



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:51 am BST

PDB ID : 2RCR  
Title : STRUCTURE OF THE MEMBRANE-BOUND PROTEIN PHOTOSYN-  
THETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES  
Authors : Chang, C.-H.; Norris, J.; Schiffer, M.  
Deposited on : 1991-02-04  
Resolution : 3.10 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

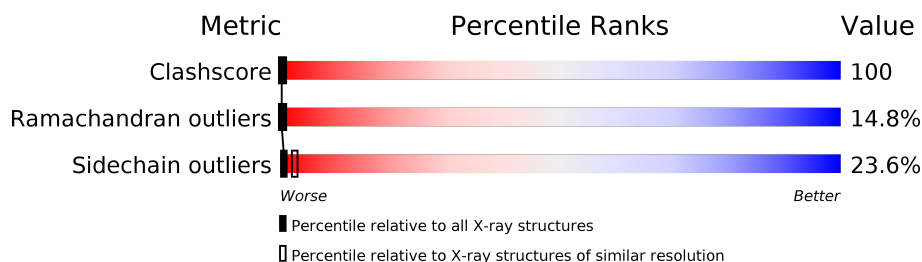
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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	L	281	
2	M	307	
3	H	260	

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
4	BCL	L	350	-	-	X	-
4	BCL	L	450	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	M	400	-	-	X	-
4	BCL	M	601	-	-	X	-
5	BPH	M	500	-	-	X	-
6	UQ	L	800	-	-	X	-
6	UQ	M	750	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7049 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 PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	278	2203	1491	349	355	8	0	0	0

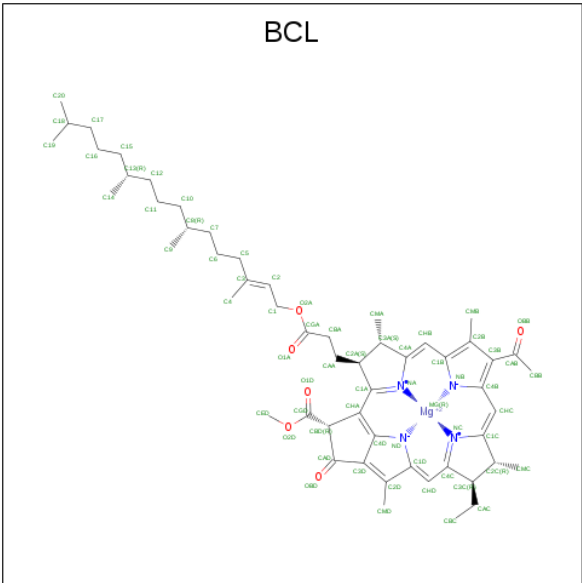
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	305	2428	1620	397	400	11	0	0	0

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

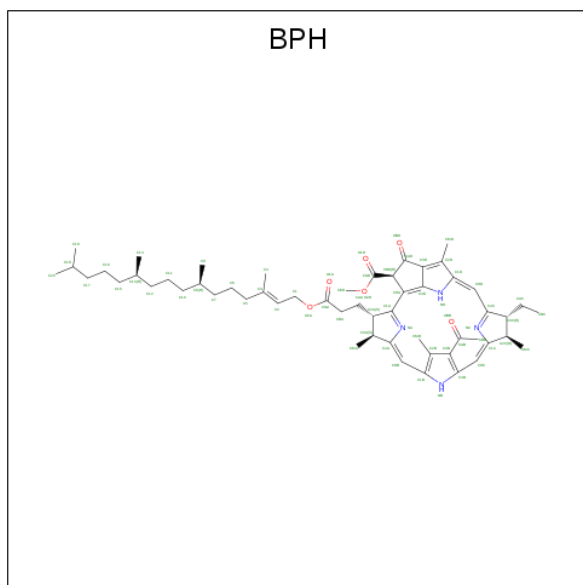
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	255	1927	1232	330	354	11	73	0	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



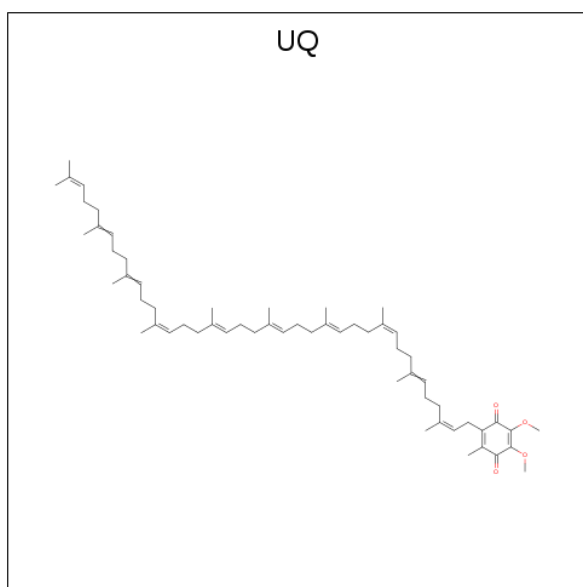
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	6	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	7	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	3	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	7	0
			65	55	4	6		

- Molecule 6 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula:  $C_{59}H_{90}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	16	0
			48	44	4		
6	M	1	Total	C	O	16	0
			48	44	4		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

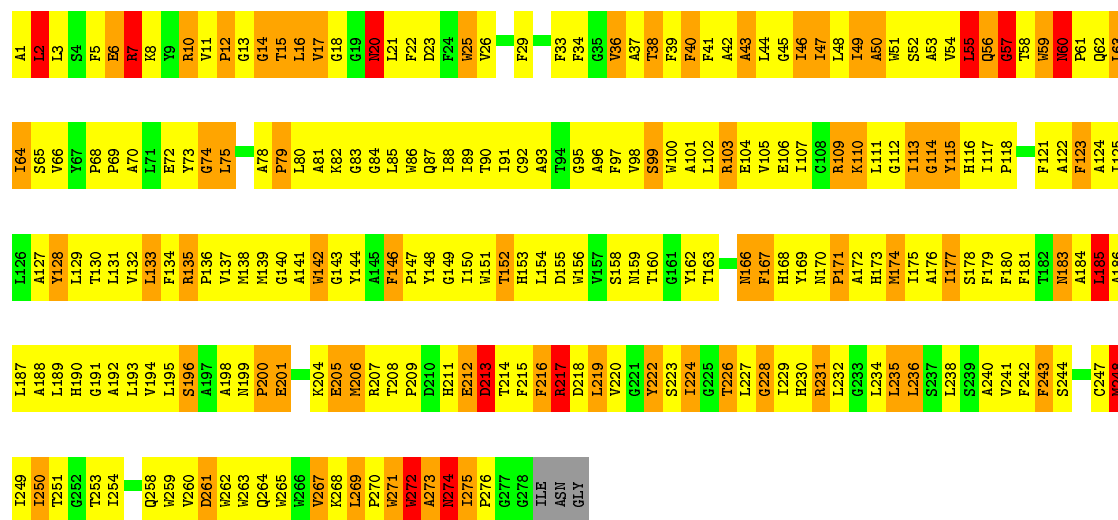
### 3 Residue-property plots

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.

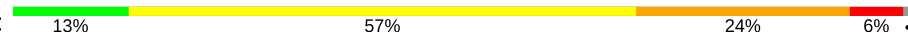
Note EDS was not executed.

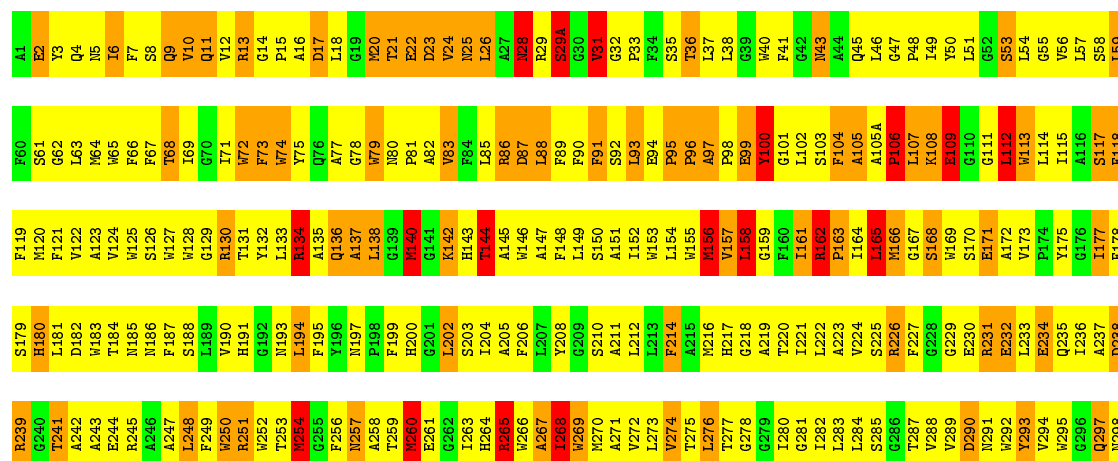
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

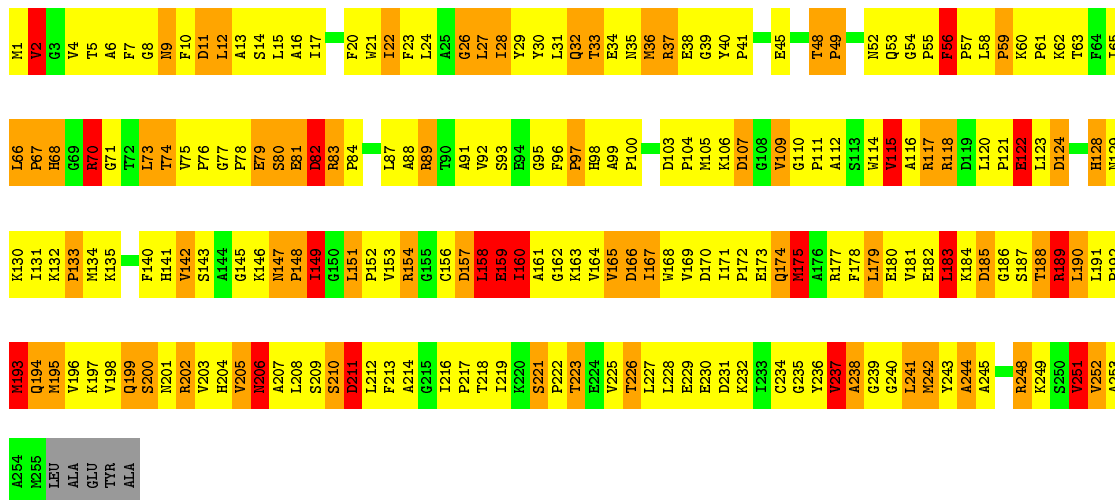
Chain L: 



#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

Chain M: 







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.20Å 139.60Å 78.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, UQ, FE

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	L	1.00	2/2291 (0.1%)	1.47	24/3137 (0.8%)
2	M	1.21	6/2521 (0.2%)	1.57	36/3442 (1.0%)
3	H	0.96	4/1977 (0.2%)	1.52	23/2689 (0.9%)
All	All	1.07	12/6789 (0.2%)	1.52	83/9268 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	250	TRP	CA-CB	-17.94	1.14	1.53
2	M	93	LEU	C-O	16.21	1.54	1.23
2	M	93	LEU	CA-C	-12.85	1.19	1.52
2	M	93	LEU	C-N	10.05	1.57	1.34
2	M	112	LEU	C-N	8.74	1.54	1.34
1	L	217	ARG	CG-CD	7.77	1.71	1.51
2	M	269	TRP	CA-CB	-7.45	1.37	1.53
3	H	56	PHE	CB-CG	7.35	1.63	1.51
1	L	166	ASN	CA-CB	-6.74	1.35	1.53
3	H	54	GLY	CA-C	6.66	1.62	1.51
3	H	56	PHE	N-CA	6.58	1.59	1.46
3	H	55	PRO	N-CA	5.17	1.56	1.47

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	112	LEU	O-C-N	-24.12	84.11	122.70
1	L	166	ASN	CA-CB-CG	18.90	154.98	113.40
1	L	166	ASN	N-CA-CB	17.93	142.88	110.60
2	M	109	GLU	CA-C-N	-15.78	84.64	116.20
2	M	112	LEU	CA-C-N	13.93	147.85	117.20
2	M	109	GLU	N-CA-C	12.44	144.58	111.00
3	H	83	ARG	NE-CZ-NH1	11.32	125.96	120.30
3	H	56	PHE	CB-CG-CD2	11.16	128.62	120.80
2	M	108	LYS	C-N-CA	-10.30	95.95	121.70
2	M	109	GLU	CB-CA-C	-9.78	90.84	110.40
1	L	135	ARG	CD-NE-CZ	9.67	137.14	123.60
3	H	83	ARG	CD-NE-CZ	9.44	136.82	123.60
1	L	135	ARG	NE-CZ-NH1	9.32	124.96	120.30
2	M	112	LEU	CB-CG-CD2	9.28	126.78	111.00
2	M	112	LEU	CB-CG-CD1	9.26	126.74	111.00
2	M	250	TRP	CB-CA-C	-9.23	91.95	110.40
3	H	154	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	L	213	ASP	CB-CG-OD1	8.68	126.11	118.30
3	H	142	VAL	CA-CB-CG2	8.54	123.71	110.90
2	M	108	LYS	O-C-N	-8.44	109.20	122.70
1	L	217	ARG	CG-CD-NE	8.26	129.14	111.80
2	M	250	TRP	N-CA-CB	7.78	124.60	110.60
2	M	130	ARG	NE-CZ-NH2	7.60	124.10	120.30
3	H	70	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	L	7	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	L	207	ARG	NE-CZ-NH2	7.53	124.06	120.30
2	M	13	ARG	CD-NE-CZ	7.52	134.13	123.60
2	M	269	TRP	N-CA-CB	-7.47	97.16	110.60
1	L	217	ARG	NE-CZ-NH2	7.45	124.03	120.30
2	M	162	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	L	231	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	L	109	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	L	103	ARG	NE-CZ-NH2	7.34	123.97	120.30
2	M	245	ARG	NE-CZ-NH2	7.33	123.97	120.30
3	H	248	ARG	NE-CZ-NH2	7.33	123.97	120.30
2	M	86	ARG	NE-CZ-NH2	7.29	123.95	120.30
2	M	13	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	M	226	ARG	NE-CZ-NH2	7.24	123.92	120.30
2	M	239	ARG	NE-CZ-NH2	7.18	123.89	120.30
3	H	89	ARG	NE-CZ-NH2	7.14	123.87	120.30
2	M	251	ARG	NE-CZ-NH2	7.03	123.81	120.30
3	H	202	ARG	NE-CZ-NH1	6.99	123.80	120.30
3	H	142	VAL	N-CA-CB	-6.73	96.69	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	134	ARG	NE-CZ-NH2	6.70	123.65	120.30
2	M	112	LEU	C-N-CA	6.69	138.43	121.70
3	H	185	ASP	CB-CG-OD1	6.63	124.27	118.30
3	H	211	ASP	CB-CG-OD2	6.60	124.24	118.30
3	H	118	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	L	273	ALA	O-C-N	6.46	133.04	122.70
3	H	159	GLU	O-C-N	6.27	132.73	122.70
2	M	140	MET	CG-SD-CE	6.25	110.19	100.20
2	M	156	MET	CG-SD-CE	6.25	110.19	100.20
2	M	254	MET	CG-SD-CE	6.22	110.16	100.20
3	H	115	VAL	CB-CA-C	6.19	123.17	111.40
1	L	206	MET	CG-SD-CE	6.17	110.07	100.20
1	L	248	MET	CG-SD-CE	6.14	110.02	100.20
3	H	195	MET	CG-SD-CE	6.14	110.02	100.20
2	M	120	MET	CG-SD-CE	6.13	110.00	100.20
3	H	36	MET	CG-SD-CE	6.12	109.99	100.20
3	H	175	MET	CG-SD-CE	6.12	109.99	100.20
1	L	139	MET	CG-SD-CE	6.11	109.97	100.20
3	H	193	MET	CG-SD-CE	6.09	109.95	100.20
2	M	106	PRO	O-C-N	6.08	132.42	122.70
1	L	59	TRP	O-C-N	6.07	132.41	122.70
2	M	166	MET	CG-SD-CE	6.04	109.86	100.20
2	M	73	PHE	O-C-N	5.89	132.12	122.70
2	M	108	LYS	CA-C-N	5.86	130.10	117.20
3	H	226	THR	N-CA-CB	5.86	121.44	110.30
2	M	260	MET	CG-SD-CE	5.76	109.41	100.20
1	L	185	LEU	O-C-N	5.62	131.69	122.70
1	L	10	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	L	174	MET	CG-SD-CE	5.56	109.09	100.20
3	H	37	ARG	NE-CZ-NH1	5.47	123.04	120.30
3	H	223	THR	CA-CB-CG2	5.44	120.02	112.40
1	L	57	GLY	N-CA-C	-5.41	99.58	113.10
1	L	212	GLU	CG-CD-OE1	-5.37	107.56	118.30
2	M	93	LEU	C-N-CA	5.36	135.09	121.70
1	L	25	TRP	CA-CB-CG	5.30	123.77	113.70
1	L	148	TYR	CB-CG-CD2	-5.22	117.87	121.00
3	H	56	PHE	CA-CB-CG	5.18	126.33	113.90
2	M	96	PRO	O-C-N	5.17	130.98	122.70
2	M	23	ASP	O-C-N	5.06	130.79	122.70
2	M	136	GLN	N-CA-CB	5.05	119.68	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	109	GLU	Mainchain,Peptide
2	M	112	LEU	Mainchain,Peptide
2	M	265	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2203	0	2156	482	1
2	M	2428	0	2342	596	1
3	H	1927	0	1927	364	2
4	L	132	0	148	46	0
4	M	132	0	148	63	0
5	L	65	0	76	16	0
5	M	65	0	76	33	0
6	L	48	0	59	21	0
6	M	48	0	63	33	0
7	M	1	0	0	0	0
All	All	7049	0	6995	1373	2

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 100.

All (1373) 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)
6:M:750:UQ:C13	6:M:750:UQ:C12	1.84	1.50
1:L:183:ASN:ND2	1:L:236:LEU:HB2	1.24	1.48
2:M:96:PRO:HG2	2:M:170:SER:CA	1.57	1.33
1:L:183:ASN:HD22	1:L:236:LEU:CB	1.44	1.30
2:M:96:PRO:CG	2:M:170:SER:HA	1.75	1.17
1:L:229:ILE:HD13	6:L:800:UQ:HM53	1.24	1.16
3:H:33:THR:HG22	3:H:34:GLU:H	1.08	1.16
1:L:185:LEU:CD2	6:L:800:UQ:H153	1.75	1.16
1:L:187:LEU:HD21	2:M:267:ALA:CB	1.77	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:102:LEU:HA	2:M:169:TRP:HD1	1.04	1.15
1:L:172:ALA:HB3	1:L:247:CYS:HB2	1.16	1.15
1:L:114:GLY:HA3	2:M:223:ALA:HB1	1.17	1.15
3:H:182:GLU:HG3	3:H:187:SER:HA	1.15	1.13
1:L:193:LEU:HD11	1:L:216:PHE:CE1	1.84	1.12
1:L:183:ASN:ND2	1:L:236:LEU:CB	2.05	1.12
4:L:350:BCL:HBD	4:L:450:BCL:HBC1	1.16	1.12
2:M:69:ILE:HA	2:M:93:LEU:HD11	1.23	1.11
3:H:168:TRP:HZ3	3:H:180:GLU:HB2	1.16	1.11
1:L:187:LEU:CD2	2:M:267:ALA:HB1	1.80	1.11
4:M:400:BCL:HBA1	4:M:400:BCL:HBD	1.14	1.10
4:L:350:BCL:HBD	4:L:450:BCL:CBC	1.81	1.10
2:M:254:MET:HE1	6:M:750:UQ:H112	1.27	1.10
2:M:102:LEU:HA	2:M:169:TRP:CD1	1.86	1.10
2:M:69:ILE:HA	2:M:93:LEU:CD1	1.80	1.10
2:M:162:ARG:HG3	2:M:282:ILE:HG22	1.34	1.09
1:L:117:ILE:HD13	2:M:249:PHE:CD2	1.86	1.08
1:L:58:THR:HG22	1:L:59:TRP:H	1.12	1.06
2:M:99:GLU:O	2:M:100:TYR:HB2	1.52	1.06
3:H:61:PRO:HA	3:H:76:PRO:HG3	1.07	1.06
1:L:74:GLY:HA2	1:L:141:ALA:HB2	1.38	1.06
1:L:37:ALA:O	1:L:40:PHE:HB2	1.53	1.05
3:H:245:ALA:HB3	3:H:248:ARG:HG3	1.37	1.05
1:L:117:ILE:HD13	2:M:249:PHE:CE2	1.91	1.05
1:L:218:ASP:OD2	2:M:50:TYR:HE1	1.37	1.04
1:L:185:LEU:HD21	6:L:800:UQ:H153	1.33	1.03
2:M:101:GLY:HA2	2:M:168:SER:HA	1.40	1.03
2:M:162:ARG:HB3	2:M:163:PRO:HD3	1.39	1.03
2:M:274:VAL:HG12	2:M:275:THR:N	1.68	1.03
1:L:218:ASP:OD2	2:M:50:TYR:CE1	2.12	1.01
1:L:195:LEU:HD13	2:M:265:ARG:HH11	1.19	1.01
1:L:3:LEU:HB3	1:L:6:GLU:HB2	1.39	1.01
2:M:24:VAL:HG12	2:M:26:LEU:H	1.25	1.01
4:M:601:BCL:C1	5:M:500:BPH:HMB2	1.89	1.01
3:H:198:VAL:HA	3:H:203:VAL:HG22	1.43	1.00
3:H:61:PRO:CA	3:H:76:PRO:HG3	1.90	1.00
2:M:111:GLY:O	2:M:114:LEU:HB3	1.62	0.99
4:M:601:BCL:H11	5:M:500:BPH:CMB	1.93	0.99
2:M:96:PRO:HG2	2:M:170:SER:HA	1.00	0.99
2:M:204:ILE:HG23	4:M:400:BCL:HMB3	1.41	0.99
1:L:231:ARG:NE	2:M:6:ILE:H	1.59	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:350:BCL:H152	5:L:550:BPH:CGA	1.93	0.98
3:H:154:ARG:HD3	3:H:202:ARG:HH11	1.26	0.98
2:M:113:TRP:O	2:M:117:SER:HB2	1.62	0.98
2:M:294:VAL:O	2:M:298:ASN:HB2	1.64	0.98
2:M:4:GLN:HG3	3:H:193:MET:O	1.64	0.98
1:L:44:LEU:HD23	1:L:47:ILE:HG21	1.43	0.98
2:M:31:VAL:HG22	2:M:33:PRO:HD3	1.46	0.97
2:M:111:GLY:O	2:M:114:LEU:CB	2.12	0.97
3:H:67:PRO:HG2	3:H:123:LEU:HD21	1.43	0.96
2:M:103:SER:C	2:M:105:ALA:H	1.61	0.96
3:H:33:THR:HG22	3:H:34:GLU:N	1.79	0.96
2:M:97:ALA:HB3	2:M:98:PRO:HD3	1.48	0.95
1:L:180:PHE:CE1	1:L:240:ALA:HB1	2.02	0.95
3:H:130:LYS:HG3	3:H:172:PRO:HG2	1.49	0.95
2:M:16:ALA:HB1	2:M:45:GLN:HE22	1.28	0.95
3:H:151:LEU:HD21	3:H:203:VAL:CG2	1.96	0.94
2:M:183:TRP:CZ3	4:M:601:BCL:HMC1	2.02	0.94
4:M:601:BCL:H11	5:M:500:BPH:HMB2	0.97	0.94
2:M:96:PRO:HG2	2:M:170:SER:N	1.83	0.94
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.32	0.94
1:L:231:ARG:HE	2:M:6:ILE:H	0.98	0.93
2:M:186:ASN:O	2:M:190:VAL:HG23	1.67	0.93
1:L:231:ARG:HE	2:M:6:ILE:N	1.67	0.93
2:M:31:VAL:CG2	2:M:33:PRO:HD3	1.97	0.93
1:L:218:ASP:HB3	2:M:50:TYR:CE1	2.02	0.93
3:H:164:VAL:O	3:H:165:VAL:HG23	1.66	0.93
3:H:160:ILE:O	3:H:160:ILE:HG23	1.67	0.92
2:M:69:ILE:CA	2:M:93:LEU:HD11	2.00	0.92
2:M:78:GLY:O	2:M:79:TRP:HB2	1.70	0.92
2:M:157:VAL:HA	2:M:161:ILE:HG22	1.50	0.92
1:L:114:GLY:HA3	2:M:223:ALA:CB	1.98	0.92
1:L:229:ILE:CD1	6:L:800:UQ:HM53	1.99	0.92
3:H:168:TRP:CZ3	3:H:180:GLU:HB2	2.05	0.92
3:H:111:PRO:HD2	3:H:243:TYR:CE2	2.04	0.91
3:H:56:PHE:H	3:H:57:PRO:HD2	1.34	0.91
1:L:58:THR:CG2	1:L:59:TRP:H	1.83	0.91
2:M:254:MET:CE	6:M:750:UQ:H112	1.99	0.91
1:L:195:LEU:HD11	2:M:265:ARG:HG3	1.50	0.91
3:H:182:GLU:HG3	3:H:187:SER:CA	2.00	0.91
3:H:103:ASP:O	3:H:107:ASP:HB2	1.70	0.91
3:H:170:ASP:OD2	3:H:173:GLU:HB3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:ALA:HB2	1:L:7:ARG:HG2	1.53	0.90
2:M:106:PRO:C	2:M:108:LYS:H	1.74	0.90
1:L:183:ASN:HD22	1:L:236:LEU:CG	1.83	0.90
1:L:37:ALA:O	1:L:40:PHE:CB	2.20	0.90
1:L:58:THR:HG22	1:L:59:TRP:N	1.87	0.90
3:H:207:ALA:O	3:H:240:GLY:HA3	1.72	0.89
2:M:113:TRP:CZ3	2:M:169:TRP:HE3	1.91	0.89
2:M:254:MET:HE1	6:M:750:UQ:C11	2.03	0.88
1:L:1:ALA:O	1:L:2:LEU:HB2	1.70	0.88
2:M:101:GLY:CA	2:M:168:SER:HA	2.03	0.88
2:M:128:TRP:HE1	2:M:145:ALA:HB1	1.36	0.88
3:H:131:ILE:HG22	3:H:168:TRP:HD1	1.37	0.88
3:H:164:VAL:O	3:H:165:VAL:CG2	2.21	0.88
2:M:258:ALA:HA	3:H:35:ASN:HB3	1.54	0.88
2:M:95:PRO:HB2	2:M:96:PRO:HD2	1.55	0.87
3:H:182:GLU:CG	3:H:187:SER:HA	2.01	0.87
1:L:264:GLN:HA	1:L:267:VAL:HG23	1.56	0.87
4:L:350:BCL:H72	4:L:450:BCL:CBB	2.03	0.87
3:H:183:LEU:HD11	3:H:189:ARG:HD3	1.57	0.87
3:H:5:THR:HA	3:H:11:ASP:HA	1.57	0.87
2:M:158:LEU:HD21	2:M:183:TRP:CZ3	2.10	0.87
1:L:114:GLY:CA	2:M:223:ALA:HB1	2.02	0.86
4:M:400:BCL:HBA1	4:M:400:BCL:CBF	2.03	0.86
1:L:53:ALA:HB2	1:L:64:ILE:CD1	2.05	0.86
1:L:37:ALA:C	1:L:40:PHE:HB2	1.94	0.86
1:L:230:HIS:CE1	2:M:221:ILE:HG21	2.09	0.86
2:M:157:VAL:CG1	2:M:162:ARG:HB2	2.06	0.86
2:M:103:SER:C	2:M:105:ALA:N	2.28	0.85
2:M:227:PHE:HE2	3:H:235:GLY:HA2	1.41	0.85
1:L:121:PHE:O	1:L:124:ALA:HB3	1.76	0.85
2:M:20:MET:HG3	2:M:21:THR:H	1.40	0.85
2:M:128:TRP:NE1	2:M:145:ALA:HB1	1.91	0.85
3:H:157:ASP:O	3:H:158:LEU:HB2	1.75	0.85
3:H:191:LEU:HD11	3:H:213:PHE:CE2	2.12	0.85
3:H:56:PHE:H	3:H:57:PRO:CD	1.90	0.84
1:L:130:THR:HB	1:L:249:ILE:HD11	1.60	0.84
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.58	0.84
2:M:274:VAL:HG12	2:M:275:THR:H	1.40	0.84
2:M:54:LEU:H	2:M:54:LEU:HD12	1.43	0.84
3:H:81:GLU:O	3:H:82:ASP:HB2	1.77	0.83
3:H:160:ILE:O	3:H:160:ILE:CG2	2.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:250:TRP:O	2:M:254:MET:HG3	1.77	0.83
1:L:187:LEU:HD21	2:M:267:ALA:HB1	0.91	0.83
2:M:271:ALA:O	2:M:274:VAL:HB	1.77	0.83
3:H:8:GLY:O	3:H:9:ASN:HB2	1.78	0.83
2:M:105(A):ALA:O	2:M:106:PRO:O	1.96	0.83
2:M:50:TYR:O	2:M:51:LEU:HG	1.78	0.83
1:L:62:GLN:HB3	1:L:151:TRP:HD1	1.42	0.83
2:M:68:THR:HG23	2:M:112:LEU:HD13	1.60	0.83
3:H:154:ARG:HD3	3:H:202:ARG:NH1	1.94	0.82
3:H:75:VAL:N	3:H:76:PRO:HD2	1.94	0.82
2:M:13:ARG:HG2	2:M:14:GLY:H	1.44	0.82
1:L:183:ASN:HD22	1:L:236:LEU:CD1	1.91	0.82
2:M:113:TRP:HZ3	2:M:169:TRP:HE3	1.24	0.82
1:L:227:LEU:HD21	1:L:231:ARG:NH2	1.95	0.82
2:M:97:ALA:C	2:M:99:GLU:H	1.80	0.82
3:H:17:ILE:HG23	3:H:21:TRP:CD1	2.14	0.82
4:M:400:BCL:H43	5:M:500:BPH:CAB	2.09	0.82
1:L:149:GLY:HA3	1:L:152:THR:CG2	2.09	0.82
1:L:229:ILE:HB	6:L:800:UQ:CM5	2.10	0.82
1:L:264:GLN:OE1	1:L:267:VAL:HG21	1.78	0.82
3:H:252:VAL:HG12	3:H:253:ALA:N	1.93	0.81
2:M:153:TRP:CZ2	2:M:283:LEU:HD12	2.14	0.81
1:L:104:GLU:HA	1:L:107:ILE:HD12	1.63	0.81
1:L:230:HIS:ND1	2:M:221:ILE:HG21	1.95	0.81
1:L:169:TYR:CG	1:L:260:VAL:HG22	2.15	0.81
1:L:212:GLU:N	2:M:140:MET:HE3	1.94	0.81
1:L:5:PHE:HB2	2:M:244:GLU:OE1	1.79	0.81
3:H:61:PRO:HA	3:H:76:PRO:CG	2.01	0.81
2:M:162:ARG:HG3	2:M:282:ILE:CG2	2.10	0.81
2:M:251:ARG:HG3	2:M:251:ARG:HH11	1.45	0.81
2:M:5:ASN:O	2:M:6:ILE:HB	1.80	0.81
1:L:150:ILE:HG12	5:L:550:BPH:H193	1.61	0.81
3:H:173:GLU:O	3:H:174:GLN:HB2	1.81	0.81
2:M:89:PHE:HB3	2:M:178:PHE:CD1	2.15	0.81
2:M:165:LEU:N	2:M:165:LEU:HD23	1.94	0.81
2:M:69:ILE:HG12	2:M:93:LEU:HD12	1.63	0.81
2:M:161:ILE:CG2	2:M:283:LEU:HD21	2.11	0.80
1:L:195:LEU:HD13	2:M:265:ARG:NH1	1.97	0.80
1:L:86:TRP:CZ2	1:L:132:VAL:HG13	2.16	0.80
4:L:350:BCL:HAA2	4:L:450:BCL:HBC1	1.64	0.80
1:L:268:LYS:HD3	1:L:272:TRP:CZ2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:250:TRP:HE1	6:M:750:UQ:HM53	1.47	0.80
3:H:164:VAL:HG12	3:H:165:VAL:H	1.47	0.79
2:M:97:ALA:HB3	2:M:98:PRO:CD	2.11	0.79
2:M:200:HIS:CE1	2:M:204:ILE:HD11	2.16	0.79
3:H:245:ALA:HB3	3:H:248:ARG:CG	2.10	0.79
2:M:183:TRP:HZ3	4:M:601:BCL:HMC1	1.43	0.79
1:L:215:PHE:HA	2:M:138:LEU:HD22	1.64	0.79
2:M:115:ILE:HG23	2:M:119:PHE:HE2	1.48	0.79
2:M:89:PHE:O	2:M:178:PHE:HB2	1.82	0.79
3:H:164:VAL:C	3:H:165:VAL:HG23	2.03	0.79
2:M:105(A):ALA:HB3	2:M:109:GLU:HG2	1.64	0.79
4:M:400:BCL:CBB	4:M:400:BCL:HMB1	2.12	0.79
3:H:66:LEU:HB3	3:H:67:PRO:HD2	1.64	0.79
1:L:74:GLY:HA2	1:L:141:ALA:CB	2.12	0.79
1:L:117:ILE:CD1	2:M:249:PHE:CD2	2.65	0.79
2:M:109:GLU:N	2:M:111:GLY:H	1.81	0.79
2:M:72:TRP:HB3	2:M:93:LEU:HD13	1.64	0.79
3:H:37:ARG:HH21	3:H:62:LYS:HG3	1.44	0.78
1:L:111:LEU:HB2	1:L:113:ILE:HG12	1.64	0.78
1:L:80:LEU:HD11	1:L:85:LEU:HD21	1.64	0.78
1:L:183:ASN:ND2	1:L:236:LEU:HD12	1.99	0.78
2:M:152:ILE:O	2:M:156:MET:HB2	1.82	0.78
1:L:53:ALA:HB2	1:L:64:ILE:HD11	1.64	0.78
2:M:101:GLY:HA2	2:M:168:SER:CA	2.13	0.78
2:M:181:LEU:O	2:M:184:THR:HG22	1.82	0.78
1:L:229:ILE:HB	6:L:800:UQ:HM52	1.63	0.78
2:M:113:TRP:HZ2	2:M:172:ALA:HB1	1.47	0.78
1:L:229:ILE:HG13	2:M:214:PHE:HZ	1.47	0.78
1:L:117:ILE:HD13	2:M:249:PHE:HD2	1.46	0.78
3:H:161:ALA:HA	3:H:210:SER:HB3	1.65	0.78
3:H:28:ILE:HG22	3:H:29:TYR:N	1.98	0.78
2:M:103:SER:O	2:M:105:ALA:N	2.17	0.77
2:M:202:LEU:O	2:M:205:ALA:HB3	1.83	0.77
3:H:135:LYS:NZ	3:H:165:VAL:HG12	1.98	0.77
2:M:102:LEU:O	2:M:102:LEU:HD12	1.84	0.77
1:L:117:ILE:CD1	2:M:249:PHE:CE2	2.66	0.77
4:L:350:BCL:H72	4:L:450:BCL:HBB1	1.65	0.77
2:M:113:TRP:CZ2	2:M:172:ALA:CB	2.67	0.77
2:M:235:GLN:NE2	2:M:243:ALA:HB2	1.98	0.77
2:M:24:VAL:HG11	2:M:26:LEU:HD13	1.67	0.77
3:H:219:ILE:HG12	3:H:221:SER:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:SER:HB2	1:L:152:THR:HG21	1.67	0.77
2:M:288:VAL:O	3:H:4:VAL:HG11	1.84	0.77
2:M:202:LEU:HD23	3:H:20:PHE:HE2	1.49	0.77
1:L:198:ALA:HB2	2:M:233:LEU:HD13	1.66	0.77
4:M:601:BCL:HMA1	4:M:400:BCL:H202	1.65	0.77
2:M:162:ARG:HB3	2:M:163:PRO:CD	2.15	0.77
2:M:32:GLY:HA2	2:M:46:LEU:O	1.84	0.77
2:M:226:ARG:HH21	3:H:238:ALA:HB1	1.51	0.77
2:M:224:VAL:HG12	2:M:242:ALA:HB1	1.67	0.76
4:M:400:BCL:C14	5:M:500:BPH:H2	2.15	0.76
1:L:41:PHE:CD2	1:L:92:CYS:HA	2.21	0.76
2:M:154:LEU:HD13	2:M:275:THR:HG22	1.66	0.76
3:H:128:HIS:CD2	3:H:129:ASN:H	2.03	0.76
3:H:199:GLN:HG2	3:H:200:SER:H	1.50	0.76
1:L:150:ILE:HG12	5:L:550:BPH:C19	2.15	0.76
1:L:218:ASP:CG	2:M:50:TYR:HE1	1.87	0.76
1:L:98:VAL:O	1:L:101:ALA:HB3	1.86	0.76
4:M:601:BCL:HBC1	4:M:400:BCL:HBD	1.68	0.76
3:H:131:ILE:HG22	3:H:168:TRP:CD1	2.20	0.76
3:H:33:THR:CG2	3:H:34:GLU:H	1.91	0.76
1:L:128:TYR:CE2	4:L:450:BCL:HBB1	2.20	0.76
2:M:216:MET:HG2	2:M:250:TRP:HZ2	1.50	0.76
3:H:130:LYS:HG3	3:H:172:PRO:CG	2.16	0.76
1:L:274:ASN:O	1:L:275:ILE:HB	1.83	0.76
3:H:205:VAL:HG12	3:H:206:ASN:H	1.51	0.76
4:L:350:BCL:HMB1	4:L:350:BCL:HBB3	1.66	0.76
1:L:151:TRP:O	2:M:303:PRO:HB3	1.86	0.75
3:H:91:ALA:HB3	3:H:96:PHE:CB	2.17	0.75
1:L:275:ILE:O	1:L:275:ILE:HG22	1.85	0.75
2:M:102:LEU:CA	2:M:169:TRP:HD1	1.93	0.75
1:L:128:TYR:CE1	1:L:132:VAL:HG21	2.22	0.75
2:M:157:VAL:HG12	2:M:162:ARG:HB2	1.67	0.75
1:L:128:TYR:HE1	1:L:132:VAL:HG21	1.51	0.75
2:M:16:ALA:HB1	2:M:45:GLN:NE2	2.00	0.75
3:H:67:PRO:CG	3:H:123:LEU:HD21	2.17	0.75
1:L:70:ALA:HB3	1:L:73:TYR:CD2	2.22	0.75
1:L:231:ARG:HD3	2:M:6:ILE:HD13	1.69	0.75
3:H:27:LEU:HG	3:H:28:ILE:N	2.02	0.74
1:L:271:TRP:HB2	1:L:274:ASN:HD22	1.52	0.74
1:L:20:ASN:C	1:L:22:PHE:H	1.90	0.74
1:L:218:ASP:CB	2:M:50:TYR:CE1	2.71	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:259:THR:C	2:M:261:GLU:H	1.88	0.74
1:L:13:GLY:H	1:L:110:LYS:HE2	1.53	0.74
1:L:212:GLU:HB3	6:L:800:UQ:O2	1.86	0.74
1:L:198:ALA:HB2	2:M:233:LEU:CD1	2.18	0.74
2:M:274:VAL:CG1	2:M:275:THR:N	2.39	0.74
2:M:130:ARG:O	2:M:134:ARG:HB2	1.88	0.74
2:M:161:ILE:HG23	2:M:283:LEU:HD21	1.69	0.74
3:H:5:THR:HG23	3:H:10:PHE:H	1.51	0.74
4:L:350:BCL:H52	4:L:450:BCL:OBB	1.88	0.73
1:L:75:LEU:HG	1:L:140:GLY:O	1.87	0.73
2:M:87:ASP:HB3	2:M:90:PHE:HB2	1.69	0.73
3:H:240:GLY:O	3:H:244:ALA:HB3	1.87	0.73
1:L:158:SER:O	1:L:162:TYR:HD2	1.69	0.73
2:M:111:GLY:O	2:M:114:LEU:HB2	1.88	0.73
3:H:192:PRO:CG	3:H:237:VAL:HG21	2.17	0.73
3:H:135:LYS:NZ	3:H:165:VAL:CG1	2.51	0.73
1:L:70:ALA:HB3	1:L:73:TYR:HD2	1.54	0.73
3:H:122:GLU:O	3:H:123:LEU:HG	1.88	0.73
2:M:22:GLU:HB3	2:M:137:ALA:HA	1.69	0.73
1:L:176:ALA:O	1:L:180:PHE:HD1	1.72	0.73
2:M:204:ILE:CG2	4:M:400:BCL:HMB3	2.18	0.73
1:L:162:TYR:CE2	4:L:350:BCL:HBC1	2.23	0.72
3:H:37:ARG:NH2	3:H:62:LYS:HG3	2.04	0.72
1:L:211:HIS:HD2	2:M:138:LEU:O	1.72	0.72
2:M:142:LYS:HG2	2:M:142:LYS:O	1.88	0.72
2:M:226:ARG:NH2	3:H:238:ALA:HB1	2.05	0.72
2:M:24:VAL:CG1	2:M:26:LEU:HB2	2.20	0.72
1:L:211:HIS:C	2:M:140:MET:HE3	2.09	0.72
1:L:183:ASN:OD1	2:M:214:PHE:HD2	1.73	0.72
1:L:10:ARG:HG3	1:L:25:TRP:CH2	2.24	0.72
2:M:96:PRO:CD	2:M:170:SER:HA	2.20	0.72
2:M:162:ARG:NH2	2:M:187:PHE:CE1	2.58	0.72
3:H:151:LEU:HD21	3:H:203:VAL:HG23	1.71	0.72
1:L:211:HIS:CD2	2:M:138:LEU:O	2.42	0.72
1:L:166:ASN:OD1	2:M:185:ASN:ND2	2.22	0.72
2:M:72:TRP:HB3	2:M:93:LEU:CD1	2.19	0.72
2:M:106:PRO:C	2:M:108:LYS:N	2.43	0.72
3:H:111:PRO:HG3	3:H:242:MET:SD	2.30	0.72
3:H:148:PRO:HA	3:H:151:LEU:HB3	1.70	0.72
2:M:35:SER:HB3	2:M:38:LEU:HB3	1.70	0.72
2:M:80:ASN:HB3	2:M:81:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:TYR:HD1	1:L:223:SER:N	1.88	0.71
1:L:212:GLU:HA	6:L:800:UQ:HM21	1.71	0.71
1:L:86:TRP:O	1:L:90:THR:HG22	1.90	0.71
2:M:113:TRP:CZ2	2:M:172:ALA:HB3	2.25	0.71
2:M:144:THR:O	2:M:147:ALA:HB3	1.88	0.71
4:L:350:BCL:HBA2	2:M:208:TYR:HE1	1.55	0.71
3:H:37:ARG:HB3	3:H:75:VAL:CG1	2.20	0.71
1:L:185:LEU:CA	5:M:500:BPH:HMC2	2.20	0.71
4:L:450:BCL:HBB2	4:L:450:BCL:HMB1	1.70	0.71
2:M:115:ILE:CG2	2:M:119:PHE:HE2	2.02	0.71
2:M:165:LEU:H	2:M:165:LEU:HD23	1.53	0.71
1:L:54:VAL:C	1:L:55:LEU:O	2.24	0.71
3:H:245:ALA:CB	3:H:248:ARG:HG3	2.17	0.71
2:M:235:GLN:HE21	2:M:260:MET:CE	2.03	0.71
3:H:151:LEU:HD21	3:H:203:VAL:HG21	1.70	0.71
1:L:217:ARG:NH2	2:M:17:ASP:OD2	2.24	0.71
1:L:222:TYR:CE2	2:M:38:LEU:HD21	2.26	0.71
2:M:195:PHE:CE2	4:M:400:BCL:HMC2	2.26	0.71
3:H:241:LEU:O	3:H:242:MET:HB2	1.90	0.71
1:L:20:ASN:ND2	1:L:23:ASP:HB3	2.06	0.70
2:M:288:VAL:HB	3:H:4:VAL:HG13	1.72	0.70
4:M:400:BCL:H42	5:M:500:BPH:CHC	2.21	0.70
1:L:187:LEU:HD23	1:L:187:LEU:C	2.12	0.70
1:L:274:ASN:O	1:L:275:ILE:CB	2.39	0.70
4:L:350:BCL:C7	4:L:450:BCL:CBB	2.69	0.70
2:M:13:ARG:CG	2:M:14:GLY:H	2.01	0.70
2:M:87:ASP:HB2	2:M:91:PHE:CE2	2.27	0.70
1:L:168:HIS:NE2	4:M:601:BCL:HMD3	2.07	0.70
2:M:256:PHE:HE1	6:M:750:UQ:H252	1.55	0.70
3:H:154:ARG:HH11	3:H:158:LEU:HG	1.56	0.70
3:H:33:THR:CG2	3:H:34:GLU:N	2.49	0.70
4:L:350:BCL:HBA2	2:M:208:TYR:CE1	2.26	0.70
2:M:280:ILE:O	2:M:284:LEU:HG	1.92	0.70
1:L:264:GLN:HA	1:L:267:VAL:CG2	2.21	0.70
1:L:185:LEU:HD22	6:L:800:UQ:H153	1.69	0.70
2:M:117:SER:HA	2:M:175:TYR:OH	1.92	0.70
2:M:182:ASP:O	2:M:185:ASN:HB3	1.90	0.70
3:H:167:ILE:HG23	3:H:179:LEU:HD12	1.74	0.70
2:M:68:THR:O	2:M:72:TRP:HB2	1.92	0.70
1:L:68:PRO:HD3	1:L:147:PRO:HA	1.72	0.69
2:M:171:GLU:O	2:M:172:ALA:HB3	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:450:BCL:HMD2	4:M:400:BCL:HBB3	1.73	0.69
4:M:400:BCL:HBD	4:M:400:BCL:CBA	2.08	0.69
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.74	0.69
1:L:172:ALA:HB3	1:L:247:CYS:CB	2.09	0.69
3:H:153:VAL:O	3:H:161:ALA:HB3	1.92	0.69
1:L:189:LEU:HD22	1:L:216:PHE:HZ	1.57	0.69
4:M:400:BCL:H43	5:M:500:BPH:CBB	2.23	0.69
3:H:149:ILE:CA	3:H:164:VAL:HB	2.22	0.69
1:L:1:ALA:CB	1:L:7:ARG:HG2	2.21	0.69
6:L:800:UQ:C25	2:M:127:TRP:CZ2	2.76	0.69
2:M:24:VAL:HG11	2:M:26:LEU:HB2	1.74	0.69
2:M:250:TRP:HE1	6:M:750:UQ:CM5	2.05	0.69
3:H:134:MET:HE1	3:H:142:VAL:HG22	1.75	0.69
1:L:65:SER:OG	1:L:66:VAL:N	2.26	0.69
3:H:80:SER:O	3:H:81:GLU:HB2	1.91	0.69
2:M:74:TRP:O	2:M:77:ALA:HB3	1.93	0.69
1:L:188:ALA:HB2	2:M:271:ALA:CB	2.23	0.68
2:M:113:TRP:HZ2	2:M:172:ALA:CB	2.04	0.68
2:M:227:PHE:HB2	2:M:242:ALA:HB2	1.75	0.68
4:L:450:BCL:CBB	4:L:450:BCL:HMB1	2.23	0.68
2:M:153:TRP:CH2	2:M:283:LEU:CD1	2.76	0.68
3:H:135:LYS:HG3	3:H:166:ASP:OD2	1.94	0.68
1:L:187:LEU:HD23	1:L:187:LEU:O	1.94	0.68
2:M:97:ALA:C	2:M:99:GLU:N	2.47	0.68
3:H:135:LYS:HZ3	3:H:165:VAL:CG1	2.06	0.68
1:L:212:GLU:CA	6:L:800:UQ:HM21	2.23	0.68
2:M:95:PRO:HB2	2:M:96:PRO:CD	2.24	0.68
1:L:189:LEU:O	1:L:193:LEU:HB2	1.94	0.68
3:H:27:LEU:HD21	3:H:32:GLN:NE2	2.09	0.68
1:L:168:HIS:CE1	4:L:350:BCL:HMC2	2.29	0.68
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.75	0.68
2:M:95:PRO:CB	2:M:96:PRO:HD2	2.24	0.68
1:L:180:PHE:CD1	1:L:240:ALA:HB1	2.28	0.67
1:L:214:THR:O	1:L:218:ASP:HB2	1.93	0.67
2:M:216:MET:HG2	2:M:250:TRP:CZ2	2.29	0.67
2:M:72:TRP:CE3	2:M:72:TRP:HA	2.28	0.67
2:M:50:TYR:C	2:M:51:LEU:HG	2.13	0.67
3:H:22:ILE:HG23	3:H:23:PHE:CD1	2.28	0.67
1:L:183:ASN:ND2	1:L:236:LEU:CD1	2.57	0.67
2:M:224:VAL:CG1	2:M:242:ALA:HB1	2.24	0.67
3:H:104:PRO:HB3	3:H:243:TYR:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:400:BCL:C4	5:M:500:BPH:CAB	2.73	0.67
1:L:59:TRP:O	1:L:60:ASN:HB2	1.95	0.67
3:H:63:THR:HA	3:H:74:THR:HG23	1.77	0.66
4:L:350:BCL:C2	5:L:550:BPH:HBB3	2.25	0.66
4:M:400:BCL:H142	5:M:500:BPH:H2	1.75	0.66
1:L:185:LEU:CD2	6:L:800:UQ:C15	2.64	0.66
1:L:80:LEU:CD1	1:L:85:LEU:HD21	2.26	0.66
2:M:29:ARG:HG2	2:M:29:ARG:HH11	1.61	0.66
1:L:34:PHE:HA	1:L:37:ALA:HB3	1.77	0.66
2:M:101:GLY:C	2:M:168:SER:HA	2.15	0.66
3:H:27:LEU:CD1	3:H:32:GLN:HB2	2.25	0.66
2:M:54:LEU:HD22	2:M:129:GLY:HA3	1.77	0.66
2:M:235:GLN:HB2	2:M:260:MET:HE2	1.76	0.66
2:M:72:TRP:CD1	2:M:112:LEU:HB3	2.30	0.66
2:M:102:LEU:CA	2:M:169:TRP:CD1	2.71	0.66
2:M:72:TRP:HZ3	2:M:75:TYR:HB2	1.61	0.66
2:M:4:GLN:HG3	3:H:193:MET:C	2.16	0.66
1:L:172:ALA:HB1	1:L:243:PHE:O	1.96	0.66
4:L:450:BCL:HMD2	4:M:400:BCL:CBB	2.26	0.66
1:L:183:ASN:CG	1:L:236:LEU:HB2	2.13	0.65
2:M:265:ARG:O	2:M:269:TRP:CD1	2.49	0.65
2:M:58:SER:OG	5:M:500:BPH:H4C2	1.96	0.65
1:L:117:ILE:HD13	2:M:249:PHE:HE2	1.57	0.65
1:L:213:ASP:O	1:L:217:ARG:HB2	1.95	0.65
2:M:239:ARG:HD3	3:H:38:GLU:OE1	1.96	0.65
3:H:244:ALA:O	3:H:245:ALA:C	2.32	0.65
1:L:127:ALA:O	1:L:131:LEU:HG	1.96	0.65
3:H:199:GLN:HG2	3:H:200:SER:N	2.11	0.65
3:H:88:ALA:O	3:H:98:HIS:HB3	1.97	0.65
4:L:450:BCL:HMD3	2:M:195:PHE:HE1	1.61	0.65
1:L:218:ASP:CG	2:M:50:TYR:CE1	2.68	0.65
2:M:226:ARG:HA	3:H:194:GLN:HG3	1.77	0.65
2:M:36:THR:HG22	2:M:37:LEU:N	2.11	0.65
3:H:133:PRO:HA	3:H:167:ILE:O	1.97	0.65
3:H:209:SER:C	3:H:211:ASP:H	1.98	0.65
1:L:193:LEU:HD21	1:L:215:PHE:CE2	2.32	0.65
2:M:49:ILE:HG12	2:M:50:TYR:O	1.97	0.65
1:L:20:ASN:HD22	1:L:23:ASP:HB3	1.62	0.64
2:M:158:LEU:HD21	2:M:183:TRP:CH2	2.32	0.64
2:M:254:MET:CE	6:M:750:UQ:C11	2.67	0.64
1:L:74:GLY:O	1:L:75:LEU:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:265:ARG:O	2:M:269:TRP:HD1	1.81	0.64
2:M:157:VAL:HG13	2:M:162:ARG:HB2	1.77	0.64
3:H:115:VAL:HG12	3:H:116:ALA:H	1.62	0.64
3:H:216:ILE:HG12	3:H:236:TYR:CE1	2.32	0.64
3:H:154:ARG:NH1	3:H:158:LEU:HG	2.12	0.64
2:M:204:ILE:HG12	4:M:400:BCL:CHB	2.28	0.64
2:M:154:LEU:HD22	4:M:400:BCL:H2	1.80	0.64
1:L:86:TRP:HZ3	1:L:142:TRP:HB3	1.63	0.63
2:M:81:PRO:C	2:M:85:LEU:HD12	2.19	0.63
3:H:5:THR:HG23	3:H:10:PHE:N	2.13	0.63
2:M:199:PHE:CE1	2:M:280:ILE:HG22	2.33	0.63
1:L:43:ALA:O	1:L:47:ILE:HB	1.98	0.63
2:M:31:VAL:HG23	2:M:33:PRO:HD3	1.81	0.63
1:L:141:ALA:C	1:L:143:GLY:H	2.02	0.63
1:L:181:PHE:O	1:L:184:ALA:HB3	1.99	0.63
2:M:150:SER:O	2:M:153:TRP:HB3	1.98	0.63
1:L:41:PHE:HD2	1:L:92:CYS:HA	1.63	0.63
1:L:218:ASP:CB	2:M:50:TYR:HE1	2.08	0.63
2:M:72:TRP:HE3	2:M:72:TRP:HA	1.64	0.63
6:M:750:UQ:C25	6:M:750:UQ:H211	2.28	0.63
3:H:118:ARG:NH2	3:H:120:LEU:HD21	2.13	0.63
3:H:152:PRO:HG2	3:H:201:ASN:O	1.98	0.63
1:L:218:ASP:HB3	2:M:50:TYR:HE1	1.62	0.63
1:L:172:ALA:O	1:L:175:ILE:N	2.32	0.63
4:L:350:BCL:CBB	4:L:350:BCL:HMB1	2.29	0.63
1:L:156:TRP:CH2	1:L:248:MET:HE3	2.34	0.63
2:M:264:HIS:O	2:M:267:ALA:HB3	1.99	0.63
3:H:36:MET:O	3:H:40:TYR:HB2	1.99	0.62
1:L:175:ILE:HG21	1:L:243:PHE:CD2	2.33	0.62
2:M:108:LYS:HG2	2:M:108:LYS:O	1.97	0.62
2:M:113:TRP:CZ3	2:M:169:TRP:CE3	2.82	0.62
2:M:45:GLN:HG2	2:M:47:GLY:O	1.99	0.62
1:L:185:LEU:HA	5:M:500:BPH:HMC2	1.79	0.62
4:L:350:BCL:C2	5:L:550:BPH:CBB	2.76	0.62
2:M:234:GLU:OE2	3:H:123:LEU:HD11	1.99	0.62
3:H:149:ILE:C	3:H:164:VAL:HB	2.20	0.62
1:L:44:LEU:HA	1:L:47:ILE:CG2	2.29	0.62
1:L:193:LEU:HD11	1:L:216:PHE:CD1	2.33	0.62
1:L:269:LEU:HG	1:L:270:PRO:HD2	1.81	0.62
1:L:112:GLY:O	2:M:226:ARG:NH2	2.33	0.62
2:M:199:PHE:HB3	2:M:277:THR:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:400:BCL:H143	5:M:500:BPH:O1A	1.99	0.62
3:H:75:VAL:N	3:H:76:PRO:CD	2.63	0.62
1:L:218:ASP:HB3	2:M:50:TYR:CD1	2.33	0.62
1:L:264:GLN:HG3	1:L:264:GLN:O	2.00	0.62
2:M:161:ILE:HG22	2:M:162:ARG:N	2.15	0.62
1:L:206:MET:CE	2:M:237:ALA:HB2	2.29	0.62
4:M:601:BCL:HBC1	4:M:400:BCL:CB D	2.29	0.62
1:L:152:THR:C	1:L:154:LEU:H	2.03	0.62
2:M:188:SER:OG	2:M:194:LEU:HB2	1.99	0.62
1:L:222:TYR:HE2	2:M:38:LEU:HD21	1.62	0.62
1:L:130:THR:HA	1:L:134:PHE:HB2	1.80	0.62
4:L:350:BCL:C7	4:L:450:BCL:HBB2	2.30	0.62
1:L:235:LEU:O	1:L:238:LEU:HB2	2.00	0.62
2:M:130:ARG:O	2:M:134:ARG:CB	2.47	0.62
2:M:216:MET:CE	6:M:750:UQ:H13	2.30	0.62
2:M:83:VAL:HG22	2:M:86:ARG:HH12	1.63	0.62
2:M:158:LEU:HD21	2:M:183:TRP:HZ3	1.62	0.61
2:M:199:PHE:HB2	2:M:281:GLY:HA3	1.81	0.61
2:M:68:THR:CG2	2:M:112:LEU:HD13	2.30	0.61
2:M:6:ILE:O	2:M:7:PHE:HB3	1.99	0.61
1:L:41:PHE:HB3	1:L:92:CYS:HB3	1.82	0.61
1:L:41:PHE:HB3	1:L:92:CYS:O	1.99	0.61
2:M:199:PHE:CD2	2:M:281:GLY:HA2	2.35	0.61
2:M:212:LEU:HD21	6:M:750:UQ:H162	1.80	0.61
1:L:190:HIS:CB	1:L:229:ILE:HG12	2.29	0.61
3:H:130:LYS:HG3	3:H:172:PRO:HD2	1.82	0.61
3:H:17:ILE:HG23	3:H:21:TRP:NE1	2.16	0.61
3:H:27:LEU:CG	3:H:28:ILE:N	2.62	0.61
1:L:51:TRP:O	1:L:54:VAL:HB	2.00	0.61
5:L:550:BPH:CBB	5:L:550:BPH:HHC	2.30	0.61
2:M:235:GLN:CB	2:M:260:MET:HE2	2.30	0.61
4:M:400:BCL:H42	5:M:500:BPH:HHC	1.81	0.61
2:M:18:LEU:HD13	2:M:48:PRO:HG3	1.83	0.61
3:H:130:LYS:HG3	3:H:172:PRO:CD	2.30	0.61
1:L:101:ALA:O	1:L:104:GLU:HB2	2.00	0.61
1:L:111:LEU:HD13	1:L:113:ILE:HD11	1.83	0.61
2:M:102:LEU:HB3	2:M:167:GLY:O	1.99	0.61
3:H:130:LYS:HB3	3:H:131:ILE:HD13	1.82	0.61
3:H:171:ILE:CB	3:H:172:PRO:HD3	2.31	0.61
3:H:192:PRO:CD	3:H:237:VAL:HG21	2.30	0.61
2:M:4:GLN:HB2	3:H:194:GLN:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:THR:O	3:H:34:GLU:HB2	1.99	0.61
3:H:36:MET:HG2	3:H:40:TYR:CZ	2.35	0.61
1:L:93:ALA:O	1:L:97:PHE:CD2	2.54	0.61
1:L:132:VAL:O	1:L:136:PRO:HG2	2.00	0.61
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.82	0.61
1:L:171:PRO:O	1:L:175:ILE:HG12	2.01	0.61
1:L:17:VAL:HG22	1:L:33:PHE:CB	2.30	0.61
2:M:29(A):SER:OG	2:M:51:LEU:HD11	2.01	0.61
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.83	0.61
3:H:56:PHE:N	3:H:57:PRO:CD	2.63	0.61
3:H:63:THR:CA	3:H:74:THR:HG23	2.30	0.61
6:M:750:UQ:C12	6:M:750:UQ:C14	2.71	0.61
1:L:200:PRO:HG2	1:L:205:GLU:O	2.01	0.60
2:M:113:TRP:HZ3	2:M:169:TRP:CE3	2.13	0.60
3:H:123:LEU:O	3:H:124:ASP:HB2	2.00	0.60
3:H:165:VAL:O	3:H:166:ASP:HB2	2.00	0.60
2:M:278:GLY:O	2:M:282:ILE:HG12	2.01	0.60
3:H:148:PRO:HB2	3:H:164:VAL:HG11	1.81	0.60
2:M:4:GLN:CD	3:H:193:MET:HG3	2.22	0.60
3:H:37:ARG:HB3	3:H:75:VAL:HG12	1.82	0.60
2:M:164:ILE:C	2:M:166:MET:H	2.04	0.60
2:M:256:PHE:CE1	6:M:750:UQ:H252	2.34	0.60
4:M:400:BCL:HMB1	4:M:400:BCL:HBB2	1.82	0.60
1:L:17:VAL:HG22	1:L:33:PHE:HB2	1.82	0.60
1:L:44:LEU:HA	1:L:47:ILE:HB	1.83	0.60
2:M:96:PRO:CG	2:M:170:SER:N	2.63	0.60
3:H:87:LEU:HG	3:H:109:VAL:HG11	1.82	0.60
4:M:601:BCL:HBC1	4:M:400:BCL:HBA1	1.82	0.60
1:L:133:LEU:O	1:L:137:VAL:HG23	2.01	0.60
2:M:157:VAL:HA	2:M:161:ILE:CG2	2.30	0.60
2:M:95:PRO:CB	2:M:96:PRO:CD	2.79	0.60
2:M:204:ILE:HG12	4:M:400:BCL:C1B	2.32	0.60
1:L:194:VAL:O	1:L:195:LEU:C	2.39	0.60
1:L:227:LEU:CD2	1:L:231:ARG:NH2	2.63	0.60
1:L:274:ASN:O	1:L:275:ILE:HG12	2.01	0.60
4:M:400:BCL:H43	5:M:500:BPH:HBB2	1.83	0.60
2:M:4:GLN:CG	3:H:193:MET:O	2.43	0.60
3:H:70:ARG:HG2	3:H:70:ARG:HH11	1.67	0.60
1:L:127:ALA:HB3	4:L:350:BCL:C4	2.31	0.60
2:M:251:ARG:NH1	2:M:251:ARG:HG3	2.16	0.60
2:M:128:TRP:HE1	2:M:145:ALA:CB	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:THR:HG23	2:M:50:TYR:OH	2.01	0.59
2:M:244:GLU:O	2:M:247:ALA:N	2.36	0.59
1:L:97:PHE:O	1:L:100:TRP:HB3	2.02	0.59
1:L:1:ALA:HB2	1:L:7:ARG:CG	2.28	0.59
1:L:152:THR:HA	2:M:303:PRO:HB3	1.85	0.59
2:M:71:ILE:O	2:M:74:TRP:HB3	2.02	0.59
1:L:53:ALA:CB	1:L:64:ILE:HG13	2.33	0.59
2:M:235:GLN:NE2	2:M:260:MET:CE	2.64	0.59
1:L:104:GLU:HA	1:L:107:ILE:CD1	2.32	0.59
2:M:158:LEU:HD23	2:M:173:VAL:CG2	2.32	0.59
6:M:750:UQ:H252	6:M:750:UQ:H211	1.83	0.59
3:H:192:PRO:HD3	3:H:237:VAL:HG21	1.85	0.59
3:H:37:ARG:HB3	3:H:75:VAL:HG11	1.83	0.59
1:L:187:LEU:O	1:L:191:GLY:N	2.35	0.59
2:M:282:ILE:HG12	4:M:400:BCL:HED1	1.85	0.59
3:H:111:PRO:HD2	3:H:243:TYR:CZ	2.37	0.59
1:L:86:TRP:CZ3	1:L:142:TRP:HB3	2.37	0.59
2:M:154:LEU:CD1	2:M:275:THR:HG22	2.31	0.59
2:M:59:LEU:O	2:M:63:LEU:HB2	2.03	0.59
3:H:237:VAL:O	3:H:239:GLY:N	2.36	0.59
1:L:185:LEU:CG	1:L:186:ALA:N	2.62	0.58
1:L:51:TRP:CZ2	1:L:80:LEU:HD21	2.39	0.58
3:H:66:LEU:HB2	3:H:71:GLY:HA2	1.85	0.58
2:M:158:LEU:HD23	2:M:173:VAL:HG21	1.85	0.58
3:H:170:ASP:CG	3:H:173:GLU:HB3	2.23	0.58
2:M:193:ASN:C	2:M:195:PHE:H	2.07	0.58
1:L:116:HIS:HB2	2:M:223:ALA:HB2	1.85	0.58
2:M:259:THR:O	2:M:261:GLU:N	2.36	0.58
1:L:231:ARG:NE	2:M:6:ILE:N	2.37	0.58
1:L:55:LEU:HG	1:L:56:GLN:N	2.17	0.58
3:H:65:ILE:O	3:H:66:LEU:O	2.22	0.58
1:L:185:LEU:HD23	1:L:186:ALA:N	2.18	0.58
2:M:92:SER:HA	2:M:175:TYR:O	2.04	0.58
1:L:185:LEU:HD22	6:L:800:UQ:C15	2.31	0.58
2:M:97:ALA:CB	2:M:98:PRO:CD	2.82	0.58
3:H:22:ILE:HG23	3:H:23:PHE:HD1	1.68	0.58
1:L:172:ALA:HA	1:L:175:ILE:HG12	1.86	0.58
2:M:21:THR:HA	2:M:137:ALA:O	2.04	0.58
1:L:222:TYR:CD1	1:L:223:SER:N	2.71	0.58
3:H:114:TRP:CG	3:H:232:LYS:HG3	2.39	0.57
2:M:165:LEU:N	2:M:165:LEU:CD2	2.64	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:218:GLY:O	2:M:222:LEU:HD12	2.03	0.57
3:H:207:ALA:HB3	3:H:237:VAL:HG12	1.85	0.57
1:L:229:ILE:HB	6:L:800:UQ:HM53	1.86	0.57
1:L:3:LEU:CB	1:L:6:GLU:HB2	2.24	0.57
2:M:113:TRP:CZ2	2:M:172:ALA:HB1	2.30	0.57
2:M:259:THR:C	2:M:261:GLU:N	2.57	0.57
2:M:97:ALA:CB	2:M:98:PRO:HD3	2.31	0.57
3:H:122:GLU:HA	3:H:227:LEU:HD21	1.86	0.57
3:H:111:PRO:HD2	3:H:243:TYR:HE2	1.60	0.57
3:H:67:PRO:HG2	3:H:123:LEU:CD2	2.28	0.57
4:L:350:BCL:CAA	4:L:450:BCL:HBC1	2.34	0.57
4:L:350:BCL:CBD	4:L:450:BCL:HBC1	2.11	0.57
2:M:148:PHE:CZ	2:M:152:ILE:HD11	2.40	0.57
2:M:238:ASP:OD2	3:H:117:ARG:HG3	2.04	0.57
1:L:13:GLY:HA3	3:H:242:MET:HE1	1.86	0.57
2:M:124:VAL:CG1	2:M:152:ILE:HD12	2.34	0.57
1:L:169:TYR:CD2	1:L:260:VAL:HG22	2.38	0.57
2:M:97:ALA:O	2:M:99:GLU:N	2.38	0.57
1:L:206:MET:HE1	2:M:237:ALA:HB2	1.85	0.57
2:M:106:PRO:O	2:M:108:LYS:N	2.38	0.57
2:M:217:HIS:HD1	2:M:263:ILE:HG12	1.70	0.57
2:M:278:GLY:CA	4:M:400:BCL:HED3	2.33	0.57
3:H:121:PRO:O	3:H:122:GLU:C	2.43	0.57
2:M:216:MET:CG	2:M:250:TRP:CZ2	2.88	0.57
3:H:131:ILE:HD13	3:H:131:ILE:N	2.20	0.57
3:H:141:HIS:HE1	3:H:143:SER:HB2	1.69	0.57
1:L:11:VAL:HG21	3:H:111:PRO:HD3	1.87	0.57
1:L:169:TYR:CD1	1:L:260:VAL:HG22	2.40	0.57
2:M:87:ASP:O	2:M:88:LEU:HB3	2.03	0.57
3:H:208:LEU:HD13	3:H:216:ILE:HD11	1.86	0.57
3:H:5:THR:HG21	3:H:9:ASN:HA	1.86	0.57
1:L:156:TRP:CH2	1:L:248:MET:CE	2.87	0.57
2:M:164:ILE:O	2:M:166:MET:N	2.38	0.57
2:M:79:TRP:HB3	2:M:80:ASN:OD1	2.05	0.57
3:H:124:ASP:HB3	3:H:128:HIS:O	2.05	0.57
3:H:27:LEU:HG	3:H:32:GLN:HB2	1.87	0.57
1:L:154:LEU:HD23	2:M:195:PHE:HD1	1.70	0.57
1:L:215:PHE:CA	2:M:138:LEU:HD22	2.33	0.57
2:M:89:PHE:HB3	2:M:178:PHE:CE1	2.40	0.57
2:M:250:TRP:NE1	6:M:750:UQ:HM53	2.17	0.57
3:H:134:MET:CE	3:H:142:VAL:HG22	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:149:ILE:H	3:H:164:VAL:HG11	1.70	0.56
2:M:164:ILE:C	2:M:166:MET:N	2.56	0.56
2:M:25:ASN:N	2:M:25:ASN:ND2	2.54	0.56
2:M:274:VAL:CG1	2:M:275:THR:H	2.06	0.56
3:H:128:HIS:CG	3:H:129:ASN:H	2.21	0.56
3:H:130:LYS:HE2	3:H:170:ASP:OD1	2.06	0.56
3:H:205:VAL:HG12	3:H:206:ASN:N	2.20	0.56
1:L:13:GLY:N	1:L:110:LYS:HE2	2.20	0.56
2:M:202:LEU:HD23	3:H:20:PHE:CE2	2.36	0.56
1:L:10:ARG:HG3	1:L:25:TRP:CZ3	2.39	0.56
2:M:184:THR:CG2	2:M:185:ASN:N	2.68	0.56
2:M:221:ILE:O	2:M:225:SER:OG	2.21	0.56
2:M:272:VAL:C	2:M:274:VAL:N	2.59	0.56
3:H:216:ILE:HG23	3:H:217:PRO:HD2	1.86	0.56
1:L:44:LEU:CA	1:L:47:ILE:HB	2.36	0.56
2:M:250:TRP:NE1	6:M:750:UQ:CM5	2.67	0.56
3:H:159:GLU:CG	3:H:160:ILE:H	2.19	0.56
1:L:222:TYR:HE1	1:L:224:ILE:HA	1.71	0.56
1:L:260:VAL:O	1:L:263:TRP:HB2	2.04	0.56
1:L:17:VAL:CG2	1:L:33:PHE:HB2	2.35	0.56
2:M:254:MET:SD	6:M:750:UQ:H203	2.45	0.56
3:H:83:ARG:HB3	3:H:84:PRO:HD2	1.88	0.56
2:M:272:VAL:C	2:M:274:VAL:H	2.09	0.56
3:H:147:ASN:O	3:H:148:PRO:O	2.23	0.56
3:H:154:ARG:HH11	3:H:158:LEU:CG	2.18	0.56
5:L:550:BPH:HBB2	5:L:550:BPH:HHC	1.86	0.56
2:M:166:MET:SD	2:M:171:GLU:OE1	2.64	0.56
2:M:62:GLY:O	2:M:65:TRP:HE3	1.88	0.56
5:M:500:BPH:O1A	5:M:500:BPH:H3A	2.06	0.56
3:H:1:MET:CG	3:H:2:VAL:H	2.19	0.56
1:L:122:ALA:O	1:L:123:PHE:C	2.44	0.56
1:L:61:PRO:HA	1:L:64:ILE:HG22	1.87	0.56
2:M:99:GLU:O	2:M:100:TYR:CB	2.37	0.56
2:M:15:PRO:HD2	3:H:140:PHE:CD1	2.42	0.55
3:H:151:LEU:O	3:H:164:VAL:HG23	2.06	0.55
2:M:171:GLU:O	2:M:172:ALA:CB	2.55	0.55
2:M:74:TRP:C	2:M:74:TRP:CD1	2.80	0.55
1:L:25:TRP:HB3	1:L:29:PHE:O	2.06	0.55
1:L:60:ASN:C	1:L:62:GLN:H	2.08	0.55
2:M:96:PRO:CG	2:M:170:SER:CA	2.50	0.55
3:H:181:VAL:HB	3:H:189:ARG:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:111:LEU:HB2	1:L:113:ILE:CG1	2.36	0.55
1:L:127:ALA:HB3	4:L:350:BCL:H42	1.87	0.55
2:M:183:TRP:CZ3	4:M:601:BCL:CMC	2.85	0.55
2:M:199:PHE:CD1	2:M:280:ILE:HG22	2.42	0.55
3:H:154:ARG:HH12	3:H:158:LEU:HD11	1.71	0.55
2:M:250:TRP:HB3	2:M:254:MET:CG	2.36	0.55
3:H:7:PHE:C	3:H:9:ASN:H	2.08	0.55
3:H:4:VAL:HG12	3:H:11:ASP:OD1	2.07	0.55
2:M:72:TRP:CE3	2:M:72:TRP:O	2.60	0.55
2:M:157:VAL:HG22	2:M:283:LEU:HD11	1.89	0.55
1:L:174:MET:HE2	4:M:601:BCL:HED2	1.89	0.55
3:H:40:TYR:HA	3:H:41:PRO:C	2.27	0.55
3:H:74:THR:C	3:H:76:PRO:HD2	2.27	0.55
1:L:58:THR:CG2	1:L:59:TRP:N	2.53	0.55
3:H:197:LYS:N	3:H:204:HIS:O	2.39	0.55
3:H:217:PRO:HD3	3:H:236:TYR:CD2	2.42	0.55
2:M:108:LYS:O	2:M:109:GLU:CB	2.43	0.55
3:H:167:ILE:HG23	3:H:179:LEU:CD1	2.35	0.54
1:L:117:ILE:N	1:L:118:PRO:CD	2.70	0.54
1:L:86:TRP:HZ2	1:L:132:VAL:HG13	1.71	0.54
1:L:50:ALA:O	1:L:54:VAL:HG23	2.07	0.54
2:M:114:LEU:O	2:M:118:PHE:HD2	1.89	0.54
2:M:161:ILE:CG2	2:M:162:ARG:N	2.70	0.54
2:M:173:VAL:HG21	4:M:601:BCL:HMC2	1.89	0.54
1:L:185:LEU:HB2	5:M:500:BPH:HMC2	1.88	0.54
1:L:185:LEU:O	1:L:188:ALA:HB3	2.07	0.54
3:H:154:ARG:NH1	3:H:158:LEU:CG	2.70	0.54
1:L:95:GLY:O	1:L:99:SER:HB2	2.07	0.54
1:L:107:ILE:HD12	2:M:249:PHE:HE1	1.72	0.54
1:L:122:ALA:HA	1:L:125:ILE:HG13	1.89	0.54
2:M:157:VAL:HG12	2:M:158:LEU:N	2.23	0.54
1:L:185:LEU:CB	5:M:500:BPH:HMC2	2.37	0.54
3:H:209:SER:O	3:H:213:PHE:HD1	1.90	0.54
2:M:227:PHE:CD2	3:H:234:CYS:HB3	2.42	0.54
3:H:37:ARG:HH12	3:H:59:PRO:HG2	1.72	0.54
1:L:180:PHE:CE1	4:L:350:BCL:HMA2	2.42	0.54
2:M:254:MET:HB3	6:M:750:UQ:C20	2.37	0.54
2:M:191:HIS:CD2	2:M:285:SER:OG	2.61	0.54
2:M:21:THR:O	2:M:22:GLU:C	2.45	0.54
2:M:178:PHE:HA	2:M:181:LEU:HD12	1.90	0.54
2:M:289:VAL:HG12	2:M:291:ASN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:294:VAL:O	2:M:298:ASN:N	2.41	0.54
3:H:192:PRO:HG3	3:H:237:VAL:HG21	1.87	0.54
3:H:36:MET:HG2	3:H:40:TYR:CE2	2.42	0.54
3:H:75:VAL:C	3:H:77:GLY:H	2.11	0.54
1:L:141:ALA:C	1:L:143:GLY:N	2.61	0.54
3:H:189:ARG:HH21	3:H:218:THR:CG2	2.21	0.54
2:M:92:SER:O	2:M:93:LEU:HD23	2.08	0.53
3:H:151:LEU:CD2	3:H:203:VAL:HG21	2.37	0.53
1:L:190:HIS:CG	1:L:229:ILE:HG12	2.43	0.53
1:L:190:HIS:O	1:L:194:VAL:HG23	2.08	0.53
1:L:20:ASN:CG	1:L:21:LEU:H	2.12	0.53
1:L:37:ALA:CA	1:L:40:PHE:HB2	2.37	0.53
1:L:107:ILE:HD13	2:M:253:THR:OG1	2.09	0.53
2:M:179:SER:C	2:M:181:LEU:N	2.61	0.53
2:M:96:PRO:HD2	2:M:170:SER:HA	1.91	0.53
3:H:105:MET:CE	3:H:212:LEU:HD22	2.37	0.53
1:L:174:MET:CE	4:M:601:BCL:HED2	2.38	0.53
3:H:105:MET:HE1	3:H:212:LEU:HD13	1.90	0.53
4:L:350:BCL:H152	5:L:550:BPH:O2A	2.06	0.53
1:L:54:VAL:O	1:L:55:LEU:O	2.26	0.53
2:M:216:MET:CG	2:M:250:TRP:HZ2	2.21	0.53
2:M:25:ASN:HD22	2:M:25:ASN:H	1.56	0.53
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.90	0.53
3:H:28:ILE:HG22	3:H:29:TYR:H	1.73	0.53
3:H:83:ARG:HB3	3:H:84:PRO:CD	2.38	0.53
1:L:175:ILE:HG22	1:L:179:PHE:CE1	2.44	0.53
3:H:66:LEU:HB2	3:H:71:GLY:CA	2.38	0.53
1:L:41:PHE:HB2	1:L:96:ALA:HB2	1.89	0.53
3:H:103:ASP:HB2	3:H:106:LYS:HB3	1.90	0.53
2:M:272:VAL:O	2:M:274:VAL:N	2.41	0.53
3:H:174:GLN:O	3:H:175:MET:HB2	2.09	0.53
1:L:169:TYR:CD2	1:L:260:VAL:HG13	2.44	0.53
1:L:12:PRO:HD3	3:H:97:PRO:HB2	1.91	0.52
1:L:103:ARG:O	1:L:107:ILE:HG13	2.09	0.52
1:L:158:SER:O	1:L:162:TYR:CD2	2.58	0.52
1:L:241:VAL:HA	1:L:244:SER:HB3	1.89	0.52
2:M:119:PHE:HA	2:M:122:VAL:HG23	1.91	0.52
2:M:187:PHE:HD2	4:M:400:BCL:HMD3	1.75	0.52
1:L:177:ILE:HG22	1:L:178:SER:N	2.23	0.52
1:L:216:PHE:O	1:L:219:LEU:CB	2.57	0.52
2:M:58:SER:HA	2:M:123:ALA:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:30:TYR:O	3:H:33:THR:HB	2.09	0.52
1:L:62:GLN:HA	1:L:150:ILE:HB	1.90	0.52
1:L:162:TYR:O	1:L:163:THR:C	2.48	0.52
2:M:216:MET:HE3	6:M:750:UQ:H13	1.92	0.52
3:H:13:ALA:O	3:H:16:ALA:HB3	2.10	0.52
3:H:27:LEU:CG	3:H:32:GLN:HB2	2.39	0.52
1:L:177:ILE:HD13	4:L:350:BCL:HMB3	1.92	0.52
2:M:158:LEU:CD2	2:M:183:TRP:CH2	2.92	0.52
3:H:66:LEU:HB3	3:H:67:PRO:CD	2.37	0.52
1:L:48:LEU:O	1:L:51:TRP:HB3	2.09	0.52
1:L:93:ALA:HB1	1:L:97:PHE:CE2	2.45	0.52
2:M:66:PHE:CD2	5:M:500:BPH:H111	2.45	0.52
3:H:115:VAL:CG1	3:H:116:ALA:H	2.22	0.52
2:M:265:ARG:O	2:M:269:TRP:HB2	2.10	0.52
3:H:204:HIS:CD2	3:H:205:VAL:O	2.62	0.52
1:L:111:LEU:CD1	1:L:113:ILE:HD11	2.40	0.52
1:L:174:MET:O	1:L:177:ILE:HB	2.10	0.52
2:M:5:ASN:HD21	2:M:225:SER:CB	2.22	0.52
2:M:12:VAL:HG21	3:H:169:VAL:HG11	1.92	0.52
2:M:153:TRP:CH2	2:M:283:LEU:HD12	2.45	0.52
2:M:293:TYR:CE2	2:M:297:GLN:NE2	2.78	0.52
2:M:72:TRP:CB	2:M:93:LEU:HD13	2.39	0.52
3:H:141:HIS:CE1	3:H:143:SER:HB2	2.45	0.52
1:L:44:LEU:HA	1:L:47:ILE:HG21	1.92	0.52
3:H:6:ALA:HB3	3:H:10:PHE:O	2.10	0.52
3:H:61:PRO:CB	3:H:76:PRO:HG3	2.39	0.52
1:L:172:ALA:O	1:L:173:HIS:C	2.47	0.52
1:L:242:PHE:C	1:L:242:PHE:CD1	2.83	0.52
6:L:800:UQ:H251	2:M:127:TRP:CZ2	2.45	0.52
2:M:162:ARG:HD2	2:M:163:PRO:N	2.25	0.52
2:M:179:SER:O	2:M:180:HIS:C	2.45	0.52
2:M:250:TRP:HB3	2:M:254:MET:HG3	1.91	0.52
1:L:183:ASN:HA	1:L:186:ALA:HB3	1.92	0.51
2:M:4:GLN:CB	3:H:194:GLN:HA	2.40	0.51
3:H:153:VAL:HG12	3:H:161:ALA:HB3	1.92	0.51
1:L:274:ASN:O	1:L:275:ILE:CG1	2.58	0.51
6:L:800:UQ:H253	2:M:127:TRP:CZ2	2.44	0.51
3:H:27:LEU:O	3:H:28:ILE:O	2.27	0.51
1:L:176:ALA:O	1:L:180:PHE:CD1	2.60	0.51
2:M:113:TRP:CH2	2:M:172:ALA:HB3	2.44	0.51
2:M:291:ASN:OD1	2:M:294:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:114:TRP:HB3	3:H:232:LYS:HA	1.92	0.51
3:H:251:VAL:O	3:H:252:VAL:HB	2.10	0.51
1:L:215:PHE:HA	2:M:138:LEU:CD2	2.38	0.51
1:L:190:HIS:HB2	1:L:229:ILE:HG12	1.92	0.51
1:L:62:GLN:HB3	1:L:151:TRP:CD1	2.33	0.51
1:L:80:LEU:CD1	1:L:85:LEU:CD2	2.89	0.51
1:L:217:ARG:N	1:L:223:SER:HB2	2.25	0.51
1:L:272:TRP:O	1:L:273:ALA:HB3	2.11	0.51
1:L:97:PHE:CD1	4:L:350:BCL:H121	2.46	0.51
1:L:53:ALA:HB2	1:L:64:ILE:CG1	2.40	0.51
1:L:127:ALA:CB	4:L:350:BCL:H42	2.41	0.51
1:L:41:PHE:CB	1:L:92:CYS:O	2.58	0.51
3:H:22:ILE:HG23	3:H:23:PHE:N	2.24	0.51
3:H:70:ARG:NH1	3:H:70:ARG:HG2	2.26	0.51
1:L:128:TYR:HD1	1:L:128:TYR:O	1.94	0.51
1:L:274:ASN:C	1:L:275:ILE:HG12	2.31	0.51
2:M:5:ASN:HD21	2:M:225:SER:HB2	1.76	0.51
3:H:148:PRO:O	3:H:149:ILE:HB	2.11	0.51
2:M:2:GLU:O	2:M:3:TYR:HB2	2.11	0.51
3:H:194:GLN:O	3:H:195:MET:HG2	2.11	0.51
3:H:37:ARG:NH1	3:H:59:PRO:HG2	2.26	0.51
1:L:189:LEU:HD22	1:L:216:PHE:CZ	2.43	0.51
1:L:230:HIS:CD2	2:M:217:HIS:CD2	2.99	0.51
3:H:196:VAL:CG2	3:H:203:VAL:HG13	2.41	0.51
3:H:252:VAL:HG12	3:H:253:ALA:CB	2.41	0.51
1:L:160:THR:O	1:L:163:THR:HB	2.11	0.51
2:M:158:LEU:HD21	4:M:601:BCL:HMC1	1.92	0.51
2:M:72:TRP:CZ3	2:M:75:TYR:CB	2.94	0.51
1:L:117:ILE:N	1:L:118:PRO:HD2	2.26	0.50
1:L:20:ASN:C	1:L:22:PHE:N	2.60	0.50
1:L:227:LEU:CD2	1:L:231:ARG:CZ	2.89	0.50
1:L:183:ASN:ND2	1:L:236:LEU:CG	2.57	0.50
2:M:264:HIS:O	2:M:268:ILE:HG22	2.10	0.50
3:H:228:LEU:HD23	3:H:228:LEU:C	2.30	0.50
1:L:158:SER:OG	1:L:162:TYR:CE2	2.62	0.50
1:L:17:VAL:HG23	1:L:106:GLU:OE2	2.11	0.50
1:L:181:PHE:HE1	4:M:400:BCL:HAA1	1.75	0.50
2:M:8:SER:O	2:M:9:GLN:HB2	2.11	0.50
3:H:37:ARG:HH21	3:H:62:LYS:CG	2.22	0.50
2:M:224:VAL:C	2:M:226:ARG:H	2.13	0.50
3:H:61:PRO:HB2	3:H:74:THR:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:TYR:CE2	4:L:350:BCL:CBC	2.94	0.50
4:M:400:BCL:C4	5:M:500:BPH:CHC	2.89	0.50
3:H:242:MET:HG2	3:H:249:LYS:HB3	1.94	0.50
1:L:47:ILE:HG22	1:L:48:LEU:HG	1.93	0.50
2:M:179:SER:O	2:M:181:LEU:N	2.45	0.50
2:M:72:TRP:HB3	2:M:93:LEU:HD22	1.93	0.50
1:L:271:TRP:HB2	1:L:274:ASN:ND2	2.25	0.50
2:M:244:GLU:O	2:M:247:ALA:HB3	2.12	0.50
2:M:56:VAL:HG13	2:M:57:LEU:N	2.25	0.50
2:M:72:TRP:CE3	2:M:72:TRP:CA	2.95	0.50
2:M:72:TRP:HZ3	2:M:75:TYR:CB	2.25	0.50
3:H:135:LYS:CE	3:H:165:VAL:HG12	2.41	0.50
3:H:183:LEU:CD1	3:H:189:ARG:HD3	2.35	0.50
3:H:91:ALA:HB3	3:H:96:PHE:CG	2.47	0.50
2:M:101:GLY:O	2:M:169:TRP:N	2.40	0.50
4:M:400:BCL:HBB3	4:M:400:BCL:HMB1	1.91	0.50
2:M:77:ALA:O	2:M:83:VAL:HG11	2.12	0.50
1:L:100:TRP:CZ2	1:L:103:ARG:NH2	2.80	0.50
1:L:116:HIS:C	1:L:118:PRO:HD2	2.31	0.50
1:L:122:ALA:C	1:L:124:ALA:N	2.64	0.50
1:L:208:THR:HB	1:L:209:PRO:HD2	1.92	0.50
1:L:230:HIS:O	2:M:222:LEU:HD11	2.12	0.50
2:M:263:ILE:HG23	2:M:264:HIS:N	2.27	0.50
2:M:271:ALA:O	2:M:274:VAL:CB	2.57	0.50
2:M:69:ILE:CG1	2:M:93:LEU:HD12	2.38	0.50
3:H:170:ASP:HB2	3:H:175:MET:O	2.11	0.49
3:H:8:GLY:O	3:H:9:ASN:CB	2.57	0.49
3:H:91:ALA:HB3	3:H:96:PHE:HB3	1.93	0.49
1:L:118:PRO:O	1:L:121:PHE:HB3	2.12	0.49
4:M:601:BCL:HAC1	4:M:400:BCL:C3D	2.42	0.49
4:M:601:BCL:HMA1	4:M:400:BCL:C20	2.41	0.49
2:M:8:SER:O	2:M:9:GLN:CB	2.58	0.49
3:H:36:MET:HG2	3:H:40:TYR:CE1	2.47	0.49
1:L:13:GLY:H	1:L:110:LYS:CE	2.21	0.49
1:L:152:THR:O	1:L:154:LEU:N	2.45	0.49
4:L:350:BCL:H122	5:L:550:BPH:HBA1	1.93	0.49
1:L:93:ALA:O	1:L:96:ALA:HB3	2.12	0.49
2:M:12:VAL:HG11	3:H:169:VAL:HG21	1.94	0.49
2:M:184:THR:HG23	2:M:185:ASN:N	2.27	0.49
2:M:266:TRP:HE1	3:H:35:ASN:HD21	1.59	0.49
1:L:181:PHE:CE1	4:M:400:BCL:HAA1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:218:ASP:CB	2:M:50:TYR:CD1	2.95	0.49
3:H:135:LYS:HZ1	3:H:165:VAL:CG1	2.25	0.49
3:H:134:MET:SD	3:H:142:VAL:HG22	2.52	0.49
1:L:158:SER:C	1:L:162:TYR:HD2	2.16	0.49
4:L:350:BCL:H71	4:L:450:BCL:HBB2	1.93	0.49
3:H:190:LEU:H	3:H:190:LEU:HD23	1.76	0.49
1:L:234:LEU:O	1:L:238:LEU:HB2	2.12	0.49
1:L:275:ILE:C	1:L:276:PRO:O	2.50	0.49
2:M:37:LEU:HA	2:M:40:TRP:CD1	2.48	0.49
2:M:72:TRP:HB3	2:M:93:LEU:CD2	2.42	0.49
3:H:110:GLY:C	3:H:112:ALA:H	2.15	0.49
3:H:160:ILE:C	3:H:162:GLY:N	2.64	0.49
3:H:67:PRO:HB2	3:H:68:HIS:CE1	2.47	0.49
2:M:54:LEU:CD2	2:M:129:GLY:HA3	2.43	0.49
3:H:188:THR:HG21	3:H:219:ILE:HG22	1.93	0.49
1:L:13:GLY:HA3	3:H:242:MET:CE	2.43	0.49
1:L:51:TRP:O	1:L:54:VAL:N	2.44	0.49
1:L:13:GLY:O	1:L:14:GLY:C	2.50	0.49
1:L:128:TYR:CD2	4:L:450:BCL:HBB1	2.47	0.49
2:M:162:ARG:HD3	2:M:166:MET:CE	2.43	0.49
3:H:70:ARG:HG2	3:H:70:ARG:O	2.13	0.49
1:L:42:ALA:O	1:L:46:ILE:HG23	2.13	0.49
2:M:69:ILE:HD11	2:M:175:TYR:CG	2.48	0.49
2:M:202:LEU:HD12	2:M:205:ALA:HB3	1.95	0.49
3:H:149:ILE:N	3:H:164:VAL:HB	2.28	0.49
3:H:171:ILE:CB	3:H:172:PRO:CD	2.91	0.49
1:L:128:TYR:HD1	1:L:128:TYR:C	2.16	0.49
1:L:131:LEU:HD23	1:L:131:LEU:N	2.28	0.49
2:M:178:PHE:O	2:M:181:LEU:HB2	2.13	0.49
2:M:56:VAL:CG1	2:M:57:LEU:N	2.76	0.49
2:M:73:PHE:CG	2:M:91:PHE:HB3	2.48	0.49
3:H:1:MET:HG2	3:H:2:VAL:H	1.77	0.48
3:H:209:SER:C	3:H:211:ASP:N	2.66	0.48
2:M:208:TYR:O	2:M:211:ALA:HB3	2.13	0.48
1:L:97:PHE:CE1	4:L:350:BCL:H112	2.48	0.48
1:L:43:ALA:C	1:L:45:GLY:N	2.66	0.48
2:M:284:LEU:O	2:M:288:VAL:HG22	2.12	0.48
2:M:69:ILE:O	2:M:73:PHE:N	2.45	0.48
1:L:150:ILE:HG12	5:L:550:BPH:H191	1.95	0.48
1:L:212:GLU:HA	2:M:140:MET:CE	2.44	0.48
2:M:250:TRP:CD1	6:M:750:UQ:HM51	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:235:GLN:NE2	2:M:260:MET:HE1	2.28	0.48
2:M:36:THR:CG2	2:M:37:LEU:N	2.75	0.48
1:L:17:VAL:HG12	1:L:18:GLY:N	2.28	0.48
4:L:450:BCL:HMD3	2:M:195:PHE:CE1	2.45	0.48
2:M:212:LEU:C	2:M:212:LEU:HD23	2.33	0.48
1:L:141:ALA:O	1:L:143:GLY:N	2.32	0.48
1:L:80:LEU:HD12	1:L:85:LEU:CD2	2.44	0.48
2:M:157:VAL:HA	2:M:162:ARG:H	1.77	0.48
2:M:4:GLN:OE1	3:H:193:MET:HG3	2.12	0.48
3:H:208:LEU:CD1	3:H:216:ILE:HD11	2.44	0.48
3:H:24:LEU:C	3:H:26:GLY:N	2.66	0.48
2:M:136:GLN:O	2:M:137:ALA:HB2	2.13	0.48
2:M:161:ILE:HG22	2:M:162:ARG:H	1.79	0.48
2:M:113:TRP:CH2	2:M:172:ALA:CB	2.96	0.48
3:H:80:SER:OG	3:H:81:GLU:N	2.45	0.48
1:L:61:PRO:O	1:L:150:ILE:HD12	2.14	0.48
1:L:155:ASP:O	1:L:159:ASN:HB2	2.13	0.48
1:L:168:HIS:CD2	4:M:601:BCL:HMD3	2.48	0.48
1:L:85:LEU:O	1:L:89:ILE:HD12	2.12	0.48
5:M:500:BPH:H1C2	5:M:500:BPH:HAA2	1.95	0.48
2:M:83:VAL:HG22	2:M:86:ARG:NH1	2.26	0.48
1:L:105:VAL:HG13	1:L:115:TYR:CZ	2.48	0.48
1:L:44:LEU:O	1:L:48:LEU:HD12	2.14	0.48
1:L:212:GLU:HB3	6:L:800:UQ:CM2	2.44	0.48
5:M:500:BPH:H13	5:M:500:BPH:H101	1.69	0.48
3:H:177:ARG:O	3:H:193:MET:CB	2.61	0.48
1:L:13:GLY:HA2	3:H:242:MET:HE3	1.95	0.48
1:L:74:GLY:CA	1:L:141:ALA:HB2	2.26	0.48
1:L:212:GLU:CB	6:L:800:UQ:HM21	2.44	0.48
1:L:86:TRP:CZ3	1:L:142:TRP:HE3	2.32	0.48
2:M:148:PHE:O	2:M:152:ILE:HG12	2.14	0.48
2:M:151:ALA:O	4:M:400:BCL:H52	2.13	0.48
2:M:74:TRP:O	2:M:77:ALA:N	2.47	0.48
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.13	0.48
1:L:212:GLU:CA	2:M:140:MET:HE3	2.44	0.48
2:M:188:SER:CB	2:M:194:LEU:HB2	2.43	0.48
3:H:22:ILE:CG2	3:H:23:PHE:N	2.77	0.47
1:L:128:TYR:C	1:L:128:TYR:CD1	2.87	0.47
1:L:151:TRP:O	2:M:303:PRO:CB	2.58	0.47
2:M:114:LEU:O	2:M:118:PHE:CD2	2.67	0.47
2:M:89:PHE:CD2	2:M:177:ILE:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:ASN:OD1	2:M:214:PHE:CD2	2.61	0.47
2:M:2:GLU:HG2	2:M:3:TYR:H	1.79	0.47
2:M:16:ALA:CB	2:M:45:GLN:NE2	2.73	0.47
3:H:230:GLU:O	3:H:234:CYS:SG	2.71	0.47
3:H:96:PHE:HA	3:H:97:PRO:HD2	1.67	0.47
2:M:13:ARG:CG	2:M:14:GLY:N	2.74	0.47
3:H:209:SER:C	3:H:213:PHE:HD1	2.17	0.47
1:L:14:GLY:HA2	1:L:109:ARG:HB2	1.97	0.47
3:H:146:LYS:O	3:H:148:PRO:HD3	2.13	0.47
2:M:153:TRP:CZ2	2:M:283:LEU:CD1	2.88	0.47
2:M:53:SER:HB3	2:M:54:LEU:HD12	1.97	0.47
1:L:37:ALA:O	1:L:40:PHE:HB3	2.10	0.47
2:M:218:GLY:C	2:M:222:LEU:HD12	2.35	0.47
2:M:247:ALA:HB1	2:M:257:ASN:HD22	1.80	0.47
2:M:24:VAL:CG1	2:M:26:LEU:HD13	2.41	0.47
2:M:294:VAL:O	2:M:298:ASN:CB	2.50	0.47
4:M:400:BCL:C4	5:M:500:BPH:C3B	2.93	0.47
2:M:55:GLY:CA	2:M:130:ARG:HH11	2.27	0.47
3:H:117:ARG:HG2	3:H:227:LEU:HB3	1.95	0.47
1:L:209:PRO:HA	1:L:212:GLU:OE1	2.15	0.47
3:H:124:ASP:OD2	3:H:129:ASN:O	2.32	0.47
3:H:128:HIS:NE2	3:H:132:LYS:NZ	2.62	0.47
3:H:99:ALA:HB1	3:H:100:PRO:HD2	1.97	0.47
1:L:169:TYR:CE2	1:L:260:VAL:HG13	2.50	0.47
1:L:92:CYS:O	1:L:96:ALA:HB2	2.15	0.47
2:M:10:VAL:HG13	2:M:11:GLN:N	2.29	0.47
2:M:234:GLU:OE2	3:H:123:LEU:CD1	2.62	0.47
3:H:171:ILE:HB	3:H:172:PRO:CD	2.43	0.47
3:H:27:LEU:O	3:H:28:ILE:C	2.53	0.47
1:L:152:THR:C	1:L:154:LEU:N	2.67	0.47
1:L:193:LEU:HD21	1:L:215:PHE:HE2	1.77	0.47
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.97	0.47
2:M:135:ALA:HA	2:M:138:LEU:HD11	1.97	0.47
2:M:293:TYR:OH	2:M:297:GLN:NE2	2.46	0.47
2:M:254:MET:HB3	6:M:750:UQ:H203	1.95	0.47
2:M:227:PHE:HD2	3:H:234:CYS:HB3	1.78	0.47
2:M:2:GLU:CG	2:M:3:TYR:H	2.28	0.47
3:H:170:ASP:N	3:H:175:MET:O	2.43	0.47
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.79	0.47
1:L:97:PHE:CE1	4:L:350:BCL:H121	2.50	0.47
1:L:177:ILE:HD12	4:M:601:BCL:HMD1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:40:TYR:HA	3:H:41:PRO:O	2.15	0.46
2:M:169:TRP:O	2:M:171:GLU:O	2.33	0.46
3:H:195:MET:CE	3:H:238:ALA:HB2	2.45	0.46
3:H:62:LYS:N	3:H:74:THR:HG22	2.30	0.46
1:L:167:PHE:O	1:L:170:ASN:N	2.48	0.46
1:L:56:GLN:C	1:L:57:GLY:O	2.52	0.46
3:H:154:ARG:NH1	3:H:158:LEU:CD1	2.78	0.46
2:M:68:THR:HG23	2:M:112:LEU:CD1	2.39	0.46
3:H:5:THR:CG2	3:H:10:PHE:H	2.23	0.46
1:L:141:ALA:H	1:L:144:TYR:HE1	1.64	0.46
1:L:185:LEU:HG	1:L:186:ALA:N	2.22	0.46
2:M:265:ARG:O	2:M:268:ILE:HG23	2.15	0.46
2:M:269:TRP:HA	2:M:269:TRP:CE3	2.49	0.46
1:L:231:ARG:CZ	2:M:6:ILE:H	2.24	0.46
3:H:170:ASP:OD2	3:H:173:GLU:CB	2.55	0.46
1:L:132:VAL:HG22	1:L:146:PHE:CE1	2.50	0.46
1:L:171:PRO:O	1:L:174:MET:HB3	2.15	0.46
1:L:84:GLY:O	1:L:87:GLN:HB2	2.16	0.46
2:M:130:ARG:C	2:M:132:TYR:H	2.19	0.46
1:L:215:PHE:HD1	2:M:138:LEU:CD2	2.27	0.46
4:L:450:BCL:HBA1	4:L:450:BCL:H3A	1.73	0.46
1:L:49:ILE:HG22	1:L:50:ALA:N	2.31	0.46
2:M:148:PHE:HB2	5:M:500:BPH:C2D	2.46	0.46
2:M:278:GLY:O	4:M:400:BCL:HED3	2.15	0.46
2:M:65:TRP:CD2	2:M:66:PHE:N	2.83	0.46
3:H:27:LEU:HD23	3:H:28:ILE:H	1.81	0.46
1:L:226:THR:O	1:L:229:ILE:HG22	2.16	0.46
1:L:117:ILE:HG21	2:M:250:TRP:CH2	2.50	0.46
2:M:191:HIS:HA	2:M:290:ASP:O	2.16	0.46
2:M:32:GLY:N	2:M:33:PRO:CD	2.78	0.46
2:M:204:ILE:HG12	4:M:400:BCL:C2B	2.46	0.46
1:L:177:ILE:HD12	4:M:601:BCL:CMD	2.46	0.46
6:M:750:UQ:HM23	6:M:750:UQ:O3	2.16	0.46
2:M:81:PRO:O	2:M:82:ALA:C	2.54	0.46
2:M:104:PHE:CD2	2:M:114:LEU:HD21	2.50	0.46
2:M:14:GLY:HA3	2:M:15:PRO:HD2	1.72	0.46
2:M:162:ARG:CB	2:M:163:PRO:CD	2.88	0.46
2:M:199:PHE:HA	2:M:277:THR:HG22	1.98	0.46
4:M:400:BCL:H41	4:M:400:BCL:H62	1.39	0.46
1:L:181:PHE:HZ	4:M:400:BCL:HAA2	1.80	0.46
3:H:164:VAL:O	3:H:165:VAL:HG22	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:111:PRO:CD	3:H:243:TYR:CE2	2.90	0.46
1:L:189:LEU:O	1:L:193:LEU:CB	2.64	0.46
1:L:250:ILE:HA	1:L:254:ILE:HB	1.97	0.46
1:L:74:GLY:O	1:L:75:LEU:CB	2.64	0.46
2:M:224:VAL:HG11	2:M:242:ALA:O	2.15	0.46
3:H:67:PRO:CG	3:H:123:LEU:CD2	2.89	0.46
3:H:182:GLU:HG3	3:H:187:SER:C	2.36	0.46
3:H:7:PHE:HB3	3:H:8:GLY:H	1.61	0.46
1:L:100:TRP:CH2	1:L:103:ARG:NH2	2.84	0.46
3:H:118:ARG:HG3	3:H:227:LEU:HD12	1.98	0.45
2:M:148:PHE:CD1	5:M:500:BPH:C4D	2.99	0.45
2:M:162:ARG:HD3	2:M:166:MET:HE3	1.98	0.45
2:M:241:THR:HB	3:H:115:VAL:HG23	1.98	0.45
2:M:221:ILE:HD11	6:M:750:UQ:HM31	1.98	0.45
2:M:237:ALA:O	3:H:73:LEU:HD22	2.15	0.45
3:H:78:PRO:HG2	3:H:79:GLU:H	1.81	0.45
1:L:130:THR:OG1	1:L:131:LEU:HD23	2.16	0.45
1:L:175:ILE:HG13	1:L:243:PHE:CE2	2.51	0.45
1:L:44:LEU:HA	1:L:47:ILE:CB	2.45	0.45
2:M:24:VAL:HG12	2:M:26:LEU:N	2.10	0.45
3:H:154:ARG:NH1	3:H:158:LEU:HD11	2.31	0.45
3:H:183:LEU:N	3:H:186:GLY:O	2.50	0.45
3:H:79:GLU:O	3:H:80:SER:HB3	2.16	0.45
1:L:150:ILE:HA	5:L:550:BPH:H193	1.99	0.45
1:L:185:LEU:CD2	1:L:186:ALA:N	2.79	0.45
2:M:212:LEU:CD1	6:M:750:UQ:H161	2.47	0.45
3:H:188:THR:O	3:H:189:ARG:CD	2.64	0.45
3:H:27:LEU:HD21	3:H:32:GLN:HE21	1.82	0.45
1:L:25:TRP:NE1	2:M:252:TRP:CD2	2.80	0.45
2:M:53:SER:O	2:M:56:VAL:HG12	2.16	0.45
3:H:177:ARG:O	3:H:193:MET:HB3	2.16	0.45
3:H:111:PRO:CG	3:H:242:MET:SD	3.01	0.45
3:H:28:ILE:CG2	3:H:29:TYR:H	2.28	0.45
3:H:91:ALA:HB3	3:H:96:PHE:HB2	1.98	0.45
2:M:157:VAL:O	2:M:159:GLY:N	2.50	0.45
2:M:199:PHE:CB	2:M:281:GLY:HA3	2.45	0.45
3:H:200:SER:O	3:H:201:ASN:HB3	2.17	0.45
1:L:190:HIS:HE1	2:M:232:GLU:OE2	2.00	0.45
1:L:86:TRP:O	1:L:90:THR:CG2	2.64	0.45
2:M:212:LEU:HD21	6:M:750:UQ:C16	2.45	0.45
3:H:103:ASP:O	3:H:107:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:148:PRO:C	3:H:149:ILE:CG1	2.80	0.45
2:M:227:PHE:CE2	3:H:235:GLY:HA2	2.33	0.45
3:H:27:LEU:HD11	3:H:32:GLN:HB2	1.97	0.45
3:H:79:GLU:HB3	3:H:80:SER:H	1.43	0.45
1:L:13:GLY:O	1:L:15:THR:HG23	2.16	0.45
1:L:251:THR:HG22	1:L:259:TRP:CZ2	2.52	0.45
2:M:28:ASN:ND2	2:M:29:ARG:H	2.15	0.45
4:M:601:BCL:O2D	4:M:601:BCL:H2A	2.17	0.45
2:M:67:PHE:O	2:M:69:ILE:N	2.50	0.45
2:M:88:LEU:HG	2:M:89:PHE:N	2.31	0.45
1:L:193:LEU:HD11	1:L:216:PHE:HE1	1.66	0.45
1:L:240:ALA:O	1:L:244:SER:HB2	2.17	0.45
1:L:53:ALA:HB2	1:L:64:ILE:HG13	1.97	0.45
2:M:225:SER:HA	2:M:229:GLY:H	1.82	0.45
3:H:105:MET:CE	3:H:212:LEU:HD13	2.47	0.45
3:H:134:MET:SD	3:H:142:VAL:CG2	3.04	0.45
3:H:130:LYS:HE3	3:H:172:PRO:HG2	1.99	0.45
1:L:216:PHE:O	1:L:219:LEU:HB2	2.17	0.45
1:L:228:GLY:C	1:L:232:LEU:HD13	2.38	0.45
2:M:118:PHE:O	2:M:121:PHE:HB3	2.17	0.45
2:M:12:VAL:HG21	3:H:169:VAL:CG1	2.46	0.45
2:M:282:ILE:CG1	4:M:400:BCL:HED1	2.46	0.45
3:H:182:GLU:HG3	3:H:187:SER:O	2.17	0.45
3:H:226:THR:O	3:H:229:GLU:HB2	2.16	0.45
1:L:26:VAL:O	1:L:26:VAL:HG13	2.17	0.45
1:L:275:ILE:N	1:L:276:PRO:CD	2.80	0.45
1:L:58:THR:HG21	1:L:63:LEU:HD11	1.99	0.45
2:M:66:PHE:HD1	2:M:67:PHE:HD1	1.65	0.45
2:M:74:TRP:O	2:M:77:ALA:CB	2.63	0.45
3:H:149:ILE:H	3:H:164:VAL:CG1	2.29	0.44
1:L:261:ASP:O	1:L:264:GLN:N	2.43	0.44
2:M:216:MET:HE2	2:M:216:MET:HB3	1.86	0.44
1:L:185:LEU:HD23	1:L:186:ALA:CA	2.47	0.44
1:L:188:ALA:HB2	2:M:271:ALA:HB1	1.96	0.44
2:M:248:LEU:HD21	2:M:252:TRP:CZ2	2.51	0.44
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.99	0.44
1:L:106:GLU:O	1:L:109:ARG:HB2	2.17	0.44
1:L:48:LEU:O	1:L:49:ILE:C	2.55	0.44
2:M:153:TRP:CH2	2:M:283:LEU:HD11	2.53	0.44
4:M:400:BCL:C4	5:M:500:BPH:C4B	2.96	0.44
2:M:87:ASP:HB2	2:M:91:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:107:ILE:O	1:L:111:LEU:HD12	2.18	0.44
1:L:86:TRP:HZ3	1:L:142:TRP:HE3	1.64	0.44
1:L:226:THR:CG2	2:M:230:GLU:HB2	2.47	0.44
2:M:24:VAL:HG12	2:M:26:LEU:HB2	1.97	0.44
2:M:276:LEU:HD23	2:M:276:LEU:HA	1.76	0.44
2:M:67:PHE:C	2:M:69:ILE:N	2.68	0.44
1:L:129:LEU:HB3	1:L:134:PHE:CD2	2.51	0.44
1:L:215:PHE:HD1	2:M:138:LEU:CD1	2.30	0.44
1:L:12:PRO:CD	3:H:97:PRO:HB2	2.47	0.44
1:L:269:LEU:HG	1:L:270:PRO:CD	2.48	0.44
2:M:251:ARG:HB2	2:M:257:ASN:HB3	2.00	0.44
2:M:81:PRO:O	2:M:85:LEU:HD12	2.18	0.44
3:H:195:MET:HE1	3:H:238:ALA:HB2	2.00	0.44
1:L:117:ILE:CG2	2:M:250:TRP:CH2	3.00	0.44
2:M:121:PHE:O	2:M:125:TRP:HD1	2.01	0.44
2:M:130:ARG:C	2:M:132:TYR:N	2.71	0.44
2:M:13:ARG:O	3:H:140:PHE:CD2	2.71	0.44
1:L:206:MET:HE2	2:M:237:ALA:HB2	1.97	0.44
2:M:35:SER:HB3	2:M:38:LEU:CD2	2.48	0.44
1:L:69:PRO:HD2	1:L:142:TRP:O	2.18	0.44
1:L:152:THR:HA	2:M:303:PRO:CB	2.47	0.44
1:L:192:ALA:HB1	2:M:143:HIS:HB3	1.99	0.44
1:L:168:HIS:HE1	4:L:350:BCL:HMC2	1.80	0.44
1:L:5:PHE:HB2	2:M:244:GLU:CD	2.38	0.44
2:M:152:ILE:O	2:M:156:MET:N	2.46	0.44
3:H:103:ASP:CB	3:H:106:LYS:HB3	2.48	0.44
1:L:149:GLY:HA3	1:L:152:THR:HG23	1.93	0.44
2:M:24:VAL:HG12	2:M:25:ASN:N	2.33	0.44
2:M:29:ARG:HG2	2:M:29:ARG:NH1	2.29	0.44
2:M:16:ALA:CB	2:M:45:GLN:HE22	2.15	0.44
3:H:135:LYS:HZ3	3:H:165:VAL:HG12	1.72	0.43
3:H:245:ALA:HB3	3:H:248:ARG:CD	2.48	0.43
3:H:28:ILE:CG2	3:H:29:TYR:N	2.64	0.43
1:L:100:TRP:O	1:L:103:ARG:HB3	2.18	0.43
1:L:189:LEU:HD13	5:M:500:BPH:HED1	2.00	0.43
1:L:226:THR:HG21	2:M:231:ARG:H	1.83	0.43
1:L:226:THR:HG22	2:M:230:GLU:HB2	1.99	0.43
1:L:230:HIS:ND1	2:M:221:ILE:CG2	2.76	0.43
1:L:224:ILE:HG22	6:L:800:UQ:H103	1.99	0.43
2:M:121:PHE:O	2:M:125:TRP:HB2	2.18	0.43
2:M:134:ARG:HD3	2:M:134:ARG:HA	1.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:158:LEU:HG	2:M:183:TRP:HH2	1.83	0.43
2:M:250:TRP:CD1	6:M:750:UQ:CM5	3.01	0.43
3:H:103:ASP:HB3	3:H:106:LYS:CB	2.48	0.43
3:H:237:VAL:O	3:H:238:ALA:C	2.57	0.43
3:H:239:GLY:O	3:H:243:TYR:HB2	2.17	0.43
1:L:172:ALA:O	1:L:175:ILE:HB	2.18	0.43
2:M:235:GLN:HE22	2:M:243:ALA:N	2.16	0.43
2:M:65:TRP:O	2:M:66:PHE:C	2.57	0.43
3:H:183:LEU:C	3:H:185:ASP:H	2.20	0.43
1:L:75:LEU:CG	1:L:140:GLY:O	2.61	0.43
1:L:268:LYS:HZ3	1:L:272:TRP:HZ2	1.61	0.43
2:M:162:ARG:NH2	2:M:187:PHE:CD1	2.86	0.43
2:M:64:MET:SD	2:M:119:PHE:CE1	3.11	0.43
2:M:234:GLU:HG2	3:H:123:LEU:HD12	1.99	0.43
3:H:181:VAL:CB	3:H:189:ARG:O	2.67	0.43
3:H:118:ARG:CG	3:H:227:LEU:HD12	2.48	0.43
2:M:193:ASN:C	2:M:195:PHE:N	2.70	0.43
2:M:230:GLU:O	2:M:231:ARG:C	2.55	0.43
2:M:35:SER:CB	2:M:38:LEU:HB3	2.43	0.43
3:H:207:ALA:CB	3:H:237:VAL:HG12	2.48	0.43
3:H:240:GLY:O	3:H:244:ALA:CB	2.62	0.43
1:L:13:GLY:CA	3:H:242:MET:CE	2.96	0.43
1:L:130:THR:CB	1:L:249:ILE:HD11	2.40	0.43
2:M:108:LYS:O	2:M:109:GLU:HB3	2.16	0.43
1:L:215:PHE:CB	2:M:138:LEU:HD22	2.48	0.43
2:M:195:PHE:CE2	4:M:400:BCL:CMC	3.01	0.43
2:M:216:MET:HE1	6:M:750:UQ:H13	1.99	0.43
2:M:282:ILE:O	2:M:284:LEU:N	2.52	0.43
3:H:212:LEU:C	3:H:214:ALA:N	2.72	0.43
1:L:12:PRO:HG3	3:H:97:PRO:HB2	2.01	0.43
1:L:189:LEU:CD1	5:M:500:BPH:HED1	2.48	0.43
5:L:550:BPH:H2	5:L:550:BPH:H6C1	1.72	0.43
2:M:166:MET:SD	2:M:171:GLU:OE2	2.76	0.43
2:M:217:HIS:HE1	2:M:264:HIS:CE1	2.36	0.43
2:M:218:GLY:O	2:M:222:LEU:CD1	2.66	0.43
2:M:61:SER:O	2:M:62:GLY:C	2.57	0.43
3:H:179:LEU:O	3:H:190:LEU:HA	2.18	0.43
1:L:113:ILE:HG21	2:M:224:VAL:HG22	1.99	0.43
1:L:61:PRO:HA	1:L:64:ILE:CG2	2.48	0.43
2:M:216:MET:O	2:M:220:THR:HG23	2.19	0.43
1:L:14:GLY:HA2	1:L:109:ARG:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:ILE:HG22	1:L:179:PHE:CD1	2.54	0.43
2:M:235:GLN:HE21	2:M:243:ALA:HB2	1.80	0.43
3:H:27:LEU:HD11	3:H:32:GLN:CD	2.39	0.43
3:H:39:GLY:O	3:H:40:TYR:CD1	2.71	0.43
1:L:166:ASN:O	1:L:168:HIS:N	2.51	0.43
1:L:187:LEU:C	1:L:187:LEU:CD2	2.82	0.43
1:L:235:LEU:O	1:L:238:LEU:N	2.51	0.43
1:L:41:PHE:HD2	1:L:92:CYS:CA	2.30	0.43
2:M:142:LYS:O	2:M:143:HIS:C	2.53	0.43
1:L:230:HIS:NE2	2:M:217:HIS:CD2	2.86	0.43
2:M:227:PHE:HE2	3:H:235:GLY:CA	2.20	0.43
2:M:263:ILE:HG23	2:M:264:HIS:ND1	2.33	0.43
2:M:127:TRP:CD1	5:M:500:BPH:HAA1	2.54	0.43
2:M:62:GLY:O	2:M:65:TRP:HB3	2.19	0.43
3:H:130:LYS:O	3:H:171:ILE:HB	2.18	0.43
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.40	0.43
1:L:268:LYS:NZ	1:L:272:TRP:HZ2	2.16	0.43
1:L:36:VAL:HA	1:L:39:PHE:HB3	2.00	0.43
1:L:46:ILE:O	1:L:46:ILE:HG13	2.17	0.43
1:L:117:ILE:HG21	2:M:249:PHE:HE2	1.84	0.43
2:M:285:SER:HB2	2:M:292:TRP:HE1	1.83	0.43
6:M:750:UQ:H222	6:M:750:UQ:H201	1.64	0.43
3:H:20:PHE:CD2	3:H:21:TRP:CD1	3.07	0.42
3:H:237:VAL:C	3:H:239:GLY:N	2.71	0.42
2:M:250:TRP:NE1	6:M:750:UQ:HM51	2.34	0.42
3:H:33:THR:C	3:H:35:ASN:H	2.21	0.42
2:M:104:PHE:HD2	2:M:114:LEU:HD21	1.83	0.42
2:M:202:LEU:O	2:M:206:PHE:N	2.48	0.42
3:H:135:LYS:HZ1	3:H:165:VAL:HG12	1.82	0.42
3:H:60:LYS:HG2	3:H:60:LYS:H	1.63	0.42
1:L:123:PHE:CZ	1:L:242:PHE:HD2	2.37	0.42
2:M:243:ALA:O	6:M:750:UQ:CM2	2.67	0.42
2:M:24:VAL:HG11	2:M:26:LEU:CD1	2.44	0.42
2:M:282:ILE:C	2:M:284:LEU:N	2.72	0.42
1:L:11:VAL:CG2	3:H:111:PRO:HD3	2.50	0.42
1:L:121:PHE:HD1	5:L:550:BPH:C4D	2.32	0.42
1:L:125:ILE:HG21	1:L:125:ILE:HD13	1.83	0.42
1:L:190:HIS:HB2	1:L:229:ILE:CD1	2.50	0.42
5:L:550:BPH:HBA1	5:L:550:BPH:H3A	1.22	0.42
2:M:199:PHE:HB3	2:M:277:THR:HG22	2.01	0.42
2:M:29(A):SER:HB2	2:M:49:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:601:BCL:CAA	4:M:601:BCL:HBD	2.49	0.42
1:L:251:THR:CG2	1:L:259:TRP:HE1	2.32	0.42
1:L:3:LEU:HB3	1:L:6:GLU:CB	2.29	0.42
1:L:80:LEU:O	1:L:82:LYS:N	2.53	0.42
2:M:4:GLN:HG3	3:H:194:GLN:HA	2.00	0.42
1:L:185:LEU:HD12	5:M:500:BPH:NC	2.35	0.42
2:M:66:PHE:O	2:M:69:ILE:HB	2.19	0.42
1:L:167:PHE:HD1	1:L:173:HIS:CD2	2.38	0.42
1:L:187:LEU:HD21	2:M:267:ALA:CA	2.44	0.42
1:L:80:LEU:C	1:L:82:LYS:N	2.72	0.42
2:M:105:ALA:HB1	2:M:105(A):ALA:H	1.43	0.42
2:M:163:PRO:HB3	2:M:171:GLU:HB2	2.01	0.42
2:M:170:SER:C	2:M:171:GLU:O	2.58	0.42
2:M:212:LEU:CD2	6:M:750:UQ:C16	2.97	0.42
2:M:148:PHE:HB2	5:M:500:BPH:HMD3	2.02	0.42
1:L:211:HIS:O	1:L:215:PHE:CB	2.68	0.42
1:L:240:ALA:O	1:L:244:SER:CB	2.68	0.42
2:M:115:ILE:CG2	2:M:119:PHE:CE2	2.92	0.42
2:M:219:ALA:C	2:M:221:ILE:H	2.23	0.42
1:L:232:LEU:HD12	2:M:41:PHE:CE2	2.55	0.42
2:M:72:TRP:CD1	2:M:112:LEU:CB	3.01	0.42
2:M:263:ILE:HG21	6:M:750:UQ:HM33	2.00	0.42
3:H:104:PRO:CB	3:H:243:TYR:CD1	3.03	0.42
2:M:241:THR:HG22	3:H:231:ASP:OD1	2.20	0.42
1:L:261:ASP:O	1:L:262:TRP:C	2.56	0.42
1:L:43:ALA:O	1:L:47:ILE:N	2.52	0.42
1:L:88:ILE:HA	1:L:88:ILE:HD13	1.88	0.42
2:M:204:ILE:HG12	4:M:400:BCL:HMB3	2.00	0.42
2:M:129:GLY:O	2:M:133:LEU:HB2	2.20	0.42
2:M:186:ASN:O	2:M:190:VAL:CG2	2.54	0.42
1:L:181:PHE:CZ	4:M:400:BCL:HAA2	2.54	0.42
5:M:500:BPH:H9C1	5:M:500:BPH:H112	1.69	0.42
3:H:104:PRO:CB	3:H:243:TYR:CE1	3.00	0.41
1:L:181:PHE:CE1	4:M:400:BCL:O1A	2.73	0.41
1:L:201:GLU:HB2	1:L:204:LYS:HB2	2.02	0.41
2:M:102:LEU:O	2:M:102:LEU:CD1	2.63	0.41
2:M:197:ASN:OD1	2:M:199:PHE:HD2	2.03	0.41
1:L:195:LEU:CD1	2:M:265:ARG:HG3	2.34	0.41
1:L:273:ALA:CB	2:M:82:ALA:O	2.68	0.41
2:M:69:ILE:O	2:M:93:LEU:HD11	2.20	0.41
3:H:31:LEU:HD12	3:H:31:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:32:GLN:O	3:H:32:GLN:HG3	2.20	0.41
1:L:111:LEU:CB	1:L:113:ILE:HG12	2.42	0.41
1:L:235:LEU:O	1:L:236:LEU:C	2.59	0.41
2:M:150:SER:OG	2:M:276:LEU:HD23	2.20	0.41
3:H:216:ILE:CG2	3:H:217:PRO:HD2	2.48	0.41
1:L:275:ILE:O	1:L:275:ILE:CG2	2.56	0.41
1:L:17:VAL:HG22	1:L:33:PHE:HB3	1.99	0.41
1:L:34:PHE:O	1:L:38:THR:HB	2.19	0.41
1:L:78:ALA:HB1	1:L:79:PRO:CD	2.51	0.41
2:M:65:TRP:CG	2:M:66:PHE:N	2.88	0.41
3:H:183:LEU:HD11	3:H:213:PHE:O	2.20	0.41
3:H:36:MET:HA	3:H:40:TYR:CD1	2.56	0.41
1:L:16:LEU:HD11	1:L:105:VAL:CG1	2.50	0.41
1:L:200:PRO:HB2	1:L:201:GLU:H	1.35	0.41
1:L:227:LEU:HD23	1:L:231:ARG:NH1	2.36	0.41
1:L:53:ALA:CB	1:L:64:ILE:CD1	2.90	0.41
1:L:193:LEU:HD22	6:L:800:UQ:HM23	2.03	0.41
2:M:149:LEU:HA	2:M:149:LEU:HD12	1.84	0.41
3:H:93:SER:HB3	3:H:96:PHE:HD2	1.84	0.41
1:L:166:ASN:C	1:L:168:HIS:N	2.73	0.41
1:L:183:ASN:HB2	1:L:236:LEU:HB3	2.01	0.41
6:L:800:UQ:C8	6:L:800:UQ:HM51	2.50	0.41
1:L:104:GLU:HG2	2:M:249:PHE:CZ	2.54	0.41
2:M:251:ARG:CG	2:M:251:ARG:NH1	2.81	0.41
2:M:69:ILE:C	2:M:93:LEU:HD11	2.38	0.41
2:M:231:ARG:NH1	3:H:122:GLU:OE1	2.54	0.41
3:H:124:ASP:HB2	3:H:129:ASN:O	2.21	0.41
3:H:148:PRO:O	3:H:149:ILE:CB	2.68	0.41
3:H:173:GLU:O	3:H:173:GLU:CG	2.69	0.41
3:H:2:VAL:CG1	3:H:2:VAL:O	2.68	0.41
1:L:158:SER:OG	1:L:162:TYR:HE2	1.99	0.41
1:L:215:PHE:CD1	2:M:138:LEU:CD2	3.04	0.41
2:M:288:VAL:HB	3:H:4:VAL:CG1	2.45	0.41
2:M:6:ILE:HA	2:M:6:ILE:HD13	1.94	0.41
3:H:115:VAL:HG12	3:H:116:ALA:N	2.34	0.41
3:H:206:ASN:HD22	3:H:206:ASN:HA	1.71	0.41
3:H:17:ILE:CG2	3:H:21:TRP:CD1	2.95	0.41
1:L:122:ALA:O	1:L:124:ALA:N	2.53	0.41
1:L:172:ALA:HA	1:L:175:ILE:CG1	2.50	0.41
1:L:194:VAL:O	1:L:196:SER:N	2.53	0.41
4:L:350:BCL:H93	4:L:350:BCL:H62	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:74:TRP:CD1	2:M:79:TRP:CD1	3.08	0.41
3:H:209:SER:O	3:H:213:PHE:CD1	2.72	0.41
1:L:129:LEU:HB3	1:L:134:PHE:CE2	2.56	0.41
1:L:80:LEU:O	1:L:83:GLY:N	2.54	0.41
2:M:158:LEU:CG	2:M:183:TRP:HH2	2.34	0.41
2:M:21:THR:CG2	2:M:50:TYR:OH	2.67	0.41
2:M:224:VAL:C	2:M:226:ARG:N	2.74	0.41
3:H:167:ILE:CG2	3:H:179:LEU:HD12	2.46	0.41
3:H:182:GLU:C	3:H:184:LYS:H	2.24	0.41
1:L:16:LEU:HD11	1:L:105:VAL:HG12	2.03	0.41
5:L:550:BPH:H203	5:L:550:BPH:H152	2.02	0.41
2:M:162:ARG:O	2:M:164:ILE:N	2.54	0.41
2:M:267:ALA:O	2:M:268:ILE:C	2.58	0.41
1:L:177:ILE:CD1	4:L:350:BCL:HMB3	2.51	0.41
1:L:36:VAL:O	1:L:40:PHE:HD1	2.04	0.41
1:L:42:ALA:CB	5:L:550:BPH:H5C1	2.50	0.41
2:M:105(A):ALA:HB1	2:M:109:GLU:OE1	2.21	0.41
1:L:234:LEU:HD13	2:M:222:LEU:CD1	2.50	0.41
2:M:65:TRP:CE3	2:M:66:PHE:N	2.89	0.41
3:H:156:CYS:O	3:H:157:ASP:O	2.38	0.41
3:H:63:THR:N	3:H:74:THR:HG23	2.35	0.41
1:L:128:TYR:O	1:L:132:VAL:HG23	2.21	0.41
1:L:215:PHE:CD1	2:M:138:LEU:HD21	2.56	0.41
2:M:216:MET:O	2:M:219:ALA:HB3	2.21	0.41
2:M:43:ASN:HA	2:M:43:ASN:HD22	1.68	0.41
3:H:12:LEU:HD13	3:H:12:LEU:HA	1.86	0.40
1:L:222:TYR:HD2	2:M:46:LEU:HD21	1.86	0.40
2:M:105(A):ALA:O	2:M:106:PRO:C	2.47	0.40
2:M:202:LEU:HA	2:M:205:ALA:HB3	2.04	0.40
1:L:113:ILE:CG2	2:M:224:VAL:HG22	2.50	0.40
2:M:243:ALA:O	6:M:750:UQ:HM22	2.21	0.40
2:M:80:ASN:HB3	2:M:81:PRO:CD	2.44	0.40
4:L:450:BCL:OBD	4:L:450:BCL:O2D	2.39	0.40
2:M:25:ASN:O	2:M:26:LEU:C	2.59	0.40
3:H:170:ASP:OD2	3:H:177:ARG:NH2	2.54	0.40
3:H:177:ARG:O	3:H:193:MET:HB2	2.21	0.40
3:H:66:LEU:CB	3:H:67:PRO:CD	2.99	0.40
1:L:175:ILE:C	1:L:177:ILE:N	2.74	0.40
1:L:248:MET:HE3	4:L:350:BCL:HMD1	2.03	0.40
2:M:217:HIS:ND1	2:M:263:ILE:HG12	2.34	0.40
2:M:282:ILE:C	2:M:284:LEU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:131:THR:HG21	5:M:500:BPH:OBD	2.21	0.40
1:L:93:ALA:HB1	1:L:97:PHE:HE2	1.87	0.40
2:M:55:GLY:HA3	2:M:130:ARG:HH11	1.87	0.40
2:M:131:THR:HG22	2:M:144:THR:HB	2.04	0.40
2:M:170:SER:O	2:M:171:GLU:O	2.39	0.40
2:M:173:VAL:HG22	2:M:183:TRP:CZ3	2.56	0.40
3:H:212:LEU:C	3:H:214:ALA:H	2.25	0.40
1:L:11:VAL:HG12	3:H:98:HIS:O	2.22	0.40
4:L:450:BCL:H102	4:L:450:BCL:H13	1.71	0.40
2:M:121:PHE:O	2:M:125:TRP:CD1	2.74	0.40
2:M:96:PRO:HG2	2:M:170:SER:CB	2.40	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:293:TYR:OH	3:H:166:ASP:OD1[4_445]	1.59	0.61
1:L:265:TRP:CB	3:H:49:PRO:O[1_556]	2.17	0.03

## 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	L	276/281 (98%)	187 (68%)	52 (19%)	37 (13%)	0	1
2	M	303/307 (99%)	189 (62%)	72 (24%)	42 (14%)	0	1
3	H	253/260 (97%)	144 (57%)	65 (26%)	44 (17%)	0	0
All	All	832/848 (98%)	520 (62%)	189 (23%)	123 (15%)	0	0

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	20	ASN
1	L	55	LEU
1	L	60	ASN
1	L	74	GLY
1	L	79	PRO
1	L	200	PRO
1	L	205	GLU
1	L	226	THR
1	L	235	LEU
1	L	272	TRP
1	L	274	ASN
1	L	275	ILE
2	M	20	MET
2	M	21	THR
2	M	24	VAL
2	M	28	ASN
2	M	29(A)	SER
2	M	100	TYR
2	M	113	TRP
2	M	137	ALA
2	M	157	VAL
2	M	158	LEU
2	M	171	GLU
2	M	260	MET
2	M	274	VAL
3	H	2	VAL
3	H	9	ASN
3	H	28	ILE
3	H	48	THR
3	H	49	PRO
3	H	53	GLN
3	H	56	PHE
3	H	66	LEU
3	H	81	GLU
3	H	82	ASP
3	H	122	GLU
3	H	124	ASP
3	H	128	HIS
3	H	148	PRO
3	H	149	ILE
3	H	157	ASP
3	H	158	LEU

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Mol	Chain	Res	Type
3	H	165	VAL
3	H	189	ARG
3	H	242	MET
3	H	244	ALA
3	H	252	VAL
1	L	2	LEU
1	L	8	LYS
1	L	14	GLY
1	L	17	VAL
1	L	49	ILE
1	L	50	ALA
1	L	75	LEU
1	L	81	ALA
1	L	153	HIS
1	L	271	TRP
2	M	2	GLU
2	M	6	ILE
2	M	9	GLN
2	M	31	VAL
2	M	36	THR
2	M	53	SER
2	M	68	THR
2	M	79	TRP
2	M	104	PHE
2	M	106	PRO
2	M	107	LEU
2	M	140	MET
2	M	156	MET
3	H	33	THR
3	H	80	SER
3	H	115	VAL
3	H	166	ASP
3	H	206	ASN
3	H	238	ALA
3	H	251	VAL
1	L	167	PHE
1	L	201	GLU
1	L	236	LEU
2	M	95	PRO
2	M	97	ALA
2	M	165	LEU
2	M	194	LEU

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Mol	Chain	Res	Type
2	M	231	ARG
3	H	59	PRO
3	H	95	GLY
3	H	174	GLN
3	H	175	MET
3	H	199	GLN
3	H	205	VAL
3	H	237	VAL
1	L	57	GLY
1	L	142	TRP
1	L	258	GLN
2	M	105	ALA
2	M	144	THR
2	M	267	ALA
2	M	273	LEU
1	L	6	GLU
1	L	15	THR
1	L	43	ALA
1	L	171	PRO
1	L	267	VAL
2	M	91	PHE
2	M	99	GLU
2	M	163	PRO
3	H	183	LEU
3	H	222	PRO
3	H	26	GLY
3	H	145	GLY
1	L	12	PRO
2	M	268	ILE
2	M	300	GLY
3	H	67	PRO
1	L	228	GLY
2	M	302	ALA
2	M	83	VAL
3	H	160	ILE
1	L	114	GLY
3	H	133	PRO
3	H	97	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	L	216 / 220 (98%)	169 (78%)	47 (22%)	1	4
2	M	238 / 240 (99%)	179 (75%)	59 (25%)	0	2
3	H	203 / 208 (98%)	154 (76%)	49 (24%)	0	2
All	All	657 / 668 (98%)	502 (76%)	155 (24%)	1	2

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	7	ARG
1	L	16	LEU
1	L	20	ASN
1	L	36	VAL
1	L	38	THR
1	L	40	PHE
1	L	46	ILE
1	L	47	ILE
1	L	55	LEU
1	L	56	GLN
1	L	60	ASN
1	L	63	LEU
1	L	64	ILE
1	L	72	GLU
1	L	91	ILE
1	L	99	SER
1	L	102	LEU
1	L	110	LYS
1	L	113	ILE
1	L	115	TYR
1	L	123	PHE
1	L	128	TYR
1	L	133	LEU
1	L	138	MET
1	L	146	PHE

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Mol	Chain	Res	Type
1	L	152	THR
1	L	177	ILE
1	L	183	ASN
1	L	185	LEU
1	L	196	SER
1	L	199	ASN
1	L	213	ASP
1	L	216	PHE
1	L	217	ARG
1	L	219	LEU
1	L	220	VAL
1	L	222	TYR
1	L	224	ILE
1	L	243	PHE
1	L	248	MET
1	L	250	ILE
1	L	253	THR
1	L	261	ASP
1	L	269	LEU
1	L	272	TRP
1	L	274	ASN
2	M	10	VAL
2	M	11	GLN
2	M	17	ASP
2	M	22	GLU
2	M	23	ASP
2	M	25	ASN
2	M	26	LEU
2	M	28	ASN
2	M	29(A)	SER
2	M	31	VAL
2	M	43	ASN
2	M	59	LEU
2	M	72	TRP
2	M	74	TRP
2	M	87	ASP
2	M	88	LEU
2	M	94	GLU
2	M	100	TYR
2	M	107	LEU
2	M	112	LEU
2	M	117	SER

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Mol	Chain	Res	Type
2	M	118	PHE
2	M	126	SER
2	M	134	ARG
2	M	138	LEU
2	M	142	LYS
2	M	144	THR
2	M	146	TRP
2	M	155	TRP
2	M	156	MET
2	M	158	LEU
2	M	161	ILE
2	M	162	ARG
2	M	165	LEU
2	M	168	SER
2	M	177	ILE
2	M	180	HIS
2	M	202	LEU
2	M	203	SER
2	M	210	SER
2	M	214	PHE
2	M	232	GLU
2	M	234	GLU
2	M	236	ILE
2	M	238	ASP
2	M	241	THR
2	M	248	LEU
2	M	254	MET
2	M	257	ASN
2	M	260	MET
2	M	265	ARG
2	M	268	ILE
2	M	270	MET
2	M	276	LEU
2	M	287	THR
2	M	290	ASP
2	M	293	TYR
2	M	295	TRP
2	M	297	GLN
3	H	2	VAL
3	H	11	ASP
3	H	12	LEU
3	H	14	SER

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Mol	Chain	Res	Type
3	H	15	LEU
3	H	22	ILE
3	H	27	LEU
3	H	32	GLN
3	H	45	GLU
3	H	48	THR
3	H	52	ASN
3	H	58	LEU
3	H	68	HIS
3	H	70	ARG
3	H	73	LEU
3	H	74	THR
3	H	79	GLU
3	H	82	ASP
3	H	89	ARG
3	H	92	VAL
3	H	107	ASP
3	H	109	VAL
3	H	117	ARG
3	H	122	GLU
3	H	147	ASN
3	H	149	ILE
3	H	151	LEU
3	H	158	LEU
3	H	159	GLU
3	H	160	ILE
3	H	163	LYS
3	H	167	ILE
3	H	179	LEU
3	H	183	LEU
3	H	188	THR
3	H	189	ARG
3	H	190	LEU
3	H	193	MET
3	H	194	GLN
3	H	200	SER
3	H	206	ASN
3	H	210	SER
3	H	211	ASP
3	H	221	SER
3	H	223	THR
3	H	225	VAL

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Mol	Chain	Res	Type
3	H	237	VAL
3	H	241	LEU
3	H	251	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	183	ASN
1	L	211	HIS
1	L	274	ASN
2	M	4	GLN
2	M	5	ASN
2	M	9	GLN
2	M	25	ASN
2	M	28	ASN
2	M	43	ASN
2	M	45	GLN
2	M	185	ASN
2	M	191	HIS
2	M	235	GLN
2	M	257	ASN
2	M	297	GLN
3	H	9	ASN
3	H	35	ASN
3	H	129	ASN
3	H	206	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	$\# Z  > 2$
6	UQ	L	800	-	48,48,63	2.39	15 (31%)	58,61,79	2.43	24 (41%)
6	UQ	M	750	-	48,48,63	2.22	9 (18%)	58,61,79	2.04	17 (29%)
4	BCL	M	601	2	58,74,74	1.37	9 (15%)	69,115,115	1.63	12 (17%)
5	BPH	L	550	-	64,70,70	1.17	7 (10%)	76,101,101	1.42	13 (17%)
4	BCL	L	450	-	58,74,74	1.28	7 (12%)	69,115,115	1.56	11 (15%)
4	BCL	L	350	-	58,74,74	1.57	8 (13%)	69,115,115	1.82	14 (20%)
4	BCL	M	400	2	58,74,74	1.75	9 (15%)	69,115,115	1.73	14 (20%)
5	BPH	M	500	-	64,70,70	1.22	7 (10%)	76,101,101	1.30	10 (13%)

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
6	UQ	L	800	-	-	14/45/69/87	0/1/1/1
6	UQ	M	750	-	-	18/45/69/87	0/1/1/1
4	BCL	M	601	2	-	17/37/137/137	-
5	BPH	L	550	-	-	15/54/105/105	0/5/6/6
4	BCL	L	450	-	-	15/37/137/137	-
4	BCL	L	350	-	-	20/37/137/137	-
4	BCL	M	400	2	-	26/37/137/137	-
5	BPH	M	500	-	-	20/54/105/105	0/5/6/6

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	750	UQ	C12-C13	10.31	1.84	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	800	UQ	C16-C17	-8.80	1.24	1.53
4	M	400	BCL	MG-NA	8.79	2.27	2.06
6	L	800	UQ	C7-C8	6.82	1.60	1.50
4	L	350	BCL	MG-NC	5.00	2.18	2.06
6	M	750	UQ	C7-C8	4.80	1.57	1.50
6	L	800	UQ	C26-C24	4.12	1.59	1.51
4	M	400	BCL	C4B-NB	4.10	1.38	1.35
4	L	350	BCL	MG-NA	4.08	2.16	2.06
4	L	350	BCL	C4B-NB	3.94	1.38	1.35
4	L	350	BCL	C3C-C4C	-3.89	1.46	1.51
4	M	400	BCL	C3C-C4C	-3.88	1.46	1.51
4	L	350	BCL	C1B-NB	3.86	1.38	1.35
6	L	800	UQ	C31-C29	3.86	1.59	1.51
6	L	800	UQ	C35-C34	3.67	1.60	1.50
5	L	550	BPH	C2C-C1C	-3.59	1.45	1.52
5	M	500	BPH	C2C-C1C	-3.44	1.46	1.52
4	L	450	BCL	C3C-C4C	-3.44	1.47	1.51
5	M	500	BPH	CHC-C1C	3.41	1.43	1.36
4	L	450	BCL	C3B-C2B	-3.34	1.33	1.39
5	L	550	BPH	C3C-C4C	-3.30	1.46	1.50
4	M	601	BCL	C3C-C4C	-3.24	1.47	1.51
4	M	400	BCL	C1B-NB	3.24	1.38	1.35
4	L	450	BCL	C2C-C3C	-3.23	1.45	1.54
6	L	800	UQ	C11-C9	3.21	1.58	1.51
5	L	550	BPH	C2C-C3C	-3.20	1.45	1.54
6	L	800	UQ	C16-C14	3.18	1.57	1.51
4	M	601	BCL	C4B-NB	3.18	1.38	1.35
4	M	601	BCL	MG-NC	3.16	2.13	2.06
4	M	400	BCL	C2C-C3C	-3.14	1.45	1.54
6	L	800	UQ	C36-C34	3.12	1.57	1.51
5	M	500	BPH	C2A-C1A	-3.10	1.46	1.51
4	M	601	BCL	C2C-C3C	-3.09	1.45	1.54
4	L	350	BCL	C2C-C3C	-3.01	1.46	1.54
5	M	500	BPH	C2C-C3C	-2.98	1.46	1.54
6	M	750	UQ	C11-C9	2.98	1.57	1.51
5	M	500	BPH	C3C-C4C	-2.92	1.46	1.50
5	M	500	BPH	CBB-CAB	2.85	1.55	1.50
6	M	750	UQ	C16-C14	2.84	1.57	1.51
4	M	601	BCL	C1B-NB	2.83	1.37	1.35
6	L	800	UQ	C18-C19	-2.81	1.26	1.33
5	L	550	BPH	C2A-C1A	-2.80	1.46	1.51
4	L	350	BCL	C3B-C2B	-2.78	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	601	BCL	C3B-C2B	-2.75	1.34	1.39
6	M	750	UQ	C7-C6	2.70	1.55	1.51
5	L	550	BPH	CBB-CAB	2.66	1.55	1.50
6	L	800	UQ	C40-C39	2.62	1.57	1.50
6	M	750	UQ	C31-C29	2.60	1.56	1.51
4	M	601	BCL	MG-NA	2.59	2.12	2.06
5	L	550	BPH	CHC-C1C	2.56	1.41	1.36
6	M	750	UQ	C27-C28	2.50	1.58	1.50
6	M	750	UQ	C30-C29	2.49	1.57	1.50
4	M	601	BCL	C2A-C1A	-2.43	1.46	1.52
6	M	750	UQ	C35-C34	2.42	1.56	1.50
4	L	450	BCL	C2A-C1A	-2.42	1.46	1.52
4	M	400	BCL	C2A-C1A	-2.42	1.46	1.52
6	L	800	UQ	O3-C3	-2.39	1.31	1.36
4	M	400	BCL	C3B-C2B	-2.31	1.35	1.39
4	L	450	BCL	MG-NC	2.30	2.11	2.06
4	L	450	BCL	C1B-CHB	-2.26	1.34	1.41
6	L	800	UQ	C22-C23	2.20	1.57	1.50
5	M	500	BPH	C3D-CAD	-2.19	1.42	1.47
6	L	800	UQ	C21-C19	2.16	1.55	1.51
6	L	800	UQ	C33-C34	2.15	1.38	1.33
4	L	350	BCL	C2A-C1A	-2.09	1.47	1.52
4	L	450	BCL	C2C-C1C	-2.08	1.45	1.51
4	M	601	BCL	CBB-CAB	2.07	1.55	1.49
4	M	400	BCL	CBB-CAB	2.06	1.55	1.49
5	L	550	BPH	C3D-CAD	-2.06	1.43	1.47
4	M	400	BCL	C1-C2	2.05	1.55	1.49
6	L	800	UQ	C32-C33	2.04	1.57	1.50

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	400	BCL	C4A-NA-C1A	7.95	110.28	106.71
4	L	350	BCL	C4A-NA-C1A	7.06	109.88	106.71
4	M	601	BCL	C4A-NA-C1A	6.50	109.63	106.71
4	L	350	BCL	C4D-C3D-CAD	-5.62	105.34	108.47
6	L	800	UQ	C20-C19-C21	5.42	124.39	115.27
6	L	800	UQ	C8-C7-C6	5.28	126.29	112.05
6	M	750	UQ	C11-C12-C13	5.23	129.08	111.88
6	L	800	UQ	C10-C9-C11	5.18	123.99	115.27
6	M	750	UQ	C7-C8-C9	4.99	135.09	126.79
6	M	750	UQ	C11-C9-C8	4.84	130.91	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	450	BCL	C4D-C3D-CAD	-4.72	105.84	108.47
6	M	750	UQ	C12-C13-C14	-4.58	116.63	127.66
6	L	800	UQ	C30-C29-C28	-4.55	112.01	123.68
6	L	800	UQ	C37-C38-C39	-4.28	113.13	127.75
4	L	350	BCL	OBD-CAD-CBD	-4.20	119.89	125.89
6	L	800	UQ	C15-C14-C16	4.05	122.09	115.27
6	L	800	UQ	C25-C24-C23	-4.03	113.34	123.68
4	L	450	BCL	C4A-NA-C1A	4.01	108.51	106.71
6	L	800	UQ	C37-C36-C34	-3.97	99.93	112.98
4	L	350	BCL	C1-C2-C3	-3.88	119.33	126.04
4	M	601	BCL	C1-C2-C3	-3.87	119.35	126.04
4	L	450	BCL	OBD-CAD-CBD	-3.79	120.48	125.89
6	M	750	UQ	C10-C9-C8	-3.71	114.17	123.68
6	M	750	UQ	C5-C6-C1	-3.70	116.10	119.58
4	M	400	BCL	OBD-CAD-CBD	-3.62	120.72	125.89
5	L	550	BPH	OBD-CAD-CBD	-3.59	120.77	125.89
5	L	550	BPH	C2C-C3C-C4C	3.51	106.60	101.34
4	M	400	BCL	C1-C2-C3	-3.46	120.06	126.04
4	M	601	BCL	C4D-C3D-CAD	-3.45	106.55	108.47
5	L	550	BPH	C1-C2-C3	-3.45	120.08	126.04
6	L	800	UQ	C17-C18-C19	-3.43	119.41	127.66
6	L	800	UQ	C31-C29-C28	3.42	128.03	121.12
4	L	350	BCL	C1C-NC-C4C	3.42	108.24	106.71
6	L	800	UQ	C41-C39-C40	3.40	122.11	114.60
6	M	750	UQ	C22-C21-C19	-3.37	101.91	112.98
4	M	400	BCL	C2C-C3C-C4C	3.33	106.32	101.34
4	L	450	BCL	C2C-C3C-C4C	3.29	106.27	101.34
5	L	550	BPH	C4D-CHA-C1A	-3.27	122.46	130.51
5	M	500	BPH	C2C-C3C-C4C	3.26	106.22	101.34
6	L	800	UQ	C20-C19-C18	-3.25	115.33	123.68
4	M	400	BCL	CMD-C2D-C3D	3.25	130.76	124.68
4	L	450	BCL	C1-C2-C3	-3.24	120.44	126.04
6	M	750	UQ	O1-C1-C6	-3.24	115.87	121.55
4	M	601	BCL	OBD-CAD-CBD	-3.23	121.28	125.89
4	M	400	BCL	OBB-CAB-CBB	-3.23	112.91	120.17
5	M	500	BPH	C4-C3-C5	3.18	120.63	115.27
6	L	800	UQ	CM5-C5-C6	-3.18	119.21	124.40
4	M	601	BCL	OBB-CAB-CBB	-3.16	113.06	120.17
4	M	400	BCL	C1C-NC-C4C	3.16	108.12	106.71
4	L	450	BCL	CMD-C2D-C3D	3.14	130.56	124.68
4	M	400	BCL	C4D-C3D-CAD	-3.12	106.73	108.47
4	M	601	BCL	C4-C3-C5	3.12	120.52	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	500	BPH	C1-C2-C3	-3.11	120.67	126.04
4	M	601	BCL	C2C-C3C-C4C	3.11	105.99	101.34
6	L	800	UQ	C25-C24-C26	3.10	120.49	115.27
4	L	350	BCL	CMD-C2D-C3D	3.09	130.47	124.68
4	L	450	BCL	OBB-CAB-CBB	-3.00	113.42	120.17
4	L	350	BCL	OBB-CAB-CBB	-3.00	113.43	120.17
4	L	350	BCL	C4-C3-C5	2.97	120.27	115.27
5	L	550	BPH	C1C-NC-C4C	-2.97	107.93	110.54
5	L	550	BPH	OBB-CAB-CBB	-2.96	113.17	119.73
4	L	350	BCL	C2C-C3C-C4C	2.96	105.77	101.34
6	M	750	UQ	C20-C19-C21	2.94	120.21	115.27
5	M	500	BPH	OBB-CAB-CBB	-2.92	113.27	119.73
6	L	800	UQ	C11-C9-C8	-2.90	115.24	121.12
4	M	601	BCL	CMD-C2D-C3D	2.85	130.01	124.68
4	L	450	BCL	C4-C3-C5	2.81	120.00	115.27
6	L	800	UQ	C30-C29-C31	2.78	119.95	115.27
5	M	500	BPH	C1C-NC-C4C	-2.76	108.11	110.54
5	L	550	BPH	C4-C3-C5	2.74	119.88	115.27
6	M	750	UQ	C26-C24-C23	-2.72	115.61	121.12
5	L	550	BPH	CMD-C2D-C3D	2.70	129.73	124.68
6	L	800	UQ	O1-C1-C6	-2.70	116.81	121.55
5	M	500	BPH	OBD-CAD-C3D	2.69	132.44	127.98
5	L	550	BPH	CBD-CHA-C1A	2.61	132.44	126.40
4	L	350	BCL	OBD-CAD-C3D	2.56	132.23	127.98
6	M	750	UQ	O2-C2-C1	2.54	125.14	116.56
4	L	350	BCL	CMB-C2B-C1B	-2.54	124.57	128.46
6	L	800	UQ	C15-C14-C13	-2.54	117.17	123.68
6	M	750	UQ	C25-C24-C26	2.53	119.53	115.27
5	M	500	BPH	C4D-C3D-CAD	2.52	109.47	107.87
5	M	500	BPH	OBD-CAD-CBD	-2.52	122.30	125.89
6	M	750	UQ	C36-C34-C33	-2.52	116.02	121.12
4	M	601	BCL	CMB-C2B-C1B	-2.52	124.59	128.46
6	M	750	UQ	C3-C2-C1	-2.50	115.77	120.68
6	L	800	UQ	C26-C24-C23	2.49	126.15	121.12
4	L	350	BCL	C2A-C1A-CHA	2.45	128.15	123.86
4	L	350	BCL	CHA-C1A-NA	-2.42	120.85	126.40
5	L	550	BPH	CGD-CBD-CAD	-2.41	102.94	110.73
4	L	450	BCL	CMB-C2B-C1B	-2.40	124.78	128.46
4	M	601	BCL	C1C-NC-C4C	2.37	107.77	106.71
6	L	800	UQ	O2-C2-C1	2.37	124.57	116.56
6	L	800	UQ	CM3-O3-C3	-2.35	108.13	116.47
6	L	800	UQ	C27-C26-C24	2.35	120.71	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	400	BCL	CHA-C1A-NA	-2.34	121.03	126.40
4	M	400	BCL	C2A-C1A-CHA	2.30	127.88	123.86
5	L	550	BPH	OBD-CAD-C3D	2.30	131.79	127.98
4	L	350	BCL	C3C-C2C-C1C	2.29	105.57	101.87
4	M	400	BCL	C3C-C2C-C1C	2.28	105.55	101.87
4	M	400	BCL	CMB-C2B-C1B	-2.27	124.98	128.46
4	M	601	BCL	OBD-CAD-C3D	2.24	131.70	127.98
6	M	750	UQ	C35-C34-C36	2.24	119.04	115.27
4	L	450	BCL	CHA-C1A-NA	-2.21	121.34	126.40
4	L	450	BCL	OBD-CAD-C3D	2.20	131.64	127.98
6	L	800	UQ	CM2-O2-C2	2.20	124.25	116.47
4	M	601	BCL	CHA-C1A-NA	-2.19	121.38	126.40
5	M	500	BPH	CMD-C2D-C3D	2.17	128.74	124.68
6	L	800	UQ	O4-C4-C3	-2.16	116.34	120.93
4	M	400	BCL	C4-C3-C5	2.16	118.90	115.27
4	M	400	BCL	OBD-CAD-C3D	2.13	131.52	127.98
5	M	500	BPH	C3C-C2C-C1C	2.10	105.25	101.87
6	M	750	UQ	C6-C5-C4	2.08	120.82	119.18
5	L	550	BPH	C4A-NA-C1A	2.07	109.81	108.14
5	L	550	BPH	CBB-CAB-C3B	2.05	124.82	120.43
6	M	750	UQ	C21-C22-C23	2.00	118.46	111.88

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	800	UQ	C18-C19-C21-C22
6	L	800	UQ	C20-C19-C21-C22
6	L	800	UQ	C30-C29-C31-C32
6	L	800	UQ	C29-C31-C32-C33
6	M	750	UQ	C21-C22-C23-C24
6	M	750	UQ	C24-C26-C27-C28
6	M	750	UQ	C28-C29-C31-C32
6	M	750	UQ	C30-C29-C31-C32
6	M	750	UQ	C34-C36-C37-C38
4	M	601	BCL	C1A-C2A-CAA-CBA
4	M	601	BCL	C3A-C2A-CAA-CBA
4	M	601	BCL	C2A-CAA-CBA-CGA
4	M	601	BCL	C2C-C3C-CAC-CBC
5	L	550	BPH	C2C-C3C-CAC-CBC
5	L	550	BPH	C3A-C2A-CAA-CBA
5	L	550	BPH	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	L	550	BPH	C2A-CAA-CBA-CGA
4	L	450	BCL	C1A-C2A-CAA-CBA
4	L	450	BCL	C3A-C2A-CAA-CBA
4	L	450	BCL	C2C-C3C-CAC-CBC
4	L	450	BCL	C4C-C3C-CAC-CBC
4	L	350	BCL	C2-C3-C5-C6
4	L	350	BCL	C4-C3-C5-C6
4	L	350	BCL	C6-C7-C8-C9
4	M	400	BCL	C1A-C2A-CAA-CBA
4	M	400	BCL	CHA-CBD-CGD-O1D
4	M	400	BCL	CAD-CBD-CGD-O1D
4	M	400	BCL	CAD-CBD-CGD-O2D
4	M	400	BCL	C11-C12-C13-C14
5	M	500	BPH	C4C-C3C-CAC-CBC
5	M	500	BPH	C2C-C3C-CAC-CBC
5	M	500	BPH	C4B-C3B-CAB-CBB
5	M	500	BPH	C4B-C3B-CAB-OB
5	M	500	BPH	C2B-C3B-CAB-CBB
4	L	350	BCL	CBD-CGD-O2D-CED
4	M	400	BCL	CBD-CGD-O2D-CED
4	L	350	BCL	O1D-CGD-O2D-CED
4	L	450	BCL	C10-C11-C12-C13
4	M	400	BCL	C3-C5-C6-C7
5	M	500	BPH	C3-C5-C6-C7
6	L	800	UQ	C35-C34-C36-C37
6	L	800	UQ	C28-C29-C31-C32
4	L	350	BCL	C2A-CAA-CBA-CGA
4	M	400	BCL	O1D-CGD-O2D-CED
4	L	450	BCL	O1A-CGA-O2A-C1
5	M	500	BPH	O1A-CGA-O2A-C1
5	M	500	BPH	CBA-CGA-O2A-C1
4	L	450	BCL	CBA-CGA-O2A-C1
6	L	800	UQ	C12-C11-C9-C10
4	M	400	BCL	C4-C3-C5-C6
6	L	800	UQ	C12-C11-C9-C8
4	M	400	BCL	C2-C3-C5-C6
6	L	800	UQ	C14-C16-C17-C18
6	M	750	UQ	C12-C13-C14-C15
4	L	350	BCL	C10-C11-C12-C13
4	M	400	BCL	C6-C7-C8-C9
4	M	601	BCL	C5-C6-C7-C8
5	M	500	BPH	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	M	601	BCL	C2-C1-O2A-CGA
6	L	800	UQ	C19-C21-C22-C23
6	M	750	UQ	C9-C11-C12-C13
6	M	750	UQ	C19-C21-C22-C23
6	M	750	UQ	C29-C31-C32-C33
4	M	400	BCL	C13-C15-C16-C17
5	M	500	BPH	C5-C6-C7-C8
4	M	400	BCL	C10-C11-C12-C13
6	M	750	UQ	C12-C13-C14-C16
5	M	500	BPH	C10-C11-C12-C13
5	M	500	BPH	C2B-C3B-CAB-OBB
4	M	400	BCL	C16-C17-C18-C19
6	L	800	UQ	C33-C34-C36-C37
4	L	350	BCL	C16-C17-C18-C19
4	L	350	BCL	C16-C17-C18-C20
4	M	400	BCL	C16-C17-C18-C20
5	M	500	BPH	C16-C17-C18-C19
4	L	350	BCL	C11-C10-C8-C7
5	M	500	BPH	C16-C17-C18-C20
4	L	350	BCL	C11-C10-C8-C9
4	M	400	BCL	C8-C10-C11-C12
6	L	800	UQ	C1-C6-C7-C8
5	L	550	BPH	C11-C10-C8-C7
4	L	450	BCL	C11-C10-C8-C7
4	L	450	BCL	C11-C12-C13-C15
4	L	350	BCL	C6-C7-C8-C10
4	M	400	BCL	C6-C7-C8-C10
4	M	400	BCL	C11-C10-C8-C7
5	L	550	BPH	C11-C10-C8-C9
4	L	450	BCL	C11-C10-C8-C9
4	L	450	BCL	C11-C12-C13-C14
4	M	400	BCL	C11-C10-C8-C9
4	L	450	BCL	C4-C3-C5-C6
4	M	601	BCL	CBA-CGA-O2A-C1
5	L	550	BPH	C3-C5-C6-C7
5	L	550	BPH	C2-C1-O2A-CGA
4	L	450	BCL	C2-C3-C5-C6
4	M	601	BCL	C11-C12-C13-C14
5	M	500	BPH	C14-C13-C15-C16
5	M	500	BPH	C2A-CAA-CBA-CGA
6	M	750	UQ	C25-C24-C26-C27
4	L	350	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
4	M	400	BCL	C11-C12-C13-C15
5	M	500	BPH	C12-C13-C15-C16
5	L	550	BPH	C16-C17-C18-C20
5	L	550	BPH	CAD-CBD-CGD-O2D
5	M	500	BPH	CAD-CBD-CGD-O2D
6	M	750	UQ	C7-C8-C9-C10
4	M	601	BCL	O1A-CGA-O2A-C1
6	M	750	UQ	C1-C2-O2-CM2
4	L	350	BCL	CHA-CBD-CGD-O1D
4	L	350	BCL	CHA-CBD-CGD-O2D
6	M	750	UQ	C23-C24-C26-C27
5	L	550	BPH	C16-C17-C18-C19
6	M	750	UQ	C20-C19-C21-C22
4	L	350	BCL	CAD-CBD-CGD-O1D
4	M	400	BCL	CBA-CGA-O2A-C1
4	M	601	BCL	C11-C10-C8-C7
4	M	400	BCL	O1A-CGA-O2A-C1
4	L	350	BCL	C14-C13-C15-C16
6	M	750	UQ	C7-C8-C9-C11
4	M	601	BCL	C10-C11-C12-C13
4	M	601	BCL	C3-C5-C6-C7
4	M	601	BCL	C11-C10-C8-C9
4	L	350	BCL	C11-C12-C13-C14
4	M	400	BCL	C12-C13-C15-C16
5	L	550	BPH	CBA-CGA-O2A-C1
5	L	550	BPH	O1A-CGA-O2A-C1
6	M	750	UQ	C14-C16-C17-C18
4	M	601	BCL	C4C-C3C-CAC-CBC
4	L	450	BCL	C3-C5-C6-C7
4	L	350	BCL	CAA-CBA-CGA-O2A
4	M	400	BCL	C14-C13-C15-C16
5	L	550	BPH	C15-C16-C17-C18
4	M	601	BCL	CAD-CBD-CGD-O2D
4	L	450	BCL	CAD-CBD-CGD-O2D
6	M	750	UQ	C12-C11-C9-C10
5	M	500	BPH	CAA-CBA-CGA-O2A
4	M	400	BCL	CHA-CBD-CGD-O2D
4	M	601	BCL	CAA-CBA-CGA-O2A
6	L	800	UQ	C2-C3-O3-CM3
6	L	800	UQ	C4-C3-O3-CM3
4	L	350	BCL	CAA-CBA-CGA-O1A
5	M	500	BPH	CAA-CBA-CGA-O1A

*Continued on next page...*



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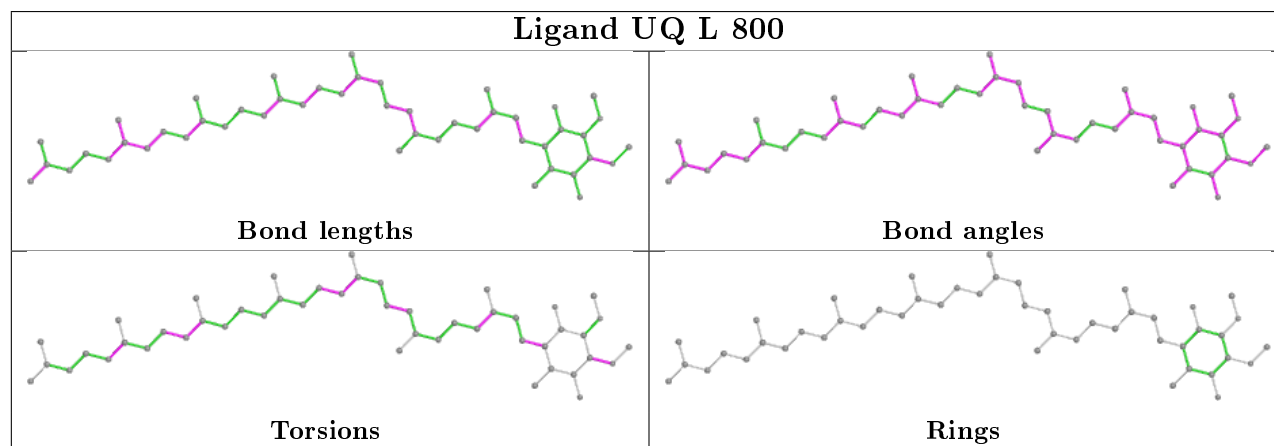
Mol	Chain	Res	Type	Atoms
5	L	550	BPH	C11-C12-C13-C14
4	M	601	BCL	CAA-CBA-CGA-O1A
4	M	400	BCL	C3A-C2A-CAA-CBA

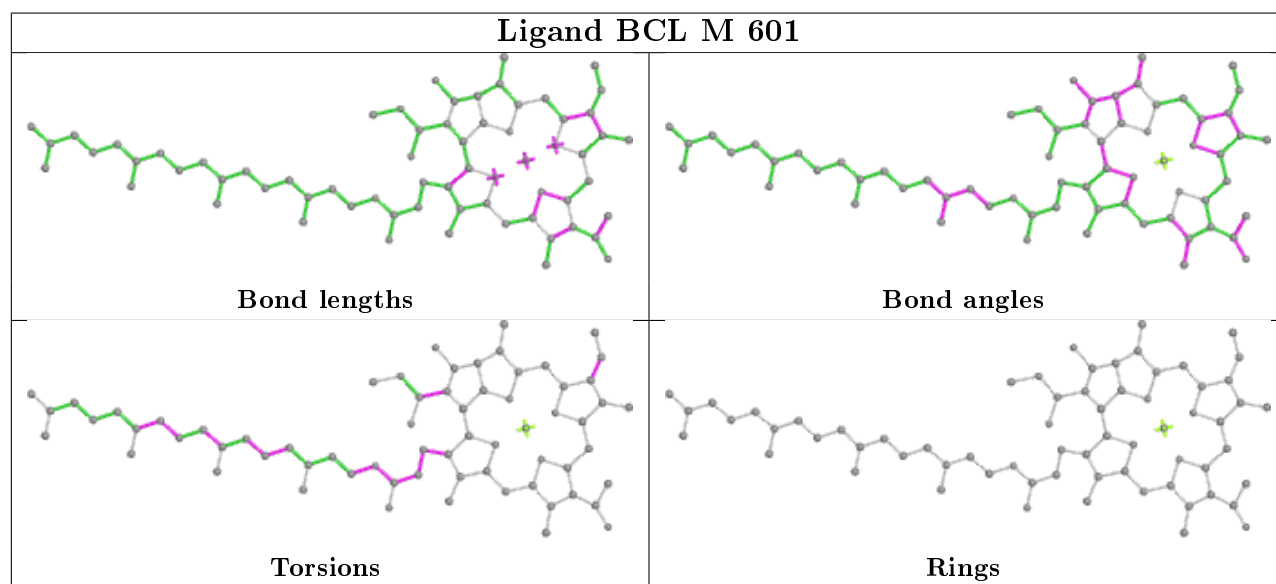
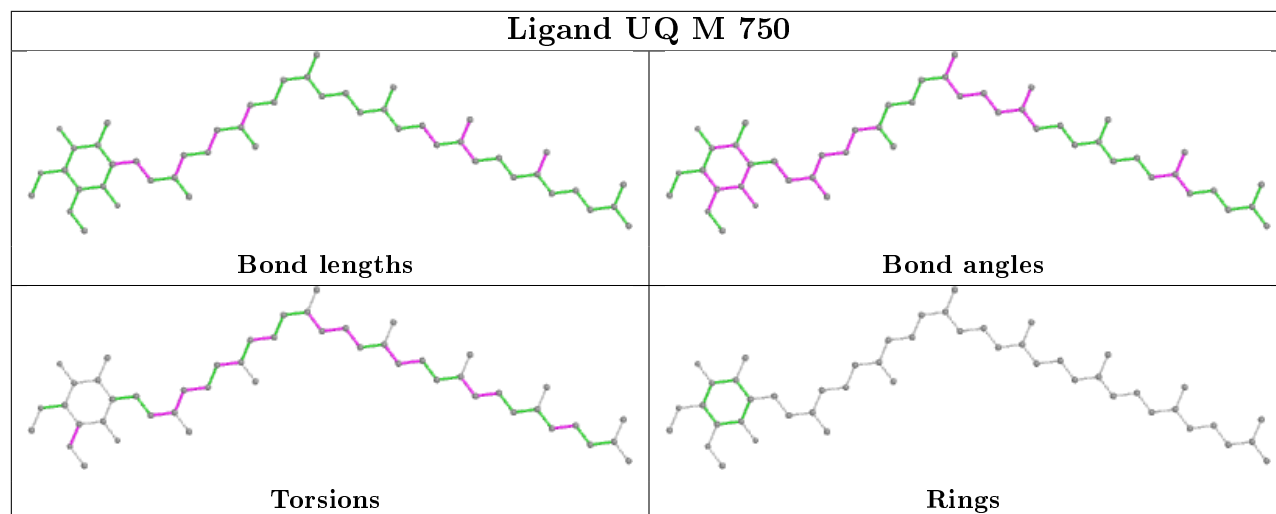
There are no ring outliers.

8 monomers are involved in 190 short contacts:

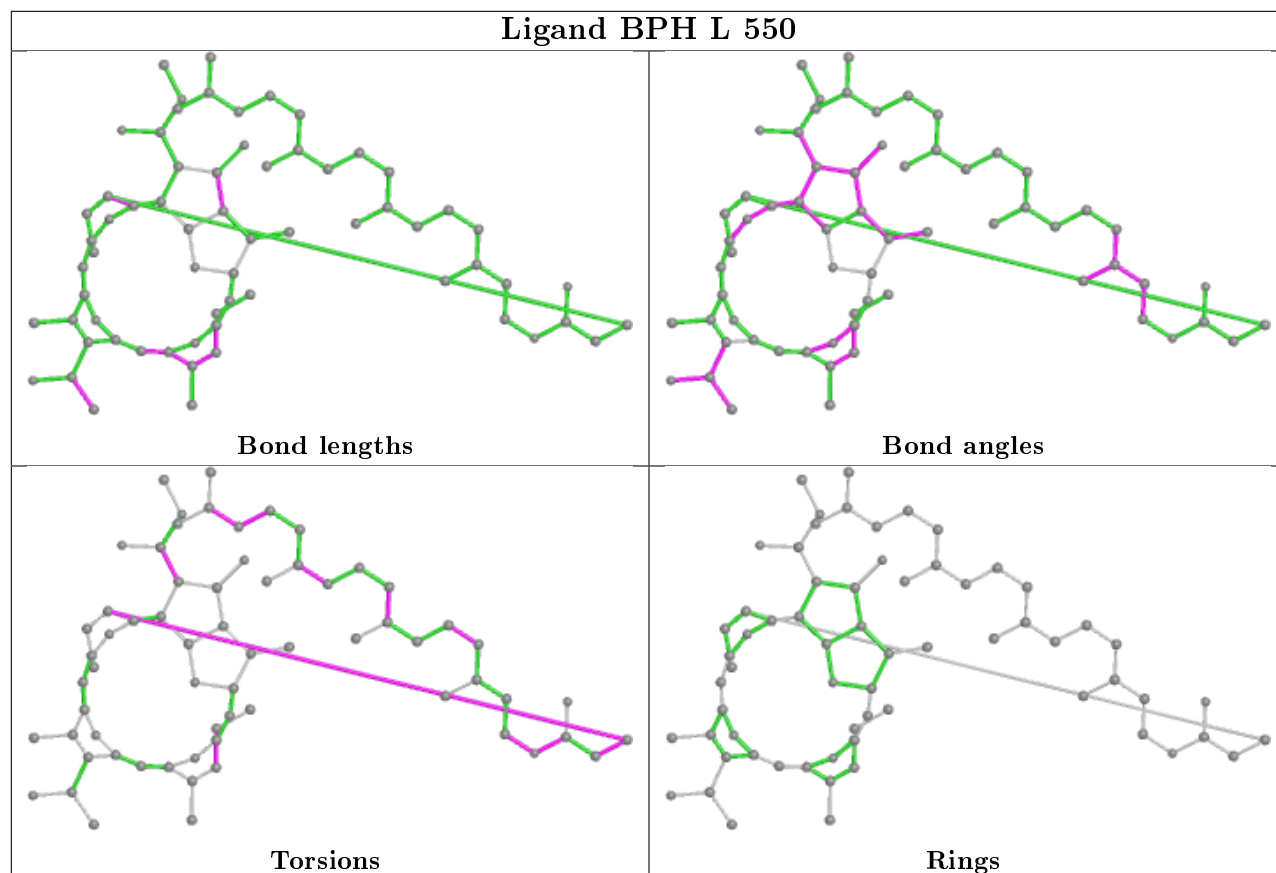
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	800	UQ	21	0
6	M	750	UQ	33	0
4	M	601	BCL	22	0
5	L	550	BPH	16	0
4	L	450	BCL	22	0
4	L	350	BCL	35	0
4	M	400	BCL	47	0
5	M	500	BPH	33	0

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.

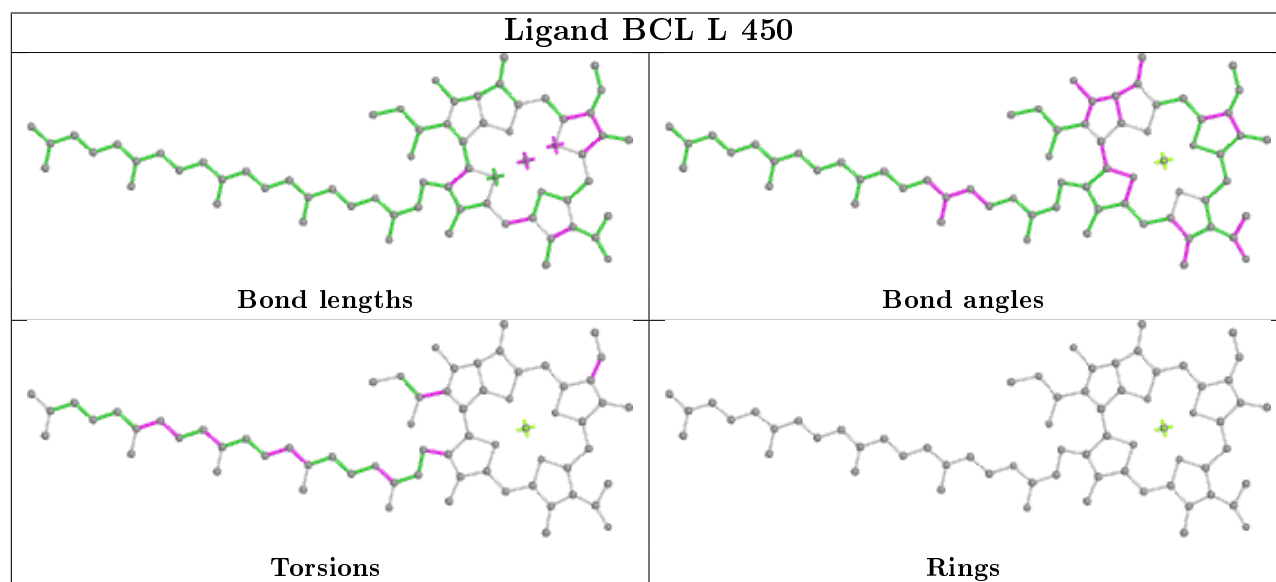


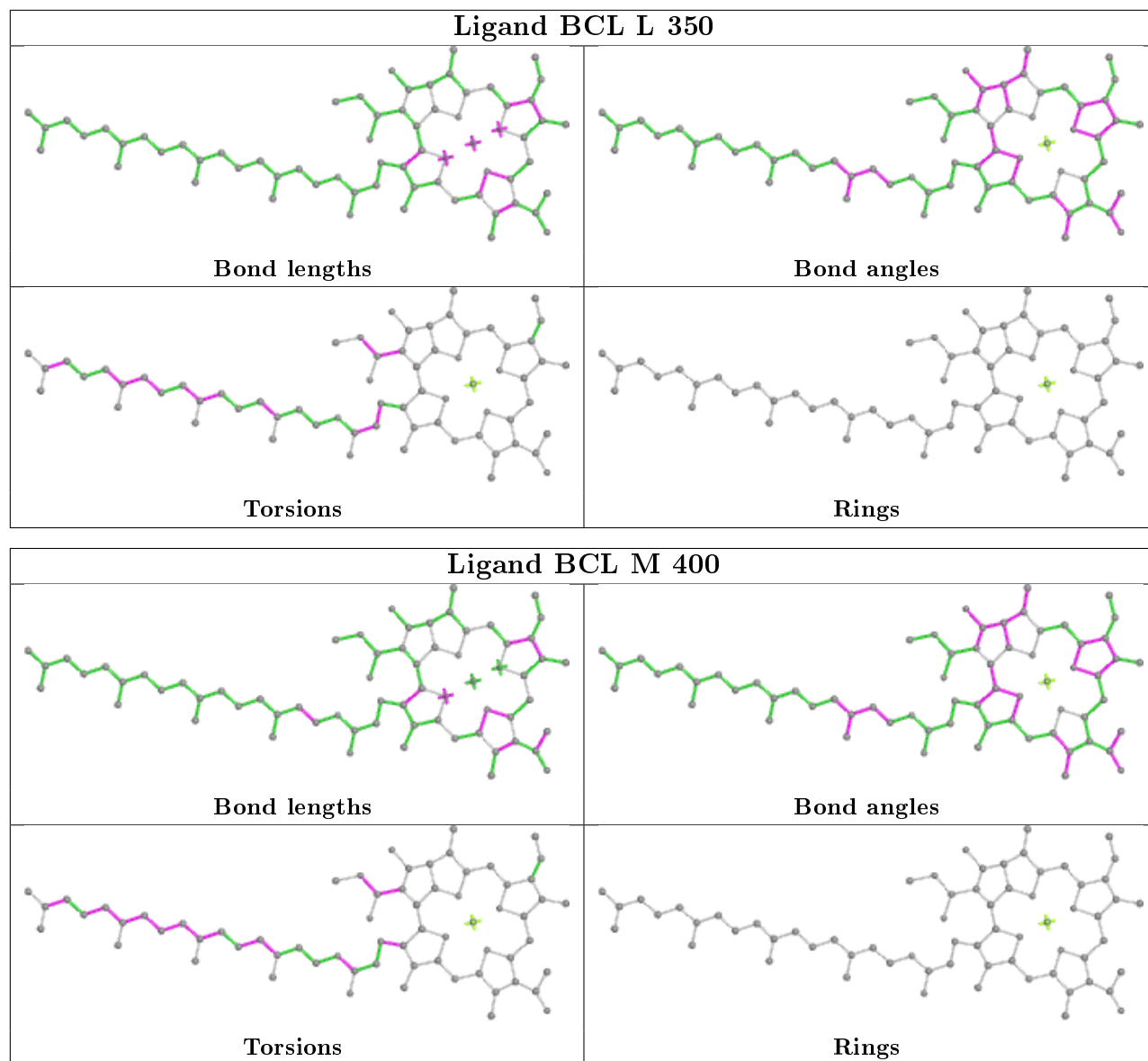


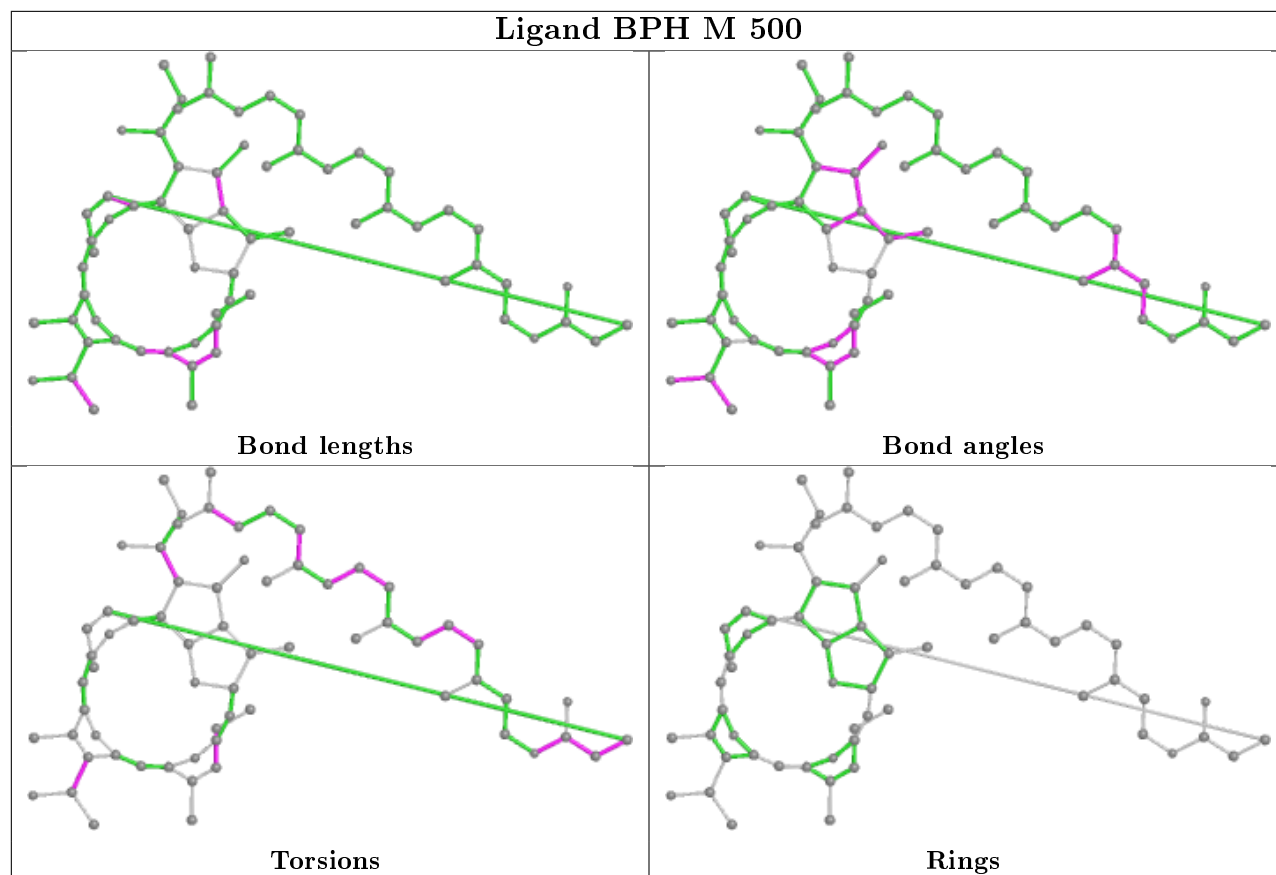
## Ligand BPH L 550



## Ligand BCL L 450







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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.