



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:23 PM UTC

PDB ID : 7N8Q / pdb_00007n8q
Title : Rhesusized RV305 DH677.3 Fab bound to Clade A/E 93TH057 HIV-1 gp120 core.
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2021-06-15
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

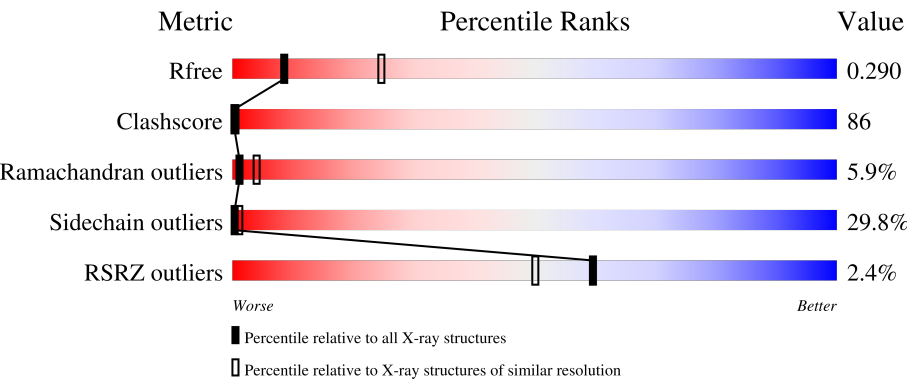
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	355	3% 21% 42% 22% • 13%
1	G	355	2% 21% 51% 21% • 5%
2	N	28	54% 36% 11%
3	C	228	4% 24% 54% 16% 5%
3	H	228	25% 50% 19% • •

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Mol	Chain	Length	Quality of chain
4	D	214	%22%55%21%•
4	L	214	2%21%52%23%••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	338	Total	C	N	O	S	0	0	0
			2646	1663	458	503	22			
1	A	308	Total	C	N	O	S	0	0	0
			2419	1516	417	465	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	42	VAL	-	expression tag	UNP A0A0M3KKW9
G	43	PRO	-	expression tag	UNP A0A0M3KKW9
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
A	42	VAL	-	expression tag	UNP A0A0M3KKW9
A	43	PRO	-	expression tag	UNP A0A0M3KKW9
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- Molecule 2 is a protein called M48U1 CD4 MIMETIC PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

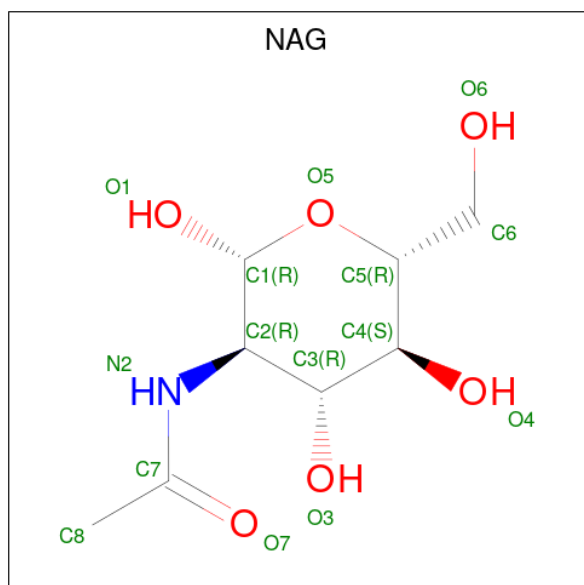
- Molecule 3 is a protein called Rhesusized DH677.3 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	218	Total	C	N	O	S	0	0	0
			1657	1049	277	323	8			
3	C	217	Total	C	N	O	S	0	0	0
			1651	1046	276	321	8			

- Molecule 4 is a protein called Rhesusized DH677.3 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1604	1008	266	325	5			
4	D	210	Total	C	N	O	S	0	0	0
			1604	1008	266	325	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

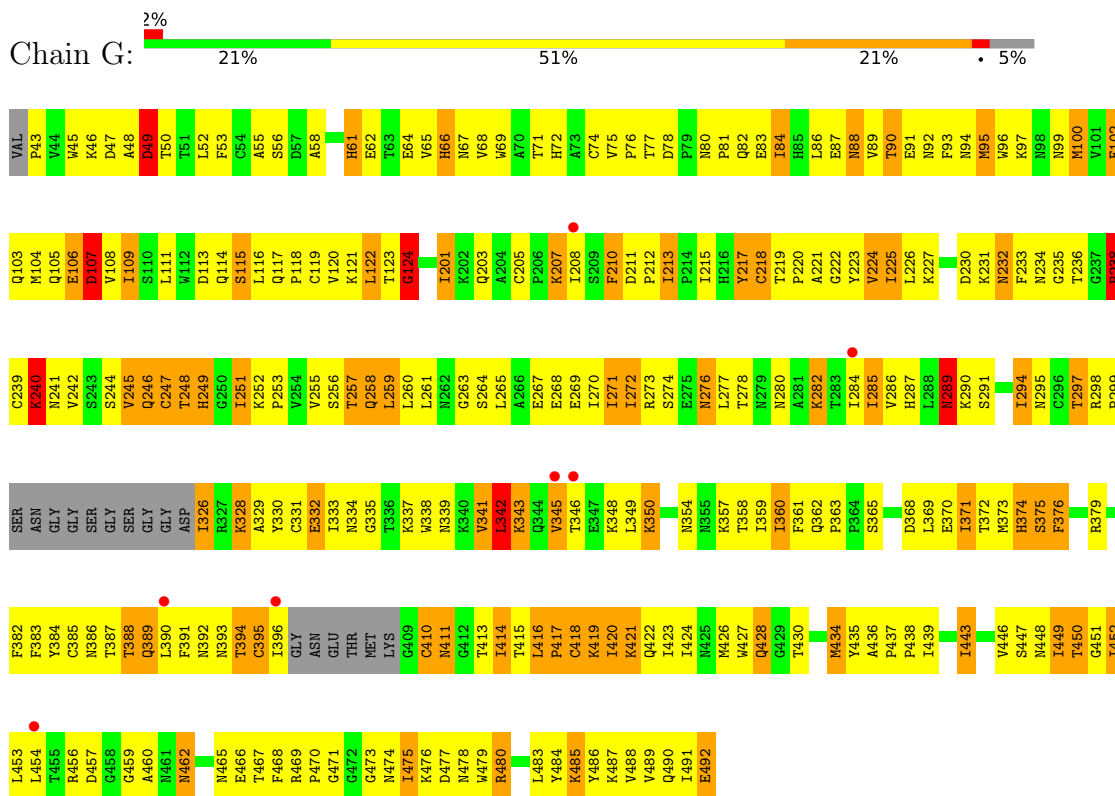
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	5	Total	O	0	0
			5	5		
6	H	3	Total	O	0	0
			3	3		
6	L	2	Total	O	0	0
			2	2		
6	A	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		

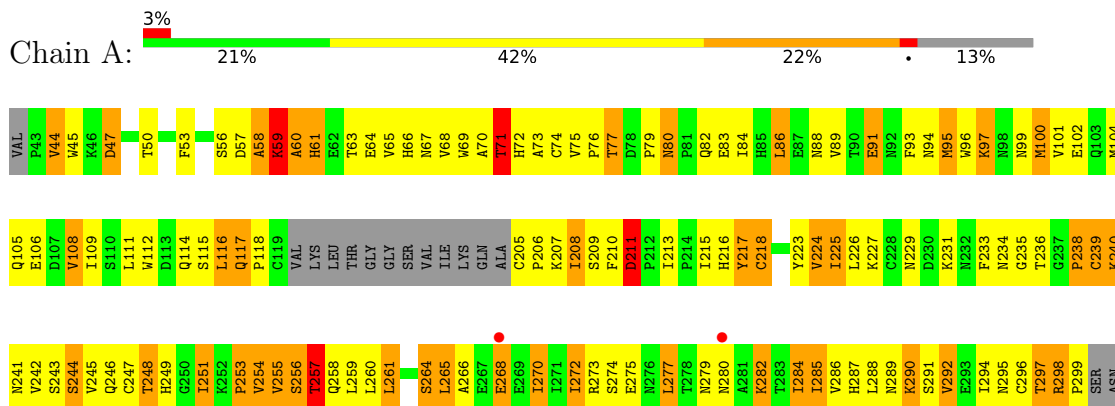
3 Residue-property plots

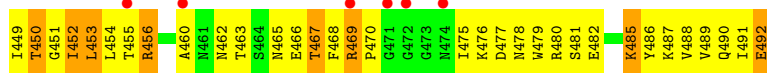
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core

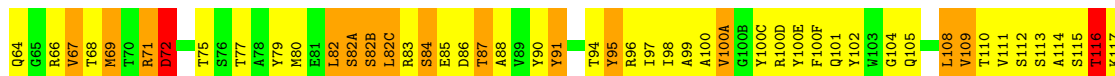




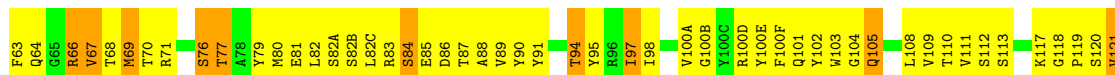
Chain N: 54% 36% 11%



Chain H: 25% 50% 19% . .

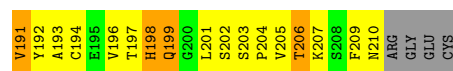
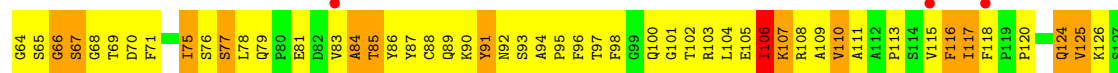
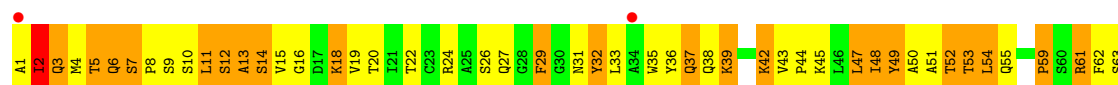
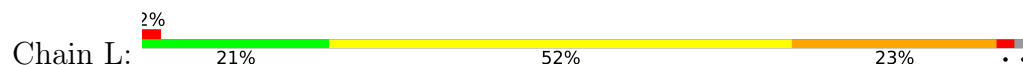


Chain C: 4% 24% 54% 16% 5%

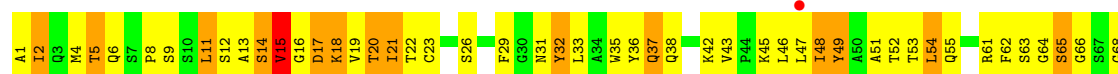




● Molecule 4: Rhesusized DH677.3 FAB LIGHT CHAIN



● Molecule 4: Rhesusized DH677.3 FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.18Å 82.66Å 111.90Å 90.00° 112.02° 90.00°	Depositor
Resolution (Å)	47.93 – 2.90 47.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.6 (47.93-2.90) 82.7 (47.93-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1	Depositor
R, R_{free}	0.255 , 0.296 0.255 , 0.290	Depositor DCC
R_{free} test set	1599 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12057	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, DPR, MPT, NH2, U2X

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.91	0/2468	1.37	9/3346 (0.3%)
1	G	0.94	1/2702 (0.0%)	1.36	12/3667 (0.3%)
2	N	0.76	0/176	0.97	0/231
3	C	0.96	0/1691	1.28	5/2304 (0.2%)
3	H	0.94	0/1697	1.29	8/2312 (0.3%)
4	D	0.99	0/1639	1.30	8/2231 (0.4%)
4	L	0.98	0/1639	1.38	10/2231 (0.4%)
All	All	0.95	1/12012 (0.0%)	1.33	52/16322 (0.3%)

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
2	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	124	GLY	C-N	9.70	1.47	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	32	TYR	CB-CA-C	-10.84	96.58	112.09
1	A	392	ASN	N-CA-C	-10.31	89.58	108.24
4	D	32	TYR	N-CA-C	-7.94	98.51	109.71
4	L	32	TYR	N-CA-C	-7.63	91.72	107.67
1	A	392	ASN	N-CA-CB	7.49	121.49	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	100(A)	VAL	CB-CA-C	-6.82	102.43	111.70
4	D	200	GLY	CA-C-N	6.66	134.26	121.54
4	D	200	GLY	C-N-CA	6.66	134.26	121.54
1	A	387	THR	CB-CA-C	-6.38	97.73	110.42
4	L	209	PHE	CA-CB-CG	6.20	120.00	113.80
4	D	32	TYR	CB-CA-C	-5.97	103.23	112.07
1	A	450	THR	CA-CB-OG1	-5.95	100.67	109.60
3	H	52(A)	PRO	N-CA-C	5.93	121.28	113.86
1	G	43	PRO	CA-N-CD	-5.90	103.74	112.00
1	G	49	ASP	CB-CA-C	5.90	120.00	109.38
1	G	107	ASP	CB-CA-C	-5.85	101.62	110.92
1	G	124	GLY	CA-C-N	-5.76	110.11	121.41
1	G	124	GLY	C-N-CA	-5.76	110.11	121.41
3	H	72	ASP	CA-C-N	5.75	127.99	120.28
3	H	72	ASP	C-N-CA	5.75	127.99	120.28
4	D	157	GLY	CA-C-O	-5.75	116.83	121.77
4	L	52	THR	CA-CB-OG1	-5.73	101.00	109.60
1	A	455	THR	CB-CA-C	-5.73	101.87	110.24
1	G	342	LEU	N-CA-C	-5.64	104.61	112.45
1	G	277	LEU	CA-C-N	5.63	127.76	120.44
1	G	277	LEU	C-N-CA	5.63	127.76	120.44
3	H	186	SER	N-CA-C	-5.62	98.83	110.80
1	G	289	ASN	CA-CB-CG	5.60	118.20	112.60
3	C	188	SER	CA-C-N	-5.55	113.62	122.29
3	C	188	SER	C-N-CA	-5.55	113.62	122.29
3	C	77	THR	CB-CA-C	-5.53	101.29	110.14
1	A	292	VAL	CA-C-N	5.51	128.67	120.90
1	A	292	VAL	C-N-CA	5.51	128.67	120.90
3	C	41	PRO	N-CA-CB	-5.47	97.50	103.25
4	L	1	ALA	CA-C-N	5.47	131.81	121.97
4	L	1	ALA	C-N-CA	5.47	131.81	121.97
1	G	217	TYR	CB-CA-C	5.43	118.61	109.48
4	D	127	SER	N-CA-C	-5.41	107.94	114.75
3	H	72	ASP	CB-CA-C	5.38	118.88	111.23
1	A	71	THR	N-CA-C	-5.38	106.56	113.01
4	L	201	LEU	CA-C-N	5.34	131.75	121.54
4	L	201	LEU	C-N-CA	5.34	131.75	121.54
4	D	208	SER	CA-C-N	5.30	131.66	121.54
4	D	208	SER	C-N-CA	5.30	131.66	121.54
1	G	470	PRO	CB-CA-C	-5.24	105.13	111.46
3	C	183	THR	CB-CA-C	5.22	118.25	109.48
1	A	217	TYR	CB-CA-C	5.19	118.73	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	197	ASN	CB-CA-C	5.16	118.64	109.72
1	G	246	GLN	N-CA-C	-5.08	107.21	113.41
4	L	116	PHE	CB-CA-C	-5.05	103.77	110.79
3	H	91	TYR	CB-CA-C	-5.01	99.46	109.33
4	L	61	ARG	N-CA-C	-5.00	107.03	113.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	1	MPT	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2419	0	2342	433	0
1	G	2646	0	2587	409	0
2	N	209	0	212	21	0
3	C	1651	0	1617	319	0
3	H	1657	0	1622	338	0
4	D	1604	0	1563	327	0
4	L	1604	0	1563	339	0
5	A	126	0	117	18	0
5	G	126	0	117	15	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	G	5	0	0	0	0
6	H	3	0	0	0	0
6	L	2	0	0	0	0
All	All	12057	0	11740	2054	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 86.

All (2054) 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:G:259:LEU:HD12	1:G:374:HIS:CD2	1.31	1.58
3:H:163:VAL:CG2	3:H:182:VAL:HG13	1.31	1.57
3:C:87:THR:CG2	3:C:111:VAL:HG22	1.29	1.56
1:G:116:LEU:HD11	1:G:210:PHE:CE2	1.39	1.55
4:D:142:ARG:HB2	4:D:173:TYR:CD2	1.47	1.49
3:C:181:VAL:HG21	4:D:135:LEU:CD1	1.48	1.43
1:G:226:LEU:CD1	1:G:489:VAL:HG21	1.51	1.40
3:H:101:GLN:NE2	3:H:102:TYR:CE2	1.90	1.38
1:G:116:LEU:HD11	1:G:210:PHE:CZ	1.63	1.33
1:A:299:PRO:CG	1:A:442:LYS:HD2	1.56	1.33
3:C:101:GLN:NE2	3:C:102:TYR:CE2	1.97	1.33
4:D:19:VAL:CG2	4:D:75:ILE:HG13	1.58	1.32
1:A:387:THR:HA	1:A:416:LEU:CD2	1.59	1.31
1:G:350:LYS:HB3	1:G:359:ILE:CD1	1.58	1.31
1:G:382:PHE:HE2	1:G:435:TYR:CD1	1.47	1.31
1:A:95:MET:CE	1:A:235:GLY:HA3	1.61	1.30
3:C:122:PHE:CD2	4:D:124:GLN:HG3	1.65	1.29
3:C:59:TYR:CE1	3:C:69:MET:HE3	1.68	1.29
4:D:119:PRO:HB3	4:D:207:LYS:NZ	1.46	1.28
1:G:226:LEU:HD12	1:G:489:VAL:CG2	1.65	1.27
4:L:38:GLN:O	4:L:84:ALA:HB1	1.25	1.26
4:L:29:PHE:HB2	4:L:92:ASN:ND2	1.50	1.26
1:G:259:LEU:CD1	1:G:374:HIS:HD2	1.50	1.25
3:C:38:ARG:HD2	3:C:90:TYR:CE1	1.72	1.25
3:H:138:LEU:HD12	3:H:211:VAL:CG2	1.63	1.25
1:A:58:ALA:HB1	1:A:67:ASN:O	1.32	1.24
1:G:384:TYR:CE2	1:G:421:LYS:HG3	1.71	1.23
1:A:65:VAL:CG2	1:A:208:ILE:HB	1.67	1.23
1:A:277:LEU:HD21	1:A:352:HIS:CD2	1.73	1.22
3:C:121:VAL:CG2	3:C:207:VAL:HG11	1.69	1.22
1:G:66:HIS:ND1	1:G:212:PRO:HA	1.52	1.22
1:G:446:VAL:HG21	5:G:506:NAG:H82	1.22	1.22
4:D:150:VAL:HG13	4:D:192:TYR:CE1	1.75	1.21
1:G:382:PHE:CE2	1:G:435:TYR:CD1	2.30	1.20
1:A:386:ASN:O	1:A:416:LEU:HD23	1.42	1.19
1:A:386:ASN:OD1	1:A:388:THR:HG22	1.37	1.19
3:C:17:SER:H	3:C:82(C):LEU:CD1	1.57	1.18
1:A:95:MET:HE2	1:A:235:GLY:HA3	1.24	1.18
4:L:87:TYR:HE1	4:L:101:GLY:HA3	1.02	1.18
3:H:154:TRP:CD1	3:H:182:VAL:HG21	1.79	1.17
1:A:277:LEU:CD2	1:A:352:HIS:CD2	2.27	1.17
1:A:335:GLY:HA3	1:A:414:ILE:CD1	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:PHE:HB2	4:D:92:ASN:ND2	1.57	1.17
1:G:382:PHE:CE2	1:G:435:TYR:CE1	2.33	1.17
4:L:87:TYR:CE1	4:L:101:GLY:HA3	1.79	1.17
3:H:154:TRP:NE1	3:H:182:VAL:HG21	1.59	1.16
1:A:299:PRO:CB	1:A:442:LYS:HD2	1.76	1.16
3:C:87:THR:CG2	3:C:111:VAL:CG2	2.24	1.16
4:D:150:VAL:CG1	4:D:192:TYR:CE1	2.28	1.16
1:G:66:HIS:CE1	1:G:212:PRO:HA	1.80	1.16
3:H:163:VAL:CG2	3:H:182:VAL:CG1	2.24	1.15
4:L:136:LEU:HD21	4:L:196:VAL:CG2	1.75	1.15
4:L:155:LYS:NZ	4:L:181:LEU:HD21	1.60	1.15
4:D:37:GLN:NE2	4:D:86:TYR:HE1	1.44	1.15
4:D:19:VAL:HG22	4:D:75:ILE:HB	1.18	1.15
3:C:137:ALA:HB3	4:D:116:PHE:CD2	1.81	1.14
3:C:112:SER:CB	3:C:146:PHE:CZ	2.30	1.14
4:D:33:LEU:HD22	4:D:71:PHE:CD1	1.82	1.14
1:G:90:THR:HB	1:G:240:LYS:HA	1.24	1.14
4:D:19:VAL:CG2	4:D:75:ILE:CG1	2.25	1.14
3:H:181:VAL:HG21	4:L:135:LEU:CD2	1.77	1.13
4:L:136:LEU:HD21	4:L:196:VAL:HG22	1.14	1.13
1:A:359:ILE:HG21	1:A:468:PHE:CE2	1.83	1.13
3:C:83:ARG:O	3:C:111:VAL:HG21	1.47	1.13
3:H:66:ARG:HD3	3:H:82(B):SER:OG	1.42	1.13
1:G:117:GLN:NE2	1:G:203:GLN:HG3	1.64	1.13
1:G:376:PHE:HE1	1:G:383:PHE:CB	1.62	1.13
4:L:87:TYR:CD1	4:L:101:GLY:HA2	1.85	1.12
1:A:225:ILE:HG22	1:A:245:VAL:HG22	1.30	1.12
4:D:37:GLN:HB2	4:D:86:TYR:CD1	1.83	1.12
3:H:181:VAL:CG2	4:L:135:LEU:HD22	1.79	1.12
4:L:150:VAL:HG22	4:L:192:TYR:HD2	1.07	1.12
1:A:377:ASN:HB2	1:A:382:PHE:CE2	1.85	1.11
1:G:390:LEU:CD1	1:G:416:LEU:HD21	1.79	1.11
3:C:38:ARG:CD	3:C:90:TYR:HE1	1.63	1.11
1:G:373:MET:HE1	1:G:386:ASN:HB2	1.12	1.11
3:H:17:SER:OG	3:H:82(A):SER:HA	1.48	1.11
1:G:84:ILE:HD12	3:H:100(A):VAL:HG13	1.26	1.11
1:G:116:LEU:CD1	1:G:210:PHE:CE2	2.33	1.11
1:G:384:TYR:CD2	1:G:421:LYS:HG3	1.84	1.10
4:L:132:VAL:HG12	4:L:148:TRP:CH2	1.86	1.10
1:A:359:ILE:CG2	1:A:468:PHE:CE2	2.34	1.10
3:C:112:SER:HB2	3:C:146:PHE:HZ	1.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:163:VAL:HG23	3:H:182:VAL:HG13	1.34	1.09
1:A:44:VAL:HG11	1:A:492:GLU:HB3	1.29	1.09
3:C:87:THR:HG21	3:C:111:VAL:HG22	1.22	1.09
1:G:259:LEU:CD1	1:G:374:HIS:CD2	2.27	1.09
3:H:154:TRP:HZ3	3:H:195:VAL:C	1.60	1.09
3:H:83:ARG:HG2	3:H:85:GLU:OE1	1.52	1.09
3:H:163:VAL:HG22	3:H:182:VAL:HG13	1.24	1.09
4:L:19:VAL:CG2	4:L:75:ILE:CG2	2.29	1.09
1:A:259:LEU:HD22	1:A:449:ILE:HD13	1.26	1.09
3:C:38:ARG:HD2	3:C:90:TYR:HE1	0.95	1.09
4:D:62:PHE:CE2	4:D:75:ILE:CD1	2.36	1.09
1:G:223:TYR:CE2	1:G:490:GLN:HB2	1.89	1.08
3:H:154:TRP:CD1	3:H:182:VAL:CG2	2.35	1.08
1:A:277:LEU:HD21	1:A:352:HIS:HD2	0.92	1.08
3:H:55:GLY:N	3:H:71:ARG:HH11	1.50	1.08
4:D:150:VAL:HG13	4:D:192:TYR:CD1	1.88	1.08
4:D:19:VAL:HG22	4:D:75:ILE:CB	1.84	1.08
4:L:33:LEU:HD23	4:L:71:PHE:CG	1.89	1.07
1:G:338:TRP:CD1	1:G:390:LEU:HD23	1.90	1.07
3:H:154:TRP:CH2	3:H:196:CYS:HB3	1.87	1.07
1:A:353:PHE:CZ	1:A:456:ARG:NH1	2.23	1.07
4:D:29:PHE:HB2	4:D:92:ASN:HD22	0.90	1.07
4:L:7:SER:HB3	4:L:8:PRO:HD3	1.08	1.07
4:L:52:THR:HG22	4:L:64:GLY:O	1.53	1.07
1:G:226:LEU:HD12	1:G:489:VAL:HG21	1.14	1.06
4:L:7:SER:HB3	4:L:8:PRO:CD	1.82	1.06
1:A:60:ALA:HB2	1:A:71:THR:HB	1.36	1.06
4:L:19:VAL:HG22	4:L:75:ILE:CG2	1.86	1.06
3:C:87:THR:HG22	3:C:111:VAL:HG22	1.29	1.06
3:C:181:VAL:CG2	4:D:135:LEU:CD1	2.32	1.06
3:H:154:TRP:CZ3	3:H:196:CYS:N	2.24	1.06
4:D:2:ILE:HD11	4:D:90:LYS:HD2	1.16	1.06
4:D:142:ARG:CB	4:D:173:TYR:CD2	2.38	1.06
1:G:383:PHE:CE2	1:G:420:ILE:HD11	1.90	1.06
2:N:5:PHE:CE1	2:N:9:ARG:NH1	2.23	1.05
4:L:19:VAL:HG23	4:L:75:ILE:HG22	1.39	1.05
4:L:37:GLN:NE2	4:L:86:TYR:HE1	1.55	1.05
1:A:359:ILE:HG21	1:A:468:PHE:HE2	1.08	1.05
1:A:387:THR:HA	1:A:416:LEU:HD22	1.35	1.05
4:D:11:LEU:HB3	4:D:104:LEU:CD1	1.87	1.05
4:D:37:GLN:NE2	4:D:86:TYR:CE1	2.21	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:142:ARG:HB2	4:D:173:TYR:CE2	1.91	1.05
4:L:31:ASN:ND2	4:L:67:SER:HB2	1.72	1.04
3:C:112:SER:HB2	3:C:146:PHE:CZ	1.91	1.04
3:H:34:ILE:HG22	3:H:51:MET:HG2	1.39	1.04
3:H:100(F):PHE:CE1	4:L:89:GLN:NE2	2.24	1.04
1:A:60:ALA:HB2	1:A:71:THR:CG2	1.87	1.04
4:L:157:GLY:C	4:L:158:ASN:HD22	1.64	1.04
1:A:376:PHE:HE1	1:A:383:PHE:CB	1.71	1.04
1:G:383:PHE:CE2	1:G:420:ILE:CD1	2.40	1.03
4:L:19:VAL:CG2	4:L:75:ILE:HG22	1.87	1.03
3:C:59:TYR:HE1	3:C:69:MET:HE3	0.90	1.03
3:C:154:TRP:CZ3	3:C:196:CYS:HB3	1.92	1.03
3:C:181:VAL:HG21	4:D:135:LEU:HD12	1.08	1.03
1:G:116:LEU:CD1	1:G:210:PHE:CZ	2.40	1.03
1:G:376:PHE:HE1	1:G:383:PHE:HB3	1.21	1.03
3:C:84:SER:HA	3:C:111:VAL:HG21	1.39	1.03
3:H:138:LEU:HD12	3:H:211:VAL:HG21	1.03	1.03
1:A:299:PRO:HG3	1:A:442:LYS:HD2	1.06	1.03
4:L:150:VAL:HG22	4:L:192:TYR:CD2	1.91	1.03
1:A:226:LEU:HD12	1:A:489:VAL:HG21	1.36	1.03
1:A:390:LEU:HD21	1:A:416:LEU:HD11	1.40	1.03
4:D:19:VAL:HG21	4:D:75:ILE:HG13	1.07	1.03
3:C:17:SER:HA	3:C:82(C):LEU:HD11	1.41	1.02
1:A:387:THR:HG22	1:A:390:LEU:HD12	1.41	1.02
1:G:226:LEU:HD11	1:G:489:VAL:HG21	1.35	1.02
3:H:138:LEU:CD1	3:H:211:VAL:CG2	2.37	1.02
3:H:198:VAL:O	3:H:206:LYS:HA	1.59	1.02
3:H:55:GLY:H	3:H:71:ARG:NH1	1.57	1.01
4:L:87:TYR:CE1	4:L:101:GLY:CA	2.43	1.01
3:C:59:TYR:CE1	3:C:69:MET:CE	2.42	1.01
3:H:154:TRP:HZ3	3:H:196:CYS:N	1.57	1.01
1:A:299:PRO:HG3	1:A:442:LYS:CD	1.89	1.01
1:G:350:LYS:HB3	1:G:359:ILE:HD12	1.40	1.01
1:G:350:LYS:CB	1:G:359:ILE:CD1	2.38	1.01
3:H:152:VAL:HG11	3:H:165:THR:CB	1.89	1.01
3:H:154:TRP:NE1	3:H:182:VAL:CG2	2.22	1.01
1:A:299:PRO:HB3	1:A:442:LYS:CD	1.90	1.01
4:L:37:GLN:HB2	4:L:86:TYR:CD1	1.96	1.00
4:L:85:THR:CG2	4:L:102:THR:C	2.34	1.00
3:C:84:SER:HA	3:C:111:VAL:CG2	1.89	1.00
1:A:65:VAL:HG21	1:A:208:ILE:HB	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:VAL:HG21	3:C:207:VAL:HG11	1.40	1.00
1:G:95:MET:O	1:G:480:ARG:HD3	1.60	1.00
1:A:65:VAL:HG23	1:A:208:ILE:HB	1.40	1.00
1:A:387:THR:CG2	1:A:390:LEU:HD12	1.90	1.00
1:G:120:VAL:HB	1:G:434:MET:HE2	1.42	1.00
1:G:223:TYR:HE2	1:G:490:GLN:HB2	1.26	0.99
3:H:181:VAL:HG21	4:L:135:LEU:HD22	1.01	0.99
3:C:121:VAL:HG21	3:C:207:VAL:CG1	1.92	0.99
4:L:6:GLN:HE22	4:L:87:TYR:HA	1.28	0.99
3:H:152:VAL:HG11	3:H:165:THR:HB	1.45	0.99
1:G:349:LEU:HD21	1:G:468:PHE:CE1	1.96	0.98
4:L:33:LEU:CD2	4:L:71:PHE:CG	2.45	0.98
1:A:44:VAL:CG1	1:A:492:GLU:HB3	1.91	0.98
1:A:299:PRO:CB	1:A:442:LYS:CD	2.40	0.98
3:H:154:TRP:CZ3	3:H:196:CYS:CA	2.47	0.98
4:L:85:THR:HG23	4:L:103:ARG:CA	1.94	0.98
1:A:340:LYS:O	1:A:343:LYS:HD2	1.61	0.98
1:G:376:PHE:CE1	1:G:383:PHE:CB	2.45	0.98
4:D:11:LEU:HB3	4:D:104:LEU:HD12	1.41	0.98
1:A:100:MET:HE1	1:A:486:TYR:HB3	1.45	0.98
4:D:48:ILE:HG12	4:D:54:LEU:HD12	1.44	0.97
1:G:362:GLN:HG3	1:G:363:PRO:CD	1.94	0.97
3:C:59:TYR:HE1	3:C:69:MET:CE	1.77	0.97
4:D:37:GLN:HB2	4:D:86:TYR:CE1	2.00	0.97
1:A:60:ALA:HB2	1:A:71:THR:CB	1.94	0.97
1:A:65:VAL:HG21	1:A:208:ILE:CB	1.94	0.96
4:D:62:PHE:CD2	4:D:75:ILE:CD1	2.47	0.96
4:D:150:VAL:HG11	4:D:192:TYR:HE1	1.29	0.96
4:L:132:VAL:HG12	4:L:148:TRP:HH2	1.27	0.96
3:C:35:ASN:CG	3:C:47:TRP:HE1	1.72	0.96
4:D:62:PHE:CE2	4:D:75:ILE:HD11	1.98	0.96
1:G:66:HIS:CE1	1:G:212:PRO:CA	2.48	0.96
4:L:29:PHE:HB2	4:L:92:ASN:HD22	1.23	0.96
1:A:387:THR:CA	1:A:416:LEU:CD2	2.43	0.96
1:A:359:ILE:CG2	1:A:468:PHE:HE2	1.76	0.96
1:G:390:LEU:HD11	1:G:416:LEU:HD21	1.47	0.96
4:D:62:PHE:CD2	4:D:75:ILE:HD13	2.01	0.96
1:A:376:PHE:CE1	1:A:383:PHE:CB	2.49	0.96
4:L:48:ILE:CD1	4:L:64:GLY:N	2.28	0.95
3:H:100(F):PHE:HE1	4:L:89:GLN:NE2	1.61	0.95
1:A:66:HIS:CE1	1:A:210:PHE:CE1	2.53	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:SER:H	3:C:82(C):LEU:HD13	1.29	0.95
4:D:85:THR:CG2	4:D:103:ARG:HG3	1.96	0.95
3:H:101:GLN:NE2	3:H:102:TYR:CZ	2.34	0.95
3:H:114:ALA:CB	3:H:146:PHE:CD1	2.49	0.95
3:H:184:VAL:HB	3:H:185:PRO:HD2	1.49	0.95
4:L:186:TYR:CE1	4:L:192:TYR:HE1	1.84	0.95
3:C:181:VAL:CG2	4:D:135:LEU:HD12	1.94	0.95
2:N:5:PHE:CZ	2:N:9:ARG:HD3	2.01	0.95
3:H:114:ALA:HB3	3:H:146:PHE:CD1	2.00	0.95
3:C:17:SER:CA	3:C:82(C):LEU:HD11	1.97	0.95
1:A:94:ASN:HD21	1:A:97:LYS:HG2	1.32	0.95
1:A:95:MET:HE2	1:A:235:GLY:CA	1.96	0.95
1:G:390:LEU:HD12	1:G:416:LEU:CD2	1.96	0.94
1:A:207:LYS:CG	1:A:208:ILE:H	1.79	0.94
1:A:364:PRO:HB3	1:A:372:THR:HG22	1.46	0.94
1:A:258:GLN:OE1	1:A:470:PRO:HB2	1.65	0.94
3:C:38:ARG:CB	3:C:90:TYR:CD1	2.50	0.94
4:D:119:PRO:HB3	4:D:207:LYS:HZ1	1.14	0.94
1:A:66:HIS:HE1	1:A:210:PHE:CE1	1.84	0.94
1:A:44:VAL:CG1	1:A:492:GLU:CB	2.44	0.94
3:C:112:SER:CB	3:C:146:PHE:HZ	1.75	0.94
3:H:96:ARG:HD3	3:H:98:ILE:HG21	1.50	0.94
4:L:108:ARG:HG3	4:L:109:ALA:H	1.32	0.94
4:D:4:MET:HE2	4:D:97:THR:HG22	1.46	0.94
1:A:329:ALA:HA	1:A:418:CYS:O	1.68	0.94
1:A:335:GLY:HA3	1:A:414:ILE:HD12	1.50	0.94
3:C:181:VAL:HG21	4:D:135:LEU:HD11	1.50	0.94
3:C:150:VAL:HG23	3:C:199:ASN:O	1.68	0.94
1:G:84:ILE:CD1	3:H:100(A):VAL:HG13	1.96	0.93
4:L:85:THR:HG22	4:L:102:THR:C	1.93	0.93
4:D:142:ARG:CB	4:D:173:TYR:CE2	2.49	0.93
3:H:163:VAL:HG21	3:H:182:VAL:HG13	1.46	0.93
1:A:112:TRP:O	1:A:116:LEU:HD12	1.69	0.93
3:C:87:THR:HG23	3:C:111:VAL:HG22	1.48	0.93
4:D:37:GLN:HB2	4:D:86:TYR:HD1	1.32	0.93
3:H:138:LEU:CD1	3:H:211:VAL:HG22	1.97	0.93
1:G:383:PHE:CD2	1:G:420:ILE:HD13	2.04	0.93
1:A:387:THR:HA	1:A:416:LEU:HD21	1.50	0.93
4:L:33:LEU:HD23	4:L:71:PHE:CD1	2.04	0.93
1:G:338:TRP:NE1	1:G:390:LEU:HD23	1.83	0.93
4:D:187:GLN:HA	4:D:187:GLN:HE21	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:11:VAL:HA	3:H:110:THR:O	1.68	0.92
4:L:87:TYR:CD1	4:L:101:GLY:CA	2.52	0.92
1:A:60:ALA:CB	1:A:71:THR:HB	1.99	0.92
1:A:207:LYS:HG2	1:A:208:ILE:N	1.85	0.92
1:G:272:ILE:H	1:G:272:ILE:HD12	1.30	0.92
3:H:96:ARG:HD3	3:H:98:ILE:CG2	1.99	0.92
1:G:350:LYS:CB	1:G:359:ILE:HD11	1.98	0.91
3:H:119:PRO:CB	3:H:142:VAL:HG12	2.00	0.91
3:C:38:ARG:HB3	3:C:90:TYR:CD1	2.04	0.91
1:A:364:PRO:CB	1:A:372:THR:HG22	1.99	0.91
4:D:4:MET:HE2	4:D:97:THR:CG2	2.00	0.91
1:G:346:THR:HG22	1:G:361:PHE:HE2	1.36	0.91
4:L:87:TYR:HD1	4:L:101:GLY:HA2	1.22	0.91
4:L:117:ILE:HG13	4:L:205:VAL:HG23	1.50	0.91
4:L:186:TYR:CE1	4:L:192:TYR:CE1	2.58	0.91
1:A:44:VAL:HG11	1:A:492:GLU:CB	2.00	0.91
3:H:181:VAL:CG2	4:L:135:LEU:CD2	2.41	0.91
3:C:17:SER:N	3:C:82(C):LEU:CD1	2.32	0.91
3:H:154:TRP:CZ3	3:H:196:CYS:HB3	2.05	0.91
1:G:362:GLN:HG3	1:G:363:PRO:HD2	1.50	0.91
4:D:150:VAL:CG1	4:D:192:TYR:HE1	1.78	0.91
1:G:376:PHE:CE1	1:G:383:PHE:HB2	2.06	0.91
4:L:37:GLN:HB2	4:L:86:TYR:CE1	2.05	0.91
4:L:85:THR:HG23	4:L:103:ARG:N	1.85	0.91
1:G:373:MET:HE1	1:G:386:ASN:CB	2.01	0.90
1:G:370:GLU:HG3	1:G:384:TYR:HE1	1.36	0.90
1:G:383:PHE:CD2	1:G:420:ILE:CD1	2.54	0.90
1:G:382:PHE:CE2	1:G:435:TYR:HD1	1.87	0.90
4:L:19:VAL:HG22	4:L:75:ILE:HG23	1.52	0.90
3:C:137:ALA:HB3	4:D:116:PHE:CE2	2.05	0.90
3:H:163:VAL:HG22	3:H:182:VAL:CG1	1.91	0.90
3:H:184:VAL:HG11	3:H:194:TYR:OH	1.70	0.90
3:C:154:TRP:HE3	3:C:195:VAL:O	1.53	0.90
1:G:224:VAL:HG22	3:H:100(A):VAL:CG2	2.01	0.90
4:L:7:SER:CB	4:L:8:PRO:HD3	2.01	0.90
4:D:119:PRO:HB3	4:D:207:LYS:HZ3	1.26	0.90
1:G:376:PHE:CE1	1:G:383:PHE:HB3	2.04	0.90
4:L:85:THR:HG23	4:L:102:THR:C	1.97	0.90
1:A:274:SER:HB2	1:A:284:ILE:HA	1.53	0.90
3:H:32:TYR:O	3:H:52(A):PRO:HG2	1.72	0.90
3:H:119:PRO:HB2	3:H:142:VAL:HG12	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ARG:O	3:C:111:VAL:CG2	2.20	0.90
3:H:6:GLN:HE22	3:H:91:TYR:HA	1.35	0.90
4:L:128:GLY:HA2	4:L:183:ASN:CG	1.96	0.90
1:G:118:PRO:HG3	1:G:435:TYR:HE2	1.36	0.89
1:G:273:ARG:HH21	1:G:287:HIS:HB2	1.36	0.89
4:D:19:VAL:O	4:D:74:THR:HA	1.72	0.89
1:A:353:PHE:HZ	1:A:456:ARG:HH11	1.05	0.89
3:C:40:ALA:HA	3:C:88:ALA:CB	2.02	0.89
3:C:40:ALA:HA	3:C:88:ALA:HB2	1.53	0.89
3:H:17:SER:OG	3:H:82(A):SER:CA	2.20	0.89
3:H:135:THR:HA	3:H:186:SER:O	1.73	0.89
1:A:335:GLY:CA	1:A:414:ILE:CD1	2.50	0.89
4:D:192:TYR:HB2	4:D:207:LYS:HD3	1.52	0.89
3:H:114:ALA:HB1	3:H:146:PHE:CG	2.08	0.89
4:D:14:SER:O	4:D:17:ASP:HB2	1.72	0.89
1:A:338:TRP:HE1	1:A:390:LEU:HB3	1.36	0.89
1:A:66:HIS:HE1	1:A:210:PHE:CZ	1.92	0.88
3:H:98:ILE:HD11	3:H:100(C):TYR:HB2	1.51	0.88
3:C:83:ARG:O	3:C:111:VAL:HG11	1.74	0.88
1:G:390:LEU:CD1	1:G:416:LEU:CD2	2.51	0.88
3:C:2:VAL:HG11	3:C:102:TYR:CE1	2.09	0.88
1:A:259:LEU:CD2	1:A:449:ILE:HD13	2.03	0.88
1:A:96:TRP:CZ2	1:A:274:SER:HA	2.09	0.88
1:G:446:VAL:CG2	5:G:506:NAG:H82	2.04	0.88
4:L:155:LYS:HZ3	4:L:181:LEU:HD21	1.38	0.88
1:A:377:ASN:HB2	1:A:382:PHE:HE2	1.37	0.87
1:G:358:THR:HB	1:G:465:ASN:HB3	1.55	0.87
2:N:9:ARG:NH2	2:N:30:CYS:SG	2.47	0.87
3:C:122:PHE:CE2	4:D:124:GLN:HG3	2.07	0.87
4:D:2:ILE:HD11	4:D:90:LYS:CD	2.03	0.87
1:G:84:ILE:CD1	3:H:100(A):VAL:CG1	2.53	0.87
3:C:101:GLN:NE2	3:C:102:TYR:HE2	1.67	0.87
1:G:273:ARG:HH21	1:G:287:HIS:CB	1.86	0.87
3:H:17:SER:OG	3:H:82(A):SER:HB2	1.74	0.87
4:L:136:LEU:CD2	4:L:196:VAL:CG2	2.53	0.87
1:A:65:VAL:HG21	1:A:208:ILE:HD13	1.56	0.87
4:D:19:VAL:CG2	4:D:75:ILE:HB	2.03	0.87
3:H:55:GLY:H	3:H:71:ARG:HH11	0.90	0.87
1:A:238:PRO:O	1:A:239:CYS:HB2	1.73	0.87
1:A:376:PHE:HE1	1:A:383:PHE:HB3	1.40	0.87
4:D:48:ILE:HG12	4:D:54:LEU:CD1	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:VAL:HG21	4:D:75:ILE:CG1	1.98	0.87
3:H:59:TYR:HE1	3:H:69:MET:SD	1.97	0.86
1:A:225:ILE:HG22	1:A:245:VAL:CG2	2.04	0.86
3:H:181:VAL:HG11	4:L:135:LEU:HD21	1.57	0.86
3:C:38:ARG:HB2	3:C:90:TYR:CD1	2.11	0.86
4:D:11:LEU:HD12	4:D:104:LEU:HD13	1.55	0.86
1:G:212:PRO:HB2	1:G:252:LYS:HG2	1.56	0.86
3:C:121:VAL:CG2	3:C:207:VAL:CG1	2.49	0.86
3:H:154:TRP:HE1	3:H:182:VAL:CG2	1.85	0.86
3:H:114:ALA:CB	3:H:146:PHE:CG	2.59	0.86
3:H:119:PRO:HB2	3:H:142:VAL:CG1	2.06	0.86
3:H:124:LEU:O	4:L:118:PHE:CD2	2.29	0.86
1:A:335:GLY:HA3	1:A:414:ILE:HD11	1.58	0.86
3:C:70:THR:HG22	3:C:71:ARG:N	1.88	0.85
3:H:35:ASN:HD21	4:L:96:PHE:HE2	1.20	0.85
3:H:135:THR:H	3:H:186:SER:HA	1.41	0.85
1:A:258:GLN:OE1	1:A:470:PRO:CB	2.24	0.85
3:C:166:PHE:CE1	4:D:174:SER:O	2.29	0.85
3:C:184:VAL:HG21	3:C:194:TYR:CE2	2.11	0.85
1:G:427:TRP:CE3	1:G:475:ILE:HG13	2.11	0.85
3:H:34:ILE:HG22	3:H:51:MET:CG	2.05	0.85
4:L:108:ARG:HG3	4:L:109:ALA:N	1.91	0.85
1:A:94:ASN:HD21	1:A:97:LYS:CG	1.88	0.85
1:A:207:LYS:CG	1:A:208:ILE:N	2.38	0.85
3:C:38:ARG:HB3	3:C:90:TYR:HD1	1.40	0.85
4:D:150:VAL:HG11	4:D:192:TYR:CE1	2.07	0.85
1:G:120:VAL:HB	1:G:434:MET:CE	2.05	0.85
1:A:106:GLU:HA	1:A:109:ILE:HD12	1.59	0.85
4:L:136:LEU:HD23	4:L:196:VAL:CG1	2.06	0.85
4:L:186:TYR:HE1	4:L:192:TYR:CE1	1.94	0.85
1:A:58:ALA:CB	1:A:67:ASN:O	2.23	0.85
1:A:59:LYS:HD2	1:A:59:LYS:H	1.41	0.85
4:D:2:ILE:CD1	4:D:90:LYS:HD2	2.04	0.85
3:H:124:LEU:O	4:L:118:PHE:HD2	1.60	0.85
4:L:49:TYR:CE1	4:L:53:THR:OG1	2.28	0.85
1:G:224:VAL:CG2	3:H:100(A):VAL:CG2	2.54	0.84
3:H:63:PHE:HB3	3:H:67:VAL:CG2	2.08	0.84
4:L:136:LEU:HD23	4:L:196:VAL:HG11	1.59	0.84
1:A:95:MET:HE3	1:A:235:GLY:HA3	1.56	0.84
1:A:376:PHE:CE1	1:A:383:PHE:HB2	2.12	0.84
3:C:112:SER:HB3	3:C:146:PHE:CZ	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:32:TYR:C	4:D:91:TYR:HE2	1.86	0.84
1:A:225:ILE:CG2	1:A:245:VAL:HG22	2.06	0.84
3:H:11:VAL:HG12	3:H:110:THR:OG1	1.77	0.84
1:G:226:LEU:CD1	1:G:489:VAL:CG2	2.35	0.84
4:L:33:LEU:HD22	4:L:71:PHE:CD2	2.12	0.84
4:D:85:THR:HG21	4:D:103:ARG:HG3	1.60	0.84
1:G:116:LEU:CD1	1:G:210:PHE:HE2	1.79	0.84
3:H:114:ALA:HB3	3:H:146:PHE:CE1	2.13	0.84
1:G:446:VAL:HG21	5:G:506:NAG:C8	2.06	0.83
1:G:52:LEU:HB2	1:G:103:GLN:OE1	1.78	0.83
1:A:258:GLN:CD	1:A:372:THR:O	2.21	0.83
4:L:29:PHE:HB2	4:L:92:ASN:HD21	1.39	0.83
1:G:480:ARG:HG3	1:G:480:ARG:HH11	1.44	0.83
4:L:106:ILE:HB	4:L:166:GLN:HE22	1.43	0.83
1:A:76:PRO:HG2	4:D:1:ALA:HA	1.61	0.83
3:H:4:LEU:CD2	3:H:24:ALA:HB2	2.08	0.82
4:L:107:LYS:O	4:L:140:TYR:CE2	2.32	0.82
1:G:338:TRP:CZ2	1:G:342:LEU:HD22	2.13	0.82
1:G:84:ILE:HD12	3:H:100(A):VAL:CG1	2.09	0.82
1:A:296:CYS:HB2	1:A:383:PHE:HE1	1.42	0.82
1:A:359:ILE:HG23	1:A:468:PHE:CE2	2.12	0.82
4:D:85:THR:HG23	4:D:103:ARG:HA	1.61	0.82
1:A:261:LEU:H	1:A:261:LEU:HD12	1.42	0.82
3:H:152:VAL:CG1	3:H:165:THR:HB	2.09	0.82
3:H:17:SER:OG	3:H:82(A):SER:CB	2.27	0.82
1:A:65:VAL:CG2	1:A:208:ILE:CB	2.51	0.82
4:L:100:GLN:OE1	4:L:100:GLN:N	2.10	0.82
4:L:157:GLY:C	4:L:158:ASN:ND2	2.37	0.82
4:D:166:GLN:HG3	4:D:173:TYR:CZ	2.15	0.82
3:H:72:ASP:O	3:H:75:THR:CG2	2.28	0.82
1:G:382:PHE:CE2	1:G:435:TYR:HE1	1.94	0.82
4:D:11:LEU:HD12	4:D:104:LEU:CD1	2.10	0.82
1:G:382:PHE:HE2	1:G:435:TYR:CE1	1.79	0.81
4:L:151:ASP:OD2	4:L:189:HIS:HB3	1.80	0.81
3:C:35:ASN:ND2	3:C:47:TRP:HE1	1.78	0.81
1:G:93:PHE:HE1	1:G:239:CYS:SG	2.04	0.81
1:G:95:MET:O	1:G:480:ARG:CD	2.28	0.81
1:G:382:PHE:CZ	1:G:435:TYR:CE1	2.68	0.81
3:H:95:TYR:CD1	3:H:100(D):ARG:HA	2.15	0.81
3:H:154:TRP:CZ3	3:H:195:VAL:C	2.52	0.81
4:L:136:LEU:CD2	4:L:196:VAL:CG1	2.57	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:N	1:A:102:GLU:OE1	2.12	0.81
3:H:154:TRP:CZ3	3:H:196:CYS:CB	2.63	0.81
1:A:299:PRO:CG	1:A:442:LYS:CD	2.48	0.81
1:G:116:LEU:HD11	1:G:210:PHE:HE2	1.04	0.81
4:L:11:LEU:O	4:L:105:GLU:HG2	1.81	0.81
4:D:61:ARG:HH11	4:D:82:ASP:CG	1.88	0.81
4:L:136:LEU:HD11	4:L:146:VAL:HG22	1.63	0.81
1:G:84:ILE:HG21	3:H:99:ALA:O	1.80	0.81
3:H:6:GLN:NE2	3:H:91:TYR:HA	1.95	0.81
4:D:141:PRO:HG3	4:D:199:GLN:NE2	1.96	0.81
1:G:90:THR:CB	1:G:240:LYS:HA	2.09	0.81
1:A:94:ASN:ND2	1:A:97:LYS:HG2	1.96	0.80
1:A:277:LEU:HD23	1:A:352:HIS:CD2	2.16	0.80
3:C:84:SER:CA	3:C:111:VAL:HG21	2.11	0.80
1:A:227:LYS:HG3	1:A:486:TYR:HE1	1.45	0.80
4:L:3:GLN:HB2	4:L:26:SER:OG	1.81	0.80
3:C:23:LYS:HG3	3:C:77:THR:HG22	1.63	0.80
4:L:65:SER:OG	4:L:66:GLY:N	2.12	0.80
1:A:299:PRO:HB3	1:A:442:LYS:HD3	1.60	0.80
1:A:395:CYS:SG	5:A:509:NAG:O6	2.38	0.80
4:D:166:GLN:HG3	4:D:173:TYR:CE1	2.17	0.80
1:A:272:ILE:CD1	1:A:272:ILE:H	1.94	0.80
1:A:60:ALA:CB	1:A:71:THR:CG2	2.60	0.80
3:H:137:ALA:HB3	4:L:116:PHE:CD2	2.17	0.80
4:L:11:LEU:O	4:L:105:GLU:CG	2.30	0.80
1:G:233:PHE:CE1	1:G:235:GLY:HA2	2.17	0.79
4:L:151:ASP:CG	4:L:189:HIS:ND1	2.40	0.79
4:D:80:PRO:O	4:D:83:VAL:HG22	1.81	0.79
1:G:382:PHE:CZ	1:G:435:TYR:HE1	1.99	0.79
1:A:65:VAL:HG21	1:A:208:ILE:CD1	2.12	0.79
1:A:57:ASP:OD1	1:A:77:THR:HB	1.83	0.79
1:A:296:CYS:CB	1:A:383:PHE:HE1	1.95	0.79
3:C:17:SER:N	3:C:82(C):LEU:HD11	1.96	0.79
3:C:184:VAL:HG11	3:C:194:TYR:HE2	1.47	0.79
1:A:226:LEU:CD1	1:A:489:VAL:HG21	2.13	0.79
1:G:456:ARG:HG2	1:G:456:ARG:HH11	1.44	0.79
1:A:58:ALA:O	1:A:60:ALA:N	2.14	0.79
1:A:68:VAL:HA	1:A:71:THR:HG23	1.63	0.79
1:G:338:TRP:CH2	1:G:342:LEU:HD22	2.17	0.79
3:H:138:LEU:CD1	3:H:211:VAL:HG21	1.98	0.79
1:A:376:PHE:CE1	1:A:383:PHE:HB3	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:HIS:HE1	1:G:376:PHE:CD2	2.01	0.79
4:D:29:PHE:CB	4:D:92:ASN:HD22	1.85	0.79
1:G:370:GLU:HG3	1:G:384:TYR:CE1	2.18	0.79
3:H:66:ARG:HD3	3:H:82(B):SER:HG	1.46	0.79
4:D:62:PHE:CD2	4:D:75:ILE:HD11	2.16	0.79
4:L:12:SER:HB2	4:L:107:LYS:HD3	1.65	0.79
4:D:48:ILE:HD13	4:D:64:GLY:CA	2.12	0.79
4:D:119:PRO:CB	4:D:207:LYS:HZ1	1.94	0.79
4:L:117:ILE:CG1	4:L:205:VAL:HG23	2.13	0.78
1:A:387:THR:HG22	1:A:390:LEU:CD1	2.13	0.78
4:D:61:ARG:HD2	4:D:82:ASP:OD2	1.82	0.78
3:C:154:TRP:CD1	3:C:163:VAL:HG22	2.19	0.78
4:D:135:LEU:HD23	4:D:135:LEU:O	1.84	0.78
1:G:226:LEU:HD12	1:G:489:VAL:HG23	1.65	0.78
4:L:38:GLN:O	4:L:84:ALA:CB	2.21	0.78
4:L:48:ILE:HD13	4:L:64:GLY:HA3	1.66	0.78
3:C:101:GLN:NE2	3:C:102:TYR:CZ	2.51	0.78
4:D:193:ALA:HB2	4:D:206:THR:HG23	1.65	0.78
1:A:56:SER:CB	1:A:70:ALA:HB1	2.13	0.78
3:H:163:VAL:HG22	3:H:182:VAL:CB	2.14	0.78
3:H:198:VAL:HG22	3:H:207:VAL:O	1.83	0.78
3:C:122:PHE:CD2	4:D:124:GLN:CG	2.59	0.78
3:C:152:VAL:HB	3:C:198:VAL:HG22	1.65	0.78
4:D:37:GLN:HE21	4:D:86:TYR:HE1	0.80	0.78
1:G:105:GLN:O	1:G:109:ILE:HG13	1.84	0.77
4:L:43:VAL:HG22	4:L:44:PRO:HD2	1.63	0.77
4:L:33:LEU:CD2	4:L:71:PHE:CD2	2.67	0.77
1:A:225:ILE:CG2	1:A:245:VAL:CG2	2.62	0.77
4:D:11:LEU:HB3	4:D:104:LEU:HD13	1.66	0.77
4:D:71:PHE:O	4:D:72:THR:OG1	2.01	0.77
1:G:116:LEU:CD1	1:G:210:PHE:HZ	1.94	0.77
3:H:135:THR:O	4:L:116:PHE:HZ	1.66	0.77
3:C:123:PRO:HD3	3:C:209:LYS:NZ	1.99	0.77
1:G:390:LEU:HD12	1:G:416:LEU:HD21	1.61	0.77
2:N:5:PHE:HE1	2:N:9:ARG:NH1	1.82	0.77
3:H:72:ASP:O	3:H:75:THR:HG23	1.84	0.77
3:C:59:TYR:CD1	3:C:69:MET:CE	2.68	0.77
1:G:217:TYR:HB2	1:G:248:THR:HG21	1.67	0.77
4:D:19:VAL:CG2	4:D:75:ILE:CB	2.53	0.77
4:D:48:ILE:HD13	4:D:64:GLY:HA3	1.65	0.77
4:D:118:PHE:HB2	4:D:133:VAL:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:CYS:N	1:G:205:CYS:SG	2.57	0.77
3:H:45:LEU:HD12	4:L:87:TYR:CD2	2.19	0.77
1:G:45:TRP:HB2	1:G:489:VAL:CG1	2.14	0.77
1:G:270:ILE:HD11	1:G:345:VAL:HG22	1.66	0.77
1:A:65:VAL:HG11	1:A:115:SER:OG	1.84	0.77
1:A:272:ILE:HG13	1:A:352:HIS:NE2	2.00	0.77
1:G:278:THR:O	1:G:456:ARG:NH2	2.17	0.76
4:L:55:GLN:NE2	4:L:55:GLN:HA	2.00	0.76
1:A:207:LYS:HG3	1:A:208:ILE:H	1.50	0.76
3:C:170:LEU:HD13	3:C:176:TYR:CE2	2.21	0.76
4:D:163:VAL:HG12	4:D:175:LEU:HD12	1.65	0.76
1:G:105:GLN:O	1:G:109:ILE:CG1	2.33	0.76
1:G:350:LYS:HB3	1:G:359:ILE:HD11	1.52	0.76
4:L:120:PRO:HG3	4:L:186:TYR:OH	1.85	0.76
1:G:373:MET:CE	1:G:386:ASN:HB2	2.06	0.76
4:L:146:VAL:HG11	4:L:177:SER:CB	2.16	0.76
3:H:181:VAL:CG1	4:L:135:LEU:HD21	2.14	0.76
3:C:4:LEU:CD1	3:C:103:TRP:O	2.33	0.76
3:H:96:ARG:HE	3:H:100(C):TYR:HD1	1.31	0.76
3:H:101:GLN:NE2	3:H:102:TYR:HE2	1.78	0.76
4:L:29:PHE:CB	4:L:92:ASN:ND2	2.42	0.76
4:L:31:ASN:ND2	4:L:67:SER:CB	2.49	0.76
1:A:65:VAL:HG21	1:A:208:ILE:CG1	2.16	0.76
3:H:59:TYR:CE1	3:H:69:MET:SD	2.78	0.76
4:L:136:LEU:CD2	4:L:196:VAL:HG13	2.16	0.76
1:A:469:ARG:O	1:A:469:ARG:HD3	1.85	0.76
3:C:70:THR:HG22	3:C:71:ARG:H	1.51	0.76
4:D:49:TYR:CE1	4:D:53:THR:HG21	2.20	0.76
4:D:91:TYR:H	4:D:91:TYR:HD2	1.34	0.76
4:D:61:ARG:HG2	4:D:75:ILE:HG23	1.66	0.76
1:A:264:SER:OG	1:A:482:GLU:HG3	1.86	0.75
3:C:145:TYR:CE1	3:C:176:TYR:C	2.65	0.75
1:G:232:ASN:OD1	1:G:268:GLU:HB2	1.85	0.75
3:C:121:VAL:HG22	3:C:207:VAL:HG11	1.68	0.75
1:G:80:ASN:OD1	3:H:52:ASN:ND2	2.20	0.75
1:G:390:LEU:HD12	1:G:416:LEU:HD22	1.66	0.75
4:L:37:GLN:HB2	4:L:86:TYR:HD1	1.47	0.75
4:D:90:LYS:NZ	4:D:95:PRO:HD2	2.01	0.75
3:H:96:ARG:CD	3:H:98:ILE:HG21	2.17	0.75
1:A:80:ASN:ND2	1:A:80:ASN:O	2.19	0.75
1:A:386:ASN:OD1	1:A:388:THR:CG2	2.28	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:270:ILE:CG2	1:G:348:LYS:HG3	2.16	0.75
3:H:119:PRO:CB	3:H:142:VAL:CG1	2.63	0.75
3:H:135:THR:N	3:H:186:SER:HA	2.02	0.75
4:L:31:ASN:HD21	4:L:67:SER:CB	2.00	0.75
1:A:369:LEU:HD11	1:A:384:TYR:CD1	2.22	0.74
3:C:37:VAL:HG23	3:C:46:GLU:O	1.88	0.74
4:D:2:ILE:HG22	4:D:26:SER:OG	1.87	0.74
3:C:145:TYR:HE1	3:C:176:TYR:C	1.95	0.74
1:G:100:MET:HE1	1:G:486:TYR:HB2	1.68	0.74
4:L:29:PHE:HE2	4:L:32:TYR:O	1.70	0.74
4:D:31:ASN:CG	4:D:68:GLY:H	1.96	0.74
4:L:120:PRO:CG	4:L:186:TYR:OH	2.34	0.74
4:L:38:GLN:C	4:L:84:ALA:HB1	2.13	0.74
3:C:167:PRO:HD2	4:D:162:SER:OG	1.88	0.74
4:D:11:LEU:CD1	4:D:104:LEU:CD1	2.65	0.74
3:H:124:LEU:HD11	4:L:133:VAL:HG21	1.68	0.74
1:G:273:ARG:NH2	1:G:287:HIS:CB	2.51	0.74
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.70	0.74
4:L:108:ARG:HH11	4:L:109:ALA:H	1.35	0.74
1:A:376:PHE:CE1	1:A:383:PHE:CD1	2.76	0.74
3:C:82(C):LEU:H	3:C:82(C):LEU:HD12	1.51	0.74
1:G:257:THR:HG21	1:G:370:GLU:O	1.88	0.74
3:H:4:LEU:HD23	3:H:24:ALA:HB2	1.68	0.74
3:H:152:VAL:HG21	3:H:180:SER:OG	1.88	0.73
1:A:444:ASN:OD1	1:A:444:ASN:C	2.30	0.73
3:C:37:VAL:CG2	3:C:46:GLU:O	2.35	0.73
3:C:150:VAL:CG2	3:C:199:ASN:O	2.36	0.73
1:G:78:ASP:OD1	1:G:81:PRO:HA	1.87	0.73
1:A:342:LEU:HA	1:A:345:VAL:HG13	1.68	0.73
1:G:217:TYR:HB2	1:G:248:THR:CG2	2.19	0.73
4:L:6:GLN:NE2	4:L:86:TYR:O	2.20	0.73
1:A:460:ALA:HB1	1:A:466:GLU:HA	1.68	0.73
3:C:2:VAL:CG1	3:C:102:TYR:CE1	2.71	0.73
4:L:55:GLN:HA	4:L:55:GLN:HE21	1.53	0.73
1:G:65:VAL:HB	1:G:115:SER:HB3	1.70	0.73
1:A:444:ASN:OD1	1:A:444:ASN:O	2.06	0.73
4:D:142:ARG:HB3	4:D:173:TYR:CE2	2.23	0.73
1:G:473:GLY:HA2	2:N:29:U2X:HD21	1.71	0.73
1:A:207:LYS:O	1:A:208:ILE:HG23	1.88	0.73
1:G:376:PHE:CD1	1:G:383:PHE:HB2	2.23	0.73
1:G:384:TYR:CE2	1:G:421:LYS:CG	2.64	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:SER:N	3:C:82(C):LEU:HD13	2.02	0.73
3:C:154:TRP:CE3	3:C:195:VAL:O	2.41	0.73
4:D:4:MET:HE1	4:D:97:THR:O	1.87	0.73
3:C:87:THR:HG22	3:C:111:VAL:CG2	2.08	0.73
1:G:260:LEU:CD2	1:G:478:ASN:OD1	2.37	0.73
1:G:330:TYR:HA	1:G:417:PRO:O	1.88	0.73
1:G:368:ASP:OD2	2:N:30:CYS:HB3	1.89	0.73
3:H:63:PHE:HB3	3:H:67:VAL:HG21	1.70	0.73
4:L:48:ILE:HD11	4:L:64:GLY:N	2.03	0.73
1:A:386:ASN:CG	1:A:388:THR:HG22	2.13	0.73
1:G:258:GLN:NE2	1:G:372:THR:O	2.22	0.72
3:H:46:GLU:OE2	3:H:62:LYS:NZ	2.21	0.72
1:A:394:THR:O	1:A:396:ILE:HG23	1.89	0.72
1:G:289:ASN:HD22	5:G:505:NAG:C7	2.01	0.72
3:H:63:PHE:O	3:H:67:VAL:HG23	1.89	0.72
3:C:137:ALA:CB	4:D:116:PHE:CE2	2.71	0.72
4:D:37:GLN:CB	4:D:86:TYR:CD1	2.67	0.72
1:G:69:TRP:HD1	1:G:114:GLN:NE2	1.87	0.72
1:G:338:TRP:CD1	1:G:390:LEU:CD2	2.70	0.72
3:H:95:TYR:CD1	3:H:100(D):ARG:C	2.67	0.72
4:L:39:LYS:HA	4:L:84:ALA:HB2	1.69	0.72
1:A:65:VAL:CG2	1:A:208:ILE:HD13	2.19	0.72
3:C:38:ARG:CD	3:C:90:TYR:CE1	2.51	0.72
3:C:38:ARG:CB	3:C:90:TYR:CE1	2.72	0.72
3:C:145:TYR:CD1	3:C:176:TYR:O	2.42	0.72
3:H:35:ASN:ND2	4:L:96:PHE:CE2	2.55	0.72
4:L:11:LEU:HD12	4:L:12:SER:N	2.04	0.72
1:A:376:PHE:HE1	1:A:383:PHE:CD1	2.07	0.72
1:G:365:SER:OG	1:G:469:ARG:NE	2.22	0.72
4:L:85:THR:HG22	4:L:102:THR:O	1.89	0.72
3:C:154:TRP:CD1	3:C:163:VAL:CG2	2.73	0.72
4:D:83:VAL:HG11	4:D:106:ILE:HD12	1.70	0.72
3:H:152:VAL:CG1	3:H:165:THR:CB	2.66	0.72
1:A:95:MET:HE1	1:A:273:ARG:HD3	1.72	0.72
1:A:233:PHE:O	1:A:273:ARG:NH2	2.20	0.72
1:A:259:LEU:HD22	1:A:449:ILE:CD1	2.13	0.72
1:A:376:PHE:CD1	1:A:383:PHE:HB2	2.24	0.72
4:D:207:LYS:NZ	4:D:207:LYS:HB2	2.05	0.72
1:G:297:THR:O	1:G:329:ALA:HB1	1.88	0.72
3:H:154:TRP:CE3	3:H:196:CYS:HA	2.25	0.72
1:A:82:GLN:NE2	3:C:100(D):ARG:HD3	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:95:TYR:CD1	3:H:100(D):ARG:CA	2.73	0.72
3:H:100(F):PHE:HE1	4:L:89:GLN:CD	1.98	0.72
4:L:48:ILE:CD1	4:L:64:GLY:H	2.02	0.72
4:L:188:SER:O	4:L:189:HIS:CD2	2.43	0.72
1:A:56:SER:OG	1:A:70:ALA:HB1	1.90	0.72
1:A:272:ILE:H	1:A:272:ILE:HD13	1.53	0.72
1:A:341:VAL:O	1:A:344:GLN:HG3	1.90	0.72
3:C:4:LEU:HD13	3:C:103:TRP:O	1.90	0.72
4:D:6:GLN:NE2	4:D:86:TYR:O	2.23	0.72
3:H:32:TYR:OH	3:H:98:ILE:N	2.23	0.72
3:C:17:SER:H	3:C:82(C):LEU:HD11	1.49	0.72
1:G:346:THR:HG22	1:G:361:PHE:CE2	2.23	0.71
3:H:61:GLN:O	3:H:64:GLN:HB2	1.90	0.71
3:H:200:HIS:ND1	3:H:203:SER:HB2	2.05	0.71
1:G:212:PRO:HB2	1:G:252:LYS:CG	2.20	0.71
4:L:85:THR:CG2	4:L:102:THR:O	2.37	0.71
1:G:84:ILE:HD11	3:H:100(A):VAL:CG1	2.20	0.71
3:H:154:TRP:HE1	3:H:182:VAL:HG23	1.52	0.71
1:A:84:ILE:CD1	3:C:100(A):VAL:HG13	2.20	0.71
4:D:207:LYS:HB2	4:D:207:LYS:HZ2	1.53	0.71
1:G:350:LYS:CA	1:G:359:ILE:HD11	2.20	0.71
1:G:118:PRO:HG3	1:G:435:TYR:CE2	2.23	0.71
1:A:95:MET:CE	1:A:235:GLY:CA	2.53	0.71
3:C:66:ARG:HH11	3:C:82:LEU:HD11	1.56	0.71
4:L:12:SER:HB2	4:L:107:LYS:CD	2.20	0.71
4:L:106:ILE:HB	4:L:166:GLN:NE2	2.04	0.71
1:A:298:ARG:NH2	1:A:441:GLY:O	2.23	0.71
1:G:223:TYR:CD2	1:G:490:GLN:HB2	2.24	0.71
4:L:120:PRO:HG3	4:L:186:TYR:CZ	2.26	0.71
3:C:70:THR:CG2	3:C:71:ARG:N	2.53	0.71
1:G:439:ILE:HD12	1:G:439:ILE:C	2.15	0.71
3:H:66:ARG:CD	3:H:82(B):SER:OG	2.31	0.71
3:H:152:VAL:HG11	3:H:165:THR:OG1	1.91	0.70
4:L:4:MET:CE	4:L:90:LYS:HB3	2.21	0.70
4:L:13:ALA:O	4:L:14:SER:O	2.09	0.70
4:L:48:ILE:CD1	4:L:64:GLY:CA	2.69	0.70
1:A:44:VAL:CG1	1:A:492:GLU:HB2	2.19	0.70
1:A:377:ASN:HB2	1:A:382:PHE:CD2	2.26	0.70
1:A:392:ASN:O	1:A:394:THR:N	2.24	0.70
3:C:136:ALA:HB2	3:C:186:SER:CB	2.22	0.70
4:L:85:THR:HG22	4:L:102:THR:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:108:ARG:NH1	4:L:109:ALA:HB3	2.06	0.70
1:G:249:HIS:HD1	1:G:486:TYR:HH	1.31	0.70
3:H:154:TRP:CD1	3:H:182:VAL:HG22	2.25	0.70
1:A:392:ASN:C	1:A:394:THR:H	2.00	0.70
4:D:49:TYR:CE1	4:D:53:THR:CG2	2.74	0.70
4:L:16:GLY:N	4:L:78:LEU:O	2.22	0.70
1:A:277:LEU:CD2	1:A:352:HIS:HD2	1.72	0.70
4:D:85:THR:HG23	4:D:103:ARG:HG3	1.72	0.70
3:H:96:ARG:CD	3:H:98:ILE:CG2	2.69	0.70
3:C:54:THR:O	3:C:54:THR:OG1	2.02	0.70
4:D:167:ASP:O	4:D:171:ASN:ND2	2.24	0.70
4:L:155:LYS:HZ1	4:L:181:LEU:HD21	1.55	0.70
4:D:11:LEU:O	4:D:105:GLU:N	2.21	0.70
1:G:49:ASP:OD2	1:A:444:ASN:ND2	2.24	0.70
1:G:66:HIS:HB3	1:G:213:ILE:HD11	1.71	0.70
1:A:72:HIS:O	1:A:74:CYS:N	2.24	0.70
1:A:369:LEU:CD1	1:A:384:TYR:CD1	2.74	0.70
3:C:83:ARG:O	3:C:111:VAL:CB	2.40	0.70
3:C:83:ARG:O	3:C:111:VAL:CG1	2.39	0.70
4:D:135:LEU:HD23	4:D:135:LEU:C	2.17	0.70
3:H:147:PRO:O	3:H:200:HIS:NE2	2.25	0.70
1:A:233:PHE:CE1	1:A:235:GLY:CA	2.75	0.70
1:G:109:ILE:HG23	1:G:428:GLN:CG	2.22	0.69
1:A:359:ILE:CG2	1:A:468:PHE:CD2	2.74	0.69
3:C:145:TYR:CE1	3:C:176:TYR:O	2.46	0.69
4:D:31:ASN:OD1	4:D:68:GLY:N	2.25	0.69
4:D:32:TYR:C	4:D:91:TYR:CE2	2.69	0.69
1:G:224:VAL:CG2	3:H:100(A):VAL:HG22	2.21	0.69
3:H:30:THR:CG2	3:H:53:LYS:HD2	2.22	0.69
1:A:59:LYS:H	1:A:59:LYS:CD	2.05	0.69
3:C:70:THR:CG2	3:C:71:ARG:H	2.04	0.69
4:D:48:ILE:CG1	4:D:54:LEU:HD12	2.20	0.69
4:D:61:ARG:NH1	4:D:82:ASP:CG	2.50	0.69
1:G:93:PHE:CE1	1:G:239:CYS:SG	2.85	0.69
1:G:375:SER:OG	1:G:384:TYR:CD1	2.46	0.69
1:G:439:ILE:HD12	1:G:439:ILE:O	1.91	0.69
3:H:38:ARG:CD	3:H:90:TYR:HE1	2.04	0.69
4:L:31:ASN:OD1	4:L:68:GLY:N	2.25	0.69
1:A:258:GLN:HG3	1:A:374:HIS:HA	1.73	0.69
1:G:338:TRP:CD1	1:G:339:ASN:HD21	2.11	0.69
1:A:233:PHE:HE1	1:A:235:GLY:CA	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:VAL:CG1	3:C:102:TYR:HE1	2.05	0.69
3:H:154:TRP:CZ3	3:H:196:CYS:HA	2.28	0.69
1:G:66:HIS:CE1	1:G:212:PRO:CB	2.75	0.69
1:G:346:THR:CG2	1:G:361:PHE:HE2	2.06	0.69
3:H:66:ARG:NH2	3:H:86:ASP:OD1	2.26	0.69
3:H:97:ILE:O	3:H:97:ILE:HG13	1.91	0.69
3:H:115:SER:O	3:H:116:THR:O	2.11	0.69
4:L:155:LYS:NZ	4:L:181:LEU:CD2	2.50	0.69
1:A:392:ASN:OD1	5:A:509:NAG:H82	1.92	0.69
4:D:183:ASN:O	4:D:187:GLN:N	2.20	0.69
1:G:66:HIS:HE1	1:G:212:PRO:CB	2.05	0.69
1:G:84:ILE:HD11	3:H:100(A):VAL:HG12	1.74	0.69
3:H:150:VAL:CG1	3:H:178:LEU:HD21	2.22	0.69
4:L:31:ASN:HD21	4:L:67:SER:HB2	1.53	0.69
4:L:136:LEU:HD13	4:L:175:LEU:HD13	1.74	0.69
1:A:370:GLU:CD	1:A:370:GLU:H	2.00	0.69
3:C:122:PHE:CE2	4:D:124:GLN:CG	2.75	0.69
4:D:61:ARG:NH1	4:D:82:ASP:OD1	2.26	0.69
4:L:151:ASP:OD2	4:L:189:HIS:ND1	2.26	0.69
1:A:94:ASN:ND2	1:A:97:LYS:CG	2.53	0.69
1:A:256:SER:OG	1:A:261:LEU:CD1	2.41	0.69
1:A:392:ASN:ND2	5:A:509:NAG:H82	2.08	0.69
3:C:10:GLU:HG2	3:C:18:VAL:HG23	1.74	0.69
4:L:48:ILE:HD13	4:L:64:GLY:CA	2.22	0.69
4:L:113:PRO:HA	4:L:137:ASN:O	1.93	0.69
1:A:261:LEU:HD12	1:A:261:LEU:N	2.08	0.69
4:D:8:PRO:O	4:D:102:THR:HB	1.93	0.69
4:L:2:ILE:HG12	4:L:2:ILE:O	1.92	0.68
3:C:121:VAL:HG21	3:C:207:VAL:HG12	1.75	0.68
3:C:122:PHE:CG	4:D:124:GLN:HG3	2.28	0.68
4:D:32:TYR:O	4:D:91:TYR:CD2	2.46	0.68
1:G:270:ILE:CD1	1:G:345:VAL:HG22	2.23	0.68
3:H:95:TYR:HD1	3:H:100(D):ARG:C	2.01	0.68
1:A:233:PHE:CE1	1:A:235:GLY:N	2.62	0.68
1:A:94:ASN:HA	1:A:236:THR:HG22	1.76	0.68
1:G:217:TYR:O	1:G:248:THR:N	2.25	0.68
4:L:4:MET:HE1	4:L:90:LYS:N	2.08	0.68
4:L:11:LEU:CD1	4:L:12:SER:H	2.05	0.68
1:G:66:HIS:HE1	1:G:212:PRO:HB3	1.59	0.68
1:G:107:ASP:CG	1:G:217:TYR:OH	2.36	0.68
4:D:61:ARG:HG2	4:D:75:ILE:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:VAL:HG21	3:H:100(A):VAL:HG22	1.76	0.68
3:H:32:TYR:CZ	3:H:97:ILE:HA	2.29	0.68
4:L:128:GLY:HA2	4:L:183:ASN:ND2	2.09	0.68
4:D:183:ASN:O	4:D:186:TYR:N	2.26	0.68
1:G:66:HIS:HB3	1:G:213:ILE:CD1	2.24	0.68
1:G:260:LEU:HD23	1:G:478:ASN:OD1	1.94	0.68
1:G:286:VAL:O	1:G:451:GLY:CA	2.42	0.68
1:A:335:GLY:N	1:A:412:GLY:O	2.24	0.68
3:C:95:TYR:CD2	3:C:100(D):ARG:C	2.72	0.68
1:G:480:ARG:HG3	1:G:480:ARG:NH1	2.09	0.68
3:C:37:VAL:HG23	3:C:46:GLU:C	2.19	0.68
4:D:100:GLN:OE1	4:D:100:GLN:N	2.25	0.68
1:G:207:LYS:NZ	1:G:437:PRO:O	2.25	0.68
3:H:85:GLU:OE1	3:H:85:GLU:N	2.25	0.68
4:L:2:ILE:HD12	4:L:90:LYS:HE2	1.76	0.68
1:A:60:ALA:CB	1:A:71:THR:CB	2.67	0.67
3:C:197:ASN:HD22	3:C:208:ASP:CG	2.03	0.67
4:L:150:VAL:CG2	4:L:192:TYR:CD2	2.74	0.67
4:L:199:GLN:HA	4:L:199:GLN:NE2	2.09	0.67
4:D:29:PHE:CB	4:D:92:ASN:ND2	2.48	0.67
4:D:32:TYR:O	4:D:91:TYR:CE2	2.46	0.67
4:L:115:VAL:HG21	4:L:203:SER:OG	1.95	0.67
4:L:146:VAL:HG11	4:L:177:SER:OG	1.94	0.67
1:A:47:ASP:OD2	1:A:47:ASP:N	2.27	0.67
1:A:60:ALA:HB2	1:A:71:THR:HG22	1.75	0.67
1:A:350:LYS:HB3	1:A:359:ILE:HD11	1.76	0.67
1:A:383:PHE:HA	1:A:420:ILE:HG22	1.76	0.67
3:C:83:ARG:C	3:C:111:VAL:HG21	2.20	0.67
4:D:8:PRO:O	4:D:102:THR:CB	2.42	0.67
4:D:37:GLN:CB	4:D:86:TYR:CE1	2.76	0.67
4:D:108:ARG:HD2	4:D:170:ASP:O	1.94	0.67
4:D:129:THR:HA	4:D:182:SER:HA	1.77	0.67
3:C:159:LEU:HD21	3:C:182:VAL:HG11	1.76	0.67
4:D:90:LYS:HZ3	4:D:95:PRO:HD2	1.57	0.67
1:G:265:LEU:HD11	1:G:291:SER:HB2	1.75	0.67
3:H:66:ARG:HG2	3:H:82(A):SER:O	1.95	0.67
4:L:107:LYS:O	4:L:140:TYR:CZ	2.48	0.67
3:H:194:TYR:HB2	3:H:211:VAL:HG13	1.76	0.67
4:L:11:LEU:O	4:L:105:GLU:CB	2.42	0.67
1:G:122:LEU:C	1:G:122:LEU:HD12	2.19	0.67
3:H:72:ASP:O	3:H:75:THR:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:151:ASP:HA	4:L:191:VAL:HG13	1.76	0.67
3:C:36:TRP:HB3	3:C:48:MET:HE3	1.77	0.67
1:A:388:THR:HG21	5:A:508:NAG:C1	2.24	0.67
3:C:66:ARG:NH1	3:C:86:ASP:OD2	2.28	0.67
1:G:338:TRP:CD1	1:G:339:ASN:ND2	2.63	0.67
4:L:135:LEU:C	4:L:135:LEU:HD12	2.19	0.67
3:C:166:PHE:CZ	4:D:174:SER:O	2.48	0.67
1:G:331:CYS:C	1:G:332:GLU:HG3	2.20	0.66
4:L:89:GLN:HG2	4:L:90:LYS:N	2.09	0.66
4:D:107:LYS:HB2	4:D:107:LYS:NZ	2.10	0.66
3:C:111:VAL:HG23	3:C:111:VAL:O	1.96	0.66
3:C:124:LEU:HD11	4:D:133:VAL:HG21	1.78	0.66
4:D:85:THR:HG23	4:D:103:ARG:CG	2.24	0.66
4:L:113:PRO:HB3	4:L:139:PHE:HB3	1.77	0.66
4:D:38:GLN:O	4:D:84:ALA:HB1	1.94	0.66
1:G:417:PRO:O	1:G:418:CYS:CB	2.43	0.66
4:L:5:THR:HA	4:L:100:GLN:HE22	1.61	0.66
4:D:11:LEU:CD1	4:D:104:LEU:HD13	2.26	0.66
4:D:116:PHE:HB2	4:D:135:LEU:HD22	1.77	0.66
1:G:270:ILE:HG22	5:G:505:NAG:H62	1.78	0.66
1:G:350:LYS:CB	1:G:359:ILE:HD12	2.16	0.66
1:G:350:LYS:HG3	1:G:350:LYS:O	1.95	0.66
4:D:11:LEU:O	4:D:104:LEU:HA	1.95	0.66
3:H:4:LEU:HD23	3:H:24:ALA:CB	2.25	0.66
4:L:85:THR:HG23	4:L:103:ARG:HA	1.74	0.66
4:D:37:GLN:CD	4:D:86:TYR:HE1	2.04	0.66
3:H:101:GLN:HE22	3:H:102:TYR:HE2	1.36	0.66
1:G:117:GLN:CD	1:G:203:GLN:HG3	2.21	0.66
2:N:5:PHE:HE1	2:N:9:ARG:HH11	1.36	0.66
4:L:108:ARG:CG	4:L:109:ALA:H	2.06	0.66
1:A:84:ILE:HD12	3:C:100(A):VAL:HG13	1.77	0.66
3:C:35:ASN:OD1	3:C:47:TRP:NE1	2.27	0.66
3:C:4:LEU:H	3:C:4:LEU:HD12	1.60	0.65
3:C:82(B):SER:O	3:C:82(B):SER:OG	2.09	0.65
1:A:226:LEU:HD12	1:A:489:VAL:CG2	2.20	0.65
1:A:256:SER:OG	1:A:261:LEU:HD11	1.97	0.65
1:A:376:PHE:HE1	1:A:383:PHE:CG	2.13	0.65
3:C:170:LEU:CD1	3:C:176:TYR:CE2	2.78	0.65
1:A:60:ALA:CB	1:A:71:THR:HG21	2.24	0.65
1:A:258:GLN:HE21	1:A:374:HIS:N	1.94	0.65
3:C:87:THR:HG21	3:C:111:VAL:CG2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:166:PHE:CZ	4:L:175:LEU:O	2.49	0.65
1:A:370:GLU:OE2	1:A:370:GLU:N	2.23	0.65
1:A:394:THR:O	1:A:396:ILE:N	2.30	0.65
3:C:97:ILE:HG13	3:C:97:ILE:O	1.94	0.65
4:D:6:GLN:HE22	4:D:87:TYR:HA	1.62	0.65
1:G:373:MET:SD	1:G:386:ASN:HA	2.36	0.65
1:G:475:ILE:O	1:G:478:ASN:N	2.28	0.65
1:G:388:THR:O	1:G:391:PHE:N	2.20	0.65
1:A:91:GLU:CD	1:A:487:LYS:HZ3	2.04	0.65
3:C:61:GLN:NE2	3:C:61:GLN:HA	2.12	0.65
4:D:48:ILE:CD1	4:D:64:GLY:N	2.60	0.65
4:D:62:PHE:HE2	4:D:75:ILE:HD11	1.61	0.65
1:G:226:LEU:O	1:G:486:TYR:HA	1.97	0.65
1:G:239:CYS:SG	1:G:239:CYS:O	2.54	0.65
1:G:338:TRP:NE1	1:G:390:LEU:CD2	2.58	0.65
1:G:78:ASP:OD2	4:L:93:SER:HB2	1.96	0.65
1:G:95:MET:HG2	1:G:235:GLY:O	1.97	0.65
1:G:475:ILE:HD13	1:G:475:ILE:N	2.11	0.65
3:C:154:TRP:CH2	3:C:196:CYS:HB3	2.30	0.65
3:H:39:GLN:O	3:H:88:ALA:HB1	1.96	0.65
1:A:91:GLU:OE1	1:A:487:LYS:NZ	2.30	0.65
1:G:122:LEU:HD12	1:G:123:THR:N	2.12	0.64
4:D:11:LEU:N	4:D:103:ARG:O	2.22	0.64
4:D:61:ARG:NH1	4:D:82:ASP:OD2	2.21	0.64
1:A:100:MET:HE1	1:A:486:TYR:CB	2.25	0.64
3:C:100(E):TYR:N	4:D:91:TYR:HD1	1.96	0.64
4:D:19:VAL:HG23	4:D:75:ILE:HG13	1.74	0.64
3:C:100(D):ARG:O	4:D:91:TYR:HB2	1.97	0.64
4:D:37:GLN:CB	4:D:86:TYR:HD1	2.07	0.64
4:L:161:GLU:N	4:L:161:GLU:OE2	2.31	0.64
1:A:396:ILE:C	1:A:396:ILE:HD12	2.22	0.64
1:G:109:ILE:HG23	1:G:428:GLN:HG3	1.79	0.64
3:H:114:ALA:CB	3:H:146:PHE:CE1	2.77	0.64
1:A:373:MET:HG2	1:A:385:CYS:C	2.23	0.64
1:G:82:GLN:NE2	1:G:246:GLN:OE1	2.23	0.64
1:G:270:ILE:HG22	1:G:348:LYS:HG3	1.78	0.64
1:A:386:ASN:O	1:A:416:LEU:CD2	2.35	0.64
3:C:37:VAL:HG23	3:C:47:TRP:HA	1.80	0.64
3:H:32:TYR:CE2	3:H:97:ILE:HA	2.33	0.64
4:L:85:THR:HG22	4:L:102:THR:N	2.13	0.64
1:A:364:PRO:HB2	1:A:372:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:LEU:HD22	4:D:185:ASP:HB3	1.79	0.64
4:L:37:GLN:NE2	4:L:86:TYR:CE1	2.41	0.64
4:L:66:GLY:HA3	4:L:71:PHE:HA	1.78	0.64
4:L:120:PRO:HD3	4:L:132:VAL:HG22	1.79	0.64
4:L:186:TYR:CD1	4:L:192:TYR:CE1	2.86	0.64
4:L:7:SER:HB2	4:L:22:THR:HB	1.79	0.64
4:L:24:ARG:NE	4:L:70:ASP:OD2	2.31	0.64
4:D:1:ALA:HB2	4:D:95:PRO:CD	2.28	0.64
1:G:118:PRO:CG	1:G:435:TYR:HE2	2.09	0.63
3:H:154:TRP:HD1	3:H:182:VAL:HG22	1.63	0.63
1:G:104:MET:O	1:G:108:VAL:HG23	1.97	0.63
1:G:350:LYS:HB3	1:G:359:ILE:HD13	1.74	0.63
3:H:51:MET:O	3:H:51:MET:HG3	1.97	0.63
3:H:61:GLN:HA	3:H:64:GLN:HB2	1.79	0.63
1:G:386:ASN:O	1:G:416:LEU:HB3	1.99	0.63
3:H:38:ARG:HB3	3:H:90:TYR:CE1	2.33	0.63
3:H:40:ALA:HB3	3:H:43:GLN:HB2	1.80	0.63
3:C:66:ARG:NH1	3:C:82:LEU:HD11	2.13	0.63
3:C:185:PRO:HD2	3:C:189:LEU:HB2	1.80	0.63
4:L:170:ASP:HB2	4:L:172:THR:HG23	1.80	0.63
1:A:97:LYS:HA	1:A:97:LYS:HE3	1.79	0.63
1:A:362:GLN:HG3	1:A:363:PRO:HD2	1.79	0.63
3:C:23:LYS:HG3	3:C:77:THR:CG2	2.27	0.63
3:C:84:SER:HA	3:C:111:VAL:HG23	1.80	0.63
3:C:154:TRP:CE3	3:C:196:CYS:HB3	2.33	0.63
4:D:85:THR:CG2	4:D:103:ARG:CG	2.73	0.63
4:D:141:PRO:HG3	4:D:199:GLN:HE21	1.62	0.63
1:G:349:LEU:HD21	1:G:468:PHE:CD1	2.32	0.63
3:H:38:ARG:HD2	3:H:90:TYR:CE1	2.34	0.63
1:A:272:ILE:CG1	1:A:352:HIS:NE2	2.62	0.63
1:A:296:CYS:HB2	1:A:383:PHE:CE1	2.30	0.63
4:L:11:LEU:HD12	4:L:12:SER:H	1.62	0.63
4:L:132:VAL:CG1	4:L:148:TRP:CH2	2.76	0.63
1:A:258:GLN:NE2	1:A:372:THR:O	2.32	0.63
3:C:124:LEU:CD1	4:D:133:VAL:HG21	2.29	0.63
1:G:257:THR:HG22	1:G:258:GLN:HG3	1.81	0.63
1:G:384:TYR:CD2	1:G:421:LYS:CG	2.72	0.63
3:H:34:ILE:CG2	3:H:51:MET:HG2	2.22	0.63
1:A:68:VAL:HA	1:A:71:THR:CG2	2.28	0.63
4:D:5:THR:HB	4:D:100:GLN:HE22	1.64	0.63
1:G:105:GLN:OE1	1:G:479:TRP:NE1	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:ARG:NH2	1:G:287:HIS:CG	2.67	0.62
1:A:95:MET:O	1:A:480:ARG:HG2	1.98	0.62
1:A:111:LEU:HD23	1:A:111:LEU:C	2.24	0.62
4:D:19:VAL:HG23	4:D:75:ILE:CG1	2.25	0.62
1:G:276:ASN:OD1	5:G:504:NAG:N2	2.32	0.62
2:N:1:MPT:HB2	2:N:29:U2X:N	2.13	0.62
3:H:38:ARG:HD3	3:H:90:TYR:HE1	1.63	0.62
4:L:77:SER:O	4:L:77:SER:OG	2.15	0.62
3:C:39:GLN:OE1	4:D:38:GLN:NE2	2.31	0.62
1:G:224:VAL:CG2	3:H:100(A):VAL:HG23	2.30	0.62
4:L:29:PHE:CB	4:L:92:ASN:HD21	2.08	0.62
1:G:86:LEU:HB2	1:G:242:VAL:HG13	1.81	0.62
3:H:33:ASP:HB2	3:H:95:TYR:HE2	1.63	0.62
4:L:157:GLY:C	4:L:159:SER:H	2.06	0.62
4:L:158:ASN:ND2	4:L:158:ASN:N	2.48	0.62
1:A:335:GLY:HA2	1:A:338:TRP:HB3	1.79	0.62
1:A:376:PHE:CE1	1:A:383:PHE:HD1	2.15	0.62
3:C:142:VAL:O	3:C:177:SER:HA	2.00	0.62
4:D:107:LYS:HB2	4:D:107:LYS:HZ2	1.62	0.62
1:G:388:THR:OG1	1:G:389:GLN:N	2.28	0.62
3:H:98:ILE:HD11	3:H:100(C):TYR:CB	2.28	0.62
3:H:184:VAL:HB	3:H:185:PRO:CD	2.26	0.62
3:C:154:TRP:CE3	3:C:195:VAL:C	2.78	0.62
1:A:361:PHE:O	1:A:393:ASN:ND2	2.32	0.62
1:A:379:ARG:NH1	5:A:503:NAG:O4	2.32	0.62
1:A:386:ASN:C	1:A:416:LEU:HD23	2.23	0.62
3:C:23:LYS:CG	3:C:77:THR:HG22	2.29	0.62
4:D:48:ILE:CG1	4:D:54:LEU:CD1	2.77	0.62
1:A:112:TRP:CH2	1:A:382:PHE:HZ	2.17	0.62
3:C:38:ARG:NH1	3:C:90:TYR:OH	2.32	0.62
4:D:132:VAL:HG22	4:D:148:TRP:CH2	2.34	0.62
3:H:166:PHE:CD2	3:H:179:SER:HB2	2.35	0.62
4:L:11:LEU:O	4:L:105:GLU:HB2	2.00	0.62
4:L:155:LYS:HZ3	4:L:181:LEU:CD2	2.12	0.62
4:L:29:PHE:CE2	4:L:32:TYR:O	2.53	0.62
3:C:52:ASN:O	3:C:55:GLY:HA2	2.00	0.62
4:D:125:VAL:HG13	4:D:183:ASN:ND2	2.13	0.62
1:G:492:GLU:OE2	1:G:492:GLU:HA	1.99	0.61
3:H:12:LYS:O	3:H:111:VAL:HA	2.00	0.61
3:H:124:LEU:HD21	3:H:141:LEU:HB2	1.80	0.61
1:G:111:LEU:HD23	1:G:111:LEU:C	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ALA:HB1	1:G:67:ASN:HA	1.81	0.61
3:H:201:LYS:O	3:H:204:ASN:ND2	2.33	0.61
1:A:254:VAL:HG21	1:A:261:LEU:HD13	1.82	0.61
1:G:358:THR:HB	1:G:465:ASN:CB	2.30	0.61
3:H:197:ASN:HB3	3:H:208:ASP:OD1	1.98	0.61
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.36	0.61
3:C:136:ALA:HB2	3:C:186:SER:CA	2.29	0.61
3:H:197:ASN:CB	3:H:208:ASP:OD1	2.48	0.61
3:C:123:PRO:CD	3:C:209:LYS:NZ	2.63	0.61
1:G:94:ASN:HD22	5:A:507:NAG:H83	1.65	0.61
4:L:59:PRO:HD3	3:C:64:GLN:O	2.00	0.61
1:A:246:GLN:HG2	3:C:100(A):VAL:HB	1.81	0.61
4:D:131:SER:HG	4:D:180:THR:HG1	1.44	0.61
1:G:383:PHE:HE2	1:G:420:ILE:CD1	2.11	0.61
3:H:72:ASP:HB3	3:H:75:THR:HG22	1.82	0.61
3:H:195:VAL:CG2	3:H:210:ARG:HG3	2.30	0.61
3:C:85:GLU:OE2	3:C:85:GLU:N	2.28	0.61
4:D:79:GLN:HB3	4:D:80:PRO:HD2	1.83	0.61
1:G:270:ILE:HG22	5:G:505:NAG:C6	2.30	0.61
1:G:270:ILE:HB	1:G:289:ASN:OD1	2.00	0.61
1:G:446:VAL:HG11	5:G:506:NAG:H82	1.83	0.61
3:H:49:GLY:C	3:H:69:MET:HE1	2.25	0.61
1:A:93:PHE:CE2	1:A:487:LYS:HB3	2.36	0.61
3:C:136:ALA:HB2	3:C:186:SER:HB3	1.83	0.61
1:G:273:ARG:HG2	1:G:285:ILE:HG22	1.83	0.61
1:G:298:ARG:HD2	1:G:443:ILE:HG13	1.82	0.61
3:H:87:THR:HG23	3:H:109:VAL:O	2.01	0.61
3:H:184:VAL:HG11	3:H:194:TYR:HH	1.65	0.61
1:A:45:TRP:HB2	1:A:489:VAL:CG1	2.30	0.61
1:G:265:LEU:HD11	1:G:291:SER:CB	2.31	0.60
3:H:40:ALA:HA	3:H:88:ALA:CB	2.31	0.60
4:L:90:LYS:HE3	4:L:95:PRO:O	2.01	0.60
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.83	0.60
1:A:217:TYR:O	1:A:248:THR:N	2.30	0.60
3:C:41:PRO:HD2	3:C:88:ALA:HA	1.83	0.60
3:H:6:GLN:HB2	3:H:105:GLN:HG3	1.82	0.60
3:H:38:ARG:CB	3:H:90:TYR:CE1	2.84	0.60
1:G:298:ARG:O	1:G:298:ARG:HD3	2.02	0.60
1:A:337:LYS:O	1:A:341:VAL:HG23	2.01	0.60
3:C:100(E):TYR:HD2	4:D:91:TYR:CE1	2.18	0.60
1:G:203:GLN:OE1	1:G:203:GLN:HA	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:138:LEU:HD13	3:H:211:VAL:HG22	1.80	0.60
1:G:349:LEU:HD21	1:G:468:PHE:CZ	2.36	0.60
4:L:52:THR:CG2	4:L:64:GLY:O	2.42	0.60
1:A:390:LEU:CD2	1:A:416:LEU:HD11	2.25	0.60
4:D:129:THR:HG22	4:D:181:LEU:O	2.01	0.60
1:G:371:ILE:HD11	2:N:30:CYS:O	2.01	0.60
3:H:100(D):ARG:HG3	4:L:91:TYR:O	2.02	0.60
1:A:207:LYS:HG2	1:A:208:ILE:H	1.49	0.60
3:C:154:TRP:HD1	3:C:163:VAL:CG2	2.15	0.60
4:D:21:ILE:HD11	4:D:73:LEU:HD23	1.84	0.60
3:H:38:ARG:CB	3:H:90:TYR:CD1	2.85	0.60
3:H:163:VAL:HG22	3:H:182:VAL:HG22	1.83	0.60
1:A:299:PRO:CA	1:A:442:LYS:HD2	2.32	0.60
1:A:456:ARG:HG2	1:A:468:PHE:CD1	2.36	0.60
3:C:39:GLN:O	3:C:88:ALA:HB1	2.02	0.60
4:D:12:SER:HA	4:D:105:GLU:O	2.02	0.60
1:G:473:GLY:CA	2:N:29:U2X:HD21	2.31	0.60
3:H:38:ARG:CD	3:H:90:TYR:CE1	2.84	0.60
3:C:184:VAL:HG11	3:C:194:TYR:CE2	2.33	0.60
4:L:140:TYR:HA	4:L:141:PRO:O	2.01	0.59
1:A:298:ARG:N	1:A:299:PRO:HD3	2.17	0.59
1:A:387:THR:CA	1:A:416:LEU:HD21	2.21	0.59
4:D:71:PHE:C	4:D:72:THR:HG1	2.08	0.59
4:D:125:VAL:CA	4:D:183:ASN:HD21	2.15	0.59
1:G:65:VAL:CB	1:G:115:SER:HB3	2.30	0.59
1:G:223:TYR:HD2	1:G:490:GLN:HA	1.66	0.59
4:L:100:GLN:H	4:L:100:GLN:CD	2.06	0.59
1:A:270:ILE:HG13	5:A:505:NAG:H62	1.84	0.59
4:D:33:LEU:HD22	4:D:71:PHE:CE1	2.32	0.59
1:G:69:TRP:CD1	1:G:114:GLN:NE2	2.70	0.59
1:G:375:SER:OG	1:G:384:TYR:CE1	2.55	0.59
3:H:2:VAL:HB	3:H:102:TYR:CE1	2.36	0.59
4:L:11:LEU:CD1	4:L:12:SER:N	2.65	0.59
4:L:85:THR:HG23	4:L:103:ARG:CB	2.32	0.59
4:L:132:VAL:HG12	4:L:148:TRP:CZ3	2.36	0.59
4:D:189:HIS:HB2	4:D:192:TYR:OH	2.02	0.59
1:G:217:TYR:N	1:G:248:THR:OG1	2.27	0.59
3:H:94:THR:O	3:H:100(F):PHE:HA	2.03	0.59
1:G:105:GLN:O	1:G:109:ILE:HG12	2.03	0.59
1:A:336:THR:O	1:A:340:LYS:HB2	2.03	0.59
1:G:362:GLN:HG3	1:G:363:PRO:HD3	1.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:136:LEU:CD2	4:L:196:VAL:HG22	2.07	0.59
4:L:193:ALA:HB2	4:L:206:THR:HG23	1.85	0.59
3:H:163:VAL:HG22	3:H:182:VAL:CG2	2.32	0.59
4:L:108:ARG:CG	4:L:109:ALA:N	2.65	0.59
1:A:392:ASN:C	1:A:394:THR:N	2.61	0.59
3:C:49:GLY:HA3	3:C:69:MET:HE1	1.83	0.59
3:C:59:TYR:CD1	3:C:69:MET:HE1	2.36	0.59
4:D:33:LEU:CD2	4:D:71:PHE:CD1	2.73	0.59
1:G:109:ILE:HG23	1:G:428:GLN:HG2	1.85	0.59
1:G:273:ARG:HH21	1:G:287:HIS:CG	2.20	0.59
1:G:450:THR:O	1:G:450:THR:OG1	2.18	0.59
4:L:120:PRO:HD2	4:L:207:LYS:NZ	2.18	0.59
1:A:65:VAL:CB	1:A:208:ILE:HD13	2.33	0.59
3:H:38:ARG:HB3	3:H:90:TYR:CD1	2.37	0.59
1:A:392:ASN:CG	5:A:509:NAG:H82	2.28	0.59
3:H:10:GLU:HB2	3:H:109:VAL:HG22	1.84	0.59
1:A:254:VAL:CG2	1:A:261:LEU:HD13	2.33	0.59
3:C:39:GLN:C	3:C:88:ALA:HB1	2.28	0.59
1:G:286:VAL:O	1:G:451:GLY:HA2	2.02	0.58
4:L:16:GLY:HA2	4:L:77:SER:HA	1.85	0.58
4:D:37:GLN:CG	4:D:86:TYR:HE1	2.16	0.58
3:H:4:LEU:HD21	3:H:24:ALA:HB2	1.82	0.58
3:H:198:VAL:CG2	3:H:207:VAL:O	2.51	0.58
4:D:48:ILE:HG22	4:D:48:ILE:O	2.02	0.58
4:D:71:PHE:C	4:D:72:THR:OG1	2.46	0.58
1:G:88:ASN:O	1:G:240:LYS:HE2	2.03	0.58
1:G:116:LEU:HD21	1:G:210:PHE:CE2	2.37	0.58
4:D:2:ILE:HG22	4:D:26:SER:HG	1.66	0.58
1:G:423:ILE:C	1:G:424:ILE:HG23	2.29	0.58
1:A:385:CYS:HA	1:A:418:CYS:HA	1.85	0.58
1:G:49:ASP:OD1	1:G:99:ASN:ND2	2.37	0.58
1:G:270:ILE:HD11	1:G:345:VAL:CG2	2.31	0.58
3:H:151:THR:HB	3:H:199:ASN:HB3	1.84	0.58
3:C:184:VAL:CG2	3:C:194:TYR:CE2	2.85	0.58
4:D:125:VAL:HA	4:D:130:VAL:CG1	2.33	0.58
1:G:211:ASP:OD1	5:G:503:NAG:H4	2.02	0.58
1:G:448:ASN:O	1:G:450:THR:HG22	2.04	0.58
3:H:96:ARG:HD3	3:H:98:ILE:HG23	1.85	0.58
3:H:189:LEU:HD12	3:H:191:THR:HG23	1.85	0.58
4:D:19:VAL:HG11	4:D:104:LEU:HD21	1.84	0.58
4:D:83:VAL:CG1	4:D:106:ILE:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:ALA:O	2:N:29:U2X:HB3	2.03	0.58
3:H:84:SER:OG	3:H:111:VAL:O	2.21	0.58
4:L:136:LEU:HD11	4:L:146:VAL:CG2	2.33	0.58
1:G:83:GLU:HG3	1:G:245:VAL:HG22	1.86	0.58
1:G:358:THR:O	1:G:466:GLU:N	2.33	0.58
1:G:388:THR:C	1:G:390:LEU:N	2.60	0.58
4:L:61:ARG:O	4:L:75:ILE:HA	2.04	0.58
3:C:123:PRO:HD3	3:C:209:LYS:CE	2.34	0.58
1:G:223:TYR:CD2	1:G:490:GLN:HA	2.39	0.58
4:L:48:ILE:HD11	4:L:64:GLY:H	1.64	0.58
4:L:128:GLY:HA2	4:L:183:ASN:OD1	2.03	0.58
3:C:24:ALA:HB1	3:C:27:TYR:HE2	1.67	0.58
4:D:1:ALA:HB2	4:D:95:PRO:HD3	1.85	0.58
4:D:117:ILE:HG12	4:D:207:LYS:HG2	1.85	0.58
1:G:116:LEU:CG	1:G:210:PHE:HE2	2.17	0.58
1:G:270:ILE:CD1	1:G:345:VAL:CG2	2.82	0.58
1:G:456:ARG:HH11	1:G:456:ARG:CG	2.16	0.58
1:G:462:ASN:OD1	1:G:462:ASN:N	2.29	0.58
3:H:54:THR:O	3:H:54:THR:OG1	2.13	0.58
3:H:100(D):ARG:O	4:L:91:TYR:HB2	2.04	0.58
4:L:48:ILE:HD13	4:L:64:GLY:N	2.14	0.58
4:L:109:ALA:O	4:L:111:ALA:N	2.37	0.58
1:A:291:SER:OG	1:A:448:ASN:CG	2.47	0.58
3:C:100(D):ARG:C	4:D:91:TYR:HD1	2.12	0.58
4:L:33:LEU:HD22	4:L:71:PHE:CE2	2.39	0.57
3:C:123:PRO:HD3	3:C:209:LYS:HZ2	1.69	0.57
1:G:232:ASN:OD1	1:G:268:GLU:CB	2.52	0.57
3:H:80:MET:O	3:H:80:MET:HE3	2.04	0.57
1:A:227:LYS:CG	1:A:486:TYR:HE1	2.14	0.57
3:C:2:VAL:HG11	3:C:102:TYR:HE1	1.59	0.57
3:C:66:ARG:CD	3:C:82(A):SER:O	2.52	0.57
4:D:163:VAL:CG1	4:D:175:LEU:HD12	2.32	0.57
1:G:227:LYS:HB2	1:G:486:TYR:CD1	2.38	0.57
4:L:120:PRO:HG2	4:L:186:TYR:OH	2.03	0.57
1:A:285:ILE:HD11	1:A:477:ASP:HB3	1.85	0.57
1:G:272:ILE:HD12	1:G:272:ILE:N	2.08	0.57
1:G:299:PRO:CD	1:G:330:TYR:HE2	2.17	0.57
4:L:132:VAL:O	4:L:148:TRP:CH2	2.57	0.57
1:A:229:ASN:ND2	5:A:502:NAG:O5	2.36	0.57
1:A:234:ASN:HA	1:A:273:ARG:HE	1.69	0.57
4:D:105:GLU:HG3	4:D:166:GLN:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:TRP:CE3	3:H:196:CYS:CA	2.87	0.57
3:H:166:PHE:HD2	3:H:179:SER:O	1.87	0.57
1:A:272:ILE:HD13	1:A:272:ILE:O	2.05	0.57
1:G:96:TRP:CZ2	1:G:274:SER:HA	2.39	0.57
3:H:117:LYS:HG2	3:H:175:LEU:HD13	1.86	0.57
1:A:117:GLN:OE1	1:A:118:PRO:HD2	2.04	0.57
1:A:349:LEU:HD23	1:A:468:PHE:CE2	2.40	0.57
1:G:95:MET:HG2	1:G:235:GLY:HA3	1.85	0.57
3:H:6:GLN:NE2	3:H:90:TYR:O	2.38	0.57
3:H:96:ARG:HD2	3:H:98:ILE:HD13	1.86	0.57
1:A:266:ALA:HB2	1:A:287:HIS:ND1	2.20	0.57
3:C:6:GLN:OE1	3:C:91:TYR:HA	2.05	0.57
3:C:59:TYR:HD1	3:C:69:MET:HE1	1.69	0.57
4:D:187:GLN:HA	4:D:187:GLN:NE2	2.13	0.57
4:D:192:TYR:O	4:D:207:LYS:HG3	2.04	0.57
4:L:170:ASP:OD2	4:L:170:ASP:N	2.38	0.57
3:C:4:LEU:HD21	3:C:102:TYR:O	2.05	0.57
4:D:87:TYR:HD1	4:D:101:GLY:HA2	1.69	0.57
4:D:185:ASP:O	4:D:188:SER:OG	2.22	0.57
1:A:256:SER:CB	1:A:261:LEU:HD11	2.35	0.57
1:G:93:PHE:HE2	1:G:487:LYS:HB3	1.69	0.56
1:G:95:MET:SD	1:G:235:GLY:HA3	2.45	0.56
1:A:227:LYS:HG3	1:A:486:TYR:CE1	2.34	0.56
4:L:43:VAL:CG2	4:L:44:PRO:HD2	2.33	0.56
3:C:87:THR:HG23	3:C:111:VAL:CG2	2.18	0.56
1:G:72:HIS:C	1:G:74:CYS:H	2.13	0.56
1:G:239:CYS:O	1:G:240:LYS:C	2.48	0.56
1:G:357:LYS:NZ	1:G:460:ALA:O	2.34	0.56
4:L:4:MET:HE1	4:L:90:LYS:HB3	1.86	0.56
4:L:106:ILE:HG21	4:L:171:ASN:HB3	1.87	0.56
1:A:258:GLN:NE2	1:A:387:THR:OG1	2.38	0.56
3:C:38:ARG:HB3	3:C:90:TYR:CE1	2.40	0.56
3:C:41:PRO:CD	3:C:88:ALA:HA	2.36	0.56
3:C:95:TYR:CE2	3:C:100(D):ARG:O	2.58	0.56
4:D:32:TYR:HB3	4:D:91:TYR:CE2	2.40	0.56
4:D:125:VAL:O	4:D:183:ASN:ND2	2.37	0.56
1:A:387:THR:CG2	1:A:390:LEU:CD1	2.74	0.56
3:C:61:GLN:HA	3:C:61:GLN:HE21	1.70	0.56
4:D:142:ARG:HB2	4:D:173:TYR:HD2	1.53	0.56
3:H:137:ALA:HB3	4:L:116:PHE:CE2	2.40	0.56
3:H:197:ASN:OD1	3:H:208:ASP:OD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:6:GLN:HE22	4:L:87:TYR:CA	2.11	0.56
1:A:65:VAL:CG1	1:A:115:SER:OG	2.54	0.56
1:A:353:PHE:N	1:A:353:PHE:CD1	2.72	0.56
3:H:154:TRP:CE3	3:H:154:TRP:HA	2.40	0.56
1:A:207:LYS:O	1:A:208:ILE:CG2	2.54	0.56
1:A:208:ILE:HD12	1:A:208:ILE:O	2.05	0.56
1:A:217:TYR:O	1:A:247:CYS:HA	2.05	0.56
3:C:152:VAL:HB	3:C:198:VAL:CG2	2.35	0.56
4:D:186:TYR:CD1	4:D:192:TYR:CE2	2.94	0.56
3:H:117:LYS:O	3:H:145:TYR:HA	2.06	0.56
1:G:117:GLN:HE21	1:G:203:GLN:HG3	1.62	0.56
1:G:415:THR:O	1:G:415:THR:HG22	2.06	0.56
1:A:288:LEU:HD12	1:A:450:THR:C	2.30	0.56
1:A:390:LEU:HD23	1:A:414:ILE:HG21	1.88	0.56
1:G:78:ASP:OD2	4:L:93:SER:CB	2.54	0.56
1:A:362:GLN:NE2	1:A:467:THR:OG1	2.39	0.56
3:H:171:GLN:OE1	4:L:160:GLN:HG3	2.04	0.56
1:A:50:THR:HG23	1:A:50:THR:O	2.05	0.56
4:D:18:LYS:HA	4:D:75:ILE:O	2.06	0.56
1:A:44:VAL:HG13	1:A:492:GLU:HB2	1.86	0.55
4:D:106:ILE:O	4:D:106:ILE:HG22	2.05	0.55
3:H:18:VAL:HG12	3:H:82(C):LEU:HD11	1.89	0.55
3:H:100(F):PHE:N	4:L:36:TYR:OH	2.39	0.55
3:H:201:LYS:HB2	3:H:202:PRO:HD3	1.88	0.55
1:A:229:ASN:O	5:A:502:NAG:H61	2.07	0.55
3:C:166:PHE:CD1	4:D:162:SER:O	2.59	0.55
4:D:49:TYR:C	4:D:49:TYR:CD1	2.85	0.55
1:G:299:PRO:CG	1:G:330:TYR:HE2	2.19	0.55
3:H:154:TRP:CZ2	3:H:196:CYS:HB3	2.38	0.55
1:A:56:SER:HB3	1:A:70:ALA:HB1	1.89	0.55
1:A:260:LEU:N	1:A:451:GLY:O	2.31	0.55
4:D:85:THR:HG23	4:D:103:ARG:CA	2.35	0.55
4:D:87:TYR:HD1	4:D:101:GLY:CA	2.19	0.55
1:G:102:GLU:OE1	1:G:476:LYS:NZ	2.40	0.55
1:G:453:LEU:O	1:G:471:GLY:N	2.26	0.55
3:H:61:GLN:O	3:H:64:GLN:CB	2.53	0.55
4:D:87:TYR:CD1	4:D:101:GLY:HA2	2.40	0.55
4:L:129:THR:O	4:L:129:THR:OG1	2.22	0.55
1:A:58:ALA:HB2	1:A:70:ALA:HB3	1.89	0.55
4:D:48:ILE:HD13	4:D:64:GLY:N	2.22	0.55
1:G:373:MET:SD	1:G:386:ASN:CA	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:TYR:N	1:A:417:PRO:O	2.39	0.55
4:D:37:GLN:CG	4:D:86:TYR:CE1	2.90	0.55
1:G:456:ARG:HG2	1:G:456:ARG:NH1	2.20	0.55
3:H:136:ALA:N	3:H:186:SER:O	2.38	0.55
1:A:97:LYS:HA	1:A:97:LYS:CE	2.37	0.55
1:G:50:THR:O	1:G:103:GLN:NE2	2.40	0.55
3:H:135:THR:HA	3:H:186:SER:C	2.31	0.55
3:H:137:ALA:CB	4:L:116:PHE:CE2	2.90	0.55
3:H:211:VAL:HG22	3:H:211:VAL:O	2.06	0.55
3:C:3:GLN:O	3:C:3:GLN:HG2	2.07	0.55
4:D:31:ASN:ND2	4:D:68:GLY:H	2.04	0.55
4:L:156:THR:O	4:L:158:ASN:ND2	2.40	0.55
3:C:37:VAL:HG22	3:C:46:GLU:O	2.06	0.55
3:C:40:ALA:HA	3:C:88:ALA:HB1	1.85	0.55
3:C:206:LYS:N	3:C:206:LYS:HD2	2.22	0.55
2:N:3:LEU:HD13	2:N:19:CYS:SG	2.47	0.55
4:L:85:THR:HA	4:L:102:THR:O	2.07	0.55
4:L:199:GLN:NE2	4:L:199:GLN:CA	2.70	0.55
1:A:225:ILE:HG22	1:A:225:ILE:O	2.06	0.55
1:A:407:MET:SD	1:A:407:MET:N	2.79	0.55
1:A:413:THR:O	1:A:413:THR:HG22	2.04	0.55
4:D:125:VAL:HA	4:D:183:ASN:HD21	1.72	0.55
4:L:151:ASP:OD2	4:L:189:HIS:CB	2.54	0.54
3:C:163:VAL:O	3:C:163:VAL:HG12	2.06	0.54
1:G:93:PHE:CE2	1:G:487:LYS:HB3	2.41	0.54
1:G:106:GLU:HA	1:G:109:ILE:HG13	1.89	0.54
1:G:263:GLY:H	1:G:450:THR:HG21	1.73	0.54
1:A:57:ASP:OD1	1:A:77:THR:CB	2.53	0.54
1:G:47:ASP:HB3	1:G:487:LYS:HE3	1.90	0.54
1:G:474:ASN:HB3	1:G:477:ASP:OD2	2.07	0.54
1:A:68:VAL:O	1:A:69:TRP:C	2.50	0.54
1:A:387:THR:HG23	1:A:390:LEU:HD12	1.87	0.54
1:G:119:CYS:HB2	1:G:434:MET:HE3	1.89	0.54
1:G:388:THR:HG21	5:G:508:NAG:C1	2.38	0.54
1:A:291:SER:OG	1:A:448:ASN:HB3	2.07	0.54
3:H:181:VAL:HG22	4:L:135:LEU:CD2	2.33	0.54
1:A:238:PRO:O	1:A:239:CYS:CB	2.45	0.54
3:C:2:VAL:HA	3:C:26:GLY:HA3	1.90	0.54
3:C:40:ALA:CA	3:C:88:ALA:HB2	2.31	0.54
4:D:163:VAL:HG12	4:D:175:LEU:CD1	2.37	0.54
1:G:259:LEU:HD22	1:G:449:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:ILE:HG13	1:G:360:ILE:O	2.07	0.54
3:H:163:VAL:O	3:H:163:VAL:HG12	2.06	0.54
4:L:29:PHE:N	4:L:29:PHE:CD1	2.76	0.54
1:A:294:ILE:HG23	1:A:294:ILE:O	2.07	0.54
3:C:150:VAL:HG11	3:C:178:LEU:HD21	1.89	0.54
3:C:156:SER:O	3:C:156:SER:OG	2.11	0.54
3:H:144:ASP:HA	3:H:175:LEU:HB3	1.87	0.54
4:L:62:PHE:CD1	4:L:75:ILE:HD12	2.43	0.54
1:A:95:MET:N	1:A:235:GLY:O	2.40	0.54
4:D:20:THR:O	4:D:20:THR:OG1	2.21	0.54
3:H:20:LEU:HD12	3:H:80:MET:CE	2.38	0.54
3:H:119:PRO:CG	3:H:142:VAL:CG1	2.86	0.54
4:L:117:ILE:HD11	4:L:205:VAL:O	2.08	0.54
4:L:132:VAL:CG1	4:L:148:TRP:CZ3	2.91	0.54
4:L:160:GLN:OE1	4:L:160:GLN:HA	2.08	0.54
1:A:409:GLY:O	1:A:410:CYS:O	2.25	0.54
4:D:132:VAL:HG22	4:D:132:VAL:O	2.07	0.54
4:L:49:TYR:C	4:L:49:TYR:CD1	2.85	0.54
3:C:30:THR:HA	3:C:52(A):PRO:HB2	1.89	0.54
3:C:189:LEU:HD13	3:C:194:TYR:OH	2.08	0.54
1:G:388:THR:O	1:G:390:LEU:N	2.41	0.54
1:G:123:THR:O	1:G:124:GLY:C	2.51	0.53
3:H:10:GLU:O	3:H:110:THR:N	2.31	0.53
1:A:233:PHE:CE1	1:A:235:GLY:C	2.85	0.53
3:C:84:SER:O	3:C:87:THR:HG23	2.08	0.53
4:D:48:ILE:HD11	4:D:64:GLY:N	2.23	0.53
3:H:33:ASP:HA	3:H:52(A):PRO:HD3	1.90	0.53
3:H:100(D):ARG:HD2	4:L:92:ASN:O	2.08	0.53
4:D:160:GLN:HG3	4:D:160:GLN:O	2.08	0.53
3:H:135:THR:H	3:H:186:SER:CA	2.18	0.53
4:D:176:SER:O	4:D:176:SER:OG	2.24	0.53
3:H:40:ALA:HA	3:H:88:ALA:HB2	1.91	0.53
4:D:31:ASN:HD21	4:D:68:GLY:HA2	1.72	0.53
3:H:95:TYR:CE1	3:H:100(D):ARG:HB2	2.44	0.53
3:H:95:TYR:HA	3:H:100(E):TYR:O	2.09	0.53
4:L:117:ILE:HG13	4:L:205:VAL:CG2	2.30	0.53
4:L:136:LEU:CD2	4:L:196:VAL:HG21	2.37	0.53
1:A:286:VAL:HB	1:A:452:ILE:HD12	1.89	0.53
3:C:136:ALA:HB3	3:C:184:VAL:O	2.09	0.53
3:C:154:TRP:CD1	3:C:163:VAL:HG21	2.44	0.53
1:G:120:VAL:CB	1:G:434:MET:CE	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:475:ILE:O	1:G:476:LYS:C	2.50	0.53
3:H:135:THR:HA	3:H:186:SER:CA	2.38	0.53
1:A:115:SER:C	1:A:116:LEU:HG	2.33	0.53
1:A:376:PHE:CZ	1:A:383:PHE:HD1	2.26	0.53
3:C:33:ASP:CB	3:C:95:TYR:HE1	2.22	0.53
3:C:50:TRP:CD1	4:D:94:ALA:HB2	2.43	0.53
4:L:136:LEU:HD21	4:L:196:VAL:CB	2.39	0.53
1:A:294:ILE:HG22	1:A:447:SER:O	2.08	0.53
1:A:394:THR:C	1:A:396:ILE:HG23	2.32	0.53
3:C:142:VAL:HG13	3:C:198:VAL:HG11	1.90	0.53
4:D:192:TYR:CB	4:D:207:LYS:HD3	2.30	0.53
1:G:388:THR:C	1:G:390:LEU:H	2.14	0.53
4:L:110:VAL:O	4:L:110:VAL:HG12	2.08	0.53
3:C:100(B):GLY:CA	4:D:32:TYR:HE1	2.22	0.53
3:C:100(B):GLY:O	4:D:32:TYR:HE1	1.91	0.53
4:D:9:SER:HA	4:D:102:THR:HA	1.89	0.53
1:A:233:PHE:HE1	1:A:235:GLY:HA2	1.73	0.53
1:A:362:GLN:HG2	1:A:469:ARG:HB2	1.91	0.53
3:C:124:LEU:C	4:D:118:PHE:HE1	2.15	0.53
4:D:87:TYR:CD1	4:D:101:GLY:CA	2.91	0.53
3:H:30:THR:HG21	3:H:53:LYS:HD2	1.89	0.53
3:H:33:ASP:HB2	3:H:95:TYR:CE2	2.43	0.53
1:A:350:LYS:C	1:A:350:LYS:HD2	2.33	0.53
4:D:31:ASN:HD21	4:D:68:GLY:CA	2.22	0.53
4:L:33:LEU:HD23	4:L:71:PHE:CB	2.38	0.52
4:L:85:THR:CG2	4:L:103:ARG:N	2.60	0.52
4:L:124:GLN:OE1	4:L:131:SER:N	2.30	0.52
1:A:93:PHE:HE2	1:A:487:LYS:HB3	1.74	0.52
1:A:414:ILE:HD12	1:A:414:ILE:H	1.74	0.52
4:D:32:TYR:HB3	4:D:91:TYR:CD2	2.44	0.52
3:H:9:ALA:HB1	3:H:108:LEU:HB3	1.91	0.52
1:A:117:GLN:HG3	1:A:118:PRO:HD2	1.91	0.52
1:A:257:THR:OG1	1:A:375:SER:O	2.26	0.52
1:A:258:GLN:HE21	1:A:374:HIS:H	1.57	0.52
1:G:119:CYS:O	1:G:203:GLN:N	2.26	0.52
4:L:157:GLY:O	4:L:159:SER:N	2.42	0.52
4:L:199:GLN:HA	4:L:199:GLN:HE21	1.71	0.52
3:C:33:ASP:HB2	3:C:95:TYR:HE1	1.73	0.52
4:D:5:THR:HA	4:D:100:GLN:HE22	1.75	0.52
3:H:38:ARG:HB2	3:H:90:TYR:CD1	2.44	0.52
4:L:85:THR:HG23	4:L:103:ARG:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:106:ILE:CG2	4:L:171:ASN:HB3	2.39	0.52
4:L:199:GLN:C	4:L:199:GLN:CD	2.78	0.52
1:A:91:GLU:CD	1:A:487:LYS:NZ	2.67	0.52
1:A:95:MET:HE1	1:A:273:ARG:CD	2.39	0.52
1:A:258:GLN:OE1	1:A:372:THR:O	2.26	0.52
1:A:297:THR:HB	1:A:299:PRO:HD3	1.90	0.52
3:C:4:LEU:HD13	3:C:103:TRP:C	2.35	0.52
3:C:60:ALA:O	3:C:64:GLN:N	2.43	0.52
1:G:121:LYS:HE3	1:G:426:MET:HE3	1.91	0.52
1:G:374:HIS:CE1	1:G:376:PHE:CE2	2.98	0.52
1:A:258:GLN:OE1	1:A:470:PRO:HB3	2.07	0.52
1:G:121:LYS:HB3	1:G:201:ILE:HG12	1.90	0.52
1:A:225:ILE:HG21	1:A:245:VAL:CG2	2.38	0.52
1:A:338:TRP:NE1	1:A:390:LEU:HB3	2.17	0.52
1:A:388:THR:HG21	5:A:508:NAG:O5	2.10	0.52
3:C:124:LEU:HB3	4:D:118:PHE:CE1	2.45	0.52
1:G:490:GLN:O	1:G:490:GLN:HG2	2.10	0.52
3:H:30:THR:HG22	3:H:53:LYS:HD2	1.90	0.52
3:H:40:ALA:O	3:H:43:GLN:CB	2.57	0.52
4:L:146:VAL:HG11	4:L:177:SER:HB2	1.92	0.52
3:C:27:TYR:OH	3:C:94:THR:HG21	2.09	0.52
1:G:446:VAL:HG11	5:G:506:NAG:C8	2.39	0.52
3:H:9:ALA:HB1	3:H:108:LEU:O	2.10	0.52
4:L:155:LYS:NZ	4:L:181:LEU:HD11	2.25	0.52
4:D:142:ARG:HG2	4:D:142:ARG:O	2.09	0.52
4:L:108:ARG:NE	4:L:170:ASP:O	2.43	0.52
1:A:270:ILE:HG13	5:A:505:NAG:C6	2.39	0.52
1:A:338:TRP:CH2	1:A:342:LEU:HD21	2.45	0.52
3:C:62:LYS:N	3:C:62:LYS:HD3	2.24	0.52
3:H:17:SER:HG	3:H:82(A):SER:HA	1.68	0.51
3:H:111:VAL:O	3:H:111:VAL:HG12	2.10	0.51
1:A:239:CYS:O	1:A:240:LYS:C	2.51	0.51
4:D:151:ASP:HA	4:D:191:VAL:HB	1.91	0.51
1:G:84:ILE:CD1	3:H:100(A):VAL:HG12	2.34	0.51
2:N:19:CYS:HB3	2:N:21:DPR:HD3	1.93	0.51
3:C:145:TYR:HD1	3:C:176:TYR:O	1.93	0.51
4:D:201:LEU:H	4:D:201:LEU:HD22	1.75	0.51
3:H:166:PHE:HD2	3:H:179:SER:HB2	1.75	0.51
4:L:32:TYR:C	4:L:91:TYR:HE2	2.19	0.51
4:L:108:ARG:HG3	4:L:108:ARG:HH11	1.75	0.51
4:D:80:PRO:HA	4:D:106:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:VAL:HG11	4:D:177:SER:HB3	1.92	0.51
1:G:56:SER:O	1:G:77:THR:OG1	2.23	0.51
1:G:423:ILE:C	1:G:424:ILE:CG2	2.83	0.51
3:C:206:LYS:N	3:C:206:LYS:CD	2.74	0.51
1:G:299:PRO:CD	1:G:330:TYR:CE2	2.94	0.51
4:L:13:ALA:HB1	4:L:78:LEU:HD23	1.92	0.51
1:A:362:GLN:HG3	1:A:363:PRO:CD	2.39	0.51
1:A:369:LEU:HD11	1:A:384:TYR:CE1	2.45	0.51
1:A:385:CYS:N	1:A:418:CYS:SG	2.84	0.51
1:G:221:ALA:HB2	4:L:31:ASN:O	2.10	0.51
1:G:341:VAL:HG13	1:G:341:VAL:O	2.08	0.51
3:H:36:TRP:HB2	3:H:69:MET:HE3	1.92	0.51
3:H:39:GLN:HG3	3:H:44:GLY:O	2.10	0.51
4:L:120:PRO:HD2	4:L:207:LYS:HZ1	1.75	0.51
1:A:362:GLN:OE1	1:A:365:SER:OG	2.29	0.51
1:G:332:GLU:HA	1:G:414:ILE:O	2.11	0.51
1:G:338:TRP:CZ2	1:G:342:LEU:CD2	2.91	0.51
2:N:16:LEU:O	2:N:32:CYS:HA	2.10	0.51
4:L:136:LEU:HD21	4:L:196:VAL:CG1	2.41	0.51
1:A:97:LYS:CE	1:A:97:LYS:CA	2.88	0.51
1:A:207:LYS:C	1:A:208:ILE:HG23	2.36	0.51
3:C:35:ASN:ND2	3:C:47:TRP:NE1	2.55	0.51
3:C:100(E):TYR:CD2	4:D:91:TYR:CE1	2.97	0.51
4:L:194:CYS:O	4:L:204:PRO:HA	2.10	0.51
4:D:186:TYR:CE1	4:D:192:TYR:CE2	2.98	0.51
1:G:487:LYS:NZ	5:A:506:NAG:H81	2.25	0.51
3:H:185:PRO:O	3:H:186:SER:C	2.52	0.51
4:L:115:VAL:CG2	4:L:203:SER:OG	2.59	0.51
4:L:191:VAL:O	4:L:191:VAL:HG22	2.10	0.51
1:A:223:TYR:CE2	1:A:490:GLN:OE1	2.64	0.51
1:A:450:THR:O	1:A:450:THR:OG1	2.26	0.51
4:D:5:THR:CA	4:D:100:GLN:HE22	2.24	0.51
3:H:96:ARG:NE	3:H:100(C):TYR:CD1	2.77	0.50
4:L:13:ALA:C	4:L:14:SER:O	2.52	0.50
3:C:125:ALA:HB1	3:C:213:ILE:HA	1.92	0.50
1:G:249:HIS:ND1	1:G:486:TYR:OH	2.22	0.50
3:H:138:LEU:HA	4:L:118:PHE:HE2	1.76	0.50
1:A:117:GLN:HG3	1:A:118:PRO:CD	2.42	0.50
1:A:298:ARG:HH12	1:A:440:ASP:HA	1.76	0.50
3:C:47:TRP:CE2	4:D:96:PHE:HD2	2.29	0.50
1:G:224:VAL:HG22	3:H:100(A):VAL:HG21	1.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:ASP:OD1	1:G:239:CYS:C	2.54	0.50
4:L:4:MET:HE1	4:L:89:GLN:C	2.36	0.50
1:A:265:LEU:HD22	1:A:288:LEU:O	2.12	0.50
1:A:275:GLU:HB3	1:A:282:LYS:HG3	1.92	0.50
4:D:183:ASN:HA	4:D:186:TYR:HB3	1.94	0.50
3:H:166:PHE:CD2	3:H:179:SER:O	2.64	0.50
1:A:350:LYS:O	1:A:353:PHE:O	2.30	0.50
3:C:37:VAL:CG2	3:C:46:GLU:C	2.83	0.50
1:G:329:ALA:O	1:G:417:PRO:O	2.29	0.50
1:G:434:MET:O	1:G:434:MET:HG2	2.11	0.50
4:L:3:GLN:CB	4:L:26:SER:OG	2.57	0.50
4:L:12:SER:O	4:L:105:GLU:HB2	2.12	0.50
1:A:86:LEU:N	1:A:86:LEU:HD23	2.26	0.50
1:A:446:VAL:O	1:A:446:VAL:HG12	2.12	0.50
3:C:38:ARG:HB2	3:C:90:TYR:CE1	2.42	0.50
3:C:67:VAL:HA	3:C:81:GLU:O	2.12	0.50
1:A:59:LYS:HD2	1:A:59:LYS:N	2.20	0.50
1:A:456:ARG:HD2	1:A:468:PHE:HE1	1.76	0.50
3:C:201:LYS:O	3:C:204:ASN:N	2.45	0.50
4:L:6:GLN:NE2	4:L:87:TYR:HA	2.12	0.50
1:A:91:GLU:OE2	1:A:487:LYS:NZ	2.44	0.50
5:A:505:NAG:H3	5:A:505:NAG:H83	1.93	0.50
3:H:96:ARG:CD	3:H:98:ILE:HG23	2.38	0.50
4:L:166:GLN:HB2	4:L:173:TYR:CE1	2.47	0.50
1:A:286:VAL:O	1:A:451:GLY:HA2	2.12	0.50
1:A:344:GLN:NE2	5:A:505:NAG:O4	2.45	0.50
1:A:387:THR:CA	1:A:416:LEU:HD23	2.40	0.50
4:L:69:THR:HG23	4:L:70:ASP:OD1	2.11	0.50
1:A:112:TRP:CH2	1:A:382:PHE:CZ	2.99	0.50
1:A:338:TRP:HA	1:A:338:TRP:CE3	2.47	0.50
3:C:61:GLN:HE21	3:C:61:GLN:CA	2.25	0.50
1:G:120:VAL:CG2	1:G:434:MET:CE	2.90	0.49
3:H:119:PRO:HB2	3:H:142:VAL:HG13	1.89	0.49
3:H:135:THR:OG1	3:H:186:SER:N	2.41	0.49
3:H:150:VAL:HG11	3:H:178:LEU:HD21	1.93	0.49
1:A:256:SER:HB3	1:A:261:LEU:HD11	1.94	0.49
1:A:358:THR:O	1:A:465:ASN:HA	2.12	0.49
1:G:335:GLY:HA2	1:G:338:TRP:HB3	1.94	0.49
1:G:358:THR:O	1:G:465:ASN:HA	2.12	0.49
3:H:135:THR:O	4:L:116:PHE:CZ	2.56	0.49
3:H:153:SER:O	3:H:197:ASN:ND2	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:CYS:O	1:A:248:THR:O	2.30	0.49
1:A:272:ILE:HD13	1:A:272:ILE:N	2.20	0.49
3:C:29:PHE:CD1	3:C:76:SER:HA	2.47	0.49
3:C:200:HIS:ND1	3:C:203:SER:OG	2.34	0.49
1:G:45:TRP:HB2	1:G:489:VAL:HG12	1.94	0.49
1:G:52:LEU:HD11	1:G:219:THR:HG22	1.94	0.49
1:G:105:GLN:OE1	1:G:105:GLN:HA	2.12	0.49
1:G:234:ASN:HA	1:G:273:ARG:HD3	1.94	0.49
3:H:6:GLN:H	3:H:105:GLN:HG2	1.76	0.49
3:H:40:ALA:O	3:H:43:GLN:N	2.44	0.49
3:H:150:VAL:HG12	3:H:178:LEU:HD21	1.91	0.49
3:H:166:PHE:O	3:H:167:PRO:C	2.55	0.49
4:L:186:TYR:HD1	4:L:192:TYR:OH	1.95	0.49
1:G:97:LYS:O	5:A:506:NAG:O3	2.22	0.49
3:H:39:GLN:C	3:H:88:ALA:HB1	2.38	0.49
4:L:37:GLN:HB2	4:L:86:TYR:HE1	1.68	0.49
1:A:387:THR:HG22	1:A:390:LEU:CG	2.41	0.49
3:C:68:THR:O	3:C:68:THR:OG1	2.22	0.49
4:L:130:VAL:HG21	4:L:186:TYR:CB	2.43	0.49
1:A:58:ALA:C	1:A:60:ALA:N	2.69	0.49
1:A:117:GLN:CG	1:A:118:PRO:HD2	2.42	0.49
1:A:361:PHE:HB3	1:A:391:PHE:HB3	1.95	0.49
1:A:469:ARG:HD3	1:A:469:ARG:C	2.38	0.49
4:D:32:TYR:O	4:D:91:TYR:HD2	1.93	0.49
4:D:91:TYR:CD2	4:D:91:TYR:N	2.79	0.49
3:H:82(B):SER:OG	3:H:82(B):SER:O	2.19	0.49
4:L:20:THR:O	4:L:20:THR:OG1	2.27	0.49
4:L:91:TYR:N	4:L:91:TYR:CD2	2.80	0.49
4:L:146:VAL:O	4:L:146:VAL:HG12	2.11	0.49
4:L:151:ASP:HA	4:L:191:VAL:CG1	2.41	0.49
1:A:265:LEU:HD23	1:A:450:THR:OG1	2.12	0.49
1:A:279:ASN:OD1	1:A:280:ASN:N	2.46	0.49
1:A:361:PHE:CB	1:A:391:PHE:HB3	2.43	0.49
1:A:376:PHE:CD1	1:A:376:PHE:C	2.87	0.49
3:C:32:TYR:OH	3:C:98:ILE:O	2.30	0.49
3:C:51:MET:HB3	3:C:51:MET:HE2	1.67	0.49
4:D:124:GLN:OE1	4:D:131:SER:N	2.38	0.49
1:G:83:GLU:CG	1:G:245:VAL:HG22	2.43	0.49
3:H:49:GLY:CA	3:H:69:MET:HE1	2.43	0.49
1:A:112:TRP:HH2	1:A:382:PHE:CZ	2.30	0.49
1:A:329:ALA:HB1	1:A:417:PRO:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:PRO:HG2	1:A:372:THR:HB	1.95	0.49
4:D:8:PRO:O	4:D:102:THR:OG1	2.30	0.49
1:G:217:TYR:O	1:G:247:CYS:HA	2.13	0.49
3:H:61:GLN:CA	3:H:64:GLN:HB2	2.43	0.49
3:H:68:THR:O	3:H:68:THR:HG22	2.13	0.49
1:A:223:TYR:HD2	1:A:490:GLN:HA	1.77	0.49
1:A:246:GLN:CG	3:C:100(A):VAL:HB	2.43	0.49
3:C:148:GLU:HG2	3:C:176:TYR:CD1	2.48	0.49
3:C:170:LEU:HD13	3:C:176:TYR:CZ	2.48	0.49
4:D:49:TYR:C	4:D:49:TYR:HD1	2.20	0.49
1:G:100:MET:CE	1:G:486:TYR:O	2.60	0.49
1:G:456:ARG:CG	1:G:456:ARG:NH1	2.75	0.49
1:G:225:ILE:O	1:G:225:ILE:HG22	2.13	0.49
4:L:89:GLN:HB2	4:L:98:PHE:CD2	2.47	0.49
1:A:68:VAL:CA	1:A:71:THR:HG23	2.36	0.49
3:C:11:VAL:HG12	3:C:110:THR:OG1	2.12	0.49
3:C:137:ALA:HB3	4:D:116:PHE:HD2	1.62	0.49
1:G:109:ILE:CG2	1:G:428:GLN:HG2	2.43	0.48
1:G:374:HIS:CE1	1:G:376:PHE:CD2	2.91	0.48
1:G:374:HIS:C	1:G:374:HIS:ND1	2.71	0.48
3:H:119:PRO:CB	3:H:145:TYR:HB3	2.43	0.48
1:A:296:CYS:HA	1:A:331:CYS:HA	1.94	0.48
1:A:298:ARG:NH1	1:A:440:ASP:HA	2.28	0.48
3:C:100(B):GLY:CA	4:D:32:TYR:CE1	2.96	0.48
3:C:100(B):GLY:O	4:D:32:TYR:CE1	2.66	0.48
4:D:4:MET:CE	4:D:97:THR:HG22	2.30	0.48
4:D:19:VAL:O	4:D:19:VAL:HG23	2.13	0.48
4:D:141:PRO:HD2	4:D:198:HIS:CE1	2.48	0.48
1:G:270:ILE:HG22	5:G:505:NAG:O6	2.13	0.48
1:G:383:PHE:HD2	1:G:420:ILE:HD13	1.68	0.48
3:H:195:VAL:HG22	3:H:210:ARG:HG3	1.95	0.48
4:L:157:GLY:C	4:L:159:SER:N	2.71	0.48
1:A:65:VAL:CG2	1:A:208:ILE:CD1	2.86	0.48
3:C:61:GLN:NE2	3:C:61:GLN:CA	2.76	0.48
4:D:89:GLN:HG2	4:D:90:LYS:H	1.78	0.48
1:G:116:LEU:HD13	1:G:210:PHE:HZ	1.75	0.48
1:G:468:PHE:C	1:G:469:ARG:HG3	2.38	0.48
3:H:137:ALA:N	4:L:116:PHE:CE2	2.81	0.48
4:D:37:GLN:NE2	4:D:86:TYR:OH	2.47	0.48
4:D:61:ARG:HD3	4:D:77:SER:O	2.12	0.48
4:D:117:ILE:HB	4:D:205:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:166:PHE:HE1	4:L:174:SER:O	1.96	0.48
3:H:38:ARG:NH1	3:H:90:TYR:OH	2.41	0.48
4:L:75:ILE:HG23	4:L:75:ILE:O	2.12	0.48
1:A:335:GLY:CA	1:A:414:ILE:HD12	2.29	0.48
1:A:338:TRP:HA	1:A:338:TRP:HE3	1.78	0.48
4:D:90:LYS:O	4:D:96:PHE:HA	2.13	0.48
4:D:195:GLU:HA	4:D:204:PRO:HA	1.94	0.48
1:G:480:ARG:NH1	1:G:480:ARG:CG	2.76	0.48
4:L:33:LEU:CD2	4:L:71:PHE:CD1	2.82	0.48
4:L:186:TYR:HE1	4:L:192:TYR:HE1	1.33	0.48
1:A:227:LYS:CG	1:A:486:TYR:CE1	2.95	0.48
1:A:359:ILE:HG21	1:A:468:PHE:CD2	2.38	0.48
3:C:154:TRP:CZ3	3:C:195:VAL:C	2.91	0.48
4:D:62:PHE:CE2	4:D:75:ILE:HD13	2.30	0.48
1:G:233:PHE:CE1	1:G:235:GLY:CA	2.94	0.48
1:G:473:GLY:HA2	2:N:29:U2X:CD2	2.42	0.48
3:H:4:LEU:O	3:H:104:GLY:HA2	2.14	0.48
1:A:225:ILE:CG2	1:A:245:VAL:HG23	2.43	0.48
1:A:377:ASN:CB	1:A:382:PHE:CD2	2.96	0.48
1:G:417:PRO:HB2	1:G:418:CYS:H	1.40	0.48
3:H:14:PRO:HA	3:H:82(C):LEU:O	2.14	0.48
1:A:299:PRO:CA	1:A:442:LYS:CD	2.90	0.48
4:D:1:ALA:CB	4:D:95:PRO:HD2	2.43	0.48
4:D:191:VAL:O	4:D:191:VAL:HG12	2.13	0.48
1:G:100:MET:CE	1:G:486:TYR:C	2.87	0.48
3:H:114:ALA:CB	3:H:146:PHE:CD2	2.97	0.48
4:L:108:ARG:HD3	4:L:171:ASN:HB2	1.96	0.48
1:A:44:VAL:HG12	1:A:492:GLU:OXT	2.14	0.48
1:A:94:ASN:HD21	1:A:97:LYS:HG3	1.72	0.48
1:A:111:LEU:C	1:A:111:LEU:CD2	2.86	0.48
1:A:354:ASN:OD1	1:A:354:ASN:N	2.46	0.48
1:A:382:PHE:O	1:A:420:ILE:HB	2.13	0.48
4:D:1:ALA:CB	4:D:95:PRO:CD	2.91	0.48
4:D:33:LEU:HD22	4:D:71:PHE:CG	2.43	0.48
4:L:62:PHE:CE1	4:L:75:ILE:CD1	2.96	0.48
1:A:291:SER:OG	1:A:448:ASN:CB	2.62	0.48
1:A:297:THR:HG23	1:A:444:ASN:HB2	1.95	0.48
1:A:364:PRO:CB	1:A:372:THR:CG2	2.82	0.48
3:C:136:ALA:O	3:C:184:VAL:N	2.45	0.48
3:C:196:CYS:O	3:C:208:ASP:HA	2.13	0.48
3:C:201:LYS:N	3:C:202:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:TRP:O	4:D:46:LEU:HD12	2.14	0.48
4:D:191:VAL:HG13	4:D:206:THR:CG2	2.43	0.48
1:G:121:LYS:HE3	1:G:426:MET:CE	2.44	0.47
1:G:299:PRO:CG	1:G:330:TYR:CE2	2.97	0.47
4:L:91:TYR:N	4:L:91:TYR:HD2	2.12	0.47
1:A:417:PRO:O	1:A:418:CYS:CB	2.62	0.47
1:A:456:ARG:HG2	1:A:468:PHE:HD1	1.77	0.47
3:C:16:ALA:H	3:C:82(C):LEU:HD13	1.79	0.47
3:C:40:ALA:CA	3:C:88:ALA:CB	2.83	0.47
4:D:107:LYS:NZ	4:D:107:LYS:CB	2.76	0.47
1:G:427:TRP:CE3	1:G:475:ILE:CG1	2.90	0.47
4:L:19:VAL:CG2	4:L:75:ILE:HG21	2.34	0.47
3:C:166:PHE:HD1	4:D:162:SER:O	1.96	0.47
1:G:343:LYS:O	1:G:346:THR:OG1	2.33	0.47
3:H:50:TRP:CD1	4:L:94:ALA:CB	2.96	0.47
3:H:197:ASN:ND2	3:H:197:ASN:N	2.62	0.47
4:L:11:LEU:HD13	4:L:12:SER:H	1.76	0.47
4:L:48:ILE:CD1	4:L:64:GLY:HA3	2.35	0.47
1:A:409:GLY:C	1:A:410:CYS:O	2.58	0.47
3:C:67:VAL:HG21	3:C:80:MET:HE2	1.95	0.47
3:C:124:LEU:C	4:D:118:PHE:CE1	2.93	0.47
1:G:53:PHE:CE2	1:G:218:CYS:HB3	2.49	0.47
4:L:5:THR:O	4:L:5:THR:OG1	2.24	0.47
1:A:296:CYS:HB3	1:A:383:PHE:HE1	1.74	0.47
1:A:353:PHE:N	1:A:353:PHE:HD1	2.12	0.47
3:C:95:TYR:HD2	3:C:100(D):ARG:C	2.21	0.47
1:G:205:CYS:HB3	1:G:436:ALA:HB2	1.95	0.47
1:A:97:LYS:HE3	1:A:97:LYS:CA	2.43	0.47
1:A:223:TYR:CZ	1:A:490:GLN:OE1	2.66	0.47
1:G:212:PRO:HB3	1:G:253:PRO:HD2	1.96	0.47
4:L:39:LYS:HE2	4:L:81:GLU:O	2.14	0.47
4:L:130:VAL:HG21	4:L:186:TYR:CG	2.49	0.47
1:A:264:SER:OG	1:A:482:GLU:CG	2.60	0.47
1:G:92:ASN:OD1	1:G:238:PRO:N	2.48	0.47
1:G:298:ARG:HB3	1:G:443:ILE:HG13	1.97	0.47
3:H:82:LEU:CD1	3:H:82:LEU:C	2.88	0.47
4:L:139:PHE:N	4:L:139:PHE:CD1	2.83	0.47
1:A:297:THR:CG2	1:A:443:ILE:O	2.63	0.47
3:C:35:ASN:ND2	3:C:100(F):PHE:CZ	2.83	0.47
4:D:21:ILE:CD1	4:D:73:LEU:HD23	2.44	0.47
4:D:128:GLY:O	4:D:182:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:201:LEU:HD22	4:D:201:LEU:N	2.28	0.47
4:D:207:LYS:NZ	4:D:207:LYS:CB	2.77	0.47
3:H:183:THR:HG21	4:L:137:ASN:ND2	2.30	0.47
1:A:335:GLY:CA	1:A:414:ILE:HD13	2.40	0.47
3:C:33:ASP:CB	3:C:95:TYR:CE1	2.98	0.47
3:C:34:ILE:HB	3:C:51:MET:HE2	1.96	0.47
3:C:145:TYR:CE1	3:C:176:TYR:HB2	2.49	0.47
4:D:5:THR:O	4:D:5:THR:OG1	2.27	0.47
1:A:80:ASN:ND2	1:A:80:ASN:C	2.73	0.47
3:C:6:GLN:HE21	3:C:6:GLN:HB3	1.52	0.47
3:C:166:PHE:HB3	3:C:167:PRO:CD	2.44	0.47
4:D:48:ILE:CD1	4:D:64:GLY:CA	2.88	0.47
1:A:350:LYS:C	1:A:350:LYS:CD	2.88	0.47
3:H:124:LEU:O	4:L:118:PHE:CE2	2.68	0.46
1:A:349:LEU:CD2	1:A:468:PHE:CE2	2.98	0.46
4:D:19:VAL:O	4:D:74:THR:CA	2.56	0.46
4:D:37:GLN:HA	4:D:86:TYR:CD1	2.50	0.46
4:D:125:VAL:C	4:D:183:ASN:HD21	2.22	0.46
1:G:371:ILE:H	1:G:371:ILE:HG13	1.55	0.46
4:L:186:TYR:HD1	4:L:192:TYR:CZ	2.33	0.46
1:A:482:GLU:O	1:A:485:LYS:NZ	2.48	0.46
3:H:123:PRO:C	3:H:124:LEU:HD23	2.40	0.46
4:L:62:PHE:CE1	4:L:75:ILE:HD12	2.49	0.46
1:A:95:MET:HE1	1:A:273:ARG:HG2	1.96	0.46
4:D:4:MET:CE	4:D:97:THR:O	2.59	0.46
1:G:84:ILE:HD13	3:H:100:ALA:C	2.40	0.46
1:G:219:THR:HG23	1:G:225:ILE:HD12	1.98	0.46
1:A:249:HIS:HD2	1:A:486:TYR:HE2	1.63	0.46
3:C:137:ALA:CB	4:D:116:PHE:CD2	2.74	0.46
1:G:52:LEU:HD21	1:G:225:ILE:HD11	1.98	0.46
3:H:167:PRO:HG2	4:L:163:VAL:O	2.15	0.46
3:H:171:GLN:OE1	4:L:160:GLN:NE2	2.44	0.46
1:A:61:HIS:C	1:A:61:HIS:HD1	2.24	0.46
1:A:112:TRP:CZ2	1:A:255:VAL:HG21	2.51	0.46
1:A:456:ARG:HG2	1:A:468:PHE:CE1	2.49	0.46
3:C:47:TRP:HZ2	3:C:50:TRP:HB3	1.81	0.46
4:D:141:PRO:HG3	4:D:199:GLN:HE22	1.78	0.46
1:G:120:VAL:CG2	1:G:434:MET:HE1	2.46	0.46
4:L:153:VAL:HG13	4:L:154:LEU:H	1.81	0.46
4:L:186:TYR:O	4:L:192:TYR:OH	2.30	0.46
1:A:218:CYS:HA	1:A:246:GLN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ALA:N	3:C:184:VAL:O	2.45	0.46
4:D:36:TYR:O	4:D:86:TYR:HA	2.16	0.46
3:H:83:ARG:CG	3:H:85:GLU:OE1	2.44	0.46
1:A:64:GLU:HB2	1:A:67:ASN:HB2	1.97	0.46
1:A:68:VAL:O	1:A:71:THR:HG23	2.14	0.46
3:C:52(A):PRO:HA	3:C:71:ARG:HD3	1.98	0.46
3:C:59:TYR:HE1	3:C:69:MET:HB2	1.81	0.46
4:L:136:LEU:CD1	4:L:146:VAL:CG2	2.93	0.46
4:L:205:VAL:HG23	4:L:205:VAL:O	2.16	0.46
3:C:100(F):PHE:N	4:D:36:TYR:OH	2.49	0.46
4:D:201:LEU:N	4:D:201:LEU:CD2	2.79	0.46
1:G:45:TRP:HB2	1:G:489:VAL:HG11	1.93	0.46
1:G:232:ASN:HB3	1:G:271:ILE:HD11	1.98	0.46
3:H:163:VAL:HG22	3:H:182:VAL:HA	1.97	0.46
3:H:168:ALA:HA	3:H:178:LEU:HB3	1.97	0.46
3:H:189:LEU:HD12	3:H:191:THR:CG2	2.45	0.46
1:A:91:GLU:OE1	1:A:487:LYS:HD3	2.16	0.46
3:C:69:MET:HE3	3:C:69:MET:HB2	1.80	0.46
3:C:137:ALA:N	4:D:116:PHE:HE2	2.14	0.46
1:G:61:HIS:ND1	1:G:61:HIS:C	2.73	0.46
1:G:102:GLU:OE1	1:G:476:LYS:HE3	2.16	0.46
3:H:169:VAL:CG2	4:L:162:SER:HB2	2.46	0.46
4:L:125:VAL:HG13	4:L:125:VAL:O	2.16	0.46
4:L:170:ASP:HB2	4:L:172:THR:CG2	2.45	0.46
1:A:233:PHE:HE1	1:A:235:GLY:C	2.22	0.46
3:C:50:TRP:NE1	3:C:58:GLY:HA3	2.31	0.46
3:C:117:LYS:O	3:C:145:TYR:HA	2.17	0.46
1:G:218:CYS:HA	1:G:246:GLN:O	2.15	0.45
4:L:136:LEU:HD12	4:L:136:LEU:H	1.80	0.45
1:A:266:ALA:N	1:A:287:HIS:CE1	2.84	0.45
1:A:386:ASN:CG	1:A:388:THR:CG2	2.83	0.45
4:D:52:THR:HG22	4:D:64:GLY:O	2.17	0.45
1:G:95:MET:CG	1:G:235:GLY:HA3	2.46	0.45
1:G:121:LYS:HE3	1:G:426:MET:SD	2.57	0.45
3:H:91:TYR:CE1	4:L:43:VAL:HG23	2.51	0.45
3:H:163:VAL:HG21	3:H:182:VAL:CG1	2.22	0.45
4:L:42:LYS:HA	4:L:42:LYS:HD3	1.38	0.45
1:A:239:CYS:O	1:A:239:CYS:SG	2.75	0.45
3:C:143:LYS:HE3	3:C:143:LYS:HB3	1.33	0.45
4:D:33:LEU:O	4:D:51:ALA:N	2.44	0.45
4:D:161:GLU:HG2	4:D:177:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:HIS:O	1:G:74:CYS:N	2.48	0.45
1:G:111:LEU:C	1:G:111:LEU:CD2	2.88	0.45
1:G:294:ILE:CG1	1:G:295:ASN:N	2.80	0.45
3:H:196:CYS:O	3:H:208:ASP:HA	2.15	0.45
3:C:123:PRO:CD	3:C:209:LYS:HZ3	2.29	0.45
4:D:37:GLN:HB2	4:D:86:TYR:HE1	1.70	0.45
1:G:111:LEU:HD23	1:G:111:LEU:O	2.17	0.45
1:G:417:PRO:O	1:G:418:CYS:HB2	2.15	0.45
4:L:89:GLN:NE2	4:L:98:PHE:CZ	2.85	0.45
4:L:186:TYR:CD1	4:L:192:TYR:CZ	3.04	0.45
1:A:84:ILE:O	1:A:243:SER:HB2	2.17	0.45
4:D:166:GLN:CG	4:D:173:TYR:CE1	2.96	0.45
3:H:45:LEU:HD12	4:L:87:TYR:HD2	1.73	0.45
3:H:95:TYR:CG	3:H:100(D):ARG:HA	2.52	0.45
3:H:135:THR:CA	3:H:186:SER:O	2.56	0.45
1:A:216:HIS:ND1	1:A:216:HIS:N	2.64	0.45
1:A:396:ILE:C	1:A:396:ILE:CD1	2.88	0.45
3:C:189:LEU:CD1	3:C:194:TYR:OH	2.65	0.45
1:G:446:VAL:CG1	5:G:506:NAG:H82	2.46	0.45
3:C:66:ARG:HD2	3:C:82(B):SER:CB	2.46	0.45
1:G:100:MET:HB2	1:G:483:LEU:HD13	1.98	0.45
1:G:102:GLU:OE1	1:G:476:LYS:CE	2.65	0.45
1:G:282:LYS:HD3	1:G:282:LYS:HA	1.77	0.45
3:H:85:GLU:N	3:H:85:GLU:CD	2.74	0.45
1:A:66:HIS:HB2	1:A:211:ASP:O	2.17	0.45
1:A:286:VAL:HG21	1:A:454:LEU:HD11	1.99	0.45
3:C:19:LYS:HE3	3:C:19:LYS:O	2.16	0.45
3:C:123:PRO:CD	3:C:209:LYS:HZ2	2.29	0.45
4:D:91:TYR:HA	4:D:96:PHE:HD1	1.81	0.45
3:H:201:LYS:CB	3:H:202:PRO:HD3	2.47	0.45
4:L:33:LEU:CD2	4:L:71:PHE:CB	2.95	0.45
1:A:233:PHE:CD1	1:A:235:GLY:N	2.76	0.45
3:C:100(B):GLY:HA2	4:D:32:TYR:CE1	2.52	0.45
1:G:417:PRO:O	1:G:418:CYS:HB3	2.17	0.45
3:H:22:CYS:O	3:H:77:THR:HG23	2.16	0.45
3:H:96:ARG:HB2	3:H:100(E):TYR:CE1	2.51	0.45
3:H:198:VAL:O	3:H:206:LYS:CA	2.49	0.45
4:L:54:LEU:HD21	4:L:62:PHE:O	2.17	0.45
1:A:260:LEU:HD21	1:A:453:LEU:HD13	1.99	0.45
3:C:112:SER:CB	3:C:146:PHE:CE2	2.93	0.45
4:D:38:GLN:C	4:D:84:ALA:HB1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:ARG:NH1	1:G:439:ILE:O	2.50	0.45
3:H:122:PHE:CD1	4:L:124:GLN:HG3	2.52	0.45
1:A:258:GLN:NE2	1:A:374:HIS:N	2.63	0.45
1:A:410:CYS:O	1:A:411:ASN:O	2.34	0.45
4:D:37:GLN:CB	4:D:47:LEU:HD11	2.47	0.45
1:G:95:MET:HG2	1:G:235:GLY:CA	2.47	0.44
1:G:286:VAL:O	1:G:451:GLY:HA3	2.17	0.44
1:G:299:PRO:HG3	1:G:330:TYR:OH	2.17	0.44
3:H:104:GLY:O	4:L:43:VAL:HG21	2.17	0.44
1:A:66:HIS:CD2	1:A:111:LEU:HD11	2.52	0.44
1:A:108:VAL:HG12	1:A:112:TRP:CD1	2.52	0.44
3:C:170:LEU:HD12	3:C:176:TYR:CE2	2.51	0.44
1:G:339:ASN:HB3	1:G:395:CYS:O	2.17	0.44
1:G:349:LEU:CD2	1:G:468:PHE:CZ	3.00	0.44
1:G:359:ILE:HG23	1:G:468:PHE:CE2	2.52	0.44
3:H:100(F):PHE:O	4:L:36:TYR:OH	2.35	0.44
3:H:163:VAL:HG22	3:H:182:VAL:CA	2.47	0.44
3:C:142:VAL:CG1	3:C:198:VAL:HG11	2.47	0.44
4:D:183:ASN:O	4:D:184:THR:C	2.59	0.44
1:G:212:PRO:CB	1:G:252:LYS:HG2	2.37	0.44
1:A:114:GLN:HE21	1:A:114:GLN:HB3	1.62	0.44
1:A:229:ASN:HB3	1:A:241:ASN:ND2	2.32	0.44
3:C:6:GLN:HG3	3:C:104:GLY:HA3	1.99	0.44
3:H:66:ARG:CG	3:H:82(A):SER:O	2.62	0.44
4:L:108:ARG:HH11	4:L:109:ALA:N	2.08	0.44
1:A:376:PHE:CD1	1:A:376:PHE:N	2.85	0.44
3:C:148:GLU:OE2	3:C:176:TYR:CE2	2.70	0.44
3:H:20:LEU:HD12	3:H:80:MET:HE1	1.98	0.44
1:A:286:VAL:CB	1:A:452:ILE:HD12	2.48	0.44
1:A:373:MET:HG3	1:A:386:ASN:HA	1.98	0.44
3:H:100(F):PHE:N	3:H:100(F):PHE:CD1	2.85	0.44
3:H:100(F):PHE:O	4:L:36:TYR:CE1	2.71	0.44
3:C:38:ARG:CB	3:C:90:TYR:HD1	2.02	0.44
4:D:129:THR:CG2	4:D:181:LEU:O	2.65	0.44
1:G:65:VAL:CG1	1:G:115:SER:HB3	2.47	0.44
1:G:94:ASN:ND2	5:A:507:NAG:H83	2.33	0.44
1:G:298:ARG:HH12	1:G:439:ILE:C	2.26	0.44
1:G:427:TRP:CD1	1:G:427:TRP:H	2.35	0.44
1:A:362:GLN:CB	1:A:363:PRO:CD	2.95	0.44
4:D:92:ASN:OD1	4:D:93:SER:N	2.51	0.44
4:D:196:VAL:O	4:D:202:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:390:LEU:HD11	1:G:416:LEU:HD11	1.99	0.44
1:A:268:GLU:O	1:A:289:ASN:ND2	2.39	0.44
1:A:298:ARG:N	1:A:299:PRO:CD	2.81	0.44
3:C:87:THR:HG22	3:C:111:VAL:HG13	1.99	0.44
1:G:227:LYS:HE3	1:G:486:TYR:CE1	2.53	0.44
3:H:61:GLN:O	3:H:64:GLN:N	2.39	0.44
3:H:100(D):ARG:C	4:L:91:TYR:HD1	2.25	0.44
4:L:37:GLN:CB	4:L:86:TYR:HD1	2.23	0.44
4:L:78:LEU:HD12	4:L:79:GLN:H	1.82	0.44
1:A:298:ARG:HE	1:A:298:ARG:HB3	1.65	0.44
3:C:184:VAL:CG1	3:C:194:TYR:HE2	2.23	0.44
4:D:5:THR:CB	4:D:100:GLN:HE22	2.29	0.44
4:D:14:SER:C	4:D:15:VAL:O	2.58	0.44
1:G:251:ILE:O	1:G:251:ILE:HG12	2.17	0.43
4:L:18:LYS:HG3	4:L:18:LYS:O	2.17	0.43
1:A:376:PHE:HD1	1:A:376:PHE:O	2.01	0.43
3:C:23:LYS:HA	3:C:77:THR:HA	2.00	0.43
4:D:65:SER:OG	4:D:66:GLY:N	2.50	0.43
4:D:110:VAL:O	4:D:110:VAL:HG12	2.18	0.43
1:G:439:ILE:C	1:G:439:ILE:CD1	2.85	0.43
1:G:473:GLY:HA3	2:N:20:ALA:O	2.18	0.43
3:H:21:SER:HG	3:H:79:TYR:HE1	1.63	0.43
3:H:54:THR:O	3:H:56:ASN:N	2.48	0.43
4:L:32:TYR:HB3	4:L:91:TYR:CE2	2.53	0.43
1:A:376:PHE:CZ	1:A:383:PHE:CD1	3.05	0.43
4:D:51:ALA:CB	4:D:71:PHE:HE1	2.32	0.43
4:D:117:ILE:HG13	4:D:118:PHE:N	2.32	0.43
1:G:86:LEU:HD23	1:G:86:LEU:HA	1.83	0.43
1:G:349:LEU:CD2	1:G:468:PHE:CE1	2.86	0.43
1:G:484:TYR:CD1	1:G:484:TYR:C	2.96	0.43
3:H:166:PHE:C	3:H:167:PRO:O	2.60	0.43
4:L:140:TYR:CD2	4:L:141:PRO:HA	2.53	0.43
3:C:87:THR:CG2	3:C:111:VAL:H	2.32	0.43
3:C:136:ALA:HB2	3:C:186:SER:HA	1.98	0.43
4:D:16:GLY:HA2	4:D:77:SER:HB2	1.99	0.43
1:G:232:ASN:HA	1:G:271:ILE:HD11	2.00	0.43
1:G:326:ILE:HD12	1:G:326:ILE:HA	1.76	0.43
4:L:210:ASN:OD1	4:L:210:ASN:N	2.44	0.43
1:A:340:LYS:HG3	1:A:343:LYS:CE	2.48	0.43
1:A:376:PHE:CE1	1:A:383:PHE:CG	2.96	0.43
3:C:63:PHE:O	3:C:67:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100(F):PHE:CE1	4:D:89:GLN:NE2	2.86	0.43
1:G:270:ILE:CG2	5:G:505:NAG:H62	2.48	0.43
3:H:195:VAL:HG23	3:H:210:ARG:HG3	2.01	0.43
4:L:150:VAL:O	4:L:153:VAL:HG12	2.19	0.43
1:A:290:LYS:HD2	1:A:290:LYS:HA	1.82	0.43
1:A:382:PHE:O	1:A:420:ILE:CB	2.67	0.43
4:D:85:THR:HG21	4:D:103:ARG:CG	2.39	0.43
1:G:273:ARG:NH2	1:G:287:HIS:HB2	2.17	0.43
3:H:40:ALA:HA	3:H:88:ALA:HB1	2.00	0.43
4:L:16:GLY:HA2	4:L:78:LEU:N	2.34	0.43
4:L:67:SER:HA	4:L:71:PHE:CE1	2.53	0.43
1:A:299:PRO:CB	1:A:442:LYS:HD3	2.29	0.43
4:D:49:TYR:CD1	4:D:53:THR:HB	2.54	0.43
4:D:90:LYS:HE2	4:D:93:SER:O	2.19	0.43
1:G:368:ASP:H	1:G:371:ILE:HD11	1.83	0.43
2:N:20:ALA:N	2:N:29:U2X:O	2.46	0.43
4:L:48:ILE:HD12	4:L:64:GLY:CA	2.49	0.43
4:L:124:GLN:O	4:L:129:THR:O	2.37	0.43
1:A:256:SER:OG	1:A:261:LEU:HD12	2.19	0.43
1:A:370:GLU:CD	1:A:370:GLU:N	2.74	0.43
1:G:66:HIS:CE1	1:G:212:PRO:HG3	2.54	0.43
3:H:20:LEU:HD11	3:H:90:TYR:HB2	2.01	0.43
1:A:96:TRP:HZ2	1:A:274:SER:HA	1.76	0.43
3:C:27:TYR:HE1	3:C:32:TYR:HB2	1.84	0.43
3:C:66:ARG:HH12	3:C:86:ASP:CG	2.27	0.43
3:C:118:GLY:HA3	3:C:205:THR:HG21	2.00	0.43
3:C:148:GLU:OE1	3:C:168:ALA:HB3	2.18	0.43
3:C:189:LEU:HB3	3:C:194:TYR:OH	2.18	0.43
3:C:203:SER:HB2	3:C:205:THR:HG23	2.00	0.43
1:G:118:PRO:HB3	1:G:435:TYR:CE2	2.54	0.43
1:G:294:ILE:HG12	1:G:295:ASN:N	2.34	0.43
1:G:343:LYS:HB2	1:G:396:ILE:HG23	1.99	0.43
1:G:454:LEU:HA	1:G:469:ARG:O	2.19	0.43
1:A:105:GLN:HG3	1:A:109:ILE:HD11	1.99	0.43
1:A:223:TYR:HE2	1:A:490:GLN:HB2	1.83	0.43
1:A:362:GLN:HG3	1:A:363:PRO:O	2.19	0.43
1:A:376:PHE:CD1	1:A:383:PHE:CB	2.92	0.43
1:A:453:LEU:O	1:A:470:PRO:HA	2.18	0.43
3:C:121:VAL:HG23	3:C:207:VAL:HG11	1.86	0.43
3:C:140:CYS:O	3:C:179:SER:HA	2.18	0.43
4:D:11:LEU:CB	4:D:104:LEU:CD1	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:SER:O	4:D:15:VAL:C	2.62	0.43
4:D:21:ILE:HG12	4:D:73:LEU:HB3	2.01	0.43
4:D:122:GLU:H	4:D:122:GLU:HG2	1.57	0.43
1:G:100:MET:HE1	1:G:486:TYR:CB	2.44	0.43
3:H:119:PRO:HB3	3:H:142:VAL:HG12	1.92	0.43
3:H:152:VAL:CG1	3:H:165:THR:HG21	2.49	0.43
4:L:4:MET:HE1	4:L:90:LYS:CB	2.48	0.43
3:C:105:GLN:H	3:C:105:GLN:HG2	1.43	0.43
4:D:37:GLN:HB3	4:D:47:LEU:HD11	2.01	0.43
1:G:48:ALA:O	1:G:488:VAL:HG12	2.19	0.42
1:G:255:VAL:HG12	2:N:29:U2X:H12	1.99	0.42
1:G:260:LEU:HD21	1:G:478:ASN:OD1	2.15	0.42
1:G:384:TYR:HE2	1:G:421:LYS:HB2	1.84	0.42
4:L:136:LEU:HD13	4:L:175:LEU:CD1	2.47	0.42
4:L:160:GLN:N	4:L:178:THR:O	2.45	0.42
1:A:66:HIS:CE1	1:A:210:PHE:CZ	2.84	0.42
1:A:112:TRP:O	1:A:116:LEU:CD1	2.55	0.42
1:A:377:ASN:CB	1:A:382:PHE:CE2	2.78	0.42
3:C:51:MET:HE1	3:C:52(A):PRO:HG3	2.01	0.42
3:C:100(E):TYR:N	4:D:91:TYR:CD1	2.81	0.42
4:D:13:ALA:C	4:D:107:LYS:HB3	2.43	0.42
1:G:66:HIS:ND1	1:G:212:PRO:CA	2.47	0.42
1:G:382:PHE:CD2	1:G:435:TYR:HD1	2.32	0.42
3:H:11:VAL:O	3:H:11:VAL:HG23	2.19	0.42
3:H:114:ALA:HB2	3:H:146:PHE:CE2	2.54	0.42
3:H:124:LEU:HB3	4:L:118:PHE:CD2	2.54	0.42
3:H:146:PHE:HA	3:H:147:PRO:HA	1.79	0.42
4:L:32:TYR:C	4:L:91:TYR:CE2	2.97	0.42
3:C:4:LEU:HD23	3:C:94:THR:OG1	2.19	0.42
4:D:206:THR:HG22	4:D:207:LYS:H	1.84	0.42
3:H:4:LEU:HD23	3:H:4:LEU:HA	1.81	0.42
1:A:338:TRP:CE3	1:A:338:TRP:O	2.72	0.42
3:C:15:GLY:N	3:C:82(C):LEU:O	2.53	0.42
4:D:37:GLN:CA	4:D:86:TYR:HD1	2.32	0.42
1:G:330:TYR:HE1	1:G:332:GLU:OE2	2.01	0.42
1:G:411:ASN:C	1:G:411:ASN:HD22	2.28	0.42
3:H:135:THR:CA	3:H:186:SER:CA	2.97	0.42
1:A:239:CYS:O	1:A:241:ASN:N	2.52	0.42
3:C:154:TRP:HD1	3:C:163:VAL:HG21	1.83	0.42
4:D:9:SER:O	4:D:103:ARG:N	2.29	0.42
4:D:51:ALA:HB2	4:D:71:PHE:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:VAL:HG11	4:D:177:SER:CB	2.50	0.42
1:G:383:PHE:CE2	1:G:420:ILE:HD12	2.48	0.42
1:G:394:THR:HG22	1:G:395:CYS:N	2.34	0.42
3:H:166:PHE:O	3:H:167:PRO:O	2.37	0.42
4:L:12:SER:HA	4:L:105:GLU:HB2	2.01	0.42
4:L:49:TYR:C	4:L:49:TYR:HD1	2.25	0.42
4:L:132:VAL:O	4:L:148:TRP:CZ2	2.73	0.42
3:C:18:VAL:O	3:C:81:GLU:HA	2.19	0.42
1:G:485:LYS:HB3	1:G:485:LYS:HE3	1.74	0.42
3:H:167:PRO:CG	4:L:163:VAL:O	2.68	0.42
4:L:13:ALA:HB1	4:L:78:LEU:CD2	2.49	0.42
1:A:45:TRP:HB2	1:A:489:VAL:HG13	1.99	0.42
1:A:223:TYR:CE2	1:A:490:GLN:CG	3.02	0.42
1:A:295:ASN:HB2	1:A:446:VAL:HG22	2.01	0.42
3:C:66:ARG:NE	3:C:82(A):SER:O	2.53	0.42
4:D:11:LEU:CB	4:D:104:LEU:HD13	2.42	0.42
1:G:297:THR:HA	1:G:443:ILE:O	2.19	0.42
1:G:394:THR:HB	1:G:395:CYS:H	1.48	0.42
1:A:225:ILE:HG21	1:A:245:VAL:HG23	2.01	0.42
1:A:264:SER:HG	1:A:482:GLU:HG3	1.80	0.42
1:A:299:PRO:HG3	1:A:442:LYS:CE	2.47	0.42
3:C:30:THR:O	3:C:30:THR:OG1	2.37	0.42
3:C:37:VAL:HG23	3:C:47:TRP:CA	2.48	0.42
3:C:66:ARG:CZ	3:C:86:ASP:OD2	2.68	0.42
4:D:6:GLN:NE2	4:D:87:TYR:HA	2.31	0.42
1:G:255:VAL:HG12	2:N:29:U2X:H21	2.02	0.42
1:G:385:CYS:HA	1:G:418:CYS:HA	2.02	0.42
4:L:117:ILE:CG1	4:L:205:VAL:CG2	2.91	0.42
4:L:151:ASP:OD2	4:L:189:HIS:CG	2.72	0.42
1:A:104:MET:HE1	1:A:251:ILE:HD11	2.01	0.42
3:C:140:CYS:SG	3:C:154:TRP:CH2	3.13	0.42
1:G:45:TRP:CG	1:G:489:VAL:HG11	2.55	0.42
1:G:223:TYR:HD2	1:G:490:GLN:CA	2.31	0.42
3:H:143:LYS:CG	3:H:177:SER:OG	2.68	0.42
3:H:197:ASN:CG	3:H:208:ASP:OD1	2.62	0.42
4:L:106:ILE:O	4:L:106:ILE:HG23	2.19	0.42
1:A:375:SER:HA	1:A:384:TYR:HA	2.02	0.42
3:C:33:ASP:OD1	3:C:51:MET:O	2.37	0.42
3:C:95:TYR:CD2	3:C:100(D):ARG:O	2.73	0.42
3:C:166:PHE:HE1	4:D:174:SER:O	1.92	0.42
3:C:201:LYS:HA	3:C:204:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:TYR:HD1	4:D:192:TYR:CE2	2.38	0.42
4:L:104:LEU:HD23	4:L:104:LEU:HA	1.74	0.42
1:A:72:HIS:O	1:A:74:CYS:O	2.38	0.42
4:D:23:CYS:O	4:D:71:PHE:HB2	2.19	0.42
4:D:48:ILE:HD12	4:D:73:LEU:HD13	2.02	0.42
1:G:451:GLY:C	1:G:452:ILE:HG13	2.45	0.41
4:L:106:ILE:HD12	4:L:166:GLN:NE2	2.35	0.41
1:A:45:TRP:HB2	1:A:489:VAL:HG11	2.00	0.41
3:C:2:VAL:HG13	3:C:102:TYR:CE1	2.51	0.41
3:H:98:ILE:CD1	3:H:100(C):TYR:CG	3.03	0.41
3:H:100(F):PHE:CE1	4:L:89:GLN:CD	2.85	0.41
3:H:154:TRP:CE3	3:H:196:CYS:CB	3.02	0.41
4:L:132:VAL:HG12	4:L:132:VAL:O	2.19	0.41
1:A:286:VAL:CG2	1:A:452:ILE:HD12	2.50	0.41
1:A:479:TRP:HA	1:A:479:TRP:HE3	1.85	0.41
3:C:2:VAL:HG13	3:C:102:TYR:HE1	1.80	0.41
3:C:124:LEU:O	4:D:118:PHE:HE1	2.04	0.41
4:D:14:SER:O	4:D:15:VAL:O	2.38	0.41
1:G:330:TYR:N	1:G:330:TYR:CD2	2.88	0.41
1:G:422:GLN:HE21	1:G:422:GLN:HB2	1.68	0.41
1:G:468:PHE:N	1:G:468:PHE:CD2	2.88	0.41
3:H:38:ARG:HB2	3:H:90:TYR:CE1	2.55	0.41
3:H:114:ALA:HB2	3:H:146:PHE:CD2	2.55	0.41
4:L:19:VAL:HG23	4:L:75:ILE:CG2	2.14	0.41
4:L:108:ARG:HH12	4:L:109:ALA:HB3	1.79	0.41
1:A:223:TYR:CD2	1:A:490:GLN:HA	2.55	0.41
1:A:224:VAL:CG2	1:A:244:SER:OG	2.68	0.41
3:C:32:TYR:OH	3:C:98:ILE:N	2.53	0.41
3:C:100(E):TYR:CD2	4:D:49:TYR:HB2	2.54	0.41
3:C:181:VAL:CG2	4:D:135:LEU:HD13	2.40	0.41
1:G:217:TYR:CB	1:G:248:THR:HG23	2.50	0.41
1:A:227:LYS:HA	1:A:485:LYS:O	2.20	0.41
1:A:394:THR:CG2	1:A:395:CYS:N	2.83	0.41
1:A:475:ILE:HG23	1:A:478:ASN:HD21	1.84	0.41
1:A:479:TRP:HA	1:A:479:TRP:CE3	2.55	0.41
3:C:40:ALA:O	3:C:43:GLN:HB2	2.21	0.41
3:C:145:TYR:CD1	3:C:145:TYR:N	2.89	0.41
3:H:38:ARG:HB3	3:H:90:TYR:HE1	1.84	0.41
3:H:98:ILE:CD1	3:H:100(C):TYR:HB2	2.38	0.41
1:A:369:LEU:C	1:A:369:LEU:HD12	2.45	0.41
3:C:19:LYS:HE3	3:C:19:LYS:HB3	1.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:VAL:O	3:C:176:TYR:HA	2.21	0.41
4:D:203:SER:O	4:D:203:SER:OG	2.27	0.41
1:G:75:VAL:HB	1:G:76:PRO:CD	2.51	0.41
3:H:152:VAL:CG1	3:H:165:THR:CG2	2.99	0.41
4:L:49:TYR:CD1	4:L:53:THR:OG1	2.71	0.41
4:L:50:ALA:O	4:L:51:ALA:HB3	2.20	0.41
4:L:155:LYS:HZ1	4:L:181:LEU:CD2	2.28	0.41
3:C:33:ASP:HB2	3:C:95:TYR:CE1	2.55	0.41
3:C:66:ARG:CG	3:C:82(A):SER:O	2.68	0.41
3:C:119:PRO:CA	3:C:145:TYR:HB3	2.51	0.41
4:D:209:PHE:HB2	4:D:210:ASN:H	1.67	0.41
1:G:217:TYR:HB2	1:G:248:THR:HG23	1.97	0.41
1:G:269:GLU:HB3	5:G:505:NAG:O6	2.21	0.41
3:H:27:TYR:HD1	3:H:97:ILE:CG2	2.34	0.41
3:H:45:LEU:CD1	4:L:87:TYR:CD2	2.97	0.41
3:H:87:THR:HA	3:H:109:VAL:O	2.21	0.41
3:H:116:THR:HA	3:H:146:PHE:O	2.21	0.41
3:H:139:GLY:HA3	3:H:180:SER:O	2.21	0.41
4:L:91:TYR:HD2	4:L:91:TYR:H	1.68	0.41
1:A:105:GLN:NE2	1:A:109:ILE:HD11	2.36	0.41
1:A:338:TRP:O	1:A:338:TRP:CD2	2.74	0.41
3:C:95:TYR:HA	3:C:100(E):TYR:O	2.21	0.41
3:C:100(E):TYR:CD2	4:D:91:TYR:HE1	2.37	0.41
1:G:487:LYS:HZ2	5:A:506:NAG:H81	1.85	0.41
3:H:20:LEU:CD1	3:H:90:TYR:CB	2.99	0.41
3:C:50:TRP:CE2	3:C:58:GLY:HA3	2.55	0.41
3:C:70:THR:HB	3:C:79:TYR:HB2	2.02	0.41
4:D:49:TYR:CE1	4:D:53:THR:HB	2.55	0.41
1:G:95:MET:O	1:G:480:ARG:NE	2.53	0.41
1:G:223:TYR:HA	1:G:489:VAL:O	2.21	0.41
1:G:328:LYS:HE2	1:G:419:LYS:HG3	2.02	0.41
1:G:333:ILE:O	1:G:335:GLY:N	2.54	0.41
3:H:3:GLN:O	3:H:24:ALA:HA	2.20	0.41
3:H:80:MET:O	3:H:80:MET:SD	2.79	0.41
3:H:87:THR:OG1	3:H:111:VAL:N	2.53	0.41
3:C:33:ASP:HB3	3:C:95:TYR:CE1	2.55	0.41
3:C:100(E):TYR:CE2	4:D:49:TYR:CD2	3.09	0.41
4:D:35:TRP:CZ3	4:D:88:CYS:HB3	2.56	0.41
3:H:12:LYS:HG3	3:H:18:VAL:HB	2.03	0.41
4:L:143:GLU:O	4:L:143:GLU:HG2	2.17	0.41
1:A:66:HIS:CE1	1:A:210:PHE:HE1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:HG22	1:A:465:ASN:HB3	2.03	0.41
3:C:12:LYS:O	3:C:111:VAL:HA	2.20	0.41
3:C:151:THR:O	3:C:151:THR:HG22	2.21	0.41
3:C:171:GLN:HG2	4:D:160:GLN:HE22	1.86	0.41
3:C:189:LEU:HD23	3:C:189:LEU:HA	1.87	0.41
3:C:197:ASN:HA	3:C:208:ASP:OD2	2.21	0.41
4:D:62:PHE:CE2	4:D:75:ILE:HD12	2.43	0.41
1:G:121:LYS:CD	1:G:201:ILE:HD11	2.51	0.40
2:N:3:LEU:C	2:N:5:PHE:N	2.77	0.40
3:H:124:LEU:C	4:L:118:PHE:HD2	2.26	0.40
4:L:39:LYS:HA	4:L:84:ALA:CB	2.46	0.40
3:C:87:THR:O	3:C:87:THR:OG1	2.37	0.40
4:D:5:THR:HA	4:D:100:GLN:NE2	2.35	0.40
4:D:155:LYS:HA	4:D:155:LYS:HD2	1.73	0.40
4:D:159:SER:HA	4:D:178:THR:O	2.21	0.40
3:H:61:GLN:C	3:H:64:GLN:HB2	2.46	0.40
1:A:272:ILE:HG13	1:A:352:HIS:CE1	2.54	0.40
1:A:286:VAL:CG2	1:A:454:LEU:HD11	2.51	0.40
3:C:50:TRP:CD1	4:D:94:ALA:CB	3.04	0.40
3:C:66:ARG:HG2	3:C:82(A):SER:O	2.20	0.40
3:C:87:THR:HG22	3:C:111:VAL:CB	2.49	0.40
4:D:2:ILE:H	4:D:2:ILE:HG13	1.53	0.40
1:G:116:LEU:CG	1:G:210:PHE:CE2	2.99	0.40
1:G:116:LEU:CD2	1:G:210:PHE:CE2	3.03	0.40
1:G:390:LEU:CD1	1:G:416:LEU:HD11	2.52	0.40
3:H:35:ASN:OD1	3:H:47:TRP:NE1	2.25	0.40
3:H:82(C):LEU:HD23	3:H:82(C):LEU:HA	1.92	0.40
1:A:53:PHE:CZ	1:A:218:CYS:HB3	2.57	0.40
1:A:210:PHE:HB2	1:A:380:GLY:N	2.36	0.40
1:A:338:TRP:HE1	1:A:390:LEU:CB	2.21	0.40
3:C:38:ARG:HD2	3:C:90:TYR:CZ	2.42	0.40
3:C:154:TRP:CE3	3:C:196:CYS:CB	3.03	0.40
1:G:121:LYS:HD2	1:G:201:ILE:HD11	2.02	0.40
2:N:1:MPT:HB2	2:N:22:THR:C	2.47	0.40
3:H:51:MET:HE2	3:H:51:MET:HB2	1.50	0.40
3:H:114:ALA:HB1	3:H:146:PHE:CD1	2.35	0.40
4:L:186:TYR:CD1	4:L:192:TYR:OH	2.68	0.40
1:G:65:VAL:HB	1:G:115:SER:CB	2.46	0.40
1:G:222:GLY:HA3	1:G:492:GLU:OE2	2.21	0.40
1:G:427:TRP:HE3	1:G:475:ILE:CG1	2.34	0.40
4:L:35:TRP:O	4:L:47:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:111:ALA:O	4:L:198:HIS:CE1	2.75	0.40
4:D:89:GLN:HG3	4:D:98:PHE:CE1	2.57	0.40
4:D:90:LYS:NZ	4:D:95:PRO:O	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/355 (84%)	224 (75%)	46 (15%)	28 (9%)	0	1
1	G	332/355 (94%)	272 (82%)	34 (10%)	26 (8%)	1	2
2	N	24/28 (86%)	20 (83%)	3 (12%)	1 (4%)	2	9
3	C	213/228 (93%)	173 (81%)	36 (17%)	4 (2%)	6	23
3	H	214/228 (94%)	176 (82%)	31 (14%)	7 (3%)	3	13
4	D	208/214 (97%)	175 (84%)	26 (12%)	7 (3%)	3	12
4	L	208/214 (97%)	159 (76%)	33 (16%)	16 (8%)	1	2
All	All	1497/1622 (92%)	1199 (80%)	209 (14%)	89 (6%)	1	4

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	240	LYS
1	G	248	THR
1	G	393	ASN
1	G	395	CYS
1	G	417	PRO
3	H	116	THR
4	L	7	SER
4	L	14	SER

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Mol	Chain	Res	Type
4	L	106	ILE
4	L	110	VAL
4	L	198	HIS
1	A	58	ALA
1	A	59	LYS
1	A	60	ALA
1	A	73	ALA
1	A	209	SER
1	A	239	CYS
1	A	240	LYS
1	A	248	THR
1	A	393	ASN
1	A	395	CYS
1	A	411	ASN
1	A	417	PRO
3	C	55	GLY
1	G	87	GLU
1	G	124	GLY
1	G	334	ASN
1	G	388	THR
1	G	392	ASN
1	G	394	THR
1	G	418	CYS
1	G	459	GLY
3	H	55	GLY
3	H	158	SER
4	L	12	SER
4	L	154	LEU
1	A	354	ASN
1	A	374	HIS
1	A	410	CYS
1	A	462	ASN
4	D	15	VAL
4	D	110	VAL
4	D	154	LEU
4	D	201	LEU
4	D	209	PHE
1	G	55	ALA
1	G	241	ASN
1	G	387	THR
1	G	389	GLN
3	H	159	LEU

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Mol	Chain	Res	Type
3	H	167	PRO
4	L	84	ALA
4	L	107	LYS
4	L	143	GLU
1	A	238	PRO
1	A	418	CYS
1	A	476	LYS
3	C	41	PRO
3	C	144	ASP
1	G	88	ASN
1	G	231	LYS
1	G	238	PRO
1	G	258	GLN
1	G	379	ARG
3	H	126	PRO
4	L	2	ILE
4	L	66	GLY
4	L	158	ASN
4	L	202	SER
1	A	257	THR
1	A	412	GLY
1	A	463	THR
3	C	17	SER
1	G	410	CYS
1	G	438	PRO
2	N	33	VAL
3	H	147	PRO
4	L	13	ALA
1	A	208	ILE
4	D	143	GLU
4	D	138	ASN
1	A	364	PRO
1	A	206	PRO
1	A	211	ASP
1	G	220	PRO
1	A	79	PRO
1	A	253	PRO
1	G	89	VAL
4	L	141	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/313 (89%)	194 (70%)	85 (30%)	0	1
1	G	302/313 (96%)	207 (68%)	95 (32%)	0	1
2	N	20/20 (100%)	19 (95%)	1 (5%)	22	53
3	C	183/192 (95%)	131 (72%)	52 (28%)	0	1
3	H	184/192 (96%)	131 (71%)	53 (29%)	0	1
4	D	184/187 (98%)	127 (69%)	57 (31%)	0	1
4	L	184/187 (98%)	129 (70%)	55 (30%)	0	1
All	All	1336/1404 (95%)	938 (70%)	398 (30%)	0	1

All (398) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	46	LYS
1	G	49	ASP
1	G	61	HIS
1	G	62	GLU
1	G	64	GLU
1	G	66	HIS
1	G	68	VAL
1	G	71	THR
1	G	84	ILE
1	G	90	THR
1	G	91	GLU
1	G	95	MET
1	G	100	MET
1	G	102	GLU
1	G	106	GLU
1	G	107	ASP
1	G	109	ILE
1	G	113	ASP
1	G	115	SER
1	G	122	LEU

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Mol	Chain	Res	Type
1	G	201	ILE
1	G	207	LYS
1	G	208	ILE
1	G	210	PHE
1	G	213	ILE
1	G	215	ILE
1	G	218	CYS
1	G	224	VAL
1	G	225	ILE
1	G	232	ASN
1	G	236	THR
1	G	238	PRO
1	G	240	LYS
1	G	244	SER
1	G	245	VAL
1	G	247	CYS
1	G	249	HIS
1	G	251	ILE
1	G	256	SER
1	G	257	THR
1	G	259	LEU
1	G	261	LEU
1	G	264	SER
1	G	267	GLU
1	G	271	ILE
1	G	272	ILE
1	G	276	ASN
1	G	280	ASN
1	G	282	LYS
1	G	284	ILE
1	G	285	ILE
1	G	289	ASN
1	G	290	LYS
1	G	294	ILE
1	G	297	THR
1	G	326	ILE
1	G	328	LYS
1	G	332	GLU
1	G	337	LYS
1	G	341	VAL
1	G	342	LEU
1	G	343	LYS

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Mol	Chain	Res	Type
1	G	345	VAL
1	G	350	LYS
1	G	354	ASN
1	G	360	ILE
1	G	369	LEU
1	G	371	ILE
1	G	374	HIS
1	G	375	SER
1	G	376	PHE
1	G	410	CYS
1	G	411	ASN
1	G	413	THR
1	G	414	ILE
1	G	416	LEU
1	G	419	LYS
1	G	420	ILE
1	G	421	LYS
1	G	428	GLN
1	G	430	THR
1	G	434	MET
1	G	443	ILE
1	G	447	SER
1	G	449	ILE
1	G	450	THR
1	G	452	ILE
1	G	457	ASP
1	G	462	ASN
1	G	467	THR
1	G	475	ILE
1	G	480	ARG
1	G	485	LYS
1	G	491	ILE
1	G	492	GLU
2	N	30	CYS
3	H	3	GLN
3	H	4	LEU
3	H	21	SER
3	H	25	SER
3	H	27	TYR
3	H	28	THR
3	H	30	THR
3	H	34	ILE

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Mol	Chain	Res	Type
3	H	37	VAL
3	H	43	GLN
3	H	51	MET
3	H	67	VAL
3	H	69	MET
3	H	71	ARG
3	H	72	ASP
3	H	82	LEU
3	H	82(A)	SER
3	H	82(B)	SER
3	H	82(C)	LEU
3	H	84	SER
3	H	87	THR
3	H	95	TYR
3	H	108	LEU
3	H	109	VAL
3	H	112	SER
3	H	113	SER
3	H	116	THR
3	H	121	VAL
3	H	124	LEU
3	H	133	GLU
3	H	135	THR
3	H	138	LEU
3	H	141	LEU
3	H	143	LYS
3	H	154	TRP
3	H	158	SER
3	H	159	LEU
3	H	163	VAL
3	H	164	HIS
3	H	172	SER
3	H	175	LEU
3	H	178	LEU
3	H	186	SER
3	H	191	THR
3	H	192	GLN
3	H	197	ASN
3	H	201	LYS
3	H	206	LYS
3	H	207	VAL
3	H	209	LYS

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Mol	Chain	Res	Type
3	H	210	ARG
3	H	211	VAL
3	H	213	ILE
4	L	2	ILE
4	L	3	GLN
4	L	5	THR
4	L	6	GLN
4	L	9	SER
4	L	10	SER
4	L	11	LEU
4	L	15	VAL
4	L	18	LYS
4	L	27	GLN
4	L	29	PHE
4	L	37	GLN
4	L	39	LYS
4	L	42	LYS
4	L	45	LYS
4	L	47	LEU
4	L	48	ILE
4	L	49	TYR
4	L	53	THR
4	L	54	LEU
4	L	59	PRO
4	L	63	SER
4	L	67	SER
4	L	75	ILE
4	L	76	SER
4	L	77	SER
4	L	83	VAL
4	L	85	THR
4	L	91	TYR
4	L	97	THR
4	L	106	ILE
4	L	117	ILE
4	L	124	GLN
4	L	125	VAL
4	L	126	LYS
4	L	131	SER
4	L	135	LEU
4	L	139	PHE
4	L	142	ARG

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Mol	Chain	Res	Type
4	L	147	LYS
4	L	153	VAL
4	L	154	LEU
4	L	155	LYS
4	L	158	ASN
4	L	159	SER
4	L	167	ASP
4	L	170	ASP
4	L	175	LEU
4	L	179	LEU
4	L	184	THR
4	L	190	ASN
4	L	191	VAL
4	L	197	THR
4	L	199	GLN
4	L	206	THR
1	A	44	VAL
1	A	47	ASP
1	A	59	LYS
1	A	61	HIS
1	A	63	THR
1	A	71	THR
1	A	75	VAL
1	A	77	THR
1	A	80	ASN
1	A	83	GLU
1	A	86	LEU
1	A	88	ASN
1	A	89	VAL
1	A	91	GLU
1	A	95	MET
1	A	97	LYS
1	A	99	ASN
1	A	100	MET
1	A	108	VAL
1	A	116	LEU
1	A	117	GLN
1	A	205	CYS
1	A	211	ASP
1	A	213	ILE
1	A	215	ILE
1	A	218	CYS

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Mol	Chain	Res	Type
1	A	224	VAL
1	A	225	ILE
1	A	231	LYS
1	A	242	VAL
1	A	244	SER
1	A	251	ILE
1	A	253	PRO
1	A	254	VAL
1	A	255	VAL
1	A	256	SER
1	A	257	THR
1	A	261	LEU
1	A	264	SER
1	A	265	LEU
1	A	268	GLU
1	A	270	ILE
1	A	272	ILE
1	A	277	LEU
1	A	282	LYS
1	A	284	ILE
1	A	285	ILE
1	A	290	LYS
1	A	292	VAL
1	A	297	THR
1	A	298	ARG
1	A	332	GLU
1	A	342	LEU
1	A	343	LYS
1	A	344	GLN
1	A	345	VAL
1	A	350	LYS
1	A	353	PHE
1	A	354	ASN
1	A	358	THR
1	A	360	ILE
1	A	362	GLN
1	A	368	ASP
1	A	369	LEU
1	A	371	ILE
1	A	373	MET
1	A	376	PHE
1	A	381	GLU

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Mol	Chain	Res	Type
1	A	387	THR
1	A	388	THR
1	A	394	THR
1	A	396	ILE
1	A	442	LYS
1	A	444	ASN
1	A	447	SER
1	A	452	ILE
1	A	453	LEU
1	A	456	ARG
1	A	467	THR
1	A	469	ARG
1	A	481	SER
1	A	485	LYS
1	A	488	VAL
1	A	491	ILE
1	A	492	GLU
3	C	2	VAL
3	C	3	GLN
3	C	4	LEU
3	C	7	SER
3	C	11	VAL
3	C	12	LYS
3	C	13	LYS
3	C	19	LYS
3	C	21	SER
3	C	27	TYR
3	C	28	THR
3	C	34	ILE
3	C	41	PRO
3	C	51	MET
3	C	53	LYS
3	C	54	THR
3	C	61	GLN
3	C	62	LYS
3	C	66	ARG
3	C	67	VAL
3	C	69	MET
3	C	76	SER
3	C	84	SER
3	C	89	VAL
3	C	94	THR

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Mol	Chain	Res	Type
3	C	97	ILE
3	C	105	GLN
3	C	108	LEU
3	C	109	VAL
3	C	113	SER
3	C	120	SER
3	C	121	VAL
3	C	141	LEU
3	C	142	VAL
3	C	143	LYS
3	C	145	TYR
3	C	148	GLU
3	C	149	PRO
3	C	151	THR
3	C	152	VAL
3	C	153	SER
3	C	163	VAL
3	C	172	SER
3	C	178	LEU
3	C	181	VAL
3	C	187	SER
3	C	188	SER
3	C	189	LEU
3	C	192	GLN
3	C	195	VAL
3	C	209	LYS
3	C	212	GLU
4	D	2	ILE
4	D	5	THR
4	D	11	LEU
4	D	14	SER
4	D	15	VAL
4	D	17	ASP
4	D	18	LYS
4	D	20	THR
4	D	21	ILE
4	D	22	THR
4	D	37	GLN
4	D	42	LYS
4	D	43	VAL
4	D	45	LYS
4	D	48	ILE

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Mol	Chain	Res	Type
4	D	49	TYR
4	D	54	LEU
4	D	55	GLN
4	D	63	SER
4	D	65	SER
4	D	69	THR
4	D	75	ILE
4	D	78	LEU
4	D	81	GLU
4	D	83	VAL
4	D	85	THR
4	D	91	TYR
4	D	92	ASN
4	D	97	THR
4	D	105	GLU
4	D	106	ILE
4	D	107	LYS
4	D	108	ARG
4	D	114	SER
4	D	122	GLU
4	D	123	ASP
4	D	124	GLN
4	D	125	VAL
4	D	129	THR
4	D	132	VAL
4	D	133	VAL
4	D	135	LEU
4	D	143	GLU
4	D	145	SER
4	D	155	LYS
4	D	163	VAL
4	D	164	THR
4	D	165	GLU
4	D	168	SER
4	D	170	ASP
4	D	172	THR
4	D	180	THR
4	D	184	THR
4	D	187	GLN
4	D	195	GLU
4	D	206	THR
4	D	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	66	HIS
1	G	72	HIS
1	G	80	ASN
1	G	114	GLN
1	G	117	GLN
1	G	216	HIS
1	G	280	ASN
1	G	339	ASN
1	G	374	HIS
1	G	411	ASN
1	G	422	GLN
1	G	490	GLN
3	H	52	ASN
3	H	101	GLN
3	H	105	GLN
3	H	192	GLN
3	H	197	ASN
3	H	204	ASN
4	L	6	GLN
4	L	55	GLN
4	L	158	ASN
4	L	166	GLN
4	L	199	GLN
1	A	66	HIS
1	A	72	HIS
1	A	82	GLN
1	A	114	GLN
1	A	258	GLN
1	A	280	ASN
1	A	344	GLN
1	A	362	GLN
3	C	3	GLN
3	C	164	HIS
3	C	192	GLN
4	D	31	ASN
4	D	160	GLN
4	D	183	ASN
4	D	187	GLN
4	D	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
2	U2X	N	29	2	19,20,21	1.34	2 (10%)	20,25,27	1.47	4 (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
2	U2X	N	29	2	-	5/10/19/21	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	29	U2X	OH-CZ	3.75	1.46	1.37
2	N	29	U2X	CE1-CD1	2.20	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	29	U2X	CB-CG-CD2	-3.59	114.22	120.90
2	N	29	U2X	CB-CG-CD1	2.35	125.27	120.90
2	N	29	U2X	CE1-CD1-CG	-2.10	118.24	121.00
2	N	29	U2X	C7-OH-CZ	-2.09	113.26	117.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	29	U2X	N-CA-CB-CG
2	N	29	U2X	CA-CB-CG-CD2
2	N	29	U2X	CA-CB-CG-CD1
2	N	29	U2X	C4-C3-C7-OH
2	N	29	U2X	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	29	U2X	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
5	NAG	A	505	1	14,14,15	0.28	0	17,19,21	1.78	3 (17%)
5	NAG	G	502	1	14,14,15	0.40	0	17,19,21	1.54	1 (5%)
5	NAG	G	501	1	14,14,15	0.23	0	17,19,21	0.58	0
5	NAG	G	509	1	14,14,15	0.46	0	17,19,21	0.59	0
5	NAG	A	508	1	14,14,15	0.22	0	17,19,21	0.92	1 (5%)
5	NAG	G	507	1	14,14,15	0.26	0	17,19,21	0.36	0
5	NAG	A	507	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	A	501	1	14,14,15	0.34	0	17,19,21	0.63	0
5	NAG	A	503	1	14,14,15	0.45	0	17,19,21	0.80	1 (5%)
5	NAG	A	504	1	14,14,15	0.18	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	505	1	14,14,15	1.37	2 (14%)	17,19,21	1.80	2 (11%)
5	NAG	A	506	1	14,14,15	0.40	0	17,19,21	0.72	0
5	NAG	G	506	1	14,14,15	0.88	1 (7%)	17,19,21	1.20	2 (11%)
5	NAG	A	509	1	14,14,15	0.50	0	17,19,21	0.86	2 (11%)
5	NAG	A	502	1	14,14,15	0.69	1 (7%)	17,19,21	1.87	1 (5%)
5	NAG	G	508	1	14,14,15	0.28	0	17,19,21	0.68	0
5	NAG	G	503	1	14,14,15	0.31	0	17,19,21	0.61	0
5	NAG	G	504	1	14,14,15	0.34	0	17,19,21	1.08	3 (17%)

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
5	NAG	A	505	1	-	6/6/23/26	0/1/1/1
5	NAG	G	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	501	1	-	0/6/23/26	0/1/1/1
5	NAG	G	509	1	-	2/6/23/26	0/1/1/1
5	NAG	A	508	1	-	2/6/23/26	0/1/1/1
5	NAG	G	507	1	-	2/6/23/26	0/1/1/1
5	NAG	A	507	1	-	0/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	G	505	1	-	2/6/23/26	0/1/1/1
5	NAG	A	506	1	-	2/6/23/26	0/1/1/1
5	NAG	G	506	1	-	0/6/23/26	0/1/1/1
5	NAG	A	509	1	-	2/6/23/26	0/1/1/1
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	508	1	-	2/6/23/26	0/1/1/1
5	NAG	G	503	1	-	0/6/23/26	0/1/1/1
5	NAG	G	504	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	505	NAG	O5-C1	3.99	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	506	NAG	O5-C1	-2.81	1.39	1.43
5	A	502	NAG	O5-C1	2.22	1.47	1.43
5	G	505	NAG	C1-C2	2.17	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	NAG	C1-O5-C5	7.45	122.17	112.19
5	G	502	NAG	C1-O5-C5	5.93	120.13	112.19
5	G	505	NAG	O5-C1-C2	-5.75	102.39	111.29
5	A	505	NAG	C2-N2-C7	4.59	129.04	122.90
5	A	508	NAG	C1-O5-C5	3.38	116.71	112.19
5	A	505	NAG	C1-C2-N2	3.36	115.73	110.43
5	G	506	NAG	C3-C4-C5	2.75	115.22	110.23
5	G	504	NAG	C1-O5-C5	2.58	115.64	112.19
5	G	504	NAG	C4-C3-C2	-2.39	107.52	111.02
5	A	505	NAG	C8-C7-N2	2.35	120.02	116.12
5	A	503	NAG	C1-O5-C5	2.34	115.32	112.19
5	G	506	NAG	O5-C1-C2	-2.33	107.68	111.29
5	A	509	NAG	C2-N2-C7	-2.30	119.81	122.90
5	A	504	NAG	C1-O5-C5	2.26	115.21	112.19
5	A	509	NAG	O7-C7-C8	-2.02	118.45	122.05
5	G	505	NAG	C4-C3-C2	-2.02	108.06	111.02
5	G	504	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	509	NAG	C8-C7-N2-C2
5	A	509	NAG	O7-C7-N2-C2
5	A	501	NAG	O5-C5-C6-O6
5	A	506	NAG	O5-C5-C6-O6
5	G	502	NAG	O5-C5-C6-O6
5	A	502	NAG	O5-C5-C6-O6
5	A	505	NAG	O5-C5-C6-O6
5	A	508	NAG	O5-C5-C6-O6
5	G	509	NAG	O5-C5-C6-O6
5	A	502	NAG	C4-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	A	506	NAG	C4-C5-C6-O6
5	A	505	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	502	NAG	C4-C5-C6-O6
5	G	509	NAG	C4-C5-C6-O6
5	A	505	NAG	C8-C7-N2-C2
5	A	505	NAG	O7-C7-N2-C2
5	A	503	NAG	O5-C5-C6-O6
5	G	508	NAG	C4-C5-C6-O6
5	A	508	NAG	C4-C5-C6-O6
5	G	508	NAG	O5-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	G	505	NAG	O5-C5-C6-O6
5	G	505	NAG	C4-C5-C6-O6
5	A	505	NAG	C3-C2-N2-C7
5	G	507	NAG	C4-C5-C6-O6
5	A	505	NAG	C1-C2-N2-C7
5	G	507	NAG	O5-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	NAG	4	0
5	A	508	NAG	2	0
5	A	507	NAG	2	0
5	A	503	NAG	1	0
5	G	505	NAG	6	0
5	A	506	NAG	3	0
5	G	506	NAG	6	0
5	A	509	NAG	4	0
5	A	502	NAG	2	0
5	G	508	NAG	1	0
5	G	503	NAG	1	0
5	G	504	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	308/355 (86%)	0.49	12 (3%) 43 35	44, 80, 126, 169	0
1	G	338/355 (95%)	0.21	7 (2%) 63 54	31, 68, 102, 119	0
2	N	24/28 (85%)	0.07	0 100 100	37, 56, 80, 98	0
3	C	217/228 (95%)	0.24	8 (3%) 45 37	36, 63, 88, 116	0
3	H	218/228 (95%)	0.19	1 (0%) 87 83	48, 70, 99, 116	0
4	D	210/214 (98%)	0.16	3 (1%) 73 65	36, 60, 79, 95	0
4	L	210/214 (98%)	0.24	5 (2%) 59 50	51, 69, 90, 111	0
All	All	1525/1622 (94%)	0.26	36 (2%) 59 50	31, 68, 106, 169	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	454	LEU	4.4
1	G	345	VAL	4.0
1	G	396	ILE	3.6
4	L	34	ALA	3.4
1	A	396	ILE	3.3
1	A	455	THR	3.3
3	C	187	SER	3.1
4	L	83	VAL	3.0
1	A	268	GLU	3.0
1	A	474	ASN	3.0
1	G	346	THR	3.0
1	A	469	ARG	2.9
1	A	280	ASN	2.9
3	C	139	GLY	2.8
3	C	180	SER	2.8
4	D	47	LEU	2.8
1	A	395	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	284	ILE	2.7
1	A	471	GLY	2.7
3	C	192	GLN	2.6
1	A	367	GLY	2.5
4	D	201	LEU	2.5
4	D	200	GLY	2.5
1	G	208	ILE	2.4
3	H	188	SER	2.4
4	L	118	PHE	2.4
1	A	460	ALA	2.4
3	C	40	ALA	2.3
1	A	361	PHE	2.3
4	L	1	ALA	2.3
3	C	181	VAL	2.3
4	L	115	VAL	2.2
3	C	25	SER	2.1
1	G	390	LEU	2.1
3	C	193	THR	2.1
1	A	472	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DPR	N	21	7/8	0.85	0.17	47,51,61,75	0
2	U2X	N	29	19/20	0.90	0.10	25,30,52,53	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	502	14/15	0.60	0.13	69,74,80,84	0
5	NAG	G	504	14/15	0.62	0.15	96,106,115,116	0
5	NAG	G	509	14/15	0.68	0.13	65,81,89,94	0
5	NAG	A	509	14/15	0.69	0.15	86,92,102,103	0
5	NAG	A	502	14/15	0.70	0.10	70,76,82,83	0
5	NAG	A	508	14/15	0.72	0.11	70,82,101,101	0
5	NAG	G	507	14/15	0.73	0.11	58,65,92,92	0
5	NAG	A	501	14/15	0.75	0.12	47,52,66,80	0
5	NAG	A	505	14/15	0.75	0.15	50,63,79,86	0
5	NAG	A	507	14/15	0.78	0.13	60,75,89,99	0
5	NAG	G	501	14/15	0.79	0.11	44,57,69,70	0
5	NAG	A	504	14/15	0.80	0.14	66,73,86,93	0
5	NAG	G	506	14/15	0.82	0.14	76,85,97,97	0
5	NAG	G	508	14/15	0.82	0.12	60,64,72,80	0
5	NAG	A	506	14/15	0.83	0.14	62,72,77,85	0
5	NAG	G	505	14/15	0.83	0.17	27,33,37,37	0
5	NAG	G	503	14/15	0.92	0.09	44,54,68,75	0
5	NAG	A	503	14/15	0.93	0.06	39,43,56,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.