Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 09:42 PM EST

PDB ID	:	7N8Q
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:

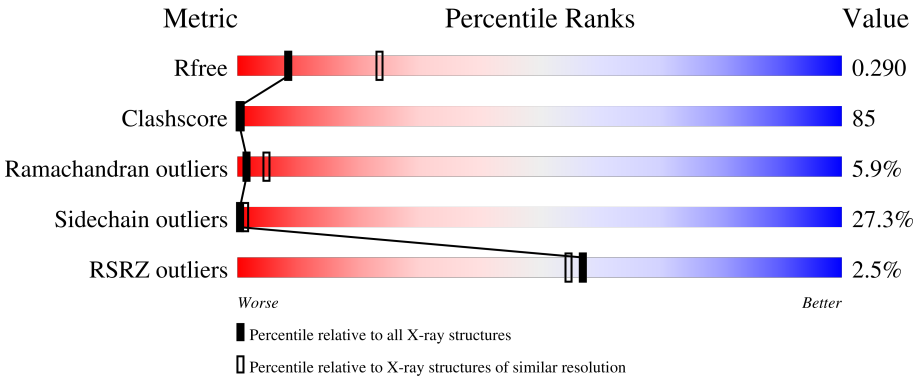
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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% 22% 43% 21% · 13%
1	G	355	2% 23% 54% 18% · 5%
2	N	28	4% 57% 32% 11%
3	C	228	3% 28% 50% 17% 5%
3	H	228	3% 25% 52% 18% ·

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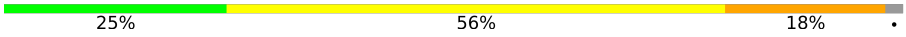
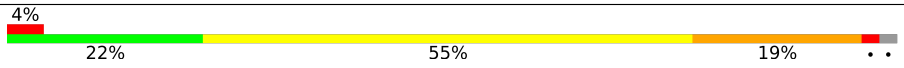
Mol	Chain	Length	Quality of chain
4	D	214	
4	L	214	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	509	-	-	-	X

2 Entry composition (i)

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			

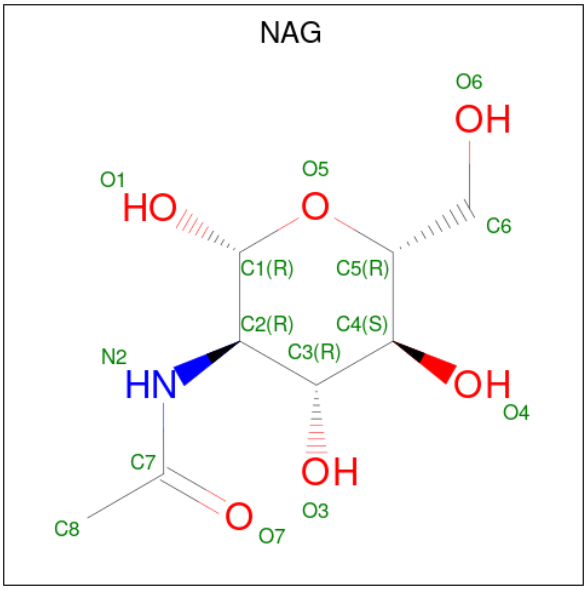
- Molecule 3 is a protein called Rhesusized DH677.3 FAB HEAVY CHAIN.

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 (three-letter code: 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		
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 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

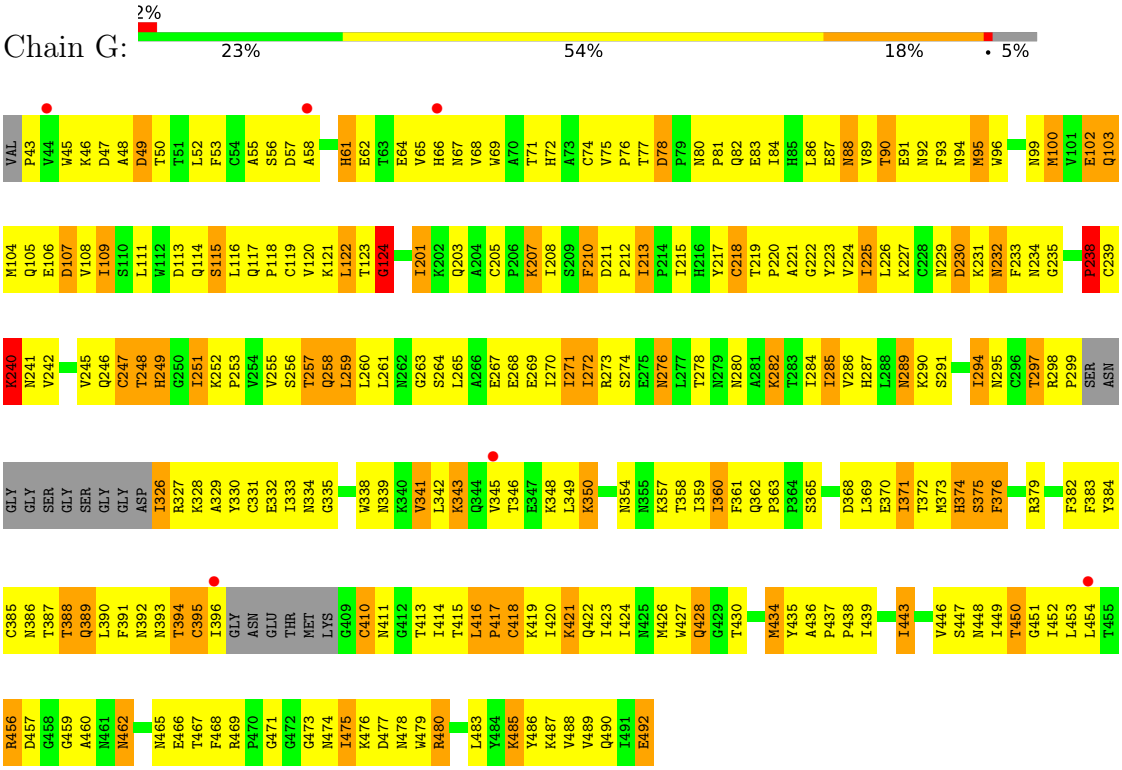
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	5	Total O 5 5	0	0
6	H	3	Total O 3 3	0	0
6	L	2	Total O 2 2	0	0
6	A	2	Total O 2 2	0	0
6	C	1	Total O 1 1	0	0
6	D	2	Total O 2 2	0	0

3 Residue-property plots (i)

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.

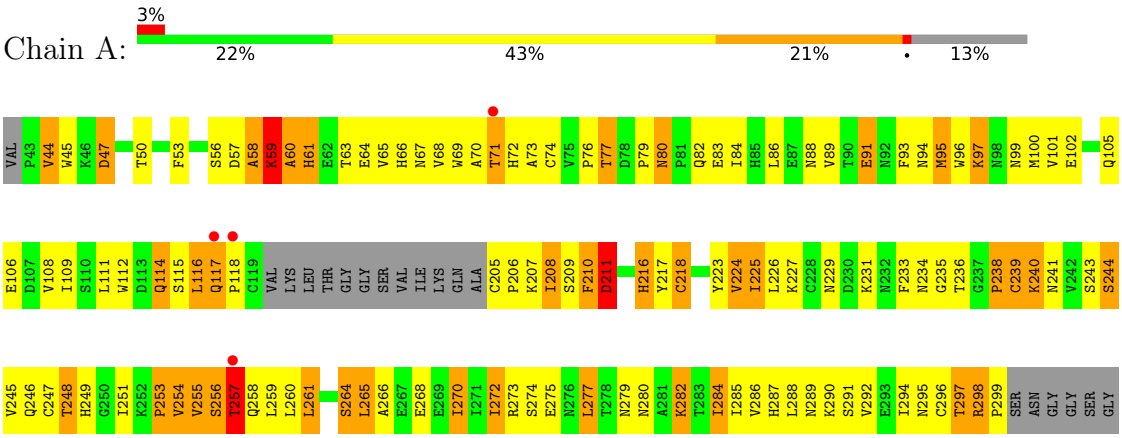
• Molecule 1: clade A/E 93TH057 HIV-1 gp120 core

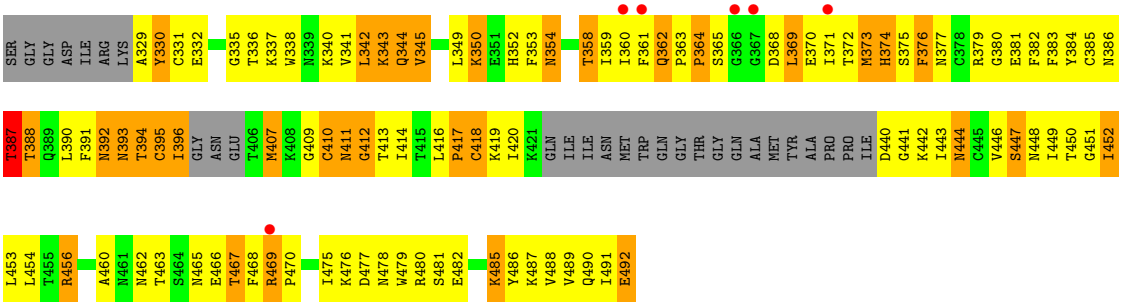
Chain G:



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

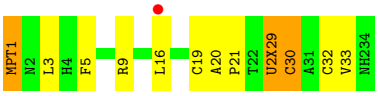
Chain A:





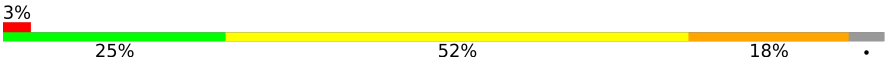
• Molecule 2: M48U1 CD4 MIMETIC PEPTIDE

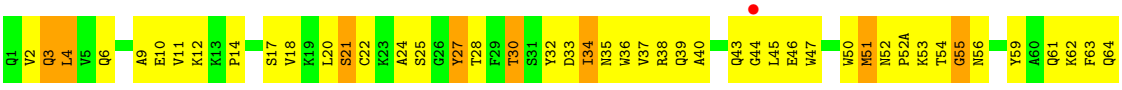
Chain N:

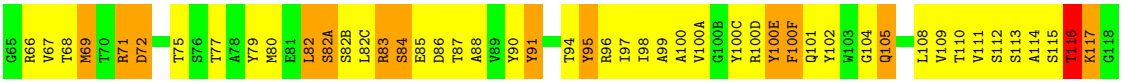


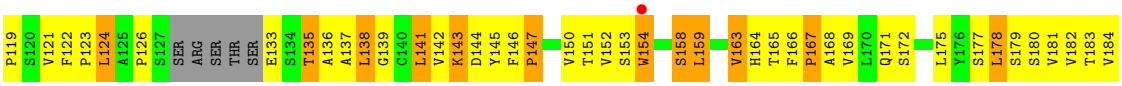
• Molecule 3: Rhesusized DH677.3 FAB HEAVY CHAIN

Chain H:



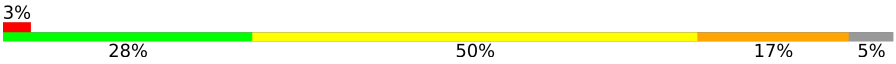


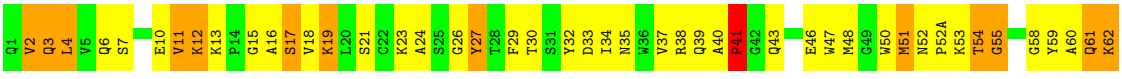


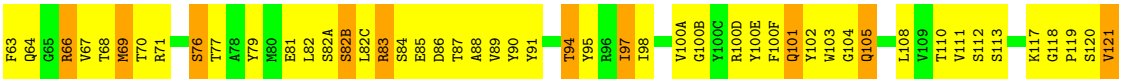


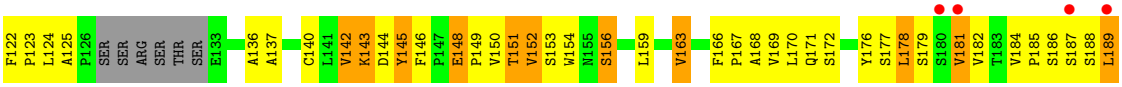
• Molecule 3: Rhesusized DH677.3 FAB HEAVY CHAIN

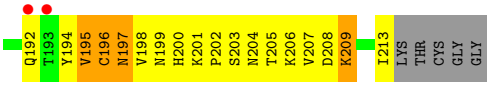
Chain C:





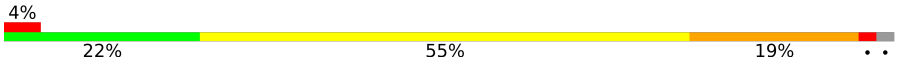


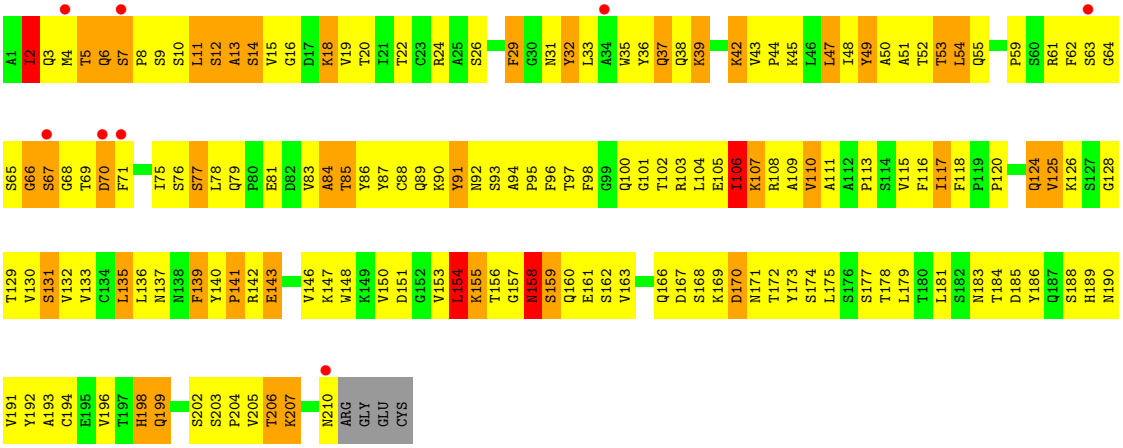




• Molecule 4: Rhesusized DH677.3 FAB LIGHT CHAIN

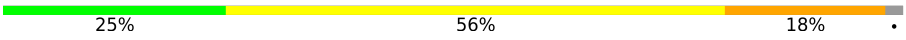
Chain L:

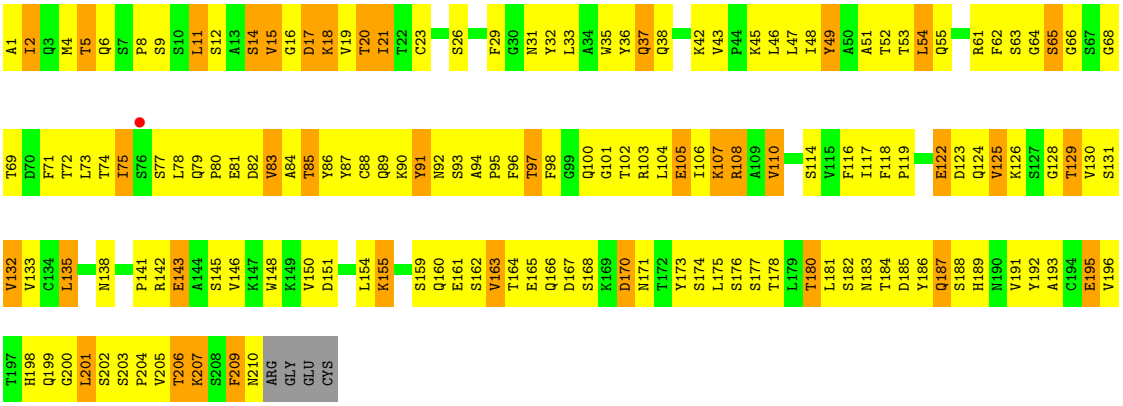




• Molecule 4: Rhesusized DH677.3 FAB LIGHT CHAIN

Chain D:





4 Data and refinement statistics (i)

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 47.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.6 (47.93-2.90) 82.7 (47.88-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.15%)	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)	0.26 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, U2X, MPT, DPR, NH2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.62	0/2468	0.88	3/3346 (0.1%)
1	G	0.63	1/2702 (0.0%)	0.84	2/3667 (0.1%)
2	N	0.56	0/176	0.72	0/231
3	C	0.65	0/1691	0.83	0/2304
3	H	0.65	0/1697	0.87	1/2312 (0.0%)
4	D	0.67	0/1639	0.83	1/2231 (0.0%)
4	L	0.67	0/1639	0.89	2/2231 (0.1%)
All	All	0.64	1/12012 (0.0%)	0.86	9/16322 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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	8.12	1.47	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	392	ASN	N-CA-C	-7.93	89.58	111.00
4	L	32	TYR	N-CA-C	-7.14	91.72	111.00
4	L	32	TYR	CB-CA-C	-6.91	96.58	110.40
1	A	392	ASN	N-CA-CB	6.05	121.49	110.60
1	G	124	GLY	C-N-CA	-5.80	110.11	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	43	PRO	CA-N-CD	-5.54	103.74	111.50
3	H	91	TYR	CB-CA-C	-5.47	99.46	110.40
1	A	387	THR	CB-CA-C	-5.14	97.73	111.60
4	D	200	GLY	C-N-CA	5.02	134.26	121.70

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2419	0	2342	433	0
1	G	2646	0	2587	404	0
2	N	209	0	212	19	0
3	C	1651	0	1617	315	0
3	H	1657	0	1622	329	0
4	D	1604	0	1563	324	0
4	L	1604	0	1563	335	0
5	A	126	0	117	17	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	2030	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 85.

All (2030) 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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:87:TYR:CE1	4:L:101:GLY:HA3	1.79	1.17
1:A:95:MET:HE3	1:A:235:GLY:HA3	1.20	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
3:C:59:TYR:CE1	3:C:69:MET:HE3	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
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
3:H:163:VAL:HG23	3:H:182:VAL:HG13	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:154:TRP:HZ3	3:H:195:VAL:C	1.60	1.04
1:A:60:ALA:HB2	1:A:71:THR:CG2	1.87	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:TYR:HE2	1:G:490:GLN:HB2	1.26	0.99
4:L:157:GLY:C	4:L:158:ASN:HD22	1.64	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
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
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
4:L:85:THR:CG2	4:L:102:THR:C	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
3:C:35:ASN:CG	3:C:47:TRP:HE1	1.72	0.93
4:D:187:GLN:HA	4:D:187:GLN:HE21	1.32	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:L:85:THR:HG22	4:L:102:THR:C	1.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:119:PRO:HB2	3:H:142:VAL:CG1	2.06	0.86
3:C:59:TYR:CD1	3:C:69:MET:HE3	2.10	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
1:G:373:MET:CE	1:G:386:ASN:HB2	2.06	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
4:L:85:THR:HG23	4:L:102:THR:C	1.97	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:128:GLY:HA2	4:L:183:ASN:CG	1.96	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
4:D:4:MET:HE1	4:D:97:THR:O	1.77	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:95:MET:CE	1:A:235:GLY:CA	2.53	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: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
4:L:136:LEU:CD2	4:L:196:VAL:CG1	2.57	0.81
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
4:D:4:MET:HE2	4:D:97:THR:CG2	2.11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:32:TYR:C	4:D:91:TYR:HE2	1.86	0.80
1:G:233:PHE:CE1	1:G:235:GLY:HA2	2.17	0.79
1:A:95:MET:HE2	1:A:235:GLY:HA3	1.62	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:117:ILE:CG1	4:L:205:VAL:HG23	2.13	0.78
1:A:258:GLN:CD	1:A:372:THR:O	2.21	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
4:L:157:GLY:C	4:L:158:ASN:ND2	2.37	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
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
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:120:VAL:HB	1:G:434:MET:HE1	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:ARG:HH11	4:D:82:ASP:CG	1.88	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
4:L:146:VAL:HG11	4:L:177:SER:CB	2.16	0.76
1:A:95:MET:HE3	1:A:235:GLY:CA	2.10	0.76
3:H:181:VAL:CG1	4:L:135:LEU:HD21	2.14	0.76
1:G:373:MET:HE1	1:G:386:ASN:HB2	1.65	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
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
3:C:59:TYR:CD1	3:C:69:MET:CE	2.68	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:151:ASP:CG	4:L:189:HIS:ND1	2.40	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
4:L:29:PHE:HE2	4:L:32:TYR:O	1.70	0.74
4:L:120:PRO:CG	4:L:186:TYR:OH	2.34	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
4:D:4:MET:HE2	4:D:97:THR:HG22	1.70	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
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
3:C:59:TYR:HE1	3:C:69:MET:HE3	1.30	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
3:H:95:TYR:CD1	3:H:100(D):ARG:CA	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:91:GLU:CD	1:A:487:LYS:HZ3	1.93	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
3:H:66:ARG:CD	3:H:82(B):SER:OG	2.31	0.71
3:H:154:TRP:CZ3	3:H:195:VAL:C	2.52	0.71
3:C:145:TYR:CE1	3:C:176:TYR:C	2.65	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:145:TYR:HE1	3:C:176:TYR:C	1.95	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
4:D:31:ASN:CG	4:D:68:GLY:H	1.96	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
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
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:O	1:G:439:ILE:HD12	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
3:H:97:ILE:O	3:H:97:ILE:HG13	1.91	0.69
1:A:233:PHE:HE1	1:A:235:GLY:CA	2.05	0.69
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:4:MET:HE1	4:L:90:LYS:N	2.08	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:444:ASN:OD1	1:A:444:ASN:C	2.30	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
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: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:A:386:ASN:CG	1:A:388:THR:HG22	2.13	0.68
4:D:61:ARG:HG2	4:D:75:ILE:CG2	2.23	0.68
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:59:TYR:CE1	3:C:69:MET:HE2	2.27	0.68
1:G:480:ARG:HG3	1:G:480:ARG:NH1	2.09	0.68
4:D:100:GLN:OE1	4:D:100:GLN:N	2.25	0.68
3:H:85:GLU:OE1	3:H:85:GLU:N	2.25	0.68
3:H:95:TYR:CD1	3:H:100(D):ARG:C	2.67	0.68
4:L:2:ILE:HD12	4:L:90:LYS:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:CB	1:A:71:THR:CB	2.67	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:D:90:LYS:HZ3	4:D:95:PRO:HD2	1.59	0.67
1:G:207:LYS:NZ	1:G:437:PRO:O	2.25	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
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
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
3:H:100(F):PHE:HE1	4:L:89:GLN:CD	1.98	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
3:H:72:ASP:O	3:H:75:THR:HG22	1.94	0.67
4:L:151:ASP:HA	4:L:191:VAL:HG13	1.76	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
3:C:166:PHE:CZ	4:D:174:SER:O	2.48	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:388:THR:OG1	1:G:389:GLN:N	2.28	0.66
4:D:11:LEU:O	4:D:104:LEU:HA	1.95	0.66
1:G:439:ILE:HD12	1:G:439:ILE:C	2.15	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
3:H:101:GLN:HE22	3:H:102:TYR:HE2	1.36	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
1:A:392:ASN:C	1:A:394:THR:H	2.00	0.66
3:C:35:ASN:OD1	3:C:47:TRP:NE1	2.27	0.66
1:G:239:CYS:SG	1:G:239:CYS:O	2.54	0.65
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
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
4:D:135:LEU:HD23	4:D:135:LEU:C	2.17	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
3:C:61:GLN:NE2	3:C:61:GLN:HA	2.12	0.65
4:D:32:TYR:C	4:D:91:TYR:CE2	2.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:61:ARG:NH1	4:D:82:ASP:CG	2.50	0.65
3:H:39:GLN:O	3:H:88:ALA:HB1	1.96	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
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: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:370:GLU:H	1:A:370:GLU:CD	2.00	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:77:SER:O	4:L:77:SER:OG	2.15	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
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
3:H:95:TYR:HD1	3:H:100(D):ARG:C	2.01	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
1:G:122:LEU:HD12	1:G:122:LEU:C	2.19	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:107:ASP:CG	1:G:217:TYR:OH	2.36	0.63
1:G:386:ASN:O	1:G:416:LEU:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:TYR:CD2	3:C:100(D):ARG:C	2.72	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:L:85:THR:CG2	4:L:103:ARG:N	2.60	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
3:H:54:THR:O	3:H:54:THR:OG1	2.13	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
3:C:37:VAL:HG23	3:C:46:GLU:C	2.19	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
3:C:197:ASN:HD22	3:C:208:ASP:CG	2.03	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
1:G:273:ARG:NH2	1:G:287:HIS:CG	2.67	0.62
1:G:331:CYS:C	1:G:332:GLU:HG3	2.20	0.62
4:L:4:MET:HE1	4:L:90:LYS:HB3	1.80	0.62
1:A:95:MET:O	1:A:480:ARG:HG2	1.98	0.62
3:C:83:ARG:C	3:C:111:VAL:HG21	2.20	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
3:C:39:GLN:OE1	4:D:38:GLN:NE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
4:L:38:GLN:C	4:L:84:ALA:HB1	2.13	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
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:80:MET:O	3:H:80:MET:HE3	2.00	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:135:LEU:C	4:L:135:LEU:HD12	2.19	0.62
4:L:155:LYS:HZ3	4:L:181:LEU:CD2	2.12	0.62
3:C:59:TYR:HE1	3:C:69:MET:HE2	1.60	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: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
4:D:131:SER:HG	4:D:180:THR:HG1	1.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:117:GLN:CD	1:G:203:GLN:HG3	2.21	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
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
1:A:45:TRP:HB2	1:A:489:VAL:CG1	2.30	0.61
4:D:4:MET:CE	4:D:97:THR:HG22	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:91:GLU:OE1	1:A:487:LYS:NZ	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:270:ILE:HG13	5:A:505:NAG:H62	1.84	0.59
1:A:396:ILE:C	1:A:396:ILE:HD12	2.22	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
1:A:373:MET:HG2	1:A:385:CYS:C	2.23	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
3:C:156:SER:O	3:C:156:SER:OG	2.11	0.59
1:G:362:GLN:HG3	1:G:363:PRO:HD3	1.80	0.59
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
3:C:123:PRO:HD3	3:C:209:LYS:HZ2	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:120:VAL:HB	1:G:434:MET:HE2	1.83	0.58
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
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: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
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
4:L:61:ARG:O	4:L:75:ILE:HA	2.04	0.58
1:A:111:LEU:HD23	1:A:111:LEU:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:L:33:LEU:HD22	4:L:71:PHE:CE2	2.39	0.57
1:G:232:ASN:OD1	1:G:268:GLU:CB	2.52	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:100:MET:HE1	1:A:486:TYR:HB3	1.86	0.57
1:A:386:ASN:C	1:A:416:LEU:HD23	2.23	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
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
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
1:G:111:LEU:HD23	1:G:111:LEU:C	2.25	0.57
4:L:157:GLY:C	4:L:159:SER:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:413:THR:O	1:A:413:THR:HG22	2.04	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
3:C:154:TRP:CE3	3:C:195:VAL:C	2.78	0.56
1:G:373:MET:HE3	1:G:386:ASN:HB2	1.87	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
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
4:D:37:GLN:CD	4:D:86:TYR:HE1	2.04	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
4:L:5:THR:O	4:L:5:THR:OG1	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:A:294:ILE:HG23	1:A:294:ILE:O	2.07	0.55
1:G:50:THR:O	1:G:103:GLN:NE2	2.40	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
4:L:100:GLN:H	4:L:100:GLN:CD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:387:THR:HG23	1:A:390:LEU:HD12	1.87	0.54
1:A:392:ASN:C	1:A:394:THR:N	2.61	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
1:A:392:ASN:CG	5:A:509:NAG:H82	2.28	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
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
4:L:110:VAL:O	4:L:110:VAL:HG12	2.08	0.54
3:C:150:VAL:HG11	3:C:178:LEU:HD21	1.89	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:71:PHE:C	4:D:72:THR:OG1	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:VAL:HG22	4:D:132:VAL:O	2.07	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:423:ILE:C	1:G:424:ILE:HG23	2.29	0.53
3:H:10:GLU:O	3:H:110:THR:N	2.31	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
1:G:388:THR:C	1:G:390:LEU:N	2.60	0.53
3:H:135:THR:H	3:H:186:SER:CA	2.18	0.53
1:A:291:SER:OG	1:A:448:ASN:CG	2.47	0.53
3:C:39:GLN:C	3:C:88:ALA:HB1	2.28	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
3:H:135:THR:HA	3:H:186:SER:CA	2.38	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
3:C:100(D):ARG:C	4:D:91:TYR:HD1	2.12	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
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
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
4:D:87:TYR:CD1	4:D:101:GLY:CA	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:100:MET:CE	1:A:486:TYR:HB3	2.39	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
4:L:106:ILE:CG2	4:L:171:ASN:HB3	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:60:ALA:O	3:C:64:GLN:N	2.43	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
1:G:239:CYS:O	1:G:240:LYS:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:HIS:C	1:G:74:CYS:H	2.13	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
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
1:G:100:MET:HE1	1:G:486:TYR:HB2	1.92	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: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
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:A:288:LEU:HD12	1:A:450:THR:C	2.30	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:39:GLN:HG3	3:H:44:GLY:O	2.10	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
1:G:357:LYS:NZ	1:G:460:ALA:O	2.34	0.51
2:N:16:LEU:O	2:N:32:CYS:HA	2.10	0.51
4:L:115:VAL:HG21	4:L:203:SER:HG	1.74	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
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:49:TYR:C	4:D:49:TYR:CD1	2.85	0.51
4:D:186:TYR:CE1	4:D:192:TYR:CE2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:487:LYS:NZ	5:A:506:NAG:H81	2.25	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
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:95:MET:HE2	1:A:235:GLY:CA	2.29	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
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
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
3:H:135:THR:HA	3:H:186:SER:C	2.31	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
1:G:373:MET:CE	1:G:386:ASN:CB	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:TYR:C	4:L:49:TYR:CD1	2.85	0.50
4:L:69:THR:HG23	4:L:70:ASP:OD1	2.11	0.50
4:L:120:PRO:HD2	4:L:207:LYS:HZ1	1.76	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:68:VAL:O	1:A:69:TRP:C	2.50	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
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
4:L:186:TYR:HD1	4:L:192:TYR:OH	1.95	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:95:MET:HE1	1:A:273:ARG:HG2	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:32:TYR:OH	3:C:98:ILE:O	2.30	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
1:A:112:TRP:HH2	1:A:382:PHE:CZ	2.30	0.49
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:233:PHE:CE1	1:A:235:GLY:C	2.85	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
1:G:100:MET:CE	1:G:486:TYR:O	2.60	0.49
1:G:123:THR:O	1:G:124:GLY:C	2.51	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
1:A:354:ASN:OD1	1:A:354:ASN:N	2.46	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:388:THR:C	1:G:390:LEU:H	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:137:ALA:N	4:L:116:PHE:CE2	2.81	0.48
1:A:239:CYS:O	1:A:240:LYS:C	2.51	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
1:G:475:ILE:O	1:G:476:LYS:C	2.50	0.48
3:H:166:PHE:HE1	4:L:174:SER:O	1.96	0.48
4:L:4:MET:HE1	4:L:90:LYS:CB	2.42	0.48
1:A:115:SER:C	1:A:116:LEU:HG	2.33	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
1:A:394:THR:C	1:A:396:ILE:HG23	2.32	0.48
3:C:124:LEU:C	4:D:118:PHE:HE1	2.15	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
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
1:A:350:LYS:C	1:A:350:LYS:HD2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:HD21	1:A:97:LYS:HG3	1.72	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
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:4:LEU:HD13	3:C:103:TRP:C	2.35	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
3:C:51:MET:HB3	3:C:51:MET:HE2	1.61	0.47
1:G:53:PHE:CE2	1:G:218:CYS:HB3	2.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
3:H:36:TRP:CD1	3:H:69:MET:HE3	2.49	0.47
3:H:185:PRO:O	3:H:186:SER:C	2.52	0.47
4:L:32:TYR:C	4:L:91:TYR:HE2	2.19	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:G:423:ILE:C	1:G:424:ILE:CG2	2.83	0.46
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
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:C:112:SER:OG	3:C:146:PHE:CE2	2.66	0.46
3:C:123:PRO:CD	3:C:209:LYS:HZ2	2.28	0.46
4:L:62:PHE:CE1	4:L:75:ILE:HD12	2.49	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:20:LEU:HD12	3:H:80:MET:HE1	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:PRO:HG3	4:D:199:GLN:HE22	1.78	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:91:GLU:CD	1:A:487:LYS:NZ	2.67	0.46
1:A:207:LYS:C	1:A:208:ILE:HG23	2.36	0.46
1:A:218:CYS:HA	1:A:246:GLN:O	2.16	0.46
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:13:ALA:C	4:L:14:SER:O	2.52	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:4:MET:CE	4:D:97:THR:CG2	2.88	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
1:G:388:THR:HG1	1:G:389:GLN:H	1.64	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:137:ALA:N	4:D:116:PHE:HE2	2.14	0.46
1:G:102:GLU:OE1	1:G:476:LYS:HE3	2.16	0.46
1:G:230:ASP:OD1	1:G:239:CYS:C	2.54	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:373:MET:HE3	1:A:373:MET:HB2	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:36:TRP:HB2	3:H:69:MET:HE3	1.98	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
1:G:72:HIS:O	1:G:74:CYS:N	2.48	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
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
3:C:48:MET:HE1	3:C:90:TYR:CD1	2.51	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
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
4:L:143:GLU:O	4:L:143:GLU:HG2	2.17	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
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
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
4:L:186:TYR:CD1	4:L:192:TYR:OH	2.68	0.45
1:A:233:PHE:CD1	1:A:235:GLY:N	2.76	0.45
3:C:37:VAL:CG2	3:C:46:GLU:C	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:166:PHE:O	3:H:167:PRO:C	2.55	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
1:A:376:PHE:CD1	1:A:376:PHE:C	2.87	0.45
3:C:112:SER:CB	3:C:146:PHE:CE2	2.93	0.45
4:D:117:ILE:HG13	4:D:118:PHE:N	2.32	0.45
1:G:298:ARG:NH1	1:G:439:ILE:O	2.50	0.45
3:H:39:GLN:C	3:H:88:ALA:HB1	2.38	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:58:ALA:C	1:A:60:ALA:N	2.69	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
1:A:469:ARG:HD3	1:A:469:ARG:C	2.38	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
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:C:154:TRP:CZ3	3:C:195:VAL:C	2.91	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
4:D:49:TYR:C	4:D:49:TYR:HD1	2.20	0.44
1:A:286:VAL:CB	1:A:452:ILE:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ALA:HB1	1:A:417:PRO:C	2.38	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
1:A:369:LEU:HB2	1:A:373:MET:HE3	1.99	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:374:HIS:C	1:G:374:HIS:ND1	2.71	0.44
3:H:21:SER:HG	3:H:79:TYR:HE1	1.63	0.44
4:L:157:GLY:C	4:L:159:SER:N	2.71	0.44
1:A:362:GLN:CB	1:A:363:PRO:CD	2.95	0.44
3:C:123:PRO:CD	3:C:209:LYS:HZ3	2.30	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
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
1:G:468:PHE:C	1:G:469:ARG:HG3	2.38	0.44
3:H:61:GLN:O	3:H:64:GLN:N	2.39	0.44
4:L:18:LYS:HG3	4:L:18:LYS:O	2.17	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
1:G:251:ILE:O	1:G:251:ILE:HG12	2.17	0.43
1:A:111:LEU:C	1:A:111:LEU:CD2	2.86	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:4:MET:CE	4:D:97:THR:O	2.59	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:473:GLY:HA3	2:N:20:ALA:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:100:MET:CE	1:G:486:TYR:C	2.87	0.43
1:G:273:ARG:NH2	1:G:287:HIS:HB2	2.17	0.43
1:G:373:MET:HE3	1:G:386:ASN:N	2.34	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
4:D:4:MET:HE2	4:D:97:THR:HG23	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:409:GLY:C	1:A:410:CYS:O	2.58	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:95:MET:HE3	1:A:95:MET:HB3	1.52	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:95:TYR:HD2	3:C:100(D):ARG:C	2.21	0.42
3:C:100(E):TYR:N	4:D:91:TYR:CD1	2.81	0.42
3:C:124:LEU:C	4:D:118:PHE:CE1	2.93	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:132:VAL:HG12	4:L:132:VAL:O	2.19	0.42
3:C:4:LEU:HD23	3:C:94:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:82:LEU:C	3:H:82:LEU:CD1	2.88	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
4:D:146:VAL:HG11	4:D:177:SER:CB	2.50	0.42
1:G:120:VAL:HG23	1:G:434:MET:HE3	2.01	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:50:ALA:O	4:L:51:ALA:HB3	2.20	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
1:G:487:LYS:HZ1	5:A:506:NAG:H81	1.85	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:80:ASN:ND2	1:A:80:ASN:C	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:350:LYS:C	1:A:350:LYS:CD	2.88	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
4:L:106:ILE:HG23	4:L:106:ILE:O	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
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
4:L:199:GLN:C	4:L:199:GLN:CD	2.78	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
3:H:123:PRO:C	3:H:124:LEU:HD23	2.40	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
1:G:84:ILE:HD13	3:H:100:ALA:C	2.40	0.41
3:H:98:ILE:CD1	3:H:100(C):TYR:CG	3.03	0.41
3:H:154:TRP:CE3	3:H:196:CYS:CB	3.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:100:MET:HE1	1:G:486:TYR:C	2.41	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:386:ASN:CG	1:A:388:THR:CG2	2.83	0.41
3:C:19:LYS:HE3	3:C:19:LYS:HB3	1.40	0.41
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:155:LYS:HZ1	4:L:181:LEU:CD2	2.28	0.41
1:A:233:PHE:HE1	1:A:235:GLY:C	2.22	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
4:D:4:MET:HE2	4:D:4:MET:HB2	1.66	0.41
1:G:61:HIS:ND1	1:G:61:HIS:C	2.73	0.41
3:H:20:LEU:CD1	3:H:90:TYR:CB	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:L:4:MET:HE1	4:L:89:GLN:C	2.39	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
1:G:111:LEU:C	1:G:111:LEU:CD2	2.88	0.41
1:G:120:VAL:CB	1:G:434:MET:HE1	2.44	0.41
3:H:12:LYS:HG3	3:H:18:VAL:HB	2.03	0.41
1:A:66:HIS:CE1	1:A:210:PHE:HE1	2.31	0.41
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
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
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
1:A:396:ILE:C	1:A:396:ILE:CD1	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:465:ASN:N	1:A:465:ASN:OD1	2.54	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
4:D:125:VAL:C	4:D:183:ASN:HD21	2.22	0.40
1:G:121:LYS:HD2	1:G:201:ILE:HD11	2.02	0.40
3:H:114:ALA:HB1	3:H:146:PHE:CD1	2.35	0.40
1:A:61:HIS:HD1	1:A:61:HIS:C	2.24	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
3:H:85:GLU:N	3:H:85:GLU:CD	2.74	0.40
4:L:35:TRP:O	4:L:47:LEU:HB2	2.21	0.40
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%)	3 10
3	C	213/228 (93%)	173 (81%)	36 (17%)	4 (2%)	8 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	H	214/228 (94%)	176 (82%)	31 (14%)	7 (3%)	4 15
4	D	208/214 (97%)	175 (84%)	26 (12%)	7 (3%)	3 15
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 5

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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%)	202 (72%)	77 (28%)	0 1
1	G	302/313 (96%)	217 (72%)	85 (28%)	0 1
2	N	20/20 (100%)	19 (95%)	1 (5%)	24 57
3	C	183/192 (95%)	131 (72%)	52 (28%)	0 1
3	H	184/192 (96%)	135 (73%)	49 (27%)	0 1
4	D	184/187 (98%)	134 (73%)	50 (27%)	0 1
4	L	184/187 (98%)	133 (72%)	51 (28%)	0 1
All	All	1336/1404 (95%)	971 (73%)	365 (27%)	0 1

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	46	LYS
1	G	49	ASP
1	G	57	ASP

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Mol	Chain	Res	Type
1	G	61	HIS
1	G	62	GLU
1	G	64	GLU
1	G	68	VAL
1	G	71	THR
1	G	78	ASP
1	G	90	THR
1	G	91	GLU
1	G	95	MET
1	G	100	MET
1	G	102	GLU
1	G	103	GLN
1	G	107	ASP
1	G	109	ILE
1	G	113	ASP
1	G	115	SER
1	G	122	LEU
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	225	ILE
1	G	229	ASN
1	G	230	ASP
1	G	232	ASN
1	G	238	PRO
1	G	240	LYS
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

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Mol	Chain	Res	Type
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	327	ARG
1	G	341	VAL
1	G	343	LYS
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	416	LEU
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	450	THR
1	G	452	ILE
1	G	456	ARG
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	492	GLU
2	N	30	CYS
3	H	3	GLN

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Mol	Chain	Res	Type
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
3	H	37	VAL
3	H	51	MET
3	H	69	MET
3	H	71	ARG
3	H	72	ASP
3	H	82	LEU
3	H	82(A)	SER
3	H	83	ARG
3	H	84	SER
3	H	95	TYR
3	H	100(E)	TYR
3	H	100(F)	PHE
3	H	105	GLN
3	H	112	SER
3	H	113	SER
3	H	116	THR
3	H	117	LYS
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	178	LEU
3	H	186	SER
3	H	191	THR
3	H	192	GLN
3	H	197	ASN

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Mol	Chain	Res	Type
3	H	201	LYS
3	H	206	LYS
3	H	207	VAL
3	H	209	LYS
3	H	210	ARG
3	H	211	VAL
4	L	2	ILE
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	29	PHE
4	L	37	GLN
4	L	39	LYS
4	L	42	LYS
4	L	45	LYS
4	L	47	LEU
4	L	49	TYR
4	L	53	THR
4	L	54	LEU
4	L	63	SER
4	L	67	SER
4	L	70	ASP
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
4	L	147	LYS

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Mol	Chain	Res	Type
4	L	154	LEU
4	L	155	LYS
4	L	158	ASN
4	L	159	SER
4	L	167	ASP
4	L	168	SER
4	L	169	LYS
4	L	170	ASP
4	L	179	LEU
4	L	184	THR
4	L	185	ASP
4	L	190	ASN
4	L	199	GLN
4	L	206	THR
4	L	207	LYS
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	77	THR
1	A	80	ASN
1	A	83	GLU
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	114	GLN
1	A	116	LEU
1	A	117	GLN
1	A	205	CYS
1	A	210	PHE
1	A	211	ASP
1	A	216	HIS
1	A	218	CYS
1	A	224	VAL
1	A	225	ILE
1	A	231	LYS
1	A	244	SER

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Mol	Chain	Res	Type
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	270	ILE
1	A	272	ILE
1	A	277	LEU
1	A	282	LYS
1	A	284	ILE
1	A	292	VAL
1	A	297	THR
1	A	298	ARG
1	A	330	TYR
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	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
1	A	387	THR
1	A	388	THR
1	A	394	THR
1	A	396	ILE
1	A	407	MET
1	A	419	LYS
1	A	444	ASN
1	A	447	SER
1	A	452	ILE

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Mol	Chain	Res	Type
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	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	69	MET
3	C	76	SER
3	C	82(B)	SER
3	C	83	ARG
3	C	89	VAL
3	C	94	THR
3	C	97	ILE
3	C	101	GLN
3	C	105	GLN
3	C	108	LEU
3	C	113	SER
3	C	120	SER
3	C	121	VAL
3	C	142	VAL
3	C	143	LYS
3	C	145	TYR

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Mol	Chain	Res	Type
3	C	148	GLU
3	C	149	PRO
3	C	151	THR
3	C	152	VAL
3	C	153	SER
3	C	156	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	196	CYS
3	C	197	ASN
3	C	209	LYS
4	D	2	ILE
4	D	5	THR
4	D	11	LEU
4	D	14	SER
4	D	17	ASP
4	D	18	LYS
4	D	20	THR
4	D	21	ILE
4	D	37	GLN
4	D	42	LYS
4	D	43	VAL
4	D	45	LYS
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

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Mol	Chain	Res	Type
4	D	97	THR
4	D	105	GLU
4	D	107	LYS
4	D	108	ARG
4	D	114	SER
4	D	122	GLU
4	D	123	ASP
4	D	125	VAL
4	D	126	LYS
4	D	129	THR
4	D	132	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	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 (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	66	HIS
1	G	80	ASN
1	G	98	ASN
1	G	99	ASN
1	G	114	GLN
1	G	117	GLN
1	G	339	ASN
1	G	374	HIS
1	G	411	ASN
1	G	422	GLN
3	H	52	ASN
3	H	192	GLN

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Mol	Chain	Res	Type
3	H	197	ASN
3	H	204	ASN
4	L	6	GLN
4	L	55	GLN
4	L	89	GLN
4	L	158	ASN
4	L	166	GLN
4	L	199	GLN
1	A	66	HIS
1	A	72	HIS
1	A	114	GLN
1	A	249	HIS
1	A	258	GLN
1	A	344	GLN
1	A	362	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 (i)

There are no RNA molecules in this entry.

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

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	1.29	1 (5%)	22,25,27	1.56	5 (22%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	29	U2X	OH-CZ	3.69	1.46	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	29	U2X	CB-CG-CD2	-3.37	114.22	120.91
2	N	29	U2X	CG-CB-CA	2.85	119.86	114.10
2	N	29	U2X	C7-OH-CZ	-2.20	113.26	117.93
2	N	29	U2X	CB-CG-CD1	2.20	125.27	120.91
2	N	29	U2X	CE1-CD1-CG	-2.02	118.24	121.03

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	C-CA-CB-CG
2	N	29	U2X	C4-C3-C7-OH

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 monosaccharides 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	G	509	1	14,14,15	0.43	0	17,19,21	0.61	0
5	NAG	A	506	1	14,14,15	0.41	0	17,19,21	0.71	0
5	NAG	A	509	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	A	508	1	14,14,15	0.22	0	17,19,21	0.90	1 (5%)
5	NAG	G	501	1	14,14,15	0.23	0	17,19,21	0.56	0
5	NAG	G	502	1	14,14,15	0.40	0	17,19,21	1.52	1 (5%)
5	NAG	G	503	1	14,14,15	0.30	0	17,19,21	0.60	0
5	NAG	A	505	1	14,14,15	0.28	0	17,19,21	1.70	3 (17%)
5	NAG	A	502	1	14,14,15	0.70	1 (7%)	17,19,21	1.85	1 (5%)
5	NAG	G	504	1	14,14,15	0.34	0	17,19,21	1.05	2 (11%)
5	NAG	A	503	1	14,14,15	0.44	0	17,19,21	0.79	1 (5%)
5	NAG	G	508	1	14,14,15	0.28	0	17,19,21	0.67	0
5	NAG	G	507	1	14,14,15	0.26	0	17,19,21	0.38	0
5	NAG	A	504	1	14,14,15	0.18	0	17,19,21	0.87	1 (5%)
5	NAG	A	507	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	G	505	1	14,14,15	1.38	1 (7%)	17,19,21	1.80	2 (11%)
5	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.62	0
5	NAG	G	506	1	14,14,15	0.91	1 (7%)	17,19,21	1.20	2 (11%)

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	G	509	1	-	2/6/23/26	0/1/1/1
5	NAG	A	506	1	-	2/6/23/26	0/1/1/1
5	NAG	A	509	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	508	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	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	503	1	-	0/6/23/26	0/1/1/1
5	NAG	A	505	1	-	5/6/23/26	0/1/1/1
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	504	1	-	0/6/23/26	0/1/1/1
5	NAG	A	503	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	507	1	-	2/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	A	507	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	501	1	-	2/6/23/26	0/1/1/1
5	NAG	G	506	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	505	NAG	O5-C1	4.19	1.50	1.43
5	G	506	NAG	O5-C1	-2.97	1.39	1.43
5	A	502	NAG	O5-C1	2.32	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	502	NAG	C1-O5-C5	7.37	122.17	112.19
5	G	502	NAG	C1-O5-C5	5.86	120.13	112.19
5	G	505	NAG	O5-C1-C2	-5.63	102.39	111.29
5	A	505	NAG	C2-N2-C7	4.31	129.04	122.90
5	A	508	NAG	C1-O5-C5	3.34	116.71	112.19
5	A	505	NAG	C1-C2-N2	3.07	115.73	110.49
5	G	506	NAG	C3-C4-C5	2.79	115.22	110.24
5	G	504	NAG	C1-O5-C5	2.55	115.64	112.19
5	G	504	NAG	C4-C3-C2	-2.39	107.52	111.02
5	A	505	NAG	C8-C7-N2	2.31	120.02	116.10
5	A	503	NAG	C1-O5-C5	2.31	115.32	112.19
5	G	506	NAG	O5-C1-C2	-2.28	107.68	111.29
5	A	504	NAG	C1-O5-C5	2.23	115.21	112.19
5	A	509	NAG	C2-N2-C7	-2.17	119.81	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	505	NAG	C4-C3-C2	-2.02	108.06	111.02

There are no chirality outliers.

All (27) 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	G	502	NAG	O5-C5-C6-O6
5	A	506	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
5	A	505	NAG	C8-C7-N2-C2
5	A	505	NAG	O7-C7-N2-C2
5	G	502	NAG	C4-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	G	508	NAG	C4-C5-C6-O6
5	G	509	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	G	507	NAG	O5-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	NAG	2	0
5	A	509	NAG	4	0
5	A	508	NAG	2	0

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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, 95^{th} 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%)	0.17	10 (3%)	47	43	44, 80, 126, 169	0
1	G	338/355 (95%)	-0.13	6 (1%)	68	67	31, 68, 102, 119	0
2	N	24/28 (85%)	0.13	1 (4%)	36	32	37, 56, 80, 98	0
3	C	217/228 (95%)	-0.03	6 (2%)	53	49	36, 63, 88, 116	0
3	H	218/228 (95%)	0.01	6 (2%)	53	49	48, 70, 99, 116	0
4	D	210/214 (98%)	-0.14	1 (0%)	91	91	36, 60, 79, 95	0
4	L	210/214 (98%)	0.06	8 (3%)	40	36	51, 69, 90, 111	0
All	All	1525/1622 (94%)	-0.01	38 (2%)	57	55	31, 68, 106, 169	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	189	LEU	5.4
1	A	118	PRO	4.4
1	A	367	GLY	4.3
1	A	71	THR	4.0
3	H	194	TYR	3.9
1	A	117	GLN	3.7
4	L	34	ALA	3.6
3	H	185	PRO	3.6
3	C	192	GLN	3.5
1	G	44	VAL	3.2
1	G	396	ILE	3.1
4	L	67	SER	3.0
1	G	58	ALA	3.0
3	C	180	SER	2.9
4	L	70	ASP	2.9
3	H	211	VAL	2.7
1	A	371	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	76	SER	2.6
4	L	7	SER	2.6
4	L	71	PHE	2.6
1	A	257	THR	2.5
3	H	154	TRP	2.5
1	G	454	LEU	2.4
1	A	366	GLY	2.4
1	G	345	VAL	2.3
3	H	195	VAL	2.3
3	C	181	VAL	2.2
2	N	16	LEU	2.2
3	C	193	THR	2.2
1	A	361	PHE	2.2
1	A	360	ILE	2.2
3	C	187	SER	2.2
1	G	66	HIS	2.1
3	H	44	GLY	2.1
4	L	63	SER	2.1
4	L	4	MET	2.1
1	A	469	ARG	2.1
4	L	210	ASN	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.92	0.27	47,51,61,75	0
2	U2X	N	29	19/20	0.94	0.18	25,30,52,53	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} 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
5	NAG	G	509	14/15	0.74	0.41	65,81,89,94	0
5	NAG	A	509	14/15	0.77	0.21	86,92,102,103	0
5	NAG	G	506	14/15	0.80	0.26	76,85,97,97	0
5	NAG	G	502	14/15	0.81	0.22	69,74,80,84	0
5	NAG	A	505	14/15	0.84	0.26	50,63,79,86	0
5	NAG	G	504	14/15	0.85	0.23	96,106,115,116	0
5	NAG	G	505	14/15	0.85	0.18	27,33,37,37	0
5	NAG	A	507	14/15	0.86	0.23	60,75,89,99	0
5	NAG	A	504	14/15	0.87	0.26	66,73,86,93	0
5	NAG	G	508	14/15	0.88	0.18	60,64,72,80	0
5	NAG	A	506	14/15	0.88	0.23	62,72,77,85	0
5	NAG	A	508	14/15	0.89	0.26	70,82,101,101	0
5	NAG	G	507	14/15	0.90	0.17	58,65,92,92	0
5	NAG	A	502	14/15	0.90	0.18	70,76,82,83	0
5	NAG	A	501	14/15	0.91	0.19	47,52,66,80	0
5	NAG	G	501	14/15	0.92	0.16	44,57,69,70	0
5	NAG	G	503	14/15	0.95	0.18	44,54,68,75	0
5	NAG	A	503	14/15	0.95	0.15	39,43,56,59	0

6.5 Other polymers (i)

There are no such residues in this entry.