wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:55 PM BST

PDB ID	:	3J6Q
EMDB ID:	:	EMD-5926
Title	:	Identification of the active sites in the methyltransferases of a transcribing dsRNA virus
Authors	:	Zhu, B.; Yang, C.; Liu, H.; Cheng, L.; Song, F.; Zeng, S.; Huang, X.; Ji, G.; Zhu, P.
Deposited on	:	2014-03-20
Resolution	:	3.80 Å(reported)

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

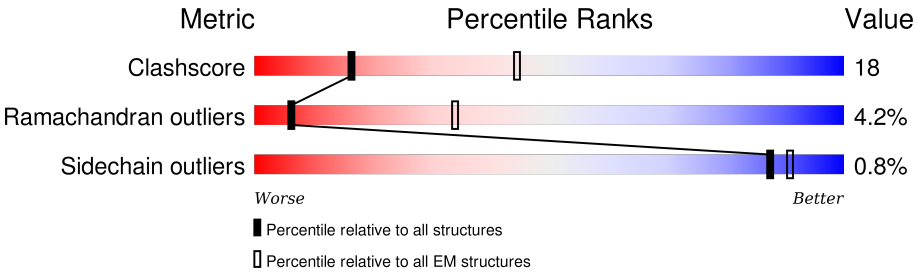
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1058	80% 16%
1	B	1058	80% 16%
1	C	1058	80% 16%
1	D	1058	81% 16%
1	E	1058	81% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	GPL	B	234	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAH	A	1101	-	-	X	-
2	SAH	A	1102	-	-	X	-
2	SAH	B	1101	-	-	X	-
2	SAH	B	1102	-	-	X	-
2	SAH	C	1101	-	-	X	-
2	SAH	C	1102	-	-	X	-
2	SAH	D	1101	-	-	X	-
2	SAH	D	1102	-	-	X	-
2	SAH	E	1101	-	-	X	-
2	SAH	E	1102	-	-	X	-

2 Entry composition

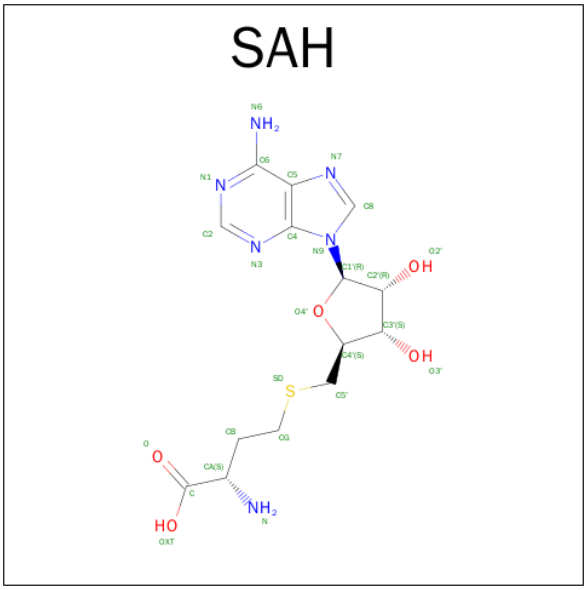
There are 2 unique types of molecules in this entry. The entry contains 42575 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Structural protein VP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	B	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	C	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	D	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		
1	E	1058	Total	C	N	O	P	S	0	0
			8463	5358	1463	1596	1	45		

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			52	28	12	10	2	

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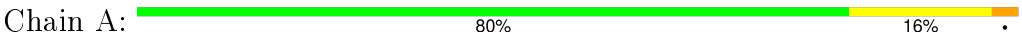
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	B	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	B	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	C	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	C	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	D	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	D	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	E	1	Total	C	N	O	S	0
			52	28	12	10	2	
2	E	1	Total	C	N	O	S	0
			52	28	12	10	2	

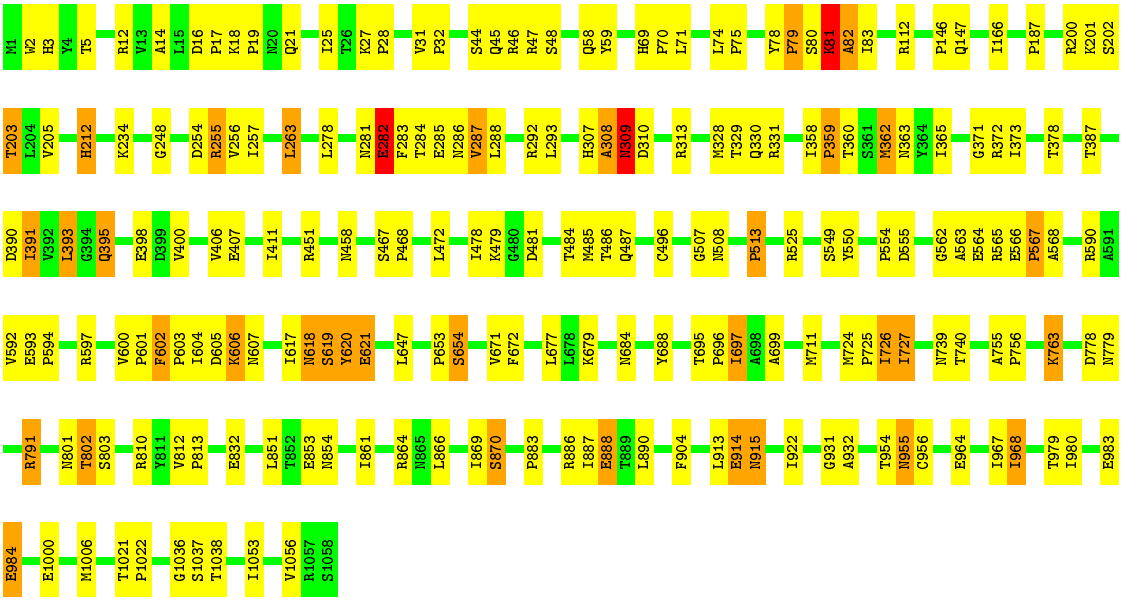
3 Residue-property plots (i)

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

- Molecule 1: Structural protein VP3

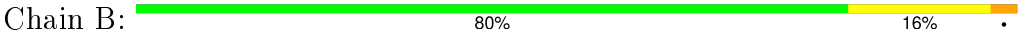
Chain A:

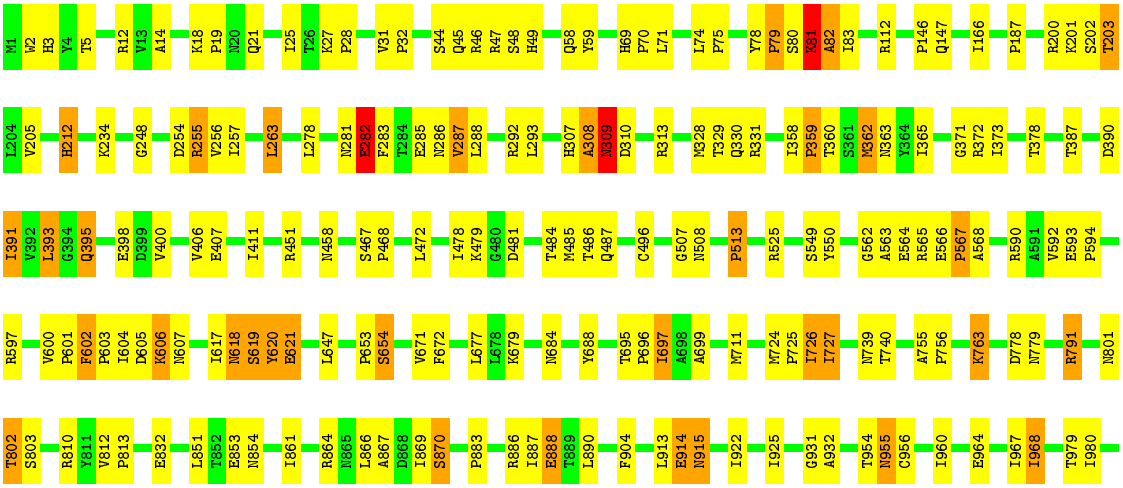


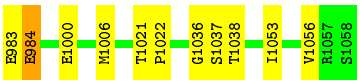


- Molecule 1: Structural protein VP3

Chain B:

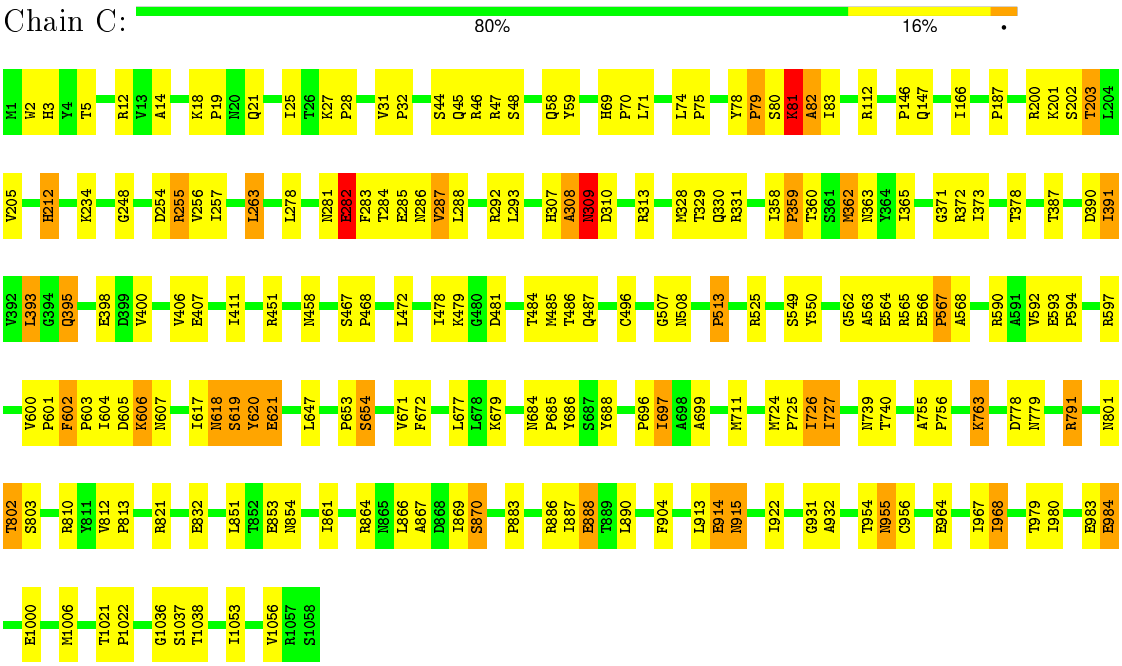






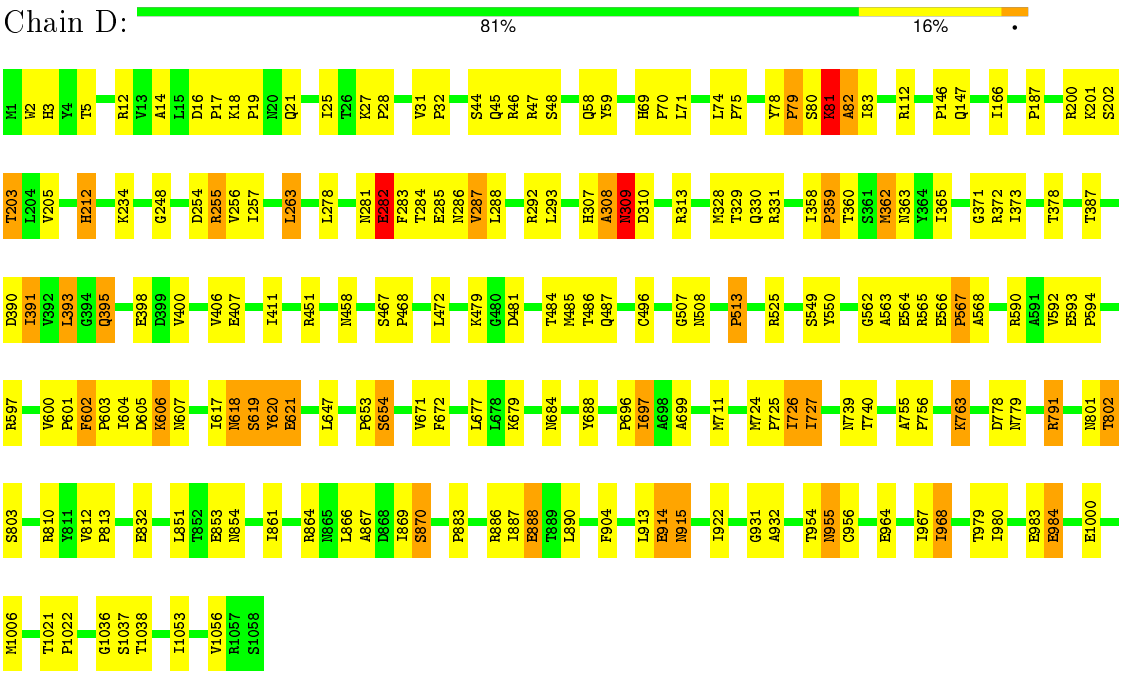
• Molecule 1: Structural protein VP3

Chain C:



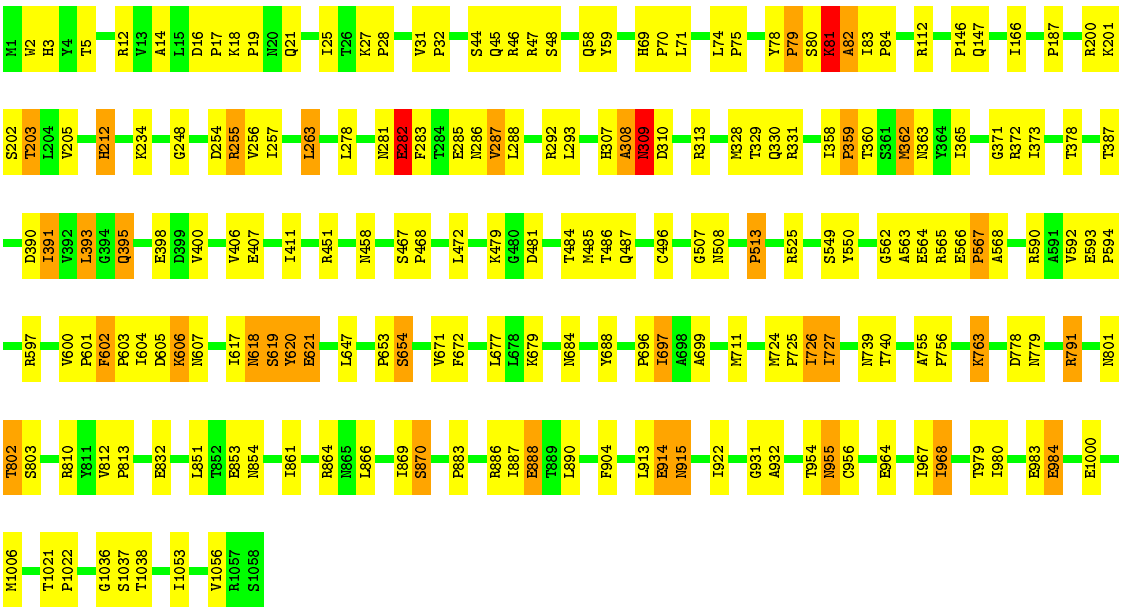
• Molecule 1: Structural protein VP3

Chain D:



• Molecule 1: Structural protein VP3

Chain E:


M1 W2 H3 Y4 T5 R12 V13 A14 L15 D16 P17 K18 P19 N20 Q21 I25 T26 K27 P28 V31 P32 S44 Q45 R46 R47 S48 Q58 Y59 H69 P70 L71 L74 P75 Y78 P79 S80 K81 A82 I83 P84 R112 P146 Q147 I166 P187 R200 K201
S202 T203 L204 V205 H212 K234 G248 D254 R255 V256 I257 L263 L278 N281 E282 F283 T284 E285 N286 V287 L288 R292 L293 H307 A308 N309 D310 R313 N328 T329 Q330 R331 I358 P359 T360 S361 N362 N363 Y364 I365 G371 R372 I373 T378 T387
D390 I391 V392 L393 G394 Q395 E398 D399 V400 V406 E407 I411 R451 N458 S467 P468 L472 K479 G480 D481 T484 M485 T486 Q487 C496 G507 N508 P513 R525 S549 Y550 G562 A563 E564 R565 E566 P567 A568 R590 A591 V592 E593 P594
R597 V600 P601 F602 P603 I604 D605 K606 N607 I617 N618 S619 Y620 E621 L647 P653 S654 V671 F672 L677 L678 K679 N684 Y688 P696 I697 A698 A699 M711 M724 P725 I726 I727 N739 T740 A755 F756 K763 D778 N779 R791 N801
T802 S803 R810 Y811 V812 P813 E832 L851 T852 E853 N854 I861 R864 N865 L866 I869 S870 P883 R886 I887 E888 T889 L890 F904 L913 E914 N915 I922 G931 A932 T954 N955 C956 E964 I967 I968 T979 I980 E983 E984 E1000
M1006 T1021 P1022 G1036 S1037 T1038 I1053 V1056 R1057 S1058

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	30000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	EMAN	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GPL, SAH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.61	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	B	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	C	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	D	0.62	3/8615 (0.0%)	0.54	2/11731 (0.0%)
1	E	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
All	All	0.62	15/43075 (0.0%)	0.55	10/58655 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
All	All	0	25

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	513	PRO	N-CD	6.56	1.57	1.47
1	D	513	PRO	N-CD	6.55	1.57	1.47
1	B	513	PRO	N-CD	6.54	1.57	1.47
1	A	513	PRO	N-CD	6.54	1.57	1.47
1	C	513	PRO	N-CD	6.47	1.56	1.47
1	E	79	PRO	N-CD	6.36	1.56	1.47
1	C	79	PRO	N-CD	6.31	1.56	1.47
1	A	79	PRO	N-CD	6.24	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	PRO	N-CD	6.18	1.56	1.47
1	D	79	PRO	N-CD	6.16	1.56	1.47
1	E	359	PRO	N-CD	5.90	1.56	1.47
1	C	359	PRO	N-CD	5.89	1.56	1.47
1	A	359	PRO	N-CD	5.88	1.56	1.47
1	D	359	PRO	N-CD	5.85	1.56	1.47
1	B	359	PRO	N-CD	5.84	1.56	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	79	PRO	CA-N-CD	-5.23	104.17	111.50
1	C	79	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	79	PRO	CA-N-CD	-5.22	104.19	111.50
1	D	79	PRO	CA-N-CD	-5.21	104.20	111.50
1	B	79	PRO	CA-N-CD	-5.19	104.23	111.50
1	C	359	PRO	CA-N-CD	-5.19	104.24	111.50
1	B	359	PRO	CA-N-CD	-5.17	104.27	111.50
1	A	359	PRO	CA-N-CD	-5.13	104.32	111.50
1	D	359	PRO	CA-N-CD	-5.11	104.35	111.50
1	E	359	PRO	CA-N-CD	-5.11	104.34	111.50

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	ALA	Peptide
1	A	309	ASN	Peptide
1	A	362	MET	Peptide
1	A	71	LEU	Peptide
1	A	81	LYS	Peptide
1	B	308	ALA	Peptide
1	B	309	ASN	Peptide
1	B	362	MET	Peptide
1	B	71	LEU	Peptide
1	B	81	LYS	Peptide
1	C	308	ALA	Peptide
1	C	309	ASN	Peptide
1	C	362	MET	Peptide
1	C	71	LEU	Peptide
1	C	81	LYS	Peptide
1	D	308	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	D	309	ASN	Peptide
1	D	362	MET	Peptide
1	D	71	LEU	Peptide
1	D	81	LYS	Peptide
1	E	308	ALA	Peptide
1	E	309	ASN	Peptide
1	E	362	MET	Peptide
1	E	71	LEU	Peptide
1	E	81	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8463	0	8411	385	0
1	B	8463	0	8411	400	0
1	C	8463	0	8411	390	0
1	D	8463	0	8411	385	0
1	E	8463	0	8411	385	0
2	A	52	0	38	28	0
2	B	52	0	38	29	0
2	C	52	0	38	29	0
2	D	52	0	38	28	0
2	E	52	0	38	29	0
All	All	42575	0	42245	1567	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 (1567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLN:CG	1:B:112:ARG:NH2	1.75	1.48
1:B:395:GLN:CG	1:C:112:ARG:NH2	1.77	1.48
1:C:395:GLN:CG	1:D:112:ARG:NH2	1.74	1.46
1:A:112:ARG:NH2	1:E:395:GLN:CG	1.74	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:GLN:CG	1:E:112:ARG:NH2	1.76	1.45
1:B:44:SER:CB	1:B:46:ARG:HE	1.28	1.43
1:C:618:ASN:O	2:C:1101:SAH:H5'1	1.22	1.33
1:C:604:ILE:HG22	1:D:890:LEU:CD1	1.58	1.33
1:B:604:ILE:HG22	1:C:890:LEU:CD1	1.57	1.33
1:D:618:ASN:O	2:D:1101:SAH:H5'1	1.22	1.32
1:A:890:LEU:CD1	1:E:604:ILE:HG22	1.58	1.31
1:A:604:ILE:HG22	1:B:890:LEU:CD1	1.59	1.31
1:D:604:ILE:HG22	1:E:890:LEU:CD1	1.58	1.30
1:D:44:SER:C	1:D:46:ARG:HG2	1.52	1.29
1:B:618:ASN:O	2:B:1101:SAH:H5'1	1.22	1.29
1:E:618:ASN:O	2:E:1101:SAH:H5'1	1.22	1.28
1:D:44:SER:CA	1:D:46:ARG:HG2	1.65	1.27
1:D:602:PHE:O	1:E:886:ARG:NH1	1.66	1.27
1:B:602:PHE:O	1:C:886:ARG:NH1	1.65	1.27
1:A:618:ASN:O	2:A:1101:SAH:H5'1	1.22	1.27
1:E:44:SER:C	1:E:46:ARG:HG2	1.52	1.27
1:E:44:SER:CA	1:E:46:ARG:HG2	1.64	1.26
1:A:44:SER:HB3	1:A:46:ARG:NE	1.49	1.26
1:A:602:PHE:O	1:B:886:ARG:NH1	1.68	1.25
1:A:12:ARG:NH2	1:A:234:GPL:HN22	1.36	1.24
1:B:44:SER:HB3	1:B:46:ARG:NE	1.49	1.24
1:B:12:ARG:NH2	1:B:234:GPL:HN22	1.36	1.24
1:C:12:ARG:NH2	1:C:234:GPL:HN22	1.36	1.23
1:D:12:ARG:NH2	1:D:234:GPL:HN22	1.36	1.23
1:A:886:ARG:NH1	1:E:602:PHE:O	1.70	1.23
1:A:890:LEU:CD1	1:E:604:ILE:CG2	2.17	1.23
1:C:602:PHE:O	1:D:886:ARG:NH1	1.70	1.23
1:B:604:ILE:CG2	1:C:890:LEU:CD1	2.17	1.22
1:D:604:ILE:CG2	1:E:890:LEU:CD1	2.17	1.22
1:E:12:ARG:NH2	1:E:234:GPL:HN22	1.36	1.22
1:C:593:GLU:CB	1:D:372:ARG:O	1.87	1.22
1:A:864:ARG:NE	1:E:607:ASN:HA	1.55	1.22
1:D:593:GLU:CB	1:E:372:ARG:O	1.89	1.21
1:A:604:ILE:CG2	1:B:890:LEU:CD1	2.19	1.21
1:C:604:ILE:CG2	1:D:890:LEU:CD1	2.17	1.21
1:A:372:ARG:O	1:E:593:GLU:CB	1.87	1.21
1:A:593:GLU:CB	1:B:372:ARG:O	1.89	1.21
1:C:607:ASN:HA	1:D:864:ARG:NE	1.55	1.21
1:B:607:ASN:HA	1:C:864:ARG:NE	1.55	1.21
1:A:607:ASN:HA	1:B:864:ARG:NE	1.56	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:ASN:HA	1:E:864:ARG:NE	1.56	1.20
1:B:593:GLU:CB	1:C:372:ARG:O	1.89	1.19
1:D:395:GLN:HG3	1:E:112:ARG:NH2	0.85	1.17
1:B:395:GLN:HG3	1:C:112:ARG:NH2	0.86	1.17
1:C:593:GLU:HB2	1:D:372:ARG:O	1.44	1.17
1:C:604:ILE:HG22	1:D:890:LEU:HD11	1.18	1.16
1:A:44:SER:CB	1:A:46:ARG:HE	1.58	1.16
1:C:44:SER:C	1:C:46:ARG:HG3	1.64	1.16
1:A:112:ARG:NH2	1:E:395:GLN:HG3	0.83	1.15
1:D:590:ARG:HD3	1:E:365:ILE:HD11	1.28	1.15
1:C:395:GLN:HG3	1:D:112:ARG:NH2	0.82	1.15
1:A:593:GLU:HB2	1:B:372:ARG:O	1.45	1.15
1:A:395:GLN:HG3	1:B:112:ARG:NH2	0.84	1.14
1:A:44:SER:C	1:A:46:ARG:HG3	1.68	1.14
1:D:593:GLU:HB2	1:E:372:ARG:O	1.44	1.14
1:D:604:ILE:HG22	1:E:890:LEU:HD11	1.16	1.13
1:B:593:GLU:HB2	1:C:372:ARG:O	1.45	1.12
1:E:44:SER:CB	1:E:46:ARG:HE	1.61	1.12
1:C:590:ARG:HD3	1:D:365:ILE:HD11	1.29	1.12
1:E:618:ASN:O	2:E:1101:SAH:C5'	1.98	1.11
1:A:618:ASN:O	2:A:1101:SAH:C5'	1.98	1.11
1:D:618:ASN:O	2:D:1101:SAH:C5'	1.98	1.11
1:C:395:GLN:HG3	1:D:112:ARG:CZ	1.81	1.11
1:D:44:SER:CB	1:D:46:ARG:HE	1.62	1.10
1:A:44:SER:HA	1:A:46:ARG:HG2	1.11	1.10
1:C:618:ASN:O	2:C:1101:SAH:C5'	1.98	1.10
1:B:590:ARG:HD3	1:C:365:ILE:HD11	1.26	1.10
1:B:618:ASN:O	2:B:1101:SAH:C5'	1.98	1.10
1:A:372:ARG:O	1:E:593:GLU:HB2	1.44	1.10
1:C:44:SER:CB	1:C:46:ARG:HE	1.64	1.10
1:C:44:SER:CA	1:C:46:ARG:HG2	1.82	1.10
1:A:112:ARG:CZ	1:E:395:GLN:HG3	1.82	1.09
1:D:395:GLN:HG3	1:E:112:ARG:CZ	1.82	1.08
1:D:44:SER:HB3	1:D:46:ARG:HE	0.97	1.08
1:A:890:LEU:HD11	1:E:604:ILE:HG22	1.18	1.08
1:E:44:SER:HB3	1:E:46:ARG:HE	0.96	1.08
1:A:590:ARG:HD3	1:B:365:ILE:HD11	1.29	1.08
1:A:604:ILE:HG22	1:B:890:LEU:HD11	1.18	1.07
1:A:395:GLN:HG3	1:B:112:ARG:CZ	1.81	1.07
1:B:44:SER:C	1:B:46:ARG:HG3	1.73	1.07
1:C:44:SER:HA	1:C:46:ARG:HG2	1.07	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:SER:HB3	1:C:46:ARG:HE	0.93	1.06
1:B:395:GLN:HG3	1:C:112:ARG:CZ	1.83	1.06
1:B:604:ILE:HG22	1:C:890:LEU:HD11	1.15	1.06
1:A:600:VAL:HB	2:A:1101:SAH:HN61	1.20	1.05
1:A:365:ILE:HD11	1:E:590:ARG:HD3	1.29	1.05
1:D:44:SER:HA	1:D:46:ARG:HG2	1.36	1.05
1:A:44:SER:CA	1:A:46:ARG:HG2	1.86	1.04
1:E:600:VAL:HB	2:E:1101:SAH:HN61	1.20	1.04
1:B:600:VAL:HB	2:B:1101:SAH:HN61	1.20	1.04
1:A:890:LEU:HD13	1:E:604:ILE:CG2	1.87	1.04
1:E:44:SER:HA	1:E:46:ARG:HG2	1.35	1.04
1:D:590:ARG:HD3	1:E:365:ILE:CD1	1.88	1.03
1:C:44:SER:HA	1:C:46:ARG:CG	1.88	1.03
1:C:590:ARG:HD3	1:D:365:ILE:CD1	1.89	1.03
1:B:590:ARG:HD3	1:C:365:ILE:CD1	1.87	1.03
1:B:44:SER:HA	1:B:46:ARG:CG	1.87	1.03
1:B:44:SER:CB	1:B:46:ARG:NE	2.10	1.03
1:D:600:VAL:HB	2:D:1101:SAH:HN61	1.20	1.02
1:C:593:GLU:HB3	1:D:372:ARG:O	1.60	1.01
1:D:604:ILE:CG2	1:E:890:LEU:HD13	1.89	1.01
1:A:365:ILE:CD1	1:E:590:ARG:HD3	1.88	1.01
1:C:604:ILE:CG2	1:D:890:LEU:HD13	1.87	1.01
1:A:604:ILE:CG2	1:B:890:LEU:HD13	1.90	1.00
1:C:600:VAL:HB	2:C:1101:SAH:HN61	1.20	1.00
1:A:886:ARG:HH12	1:E:601:PRO:C	1.65	1.00
1:C:601:PRO:C	1:D:886:ARG:HH12	1.65	0.99
1:D:44:SER:C	1:D:46:ARG:CG	2.30	0.99
1:E:44:SER:C	1:E:46:ARG:CG	2.30	0.99
1:B:604:ILE:CG2	1:C:890:LEU:HD13	1.89	0.99
1:A:590:ARG:HD3	1:B:365:ILE:CD1	1.90	0.99
1:C:44:SER:C	1:C:46:ARG:CG	2.30	0.99
1:A:601:PRO:C	1:B:886:ARG:HH12	1.67	0.99
1:C:861:ILE:CG2	2:C:1102:SAH:H2	1.93	0.98
1:B:861:ILE:CG2	2:B:1102:SAH:H2	1.93	0.98
1:A:372:ARG:O	1:E:593:GLU:HB3	1.60	0.98
1:D:861:ILE:CG2	2:D:1102:SAH:H2	1.93	0.98
1:D:593:GLU:HB3	1:E:372:ARG:O	1.62	0.98
1:D:46:ARG:HB3	1:D:47:ARG:HA	1.45	0.98
1:D:601:PRO:C	1:E:886:ARG:HH12	1.67	0.97
1:E:46:ARG:HB3	1:E:47:ARG:HA	1.44	0.97
1:A:593:GLU:HB3	1:B:372:ARG:O	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:ILE:CG2	2:A:1102:SAH:H2	1.93	0.97
1:E:861:ILE:CG2	2:E:1102:SAH:H2	1.93	0.97
1:A:395:GLN:HG3	1:B:112:ARG:HH22	1.17	0.97
1:B:44:SER:CA	1:B:46:ARG:HG3	1.94	0.97
1:B:593:GLU:HB3	1:C:372:ARG:O	1.62	0.96
1:C:44:SER:HB3	1:C:46:ARG:NE	1.79	0.96
1:B:607:ASN:HA	1:C:864:ARG:HE	1.27	0.96
1:B:601:PRO:C	1:C:886:ARG:HH12	1.68	0.96
1:A:44:SER:HA	1:A:46:ARG:CG	1.94	0.96
1:B:604:ILE:HG22	1:C:890:LEU:HD13	1.47	0.95
1:C:607:ASN:HA	1:D:864:ARG:HE	1.26	0.95
1:B:791:ARG:HB3	1:B:791:ARG:HH11	1.32	0.95
1:D:395:GLN:HG3	1:E:112:ARG:HH22	1.19	0.95
1:A:44:SER:CA	1:A:46:ARG:CG	2.44	0.95
1:A:791:ARG:HH11	1:A:791:ARG:HB3	1.32	0.95
1:C:791:ARG:HH11	1:C:791:ARG:HB3	1.32	0.94
1:A:607:ASN:HA	1:B:864:ARG:HE	1.27	0.94
1:C:282:GLU:O	1:C:282:GLU:OE1	1.86	0.94
1:A:886:ARG:NH1	1:E:601:PRO:HG2	1.83	0.94
1:C:44:SER:CA	1:C:46:ARG:CG	2.42	0.94
1:B:282:GLU:OE1	1:B:282:GLU:O	1.86	0.94
1:E:44:SER:HB3	1:E:46:ARG:NE	1.82	0.94
1:A:601:PRO:HG2	1:B:886:ARG:NH1	1.83	0.94
1:E:791:ARG:HB3	1:E:791:ARG:HH11	1.32	0.94
1:D:791:ARG:HH11	1:D:791:ARG:HB3	1.32	0.93
1:A:604:ILE:HG22	1:B:890:LEU:HD13	1.48	0.93
1:D:282:GLU:OE1	1:D:282:GLU:O	1.86	0.93
1:A:864:ARG:HE	1:E:607:ASN:HA	1.26	0.93
1:E:282:GLU:O	1:E:282:GLU:OE1	1.86	0.92
1:A:282:GLU:OE1	1:A:282:GLU:O	1.86	0.92
1:D:44:SER:HB3	1:D:46:ARG:NE	1.83	0.92
1:B:395:GLN:HG3	1:C:112:ARG:HH22	1.20	0.92
1:A:44:SER:C	1:A:46:ARG:CG	2.37	0.92
1:C:395:GLN:HG3	1:D:112:ARG:HH22	1.16	0.91
1:A:861:ILE:HG22	2:A:1102:SAH:H2	1.52	0.91
1:D:883:PRO:HG3	2:D:1102:SAH:C8	2.01	0.90
1:B:601:PRO:HG2	1:C:886:ARG:NH1	1.86	0.90
1:B:883:PRO:HG3	2:B:1102:SAH:C8	2.01	0.90
1:A:112:ARG:HH22	1:E:395:GLN:HG3	1.17	0.90
1:E:883:PRO:HG3	2:E:1102:SAH:C8	2.01	0.90
1:C:601:PRO:HG2	1:D:886:ARG:NH1	1.83	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:HB3	1:C:47:ARG:CA	2.02	0.90
1:C:44:SER:O	1:C:46:ARG:HG3	1.71	0.90
1:C:46:ARG:HB3	1:C:47:ARG:HA	1.54	0.90
1:C:861:ILE:HG22	2:C:1102:SAH:H2	1.52	0.90
1:A:883:PRO:HG3	2:A:1102:SAH:C8	2.01	0.90
1:C:883:PRO:HG3	2:C:1102:SAH:C8	2.01	0.89
1:D:861:ILE:HG22	2:D:1102:SAH:H2	1.52	0.89
1:E:45:GLN:HB2	1:E:46:ARG:HA	1.54	0.89
1:D:45:GLN:HB2	1:D:46:ARG:HA	1.55	0.89
1:E:861:ILE:HG22	2:E:1102:SAH:H2	1.52	0.88
1:D:607:ASN:HA	1:E:864:ARG:HE	1.28	0.88
1:A:890:LEU:HD13	1:E:604:ILE:HG22	1.46	0.88
1:B:861:ILE:HG22	2:B:1102:SAH:H2	1.52	0.88
1:C:395:GLN:CG	1:D:112:ARG:HH22	1.72	0.87
1:E:619:SER:OG	2:E:1101:SAH:H3'	1.75	0.87
1:A:44:SER:CB	1:A:46:ARG:NE	2.27	0.87
1:B:44:SER:HA	1:B:46:ARG:HG2	1.57	0.87
1:C:619:SER:OG	2:C:1101:SAH:H3'	1.75	0.86
1:D:619:SER:OG	2:D:1101:SAH:H3'	1.75	0.86
1:A:378:THR:HG21	1:E:603:PRO:HG2	1.57	0.86
1:D:601:PRO:HG2	1:E:886:ARG:NH1	1.85	0.86
1:A:619:SER:OG	2:A:1101:SAH:H3'	1.75	0.86
1:A:603:PRO:HG2	1:B:378:THR:HG21	1.57	0.86
1:B:619:SER:OG	2:B:1101:SAH:H3'	1.75	0.86
1:E:600:VAL:HB	2:E:1101:SAH:N6	1.91	0.86
1:B:600:VAL:HB	2:B:1101:SAH:N6	1.91	0.86
1:B:44:SER:HB3	1:B:46:ARG:HE	0.70	0.86
1:C:603:PRO:HG2	1:D:378:THR:HG21	1.57	0.85
1:E:44:SER:CB	1:E:46:ARG:NE	2.37	0.85
1:A:602:PHE:N	1:B:886:ARG:HH12	1.74	0.85
1:C:600:VAL:HB	2:C:1101:SAH:N6	1.91	0.85
1:D:604:ILE:HG22	1:E:890:LEU:HD13	1.47	0.85
1:C:45:GLN:HB2	1:C:46:ARG:HA	1.59	0.85
1:A:600:VAL:HB	2:A:1101:SAH:N6	1.91	0.84
1:A:45:GLN:HB2	1:A:46:ARG:HA	1.59	0.84
1:B:46:ARG:HB3	1:B:47:ARG:HB3	1.57	0.84
1:B:607:ASN:CA	1:C:864:ARG:NE	2.41	0.84
1:C:604:ILE:CG2	1:D:890:LEU:HD11	1.99	0.84
1:D:602:PHE:N	1:E:886:ARG:HH12	1.75	0.84
1:D:600:VAL:HB	2:D:1101:SAH:N6	1.91	0.84
1:D:44:SER:CB	1:D:46:ARG:NE	2.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ARG:HH12	1:E:602:PHE:N	1.74	0.84
1:B:602:PHE:N	1:C:886:ARG:HH12	1.75	0.83
1:C:602:PHE:N	1:D:886:ARG:HH12	1.74	0.83
1:D:603:PRO:HG2	1:E:378:THR:HG21	1.58	0.83
1:D:607:ASN:CA	1:E:864:ARG:NE	2.41	0.83
1:B:603:PRO:HG2	1:C:378:THR:HG21	1.58	0.83
1:C:44:SER:CB	1:C:46:ARG:NE	2.38	0.82
1:B:45:GLN:NE2	1:B:48:SER:OG	2.12	0.82
1:C:604:ILE:HG21	1:D:890:LEU:HD13	1.61	0.82
1:C:607:ASN:CA	1:D:864:ARG:NE	2.41	0.82
1:A:864:ARG:NE	1:E:607:ASN:CA	2.42	0.81
1:C:604:ILE:HG22	1:D:890:LEU:HD13	1.45	0.81
1:E:861:ILE:CG2	2:E:1102:SAH:C2	2.59	0.81
1:B:44:SER:CA	1:B:46:ARG:CG	2.57	0.81
1:A:890:LEU:HD13	1:E:604:ILE:HG21	1.61	0.81
1:A:861:ILE:CG2	2:A:1102:SAH:C2	2.59	0.80
1:D:861:ILE:CG2	2:D:1102:SAH:C2	2.59	0.80
1:D:604:ILE:HG21	1:E:890:LEU:HD13	1.62	0.80
1:B:395:GLN:HG3	1:C:112:ARG:HH21	0.98	0.80
1:D:395:GLN:CG	1:E:112:ARG:HH22	1.75	0.80
1:B:46:ARG:HB3	1:B:47:ARG:CB	2.10	0.79
1:A:607:ASN:CA	1:B:864:ARG:NE	2.42	0.79
1:B:861:ILE:CG2	2:B:1102:SAH:C2	2.59	0.79
1:A:395:GLN:HG3	1:B:112:ARG:HH21	0.98	0.79
1:A:883:PRO:HG3	2:A:1102:SAH:H8	1.64	0.79
1:C:861:ILE:CG2	2:C:1102:SAH:C2	2.59	0.79
1:A:112:ARG:HH21	1:E:395:GLN:HG3	0.96	0.79
1:B:604:ILE:HG21	1:C:890:LEU:HD13	1.62	0.79
1:C:46:ARG:HB3	1:C:47:ARG:CB	2.12	0.79
1:C:3:HIS:O	1:C:3:HIS:ND1	2.16	0.79
1:E:3:HIS:ND1	1:E:3:HIS:O	2.16	0.79
1:B:3:HIS:ND1	1:B:3:HIS:O	2.16	0.79
1:D:45:GLN:CB	1:D:46:ARG:HA	2.13	0.78
1:D:883:PRO:HG3	2:D:1102:SAH:H8	1.64	0.78
1:D:869:ILE:O	1:D:870:SER:CB	2.32	0.78
1:C:395:GLN:HE21	1:D:112:ARG:CZ	1.97	0.78
1:A:3:HIS:ND1	1:A:3:HIS:O	2.16	0.78
1:B:869:ILE:O	1:B:870:SER:CB	2.32	0.78
1:E:883:PRO:HG3	2:E:1102:SAH:H8	1.64	0.78
1:A:869:ILE:O	1:A:870:SER:CB	2.32	0.78
1:A:112:ARG:HH22	1:E:395:GLN:CG	1.72	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:ILE:CG2	1:E:890:LEU:HD11	1.98	0.78
1:C:869:ILE:O	1:C:870:SER:CB	2.32	0.78
1:D:3:HIS:O	1:D:3:HIS:ND1	2.16	0.78
1:B:604:ILE:CG2	1:C:890:LEU:HD11	1.97	0.78
1:B:883:PRO:HG3	2:B:1102:SAH:H8	1.64	0.77
1:A:395:GLN:CG	1:B:112:ARG:HH22	1.73	0.77
1:C:883:PRO:HG3	2:C:1102:SAH:H8	1.64	0.77
1:A:604:ILE:CG2	1:B:890:LEU:HD11	2.00	0.77
1:D:44:SER:CA	1:D:46:ARG:CG	2.58	0.77
1:B:44:SER:OG	1:B:46:ARG:NH2	2.18	0.77
1:A:604:ILE:HG21	1:B:890:LEU:HD13	1.64	0.77
1:E:869:ILE:O	1:E:870:SER:CB	2.31	0.77
1:D:395:GLN:HG3	1:E:112:ARG:HH21	0.97	0.77
1:D:883:PRO:CG	2:D:1102:SAH:C8	2.63	0.77
1:A:112:ARG:CZ	1:E:395:GLN:HE21	1.97	0.77
1:C:861:ILE:HG22	2:C:1102:SAH:C2	2.15	0.77
1:D:861:ILE:HG22	2:D:1102:SAH:C2	2.15	0.76
1:B:395:GLN:HE21	1:C:112:ARG:CZ	1.98	0.76
1:B:45:GLN:HB2	1:B:46:ARG:HA	1.67	0.76
1:E:883:PRO:CG	2:E:1102:SAH:C8	2.63	0.76
1:A:395:GLN:HE21	1:B:112:ARG:CZ	1.98	0.76
1:A:861:ILE:HG22	2:A:1102:SAH:C2	2.15	0.76
1:E:44:SER:CA	1:E:46:ARG:CG	2.58	0.76
1:B:883:PRO:CG	2:B:1102:SAH:C8	2.63	0.76
1:C:883:PRO:CG	2:C:1102:SAH:C8	2.63	0.76
1:A:883:PRO:CG	2:A:1102:SAH:C8	2.63	0.76
1:B:395:GLN:CG	1:C:112:ARG:HH22	1.75	0.76
1:C:395:GLN:HG3	1:D:112:ARG:HH21	0.96	0.76
1:B:861:ILE:HG22	2:B:1102:SAH:C2	2.15	0.76
1:D:395:GLN:HE21	1:E:112:ARG:CZ	1.98	0.75
1:E:46:ARG:HB3	1:E:47:ARG:CA	2.16	0.75
1:C:590:ARG:CD	1:D:365:ILE:HD11	2.15	0.75
1:E:861:ILE:HG22	2:E:1102:SAH:C2	2.15	0.75
1:A:890:LEU:HD11	1:E:604:ILE:CG2	1.98	0.75
1:A:44:SER:O	1:A:46:ARG:HG3	1.86	0.74
1:D:46:ARG:HB3	1:D:47:ARG:CA	2.16	0.74
1:D:619:SER:OG	2:D:1101:SAH:H5'1	1.88	0.74
1:C:45:GLN:HB2	1:C:46:ARG:CA	2.17	0.74
1:B:604:ILE:HG21	1:C:890:LEU:CD1	2.17	0.74
1:D:590:ARG:CD	1:E:365:ILE:HD11	2.14	0.74
1:E:619:SER:OG	2:E:1101:SAH:H5'1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:SER:HA	1:E:46:ARG:CG	2.15	0.74
1:C:619:SER:OG	2:C:1101:SAH:H5'1	1.88	0.74
1:C:592:VAL:HA	1:D:373:ILE:HG12	1.69	0.74
1:A:619:SER:OG	2:A:1101:SAH:H5'1	1.88	0.74
1:D:604:ILE:HG21	1:E:890:LEU:CD1	2.17	0.74
1:A:373:ILE:HG12	1:E:592:VAL:HA	1.69	0.74
1:B:592:VAL:HA	1:C:373:ILE:HG12	1.70	0.74
1:E:45:GLN:CB	1:E:46:ARG:HA	2.13	0.73
1:D:592:VAL:HA	1:E:373:ILE:HG12	1.70	0.73
1:B:619:SER:OG	2:B:1101:SAH:H5'1	1.87	0.73
1:A:618:ASN:O	1:A:619:SER:CB	2.37	0.73
1:A:590:ARG:CD	1:B:365:ILE:HD11	2.16	0.73
1:C:45:GLN:CB	1:C:46:ARG:HA	2.15	0.73
1:E:618:ASN:O	1:E:619:SER:CB	2.37	0.73
1:A:592:VAL:HA	1:B:373:ILE:HG12	1.71	0.73
1:C:618:ASN:O	1:C:619:SER:CB	2.37	0.72
1:D:391:ILE:O	1:D:391:ILE:HG23	1.89	0.72
1:A:112:ARG:CZ	1:E:395:GLN:NE2	2.53	0.72
1:B:618:ASN:O	1:B:619:SER:CB	2.37	0.72
1:C:605:ASP:O	1:C:606:LYS:CB	2.37	0.72
1:D:46:ARG:CB	1:D:47:ARG:HA	2.10	0.72
1:B:607:ASN:HA	1:C:864:ARG:CZ	2.19	0.72
1:B:904:PHE:N	2:B:1102:SAH:N6	2.38	0.72
1:C:395:GLN:HE21	1:D:112:ARG:NH1	1.87	0.72
1:E:605:ASP:O	1:E:606:LYS:CB	2.37	0.72
1:E:904:PHE:N	2:E:1102:SAH:N6	2.38	0.72
1:B:590:ARG:CD	1:C:365:ILE:HD11	2.13	0.72
1:A:904:PHE:N	2:A:1102:SAH:N6	2.38	0.72
1:D:45:GLN:HB2	1:D:46:ARG:CA	2.19	0.72
1:E:45:GLN:HB2	1:E:46:ARG:CA	2.19	0.72
1:E:391:ILE:O	1:E:391:ILE:HG23	1.89	0.72
1:B:391:ILE:HG23	1:B:391:ILE:O	1.89	0.72
1:D:618:ASN:O	1:D:619:SER:CB	2.37	0.72
1:C:904:PHE:N	2:C:1102:SAH:N6	2.38	0.72
1:C:395:GLN:NE2	1:D:112:ARG:CZ	2.52	0.72
1:A:605:ASP:O	1:A:606:LYS:CB	2.37	0.72
1:A:12:ARG:CZ	1:A:234:GPL:HN22	2.03	0.71
1:D:904:PHE:N	2:D:1102:SAH:N6	2.38	0.71
1:C:592:VAL:HG13	1:D:373:ILE:HG13	1.73	0.71
1:B:12:ARG:CZ	1:B:234:GPL:HN22	2.04	0.71
1:B:605:ASP:O	1:B:606:LYS:CB	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:ASP:O	1:D:606:LYS:CB	2.37	0.71
1:A:365:ILE:HD11	1:E:590:ARG:CD	2.15	0.71
1:A:619:SER:HG	2:A:1101:SAH:H5'1	1.55	0.71
1:A:395:GLN:HE21	1:B:112:ARG:NH1	1.89	0.71
1:D:607:ASN:HA	1:E:864:ARG:CZ	2.20	0.71
1:C:604:ILE:HG21	1:D:890:LEU:CD1	2.18	0.71
1:D:44:SER:HA	1:D:46:ARG:CG	2.16	0.71
1:D:398:GLU:HB2	1:E:14:ALA:O	1.91	0.71
1:A:112:ARG:NH1	1:E:395:GLN:HE21	1.88	0.70
1:D:12:ARG:CZ	1:D:234:GPL:HN22	2.04	0.70
1:A:373:ILE:HG13	1:E:592:VAL:HG13	1.73	0.70
1:C:391:ILE:O	1:C:391:ILE:HG23	1.89	0.70
2:B:1101:SAH:H2'	2:B:1101:SAH:N3	2.07	0.70
1:B:398:GLU:HB2	1:C:14:ALA:O	1.91	0.70
1:B:395:GLN:CG	1:C:112:ARG:CZ	2.57	0.70
1:D:619:SER:HG	2:D:1101:SAH:H5'1	1.56	0.70
1:A:607:ASN:HA	1:B:864:ARG:CZ	2.22	0.70
1:A:395:GLN:NE2	1:B:112:ARG:CZ	2.54	0.70
1:E:861:ILE:HG21	2:E:1102:SAH:H2	1.74	0.70
1:B:45:GLN:N	1:B:46:ARG:HA	2.05	0.70
1:C:725:PRO:HG3	1:D:5:THR:HG21	1.74	0.70
1:A:391:ILE:O	1:A:391:ILE:HG23	1.89	0.70
1:A:864:ARG:CZ	1:E:607:ASN:HA	2.22	0.70
1:A:861:ILE:HG21	2:A:1102:SAH:H2	1.74	0.70
1:D:406:VAL:HB	1:D:407:GLU:CA	2.22	0.70
1:E:406:VAL:HB	1:E:407:GLU:CA	2.22	0.70
1:E:12:ARG:CZ	1:E:234:GPL:HN22	2.04	0.69
1:B:395:GLN:NE2	1:C:112:ARG:CZ	2.55	0.69
1:C:406:VAL:HB	1:C:407:GLU:CA	2.22	0.69
1:C:254:ASP:O	1:C:255:ARG:CB	2.41	0.69
1:A:212:HIS:NE2	1:A:234:GPL:O3'	2.26	0.69
1:A:592:VAL:HG13	1:B:373:ILE:HG13	1.74	0.69
1:A:398:GLU:HB2	1:B:14:ALA:O	1.93	0.69
1:A:5:THR:HG21	1:E:725:PRO:HG3	1.74	0.69
2:C:1101:SAH:H2'	2:C:1101:SAH:N3	2.07	0.69
2:A:1101:SAH:H2'	2:A:1101:SAH:N3	2.07	0.69
1:C:12:ARG:CZ	1:C:234:GPL:HN22	2.04	0.69
1:C:398:GLU:HB2	1:D:14:ALA:O	1.93	0.69
1:C:607:ASN:HA	1:D:864:ARG:CZ	2.22	0.69
1:B:592:VAL:HG13	1:C:373:ILE:HG13	1.74	0.69
1:D:395:GLN:HE21	1:E:112:ARG:NH1	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:VAL:HB	1:B:407:GLU:CA	2.22	0.69
1:A:14:ALA:O	1:E:398:GLU:HB2	1.93	0.69
1:D:725:PRO:HG3	1:E:5:THR:HG21	1.75	0.69
1:A:395:GLN:CG	1:B:112:ARG:CZ	2.56	0.69
1:B:395:GLN:HE21	1:C:112:ARG:NH1	1.91	0.69
1:C:212:HIS:NE2	1:C:234:GPL:O3'	2.26	0.69
1:D:592:VAL:HG13	1:E:373:ILE:HG13	1.75	0.69
1:B:254:ASP:O	1:B:255:ARG:CB	2.41	0.69
1:E:869:ILE:O	1:E:870:SER:HB3	1.93	0.69
1:E:254:ASP:O	1:E:255:ARG:CB	2.41	0.69
1:D:254:ASP:O	1:D:255:ARG:CB	2.41	0.69
1:A:562:GLY:CA	1:A:563:ALA:HB3	2.23	0.69
1:B:212:HIS:NE2	1:B:234:GPL:O3'	2.26	0.69
1:D:406:VAL:HB	1:D:407:GLU:HA	1.75	0.69
1:D:395:GLN:NE2	1:E:112:ARG:CZ	2.55	0.68
1:D:212:HIS:NE2	1:D:234:GPL:O3'	2.26	0.68
1:B:406:VAL:HB	1:B:407:GLU:HA	1.74	0.68
1:A:725:PRO:HG3	1:B:5:THR:HG21	1.74	0.68
1:C:562:GLY:HA2	1:C:563:ALA:HB3	1.76	0.68
1:A:619:SER:HG	2:A:1101:SAH:H3'	1.58	0.68
1:B:861:ILE:HG21	2:B:1102:SAH:H2	1.74	0.68
1:A:562:GLY:HA2	1:A:563:ALA:HB3	1.76	0.68
1:D:562:GLY:CA	1:D:563:ALA:HB3	2.24	0.68
1:D:869:ILE:O	1:D:870:SER:HB3	1.93	0.68
1:A:406:VAL:HB	1:A:407:GLU:CA	2.22	0.68
1:B:562:GLY:CA	1:B:563:ALA:HB3	2.23	0.68
1:E:212:HIS:NE2	1:E:234:GPL:O3'	2.26	0.68
1:B:869:ILE:O	1:B:870:SER:HB3	1.93	0.68
1:A:869:ILE:O	1:A:870:SER:HB3	1.93	0.68
1:A:406:VAL:HB	1:A:407:GLU:HA	1.75	0.68
1:C:406:VAL:HB	1:C:407:GLU:HA	1.75	0.68
1:C:562:GLY:CA	1:C:563:ALA:HB3	2.24	0.68
1:E:562:GLY:HA2	1:E:563:ALA:HB3	1.76	0.68
1:A:44:SER:HB3	1:A:46:ARG:HE	0.67	0.68
1:C:869:ILE:O	1:C:870:SER:HB3	1.93	0.68
2:E:1101:SAH:N3	2:E:1101:SAH:H2'	2.07	0.68
1:B:562:GLY:HA2	1:B:563:ALA:HB3	1.75	0.68
1:A:46:ARG:HB3	1:A:47:ARG:HB3	1.74	0.67
1:A:112:ARG:CZ	1:E:395:GLN:CG	2.56	0.67
1:E:562:GLY:CA	1:E:563:ALA:HB3	2.23	0.67
1:B:12:ARG:HH22	1:B:234:GPL:HN22	0.69	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:HH22	1:C:234:GPL:HN22	0.69	0.67
1:B:725:PRO:HG3	1:C:5:THR:HG21	1.76	0.67
2:D:1101:SAH:N3	2:D:1101:SAH:H2'	2.07	0.67
1:D:954:THR:O	1:D:955:ASN:C	2.33	0.67
1:A:248:GLY:O	1:E:458:ASN:OD1	2.13	0.67
1:A:254:ASP:O	1:A:255:ARG:CB	2.40	0.67
1:D:458:ASN:OD1	1:E:248:GLY:O	2.12	0.67
1:E:406:VAL:HB	1:E:407:GLU:HA	1.75	0.67
1:B:458:ASN:OD1	1:C:248:GLY:O	2.12	0.67
1:B:954:THR:O	1:B:955:ASN:C	2.33	0.67
1:A:954:THR:O	1:A:955:ASN:C	2.33	0.67
1:C:45:GLN:NE2	1:C:48:SER:OG	2.28	0.66
1:C:395:GLN:CG	1:D:112:ARG:CZ	2.55	0.66
1:B:44:SER:CA	1:B:46:ARG:HE	2.07	0.66
1:C:601:PRO:O	1:C:602:PHE:CB	2.43	0.66
1:D:619:SER:HG	2:D:1101:SAH:H3'	1.58	0.66
1:D:562:GLY:HA2	1:D:563:ALA:HB3	1.76	0.66
1:B:619:SER:HG	2:B:1101:SAH:H3'	1.59	0.66
1:E:601:PRO:O	1:E:602:PHE:CB	2.43	0.66
1:C:954:THR:O	1:C:955:ASN:C	2.33	0.66
1:A:864:ARG:CD	1:E:607:ASN:H	2.08	0.66
1:A:601:PRO:O	1:A:602:PHE:CB	2.43	0.66
1:C:12:ARG:NH2	1:C:234:GPL:N2	2.13	0.66
1:D:601:PRO:O	1:D:602:PHE:CB	2.43	0.66
1:A:12:ARG:HH22	1:A:234:GPL:HN22	0.69	0.66
1:C:607:ASN:H	1:D:864:ARG:CD	2.08	0.66
1:A:458:ASN:OD1	1:B:248:GLY:O	2.14	0.66
1:E:954:THR:O	1:E:955:ASN:C	2.33	0.66
1:B:12:ARG:NH2	1:B:234:GPL:N2	2.13	0.66
1:B:607:ASN:H	1:C:864:ARG:CD	2.09	0.66
1:A:607:ASN:H	1:B:864:ARG:CD	2.09	0.66
1:B:883:PRO:CG	2:B:1102:SAH:H8	2.26	0.66
1:D:12:ARG:HH22	1:D:234:GPL:HN22	0.69	0.66
1:D:607:ASN:H	1:E:864:ARG:CD	2.09	0.65
1:C:861:ILE:HG21	2:C:1102:SAH:H2	1.74	0.65
1:C:883:PRO:CG	2:C:1102:SAH:H8	2.26	0.65
1:C:78:TYR:N	1:C:79:PRO:HA	2.11	0.65
1:D:861:ILE:HG21	2:D:1102:SAH:H2	1.74	0.65
1:E:619:SER:HG	2:E:1101:SAH:H3'	1.59	0.65
1:A:45:GLN:N	1:A:46:ARG:HA	2.10	0.65
1:E:390:ASP:O	1:E:391:ILE:C	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ASP:O	1:A:391:ILE:C	2.35	0.65
1:C:458:ASN:OD1	1:D:248:GLY:O	2.13	0.65
1:A:604:ILE:HG21	1:B:890:LEU:CD1	2.19	0.65
1:A:45:GLN:HB2	1:A:46:ARG:CA	2.27	0.65
1:B:78:TYR:N	1:B:79:PRO:HA	2.11	0.65
1:A:883:PRO:CG	2:A:1102:SAH:H8	2.26	0.65
1:B:390:ASP:O	1:B:391:ILE:C	2.35	0.65
1:C:329:THR:O	1:C:331:ARG:N	2.30	0.65
1:D:44:SER:O	1:D:46:ARG:CG	2.45	0.65
1:E:12:ARG:HH22	1:E:234:GPL:HN22	0.69	0.65
1:B:601:PRO:O	1:B:602:PHE:CB	2.43	0.65
1:C:390:ASP:O	1:C:391:ILE:C	2.35	0.65
1:B:329:THR:O	1:B:331:ARG:N	2.30	0.64
1:B:45:GLN:CD	1:B:48:SER:OG	2.35	0.64
1:A:78:TYR:N	1:A:79:PRO:HA	2.11	0.64
1:D:329:THR:O	1:D:331:ARG:N	2.30	0.64
1:A:329:THR:O	1:A:331:ARG:N	2.30	0.64
1:E:78:TYR:N	1:E:79:PRO:HA	2.11	0.64
1:A:45:GLN:NE2	1:A:48:SER:OG	2.30	0.64
1:C:601:PRO:C	1:D:886:ARG:NH1	2.46	0.64
1:C:619:SER:HG	2:C:1101:SAH:H3'	1.59	0.64
1:B:883:PRO:CD	2:B:1102:SAH:C8	2.76	0.64
1:A:883:PRO:CD	2:A:1102:SAH:C8	2.76	0.64
1:E:329:THR:O	1:E:331:ARG:N	2.30	0.64
1:E:619:SER:HG	2:E:1101:SAH:H5'1	1.63	0.64
1:E:46:ARG:CB	1:E:47:ARG:HA	2.10	0.64
1:B:406:VAL:H	1:B:407:GLU:HA	1.63	0.63
1:E:563:ALA:HA	2:E:1101:SAH:HN1	1.63	0.63
1:C:46:ARG:CB	1:C:47:ARG:HA	2.17	0.63
1:B:362:MET:HB3	1:B:363:ASN:HA	1.80	0.63
1:D:390:ASP:O	1:D:391:ILE:C	2.35	0.63
1:A:362:MET:HB3	1:A:363:ASN:HA	1.80	0.63
1:D:362:MET:HB3	1:D:363:ASN:HA	1.81	0.63
1:D:395:GLN:CG	1:E:112:ARG:CZ	2.56	0.63
1:B:619:SER:HG	2:B:1101:SAH:H5'1	1.63	0.63
1:A:890:LEU:CD1	1:E:604:ILE:HG21	2.18	0.63
1:B:563:ALA:HA	2:B:1101:SAH:HN1	1.64	0.63
1:C:592:VAL:HG22	1:D:373:ILE:CG1	2.29	0.63
1:D:883:PRO:CG	2:D:1102:SAH:H8	2.26	0.63
1:D:883:PRO:CD	2:D:1102:SAH:C8	2.76	0.63
1:A:406:VAL:H	1:A:407:GLU:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:CB	1:D:47:ARG:CA	2.75	0.63
1:A:373:ILE:HG12	1:E:592:VAL:HG22	1.81	0.63
1:C:406:VAL:H	1:C:407:GLU:HA	1.63	0.63
1:A:45:GLN:CD	1:A:48:SER:OG	2.37	0.63
1:C:592:VAL:HG22	1:D:373:ILE:HG12	1.81	0.63
1:E:883:PRO:CG	2:E:1102:SAH:H8	2.26	0.63
1:A:406:VAL:N	1:A:407:GLU:HA	2.14	0.63
1:C:883:PRO:CD	2:C:1102:SAH:C8	2.76	0.63
1:D:78:TYR:N	1:D:79:PRO:HA	2.11	0.63
1:C:563:ALA:HA	2:C:1101:SAH:HN1	1.64	0.62
1:C:362:MET:HB3	1:C:363:ASN:HA	1.81	0.62
1:A:365:ILE:HD11	1:E:590:ARG:HH11	1.64	0.62
1:E:362:MET:HB3	1:E:363:ASN:HA	1.81	0.62
1:A:46:ARG:HB3	1:A:47:ARG:CA	2.29	0.62
1:A:373:ILE:CG1	1:E:592:VAL:HG22	2.29	0.62
1:C:590:ARG:HH11	1:D:365:ILE:HD11	1.65	0.62
1:E:406:VAL:H	1:E:407:GLU:HA	1.63	0.62
1:E:883:PRO:CD	2:E:1102:SAH:C8	2.76	0.62
1:D:406:VAL:H	1:D:407:GLU:HA	1.63	0.62
1:D:563:ALA:HA	2:D:1101:SAH:HN1	1.64	0.62
1:A:563:ALA:HA	2:A:1101:SAH:HN1	1.64	0.62
1:E:406:VAL:N	1:E:407:GLU:HA	2.14	0.62
1:D:607:ASN:CA	1:E:864:ARG:HE	2.08	0.62
1:D:406:VAL:N	1:D:407:GLU:HA	2.14	0.62
1:B:46:ARG:HB3	1:B:47:ARG:CA	2.30	0.61
1:C:619:SER:HG	2:C:1101:SAH:H5'1	1.63	0.61
1:E:44:SER:O	1:E:46:ARG:CG	2.46	0.61
1:A:886:ARG:NH1	1:E:601:PRO:C	2.47	0.61
1:C:406:VAL:N	1:C:407:GLU:HA	2.14	0.61
1:B:44:SER:OG	1:B:46:ARG:CZ	2.47	0.61
1:B:44:SER:OG	1:B:46:ARG:NE	2.32	0.61
1:B:395:GLN:HG2	1:C:112:ARG:NH2	2.07	0.61
1:B:601:PRO:CG	1:C:886:ARG:NH1	2.56	0.61
1:A:864:ARG:HE	1:E:607:ASN:CA	2.08	0.61
1:B:607:ASN:CA	1:C:864:ARG:HE	2.08	0.61
1:A:112:ARG:HH22	1:E:395:GLN:HG2	1.62	0.61
1:B:45:GLN:N	1:B:46:ARG:HG3	2.14	0.61
1:E:791:ARG:NH1	1:E:791:ARG:HB3	2.12	0.61
1:C:45:GLN:CD	1:C:48:SER:OG	2.38	0.61
1:C:395:GLN:HG2	1:D:112:ARG:HH22	1.62	0.61
1:B:406:VAL:N	1:B:407:GLU:HA	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:967:ILE:O	1:D:968:ILE:C	2.39	0.61
1:A:590:ARG:HH11	1:B:365:ILE:HD11	1.66	0.61
1:A:592:VAL:HG22	1:B:373:ILE:HG12	1.82	0.60
1:B:791:ARG:HB3	1:B:791:ARG:NH1	2.12	0.60
1:A:255:ARG:O	1:A:256:VAL:HB	2.01	0.60
1:B:967:ILE:O	1:B:968:ILE:C	2.39	0.60
1:D:81:LYS:CA	1:D:82:ALA:HB3	2.31	0.60
1:E:46:ARG:CB	1:E:47:ARG:CA	2.75	0.60
1:A:592:VAL:HG22	1:B:373:ILE:CG1	2.31	0.60
1:E:255:ARG:O	1:E:256:VAL:HB	2.01	0.60
1:C:81:LYS:CA	1:C:82:ALA:HB3	2.31	0.60
1:B:81:LYS:CA	1:B:82:ALA:HB3	2.31	0.60
1:A:600:VAL:CB	2:A:1101:SAH:HN61	2.06	0.60
1:C:255:ARG:O	1:C:256:VAL:HB	2.01	0.60
1:A:967:ILE:O	1:A:968:ILE:C	2.39	0.60
1:A:212:HIS:CD2	1:A:234:GPL:O3'	2.55	0.60
1:C:967:ILE:O	1:C:968:ILE:C	2.39	0.60
1:E:281:ASN:O	1:E:283:PHE:N	2.34	0.60
1:B:281:ASN:O	1:B:283:PHE:N	2.35	0.60
1:A:81:LYS:HA	1:A:82:ALA:HB3	1.84	0.60
1:E:696:PRO:O	1:E:697:ILE:O	2.20	0.60
1:E:212:HIS:CD2	1:E:234:GPL:O3'	2.55	0.60
1:D:590:ARG:HH11	1:E:365:ILE:HD11	1.67	0.60
1:B:81:LYS:HA	1:B:82:ALA:HB3	1.84	0.60
1:A:81:LYS:CA	1:A:82:ALA:HB3	2.32	0.60
1:A:308:ALA:HB3	1:A:309:ASN:HB2	1.84	0.60
1:A:358:ILE:H	1:A:359:PRO:HA	1.67	0.60
1:D:25:ILE:C	1:D:25:ILE:HD12	2.23	0.60
1:A:696:PRO:O	1:A:697:ILE:O	2.20	0.60
1:A:395:GLN:HG2	1:B:112:ARG:NH2	2.06	0.60
1:B:592:VAL:HG22	1:C:373:ILE:HG12	1.84	0.60
1:D:696:PRO:O	1:D:697:ILE:O	2.20	0.60
1:C:604:ILE:CB	1:D:890:LEU:CD1	2.80	0.59
1:D:44:SER:O	1:D:46:ARG:HG3	2.01	0.59
1:A:46:ARG:HB3	1:A:47:ARG:CB	2.32	0.59
1:E:601:PRO:O	1:E:602:PHE:HB3	2.02	0.59
1:C:308:ALA:HB3	1:C:309:ASN:HB2	1.84	0.59
1:B:308:ALA:HB3	1:B:309:ASN:HB2	1.84	0.59
1:B:212:HIS:CD2	1:B:234:GPL:O3'	2.55	0.59
1:D:212:HIS:CD2	1:D:234:GPL:O3'	2.55	0.59
1:D:592:VAL:HG22	1:E:373:ILE:CG1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:PRO:O	1:B:697:ILE:O	2.20	0.59
1:C:281:ASN:O	1:C:283:PHE:N	2.34	0.59
1:C:696:PRO:O	1:C:697:ILE:O	2.20	0.59
1:A:83:ILE:O	1:A:83:ILE:HG22	2.02	0.59
1:B:25:ILE:HD12	1:B:25:ILE:C	2.22	0.59
1:D:1056:VAL:O	1:D:1056:VAL:HG13	2.03	0.59
1:C:25:ILE:HD12	1:C:25:ILE:C	2.23	0.59
1:E:308:ALA:HB3	1:E:309:ASN:HB2	1.84	0.59
1:E:308:ALA:H	1:E:309:ASN:HB2	1.66	0.59
1:A:281:ASN:O	1:A:283:PHE:N	2.34	0.59
1:E:967:ILE:O	1:E:968:ILE:C	2.39	0.59
1:D:358:ILE:H	1:D:359:PRO:HA	1.67	0.59
1:D:395:GLN:HG2	1:E:112:ARG:HH22	1.64	0.59
1:E:44:SER:O	1:E:46:ARG:HG3	2.02	0.59
1:C:212:HIS:CD2	1:C:234:GPL:O3'	2.55	0.59
1:B:255:ARG:O	1:B:256:VAL:HB	2.02	0.59
1:D:255:ARG:O	1:D:256:VAL:HB	2.02	0.59
1:C:81:LYS:HA	1:C:82:ALA:HB3	1.84	0.59
1:E:358:ILE:H	1:E:359:PRO:HA	1.67	0.59
1:A:308:ALA:H	1:A:309:ASN:HB2	1.66	0.59
1:D:308:ALA:HB3	1:D:309:ASN:HB2	1.84	0.59
1:B:358:ILE:H	1:B:359:PRO:HA	1.67	0.59
1:A:601:PRO:O	1:A:602:PHE:HB3	2.03	0.59
1:E:81:LYS:HA	1:E:82:ALA:HB3	1.84	0.59
1:E:25:ILE:HD12	1:E:25:ILE:C	2.23	0.59
1:A:395:GLN:HG2	1:B:112:ARG:HH22	1.63	0.59
1:D:601:PRO:O	1:D:602:PHE:HB3	2.03	0.59
1:C:590:ARG:NH1	1:D:365:ILE:HD11	2.18	0.59
1:D:27:LYS:N	1:D:28:PRO:CD	2.66	0.59
1:B:83:ILE:HG22	1:B:83:ILE:O	2.03	0.59
1:B:592:VAL:HG22	1:C:373:ILE:CG1	2.33	0.59
1:E:81:LYS:CA	1:E:82:ALA:HB3	2.32	0.59
1:D:778:ASP:O	1:D:779:ASN:HB2	2.03	0.59
1:B:1056:VAL:O	1:B:1056:VAL:HG13	2.03	0.59
1:E:27:LYS:N	1:E:28:PRO:CD	2.66	0.59
1:B:601:PRO:C	1:C:886:ARG:NH1	2.49	0.59
1:B:601:PRO:O	1:B:602:PHE:HB3	2.03	0.59
1:A:601:PRO:C	1:B:886:ARG:NH1	2.48	0.59
1:D:12:ARG:NH2	1:D:234:GPL:N2	2.13	0.59
1:C:308:ALA:H	1:C:309:ASN:HB2	1.66	0.59
1:C:887:ILE:O	1:C:888:GLU:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:VAL:O	1:A:1056:VAL:HG13	2.02	0.59
1:A:25:ILE:HD12	1:A:25:ILE:C	2.22	0.59
1:D:281:ASN:O	1:D:283:PHE:N	2.34	0.59
1:A:887:ILE:O	1:A:888:GLU:HB3	2.03	0.59
1:D:308:ALA:H	1:D:309:ASN:HB2	1.66	0.59
1:B:590:ARG:HH11	1:C:365:ILE:HD11	1.67	0.58
1:B:308:ALA:H	1:B:309:ASN:HB2	1.66	0.58
1:E:887:ILE:O	1:E:888:GLU:HB3	2.03	0.58
1:D:593:GLU:OE1	1:E:372:ARG:HB3	2.03	0.58
1:D:592:VAL:HG22	1:E:373:ILE:HG12	1.83	0.58
1:B:593:GLU:OE1	1:C:372:ARG:HB3	2.03	0.58
1:B:27:LYS:N	1:B:28:PRO:CD	2.66	0.58
1:C:27:LYS:N	1:C:28:PRO:CD	2.66	0.58
1:A:890:LEU:CD1	1:E:604:ILE:CB	2.80	0.58
1:C:45:GLN:N	1:C:46:ARG:HA	2.17	0.58
1:A:778:ASP:O	1:A:779:ASN:HB2	2.03	0.58
1:C:358:ILE:H	1:C:359:PRO:HA	1.67	0.58
1:C:1056:VAL:O	1:C:1056:VAL:HG13	2.02	0.58
1:A:27:LYS:N	1:A:28:PRO:CD	2.66	0.58
1:C:601:PRO:O	1:C:602:PHE:HB3	2.03	0.58
1:A:365:ILE:HD11	1:E:590:ARG:NH1	2.18	0.58
1:D:81:LYS:HA	1:D:82:ALA:HB3	1.84	0.58
1:A:112:ARG:NH2	1:E:395:GLN:HG2	2.05	0.58
1:C:778:ASP:O	1:C:779:ASN:HB2	2.03	0.58
1:A:362:MET:N	1:A:363:ASN:HA	2.19	0.58
1:B:887:ILE:O	1:B:888:GLU:HB3	2.03	0.58
1:A:12:ARG:NH2	1:A:234:GPL:N2	2.13	0.58
1:C:146:PRO:O	1:C:147:GLN:HB3	2.04	0.58
1:D:146:PRO:O	1:D:147:GLN:HB3	2.04	0.58
1:E:83:ILE:HG22	1:E:83:ILE:O	2.03	0.58
1:E:605:ASP:O	1:E:606:LYS:HB3	2.04	0.58
1:C:592:VAL:HG22	1:D:373:ILE:HD11	1.86	0.58
1:B:146:PRO:O	1:B:147:GLN:HB3	2.04	0.58
1:D:83:ILE:HG22	1:D:83:ILE:O	2.02	0.58
1:B:778:ASP:O	1:B:779:ASN:HB2	2.03	0.58
1:A:605:ASP:O	1:A:606:LYS:HB3	2.04	0.58
1:D:605:ASP:O	1:D:606:LYS:HB3	2.04	0.58
1:A:372:ARG:HB3	1:E:593:GLU:OE1	2.04	0.58
1:A:607:ASN:CA	1:B:864:ARG:HE	2.08	0.57
1:D:254:ASP:O	1:D:255:ARG:HB3	2.04	0.57
1:E:1056:VAL:HG13	1:E:1056:VAL:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASP:O	1:C:255:ARG:HB3	2.05	0.57
1:A:358:ILE:HB	1:A:359:PRO:HA	1.86	0.57
1:E:778:ASP:O	1:E:779:ASN:HB2	2.03	0.57
1:E:146:PRO:O	1:E:147:GLN:HB3	2.04	0.57
1:B:254:ASP:O	1:B:255:ARG:HB3	2.04	0.57
1:A:146:PRO:O	1:A:147:GLN:HB3	2.04	0.57
1:E:358:ILE:N	1:E:359:PRO:HA	2.20	0.57
1:D:887:ILE:O	1:D:888:GLU:HB3	2.03	0.57
1:D:618:ASN:O	1:D:619:SER:HB3	2.05	0.57
1:E:600:VAL:CB	2:E:1101:SAH:HN61	2.06	0.57
1:A:590:ARG:NH1	1:B:365:ILE:HD11	2.20	0.57
1:C:83:ILE:O	1:C:83:ILE:HG22	2.03	0.57
1:A:358:ILE:N	1:A:359:PRO:HA	2.20	0.57
1:C:605:ASP:O	1:C:606:LYS:HB3	2.04	0.57
1:D:604:ILE:CB	1:E:890:LEU:CD1	2.82	0.57
1:B:358:ILE:N	1:B:359:PRO:HA	2.19	0.57
1:B:362:MET:N	1:B:363:ASN:HA	2.19	0.57
1:E:362:MET:N	1:E:363:ASN:HA	2.19	0.57
1:E:74:LEU:N	1:E:75:PRO:CD	2.68	0.57
1:A:166:ILE:HA	1:A:234:GPL:O6	2.05	0.57
1:E:254:ASP:O	1:E:255:ARG:HB3	2.04	0.57
1:E:810:ARG:HG2	1:E:810:ARG:O	2.05	0.57
1:E:618:ASN:O	1:E:619:SER:HB3	2.05	0.56
1:C:46:ARG:HB3	1:C:47:ARG:HB3	1.84	0.56
1:D:362:MET:N	1:D:363:ASN:HA	2.19	0.56
1:C:358:ILE:N	1:C:359:PRO:HA	2.20	0.56
1:C:810:ARG:O	1:C:810:ARG:HG2	2.05	0.56
1:B:395:GLN:HG2	1:C:112:ARG:HH22	1.65	0.56
1:C:618:ASN:O	1:C:619:SER:HB3	2.05	0.56
1:B:166:ILE:HA	1:B:234:GPL:O6	2.05	0.56
1:E:166:ILE:HA	1:E:234:GPL:O6	2.05	0.56
1:D:592:VAL:HG11	1:E:371:GLY:HA3	1.88	0.56
1:A:593:GLU:OE1	1:B:372:ARG:HB3	2.05	0.56
1:A:592:VAL:HG11	1:B:371:GLY:HA3	1.87	0.56
1:C:607:ASN:CA	1:D:864:ARG:HE	2.07	0.56
1:A:81:LYS:HG3	1:A:82:ALA:O	2.05	0.56
1:D:358:ILE:HB	1:D:359:PRO:HA	1.86	0.56
1:B:358:ILE:HB	1:B:359:PRO:HA	1.87	0.56
1:D:486:THR:O	1:D:487:GLN:HB2	2.06	0.56
1:D:69:HIS:HB2	1:D:70:PRO:HD3	1.87	0.56
1:D:74:LEU:N	1:D:75:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:810:ARG:HG2	1:D:810:ARG:O	2.05	0.56
1:B:74:LEU:N	1:B:75:PRO:CD	2.68	0.56
1:A:74:LEU:N	1:A:75:PRO:CD	2.68	0.56
1:A:400:VAL:HG22	1:B:21:GLN:HE22	1.70	0.56
1:C:600:VAL:CB	2:C:1101:SAH:HN61	2.06	0.56
1:B:605:ASP:O	1:B:606:LYS:HB3	2.04	0.56
1:A:46:ARG:HB3	1:A:47:ARG:HA	1.87	0.56
1:A:373:ILE:HD11	1:E:592:VAL:HG22	1.86	0.56
1:A:365:ILE:CG1	1:E:590:ARG:HD3	2.36	0.56
1:D:791:ARG:NH1	1:D:791:ARG:HB3	2.12	0.56
1:E:358:ILE:HB	1:E:359:PRO:HA	1.86	0.56
1:B:45:GLN:HB2	1:B:46:ARG:CA	2.34	0.56
1:C:358:ILE:HB	1:C:359:PRO:HA	1.87	0.56
1:C:202:SER:O	1:C:203:THR:C	2.44	0.56
1:B:688:TYR:CD1	1:B:688:TYR:O	2.59	0.56
1:B:618:ASN:O	1:B:619:SER:HB3	2.05	0.56
1:C:166:ILE:HA	1:C:234:GPL:O6	2.05	0.56
1:D:358:ILE:N	1:D:359:PRO:HA	2.19	0.56
1:E:69:HIS:HB2	1:E:70:PRO:HD3	1.87	0.56
1:A:486:THR:O	1:A:487:GLN:HB2	2.06	0.56
1:D:400:VAL:HG22	1:E:21:GLN:HE22	1.70	0.56
1:C:593:GLU:OE1	1:D:372:ARG:HB3	2.05	0.56
1:C:81:LYS:HG3	1:C:82:ALA:O	2.05	0.56
1:D:202:SER:O	1:D:203:THR:C	2.44	0.56
1:A:763:LYS:HD2	1:A:763:LYS:C	2.26	0.56
1:A:45:GLN:CB	1:A:46:ARG:HA	2.22	0.56
1:D:81:LYS:HG3	1:D:82:ALA:O	2.05	0.56
1:C:688:TYR:O	1:C:688:TYR:CD1	2.59	0.56
1:C:592:VAL:HG11	1:D:371:GLY:HA3	1.88	0.56
1:D:590:ARG:NH1	1:E:365:ILE:HD11	2.21	0.56
1:C:791:ARG:NH1	1:C:791:ARG:HB3	2.12	0.56
1:E:202:SER:O	1:E:203:THR:C	2.44	0.56
1:B:604:ILE:CB	1:C:890:LEU:CD1	2.82	0.56
1:D:166:ILE:HA	1:D:234:GPL:O6	2.05	0.56
1:A:371:GLY:HA3	1:E:592:VAL:HG11	1.88	0.56
1:B:81:LYS:HG3	1:B:82:ALA:O	2.05	0.56
1:E:81:LYS:HG3	1:E:82:ALA:O	2.05	0.56
1:A:400:VAL:CG2	1:B:21:GLN:HE22	2.18	0.56
1:C:74:LEU:N	1:C:75:PRO:CD	2.68	0.56
1:A:604:ILE:CB	1:B:890:LEU:CD1	2.83	0.55
1:A:618:ASN:O	1:A:619:SER:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ARG:NH1	1:C:365:ILE:HD11	2.21	0.55
1:A:791:ARG:NH1	1:A:791:ARG:HB3	2.12	0.55
1:D:400:VAL:CG2	1:E:21:GLN:HE22	2.19	0.55
1:A:202:SER:O	1:A:203:THR:C	2.44	0.55
1:B:592:VAL:HG11	1:C:371:GLY:HA3	1.88	0.55
1:B:592:VAL:HG22	1:C:373:ILE:HD11	1.88	0.55
1:B:763:LYS:HD2	1:B:763:LYS:C	2.27	0.55
1:D:688:TYR:O	1:D:688:TYR:CD1	2.59	0.55
1:B:810:ARG:HG2	1:B:810:ARG:O	2.05	0.55
1:B:202:SER:O	1:B:203:THR:C	2.44	0.55
1:D:395:GLN:HG2	1:E:112:ARG:NH2	2.06	0.55
1:D:600:VAL:CB	2:D:1101:SAH:HN61	2.06	0.55
1:E:45:GLN:NE2	1:E:48:SER:OG	2.39	0.55
1:C:362:MET:N	1:C:363:ASN:HA	2.19	0.55
1:D:755:ALA:N	1:D:756:PRO:HD2	2.21	0.55
1:E:688:TYR:O	1:E:688:TYR:CD1	2.59	0.55
1:A:254:ASP:O	1:A:255:ARG:HB3	2.04	0.55
1:D:763:LYS:HD2	1:D:763:LYS:C	2.26	0.55
1:E:486:THR:O	1:E:487:GLN:HB2	2.06	0.55
1:A:755:ALA:N	1:A:756:PRO:HD2	2.21	0.55
1:A:810:ARG:O	1:A:810:ARG:HG2	2.05	0.55
1:D:45:GLN:CD	1:D:48:SER:OG	2.45	0.55
1:D:592:VAL:HG22	1:E:373:ILE:HD11	1.88	0.55
1:A:592:VAL:HG22	1:B:373:ILE:HD11	1.88	0.55
1:B:400:VAL:CG2	1:C:21:GLN:HE22	2.20	0.55
1:C:400:VAL:CG2	1:D:21:GLN:HE22	2.20	0.55
1:C:763:LYS:HD2	1:C:763:LYS:C	2.26	0.55
1:E:763:LYS:HD2	1:E:763:LYS:C	2.27	0.55
1:E:866:LEU:HD12	1:E:866:LEU:C	2.27	0.55
1:C:486:THR:O	1:C:487:GLN:HB2	2.06	0.55
1:C:69:HIS:HB2	1:C:70:PRO:HD3	1.87	0.55
1:B:618:ASN:O	2:B:1101:SAH:H5'2	2.03	0.55
1:A:602:PHE:C	1:B:886:ARG:NH1	2.57	0.55
1:B:69:HIS:HB2	1:B:70:PRO:HD3	1.87	0.55
1:D:45:GLN:NE2	1:D:48:SER:OG	2.39	0.55
1:B:590:ARG:HD3	1:C:365:ILE:CG1	2.36	0.55
1:E:12:ARG:NH2	1:E:234:GPL:N2	2.13	0.55
1:A:21:GLN:HE22	1:E:400:VAL:HG22	1.72	0.55
1:E:677:LEU:C	1:E:677:LEU:HD12	2.27	0.55
1:B:44:SER:CB	1:B:46:ARG:CZ	2.84	0.55
1:E:618:ASN:O	1:E:619:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:PRO:C	1:E:886:ARG:NH1	2.49	0.55
1:E:755:ALA:N	1:E:756:PRO:HD2	2.21	0.55
1:A:688:TYR:O	1:A:688:TYR:CD1	2.59	0.55
1:A:69:HIS:HB2	1:A:70:PRO:HD3	1.87	0.55
1:A:677:LEU:C	1:A:677:LEU:HD12	2.27	0.55
1:C:755:ALA:N	1:C:756:PRO:HD2	2.21	0.55
1:B:602:PHE:C	1:C:886:ARG:NH1	2.56	0.54
1:E:201:LYS:O	1:E:201:LYS:HG3	2.07	0.54
1:D:983:GLU:O	1:D:984:GLU:C	2.46	0.54
1:A:866:LEU:C	1:A:866:LEU:HD12	2.27	0.54
1:D:913:LEU:O	1:D:914:GLU:HB2	2.07	0.54
1:B:866:LEU:C	1:B:866:LEU:HD12	2.27	0.54
1:A:395:GLN:OE1	1:B:18:LYS:NZ	2.39	0.54
1:E:45:GLN:CD	1:E:48:SER:OG	2.45	0.54
1:C:866:LEU:C	1:C:866:LEU:HD12	2.27	0.54
1:B:618:ASN:O	1:B:619:SER:OG	2.25	0.54
1:C:592:VAL:HG22	1:D:373:ILE:CD1	2.38	0.54
1:D:593:GLU:HG3	1:D:594:PRO:HA	1.90	0.54
1:C:590:ARG:HD3	1:D:365:ILE:CG1	2.36	0.54
1:A:618:ASN:O	1:A:619:SER:OG	2.25	0.54
1:D:590:ARG:HD3	1:E:365:ILE:CG1	2.36	0.54
1:D:677:LEU:C	1:D:677:LEU:HD12	2.27	0.54
1:C:913:LEU:O	1:C:914:GLU:HB2	2.08	0.54
1:E:983:GLU:O	1:E:984:GLU:C	2.46	0.54
1:B:395:GLN:OE1	1:C:18:LYS:NZ	2.40	0.54
1:B:45:GLN:CB	1:B:46:ARG:HA	2.28	0.54
1:D:618:ASN:O	2:D:1101:SAH:H5'2	2.03	0.54
1:D:45:GLN:N	1:D:46:ARG:HA	2.21	0.54
1:E:593:GLU:HG3	1:E:594:PRO:HA	1.90	0.54
1:B:400:VAL:HG22	1:C:21:GLN:HE22	1.71	0.54
1:C:400:VAL:HG22	1:D:21:GLN:HE22	1.72	0.54
1:D:201:LYS:HG3	1:D:201:LYS:O	2.08	0.54
1:B:486:THR:O	1:B:487:GLN:HB2	2.06	0.54
1:C:677:LEU:HD12	1:C:677:LEU:C	2.28	0.54
1:C:618:ASN:O	1:C:619:SER:OG	2.25	0.54
1:A:373:ILE:CD1	1:E:592:VAL:HG22	2.38	0.54
1:B:755:ALA:N	1:B:756:PRO:HD2	2.21	0.54
1:C:395:GLN:OE1	1:D:18:LYS:NZ	2.41	0.54
1:E:45:GLN:N	1:E:46:ARG:HA	2.21	0.54
1:A:593:GLU:HG3	1:A:594:PRO:HA	1.90	0.54
1:A:46:ARG:CB	1:A:47:ARG:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:GLU:HG3	1:C:594:PRO:HA	1.90	0.53
1:E:696:PRO:C	1:E:697:ILE:HG13	2.28	0.53
1:A:201:LYS:HG3	1:A:201:LYS:O	2.08	0.53
1:A:18:LYS:NZ	1:E:395:GLN:OE1	2.41	0.53
1:A:358:ILE:HB	1:A:359:PRO:CA	2.38	0.53
1:D:866:LEU:C	1:D:866:LEU:HD12	2.27	0.53
1:E:507:GLY:O	1:E:508:ASN:HB2	2.09	0.53
1:A:590:ARG:HD3	1:B:365:ILE:CG1	2.37	0.53
1:E:467:SER:N	1:E:468:PRO:CD	2.72	0.53
1:B:983:GLU:O	1:B:984:GLU:C	2.46	0.53
1:D:618:ASN:O	1:D:619:SER:OG	2.25	0.53
1:A:467:SER:N	1:A:468:PRO:CD	2.72	0.53
1:D:467:SER:N	1:D:468:PRO:CD	2.72	0.53
1:D:395:GLN:OE1	1:E:18:LYS:NZ	2.40	0.53
1:A:696:PRO:C	1:A:697:ILE:HG13	2.29	0.53
1:B:358:ILE:HB	1:B:359:PRO:CA	2.38	0.53
1:A:869:ILE:O	1:A:870:SER:OG	2.27	0.53
1:C:201:LYS:O	1:C:201:LYS:HG3	2.08	0.53
1:E:913:LEU:O	1:E:914:GLU:HB2	2.07	0.53
1:B:913:LEU:O	1:B:914:GLU:HB2	2.08	0.53
1:B:677:LEU:C	1:B:677:LEU:HD12	2.27	0.53
1:C:618:ASN:O	2:C:1101:SAH:H5'2	2.03	0.53
1:C:308:ALA:N	1:C:309:ASN:HB2	2.24	0.53
1:C:467:SER:N	1:C:468:PRO:CD	2.72	0.53
1:A:913:LEU:O	1:A:914:GLU:HB2	2.07	0.53
1:A:507:GLY:O	1:A:508:ASN:HB2	2.09	0.53
1:B:308:ALA:N	1:B:309:ASN:HB2	2.24	0.53
1:B:696:PRO:C	1:B:697:ILE:HG13	2.29	0.53
1:B:467:SER:N	1:B:468:PRO:CD	2.72	0.53
1:B:600:VAL:CB	2:B:1101:SAH:HN61	2.06	0.53
1:B:593:GLU:HG3	1:B:594:PRO:HA	1.90	0.53
1:C:358:ILE:HB	1:C:359:PRO:CA	2.38	0.53
1:B:507:GLY:O	1:B:508:ASN:HB2	2.09	0.53
1:B:201:LYS:HG3	1:B:201:LYS:O	2.08	0.53
1:D:507:GLY:O	1:D:508:ASN:HB2	2.09	0.52
1:B:562:GLY:O	2:B:1101:SAH:H8	2.10	0.52
1:B:869:ILE:O	1:B:870:SER:OG	2.27	0.52
1:E:869:ILE:O	1:E:870:SER:OG	2.27	0.52
1:D:358:ILE:HB	1:D:359:PRO:CA	2.38	0.52
1:A:21:GLN:HE22	1:E:400:VAL:CG2	2.20	0.52
1:A:983:GLU:O	1:A:984:GLU:C	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:GLY:O	1:C:508:ASN:HB2	2.09	0.52
1:D:696:PRO:C	1:D:697:ILE:HG13	2.29	0.52
1:E:358:ILE:HB	1:E:359:PRO:CA	2.38	0.52
1:C:983:GLU:O	1:C:984:GLU:C	2.46	0.52
1:A:890:LEU:HD12	1:E:604:ILE:HB	1.92	0.52
1:A:592:VAL:HG22	1:B:373:ILE:CD1	2.40	0.52
1:D:869:ILE:O	1:D:870:SER:OG	2.27	0.52
1:A:2:TRP:CE2	1:E:451:ARG:CD	2.93	0.52
1:B:484:THR:O	1:B:485:MET:HB3	2.10	0.52
1:E:3:HIS:CG	1:E:3:HIS:O	2.63	0.52
1:A:308:ALA:N	1:A:309:ASN:HB2	2.24	0.52
1:A:292:ARG:O	1:A:293:LEU:HB3	2.10	0.52
1:B:3:HIS:CG	1:B:3:HIS:O	2.63	0.52
1:E:308:ALA:N	1:E:309:ASN:HB2	2.24	0.52
1:D:592:VAL:HG22	1:E:373:ILE:CD1	2.40	0.52
1:C:451:ARG:CD	1:D:2:TRP:CE2	2.93	0.52
1:B:27:LYS:HB3	1:B:28:PRO:HD3	1.92	0.52
1:A:27:LYS:HB3	1:A:28:PRO:HD3	1.92	0.52
1:D:292:ARG:O	1:D:293:LEU:HB3	2.10	0.52
1:C:484:THR:O	1:C:485:MET:HB3	2.10	0.52
1:E:484:THR:O	1:E:485:MET:HB3	2.10	0.51
1:D:562:GLY:O	2:D:1101:SAH:H8	2.10	0.51
1:A:365:ILE:CD1	1:E:590:ARG:HH11	2.23	0.51
1:D:308:ALA:N	1:D:309:ASN:HB2	2.24	0.51
1:B:44:SER:HB3	1:B:46:ARG:CZ	2.32	0.51
1:E:562:GLY:O	2:E:1101:SAH:H8	2.10	0.51
1:C:869:ILE:O	1:C:870:SER:OG	2.27	0.51
1:A:307:HIS:HB3	1:A:308:ALA:HB2	1.93	0.51
1:C:562:GLY:O	2:C:1101:SAH:H8	2.10	0.51
1:C:592:VAL:HG13	1:D:373:ILE:CG1	2.40	0.51
1:A:3:HIS:O	1:A:3:HIS:CG	2.63	0.51
1:B:307:HIS:CB	1:B:308:ALA:HA	2.41	0.51
1:C:696:PRO:C	1:C:697:ILE:HG13	2.29	0.51
1:C:619:SER:HB2	1:C:620:TYR:CB	2.41	0.51
1:A:562:GLY:O	2:A:1101:SAH:H8	2.10	0.51
1:A:362:MET:HB3	1:A:363:ASN:CA	2.40	0.51
1:B:307:HIS:HB3	1:B:308:ALA:HB2	1.92	0.51
1:D:619:SER:HB2	1:D:620:TYR:CB	2.41	0.51
1:A:378:THR:HG21	1:E:603:PRO:CG	2.36	0.51
1:B:592:VAL:HG22	1:C:373:ILE:CD1	2.41	0.51
1:D:398:GLU:CB	1:E:14:ALA:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:HIS:HB3	1:D:308:ALA:HB2	1.93	0.51
1:D:27:LYS:HB3	1:D:28:PRO:HD3	1.92	0.51
1:B:292:ARG:O	1:B:293:LEU:HB3	2.10	0.51
1:E:619:SER:HB2	1:E:620:TYR:CB	2.41	0.51
1:A:619:SER:HB2	1:A:620:TYR:CB	2.41	0.51
1:C:590:ARG:HH11	1:D:365:ILE:CD1	2.23	0.51
1:C:362:MET:HB3	1:C:363:ASN:CA	2.41	0.51
1:E:27:LYS:HB3	1:E:28:PRO:HD3	1.92	0.51
1:D:484:THR:O	1:D:485:MET:HB3	2.10	0.51
1:C:607:ASN:N	1:D:864:ARG:CD	2.74	0.51
1:E:362:MET:HB3	1:E:363:ASN:CA	2.40	0.51
1:E:292:ARG:O	1:E:293:LEU:HB3	2.10	0.51
1:D:31:VAL:HB	1:D:32:PRO:HD3	1.93	0.51
1:D:3:HIS:O	1:D:3:HIS:CG	2.63	0.50
1:B:398:GLU:CB	1:C:14:ALA:O	2.59	0.50
1:E:307:HIS:CB	1:E:308:ALA:HA	2.41	0.50
1:C:292:ARG:O	1:C:293:LEU:HB3	2.10	0.50
1:B:604:ILE:CG2	1:C:890:LEU:HD12	2.33	0.50
1:B:31:VAL:HB	1:B:32:PRO:HD3	1.94	0.50
1:A:373:ILE:HD13	1:E:597:ARG:NH2	2.26	0.50
1:C:590:ARG:O	1:C:590:ARG:HG2	2.11	0.50
1:A:451:ARG:CD	1:B:2:TRP:CE2	2.94	0.50
1:B:80:SER:O	1:B:81:LYS:C	2.50	0.50
1:A:307:HIS:CB	1:A:308:ALA:HA	2.41	0.50
1:D:362:MET:HB3	1:D:363:ASN:CA	2.40	0.50
1:E:1021:THR:N	1:E:1022:PRO:CD	2.75	0.50
1:A:1021:THR:N	1:A:1022:PRO:CD	2.75	0.50
1:C:604:ILE:HB	1:D:890:LEU:HD12	1.92	0.50
1:C:80:SER:O	1:C:81:LYS:C	2.50	0.50
1:C:307:HIS:HB3	1:C:308:ALA:HB2	1.93	0.50
1:C:308:ALA:CA	1:C:309:ASN:HB2	2.41	0.50
1:E:80:SER:O	1:E:81:LYS:C	2.49	0.50
1:C:27:LYS:HB3	1:C:28:PRO:HD3	1.92	0.50
1:D:564:GLU:HB3	1:D:565:ARG:HA	1.94	0.50
1:E:549:SER:O	1:E:550:TYR:HB2	2.12	0.50
1:A:617:ILE:O	1:A:618:ASN:CB	2.60	0.50
1:D:590:ARG:O	1:D:590:ARG:HG2	2.12	0.50
1:A:484:THR:O	1:A:485:MET:HB3	2.10	0.50
1:A:590:ARG:HH11	1:B:365:ILE:CD1	2.25	0.50
1:C:307:HIS:CB	1:C:308:ALA:HA	2.41	0.50
1:D:307:HIS:CB	1:D:308:ALA:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:SER:HB2	1:B:620:TYR:CB	2.41	0.50
1:A:373:ILE:CG1	1:E:592:VAL:HG13	2.40	0.50
1:E:590:ARG:O	1:E:590:ARG:HG2	2.12	0.50
1:E:406:VAL:CB	1:E:407:GLU:CA	2.88	0.50
1:C:1021:THR:N	1:C:1022:PRO:CD	2.75	0.50
1:B:1021:THR:N	1:B:1022:PRO:CD	2.75	0.50
1:E:617:ILE:O	1:E:618:ASN:CB	2.60	0.50
1:B:308:ALA:CA	1:B:309:ASN:HB2	2.41	0.50
1:E:308:ALA:CA	1:E:309:ASN:HB2	2.41	0.50
1:E:564:GLU:HB3	1:E:565:ARG:HA	1.94	0.50
1:E:44:SER:OG	1:E:46:ARG:NE	2.45	0.49
1:B:212:HIS:HE2	1:B:234:GPL:HO3'	1.58	0.49
1:B:590:ARG:HG2	1:B:590:ARG:O	2.11	0.49
1:E:31:VAL:HB	1:E:32:PRO:HD3	1.94	0.49
1:D:1021:THR:N	1:D:1022:PRO:CD	2.75	0.49
1:B:564:GLU:HB3	1:B:565:ARG:HA	1.94	0.49
1:C:597:ARG:NH2	1:D:373:ILE:HD13	2.26	0.49
1:A:549:SER:O	1:A:550:TYR:HB2	2.12	0.49
1:C:549:SER:O	1:C:550:TYR:HB2	2.12	0.49
1:B:362:MET:HB3	1:B:363:ASN:CA	2.40	0.49
1:D:80:SER:O	1:D:81:LYS:C	2.50	0.49
1:E:307:HIS:HB3	1:E:308:ALA:HB2	1.93	0.49
1:A:886:ARG:NH1	1:E:601:PRO:CG	2.51	0.49
1:B:904:PHE:N	2:B:1102:SAH:HN62	2.10	0.49
1:A:904:PHE:N	2:A:1102:SAH:HN62	2.10	0.49
1:A:80:SER:O	1:A:81:LYS:C	2.49	0.49
1:D:617:ILE:O	1:D:618:ASN:CB	2.60	0.49
1:A:864:ARG:CD	1:E:607:ASN:N	2.74	0.49
1:D:593:GLU:CG	1:D:594:PRO:HA	2.43	0.49
1:A:391:ILE:O	1:A:391:ILE:CG2	2.61	0.49
1:D:604:ILE:HB	1:E:890:LEU:HD12	1.95	0.49
1:A:597:ARG:NH2	1:B:373:ILE:HD13	2.27	0.49
1:B:592:VAL:HG13	1:C:373:ILE:CG1	2.41	0.49
1:B:590:ARG:HH11	1:C:365:ILE:CD1	2.26	0.49
1:A:590:ARG:HG2	1:A:590:ARG:O	2.12	0.49
1:A:31:VAL:HB	1:A:32:PRO:HD3	1.94	0.49
1:A:45:GLN:CB	1:A:46:ARG:CA	2.90	0.49
1:E:593:GLU:CG	1:E:594:PRO:HA	2.43	0.49
1:A:308:ALA:CA	1:A:309:ASN:HB2	2.42	0.49
1:B:549:SER:O	1:B:550:TYR:HB2	2.12	0.49
1:B:605:ASP:O	1:B:606:LYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:HIS:CG	1:C:3:HIS:O	2.63	0.49
1:D:308:ALA:CA	1:D:309:ASN:HB2	2.42	0.49
1:C:31:VAL:HB	1:C:32:PRO:HD3	1.94	0.49
1:D:451:ARG:CD	1:E:2:TRP:CE2	2.96	0.49
1:C:398:GLU:CB	1:D:14:ALA:O	2.61	0.49
1:C:564:GLU:HB3	1:C:565:ARG:HA	1.94	0.49
1:C:617:ILE:O	1:C:618:ASN:CB	2.60	0.49
1:C:603:PRO:CG	1:D:378:THR:HG21	2.37	0.49
1:B:46:ARG:CB	1:B:47:ARG:CA	2.90	0.48
1:A:14:ALA:O	1:E:398:GLU:CB	2.60	0.48
1:B:604:ILE:HB	1:C:890:LEU:HD12	1.95	0.48
1:D:212:HIS:HE2	1:D:234:GPL:HO3'	1.57	0.48
1:C:602:PHE:C	1:D:886:ARG:NH1	2.59	0.48
1:C:593:GLU:CG	1:C:594:PRO:HA	2.43	0.48
1:A:592:VAL:HG13	1:B:373:ILE:CG1	2.42	0.48
1:D:883:PRO:HG3	2:D:1102:SAH:N7	2.29	0.48
1:A:362:MET:H	1:A:363:ASN:HA	1.78	0.48
1:B:607:ASN:N	1:C:864:ARG:CD	2.74	0.48
1:E:362:MET:H	1:E:363:ASN:HA	1.78	0.48
1:D:592:VAL:HG13	1:E:373:ILE:CG1	2.41	0.48
1:A:607:ASN:N	1:B:864:ARG:CD	2.75	0.48
1:C:904:PHE:N	2:C:1102:SAH:HN62	2.10	0.48
1:E:883:PRO:HG3	2:E:1102:SAH:N7	2.29	0.48
1:D:887:ILE:O	1:D:888:GLU:CB	2.61	0.48
1:A:755:ALA:N	1:A:756:PRO:CD	2.76	0.48
1:E:755:ALA:N	1:E:756:PRO:CD	2.76	0.48
1:C:755:ALA:N	1:C:756:PRO:CD	2.76	0.48
1:A:564:GLU:HB3	1:A:565:ARG:HA	1.94	0.48
1:D:549:SER:O	1:D:550:TYR:HB2	2.12	0.48
1:C:605:ASP:O	1:C:606:LYS:HB2	2.12	0.48
1:D:605:ASP:O	1:D:606:LYS:HB2	2.13	0.48
1:D:44:SER:OG	1:D:46:ARG:NE	2.46	0.48
1:D:607:ASN:N	1:E:864:ARG:CD	2.75	0.48
1:D:590:ARG:HH11	1:E:365:ILE:CD1	2.26	0.48
1:A:887:ILE:O	1:A:888:GLU:CB	2.61	0.48
1:C:27:LYS:H	1:C:28:PRO:HD3	1.79	0.48
1:D:755:ALA:N	1:D:756:PRO:CD	2.76	0.48
1:A:853:GLU:HG3	1:A:854:ASN:N	2.29	0.48
1:B:853:GLU:HG3	1:B:854:ASN:N	2.28	0.48
1:A:605:ASP:O	1:A:606:LYS:HB2	2.12	0.48
1:B:593:GLU:CG	1:B:594:PRO:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:PRO:CG	1:B:378:THR:HG21	2.37	0.48
1:C:307:HIS:HB3	1:C:308:ALA:CA	2.44	0.48
1:E:887:ILE:O	1:E:888:GLU:CB	2.61	0.48
1:A:27:LYS:H	1:A:28:PRO:HD3	1.79	0.48
1:B:617:ILE:O	1:B:618:ASN:CB	2.60	0.48
1:C:883:PRO:HG3	2:C:1102:SAH:N7	2.29	0.48
1:B:451:ARG:CD	1:C:2:TRP:CE2	2.97	0.48
1:B:679:LYS:HG2	1:B:711:MET:SD	2.54	0.48
1:A:593:GLU:CG	1:A:594:PRO:HA	2.43	0.48
1:B:406:VAL:HB	1:B:407:GLU:C	2.34	0.48
1:B:81:LYS:HA	1:B:82:ALA:C	2.34	0.48
1:E:307:HIS:HB3	1:E:308:ALA:CA	2.44	0.48
1:D:81:LYS:HA	1:D:82:ALA:C	2.34	0.48
1:C:81:LYS:HA	1:C:82:ALA:C	2.34	0.48
1:D:307:HIS:HB3	1:D:308:ALA:CA	2.44	0.48
1:D:27:LYS:H	1:D:28:PRO:HD3	1.79	0.48
1:A:677:LEU:O	1:A:677:LEU:HD12	2.14	0.48
1:C:677:LEU:HD12	1:C:677:LEU:O	2.14	0.48
1:C:853:GLU:HG3	1:C:854:ASN:N	2.28	0.48
1:D:679:LYS:HG2	1:D:711:MET:SD	2.54	0.48
1:A:373:ILE:HA	1:E:593:GLU:H	1.79	0.48
1:A:2:TRP:CE2	1:E:451:ARG:HD3	2.49	0.48
1:D:914:GLU:O	1:D:915:ASN:C	2.52	0.48
1:E:853:GLU:HG3	1:E:854:ASN:N	2.29	0.48
1:D:602:PHE:C	1:E:886:ARG:NH1	2.56	0.47
1:E:27:LYS:H	1:E:28:PRO:HD3	1.79	0.47
1:B:887:ILE:O	1:B:888:GLU:CB	2.61	0.47
1:B:914:GLU:O	1:B:915:ASN:C	2.52	0.47
1:D:853:GLU:HG3	1:D:854:ASN:N	2.29	0.47
1:E:393:LEU:O	1:E:393:LEU:HD12	2.14	0.47
1:B:46:ARG:CB	1:B:47:ARG:HA	2.43	0.47
1:A:604:ILE:HB	1:B:890:LEU:HD12	1.95	0.47
1:C:406:VAL:HB	1:C:407:GLU:C	2.34	0.47
1:A:406:VAL:HB	1:A:407:GLU:C	2.34	0.47
1:B:362:MET:H	1:B:363:ASN:HA	1.78	0.47
1:D:362:MET:H	1:D:363:ASN:HA	1.78	0.47
1:E:677:LEU:O	1:E:677:LEU:HD12	2.14	0.47
1:C:679:LYS:HG2	1:C:711:MET:SD	2.54	0.47
1:D:1036:GLY:O	1:D:1038:THR:N	2.47	0.47
1:C:393:LEU:HD12	1:C:393:LEU:O	2.14	0.47
1:D:597:ARG:NH2	1:E:373:ILE:HD13	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1102:SAH:HG2	2:B:1102:SAH:H4'	1.77	0.47
1:C:391:ILE:CG2	1:C:391:ILE:O	2.61	0.47
1:A:398:GLU:CB	1:B:14:ALA:O	2.61	0.47
1:B:458:ASN:ND2	1:C:248:GLY:O	2.47	0.47
1:C:362:MET:H	1:C:363:ASN:HA	1.78	0.47
1:D:677:LEU:O	1:D:677:LEU:HD12	2.14	0.47
1:A:914:GLU:O	1:A:915:ASN:C	2.52	0.47
1:A:679:LYS:HG2	1:A:711:MET:SD	2.54	0.47
1:E:679:LYS:HG2	1:E:711:MET:SD	2.54	0.47
1:A:1053:ILE:O	1:A:1053:ILE:HG23	2.15	0.47
1:D:393:LEU:O	1:D:393:LEU:HD12	2.14	0.47
1:A:451:ARG:HD3	1:B:2:TRP:CE2	2.50	0.47
1:C:887:ILE:O	1:C:888:GLU:CB	2.61	0.47
1:B:27:LYS:H	1:B:28:PRO:HD3	1.79	0.47
1:B:755:ALA:N	1:B:756:PRO:CD	2.76	0.47
1:E:1053:ILE:HG23	1:E:1053:ILE:O	2.15	0.47
1:C:562:GLY:HA3	1:C:563:ALA:C	2.35	0.47
1:A:81:LYS:HA	1:A:82:ALA:C	2.34	0.47
1:E:81:LYS:HA	1:E:82:ALA:C	2.34	0.47
1:B:69:HIS:N	1:B:70:PRO:CD	2.78	0.47
1:B:393:LEU:HD12	1:B:393:LEU:O	2.14	0.47
1:B:1036:GLY:O	1:B:1038:THR:N	2.47	0.47
2:D:1101:SAH:H4'	2:D:1101:SAH:HG2	1.58	0.47
1:A:562:GLY:HA3	1:A:563:ALA:C	2.35	0.47
1:C:602:PHE:N	1:D:886:ARG:NH1	2.55	0.47
1:D:603:PRO:HG2	1:E:378:THR:CG2	2.39	0.47
1:B:677:LEU:O	1:B:677:LEU:HD12	2.14	0.47
1:C:1036:GLY:O	1:C:1038:THR:N	2.47	0.47
1:A:1036:GLY:O	1:A:1038:THR:N	2.47	0.47
1:E:1036:GLY:O	1:E:1038:THR:N	2.47	0.47
1:B:653:PRO:O	1:B:654:SER:C	2.53	0.47
1:B:1053:ILE:HG23	1:B:1053:ILE:O	2.14	0.47
1:C:567:PRO:O	1:C:568:ALA:HB3	2.15	0.47
1:D:562:GLY:HA3	1:D:563:ALA:C	2.35	0.47
1:E:605:ASP:O	1:E:606:LYS:HB2	2.13	0.47
1:B:562:GLY:HA3	1:B:563:ALA:C	2.35	0.47
1:A:864:ARG:O	1:A:864:ARG:HG2	2.15	0.47
1:C:451:ARG:HD3	1:D:2:TRP:CE2	2.49	0.47
1:E:391:ILE:CG2	1:E:391:ILE:O	2.61	0.47
1:C:255:ARG:O	1:C:256:VAL:CB	2.63	0.47
1:B:406:VAL:CB	1:B:407:GLU:HA	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ARG:O	1:D:256:VAL:CB	2.63	0.47
1:A:358:ILE:HB	1:A:359:PRO:C	2.35	0.47
1:B:307:HIS:HB3	1:B:308:ALA:CA	2.44	0.47
1:D:358:ILE:HB	1:D:359:PRO:C	2.35	0.47
1:E:358:ILE:HB	1:E:359:PRO:C	2.35	0.47
1:C:358:ILE:HB	1:C:359:PRO:C	2.34	0.47
1:C:69:HIS:N	1:C:70:PRO:CD	2.78	0.47
1:A:69:HIS:N	1:A:70:PRO:CD	2.78	0.47
1:D:310:ASP:O	1:D:313:ARG:N	2.47	0.47
1:D:278:LEU:C	1:D:278:LEU:HD12	2.35	0.47
1:C:1053:ILE:O	1:C:1053:ILE:HG23	2.15	0.47
1:D:406:VAL:HB	1:D:407:GLU:C	2.34	0.47
1:E:69:HIS:N	1:E:70:PRO:CD	2.78	0.47
1:C:914:GLU:O	1:C:915:ASN:C	2.52	0.47
1:D:567:PRO:O	1:D:568:ALA:HB3	2.15	0.47
1:C:310:ASP:O	1:C:313:ARG:N	2.48	0.47
1:D:812:VAL:HG13	1:D:813:PRO:HA	1.97	0.47
1:C:812:VAL:HG13	1:C:813:PRO:HA	1.97	0.47
1:A:393:LEU:HD12	1:A:393:LEU:O	2.14	0.47
1:D:458:ASN:ND2	1:E:248:GLY:O	2.48	0.47
1:A:307:HIS:HB3	1:A:308:ALA:CA	2.44	0.47
1:E:25:ILE:O	1:E:25:ILE:HD12	2.15	0.47
1:E:1021:THR:HB	1:E:1022:PRO:HD3	1.97	0.47
1:D:653:PRO:O	1:D:654:SER:C	2.53	0.47
1:D:562:GLY:CA	1:D:563:ALA:CB	2.91	0.47
1:E:212:HIS:CD2	1:E:234:GPL:HO3'	2.33	0.47
1:E:255:ARG:O	1:E:256:VAL:CB	2.63	0.47
1:B:310:ASP:O	1:B:313:ARG:N	2.48	0.47
1:E:653:PRO:O	1:E:654:SER:C	2.53	0.47
1:B:812:VAL:HG13	1:B:813:PRO:HA	1.97	0.47
1:B:864:ARG:O	1:B:864:ARG:HG2	2.15	0.46
1:B:597:ARG:NH2	1:C:373:ILE:HD13	2.30	0.46
1:E:904:PHE:N	2:E:1102:SAH:HN62	2.10	0.46
1:A:25:ILE:HD12	1:A:25:ILE:O	2.15	0.46
1:D:69:HIS:N	1:D:70:PRO:CD	2.78	0.46
1:E:278:LEU:HD12	1:E:278:LEU:C	2.35	0.46
1:C:653:PRO:O	1:C:654:SER:C	2.53	0.46
1:C:212:HIS:HE2	1:C:234:GPL:HO3'	1.57	0.46
1:E:406:VAL:HB	1:E:407:GLU:C	2.34	0.46
1:C:25:ILE:HD12	1:C:25:ILE:O	2.15	0.46
1:B:567:PRO:O	1:B:568:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HD12	1:B:278:LEU:C	2.35	0.46
1:B:25:ILE:O	1:B:25:ILE:HD12	2.15	0.46
1:A:1021:THR:HB	1:A:1022:PRO:HD3	1.97	0.46
1:B:1021:THR:HB	1:B:1022:PRO:HD3	1.97	0.46
1:E:567:PRO:O	1:E:568:ALA:HB3	2.15	0.46
1:A:278:LEU:HD12	1:A:278:LEU:C	2.35	0.46
1:C:278:LEU:HD12	1:C:278:LEU:C	2.35	0.46
1:C:562:GLY:CA	1:C:563:ALA:CB	2.91	0.46
1:C:604:ILE:CG2	1:D:890:LEU:HD12	2.35	0.46
1:E:864:ARG:HG2	1:E:864:ARG:O	2.15	0.46
1:D:25:ILE:O	1:D:25:ILE:HD12	2.15	0.46
1:B:358:ILE:HB	1:B:359:PRO:C	2.35	0.46
1:B:621:GLU:O	1:B:621:GLU:CD	2.54	0.46
1:C:621:GLU:O	1:C:621:GLU:CD	2.54	0.46
1:A:604:ILE:O	1:A:605:ASP:HB3	2.16	0.46
1:A:567:PRO:O	1:A:568:ALA:HB3	2.15	0.46
1:C:604:ILE:O	1:C:605:ASP:HB3	2.15	0.46
2:E:1101:SAH:H4'	2:E:1101:SAH:HG2	1.58	0.46
1:C:593:GLU:H	1:D:373:ILE:HA	1.79	0.46
1:D:904:PHE:N	2:D:1102:SAH:HN62	2.10	0.46
1:A:398:GLU:HG2	1:A:398:GLU:O	2.16	0.46
1:A:310:ASP:O	1:A:313:ARG:N	2.48	0.46
1:A:964:GLU:HG3	1:A:1000:GLU:HB2	1.98	0.46
1:E:812:VAL:HG13	1:E:813:PRO:HA	1.97	0.46
1:B:45:GLN:CB	1:B:46:ARG:CA	2.92	0.46
1:E:621:GLU:CD	1:E:621:GLU:O	2.54	0.46
1:D:864:ARG:O	1:D:864:ARG:HG2	2.15	0.46
1:C:398:GLU:O	1:C:398:GLU:HG2	2.16	0.46
1:C:286:ASN:O	1:C:287:VAL:HB	2.16	0.46
1:E:964:GLU:HG3	1:E:1000:GLU:HB2	1.98	0.46
1:D:964:GLU:HG3	1:D:1000:GLU:HB2	1.98	0.46
1:D:603:PRO:CG	1:E:378:THR:HG21	2.38	0.46
1:E:914:GLU:O	1:E:915:ASN:C	2.52	0.46
1:A:653:PRO:O	1:A:654:SER:C	2.53	0.46
1:D:647:LEU:C	1:D:647:LEU:HD23	2.36	0.46
1:D:1053:ILE:HG23	1:D:1053:ILE:O	2.15	0.46
1:E:562:GLY:HA3	1:E:563:ALA:C	2.35	0.46
1:A:44:SER:CA	1:A:46:ARG:HG3	2.25	0.46
1:A:255:ARG:O	1:A:256:VAL:CB	2.63	0.46
1:A:566:GLU:O	1:A:567:PRO:O	2.34	0.46
1:A:812:VAL:HG13	1:A:813:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:O	1:A:287:VAL:HB	2.16	0.46
1:E:647:LEU:HD23	1:E:647:LEU:C	2.36	0.46
1:A:647:LEU:HD23	1:A:647:LEU:C	2.37	0.46
1:C:864:ARG:O	1:C:864:ARG:HG2	2.15	0.46
1:B:391:ILE:O	1:B:391:ILE:CG2	2.61	0.46
1:D:31:VAL:HB	1:D:32:PRO:CD	2.46	0.46
1:D:566:GLU:O	1:D:567:PRO:O	2.34	0.46
1:E:310:ASP:O	1:E:313:ARG:N	2.48	0.46
1:B:45:GLN:N	1:B:46:ARG:CA	2.77	0.45
1:E:619:SER:HB2	1:E:620:TYR:CA	2.46	0.45
1:A:621:GLU:O	1:A:621:GLU:CD	2.54	0.45
1:B:398:GLU:O	1:B:398:GLU:HG2	2.16	0.45
1:D:74:LEU:HB2	1:D:75:PRO:HD3	1.98	0.45
1:B:31:VAL:HB	1:B:32:PRO:CD	2.46	0.45
1:C:566:GLU:O	1:C:567:PRO:O	2.34	0.45
1:B:647:LEU:C	1:B:647:LEU:HD23	2.36	0.45
1:E:604:ILE:O	1:E:605:ASP:HB3	2.16	0.45
1:E:619:SER:HB2	1:E:620:TYR:HA	1.98	0.45
1:C:307:HIS:HB3	1:C:308:ALA:HA	1.98	0.45
1:C:1021:THR:HB	1:C:1022:PRO:HD3	1.97	0.45
1:D:1021:THR:HB	1:D:1022:PRO:HD3	1.97	0.45
1:E:566:GLU:O	1:E:567:PRO:O	2.34	0.45
1:B:604:ILE:O	1:B:605:ASP:HB3	2.15	0.45
1:D:621:GLU:O	1:D:621:GLU:CD	2.54	0.45
1:A:458:ASN:ND2	1:B:248:GLY:O	2.50	0.45
1:B:964:GLU:HG3	1:B:1000:GLU:HB2	1.98	0.45
1:C:647:LEU:HD23	1:C:647:LEU:C	2.36	0.45
1:E:726:ILE:O	1:E:727:ILE:HB	2.16	0.45
1:D:604:ILE:CG2	1:E:890:LEU:HD12	2.34	0.45
1:B:619:SER:HB2	1:B:620:TYR:CA	2.47	0.45
1:B:883:PRO:HG3	2:B:1102:SAH:N7	2.29	0.45
1:B:307:HIS:HB3	1:B:308:ALA:HA	1.98	0.45
1:A:74:LEU:HB2	1:A:75:PRO:HD3	1.98	0.45
1:C:31:VAL:HB	1:C:32:PRO:CD	2.46	0.45
1:B:566:GLU:O	1:B:567:PRO:O	2.34	0.45
1:B:47:ARG:HG3	1:B:49:HIS:NE2	2.31	0.45
1:D:593:GLU:H	1:E:373:ILE:HA	1.81	0.45
1:A:2:TRP:CZ2	1:E:451:ARG:HD2	2.52	0.45
1:D:307:HIS:HB3	1:D:308:ALA:HA	1.98	0.45
1:A:69:HIS:CB	1:A:70:PRO:HD3	2.47	0.45
1:B:726:ILE:O	1:B:727:ILE:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:O	1:C:727:ILE:HB	2.16	0.45
1:C:619:SER:HB2	1:C:620:TYR:CA	2.47	0.45
1:C:604:ILE:O	1:C:605:ASP:CB	2.65	0.45
1:D:604:ILE:O	1:D:605:ASP:HB3	2.15	0.45
1:E:619:SER:HA	1:E:620:TYR:HA	1.83	0.45
1:C:451:ARG:NE	1:D:2:TRP:NE1	2.65	0.45
1:D:398:GLU:O	1:D:398:GLU:HG2	2.16	0.45
1:D:726:ILE:O	1:D:727:ILE:HB	2.17	0.45
1:B:562:GLY:CA	1:B:563:ALA:CB	2.91	0.45
2:A:1101:SAH:HG2	2:A:1101:SAH:H4'	1.58	0.45
1:A:562:GLY:CA	1:A:563:ALA:CB	2.91	0.45
1:A:619:SER:HB2	1:A:620:TYR:CA	2.47	0.45
1:E:74:LEU:HB2	1:E:75:PRO:HD3	1.97	0.45
1:E:69:HIS:CB	1:E:70:PRO:HD3	2.47	0.45
1:A:31:VAL:HB	1:A:32:PRO:CD	2.46	0.45
1:C:964:GLU:HG3	1:C:1000:GLU:HB2	1.98	0.45
1:D:619:SER:HB2	1:D:620:TYR:HA	1.98	0.45
1:A:619:SER:HB2	1:A:620:TYR:HA	1.99	0.45
1:C:46:ARG:CB	1:C:47:ARG:CA	2.74	0.45
2:E:1102:SAH:HG2	2:E:1102:SAH:H4'	1.77	0.45
1:C:451:ARG:HD2	1:D:2:TRP:CZ2	2.52	0.45
1:A:307:HIS:HB3	1:A:308:ALA:HA	1.98	0.45
1:C:74:LEU:HB2	1:C:75:PRO:HD3	1.97	0.45
1:E:31:VAL:HB	1:E:32:PRO:CD	2.46	0.45
1:E:286:ASN:O	1:E:287:VAL:HB	2.16	0.45
1:A:285:GLU:H	1:A:285:GLU:CD	2.20	0.45
1:A:864:ARG:HD2	1:E:607:ASN:N	2.31	0.45
1:C:607:ASN:N	1:D:864:ARG:HD2	2.31	0.45
1:B:27:LYS:N	1:B:28:PRO:HD3	2.32	0.45
1:E:146:PRO:O	1:E:147:GLN:CB	2.65	0.45
1:B:74:LEU:HB2	1:B:75:PRO:HD3	1.98	0.45
1:C:69:HIS:CB	1:C:70:PRO:HD3	2.47	0.45
1:D:671:VAL:O	1:D:671:VAL:HG12	2.17	0.45
1:B:697:ILE:HD12	1:B:697:ILE:C	2.37	0.45
1:D:27:LYS:N	1:D:28:PRO:HD3	2.32	0.45
1:C:27:LYS:N	1:C:28:PRO:HD3	2.32	0.45
1:B:69:HIS:CB	1:B:70:PRO:HD3	2.47	0.45
1:B:286:ASN:O	1:B:287:VAL:HB	2.16	0.45
1:B:603:PRO:CG	1:C:378:THR:HG21	2.39	0.44
1:B:451:ARG:HD3	1:C:2:TRP:CE2	2.52	0.44
1:E:398:GLU:HG2	1:E:398:GLU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:H	1:C:28:PRO:CD	2.30	0.44
1:E:285:GLU:H	1:E:285:GLU:CD	2.21	0.44
1:B:18:LYS:HB3	1:B:19:PRO:HD2	1.99	0.44
1:D:619:SER:HB2	1:D:620:TYR:CA	2.46	0.44
1:D:604:ILE:O	1:D:605:ASP:CB	2.65	0.44
1:B:619:SER:HB2	1:B:620:TYR:HA	1.99	0.44
1:C:601:PRO:CG	1:D:886:ARG:NH1	2.51	0.44
1:C:607:ASN:H	1:D:864:ARG:HD2	1.81	0.44
1:B:255:ARG:O	1:B:256:VAL:CB	2.63	0.44
1:A:248:GLY:O	1:E:458:ASN:ND2	2.50	0.44
1:C:458:ASN:ND2	1:D:248:GLY:O	2.51	0.44
1:B:27:LYS:H	1:B:28:PRO:CD	2.30	0.44
1:B:285:GLU:H	1:B:285:GLU:CD	2.21	0.44
1:B:604:ILE:O	1:B:605:ASP:CB	2.65	0.44
1:B:593:GLU:H	1:C:373:ILE:HA	1.81	0.44
1:A:2:TRP:CZ2	1:E:451:ARG:CD	3.00	0.44
1:E:697:ILE:C	1:E:697:ILE:HD12	2.38	0.44
1:B:671:VAL:HG12	1:B:671:VAL:O	2.18	0.44
1:B:44:SER:CB	1:B:46:ARG:HH21	2.29	0.44
1:B:44:SER:CA	1:B:46:ARG:NE	2.74	0.44
1:A:603:PRO:HG2	1:B:378:THR:CG2	2.38	0.44
1:A:2:TRP:NE1	1:E:451:ARG:NE	2.65	0.44
1:A:308:ALA:CB	1:A:309:ASN:HB2	2.48	0.44
1:D:27:LYS:H	1:D:28:PRO:CD	2.30	0.44
1:B:146:PRO:O	1:B:147:GLN:CB	2.65	0.44
1:B:853:GLU:HG3	1:B:854:ASN:H	1.82	0.44
1:A:18:LYS:HB3	1:A:19:PRO:HD2	1.99	0.44
1:E:618:ASN:O	2:E:1101:SAH:H5'2	2.03	0.44
1:A:886:ARG:NH1	1:E:602:PHE:C	2.59	0.44
1:A:406:VAL:CB	1:A:407:GLU:CA	2.88	0.44
1:A:78:TYR:N	1:A:79:PRO:CA	2.80	0.44
1:A:697:ILE:C	1:A:697:ILE:HD12	2.38	0.44
1:D:853:GLU:HG3	1:D:854:ASN:H	1.82	0.44
1:D:286:ASN:O	1:D:287:VAL:HB	2.16	0.44
1:A:617:ILE:O	1:A:618:ASN:HB2	2.18	0.44
1:D:451:ARG:HD3	1:E:2:TRP:CE2	2.51	0.44
1:C:406:VAL:CB	1:C:407:GLU:HA	2.37	0.44
1:D:80:SER:O	1:D:82:ALA:CB	2.66	0.44
1:E:307:HIS:HB3	1:E:308:ALA:HA	1.98	0.44
1:E:671:VAL:O	1:E:671:VAL:HG12	2.17	0.44
1:D:18:LYS:HB3	1:D:19:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ILE:O	1:D:618:ASN:HB2	2.18	0.44
1:D:602:PHE:N	1:E:886:ARG:NH1	2.56	0.44
1:A:593:GLU:H	1:B:373:ILE:HA	1.81	0.44
1:C:697:ILE:C	1:C:697:ILE:HD12	2.38	0.44
1:D:283:PHE:HA	1:D:284:THR:HA	1.81	0.44
1:A:726:ILE:O	1:A:727:ILE:HB	2.16	0.44
1:A:451:ARG:CD	1:B:2:TRP:CZ2	3.01	0.44
1:C:451:ARG:CD	1:D:2:TRP:CZ2	3.00	0.44
1:A:853:GLU:HG3	1:A:854:ASN:H	1.83	0.44
1:C:853:GLU:HG3	1:C:854:ASN:H	1.82	0.44
1:C:205:VAL:HG23	1:C:263:LEU:HB2	2.00	0.44
1:C:285:GLU:CD	1:C:285:GLU:H	2.20	0.44
1:A:671:VAL:HG12	1:A:671:VAL:O	2.17	0.44
1:C:18:LYS:HB3	1:C:19:PRO:HD2	2.00	0.44
1:A:883:PRO:HG3	2:A:1102:SAH:N7	2.29	0.44
1:C:406:VAL:CB	1:C:407:GLU:CA	2.88	0.44
1:A:724:MET:HB2	1:A:725:PRO:HD2	2.00	0.44
1:C:283:PHE:HA	1:C:284:THR:HA	1.81	0.44
1:C:358:ILE:HB	1:C:359:PRO:O	2.18	0.44
1:E:18:LYS:HB3	1:E:19:PRO:HD2	2.00	0.43
1:C:619:SER:HB2	1:C:620:TYR:HA	1.99	0.43
1:A:45:GLN:N	1:A:46:ARG:CA	2.79	0.43
1:B:724:MET:HB2	1:B:725:PRO:HD2	2.00	0.43
1:C:80:SER:O	1:C:82:ALA:CB	2.66	0.43
1:A:358:ILE:HB	1:A:359:PRO:O	2.18	0.43
1:D:697:ILE:HD12	1:D:697:ILE:C	2.37	0.43
1:D:285:GLU:H	1:D:285:GLU:CD	2.20	0.43
1:E:724:MET:HB2	1:E:725:PRO:HD2	2.00	0.43
1:B:362:MET:CB	1:B:363:ASN:HA	2.44	0.43
1:A:27:LYS:N	1:A:28:PRO:HD3	2.32	0.43
1:C:146:PRO:O	1:C:147:GLN:CB	2.65	0.43
1:C:604:ILE:HB	1:D:890:LEU:CD1	2.47	0.43
1:A:27:LYS:H	1:A:28:PRO:CD	2.30	0.43
1:A:739:ASN:O	1:A:740:THR:HB	2.19	0.43
1:C:671:VAL:HG12	1:C:671:VAL:O	2.17	0.43
1:A:283:PHE:HA	1:A:284:THR:HA	1.81	0.43
1:E:80:SER:O	1:E:82:ALA:CB	2.66	0.43
1:D:16:ASP:HA	1:D:17:PRO:HD3	1.91	0.43
1:C:617:ILE:O	1:C:618:ASN:HB2	2.18	0.43
1:A:618:ASN:O	2:A:1101:SAH:H5'2	2.03	0.43
1:A:602:PHE:N	1:B:886:ARG:NH1	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1102:SAH:H4'	2:C:1102:SAH:HG2	1.77	0.43
1:D:308:ALA:CB	1:D:309:ASN:HB2	2.48	0.43
1:B:739:ASN:O	1:B:740:THR:HB	2.19	0.43
1:C:58:GLN:O	1:C:59:TYR:HB2	2.19	0.43
1:E:604:ILE:O	1:E:605:ASP:CB	2.65	0.43
1:B:617:ILE:O	1:B:618:ASN:HB2	2.18	0.43
1:A:378:THR:CG2	1:E:603:PRO:HG2	2.37	0.43
1:A:451:ARG:HD2	1:B:2:TRP:CZ2	2.53	0.43
1:C:724:MET:HB2	1:C:725:PRO:HD2	2.00	0.43
1:D:254:ASP:O	1:D:255:ARG:HB2	2.19	0.43
1:D:458:ASN:CG	1:E:248:GLY:O	2.57	0.43
1:A:80:SER:O	1:A:82:ALA:CB	2.66	0.43
1:E:308:ALA:CB	1:E:309:ASN:HB2	2.47	0.43
1:E:358:ILE:HB	1:E:359:PRO:O	2.18	0.43
1:E:27:LYS:N	1:E:28:PRO:HD3	2.32	0.43
1:D:58:GLN:O	1:D:59:TYR:HB2	2.19	0.43
1:E:58:GLN:O	1:E:59:TYR:HB2	2.18	0.43
1:E:205:VAL:HG23	1:E:263:LEU:HB2	2.00	0.43
1:A:890:LEU:HD12	1:E:604:ILE:CG2	2.35	0.43
1:B:358:ILE:HB	1:B:359:PRO:O	2.18	0.43
1:A:604:ILE:O	1:A:605:ASP:CB	2.65	0.43
2:D:1102:SAH:HG2	2:D:1102:SAH:H4'	1.77	0.43
1:B:80:SER:O	1:B:82:ALA:CB	2.66	0.43
1:A:359:PRO:HD2	1:A:360:THR:H	1.84	0.43
1:D:146:PRO:O	1:D:147:GLN:CB	2.65	0.43
1:E:739:ASN:O	1:E:740:THR:HB	2.19	0.43
1:A:58:GLN:O	1:A:59:TYR:HB2	2.19	0.43
1:D:739:ASN:O	1:D:740:THR:HB	2.19	0.43
1:C:395:GLN:CD	1:D:112:ARG:CZ	2.87	0.43
1:B:607:ASN:N	1:C:864:ARG:HD2	2.34	0.43
1:D:724:MET:HB2	1:D:725:PRO:HD2	2.00	0.43
1:D:358:ILE:HB	1:D:359:PRO:O	2.18	0.43
1:D:802:THR:O	1:D:803:SER:CB	2.67	0.43
1:D:205:VAL:HG23	1:D:263:LEU:HB2	2.00	0.43
1:D:78:TYR:CB	1:D:79:PRO:CA	2.97	0.43
1:E:200:ARG:O	1:E:201:LYS:C	2.57	0.43
1:E:257:ILE:HD11	1:E:328:MET:HG2	2.01	0.43
1:B:212:HIS:CD2	1:B:234:GPL:HO3'	2.36	0.42
1:D:607:ASN:N	1:E:864:ARG:HD2	2.34	0.42
1:A:451:ARG:NE	1:B:2:TRP:NE1	2.67	0.42
1:D:200:ARG:O	1:D:201:LYS:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:853:GLU:HG3	1:E:854:ASN:H	1.83	0.42
1:C:801:ASN:O	1:C:802:THR:C	2.58	0.42
1:E:16:ASP:HA	1:E:17:PRO:HD3	1.91	0.42
1:A:257:ILE:HD11	1:A:328:MET:HG2	2.01	0.42
1:A:604:ILE:CG2	1:B:890:LEU:HD12	2.36	0.42
1:A:607:ASN:N	1:B:864:ARG:HD2	2.33	0.42
1:B:458:ASN:CG	1:C:248:GLY:O	2.57	0.42
1:A:695:THR:HA	1:A:696:PRO:HD3	1.85	0.42
1:B:257:ILE:HD11	1:B:328:MET:HG2	2.01	0.42
1:E:479:LYS:HD3	1:E:479:LYS:O	2.19	0.42
1:C:739:ASN:O	1:C:740:THR:HB	2.18	0.42
1:D:46:ARG:HB3	1:D:47:ARG:CB	2.49	0.42
1:E:617:ILE:O	1:E:618:ASN:HB2	2.18	0.42
1:E:791:ARG:CB	1:E:791:ARG:HH11	2.18	0.42
1:D:869:ILE:HG23	1:D:869:ILE:O	2.19	0.42
1:C:78:TYR:CB	1:C:79:PRO:CA	2.97	0.42
1:B:78:TYR:N	1:B:79:PRO:CA	2.80	0.42
1:D:359:PRO:CD	1:D:360:THR:H	2.33	0.42
1:C:802:THR:O	1:C:803:SER:CB	2.67	0.42
1:E:802:THR:O	1:E:803:SER:CB	2.67	0.42
1:A:112:ARG:CZ	1:E:395:GLN:CD	2.87	0.42
1:B:307:HIS:HB3	1:B:308:ALA:CB	2.50	0.42
1:D:359:PRO:HD2	1:D:360:THR:H	1.84	0.42
1:E:801:ASN:O	1:E:802:THR:C	2.58	0.42
1:B:58:GLN:O	1:B:59:TYR:HB2	2.18	0.42
1:B:801:ASN:O	1:B:802:THR:C	2.58	0.42
1:D:257:ILE:HD11	1:D:328:MET:HG2	2.01	0.42
1:D:45:GLN:N	1:D:46:ARG:CA	2.82	0.42
1:C:603:PRO:HG2	1:D:378:THR:CG2	2.38	0.42
1:D:391:ILE:CG2	1:D:391:ILE:O	2.61	0.42
1:E:359:PRO:HD2	1:E:360:THR:H	1.84	0.42
1:C:359:PRO:HD2	1:C:360:THR:H	1.84	0.42
1:E:467:SER:HB2	1:E:468:PRO:HD3	2.02	0.42
1:C:257:ILE:HD11	1:C:328:MET:HG2	2.01	0.42
1:C:479:LYS:HD3	1:C:479:LYS:O	2.20	0.42
1:B:602:PHE:N	1:C:886:ARG:NH1	2.56	0.42
1:B:607:ASN:H	1:C:864:ARG:HD3	1.85	0.42
1:D:451:ARG:NE	1:E:2:TRP:NE1	2.67	0.42
1:A:78:TYR:CB	1:A:79:PRO:CA	2.97	0.42
1:C:308:ALA:CB	1:C:309:ASN:HB2	2.47	0.42
1:B:359:PRO:HD2	1:B:360:THR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:O	1:A:201:LYS:C	2.57	0.42
1:B:205:VAL:HG23	1:B:263:LEU:HB2	2.00	0.42
1:E:45:GLN:N	1:E:46:ARG:CA	2.82	0.42
1:D:451:ARG:HD2	1:E:2:TRP:CZ2	2.55	0.42
1:E:254:ASP:O	1:E:255:ARG:HB2	2.19	0.42
1:B:78:TYR:CB	1:B:79:PRO:CA	2.97	0.42
1:E:359:PRO:CD	1:E:360:THR:H	2.33	0.42
1:C:467:SER:HB2	1:C:468:PRO:HD3	2.02	0.42
1:B:467:SER:HB2	1:B:468:PRO:HD3	2.02	0.42
1:D:479:LYS:O	1:D:479:LYS:HD3	2.19	0.42
1:A:307:HIS:HB3	1:A:308:ALA:CB	2.50	0.42
1:E:358:ILE:CB	1:E:359:PRO:CA	2.98	0.42
1:A:467:SER:HB2	1:A:468:PRO:HD3	2.02	0.42
1:D:467:SER:HB2	1:D:468:PRO:HD3	2.02	0.42
1:C:979:THR:O	1:C:980:ILE:CG1	2.68	0.42
1:A:205:VAL:HG23	1:A:263:LEU:HB2	2.00	0.42
2:B:1101:SAH:HG2	2:B:1101:SAH:H4'	1.58	0.42
1:A:359:PRO:CD	1:A:360:THR:H	2.33	0.42
1:D:69:HIS:CB	1:D:70:PRO:HD3	2.47	0.42
1:D:468:PRO:O	1:D:472:LEU:HG	2.20	0.42
1:B:619:SER:HA	1:B:620:TYR:HA	1.83	0.42
1:E:46:ARG:HB3	1:E:47:ARG:CB	2.49	0.42
1:B:603:PRO:HG2	1:C:378:THR:CG2	2.40	0.42
1:B:869:ILE:O	1:B:869:ILE:HG23	2.19	0.42
1:E:78:TYR:CB	1:E:79:PRO:CA	2.97	0.42
1:E:287:VAL:O	1:E:288:LEU:HB3	2.20	0.42
1:B:287:VAL:O	1:B:288:LEU:HB3	2.20	0.42
1:B:479:LYS:HD3	1:B:479:LYS:O	2.20	0.42
1:A:607:ASN:H	1:B:864:ARG:HD2	1.83	0.41
1:D:451:ARG:CD	1:E:2:TRP:CZ2	3.03	0.41
1:E:869:ILE:O	1:E:869:ILE:HG23	2.19	0.41
1:D:358:ILE:CB	1:D:359:PRO:CA	2.98	0.41
1:A:468:PRO:O	1:A:472:LEU:HG	2.20	0.41
1:C:200:ARG:O	1:C:201:LYS:C	2.57	0.41
1:D:801:ASN:O	1:D:802:THR:C	2.58	0.41
1:B:979:THR:O	1:B:980:ILE:CG1	2.68	0.41
1:A:801:ASN:O	1:A:802:THR:C	2.58	0.41
1:B:44:SER:CB	1:B:46:ARG:NH2	2.83	0.41
1:C:2:TRP:O	1:C:3:HIS:C	2.59	0.41
1:C:869:ILE:HG23	1:C:869:ILE:O	2.19	0.41
1:A:954:THR:O	1:A:956:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASN:CG	1:B:248:GLY:O	2.59	0.41
1:C:359:PRO:CD	1:C:360:THR:H	2.33	0.41
1:B:468:PRO:O	1:B:472:LEU:HG	2.20	0.41
1:A:479:LYS:HD3	1:A:479:LYS:O	2.20	0.41
1:A:395:GLN:CD	1:B:112:ARG:CZ	2.88	0.41
1:C:44:SER:OG	1:C:46:ARG:NE	2.53	0.41
1:B:2:TRP:O	1:B:3:HIS:C	2.59	0.41
1:A:2:TRP:O	1:A:3:HIS:C	2.59	0.41
1:C:468:PRO:O	1:C:472:LEU:HG	2.20	0.41
1:C:607:ASN:H	1:D:864:ARG:HD3	1.85	0.41
1:E:2:TRP:O	1:E:3:HIS:C	2.59	0.41
1:B:954:THR:O	1:B:956:CYS:HB2	2.21	0.41
1:C:287:VAL:O	1:C:288:LEU:HB3	2.20	0.41
1:E:979:THR:O	1:E:980:ILE:CG1	2.68	0.41
1:E:620:TYR:O	1:E:621:GLU:O	2.39	0.41
1:B:607:ASN:H	1:C:864:ARG:HD2	1.84	0.41
1:C:254:ASP:O	1:C:255:ARG:HB2	2.19	0.41
1:B:358:ILE:CB	1:B:359:PRO:CA	2.98	0.41
1:E:27:LYS:H	1:E:28:PRO:CD	2.30	0.41
1:A:802:THR:O	1:A:803:SER:CB	2.67	0.41
1:D:979:THR:O	1:D:980:ILE:CG1	2.68	0.41
1:A:979:THR:O	1:A:980:ILE:CG1	2.68	0.41
1:B:604:ILE:HB	1:C:890:LEU:CD1	2.50	0.41
1:D:620:TYR:O	1:D:621:GLU:O	2.39	0.41
1:B:593:GLU:HA	1:B:594:PRO:C	2.41	0.41
1:A:869:ILE:HG23	1:A:869:ILE:O	2.19	0.41
1:D:954:THR:O	1:D:956:CYS:HB2	2.21	0.41
1:C:954:THR:O	1:C:956:CYS:HB2	2.21	0.41
1:E:954:THR:O	1:E:956:CYS:HB2	2.21	0.41
2:C:1101:SAH:H4'	2:C:1101:SAH:HG2	1.58	0.41
1:C:307:HIS:HB3	1:C:308:ALA:CB	2.50	0.41
1:C:866:LEU:O	1:C:867:ALA:HB3	2.21	0.41
1:B:802:THR:O	1:B:803:SER:CB	2.67	0.41
1:A:248:GLY:O	1:E:458:ASN:CG	2.59	0.41
1:B:308:ALA:CB	1:B:309:ASN:HB2	2.48	0.41
1:B:200:ARG:O	1:B:201:LYS:C	2.57	0.41
1:A:287:VAL:O	1:A:288:LEU:HB3	2.21	0.41
2:C:1101:SAH:C2'	2:C:1101:SAH:N3	2.81	0.41
1:A:620:TYR:O	1:A:621:GLU:O	2.39	0.41
1:A:212:HIS:CD2	1:A:234:GPL:HO3'	2.34	0.41
1:C:44:SER:C	1:C:46:ARG:HG2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ARG:NE	1:C:2:TRP:NE1	2.69	0.41
1:E:696:PRO:C	1:E:697:ILE:O	2.59	0.41
1:B:695:THR:HA	1:B:696:PRO:HD3	1.85	0.41
1:D:307:HIS:HB3	1:D:308:ALA:CB	2.50	0.41
1:C:358:ILE:CB	1:C:359:PRO:CA	2.98	0.41
1:A:146:PRO:O	1:A:147:GLN:CB	2.65	0.41
1:B:866:LEU:O	1:B:867:ALA:HB3	2.21	0.41
1:E:468:PRO:O	1:E:472:LEU:HG	2.20	0.41
1:D:31:VAL:N	1:D:32:PRO:HD2	2.36	0.41
1:E:31:VAL:N	1:E:32:PRO:HD2	2.36	0.41
1:C:31:VAL:N	1:C:32:PRO:HD2	2.36	0.41
1:B:478:ILE:O	1:B:479:LYS:CB	2.69	0.41
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.91	0.41
1:C:592:VAL:CA	1:D:373:ILE:HG12	2.44	0.41
1:A:619:SER:CB	1:A:620:TYR:CA	3.00	0.40
1:E:593:GLU:HA	1:E:594:PRO:C	2.41	0.40
1:B:451:ARG:CD	1:C:2:TRP:CZ2	3.04	0.40
1:D:2:TRP:O	1:D:3:HIS:C	2.59	0.40
1:E:307:HIS:HB3	1:E:308:ALA:CB	2.50	0.40
1:C:478:ILE:O	1:C:479:LYS:CB	2.69	0.40
1:D:81:LYS:HA	1:D:82:ALA:CB	2.48	0.40
1:B:359:PRO:CD	1:B:360:THR:H	2.33	0.40
1:E:83:ILE:N	1:E:84:PRO:HD3	2.36	0.40
1:B:286:ASN:C	1:B:288:LEU:H	2.25	0.40
1:D:287:VAL:O	1:D:288:LEU:HB3	2.20	0.40
1:A:904:PHE:CA	2:A:1102:SAH:HN62	2.35	0.40
1:E:904:PHE:CA	2:E:1102:SAH:HN62	2.35	0.40
1:A:791:ARG:CB	1:A:791:ARG:HH11	2.18	0.40
1:B:451:ARG:HD2	1:C:2:TRP:CZ2	2.56	0.40
1:C:458:ASN:CG	1:D:248:GLY:O	2.59	0.40
1:C:696:PRO:O	1:C:697:ILE:HD12	2.22	0.40
1:B:31:VAL:N	1:B:32:PRO:HD2	2.36	0.40
1:A:31:VAL:N	1:A:32:PRO:HD2	2.36	0.40
1:D:395:GLN:CD	1:E:112:ARG:CZ	2.89	0.40
1:B:904:PHE:CA	2:B:1102:SAH:HN62	2.35	0.40
1:B:81:LYS:CA	1:B:82:ALA:CB	2.98	0.40
1:C:286:ASN:C	1:C:288:LEU:H	2.25	0.40
1:E:286:ASN:C	1:E:288:LEU:H	2.25	0.40
1:C:685:PRO:O	1:C:686:TYR:C	2.60	0.40
1:D:619:SER:CB	1:D:620:TYR:CA	2.99	0.40
1:B:619:SER:CB	1:B:620:TYR:CA	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:SER:CB	1:E:620:TYR:CA	2.99	0.40
1:D:866:LEU:O	1:D:867:ALA:HB3	2.21	0.40
1:A:478:ILE:O	1:A:479:LYS:CB	2.69	0.40
1:B:925:ILE:HD13	1:B:960:ILE:HG23	2.04	0.40
1:A:554:PRO:O	1:A:555:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1055/1058 (100%)	889 (84%)	122 (12%)	44 (4%)	3 36
1	B	1055/1058 (100%)	889 (84%)	122 (12%)	44 (4%)	3 36
1	C	1055/1058 (100%)	887 (84%)	123 (12%)	45 (4%)	3 35
1	D	1055/1058 (100%)	887 (84%)	124 (12%)	44 (4%)	3 36
1	E	1055/1058 (100%)	887 (84%)	124 (12%)	44 (4%)	3 36
All	All	5275/5290 (100%)	4439 (84%)	615 (12%)	221 (4%)	6 36

All (221) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	A	282	GLU
1	A	287	VAL
1	A	309	ASN
1	A	330	GLN
1	A	391	ILE
1	A	567	PRO
1	A	618	ASN
1	A	619	SER

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Mol	Chain	Res	Type
1	A	697	ILE
1	A	915	ASN
1	A	922	ILE
1	A	968	ILE
1	B	212	HIS
1	B	282	GLU
1	B	287	VAL
1	B	309	ASN
1	B	330	GLN
1	B	391	ILE
1	B	567	PRO
1	B	618	ASN
1	B	619	SER
1	B	697	ILE
1	B	915	ASN
1	B	922	ILE
1	B	968	ILE
1	C	212	HIS
1	C	282	GLU
1	C	287	VAL
1	C	309	ASN
1	C	330	GLN
1	C	391	ILE
1	C	567	PRO
1	C	618	ASN
1	C	619	SER
1	C	697	ILE
1	C	915	ASN
1	C	922	ILE
1	C	968	ILE
1	D	212	HIS
1	D	282	GLU
1	D	287	VAL
1	D	309	ASN
1	D	330	GLN
1	D	391	ILE
1	D	567	PRO
1	D	618	ASN
1	D	619	SER
1	D	697	ILE
1	D	915	ASN
1	D	922	ILE

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Mol	Chain	Res	Type
1	D	968	ILE
1	E	212	HIS
1	E	282	GLU
1	E	287	VAL
1	E	309	ASN
1	E	330	GLN
1	E	391	ILE
1	E	567	PRO
1	E	618	ASN
1	E	619	SER
1	E	697	ILE
1	E	915	ASN
1	E	922	ILE
1	E	968	ILE
1	A	82	ALA
1	A	255	ARG
1	A	606	LYS
1	A	621	GLU
1	A	726	ILE
1	A	832	GLU
1	A	870	SER
1	A	888	GLU
1	A	932	ALA
1	A	955	ASN
1	A	984	GLU
1	B	82	ALA
1	B	255	ARG
1	B	606	LYS
1	B	621	GLU
1	B	726	ILE
1	B	832	GLU
1	B	870	SER
1	B	888	GLU
1	B	932	ALA
1	B	955	ASN
1	B	984	GLU
1	C	82	ALA
1	C	255	ARG
1	C	606	LYS
1	C	621	GLU
1	C	726	ILE
1	C	832	GLU

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Mol	Chain	Res	Type
1	C	870	SER
1	C	888	GLU
1	C	932	ALA
1	C	955	ASN
1	C	984	GLU
1	D	82	ALA
1	D	255	ARG
1	D	606	LYS
1	D	621	GLU
1	D	726	ILE
1	D	832	GLU
1	D	870	SER
1	D	888	GLU
1	D	932	ALA
1	D	955	ASN
1	D	984	GLU
1	E	82	ALA
1	E	255	ARG
1	E	606	LYS
1	E	621	GLU
1	E	726	ILE
1	E	832	GLU
1	E	870	SER
1	E	888	GLU
1	E	932	ALA
1	E	955	ASN
1	E	984	GLU
1	A	81	LYS
1	A	203	THR
1	A	263	LEU
1	A	387	THR
1	A	395	GLN
1	A	513	PRO
1	A	654	SER
1	A	1037	SER
1	B	81	LYS
1	B	203	THR
1	B	263	LEU
1	B	387	THR
1	B	395	GLN
1	B	513	PRO
1	B	654	SER

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Mol	Chain	Res	Type
1	B	1037	SER
1	C	81	LYS
1	C	203	THR
1	C	263	LEU
1	C	387	THR
1	C	395	GLN
1	C	513	PRO
1	C	654	SER
1	C	1037	SER
1	D	81	LYS
1	D	203	THR
1	D	263	LEU
1	D	387	THR
1	D	395	GLN
1	D	513	PRO
1	D	654	SER
1	D	1037	SER
1	E	81	LYS
1	E	203	THR
1	E	263	LEU
1	E	387	THR
1	E	395	GLN
1	E	513	PRO
1	E	654	SER
1	E	1037	SER
1	A	496	CYS
1	A	602	PHE
1	A	727	ILE
1	A	802	THR
1	A	851	LEU
1	A	914	GLU
1	A	931	GLY
1	B	496	CYS
1	B	602	PHE
1	B	727	ILE
1	B	802	THR
1	B	851	LEU
1	B	914	GLU
1	B	931	GLY
1	C	496	CYS
1	C	602	PHE
1	C	727	ILE

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Mol	Chain	Res	Type
1	C	802	THR
1	C	851	LEU
1	C	914	GLU
1	C	931	GLY
1	D	496	CYS
1	D	602	PHE
1	D	727	ILE
1	D	802	THR
1	D	851	LEU
1	D	914	GLU
1	D	931	GLY
1	E	496	CYS
1	E	602	PHE
1	E	727	ILE
1	E	802	THR
1	E	851	LEU
1	E	914	GLU
1	E	931	GLY
1	A	187	PRO
1	A	672	PHE
1	A	684	ASN
1	A	699	ALA
1	B	187	PRO
1	B	672	PHE
1	B	684	ASN
1	B	699	ALA
1	C	187	PRO
1	C	672	PHE
1	C	684	ASN
1	C	699	ALA
1	D	187	PRO
1	D	672	PHE
1	D	684	ASN
1	D	699	ALA
1	E	187	PRO
1	E	672	PHE
1	E	684	ASN
1	E	699	ALA
1	C	821	ARG
1	A	411	ILE
1	B	411	ILE
1	C	411	ILE

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Mol	Chain	Res	Type
1	D	411	ILE
1	E	411	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	942/942 (100%)	934 (99%)	8 (1%)	86 94
1	B	942/942 (100%)	934 (99%)	8 (1%)	86 94
1	C	942/942 (100%)	934 (99%)	8 (1%)	86 94
1	D	942/942 (100%)	934 (99%)	8 (1%)	86 94
1	E	942/942 (100%)	934 (99%)	8 (1%)	86 94
All	All	4710/4710 (100%)	4670 (99%)	40 (1%)	87 94

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	GLU
1	A	393	LEU
1	A	481	ASP
1	A	525	ARG
1	A	620	TYR
1	A	763	LYS
1	A	791	ARG
1	A	1006	MET
1	B	282	GLU
1	B	393	LEU
1	B	481	ASP
1	B	525	ARG
1	B	620	TYR
1	B	763	LYS
1	B	791	ARG
1	B	1006	MET
1	C	282	GLU

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Mol	Chain	Res	Type
1	C	393	LEU
1	C	481	ASP
1	C	525	ARG
1	C	620	TYR
1	C	763	LYS
1	C	791	ARG
1	C	1006	MET
1	D	282	GLU
1	D	393	LEU
1	D	481	ASP
1	D	525	ARG
1	D	620	TYR
1	D	763	LYS
1	D	791	ARG
1	D	1006	MET
1	E	282	GLU
1	E	393	LEU
1	E	481	ASP
1	E	525	ARG
1	E	620	TYR
1	E	763	LYS
1	E	791	ARG
1	E	1006	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	45	GLN
1	B	21	GLN
1	B	45	GLN
1	C	45	GLN
1	D	21	GLN
1	D	45	GLN
1	E	45	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are 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	$\#\|Z\|>2$
1	GPL	A	234	1	28,34,35	2.80	4 (14%)	30,49,51	1.79	6 (20%)
1	GPL	B	234	1	28,34,35	2.80	4 (14%)	30,49,51	1.79	6 (20%)
1	GPL	C	234	1	28,34,35	2.81	4 (14%)	30,49,51	1.78	6 (20%)
1	GPL	D	234	1	28,34,35	2.79	4 (14%)	30,49,51	1.78	6 (20%)
1	GPL	E	234	1	28,34,35	2.81	4 (14%)	30,49,51	1.78	6 (20%)

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
1	GPL	A	234	1	-	0/14/37/39	0/3/3/3
1	GPL	B	234	1	-	0/14/37/39	0/3/3/3
1	GPL	C	234	1	-	0/14/37/39	0/3/3/3
1	GPL	D	234	1	-	0/14/37/39	0/3/3/3
1	GPL	E	234	1	-	0/14/37/39	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	234	GPL	P-O1P	2.04	1.48	1.46
1	D	234	GPL	P-O1P	2.07	1.48	1.46
1	A	234	GPL	P-O1P	2.08	1.48	1.46
1	C	234	GPL	P-O1P	2.16	1.48	1.46
1	B	234	GPL	P-O1P	2.18	1.48	1.46
1	D	234	GPL	C5-C4	3.10	1.47	1.40
1	C	234	GPL	C5-C4	3.10	1.47	1.40
1	B	234	GPL	C5-C4	3.12	1.47	1.40
1	E	234	GPL	C5-C4	3.14	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GPL	C5-C4	3.15	1.47	1.40
1	A	234	GPL	C6-C5	3.62	1.48	1.41
1	D	234	GPL	C6-C5	3.65	1.48	1.41
1	C	234	GPL	C6-C5	3.66	1.48	1.41
1	B	234	GPL	C6-C5	3.68	1.48	1.41
1	E	234	GPL	C6-C5	3.73	1.48	1.41
1	D	234	GPL	P-NZ	13.29	1.75	1.61
1	B	234	GPL	P-NZ	13.34	1.75	1.61
1	E	234	GPL	P-NZ	13.38	1.75	1.61
1	A	234	GPL	P-NZ	13.41	1.75	1.61
1	C	234	GPL	P-NZ	13.43	1.75	1.61

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	234	GPL	C5-C6-N1	-4.29	117.91	123.52
1	E	234	GPL	C5-C6-N1	-4.26	117.95	123.52
1	C	234	GPL	C5-C6-N1	-4.26	117.96	123.52
1	D	234	GPL	C5-C6-N1	-4.25	117.96	123.52
1	A	234	GPL	C5-C6-N1	-4.20	118.03	123.52
1	D	234	GPL	N3-C2-N1	-3.44	122.88	127.56
1	B	234	GPL	N3-C2-N1	-3.43	122.90	127.56
1	A	234	GPL	N3-C2-N1	-3.40	122.93	127.56
1	C	234	GPL	N3-C2-N1	-3.40	122.93	127.56
1	E	234	GPL	N3-C2-N1	-3.36	122.99	127.56
1	A	234	GPL	C6-C5-C4	-3.27	117.12	120.86
1	E	234	GPL	C6-C5-C4	-3.24	117.15	120.86
1	B	234	GPL	C6-C5-C4	-3.18	117.22	120.86
1	D	234	GPL	C6-C5-C4	-3.15	117.25	120.86
1	C	234	GPL	C6-C5-C4	-3.15	117.26	120.86
1	A	234	GPL	O-C-CA	-2.18	119.87	125.72
1	B	234	GPL	O-C-CA	-2.18	119.88	125.72
1	C	234	GPL	O-C-CA	-2.17	119.89	125.72
1	E	234	GPL	O-C-CA	-2.17	119.92	125.72
1	D	234	GPL	O-C-CA	-2.15	119.96	125.72
1	E	234	GPL	C4'-O4'-C1'	2.05	111.81	109.64
1	D	234	GPL	C4'-O4'-C1'	2.09	111.85	109.64
1	B	234	GPL	C4'-O4'-C1'	2.09	111.86	109.64
1	C	234	GPL	C4'-O4'-C1'	2.09	111.86	109.64
1	A	234	GPL	C4'-O4'-C1'	2.19	111.97	109.64
1	A	234	GPL	C6-N1-C2	5.49	122.32	115.88
1	C	234	GPL	C6-N1-C2	5.49	122.32	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	234	GPL	C6-N1-C2	5.50	122.33	115.88
1	E	234	GPL	C6-N1-C2	5.51	122.34	115.88
1	B	234	GPL	C6-N1-C2	5.53	122.36	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	234	GPL	8	0
1	B	234	GPL	9	0
1	C	234	GPL	8	0
1	D	234	GPL	8	0
1	E	234	GPL	8	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 ligands are 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	$\#\|Z\| > 2$
2	SAH	A	1101	-	22,28,28	1.12	2 (9%)	18,40,40	1.86	1 (5%)
2	SAH	A	1102	-	22,28,28	1.11	2 (9%)	18,40,40	2.01	2 (11%)
2	SAH	B	1101	-	22,28,28	1.11	2 (9%)	18,40,40	1.87	1 (5%)
2	SAH	B	1102	-	22,28,28	1.10	2 (9%)	18,40,40	1.98	2 (11%)
2	SAH	C	1101	-	22,28,28	1.12	2 (9%)	18,40,40	1.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SAH	C	1102	-	22,28,28	1.09	2 (9%)	18,40,40	1.97	1 (5%)
2	SAH	D	1101	-	22,28,28	1.12	2 (9%)	18,40,40	1.86	1 (5%)
2	SAH	D	1102	-	22,28,28	1.11	2 (9%)	18,40,40	1.99	1 (5%)
2	SAH	E	1101	-	22,28,28	1.11	2 (9%)	18,40,40	1.85	1 (5%)
2	SAH	E	1102	-	22,28,28	1.11	2 (9%)	18,40,40	1.98	1 (5%)

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
2	SAH	A	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	A	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	B	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	B	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	C	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	C	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	D	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	D	1102	-	-	0/7/31/31	0/3/3/3
2	SAH	E	1101	-	-	0/7/31/31	0/3/3/3
2	SAH	E	1102	-	-	0/7/31/31	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	SAH	C5'-SD	-2.45	1.76	1.81
2	E	1102	SAH	C5'-SD	-2.43	1.76	1.81
2	B	1102	SAH	C5'-SD	-2.41	1.76	1.81
2	D	1102	SAH	C5'-SD	-2.41	1.76	1.81
2	C	1102	SAH	C5'-SD	-2.41	1.76	1.81
2	D	1101	SAH	C5'-SD	-2.38	1.76	1.81
2	B	1101	SAH	C5'-SD	-2.37	1.76	1.81
2	A	1101	SAH	C5'-SD	-2.34	1.76	1.81
2	C	1101	SAH	C5'-SD	-2.34	1.76	1.81
2	E	1101	SAH	C5'-SD	-2.32	1.76	1.81
2	A	1102	SAH	C5-C4	2.88	1.47	1.40
2	C	1102	SAH	C5-C4	2.92	1.47	1.40
2	E	1102	SAH	C5-C4	2.93	1.47	1.40
2	B	1102	SAH	C5-C4	2.94	1.47	1.40
2	D	1102	SAH	C5-C4	2.96	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	SAH	C5-C4	3.04	1.47	1.40
2	E	1101	SAH	C5-C4	3.06	1.47	1.40
2	A	1101	SAH	C5-C4	3.08	1.47	1.40
2	D	1101	SAH	C5-C4	3.09	1.47	1.40
2	C	1101	SAH	C5-C4	3.15	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1102	SAH	N3-C2-N1	-6.95	123.41	128.87
2	D	1102	SAH	N3-C2-N1	-6.87	123.47	128.87
2	E	1102	SAH	N3-C2-N1	-6.83	123.50	128.87
2	B	1102	SAH	N3-C2-N1	-6.82	123.52	128.87
2	C	1102	SAH	N3-C2-N1	-6.81	123.52	128.87
2	C	1101	SAH	N3-C2-N1	-6.70	123.61	128.87
2	B	1101	SAH	N3-C2-N1	-6.61	123.68	128.87
2	D	1101	SAH	N3-C2-N1	-6.60	123.69	128.87
2	A	1101	SAH	N3-C2-N1	-6.57	123.71	128.87
2	E	1101	SAH	N3-C2-N1	-6.50	123.77	128.87
2	A	1102	SAH	O4'-C1'-N9	2.02	111.91	108.11
2	B	1102	SAH	O4'-C1'-N9	2.05	111.99	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 143 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	SAH	14	0
2	A	1102	SAH	14	0
2	B	1101	SAH	14	0
2	B	1102	SAH	15	0
2	C	1101	SAH	15	0
2	C	1102	SAH	14	0
2	D	1101	SAH	14	0
2	D	1102	SAH	14	0
2	E	1101	SAH	14	0
2	E	1102	SAH	15	0

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.