



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:56 am BST

PDB ID : 1CWQ  
Title : M INTERMEDIATE STRUCTURE OF THE WILD TYPE BACTERIORHODOPSIN IN COMBINATION WITH THE GROUND STATE STRUCTURE  
Authors : Sass, H.J.; Berendzen, J.; Neff, D.; Gessenich, R.; Ormos, P.; Bueldt, G.  
Deposited on : 1999-08-26  
Resolution : 2.25 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](mailto: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.

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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) : **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) : 2.11

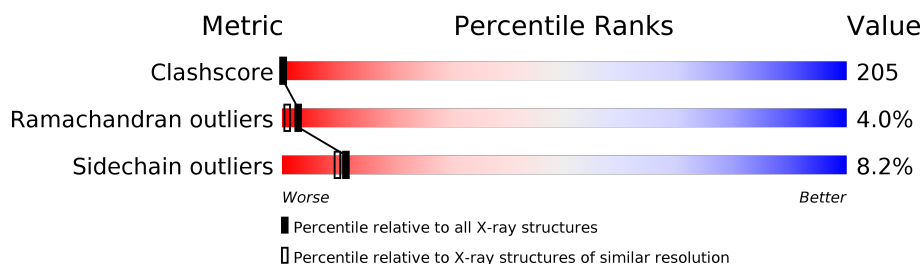
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	
1	B	248	

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
2	RET	A	601	-	-	X	-
2	RET	B	601	-	-	X	-
3	UND	A	1604	-	-	X	-
3	UND	A	604	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UND	B	1616	-	-	X	-
3	UND	B	614	-	-	X	-
4	OCT	A	1605	-	-	X	-
4	OCT	A	1621	-	-	X	-
4	OCT	A	1623	-	-	X	-
4	OCT	A	623	-	-	X	-
4	OCT	B	1607	-	-	X	-
4	OCT	B	1609	-	-	X	-
4	OCT	B	1613	-	-	X	-
4	OCT	B	1618	-	-	X	-
4	OCT	B	607	-	-	X	-
4	OCT	B	609	-	-	X	-
4	OCT	B	618	-	-	X	-
4	OCT	B	621	-	-	X	-
5	HEX	A	1606	-	-	X	-
5	HEX	A	1610	-	-	X	-
5	HEX	A	1622	-	-	X	-
5	HEX	A	606	-	-	X	-
5	HEX	A	620	-	-	X	-
5	HEX	B	1620	-	-	X	-
5	HEX	B	622	-	-	X	-
6	TRD	A	1615	-	-	X	-
6	TRD	B	611	-	-	X	-
6	TRD	B	615	-	-	X	-

## 2 Entry composition [i](#)

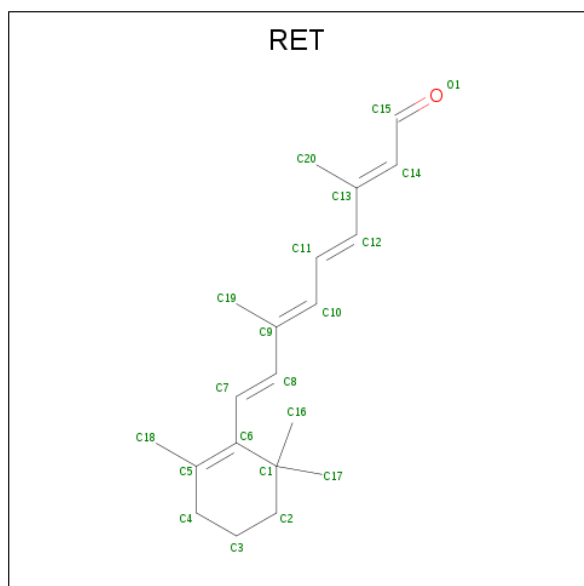
There are 7 unique types of molecules in this entry. The entry contains 4230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BACTERIORHODOPSIN ("M" STATE INTERMEDIATE IN COMBINATION WITH GROUND STATE).

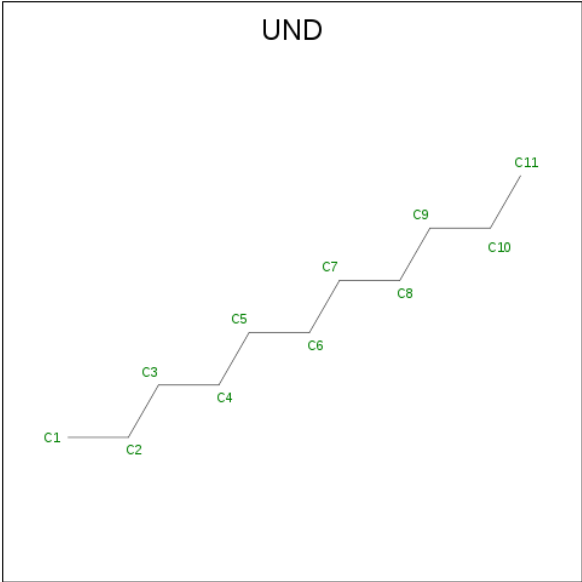
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1835	1228	280	318	9			
1	B	238	Total	C	N	O	S	0	0	0
			1835	1228	280	318	9			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



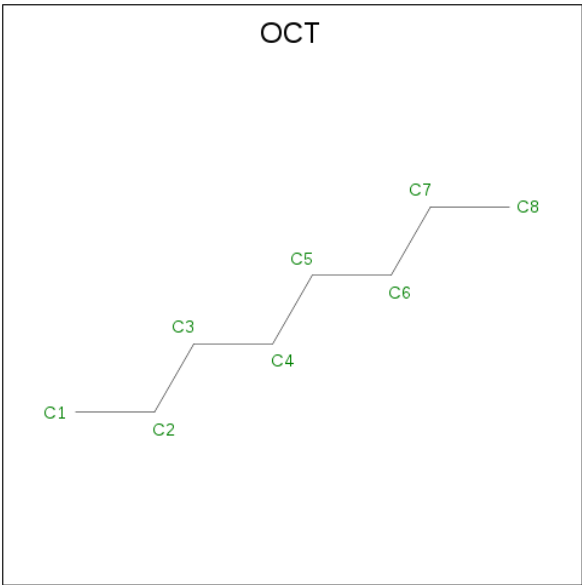
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		

- Molecule 3 is UNDECANE (three-letter code: UND) (formula: C<sub>11</sub>H<sub>24</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 11 11	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 11 11	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 11 11	0	0

- Molecule 4 is N-OCTANE (three-letter code: OCT) (formula: C<sub>8</sub>H<sub>18</sub>).



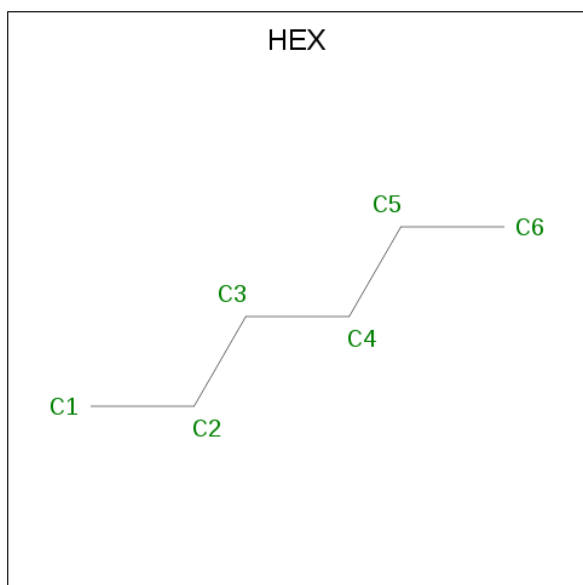
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 8 8	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 8 8	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 8 8	0	0
4	B	1	Total C 8 8	0	0

- Molecule 5 is HEXANE (three-letter code: HEX) (formula: C<sub>6</sub>H<sub>14</sub>).



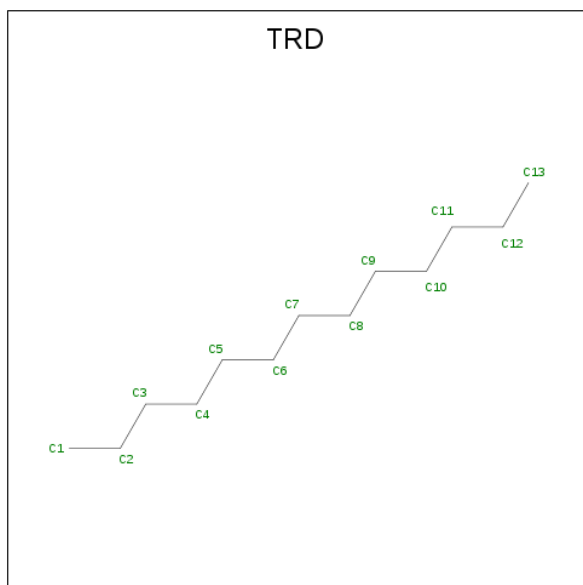
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 6 6	0	0
5	B	1	Total C 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C 6 6	0	0
5	B	1	Total C 6 6	0	0
5	B	1	Total C 6 6	0	0

- Molecule 6 is TRIDECANE (three-letter code: TRD) (formula:  $C_{13}H_{28}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 13 13	0	0
6	A	1	Total C 13 13	0	0
6	A	1	Total C 13 13	0	0
6	B	1	Total C 13 13	0	0
6	B	1	Total C 13 13	0	0
6	B	1	Total C 13 13	0	0

- Molecule 7 is water.



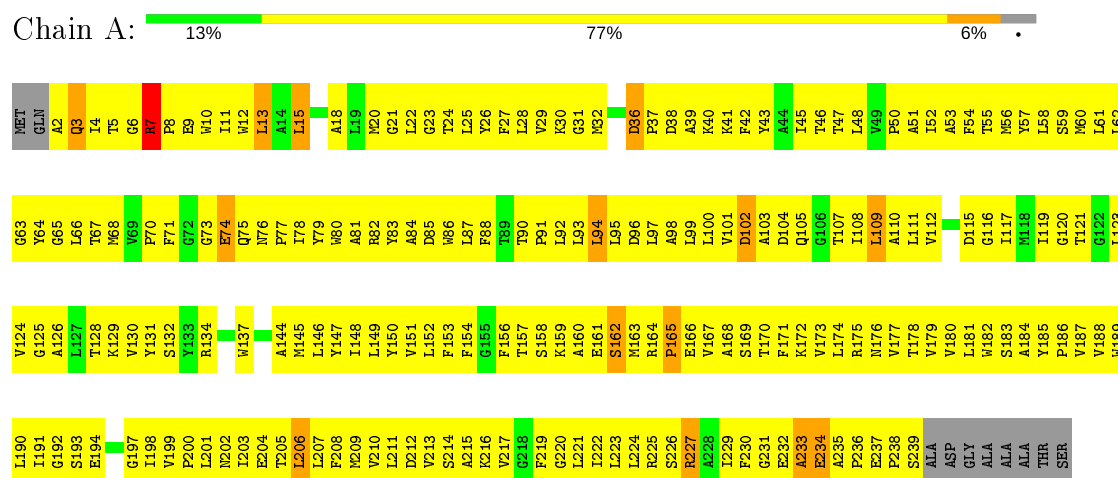
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	79	Total 79	O 79	0	0
7	B	75	Total 75	O 75	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: BACTERIORHODOPSIN ("M" STATE INTERMEDIATE IN COMBINATION WITH GROUND STATE)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.08 Å 61.08 Å 110.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	13.00 – 2.25	Depositor
% Data completeness (in resolution range)	97.5 (13.00-2.25)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	8.20	Depositor
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.167 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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: UND, HEX, TRD, RET, OCT

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	0.37	0/1885	0.53	0/2576
1	B	0.46	0/1885	0.66	0/2576
All	All	0.41	0/3770	0.60	0/5152

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	43	TYR	Sidechain

### 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	1835	0	1706	1222	0
1	B	1835	0	1721	1347	0
2	A	20	0	20	9	0
2	B	20	0	21	11	0
3	A	44	0	49	33	0
3	B	44	0	49	17	0
4	A	56	0	66	42	0
4	B	72	0	112	96	0
5	A	48	0	55	53	0
5	B	24	0	31	31	0
6	A	39	0	46	11	0
6	B	39	0	50	28	0
7	A	79	0	0	39	0
7	B	75	0	0	53	0
All	All	4230	0	3926	1634	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 205.

All (1634) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HG3	1:B:74:GLU:CG	1.23	1.64
4:A:623:OCT:C8	4:A:1623:OCT:H83	1.18	1.61
4:A:623:OCT:H82	4:A:1623:OCT:C8	1.15	1.61
1:A:153:PHE:CD1	1:B:175:ARG:HD2	1.26	1.60
1:A:74:GLU:CG	1:B:74:GLU:CG	1.81	1.58
1:A:45:ILE:CD1	1:B:95:LEU:CD2	1.74	1.58
4:B:609:OCT:H41	4:B:1609:OCT:C4	1.35	1.56
4:B:618:OCT:C7	4:B:1618:OCT:H72	1.36	1.56
1:A:161:GLU:HA	1:B:161:GLU:CG	1.34	1.54
1:A:74:GLU:CG	1:B:74:GLU:HG2	1.33	1.54
1:A:165:PRO:CG	1:B:161:GLU:HA	1.11	1.53
1:A:45:ILE:HD13	1:B:95:LEU:CD2	1.08	1.53
1:A:165:PRO:HG3	1:B:161:GLU:CA	1.35	1.53
1:A:161:GLU:C	1:B:161:GLU:HB2	1.26	1.52
1:A:227:ARG:CZ	1:B:238:PRO:HA	1.37	1.52
1:A:153:PHE:CE1	1:B:175:ARG:NE	1.77	1.50
1:A:161:GLU:CA	1:B:161:GLU:CB	1.84	1.50
1:A:161:GLU:HA	1:B:161:GLU:CB	1.40	1.46
1:B:48:LEU:CD2	6:B:611:TRD:H111	1.45	1.45
1:A:28:LEU:HD12	1:B:28:LEU:CD2	1.32	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LYS:HB2	1:B:159:LYS:CB	1.30	1.44
1:A:28:LEU:CD1	1:B:28:LEU:HD13	1.37	1.44
1:A:153:PHE:CE1	1:B:175:ARG:CD	1.98	1.44
4:B:618:OCT:H71	4:B:1618:OCT:C7	1.47	1.44
4:B:609:OCT:C2	4:B:1609:OCT:H22	1.46	1.43
1:A:201:LEU:CD1	1:B:204:GLU:OE2	1.68	1.41
5:A:620:HEX:H63	5:B:1620:HEX:C6	1.30	1.41
1:A:165:PRO:HB3	1:B:161:GLU:N	1.28	1.40
5:A:1622:HEX:C6	5:B:622:HEX:H63	1.11	1.40
1:A:28:LEU:HD13	1:B:28:LEU:CD1	1.18	1.39
1:A:45:ILE:CD1	1:B:95:LEU:HD21	1.41	1.39
4:A:1621:OCT:H12	4:B:621:OCT:C3	1.16	1.39
3:A:604:UND:C9	3:A:1604:UND:H91	1.33	1.39
1:A:74:GLU:OE2	1:B:74:GLU:CG	1.72	1.36
3:A:604:UND:H82	3:A:1604:UND:C10	1.50	1.36
1:A:153:PHE:HE1	1:B:175:ARG:NE	1.12	1.35
4:B:609:OCT:H41	4:B:1609:OCT:C3	1.53	1.35
1:A:74:GLU:CG	1:B:74:GLU:CB	2.03	1.34
1:A:164:ARG:O	1:B:159:LYS:CD	1.76	1.33
1:B:48:LEU:HD23	6:B:611:TRD:C11	1.49	1.33
1:A:161:GLU:CA	1:B:161:GLU:HB2	1.51	1.33
4:B:609:OCT:C4	4:B:1609:OCT:C4	2.05	1.32
5:A:620:HEX:C6	5:B:1620:HEX:H62	1.23	1.32
1:A:176:ASN:N	1:B:173:VAL:O	1.57	1.32
4:B:609:OCT:H41	4:B:1609:OCT:C5	1.59	1.31
1:A:153:PHE:CD1	1:B:175:ARG:CD	2.12	1.31
1:A:181:LEU:O	1:B:184:ALA:HB3	1.31	1.30
1:A:74:GLU:CD	1:B:74:GLU:CG	2.00	1.30
1:A:74:GLU:CD	1:B:74:GLU:HG2	1.47	1.30
1:A:164:ARG:O	1:B:159:LYS:HD2	1.17	1.29
4:B:609:OCT:C8	4:B:1609:OCT:H83	1.61	1.29
1:A:222:ILE:HD13	3:A:1604:UND:C11	1.60	1.29
4:A:1621:OCT:C1	4:B:621:OCT:H32	0.96	1.29
4:B:609:OCT:H21	4:B:1609:OCT:C2	1.62	1.28
1:A:68:MET:SD	1:B:77:PRO:HG3	1.75	1.27
1:A:159:LYS:C	1:B:160:ALA:HA	1.54	1.27
1:B:48:LEU:CD2	6:B:611:TRD:C12	2.10	1.27
1:A:74:GLU:CD	1:B:74:GLU:CB	2.03	1.26
1:A:160:ALA:N	1:B:160:ALA:HA	1.51	1.25
1:A:227:ARG:CB	1:B:236:PRO:O	1.84	1.25
6:A:1615:TRD:C11	6:B:615:TRD:H111	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:CD2	1:B:99:LEU:HD13	1.65	1.25
4:B:618:OCT:C7	4:B:1618:OCT:C7	2.08	1.25
1:A:87:LEU:HD11	5:A:1610:HEX:C1	1.66	1.24
1:A:28:LEU:CD1	1:B:28:LEU:HD22	1.52	1.24
1:A:45:ILE:CD1	1:B:95:LEU:HD22	1.50	1.24
1:B:48:LEU:HD21	6:B:611:TRD:C12	1.65	1.24
1:A:159:LYS:CA	1:B:159:LYS:CG	2.13	1.23
1:A:239:SER:CA	1:B:239:SER:HA	1.68	1.23
1:A:227:ARG:CZ	1:B:238:PRO:CA	2.17	1.23
1:A:91:PRO:HG3	1:B:115:ASP:OD2	1.36	1.23
4:B:618:OCT:C6	4:B:1618:OCT:C7	2.14	1.23
6:A:1615:TRD:H112	6:B:615:TRD:C11	1.69	1.23
1:A:206:LEU:C	1:B:206:LEU:HD13	1.59	1.22
1:A:28:LEU:CD1	1:B:28:LEU:CD1	1.95	1.22
4:B:618:OCT:H22	5:B:1620:HEX:C6	1.67	1.22
1:A:219:PHE:CE1	1:B:223:LEU:HD23	1.74	1.22
1:A:164:ARG:CG	1:B:159:LYS:HA	1.69	1.22
1:A:165:PRO:CG	1:B:161:GLU:CA	2.01	1.21
1:A:227:ARG:HB3	1:B:236:PRO:O	1.07	1.21
1:B:48:LEU:HD21	6:B:611:TRD:C11	1.60	1.21
4:B:613:OCT:C5	4:B:1613:OCT:H51	1.44	1.21
4:B:609:OCT:C8	4:B:1609:OCT:C8	2.19	1.20
4:A:623:OCT:C7	4:A:1623:OCT:H83	1.70	1.20
5:A:606:HEX:C1	5:A:1606:HEX:H13	1.55	1.20
1:A:165:PRO:CB	1:B:161:GLU:HA	1.70	1.20
1:B:48:LEU:CD2	6:B:611:TRD:H121	1.69	1.19
1:A:153:PHE:CE1	1:B:175:ARG:HD2	1.65	1.19
1:A:227:ARG:NH1	1:B:238:PRO:HA	1.57	1.19
1:A:161:GLU:CA	1:B:161:GLU:HG3	1.55	1.19
1:A:94:LEU:HD13	1:B:94:LEU:CD1	1.60	1.18
1:A:87:LEU:CG	5:A:1610:HEX:H11	1.72	1.18
1:B:82:ARG:HG3	7:B:716:HOH:O	1.41	1.18
1:A:159:LYS:CA	1:B:159:LYS:HG3	1.63	1.18
1:A:206:LEU:O	1:B:210:VAL:HG23	1.42	1.18
1:A:165:PRO:CB	1:B:161:GLU:H	1.57	1.17
1:A:223:LEU:CD2	1:B:223:LEU:HD22	1.76	1.16
4:B:618:OCT:H71	4:B:1618:OCT:C8	1.75	1.16
1:A:229:ILE:HD13	1:B:229:ILE:HD11	1.19	1.16
4:B:618:OCT:C2	5:B:1620:HEX:H63	1.76	1.16
1:A:161:GLU:C	1:B:161:GLU:CB	2.01	1.16
1:A:78:ILE:HG12	1:B:76:ASN:O	1.44	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:CA	1:B:174:LEU:HD12	1.74	1.16
5:A:1622:HEX:H13	5:B:622:HEX:C1	1.60	1.16
1:A:204:GLU:CD	1:B:204:GLU:OE1	1.84	1.16
1:A:219:PHE:CD1	1:B:223:LEU:HD23	1.79	1.15
1:B:48:LEU:CG	6:B:611:TRD:H121	1.75	1.15
1:A:94:LEU:CD1	1:B:94:LEU:CD1	2.06	1.15
1:A:95:LEU:CD2	1:B:99:LEU:CD1	2.24	1.15
1:A:165:PRO:CB	1:B:161:GLU:N	2.11	1.14
5:A:1622:HEX:C1	5:B:622:HEX:C1	2.23	1.14
1:A:182:TRP:CE2	2:B:601:RET:H202	1.81	1.14
1:A:233:ALA:O	1:B:234:GLU:HB3	1.43	1.14
1:A:169:SER:OG	1:B:169:SER:CB	1.94	1.13
1:A:204:GLU:OE1	1:B:204:GLU:CG	1.78	1.13
1:A:239:SER:HB2	1:B:239:SER:C	1.69	1.13
1:A:74:GLU:O	1:B:70:PRO:HA	1.48	1.13
4:B:609:OCT:C4	4:B:1609:OCT:H42	1.79	1.13
1:A:204:GLU:CD	1:B:204:GLU:CD	2.01	1.13
1:A:3:GLN:NE2	1:B:3:GLN:OE1	1.57	1.12
1:A:171:PHE:HA	1:B:174:LEU:CD1	1.78	1.12
1:A:164:ARG:HG3	1:B:159:LYS:HA	1.14	1.12
1:A:165:PRO:HD3	1:B:162:SER:H	1.10	1.12
6:A:1615:TRD:C11	6:B:615:TRD:C11	2.26	1.12
1:A:166:GLU:CG	1:B:234:GLU:HA	1.78	1.12
1:A:74:GLU:HG3	1:B:74:GLU:HG3	1.19	1.12
1:A:74:GLU:OE2	1:B:74:GLU:OE1	1.65	1.12
5:A:1622:HEX:H61	5:B:622:HEX:C6	1.73	1.11
1:A:95:LEU:HD23	1:B:99:LEU:HD13	1.19	1.11
1:A:173:VAL:HG11	3:A:1604:UND:H111	1.32	1.11
4:A:623:OCT:C7	4:A:1623:OCT:C8	2.26	1.11
1:A:165:PRO:CB	1:B:161:GLU:CA	2.28	1.11
5:A:620:HEX:H63	5:B:1620:HEX:H63	1.15	1.11
1:A:153:PHE:CZ	1:B:153:PHE:CE2	2.23	1.11
1:A:225:ARG:HH21	1:B:225:ARG:NE	1.49	1.11
1:A:74:GLU:OE2	1:B:74:GLU:CD	1.88	1.10
5:A:606:HEX:H13	5:A:1606:HEX:C1	1.64	1.10
1:A:160:ALA:N	1:B:160:ALA:CA	2.14	1.10
4:B:609:OCT:H81	4:B:1609:OCT:H83	1.16	1.09
1:A:167:VAL:HB	1:B:166:GLU:HB3	1.10	1.09
1:A:223:LEU:HD22	1:B:223:LEU:HD22	1.11	1.09
1:A:173:VAL:HG11	3:A:1604:UND:C11	1.82	1.09
1:A:225:ARG:NH2	1:B:225:ARG:NE	1.99	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LYS:CB	1:B:159:LYS:HG2	1.57	1.09
1:A:209:MET:SD	1:B:15:LEU:HD12	1.92	1.08
4:A:623:OCT:H81	4:A:1623:OCT:H83	1.28	1.08
1:A:134:ARG:CG	1:B:128:THR:HB	1.82	1.08
1:A:94:LEU:HD13	1:B:94:LEU:HD12	1.17	1.08
1:A:215:ALA:CA	1:B:181:LEU:HD11	1.82	1.08
1:A:166:GLU:OE1	1:B:234:GLU:HB2	1.53	1.08
1:A:28:LEU:CD1	1:B:28:LEU:CD2	2.05	1.07
1:A:161:GLU:HA	1:B:161:GLU:CA	1.84	1.07
5:A:620:HEX:H62	1:B:187:VAL:HG22	1.36	1.07
1:A:66:LEU:HD11	1:B:77:PRO:HB3	1.32	1.07
1:A:229:ILE:HD13	1:B:229:ILE:CD1	1.77	1.07
1:A:239:SER:HA	1:B:239:SER:HA	1.31	1.07
1:A:41:LYS:O	1:B:45:ILE:HD13	1.52	1.07
3:A:604:UND:H91	3:A:1604:UND:H91	1.36	1.07
1:A:166:GLU:HG2	1:B:234:GLU:CA	1.84	1.07
1:A:233:ALA:CB	1:B:234:GLU:OE1	2.03	1.07
1:A:101:VAL:HB	1:B:163:MET:CA	1.84	1.07
1:A:73:GLY:CA	1:B:73:GLY:HA2	1.81	1.07
1:A:169:SER:H	1:B:167:VAL:C	1.42	1.06
1:A:161:GLU:CA	1:B:161:GLU:CG	1.95	1.06
1:A:167:VAL:CB	1:B:166:GLU:HB3	1.49	1.06
1:A:90:THR:O	1:B:94:LEU:HD13	1.54	1.06
1:A:91:PRO:HD3	1:B:90:THR:OG1	1.55	1.06
1:A:169:SER:OG	1:B:169:SER:HB3	1.09	1.05
1:A:215:ALA:HA	1:B:181:LEU:HD11	1.34	1.05
1:A:161:GLU:CA	1:B:161:GLU:N	2.14	1.05
1:A:175:ARG:HD3	1:B:171:PHE:CE2	1.91	1.05
1:A:83:TYR:O	1:B:87:LEU:HB2	1.57	1.05
4:A:623:OCT:H71	4:A:1605:OCT:C1	1.86	1.05
1:A:219:PHE:CE1	1:B:223:LEU:CD2	2.39	1.04
1:A:7:ARG:N	1:B:8:PRO:CD	2.16	1.04
1:B:48:LEU:HD21	6:B:611:TRD:H121	1.26	1.04
5:A:1622:HEX:H61	5:B:622:HEX:H62	1.39	1.04
1:A:164:ARG:HG3	1:B:159:LYS:CA	1.87	1.04
4:B:613:OCT:H52	4:B:1613:OCT:H51	1.39	1.04
1:A:167:VAL:CB	1:B:166:GLU:CB	2.24	1.04
3:A:604:UND:H32	3:A:1604:UND:H32	1.38	1.04
1:A:207:LEU:N	1:B:206:LEU:HD13	1.71	1.04
1:A:94:LEU:HD12	1:B:97:LEU:CD1	1.86	1.04
4:A:623:OCT:H71	4:A:1605:OCT:H11	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD22	1:B:43:TYR:CE2	1.92	1.03
1:A:178:THR:HG23	1:B:182:TRP:NE1	1.72	1.03
1:A:66:LEU:HD11	1:B:77:PRO:CB	1.87	1.03
1:A:159:LYS:CE	1:B:159:LYS:CD	2.27	1.03
4:B:609:OCT:C4	4:B:1609:OCT:C3	2.31	1.03
1:A:166:GLU:HG2	1:B:234:GLU:HA	1.05	1.03
1:A:182:TRP:NE1	2:B:601:RET:C20	2.22	1.02
5:A:1622:HEX:H13	5:B:622:HEX:H11	1.06	1.02
1:A:179:VAL:HG22	1:B:149:LEU:HD22	1.35	1.02
1:A:215:ALA:CB	1:B:181:LEU:HD13	1.88	1.02
1:A:15:LEU:HD13	1:B:15:LEU:CD1	1.85	1.02
1:A:101:VAL:HB	1:B:163:MET:HA	1.40	1.02
1:A:215:ALA:CB	1:B:181:LEU:CD1	2.36	1.02
1:A:87:LEU:CD1	5:A:1610:HEX:C1	2.38	1.02
1:A:151:VAL:HG11	1:B:111:LEU:HD21	1.38	1.01
1:A:227:ARG:NH1	1:B:227:ARG:NE	1.96	1.01
1:A:157:THR:HB	1:B:164:ARG:HG2	1.43	1.01
3:A:604:UND:C8	3:A:1604:UND:C10	2.07	1.01
4:B:618:OCT:C7	4:B:1618:OCT:C8	2.36	1.01
1:A:187:VAL:O	1:B:191:ILE:HG12	1.60	1.01
1:A:45:ILE:HD11	1:B:95:LEU:HD21	1.02	1.01
4:B:609:OCT:C3	4:B:1609:OCT:H22	1.89	1.01
1:A:41:LYS:O	1:B:45:ILE:CD1	2.07	1.01
1:A:159:LYS:HB2	1:B:159:LYS:HG2	1.14	1.01
1:A:74:GLU:O	1:B:70:PRO:CA	2.09	1.01
1:A:83:TYR:HB2	1:B:123:LEU:HD22	1.41	1.01
1:A:156:PHE:CZ	1:B:101:VAL:HG21	1.95	1.01
1:A:169:SER:N	1:B:167:VAL:C	2.04	1.01
1:A:215:ALA:HB2	1:B:181:LEU:CD1	1.89	1.01
1:A:173:VAL:CG1	3:A:1604:UND:H102	1.91	1.01
1:A:74:GLU:CG	1:B:74:GLU:CA	1.77	1.00
1:A:169:SER:N	1:B:167:VAL:O	1.95	1.00
6:A:1615:TRD:C10	6:B:615:TRD:C11	2.22	1.00
1:A:75:GLN:NE2	1:B:70:PRO:HB3	1.76	1.00
1:A:166:GLU:C	1:B:165:PRO:O	1.83	1.00
5:A:620:HEX:H11	4:A:1617:OCT:H31	1.40	0.99
1:A:134:ARG:HG2	1:B:128:THR:HB	1.01	0.99
1:B:94:LEU:HD11	1:B:182:TRP:CH2	1.97	0.99
1:A:173:VAL:O	1:B:177:VAL:HG23	1.63	0.99
1:A:190:LEU:O	1:B:196:ALA:N	1.95	0.99
1:A:82:ARG:CZ	7:A:1716:HOH:O	2.09	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PHE:HA	1:B:174:LEU:HD12	1.43	0.99
1:A:164:ARG:CG	1:B:159:LYS:CA	2.41	0.99
1:A:11:ILE:HD12	1:B:11:ILE:HD13	1.44	0.99
1:A:159:LYS:CD	1:B:159:LYS:HG2	1.82	0.99
1:A:68:MET:SD	1:B:5:THR:HG22	2.02	0.99
1:A:82:ARG:NH2	7:A:1716:HOH:O	1.96	0.98
1:A:87:LEU:HG	5:A:1610:HEX:H11	1.44	0.98
1:A:68:MET:HE1	1:B:5:THR:HB	1.45	0.98
3:A:604:UND:H32	3:A:1604:UND:C3	1.42	0.98
4:B:618:OCT:H62	4:B:1618:OCT:C8	1.93	0.98
1:A:74:GLU:CD	1:B:74:GLU:CA	2.26	0.98
4:A:1621:OCT:H82	4:B:621:OCT:H71	1.44	0.98
1:B:94:LEU:HD11	1:B:182:TRP:HH2	1.25	0.98
1:A:153:PHE:HE1	1:B:175:ARG:CZ	1.76	0.98
5:B:619:HEX:C6	5:B:1619:HEX:C6	2.42	0.98
1:A:156:PHE:CE2	1:B:101:VAL:HG11	1.99	0.98
1:A:159:LYS:C	1:B:160:ALA:CA	2.29	0.97
1:A:181:LEU:O	1:B:184:ALA:CB	2.12	0.97
1:A:74:GLU:CD	1:B:74:GLU:HA	1.84	0.97
1:A:178:THR:HG23	1:B:182:TRP:CD1	1.98	0.97
1:B:48:LEU:HD21	6:B:611:TRD:C10	1.95	0.97
1:A:57:TYR:OH	1:B:209:MET:HA	1.63	0.97
1:A:223:LEU:CD2	1:B:223:LEU:CD2	2.33	0.97
1:A:209:MET:O	1:B:209:MET:HE3	1.65	0.97
1:A:159:LYS:CB	1:B:159:LYS:CB	1.98	0.96
1:A:74:GLU:OE2	1:B:74:GLU:CB	2.08	0.96
1:A:223:LEU:HD22	1:B:223:LEU:CD2	1.95	0.96
1:A:159:LYS:CE	1:B:159:LYS:HG2	1.95	0.96
1:A:227:ARG:NH1	1:B:238:PRO:CA	2.22	0.96
1:B:48:LEU:CG	6:B:611:TRD:C12	2.41	0.96
1:B:203:ILE:O	1:B:207:LEU:HG	1.65	0.96
1:A:153:PHE:CE1	1:B:153:PHE:CE2	2.32	0.96
6:A:1615:TRD:H112	6:B:615:TRD:H111	0.97	0.96
1:A:101:VAL:CG1	1:B:163:MET:O	2.13	0.96
1:A:170:THR:OG1	1:B:226:SER:OG	1.82	0.96
1:A:82:ARG:NH2	7:A:1713:HOH:O	1.88	0.96
1:A:87:LEU:CD1	5:A:1610:HEX:H11	1.95	0.96
1:A:223:LEU:HD11	1:B:229:ILE:HG21	1.45	0.96
1:A:161:GLU:CA	1:B:161:GLU:CA	2.43	0.95
1:A:83:TYR:CD2	1:B:123:LEU:HD13	2.01	0.95
1:A:166:GLU:HG3	1:B:166:GLU:OE2	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:607:OCT:C1	4:B:1607:OCT:H11	1.45	0.95
1:A:64:TYR:CD1	1:B:64:TYR:C	2.36	0.95
1:A:159:LYS:HE3	1:B:159:LYS:HG2	1.49	0.95
1:A:222:ILE:CD1	3:A:1604:UND:C11	2.43	0.95
1:A:172:LYS:HB3	1:B:169:SER:O	1.66	0.95
1:A:204:GLU:OE1	1:B:204:GLU:HG2	1.14	0.95
4:B:609:OCT:H82	4:B:1609:OCT:C8	1.95	0.94
1:A:182:TRP:CE2	2:B:601:RET:C20	2.51	0.94
1:A:159:LYS:HE3	1:B:159:LYS:CG	1.97	0.94
1:A:164:ARG:NE	1:B:159:LYS:HB2	1.83	0.94
1:A:42:PHE:CD2	1:B:229:ILE:HB	2.02	0.94
1:A:206:LEU:C	1:B:206:LEU:CD1	2.31	0.94
4:A:1621:OCT:C8	4:B:621:OCT:H71	1.96	0.94
1:A:194:GLU:OE2	1:B:82:ARG:NH2	1.99	0.94
1:B:216:LYS:CE	7:B:710:HOH:O	2.15	0.94
1:A:11:ILE:HD12	1:B:11:ILE:CD1	1.97	0.93
1:A:175:ARG:HD3	1:B:171:PHE:CZ	2.02	0.93
1:A:163:MET:O	1:B:165:PRO:HD3	1.69	0.93
1:A:173:VAL:CG1	3:A:1604:UND:C11	2.46	0.93
4:B:618:OCT:H22	5:B:1620:HEX:H63	0.93	0.93
1:A:169:SER:HB3	1:B:167:VAL:CG1	1.98	0.93
5:A:1622:HEX:C1	5:B:622:HEX:H11	1.90	0.93
1:A:159:LYS:HA	1:B:159:LYS:HD2	1.51	0.93
1:A:68:MET:CE	1:B:77:PRO:HG3	1.99	0.93
1:A:197:GLY:HA2	1:B:193:SER:HA	1.51	0.93
4:B:609:OCT:C4	4:B:1609:OCT:C2	2.47	0.93
1:A:66:LEU:HD21	1:B:5:THR:HB	1.51	0.93
1:A:165:PRO:HD3	1:B:162:SER:N	1.84	0.92
1:A:182:TRP:HD1	1:B:181:LEU:HB3	1.33	0.92
5:A:1622:HEX:H63	5:B:622:HEX:C6	1.72	0.92
4:A:1621:OCT:H13	4:B:621:OCT:H32	1.51	0.92
1:B:48:LEU:CD2	6:B:611:TRD:C10	2.48	0.92
1:A:217:VAL:O	1:B:221:LEU:CD2	2.17	0.92
1:A:101:VAL:HG12	1:B:163:MET:O	1.68	0.92
4:B:618:OCT:H81	3:B:1616:UND:H113	1.48	0.92
4:B:618:OCT:H62	4:B:1618:OCT:H82	1.50	0.92
1:A:68:MET:HE1	1:B:5:THR:CG2	2.00	0.92
1:A:166:GLU:OE1	1:B:234:GLU:CB	2.18	0.92
4:B:609:OCT:H42	4:B:1609:OCT:H42	1.52	0.92
1:A:94:LEU:HD12	1:B:97:LEU:HD12	1.49	0.92
1:A:32:MET:CE	1:B:32:MET:CE	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:O	1:B:165:PRO:CD	2.17	0.91
1:A:84:ALA:O	1:B:88:PHE:HD2	1.51	0.91
1:A:201:LEU:HD12	1:B:204:GLU:OE2	0.74	0.91
1:A:85:ASP:OD1	1:B:85:ASP:C	2.08	0.91
1:B:48:LEU:HG	6:B:611:TRD:C12	1.99	0.91
5:A:1622:HEX:C6	5:B:622:HEX:H62	1.94	0.91
4:B:618:OCT:C6	4:B:1618:OCT:H72	1.87	0.91
1:A:224:LEU:HD22	1:B:43:TYR:CZ	2.06	0.90
1:A:235:ALA:H	1:B:234:GLU:H	1.16	0.90
1:A:66:LEU:HD21	1:B:5:THR:CB	2.01	0.90
1:B:201:LEU:HB3	7:B:1800:HOH:O	1.72	0.90
1:A:68:MET:CE	1:B:5:THR:CG2	2.48	0.90
1:A:201:LEU:HD12	1:B:204:GLU:CD	1.90	0.90
1:A:95:LEU:HD21	1:B:99:LEU:HD11	1.52	0.90
1:A:159:LYS:HE3	1:B:159:LYS:CD	1.99	0.90
1:A:46:THR:HG23	7:A:1724:HOH:O	1.70	0.90
1:A:64:TYR:CD1	1:B:64:TYR:O	2.25	0.90
1:A:150:TYR:CD2	1:B:150:TYR:O	2.25	0.90
1:A:165:PRO:HB3	1:B:161:GLU:CA	1.95	0.90
1:A:173:VAL:CG1	3:A:1604:UND:H111	2.01	0.90
1:A:158:SER:HB3	1:B:160:ALA:HB3	1.52	0.90
1:A:162:SER:HB3	1:B:160:ALA:HB3	1.54	0.89
1:B:232:GLU:CA	7:B:740:HOH:O	2.21	0.89
1:A:74:GLU:CG	1:B:74:GLU:HA	1.61	0.89
1:A:173:VAL:CG1	3:A:1604:UND:C10	2.51	0.89
1:A:4:ILE:CD1	1:B:3:GLN:NE2	2.36	0.89
1:A:227:ARG:HH11	1:B:227:ARG:NE	1.69	0.89
1:A:159:LYS:CE	1:B:159:LYS:CG	2.50	0.89
1:A:223:LEU:HD11	1:B:229:ILE:CG2	2.01	0.89
4:B:609:OCT:H41	4:B:1609:OCT:H31	1.52	0.89
1:B:80:TRP:CZ3	5:B:622:HEX:H31	2.06	0.89
1:A:154:PHE:CD1	1:B:153:PHE:HB3	2.07	0.89
1:A:210:VAL:HG22	5:A:606:HEX:H11	1.52	0.89
1:A:83:TYR:CB	1:B:123:LEU:HD22	2.01	0.89
1:A:79:TYR:CE1	1:B:66:LEU:HD22	2.07	0.89
1:A:233:ALA:HB1	1:B:234:GLU:OE1	1.69	0.89
1:A:134:ARG:NH1	1:B:126:ALA:O	2.04	0.89
4:B:618:OCT:H71	4:B:1618:OCT:H72	0.91	0.89
1:A:166:GLU:O	1:B:165:PRO:O	1.90	0.89
4:A:1621:OCT:H13	4:B:621:OCT:H12	1.53	0.89
1:A:169:SER:HB3	1:B:167:VAL:HG12	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASP:OD2	7:B:850:HOH:O	1.90	0.88
5:A:606:HEX:C1	5:A:1606:HEX:C1	2.11	0.88
4:A:623:OCT:C7	4:A:1605:OCT:H11	2.02	0.88
1:A:153:PHE:CE2	1:B:179:VAL:CG2	2.56	0.88
1:A:68:MET:HE1	1:B:5:THR:CB	2.02	0.88
1:B:94:LEU:HA	1:B:97:LEU:HD12	1.56	0.88
1:A:103:ALA:HB2	1:B:101:VAL:CG2	2.03	0.88
1:B:7:ARG:NE	7:B:816:HOH:O	2.04	0.88
1:A:77:PRO:HD3	1:B:75:GLN:O	1.74	0.88
1:A:82:ARG:NH1	7:A:1713:HOH:O	2.05	0.88
1:A:150:TYR:CG	1:B:150:TYR:O	2.25	0.88
1:A:161:GLU:HA	1:B:161:GLU:N	1.85	0.88
1:A:239:SER:N	1:B:239:SER:HA	1.89	0.88
1:A:234:GLU:OE2	1:B:234:GLU:OE1	1.90	0.88
1:A:219:PHE:HE1	1:B:223:LEU:CD2	1.87	0.87
1:A:165:PRO:HG3	1:B:161:GLU:C	1.93	0.87
4:B:609:OCT:C4	4:B:1609:OCT:H51	1.66	0.87
1:A:95:LEU:HD21	1:B:99:LEU:CD1	2.04	0.87
1:A:194:GLU:OE1	7:A:1717:HOH:O	1.92	0.87
1:A:79:TYR:CD1	1:B:66:LEU:HD13	2.10	0.87
4:B:618:OCT:H81	3:B:1616:UND:C11	2.05	0.87
1:A:95:LEU:HD23	1:B:99:LEU:CD1	1.95	0.87
1:A:83:TYR:O	1:B:87:LEU:CB	2.22	0.87
1:A:161:GLU:CB	1:B:161:GLU:HB2	2.03	0.87
1:A:153:PHE:CD1	1:B:153:PHE:CZ	2.53	0.86
1:A:200:PRO:HD2	1:B:199:VAL:HG12	1.55	0.86
5:A:620:HEX:H61	5:B:1620:HEX:H62	0.90	0.86
1:B:45:ILE:HG12	1:B:95:LEU:HD22	1.55	0.86
1:A:232:GLU:OE1	1:B:232:GLU:OE1	1.91	0.86
1:A:215:ALA:HA	1:B:181:LEU:CD1	2.05	0.86
1:A:183:SER:O	1:B:187:VAL:HG23	1.75	0.86
1:A:67:THR:O	1:B:77:PRO:HA	1.75	0.86
1:A:94:LEU:CD1	1:B:94:LEU:HD12	1.84	0.86
4:B:618:OCT:C8	3:B:1616:UND:H113	2.04	0.86
1:B:31:GLY:HA3	7:B:864:HOH:O	1.76	0.86
1:B:98:ALA:HB1	1:B:108:ILE:HD11	1.55	0.86
1:A:224:LEU:HD12	1:B:27:PHE:CD1	2.11	0.86
1:A:189:TRP:NE1	1:B:83:TYR:OH	2.08	0.86
1:A:217:VAL:O	1:B:221:LEU:HD22	1.74	0.86
1:B:25:LEU:HA	1:B:28:LEU:HD12	1.55	0.85
1:A:209:MET:C	1:B:209:MET:HE3	1.96	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:O	1:B:94:LEU:CD1	2.24	0.85
1:A:166:GLU:HB3	1:B:166:GLU:CB	1.97	0.85
1:A:227:ARG:HH11	1:B:227:ARG:HE	1.21	0.85
1:A:164:ARG:HG2	1:B:159:LYS:HA	1.57	0.85
1:A:209:MET:SD	1:B:15:LEU:CD1	2.63	0.85
1:A:157:THR:HA	1:B:163:MET:CG	2.05	0.85
1:A:157:THR:HB	1:B:164:ARG:CG	2.06	0.85
1:A:164:ARG:HE	1:B:159:LYS:HB2	1.42	0.85
1:A:174:LEU:HD11	1:B:223:LEU:CB	2.06	0.85
1:A:130:VAL:HB	1:B:133:TYR:CD2	2.11	0.85
1:A:101:VAL:O	1:B:163:MET:HA	1.75	0.85
1:A:238:PRO:C	1:B:239:SER:N	2.16	0.85
1:A:158:SER:CB	1:B:160:ALA:HB3	2.06	0.85
1:A:97:LEU:HD21	1:B:174:LEU:HB3	1.58	0.84
4:B:607:OCT:C1	4:B:1607:OCT:H12	1.33	0.84
4:B:609:OCT:H21	4:B:1609:OCT:H22	0.87	0.84
1:A:74:GLU:OE2	1:B:74:GLU:HB3	1.78	0.84
1:A:74:GLU:CD	1:B:74:GLU:HB3	1.97	0.84
1:A:25:LEU:HD23	1:B:28:LEU:HD12	1.58	0.84
1:A:20:MET:HE1	1:B:216:LYS:HB2	1.58	0.84
1:A:111:LEU:HD11	1:B:156:PHE:CE1	2.12	0.84
1:A:153:PHE:HE2	1:B:179:VAL:CG2	1.90	0.84
1:A:22:LEU:HD22	1:B:22:LEU:N	1.91	0.84
1:B:48:LEU:HG	6:B:611:TRD:H121	1.56	0.84
1:A:178:THR:OG1	7:A:1721:HOH:O	1.95	0.84
1:A:221:LEU:HD22	1:B:27:PHE:HZ	1.43	0.84
1:A:173:VAL:HG13	3:A:1604:UND:H102	1.58	0.83
1:A:215:ALA:CA	1:B:181:LEU:CD1	2.56	0.83
4:B:618:OCT:C6	4:B:1618:OCT:H82	2.08	0.83
1:A:215:ALA:HB2	1:B:181:LEU:HD13	1.53	0.83
1:B:90:THR:O	1:B:94:LEU:HD13	1.78	0.83
1:A:134:ARG:HG2	1:B:128:THR:CB	1.97	0.83
1:A:206:LEU:O	1:B:206:LEU:HD22	1.78	0.83
1:A:238:PRO:C	1:B:239:SER:CA	2.47	0.83
1:A:94:LEU:HD12	1:B:97:LEU:HD11	1.60	0.83
1:B:216:LYS:HE2	7:B:710:HOH:O	1.74	0.83
1:A:163:MET:C	1:B:165:PRO:HD3	1.99	0.83
1:A:227:ARG:NH1	1:B:238:PRO:CB	2.42	0.82
1:A:74:GLU:OE1	7:A:1829:HOH:O	1.97	0.82
6:A:1615:TRD:C10	6:B:615:TRD:H111	1.97	0.82
1:B:138:TRP:HH2	4:B:618:OCT:C1	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:O	1:B:66:LEU:HD12	1.79	0.82
4:A:623:OCT:H72	4:A:1623:OCT:H83	1.60	0.82
1:A:71:PHE:HB3	1:B:129:LYS:HA	1.59	0.82
1:A:159:LYS:CE	1:B:159:LYS:HD3	2.09	0.82
3:A:604:UND:C9	3:A:1604:UND:H92	1.83	0.82
1:A:238:PRO:O	1:B:239:SER:CA	2.27	0.82
1:A:74:GLU:HA	7:B:820:HOH:O	1.78	0.82
1:B:22:LEU:HG	4:B:1613:OCT:H41	1.62	0.82
1:A:101:VAL:CB	1:B:163:MET:HA	2.09	0.82
7:A:743:HOH:O	1:B:11:ILE:HD11	1.77	0.82
1:B:29:VAL:HG21	3:B:614:UND:C1	2.10	0.82
1:A:173:VAL:O	1:B:177:VAL:CG2	2.27	0.81
1:A:217:VAL:HG11	5:A:608:HEX:H32	1.62	0.81
1:A:234:GLU:CD	1:B:234:GLU:OE1	2.09	0.81
1:A:45:ILE:H	1:B:45:ILE:HD12	1.45	0.81
1:A:159:LYS:HE3	1:B:164:ARG:NH2	1.94	0.81
4:A:623:OCT:H82	4:A:1623:OCT:H82	0.83	0.81
1:A:230:PHE:O	7:A:742:HOH:O	1.98	0.81
1:A:227:ARG:HG3	1:B:237:GLU:O	1.81	0.81
1:A:162:SER:N	1:B:161:GLU:C	1.98	0.81
1:A:204:GLU:OE2	1:B:204:GLU:OE1	1.96	0.81
1:A:103:ALA:HB2	1:B:101:VAL:HG23	1.60	0.81
1:A:161:GLU:O	1:B:161:GLU:HB2	1.80	0.81
1:A:66:LEU:O	7:A:1826:HOH:O	1.98	0.81
1:A:227:ARG:NE	1:B:238:PRO:HA	1.96	0.81
4:A:1621:OCT:H12	4:B:621:OCT:H31	1.58	0.81
1:A:7:ARG:CB	1:B:8:PRO:HD3	2.08	0.80
1:A:222:ILE:HD13	3:A:1604:UND:H111	1.64	0.80
1:A:161:GLU:HA	1:B:161:GLU:HG3	1.06	0.80
1:A:68:MET:CE	1:B:77:PRO:HB3	2.10	0.80
1:A:177:VAL:O	1:B:181:LEU:HB2	1.81	0.80
1:A:38:ASP:OD1	7:A:1745:HOH:O	2.00	0.80
1:A:159:LYS:HB3	1:B:159:LYS:HG3	0.81	0.80
1:A:229:ILE:CD1	1:B:229:ILE:CD1	2.50	0.80
1:A:224:LEU:N	1:B:223:LEU:HD12	1.91	0.80
1:A:61:LEU:O	1:B:61:LEU:HD12	1.80	0.80
1:A:158:SER:HB3	1:B:160:ALA:CB	2.11	0.80
1:A:221:LEU:HD22	1:B:27:PHE:CZ	2.16	0.80
4:B:609:OCT:C7	4:B:1609:OCT:H83	2.09	0.80
1:A:164:ARG:O	1:B:159:LYS:HD3	1.79	0.80
1:B:3:GLN:HB3	7:B:832:HOH:O	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:C	1:B:239:SER:HA	2.02	0.80
1:A:25:LEU:HA	1:B:28:LEU:HD12	1.64	0.79
1:A:76:ASN:HB2	1:B:69:VAL:O	1.82	0.79
1:A:68:MET:CE	1:B:77:PRO:CB	2.59	0.79
1:A:233:ALA:HB3	1:B:234:GLU:OE1	1.79	0.79
1:A:153:PHE:CE1	1:B:175:ARG:CZ	2.59	0.79
1:A:94:LEU:HD13	1:B:182:TRP:CZ2	2.18	0.79
1:B:48:LEU:HD21	6:B:611:TRD:H102	1.64	0.79
1:A:189:TRP:CD1	1:B:83:TYR:OH	2.35	0.79
1:A:170:THR:O	1:B:174:LEU:HG	1.81	0.79
1:A:160:ALA:N	1:B:160:ALA:CB	2.45	0.79
4:B:609:OCT:H41	4:B:1609:OCT:H51	1.35	0.79
1:A:234:GLU:C	1:B:234:GLU:OE2	2.18	0.79
4:A:623:OCT:C6	4:A:1605:OCT:H11	2.13	0.79
1:A:87:LEU:CD2	5:A:1610:HEX:H11	2.11	0.79
1:A:182:TRP:HA	1:B:185:TYR:HD1	1.45	0.79
1:A:80:TRP:CZ3	5:B:622:HEX:H31	2.16	0.79
1:A:215:ALA:CB	1:B:181:LEU:HD11	2.07	0.79
1:A:224:LEU:HB3	1:B:43:TYR:OH	1.83	0.79
1:A:98:ALA:HB2	1:B:156:PHE:HZ	1.45	0.79
1:A:203:ILE:O	1:B:207:LEU:HG	1.79	0.79
1:A:170:THR:CG2	1:B:226:SER:OG	2.30	0.78
1:A:123:LEU:HD21	5:A:1622:HEX:H22	1.65	0.78
1:A:154:PHE:CE1	1:B:153:PHE:HB3	2.17	0.78
1:A:20:MET:CE	1:B:216:LYS:HD3	2.13	0.78
4:B:618:OCT:C6	4:B:1618:OCT:C8	2.53	0.78
1:A:166:GLU:HG3	1:B:166:GLU:CD	2.04	0.78
1:A:161:GLU:C	1:B:161:GLU:CA	2.32	0.78
1:A:225:ARG:HH21	1:B:225:ARG:HE	1.28	0.78
1:A:4:ILE:HD13	1:B:4:ILE:CG1	2.14	0.78
1:A:166:GLU:HG2	1:B:166:GLU:HG2	1.65	0.78
4:B:609:OCT:C4	4:B:1609:OCT:H22	2.12	0.78
1:A:151:VAL:O	1:B:156:PHE:HB2	1.83	0.77
1:A:172:LYS:NZ	1:B:172:LYS:NZ	2.27	0.77
1:A:74:GLU:HG3	1:B:74:GLU:HG2	1.02	0.77
1:A:68:MET:CE	1:B:77:PRO:CG	2.62	0.77
6:A:1615:TRD:C11	6:B:615:TRD:C12	2.53	0.77
1:A:166:GLU:CB	1:B:166:GLU:N	2.22	0.77
5:A:1622:HEX:H63	5:B:622:HEX:H63	0.78	0.77
1:A:153:PHE:CG	1:B:175:ARG:HD2	2.15	0.77
1:B:183:SER:O	1:B:186:PRO:HD2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:O	1:B:162:SER:O	1.83	0.77
1:A:153:PHE:CZ	1:B:179:VAL:HG21	2.19	0.77
1:A:223:LEU:CD1	1:B:229:ILE:HG21	2.15	0.77
1:A:182:TRP:CZ2	2:B:601:RET:H202	2.20	0.77
1:A:201:LEU:HA	1:B:204:GLU:HG3	1.66	0.77
1:A:76:ASN:ND2	1:B:76:ASN:ND2	0.77	0.77
1:A:165:PRO:O	1:B:159:LYS:NZ	2.17	0.77
1:A:3:GLN:HB3	1:A:4:ILE:HD12	1.66	0.77
1:A:206:LEU:HD13	1:B:206:LEU:CD1	2.15	0.77
5:A:620:HEX:H62	1:B:187:VAL:CG2	2.14	0.76
1:A:7:ARG:N	1:B:8:PRO:HD2	1.98	0.76
1:A:222:ILE:HD13	3:A:1604:UND:C10	2.15	0.76
1:A:32:MET:HE3	1:B:32:MET:CE	2.13	0.76
1:A:32:MET:HE2	1:B:32:MET:CE	2.16	0.76
1:A:225:ARG:HH21	1:B:225:ARG:CZ	1.97	0.76
1:A:22:LEU:HD23	1:B:18:ALA:O	1.85	0.76
1:A:28:LEU:HD12	1:B:28:LEU:HD22	0.77	0.76
1:B:72:GLY:HA2	7:B:1815:HOH:O	1.85	0.76
1:A:179:VAL:HG23	1:B:175:ARG:O	1.85	0.76
1:A:225:ARG:CZ	1:B:225:ARG:NE	2.42	0.76
1:A:68:MET:HE2	1:B:77:PRO:HA	1.68	0.76
5:A:1622:HEX:H12	5:B:622:HEX:C1	2.13	0.76
1:A:166:GLU:HB3	1:B:166:GLU:N	1.86	0.76
1:A:222:ILE:CD1	3:A:1604:UND:C10	2.64	0.76
1:B:97:LEU:HD13	1:B:152:LEU:HD21	1.68	0.76
1:B:176:ASN:OD1	4:B:609:OCT:H83	1.86	0.75
4:B:618:OCT:C7	4:B:1618:OCT:H82	2.16	0.75
1:A:67:THR:O	1:B:78:ILE:N	2.19	0.75
1:A:91:PRO:C	1:B:90:THR:O	2.16	0.75
4:B:609:OCT:H42	4:B:1609:OCT:C2	2.16	0.75
1:A:161:GLU:CB	1:B:161:GLU:CB	2.46	0.75
1:A:76:ASN:HD21	1:B:76:ASN:HD21	0.76	0.75
1:A:15:LEU:C	1:B:15:LEU:HD13	2.06	0.75
1:B:25:LEU:HD13	3:B:614:UND:H41	1.67	0.75
1:A:85:ASP:OD1	1:B:85:ASP:O	2.04	0.75
1:A:148:ILE:O	1:A:152:LEU:HD13	1.87	0.75
1:A:157:THR:CB	1:B:164:ARG:HG2	2.16	0.75
1:A:84:ALA:O	1:B:88:PHE:CD2	2.38	0.75
1:A:157:THR:HB	1:B:164:ARG:CD	2.17	0.75
1:A:101:VAL:O	1:B:102:ASP:CB	2.28	0.75
1:A:164:ARG:HE	1:B:159:LYS:CB	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLN:CB	7:B:832:HOH:O	2.34	0.75
1:A:153:PHE:CZ	1:B:153:PHE:HE2	1.86	0.74
1:A:150:TYR:CD2	1:B:150:TYR:C	2.60	0.74
1:A:161:GLU:N	1:B:160:ALA:HA	2.02	0.74
5:A:606:HEX:H13	5:A:1606:HEX:H13	0.79	0.74
1:A:156:PHE:CE1	1:B:101:VAL:HG21	2.22	0.74
1:A:153:PHE:CE2	1:B:179:VAL:HG21	2.22	0.74
1:A:222:ILE:CD1	3:A:1604:UND:H101	2.16	0.74
1:A:97:LEU:O	1:B:101:VAL:HG13	1.85	0.74
1:A:101:VAL:O	1:B:102:ASP:HB3	1.87	0.74
1:B:232:GLU:CB	7:B:740:HOH:O	2.33	0.74
4:A:623:OCT:C8	4:A:1623:OCT:H82	1.78	0.74
1:A:227:ARG:HH22	1:B:238:PRO:HB3	1.52	0.74
4:B:607:OCT:H22	4:B:1607:OCT:C2	1.22	0.74
1:A:18:ALA:O	1:A:22:LEU:HD23	1.87	0.74
4:A:623:OCT:H62	4:A:1605:OCT:H11	1.69	0.74
1:A:74:GLU:OE1	7:A:831:HOH:O	2.05	0.74
1:A:159:LYS:HE3	1:B:159:LYS:HD3	1.66	0.74
1:B:101:VAL:O	1:B:163:MET:HA	1.88	0.74
1:A:237:GLU:OE1	1:B:237:GLU:OE1	1.95	0.74
1:A:71:PHE:HB2	1:B:129:LYS:O	1.88	0.74
1:A:159:LYS:CE	1:B:164:ARG:HH21	2.00	0.74
1:B:138:TRP:CH2	4:B:618:OCT:C1	2.70	0.74
1:A:66:LEU:CD1	1:B:77:PRO:HB3	2.16	0.74
1:B:82:ARG:HA	7:B:1712:HOH:O	1.87	0.74
1:A:160:ALA:H	1:B:160:ALA:HB2	1.53	0.73
1:A:211:LEU:O	1:B:214:SER:HB2	1.87	0.73
1:A:159:LYS:CA	1:B:159:LYS:CD	2.49	0.73
1:A:217:VAL:O	1:B:221:LEU:HD23	1.86	0.73
1:A:76:ASN:HD22	1:B:76:ASN:HD22	0.77	0.73
1:A:161:GLU:N	1:B:161:GLU:N	2.36	0.73
1:A:29:VAL:HG23	1:B:25:LEU:O	1.88	0.73
1:B:82:ARG:NH2	7:B:715:HOH:O	2.21	0.73
1:A:153:PHE:CE1	1:B:153:PHE:CZ	2.74	0.73
1:A:227:ARG:NH2	1:B:238:PRO:CA	2.50	0.73
1:A:215:ALA:HB1	1:B:181:LEU:HD13	1.70	0.73
1:A:227:ARG:HH12	1:B:238:PRO:CB	2.01	0.73
1:A:119:ILE:CG2	1:B:87:LEU:HD13	2.18	0.73
1:A:227:ARG:CG	1:B:236:PRO:O	2.36	0.73
1:A:68:MET:CE	1:B:5:THR:HG21	2.18	0.73
1:A:160:ALA:CA	1:B:160:ALA:HA	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:620:HEX:C1	4:A:1617:OCT:H31	2.19	0.73
1:A:79:TYR:N	7:A:1714:HOH:O	2.10	0.73
1:A:71:PHE:CD2	1:B:69:VAL:HG12	2.23	0.73
1:A:223:LEU:HD23	1:B:223:LEU:CD2	2.09	0.73
1:A:45:ILE:N	1:B:45:ILE:HD12	2.04	0.73
1:A:224:LEU:HD12	1:B:27:PHE:CE1	2.23	0.73
1:A:94:LEU:HD13	1:B:94:LEU:HD11	1.67	0.73
1:A:168:ALA:CB	1:B:164:ARG:HB2	2.17	0.73
1:A:178:THR:CG2	1:B:182:TRP:CD1	2.72	0.73
1:A:233:ALA:O	1:B:234:GLU:CB	2.18	0.73
1:A:215:ALA:HB1	7:A:1722:HOH:O	1.86	0.73
1:A:171:PHE:O	1:B:174:LEU:HB2	1.89	0.73
1:A:71:PHE:HD2	1:B:69:VAL:HG12	1.53	0.72
1:A:166:GLU:CG	1:B:166:GLU:OE2	2.37	0.72
1:A:209:MET:C	1:B:209:MET:CE	2.57	0.72
1:A:38:ASP:OD2	7:A:1742:HOH:O	2.07	0.72
1:A:204:GLU:OE1	1:B:204:GLU:CD	2.13	0.72
1:A:75:GLN:OE1	1:B:75:GLN:OE1	2.01	0.72
1:A:172:LYS:HE2	1:B:169:SER:OG	1.89	0.72
1:A:134:ARG:NH1	1:B:128:THR:O	2.20	0.72
4:B:618:OCT:H51	5:B:1620:HEX:C4	2.19	0.72
1:A:68:MET:SD	1:B:5:THR:CG2	2.76	0.72
1:A:25:LEU:HD13	3:B:614:UND:H41	1.70	0.72
1:B:212:ASP:OD2	7:B:716:HOH:O	2.07	0.72
1:A:87:LEU:HD11	5:A:610:HEX:C1	2.19	0.72
1:A:222:ILE:HD11	3:A:604:UND:H81	1.70	0.72
1:B:48:LEU:HG	6:B:611:TRD:H122	1.70	0.72
1:A:159:LYS:CE	1:B:164:ARG:NH2	2.53	0.72
1:A:203:ILE:HD12	4:A:1623:OCT:H22	1.72	0.72
1:A:164:ARG:HG2	1:B:159:LYS:N	2.05	0.72
1:A:97:LEU:CD2	1:B:174:LEU:HB3	2.20	0.72
1:A:159:LYS:HB3	1:B:159:LYS:CG	1.48	0.72
1:A:174:LEU:HD11	1:B:223:LEU:HB3	1.72	0.72
2:A:601:RET:H14	1:B:86:TRP:CD1	2.25	0.71
1:A:68:MET:HE1	1:B:77:PRO:HB3	1.69	0.71
1:A:185:TYR:O	1:B:185:TYR:O	0.72	0.71
1:A:101:VAL:HB	1:B:163:MET:CB	2.20	0.71
1:A:32:MET:HE2	1:B:32:MET:HE2	1.70	0.71
1:A:61:LEU:C	1:B:61:LEU:HD12	2.11	0.71
1:A:239:SER:HB2	1:B:239:SER:CA	2.21	0.71
1:A:153:PHE:HE2	1:B:179:VAL:HG22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:CD2	1:B:99:LEU:HD11	2.10	0.71
1:A:22:LEU:CD2	1:B:22:LEU:N	2.54	0.71
3:A:604:UND:C8	3:A:1604:UND:H92	0.50	0.71
1:A:169:SER:HG	1:B:169:SER:HB3	1.44	0.71
1:A:235:ALA:N	1:B:234:GLU:H	1.88	0.71
1:A:93:LEU:O	1:B:96:ASP:HB2	1.91	0.71
1:A:60:MET:C	1:B:13:LEU:HD23	2.11	0.71
1:A:107:THR:O	1:B:107:THR:HG22	1.91	0.71
1:B:175:ARG:O	1:B:179:VAL:HG23	1.90	0.71
1:A:164:ARG:HG2	1:B:159:LYS:CA	2.16	0.71
1:B:75:GLN:O	1:B:77:PRO:HD3	1.90	0.71
1:A:153:PHE:HE1	1:B:175:ARG:HE	1.23	0.70
1:A:224:LEU:HD22	1:B:43:TYR:CD2	2.25	0.70
1:A:94:LEU:HA	1:B:97:LEU:CD1	2.21	0.70
1:A:165:PRO:CD	1:B:162:SER:H	1.97	0.70
1:A:178:THR:C	1:B:177:VAL:O	2.27	0.70
1:A:178:THR:O	1:B:182:TRP:N	2.24	0.70
1:A:171:PHE:HA	1:B:174:LEU:HD12	0.82	0.70
1:A:174:LEU:CD1	1:B:223:LEU:HB3	2.21	0.70
1:A:74:GLU:OE2	1:B:74:GLU:HG2	1.56	0.70
1:A:157:THR:HA	1:B:163:MET:HB2	1.72	0.70
1:A:217:VAL:HG12	1:B:221:LEU:HD21	1.73	0.70
1:A:76:ASN:ND2	1:B:76:ASN:HD21	0.63	0.70
1:A:156:PHE:O	1:B:163:MET:HB2	1.91	0.70
1:A:182:TRP:HA	1:B:185:TYR:CD1	2.25	0.70
1:A:22:LEU:CD2	1:B:22:LEU:H	2.04	0.70
1:A:53:ALA:HA	1:B:85:ASP:OD1	1.92	0.70
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.26	0.70
1:A:74:GLU:CD	7:A:1829:HOH:O	2.28	0.70
1:A:147:TYR:HE1	1:B:147:TYR:CE1	1.40	0.70
1:A:28:LEU:HD23	1:B:29:VAL:N	2.06	0.70
1:A:182:TRP:CD1	2:B:601:RET:H203	2.27	0.70
1:A:98:ALA:HA	1:B:101:VAL:HG22	1.71	0.70
1:A:204:GLU:CG	1:B:204:GLU:OE1	2.20	0.70
4:A:1621:OCT:H13	4:B:621:OCT:C1	2.21	0.70
1:A:68:MET:HE2	1:B:77:PRO:CB	2.20	0.70
1:A:4:ILE:HD13	1:B:4:ILE:HD13	1.72	0.69
1:A:76:ASN:HD22	1:B:76:ASN:ND2	1.28	0.69
1:A:145:MET:HE1	1:B:186:PRO:HG2	1.74	0.69
1:B:209:MET:O	1:B:209:MET:HE3	1.87	0.69
1:A:4:ILE:CD1	1:B:3:GLN:CD	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD22	1:B:22:LEU:H	1.57	0.69
4:B:618:OCT:H72	4:B:1618:OCT:H72	1.63	0.69
1:A:182:TRP:O	1:B:186:PRO:HD3	1.91	0.69
1:A:192:GLY:O	1:B:193:SER:C	2.16	0.69
1:A:94:LEU:HA	1:B:97:LEU:HD12	1.68	0.69
1:A:153:PHE:CD1	1:B:153:PHE:CE1	2.67	0.69
1:A:227:ARG:NH1	1:B:227:ARG:HE	1.80	0.69
1:A:91:PRO:CG	1:B:115:ASP:OD2	2.29	0.69
1:B:48:LEU:CD2	6:B:611:TRD:H102	2.20	0.69
1:A:20:MET:HE3	1:B:216:LYS:HD3	1.72	0.69
1:B:162:SER:HB3	7:B:850:HOH:O	1.90	0.69
1:A:239:SER:CA	1:B:239:SER:CA	2.61	0.69
4:B:609:OCT:H81	4:B:1609:OCT:C8	2.02	0.69
1:A:168:ALA:C	1:B:167:VAL:O	2.25	0.69
1:A:219:PHE:CD1	1:B:223:LEU:CD2	2.66	0.69
1:A:107:THR:O	1:B:111:LEU:HG	1.93	0.69
5:B:619:HEX:C6	5:B:1619:HEX:H61	2.21	0.69
1:A:66:LEU:HD11	1:B:77:PRO:HB2	1.74	0.69
1:A:182:TRP:CD1	1:B:182:TRP:N	2.56	0.69
1:A:111:LEU:CD1	1:B:156:PHE:CE1	2.75	0.69
4:A:1621:OCT:C1	4:B:621:OCT:C2	2.69	0.69
1:A:46:THR:OG1	7:A:1724:HOH:O	2.08	0.69
1:A:153:PHE:CE1	1:B:175:ARG:CG	2.75	0.69
1:A:233:ALA:O	1:B:234:GLU:CA	2.40	0.69
1:A:46:THR:CB	7:A:1724:HOH:O	2.41	0.69
1:A:166:GLU:CG	1:B:166:GLU:HG2	2.23	0.69
1:A:159:LYS:CA	1:B:159:LYS:HD2	2.13	0.69
1:A:4:ILE:HD12	1:B:3:GLN:NE2	2.08	0.69
1:A:165:PRO:CD	1:B:162:SER:N	2.56	0.68
1:B:216:LYS:HE3	7:B:710:HOH:O	1.88	0.68
1:A:239:SER:CB	1:B:239:SER:HA	2.22	0.68
4:B:607:OCT:C1	4:B:1607:OCT:H13	1.17	0.68
1:A:71:PHE:CD1	1:B:71:PHE:C	2.63	0.68
1:B:68:MET:SD	1:B:75:GLN:HB3	2.33	0.68
1:A:169:SER:HB3	1:B:167:VAL:HG13	1.75	0.68
1:A:46:THR:CG2	7:A:1724:HOH:O	2.35	0.68
1:A:81:ALA:HB2	1:B:65:GLY:HA3	1.74	0.68
1:A:154:PHE:CD1	1:B:153:PHE:C	2.66	0.68
1:A:199:VAL:CG1	1:B:203:ILE:HB	2.24	0.68
1:B:27:PHE:CE1	1:B:224:LEU:HD12	2.28	0.68
1:A:41:LYS:O	1:B:45:ILE:HD12	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:CB	1:B:8:PRO:CD	2.72	0.68
1:B:25:LEU:HB3	3:B:614:UND:C2	2.23	0.68
1:A:68:MET:CE	1:B:5:THR:HG22	2.23	0.68
1:A:68:MET:SD	1:B:77:PRO:CG	2.69	0.68
1:A:60:MET:HG2	1:B:79:TYR:HD1	1.58	0.68
1:A:238:PRO:O	1:B:239:SER:HA	1.93	0.68
1:A:165:PRO:C	1:B:159:LYS:NZ	2.48	0.68
1:A:160:ALA:C	1:B:160:ALA:HA	2.13	0.68
1:A:239:SER:CB	1:B:239:SER:C	2.56	0.68
1:B:5:THR:HA	1:B:77:PRO:HG2	1.74	0.68
1:A:81:ALA:C	1:B:80:TRP:O	2.29	0.68
1:A:86:TRP:CD1	1:B:86:TRP:N	2.47	0.68
1:A:184:ALA:O	1:B:188:VAL:N	2.27	0.67
1:A:20:MET:CE	1:B:216:LYS:HB2	2.24	0.67
1:A:157:THR:HA	1:B:163:MET:CB	2.23	0.67
1:A:56:MET:O	1:B:60:MET:HG3	1.94	0.67
1:A:75:GLN:HE21	1:B:70:PRO:HB3	1.57	0.67
1:B:27:PHE:HE1	1:B:224:LEU:HD12	1.59	0.67
1:B:68:MET:HG2	1:B:75:GLN:OE1	1.94	0.67
1:A:82:ARG:CZ	7:A:1713:HOH:O	2.25	0.67
1:B:126:ALA:O	1:B:134:ARG:NH1	2.21	0.67
1:A:162:SER:HB3	1:B:160:ALA:CB	2.23	0.67
1:A:101:VAL:CA	1:B:163:MET:HA	2.24	0.67
1:A:74:GLU:O	1:B:70:PRO:CB	2.42	0.67
1:A:164:ARG:HE	1:B:159:LYS:H	1.42	0.67
1:A:200:PRO:HD2	1:B:199:VAL:CG1	2.24	0.67
1:A:68:MET:HE2	1:B:77:PRO:CA	2.24	0.67
1:A:219:PHE:HE1	1:B:223:LEU:HD22	1.60	0.67
1:A:65:GLY:O	1:B:79:TYR:HA	1.95	0.67
1:A:176:ASN:CA	1:B:173:VAL:O	2.42	0.67
1:A:11:ILE:CD1	1:B:11:ILE:CD1	2.68	0.67
1:A:164:ARG:C	1:B:159:LYS:HD2	2.09	0.67
1:A:15:LEU:HD22	1:B:19:LEU:HD11	1.75	0.67
1:B:206:LEU:HD12	1:B:207:LEU:HD23	1.77	0.67
1:B:25:LEU:HD13	3:B:614:UND:C4	2.25	0.67
1:B:83:TYR:HE2	7:B:715:HOH:O	1.78	0.67
1:A:174:LEU:HD21	1:B:222:ILE:HG22	1.76	0.66
1:A:94:LEU:CD1	1:B:94:LEU:HD11	2.22	0.66
1:B:9:GLU:O	1:B:13:LEU:HD13	1.95	0.66
1:A:159:LYS:HD2	1:B:159:LYS:HG2	1.76	0.66
1:A:4:ILE:HD13	1:B:4:ILE:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:O	1:B:88:PHE:N	2.26	0.66
1:A:165:PRO:C	1:B:159:LYS:HZ1	1.97	0.66
1:A:88:PHE:C	1:B:91:PRO:HD2	2.15	0.66
1:A:232:GLU:O	1:B:233:ALA:O	1.96	0.66
1:A:217:VAL:HG12	1:B:221:LEU:CD2	2.25	0.66
1:A:57:TYR:HA	1:B:60:MET:CE	2.26	0.66
1:A:207:LEU:N	1:B:206:LEU:CD1	2.51	0.66
1:A:175:ARG:NH1	1:B:171:PHE:HE2	1.94	0.66
1:A:223:LEU:HD21	1:B:42:PHE:CD1	2.31	0.66
1:A:154:PHE:CG	1:B:153:PHE:C	2.66	0.66
1:A:225:ARG:NH2	1:B:225:ARG:HE	1.88	0.66
1:A:171:PHE:C	1:B:170:THR:O	2.27	0.66
1:A:179:VAL:HG22	1:B:149:LEU:CD2	2.19	0.66
1:A:182:TRP:CH2	1:B:90:THR:HG22	2.30	0.66
1:A:223:LEU:CD1	1:B:229:ILE:CG2	2.74	0.66
1:A:227:ARG:CZ	1:B:238:PRO:CB	2.74	0.66
1:A:227:ARG:NH2	1:B:238:PRO:HB3	2.09	0.66
1:A:224:LEU:HD13	1:B:43:TYR:CE1	2.30	0.65
1:A:92:LEU:HB2	1:B:89:THR:O	1.96	0.65
1:A:153:PHE:CZ	1:B:175:ARG:HG2	2.31	0.65
1:A:166:GLU:CG	1:B:166:GLU:CG	2.75	0.65
1:A:188:VAL:HG12	1:B:188:VAL:O	1.95	0.65
5:A:620:HEX:H61	5:B:1620:HEX:C6	1.84	0.65
1:A:6:GLY:O	1:B:7:ARG:HB2	1.95	0.65
1:A:173:VAL:HG12	3:A:1604:UND:C10	2.27	0.65
7:A:1829:HOH:O	1:B:74:GLU:HB3	1.96	0.65
1:A:112:VAL:HG11	5:A:1610:HEX:H62	1.78	0.65
1:A:24:THR:O	1:B:28:LEU:HG	1.95	0.65
1:A:201:LEU:HA	1:B:204:GLU:CG	2.26	0.65
1:A:45:ILE:HD13	1:B:95:LEU:HD23	1.59	0.65
1:A:57:TYR:HA	1:B:60:MET:HE3	1.79	0.65
1:B:202:ASN:N	7:B:1800:HOH:O	2.30	0.65
1:B:102:ASP:CG	7:B:850:HOH:O	2.30	0.65
1:A:175:ARG:CD	1:B:171:PHE:CE2	2.77	0.65
1:A:7:ARG:N	1:B:8:PRO:HD3	2.09	0.65
1:A:238:PRO:O	1:B:239:SER:HB3	1.96	0.65
1:A:166:GLU:HG3	1:B:166:GLU:HA	1.77	0.64
1:A:172:LYS:HZ1	1:B:172:LYS:NZ	1.95	0.64
1:A:154:PHE:CG	1:B:153:PHE:O	2.50	0.64
1:A:66:LEU:HD21	1:B:5:THR:OG1	1.97	0.64
1:A:126:ALA:HB3	1:B:123:LEU:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:B:133:TYR:CE2	2.33	0.64
1:A:175:ARG:HD2	1:B:152:LEU:O	1.96	0.64
7:A:1864:HOH:O	1:B:31:GLY:HA3	1.96	0.64
4:B:607:OCT:C1	4:B:1607:OCT:C1	0.64	0.64
1:A:102:ASP:OD2	1:B:232:GLU:HG3	1.97	0.64
1:A:4:ILE:HD11	1:B:3:GLN:NE2	2.11	0.64
1:A:186:PRO:HD2	1:B:183:SER:O	1.98	0.64
1:A:164:ARG:HG3	1:B:159:LYS:CB	2.28	0.64
1:B:212:ASP:O	1:B:216:LYS:HD2	1.98	0.64
4:A:605:OCT:H62	4:A:623:OCT:H22	1.78	0.64
1:A:163:MET:CE	1:B:158:SER:HB2	2.28	0.64
1:B:25:LEU:O	1:B:29:VAL:HG23	1.95	0.64
1:A:73:GLY:HA3	1:B:73:GLY:HA2	1.78	0.64
1:B:80:TRP:CE3	5:B:622:HEX:H31	2.33	0.63
1:A:109:LEU:HD13	1:B:109:LEU:C	2.17	0.63
1:A:41:LYS:HD2	1:A:99:LEU:HD21	1.81	0.63
1:A:74:GLU:OE1	1:B:74:GLU:HA	1.98	0.63
1:B:203:ILE:HG23	1:B:207:LEU:HD21	1.80	0.63
1:A:147:TYR:CE1	1:B:147:TYR:CE1	0.81	0.63
1:A:160:ALA:N	1:B:160:ALA:HB2	2.10	0.63
1:A:86:TRP:O	1:B:90:THR:OG1	2.16	0.63
1:A:201:LEU:HB3	7:B:1800:HOH:O	1.84	0.63
1:A:68:MET:HE2	1:B:77:PRO:HB3	1.78	0.63
1:A:157:THR:CA	1:B:163:MET:CG	2.77	0.63
1:A:15:LEU:HD13	1:B:15:LEU:HD11	1.75	0.63
1:A:26:TYR:O	1:B:30:LYS:HB2	1.97	0.63
1:A:68:MET:HE1	1:B:77:PRO:CG	2.27	0.63
1:A:145:MET:SD	1:B:186:PRO:HG2	2.39	0.63
1:A:87:LEU:HD21	5:A:1610:HEX:H11	1.78	0.63
1:A:227:ARG:O	1:B:230:PHE:HB2	1.99	0.63
2:A:601:RET:H41	1:B:141:SER:HB3	1.80	0.63
1:A:94:LEU:CD1	1:B:182:TRP:CZ2	2.82	0.63
1:A:9:GLU:OE1	1:B:9:GLU:N	2.26	0.63
1:B:206:LEU:CD1	1:B:207:LEU:HD23	2.28	0.63
1:A:168:ALA:HB1	1:B:164:ARG:HB2	1.81	0.62
1:A:215:ALA:HB2	1:B:181:LEU:HD11	1.74	0.62
1:A:160:ALA:C	1:B:160:ALA:CA	2.67	0.62
1:A:68:MET:HE1	1:B:77:PRO:CB	2.28	0.62
1:A:110:ALA:N	1:B:107:THR:O	2.32	0.62
1:A:151:VAL:CG1	1:B:111:LEU:HD21	2.22	0.62
1:A:26:TYR:C	1:B:26:TYR:CD2	2.70	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1745:HOH:O	1:B:37:PRO:HB2	2.00	0.62
1:A:4:ILE:HD12	1:B:3:GLN:CG	2.28	0.62
1:A:156:PHE:CZ	1:B:101:VAL:CG2	2.79	0.62
1:A:157:THR:CA	1:B:163:MET:HG3	2.29	0.62
5:A:608:HEX:H32	1:B:217:VAL:HG11	1.81	0.62
1:A:4:ILE:HD12	1:B:3:GLN:CD	2.19	0.62
1:A:163:MET:O	1:B:165:PRO:HD2	1.98	0.61
1:A:184:ALA:O	1:B:188:VAL:HG23	2.00	0.61
1:A:222:ILE:O	1:B:225:ARG:N	2.32	0.61
1:A:172:LYS:HZ1	1:B:172:LYS:HZ3	1.47	0.61
1:A:176:ASN:HB2	1:B:173:VAL:O	2.00	0.61
4:B:618:OCT:H71	4:B:1618:OCT:H81	1.74	0.61
1:A:78:ILE:CG1	1:B:76:ASN:O	2.35	0.61
2:A:601:RET:H162	1:B:83:TYR:HE1	1.65	0.61
1:A:20:MET:HE1	1:B:216:LYS:HD3	1.80	0.61
1:A:131:TYR:O	1:B:134:ARG:HB2	2.01	0.61
1:A:221:LEU:O	1:B:225:ARG:N	2.31	0.61
1:A:115:ASP:OD2	1:B:90:THR:HB	2.00	0.61
1:A:225:ARG:NH2	1:B:225:ARG:CZ	2.60	0.61
1:A:15:LEU:HD22	1:B:19:LEU:CD1	2.30	0.61
1:A:100:LEU:HG	1:B:42:PHE:CZ	2.36	0.61
1:A:123:LEU:CD2	5:A:1622:HEX:H22	2.29	0.61
1:A:174:LEU:CD2	1:B:222:ILE:HG22	2.31	0.61
1:A:2:ALA:CB	7:B:1809:HOH:O	2.47	0.61
1:B:194:GLU:OE2	7:B:715:HOH:O	2.16	0.61
1:B:48:LEU:CD1	6:B:611:TRD:H121	2.29	0.61
1:A:85:ASP:C	1:B:84:ALA:O	2.34	0.61
1:A:161:GLU:N	1:B:160:ALA:CA	2.63	0.61
1:A:159:LYS:HA	1:B:159:LYS:CD	2.18	0.61
1:A:153:PHE:CZ	1:B:179:VAL:CG2	2.80	0.60
1:A:121:THR:HA	1:A:124:VAL:HG22	1.83	0.60
1:A:185:TYR:CZ	1:B:211:LEU:HB3	2.36	0.60
1:B:212:ASP:HB3	1:B:216:LYS:HD3	1.83	0.60
1:A:148:ILE:O	1:B:152:LEU:HD13	1.96	0.60
1:A:36:ASP:HB2	1:A:39:ALA:HB3	1.83	0.60
1:B:53:ALA:HB2	1:B:216:LYS:HG2	1.83	0.60
1:B:232:GLU:N	7:B:740:HOH:O	2.29	0.60
1:A:4:ILE:HD11	1:B:3:GLN:CD	2.20	0.60
1:A:45:ILE:H	1:B:45:ILE:CD1	2.13	0.60
1:A:227:ARG:CB	1:B:227:ARG:O	2.31	0.60
1:A:227:ARG:NH2	1:B:238:PRO:CB	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLU:N	1:B:160:ALA:C	2.55	0.60
1:A:172:LYS:NZ	1:B:172:LYS:HZ2	1.99	0.60
1:B:169:SER:O	1:B:173:VAL:HG23	2.01	0.60
1:A:200:PRO:O	1:B:201:LEU:C	2.37	0.60
1:A:212:ASP:OD2	1:B:57:TYR:OH	2.18	0.60
1:A:215:ALA:HB2	1:B:181:LEU:CD2	2.31	0.60
1:B:113:GLY:HA2	4:B:607:OCT:H22	1.84	0.60
1:A:101:VAL:HB	1:B:163:MET:C	2.21	0.60
1:A:159:LYS:HE3	1:B:164:ARG:HH21	1.60	0.60
1:A:212:ASP:O	1:B:216:LYS:N	2.34	0.60
1:A:32:MET:HE3	1:B:32:MET:HE1	1.83	0.60
1:A:173:VAL:HG12	3:A:1604:UND:H102	1.80	0.60
1:A:239:SER:CB	1:B:239:SER:CA	2.79	0.60
1:A:227:ARG:HH12	1:B:238:PRO:HB3	1.66	0.60
1:B:165:PRO:HG2	1:B:166:GLU:H	1.65	0.60
1:A:172:LYS:N	1:B:170:THR:C	2.40	0.60
1:A:111:LEU:CD1	1:B:156:PHE:CZ	2.85	0.60
1:A:168:ALA:HB2	1:B:164:ARG:C	2.23	0.60
1:A:112:VAL:O	1:B:115:ASP:HB3	2.02	0.59
4:A:623:OCT:H72	4:A:1623:OCT:C8	2.07	0.59
1:A:227:ARG:NH1	1:B:227:ARG:CZ	2.63	0.59
1:A:176:ASN:CB	1:B:173:VAL:O	2.50	0.59
1:A:238:PRO:O	1:B:239:SER:CB	2.49	0.59
3:A:604:UND:C8	3:A:1604:UND:H91	1.11	0.59
1:B:159:LYS:HB3	7:B:858:HOH:O	2.01	0.59
1:A:182:TRP:NE1	2:B:601:RET:H203	2.12	0.59
1:B:97:LEU:O	1:B:101:VAL:HG13	2.02	0.59
1:A:123:LEU:HD21	5:A:1622:HEX:C2	2.33	0.59
1:A:166:GLU:CG	1:B:166:GLU:HA	2.10	0.59
1:B:25:LEU:CD1	3:B:614:UND:H41	2.33	0.59
1:A:5:THR:HG22	1:B:68:MET:HE2	1.85	0.59
1:A:171:PHE:N	1:B:170:THR:HG22	2.04	0.59
1:A:163:MET:HE1	1:B:158:SER:HB2	1.84	0.59
1:A:45:ILE:HD13	1:B:95:LEU:HD22	0.59	0.59
1:B:66:LEU:HD12	1:B:78:ILE:O	2.02	0.59
1:A:156:PHE:CD2	1:B:101:VAL:HG11	2.38	0.59
4:A:1623:OCT:H71	1:B:206:LEU:HD11	1.85	0.59
1:A:92:LEU:N	1:B:89:THR:O	2.36	0.59
1:A:166:GLU:HG2	1:B:234:GLU:C	2.24	0.58
1:B:48:LEU:HD23	6:B:611:TRD:H111	0.65	0.58
1:A:227:ARG:NH1	1:B:238:PRO:HG3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PRO:HG3	1:B:161:GLU:HA	0.58	0.58
1:B:201:LEU:HA	1:B:204:GLU:HG3	1.79	0.58
1:A:25:LEU:HD23	1:B:28:LEU:CD1	2.32	0.58
1:A:4:ILE:CD1	1:B:4:ILE:CG1	2.81	0.58
4:B:607:OCT:C2	4:B:1607:OCT:C2	0.82	0.58
1:B:80:TRP:CH2	5:B:622:HEX:H31	2.37	0.58
1:A:126:ALA:N	1:B:123:LEU:O	2.36	0.58
1:A:200:PRO:C	1:B:202:ASN:N	2.48	0.58
1:A:71:PHE:CB	1:B:129:LYS:O	2.51	0.58
1:A:160:ALA:C	1:B:160:ALA:HB1	2.24	0.58
1:A:239:SER:N	1:B:239:SER:CA	2.61	0.58
4:B:609:OCT:H82	4:B:1609:OCT:H82	1.81	0.58
1:A:145:MET:CE	1:B:186:PRO:HG2	2.32	0.58
1:A:227:ARG:HH12	1:B:238:PRO:CG	2.16	0.58
1:A:7:ARG:CZ	7:A:1817:HOH:O	2.52	0.58
1:A:111:LEU:N	1:B:107:THR:O	2.33	0.58
1:A:98:ALA:CB	1:B:156:PHE:HZ	2.13	0.58
1:A:222:ILE:C	1:B:221:LEU:O	2.31	0.58
1:A:167:VAL:HB	1:B:166:GLU:CB	2.04	0.58
1:B:68:MET:SD	1:B:77:PRO:HG3	2.39	0.58
1:A:111:LEU:HD11	1:B:156:PHE:CZ	2.38	0.58
1:A:107:THR:HG21	1:B:156:PHE:HD1	1.69	0.58
1:A:157:THR:HB	1:B:164:ARG:HD3	1.86	0.58
1:B:66:LEU:HD13	1:B:79:TYR:CG	2.39	0.58
1:B:209:MET:HB2	7:B:713:HOH:O	2.03	0.58
1:A:170:THR:CB	1:B:226:SER:OG	2.51	0.58
1:A:164:ARG:O	1:B:159:LYS:CE	2.50	0.58
1:A:165:PRO:CG	1:B:161:GLU:N	2.56	0.58
1:A:58:LEU:HG	1:B:62:LEU:CD1	2.34	0.58
1:A:109:LEU:CD1	1:B:109:LEU:C	2.72	0.57
4:B:607:OCT:C1	4:B:1607:OCT:C2	0.93	0.57
1:A:204:GLU:C	1:B:203:ILE:O	2.37	0.57
1:A:227:ARG:HH12	1:B:238:PRO:HG3	1.67	0.57
1:A:156:PHE:CE2	1:B:101:VAL:HG21	2.39	0.57
1:A:214:SER:O	1:B:219:PHE:N	2.31	0.57
1:A:4:ILE:HD13	1:B:4:ILE:HG12	1.85	0.57
1:A:165:PRO:CD	1:B:161:GLU:CA	2.82	0.57
1:A:168:ALA:HB2	1:B:164:ARG:CA	2.33	0.57
1:A:20:MET:HE1	1:B:212:ASP:O	2.04	0.57
1:A:7:ARG:NH1	1:B:7:ARG:HG3	2.18	0.57
1:A:193:SER:OG	1:B:194:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PRO:O	1:B:41:LYS:HG3	2.04	0.57
1:A:182:TRP:CD1	2:B:601:RET:C20	2.86	0.57
1:A:159:LYS:HE2	1:B:159:LYS:HD3	1.79	0.57
5:A:620:HEX:H11	4:A:1617:OCT:C3	2.25	0.57
1:A:81:ALA:N	1:B:79:TYR:C	2.50	0.57
1:A:172:LYS:HZ2	1:B:172:LYS:HZ2	1.53	0.57
1:A:7:ARG:HB2	1:B:8:PRO:HD3	1.84	0.57
1:B:113:GLY:O	1:B:117:ILE:HD13	2.05	0.57
1:A:147:TYR:HB3	1:B:144:ALA:O	2.05	0.57
1:B:187:VAL:O	1:B:191:ILE:HG12	2.03	0.57
1:A:38:ASP:HA	1:B:41:LYS:NZ	2.20	0.57
1:A:199:VAL:HG13	1:B:203:ILE:HB	1.87	0.57
1:A:207:LEU:HD23	4:A:1623:OCT:H71	1.87	0.57
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.85	0.57
1:A:227:ARG:NH1	1:B:238:PRO:CG	2.67	0.57
1:A:170:THR:HG21	1:B:226:SER:OG	2.03	0.57
1:A:23:GLY:O	1:B:27:PHE:CD2	2.58	0.57
1:A:70:PRO:O	1:B:129:LYS:HB3	2.04	0.57
1:B:50:PRO:HA	1:B:53:ALA:HB3	1.87	0.57
1:B:68:MET:HE3	1:B:75:GLN:HB3	1.87	0.57
3:A:1604:UND:H101	1:B:222:ILE:HD13	1.86	0.57
1:A:43:TYR:CD2	1:B:34:VAL:HG11	2.40	0.57
1:A:227:ARG:NH1	1:B:238:PRO:HB3	2.19	0.56
1:A:134:ARG:NH2	1:B:126:ALA:HA	2.20	0.56
1:B:176:ASN:OD1	4:B:609:OCT:C8	2.53	0.56
1:B:131:TYR:HE2	7:B:824:HOH:O	1.87	0.56
1:A:161:GLU:HB3	1:B:161:GLU:CB	2.20	0.56
1:A:206:LEU:CD1	1:B:206:LEU:CD1	2.56	0.56
1:B:65:GLY:HA3	1:B:81:ALA:HB2	1.87	0.56
1:A:119:ILE:HG21	1:B:87:LEU:HD13	1.87	0.56
1:A:201:LEU:O	1:B:205:THR:OG1	2.22	0.56
1:B:203:ILE:HG22	1:B:207:LEU:HD11	1.87	0.56
1:B:93:LEU:O	1:B:97:LEU:HG	2.06	0.56
1:A:180:VAL:HG23	1:B:176:ASN:O	2.06	0.56
1:A:206:LEU:HD13	1:B:206:LEU:HD12	1.88	0.56
1:A:229:ILE:HG13	1:B:230:PHE:CD1	2.40	0.56
1:A:210:VAL:CG2	5:A:606:HEX:H11	2.30	0.56
1:A:179:VAL:CG2	1:B:175:ARG:O	2.53	0.56
1:A:39:ALA:O	1:B:40:LYS:C	2.34	0.56
1:B:94:LEU:N	1:B:94:LEU:HD12	2.20	0.56
1:A:145:MET:SD	1:B:186:PRO:CG	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HD3	1:B:90:THR:CB	2.36	0.56
1:A:50:PRO:O	1:B:53:ALA:HB3	2.06	0.56
1:B:100:LEU:HD23	7:B:1743:HOH:O	2.04	0.56
1:A:161:GLU:HB3	1:B:161:GLU:HB2	1.80	0.56
1:A:166:GLU:HB3	1:B:166:GLU:HB2	1.83	0.56
1:A:131:TYR:C	1:B:130:VAL:O	2.41	0.56
1:A:174:LEU:HD21	1:B:223:LEU:N	2.21	0.56
1:A:198:ILE:CG1	1:B:197:GLY:O	2.52	0.56
1:A:20:MET:HE1	1:B:216:LYS:CD	2.35	0.56
1:B:223:LEU:HD12	1:B:224:LEU:HD23	1.88	0.56
1:A:52:ILE:O	1:B:56:MET:HG2	2.05	0.56
1:A:204:GLU:HG2	1:B:204:GLU:OE1	2.06	0.56
1:A:224:LEU:CD1	1:B:27:PHE:CD1	2.86	0.56
1:A:162:SER:CB	1:B:160:ALA:HB3	2.32	0.56
1:A:224:LEU:HD11	1:B:46:THR:HB	1.86	0.56
1:B:101:VAL:C	1:B:163:MET:HA	2.25	0.56
1:A:81:ALA:HB2	1:B:65:GLY:CA	2.36	0.56
1:A:63:GLY:O	7:A:1826:HOH:O	2.17	0.55
1:A:101:VAL:C	1:B:163:MET:HA	2.26	0.55
1:A:182:TRP:C	1:B:184:ALA:N	2.47	0.55
1:A:134:ARG:HH11	1:B:134:ARG:HH11	0.56	0.55
1:A:45:ILE:HG23	1:B:92:LEU:HB3	1.89	0.55
1:A:121:THR:O	1:A:124:VAL:HG22	2.05	0.55
1:B:142:THR:O	1:B:145:MET:HB3	2.07	0.55
1:B:15:LEU:HD22	1:B:19:LEU:HG	1.87	0.55
1:A:172:LYS:CB	1:B:169:SER:O	2.46	0.55
1:A:153:PHE:HZ	1:B:179:VAL:HG21	1.71	0.55
1:A:94:LEU:CD1	1:B:182:TRP:CH2	2.89	0.55
1:A:130:VAL:O	1:B:128:THR:HG22	2.06	0.55
1:A:22:LEU:HG	4:B:1613:OCT:H41	1.85	0.55
1:A:22:LEU:O	1:B:23:GLY:C	2.35	0.55
1:A:28:LEU:HD23	1:B:28:LEU:C	2.26	0.55
1:A:223:LEU:HD21	1:B:42:PHE:HD1	1.71	0.55
1:B:14:ALA:HA	1:B:61:LEU:HD22	1.89	0.55
1:A:157:THR:HA	1:B:163:MET:HG3	1.84	0.55
1:A:206:LEU:C	1:B:206:LEU:HD22	2.24	0.55
3:A:604:UND:H81	3:A:1604:UND:C10	2.06	0.55
1:A:159:LYS:HB2	1:B:159:LYS:CG	0.25	0.55
1:A:4:ILE:HD12	1:A:4:ILE:N	2.21	0.55
4:B:618:OCT:C4	4:B:1618:OCT:H72	2.37	0.55
1:A:185:TYR:HD1	1:B:185:TYR:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:O	1:B:218:GLY:C	2.38	0.55
1:A:4:ILE:CD1	1:B:4:ILE:HG12	2.37	0.55
1:A:227:ARG:NH2	1:B:238:PRO:C	2.60	0.55
1:B:66:LEU:HD12	1:B:78:ILE:C	2.26	0.55
1:A:77:PRO:CD	1:B:75:GLN:O	2.52	0.55
1:A:226:SER:N	1:B:224:LEU:C	2.46	0.54
1:A:25:LEU:C	1:B:24:THR:O	2.35	0.54
1:A:86:TRP:C	1:B:88:PHE:N	2.50	0.54
1:A:8:PRO:O	1:B:8:PRO:O	0.54	0.54
1:A:182:TRP:O	1:B:186:PRO:CD	2.55	0.54
1:A:23:GLY:O	1:B:27:PHE:HD2	1.90	0.54
1:A:5:THR:HB	1:A:68:MET:HE1	1.74	0.54
1:A:188:VAL:CG1	1:B:188:VAL:O	2.49	0.54
1:A:174:LEU:HD11	1:B:223:LEU:HB2	1.88	0.54
1:B:94:LEU:HD11	1:B:182:TRP:CZ2	2.39	0.54
1:A:223:LEU:O	1:B:229:ILE:CD1	2.55	0.54
1:A:236:PRO:C	1:B:236:PRO:O	2.43	0.54
1:A:95:LEU:HD22	1:B:99:LEU:HD13	1.77	0.54
1:B:70:PRO:HA	1:B:74:GLU:O	2.07	0.54
1:A:11:ILE:HD12	1:B:11:ILE:HD12	1.86	0.54
1:A:227:ARG:CZ	1:B:238:PRO:C	2.75	0.54
1:A:95:LEU:CD2	1:A:99:LEU:HD22	2.36	0.54
1:A:182:TRP:CD1	1:B:181:LEU:HB3	2.26	0.54
1:A:95:LEU:HD23	1:B:95:LEU:O	2.08	0.54
1:A:94:LEU:HD13	1:B:182:TRP:HZ2	1.67	0.54
1:A:101:VAL:CB	1:B:163:MET:O	2.56	0.54
1:A:217:VAL:CG1	1:B:221:LEU:HD21	2.37	0.54
1:B:225:ARG:O	1:B:225:ARG:HD3	2.07	0.54
1:A:224:LEU:CD2	1:B:43:TYR:CE2	2.81	0.54
1:B:5:THR:HG22	1:B:77:PRO:HG3	1.89	0.54
1:A:130:VAL:HG11	1:B:133:TYR:CE2	2.43	0.54
1:A:134:ARG:HH11	1:B:134:ARG:NH1	1.18	0.54
1:A:134:ARG:CZ	1:B:126:ALA:O	2.55	0.53
1:A:164:ARG:NE	1:B:159:LYS:H	2.06	0.53
1:B:201:LEU:HA	1:B:204:GLU:CG	2.35	0.53
1:A:101:VAL:O	1:B:163:MET:CA	2.53	0.53
1:A:120:GLY:O	1:B:124:VAL:HG12	2.08	0.53
1:A:77:PRO:C	1:B:76:ASN:O	2.43	0.53
1:A:182:TRP:HH2	1:B:94:LEU:HD11	1.72	0.53
1:A:130:VAL:CB	1:B:133:TYR:CD2	2.88	0.53
1:A:185:TYR:CE1	1:B:211:LEU:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1621:OCT:C1	4:B:621:OCT:C1	2.85	0.53
7:A:1829:HOH:O	1:B:75:GLN:N	2.41	0.53
1:B:7:ARG:CD	7:B:816:HOH:O	2.50	0.53
1:A:220:GLY:O	1:B:224:LEU:HG	2.09	0.53
1:A:67:THR:OG1	1:B:68:MET:N	2.39	0.53
1:A:109:LEU:HD13	1:B:109:LEU:O	2.07	0.53
1:B:117:ILE:HD12	4:B:1607:OCT:H62	1.89	0.53
1:A:101:VAL:CB	1:B:163:MET:CA	2.72	0.53
1:A:76:ASN:CB	1:B:69:VAL:O	2.56	0.53
1:A:172:LYS:C	1:B:171:PHE:O	2.43	0.53
1:A:225:ARG:NH2	1:B:225:ARG:CD	2.61	0.53
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.66	0.53
1:A:117:ILE:HG13	1:B:113:GLY:O	2.09	0.53
1:A:187:VAL:O	1:B:191:ILE:N	2.41	0.53
1:A:160:ALA:C	1:B:160:ALA:CB	2.77	0.53
1:A:224:LEU:HB3	1:B:43:TYR:CZ	2.43	0.53
1:A:235:ALA:N	1:B:234:GLU:OE2	2.41	0.53
1:A:185:TYR:CD1	1:B:185:TYR:N	2.75	0.53
7:A:1722:HOH:O	1:B:93:LEU:CD1	2.56	0.53
1:A:160:ALA:CA	1:B:160:ALA:CB	2.87	0.53
1:A:43:TYR:CE2	1:B:34:VAL:HG21	2.43	0.53
1:A:110:ALA:HB3	1:B:107:THR:O	2.08	0.53
1:B:147:TYR:O	1:B:150:TYR:HB3	2.08	0.53
1:A:224:LEU:CD1	1:B:46:THR:HG21	2.39	0.53
1:B:71:PHE:C	1:B:73:GLY:N	2.61	0.53
1:A:185:TYR:CD2	1:B:208:PHE:CE1	2.97	0.53
1:A:134:ARG:NH1	1:B:134:ARG:NH1	0.53	0.53
1:B:175:ARG:NH1	7:B:866:HOH:O	2.41	0.52
1:A:75:GLN:NE2	1:B:70:PRO:CB	2.61	0.52
1:A:227:ARG:HG3	1:A:238:PRO:HA	1.90	0.52
1:A:158:SER:HB2	1:B:160:ALA:HB3	1.91	0.52
1:A:158:SER:N	1:B:163:MET:HG2	2.23	0.52
1:B:31:GLY:C	7:B:864:HOH:O	2.47	0.52
1:B:72:GLY:HA3	7:B:814:HOH:O	2.09	0.52
1:B:83:TYR:HE1	2:B:601:RET:H162	1.74	0.52
1:A:88:PHE:O	1:B:92:LEU:HG	2.09	0.52
1:A:134:ARG:NH2	1:B:126:ALA:O	2.41	0.52
1:A:68:MET:HE2	1:B:67:THR:O	2.10	0.52
1:B:23:GLY:O	1:B:26:TYR:HB3	2.10	0.52
1:A:223:LEU:O	1:B:229:ILE:HD13	2.08	0.52
1:A:235:ALA:N	1:B:234:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:GLY:O	1:B:223:LEU:HG	2.10	0.52
1:A:172:LYS:HD3	7:A:1866:HOH:O	2.10	0.52
1:A:165:PRO:HA	1:B:159:LYS:CE	2.40	0.52
1:B:159:LYS:HB2	1:B:164:ARG:CZ	2.39	0.52
1:A:164:ARG:HE	1:B:159:LYS:N	2.07	0.52
1:A:5:THR:CG2	1:B:4:ILE:O	2.53	0.52
1:A:58:LEU:HG	1:B:62:LEU:HD11	1.90	0.52
1:A:12:TRP:HZ3	5:A:1606:HEX:C6	2.22	0.52
1:A:164:ARG:CG	1:B:159:LYS:N	2.70	0.52
1:A:58:LEU:O	1:B:59:SER:C	2.42	0.52
1:A:175:ARG:O	1:B:178:THR:N	2.43	0.52
1:B:101:VAL:O	1:B:163:MET:CA	2.56	0.52
1:B:57:TYR:OH	1:B:212:ASP:OD2	2.27	0.52
1:A:231:GLY:HA3	1:A:235:ALA:O	2.10	0.51
1:A:32:MET:CE	1:B:32:MET:HE1	2.37	0.51
1:A:191:ILE:HA	1:B:196:ALA:HB3	1.92	0.51
1:A:51:ALA:HB3	1:B:48:LEU:O	2.09	0.51
1:A:190:LEU:O	1:B:196:ALA:CB	2.59	0.51
1:A:60:MET:CG	1:B:79:TYR:HD1	2.23	0.51
4:B:609:OCT:C2	4:B:1609:OCT:C2	2.40	0.51
4:B:609:OCT:H21	4:B:1609:OCT:C1	2.37	0.51
1:A:64:TYR:CG	1:B:64:TYR:O	2.51	0.51
1:A:227:ARG:HB2	1:B:227:ARG:O	1.89	0.51
1:B:107:THR:O	1:B:111:LEU:HG	2.09	0.51
4:B:618:OCT:H61	5:B:1620:HEX:C2	2.40	0.51
1:A:45:ILE:HD11	1:B:95:LEU:CD2	1.81	0.51
1:A:31:GLY:HA2	1:B:34:VAL:HG21	1.91	0.51
1:A:43:TYR:O	1:B:44:ALA:C	2.48	0.51
1:B:67:THR:O	1:B:77:PRO:HA	2.11	0.51
1:A:151:VAL:C	1:B:153:PHE:H	2.14	0.51
1:A:165:PRO:HA	1:B:159:LYS:HE3	1.91	0.51
1:A:66:LEU:CD2	1:B:5:THR:OG1	2.58	0.51
1:A:81:ALA:O	1:B:84:ALA:HB3	2.10	0.51
1:A:85:ASP:O	1:B:88:PHE:HB2	2.11	0.51
1:A:162:SER:OG	1:B:162:SER:HB2	2.11	0.51
1:B:159:LYS:HB2	1:B:164:ARG:NE	2.26	0.51
1:B:43:TYR:OH	1:B:224:LEU:HD13	2.10	0.51
1:A:98:ALA:O	1:B:101:VAL:HG22	2.11	0.51
1:A:105:GLN:C	1:B:104:ASP:O	2.47	0.51
1:B:225:ARG:NH1	1:B:227:ARG:HH12	2.08	0.51
1:A:194:GLU:HB2	1:B:189:TRP:NE1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:OD1	1:B:36:ASP:N	2.42	0.51
1:A:60:MET:SD	1:B:79:TYR:HB3	2.51	0.51
1:A:98:ALA:HA	1:B:156:PHE:CZ	2.45	0.51
1:B:136:VAL:O	1:B:139:ALA:HB3	2.10	0.51
1:B:31:GLY:CA	7:B:864:HOH:O	2.45	0.51
1:A:192:GLY:O	1:B:194:GLU:N	2.44	0.50
1:A:86:TRP:O	1:B:87:LEU:C	2.44	0.50
1:B:145:MET:HE3	1:B:183:SER:HA	1.93	0.50
1:A:156:PHE:CE2	1:B:101:VAL:CG1	2.85	0.50
1:A:31:GLY:HA2	1:B:34:VAL:CG2	2.42	0.50
1:B:232:GLU:HA	7:B:740:HOH:O	1.99	0.50
1:A:236:PRO:O	1:B:236:PRO:O	2.30	0.50
1:A:54:PHE:CD2	1:B:54:PHE:C	2.77	0.50
4:B:613:OCT:C4	4:B:1613:OCT:C6	2.69	0.50
1:A:91:PRO:CD	1:B:90:THR:OG1	2.44	0.50
1:A:80:TRP:CZ2	1:B:65:GLY:HA2	2.46	0.50
1:B:98:ALA:CB	1:B:108:ILE:HD11	2.34	0.50
1:A:15:LEU:O	1:B:19:LEU:HG	2.11	0.50
1:B:96:ASP:OD1	1:B:223:LEU:HD22	2.11	0.50
1:A:124:VAL:HG22	1:B:121:THR:O	2.09	0.50
1:B:3:GLN:N	7:B:832:HOH:O	2.19	0.50
1:A:68:MET:HE1	1:B:77:PRO:HG3	1.83	0.50
1:A:20:MET:SD	1:B:216:LYS:HB2	2.52	0.50
1:A:137:TRP:CH2	1:B:137:TRP:HH2	1.20	0.50
1:A:134:ARG:HH12	1:B:134:ARG:HH12	0.51	0.50
1:A:15:LEU:CD1	1:B:15:LEU:CD1	2.42	0.50
1:B:169:SER:HB2	7:B:1856:HOH:O	2.11	0.50
1:A:207:LEU:HD23	4:A:1623:OCT:C7	2.42	0.50
1:A:80:TRP:CE3	1:B:80:TRP:CE3	0.66	0.50
1:A:80:TRP:CE3	1:B:80:TRP:HE3	1.21	0.50
1:A:100:LEU:HD12	1:B:174:LEU:CD1	2.42	0.50
1:A:194:GLU:HB2	1:B:189:TRP:CE2	2.47	0.50
1:A:223:LEU:HG	1:B:229:ILE:HD13	1.94	0.50
1:A:38:ASP:C	1:B:37:PRO:O	2.42	0.50
1:A:38:ASP:OD1	1:B:41:LYS:NZ	2.45	0.50
4:B:618:OCT:H22	5:B:1620:HEX:H61	1.83	0.50
1:A:150:TYR:HB3	1:B:147:TYR:O	2.12	0.50
1:B:224:LEU:C	1:B:226:SER:N	2.65	0.50
1:A:4:ILE:HD12	1:B:3:GLN:HG2	1.94	0.50
1:B:68:MET:CE	1:B:75:GLN:HB3	2.42	0.50
1:A:6:GLY:O	1:B:7:ARG:CB	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:N	1:B:13:LEU:HD23	2.27	0.49
1:A:76:ASN:ND2	1:B:71:PHE:CD2	2.80	0.49
1:B:151:VAL:O	1:B:156:PHE:HB2	1.93	0.49
1:A:164:ARG:HG3	1:B:159:LYS:CD	2.42	0.49
1:A:37:PRO:O	1:A:40:LYS:HB2	2.12	0.49
4:B:613:OCT:H52	4:B:1613:OCT:C5	2.10	0.49
1:A:87:LEU:O	1:B:91:PRO:HG2	2.12	0.49
1:A:15:LEU:HD13	1:B:15:LEU:HD12	1.85	0.49
1:A:54:PHE:C	1:B:53:ALA:O	2.45	0.49
1:B:117:ILE:HD12	4:B:607:OCT:H72	1.94	0.49
1:A:207:LEU:CA	1:B:206:LEU:HD13	2.40	0.49
1:A:207:LEU:N	1:B:207:LEU:HD23	2.27	0.49
1:A:119:ILE:HG21	1:B:87:LEU:CB	2.42	0.49
1:A:205:THR:O	1:B:206:LEU:C	2.42	0.49
1:A:55:THR:HG22	1:A:56:MET:HE3	1.95	0.49
1:A:60:MET:O	1:B:13:LEU:HD23	2.12	0.49
1:A:117:ILE:C	1:B:116:GLY:O	2.48	0.49
1:A:61:LEU:HA	1:B:13:LEU:HD23	1.92	0.49
1:A:208:PHE:O	1:B:209:MET:C	2.45	0.49
1:A:48:LEU:O	1:B:49:VAL:C	2.45	0.49
1:B:135:PHE:O	1:B:138:TRP:HB3	2.13	0.49
1:A:156:PHE:N	1:B:157:THR:O	2.45	0.49
1:B:29:VAL:CG2	3:B:614:UND:C1	2.87	0.49
1:A:216:LYS:HE2	1:B:89:THR:HG21	1.94	0.49
3:A:604:UND:H81	3:A:1604:UND:H92	0.49	0.49
1:A:2:ALA:HB1	7:B:1809:HOH:O	2.11	0.49
4:B:618:OCT:C8	3:B:1616:UND:C11	2.78	0.49
1:A:100:LEU:CD1	1:B:174:LEU:CD1	2.91	0.49
1:A:166:GLU:HB3	1:B:166:GLU:H	1.73	0.49
1:A:168:ALA:O	1:B:170:THR:N	2.46	0.49
1:B:145:MET:SD	1:B:186:PRO:HG2	2.47	0.49
1:A:225:ARG:HB3	1:B:225:ARG:CD	2.33	0.48
1:A:12:TRP:HA	1:B:12:TRP:HE3	1.78	0.48
1:B:212:ASP:CG	7:B:710:HOH:O	2.51	0.48
4:B:618:OCT:C4	4:B:1618:OCT:C7	2.65	0.48
1:A:82:ARG:HH11	1:B:82:ARG:CG	2.19	0.48
1:A:159:LYS:CB	1:B:159:LYS:CG	0.88	0.48
1:A:160:ALA:O	1:B:160:ALA:HB1	2.13	0.48
1:B:162:SER:CB	7:B:850:HOH:O	2.55	0.48
1:A:163:MET:C	1:B:165:PRO:CD	2.74	0.48
1:A:98:ALA:CB	1:B:156:PHE:CZ	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:MET:HE3	1:B:5:THR:HG21	1.95	0.48
1:A:159:LYS:HB3	7:B:858:HOH:O	2.13	0.48
1:A:166:GLU:CG	1:B:234:GLU:CA	2.64	0.48
1:A:172:LYS:CE	1:B:169:SER:OG	2.61	0.48
1:A:206:LEU:O	1:B:206:LEU:HD13	2.07	0.48
1:A:181:LEU:C	1:B:180:VAL:O	2.47	0.48
1:A:178:THR:CG2	1:B:182:TRP:NE1	2.63	0.48
1:A:107:THR:O	1:B:107:THR:CG2	2.55	0.48
2:A:601:RET:C12	1:B:185:TYR:CE2	2.97	0.48
1:B:227:ARG:HG2	1:B:238:PRO:HA	1.95	0.48
1:A:226:SER:OG	1:B:228:ALA:N	2.47	0.48
1:B:29:VAL:HG21	3:B:614:UND:H11	1.91	0.48
1:A:164:ARG:O	1:A:164:ARG:HG3	2.13	0.48
1:A:59:SER:N	1:B:56:MET:O	2.47	0.48
1:B:188:VAL:HG12	1:B:188:VAL:O	2.13	0.48
1:A:227:ARG:CZ	1:B:238:PRO:HB3	2.42	0.48
1:A:116:GLY:HA2	7:B:872:HOH:O	2.12	0.48
1:A:126:ALA:HB3	1:B:123:LEU:HD12	1.95	0.48
1:B:101:VAL:O	1:B:163:MET:HB3	2.13	0.48
1:A:158:SER:CB	1:B:160:ALA:CB	2.80	0.48
4:B:618:OCT:H51	5:B:1620:HEX:C5	2.42	0.48
1:A:94:LEU:HD13	1:B:182:TRP:CH2	2.49	0.48
1:B:83:TYR:CE1	2:B:601:RET:H162	2.48	0.48
1:A:119:ILE:HG21	1:B:87:LEU:HB2	1.95	0.48
4:A:1621:OCT:H82	4:B:621:OCT:C7	2.28	0.48
1:A:93:LEU:HA	1:B:93:LEU:HD23	1.55	0.48
4:B:609:OCT:H42	4:B:1609:OCT:H21	1.94	0.48
1:A:46:THR:N	1:B:45:ILE:HG22	2.29	0.47
1:A:130:VAL:HG11	1:B:133:TYR:CZ	2.49	0.47
1:A:169:SER:CB	1:B:167:VAL:HG12	2.37	0.47
1:A:29:VAL:O	1:B:30:LYS:C	2.45	0.47
1:A:112:VAL:CG1	5:A:1610:HEX:H62	2.44	0.47
1:A:174:LEU:CD1	1:B:223:LEU:CB	2.82	0.47
1:A:43:TYR:N	1:B:40:LYS:O	2.45	0.47
1:A:131:TYR:HD1	1:B:71:PHE:CD1	2.31	0.47
1:A:92:LEU:O	1:B:95:LEU:HB3	2.14	0.47
1:A:104:ASP:OD1	1:B:104:ASP:CG	2.47	0.47
1:A:12:TRP:CA	1:B:12:TRP:CE3	2.97	0.47
1:A:194:GLU:CA	1:B:134:ARG:HH21	2.27	0.47
1:A:36:ASP:HB2	1:A:39:ALA:CB	2.44	0.47
2:A:601:RET:C18	1:B:142:THR:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:OG1	1:B:117:ILE:O	2.33	0.47
1:A:165:PRO:HB3	1:B:161:GLU:H	0.61	0.47
1:A:227:ARG:CZ	1:B:227:ARG:CZ	2.84	0.47
1:A:199:VAL:HG23	1:B:198:ILE:HG22	1.96	0.47
1:A:217:VAL:O	1:B:218:GLY:O	2.32	0.47
1:A:78:ILE:N	1:B:76:ASN:O	2.48	0.47
1:A:164:ARG:O	1:B:159:LYS:NZ	2.47	0.47
1:A:55:THR:HG22	1:A:56:MET:CE	2.44	0.47
1:A:103:ALA:CB	1:B:101:VAL:HG23	2.38	0.47
1:B:182:TRP:O	1:B:186:PRO:HD3	2.06	0.47
1:A:12:TRP:HA	1:B:12:TRP:CE3	2.50	0.47
1:A:159:LYS:HE2	1:B:159:LYS:HZ3	1.79	0.47
1:B:29:VAL:CG2	3:B:614:UND:H11	2.44	0.47
1:A:197:GLY:O	7:A:1832:HOH:O	2.20	0.47
1:A:134:ARG:NH1	1:B:134:ARG:HH12	0.68	0.47
1:A:174:LEU:HD23	1:B:222:ILE:CG2	2.45	0.47
1:A:191:ILE:C	1:B:192:GLY:O	2.48	0.47
1:A:213:VAL:O	1:B:214:SER:C	2.45	0.47
1:B:43:TYR:CZ	1:B:224:LEU:HD13	2.50	0.47
1:A:107:THR:HG21	1:B:156:PHE:CD1	2.49	0.47
1:A:60:MET:SD	1:B:82:ARG:HB2	2.55	0.47
1:B:183:SER:C	1:B:186:PRO:HD2	2.35	0.47
1:A:188:VAL:HA	1:B:191:ILE:CG1	2.45	0.47
4:B:609:OCT:H72	4:B:1609:OCT:C8	2.00	0.47
1:A:128:THR:HG22	1:B:128:THR:HG22	0.66	0.47
1:A:168:ALA:O	1:B:169:SER:C	2.52	0.47
1:A:25:LEU:O	1:B:26:TYR:C	2.46	0.47
1:A:166:GLU:CD	1:B:234:GLU:HB2	2.31	0.47
1:A:79:TYR:HE1	1:B:66:LEU:HD22	1.74	0.47
1:A:101:VAL:HB	1:B:163:MET:O	2.14	0.47
1:B:159:LYS:NZ	1:B:165:PRO:O	2.48	0.47
1:A:56:MET:HE3	1:B:55:THR:CG2	2.45	0.47
1:A:172:LYS:NZ	1:B:172:LYS:HZ3	2.04	0.46
1:A:217:VAL:CG1	5:A:608:HEX:H32	2.38	0.46
1:B:164:ARG:HB2	1:B:168:ALA:HB1	1.96	0.46
1:A:161:GLU:HA	1:A:165:PRO:HB3	1.95	0.46
1:A:185:TYR:O	1:B:189:TRP:N	2.48	0.46
1:A:76:ASN:ND2	1:B:76:ASN:HD22	1.01	0.46
1:A:119:ILE:HG21	1:B:87:LEU:CA	2.45	0.46
5:A:1610:HEX:H62	1:B:112:VAL:HG11	1.92	0.46
1:A:179:VAL:C	1:B:178:THR:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:CE	1:B:56:MET:HA	2.46	0.46
1:A:87:LEU:HA	1:B:87:LEU:HD12	1.39	0.46
1:A:87:LEU:HD21	5:A:1610:HEX:C1	2.45	0.46
1:A:175:ARG:CZ	1:B:171:PHE:HE2	2.27	0.46
2:A:601:RET:C12	1:B:185:TYR:CZ	2.98	0.46
1:A:198:ILE:HG13	1:B:197:GLY:O	2.09	0.46
1:B:201:LEU:O	1:B:204:GLU:HG3	2.16	0.46
1:A:202:ASN:O	1:B:202:ASN:O	0.46	0.46
1:B:68:MET:HE3	1:B:75:GLN:CB	2.46	0.46
7:A:1817:HOH:O	1:B:7:ARG:HG2	2.15	0.46
1:A:56:MET:HE3	1:B:55:THR:HG22	1.98	0.46
1:B:232:GLU:HG2	7:B:740:HOH:O	2.16	0.46
1:A:203:ILE:CD1	4:A:1623:OCT:H22	2.44	0.46
1:A:219:PHE:CE1	1:B:223:LEU:HD22	2.35	0.46
1:A:235:ALA:O	1:B:235:ALA:O	2.31	0.46
1:A:12:TRP:N	1:B:11:ILE:HG13	2.31	0.46
1:A:187:VAL:HG12	1:B:191:ILE:CD1	2.46	0.46
1:B:68:MET:CG	1:B:75:GLN:HB3	2.46	0.46
1:A:130:VAL:HG21	1:B:133:TYR:HE2	1.77	0.46
1:A:98:ALA:HB2	1:B:156:PHE:CZ	2.37	0.46
2:A:601:RET:H193	1:B:185:TYR:HB2	1.97	0.46
1:B:188:VAL:HG12	1:B:208:PHE:CE2	2.50	0.46
1:A:185:TYR:CD2	1:B:208:PHE:HE1	2.33	0.46
1:A:174:LEU:CD2	1:B:222:ILE:CG2	2.93	0.46
1:A:53:ALA:O	1:B:57:TYR:HB2	2.16	0.46
5:A:610:HEX:H63	5:A:1610:HEX:H62	0.81	0.46
1:A:183:SER:C	1:B:186:PRO:HD2	2.33	0.46
1:A:13:LEU:HD13	1:A:205:THR:HG21	1.98	0.46
1:B:233:ALA:HB1	1:B:234:GLU:OE1	2.15	0.46
1:A:9:GLU:OE2	1:B:6:GLY:HA2	2.16	0.46
1:A:184:ALA:O	1:A:188:VAL:HG23	2.13	0.46
1:A:94:LEU:HD11	1:B:182:TRP:CH2	2.51	0.46
1:A:162:SER:CB	1:B:160:ALA:CB	2.90	0.46
4:B:618:OCT:C7	3:B:1616:UND:H113	2.46	0.46
1:A:201:LEU:CA	1:B:204:GLU:HG3	2.41	0.46
1:A:79:TYR:OH	1:B:9:GLU:OE2	2.34	0.46
1:A:53:ALA:HB2	1:B:216:LYS:HG2	1.97	0.45
1:A:87:LEU:HG	5:A:1610:HEX:C1	2.29	0.45
4:A:1621:OCT:H13	4:B:621:OCT:C3	2.23	0.45
1:A:203:ILE:HA	1:B:203:ILE:HD13	1.36	0.45
2:A:601:RET:H162	1:B:83:TYR:CE1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:C	1:B:149:LEU:O	2.48	0.45
1:B:29:VAL:HG13	5:B:619:HEX:H12	1.98	0.45
1:A:224:LEU:HB3	1:B:43:TYR:HH	1.81	0.45
7:A:1741:HOH:O	1:B:100:LEU:HD22	2.15	0.45
1:B:55:THR:HG22	1:B:56:MET:N	2.30	0.45
4:B:618:OCT:H81	3:B:1616:UND:H111	1.96	0.45
1:A:119:ILE:HG21	1:B:87:LEU:CD1	2.45	0.45
1:A:134:ARG:CG	1:B:128:THR:CB	2.74	0.45
5:A:620:HEX:C1	4:A:1617:OCT:H22	2.45	0.45
1:A:158:SER:HB2	1:A:162:SER:HB3	1.98	0.45
1:A:100:LEU:CD1	1:B:174:LEU:HD11	2.46	0.45
1:B:145:MET:CE	1:B:183:SER:HA	2.47	0.45
1:B:190:LEU:O	1:B:196:ALA:HB3	2.17	0.45
1:B:223:LEU:O	1:B:226:SER:HB3	2.17	0.45
1:A:170:THR:CB	1:B:226:SER:HG	2.28	0.45
1:B:5:THR:HG22	1:B:68:MET:CE	2.46	0.45
1:A:109:LEU:O	1:B:110:ALA:C	2.52	0.45
1:A:168:ALA:O	1:B:171:PHE:N	2.50	0.45
1:A:177:VAL:HG22	3:A:1604:UND:H81	1.99	0.45
1:A:58:LEU:HD11	1:B:62:LEU:HD21	1.98	0.45
1:A:172:LYS:HZ2	1:B:172:LYS:NZ	2.07	0.45
1:A:215:ALA:O	1:B:219:PHE:HB3	2.17	0.45
1:A:216:LYS:CE	1:B:89:THR:HG21	2.47	0.45
1:A:30:LYS:C	1:B:32:MET:N	2.70	0.45
1:A:160:ALA:CA	1:B:160:ALA:CA	2.89	0.45
1:A:166:GLU:CG	1:B:166:GLU:CD	2.76	0.45
1:A:76:ASN:ND2	1:B:71:PHE:N	2.64	0.45
1:A:59:SER:O	1:B:64:TYR:N	2.50	0.45
1:A:71:PHE:HD2	1:B:69:VAL:CG1	2.28	0.45
1:A:147:TYR:HE1	1:B:147:TYR:HE1	0.98	0.45
1:A:166:GLU:CB	1:B:234:GLU:HA	2.41	0.45
1:B:40:LYS:O	1:B:41:LYS:C	2.55	0.45
1:A:144:ALA:O	1:B:148:ILE:HG13	2.16	0.45
1:A:206:LEU:HD11	4:A:1605:OCT:H22	1.98	0.45
1:B:198:ILE:HG22	1:B:199:VAL:CG2	2.47	0.45
1:A:147:TYR:CE1	1:B:147:TYR:HE1	1.15	0.45
1:B:163:MET:O	1:B:164:ARG:HB3	2.17	0.45
1:B:198:ILE:HG22	1:B:199:VAL:HG22	1.99	0.45
1:A:224:LEU:HA	1:B:229:ILE:HD11	1.99	0.45
1:B:24:THR:HG22	1:B:28:LEU:HD11	1.98	0.45
1:A:29:VAL:O	1:B:32:MET:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:C	1:B:133:TYR:O	2.55	0.44
1:B:42:PHE:CE2	1:B:229:ILE:HG22	2.52	0.44
1:A:224:LEU:HD11	1:B:46:THR:CG2	2.48	0.44
1:B:97:LEU:HD13	1:B:152:LEU:CD2	2.42	0.44
1:A:159:LYS:NZ	1:B:164:ARG:NH2	2.65	0.44
1:A:125:GLY:O	1:B:126:ALA:C	2.52	0.44
1:A:212:ASP:O	1:B:215:ALA:N	2.51	0.44
1:A:232:GLU:OE1	1:B:232:GLU:O	2.36	0.44
1:A:54:PHE:CD2	1:B:55:THR:N	2.84	0.44
4:A:1621:OCT:C8	4:B:621:OCT:C7	2.79	0.44
4:A:1623:OCT:H71	1:B:206:LEU:CD1	2.47	0.44
1:A:176:ASN:OD1	1:B:172:LYS:O	2.35	0.44
1:A:53:ALA:CA	1:B:85:ASP:OD1	2.64	0.44
1:A:137:TRP:CH2	1:B:137:TRP:CH2	0.65	0.44
1:A:164:ARG:HB2	1:A:168:ALA:CB	2.47	0.44
1:A:187:VAL:HG12	1:B:191:ILE:HD13	1.98	0.44
1:A:29:VAL:C	1:B:31:GLY:N	2.56	0.44
1:A:159:LYS:CB	1:B:159:LYS:HG3	0.18	0.44
1:A:169:SER:O	1:B:173:VAL:HG23	2.16	0.44
1:A:88:PHE:O	1:B:91:PRO:HD2	2.16	0.44
1:A:10:TRP:CE2	1:B:11:ILE:HG22	2.52	0.44
1:A:191:ILE:HB	1:B:198:ILE:HB	1.98	0.44
1:A:202:ASN:N	7:B:1800:HOH:O	2.43	0.44
1:A:207:LEU:CD2	4:A:1623:OCT:H72	2.48	0.44
1:A:91:PRO:CD	1:B:90:THR:CB	2.89	0.44
1:A:21:GLY:O	1:B:24:THR:HB	2.17	0.44
1:A:120:GLY:O	1:B:124:VAL:CG1	2.65	0.44
1:A:182:TRP:O	1:B:185:TYR:N	2.50	0.44
1:A:79:TYR:CG	1:B:66:LEU:HD13	2.45	0.44
1:A:182:TRP:CH2	1:B:94:LEU:HD11	2.48	0.44
1:A:95:LEU:HD23	1:A:95:LEU:O	2.13	0.44
1:A:95:LEU:O	1:A:99:LEU:HB2	2.17	0.44
1:A:103:ALA:C	1:B:102:ASP:O	2.55	0.44
1:B:203:ILE:CG2	1:B:207:LEU:HD21	2.47	0.44
1:B:237:GLU:N	1:B:238:PRO:HD3	2.32	0.44
1:A:78:ILE:CG1	1:B:69:VAL:HB	2.47	0.44
1:A:119:ILE:HG21	1:B:87:LEU:HA	2.00	0.44
1:A:157:THR:HA	1:B:163:MET:HG2	1.94	0.44
3:A:604:UND:C8	3:A:1604:UND:C9	0.78	0.44
5:A:620:HEX:H61	1:B:186:PRO:HB2	2.00	0.44
1:A:235:ALA:H	1:B:234:GLU:N	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HA	1:B:146:LEU:HD23	1.53	0.43
1:A:137:TRP:HH2	1:B:137:TRP:CH2	1.14	0.43
1:A:101:VAL:HG11	1:B:163:MET:O	2.12	0.43
1:A:5:THR:HG22	1:B:68:MET:CE	2.47	0.43
1:A:83:TYR:CG	1:B:123:LEU:HB2	2.53	0.43
1:A:101:VAL:CB	1:B:163:MET:C	2.86	0.43
1:B:174:LEU:O	1:B:178:THR:OG1	2.36	0.43
1:A:239:SER:N	1:B:239:SER:N	2.66	0.43
1:B:48:LEU:HD11	6:B:611:TRD:H121	1.98	0.43
1:A:99:LEU:HD12	1:B:99:LEU:HA	1.74	0.43
1:A:164:ARG:HG3	1:B:159:LYS:HD2	2.01	0.43
1:B:29:VAL:HG21	3:B:1614:UND:C1	2.47	0.43
5:A:620:HEX:C6	1:B:187:VAL:HG22	2.26	0.43
1:B:209:MET:HE3	1:B:213:VAL:HG23	1.99	0.43
1:A:237:GLU:OE2	1:B:36:ASP:OD2	2.37	0.43
4:B:609:OCT:C3	4:B:1609:OCT:C2	2.71	0.43
1:B:65:GLY:HA3	1:B:81:ALA:CB	2.47	0.43
3:A:604:UND:H82	3:A:1604:UND:C9	0.23	0.43
1:A:94:LEU:CD2	1:B:182:TRP:HH2	2.31	0.43
1:A:96:ASP:O	1:B:42:PHE:CE1	2.71	0.43
1:A:25:LEU:HD23	1:B:25:LEU:HA	1.69	0.43
1:A:168:ALA:HB2	1:B:164:ARG:HB2	2.00	0.43
1:B:15:LEU:HD21	1:B:19:LEU:HD11	2.00	0.43
1:A:64:TYR:HD1	1:B:64:TYR:C	2.10	0.43
1:A:5:THR:OG1	1:B:6:GLY:N	2.52	0.43
1:B:159:LYS:HD3	1:B:164:ARG:HE	1.84	0.43
1:B:4:ILE:CG1	7:B:1805:HOH:O	2.66	0.43
1:A:13:LEU:HD13	1:A:205:THR:CG2	2.48	0.43
1:A:43:TYR:HB2	1:B:40:LYS:O	2.17	0.43
1:B:148:ILE:O	1:B:152:LEU:HD13	2.11	0.43
1:A:167:VAL:CG2	1:B:166:GLU:CA	2.79	0.43
1:A:174:LEU:N	1:B:173:VAL:HB	2.20	0.43
1:A:188:VAL:HA	1:B:191:ILE:HG13	2.00	0.43
1:A:3:GLN:NE2	1:A:4:ILE:HD11	2.34	0.43
1:B:177:VAL:O	1:B:178:THR:C	2.50	0.43
1:A:211:LEU:HD11	1:B:188:VAL:HG21	2.01	0.43
1:B:43:TYR:CE2	1:B:224:LEU:HD22	2.53	0.43
3:A:604:UND:H82	3:A:1604:UND:H91	0.99	0.43
6:A:612:TRD:H92	6:A:1612:TRD:H91	1.36	0.43
1:A:92:LEU:N	1:B:90:THR:C	2.65	0.43
1:A:166:GLU:HA	7:A:1854:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:CG2	1:B:226:SER:CB	2.97	0.42
1:A:224:LEU:HD22	1:B:43:TYR:CE1	2.51	0.42
1:A:27:PHE:N	1:B:26:TYR:CD2	2.87	0.42
1:B:126:ALA:HA	1:B:134:ARG:NH2	2.30	0.42
1:B:24:THR:O	1:B:28:LEU:HG	2.16	0.42
1:A:94:LEU:N	1:B:94:LEU:HD12	2.29	0.42
1:A:182:TRP:HB2	1:B:182:TRP:HB2	0.85	0.42
1:A:71:PHE:HD1	1:B:72:GLY:N	2.17	0.42
1:A:82:ARG:NH1	7:A:1716:HOH:O	2.41	0.42
1:B:128:THR:HG21	1:B:133:TYR:HB2	2.01	0.42
1:B:171:PHE:CE2	1:B:175:ARG:HB2	2.54	0.42
1:A:219:PHE:HE1	1:B:96:ASP:OD1	2.02	0.42
1:A:107:THR:HB	1:B:103:ALA:HB1	2.01	0.42
1:A:124:VAL:HG22	1:B:121:THR:C	2.40	0.42
1:A:158:SER:HB3	1:B:160:ALA:HB2	1.99	0.42
3:A:1604:UND:H22	6:A:1612:TRD:H61	2.02	0.42
1:B:94:LEU:CD1	1:B:182:TRP:CH2	2.87	0.42
1:B:28:LEU:HD23	1:B:47:THR:HG21	2.00	0.42
1:A:74:GLU:O	1:B:71:PHE:N	2.53	0.42
1:A:154:PHE:CD1	1:B:154:PHE:N	2.85	0.42
1:A:58:LEU:CG	1:B:62:LEU:HD11	2.47	0.42
1:A:100:LEU:HD12	1:B:174:LEU:HD13	2.00	0.42
1:A:211:LEU:HA	1:B:211:LEU:HD23	1.61	0.42
1:A:43:TYR:CD2	1:B:34:VAL:HG21	2.53	0.42
1:A:67:THR:H	1:B:66:LEU:HD12	1.84	0.42
1:B:13:LEU:N	1:B:13:LEU:HD12	2.34	0.42
1:B:18:ALA:O	1:B:22:LEU:HD23	2.12	0.42
1:B:232:GLU:HB2	7:B:740:HOH:O	2.11	0.42
6:A:1615:TRD:H101	6:B:615:TRD:C12	2.47	0.42
1:A:175:ARG:HB3	1:B:172:LYS:O	2.19	0.42
1:A:211:LEU:C	1:B:210:VAL:O	2.53	0.42
1:A:12:TRP:CE2	1:B:11:ILE:HD11	2.55	0.42
1:A:164:ARG:CD	1:B:159:LYS:HB2	2.47	0.42
1:A:175:ARG:N	1:B:173:VAL:O	2.51	0.42
1:A:207:LEU:O	1:B:210:VAL:HB	2.19	0.42
1:B:4:ILE:HG12	7:B:1805:HOH:O	2.19	0.42
4:A:605:OCT:C6	4:A:623:OCT:H22	2.46	0.42
1:A:108:ILE:HG21	1:B:108:ILE:HD13	1.65	0.42
1:A:179:VAL:N	1:B:177:VAL:C	2.68	0.42
1:A:180:VAL:O	1:B:180:VAL:HG12	2.18	0.42
1:A:192:GLY:CA	7:A:1717:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:605:OCT:H51	4:A:1605:OCT:H22	1.28	0.42
1:A:159:LYS:HE2	1:B:159:LYS:NZ	2.12	0.42
1:B:212:ASP:O	1:B:216:LYS:N	2.52	0.42
1:B:26:TYR:CD2	1:B:27:PHE:N	2.88	0.42
1:A:64:TYR:O	1:B:66:LEU:N	2.43	0.42
1:B:151:VAL:C	1:B:153:PHE:H	2.17	0.42
1:B:15:LEU:HD11	1:B:19:LEU:CD1	2.49	0.42
1:B:61:LEU:HD12	1:B:61:LEU:C	2.30	0.42
1:A:170:THR:O	1:B:174:LEU:CG	2.61	0.42
1:A:57:TYR:HA	1:B:60:MET:HE2	1.99	0.42
1:A:149:LEU:HA	1:B:149:LEU:HD23	1.55	0.42
3:B:616:UND:H111	3:B:1616:UND:H112	0.73	0.42
1:A:7:ARG:HB3	1:B:8:PRO:CD	2.50	0.42
1:A:70:PRO:O	1:B:129:LYS:CB	2.68	0.41
1:A:83:TYR:CD1	1:B:123:LEU:HB2	2.55	0.41
1:B:117:ILE:HD12	4:B:607:OCT:C7	2.50	0.41
1:B:29:VAL:O	1:B:32:MET:HG2	2.20	0.41
1:A:174:LEU:O	1:B:219:PHE:CE1	2.73	0.41
4:B:609:OCT:H82	4:B:1609:OCT:H61	1.22	0.41
1:B:162:SER:O	1:B:232:GLU:OE2	2.37	0.41
1:B:162:SER:HB2	1:B:163:MET:SD	2.60	0.41
1:B:34:VAL:HA	7:B:1867:HOH:O	2.20	0.41
6:A:1615:TRD:H41	6:B:615:TRD:H42	0.80	0.41
5:B:622:HEX:C1	7:B:821:HOH:O	2.68	0.41
1:A:131:TYR:HD1	1:B:71:PHE:HD1	1.68	0.41
1:A:174:LEU:HD11	1:B:223:LEU:CA	2.51	0.41
1:A:203:ILE:O	1:B:203:ILE:CG2	2.68	0.41
1:A:2:ALA:HB3	7:B:1809:HOH:O	2.17	0.41
1:A:42:PHE:CD2	1:B:229:ILE:CB	2.89	0.41
1:A:47:THR:HG22	1:B:47:THR:O	2.16	0.41
1:A:12:TRP:N	1:B:11:ILE:CG1	2.84	0.41
1:A:53:ALA:HA	1:B:85:ASP:CG	2.41	0.41
1:A:76:ASN:HA	1:A:77:PRO:HD3	1.82	0.41
1:A:77:PRO:HG3	7:B:1834:HOH:O	2.19	0.41
7:A:742:HOH:O	1:B:231:GLY:HA2	2.19	0.41
1:B:30:LYS:O	1:B:32:MET:N	2.54	0.41
1:B:86:TRP:O	1:B:90:THR:OG1	2.34	0.41
1:A:172:LYS:N	1:B:170:THR:O	2.52	0.41
1:B:45:ILE:HG23	1:B:92:LEU:HB3	2.01	0.41
1:A:7:ARG:NH2	7:A:1811:HOH:O	2.53	0.41
1:B:130:VAL:HG11	1:B:133:TYR:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LEU:O	1:B:196:ALA:CB	2.68	0.41
1:B:225:ARG:HH12	1:B:227:ARG:HH12	1.68	0.41
1:A:29:VAL:HG23	1:B:29:VAL:H	1.56	0.41
1:B:38:ASP:HA	1:B:41:LYS:NZ	2.35	0.41
1:B:95:LEU:HD23	1:B:95:LEU:C	2.41	0.41
5:A:606:HEX:H12	5:A:1606:HEX:H22	1.21	0.41
1:A:192:GLY:HA3	7:A:1717:HOH:O	2.21	0.41
1:A:78:ILE:HG12	1:B:69:VAL:HB	2.03	0.41
1:A:129:LYS:N	7:A:1816:HOH:O	2.15	0.41
1:A:20:MET:CE	1:B:216:LYS:CD	2.90	0.41
1:A:22:LEU:HD13	1:B:22:LEU:HA	1.66	0.41
1:A:36:ASP:C	1:B:35:SER:O	2.47	0.41
1:A:172:LYS:HB3	1:B:169:SER:C	2.37	0.41
1:A:61:LEU:CA	1:B:13:LEU:HD23	2.50	0.41
1:B:15:LEU:HD11	1:B:19:LEU:HD12	2.03	0.41
1:B:164:ARG:O	1:B:168:ALA:HB2	2.20	0.41
4:B:618:OCT:H62	4:B:1618:OCT:H61	1.20	0.41
1:B:102:ASP:CB	7:B:850:HOH:O	2.69	0.41
1:A:224:LEU:CD1	1:B:46:THR:CG2	2.99	0.41
1:A:121:THR:O	1:A:124:VAL:CG2	2.69	0.41
1:A:232:GLU:HB2	7:B:740:HOH:O	1.92	0.41
2:A:601:RET:H8	2:B:601:RET:H171	2.03	0.41
1:A:132:SER:HG	1:B:132:SER:HB3	0.70	0.41
1:A:179:VAL:HG23	1:B:179:VAL:H	1.45	0.41
1:B:207:LEU:O	1:B:211:LEU:HG	2.21	0.41
1:A:56:MET:HE2	1:B:56:MET:HA	2.02	0.41
1:A:62:LEU:HD23	1:B:62:LEU:HA	1.41	0.41
1:A:79:TYR:HA	1:B:66:LEU:CD1	2.51	0.41
1:A:152:LEU:CD2	1:B:178:THR:HG21	2.51	0.40
1:A:202:ASN:C	1:B:202:ASN:ND2	2.69	0.40
1:A:126:ALA:CB	1:B:123:LEU:O	2.66	0.40
1:B:225:ARG:NH1	1:B:227:ARG:NH1	2.68	0.40
1:A:189:TRP:CD1	2:B:601:RET:H22	2.56	0.40
1:B:94:LEU:N	1:B:94:LEU:CD1	2.79	0.40
1:A:81:ALA:HB3	1:B:60:MET:HG2	2.03	0.40
1:A:83:TYR:O	1:B:87:LEU:HB3	2.15	0.40
1:A:9:GLU:OE1	1:B:8:PRO:HD2	2.21	0.40
1:A:120:GLY:N	1:B:116:GLY:O	2.55	0.40
1:A:21:GLY:O	1:B:24:THR:N	2.55	0.40
1:A:43:TYR:HD2	1:B:34:VAL:HG11	1.84	0.40
4:B:607:OCT:C1	4:B:1607:OCT:H32	2.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:MET:SD	1:B:77:PRO:CD	3.10	0.40
1:A:219:PHE:O	1:B:220:GLY:C	2.57	0.40
1:A:183:SER:CB	5:A:620:HEX:H31	2.51	0.40
1:A:7:ARG:O	1:A:10:TRP:HD1	2.05	0.40
1:A:162:SER:CA	1:B:161:GLU:O	2.59	0.40
1:A:207:LEU:C	1:B:206:LEU:O	2.59	0.40
1:A:76:ASN:ND2	1:B:74:GLU:O	2.54	0.40
1:A:80:TRP:HE3	1:B:80:TRP:CE3	1.10	0.40
1:A:175:ARG:O	1:B:177:VAL:N	2.51	0.40
1:A:229:ILE:HG13	1:A:230:PHE:CD1	2.57	0.40
1:A:28:LEU:HD13	1:B:28:LEU:HD13	0.44	0.40
1:A:83:TYR:N	1:B:80:TRP:O	2.55	0.40
1:A:98:ALA:CA	1:B:101:VAL:HG22	2.46	0.40
1:A:147:TYR:C	1:B:146:LEU:O	2.56	0.40
1:A:20:MET:SD	1:B:216:LYS:CB	3.09	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236 / 248 (95%)	218 (92%)	14 (6%)	4 (2%)	9	4
1	B	236 / 248 (95%)	184 (78%)	37 (16%)	15 (6%)	1	0
All	All	472 / 496 (95%)	402 (85%)	51 (11%)	19 (4%)	3	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	SER
1	B	159	LYS
1	B	165	PRO

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Mol	Chain	Res	Type
1	B	166	GLU
1	B	238	PRO
1	A	233	ALA
1	B	4	ILE
1	B	31	GLY
1	B	118	MET
1	B	164	ARG
1	B	234	GLU
1	A	7	ARG
1	B	7	ARG
1	B	161	GLU
1	B	71	PHE
1	B	162	SER
1	B	179	VAL
1	A	162	SER
1	A	165	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/195 (97%)	178 (94%)	12 (6%)	18	17
1	B	190/195 (97%)	171 (90%)	19 (10%)	7	5
All	All	380/390 (97%)	349 (92%)	31 (8%)	11	10

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	ARG
1	A	13	LEU
1	A	15	LEU
1	A	36	ASP
1	A	74	GLU
1	A	94	LEU

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Mol	Chain	Res	Type
1	A	102	ASP
1	A	109	LEU
1	A	206	LEU
1	A	227	ARG
1	A	234	GLU
1	B	7	ARG
1	B	55	THR
1	B	61	LEU
1	B	90	THR
1	B	105	GLN
1	B	109	LEU
1	B	124	VAL
1	B	153	PHE
1	B	156	PHE
1	B	157	THR
1	B	163	MET
1	B	166	GLU
1	B	181	LEU
1	B	202	ASN
1	B	206	LEU
1	B	209	MET
1	B	225	ARG
1	B	227	ARG
1	B	234	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	76	ASN
1	B	3	GLN
1	B	105	GLN
1	B	176	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

44 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	HEX	A	1610	5	5,5,5	0.31	0	4,4,4	0.20	0
5	HEX	B	622	5	5,5,5	0.20	0	4,4,4	0.28	0
4	OCT	B	618	4	7,7,7	0.51	0	6,6,6	0.52	0
4	OCT	B	613	4	7,7,7	0.19	0	6,6,6	0.32	0
4	OCT	A	623	4	7,7,7	0.42	0	6,6,6	0.45	0
5	HEX	A	606	5	5,5,5	0.24	0	4,4,4	0.13	0
4	OCT	A	1621	4	7,7,7	0.21	0	6,6,6	0.16	0
6	TRD	B	615	6	12,12,12	0.28	0	11,11,11	0.32	0
5	HEX	B	619	5	5,5,5	0.62	0	4,4,4	0.25	0
6	TRD	B	611	1,6	12,12,12	0.32	0	11,11,11	0.93	0
5	HEX	A	608	5	5,5,5	0.58	0	4,4,4	0.16	0
3	UND	B	616	3	10,10,10	0.26	0	9,9,9	0.45	0
5	HEX	A	610	5	5,5,5	0.37	0	4,4,4	0.28	0
5	HEX	A	1606	5	5,5,5	0.22	0	4,4,4	0.14	0
3	UND	A	1624	3	10,10,10	0.24	0	9,9,9	0.31	0
4	OCT	B	1613	4	7,7,7	0.20	0	6,6,6	0.13	0
6	TRD	A	1612	6	12,12,12	0.20	0	11,11,11	0.24	0
6	TRD	B	1611	6	12,12,12	0.22	0	11,11,11	0.36	0
5	HEX	A	1608	5	5,5,5	0.26	0	4,4,4	0.17	0
4	OCT	B	621	4	7,7,7	0.39	0	6,6,6	0.54	0
2	RET	A	601	1,2	20,20,21	2.23	5 (25%)	27,27,28	1.68	6 (22%)
2	RET	B	601	1,2	20,20,21	2.87	6 (30%)	27,27,28	2.19	10 (37%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UND	A	624	3	10,10,10	0.31	0	9,9,9	0.70	0
3	UND	A	1604	3	10,10,10	0.20	0	9,9,9	0.28	0
4	OCT	A	1617	4	7,7,7	0.15	0	6,6,6	0.18	0
5	HEX	A	620	5	5,5,5	0.39	0	4,4,4	0.19	0
4	OCT	A	605	4	7,7,7	0.15	0	6,6,6	0.41	0
3	UND	B	1614	3	10,10,10	0.24	0	9,9,9	0.28	0
3	UND	B	1616	3	10,10,10	0.23	0	9,9,9	0.11	0
5	HEX	A	1622	5	5,5,5	0.21	0	4,4,4	0.19	0
6	TRD	A	612	6	12,12,12	0.25	0	11,11,11	0.42	0
4	OCT	B	1618	4	7,7,7	0.20	0	6,6,6	0.12	0
4	OCT	B	607	4	7,7,7	0.42	0	6,6,6	0.50	0
5	HEX	B	1620	5	5,5,5	0.28	0	4,4,4	0.16	0
6	TRD	A	1615	6	12,12,12	0.21	0	11,11,11	0.39	0
4	OCT	A	1623	4	7,7,7	0.27	0	6,6,6	0.12	0
4	OCT	A	617	4	7,7,7	0.41	0	6,6,6	0.69	0
3	UND	B	614	3	10,10,10	0.32	0	9,9,9	0.49	0
4	OCT	B	609	4	7,7,7	0.44	0	6,6,6	0.47	0
4	OCT	A	1605	4	7,7,7	0.22	0	6,6,6	0.21	0
3	UND	A	604	3	10,10,10	0.52	0	9,9,9	0.69	0
5	HEX	B	1619	5	5,5,5	0.18	0	4,4,4	0.18	0
4	OCT	B	1609	4	7,7,7	0.17	0	6,6,6	0.20	0
4	OCT	B	1607	4	7,7,7	0.17	0	6,6,6	0.23	0

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	HEX	A	1610	5	-	2/3/3/3	-
5	HEX	B	622	5	-	2/3/3/3	-
4	OCT	B	618	4	-	4/5/5/5	-
4	OCT	B	613	4	-	3/5/5/5	-
4	OCT	A	623	4	-	3/5/5/5	-
5	HEX	A	606	5	-	2/3/3/3	-
4	OCT	A	1621	4	-	4/5/5/5	-
6	TRD	B	615	6	-	4/10/10/10	-
5	HEX	B	619	5	-	1/3/3/3	-
6	TRD	B	611	1,6	-	3/10/10/10	-
5	HEX	A	608	5	-	2/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UND	B	616	3	-	4/8/8/8	-
5	HEX	A	610	5	-	2/3/3/3	-
5	HEX	A	1606	5	-	2/3/3/3	-
3	UND	A	1624	3	-	5/8/8/8	-
4	OCT	B	1613	4	-	4/5/5/5	-
6	TRD	A	1612	6	-	3/10/10/10	-
6	TRD	B	1611	6	-	5/10/10/10	-
5	HEX	A	1608	5	-	2/3/3/3	-
4	OCT	B	621	4	-	3/5/5/5	-
2	RET	A	601	1,2	-	0/13/30/31	0/1/1/1
2	RET	B	601	1,2	-	1/13/30/31	0/1/1/1
3	UND	A	624	3	-	2/8/8/8	-
3	UND	A	1604	3	-	2/8/8/8	-
4	OCT	A	1617	4	-	4/5/5/5	-
5	HEX	A	620	5	-	2/3/3/3	-
4	OCT	A	605	4	-	3/5/5/5	-
3	UND	B	1614	3	-	4/8/8/8	-
3	UND	B	1616	3	-	5/8/8/8	-
5	HEX	A	1622	5	-	2/3/3/3	-
6	TRD	A	612	6	-	3/10/10/10	-
4	OCT	B	1618	4	-	4/5/5/5	-
4	OCT	B	607	4	-	4/5/5/5	-
5	HEX	B	1620	5	-	1/3/3/3	-
6	TRD	A	1615	6	-	5/10/10/10	-
4	OCT	A	1623	4	-	2/5/5/5	-
4	OCT	A	617	4	-	3/5/5/5	-
3	UND	B	614	3	-	4/8/8/8	-
4	OCT	B	609	4	-	3/5/5/5	-
4	OCT	A	1605	4	-	3/5/5/5	-
3	UND	A	604	3	-	3/8/8/8	-
5	HEX	B	1619	5	-	2/3/3/3	-
4	OCT	B	1609	4	-	3/5/5/5	-
4	OCT	B	1607	4	-	4/5/5/5	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	RET	C14-C13	8.93	1.40	1.33
2	A	601	RET	C1-C6	7.29	1.63	1.53
2	B	601	RET	C1-C6	6.65	1.62	1.53
2	A	601	RET	C5-C6	3.03	1.39	1.34
2	A	601	RET	C7-C6	2.92	1.55	1.45
2	A	601	RET	C2-C3	-2.80	1.45	1.52
2	B	601	RET	C5-C6	2.74	1.39	1.34
2	A	601	RET	C2-C1	2.64	1.60	1.54
2	B	601	RET	C20-C13	2.31	1.55	1.50
2	B	601	RET	C2-C3	-2.30	1.46	1.52
2	B	601	RET	C2-C1	2.21	1.59	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	RET	C8-C7-C6	5.10	141.53	127.20
2	B	601	RET	C18-C5-C6	4.33	129.39	124.53
2	B	601	RET	C2-C3-C4	3.70	119.64	111.38
2	B	601	RET	C17-C1-C6	3.53	116.03	110.30
2	B	601	RET	C11-C10-C9	3.46	132.24	127.31
2	B	601	RET	C18-C5-C4	-3.34	107.19	113.62
2	A	601	RET	C18-C5-C6	3.15	128.06	124.53
2	A	601	RET	C17-C1-C6	2.99	115.15	110.30
2	A	601	RET	C20-C13-C12	2.79	122.47	118.08
2	B	601	RET	C10-C11-C12	2.61	131.35	123.22
2	A	601	RET	C18-C5-C4	-2.50	108.82	113.62
2	B	601	RET	C8-C9-C10	-2.34	115.35	118.94
2	A	601	RET	C7-C8-C9	2.31	129.73	126.23
2	B	601	RET	C2-C1-C6	2.23	113.91	110.48
2	B	601	RET	C17-C1-C2	-2.21	100.07	108.91
2	A	601	RET	C12-C13-C14	-2.01	112.43	118.80

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	617	OCT	C2-C3-C4-C5
6	B	611	TRD	C4-C5-C6-C7
3	B	616	UND	C2-C3-C4-C5
4	A	605	OCT	C2-C3-C4-C5
4	B	618	OCT	C4-C5-C6-C7
5	A	1608	HEX	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	616	UND	C6-C7-C8-C9
3	B	614	UND	C6-C7-C8-C9
3	B	1614	UND	C6-C7-C8-C9
3	A	1624	UND	C2-C3-C4-C5
6	A	1615	TRD	C6-C7-C8-C9
6	B	615	TRD	C2-C3-C4-C5
5	A	1610	HEX	C2-C3-C4-C5
6	A	612	TRD	C11-C10-C9-C8
4	B	1609	OCT	C2-C3-C4-C5
4	B	1618	OCT	C4-C5-C6-C7
4	B	607	OCT	C2-C3-C4-C5
4	A	605	OCT	C4-C5-C6-C7
4	A	623	OCT	C2-C3-C4-C5
6	B	1611	TRD	C6-C7-C8-C9
3	A	1624	UND	C6-C7-C8-C9
4	A	1617	OCT	C4-C5-C6-C7
4	B	607	OCT	C4-C5-C6-C7
5	A	1622	HEX	C2-C3-C4-C5
3	B	1616	UND	C2-C3-C4-C5
5	A	606	HEX	C2-C3-C4-C5
4	B	1607	OCT	C2-C3-C4-C5
6	B	1611	TRD	C11-C10-C9-C8
4	B	613	OCT	C4-C5-C6-C7
3	B	1614	UND	C2-C3-C4-C5
3	A	1624	UND	C4-C5-C6-C7
6	B	1611	TRD	C4-C5-C6-C7
3	A	1604	UND	C2-C3-C4-C5
6	A	1612	TRD	C4-C5-C6-C7
6	B	1611	TRD	C2-C3-C4-C5
4	B	609	OCT	C2-C3-C4-C5
4	B	1613	OCT	C4-C5-C6-C7
3	A	624	UND	C4-C5-C6-C7
3	A	1624	UND	C11-C10-C9-C8
3	B	614	UND	C11-C10-C9-C8
5	A	1606	HEX	C2-C3-C4-C5
6	B	611	TRD	C2-C3-C4-C5
4	B	1613	OCT	C2-C3-C4-C5
4	A	1621	OCT	C2-C3-C4-C5
6	B	615	TRD	C4-C5-C6-C7
3	B	1616	UND	C11-C10-C9-C8
6	A	1615	TRD	C2-C3-C4-C5
5	A	620	HEX	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	1617	OCT	C2-C3-C4-C5
4	A	1605	OCT	C4-C5-C6-C7
5	A	610	HEX	C2-C3-C4-C5
6	A	1615	TRD	C10-C11-C12-C13
4	B	621	OCT	C4-C5-C6-C7
3	A	604	UND	C11-C10-C9-C8
6	A	612	TRD	C6-C7-C8-C9
5	A	608	HEX	C2-C3-C4-C5
3	B	1616	UND	C6-C7-C8-C9
6	B	615	TRD	C10-C11-C12-C13
3	A	624	UND	C2-C3-C4-C5
3	B	1616	UND	C4-C5-C6-C7
4	B	1607	OCT	C4-C5-C6-C7
4	B	618	OCT	C5-C6-C7-C8
4	A	1621	OCT	C4-C5-C6-C7
4	B	1618	OCT	C2-C3-C4-C5
3	B	614	UND	C2-C3-C4-C5
4	B	607	OCT	C5-C6-C7-C8
4	B	621	OCT	C1-C2-C3-C4
2	B	601	RET	C9-C10-C11-C12
5	A	608	HEX	C1-C2-C3-C4
6	A	1612	TRD	C2-C3-C4-C5
4	B	609	OCT	C5-C6-C7-C8
5	A	606	HEX	C1-C2-C3-C4
4	B	618	OCT	C1-C2-C3-C4
4	A	617	OCT	C5-C6-C7-C8
3	A	604	UND	C2-C3-C4-C5
4	A	1621	OCT	C5-C6-C7-C8
4	A	605	OCT	C5-C6-C7-C8
3	B	616	UND	C1-C2-C3-C4
4	A	1605	OCT	C5-C6-C7-C8
4	B	621	OCT	C5-C6-C7-C8
3	A	604	UND	C1-C2-C3-C4
4	B	609	OCT	C1-C2-C3-C4
4	A	1617	OCT	C5-C6-C7-C8
6	A	1615	TRD	C1-C2-C3-C4
5	A	610	HEX	C1-C2-C3-C4
4	B	1613	OCT	C1-C2-C3-C4
4	B	1618	OCT	C1-C2-C3-C4
3	B	614	UND	C1-C2-C3-C4
5	A	1606	HEX	C1-C2-C3-C4
3	B	616	UND	C11-C10-C9-C8

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
4	B	1618	OCT	C5-C6-C7-C8
5	B	1620	HEX	C1-C2-C3-C4
4	B	1607	OCT	C5-C6-C7-C8
5	A	1610	HEX	C1-C2-C3-C4
3	A	1604	UND	C1-C2-C3-C4
3	B	1616	UND	C1-C2-C3-C4
5	B	1619	HEX	C2-C3-C4-C5
5	B	619	HEX	C1-C2-C3-C4
6	B	611	TRD	C1-C2-C3-C4
4	B	1613	OCT	C5-C6-C7-C8
6	B	1611	TRD	C1-C2-C3-C4
5	A	1608	HEX	C1-C2-C3-C4
3	B	1614	UND	C1-C2-C3-C4
4	A	1617	OCT	C1-C2-C3-C4
4	B	1609	OCT	C5-C6-C7-C8
4	A	1621	OCT	C1-C2-C3-C4
5	B	622	HEX	C1-C2-C3-C4
6	A	1612	TRD	C1-C2-C3-C4
5	A	620	HEX	C1-C2-C3-C4
5	B	622	HEX	C2-C3-C4-C5
5	B	1619	HEX	C1-C2-C3-C4
5	A	1622	HEX	C1-C2-C3-C4
4	A	1605	OCT	C1-C2-C3-C4
4	B	1609	OCT	C1-C2-C3-C4
4	A	1623	OCT	C1-C2-C3-C4
4	B	1607	OCT	C1-C2-C3-C4
4	B	613	OCT	C1-C2-C3-C4
4	B	613	OCT	C5-C6-C7-C8
4	B	607	OCT	C1-C2-C3-C4
4	A	1623	OCT	C5-C6-C7-C8
6	A	612	TRD	C1-C2-C3-C4
6	B	615	TRD	C1-C2-C3-C4
3	A	1624	UND	C1-C2-C3-C4
4	A	623	OCT	C5-C6-C7-C8
4	B	618	OCT	C2-C3-C4-C5
4	A	617	OCT	C1-C2-C3-C4
4	A	623	OCT	C1-C2-C3-C4
6	A	1615	TRD	C11-C10-C9-C8
3	B	1614	UND	C4-C5-C6-C7

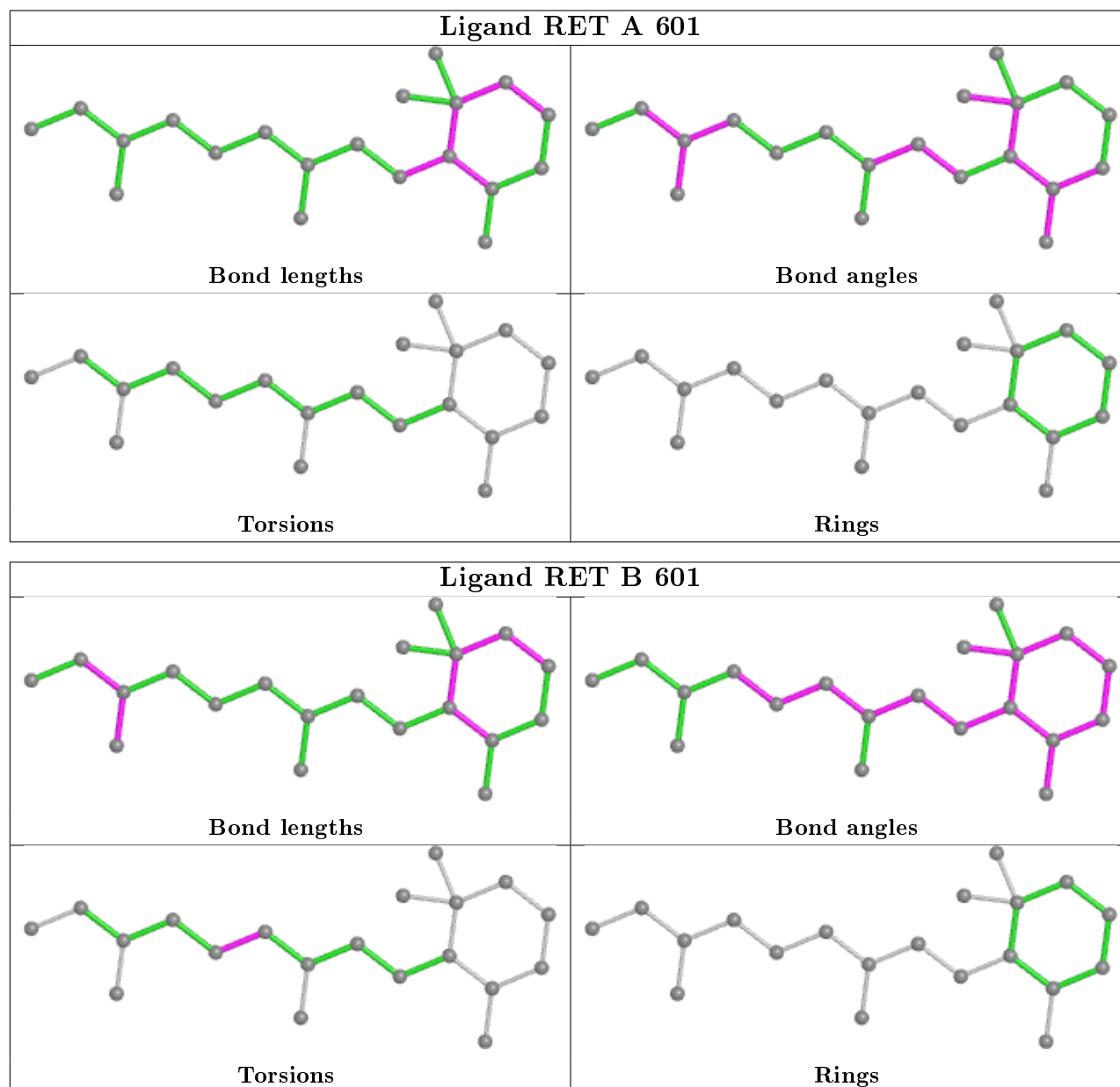
There are no ring outliers.

39 monomers are involved in 274 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1610	HEX	13	0
5	B	622	HEX	16	0
4	B	618	OCT	33	0
4	B	613	OCT	4	0
4	A	623	OCT	16	0
5	A	606	HEX	7	0
4	A	1621	OCT	13	0
6	B	615	TRD	9	0
5	B	619	HEX	3	0
6	B	611	TRD	19	0
5	A	608	HEX	3	0
3	B	616	UND	1	0
5	A	610	HEX	2	0
5	A	1606	HEX	6	0
4	B	1613	OCT	6	0
6	A	1612	TRD	2	0
4	B	621	OCT	13	0
2	A	601	RET	9	0
2	B	601	RET	11	0
3	A	1604	UND	32	0
4	A	1617	OCT	4	0
5	A	620	HEX	14	0
4	A	605	OCT	3	0
3	B	1614	UND	1	0
3	B	1616	UND	7	0
5	A	1622	HEX	14	0
6	A	612	TRD	1	0
4	B	1618	OCT	18	0
4	B	607	OCT	11	0
5	B	1620	HEX	12	0
6	A	1615	TRD	9	0
4	A	1623	OCT	16	0
3	B	614	UND	9	0
4	B	609	OCT	32	0
4	A	1605	OCT	7	0
3	A	604	UND	15	0
5	B	1619	HEX	2	0
4	B	1609	OCT	30	0
4	B	1607	OCT	9	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 than 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.



## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.