:GLY:N	2.43	0.51
4:A:401:GLY:H	4:A:435:HIS:HD2	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:709:ASP:C	5:B:711:GLU:H	2.14	0.51
6:C:259:LEU:HD13	12:K:91:CYS:HB3	1.90	0.51
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.44	0.51
4:A:351:THR:HG21	4:A:466:SER:O	2.11	0.51
6:C:97:VAL:HG21	6:C:129:ILE:CG2	2.41	0.51
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.92	0.51
4:A:482:PHE:HD1	5:B:836:GLU:HB2	1.76	0.51
4:A:467:THR:HG22	5:B:1099:VAL:HG11	1.92	0.51
4:A:870:GLU:HB2	7:E:204:THR:HG21	1.93	0.51
5:B:955:THR:HG23	13:L:54:ARG:O	2.10	0.51
6:C:184:ASN:ND2	6:C:189:THR:O	2.44	0.51
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.93	0.51
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.76	0.51
4:A:12:ARG:HB3	5:B:1218:THR:CG2	2.41	0.51
6:C:102:GLN:HG2	6:C:154:LYS:CD	2.40	0.51
6:C:251:LEU:O	6:C:255:VAL:HG23	2.11	0.51
6:C:43:THR:CG2	6:C:44:LEU:H	2.23	0.51
7:E:29:PHE:C	7:E:30:ILE:HG13	2.31	0.51
9:H:139:ASN:O	9:H:140:ALA:HB3	2.11	0.51
4:A:512:VAL:HA	4:A:519:PRO:HA	1.93	0.50
4:A:979:SER:OG	4:A:980:ASP:N	2.45	0.50
5:B:20:ASP:O	5:B:21:GLU:C	2.48	0.50
5:B:549:THR:HG22	5:B:550:ASP:N	2.21	0.50
5:B:642:ASP:O	5:B:644:GLU:N	2.44	0.50
4:A:1017:LEU:HB2	7:E:206:GLY:H	1.75	0.50
4:A:1192:LEU:HD11	4:A:1239:ARG:HB3	1.92	0.50
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.47	0.50
4:A:563:PRO:HG2	4:A:566:ILE:HG12	1.94	0.50
5:B:1084:GLN:CD	5:B:1084:GLN:H	2.15	0.50
5:B:800:GLN:CG	11:J:52:THR:HG22	2.41	0.50
5:B:986:GLN:OE1	5:B:986:GLN:HA	2.11	0.50
6:C:180:TYR:CD1	6:C:180:TYR:O	2.64	0.50
8:F:109:VAL:CG1	8:F:110:ASP:N	2.74	0.50
4:A:678:GLU:HA	4:A:681:GLU:HG2	1.92	0.50
5:B:100:PRO:HG3	5:B:172:ILE:HG13	1.93	0.50
5:B:286:PHE:HB3	5:B:297:ILE:CD1	2.37	0.50
10:I:8:ARG:O	10:I:9:ASP:CB	2.59	0.50
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.67	0.50
4:A:567:LYS:HB3	9:H:96:VAL:N	2.15	0.50
5:B:635:ARG:HB2	5:B:636:PRO:HD3	1.94	0.50
11:J:7:CYS:HA	11:J:49:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1096:ARG:HH11	5:B:1096:ARG:CG	2.23	0.50
13:L:60:ARG:HG3	13:L:61:THR:N	2.26	0.50
4:A:1021:LEU:HD11	4:A:1025:ARG:NH1	2.26	0.50
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.93	0.50
4:A:907:THR:HG22	4:A:908:LEU:N	2.27	0.50
6:C:73:GLN:HE21	6:C:74:SER:N	2.08	0.50
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.41	0.50
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.93	0.50
4:A:345:VAL:HG12	5:B:1155:SER:HB2	1.93	0.50
5:B:1079:LYS:HE3	6:C:188:HIS:CE1	2.47	0.50
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.77	0.50
11:J:6:ARG:HA	11:J:12:LYS:O	2.12	0.50
5:B:1076:HIS:HD2	12:K:40:HIS:NE2	2.06	0.50
5:B:1096:ARG:HG2	5:B:1096:ARG:NH1	2.27	0.50
5:B:487:THR:HG22	5:B:489:SER:N	2.27	0.50
5:B:515:HIS:CD2	5:B:517:THR:H	2.30	0.50
4:A:896:ARG:HD2	4:A:897:TYR:HE1	1.76	0.49
5:B:1017:ILE:H	5:B:1018:PRO:HD3	1.78	0.49
5:B:1017:ILE:HD12	5:B:1026:LEU:HD21	1.94	0.49
6:C:31:ASN:O	6:C:35:ARG:HG3	2.12	0.49
9:H:109:LYS:HB2	9:H:111:LEU:N	2.26	0.49
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	1.97	0.49
4:A:1436:ILE:O	4:A:1439:GLY:N	2.40	0.49
4:A:401:GLY:C	4:A:435:HIS:CD2	2.86	0.49
5:B:294:ASP:N	5:B:294:ASP:OD2	2.34	0.49
4:A:1236:LEU:C	4:A:1237:ILE:HG13	2.33	0.49
4:A:809:THR:HB	4:A:810:PRO:HD2	1.94	0.49
5:B:900:ALA:O	5:B:902:GLY:N	2.45	0.49
6:C:16:ASP:O	6:C:233:GLU:HA	2.12	0.49
5:B:1073:TYR:CE2	5:B:1080:LYS:HG3	2.48	0.49
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.27	0.49
5:B:864:LYS:HB2	5:B:865:LYS:CA	2.25	0.49
7:E:198:ILE:HD12	7:E:198:ILE:H	1.78	0.49
7:E:136:ASN:OD1	7:E:137:GLU:N	2.45	0.49
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.48	0.49
4:A:523:ILE:HG23	4:A:527:THR:HB	1.95	0.49
4:A:451:HIS:HB3	4:A:453:MET:N	2.28	0.49
4:A:800:VAL:HG12	4:A:802:ASN:H	1.78	0.49
4:A:907:THR:HG22	4:A:908:LEU:H	1.78	0.49
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.42	0.49
10:I:106:CYS:SG	10:I:108:HIS:HB3	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:464:PRO:HG2	12:K:67:PHE:CD1	2.47	0.49
4:A:353:ILE:HD13	4:A:487:MET:HE2	1.93	0.49
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.95	0.49
4:A:351:THR:HG23	5:B:1103:ILE:CD1	2.43	0.49
5:B:498:THR:HB	5:B:537:LYS:O	2.13	0.49
5:B:635:ARG:NH1	5:B:635:ARG:HG3	2.28	0.49
5:B:120:ARG:HA	5:B:963:PHE:HE2	1.78	0.49
8:F:81:THR:HG1	8:F:144:GLU:CD	2.16	0.49
1:R:3:U:H2'	1:R:4:C:H6	1.77	0.49
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.95	0.48
5:B:636:PRO:HB3	5:B:743:ILE:HG12	1.95	0.48
5:B:637:LEU:HD21	5:B:742:GLU:OE2	2.04	0.48
5:B:984:HIS:CE1	5:B:1025:HIS:HA	2.48	0.48
4:A:1425:SER:O	4:A:1429:ILE:HD12	2.12	0.48
4:A:455:MET:HE2	5:B:1138:MET:SD	2.53	0.48
4:A:504:LEU:HD11	8:F:91:ALA:HB1	1.95	0.48
4:A:830:LYS:HG3	4:A:1098:VAL:HG21	1.96	0.48
5:B:1146:PHE:CZ	5:B:1150:ARG:HG3	2.48	0.48
4:A:760:GLN:HE21	4:A:765:VAL:HA	1.77	0.48
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.12	0.48
5:B:545:ILE:HG23	5:B:631:GLY:HA2	1.95	0.48
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.95	0.48
2:T:20:DC:H2'	2:T:21:DT:O4'	2.13	0.48
5:B:1072:MET:O	5:B:1081:LEU:HB2	2.13	0.48
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.96	0.48
5:B:992:ILE:HD11	12:K:67:PHE:CE2	2.47	0.48
7:E:153:HIS:O	7:E:154:ILE:HD13	2.14	0.48
8:F:97:ARG:HD2	8:F:101:ILE:CD1	2.44	0.48
12:K:12:LEU:HD12	12:K:12:LEU:H	1.78	0.48
4:A:332:LYS:C	4:A:334:GLY:H	2.17	0.48
4:A:332:LYS:H	4:A:337:ARG:HB3	1.79	0.48
5:B:1002:THR:HG23	5:B:1004:GLU:N	2.28	0.48
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.95	0.48
7:E:161:LYS:HD2	7:E:195:VAL:HG23	1.94	0.48
13:L:40:LEU:HD11	13:L:49:LYS:HE2	1.95	0.48
4:A:512:VAL:HG13	4:A:512:VAL:O	2.12	0.48
4:A:1100:ARG:NH2	4:A:1351:GLU:HG3	2.28	0.48
5:B:992:ILE:HD11	12:K:67:PHE:HE2	1.77	0.48
4:A:1161:THR:CG2	4:A:1162:VAL:N	2.76	0.48
4:A:599:SER:OG	4:A:614:PHE:CD1	2.66	0.48
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:325:GLN:NE2	10:I:12:ASN:ND2	2.58	0.48
10:I:28:GLU:HB3	10:I:35:VAL:HG22	1.95	0.48
4:A:378:GLU:OE1	4:A:434:ARG:HD3	2.14	0.48
5:B:887:HIS:HB2	5:B:908:GLU:OE2	2.13	0.48
1:R:3:U:H2'	1:R:4:C:C6	2.49	0.48
4:A:1277:GLU:O	4:A:1278:ASN:HB2	2.14	0.47
5:B:1107:ALA:O	5:B:1108:ARG:CB	2.62	0.47
5:B:893:LEU:HD22	5:B:897:GLY:O	2.13	0.47
4:A:1063:MET:SD	4:A:1436:ILE:HG12	2.54	0.47
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.94	0.47
5:B:461:LEU:O	5:B:480:SER:OG	2.29	0.47
11:J:9:SER:OG	11:J:48:ARG:NH2	2.47	0.47
4:A:55:ASP:O	4:A:58:LEU:N	2.37	0.47
5:B:1073:TYR:N	5:B:1073:TYR:CD1	2.82	0.47
5:B:195:CYS:CB	5:B:782:LEU:HD22	2.44	0.47
6:C:43:THR:HG23	6:C:74:SER:OG	2.14	0.47
9:H:25:ARG:HD2	9:H:39:THR:HG22	1.96	0.47
11:J:43:ARG:HG3	11:J:46:CYS:SG	2.54	0.47
12:K:46:ILE:HG22	12:K:50:LEU:HD12	1.97	0.47
4:A:913:LEU:CD1	4:A:915:SER:H	2.26	0.47
5:B:636:PRO:HB3	5:B:637:LEU:CB	2.34	0.47
6:C:56:THR:HG23	6:C:147:LEU:HD23	1.95	0.47
6:C:5:GLY:HA3	6:C:6:PRO:HD2	1.65	0.47
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.95	0.47
4:A:802:ASN:HD21	5:B:729:ILE:H	1.63	0.47
5:B:701:ILE:HG13	5:B:740:HIS:CE1	2.50	0.47
4:A:120:GLU:HA	4:A:123:ARG:HD3	1.96	0.47
4:A:1242:VAL:CG1	4:A:1243:VAL:H	2.21	0.47
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.15	0.47
4:A:942:PHE:C	4:A:942:PHE:CD2	2.88	0.47
5:B:955:THR:CG2	5:B:956:THR:H	2.27	0.47
4:A:1154:TYR:HD1	4:A:1191:TRP:CH2	2.33	0.47
4:A:1305:VAL:HG12	4:A:1306:LEU:N	2.30	0.47
5:B:637:LEU:HD22	5:B:742:GLU:OE2	2.01	0.47
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.97	0.47
5:B:976:ILE:HG23	5:B:977:GLY:N	2.30	0.47
8:F:109:VAL:HG13	8:F:110:ASP:N	2.30	0.47
4:A:1441:PHE:CE2	8:F:89:GLU:HA	2.49	0.47
2:T:15:DC:H2''	2:T:16:DG:O5'	2.15	0.47
4:A:507:VAL:O	4:A:508:PRO:C	2.52	0.47
4:A:847:ASP:OD2	4:A:858:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:487:THR:HG23	5:B:488:TYR:H	1.78	0.47
16:T:3000:G2P:O3G	5:B:1020:ARG:NH1	2.48	0.47
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.80	0.47
5:B:37:PHE:O	5:B:38:PHE:CB	2.54	0.47
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.43	0.47
5:B:864:LYS:HB3	5:B:871:THR:HG23	1.95	0.47
5:B:892:LYS:HG2	5:B:903:VAL:HG11	1.97	0.47
9:H:41:ASP:HB3	9:H:121:LEU:HD22	1.96	0.47
4:A:809:THR:HG1	4:A:812:GLU:CD	2.18	0.46
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.50	0.46
5:B:500:THR:HA	5:B:501:PRO:HD3	1.50	0.46
5:B:865:LYS:CB	5:B:866:TYR:CA	2.89	0.46
6:C:60:ASP:HB3	13:L:67:PHE:CE1	2.50	0.46
5:B:709:ASP:O	5:B:711:GLU:N	2.48	0.46
6:C:186:LEU:CB	6:C:188:HIS:HD2	2.28	0.46
12:K:70:ARG:O	12:K:70:ARG:HG3	2.16	0.46
4:A:256:GLN:HB3	4:A:257:ARG:HB3	1.97	0.46
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.98	0.46
5:B:363:HIS:O	5:B:364:ILE:HB	2.16	0.46
7:E:46:TYR:CE2	7:E:58:MET:HA	2.49	0.46
4:A:1209:MET:O	4:A:1212:VAL:HB	2.15	0.46
4:A:1394:THR:HG21	4:A:1398:MET:HE3	1.97	0.46
4:A:746:MET:HG2	5:B:1015:HIS:CE1	2.50	0.46
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.15	0.46
5:B:636:PRO:HB2	5:B:637:LEU:CA	2.26	0.46
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.97	0.46
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.97	0.46
6:C:102:GLN:HG2	6:C:154:LYS:HD2	1.98	0.46
13:L:68:GLU:OE1	13:L:68:GLU:O	2.34	0.46
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.98	0.46
4:A:1356:ILE:HG22	4:A:1361:SER:O	2.15	0.46
4:A:347:PHE:HB2	5:B:1150:ARG:HH22	1.80	0.46
5:B:363:HIS:HD2	5:B:585:VAL:HG22	1.80	0.46
7:E:198:ILE:N	7:E:198:ILE:HD12	2.30	0.46
4:A:115:LEU:HD22	4:A:119:ASN:HB2	1.98	0.46
4:A:511:ILE:O	4:A:519:PRO:HA	2.16	0.46
5:B:865:LYS:HB2	5:B:866:TYR:HA	1.96	0.46
4:A:55:ASP:N	4:A:56:PRO:HD2	2.30	0.46
10:I:71:SER:H	10:I:83:ASN:ND2	2.14	0.46
4:A:343:LYS:HZ1	5:B:1197:PRO:HB3	1.81	0.46
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:400:HIS:CE1	5:B:517:THR:HG21	2.51	0.46
4:A:740:LEU:HD21	6:C:193:TYR:CE2	2.51	0.46
7:E:65:THR:C	7:E:67:GLU:H	2.18	0.46
8:F:82:THR:HG22	8:F:84:TYR:HB2	1.97	0.46
4:A:90:VAL:HG11	4:A:297:GLN:HA	1.98	0.46
5:B:1064:TYR:CD1	5:B:1064:TYR:N	2.83	0.46
5:B:654:ARG:N	5:B:657:HIS:HD2	2.10	0.46
6:C:67:LEU:HD11	6:C:155:LEU:HD13	1.98	0.46
4:A:19:PHE:O	4:A:1416:ALA:HA	2.16	0.46
4:A:315:LEU:HD13	4:A:319:GLY:O	2.16	0.46
4:A:567:LYS:CB	4:A:568:PRO:CD	2.52	0.46
4:A:875:ALA:HB2	4:A:1366:ARG:CD	2.44	0.46
4:A:913:LEU:HD13	4:A:914:GLU:H	1.81	0.46
8:F:97:ARG:HD2	8:F:101:ILE:HG13	1.97	0.46
9:H:110:ASP:O	9:H:128:ASN:CG	2.55	0.46
4:A:353:ILE:HD12	4:A:482:PHE:CE2	2.51	0.45
4:A:858:ASN:ND2	4:A:858:ASN:C	2.66	0.45
6:C:57:VAL:CG2	11:J:57:ILE:HD11	2.44	0.45
4:A:1058:VAL:HG12	4:A:1062:GLU:HG3	1.98	0.45
4:A:590:ARG:NH2	4:A:621:THR:HA	2.30	0.45
4:A:67:CYS:O	4:A:70:CYS:HB3	2.16	0.45
5:B:762:ASN:ND2	5:B:1022:THR:HA	2.31	0.45
8:F:116:ASP:OD2	8:F:117:PRO:HD2	2.16	0.45
9:H:24:CYS:HB2	9:H:44:VAL:CG2	2.46	0.45
4:A:754:SER:N	4:A:757:ASN:HD22	2.13	0.45
5:B:984:HIS:CD2	5:B:1024:ALA:HB3	2.50	0.45
12:K:43:GLY:HA2	12:K:71:PHE:CZ	2.52	0.45
4:A:956:LEU:HD11	4:A:1017:LEU:HD22	1.99	0.45
4:A:313:GLN:HG3	4:A:314:ALA:H	1.82	0.45
5:B:848:ARG:HH22	5:B:996:ARG:HH11	1.59	0.45
6:C:99:LEU:CD1	6:C:120:ILE:HA	2.46	0.45
6:C:66:ARG:HH21	11:J:5:VAL:H	1.64	0.45
10:I:69:PRO:HB2	10:I:85:PHE:CE2	2.51	0.45
12:K:47:ARG:HG3	12:K:60:ALA:HA	1.98	0.45
4:A:472:LEU:O	4:A:475:THR:HB	2.17	0.45
4:A:446:ARG:HH21	4:A:485:ASP:CG	2.20	0.45
5:B:979:LYS:C	5:B:980:PHE:CD1	2.89	0.45
6:C:15:LYS:O	6:C:240:VAL:HG22	2.16	0.45
7:E:77:SER:HB2	7:E:105:PHE:HD2	1.81	0.45
9:H:59:ILE:HD13	9:H:142:LEU:HD12	1.99	0.45
5:B:706:GLN:O	5:B:707:PRO:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:137:LYS:HE3	6:C:137:LYS:HB3	1.78	0.45
12:K:7:PHE:CD1	12:K:7:PHE:C	2.89	0.45
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.81	0.45
5:B:1065:GLN:NE2	5:B:1067:ARG:H	2.15	0.45
4:A:343:LYS:NZ	5:B:1156:ASP:OD2	2.49	0.45
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.82	0.45
6:C:180:TYR:O	6:C:181:ASP:HB3	2.16	0.45
8:F:107:VAL:HG12	8:F:109:VAL:H	1.81	0.45
12:K:90:ALA:O	12:K:94:ILE:HD12	2.16	0.45
2:T:26:DA:C6	2:T:27:DT:H72	2.51	0.45
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.32	0.45
4:A:18:GLN:HG2	4:A:1418:LEU:HD12	1.98	0.45
4:A:350:ARG:HG2	4:A:486:GLU:HG2	1.99	0.45
5:B:1007:VAL:HG13	5:B:1008:PRO:HD2	1.97	0.45
5:B:549:THR:HB	5:B:628:THR:HG21	1.99	0.45
6:C:173:ALA:O	6:C:174:ALA:HB3	2.17	0.45
4:A:380:VAL:HG22	4:A:430:TRP:H	1.82	0.45
5:B:483:LEU:O	5:B:484:ASN:HB2	2.17	0.45
5:B:484:ASN:ND2	5:B:490:SER:OG	2.50	0.45
5:B:70:ILE:O	5:B:70:ILE:HG22	2.16	0.45
5:B:766:ARG:HD3	5:B:766:ARG:HA	1.77	0.45
6:C:267:GLN:OE1	6:C:267:GLN:HA	2.17	0.45
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.64	0.45
10:I:7:CYS:HB2	10:I:14:LEU:HD21	1.99	0.45
4:A:549:MET:O	4:A:550:LEU:C	2.54	0.45
5:B:273:LEU:HD21	5:B:360:PHE:CD1	2.51	0.45
6:C:4:GLU:HG3	6:C:5:GLY:H	1.81	0.45
9:H:26:ILE:HG22	9:H:40:LEU:HB3	1.99	0.45
4:A:26:GLU:O	4:A:29:ALA:N	2.45	0.44
4:A:775:ILE:HB	4:A:797:LYS:O	2.17	0.44
4:A:626:ASN:HD21	4:A:880:LYS:HB3	1.83	0.44
5:B:1065:GLN:HE21	5:B:1069:PHE:H	1.64	0.44
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.99	0.44
5:B:526:GLU:HG3	5:B:771:SER:HB3	1.98	0.44
5:B:580:VAL:HG22	5:B:624:LEU:HB3	1.98	0.44
4:A:1059:HIS:ND1	8:F:86:THR:HA	2.32	0.44
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.52	0.44
4:A:1189:SER:O	4:A:1241:ARG:HD3	2.18	0.44
4:A:960:ILE:O	4:A:961:ARG:C	2.55	0.44
6:C:123:ASN:HD21	6:C:125:MET:HG2	1.78	0.44
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2:SER:N	6:C:3:GLU:CA	2.80	0.44
7:E:171:LYS:HE2	7:E:174:GLN:NE2	2.32	0.44
9:H:102:TYR:OH	9:H:122:LEU:HD22	2.17	0.44
11:J:32:GLU:O	11:J:36:LEU:HG	2.16	0.44
4:A:577:ILE:O	4:A:580:VAL:HG23	2.18	0.44
5:B:234:ILE:H	5:B:234:ILE:HD13	1.82	0.44
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.52	0.44
10:I:59:VAL:CG1	10:I:60:GLN:H	2.24	0.44
5:B:190:TYR:CE1	11:J:62:ARG:HG2	2.53	0.44
4:A:1006:ILE:HD11	7:E:163:GLU:HG3	1.99	0.44
4:A:1188:GLN:HB3	4:A:1189:SER:H	1.56	0.44
4:A:1305:VAL:CG1	4:A:1306:LEU:N	2.80	0.44
10:I:111:THR:CG2	10:I:112:SER:N	2.80	0.44
4:A:666:ILE:CG2	5:B:1026:LEU:HB2	2.47	0.44
5:B:1084:GLN:HE22	6:C:192:TRP:N	2.13	0.44
5:B:1136:ASP:HA	5:B:1139:ILE:HD12	1.99	0.44
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.17	0.44
5:B:744:HIS:HD2	5:B:746:SER:H	1.63	0.44
5:B:973:ILE:HG22	5:B:974:PRO:HD2	1.99	0.44
6:C:229:TYR:CD1	6:C:229:TYR:N	2.86	0.44
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	1.98	0.44
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	2.00	0.44
4:A:463:ILE:CB	4:A:464:PRO:HD2	2.47	0.44
4:A:852:TYR:O	4:A:853:ASP:HB3	2.18	0.44
5:B:1106:ARG:HD3	5:B:1127:GLY:N	2.32	0.44
7:E:167:ARG:HD3	7:E:167:ARG:HA	1.78	0.44
7:E:28:TYR:HE1	7:E:78:LEU:HD13	1.82	0.44
8:F:128:LYS:HD2	8:F:148:VAL:O	2.18	0.44
4:A:1393:ASN:CG	4:A:1393:ASN:O	2.56	0.44
4:A:456:MET:HE2	4:A:478:TYR:CZ	2.53	0.44
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.50	0.44
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.98	0.44
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.99	0.44
4:A:370:ILE:HG22	4:A:374:LEU:HD11	2.00	0.44
4:A:857:ARG:HA	4:A:864:ILE:HG12	1.98	0.44
4:A:954:TRP:HA	4:A:955:PRO:HD2	1.86	0.44
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	2.32	0.44
5:B:48:LEU:O	5:B:52:ASN:ND2	2.50	0.44
10:I:104:LEU:HA	10:I:104:LEU:HD23	1.90	0.44
4:A:382:PRO:N	4:A:428:TYR:HE2	2.16	0.44
4:A:49:LYS:HZ2	4:A:60:SER:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:361:LEU:HD22	4:A:646:PHE:CD1	2.53	0.44
4:A:785:PRO:HG3	5:B:698:GLU:HG2	1.99	0.44
4:A:660:ASN:OD1	5:B:1082:MET:HG3	2.16	0.44
5:B:1200:ALA:O	5:B:1203:LEU:N	2.51	0.44
5:B:185:THR:OG1	5:B:188:ASP:OD2	2.36	0.44
5:B:327:ARG:O	5:B:331:LEU:HD12	2.18	0.44
5:B:58:THR:O	5:B:62:ILE:HG12	2.17	0.44
5:B:684:LEU:CD2	5:B:689:LEU:HD12	2.48	0.44
5:B:881:ASN:HB2	5:B:933:SER:OG	2.18	0.44
4:A:271:LYS:O	4:A:275:SER:HB2	2.18	0.43
4:A:311:GLN:HA	4:A:312:PRO:HD3	1.87	0.43
4:A:335:ARG:CD	5:B:1202:LEU:HD12	2.48	0.43
4:A:49:LYS:O	4:A:50:ILE:HG12	2.18	0.43
4:A:885:THR:O	4:A:940:ARG:HG3	2.18	0.43
4:A:901:LEU:H	4:A:926:GLN:HE21	1.66	0.43
5:B:707:PRO:HB2	5:B:708:GLU:H	1.61	0.43
9:H:44:VAL:O	9:H:44:VAL:HG12	2.18	0.43
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.18	0.43
4:A:18:GLN:HG2	4:A:1418:LEU:CD1	2.48	0.43
4:A:683:ILE:HG21	4:A:801:GLU:HG2	2.00	0.43
4:A:741:ASN:ND2	4:A:741:ASN:C	2.71	0.43
5:B:198:ASP:OD1	5:B:485:ARG:NH2	2.51	0.43
5:B:942:ARG:O	5:B:944:THR:N	2.51	0.43
5:B:97:VAL:HB	5:B:178:ASN:HD21	1.83	0.43
6:C:74:SER:O	6:C:77:ILE:HB	2.18	0.43
8:F:100:GLN:O	8:F:105:ALA:HB3	2.19	0.43
9:H:23:VAL:HG21	9:H:121:LEU:HD21	1.99	0.43
4:A:567:LYS:HE3	9:H:46:LEU:HD12	1.98	0.43
5:B:487:THR:HG22	5:B:489:SER:H	1.82	0.43
5:B:54:PHE:HA	5:B:58:THR:HB	2.00	0.43
5:B:800:GLN:CB	11:J:52:THR:HG22	2.48	0.43
5:B:980:PHE:N	5:B:980:PHE:HD1	2.14	0.43
4:A:1097:GLY:C	4:A:1099:PRO:HD2	2.39	0.43
4:A:1140:HIS:HB2	4:A:1276:VAL:O	2.17	0.43
5:B:542:MET:SD	5:B:747:MET:HE2	2.58	0.43
8:F:77:ASP:N	8:F:77:ASP:OD1	2.50	0.43
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.99	0.43
4:A:1015:VAL:O	4:A:1018:PHE:N	2.51	0.43
4:A:535:THR:HG21	4:A:617:VAL:H	1.83	0.43
4:A:828:ALA:HB2	5:B:530:GLY:HA2	2.00	0.43
5:B:487:THR:HG22	5:B:488:TYR:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.99	0.43
5:B:696:GLU:O	5:B:699:GLU:HB2	2.18	0.43
5:B:870:ILE:O	5:B:870:ILE:HG22	2.18	0.43
6:C:33:LEU:HD12	6:C:251:LEU:HD23	1.99	0.43
11:J:44:TYR:HA	11:J:47:ARG:HB2	2.01	0.43
11:J:1:MET:H3	11:J:56:LEU:HD12	1.83	0.43
4:A:1155:ASP:OD1	4:A:1162:VAL:HG23	2.18	0.43
4:A:1351:GLU:OE2	4:A:1351:GLU:HA	2.18	0.43
4:A:774:ARG:HG3	4:A:797:LYS:HE3	2.01	0.43
5:B:1200:ALA:O	5:B:1201:LYS:C	2.56	0.43
5:B:552:MET:HA	5:B:555:ILE:HB	2.00	0.43
4:A:535:THR:HG23	4:A:575:LYS:HG2	2.00	0.43
5:B:1084:GLN:N	5:B:1084:GLN:CD	2.72	0.43
5:B:577:ALA:HB1	5:B:589:VAL:CG1	2.49	0.43
6:C:63:ILE:O	6:C:66:ARG:N	2.52	0.43
4:A:834:THR:HG21	4:A:1077:THR:OG1	2.18	0.43
4:A:93:VAL:HG22	4:A:301:ALA:HA	2.01	0.43
4:A:709:THR:HG22	4:A:710:LEU:N	2.34	0.43
5:B:314:LEU:O	5:B:315:LYS:C	2.55	0.43
5:B:801:LYS:O	5:B:801:LYS:HG3	2.17	0.43
6:C:102:GLN:HG2	6:C:154:LYS:HD3	2.00	0.43
7:E:77:SER:CB	7:E:105:PHE:HD2	2.31	0.43
4:A:560:ILE:HD11	12:K:58:PHE:CD1	2.54	0.43
12:K:43:GLY:HA2	12:K:71:PHE:CE1	2.52	0.43
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	2.01	0.43
4:A:802:ASN:HD21	5:B:729:ILE:N	2.16	0.43
4:A:746:MET:HG2	5:B:1015:HIS:HE1	1.83	0.43
5:B:254:LEU:HD23	5:B:381:MET:SD	2.59	0.43
5:B:690:VAL:HG12	5:B:691:GLU:H	1.82	0.43
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.83	0.43
5:B:899:ILE:HG22	5:B:900:ALA:H	1.84	0.43
6:C:73:GLN:HE21	6:C:74:SER:H	1.67	0.43
5:B:363:HIS:HD2	5:B:585:VAL:CG2	2.32	0.43
6:C:34:ARG:NH1	6:C:35:ARG:HG2	2.34	0.43
4:A:1280:GLU:HB3	4:A:1281:ARG:H	1.54	0.42
5:B:604:ARG:HH21	5:B:614:SER:HA	1.84	0.42
5:B:624:LEU:C	5:B:624:LEU:HD12	2.39	0.42
5:B:792:MET:HE3	5:B:792:MET:N	2.34	0.42
5:B:796:LEU:HD23	5:B:799:PRO:HA	2.01	0.42
7:E:198:ILE:HD12	7:E:210:SER:O	2.18	0.42
10:I:30:ARG:HD2	10:I:30:ARG:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1154:TYR:HD1	4:A:1191:TRP:CZ3	2.37	0.42
4:A:1116:LEU:HB2	4:A:1308:THR:OG1	2.18	0.42
4:A:434:ARG:NH2	4:A:437:MET:HG3	2.34	0.42
5:B:364:ILE:HD13	5:B:585:VAL:HG13	2.00	0.42
4:A:689:LYS:HG2	4:A:689:LYS:O	2.19	0.42
4:A:320:ARG:HB2	5:B:471:LYS:HE2	2.01	0.42
5:B:479:VAL:O	5:B:480:SER:CB	2.67	0.42
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.00	0.42
7:E:160:GLU:O	7:E:163:GLU:HB3	2.20	0.42
4:A:356:ASP:HA	4:A:357:PRO:HD2	1.74	0.42
4:A:543:LEU:O	4:A:544:ASP:C	2.57	0.42
5:B:1119:VAL:O	5:B:1126:GLY:HA3	2.19	0.42
5:B:28:GLU:C	5:B:30:SER:H	2.22	0.42
5:B:800:GLN:HG2	11:J:52:THR:CG2	2.46	0.42
4:A:51:GLY:HA2	4:A:56:PRO:HG3	2.01	0.42
4:A:577:ILE:H	4:A:577:ILE:HG13	1.54	0.42
4:A:899:VAL:O	4:A:929:LEU:HD12	2.20	0.42
7:E:135:PHE:CD2	7:E:140:LEU:HD11	2.54	0.42
7:E:55:ARG:HB3	7:E:82:PHE:HB3	2.02	0.42
11:J:2:ILE:HA	11:J:2:ILE:HD12	1.79	0.42
12:K:65:HIS:CD2	12:K:67:PHE:H	2.37	0.42
5:B:287:ARG:HG2	5:B:292:ILE:HA	2.02	0.42
5:B:321:GLY:C	5:B:323:VAL:H	2.22	0.42
5:B:899:ILE:HG13	5:B:899:ILE:H	1.69	0.42
6:C:176:ILE:HG12	6:C:232:VAL:HG13	2.02	0.42
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.55	0.42
4:A:1366:ARG:H	4:A:1366:ARG:HG2	1.59	0.42
4:A:54:ASN:O	4:A:55:ASP:HB2	2.19	0.42
4:A:797:LYS:HE3	4:A:797:LYS:HB3	1.88	0.42
5:B:1117:GLN:NE2	5:B:1199:ALA:HB2	2.34	0.42
5:B:273:LEU:HD21	5:B:360:PHE:HD1	1.84	0.42
7:E:196:VAL:HG23	7:E:197:LYS:N	2.35	0.42
9:H:2:SER:O	9:H:3:ASN:HB2	2.20	0.42
4:A:347:PHE:HB2	5:B:1150:ARG:NH2	2.35	0.42
5:B:1190:ASP:O	5:B:1191:ILE:HG13	2.19	0.42
5:B:345:LYS:O	5:B:348:ARG:HG2	2.20	0.42
5:B:865:LYS:HB2	5:B:866:TYR:CA	2.49	0.42
6:C:3:GLU:HB3	12:K:104:ASN:HD21	1.85	0.42
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	2.01	0.42
4:A:455:MET:CE	5:B:1138:MET:SD	3.08	0.42
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:174:LEU:HD11	5:B:204:ILE:HG13	2.02	0.42
6:C:181:ASP:HA	6:C:182:PRO:HD2	1.82	0.42
11:J:32:GLU:CD	11:J:32:GLU:H	2.22	0.42
4:A:1193:LEU:C	4:A:1193:LEU:HD12	2.41	0.42
4:A:909:ASP:OD2	4:A:910:PRO:HD2	2.20	0.42
5:B:429:PHE:O	5:B:433:GLN:HG3	2.20	0.42
5:B:43:LEU:HD23	5:B:43:LEU:HA	1.88	0.42
5:B:739:THR:OG1	5:B:740:HIS:N	2.53	0.42
13:L:30:ILE:C	13:L:56:LEU:HD23	2.40	0.42
4:A:475:THR:HG22	4:A:476:SER:N	2.35	0.41
4:A:648:ASN:OD1	4:A:648:ASN:N	2.53	0.41
4:A:1324:PRO:HB2	7:E:142:VAL:HG11	2.02	0.41
7:E:65:THR:C	7:E:67:GLU:N	2.73	0.41
4:A:1101:LEU:O	4:A:1105:LEU:HD12	2.20	0.41
4:A:304:MET:O	4:A:305:ASP:HB2	2.20	0.41
4:A:609:ASP:O	4:A:611:GLN:N	2.53	0.41
4:A:645:LEU:CD1	4:A:649:ILE:HD11	2.50	0.41
4:A:346:ASP:H	5:B:1154:ALA:HB1	1.85	0.41
5:B:1159:ARG:CD	5:B:1193:GLN:HG3	2.46	0.41
5:B:567:GLU:CD	5:B:567:GLU:H	2.22	0.41
8:F:118:LEU:O	8:F:122:MET:HG3	2.20	0.41
12:K:32:VAL:HG22	12:K:74:ARG:HB2	2.02	0.41
4:A:256:GLN:CB	4:A:257:ARG:HB3	2.50	0.41
4:A:576:GLN:O	4:A:579:SER:HB2	2.21	0.41
4:A:668:ASP:HB3	4:A:743:VAL:CG2	2.33	0.41
4:A:902:LEU:H	4:A:902:LEU:HG	1.50	0.41
5:B:762:ASN:HD21	5:B:1022:THR:HA	1.85	0.41
5:B:113:TYR:O	5:B:114:PRO:C	2.59	0.41
5:B:1174:LYS:HB2	5:B:1179:GLN:O	2.20	0.41
5:B:846:ILE:HG23	5:B:974:PRO:HG2	2.02	0.41
5:B:874:PHE:CD2	5:B:914:LYS:HB3	2.54	0.41
4:A:1332:PHE:CE1	4:A:1348:LEU:HD13	2.55	0.41
4:A:328:ARG:HD3	4:A:335:ARG:HH12	1.84	0.41
4:A:407:ARG:HG2	4:A:430:TRP:CE2	2.55	0.41
4:A:414:ASP:OD1	4:A:416:ARG:HG2	2.20	0.41
4:A:662:PHE:O	5:B:828:ALA:HA	2.19	0.41
4:A:913:LEU:HD12	4:A:915:SER:N	2.31	0.41
5:B:711:GLU:N	5:B:712:PRO:CD	2.84	0.41
5:B:855:PHE:N	5:B:970:THR:O	2.53	0.41
12:K:73:LEU:HA	12:K:73:LEU:HD12	1.82	0.41
2:T:17:DA:OP1	4:A:337:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:986:ILE:HG21	4:A:1028:THR:HA	2.03	0.41
5:B:899:ILE:HD11	5:B:911:ILE:HG23	2.02	0.41
7:E:86:PRO:HB3	7:E:114:ASN:HD22	1.84	0.41
9:H:104:PHE:HD2	9:H:114:VAL:HG12	1.86	0.41
9:H:5:LEU:O	9:H:133:ASN:HB3	2.21	0.41
9:H:93:TYR:CD2	9:H:145:ARG:HB3	2.56	0.41
4:A:562:THR:HG22	4:A:563:PRO:HD2	2.03	0.41
6:C:42:PRO:HA	6:C:163:ILE:HG23	2.02	0.41
8:F:132:LEU:O	8:F:148:VAL:HG23	2.20	0.41
12:K:20:LYS:HE3	12:K:22:ASP:OD2	2.20	0.41
4:A:321:PRO:HB2	4:A:322:VAL:H	1.55	0.41
4:A:909:ASP:C	4:A:911:SER:N	2.74	0.41
5:B:1024:ALA:O	5:B:1027:ILE:N	2.53	0.41
5:B:416:LEU:HD23	5:B:420:LEU:HD12	2.02	0.41
5:B:800:GLN:HB3	11:J:52:THR:CG2	2.50	0.41
8:F:81:THR:HG21	8:F:136:ARG:HD3	2.02	0.41
8:F:85:MET:HE1	8:F:93:ILE:HG13	2.02	0.41
9:H:44:VAL:HG13	9:H:48:PRO:HA	2.02	0.41
9:H:42:ILE:HD12	9:H:95:TYR:CZ	2.56	0.41
4:A:84:ILE:HD11	4:A:270:LEU:HG	2.03	0.41
4:A:619:LYS:O	4:A:623:GLY:N	2.49	0.41
5:B:800:GLN:HB3	11:J:52:THR:HG22	2.03	0.41
4:A:57:ARG:C	4:A:68:GLN:HG2	2.41	0.41
4:A:65:LEU:O	4:A:71:GLN:HA	2.21	0.41
5:B:100:PRO:HA	5:B:126:SER:HB3	2.03	0.41
6:C:120:ILE:H	6:C:120:ILE:HG13	1.74	0.41
7:E:24:LYS:HB3	7:E:30:ILE:HD12	2.02	0.41
9:H:109:LYS:HB3	9:H:110:ASP:HA	0.60	0.41
6:C:235:VAL:HG21	11:J:6:ARG:HH21	1.86	0.41
4:A:848:ILE:HG22	4:A:1064:VAL:HG23	2.03	0.41
5:B:1164:GLY:HA3	5:B:1190:ASP:HB3	2.03	0.41
5:B:114:PRO:HB2	5:B:194:GLU:OE2	2.21	0.41
5:B:26:THR:O	5:B:27:ALA:C	2.59	0.41
5:B:34:ILE:O	5:B:37:PHE:O	2.38	0.41
5:B:492:LEU:HB3	5:B:751:VAL:HG21	2.02	0.41
5:B:702:LEU:H	5:B:739:THR:HG23	1.84	0.41
9:H:24:CYS:HB2	9:H:44:VAL:HG23	2.02	0.41
4:A:503:GLN:HE21	8:F:90:ARG:HH21	1.69	0.41
4:A:901:LEU:HD12	4:A:926:GLN:HG2	2.02	0.41
5:B:258:LEU:HD13	5:B:269:ILE:HG12	2.03	0.41
5:B:210:LYS:HZ2	5:B:482:VAL:HG13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:135:PHE:HD2	7:E:140:LEU:HD11	1.87	0.41
9:H:38:LEU:HD12	9:H:124:ARG:O	2.21	0.41
9:H:12:VAL:HB	9:H:53:ASP:H	1.86	0.41
11:J:8:PHE:H	11:J:49:MET:CE	2.27	0.41
12:K:12:LEU:N	12:K:12:LEU:HD12	2.35	0.41
12:K:6:ARG:O	12:K:9:LEU:HG	2.21	0.41
4:A:401:GLY:N	4:A:435:HIS:HD2	2.18	0.40
4:A:756:ILE:O	4:A:760:GLN:HG3	2.20	0.40
5:B:1045:SER:HA	5:B:1046:PRO:HD3	1.85	0.40
5:B:550:ASP:OD1	5:B:551:PRO:CD	2.69	0.40
5:B:653:VAL:HG22	5:B:689:LEU:HB3	2.03	0.40
6:C:46:ILE:H	6:C:46:ILE:HG12	1.71	0.40
4:A:1339:LEU:CD1	7:E:147:HIS:CD2	3.04	0.40
4:A:315:LEU:HD12	4:A:319:GLY:O	2.22	0.40
4:A:388:LEU:O	4:A:391:LEU:HB2	2.22	0.40
4:A:469:ARG:NH1	4:A:469:ARG:HB3	2.37	0.40
4:A:837:ILE:HA	4:A:837:ILE:HD13	1.86	0.40
5:B:899:ILE:HG22	5:B:900:ALA:N	2.37	0.40
4:A:1371:LEU:O	4:A:1372:VAL:C	2.60	0.40
4:A:224:PHE:HD2	4:A:229:SER:O	2.04	0.40
4:A:455:MET:SD	5:B:1137:CYS:HB3	2.54	0.40
5:B:839:MET:HE3	5:B:1010:LEU:HD11	2.03	0.40
5:B:724:ASP:HA	5:B:725:PRO:HD3	1.98	0.40
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.61	0.40
6:C:242:GLN:HA	6:C:245:VAL:HB	2.02	0.40
9:H:111:LEU:HD23	9:H:111:LEU:HA	1.93	0.40
12:K:1:MET:O	12:K:1:MET:HG2	2.20	0.40
4:A:1393:ASN:OD1	4:A:1393:ASN:O	2.40	0.40
4:A:443:LEU:HD23	4:A:443:LEU:HA	1.76	0.40
4:A:466:SER:O	5:B:1103:ILE:CD1	2.67	0.40
4:A:737:LEU:HD23	4:A:737:LEU:HA	1.94	0.40
5:B:117:ALA:HA	5:B:122:LEU:HB2	2.04	0.40
5:B:839:MET:HB3	5:B:1012:ILE:HG22	2.02	0.40
4:A:568:PRO:HB3	6:C:221:TYR:CE1	2.56	0.40
11:J:1:MET:N	11:J:56:LEU:H	2.20	0.40
11:J:1:MET:O	11:J:2:ILE:HG22	2.22	0.40
5:B:899:ILE:CD1	5:B:911:ILE:HG23	2.51	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	
4	A	1383/1733 (80%)	1136 (82%)	182 (13%)	65 (5%)	3	26
5	B	1087/1224 (89%)	918 (84%)	124 (11%)	45 (4%)	3	29
6	C	265/318 (83%)	222 (84%)	34 (13%)	9 (3%)	4	35
7	E	212/215 (99%)	180 (85%)	25 (12%)	7 (3%)	4	35
8	F	84/155 (54%)	73 (87%)	10 (12%)	1 (1%)	15	57
9	H	129/146 (88%)	101 (78%)	23 (18%)	5 (4%)	3	31
10	I	117/122 (96%)	95 (81%)	18 (15%)	4 (3%)	4	35
11	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	5	36
12	K	112/120 (93%)	97 (87%)	11 (10%)	4 (4%)	4	33
13	L	44/70 (63%)	25 (57%)	11 (25%)	8 (18%)	0	2
All	All	3496/4173 (84%)	2903 (83%)	443 (13%)	150 (4%)	3	28

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	55	ASP
4	A	93	VAL
4	A	248	PRO
4	A	321	PRO
4	A	399	HIS
4	A	567	LYS
4	A	597	LEU
4	A	846	GLU
4	A	853	ASP
4	A	1036	ARG
4	A	1274	ARG
4	A	1435	PRO
4	A	1437	GLY

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Mol	Chain	Res	Type
5	B	21	GLU
5	B	229	ALA
5	B	483	LEU
5	B	484	ASN
5	B	531	GLN
5	B	636	PRO
5	B	707	PRO
5	B	731	VAL
5	B	958	GLN
7	E	59	SER
7	E	206	GLY
9	H	32	THR
9	H	110	ASP
10	I	34	TYR
11	J	2	ILE
13	L	53	HIS
13	L	55	ILE
4	A	50	ILE
4	A	76	GLU
4	A	257	ARG
4	A	312	PRO
4	A	315	LEU
4	A	323	LYS
4	A	424	ILE
4	A	583	PRO
4	A	593	GLU
4	A	609	ASP
4	A	922	ASP
4	A	1221	LYS
4	A	1314	SER
5	B	466	TRP
5	B	478	GLY
5	B	643	ASP
5	B	710	LEU
5	B	712	PRO
5	B	883	LEU
6	C	90	ASP
6	C	142	VAL
6	C	267	GLN
8	F	128	LYS
9	H	139	ASN
10	I	9	ASP

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Mol	Chain	Res	Type
10	I	11	ASN
10	I	77	LYS
13	L	47	ARG
13	L	63	ARG
4	A	66	LYS
4	A	68	GLN
4	A	253	ASN
4	A	254	GLU
4	A	418	SER
4	A	568	PRO
4	A	870	GLU
4	A	958	VAL
4	A	972	HIS
4	A	1388	GLY
5	B	38	PHE
5	B	294	ASP
5	B	322	PHE
5	B	468	GLU
5	B	474	SER
5	B	879	ARG
5	B	902	GLY
5	B	943	SER
5	B	986	GLN
5	B	1096	ARG
6	C	110	THR
7	E	165	LEU
11	J	6	ARG
12	K	70	ARG
13	L	46	VAL
13	L	50	ASP
4	A	56	PRO
4	A	178	GLY
4	A	305	ASP
4	A	324	SER
4	A	332	LYS
4	A	465	TYR
4	A	544	ASP
4	A	1016	THR
4	A	1054	LEU
4	A	1270	ASN
4	A	1396	ALA
4	A	1401	SER

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Mol	Chain	Res	Type
5	B	230	ALA
5	B	467	GLY
5	B	733	HIS
5	B	864	LYS
5	B	974	PRO
5	B	1017	ILE
6	C	6	PRO
6	C	181	ASP
6	C	205	LYS
7	E	4	GLU
7	E	124	VAL
9	H	128	ASN
12	K	4	PRO
12	K	5	ASP
12	K	28	PRO
13	L	59	ALA
4	A	591	PHE
4	A	700	ASN
4	A	961	ARG
5	B	90	ILE
5	B	176	SER
5	B	290	GLY
5	B	436	VAL
5	B	648	HIS
5	B	732	SER
5	B	880	THR
5	B	901	PRO
5	B	1178	ASN
5	B	1181	GLU
6	C	182	PRO
9	H	140	ALA
13	L	56	LEU
4	A	27	VAL
4	A	364	VAL
4	A	536	LEU
4	A	610	GLY
4	A	1107	VAL
4	A	1173	HIS
5	B	292	ILE
5	B	881	ASN
4	A	793	SER
4	A	1424	VAL

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Mol	Chain	Res	Type
4	A	51	GLY
5	B	410	GLY
4	A	1324	PRO
6	C	21	ILE
4	A	35	ILE
5	B	867	GLY
7	E	76	GLY
7	E	189	GLY
4	A	400	PRO
4	A	647	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1218/1520 (80%)	1083 (89%)	135 (11%)	7	32
5	B	959/1061 (90%)	852 (89%)	107 (11%)	7	32
6	C	235/274 (86%)	215 (92%)	20 (8%)	12	45
7	E	196/197 (100%)	182 (93%)	14 (7%)	17	54
8	F	76/137 (56%)	67 (88%)	9 (12%)	6	29
9	H	117/128 (91%)	103 (88%)	14 (12%)	6	28
10	I	113/116 (97%)	96 (85%)	17 (15%)	3	19
11	J	60/65 (92%)	53 (88%)	7 (12%)	6	29
12	K	99/102 (97%)	86 (87%)	13 (13%)	5	25
13	L	40/57 (70%)	32 (80%)	8 (20%)	1	8
All	All	3113/3657 (85%)	2769 (89%)	344 (11%)	7	32

All (344) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	TYR
4	A	12	ARG
4	A	13	THR

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Mol	Chain	Res	Type
4	A	18	GLN
4	A	32	VAL
4	A	41	MET
4	A	58	LEU
4	A	70	CYS
4	A	81	PHE
4	A	93	VAL
4	A	100	LYS
4	A	105	CYS
4	A	116	ASP
4	A	133	LYS
4	A	169	ASN
4	A	184	SER
4	A	208	LEU
4	A	222	LEU
4	A	225	ASN
4	A	237	THR
4	A	249	SER
4	A	250	ILE
4	A	253	ASN
4	A	257	ARG
4	A	261	ASP
4	A	270	LEU
4	A	297	GLN
4	A	303	TYR
4	A	308	ILE
4	A	315	LEU
4	A	316	GLN
4	A	320	ARG
4	A	324	SER
4	A	335	ARG
4	A	337	ARG
4	A	391	LEU
4	A	403	LYS
4	A	434	ARG
4	A	443	LEU
4	A	449	SER
4	A	450	LEU
4	A	452	LYS
4	A	454	SER
4	A	466	SER
4	A	469	ARG

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Mol	Chain	Res	Type
4	A	470	LEU
4	A	472	LEU
4	A	475	THR
4	A	485	ASP
4	A	501	LEU
4	A	509	LEU
4	A	527	THR
4	A	538	ASP
4	A	544	ASP
4	A	550	LEU
4	A	566	ILE
4	A	576	GLN
4	A	577	ILE
4	A	596	THR
4	A	599	SER
4	A	612	ILE
4	A	618	GLU
4	A	648	ASN
4	A	702	LEU
4	A	732	LEU
4	A	741	ASN
4	A	756	ILE
4	A	760	GLN
4	A	764	CYS
4	A	795	GLU
4	A	801	GLU
4	A	803	SER
4	A	821	ARG
4	A	830	LYS
4	A	831	THR
4	A	838	GLN
4	A	855	THR
4	A	856	THR
4	A	858	ASN
4	A	867	ILE
4	A	871	ASP
4	A	880	LYS
4	A	885	THR
4	A	889	SER
4	A	902	LEU
4	A	908	LEU
4	A	913	LEU

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Mol	Chain	Res	Type
4	A	918	GLU
4	A	920	LEU
4	A	929	LEU
4	A	949	ASP
4	A	969	GLN
4	A	982	THR
4	A	996	ASN
4	A	1025	ARG
4	A	1034	GLU
4	A	1035	TYR
4	A	1058	VAL
4	A	1067	LEU
4	A	1094	VAL
4	A	1095	THR
4	A	1110	ASN
4	A	1117	THR
4	A	1129	GLU
4	A	1135	ARG
4	A	1142	THR
4	A	1146	VAL
4	A	1159	ARG
4	A	1187	GLN
4	A	1193	LEU
4	A	1206	ASP
4	A	1215	ARG
4	A	1223	ASP
4	A	1257	ASP
4	A	1262	LYS
4	A	1264	GLU
4	A	1277	GLU
4	A	1280	GLU
4	A	1281	ARG
4	A	1288	ASP
4	A	1291	VAL
4	A	1295	THR
4	A	1308	THR
4	A	1322	ILE
4	A	1325	THR
4	A	1329	THR
4	A	1333	ILE
4	A	1351	GLU
4	A	1359	ASP

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Mol	Chain	Res	Type
4	A	1366	ARG
4	A	1372	VAL
4	A	1376	THR
4	A	1385	THR
4	A	1393	ASN
4	A	1410	PHE
5	B	26	THR
5	B	28	GLU
5	B	34	ILE
5	B	35	SER
5	B	45	SER
5	B	63	ILE
5	B	66	ASP
5	B	97	VAL
5	B	98	THR
5	B	108	VAL
5	B	120	ARG
5	B	126	SER
5	B	128	LEU
5	B	134	LYS
5	B	175	ARG
5	B	199	MET
5	B	206	ASN
5	B	234	ILE
5	B	244	LEU
5	B	246	LYS
5	B	249	ARG
5	B	268	THR
5	B	294	ASP
5	B	315	LYS
5	B	347	LYS
5	B	366	GLN
5	B	387	LEU
5	B	393	LYS
5	B	404	LYS
5	B	416	LEU
5	B	424	LEU
5	B	425	THR
5	B	432	MET
5	B	461	LEU
5	B	471	LYS
5	B	474	SER

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Mol	Chain	Res	Type
5	B	479	VAL
5	B	483	LEU
5	B	500	THR
5	B	510	LYS
5	B	513	GLN
5	B	518	HIS
5	B	537	LYS
5	B	542	MET
5	B	547	VAL
5	B	552	MET
5	B	570	VAL
5	B	618	ASP
5	B	624	LEU
5	B	628	THR
5	B	635	ARG
5	B	637	LEU
5	B	642	ASP
5	B	685	LEU
5	B	694	ASP
5	B	701	ILE
5	B	736	THR
5	B	737	THR
5	B	762	ASN
5	B	764	SER
5	B	783	THR
5	B	786	ASN
5	B	790	ASP
5	B	791	THR
5	B	792	MET
5	B	807	ARG
5	B	835	GLN
5	B	844	SER
5	B	857	ARG
5	B	865	LYS
5	B	868	MET
5	B	873	THR
5	B	878	GLN
5	B	880	THR
5	B	883	LEU
5	B	886	LYS
5	B	905	VAL
5	B	916	THR

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Mol	Chain	Res	Type
5	B	939	THR
5	B	941	LEU
5	B	944	THR
5	B	963	PHE
5	B	967	ARG
5	B	970	THR
5	B	980	PHE
5	B	983	ARG
5	B	997	GLU
5	B	998	ASP
5	B	999	MET
5	B	1006	ILE
5	B	1020	ARG
5	B	1048	THR
5	B	1073	TYR
5	B	1076	HIS
5	B	1082	MET
5	B	1084	GLN
5	B	1096	ARG
5	B	1099	VAL
5	B	1102	LYS
5	B	1113	VAL
5	B	1132	GLU
5	B	1150	ARG
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1218	THR
5	B	1220	ARG
6	C	15	LYS
6	C	21	ILE
6	C	23	SER
6	C	25	VAL
6	C	27	LEU
6	C	53	THR
6	C	56	THR
6	C	77	ILE
6	C	86	CYS
6	C	129	ILE
6	C	137	LYS
6	C	140	ASN
6	C	156	THR

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Mol	Chain	Res	Type
6	C	163	ILE
6	C	183	TRP
6	C	215	GLU
6	C	240	VAL
6	C	244	VAL
6	C	265	MET
6	C	268	ASP
7	E	9	ILE
7	E	29	PHE
7	E	61	GLN
7	E	77	SER
7	E	92	THR
7	E	104	ASN
7	E	127	ILE
7	E	150	VAL
7	E	156	LEU
7	E	162	ARG
7	E	165	LEU
7	E	169	ARG
7	E	198	ILE
7	E	200	ARG
8	F	71	GLU
8	F	81	THR
8	F	90	ARG
8	F	92	ARG
8	F	97	ARG
8	F	104	ASN
8	F	118	LEU
8	F	119	ARG
8	F	123	LYS
9	H	4	THR
9	H	13	SER
9	H	24	CYS
9	H	55	LEU
9	H	61	SER
9	H	77	ARG
9	H	87	ARG
9	H	88	SER
9	H	89	LEU
9	H	91	ASP
9	H	95	TYR
9	H	102	TYR

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Mol	Chain	Res	Type
9	H	110	ASP
9	H	130	ARG
10	I	5	ARG
10	I	7	CYS
10	I	8	ARG
10	I	10	CYS
10	I	11	ASN
10	I	13	MET
10	I	18	GLU
10	I	28	GLU
10	I	30	ARG
10	I	50	THR
10	I	62	ILE
10	I	70	ARG
10	I	83	ASN
10	I	84	VAL
10	I	94	ASP
10	I	95	THR
10	I	107	SER
11	J	5	VAL
11	J	9	SER
11	J	14	VAL
11	J	31	ASP
11	J	43	ARG
11	J	48	ARG
11	J	62	ARG
12	K	6	ARG
12	K	18	LYS
12	K	21	ILE
12	K	25	THR
12	K	50	LEU
12	K	78	THR
12	K	81	TYR
12	K	93	SER
12	K	101	LEU
12	K	103	THR
12	K	107	THR
12	K	113	THR
12	K	114	LEU
13	L	26	THR
13	L	27	LEU
13	L	31	CYS

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Mol	Chain	Res	Type
13	L	50	ASP
13	L	55	ILE
13	L	61	THR
13	L	65	VAL
13	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	83	HIS
4	A	313	GLN
4	A	316	GLN
4	A	425	GLN
4	A	435	HIS
4	A	451	HIS
4	A	503	GLN
4	A	626	ASN
4	A	654	ASN
4	A	736	ASN
4	A	741	ASN
4	A	757	ASN
4	A	760	GLN
4	A	767	GLN
4	A	768	GLN
4	A	858	ASN
4	A	926	GLN
4	A	996	ASN
4	A	1078	GLN
4	A	1171	GLN
4	A	1364	ASN
4	A	1432	GLN
5	B	121	ASN
5	B	178	ASN
5	B	206	ASN
5	B	215	GLN
5	B	363	HIS
5	B	366	GLN
5	B	383	ASN
5	B	484	ASN
5	B	515	HIS
5	B	516	ASN
5	B	657	HIS

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Mol	Chain	Res	Type
5	B	667	GLN
5	B	686	ASN
5	B	734	HIS
5	B	744	HIS
5	B	762	ASN
5	B	767	ASN
5	B	794	ASN
5	B	822	ASN
5	B	842	ASN
5	B	862	GLN
5	B	878	GLN
5	B	957	ASN
5	B	984	HIS
5	B	986	GLN
5	B	1015	HIS
5	B	1025	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1084	GLN
5	B	1161	HIS
5	B	1178	ASN
5	B	1187	ASN
6	C	17	ASN
6	C	31	ASN
6	C	73	GLN
6	C	112	ASN
6	C	123	ASN
6	C	188	HIS
6	C	224	GLN
6	C	231	ASN
6	C	242	GLN
7	E	32	GLN
7	E	101	GLN
7	E	104	ASN
7	E	114	ASN
7	E	147	HIS
8	F	100	GLN
9	H	11	GLN
9	H	134	ASN
10	I	12	ASN
10	I	46	HIS
10	I	60	GLN

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Mol	Chain	Res	Type
10	I	83	ASN
12	K	65	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	C
1	R	10	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
16	G2P	T	3000	-	26,34,34	2.47	6 (23%)	26,54,54	1.40	2 (7%)

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
16	G2P	T	3000	-	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	3000	G2P	C5-C6	-7.34	1.39	1.53
16	T	3000	G2P	C4-N9	-7.13	1.38	1.47
16	T	3000	G2P	C8-N9	-2.75	1.38	1.46
16	T	3000	G2P	PB-O3B	2.75	1.61	1.58
16	T	3000	G2P	C6-N1	3.06	1.38	1.33
16	T	3000	G2P	PA-O5'	3.26	1.61	1.57

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	3000	G2P	PG-O3B-PB	-4.20	117.54	132.38
16	T	3000	G2P	C3'-C2'-C1'	2.02	105.30	101.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	3000	G2P	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	-0.03	0 100 100	98, 111, 151, 169	0
2	T	27/27 (100%)	0.37	4 (14%) 3 3	100, 203, 234, 238	0
3	N	13/13 (100%)	0.56	1 (7%) 14 13	197, 219, 252, 258	0
4	A	1395/1733 (80%)	-0.22	21 (1%) 74 66	61, 99, 161, 173	0
5	B	1105/1224 (90%)	-0.23	14 (1%) 77 69	64, 94, 139, 155	0
6	C	267/318 (83%)	-0.49	0 100 100	74, 89, 122, 144	0
7	E	214/215 (99%)	-0.23	6 (2%) 53 45	79, 116, 155, 159	0
8	F	86/155 (55%)	-0.45	0 100 100	75, 105, 145, 156	0
9	H	133/146 (91%)	-0.05	2 (1%) 74 66	100, 118, 146, 148	0
10	I	119/122 (97%)	-0.40	0 100 100	84, 103, 123, 142	0
11	J	65/70 (92%)	-0.46	0 100 100	69, 87, 107, 112	0
12	K	114/120 (95%)	-0.30	0 100 100	73, 95, 112, 115	0
13	L	46/70 (65%)	-0.10	1 (2%) 62 53	102, 147, 159, 163	0
All	All	3593/4222 (85%)	-0.24	49 (1%) 75 67	61, 99, 157, 258	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	44	THR	6.1
4	A	1176	LEU	5.7
9	H	86	ASP	5.7
4	A	286	HIS	4.0
4	A	150	THR	3.9
7	E	126	SER	3.7
4	A	149	GLU	3.7
7	E	93	MET	3.6
2	T	3	DC	3.4

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Mol	Chain	Res	Type	RSRZ
4	A	69	THR	3.4
5	B	870	ILE	3.4
4	A	316	GLN	3.2
4	A	103	CYS	3.1
5	B	883	LEU	3.0
5	B	869	SER	2.9
2	T	4	DC	2.9
5	B	250	PHE	2.9
4	A	171	GLN	2.9
4	A	144	THR	2.8
4	A	152	VAL	2.7
4	A	66	LYS	2.6
5	B	1221	SER	2.6
7	E	122	LYS	2.6
4	A	1175	SER	2.6
7	E	110	PHE	2.6
4	A	175	ARG	2.5
4	A	254	GLU	2.4
2	T	11	DC	2.4
5	B	645	SER	2.4
4	A	1126	ALA	2.3
5	B	249	ARG	2.3
5	B	708	GLU	2.3
4	A	104	GLU	2.3
7	E	49	SER	2.2
7	E	83	CYS	2.2
2	T	2	DA	2.2
3	N	14	DA	2.2
4	A	323	LYS	2.2
5	B	474	SER	2.1
9	H	85	GLY	2.1
5	B	646	LEU	2.1
4	A	166	GLY	2.1
5	B	666	TYR	2.1
5	B	66	ASP	2.1
4	A	182	VAL	2.1
5	B	882	THR	2.1
5	B	248	SER	2.0
13	L	27	LEU	2.0
4	A	1170	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	G2P	T	3000	32/32	0.80	0.26	1.64	125,129,158,158	0
14	ZN	I	203	1/1	0.99	0.12	-0.16	101,101,101,101	0
14	ZN	C	319	1/1	0.97	0.12	-0.45	90,90,90,90	0
14	ZN	I	204	1/1	0.99	0.12	-0.49	90,90,90,90	0
14	ZN	A	1735	1/1	0.94	0.15	-0.63	153,153,153,153	0
14	ZN	J	101	1/1	0.99	0.17	-1.49	77,77,77,77	0
14	ZN	A	1734	1/1	0.78	0.10	-1.52	165,165,165,165	0
14	ZN	B	1307	1/1	0.95	0.08	-2.09	138,138,138,138	0
14	ZN	L	105	1/1	0.96	0.05	-	146,146,146,146	0
15	MG	A	2001	1/1	0.96	0.18	-	67,67,67,67	0
15	MG	A	2002	1/1	0.70	0.35	-	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.