Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 08:28 PM EDT

PDB ID	:	2FIX
Title	:	Structure of human liver FBPase complexed with potent benzoxazole allosteric inhibitiors
Authors	:	Abad-Zapatero, C.
Deposited on	:	2005-12-30
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

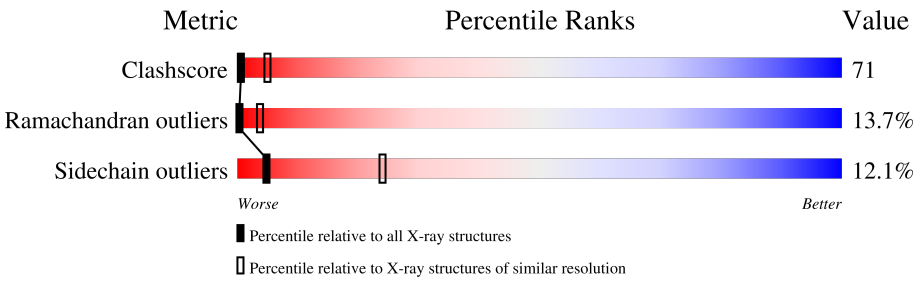
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	17% 62% 13% • 6%
1	D	338	15% 57% 21% • 6%
1	H	338	20% 60% 14% • 6%
1	L	338	20% 54% 20% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9848 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.

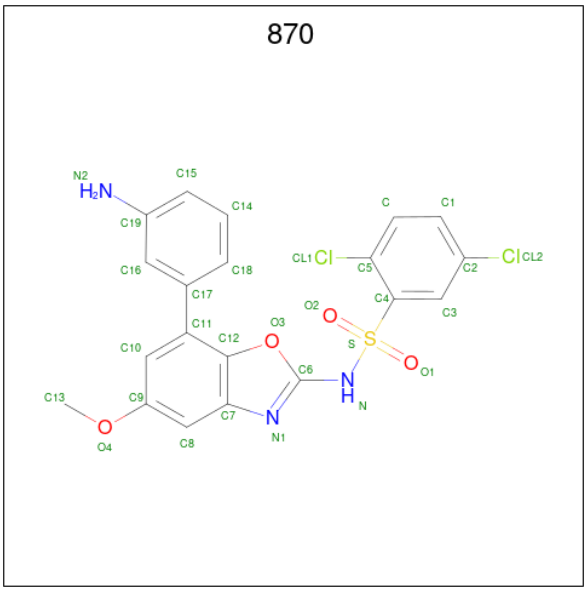
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2432	1548	408	459	17	0	0	1
1	D	319	2432	1548	408	459	17	0	0	1
1	H	319	2432	1548	408	459	17	0	0	1
1	L	319	2432	1548	408	459	17	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	ARG	variant	GB 15277851
D	217	LYS	ARG	variant	GB 15277851
H	217	LYS	ARG	variant	GB 15277851
L	217	LYS	ARG	variant	GB 15277851

- Molecule 2 is N-[7-(3-AMINOPHENYL)-5-METHOXY-1,3-BENZOXAZOL-2-YL]-2,5-DICHLOROBENZENESULFONAMIDE (three-letter code: 870) (formula: $C_{20}H_{15}Cl_2N_3O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		
2	H	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		
2	L	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		

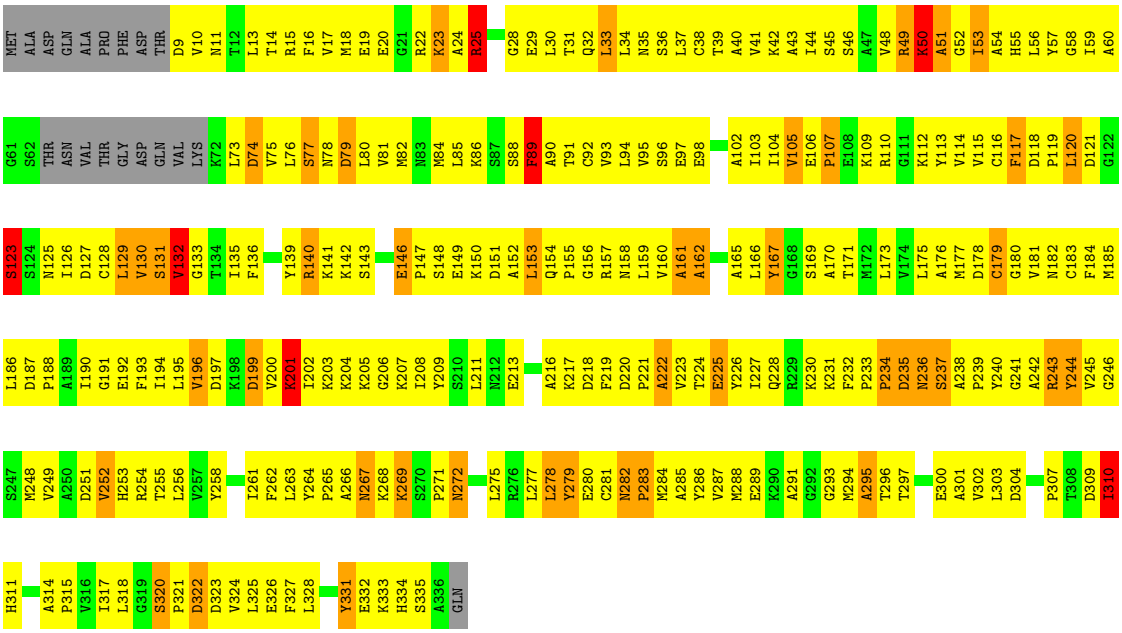
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

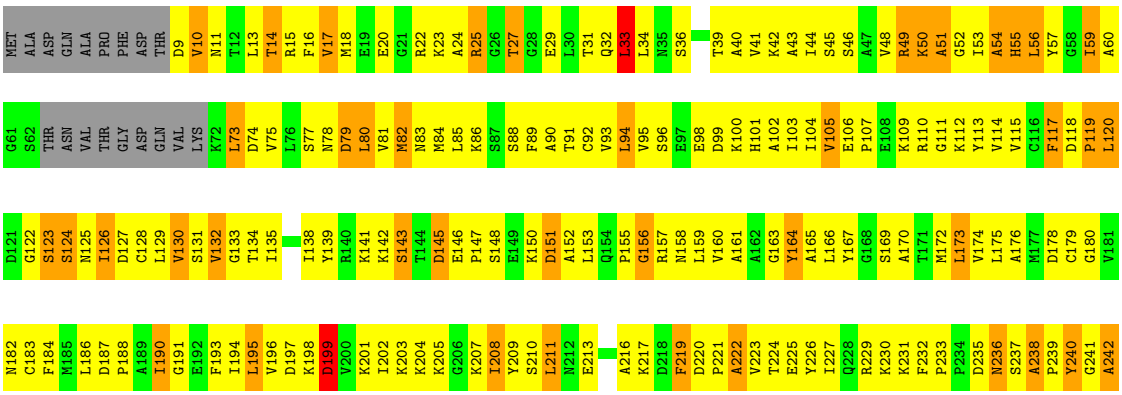
• Molecule 1: Fructose-1,6-bisphosphatase 1

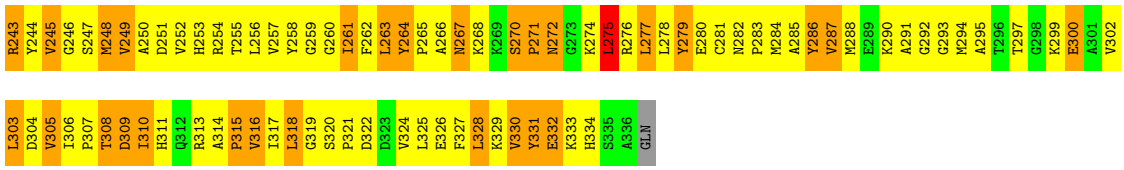
Chain A: 17% 62% 13% • 6%



• Molecule 1: Fructose-1,6-bisphosphatase 1

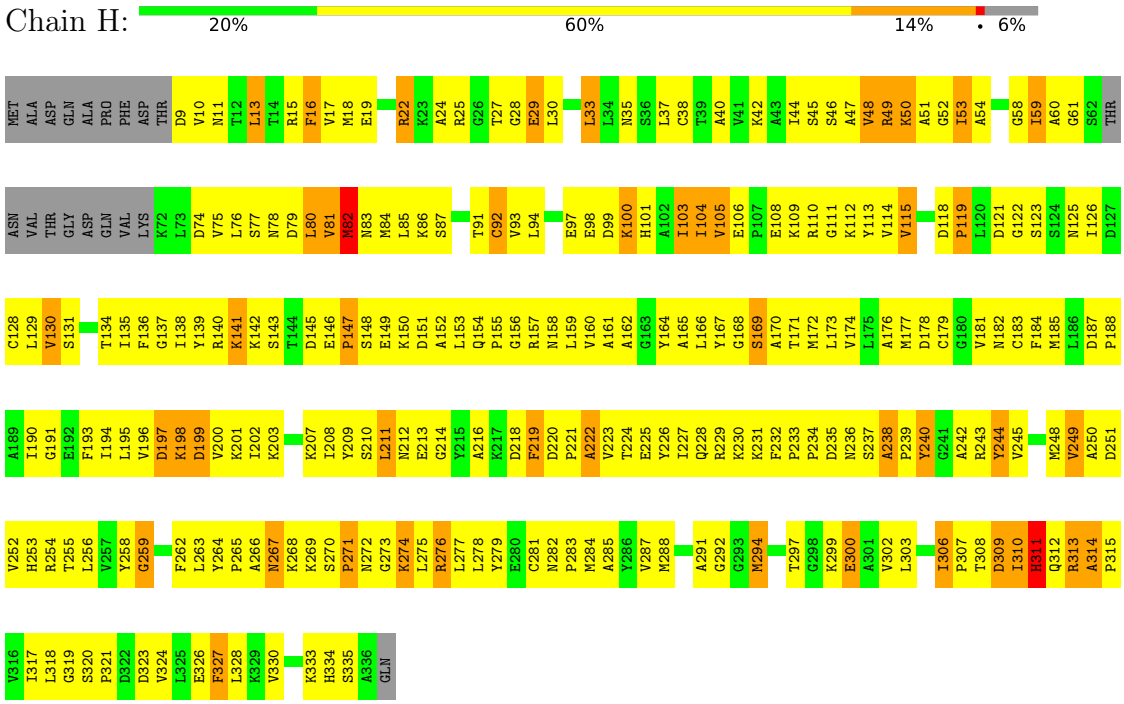
Chain D: 15% 57% 21% • 6%





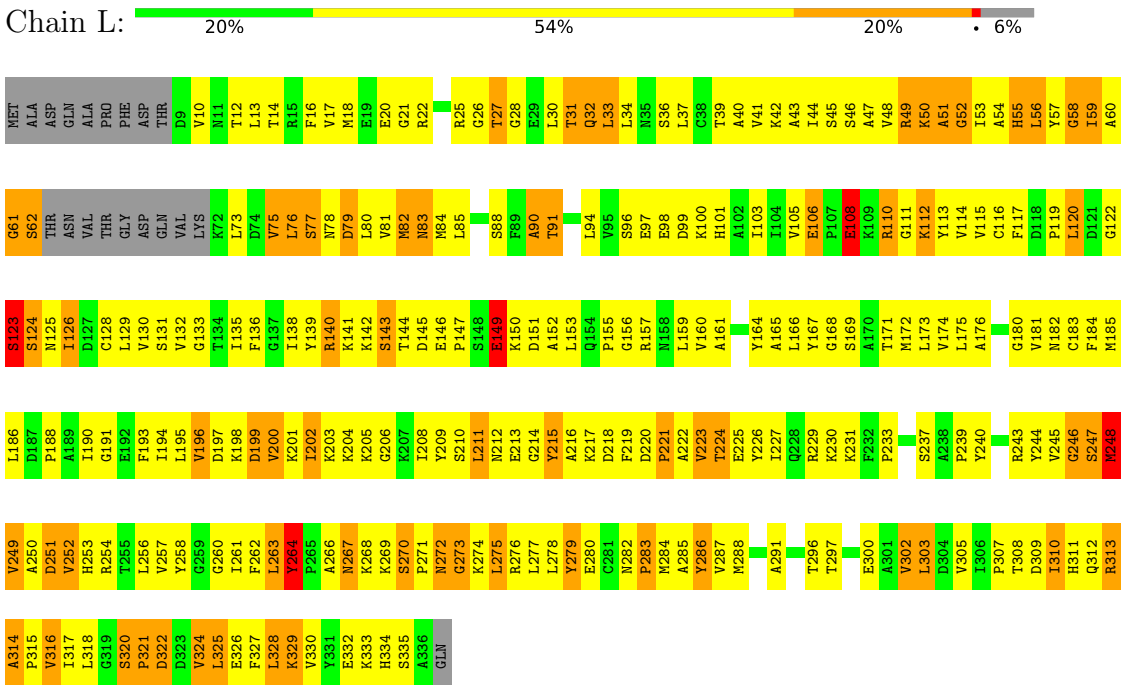
- Molecule 1: Fructose-1,6-bisphosphatase 1

Chain H:



- Molecule 1: Fructose-1,6-bisphosphatase 1

Chain L:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.40Å 108.67Å 196.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 3.50	Depositor
% Data completeness (in resolution range)	61.6 (19.88-3.50)	Depositor
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.252 , 0.355	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9848	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 870

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	0.52	0/2475	0.83	4/3343 (0.1%)
1	D	0.49	0/2475	0.78	1/3343 (0.0%)
1	H	0.48	0/2475	0.81	1/3343 (0.0%)
1	L	0.49	0/2475	0.82	2/3343 (0.1%)
All	All	0.50	0/9900	0.81	8/13372 (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
1	A	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	SER	CB-CA-C	-8.14	94.64	110.10
1	A	25	ARG	O-C-N	-7.35	110.70	123.20
1	H	29	GLU	CB-CA-C	6.30	123.00	110.40
1	L	149	GLU	CB-CA-C	-6.27	97.86	110.40
1	A	132	VAL	N-CA-CB	-5.78	98.78	111.50
1	D	33	LEU	N-CA-C	-5.67	95.70	111.00
1	L	264	TYR	N-CA-C	-5.38	96.46	111.00
1	A	131	SER	N-CA-C	5.25	125.18	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ARG	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	2432	0	2474	367	0
1	D	2432	0	2474	392	0
1	H	2432	0	2474	359	0
1	L	2432	0	2474	377	0
2	A	30	0	15	7	0
2	D	30	0	15	1	0
2	H	30	0	15	7	0
2	L	30	0	15	3	0
All	All	9848	0	9956	1406	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 71.

All (1406) 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:H:53:ILE:HD13	1:L:185:MET:HG2	1.25	1.17
1:D:91:THR:HB	1:D:94:LEU:HD21	1.38	1.05
1:H:194:ILE:HG12	1:L:54:ALA:HB2	1.31	1.05
1:D:27:THR:HA	2:H:901:870:HN22	1.18	1.03
1:A:191:GLY:HA3	1:L:191:GLY:HA3	1.37	1.02
1:D:27:THR:HA	2:H:901:870:N2	1.77	1.00
1:A:289:GLU:OE2	1:A:303:LEU:HD12	1.63	0.97
1:L:122:GLY:HA3	1:L:132:VAL:HG12	1.45	0.97
1:A:135:ILE:HD11	1:A:249:VAL:HG22	1.44	0.96
1:D:138:ILE:HB	1:D:161:ALA:HB3	1.48	0.96
1:A:11:ASN:HD21	1:A:16:PHE:HB2	1.30	0.96
1:A:85:LEU:HA	1:A:88:SER:HB3	1.47	0.95
1:L:91:THR:HG21	1:L:94:LEU:HD21	1.46	0.95
1:D:29:GLU:OE2	1:D:90:ALA:HA	1.68	0.94
1:L:156:GLY:HA3	1:L:303:LEU:HD22	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:99:ASP:HB3	1:L:103:ILE:HD11	1.50	0.91
1:D:293:GLY:HA2	1:D:321:PRO:HG3	1.51	0.91
1:H:272:ASN:O	1:H:314:ALA:HA	1.71	0.91
1:L:52:GLY:O	1:L:56:LEU:HD13	1.71	0.90
1:H:262:PHE:HB3	1:H:318:LEU:HG	1.52	0.90
1:A:82:MET:HG3	1:A:86:LYS:HE3	1.53	0.90
1:A:127:ASP:HB2	1:D:258:TYR:OH	1.72	0.90
1:H:44:ILE:HG12	1:H:80:LEU:HD12	1.52	0.89
1:A:10:VAL:HG22	1:A:11:ASN:H	1.39	0.88
1:H:190:ILE:HG13	1:H:191:GLY:N	1.87	0.88
1:A:220:ASP:HB2	1:A:221:PRO:HD2	1.54	0.88
1:H:44:ILE:HG12	1:H:80:LEU:CD1	2.04	0.88
1:A:261:ILE:HD12	1:A:323:ASP:O	1.74	0.87
1:A:17:VAL:HG13	1:A:34:LEU:HD12	1.55	0.87
1:D:242:ALA:O	1:D:243:ARG:HG2	1.75	0.87
1:L:273:GLY:H	1:L:315:PRO:HG3	1.40	0.86
1:A:282:ASN:HB2	1:A:283:PRO:HD3	1.56	0.86
1:A:245:VAL:O	1:D:243:ARG:HD2	1.74	0.85
1:D:93:VAL:O	1:D:114:VAL:HG13	1.77	0.85
1:H:150:LYS:HA	1:H:153:LEU:HD12	1.58	0.84
1:H:194:ILE:CG1	1:L:54:ALA:HB2	2.06	0.84
1:A:155:PRO:HG2	1:A:158:ASN:HD21	1.42	0.84
1:L:165:ALA:HA	1:L:173:LEU:HA	1.57	0.84
1:A:221:PRO:O	1:A:224:THR:HB	1.76	0.84
1:A:230:LYS:O	1:A:233:PRO:HD3	1.78	0.83
1:L:90:ALA:HA	1:L:111:GLY:HA3	1.58	0.83
1:A:155:PRO:HG2	1:A:158:ASN:ND2	1.94	0.83
1:L:288:MET:HG3	1:L:318:LEU:HD13	1.60	0.83
1:H:276:ARG:HH21	1:H:313:ARG:HH12	1.24	0.83
1:D:202:ILE:HG12	1:D:203:LYS:H	1.43	0.83
1:L:209:TYR:HA	1:L:261:ILE:HG22	1.60	0.83
1:L:81:VAL:HG12	1:L:85:LEU:HD12	1.59	0.82
1:D:114:VAL:HG11	1:D:152:ALA:HB2	1.60	0.82
1:L:221:PRO:HB2	1:L:334:HIS:HD2	1.43	0.82
1:L:248:MET:HE2	1:L:248:MET:HA	1.62	0.82
1:D:29:GLU:HG2	1:H:22:ARG:NH2	1.93	0.81
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.16	0.81
1:A:202:ILE:HB	1:A:256:LEU:HD12	1.61	0.81
1:A:186:LEU:O	1:A:188:PRO:HD3	1.81	0.80
1:D:202:ILE:HG12	1:D:203:LYS:N	1.95	0.80
1:D:13:LEU:HA	1:D:184:PHE:CE2	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:VAL:HG21	1:D:284:MET:HE3	1.62	0.80
1:H:15:ARG:O	1:H:19:GLU:HG2	1.81	0.80
1:A:272:ASN:N	1:A:272:ASN:HD22	1.80	0.79
1:D:27:THR:CA	2:H:901:870:HN22	1.95	0.79
1:A:139:TYR:CE1	1:A:159:LEU:HG	2.17	0.79
1:L:156:GLY:HA3	1:L:303:LEU:CD2	2.13	0.79
1:D:22:ARG:HH22	1:H:29:GLU:HG3	1.48	0.79
1:D:316:VAL:C	1:D:317:ILE:HD12	2.02	0.79
1:H:139:TYR:CE1	1:H:159:LEU:HG	2.17	0.79
1:L:153:LEU:HD21	1:L:308:THR:O	1.83	0.79
1:A:245:VAL:HG13	1:D:245:VAL:HG22	1.63	0.79
1:D:270:SER:C	1:D:272:ASN:H	1.84	0.78
1:A:30:LEU:O	1:A:33:LEU:HB3	1.83	0.78
1:H:258:TYR:OH	1:L:125:ASN:HA	1.83	0.78
1:L:82:MET:O	1:L:85:LEU:N	2.14	0.78
1:A:88:SER:O	1:A:89:PHE:HB2	1.81	0.78
1:H:50:LYS:HG2	1:H:53:ILE:HD12	1.64	0.78
1:H:245:VAL:HG22	1:L:245:VAL:HG22	1.66	0.78
1:A:285:ALA:HB3	1:A:303:LEU:HD21	1.64	0.78
1:H:82:MET:HG3	1:H:86:LYS:HE3	1.64	0.78
1:H:308:THR:HG22	1:H:312:GLN:OE1	1.83	0.77
1:A:17:VAL:CG1	1:A:34:LEU:HD12	2.14	0.77
1:H:187:ASP:OD2	1:L:53:ILE:HG22	1.85	0.77
1:L:185:MET:O	1:L:193:PHE:HA	1.85	0.77
1:D:114:VAL:HG11	1:D:152:ALA:CB	2.16	0.76
1:H:53:ILE:HD13	1:L:185:MET:CG	2.12	0.76
1:A:204:LYS:O	1:A:320:SER:HB3	1.86	0.76
1:H:229:ARG:O	1:H:233:PRO:HA	1.85	0.76
1:L:50:LYS:HD2	1:L:50:LYS:N	2.00	0.76
1:H:181:VAL:O	1:H:199:ASP:HA	1.86	0.76
1:D:93:VAL:HG23	1:D:147:PRO:HB2	1.67	0.76
1:L:91:THR:O	1:L:110:ARG:HA	1.85	0.76
1:L:50:LYS:HB3	1:L:53:ILE:HB	1.66	0.76
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.68	0.75
1:L:278:LEU:HA	1:L:282:ASN:OD1	1.86	0.75
1:H:214:GLY:C	1:H:216:ALA:H	1.90	0.75
1:L:58:GLY:HA2	1:L:62:SER:H	1.50	0.75
1:A:102:ALA:HB2	1:A:149:GLU:OE2	1.87	0.75
1:A:149:GLU:CG	1:A:310:ILE:HG21	2.17	0.75
1:D:194:ILE:N	1:D:194:ILE:HD12	2.01	0.75
1:H:190:ILE:HG13	1:H:191:GLY:H	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:O	1:A:48:VAL:HG23	1.87	0.74
1:A:129:LEU:HD22	1:D:170:ALA:HB3	1.68	0.74
1:A:234:PRO:HG2	1:A:235:ASP:H	1.52	0.74
1:D:263:LEU:HD12	1:D:263:LEU:N	2.03	0.74
1:H:195:LEU:HD21	1:H:198:LYS:HG2	1.68	0.74
1:D:157:ARG:HB2	1:D:303:LEU:O	1.88	0.74
1:H:91:THR:HB	1:H:94:LEU:HD21	1.69	0.74
1:D:11:ASN:O	1:D:194:ILE:HG23	1.88	0.74
1:D:90:ALA:C	1:D:111:GLY:HA3	2.08	0.74
1:H:94:LEU:O	1:H:103:ILE:HD12	1.87	0.74
1:A:149:GLU:OE2	1:A:310:ILE:HD13	1.87	0.73
1:L:201:LYS:HE2	1:L:201:LYS:HA	1.68	0.73
1:H:276:ARG:HG2	1:H:279:TYR:OH	1.88	0.73
1:L:141:LYS:HG3	1:L:151:ASP:CG	2.09	0.73
1:A:185:MET:HG3	1:A:186:LEU:N	2.04	0.73
1:D:186:LEU:HD13	1:D:193:PHE:CE1	2.24	0.73
1:H:194:ILE:HD12	1:H:194:ILE:N	2.04	0.73
1:D:133:GLY:HA3	1:D:249:VAL:HG11	1.71	0.73
1:D:156:GLY:O	1:D:303:LEU:HD22	1.89	0.73
1:L:128:CYS:SG	1:L:130:VAL:HB	2.29	0.72
1:H:272:ASN:O	1:H:315:PRO:HD3	1.89	0.72
1:A:155:PRO:CG	1:A:158:ASN:HD21	2.01	0.72
1:D:82:MET:HE3	1:D:94:LEU:HD12	1.70	0.72
1:H:194:ILE:HD12	1:H:194:ILE:H	1.54	0.72
1:D:119:PRO:O	1:D:134:THR:HA	1.90	0.72
1:A:95:VAL:HG13	1:A:310:ILE:HD12	1.69	0.72
1:A:104:ILE:HD11	1:A:148:SER:HA	1.71	0.72
1:A:278:LEU:HD12	1:A:310:ILE:O	1.89	0.72
1:D:29:GLU:HG2	1:H:22:ARG:HH22	1.51	0.72
1:L:272:ASN:HA	1:L:315:PRO:HD3	1.69	0.72
1:D:282:ASN:HB2	1:D:283:PRO:HD3	1.71	0.72
1:L:248:MET:HA	1:L:248:MET:CE	2.19	0.71
1:H:221:PRO:HB2	1:H:334:HIS:CE1	2.25	0.71
1:H:139:TYR:HE1	1:H:159:LEU:HG	1.55	0.71
1:A:10:VAL:HG22	1:A:11:ASN:N	2.03	0.71
1:L:53:ILE:HG23	1:L:54:ALA:N	2.04	0.71
1:A:49:ARG:NH2	1:A:171:THR:OG1	2.22	0.71
1:A:93:VAL:HG22	1:A:104:ILE:HD13	1.73	0.71
1:D:92:CYS:O	1:D:105:VAL:HB	1.90	0.71
1:L:112:LYS:HD2	1:L:140:ARG:NH1	2.06	0.71
1:L:156:GLY:CA	1:L:303:LEU:HD22	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:PRO:HA	1:D:151:ASP:OD2	1.90	0.71
1:L:183:CYS:HB2	1:L:196:VAL:HG22	1.72	0.71
1:L:276:ARG:HB2	1:L:279:TYR:CE1	2.26	0.71
1:A:141:LYS:HZ1	1:A:147:PRO:HA	1.55	0.70
1:D:186:LEU:O	1:D:188:PRO:HD3	1.91	0.70
1:H:269:LYS:NZ	1:H:274:LYS:HE2	2.06	0.70
1:L:237:SER:O	1:L:239:PRO:HD3	1.90	0.70
1:A:135:ILE:CD1	1:A:249:VAL:HG22	2.21	0.70
1:H:93:VAL:O	1:H:114:VAL:HG13	1.91	0.70
1:H:276:ARG:HD2	1:H:276:ARG:N	2.06	0.70
1:D:60:ALA:HB2	1:L:80:LEU:CD2	2.22	0.70
1:D:92:CYS:SG	1:D:93:VAL:N	2.63	0.70
1:D:107:PRO:HA	1:D:110:ARG:HE	1.56	0.70
1:D:204:LYS:HG2	1:D:322:ASP:OD1	1.92	0.70
1:D:225:GLU:O	1:D:229:ARG:HG2	1.91	0.70
1:D:270:SER:O	1:D:272:ASN:N	2.25	0.70
1:H:141:LYS:HE3	1:H:143:SER:O	1.90	0.70
1:A:11:ASN:HD21	1:A:16:PHE:CB	2.04	0.70
1:H:137:GLY:HA2	1:H:162:ALA:CB	2.22	0.70
1:A:235:ASP:OD2	1:A:237:SER:HB3	1.92	0.70
1:D:41:VAL:HG13	1:D:167:TYR:OH	1.92	0.70
1:L:313:ARG:O	1:L:314:ALA:HB2	1.91	0.70
1:H:50:LYS:HB3	1:H:53:ILE:HB	1.74	0.70
1:A:49:ARG:HH12	1:D:49:ARG:HH12	1.39	0.70
1:A:185:MET:HG3	1:A:186:LEU:H	1.56	0.70
1:H:137:GLY:HA2	1:H:162:ALA:HB2	1.73	0.70
1:D:86:LYS:O	1:D:109:LYS:HD3	1.92	0.70
1:L:318:LEU:C	1:L:318:LEU:HD12	2.12	0.70
1:A:226:TYR:O	1:A:230:LYS:CG	2.40	0.69
1:H:221:PRO:HB2	1:H:334:HIS:ND1	2.08	0.69
1:D:208:ILE:HD13	1:D:254:ARG:HD3	1.75	0.69
1:D:275:LEU:H	1:D:275:LEU:HD23	1.56	0.69
1:A:39:THR:HG22	1:A:84:MET:HE2	1.72	0.69
1:A:121:ASP:O	1:A:132:VAL:HG12	1.93	0.69
1:D:82:MET:O	1:D:85:LEU:N	2.23	0.69
1:H:53:ILE:CD1	1:L:185:MET:HG2	2.15	0.69
1:L:302:VAL:HG12	1:L:303:LEU:N	2.06	0.69
1:L:288:MET:CG	1:L:318:LEU:HD13	2.22	0.69
1:A:95:VAL:HG12	1:A:96:SER:H	1.57	0.69
1:D:49:ARG:CD	1:D:49:ARG:N	2.56	0.69
1:L:13:LEU:O	1:L:17:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:GLU:O	1:L:110:ARG:HG3	1.92	0.69
1:L:276:ARG:HB2	1:L:279:TYR:HE1	1.57	0.69
1:A:227:ILE:HG22	1:A:231:LYS:CE	2.23	0.69
1:A:82:MET:HE2	1:A:103:ILE:HG21	1.75	0.68
1:A:261:ILE:HD13	1:A:263:LEU:HD11	1.73	0.68
1:L:133:GLY:HA2	1:L:167:TYR:CD2	2.28	0.68
1:H:276:ARG:NH2	1:H:313:ARG:HH12	1.90	0.68
1:L:317:ILE:HG12	1:L:327:PHE:CE2	2.29	0.68
1:H:29:GLU:O	1:H:33:LEU:N	2.19	0.68
1:L:275:LEU:HD23	1:L:275:LEU:N	2.09	0.68
1:L:150:LYS:O	1:L:153:LEU:HB2	1.93	0.68
1:H:49:ARG:NH1	1:L:169:SER:O	2.27	0.68
1:A:226:TYR:O	1:A:230:LYS:HG2	1.92	0.68
1:L:184:PHE:HB3	1:L:193:PHE:HB3	1.76	0.68
1:D:274:LYS:O	1:D:313:ARG:HB3	1.94	0.67
1:L:183:CYS:O	1:L:195:LEU:HD12	1.93	0.67
1:A:94:LEU:CD2	1:A:115:VAL:HB	2.24	0.67
1:D:156:GLY:HA2	1:D:159:LEU:HG	1.75	0.67
1:L:133:GLY:HA2	1:L:167:TYR:HD2	1.59	0.67
1:L:198:LYS:O	1:L:200:VAL:N	2.28	0.67
1:A:116:CYS:O	1:A:117:PHE:HB3	1.93	0.67
1:A:324:VAL:HA	1:A:327:PHE:HB3	1.76	0.67
1:A:248:MET:O	1:A:252:VAL:HG23	1.94	0.67
1:L:112:LYS:HD2	1:L:140:ARG:CZ	2.25	0.67
1:L:157:ARG:HG3	1:L:157:ARG:O	1.94	0.67
1:A:176:ALA:HB2	1:A:287:VAL:HG22	1.77	0.67
1:H:210:SER:O	1:H:211:LEU:HB3	1.94	0.67
1:L:112:LYS:HB2	1:L:140:ARG:NH1	2.09	0.67
1:A:216:ALA:HA	1:A:219:PHE:HD2	1.58	0.67
1:A:39:THR:HA	1:A:42:LYS:HE3	1.76	0.67
1:L:252:VAL:HG21	1:L:284:MET:HE3	1.74	0.67
1:L:296:THR:HG21	1:L:328:LEU:HD21	1.76	0.67
1:A:227:ILE:HG22	1:A:231:LYS:HE2	1.77	0.67
1:L:270:SER:C	1:L:272:ASN:H	1.98	0.67
1:D:54:ALA:O	1:D:57:TYR:N	2.26	0.66
1:D:153:LEU:HD22	1:D:307:PRO:O	1.96	0.66
1:L:181:VAL:HB	1:L:200:VAL:HB	1.77	0.66
1:L:305:VAL:O	1:L:307:PRO:HD3	1.94	0.66
1:D:120:LEU:HD23	1:D:123:SER:HB3	1.77	0.66
1:D:264:TYR:CE1	1:D:274:LYS:HB2	2.31	0.66
1:D:182:ASN:OD1	1:D:199:ASP:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:ASP:O	1:H:237:SER:N	2.29	0.66
1:A:234:PRO:O	1:A:236:ASN:N	2.27	0.66
1:A:169:SER:O	1:D:49:ARG:NH1	2.29	0.66
1:D:16:PHE:C	1:D:18:MET:H	1.99	0.66
1:H:58:GLY:O	1:H:60:ALA:N	2.28	0.66
1:H:13:LEU:HD12	1:H:13:LEU:O	1.95	0.66
1:L:185:MET:HB2	1:L:196:VAL:CG1	2.26	0.66
1:A:283:PRO:O	1:A:286:TYR:HB3	1.96	0.66
1:D:288:MET:SD	1:D:319:GLY:HA2	2.35	0.66
1:D:308:THR:HG22	1:D:309:ASP:N	2.11	0.66
1:H:299:LYS:O	1:H:300:GLU:HB3	1.95	0.66
1:D:309:ASP:O	1:D:311:HIS:N	2.28	0.66
1:H:82:MET:O	1:H:84:MET:N	2.29	0.66
1:A:19:GLU:HB3	1:A:23:LYS:NZ	2.11	0.66
1:A:165:ALA:HB2	1:A:173:LEU:HG	1.77	0.66
1:A:218:ASP:HB3	1:A:267:ASN:HB2	1.77	0.66
1:H:266:ALA:CB	1:H:271:PRO:HA	2.26	0.65
1:A:98:GLU:CG	1:A:119:PRO:HG3	2.26	0.65
1:A:297:THR:HG22	1:A:302:VAL:HG22	1.78	0.65
1:D:60:ALA:HB2	1:L:80:LEU:HD23	1.77	0.65
1:D:278:LEU:HA	1:D:282:ASN:OD1	1.96	0.65
1:L:141:LYS:NZ	1:L:147:PRO:HA	2.11	0.65
1:L:313:ARG:HG2	1:L:313:ARG:HH11	1.60	0.65
1:D:92:CYS:SG	1:D:114:VAL:HG22	2.36	0.65
1:D:299:LYS:HG2	1:D:331:TYR:OH	1.97	0.65
1:H:218:ASP:O	1:H:267:ASN:HA	1.97	0.65
1:L:201:LYS:O	1:L:202:ILE:HB	1.97	0.65
1:D:104:ILE:HD12	1:D:148:SER:HA	1.79	0.65
1:D:73:LEU:O	1:D:75:VAL:N	2.30	0.64
1:L:111:GLY:O	1:L:113:TYR:N	2.30	0.64
1:A:196:VAL:HG12	1:D:57:TYR:CE2	2.33	0.64
1:D:46:SER:O	1:D:51:ALA:HB2	1.97	0.64
1:D:202:ILE:CG1	1:D:203:LYS:H	2.10	0.64
1:A:258:TYR:OH	1:D:125:ASN:HA	1.96	0.64
1:H:150:LYS:HD3	1:H:150:LYS:C	2.18	0.64
1:L:248:MET:HG3	1:L:249:VAL:N	2.12	0.64
1:D:207:LYS:HA	1:D:240:TYR:CE1	2.33	0.64
1:D:184:PHE:HB3	1:D:193:PHE:HB3	1.80	0.64
1:D:248:MET:O	1:D:251:ASP:N	2.31	0.64
1:H:168:GLY:C	1:H:170:ALA:H	2.01	0.64
1:A:234:PRO:C	1:A:236:ASN:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:SER:C	1:D:272:ASN:N	2.51	0.64
1:H:168:GLY:C	1:H:170:ALA:N	2.50	0.64
1:H:230:LYS:HD2	1:H:230:LYS:N	2.13	0.64
1:H:317:ILE:HG12	1:H:327:PHE:CE2	2.33	0.64
1:H:318:LEU:HD12	1:H:318:LEU:C	2.19	0.64
1:L:97:GLU:HG3	1:L:276:ARG:CZ	2.28	0.64
1:L:211:LEU:HD22	1:L:263:LEU:HD13	1.78	0.64
1:H:169:SER:O	1:L:48:VAL:HG12	1.97	0.64
1:H:248:MET:SD	1:H:275:LEU:HD13	2.37	0.64
1:D:134:THR:HG1	1:D:167:TYR:HE2	1.46	0.64
1:D:17:VAL:HG12	1:D:17:VAL:O	1.98	0.63
1:H:112:LYS:HE2	1:H:113:TYR:CE2	2.33	0.63
1:H:128:CYS:HB3	1:L:258:TYR:HE2	1.62	0.63
1:L:46:SER:O	1:L:51:ALA:HB2	1.98	0.63
1:A:82:MET:CE	1:A:103:ILE:HG21	2.28	0.63
1:A:141:LYS:HZ1	1:A:147:PRO:CA	2.11	0.63
1:D:264:TYR:OH	1:D:274:LYS:HD2	1.98	0.63
1:H:294:MET:HB3	1:H:324:VAL:HG11	1.79	0.63
1:L:141:LYS:HZ1	1:L:147:PRO:HA	1.63	0.63
1:H:252:VAL:O	1:H:255:THR:HB	1.99	0.63
1:L:149:GLU:OE1	1:L:310:ILE:HD13	1.99	0.63
1:L:243:ARG:O	1:L:254:ARG:NH1	2.31	0.63
1:A:175:LEU:HD12	1:A:176:ALA:H	1.63	0.63
1:A:282:ASN:HB2	1:A:283:PRO:CD	2.28	0.63
1:A:77:SER:O	1:A:81:VAL:HG23	1.98	0.63
1:A:150:LYS:HA	1:A:153:LEU:HD12	1.79	0.63
1:A:169:SER:OG	1:D:129:LEU:HD22	1.99	0.63
1:D:91:THR:O	1:D:111:GLY:N	2.31	0.63
1:H:51:ALA:HA	1:L:188:PRO:CG	2.29	0.63
1:L:81:VAL:O	1:L:85:LEU:HB2	1.98	0.63
1:A:11:ASN:ND2	1:A:16:PHE:HB2	2.10	0.63
1:D:93:VAL:CG2	1:D:147:PRO:HB2	2.29	0.63
1:D:302:VAL:O	1:D:304:ASP:N	2.28	0.63
1:H:243:ARG:O	1:H:244:TYR:HB2	1.98	0.63
1:L:50:LYS:CG	1:L:53:ILE:HD12	2.29	0.63
1:A:49:ARG:NH1	1:D:49:ARG:HH12	1.96	0.63
1:D:73:LEU:C	1:D:75:VAL:H	2.02	0.63
1:H:49:ARG:HH11	1:H:49:ARG:HG3	1.63	0.63
1:H:155:PRO:HD2	1:H:158:ASN:ND2	2.14	0.63
1:A:40:ALA:HB2	1:A:84:MET:HG3	1.81	0.63
1:D:107:PRO:HA	1:D:110:ARG:NE	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:CB	1:D:161:ALA:HB3	2.27	0.62
1:D:221:PRO:O	1:D:223:VAL:N	2.32	0.62
1:H:242:ALA:CB	1:L:213:GLU:HB2	2.29	0.62
1:A:141:LYS:NZ	1:A:147:PRO:HA	2.14	0.62
1:D:229:ARG:O	1:D:230:LYS:HD2	1.99	0.62
1:D:263:LEU:HA	1:D:317:ILE:HG13	1.80	0.62
1:L:203:LYS:HD2	1:L:258:TYR:O	1.99	0.62
1:A:205:LYS:HD2	1:A:240:TYR:OH	1.99	0.62
1:H:317:ILE:N	1:H:317:ILE:HD12	2.14	0.62
1:D:48:VAL:C	1:D:50:LYS:H	2.02	0.62
1:D:266:ALA:HB1	1:D:271:PRO:HA	1.82	0.62
1:H:269:LYS:HZ1	1:H:274:LYS:CE	2.12	0.62
1:L:302:VAL:O	1:L:305:VAL:HG23	1.98	0.62
1:D:27:THR:HG21	1:D:112:LYS:HZ2	1.63	0.62
1:D:91:THR:N	1:D:111:GLY:HA3	2.14	0.62
1:D:262:PHE:CE2	1:D:264:TYR:HB2	2.34	0.62
1:H:313:ARG:O	1:H:314:ALA:HB2	1.98	0.62
1:L:208:ILE:O	1:L:260:GLY:HA3	1.98	0.62
1:A:295:ALA:O	1:A:302:VAL:HG23	1.98	0.62
1:A:25:ARG:HA	2:A:701:870:C18	2.30	0.62
1:A:46:SER:O	1:A:51:ALA:HB2	1.99	0.62
1:H:201:LYS:HG2	1:H:291:ALA:O	1.99	0.62
1:L:160:VAL:O	1:L:160:VAL:HG12	1.99	0.62
1:A:95:VAL:HG12	1:A:96:SER:N	2.15	0.61
1:H:9:ASP:CG	1:H:10:VAL:H	2.03	0.61
1:L:313:ARG:O	1:L:314:ALA:CB	2.48	0.61
1:L:274:LYS:O	1:L:274:LYS:HG2	2.01	0.61
1:A:317:ILE:HG12	1:A:327:PHE:CE2	2.35	0.61
1:H:157:ARG:N	1:H:303:LEU:HB3	2.16	0.61
1:D:252:VAL:O	1:D:255:THR:HB	2.01	0.61
1:L:221:PRO:HB2	1:L:334:HIS:CD2	2.31	0.61
1:A:36:SER:O	1:A:84:MET:HE3	2.01	0.61
1:A:175:LEU:HD12	1:A:176:ALA:N	2.15	0.61
1:D:117:PHE:HD1	1:D:117:PHE:H	1.47	0.61
1:H:172:MET:HB2	1:H:185:MET:SD	2.41	0.61
1:H:234:PRO:HG2	1:H:235:ASP:OD1	2.00	0.61
1:L:139:TYR:CE2	1:L:159:LEU:HD21	2.35	0.61
1:H:297:THR:HA	1:H:315:PRO:O	2.00	0.61
1:A:183:CYS:O	1:A:195:LEU:HD12	2.00	0.61
1:A:206:GLY:O	1:A:207:LYS:HG3	1.99	0.61
1:H:29:GLU:HB2	1:H:112:LYS:NZ	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:O	1:D:16:PHE:N	2.33	0.61
1:D:88:SER:O	1:D:89:PHE:HB2	2.01	0.61
1:D:225:GLU:OE2	1:D:333:LYS:NZ	2.32	0.61
1:D:233:PRO:HG3	1:D:237:SER:O	2.00	0.61
1:D:278:LEU:HD23	1:D:282:ASN:OD1	2.01	0.61
1:H:252:VAL:HG22	1:H:318:LEU:HD21	1.83	0.61
1:L:153:LEU:HD22	1:L:307:PRO:O	2.01	0.61
1:L:308:THR:HG22	1:L:309:ASP:N	2.15	0.61
1:L:175:LEU:HD12	1:L:176:ALA:N	2.16	0.60
1:A:29:GLU:HB3	1:A:90:ALA:HB1	1.83	0.60
1:A:41:VAL:HG13	1:A:167:TYR:CE1	2.36	0.60
1:L:209:TYR:CA	1:L:261:ILE:HG22	2.29	0.60
1:D:207:LYS:HA	1:D:240:TYR:CD1	2.36	0.60
1:A:285:ALA:CB	1:A:303:LEU:HD21	2.31	0.60
1:H:177:MET:HB2	1:H:179:CYS:SG	2.41	0.60
1:L:51:ALA:O	1:L:53:ILE:N	2.32	0.60
1:A:15:ARG:HA	1:A:18:MET:HG3	1.82	0.60
1:A:42:LYS:O	1:L:190:ILE:HG22	2.02	0.60
1:D:118:ASP:HB3	1:D:135:ILE:HB	1.84	0.60
1:D:172:MET:SD	1:D:183:CYS:HB3	2.41	0.60
1:D:302:VAL:HG12	1:D:303:LEU:N	2.17	0.60
1:L:166:LEU:HD12	1:L:167:TYR:H	1.67	0.60
1:A:91:THR:O	1:A:110:ARG:HA	2.02	0.60
1:H:105:VAL:HG12	1:H:106:GLU:O	2.02	0.60
1:H:252:VAL:HB	1:H:284:MET:HE1	1.84	0.60
1:A:82:MET:HE1	1:A:94:LEU:HB2	1.84	0.60
1:A:201:LYS:HA	1:A:291:ALA:O	2.02	0.60
1:H:211:LEU:HD11	1:H:219:PHE:HZ	1.66	0.60
1:A:14:THR:HG23	1:A:35:ASN:HD22	1.67	0.60
1:D:44:ILE:HG12	1:D:77:SER:OG	2.02	0.59
1:H:134:THR:O	1:H:164:TYR:HB2	2.02	0.59
1:H:140:ARG:HB2	1:H:160:VAL:HG21	1.83	0.59
1:A:190:ILE:HG22	1:L:43:ALA:HA	1.84	0.59
1:A:266:ALA:HB2	1:A:271:PRO:O	2.01	0.59
1:H:172:MET:SD	1:L:129:LEU:HD11	2.42	0.59
1:A:94:LEU:HD23	1:A:115:VAL:HB	1.84	0.59
1:A:120:LEU:HG	1:A:120:LEU:O	2.00	0.59
1:D:242:ALA:O	1:D:243:ARG:CG	2.48	0.59
1:A:246:GLY:HA2	1:D:243:ARG:HE	1.66	0.59
1:D:195:LEU:HG	1:D:195:LEU:O	1.98	0.59
1:H:49:ARG:HD2	1:H:49:ARG:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:PRO:C	1:D:223:VAL:N	2.55	0.59
1:H:226:TYR:O	1:H:230:LYS:HG2	2.03	0.59
1:H:243:ARG:HB3	1:H:254:ARG:NH2	2.17	0.59
1:H:78:ASN:OD1	1:H:119:PRO:HG3	2.02	0.59
1:L:223:VAL:O	1:L:225:GLU:N	2.36	0.59
1:L:309:ASP:O	1:L:311:HIS:N	2.35	0.59
1:A:140:ARG:HG3	1:A:141:LYS:O	2.02	0.58
1:L:256:LEU:HD13	1:L:288:MET:CE	2.33	0.58
1:A:185:MET:H	1:A:196:VAL:HG22	1.68	0.58
1:A:322:ASP:O	1:A:326:GLU:HB2	2.04	0.58
1:H:29:GLU:HB2	1:H:112:LYS:HZ3	1.67	0.58
1:D:79:ASP:O	1:D:82:MET:N	2.36	0.58
1:D:260:GLY:N	1:D:320:SER:OG	2.35	0.58
1:L:120:LEU:HA	1:L:133:GLY:O	2.03	0.58
1:L:215:TYR:CE1	1:L:269:LYS:NZ	2.70	0.58
1:A:310:ILE:O	1:A:310:ILE:HG13	2.03	0.58
1:D:229:ARG:C	1:D:230:LYS:HD2	2.24	0.58
1:D:276:ARG:O	1:D:281:CYS:SG	2.62	0.58
1:H:112:LYS:O	1:H:141:LYS:HB2	2.03	0.58
1:H:128:CYS:HB2	1:L:254:ARG:HA	1.86	0.58
1:A:209:TYR:HA	1:A:261:ILE:HG22	1.86	0.58
1:L:205:LYS:HG2	1:L:206:GLY:N	2.18	0.58
1:L:209:TYR:CB	1:L:261:ILE:HG22	2.34	0.58
1:A:106:GLU:O	1:A:110:ARG:HG3	2.04	0.58
1:D:208:ILE:CD1	1:D:254:ARG:HD3	2.33	0.58
1:D:262:PHE:C	1:D:263:LEU:HD12	2.24	0.58
1:L:184:PHE:CB	1:L:193:PHE:HB3	2.34	0.58
1:D:73:LEU:C	1:D:75:VAL:N	2.53	0.58
1:H:130:VAL:HG21	1:H:245:VAL:HG13	1.85	0.58
1:H:222:ALA:HA	1:H:334:HIS:NE2	2.18	0.58
1:L:90:ALA:CA	1:L:111:GLY:HA3	2.32	0.58
1:L:267:ASN:OD1	1:L:269:LYS:HB2	2.03	0.58
1:H:150:LYS:HA	1:H:153:LEU:CD1	2.32	0.57
1:L:221:PRO:CB	1:L:334:HIS:HD2	2.16	0.57
1:A:317:ILE:N	1:A:317:ILE:HD12	2.18	0.57
1:D:15:ARG:NH1	1:H:87:SER:O	2.37	0.57
1:H:125:ASN:O	1:H:130:VAL:HG12	2.04	0.57
1:A:165:ALA:HA	1:A:173:LEU:HA	1.87	0.57
1:A:264:TYR:CD1	1:A:275:LEU:HG	2.38	0.57
1:A:279:TYR:O	1:A:283:PRO:HG2	2.04	0.57
1:D:294:MET:HB2	1:D:324:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:LYS:HB2	1:L:140:ARG:HH12	1.69	0.57
1:A:175:LEU:O	1:A:181:VAL:HG13	2.05	0.57
1:D:82:MET:SD	1:D:103:ILE:HD13	2.44	0.57
1:D:93:VAL:C	1:D:94:LEU:HD23	2.24	0.57
1:D:117:PHE:CD1	1:D:117:PHE:N	2.72	0.57
1:D:15:ARG:O	1:D:18:MET:HB2	2.03	0.57
1:D:276:ARG:O	1:D:280:GLU:HB2	2.05	0.57
1:H:126:ILE:HG12	1:H:126:ILE:O	2.05	0.57
1:L:26:GLY:HA3	2:L:1001:870:HN	1.69	0.57
1:L:230:LYS:HE2	1:L:240:TYR:CE2	2.39	0.57
1:A:278:LEU:HD11	1:A:310:ILE:HA	1.87	0.57
1:H:82:MET:CG	1:H:86:LYS:HE3	2.34	0.57
1:A:264:TYR:CE1	1:A:275:LEU:HG	2.39	0.57
1:D:276:ARG:HG2	1:D:279:TYR:CZ	2.40	0.57
1:H:196:VAL:HG23	1:H:197:ASP:N	2.18	0.57
1:L:103:ILE:HD12	1:L:103:ILE:N	2.20	0.57
1:A:294:MET:O	1:A:295:ALA:HB2	2.05	0.57
1:A:318:LEU:HD12	1:A:318:LEU:C	2.24	0.57
1:D:264:TYR:CD2	1:D:275:LEU:HD21	2.40	0.57
1:H:121:ASP:OD2	1:H:248:MET:HB3	2.05	0.57
1:L:165:ALA:HB2	1:L:173:LEU:HD12	1.87	0.57
1:A:190:ILE:CG2	1:L:43:ALA:HA	2.35	0.56
1:A:193:PHE:C	1:A:194:ILE:HD12	2.26	0.56
1:A:228:GLN:HE22	1:A:232:PHE:HE2	1.51	0.56
1:H:273:GLY:HA3	1:H:314:ALA:H	1.70	0.56
1:A:160:VAL:O	1:A:161:ALA:HB2	2.05	0.56
1:H:155:PRO:O	1:H:158:ASN:HB2	2.04	0.56
1:L:97:GLU:O	1:L:97:GLU:HG2	2.05	0.56
1:A:186:LEU:HD22	1:A:193:PHE:CE1	2.39	0.56
1:A:242:ALA:HB3	1:D:213:GLU:H	1.71	0.56
1:D:49:ARG:H	1:D:49:ARG:HD3	1.70	0.56
1:D:245:VAL:HG23	1:D:251:ASP:OD1	2.06	0.56
1:H:176:ALA:HB2	1:H:287:VAL:HG22	1.88	0.56
1:L:105:VAL:HG12	1:L:106:GLU:N	2.21	0.56
1:A:224:THR:O	1:A:228:GLN:HG2	2.05	0.56
1:A:31:THR:HG22	1:A:32:GLN:N	2.20	0.56
1:D:153:LEU:HD22	1:D:307:PRO:C	2.26	0.56
1:D:155:PRO:HG2	1:D:158:ASN:HD21	1.70	0.56
1:L:277:LEU:HD11	1:L:282:ASN:ND2	2.20	0.56
1:D:175:LEU:HD12	1:D:175:LEU:C	2.26	0.56
1:D:248:MET:O	1:D:250:ALA:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ASN:CB	1:D:283:PRO:HD3	2.34	0.56
1:L:332:GLU:C	1:L:334:HIS:H	2.08	0.56
1:A:53:ILE:HA	1:A:56:LEU:HD21	1.87	0.56
1:D:257:VAL:HG12	1:D:258:TYR:CD2	2.40	0.56
1:D:326:GLU:O	1:D:329:LYS:HB3	2.05	0.56
1:A:28:GLY:O	1:A:31:THR:HB	2.05	0.56
1:A:74:ASP:OD2	1:A:123:SER:OG	2.22	0.56
1:A:146:GLU:HG3	1:A:147:PRO:HD2	1.88	0.56
1:H:155:PRO:HG2	1:H:158:ASN:HB2	1.87	0.56
1:H:273:GLY:HA3	1:H:314:ALA:N	2.20	0.56
1:H:275:LEU:O	1:H:313:ARG:HA	2.06	0.56
1:D:194:ILE:N	1:D:194:ILE:CD1	2.69	0.56
1:D:278:LEU:O	1:D:283:PRO:HD3	2.06	0.56
1:L:215:TYR:HE1	1:L:269:LYS:HZ1	1.48	0.55
1:L:226:TYR:O	1:L:229:ARG:HB2	2.06	0.55
1:A:25:ARG:HA	2:A:701:870:H18	1.87	0.55
1:A:263:LEU:HD12	1:A:263:LEU:N	2.20	0.55
1:A:296:THR:HG21	1:A:328:LEU:HG	1.87	0.55
1:H:166:LEU:HB2	1:H:249:VAL:CG1	2.36	0.55
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.89	0.55
1:D:49:ARG:N	1:D:49:ARG:HD2	2.22	0.55
1:H:172:MET:SD	1:H:253:HIS:HE1	2.30	0.55
1:H:222:ALA:HA	1:H:334:HIS:CD2	2.41	0.55
1:A:14:THR:CG2	1:A:35:ASN:HD22	2.19	0.55
1:A:334:HIS:N	1:A:334:HIS:CD2	2.74	0.55
1:H:194:ILE:O	1:H:196:VAL:HG13	2.07	0.55
1:L:53:ILE:HG23	1:L:54:ALA:H	1.70	0.55
1:H:24:ALA:O	1:H:25:ARG:HB2	2.05	0.55
1:D:118:ASP:CB	1:D:135:ILE:HD12	2.37	0.55
1:L:13:LEU:HA	1:L:184:PHE:CE2	2.41	0.55
1:L:216:ALA:HA	1:L:219:PHE:CD2	2.42	0.55
1:L:321:PRO:O	1:L:322:ASP:C	2.43	0.55
1:L:325:LEU:HA	1:L:328:LEU:HB2	1.89	0.55
1:L:168:GLY:O	1:L:169:SER:C	2.44	0.55
1:L:185:MET:HB2	1:L:196:VAL:HG11	1.87	0.55
1:A:147:PRO:HA	1:A:151:ASP:OD2	2.07	0.55
1:H:168:GLY:O	1:H:170:ALA:N	2.39	0.55
1:L:30:LEU:O	1:L:33:LEU:HB3	2.06	0.55
1:A:159:LEU:HD13	1:A:286:TYR:CD2	2.42	0.55
1:H:277:LEU:HB2	1:H:312:GLN:O	2.07	0.55
1:L:77:SER:O	1:L:80:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLU:O	1:A:335:SER:N	2.38	0.54
1:D:286:TYR:O	1:D:287:VAL:C	2.45	0.54
1:H:52:GLY:O	1:H:54:ALA:N	2.40	0.54
1:H:269:LYS:HZ1	1:H:274:LYS:HE2	1.72	0.54
1:L:52:GLY:O	1:L:56:LEU:CD1	2.52	0.54
1:A:221:PRO:HG2	1:A:222:ALA:H	1.72	0.54
1:A:48:VAL:HG12	1:A:49:ARG:HD2	1.89	0.54
1:A:277:LEU:CD1	1:A:282:ASN:HD21	2.19	0.54
1:D:53:ILE:O	1:D:56:LEU:HD23	2.06	0.54
1:H:16:PHE:CD1	1:H:16:PHE:C	2.80	0.54
1:H:165:ALA:HA	1:H:173:LEU:HA	1.89	0.54
1:A:52:GLY:O	1:A:54:ALA:N	2.40	0.54
1:H:266:ALA:HB1	1:H:271:PRO:HA	1.87	0.54
1:L:173:LEU:HD23	1:L:173:LEU:O	2.08	0.54
1:A:93:VAL:HG22	1:A:104:ILE:CD1	2.36	0.54
1:A:261:ILE:HG23	1:A:261:ILE:O	2.07	0.54
1:H:200:VAL:HG12	1:H:201:LYS:H	1.72	0.54
1:A:186:LEU:HB2	1:A:193:PHE:CE1	2.43	0.54
1:A:261:ILE:HB	1:A:323:ASP:HB3	1.89	0.54
1:D:253:HIS:O	1:D:256:LEU:N	2.40	0.54
1:H:18:MET:HG2	2:H:901:870:C13	2.37	0.54
1:H:80:LEU:O	1:H:82:MET:N	2.40	0.54
1:H:333:LYS:C	1:H:335:SER:H	2.10	0.54
1:L:171:THR:HB	1:L:186:LEU:HB3	1.89	0.54
1:A:182:ASN:OD1	1:A:199:ASP:N	2.31	0.54
1:D:117:PHE:HD1	1:D:117:PHE:N	2.04	0.54
1:D:262:PHE:HE2	1:D:264:TYR:HB2	1.71	0.54
1:D:276:ARG:HG2	1:D:279:TYR:CE1	2.43	0.54
1:D:281:CYS:HB3	1:D:316:VAL:HG21	1.89	0.54
1:H:9:ASP:CG	1:H:10:VAL:N	2.61	0.54
1:L:99:ASP:CB	1:L:103:ILE:HD11	2.30	0.54
1:A:155:PRO:CD	1:A:158:ASN:HD21	2.20	0.54
1:A:252:VAL:O	1:A:255:THR:HB	2.07	0.54
1:D:22:ARG:HH22	1:H:29:GLU:CA	2.20	0.54
1:D:286:TYR:HA	1:D:303:LEU:HD11	1.90	0.54
1:H:37:LEU:O	1:H:40:ALA:N	2.41	0.54
1:H:330:VAL:HG12	1:H:330:VAL:O	2.05	0.54
1:L:256:LEU:HD13	1:L:288:MET:HE2	1.89	0.54
1:L:313:ARG:HG2	1:L:313:ARG:NH1	2.22	0.54
1:A:81:VAL:O	1:A:82:MET:C	2.47	0.54
1:D:79:ASP:O	1:D:81:VAL:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ARG:NH1	1:D:147:PRO:HG3	2.22	0.54
1:H:213:GLU:O	1:H:216:ALA:HB2	2.08	0.54
1:L:17:VAL:HG12	1:L:31:THR:OG1	2.08	0.54
1:L:55:HIS:HA	1:L:59:ILE:HG22	1.90	0.54
1:A:10:VAL:CG2	1:A:11:ASN:H	2.16	0.53
1:A:140:ARG:HG3	1:A:141:LYS:N	2.19	0.53
1:A:176:ALA:CB	1:A:287:VAL:HG22	2.39	0.53
1:D:22:ARG:O	1:D:23:LYS:C	2.47	0.53
1:H:92:CYS:SG	1:H:114:VAL:HG23	2.48	0.53
1:H:92:CYS:SG	1:H:93:VAL:N	2.81	0.53
1:L:112:LYS:HE2	1:L:113:TYR:HE2	1.74	0.53
1:L:212:ASN:HA	1:L:244:TYR:CE2	2.43	0.53
1:A:40:ALA:O	1:A:44:ILE:HG13	2.08	0.53
1:D:139:TYR:CE1	1:D:159:LEU:HG	2.42	0.53
1:D:163:GLY:HA3	1:D:174:VAL:O	2.08	0.53
1:D:308:THR:CG2	1:D:309:ASP:N	2.72	0.53
1:H:310:ILE:O	1:H:312:GLN:N	2.39	0.53
1:L:20:GLU:HA	1:L:20:GLU:OE1	2.07	0.53
1:L:268:LYS:O	1:L:268:LYS:HG2	2.08	0.53
1:D:11:ASN:ND2	1:D:15:ARG:HG2	2.23	0.53
1:L:80:LEU:O	1:L:81:VAL:C	2.45	0.53
1:L:218:ASP:O	1:L:267:ASN:HB3	2.08	0.53
1:A:49:ARG:NH1	1:D:49:ARG:NH1	2.56	0.53
1:A:153:LEU:HD22	1:A:307:PRO:O	2.09	0.53
1:H:194:ILE:HG12	1:L:54:ALA:CB	2.22	0.53
1:L:321:PRO:O	1:L:324:VAL:N	2.42	0.53
1:A:34:LEU:O	1:A:37:LEU:HB3	2.07	0.53
1:D:60:ALA:HB2	1:L:80:LEU:HD21	1.91	0.53
1:D:302:VAL:O	1:D:305:VAL:HG23	2.08	0.53
1:L:166:LEU:HD13	1:L:249:VAL:HG12	1.91	0.53
1:L:285:ALA:C	1:L:287:VAL:H	2.11	0.53
1:A:141:LYS:HE3	1:A:143:SER:O	2.09	0.53
1:A:272:ASN:N	1:A:272:ASN:ND2	2.52	0.53
1:H:150:LYS:HD3	1:H:150:LYS:O	2.08	0.53
1:H:156:GLY:O	1:H:159:LEU:HD12	2.09	0.53
1:D:329:LYS:O	1:D:331:TYR:N	2.42	0.53
1:H:82:MET:HE2	1:H:94:LEU:HD13	1.91	0.53
1:A:125:ASN:O	1:A:130:VAL:HG12	2.08	0.53
1:A:141:LYS:HG3	1:A:151:ASP:OD1	2.08	0.53
1:D:29:GLU:OE1	1:D:112:LYS:HG2	2.09	0.53
1:D:226:TYR:CD1	1:D:327:PHE:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:ILE:O	1:L:56:LEU:HB2	2.09	0.53
1:L:96:SER:C	1:L:98:GLU:H	2.12	0.53
1:L:309:ASP:O	1:L:312:GLN:N	2.42	0.53
1:D:53:ILE:HG23	1:D:54:ALA:N	2.23	0.53
1:D:244:TYR:O	1:D:246:GLY:N	2.42	0.53
1:L:36:SER:CB	1:L:88:SER:HB3	2.39	0.53
1:L:203:LYS:O	1:L:320:SER:HB3	2.09	0.53
1:L:210:SER:C	1:L:211:LEU:HD23	2.28	0.53
1:L:286:TYR:CD1	1:L:286:TYR:O	2.62	0.53
1:L:332:GLU:C	1:L:334:HIS:N	2.61	0.53
1:A:93:VAL:HG23	1:A:147:PRO:HB2	1.90	0.53
1:A:149:GLU:HG2	1:A:310:ILE:HG21	1.91	0.53
1:D:45:SER:HB2	1:D:167:TYR:HE1	1.73	0.53
1:D:191:GLY:HA3	1:H:191:GLY:HA3	1.91	0.53
1:H:29:GLU:CD	1:H:112:LYS:NZ	2.62	0.53
1:D:49:ARG:N	1:D:49:ARG:HD3	2.25	0.52
1:D:81:VAL:HG11	1:D:117:PHE:CD2	2.43	0.52
1:H:228:GLN:OE1	1:H:228:GLN:HA	2.09	0.52
1:L:41:VAL:O	1:L:44:ILE:HB	2.09	0.52
1:L:219:PHE:HB3	1:L:224:THR:OG1	2.09	0.52
1:L:272:ASN:O	1:L:273:GLY:O	2.26	0.52
1:L:277:LEU:HD11	1:L:282:ASN:HD21	1.73	0.52
1:A:125:ASN:O	1:A:128:CYS:SG	2.67	0.52
1:A:242:ALA:CB	1:D:213:GLU:HB2	2.39	0.52
1:H:165:ALA:HB2	1:H:173:LEU:HG	1.90	0.52
1:H:276:ARG:HE	1:H:313:ARG:NH1	2.06	0.52
1:L:132:VAL:O	1:L:166:LEU:HD12	2.08	0.52
1:L:139:TYR:CD2	1:L:159:LEU:HD21	2.44	0.52
1:A:185:MET:HE3	1:D:50:LYS:HG2	1.89	0.52
1:A:192:GLU:OE1	1:L:42:LYS:NZ	2.42	0.52
1:D:31:THR:CG2	1:D:31:THR:O	2.57	0.52
1:D:287:VAL:O	1:D:288:MET:C	2.48	0.52
1:H:310:ILE:HG13	1:H:311:HIS:H	1.73	0.52
1:L:14:THR:O	1:L:18:MET:HG3	2.09	0.52
1:A:196:VAL:HG12	1:D:57:TYR:CZ	2.44	0.52
1:A:331:TYR:CD1	1:A:331:TYR:C	2.83	0.52
1:D:80:LEU:O	1:D:84:MET:HB2	2.09	0.52
1:D:287:VAL:O	1:D:290:LYS:N	2.39	0.52
1:A:183:CYS:O	1:A:196:VAL:HG23	2.09	0.52
1:D:13:LEU:O	1:D:14:THR:C	2.46	0.52
1:H:91:THR:O	1:H:111:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:174:VAL:HG22	1:L:183:CYS:SG	2.49	0.52
1:A:120:LEU:HD11	1:A:132:VAL:HG11	1.92	0.52
1:L:46:SER:OG	1:L:51:ALA:HB2	2.09	0.52
1:A:105:VAL:HG11	1:A:109:LYS:O	2.10	0.52
1:A:261:ILE:CD1	1:A:263:LEU:HD11	2.39	0.52
1:D:317:ILE:HG21	1:D:327:PHE:CD2	2.45	0.52
1:H:13:LEU:CD2	1:H:173:LEU:HD13	2.39	0.52
1:H:211:LEU:CD1	1:H:219:PHE:HZ	2.23	0.52
1:L:130:VAL:HG22	1:L:131:SER:N	2.25	0.52
1:L:138:ILE:HG22	1:L:138:ILE:O	2.08	0.52
1:L:270:SER:C	1:L:272:ASN:N	2.63	0.52
1:A:93:VAL:O	1:A:114:VAL:HG13	2.09	0.52
1:D:16:PHE:C	1:D:18:MET:N	2.62	0.52
1:D:265:PRO:HA	1:D:315:PRO:HB2	1.91	0.52
1:H:44:ILE:O	1:H:48:VAL:HG23	2.10	0.52
1:H:279:TYR:N	1:H:279:TYR:CD2	2.78	0.52
1:A:19:GLU:O	1:A:23:LYS:HG3	2.10	0.52
1:D:120:LEU:HG	1:D:132:VAL:HG21	1.92	0.52
1:H:80:LEU:O	1:H:81:VAL:C	2.49	0.52
1:L:153:LEU:CD2	1:L:308:THR:O	2.57	0.52
1:A:185:MET:H	1:A:196:VAL:CG2	2.23	0.51
1:A:282:ASN:O	1:A:283:PRO:C	2.48	0.51
1:D:128:CYS:SG	1:D:130:VAL:HB	2.50	0.51
1:D:142:LYS:O	1:D:143:SER:O	2.27	0.51
1:H:277:LEU:HD23	1:H:312:GLN:NE2	2.25	0.51
1:L:185:MET:HB2	1:L:196:VAL:HG12	1.92	0.51
1:L:329:LYS:HZ3	1:L:330:VAL:N	2.08	0.51
1:A:96:SER:C	1:A:98:GLU:H	2.12	0.51
1:A:103:ILE:HG22	1:A:103:ILE:O	2.10	0.51
1:D:263:LEU:CB	1:D:317:ILE:HG13	2.40	0.51
1:H:97:GLU:HB2	1:H:279:TYR:CE1	2.45	0.51
1:H:162:ALA:O	1:H:176:ALA:HB3	2.09	0.51
1:L:40:ALA:O	1:L:44:ILE:HG13	2.10	0.51
1:L:288:MET:SD	1:L:318:LEU:HD13	2.50	0.51
1:A:31:THR:HG21	2:L:1001:870:H131	1.92	0.51
1:D:48:VAL:O	1:D:50:LYS:HD2	2.10	0.51
1:L:164:TYR:HH	1:L:253:HIS:HD1	1.55	0.51
1:L:247:SER:O	1:L:248:MET:C	2.48	0.51
1:L:296:THR:CG2	1:L:317:ILE:HB	2.41	0.51
1:A:22:ARG:O	1:A:24:ALA:N	2.43	0.51
1:A:190:ILE:HG13	1:A:191:GLY:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:HD23	1:A:211:LEU:O	2.10	0.51
1:D:202:ILE:HD13	1:D:320:SER:N	2.25	0.51
1:D:243:ARG:HG2	1:D:243:ARG:HH11	1.75	0.51
1:H:81:VAL:HG12	1:H:85:LEU:HD11	1.92	0.51
1:L:75:VAL:O	1:L:78:ASN:N	2.44	0.51
1:L:186:LEU:HB2	1:L:193:PHE:CE1	2.45	0.51
1:A:301:ALA:HB3	1:A:304:ASP:OD2	2.10	0.51
1:D:92:CYS:SG	1:D:114:VAL:CG2	2.98	0.51
1:L:270:SER:O	1:L:272:ASN:N	2.43	0.51
1:L:317:ILE:HD12	1:L:317:ILE:N	2.26	0.51
1:A:39:THR:HA	1:A:42:LYS:CE	2.41	0.51
1:A:50:LYS:O	1:D:188:PRO:HD2	2.10	0.51
1:A:187:ASP:HB2	1:D:53:ILE:CG2	2.41	0.51
1:A:288:MET:SD	1:A:318:LEU:HD13	2.50	0.51
1:D:122:GLY:HA3	1:D:247:SER:OG	2.11	0.51
1:D:160:VAL:HG12	1:D:160:VAL:O	2.10	0.51
1:H:16:PHE:HD2	1:H:195:LEU:HD13	1.76	0.51
1:H:92:CYS:SG	1:H:114:VAL:CG2	2.99	0.51
1:H:130:VAL:HG22	1:H:131:SER:N	2.26	0.51
1:H:149:GLU:O	1:H:150:LYS:C	2.48	0.51
1:H:278:LEU:HB2	1:H:279:TYR:CD2	2.46	0.51
1:L:218:ASP:HB3	1:L:267:ASN:HB2	1.92	0.51
1:L:272:ASN:HA	1:L:315:PRO:CD	2.40	0.51
1:A:49:ARG:O	1:A:50:LYS:O	2.29	0.51
1:A:74:ASP:CG	1:A:123:SER:HG	2.14	0.51
1:A:185:MET:CG	1:A:186:LEU:N	2.73	0.51
1:D:317:ILE:HD12	1:D:317:ILE:N	2.24	0.51
1:L:53:ILE:CG2	1:L:54:ALA:N	2.72	0.51
1:L:75:VAL:O	1:L:76:LEU:C	2.49	0.51
1:A:49:ARG:HG3	1:D:169:SER:O	2.10	0.51
1:A:169:SER:OG	1:D:129:LEU:HA	2.10	0.51
1:D:299:LYS:O	1:D:300:GLU:CB	2.58	0.51
1:D:299:LYS:HE2	1:D:331:TYR:OH	2.11	0.51
1:H:82:MET:HE1	1:H:94:LEU:HB3	1.92	0.51
1:L:248:MET:O	1:L:249:VAL:C	2.49	0.51
1:A:136:PHE:CE1	1:A:162:ALA:HA	2.45	0.51
1:A:175:LEU:HD11	1:A:177:MET:HG3	1.93	0.50
1:D:22:ARG:NH2	1:H:29:GLU:HG3	2.22	0.50
1:H:93:VAL:HB	1:H:114:VAL:HG22	1.93	0.50
1:H:167:TYR:CD1	1:H:171:THR:HG23	2.46	0.50
1:H:262:PHE:HB3	1:H:318:LEU:CG	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:GLY:O	1:L:60:ALA:N	2.44	0.50
1:L:263:LEU:N	1:L:263:LEU:HD12	2.26	0.50
1:D:29:GLU:HB2	1:D:112:LYS:HZ3	1.76	0.50
1:H:13:LEU:HB3	1:H:193:PHE:HB2	1.92	0.50
1:H:98:GLU:HG3	1:H:119:PRO:HG3	1.92	0.50
1:H:221:PRO:O	1:H:224:THR:HB	2.09	0.50
1:H:253:HIS:O	1:H:256:LEU:N	2.44	0.50
1:L:31:THR:HG22	1:L:32:GLN:N	2.26	0.50
1:L:223:VAL:O	1:L:224:THR:C	2.49	0.50
1:L:296:THR:HG23	1:L:317:ILE:HB	1.92	0.50
1:A:78:ASN:C	1:A:80:LEU:N	2.64	0.50
1:D:77:SER:O	1:D:78:ASN:C	2.49	0.50
1:D:105:VAL:HG13	1:D:106:GLU:N	2.27	0.50
1:D:288:MET:HG3	1:D:318:LEU:HD22	1.94	0.50
1:L:81:VAL:O	1:L:85:LEU:HD12	2.11	0.50
1:A:228:GLN:NE2	1:A:232:PHE:HE2	2.10	0.50
1:D:82:MET:CE	1:D:94:LEU:HD12	2.40	0.50
1:D:107:PRO:CA	1:D:110:ARG:HE	2.24	0.50
1:D:268:LYS:O	1:D:268:LYS:HG2	2.11	0.50
1:H:81:VAL:HG12	1:H:85:LEU:CD1	2.41	0.50
1:H:239:PRO:O	1:H:240:TYR:O	2.28	0.50
1:L:230:LYS:O	1:L:231:LYS:C	2.47	0.50
1:A:187:ASP:HB2	1:D:53:ILE:HG22	1.92	0.50
1:H:278:LEU:HD11	1:H:310:ILE:HA	1.92	0.50
1:L:73:LEU:O	1:L:73:LEU:HD12	2.12	0.50
1:D:155:PRO:HG2	1:D:158:ASN:ND2	2.27	0.50
1:H:128:CYS:O	1:H:129:LEU:HB2	2.12	0.50
1:H:143:SER:C	1:H:145:ASP:H	2.14	0.50
1:H:185:MET:HG2	1:L:50:LYS:HG2	1.93	0.50
1:L:108:GLU:CD	1:L:108:GLU:H	2.15	0.50
1:A:13:LEU:HB2	1:A:184:PHE:CD2	2.46	0.50
1:A:227:ILE:CG2	1:A:231:LYS:HE2	2.40	0.50
1:H:44:ILE:HD13	1:H:77:SER:CB	2.42	0.50
1:H:156:GLY:C	1:H:303:LEU:HD22	2.32	0.50
1:D:20:GLU:OE1	1:D:23:LYS:NZ	2.24	0.50
1:D:125:ASN:N	1:D:125:ASN:HD22	2.09	0.50
1:D:155:PRO:O	1:D:157:ARG:N	2.43	0.50
1:D:221:PRO:C	1:D:223:VAL:H	2.13	0.50
1:L:44:ILE:O	1:L:47:ALA:N	2.42	0.50
1:H:171:THR:O	1:H:171:THR:HG22	2.11	0.50
1:L:58:GLY:O	1:L:61:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:VAL:HG11	1:L:117:PHE:CD2	2.47	0.50
1:A:41:VAL:CG1	1:A:167:TYR:HE1	2.25	0.49
1:A:88:SER:O	1:A:89:PHE:CB	2.53	0.49
1:D:42:LYS:O	1:D:45:SER:HB3	2.12	0.49
1:L:233:PRO:HG3	1:L:237:SER:O	2.11	0.49
1:A:102:ALA:CB	1:A:149:GLU:OE2	2.59	0.49
1:A:152:ALA:O	1:A:154:GLN:N	2.45	0.49
1:A:153:LEU:O	1:A:154:GLN:HG3	2.12	0.49
1:A:176:ALA:HA	1:A:181:VAL:HG22	1.93	0.49
1:D:42:LYS:HA	1:D:45:SER:HB3	1.93	0.49
1:D:209:TYR:OH	1:D:231:LYS:NZ	2.45	0.49
1:D:316:VAL:O	1:D:317:ILE:HD12	2.11	0.49
1:H:299:LYS:O	1:H:300:GLU:CB	2.61	0.49
1:A:158:ASN:O	1:A:159:LEU:C	2.50	0.49
1:A:226:TYR:CE2	1:A:261:ILE:HD13	2.47	0.49
1:D:93:VAL:HG22	1:D:104:ILE:HG23	1.93	0.49
1:H:172:MET:SD	1:H:253:HIS:CE1	3.05	0.49
1:A:155:PRO:HD2	1:A:158:ASN:HD21	1.78	0.49
1:A:173:LEU:C	1:A:173:LEU:HD23	2.32	0.49
1:A:185:MET:HE1	1:D:50:LYS:HD3	1.95	0.49
1:D:17:VAL:HG13	2:D:801:870:CL2	2.48	0.49
1:D:36:SER:OG	1:H:15:ARG:HD3	2.13	0.49
1:D:264:TYR:CZ	1:D:274:LYS:HD2	2.46	0.49
1:H:15:ARG:O	1:H:19:GLU:CG	2.57	0.49
1:H:86:LYS:HG2	1:H:94:LEU:CD1	2.42	0.49
1:H:211:LEU:HD11	1:H:219:PHE:CZ	2.46	0.49
1:L:82:MET:O	1:L:83:ASN:C	2.49	0.49
1:A:149:GLU:HG3	1:A:310:ILE:HG21	1.91	0.49
1:D:22:ARG:NH2	1:H:28:GLY:C	2.66	0.49
1:D:141:LYS:C	1:D:142:LYS:HD2	2.32	0.49
1:D:216:ALA:HA	1:D:219:PHE:CD2	2.48	0.49
1:D:237:SER:O	1:D:238:ALA:C	2.51	0.49
1:L:166:LEU:HD12	1:L:167:TYR:N	2.27	0.49
1:A:51:ALA:O	1:D:187:ASP:OD1	2.31	0.49
1:H:16:PHE:HZ	1:H:182:ASN:ND2	2.11	0.49
1:H:129:LEU:O	1:H:130:VAL:O	2.29	0.49
1:H:161:ALA:O	1:H:162:ALA:HB2	2.13	0.49
1:H:200:VAL:HG12	1:H:201:LYS:N	2.26	0.49
1:A:103:ILE:O	1:A:103:ILE:CG2	2.58	0.49
1:H:212:ASN:HB2	1:H:244:TYR:CE2	2.47	0.49
1:A:52:GLY:C	1:A:54:ALA:N	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD23	1:H:60:ALA:HA	1.94	0.49
1:A:253:HIS:O	1:A:256:LEU:N	2.44	0.49
1:D:39:THR:O	1:D:40:ALA:C	2.50	0.49
1:D:132:VAL:HG23	1:D:133:GLY:N	2.28	0.49
1:H:151:ASP:O	1:H:154:GLN:NE2	2.45	0.49
1:L:59:ILE:HG12	1:L:59:ILE:O	2.13	0.49
1:L:297:THR:OG1	1:L:300:GLU:HG2	2.12	0.49
1:A:155:PRO:CG	1:A:158:ASN:ND2	2.67	0.49
1:D:186:LEU:O	1:D:188:PRO:CD	2.60	0.49
1:H:37:LEU:HD21	1:H:136:PHE:CE2	2.47	0.49
1:H:162:ALA:O	1:H:176:ALA:N	2.44	0.49
1:H:173:LEU:HD23	1:H:174:VAL:N	2.27	0.49
1:H:269:LYS:HZ2	1:H:274:LYS:HE2	1.77	0.49
1:L:77:SER:O	1:L:78:ASN:C	2.49	0.49
1:A:78:ASN:C	1:A:80:LEU:H	2.14	0.49
1:D:94:LEU:O	1:D:103:ILE:HB	2.13	0.49
1:D:202:ILE:HD11	1:D:259:GLY:HA2	1.94	0.49
1:D:225:GLU:O	1:D:229:ARG:CG	2.60	0.49
1:D:230:LYS:HE3	1:D:230:LYS:HA	1.94	0.49
1:D:299:LYS:O	1:D:300:GLU:HB3	2.13	0.49
1:H:105:VAL:HG11	1:H:110:ARG:HA	1.95	0.49
1:L:317:ILE:O	1:L:318:LEU:HB3	2.13	0.49
1:A:150:LYS:HD2	1:A:153:LEU:HD12	1.94	0.48
1:A:170:ALA:HB3	1:D:129:LEU:CD1	2.43	0.48
2:A:701:870:HN22	1:L:27:THR:HA	1.78	0.48
1:D:27:THR:CG2	1:D:112:LYS:HZ2	2.25	0.48
1:D:244:TYR:O	1:D:244:TYR:CG	2.65	0.48
1:D:252:VAL:HG21	1:D:284:MET:CE	2.40	0.48
1:H:139:TYR:CE1	1:H:159:LEU:CG	2.93	0.48
1:H:223:VAL:HG21	1:H:265:PRO:HG3	1.94	0.48
1:L:50:LYS:HD2	1:L:50:LYS:H	1.73	0.48
1:L:123:SER:O	1:L:126:ILE:HB	2.13	0.48
1:L:215:TYR:HE1	1:L:269:LYS:NZ	2.10	0.48
1:A:118:ASP:OD2	1:A:280:GLU:OE1	2.31	0.48
1:D:33:LEU:O	1:D:34:LEU:C	2.50	0.48
1:H:16:PHE:CD2	1:H:195:LEU:HD13	2.48	0.48
1:H:326:GLU:O	1:H:327:PHE:C	2.52	0.48
1:L:245:VAL:HB	1:L:251:ASP:OD1	2.13	0.48
1:L:269:LYS:O	1:L:270:SER:OG	2.30	0.48
1:D:16:PHE:O	1:D:18:MET:N	2.45	0.48
1:D:132:VAL:O	1:D:167:TYR:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LEU:O	1:D:307:PRO:HB2	2.13	0.48
1:D:224:THR:HG22	1:D:224:THR:O	2.13	0.48
1:H:75:VAL:HG12	1:H:79:ASP:OD2	2.14	0.48
1:H:143:SER:OG	1:H:151:ASP:OD1	2.30	0.48
1:H:173:LEU:O	1:H:183:CYS:HA	2.13	0.48
1:H:326:GLU:O	1:H:328:LEU:N	2.46	0.48
1:L:58:GLY:HA2	1:L:62:SER:N	2.23	0.48
1:L:195:LEU:HD21	1:L:198:LYS:HG3	1.94	0.48
1:A:251:ASP:O	1:A:252:VAL:C	2.52	0.48
1:D:242:ALA:O	1:D:243:ARG:CB	2.62	0.48
1:D:325:LEU:O	1:D:326:GLU:C	2.51	0.48
1:D:332:GLU:C	1:D:334:HIS:H	2.16	0.48
1:H:237:SER:O	1:H:238:ALA:C	2.52	0.48
1:H:308:THR:O	1:H:309:ASP:HB2	2.13	0.48
1:L:79:ASP:O	1:L:82:MET:HB3	2.13	0.48
1:D:193:PHE:C	1:D:194:ILE:HD12	2.34	0.48
1:D:198:LYS:O	1:D:199:ASP:C	2.52	0.48
1:D:292:GLY:O	1:D:321:PRO:HG2	2.14	0.48
1:H:29:GLU:CD	1:H:112:LYS:HZ2	2.16	0.48
1:H:172:MET:CE	1:H:183:CYS:HB3	2.43	0.48
1:A:117:PHE:HB2	1:A:135:ILE:O	2.12	0.48
1:A:159:LEU:HD13	1:A:286:TYR:CG	2.48	0.48
1:A:277:LEU:O	1:A:282:ASN:OD1	2.32	0.48
1:A:322:ASP:N	1:A:322:ASP:OD1	2.47	0.48
1:H:44:ILE:O	1:H:47:ALA:HB3	2.14	0.48
1:H:249:VAL:HG12	1:H:250:ALA:N	2.28	0.48
1:A:53:ILE:HA	1:A:56:LEU:CD2	2.43	0.48
1:D:114:VAL:HG21	1:D:151:ASP:O	2.13	0.48
1:D:175:LEU:HD12	1:D:176:ALA:N	2.28	0.48
1:D:201:LYS:HA	1:D:291:ALA:HB1	1.94	0.48
1:D:202:ILE:HD11	1:D:320:SER:OG	2.13	0.48
1:D:262:PHE:O	1:D:317:ILE:HA	2.14	0.48
1:H:153:LEU:O	1:H:154:GLN:HG3	2.14	0.48
1:H:164:TYR:CZ	1:H:174:VAL:HG21	2.49	0.48
1:L:285:ALA:O	1:L:287:VAL:N	2.47	0.48
1:H:167:TYR:CE1	1:H:171:THR:HG23	2.48	0.48
1:H:185:MET:O	1:H:194:ILE:HD13	2.13	0.48
1:H:194:ILE:N	1:H:194:ILE:CD1	2.75	0.48
1:H:281:CYS:O	1:H:285:ALA:N	2.41	0.48
1:L:78:ASN:HA	1:L:119:PRO:HB3	1.95	0.48
1:L:153:LEU:HD23	1:L:153:LEU:HA	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:ILE:HG22	1:L:231:LYS:HE2	1.95	0.48
1:A:157:ARG:NH1	1:A:289:GLU:OE2	2.47	0.48
1:A:185:MET:HB2	1:A:196:VAL:HG21	1.96	0.48
1:H:248:MET:SD	1:H:275:LEU:CD1	3.02	0.48
1:D:54:ALA:O	1:D:56:LEU:N	2.47	0.48
1:D:112:LYS:HG3	1:D:113:TYR:CE1	2.48	0.48
1:L:82:MET:HE3	1:L:94:LEU:CD1	2.43	0.48
1:A:39:THR:HB	1:A:84:MET:CE	2.44	0.47
1:D:263:LEU:CA	1:D:317:ILE:HG13	2.44	0.47
1:L:126:ILE:O	1:L:129:LEU:N	2.40	0.47
1:A:17:VAL:HG13	2:A:701:870:CL2	2.51	0.47
1:A:185:MET:CG	1:A:186:LEU:H	2.25	0.47
1:D:43:ALA:O	1:D:44:ILE:C	2.50	0.47
1:D:262:PHE:C	1:D:262:PHE:CD2	2.87	0.47
1:D:285:ALA:HB1	1:D:295:ALA:HB3	1.96	0.47
1:H:85:LEU:HB3	1:H:91:THR:HG21	1.95	0.47
1:H:92:CYS:HA	1:H:105:VAL:HB	1.96	0.47
1:H:225:GLU:O	1:H:228:GLN:HB2	2.14	0.47
1:H:251:ASP:O	1:H:252:VAL:C	2.53	0.47
1:H:310:ILE:C	1:H:312:GLN:H	2.18	0.47
1:L:82:MET:O	1:L:85:LEU:HB2	2.14	0.47
1:A:105:VAL:HG12	1:A:106:GLU:N	2.29	0.47
1:A:228:GLN:NE2	1:A:232:PHE:CE2	2.82	0.47
1:A:246:GLY:HA2	1:D:243:ARG:NE	2.29	0.47
1:D:209:TYR:HE2	1:D:213:GLU:OE2	1.97	0.47
1:D:226:TYR:HA	1:D:229:ARG:HB2	1.96	0.47
1:D:322:ASP:O	1:D:325:LEU:HB2	2.15	0.47
1:H:51:ALA:HA	1:L:188:PRO:HG2	1.96	0.47
1:H:84:MET:HA	1:H:87:SER:HB2	1.94	0.47
1:H:269:LYS:HZ1	1:H:274:LYS:HE3	1.79	0.47
1:L:116:CYS:HG	1:L:139:TYR:HE2	1.53	0.47
1:L:155:PRO:HB3	1:L:305:VAL:O	2.15	0.47
1:L:248:MET:HE2	1:L:248:MET:CA	2.39	0.47
1:L:277:LEU:HD12	1:L:277:LEU:O	2.14	0.47
1:A:20:GLU:HA	1:A:23:LYS:HD2	1.96	0.47
1:A:41:VAL:HG13	1:A:167:TYR:HE1	1.78	0.47
1:A:49:ARG:HH12	1:D:49:ARG:NH1	2.10	0.47
1:A:136:PHE:O	1:A:162:ALA:HB1	2.14	0.47
1:A:238:ALA:HA	1:A:239:PRO:HD3	1.74	0.47
1:D:274:LYS:O	1:D:275:LEU:O	2.33	0.47
1:H:10:VAL:HG22	1:H:11:ASN:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:97:GLU:HG3	1:L:276:ARG:NH1	2.30	0.47
1:L:149:GLU:O	1:L:152:ALA:N	2.47	0.47
1:D:105:VAL:CG1	1:D:106:GLU:N	2.75	0.47
1:D:202:ILE:CG1	1:D:203:LYS:N	2.65	0.47
1:H:258:TYR:O	1:H:259:GLY:O	2.32	0.47
1:L:112:LYS:HE2	1:L:113:TYR:CE2	2.50	0.47
1:L:225:GLU:O	1:L:226:TYR:C	2.53	0.47
1:L:266:ALA:O	1:L:267:ASN:ND2	2.47	0.47
1:A:173:LEU:C	1:A:173:LEU:CD2	2.83	0.47
1:D:138:ILE:HB	1:D:161:ALA:CB	2.33	0.47
1:H:48:VAL:C	1:H:50:LYS:H	2.16	0.47
1:A:56:LEU:H	1:A:56:LEU:HD23	1.79	0.47
1:A:141:LYS:HG2	1:A:142:LYS:N	2.30	0.47
1:A:209:TYR:OH	1:A:231:LYS:HE2	2.14	0.47
1:D:217:LYS:O	1:D:217:LYS:HG2	2.14	0.47
1:D:299:LYS:CG	1:D:331:TYR:OH	2.63	0.47
1:H:49:ARG:NH1	1:H:49:ARG:HG3	2.30	0.47
1:H:138:ILE:O	1:H:160:VAL:HB	2.15	0.47
1:H:149:GLU:O	1:H:153:LEU:HG	2.15	0.47
1:H:226:TYR:HE1	1:H:326:GLU:OE1	1.98	0.47
1:L:45:SER:O	1:L:49:ARG:HD3	2.14	0.47
1:L:261:ILE:HG23	1:L:261:ILE:O	2.15	0.47
1:A:15:ARG:NH1	1:L:36:SER:OG	2.45	0.47
1:A:297:THR:HG23	1:A:302:VAL:N	2.29	0.47
1:D:211:LEU:HD23	1:D:211:LEU:O	2.15	0.47
1:H:10:VAL:HG23	1:L:57:TYR:O	2.14	0.47
1:H:81:VAL:O	1:H:85:LEU:HG	2.15	0.47
1:H:92:CYS:O	1:H:105:VAL:HG23	2.13	0.47
1:H:276:ARG:HD2	1:H:276:ARG:H	1.78	0.47
1:A:220:ASP:HB2	1:A:221:PRO:CD	2.35	0.47
1:A:281:CYS:O	1:A:282:ASN:C	2.53	0.47
1:D:163:GLY:O	1:D:164:TYR:HB3	2.14	0.47
1:D:211:LEU:HD23	1:D:211:LEU:N	2.30	0.47
1:H:99:ASP:O	1:H:100:LYS:C	2.53	0.47
1:H:136:PHE:O	1:H:162:ALA:HB1	2.15	0.47
1:A:52:GLY:O	1:A:53:ILE:C	2.53	0.47
1:A:104:ILE:CD1	1:A:148:SER:HA	2.44	0.47
1:H:13:LEU:HD12	1:H:13:LEU:C	2.34	0.47
1:H:274:LYS:N	1:H:313:ARG:HB3	2.30	0.47
1:L:324:VAL:O	1:L:327:PHE:N	2.48	0.47
1:A:141:LYS:HZ3	1:A:147:PRO:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:278:LEU:HB2	1:H:279:TYR:HD2	1.80	0.46
1:L:34:LEU:HD13	1:L:175:LEU:HD21	1.96	0.46
1:L:82:MET:CE	1:L:94:LEU:HD12	2.44	0.46
1:L:194:ILE:N	1:L:194:ILE:HD12	2.29	0.46
1:A:39:THR:HB	1:A:84:MET:HE1	1.97	0.46
1:A:78:ASN:O	1:A:80:LEU:N	2.48	0.46
1:A:221:PRO:HG2	1:A:222:ALA:N	2.31	0.46
1:A:248:MET:O	1:A:249:VAL:C	2.54	0.46
1:D:13:LEU:HD12	1:D:184:PHE:CZ	2.50	0.46
1:D:302:VAL:HG21	1:D:316:VAL:CG1	2.46	0.46
1:H:28:GLY:HA2	2:H:901:870:O1	2.15	0.46
1:H:108:GLU:N	1:H:108:GLU:CD	2.68	0.46
1:H:195:LEU:CD2	1:H:198:LYS:HG2	2.44	0.46
1:L:58:GLY:C	1:L:60:ALA:N	2.69	0.46
1:A:58:GLY:O	1:D:10:VAL:HB	2.15	0.46
1:A:85:LEU:O	1:A:86:LYS:C	2.53	0.46
1:D:15:ARG:HA	1:D:18:MET:HB2	1.97	0.46
1:D:226:TYR:O	1:D:230:LYS:HG2	2.16	0.46
1:D:332:GLU:C	1:D:334:HIS:N	2.69	0.46
1:H:214:GLY:C	1:H:216:ALA:N	2.58	0.46
1:L:10:VAL:HG13	1:L:10:VAL:O	2.16	0.46
1:L:81:VAL:HG12	1:L:85:LEU:CD1	2.40	0.46
1:L:184:PHE:HA	1:L:194:ILE:O	2.14	0.46
1:A:234:PRO:CG	1:A:235:ASP:H	2.27	0.46
1:H:130:VAL:HG22	1:H:131:SER:H	1.80	0.46
1:H:185:MET:HB3	1:L:53:ILE:HD13	1.98	0.46
1:H:313:ARG:O	1:H:314:ALA:CB	2.64	0.46
1:L:205:LYS:HE3	1:L:240:TYR:OH	2.16	0.46
1:L:209:TYR:HB2	1:L:261:ILE:CG2	2.46	0.46
1:L:282:ASN:O	1:L:303:LEU:HD21	2.16	0.46
1:D:96:SER:C	1:D:98:GLU:H	2.18	0.46
1:D:130:VAL:HG12	1:D:130:VAL:O	2.16	0.46
1:H:148:SER:O	1:H:151:ASP:HB2	2.15	0.46
1:L:144:THR:O	1:L:144:THR:HG22	2.16	0.46
1:L:219:PHE:CB	1:L:224:THR:OG1	2.62	0.46
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.15	0.46
1:A:45:SER:O	1:A:48:VAL:N	2.49	0.46
1:H:54:ALA:O	1:H:59:ILE:HG22	2.16	0.46
1:L:101:HIS:O	1:L:103:ILE:HD12	2.15	0.46
1:L:135:ILE:HG22	1:L:283:PRO:HG2	1.98	0.46
1:L:285:ALA:C	1:L:287:VAL:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:O	1:A:325:LEU:HG	2.16	0.46
1:D:13:LEU:HA	1:D:184:PHE:HE2	1.78	0.46
1:D:22:ARG:HH22	1:H:29:GLU:CG	2.25	0.46
1:L:39:THR:HB	1:L:84:MET:HE2	1.96	0.46
1:L:75:VAL:O	1:L:78:ASN:HB3	2.16	0.46
1:L:156:GLY:C	1:L:303:LEU:HD22	2.36	0.46
1:L:201:LYS:O	1:L:202:ILE:CB	2.64	0.46
1:L:227:ILE:CG2	1:L:231:LYS:HE2	2.46	0.46
1:L:276:ARG:H	1:L:276:ARG:HD2	1.78	0.46
1:A:32:GLN:O	1:A:36:SER:N	2.39	0.46
1:A:208:ILE:HA	1:A:241:GLY:H	1.81	0.46
1:A:222:ALA:O	1:A:223:VAL:C	2.53	0.46
1:A:266:ALA:HB1	1:A:271:PRO:HA	1.98	0.46
1:D:81:VAL:HB	1:D:117:PHE:HE2	1.81	0.46
1:D:264:TYR:N	1:D:265:PRO:CD	2.79	0.46
1:L:130:VAL:CG2	1:L:131:SER:N	2.79	0.46
1:A:22:ARG:HG3	2:A:701:870:C10	2.46	0.46
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.97	0.46
1:D:22:ARG:HH22	1:H:29:GLU:HA	1.81	0.46
1:D:329:LYS:C	1:D:331:TYR:N	2.68	0.46
1:H:135:ILE:HG23	1:H:249:VAL:HG23	1.98	0.46
1:L:201:LYS:O	1:L:291:ALA:HB1	2.16	0.46
1:A:95:VAL:O	1:A:96:SER:HB2	2.16	0.46
1:A:140:ARG:HB3	1:A:160:VAL:HG21	1.98	0.46
1:A:245:VAL:HG23	1:A:251:ASP:OD1	2.15	0.46
1:D:104:ILE:CD1	1:D:148:SER:HA	2.44	0.46
1:D:248:MET:O	1:D:249:VAL:C	2.54	0.46
1:D:306:ILE:HA	1:D:307:PRO:HD3	1.63	0.46
1:H:93:VAL:HG22	1:H:147:PRO:CB	2.45	0.46
1:H:146:GLU:HA	1:H:147:PRO:HD2	1.66	0.46
1:H:273:GLY:HA3	1:H:314:ALA:C	2.36	0.46
1:H:330:VAL:O	1:H:330:VAL:CG1	2.64	0.46
1:A:48:VAL:HG21	1:A:167:TYR:CD2	2.52	0.45
1:D:166:LEU:C	1:D:166:LEU:HD12	2.36	0.45
1:D:184:PHE:HA	1:D:194:ILE:O	2.14	0.45
1:H:49:ARG:O	1:H:50:LYS:C	2.54	0.45
1:L:205:LYS:HG2	1:L:206:GLY:H	1.81	0.45
1:A:201:LYS:HA	1:A:291:ALA:CA	2.46	0.45
1:A:256:LEU:O	1:A:256:LEU:HG	2.15	0.45
1:D:22:ARG:HH12	1:H:29:GLU:HG3	1.80	0.45
1:D:29:GLU:CG	1:H:22:ARG:NH2	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:O	1:D:54:ALA:C	2.54	0.45
1:D:210:SER:O	1:D:211:LEU:HB3	2.16	0.45
1:D:293:GLY:HA2	1:D:321:PRO:CG	2.36	0.45
1:H:122:GLY:O	1:H:126:ILE:HB	2.16	0.45
1:H:264:TYR:HE1	1:H:274:LYS:HG3	1.81	0.45
1:L:222:ALA:O	1:L:225:GLU:HB3	2.15	0.45
1:L:273:GLY:H	1:L:315:PRO:CG	2.19	0.45
1:A:161:ALA:O	1:A:162:ALA:HB2	2.16	0.45
1:A:194:ILE:HD12	1:A:194:ILE:N	2.31	0.45
1:A:297:THR:CG2	1:A:302:VAL:HA	2.46	0.45
1:D:219:PHE:HD1	1:D:219:PHE:HA	1.69	0.45
1:D:328:LEU:O	1:D:331:TYR:HB3	2.17	0.45
1:L:44:ILE:O	1:L:45:SER:C	2.52	0.45
1:L:49:ARG:HG3	1:L:49:ARG:HH11	1.82	0.45
1:L:80:LEU:C	1:L:82:MET:N	2.66	0.45
1:L:261:ILE:O	1:L:261:ILE:CG2	2.64	0.45
1:L:318:LEU:C	1:L:318:LEU:CD1	2.84	0.45
1:A:288:MET:O	1:A:293:GLY:N	2.43	0.45
1:D:94:LEU:HD23	1:D:94:LEU:N	2.32	0.45
1:D:227:ILE:C	1:D:229:ARG:N	2.70	0.45
1:H:44:ILE:HG12	1:H:80:LEU:HD13	1.91	0.45
1:H:272:ASN:O	1:H:314:ALA:CA	2.55	0.45
1:L:248:MET:HE2	1:L:252:VAL:HG23	1.99	0.45
1:A:333:LYS:HG2	1:A:334:HIS:CD2	2.52	0.45
1:D:155:PRO:C	1:D:157:ARG:H	2.20	0.45
1:H:42:LYS:O	1:H:45:SER:HB3	2.17	0.45
1:H:135:ILE:HD12	1:H:279:TYR:O	2.17	0.45
1:H:320:SER:O	1:H:324:VAL:HG23	2.16	0.45
1:L:125:ASN:O	1:L:130:VAL:HG12	2.17	0.45
1:A:331:TYR:CD1	1:A:331:TYR:O	2.69	0.45
1:D:238:ALA:HA	1:D:239:PRO:HD3	1.87	0.45
1:L:30:LEU:O	1:L:33:LEU:N	2.49	0.45
1:A:91:THR:C	1:A:105:VAL:HG21	2.37	0.45
1:A:246:GLY:CA	1:D:243:ARG:HE	2.29	0.45
1:A:314:ALA:HA	1:A:315:PRO:HD3	1.66	0.45
1:D:99:ASP:OD2	1:D:103:ILE:HD11	2.17	0.45
1:D:160:VAL:O	1:D:160:VAL:CG1	2.65	0.45
1:H:256:LEU:O	1:H:256:LEU:HG	2.15	0.45
1:H:273:GLY:HA3	1:H:314:ALA:CA	2.47	0.45
1:L:251:ASP:O	1:L:254:ARG:HB3	2.16	0.45
1:L:264:TYR:CG	1:L:275:LEU:HD21	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:NZ	1:A:147:PRO:CA	2.79	0.45
1:A:149:GLU:HG2	1:A:310:ILE:CG2	2.47	0.45
1:D:48:VAL:C	1:D:50:LYS:N	2.68	0.45
1:D:123:SER:O	1:D:126:ILE:HB	2.17	0.45
1:D:132:VAL:CG2	1:D:133:GLY:N	2.77	0.45
1:D:221:PRO:O	1:D:222:ALA:C	2.53	0.45
1:H:276:ARG:NE	1:H:313:ARG:NH1	2.65	0.45
1:L:249:VAL:O	1:L:250:ALA:C	2.54	0.45
1:L:283:PRO:O	1:L:286:TYR:N	2.49	0.45
1:A:170:ALA:HB3	1:D:129:LEU:HD13	1.98	0.45
1:A:30:LEU:O	1:A:33:LEU:CB	2.60	0.45
1:A:120:LEU:HD11	1:A:132:VAL:CG1	2.47	0.45
1:A:187:ASP:OD2	1:D:52:GLY:HA2	2.17	0.45
1:A:262:PHE:C	1:A:263:LEU:HD12	2.38	0.45
1:H:13:LEU:CB	1:H:193:PHE:HB2	2.46	0.45
1:H:76:LEU:HD12	1:H:76:LEU:O	2.17	0.45
1:H:138:ILE:N	1:H:161:ALA:O	2.50	0.45
1:H:194:ILE:H	1:H:194:ILE:CD1	2.25	0.45
1:L:80:LEU:O	1:L:82:MET:N	2.50	0.45
1:A:185:MET:O	1:A:193:PHE:HD1	2.01	0.44
1:D:91:THR:HA	1:D:113:TYR:O	2.17	0.44
1:L:20:GLU:O	1:L:21:GLY:C	2.55	0.44
1:A:22:ARG:HD2	1:L:28:GLY:HA3	1.99	0.44
1:A:126:ILE:O	1:A:129:LEU:N	2.48	0.44
1:A:156:GLY:O	1:A:159:LEU:HD12	2.18	0.44
1:A:190:ILE:CG1	1:A:191:GLY:N	2.79	0.44
1:A:217:LYS:HA	1:D:232:PHE:HE1	1.82	0.44
1:A:309:ASP:C	1:A:311:HIS:H	2.20	0.44
1:D:15:ARG:C	1:D:18:MET:HB2	2.37	0.44
1:A:186:LEU:HD12	1:A:186:LEU:C	2.38	0.44
1:D:55:HIS:HA	1:D:59:ILE:CG2	2.46	0.44
1:H:113:TYR:CE1	1:H:140:ARG:HD3	2.51	0.44
1:H:123:SER:O	1:H:126:ILE:HG22	2.16	0.44
1:H:155:PRO:HG2	1:H:158:ASN:CB	2.47	0.44
1:L:221:PRO:O	1:L:222:ALA:C	2.55	0.44
1:L:266:ALA:C	1:L:267:ASN:ND2	2.71	0.44
1:A:76:LEU:O	1:A:78:ASN:N	2.51	0.44
1:A:98:GLU:HG2	1:A:119:PRO:HG3	1.96	0.44
1:A:133:GLY:HA3	1:A:249:VAL:HG11	1.99	0.44
1:A:183:CYS:HB2	1:A:197:ASP:CB	2.47	0.44
1:H:262:PHE:N	1:H:318:LEU:O	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:277:LEU:HD21	1:L:307:PRO:HG3	1.99	0.44
1:A:267:ASN:HB2	1:A:268:LYS:H	1.46	0.44
1:D:190:ILE:O	1:D:191:GLY:C	2.55	0.44
1:H:202:ILE:HD13	1:H:320:SER:HA	2.00	0.44
1:H:207:LYS:C	1:H:208:ILE:HG13	2.38	0.44
1:H:279:TYR:HA	1:H:283:PRO:HG2	1.98	0.44
1:L:53:ILE:CG2	1:L:54:ALA:H	2.31	0.44
1:A:211:LEU:HD13	1:A:227:ILE:HD11	2.00	0.44
1:D:82:MET:CE	1:D:103:ILE:HG21	2.48	0.44
1:D:263:LEU:N	1:D:263:LEU:CD1	2.74	0.44
1:H:196:VAL:CG2	1:H:197:ASP:N	2.81	0.44
1:L:225:GLU:OE2	1:L:330:VAL:CG2	2.66	0.44
1:A:92:CYS:SG	1:A:113:TYR:O	2.70	0.44
1:A:211:LEU:HB3	1:A:263:LEU:HB2	1.99	0.44
1:A:278:LEU:CD1	1:A:310:ILE:HA	2.47	0.44
1:D:50:LYS:HD2	1:D:50:LYS:N	2.33	0.44
1:H:269:LYS:NZ	1:H:274:LYS:CE	2.71	0.44
1:L:253:HIS:O	1:L:254:ARG:C	2.56	0.44
1:L:25:ARG:HA	2:L:1001:870:C14	2.48	0.44
1:L:36:SER:OG	1:L:88:SER:HB3	2.18	0.44
1:L:75:VAL:HG12	1:L:76:LEU:N	2.32	0.44
1:L:181:VAL:O	1:L:182:ASN:CG	2.57	0.44
1:A:120:LEU:CD1	1:A:132:VAL:HB	2.48	0.44
1:D:88:SER:O	1:D:89:PHE:CB	2.66	0.44
1:D:95:VAL:O	1:D:117:PHE:CD1	2.71	0.44
1:D:245:VAL:N	1:D:251:ASP:OD1	2.51	0.44
1:D:261:ILE:HD13	1:D:263:LEU:HD11	2.00	0.44
1:H:106:GLU:OE2	1:H:109:LYS:NZ	2.41	0.44
1:L:327:PHE:O	1:L:328:LEU:C	2.55	0.44
1:D:79:ASP:HB3	1:L:60:ALA:O	2.17	0.43
1:D:82:MET:HE2	1:D:103:ILE:HG21	2.00	0.43
1:H:45:SER:O	1:H:46:SER:C	2.56	0.43
1:L:42:LYS:HG3	1:L:193:PHE:CZ	2.53	0.43
1:A:13:LEU:HA	1:A:184:PHE:CE2	2.53	0.43
1:A:97:GLU:HB2	1:A:279:TYR:CE1	2.53	0.43
1:A:148:SER:O	1:A:151:ASP:HB2	2.18	0.43
1:D:22:ARG:O	1:D:25:ARG:N	2.47	0.43
1:H:154:GLN:HG2	1:H:158:ASN:HD22	1.83	0.43
1:H:156:GLY:HA3	1:H:303:LEU:CD2	2.49	0.43
1:L:98:GLU:CG	1:L:119:PRO:HG3	2.48	0.43
1:L:209:TYR:HD1	1:L:240:TYR:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:CD	1:A:158:ASN:ND2	2.81	0.43
1:A:178:ASP:C	1:A:180:GLY:H	2.21	0.43
1:D:53:ILE:HA	1:D:56:LEU:CD2	2.49	0.43
1:D:118:ASP:HB3	1:D:135:ILE:CB	2.48	0.43
1:H:252:VAL:HB	1:H:284:MET:CE	2.48	0.43
1:L:78:ASN:OD1	1:L:98:GLU:HB2	2.18	0.43
1:L:133:GLY:HA3	1:L:249:VAL:HG11	2.00	0.43
1:L:135:ILE:HG22	1:L:136:PHE:N	2.33	0.43
1:A:19:GLU:HB3	1:A:23:LYS:HZ3	1.80	0.43
1:A:235:ASP:O	1:A:236:ASN:C	2.56	0.43
1:A:289:GLU:OE2	1:A:303:LEU:CD1	2.51	0.43
1:D:133:GLY:HA2	1:D:165:ALA:O	2.18	0.43
1:D:262:PHE:CD2	1:D:263:LEU:N	2.86	0.43
1:D:276:ARG:O	1:D:281:CYS:N	2.45	0.43
1:H:164:TYR:OH	1:H:174:VAL:HG21	2.18	0.43
1:H:238:ALA:HA	1:H:239:PRO:HD3	1.69	0.43
1:H:270:SER:HA	1:H:271:PRO:HD3	1.75	0.43
1:L:164:TYR:OH	1:L:253:HIS:ND1	2.47	0.43
1:L:186:LEU:HB2	1:L:193:PHE:CD1	2.53	0.43
1:L:276:ARG:HD3	1:L:279:TYR:HE1	1.83	0.43
1:A:201:LYS:HA	1:A:291:ALA:HB1	2.01	0.43
1:D:146:GLU:HG3	1:D:147:PRO:HD2	2.00	0.43
1:H:37:LEU:O	1:H:38:CYS:C	2.56	0.43
1:H:187:ASP:CG	1:L:51:ALA:O	2.57	0.43
1:L:204:LYS:HB2	1:L:204:LYS:HE3	1.83	0.43
1:L:327:PHE:O	1:L:330:VAL:N	2.51	0.43
1:A:121:ASP:HB3	1:A:249:VAL:HG23	2.00	0.43
1:D:42:LYS:C	1:D:45:SER:HB3	2.38	0.43
1:H:24:ALA:HB1	2:H:901:870:CL1	2.55	0.43
1:H:79:ASP:O	1:H:80:LEU:O	2.37	0.43
1:H:251:ASP:HB2	1:H:262:PHE:CE1	2.54	0.43
1:L:214:GLY:C	1:L:216:ALA:H	2.22	0.43
1:L:267:ASN:OD1	1:L:269:LYS:CB	2.67	0.43
1:D:13:LEU:CA	1:D:184:PHE:CE2	2.96	0.43
1:D:179:CYS:SG	1:D:180:GLY:N	2.92	0.43
1:H:82:MET:O	1:H:85:LEU:N	2.52	0.43
1:H:141:LYS:NZ	1:H:151:ASP:OD1	2.49	0.43
1:H:185:MET:HB2	1:H:196:VAL:HG11	2.00	0.43
1:A:155:PRO:HD2	1:A:158:ASN:ND2	2.34	0.43
1:A:226:TYR:O	1:A:230:LYS:HG3	2.16	0.43
1:D:27:THR:CG2	1:D:112:LYS:NZ	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ILE:HG22	1:D:260:GLY:HA3	2.01	0.43
1:H:17:VAL:HG13	2:H:901:870:CL2	2.56	0.43
1:H:187:ASP:OD2	1:L:51:ALA:O	2.37	0.43
1:L:76:LEU:O	1:L:77:SER:C	2.57	0.43
1:L:81:VAL:O	1:L:82:MET:O	2.37	0.43
1:L:142:LYS:O	1:L:143:SER:O	2.37	0.43
1:L:202:ILE:HG22	1:L:291:ALA:O	2.19	0.43
1:L:223:VAL:C	1:L:225:GLU:N	2.71	0.43
1:L:267:ASN:HB2	1:L:268:LYS:H	1.59	0.43
1:H:135:ILE:HG23	1:H:249:VAL:CG2	2.49	0.43
1:H:277:LEU:HD11	1:H:282:ASN:HD21	1.84	0.43
1:H:288:MET:CE	1:H:288:MET:HA	2.49	0.43
1:H:318:LEU:C	1:H:318:LEU:CD1	2.87	0.43
1:L:131:SER:HB2	1:L:250:ALA:HB2	2.00	0.43
1:A:226:TYR:O	1:A:226:TYR:CG	2.72	0.43
1:A:332:GLU:O	1:A:335:SER:O	2.36	0.43
1:D:59:ILE:HD11	1:L:43:ALA:CB	2.49	0.43
1:D:150:LYS:C	1:D:152:ALA:H	2.22	0.43
1:D:195:LEU:HD11	1:D:198:LYS:HG2	2.00	0.43
1:H:294:MET:HB3	1:H:324:VAL:CG1	2.46	0.43
1:L:160:VAL:O	1:L:161:ALA:HB2	2.18	0.43
1:L:181:VAL:C	1:L:182:ASN:CG	2.78	0.43
1:D:143:SER:HB2	1:D:145:ASP:OD2	2.18	0.42
1:L:51:ALA:C	1:L:53:ILE:H	2.17	0.42
1:H:93:VAL:HB	1:H:114:VAL:CG2	2.49	0.42
1:H:184:PHE:HA	1:H:194:ILE:O	2.18	0.42
2:A:701:870:HN22	1:L:27:THR:CA	2.32	0.42
1:D:16:PHE:C	1:D:16:PHE:CD1	2.92	0.42
1:D:22:ARG:NH2	1:H:29:GLU:N	2.67	0.42
1:D:173:LEU:HG	1:D:174:VAL:N	2.34	0.42
1:H:129:LEU:HD11	1:L:172:MET:CE	2.49	0.42
1:L:16:PHE:CD1	1:L:16:PHE:C	2.93	0.42
1:A:13:LEU:O	1:A:17:VAL:HG23	2.20	0.42
1:A:31:THR:O	1:A:32:GLN:C	2.56	0.42
1:A:317:ILE:HG12	1:A:327:PHE:CZ	2.54	0.42
1:D:118:ASP:HB3	1:D:135:ILE:HD12	2.00	0.42
1:D:302:VAL:CG2	1:D:316:VAL:HG13	2.49	0.42
1:A:45:SER:HA	1:A:48:VAL:HB	2.02	0.42
1:A:53:ILE:HD11	1:A:57:TYR:CE1	2.55	0.42
1:A:162:ALA:O	1:A:176:ALA:N	2.50	0.42
1:A:186:LEU:HD22	1:A:193:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HB	1:D:117:PHE:CE2	2.55	0.42
1:H:50:LYS:O	1:L:188:PRO:HD2	2.19	0.42
1:H:268:LYS:O	1:H:269:LYS:C	2.58	0.42
1:L:135:ILE:HG22	1:L:136:PHE:H	1.84	0.42
1:L:256:LEU:HD13	1:L:288:MET:HE1	2.00	0.42
1:L:322:ASP:O	1:L:326:GLU:HB2	2.20	0.42
1:A:223:VAL:O	1:A:224:THR:C	2.58	0.42
2:A:701:870:N2	1:L:27:THR:HA	2.34	0.42
1:D:88:SER:C	1:D:89:PHE:HD1	2.23	0.42
1:D:286:TYR:CE1	1:D:290:LYS:HG3	2.55	0.42
1:H:86:LYS:HE2	1:H:94:LEU:HD12	2.01	0.42
1:H:172:MET:HE2	1:H:183:CYS:HB3	2.01	0.42
1:H:263:LEU:HD12	1:H:263:LEU:N	2.34	0.42
1:L:203:LYS:HB3	1:L:205:LYS:O	2.20	0.42
1:L:227:ILE:C	1:L:229:ARG:H	2.23	0.42
1:A:43:ALA:HA	1:L:190:ILE:CG2	2.49	0.42
1:D:31:THR:O	1:D:31:THR:HG22	2.19	0.42
1:D:205:LYS:HA	1:D:322:ASP:HB2	2.00	0.42
1:H:52:GLY:C	1:H:54:ALA:H	2.22	0.42
1:H:104:ILE:O	1:H:105:VAL:C	2.58	0.42
1:L:36:SER:HA	1:L:84:MET:HE3	2.02	0.42
1:L:50:LYS:CB	1:L:53:ILE:HD12	2.50	0.42
1:L:183:CYS:CB	1:L:196:VAL:HG22	2.46	0.42
1:L:276:ARG:CB	1:L:279:TYR:CE1	2.98	0.42
1:D:280:GLU:O	1:D:284:MET:HG2	2.19	0.42
1:D:302:VAL:HG21	1:D:316:VAL:HG11	2.01	0.42
1:H:112:LYS:HG3	1:H:113:TYR:N	2.35	0.42
1:H:115:VAL:HG13	1:H:138:ILE:HG12	2.02	0.42
1:A:20:GLU:OE2	1:A:179:CYS:SG	2.77	0.42
1:A:107:PRO:HA	1:A:110:ARG:HD2	2.01	0.42
1:A:261:ILE:CD1	1:A:323:ASP:O	2.59	0.42
1:D:134:THR:O	1:D:164:TYR:HB2	2.19	0.42
1:H:45:SER:O	1:H:48:VAL:HG23	2.19	0.42
1:H:104:ILE:H	1:H:104:ILE:HG12	1.76	0.42
1:H:135:ILE:CD1	1:H:279:TYR:O	2.68	0.42
1:D:56:LEU:HG	1:D:57:TYR:HD1	1.85	0.42
1:D:227:ILE:C	1:D:229:ARG:H	2.23	0.42
1:D:321:PRO:O	1:D:324:VAL:HB	2.20	0.42
1:L:82:MET:HE3	1:L:94:LEU:HD13	2.01	0.42
1:L:82:MET:CE	1:L:94:LEU:CD1	2.97	0.42
1:A:159:LEU:HD13	1:A:286:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:O	1:D:25:ARG:C	2.58	0.41
1:H:118:ASP:O	1:H:119:PRO:C	2.57	0.41
1:H:149:GLU:C	1:H:151:ASP:N	2.71	0.41
1:D:73:LEU:HD12	1:D:73:LEU:HA	1.83	0.41
1:D:186:LEU:HB2	1:D:193:PHE:HE1	1.85	0.41
1:D:263:LEU:HB3	1:D:317:ILE:HG13	2.02	0.41
1:D:267:ASN:CG	1:D:268:LYS:H	2.21	0.41
1:H:139:TYR:CE1	1:H:159:LEU:CD2	3.03	0.41
1:L:50:LYS:HG2	1:L:53:ILE:HD12	2.02	0.41
1:L:230:LYS:HE2	1:L:240:TYR:CD2	2.55	0.41
1:A:22:ARG:HD2	1:L:28:GLY:O	2.20	0.41
1:A:73:LEU:C	1:A:75:VAL:H	2.24	0.41
1:A:211:LEU:O	1:A:211:LEU:CG	2.68	0.41
1:A:243:ARG:O	1:A:244:TYR:HB2	2.20	0.41
1:D:275:LEU:HD23	1:D:275:LEU:N	2.27	0.41
1:D:314:ALA:HA	1:D:315:PRO:HD3	1.88	0.41
1:A:173:LEU:HD12	1:A:193:PHE:CZ	2.55	0.41
1:D:42:LYS:CA	1:D:45:SER:HB3	2.50	0.41
1:H:16:PHE:CD1	1:H:16:PHE:O	2.72	0.41
1:L:14:THR:O	1:L:18:MET:SD	2.79	0.41
1:L:333:LYS:O	1:L:333:LYS:HG2	2.19	0.41
1:A:211:LEU:HD21	1:A:213:GLU:HG2	2.02	0.41
1:D:22:ARG:NH2	1:H:29:GLU:CA	2.84	0.41
1:D:255:THR:O	1:D:259:GLY:HA2	2.20	0.41
1:H:166:LEU:HD12	1:H:167:TYR:N	2.36	0.41
1:H:253:HIS:C	1:H:255:THR:N	2.73	0.41
1:L:37:LEU:HD21	1:L:136:PHE:CE2	2.56	0.41
1:L:50:LYS:HB3	1:L:53:ILE:HD12	2.02	0.41
1:L:77:SER:O	1:L:80:LEU:HB2	2.20	0.41
1:L:115:VAL:HG22	1:L:138:ILE:HG12	2.02	0.41
1:L:248:MET:CE	1:L:248:MET:CA	2.92	0.41
1:A:324:VAL:CA	1:A:327:PHE:HB3	2.49	0.41
1:D:79:ASP:O	1:D:80:LEU:C	2.59	0.41
1:D:252:VAL:HB	1:D:284:MET:HE1	2.02	0.41
1:H:306:ILE:HA	1:H:307:PRO:HD3	1.81	0.41
1:L:91:THR:HG21	1:L:94:LEU:CD2	2.33	0.41
1:L:317:ILE:HG12	1:L:327:PHE:HE2	1.80	0.41
1:D:240:TYR:HB3	1:D:241:GLY:H	1.65	0.41
1:D:277:LEU:HB3	1:D:278:LEU:H	1.60	0.41
1:D:297:THR:HG21	1:D:305:VAL:HG21	2.02	0.41
1:D:317:ILE:N	1:D:317:ILE:CD1	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:LEU:HB2	1:H:113:TYR:CE2	2.56	0.41
1:L:198:LYS:O	1:L:199:ASP:C	2.59	0.41
1:L:276:ARG:HD3	1:L:279:TYR:CE1	2.55	0.41
1:A:82:MET:HE1	1:A:94:LEU:CB	2.48	0.41
1:D:118:ASP:CG	1:D:135:ILE:HD12	2.41	0.41
1:D:329:LYS:O	1:D:330:VAL:C	2.59	0.41
1:H:230:LYS:C	1:H:232:PHE:N	2.72	0.41
1:H:274:LYS:HA	1:H:313:ARG:HD3	2.02	0.41
1:L:114:VAL:HG12	1:L:115:VAL:N	2.36	0.41
1:L:116:CYS:SG	1:L:139:TYR:CE2	3.02	0.41
1:L:297:THR:HA	1:L:315:PRO:O	2.21	0.41
1:A:32:GLN:HE22	1:L:22:ARG:HH21	1.69	0.41
1:A:41:VAL:CG1	1:A:167:TYR:CE1	3.02	0.41
1:A:43:ALA:HA	1:L:190:ILE:HG21	2.03	0.41
1:A:91:THR:O	1:A:105:VAL:HG11	2.21	0.41
1:A:182:ASN:HB3	1:A:195:LEU:HD11	2.02	0.41
1:A:268:LYS:O	1:A:269:LYS:C	2.59	0.41
1:D:186:LEU:HD13	1:D:193:PHE:CD1	2.54	0.41
1:H:13:LEU:O	1:H:16:PHE:HB3	2.21	0.41
1:H:33:LEU:C	1:H:33:LEU:HD12	2.41	0.41
1:H:156:GLY:O	1:H:159:LEU:HB2	2.21	0.41
1:H:252:VAL:CG2	1:H:318:LEU:HD21	2.50	0.41
1:L:105:VAL:CG1	1:L:106:GLU:N	2.84	0.41
1:L:149:GLU:OE1	1:L:310:ILE:CD1	2.68	0.41
1:L:180:GLY:O	1:L:182:ASN:ND2	2.53	0.41
1:L:273:GLY:N	1:L:315:PRO:HG3	2.21	0.41
1:L:302:VAL:HG21	1:L:316:VAL:HG13	2.02	0.41
1:A:150:LYS:O	1:A:153:LEU:HB2	2.21	0.41
1:A:225:GLU:HA	1:A:228:GLN:HB2	2.02	0.41
1:H:277:LEU:HD11	1:H:282:ASN:ND2	2.35	0.41
1:H:318:LEU:HD12	1:H:319:GLY:N	2.36	0.41
1:L:138:ILE:HB	1:L:161:ALA:O	2.20	0.41
1:L:208:ILE:O	1:L:260:GLY:CA	2.69	0.41
1:L:277:LEU:CD1	1:L:282:ASN:ND2	2.84	0.41
1:A:284:MET:O	1:A:285:ALA:C	2.59	0.40
1:A:318:LEU:HD12	1:A:318:LEU:O	2.21	0.40
1:D:226:TYR:CE1	1:D:327:PHE:HB2	2.56	0.40
1:D:332:GLU:O	1:D:334:HIS:N	2.54	0.40
1:H:52:GLY:C	1:H:54:ALA:N	2.75	0.40
1:H:253:HIS:O	1:H:254:ARG:C	2.59	0.40
1:L:223:VAL:HG12	1:L:224:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLN:HE21	1:H:15:ARG:HG3	1.86	0.40
1:D:49:ARG:HH11	1:D:49:ARG:HG3	1.86	0.40
1:D:81:VAL:O	1:D:85:LEU:HG	2.21	0.40
1:D:91:THR:HB	1:D:94:LEU:CD2	2.28	0.40
1:D:235:ASP:O	1:D:237:SER:N	2.54	0.40
1:D:292:GLY:O	1:D:321:PRO:CG	2.70	0.40
1:H:45:SER:HA	1:H:167:TYR:CE1	2.56	0.40
1:H:130:VAL:CG2	1:H:245:VAL:HG13	2.50	0.40
1:H:142:LYS:HB2	1:H:154:GLN:NE2	2.36	0.40
1:H:227:ILE:HG22	1:H:231:LYS:CD	2.51	0.40
1:L:193:PHE:C	1:L:194:ILE:HD12	2.41	0.40
1:L:209:TYR:CB	1:L:261:ILE:CG2	2.99	0.40
1:L:250:ALA:O	1:L:251:ASP:C	2.59	0.40
1:A:39:THR:CG2	1:A:84:MET:HE2	2.46	0.40
1:D:43:ALA:C	1:D:45:SER:N	2.73	0.40
1:D:295:ALA:CB	1:D:318:LEU:HB3	2.52	0.40
1:H:49:ARG:N	1:H:49:ARG:CD	2.84	0.40
1:H:78:ASN:O	1:H:79:ASP:C	2.60	0.40
1:H:149:GLU:O	1:H:152:ALA:N	2.55	0.40
1:H:149:GLU:O	1:H:151:ASP:N	2.54	0.40
1:H:156:GLY:C	1:H:303:LEU:HB3	2.41	0.40
1:L:262:PHE:C	1:L:263:LEU:HD12	2.42	0.40
1:L:283:PRO:O	1:L:284:MET:C	2.60	0.40
1:A:84:MET:O	1:A:88:SER:HB3	2.22	0.40
1:A:85:LEU:C	1:A:88:SER:H	2.25	0.40
1:A:153:LEU:HD22	1:A:307:PRO:C	2.41	0.40
1:A:253:HIS:O	1:A:254:ARG:C	2.60	0.40
1:D:85:LEU:HD13	1:D:115:VAL:HG21	2.02	0.40
1:H:16:PHE:C	1:H:16:PHE:HD1	2.24	0.40
1:H:16:PHE:CZ	1:H:182:ASN:ND2	2.88	0.40
1:L:246:GLY:O	1:L:247:SER:CB	2.69	0.40
1:A:186:LEU:O	1:A:188:PRO:CD	2.61	0.40
1:D:102:ALA:HB3	1:D:104:ILE:HD11	2.04	0.40
1:D:324:VAL:O	1:D:328:LEU:HB2	2.21	0.40
1:H:128:CYS:HA	1:L:257:VAL:HG21	2.03	0.40
1:H:209:TYR:CE1	1:H:242:ALA:HB2	2.57	0.40
1:H:313:ARG:HG2	1:H:313:ARG:HH11	1.87	0.40
1:L:266:ALA:O	1:L:267:ASN:CB	2.69	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	315/338 (93%)	207 (66%)	72 (23%)	36 (11%)	0 6
1	D	315/338 (93%)	192 (61%)	74 (24%)	49 (16%)	0 2
1	H	315/338 (93%)	211 (67%)	62 (20%)	42 (13%)	0 4
1	L	315/338 (93%)	196 (62%)	73 (23%)	46 (15%)	0 3
All	All	1260/1352 (93%)	806 (64%)	281 (22%)	173 (14%)	0 4

All (173) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	51	ALA
1	A	123	SER
1	A	199	ASP
1	A	222	ALA
1	A	235	ASP
1	A	237	SER
1	A	295	ALA
1	D	10	VAL
1	D	51	ALA
1	D	80	LEU
1	D	82	MET
1	D	100	LYS
1	D	143	SER
1	D	178	ASP
1	D	236	ASN
1	D	240	TYR
1	D	243	ARG
1	D	245	VAL
1	D	249	VAL
1	D	267	ASN
1	D	270	SER

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Mol	Chain	Res	Type
1	D	275	LEU
1	D	277	LEU
1	D	287	VAL
1	D	300	GLU
1	D	303	LEU
1	D	310	ILE
1	H	59	ILE
1	H	80	LEU
1	H	81	VAL
1	H	82	MET
1	H	83	ASN
1	H	100	LYS
1	H	130	VAL
1	H	236	ASN
1	H	240	TYR
1	H	244	TYR
1	H	300	GLU
1	H	310	ILE
1	H	311	HIS
1	L	51	ALA
1	L	82	MET
1	L	112	LYS
1	L	143	SER
1	L	199	ASP
1	L	202	ILE
1	L	221	PRO
1	L	223	VAL
1	L	247	SER
1	L	248	MET
1	L	249	VAL
1	L	267	ASN
1	L	273	GLY
1	L	310	ILE
1	L	314	ALA
1	A	50	LYS
1	A	77	SER
1	A	105	VAL
1	A	153	LEU
1	A	236	ASN
1	A	244	TYR
1	A	252	VAL
1	A	267	ASN

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Mol	Chain	Res	Type
1	A	282	ASN
1	D	55	HIS
1	D	74	ASP
1	D	79	ASP
1	D	101	HIS
1	D	119	PRO
1	D	131	SER
1	D	156	GLY
1	D	222	ALA
1	D	248	MET
1	D	331	TYR
1	H	53	ILE
1	H	92	CYS
1	H	198	LYS
1	H	199	ASP
1	H	259	GLY
1	H	267	ASN
1	H	274	LYS
1	H	302	VAL
1	H	327	PHE
1	L	58	GLY
1	L	75	VAL
1	L	83	ASN
1	L	90	ALA
1	L	100	LYS
1	L	120	LEU
1	L	123	SER
1	L	124	SER
1	L	224	THR
1	L	286	TYR
1	L	302	VAL
1	L	321	PRO
1	L	322	ASP
1	L	324	VAL
1	A	117	PHE
1	A	129	LEU
1	A	161	ALA
1	A	203	LYS
1	A	331	TYR
1	D	17	VAL
1	D	54	ALA
1	D	124	SER

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Mol	Chain	Res	Type
1	D	286	TYR
1	D	330	VAL
1	H	74	ASP
1	H	313	ARG
1	L	108	GLU
1	L	303	LEU
1	A	89	PHE
1	A	120	LEU
1	A	162	ALA
1	A	234	PRO
1	A	300	GLU
1	D	25	ARG
1	D	199	ASP
1	D	242	ALA
1	D	271	PRO
1	H	22	ARG
1	H	61	GLY
1	H	101	HIS
1	H	147	PRO
1	H	203	LYS
1	H	238	ALA
1	H	271	PRO
1	H	292	GLY
1	H	321	PRO
1	L	76	LEU
1	L	110	ARG
1	L	246	GLY
1	L	283	PRO
1	A	38	CYS
1	A	53	ILE
1	A	60	ALA
1	A	79	ASP
1	A	201	LYS
1	A	269	LYS
1	A	283	PRO
1	D	59	ILE
1	D	83	ASN
1	D	211	LEU
1	H	141	LYS
1	H	169	SER
1	H	211	LEU
1	H	222	ALA

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Mol	Chain	Res	Type
1	H	309	ASP
1	L	77	SER
1	L	251	ASP
1	L	328	LEU
1	A	310	ILE
1	D	105	VAL
1	D	151	ASP
1	D	164	TYR
1	D	238	ALA
1	H	105	VAL
1	L	52	GLY
1	L	252	VAL
1	L	325	LEU
1	A	265	PRO
1	D	315	PRO
1	H	119	PRO
1	L	59	ILE
1	L	61	GLY
1	L	200	VAL
1	L	270	SER
1	H	314	ALA
1	D	305	VAL
1	H	188	PRO
1	L	271	PRO
1	D	190	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	265/281 (94%)	238 (90%)	27 (10%)	7 32
1	D	265/281 (94%)	225 (85%)	40 (15%)	3 17
1	H	265/281 (94%)	243 (92%)	22 (8%)	11 40
1	L	265/281 (94%)	226 (85%)	39 (15%)	3 18
All	All	1060/1124 (94%)	932 (88%)	128 (12%)	5 24

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	33	LEU
1	A	49	ARG
1	A	50	LYS
1	A	74	ASP
1	A	79	ASP
1	A	89	PHE
1	A	107	PRO
1	A	123	SER
1	A	130	VAL
1	A	131	SER
1	A	132	VAL
1	A	140	ARG
1	A	146	GLU
1	A	167	TYR
1	A	179	CYS
1	A	196	VAL
1	A	200	VAL
1	A	201	LYS
1	A	225	GLU
1	A	243	ARG
1	A	272	ASN
1	A	278	LEU
1	A	279	TYR
1	A	310	ILE
1	A	320	SER
1	A	322	ASP
1	D	9	ASP
1	D	14	THR
1	D	27	THR
1	D	33	LEU
1	D	49	ARG
1	D	50	LYS
1	D	56	LEU
1	D	73	LEU
1	D	94	LEU
1	D	117	PHE
1	D	120	LEU
1	D	123	SER
1	D	124	SER
1	D	126	ILE
1	D	127	ASP

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Mol	Chain	Res	Type
1	D	130	VAL
1	D	132	VAL
1	D	145	ASP
1	D	173	LEU
1	D	195	LEU
1	D	196	VAL
1	D	197	ASP
1	D	199	ASP
1	D	208	ILE
1	D	219	PHE
1	D	220	ASP
1	D	236	ASN
1	D	261	ILE
1	D	263	LEU
1	D	264	TYR
1	D	272	ASN
1	D	275	LEU
1	D	279	TYR
1	D	308	THR
1	D	309	ASP
1	D	310	ILE
1	D	316	VAL
1	D	318	LEU
1	D	328	LEU
1	D	332	GLU
1	H	13	LEU
1	H	16	PHE
1	H	27	THR
1	H	33	LEU
1	H	35	ASN
1	H	48	VAL
1	H	49	ARG
1	H	50	LYS
1	H	82	MET
1	H	103	ILE
1	H	104	ILE
1	H	115	VAL
1	H	178	ASP
1	H	197	ASP
1	H	219	PHE
1	H	220	ASP
1	H	249	VAL

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Mol	Chain	Res	Type
1	H	276	ARG
1	H	294	MET
1	H	306	ILE
1	H	311	HIS
1	H	323	ASP
1	L	12	THR
1	L	27	THR
1	L	31	THR
1	L	32	GLN
1	L	33	LEU
1	L	49	ARG
1	L	50	LYS
1	L	55	HIS
1	L	56	LEU
1	L	62	SER
1	L	79	ASP
1	L	91	THR
1	L	106	GLU
1	L	108	GLU
1	L	123	SER
1	L	124	SER
1	L	126	ILE
1	L	140	ARG
1	L	145	ASP
1	L	146	GLU
1	L	149	GLU
1	L	196	VAL
1	L	197	ASP
1	L	211	LEU
1	L	215	TYR
1	L	217	LYS
1	L	220	ASP
1	L	248	MET
1	L	263	LEU
1	L	264	TYR
1	L	272	ASN
1	L	275	LEU
1	L	279	TYR
1	L	280	GLU
1	L	313	ARG
1	L	316	VAL
1	L	320	SER

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Mol	Chain	Res	Type
1	L	329	LYS
1	L	335	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	35	ASN
1	A	158	ASN
1	A	228	GLN
1	A	236	ASN
1	A	272	ASN
1	A	282	ASN
1	A	334	HIS
1	D	32	GLN
1	D	83	ASN
1	D	125	ASN
1	D	158	ASN
1	D	272	ASN
1	H	158	ASN
1	H	272	ASN
1	H	282	ASN
1	L	35	ASN
1	L	55	HIS
1	L	228	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	870	H	901	-	30,33,33	2.47	10 (33%)	38,49,49	1.46	6 (15%)
2	870	D	801	-	30,33,33	2.22	11 (36%)	38,49,49	1.32	5 (13%)
2	870	L	1001	-	30,33,33	2.24	10 (33%)	38,49,49	1.60	6 (15%)
2	870	A	701	-	30,33,33	2.16	10 (33%)	38,49,49	1.26	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	870	H	901	-	-	2/11/17/17	0/4/4/4
2	870	D	801	-	-	2/11/17/17	0/4/4/4
2	870	L	1001	-	-	5/11/17/17	0/4/4/4
2	870	A	701	-	-	0/11/17/17	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	870	C11-C12	7.17	1.51	1.41
2	A	701	870	C11-C12	6.53	1.50	1.41
2	L	1001	870	C11-C12	6.53	1.50	1.41
2	H	901	870	C6-N	6.07	1.52	1.39
2	H	901	870	C10-C9	6.04	1.47	1.37
2	H	901	870	C11-C12	5.91	1.49	1.41
2	A	701	870	C6-N	4.67	1.49	1.39
2	L	1001	870	C6-N	4.19	1.48	1.39
2	L	1001	870	C8-C9	4.01	1.44	1.37
2	D	801	870	C10-C9	3.89	1.44	1.37
2	L	1001	870	C5-C4	3.80	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	870	C16-C19	3.68	1.45	1.39
2	A	701	870	C10-C9	3.62	1.43	1.37
2	H	901	870	C5-C4	3.26	1.44	1.40
2	H	901	870	C8-C9	3.17	1.42	1.37
2	A	701	870	C5-C4	3.03	1.44	1.40
2	H	901	870	C6-N1	2.96	1.39	1.35
2	L	1001	870	C3-C4	2.91	1.43	1.39
2	H	901	870	C1-C2	2.87	1.43	1.38
2	D	801	870	C8-C9	2.83	1.42	1.37
2	A	701	870	C6-N1	2.74	1.38	1.35
2	L	1001	870	C10-C9	2.67	1.41	1.37
2	D	801	870	C6-N	2.58	1.45	1.39
2	H	901	870	C14-C18	2.55	1.42	1.36
2	L	1001	870	C1-C2	2.55	1.42	1.38
2	A	701	870	C8-C7	-2.49	1.38	1.41
2	L	1001	870	C4-S	2.31	1.80	1.77
2	H	901	870	C8-C7	-2.28	1.38	1.41
2	A	701	870	C16-C19	2.23	1.43	1.39
2	D	801	870	C14-C15	2.22	1.43	1.38
2	L	1001	870	C14-C18	2.21	1.41	1.36
2	H	901	870	C2-CL2	-2.20	1.69	1.74
2	D	801	870	C8-C7	-2.20	1.38	1.41
2	A	701	870	C14-C18	2.16	1.41	1.36
2	D	801	870	C16-C17	2.15	1.46	1.42
2	D	801	870	O2-S	2.11	1.45	1.43
2	D	801	870	C-C5	2.06	1.43	1.38
2	D	801	870	C3-C2	2.04	1.41	1.38
2	L	1001	870	C16-C19	2.03	1.42	1.39
2	A	701	870	C-C5	2.02	1.43	1.38
2	A	701	870	C1-C	2.00	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1001	870	O2-S-O1	-5.15	113.22	119.55
2	H	901	870	C8-C7-C12	4.20	125.37	121.12
2	L	1001	870	O1-S-C4	3.87	114.03	107.66
2	A	701	870	C8-C7-C12	3.79	124.95	121.12
2	D	801	870	O2-S-O1	-3.64	115.08	119.55
2	L	1001	870	C8-C7-C12	3.49	124.65	121.12
2	A	701	870	O4-C9-C8	-3.44	115.04	124.43
2	D	801	870	C8-C7-C12	3.31	124.47	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1001	870	C-C5-C4	3.02	122.11	120.05
2	D	801	870	C-C5-C4	2.98	122.08	120.05
2	A	701	870	O2-S-O1	-2.72	116.21	119.55
2	H	901	870	C4-S-N	-2.67	104.16	107.27
2	H	901	870	O2-S-O1	-2.63	116.32	119.55
2	L	1001	870	O4-C9-C8	-2.55	117.48	124.43
2	D	801	870	O4-C9-C8	-2.51	117.58	124.43
2	H	901	870	C19-C16-C17	2.31	122.67	121.11
2	H	901	870	O4-C9-C8	-2.23	118.34	124.43
2	H	901	870	C5-C4-S	2.14	124.65	123.25
2	D	801	870	C5-C4-S	2.11	124.63	123.25
2	L	1001	870	C4-S-N	2.08	109.70	107.27

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	870	C8-C9-O4-C13
2	D	801	870	C10-C9-O4-C13
2	L	1001	870	C10-C9-O4-C13
2	L	1001	870	C8-C9-O4-C13
2	H	901	870	C8-C9-O4-C13
2	H	901	870	C10-C9-O4-C13
2	L	1001	870	C6-N-S-O2
2	L	1001	870	C6-N-S-C4
2	L	1001	870	C6-N-S-O1

There are no ring outliers.

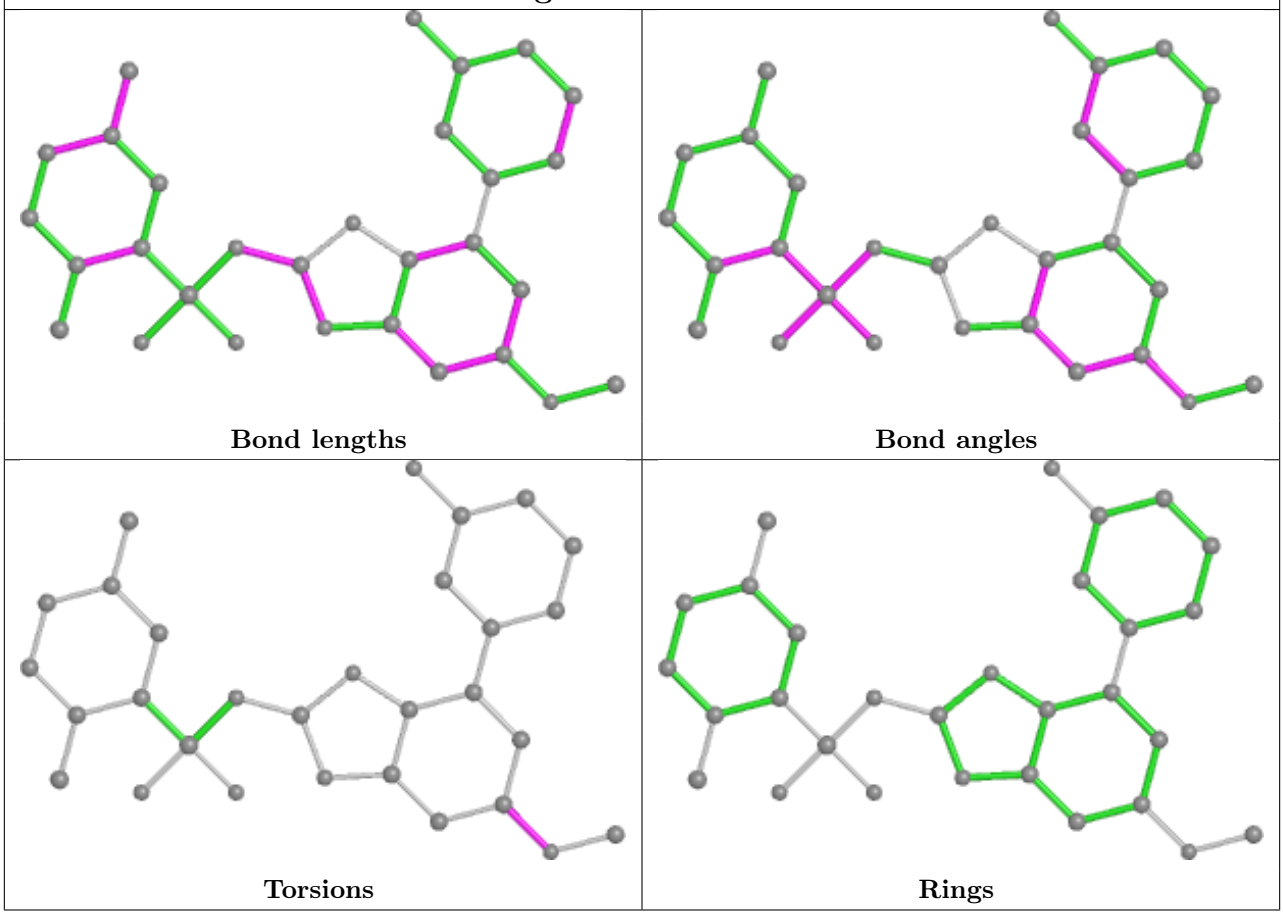
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	901	870	7	0
2	D	801	870	1	0
2	L	1001	870	3	0
2	A	701	870	7	0

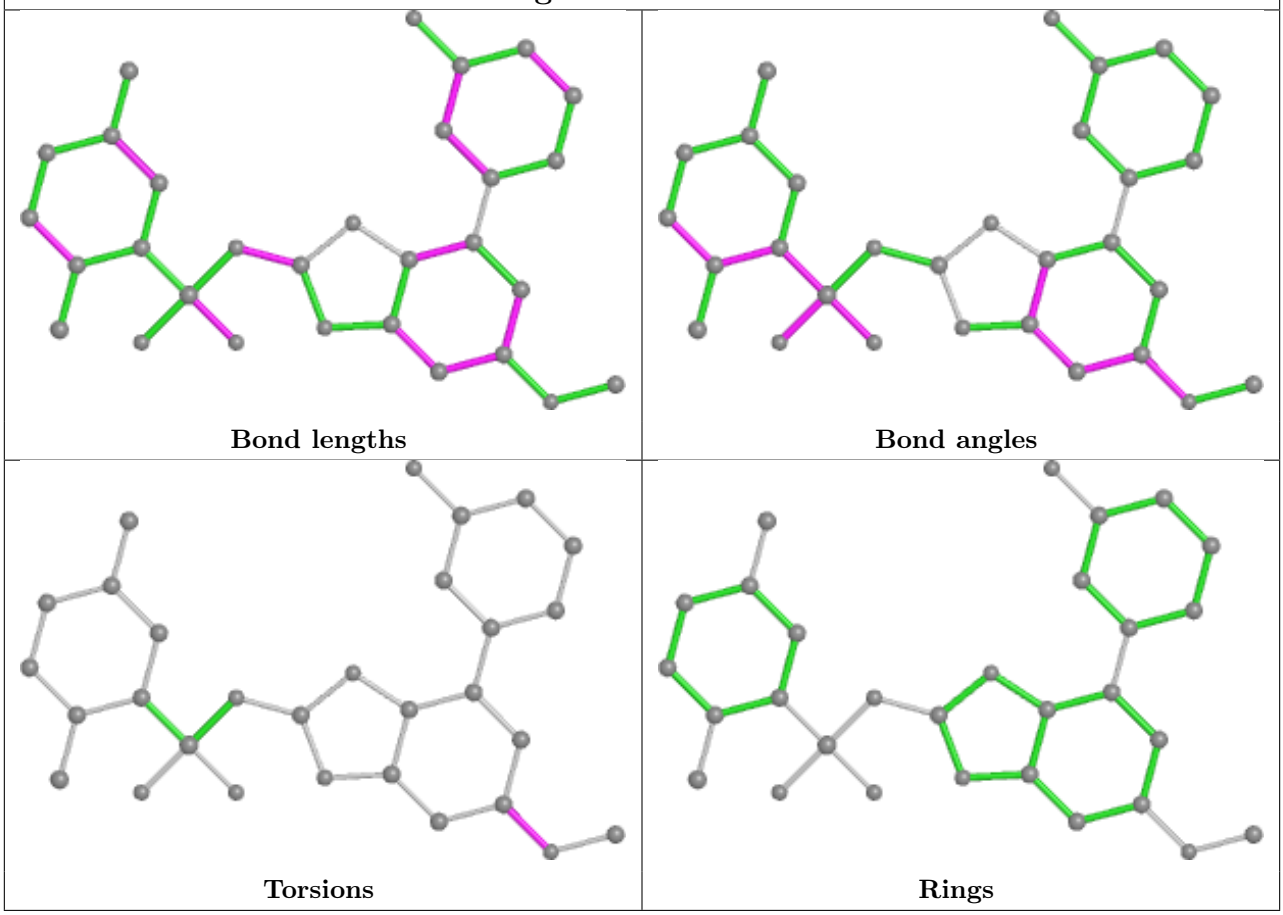
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 870 H 901



Ligand 870 D 801



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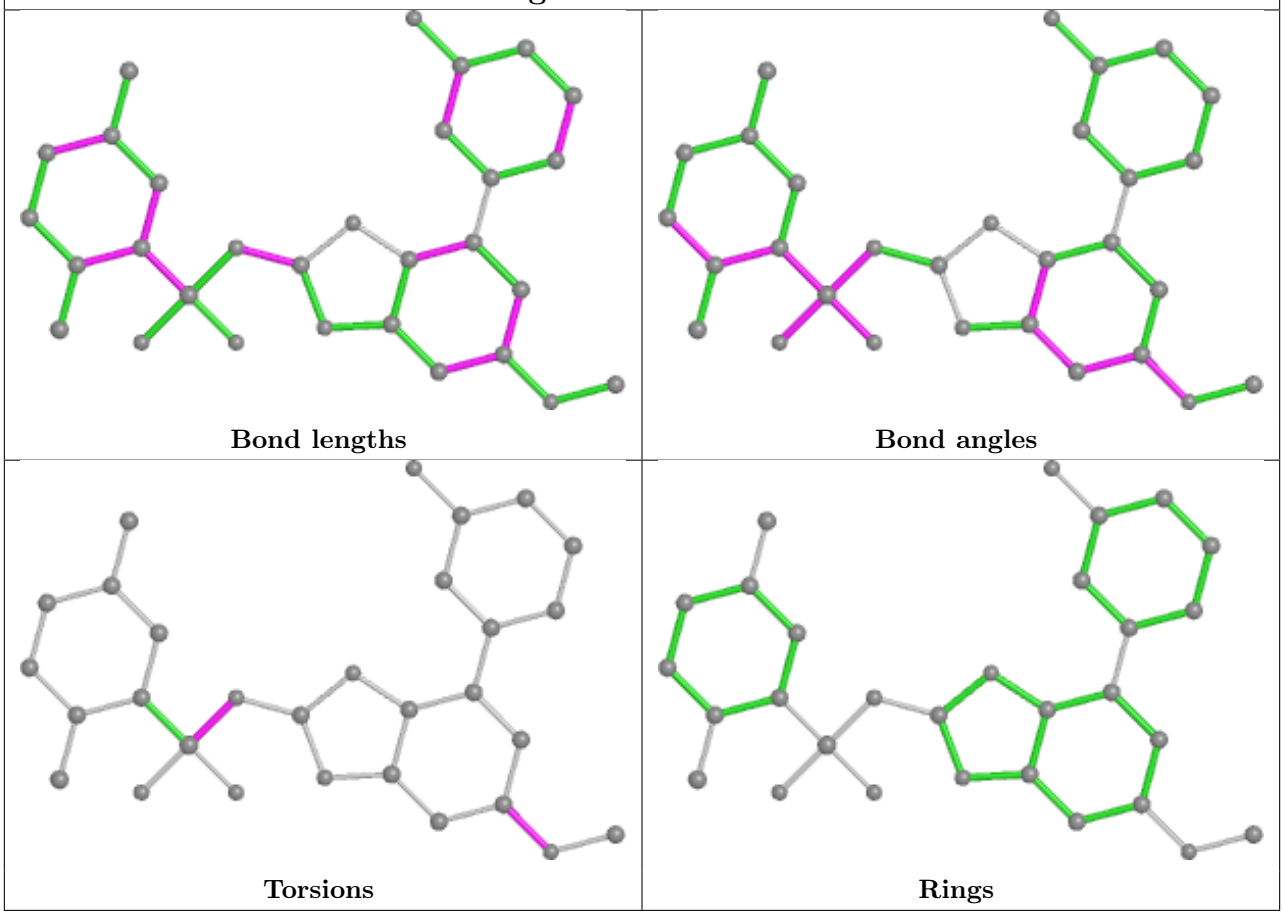
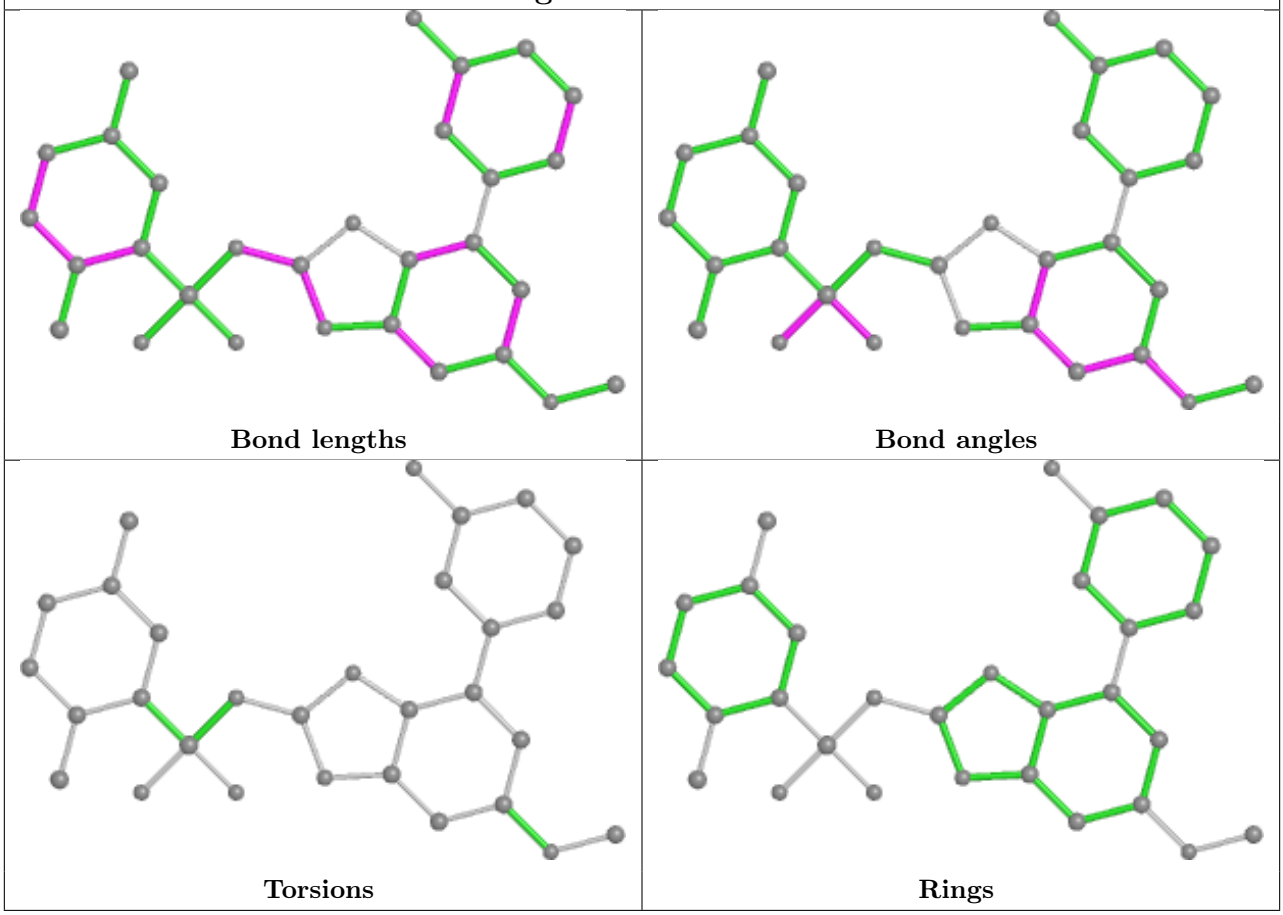


Ligand 870 A 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.