



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:14 PM EDT

PDB ID : 2RCR / pdb_00002rcr
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

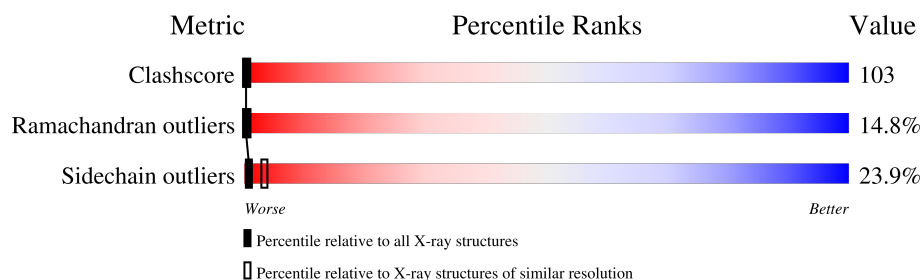
1 Overall quality at a glance

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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	M	400	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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

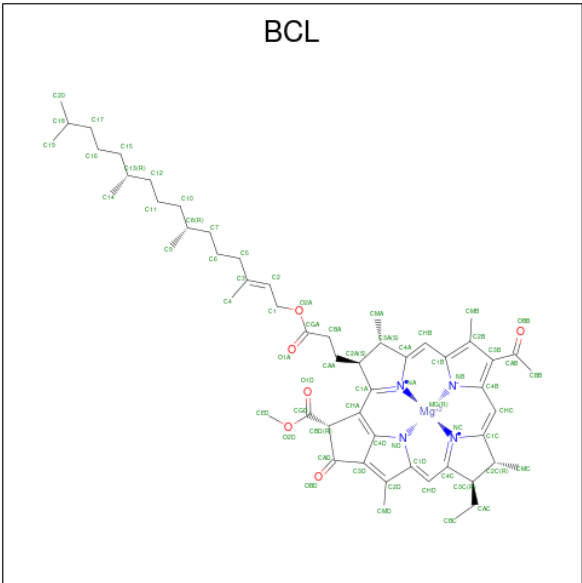
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT).

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).

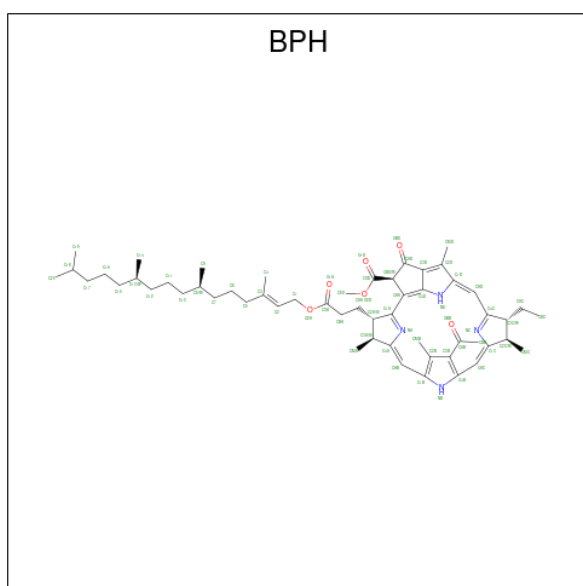
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	255	1927	1232	330	354	11	73	0	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



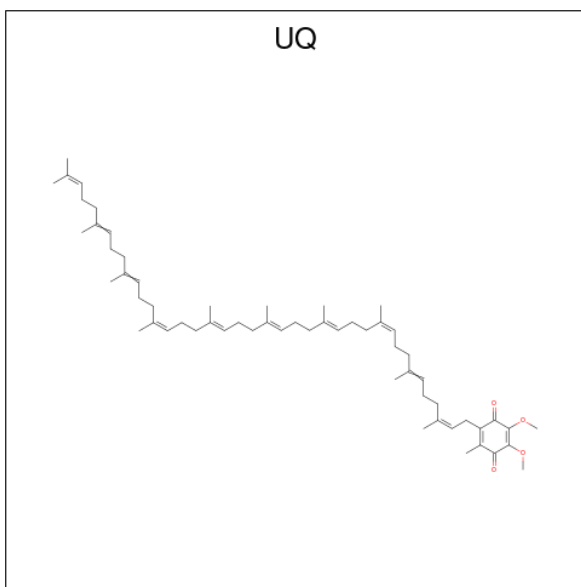
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	6	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	7	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	3	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: 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 (CCD ID: 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 (CCD ID: FE) (formula: Fe).

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

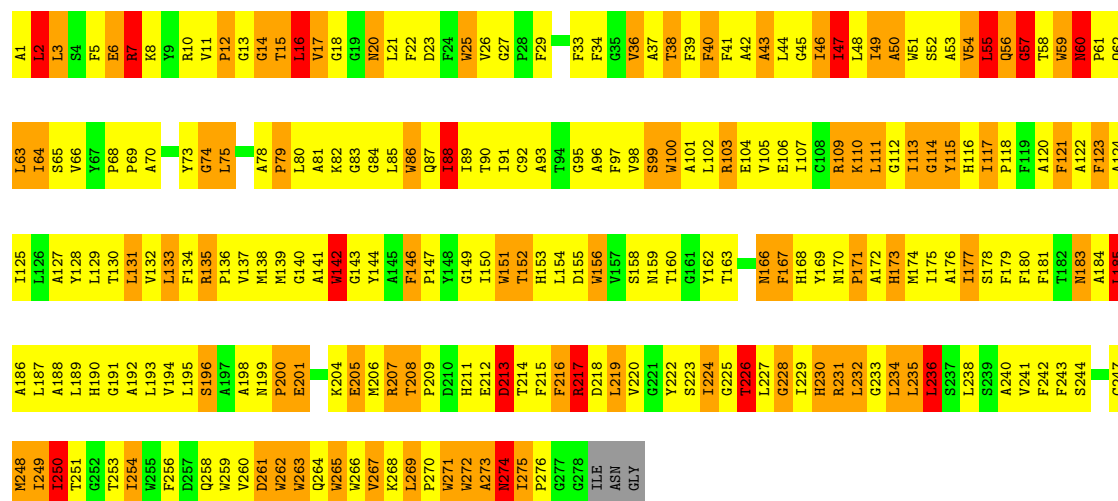
3 Residue-property plots

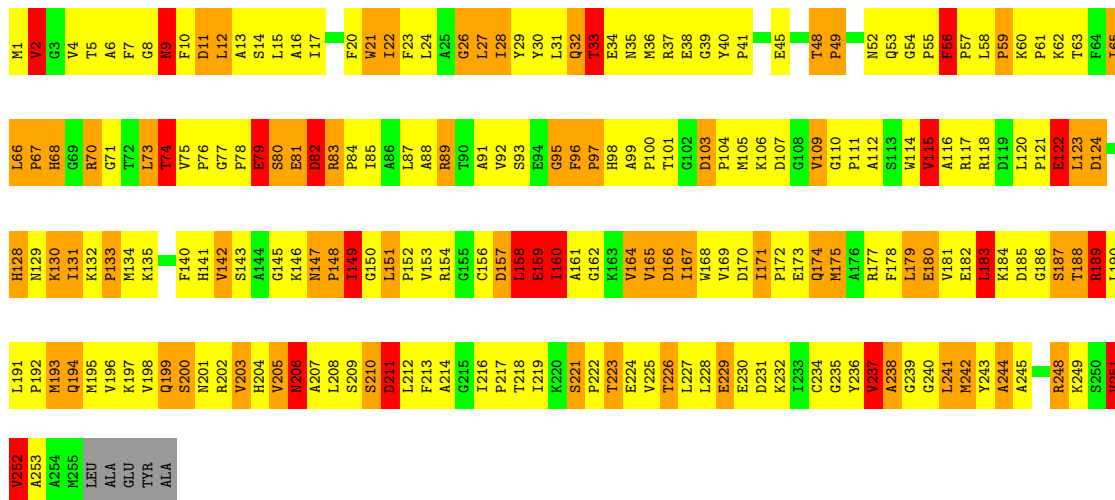
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

Chain L: 





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, α , β , γ	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 ²)	0.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.18	16/2291 (0.7%)	1.90	45/3137 (1.4%)
2	M	1.49	25/2521 (1.0%)	1.96	70/3442 (2.0%)
3	H	1.14	10/1977 (0.5%)	1.80	32/2689 (1.2%)
All	All	1.29	51/6789 (0.8%)	1.89	147/9268 (1.6%)

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 (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	93	LEU	C-O	25.26	1.54	1.23
2	M	93	LEU	CA-C	-24.86	1.19	1.53
2	M	250	TRP	CA-CB	-21.86	1.14	1.53
2	M	112	LEU	C-N	14.62	1.54	1.33
2	M	93	LEU	C-N	13.10	1.57	1.33
1	L	166	ASN	CA-CB	-10.57	1.35	1.53
2	M	269	TRP	CA-CB	-10.17	1.37	1.53
3	H	56	PHE	N-CA	9.48	1.59	1.46
3	H	54	GLY	CA-C	7.41	1.62	1.51
3	H	55	PRO	N-CA	6.81	1.56	1.47
2	M	60	PHE	N-CA	6.44	1.54	1.46
1	L	217	ARG	CG-CD	6.31	1.71	1.52
3	H	54	GLY	N-CA	6.21	1.53	1.44
2	M	59	LEU	CA-C	6.18	1.60	1.53
3	H	55	PRO	CA-C	6.15	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	230	HIS	CB-CG	6.00	1.58	1.50
1	L	231	ARG	N-CA	5.99	1.53	1.46
1	L	88	ILE	N-CA	-5.81	1.39	1.46
3	H	56	PHE	CB-CG	5.73	1.63	1.50
2	M	292	TRP	NE1-CE2	-5.73	1.31	1.37
2	M	155	TRP	NE1-CE2	-5.65	1.31	1.37
2	M	250	TRP	NE1-CE2	-5.63	1.31	1.37
2	M	128	TRP	NE1-CE2	-5.61	1.31	1.37
1	L	100	TRP	NE1-CE2	-5.59	1.31	1.37
2	M	107	LEU	CA-C	-5.58	1.45	1.52
3	H	21	TRP	NE1-CE2	-5.54	1.31	1.37
2	M	113	TRP	NE1-CE2	-5.51	1.31	1.37
1	L	263	TRP	NE1-CE2	-5.48	1.31	1.37
2	M	74	TRP	NE1-CE2	-5.47	1.31	1.37
1	L	265	TRP	NE1-CE2	-5.45	1.31	1.37
1	L	156	TRP	NE1-CE2	-5.44	1.31	1.37
1	L	151	TRP	NE1-CE2	-5.41	1.31	1.37
2	M	153	TRP	NE1-CE2	-5.40	1.31	1.37
1	L	142	TRP	NE1-CE2	-5.37	1.31	1.37
2	M	72	TRP	NE1-CE2	-5.36	1.31	1.37
2	M	127	TRP	NE1-CE2	-5.35	1.31	1.37
2	M	146	TRP	NE1-CE2	-5.34	1.31	1.37
2	M	295	TRP	NE1-CE2	-5.34	1.31	1.37
2	M	183	TRP	NE1-CE2	-5.33	1.31	1.37
2	M	79	TRP	NE1-CE2	-5.33	1.31	1.37
1	L	266	TRP	NE1-CE2	-5.31	1.31	1.37
1	L	86	TRP	NE1-CE2	-5.29	1.31	1.37
1	L	236	LEU	CA-C	5.25	1.59	1.52
2	M	125	TRP	NE1-CE2	-5.24	1.31	1.37
1	L	262	TRP	NE1-CE2	-5.22	1.31	1.37
3	H	56	PHE	CA-C	5.15	1.59	1.52
2	M	112	LEU	CG-CD2	-5.15	1.35	1.52
1	L	230	HIS	CA-C	5.06	1.59	1.52
3	H	55	PRO	C-N	5.05	1.44	1.33
2	M	252	TRP	NE1-CE2	-5.02	1.31	1.37
3	H	101	THR	CA-CB	5.01	1.58	1.53

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	166	ASN	CA-CB-CG	42.38	154.98	112.60
2	M	112	LEU	O-C-N	-36.86	84.11	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	166	ASN	N-CA-CB	19.32	142.88	111.58
2	M	109	GLU	N-CA-C	18.11	144.58	108.18
3	H	142	VAL	N-CA-CB	-14.08	96.69	111.90
2	M	109	GLU	CB-CA-C	-12.59	90.84	111.86
3	H	56	PHE	CA-CB-CG	12.53	126.33	113.80
1	L	273	ALA	O-C-N	11.37	133.04	121.89
2	M	108	LYS	CA-C-N	-11.35	95.95	122.95
2	M	108	LYS	C-N-CA	-11.35	95.95	122.95
2	M	93	LEU	CA-C-N	10.76	135.09	120.67
2	M	93	LEU	C-N-CA	10.76	135.09	120.67
2	M	108	LYS	O-C-N	-10.69	109.20	122.35
2	M	7	PHE	CA-CB-CG	9.96	123.77	113.80
2	M	60	PHE	CA-CB-CG	9.55	123.35	113.80
1	L	135	ARG	CD-NE-CZ	9.10	137.14	124.40
1	L	185	LEU	O-C-N	8.95	131.69	122.03
2	M	250	TRP	CB-CA-C	-8.93	91.95	110.17
3	H	83	ARG	CD-NE-CZ	8.87	136.82	124.40
2	M	112	LEU	CA-C-N	8.84	138.43	121.54
2	M	112	LEU	C-N-CA	8.84	138.43	121.54
2	M	269	TRP	N-CA-CB	-8.58	97.16	109.94
2	M	250	TRP	N-CA-CB	8.12	124.60	110.39
1	L	249	ILE	CA-C-O	8.01	127.76	119.35
3	H	142	VAL	CA-CB-CG2	7.83	123.71	110.40
1	L	217	ARG	CG-CD-NE	7.79	129.14	112.00
1	L	59	TRP	O-C-N	7.78	132.41	123.31
3	H	159	GLU	O-C-N	7.63	132.73	122.59
2	M	231	ARG	CA-C-N	7.26	130.33	120.38
2	M	231	ARG	C-N-CA	7.26	130.33	120.38
2	M	106	PRO	O-C-N	7.25	132.42	122.64
3	H	115	VAL	CB-CA-C	7.24	123.17	111.29
2	M	73	PHE	O-C-N	7.09	132.12	122.83
3	H	65	ILE	O-C-N	7.08	127.91	121.96
1	L	250	ILE	CB-CA-C	7.04	119.64	110.84
2	M	47	GLY	O-C-N	-7.00	114.77	121.77
2	M	13	ARG	CD-NE-CZ	6.95	134.13	124.40
2	M	282	ILE	N-CA-C	-6.94	105.08	111.67
2	M	256	PHE	CA-CB-CG	6.91	120.71	113.80
3	H	96	PHE	CB-CA-C	6.80	119.86	109.60
3	H	74	THR	CA-C-N	6.79	124.51	120.24
3	H	74	THR	C-N-CA	6.79	124.51	120.24
1	L	111	LEU	N-CA-C	-6.70	104.58	112.89
2	M	167	GLY	CA-C-N	6.60	130.12	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	167	GLY	C-N-CA	6.60	130.12	120.82
1	L	120	ALA	CA-C-N	6.59	129.11	120.28
1	L	120	ALA	C-N-CA	6.59	129.11	120.28
2	M	73	PHE	CA-CB-CG	6.51	120.31	113.80
2	M	94	GLU	O-C-N	6.49	127.77	121.28
1	L	3	LEU	CA-C-N	6.47	128.85	120.44
1	L	3	LEU	C-N-CA	6.47	128.85	120.44
2	M	268	ILE	CA-C-N	6.46	129.27	120.54
2	M	268	ILE	C-N-CA	6.46	129.27	120.54
3	H	224	GLU	CB-CG-CD	6.44	123.55	112.60
2	M	23	ASP	O-C-N	6.44	130.79	122.87
2	M	96	PRO	O-C-N	6.43	130.98	123.01
1	L	249	ILE	N-CA-CB	-6.30	104.13	112.26
1	L	249	ILE	N-CA-C	-6.27	106.88	112.90
3	H	193	MET	N-CA-C	-6.26	106.28	114.04
2	M	71	ILE	N-CA-C	-6.23	104.21	111.00
2	M	4	GLN	N-CA-C	-6.23	105.33	113.17
2	M	280	ILE	O-C-N	6.17	127.85	121.87
1	L	249	ILE	CB-CA-C	6.15	118.83	111.20
1	L	250	ILE	N-CA-CB	-6.15	105.44	112.21
3	H	79	GLU	CB-CA-C	-6.13	108.89	117.23
2	M	143	HIS	O-C-N	6.10	128.58	122.12
3	H	103	ASP	CA-CB-CG	6.09	118.69	112.60
2	M	230	GLU	CB-CG-CD	6.05	122.88	112.60
1	L	166	ASN	CB-CA-C	-6.04	103.19	111.95
2	M	215	ALA	CA-C-N	6.01	129.84	120.82
2	M	215	ALA	C-N-CA	6.01	129.84	120.82
1	L	173	HIS	O-C-N	5.99	130.55	122.59
1	L	55	LEU	N-CA-C	-5.88	98.28	110.80
3	H	180	GLU	CB-CG-CD	5.87	122.58	112.60
3	H	56	PHE	O-C-N	-5.83	114.62	121.32
2	M	105(A)	ALA	O-C-N	-5.82	115.01	121.53
3	H	226	THR	N-CA-CB	5.76	121.44	111.00
1	L	57	GLY	N-CA-C	-5.74	99.58	113.18
2	M	218	GLY	CA-C-N	5.74	128.22	120.65
2	M	218	GLY	C-N-CA	5.74	128.22	120.65
3	H	123	LEU	O-C-N	5.73	127.41	123.11
2	M	47	GLY	N-CA-C	-5.70	100.72	112.34
2	M	213	LEU	N-CA-C	5.66	118.22	111.71
2	M	60	PHE	O-C-N	5.64	128.10	122.12
2	M	136	GLN	N-CA-CB	5.63	119.68	110.39
3	H	223	THR	CA-CB-CG2	5.60	120.02	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	121	PHE	CA-CB-CG	-5.58	108.22	113.80
3	H	158	LEU	O-C-N	5.54	129.97	122.59
2	M	136	GLN	CB-CG-CD	5.54	122.02	112.60
2	M	202	LEU	N-CA-C	-5.53	105.40	111.82
1	L	208	THR	O-C-N	5.53	126.18	121.20
1	L	256	PHE	CA-CB-CG	5.48	119.28	113.80
2	M	197	ASN	O-C-N	5.48	125.67	121.23
2	M	130	ARG	NE-CZ-NH2	5.44	124.10	119.20
3	H	70	ARG	NE-CZ-NH2	5.44	124.10	119.20
3	H	83	ARG	N-CA-CB	5.43	116.61	109.55
1	L	55	LEU	O-C-N	-5.43	115.37	122.59
1	L	7	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	L	207	ARG	NE-CZ-NH2	5.41	124.06	119.20
1	L	115	TYR	N-CA-C	-5.37	106.40	113.17
1	L	217	ARG	NE-CZ-NH2	5.36	124.03	119.20
2	M	112	LEU	CB-CG-CD2	5.36	126.78	110.70
1	L	25	TRP	CA-CB-CG	5.35	123.77	113.60
2	M	112	LEU	CB-CG-CD1	5.35	126.74	110.70
2	M	162	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	L	109	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	L	231	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	L	103	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	L	117	ILE	O-C-N	5.30	127.14	121.10
2	M	245	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	H	248	ARG	NE-CZ-NH2	5.29	123.97	119.20
2	M	104	PHE	O-C-N	5.29	129.63	122.59
3	H	187	SER	N-CA-C	5.29	116.73	110.97
2	M	213	LEU	CA-C-O	-5.28	114.13	120.10
2	M	86	ARG	NE-CZ-NH2	5.27	123.95	119.20
3	H	130	LYS	CA-C-N	5.25	128.44	120.77
3	H	130	LYS	C-N-CA	5.25	128.44	120.77
1	L	16	LEU	O-C-N	5.25	129.70	122.46
2	M	226	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	M	290	ASP	N-CA-C	-5.24	107.06	113.50
1	L	232	LEU	O-C-N	5.23	127.47	122.03
2	M	216	MET	CA-C-N	5.22	127.53	120.65
2	M	216	MET	C-N-CA	5.22	127.53	120.65
2	M	239	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	H	89	ARG	NE-CZ-NH2	5.19	123.87	119.20
3	H	211	ASP	CB-CA-C	5.19	118.67	109.65
1	L	213	ASP	CA-CB-CG	5.18	117.78	112.60
1	L	47	ILE	CA-C-N	5.18	129.36	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	47	ILE	C-N-CA	5.18	129.36	120.71
2	M	269	TRP	CB-CA-C	5.18	119.10	110.81
1	L	185	LEU	CB-CA-C	-5.18	102.92	110.95
3	H	96	PHE	O-C-N	5.17	125.50	121.47
1	L	225	GLY	O-C-N	5.13	128.59	122.64
2	M	251	ARG	NE-CZ-NH2	5.13	123.81	119.20
2	M	32	GLY	O-C-N	5.12	126.89	121.77
2	M	242	ALA	CA-C-N	5.11	127.13	120.28
2	M	242	ALA	C-N-CA	5.11	127.13	120.28
3	H	54	GLY	CA-C-N	5.10	126.22	119.84
3	H	54	GLY	C-N-CA	5.10	126.22	119.84
2	M	72	TRP	CA-C-N	-5.08	115.00	122.06
2	M	72	TRP	C-N-CA	-5.08	115.00	122.06
1	L	27	GLY	O-C-N	5.05	126.82	121.77
3	H	252	VAL	O-C-N	5.03	128.86	122.57
1	L	55	LEU	CA-C-N	-5.02	114.62	122.05
1	L	55	LEU	C-N-CA	-5.02	114.62	122.05
2	M	109	GLU	CA-C-N	-5.00	116.33	123.08
2	M	109	GLU	C-N-CA	-5.00	116.33	123.08

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	109	GLU	Peptide,Mainchain
2	M	112	LEU	Peptide,Mainchain
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	497	1
2	M	2428	0	2342	608	1
3	H	1927	0	1927	383	2
4	L	132	0	148	39	0
4	M	132	0	148	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	65	0	76	16	0
5	M	65	0	76	31	0
6	L	48	0	59	22	0
6	M	48	0	63	33	0
7	M	1	0	0	0	0
All	All	7049	0	6995	1411	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 103.

All (1411) 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:C12	6:M:750:UQ:C13	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
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:229:ILE:HB	6:L:800:UQ:HM51	1.25	1.16
4:M:601:BCL:H11	5:M:500:BPH:HMB1	1.23	1.15
1:L:187:LEU:HD21	2:M:267:ALA:CB	1.77	1.15
2:M:102:LEU:HA	2:M:169:TRP:HD1	1.04	1.15
1:L:114:GLY:HA3	2:M:223:ALA:HB1	1.17	1.15
1:L:172:ALA:HB3	1:L:247:CYS:HB2	1.16	1.15
2:M:254:MET:HE1	6:M:750:UQ:C11	1.78	1.14
3:H:182:GLU:HG3	3:H:187:SER:HA	1.15	1.13
2:M:254:MET:HE1	6:M:750:UQ:H112	1.13	1.12
1:L:193:LEU:HD11	1:L:216:PHE:CE1	1.84	1.12
1:L:229:ILE:HD13	6:L:800:UQ:HM52	1.30	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
1:L:187:LEU:CD2	2:M:267:ALA:HB1	1.80	1.11
3:H:168:TRP:HZ3	3:H:180:GLU:HB2	1.16	1.11
4:M:400:BCL:HBD	4:M:400:BCL:HBA1	1.14	1.10
4:L:350:BCL:HBD	4:L:450:BCL:CBC	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:74:GLY:HA2	1:L:141:ALA:HB2	1.38	1.06
3:H:61:PRO:HA	3:H:76:PRO:HG3	1.07	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
1:L:206:MET:HE1	2:M:237:ALA:HB2	1.40	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
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
1:L:231:ARG:NE	2:M:6:ILE:H	1.59	0.99
4:L:350:BCL:H152	5:L:550:BPH:CGA	1.93	0.98
2:M:113:TRP:O	2:M:117:SER:HB2	1.62	0.98
3:H:154:ARG:HD3	3:H:202:ARG:HH11	1.26	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
2:M:250:TRP:HE1	6:M:750:UQ:HM52	1.30	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:106:PRO:C	2:M:108:LYS:H	1.74	0.95
2:M:16:ALA:HB1	2:M:45:GLN:HE22	1.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:151:LEU:HD21	3:H:203:VAL:CG2	1.96	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
1:L:218:ASP:HB3	2:M:50:TYR:CE1	2.02	0.93
2:M:31:VAL:CG2	2:M:33:PRO:HD3	1.97	0.93
2:M:216:MET:HE1	6:M:750:UQ:H13	1.50	0.93
3:H:164:VAL:O	3:H:165:VAL:HG23	1.66	0.93
2:M:69:ILE:CA	2:M:93:LEU:HD11	2.00	0.92
3:H:160:ILE:O	3:H:160:ILE:HG23	1.67	0.92
2:M:78:GLY:O	2:M:79:TRP:HB2	1.70	0.92
1:L:114:GLY:HA3	2:M:223:ALA:CB	1.98	0.92
2:M:157:VAL:HA	2:M:161:ILE:HG22	1.50	0.92
3:H:168:TRP:CZ3	3:H:180:GLU:HB2	2.05	0.92
3:H:56:PHE:H	3:H:57:PRO:HD2	1.34	0.91
3:H:111:PRO:HD2	3:H:243:TYR:CE2	2.04	0.91
1:L:58:THR:CG2	1:L:59:TRP:H	1.83	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
1:L:37:ALA:C	1:L:40:PHE:HB2	1.94	0.91
3:H:195:MET:HE1	3:H:238:ALA:HB2	1.53	0.91
1:L:1:ALA:HB2	1:L:7:ARG:HG2	1.53	0.90
1:L:183:ASN:HD22	1:L:236:LEU:CG	1.83	0.90
1:L:156:TRP:CH2	1:L:248:MET:HE1	2.05	0.90
2:M:103:SER:C	2:M:105:ALA:N	2.28	0.90
1:L:37:ALA:O	1:L:40:PHE:CB	2.20	0.90
2:M:254:MET:CE	6:M:750:UQ:H112	1.99	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
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
2:M:250:TRP:NE1	6:M:750:UQ:HM52	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:212:GLU:HA	2:M:140:MET:HE1	1.56	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
2:M:158:LEU:HD21	2:M:183:TRP:CZ3	2.10	0.87
3:H:5:THR:HA	3:H:11:ASP:HA	1.57	0.87
3:H:183:LEU:HD11	3:H:189:ARG:HD3	1.57	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:CBD	2.03	0.86
1:L:53:ALA:HB2	1:L:64:ILE:CD1	2.05	0.86
4:M:601:BCL:C1	5:M:500:BPH:HMB1	2.03	0.86
1:L:230:HIS:CE1	2:M:221:ILE:HG21	2.09	0.86
2:M:97:ALA:C	2:M:99:GLU:H	1.80	0.86
2:M:157:VAL:CG1	2:M:162:ARG:HB2	2.06	0.86
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:235:GLN:NE2	2:M:260:MET:HE1	1.92	0.85
2:M:128:TRP:NE1	2:M:145:ALA:HB1	1.91	0.85
2:M:226:ARG:HB3	3:H:195:MET:HE2	1.59	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:HD12	2:M:54:LEU:H	1.43	0.84
3:H:81:GLU:O	3:H:82:ASP:HB2	1.77	0.83
3:H:164:VAL:C	3:H:165:VAL:HG23	2.03	0.83
1:L:174:MET:HE3	4:M:601:BCL:HED2	1.57	0.83
2:M:250:TRP:O	2:M:254:MET:HG3	1.77	0.83
3:H:160:ILE:O	3:H:160:ILE:CG2	2.24	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
2:M:50:TYR:O	2:M:51:LEU:HG	1.78	0.83
2:M:105(A):ALA:O	2:M:106:PRO:O	1.96	0.83
3:H:8:GLY:O	3:H:9:ASN:HB2	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:75:VAL:N	3:H:76:PRO:HD2	1.94	0.82
3:H:154:ARG:HD3	3:H:202:ARG:NH1	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:M:400:BCL:H43	5:M:500:BPH:CAB	2.09	0.82
3:H:17:ILE:HG23	3:H:21:TRP:CD1	2.14	0.82
1:L:58:THR:HG22	1:L:59:TRP:N	1.87	0.82
1:L:149:GLY:HA3	1:L:152:THR:CG2	2.09	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
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
2:M:153:TRP:CZ2	2:M:283:LEU:HD12	2.14	0.81
1:L:5:PHE:HB2	2:M:244:GLU:OE1	1.79	0.81
1:L:169:TYR:CG	1:L:260:VAL:HG22	2.15	0.81
2:M:183:TRP:CZ3	4:M:601:BCL:HMC3	2.15	0.81
2:M:162:ARG:HG3	2:M:282:ILE:CG2	2.10	0.81
3:H:61:PRO:HA	3:H:76:PRO:CG	2.01	0.81
2:M:5:ASN:O	2:M:6:ILE:HB	1.80	0.81
2:M:251:ARG:HG3	2:M:251:ARG:HH11	1.45	0.81
1:L:150:ILE:HG12	5:L:550:BPH:H193	1.61	0.81
1:L:218:ASP:CG	2:M:50:TYR:HE1	1.87	0.81
2:M:158:LEU:HD21	4:M:601:BCL:HMC3	1.62	0.81
2:M:89:PHE:HB3	2:M:178:PHE:CD1	2.15	0.81
3:H:173:GLU:O	3:H:174:GLN:HB2	1.81	0.81
2:M:69:ILE:HG12	2:M:93:LEU:HD12	1.63	0.81
2:M:165:LEU:N	2:M:165:LEU:HD23	1.94	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
2:M:97:ALA:HB3	2:M:98:PRO:CD	2.11	0.79
3:H:164:VAL:HG12	3:H:165:VAL:H	1.47	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
1:L:20:ASN:C	1:L:22:PHE:H	1.90	0.79
2:M:259:THR:C	2:M:261:GLU:H	1.88	0.79
1:L:215:PHE:HA	2:M:138:LEU:HD22	1.64	0.79
2:M:89:PHE:O	2:M:178:PHE:HB2	1.82	0.79
2:M:115:ILE:HG23	2:M:119:PHE:HE2	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:229:ILE:CD1	6:L:800:UQ:HM52	2.12	0.79
2:M:105(A):ALA:HB3	2:M:109:GLU:HG2	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
3:H:66:LEU:HB3	3:H:67:PRO:HD2	1.64	0.79
2:M:72:TRP:HB3	2:M:93:LEU:HD13	1.64	0.79
2:M:109:GLU:N	2:M:111:GLY:H	1.81	0.79
1:L:111:LEU:HB2	1:L:113:ILE:HG12	1.64	0.78
3:H:37:ARG:HH21	3:H:62:LYS:HG3	1.44	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:117:ILE:HD13	2:M:249:PHE:HD2	1.46	0.78
1:L:229:ILE:HG13	2:M:214:PHE:HZ	1.47	0.78
2:M:113:TRP:HZ2	2:M:172:ALA:HB1	1.47	0.78
1:L:229:ILE:HB	6:L:800:UQ:CM5	2.10	0.78
3:H:28:ILE:HG22	3:H:29:TYR:N	1.98	0.78
3:H:161:ALA:HA	3:H:210:SER:HB3	1.65	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
2:M:102:LEU:HD12	2:M:102:LEU:O	1.84	0.77
3:H:135:LYS:NZ	3:H:165:VAL:HG12	1.98	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
1:L:65:SER:HB2	1:L:152:THR:HG21	1.67	0.77
3:H:219:ILE:HG12	3:H:221:SER:O	1.83	0.77
1:L:198:ALA:HB2	2:M:233:LEU:HD13	1.66	0.77
2:M:202:LEU:HD23	3:H:20:PHE:HE2	1.49	0.77
2:M:288:VAL:O	3:H:4:VAL:HG11	1.84	0.77
2:M:32:GLY:HA2	2:M:46:LEU:O	1.84	0.77
2:M:162:ARG:HB3	2:M:163:PRO:CD	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:150:ILE:HG12	5:L:550:BPH:C19	2.15	0.76
3:H:199:GLN:HG2	3:H:200:SER:H	1.50	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:33:THR:CG2	3:H:34:GLU:H	1.91	0.76
3:H:131:ILE:HG22	3:H:168:TRP:CD1	2.20	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:54:VAL:C	1:L:55:LEU:O	2.24	0.76
3:H:205:VAL:HG12	3:H:206:ASN:H	1.51	0.76
1:L:151:TRP:O	2:M:303:PRO:HB3	1.86	0.75
1:L:275:ILE:O	1:L:275:ILE:HG22	1.85	0.75
3:H:91:ALA:HB3	3:H:96:PHE:CB	2.17	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
1:L:187:LEU:C	1:L:187:LEU:HD23	2.12	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
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:67:PRO:CG	3:H:123:LEU:HD21	2.17	0.75
1:L:271:TRP:HB2	1:L:274:ASN:HD22	1.52	0.74
3:H:27:LEU:HG	3:H:28:ILE:N	2.02	0.74
1:L:218:ASP:CB	2:M:50:TYR:CE1	2.71	0.74
1:L:13:GLY:H	1:L:110:LYS:HE2	1.53	0.74
1:L:198:ALA:HB2	2:M:233:LEU:CD1	2.18	0.74
1:L:212:GLU:HB3	6:L:800:UQ:O2	1.86	0.74
1:L:274:ASN:O	1:L:275:ILE:HB	1.83	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
1:L:212:GLU:CA	2:M:140:MET:HE1	2.17	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:106:PRO:C	2:M:108:LYS:N	2.43	0.73
2:M:87:ASP:HB3	2:M:90:PHE:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:216:MET:HE1	6:M:750:UQ:C13	2.18	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:240:GLY:O	3:H:244:ALA:HB3	1.87	0.73
3:H:192:PRO:CG	3:H:237:VAL:HG21	2.17	0.73
1:L:70:ALA:HB3	1:L:73:TYR:HD2	1.54	0.73
3:H:135:LYS:NZ	3:H:165:VAL:CG1	2.51	0.73
2:M:22:GLU:HB3	2:M:137:ALA:HA	1.69	0.73
3:H:122:GLU:O	3:H:123:LEU:HG	1.88	0.73
1:L:176:ALA:O	1:L:180:PHE:HD1	1.72	0.73
1:L:162:TYR:CE2	4:L:350:BCL:HBC1	2.23	0.72
1:L:211:HIS:HD2	2:M:138:LEU:O	1.72	0.72
3:H:37:ARG:NH2	3:H:62:LYS:HG3	2.04	0.72
2:M:24:VAL:CG1	2:M:26:LEU:HB2	2.20	0.72
2:M:142:LYS:O	2:M:142:LYS:HG2	1.88	0.72
2:M:226:ARG:NH2	3:H:238:ALA:HB1	2.05	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:50:TYR:C	2:M:51:LEU:HG	2.13	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
1:L:166:ASN:OD1	2:M:185:ASN:ND2	2.22	0.72
1:L:211:HIS:CD2	2:M:138:LEU:O	2.42	0.72
3:H:151:LEU:HD21	3:H:203:VAL:HG23	1.71	0.72
2:M:72:TRP:HB3	2:M:93:LEU:CD1	2.19	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
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
1:L:222:TYR:HD1	1:L:223:SER:N	1.88	0.71
1:L:86:TRP:O	1:L:90:THR:HG22	1.90	0.71
1:L:212:GLU:HA	6:L:800:UQ:HM21	1.71	0.71
4:L:350:BCL:HBA2	2:M:208:TYR:HE1	1.55	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
2:M:115:ILE:CG2	2:M:119:PHE:HE2	2.02	0.71
2:M:165:LEU:HD23	2:M:165:LEU:H	1.53	0.71
3:H:37:ARG:HB3	3:H:75:VAL:CG1	2.20	0.71
2:M:204:ILE:HG23	4:M:400:BCL:HMB3	1.71	0.71
2:M:235:GLN:HE21	2:M:260:MET:CE	2.03	0.71
3:H:245:ALA:CB	3:H:248:ARG:HG3	2.17	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:101:GLY:C	2:M:168:SER:HA	2.15	0.71
3:H:151:LEU:HD21	3:H:203:VAL:HG21	1.70	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: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:4:GLN:HG3	3:H:193:MET:C	2.16	0.70
2:M:87:ASP:HB2	2:M:91:PHE:CE2	2.27	0.70
1:L:183:ASN:CG	1:L:236:LEU:HB2	2.13	0.70
2:M:256:PHE:HE1	6:M:750:UQ:H252	1.55	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
3:H:33:THR:CG2	3:H:34:GLU:N	2.49	0.70
3:H:154:ARG:HH11	3:H:158:LEU:HG	1.56	0.70
1:L:185:LEU:HD22	6:L:800:UQ:H153	1.69	0.70
1:L:264:GLN:HA	1:L:267:VAL:CG2	2.21	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:209:SER:C	3:H:211:ASP:H	1.98	0.70
1:L:13:GLY:CA	3:H:242:MET:HE3	2.22	0.70
3:H:244:ALA:O	3:H:245:ALA:C	2.32	0.70
2:M:68:THR:O	2:M:72:TRP:HB2	1.92	0.70
2:M:183:TRP:HZ3	4:M:601:BCL:HMC3	1.57	0.70
3:H:167:ILE:HG23	3:H:179:LEU:HD12	1.74	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
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
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:153:VAL:O	3:H:161:ALA:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:74:TRP:O	2:M:77:ALA:HB3	1.93	0.69
3:H:80:SER:O	3:H:81:GLU:HB2	1.91	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
2:M:153:TRP:CH2	2:M:283:LEU:CD1	2.76	0.68
2:M:81:PRO:C	2:M:85:LEU:HD12	2.19	0.68
2:M:250:TRP:HE1	6:M:750:UQ:CM5	2.05	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
1:L:229:ILE:HD13	6:L:800:UQ:CM5	2.19	0.68
1:L:141:ALA:C	1:L:143:GLY:H	2.02	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
3:H:135:LYS:HZ3	3:H:165:VAL:CG1	2.06	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
2:M:95:PRO:CB	2:M:96:PRO:HD2	2.24	0.68
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.75	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:72:TRP:CE3	2:M:72:TRP:HA	2.28	0.67
2:M:216:MET:HG2	2:M:250:TRP:CZ2	2.29	0.67
2:M:235:GLN:HE21	2:M:260:MET:HE1	1.57	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:22:ILE:HG23	3:H:23:PHE:CD1	2.28	0.67
4:M:400:BCL:C4	5:M:500:BPH:CAB	2.73	0.67
3:H:104:PRO:HB3	3:H:243:TYR:CE1	2.30	0.67
1:L:59:TRP:O	1:L:60:ASN:HB2	1.95	0.67
1:L:174:MET:HE3	4:M:601:BCL:CED	2.24	0.67
1:L:152:THR:C	1:L:154:LEU:H	2.03	0.67
4:L:350:BCL:C2	5:L:550:BPH:HBB3	2.25	0.66
3:H:63:THR:HA	3:H:74:THR:HG23	1.77	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:65:SER:OG	1:L:66:VAL:N	2.26	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
3:H:27:LEU:CD1	3:H:32:GLN:HB2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:54:LEU:HD22	2:M:129:GLY:HA3	1.77	0.66
2:M:72:TRP:CD1	2:M:112:LEU:HB3	2.30	0.66
2:M:158:LEU:CD2	4:M:601:BCL:HMC3	2.24	0.66
2:M:72:TRP:HZ3	2:M:75:TYR:HB2	1.61	0.66
2:M:102:LEU:CA	2:M:169:TRP:CD1	2.71	0.66
1:L:172:ALA:HB1	1:L:243:PHE:O	1.96	0.66
4:M:400:BCL:CBB	4:M:400:BCL:HMB1	2.25	0.66
3:H:149:ILE:C	3:H:164:VAL:HB	2.20	0.66
1:L:13:GLY:HA2	3:H:242:MET:HE3	1.76	0.65
2:M:58:SER:OG	5:M:500:BPH:H4C2	1.96	0.65
2:M:265:ARG:O	2:M:269:TRP:CD1	2.49	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
1:L:127:ALA:O	1:L:131:LEU:HG	1.96	0.65
2:M:4:GLN:CD	3:H:193:MET:HG3	2.22	0.65
3:H:88:ALA:O	3:H:98:HIS:HB3	1.97	0.65
3:H:199:GLN:HG2	3:H:200:SER:N	2.11	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
2:M:164:ILE:C	2:M:166:MET:H	2.04	0.65
1:L:193:LEU:HD21	1:L:215:PHE:CE2	2.32	0.65
3:H:133:PRO:HA	3:H:167:ILE:O	1.97	0.65
2:M:49:ILE:HG12	2:M:50:TYR:O	1.97	0.65
2:M:250:TRP:CD1	6:M:750:UQ:HM52	2.31	0.65
1:L:20:ASN:HD22	1:L:23:ASP:HB3	1.62	0.64
1:L:194:VAL:O	1:L:195:LEU:C	2.39	0.64
2:M:158:LEU:HD21	2:M:183:TRP:CH2	2.32	0.64
1:L:74:GLY:O	1:L:75:LEU:HB2	1.96	0.64
2:M:265:ARG:O	2:M:269:TRP:HD1	1.81	0.64
1:L:218:ASP:CG	2:M:50:TYR:CE1	2.68	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
2:M:162:ARG:HD3	2:M:166:MET:HE1	1.78	0.64
2:M:204:ILE:HG12	4:M:400:BCL:CHB	2.28	0.64
3:H:154:ARG:NH1	3:H:158:LEU:HG	2.12	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:199:PHE:CE1	2:M:280:ILE:HG22	2.33	0.63
3:H:5:THR:HG23	3:H:10:PHE:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	2:M:72:TRP:HE3	1.64	0.63
6:M:750:UQ:H211	6:M:750:UQ:C25	2.28	0.63
1:L:218:ASP:HB3	2:M:50:TYR:HE1	1.62	0.63
2:M:193:ASN:C	2:M:195:PHE:H	2.07	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
3:H:170:ASP:CG	3:H:173:GLU:HB3	2.23	0.63
1:L:172:ALA:O	1:L:175:ILE:N	2.32	0.63
2:M:264:HIS:O	2:M:267:ALA:HB3	1.99	0.63
1:L:175:ILE:HG21	1:L:243:PHE:CD2	2.33	0.62
2:M:45:GLN:HG2	2:M:47:GLY:O	1.99	0.62
2:M:108:LYS:O	2:M:108:LYS:HG2	1.97	0.62
2:M:113:TRP:CZ3	2:M:169:TRP:CE3	2.82	0.62
3:H:36:MET:O	3:H:40:TYR:HB2	1.99	0.62
4:L:350:BCL:C2	5:L:550:BPH:CBB	2.76	0.62
4:L:350:BCL:HMB1	4:L:350:BCL:HBB3	1.81	0.62
2:M:234:GLU:OE2	3:H:123:LEU:HD11	1.99	0.62
1:L:44:LEU:HA	1:L:47:ILE:CG2	2.29	0.62
2:M:97:ALA:C	2:M:99:GLU:N	2.47	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
2:M:164:ILE:C	2:M:166:MET:N	2.56	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
4:M:400:BCL:H143	5:M:500:BPH:O1A	1.99	0.62
1:L:218:ASP:HB3	2:M:50:TYR:CD1	2.33	0.62
1:L:264:GLN:O	1:L:264:GLN:HG3	2.00	0.62
2:M:161:ILE:HG22	2:M:162:ARG:N	2.15	0.62
4:M:601:BCL:HBC1	4:M:400:BCL:CBF	2.29	0.62
3:H:75:VAL:N	3:H:76:PRO:CD	2.63	0.62
1:L:222:TYR:HE2	2:M:38:LEU:HD21	1.62	0.62
2:M:188:SER:OG	2:M:194:LEU:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:130:ARG:O	2:M:134:ARG:CB	2.47	0.62
2:M:83:VAL:HG22	2:M:86:ARG:HH12	1.63	0.62
3:H:121:PRO:O	3:H:122:GLU:C	2.43	0.62
2:M:6:ILE:O	2:M:7:PHE:HB3	1.99	0.61
2:M:68:THR:CG2	2:M:112:LEU:HD13	2.30	0.61
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
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
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:18:LEU:HD13	2:M:48:PRO:HG3	1.83	0.61
4:M:400:BCL:H42	5:M:500:BPH:HHC	1.81	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
3:H:130:LYS:HG3	3:H:172:PRO:HD2	1.82	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:HG3	3:H:172:PRO:CD	2.30	0.61
2:M:4:GLN:HB2	3:H:194:GLN:HA	1.83	0.61
3:H:33:THR:O	3:H:34:GLU:HB2	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
1:L:93:ALA:O	1:L:97:PHE:CD2	2.54	0.61
3:H:36:MET:HG2	3:H:40:TYR:CZ	2.35	0.61
1:L:17:VAL:HG22	1:L:33:PHE:CB	2.30	0.61
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.82	0.61
1:L:132:VAL:O	1:L:136:PRO:HG2	2.00	0.61
1:L:171:PRO:O	1:L:175:ILE:HG12	2.01	0.61
2:M:29(A):SER:OG	2:M:51:LEU:HD11	2.01	0.61
6:M:750:UQ:C12	6:M:750:UQ:C14	2.71	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
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:278:GLY:O	2:M:282:ILE:HG12	2.01	0.60
3:H:123:LEU:O	3:H:124:ASP:HB2	2.00	0.60
1:L:122:ALA:O	1:L:123:PHE:C	2.44	0.60
2:M:256:PHE:CE1	6:M:750:UQ:H252	2.34	0.60
3:H:37:ARG:HB3	3:H:75:VAL:HG12	1.82	0.60
3:H:148:PRO:HB2	3:H:164:VAL:HG11	1.81	0.60
2:M:74:TRP:CD1	2:M:74:TRP:C	2.80	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
2:M:204:ILE:HG23	4:M:400:BCL:CMB	2.31	0.60
2:M:235:GLN:HB2	2:M:260:MET:HE2	1.83	0.60
1:L:60:ASN:C	1:L:62:GLN:H	2.08	0.60
2:M:195:PHE:CE2	4:M:400:BCL:HMC1	2.36	0.60
4:M:601:BCL:HBC1	4:M:400:BCL:HBA1	1.82	0.60
3:H:87:LEU:HG	3:H:109:VAL:HG11	1.82	0.60
1:L:133:LEU:O	1:L:137:VAL:HG23	2.01	0.60
2:M:95:PRO:CB	2:M:96:PRO:CD	2.79	0.60
2:M:157:VAL:HA	2:M:161:ILE:CG2	2.30	0.60
1:L:139:MET:HE2	1:L:144:TYR:CD2	2.36	0.60
2:M:204:ILE:HG12	4:M:400:BCL:C1B	2.32	0.60
3:H:165:VAL:O	3:H:166:ASP:HB2	2.00	0.60
1:L:156:TRP:CZ2	1:L:248:MET:HE1	2.36	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
2:M:183:TRP:CZ3	4:M:601:BCL:CMC	2.85	0.60
4:M:400:BCL:H43	5:M:500:BPH:HBB2	1.83	0.60
1:L:127:ALA:HB3	4:L:350:BCL:C4	2.31	0.60
2:M:4:GLN:CG	3:H:193:MET:O	2.43	0.60
2:M:251:ARG:HG3	2:M:251:ARG:NH1	2.16	0.60
3:H:70:ARG:HH11	3:H:70:ARG:HG2	1.67	0.60
2:M:21:THR:HG23	2:M:50:TYR:OH	2.01	0.59
2:M:128:TRP:HE1	2:M:145:ALA:CB	2.11	0.59
3:H:7:PHE:C	3:H:9:ASN:H	2.08	0.59
2:M:244:GLU:O	2:M:247:ALA:N	2.36	0.59
3:H:74:THR:C	3:H:76:PRO:HD2	2.27	0.59
1:L:1:ALA:HB2	1:L:7:ARG:CG	2.28	0.59
1:L:97:PHE:O	1:L:100:TRP:HB3	2.02	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
3:H:40:TYR:HA	3:H:41:PRO:C	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:ALA:CB	1:L:64:ILE:HG13	2.33	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
2:M:272:VAL:C	2:M:274:VAL:H	2.09	0.59
3:H:192:PRO:HD3	3:H:237:VAL:HG21	1.85	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:37:ARG:HB3	3:H:75:VAL:HG11	1.83	0.59
1:L:86:TRP:CZ3	1:L:142:TRP:HB3	2.37	0.59
2:M:59:LEU:O	2:M:63:LEU:HB2	2.03	0.59
2:M:154:LEU:CD1	2:M:275:THR:HG22	2.31	0.59
3:H:111:PRO:HD2	3:H:243:TYR:CZ	2.37	0.59
2:M:21:THR:O	2:M:22:GLU:C	2.45	0.59
3:H:237:VAL:O	3:H:239:GLY:N	2.36	0.59
1:L:51:TRP:CZ2	1:L:80:LEU:HD21	2.39	0.58
1:L:185:LEU:CG	1:L:186:ALA:N	2.62	0.58
3:H:66:LEU:HB2	3:H:71:GLY:HA2	1.85	0.58
3:H:75:VAL:C	3:H:77:GLY:H	2.11	0.58
2:M:158:LEU:HD23	2:M:173:VAL:HG21	1.85	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:55:LEU:HG	1:L:56:GLN:N	2.17	0.58
1:L:231:ARG:NE	2:M:6:ILE:N	2.37	0.58
2:M:272:VAL:C	2:M:274:VAL:N	2.59	0.58
1:L:20:ASN:CG	1:L:21:LEU:H	2.12	0.58
1:L:185:LEU:HD23	1:L:186:ALA:N	2.18	0.58
4:L:450:BCL:CBB	4:L:450:BCL:HMB1	2.34	0.58
2:M:92:SER:HA	2:M:175:TYR:O	2.04	0.58
3:H:65:ILE:O	3:H:66:LEU:O	2.22	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
2:M:259:THR:C	2:M:261:GLU:N	2.57	0.58
3:H:134:MET:CE	3:H:142:VAL:HG22	2.33	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
3:H:22:ILE:HG23	3:H:23:PHE:HD1	1.68	0.58
1:L:222:TYR:CD1	1:L:223:SER:N	2.71	0.58
4:M:400:BCL:HMB1	4:M:400:BCL:HBB3	1.84	0.58
2:M:165:LEU:N	2:M:165:LEU:CD2	2.64	0.57
2:M:218:GLY:O	2:M:222:LEU:HD12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:114:TRP:CG	3:H:232:LYS:HG3	2.39	0.57
1:L:3:LEU:CB	1:L:6:GLU:HB2	2.24	0.57
2:M:97:ALA:CB	2:M:98:PRO:HD3	2.31	0.57
2:M:113:TRP:CZ2	2:M:172:ALA:HB1	2.30	0.57
3:H:207:ALA:HB3	3:H:237:VAL:HG12	1.85	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
3:H:67:PRO:HG2	3:H:123:LEU:CD2	2.28	0.57
3:H:111:PRO:HD2	3:H:243:TYR:HE2	1.60	0.57
3:H:122:GLU:HA	3:H:227:LEU:HD21	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
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
1:L:162:TYR:O	1:L:163:THR:C	2.48	0.57
2:M:216:MET:CG	2:M:250:TRP:CZ2	2.88	0.57
1:L:11:VAL:HG21	3:H:111:PRO:HD3	1.87	0.57
1:L:168:HIS:CD2	4:M:601:BCL:HMD1	2.40	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: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:13:GLY:HA3	3:H:242:MET:HE3	1.87	0.57
2:M:79:TRP:HB3	2:M:80:ASN:OD1	2.05	0.57
2:M:164:ILE:O	2:M:166:MET:N	2.38	0.57
3:H:5:THR:HG21	3:H:9:ASN:HA	1.86	0.57
3:H:208:LEU:HD13	3:H:216:ILE:HD11	1.86	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
3:H:27:LEU:HG	3:H:32:GLN:HB2	1.87	0.57
3:H:124:ASP:HB3	3:H:128:HIS:O	2.05	0.57
2:M:254:MET:CE	6:M:750:UQ:C11	2.67	0.56
3:H:149:ILE:H	3:H:164:VAL:HG11	1.70	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
1:L:10:ARG:HG3	1:L:25:TRP:CZ3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:GLY:N	1:L:110:LYS:HE2	2.20	0.56
1:L:172:ALA:O	1:L:173:HIS:C	2.47	0.56
1:L:242:PHE:CD1	1:L:242:PHE:C	2.83	0.56
2:M:179:SER:O	2:M:180:HIS:C	2.45	0.56
2:M:184:THR:CG2	2:M:185:ASN:N	2.68	0.56
2:M:202:LEU:HD23	3:H:20:PHE:CE2	2.36	0.56
2:M:221:ILE:O	2:M:225:SER:OG	2.21	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:44:LEU:CA	1:L:47:ILE:HB	2.36	0.56
3:H:216:ILE:HG23	3:H:217:PRO:HD2	1.86	0.56
1:L:17:VAL:CG2	1:L:33:PHE:HB2	2.35	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
2:M:254:MET:SD	6:M:750:UQ:H203	2.45	0.56
3:H:159:GLU:CG	3:H:160:ILE:H	2.19	0.56
3:H:83:ARG:HB3	3:H:84:PRO:HD2	1.88	0.56
5:L:550:BPH:HHC	5:L:550:BPH:HBB2	1.86	0.56
2:M:166:MET:SD	2:M:171:GLU:OE1	2.64	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
2:M:62:GLY:O	2:M:65:TRP:HE3	1.88	0.56
1:L:211:HIS:CB	2:M:140:MET:HE3	2.36	0.56
1:L:274:ASN:C	1:L:275:ILE:HG12	2.31	0.56
5:M:500:BPH:O1A	5:M:500:BPH:H3A	2.06	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
3:H:1:MET:CG	3:H:2:VAL:H	2.19	0.56
2:M:15:PRO:HD2	3:H:140:PHE:CD1	2.42	0.55
2:M:171:GLU:O	2:M:172:ALA:CB	2.55	0.55
3:H:151:LEU:O	3:H:164:VAL:HG23	2.06	0.55
1:L:25:TRP:HB3	1:L:29:PHE:O	2.06	0.55
2:M:96:PRO:CG	2:M:170:SER:CA	2.50	0.55
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
1:L:156:TRP:CH2	1:L:248:MET:CE	2.87	0.55
2:M:199:PHE:CD1	2:M:280:ILE:HG22	2.42	0.55
3:H:181:VAL:HB	3:H:189:ARG:O	2.05	0.55
1:L:116:HIS:C	1:L:118:PRO:HD2	2.31	0.55
2:M:250:TRP:HB3	2:M:254:MET:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:ARG:HH12	3:H:158:LEU:HD11	1.71	0.55
3:H:228:LEU:C	3:H:228:LEU:HD23	2.30	0.55
1:L:177:ILE:HD12	4:M:601:BCL:HMD2	1.89	0.55
2:M:72:TRP:CE3	2:M:72:TRP:O	2.60	0.55
3:H:4:VAL:HG12	3:H:11:ASP:OD1	2.07	0.55
2:M:157:VAL:HG22	2:M:283:LEU:HD11	1.89	0.55
2:M:235:GLN:NE2	2:M:260:MET:CE	2.64	0.55
2:M:224:VAL:C	2:M:226:ARG:H	2.13	0.55
2:M:108:LYS:O	2:M:109:GLU:CB	2.43	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
1:L:50:ALA:O	1:L:54:VAL:HG23	2.07	0.54
1:L:86:TRP:HZ2	1:L:132:VAL:HG13	1.71	0.54
1:L:117:ILE:N	1:L:118:PRO:CD	2.70	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
3:H:167:ILE:HG23	3:H:179:LEU:CD1	2.35	0.54
1:L:122:ALA:C	1:L:124:ALA:N	2.64	0.54
1:L:185:LEU:O	1:L:188:ALA:HB3	2.07	0.54
1:L:95:GLY:O	1:L:99:SER:HB2	2.07	0.54
2:M:179:SER:C	2:M:181:LEU:N	2.61	0.54
3:H:154:ARG:NH1	3:H:158:LEU:CG	2.70	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:158:SER:C	1:L:162:TYR:HD2	2.16	0.54
1:L:185:LEU:HB2	5:M:500:BPH:HMC2	1.90	0.54
2:M:227:PHE:CD2	3:H:234:CYS:HB3	2.42	0.54
2:M:254:MET:HB3	6:M:750:UQ:C20	2.37	0.54
3:H:37:ARG:HH12	3:H:59:PRO:HG2	1.72	0.54
3:H:209:SER:O	3:H:213:PHE:HD1	1.90	0.54
1:L:275:ILE:C	1:L:276:PRO:O	2.50	0.54
2:M:191:HIS:CD2	2:M:285:SER:OG	2.61	0.54
2:M:178:PHE:HA	2:M:181:LEU:HD12	1.90	0.54
2:M:216:MET:CE	6:M:750:UQ:H13	2.30	0.54
2:M:289:VAL:HG12	2:M:291:ASN:O	2.07	0.54
3:H:110:GLY:C	3:H:112:ALA:H	2.15	0.54
2:M:294:VAL:O	2:M:298:ASN:N	2.41	0.54
1:L:13:GLY:O	1:L:14:GLY:C	2.50	0.54
3:H:36:MET:HG2	3:H:40:TYR:CE2	2.42	0.54
3:H:192:PRO:HG3	3:H:237:VAL:HG21	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:TYR:HD1	1:L:128:TYR:C	2.16	0.54
3:H:189:ARG:HH21	3:H:218:THR:CG2	2.21	0.54
1:L:229:ILE:CB	6:L:800:UQ:HM51	2.18	0.53
2:M:92:SER:O	2:M:93:LEU:HD23	2.08	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
1:L:141:ALA:C	1:L:143:GLY:N	2.61	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
3:H:151:LEU:CD2	3:H:203:VAL:HG21	2.37	0.53
2:M:96:PRO:HD2	2:M:170:SER:HA	1.91	0.53
2:M:212:LEU:C	2:M:212:LEU:HD23	2.33	0.53
3:H:105:MET:CE	3:H:212:LEU:HD22	2.37	0.53
1:L:54:VAL:O	1:L:55:LEU:O	2.26	0.53
4:L:350:BCL:H152	5:L:550:BPH:O2A	2.06	0.53
2:M:25:ASN:H	2:M:25:ASN:HD22	1.56	0.53
2:M:216:MET:CG	2:M:250:TRP:HZ2	2.21	0.53
1:L:175:ILE:HG22	1:L:179:PHE:CE1	2.44	0.53
4:L:450:BCL:HMD2	4:M:400:BCL:HBB3	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
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.90	0.53
1:L:41:PHE:HB2	1:L:96:ALA:HB2	1.89	0.53
1:L:156:TRP:HH2	1:L:248:MET:HE1	1.71	0.53
3:H:66:LEU:HB2	3:H:71:GLY:CA	2.38	0.53
2:M:272:VAL:O	2:M:274:VAL:N	2.41	0.53
3:H:103:ASP:HB2	3:H:106:LYS:HB3	1.90	0.53
3:H:160:ILE:C	3:H:162:GLY:N	2.64	0.53
1:L:169:TYR:CD2	1:L:260:VAL:HG13	2.44	0.53
3:H:174:GLN:O	3:H:175:MET:HB2	2.09	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:177:ILE:CD1	4:M:601:BCL:HMD2	2.39	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
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
1:L:62:GLN:HA	1:L:150:ILE:HB	1.90	0.52
1:L:128:TYR:C	1:L:128:TYR:CD1	2.87	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:211:HIS:HB2	2:M:140:MET:HE3	1.90	0.52
2:M:158:LEU:CD2	2:M:183:TRP:CH2	2.92	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: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:66:LEU:HB3	3:H:67:PRO:CD	2.37	0.52
2:M:250:TRP:NE1	6:M:750:UQ:CM5	2.67	0.52
2:M:265:ARG:O	2:M:269:TRP:HB2	2.10	0.52
3:H:115:VAL:CG1	3:H:116:ALA:H	2.22	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
3:H:204:HIS:CD2	3:H:205:VAL:O	2.62	0.52
2:M:12:VAL:HG21	3:H:169:VAL:HG11	1.92	0.52
2:M:72:TRP:CB	2:M:93:LEU:HD13	2.39	0.52
2:M:153:TRP:CH2	2:M:283:LEU:HD12	2.45	0.52
2:M:218:GLY:C	2:M:222:LEU:HD12	2.35	0.52
2:M:293:TYR:CE2	2:M:297:GLN:NE2	2.78	0.52
1:L:44:LEU:HA	1:L:47:ILE:HG21	1.92	0.52
3:H:141:HIS:CE1	3:H:143:SER:HB2	2.45	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:250:TRP:HB3	2:M:254:MET:HG3	1.91	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: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:27:LEU:O	3:H:28:ILE:C	2.53	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:153:VAL:HG12	3:H:161:ALA:HB3	1.92	0.51
3:H:209:SER:C	3:H:213:PHE:HD1	2.17	0.51
1:L:176:ALA:O	1:L:180:PHE:CD1	2.60	0.51
2:M:105(A):ALA:O	2:M:106:PRO:C	2.47	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
3:H:27:LEU:O	3:H:28:ILE:O	2.27	0.51
1:L:43:ALA:C	1:L:45:GLY:N	2.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:HIS:HB2	1:L:229:ILE:HG12	1.92	0.51
1:L:215:PHE:HA	2:M:138:LEU:CD2	2.38	0.51
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:53:ALA:HB2	1:L:64:ILE:CG1	2.40	0.51
1:L:56:GLN:C	1:L:57:GLY:O	2.52	0.51
1:L:97:PHE:CD1	4:L:350:BCL:H121	2.46	0.51
1:L:217:ARG:N	1:L:223:SER:HB2	2.25	0.51
2:M:254:MET:HE1	6:M:750:UQ:H111	1.80	0.51
1:L:41:PHE:CB	1:L:92:CYS:O	2.58	0.51
1:L:127:ALA:CB	4:L:350:BCL:H42	2.41	0.51
1:L:128:TYR:HD1	1:L:128:TYR:O	1.94	0.51
1:L:207:ARG:NH2	2:M:20:MET:HE1	2.25	0.51
2:M:5:ASN:HD21	2:M:225:SER:HB2	1.76	0.51
3:H:22:ILE:HG23	3:H:23:PHE:N	2.24	0.51
3:H:70:ARG:HG2	3:H:70:ARG:NH1	2.26	0.51
2:M:130:ARG:C	2:M:132:TYR:H	2.19	0.51
3:H:148:PRO:O	3:H:149:ILE:HB	2.11	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
2:M:2:GLU:O	2:M:3:TYR:HB2	2.11	0.51
3:H:37:ARG:NH1	3:H:59:PRO:HG2	2.26	0.51
3:H:194:GLN:O	3:H:195:MET:HG2	2.11	0.51
1:L:160:THR:O	1:L:163:THR:HB	2.11	0.51
2:M:72:TRP:CZ3	2:M:75:TYR:CB	2.94	0.51
2:M:81:PRO:O	2:M:82:ALA:C	2.54	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:117:ILE:N	1:L:118:PRO:HD2	2.26	0.50
1:L:183:ASN:ND2	1:L:236:LEU:CG	2.57	0.50
1:L:227:LEU:CD2	1:L:231:ARG:CZ	2.89	0.50
2:M:229:GLY:O	2:M:260:MET:HE3	2.11	0.50
2:M:264:HIS:O	2:M:268:ILE:HG22	2.10	0.50
1:L:17:VAL:HG23	1:L:106:GLU:OE2	2.11	0.50
1:L:158:SER:OG	1:L:162:TYR:CE2	2.62	0.50
1:L:181:PHE:HE1	4:M:400:BCL:HAA1	1.75	0.50
3:H:182:GLU:HG3	3:H:187:SER:C	2.36	0.50
2:M:8:SER:O	2:M:9:GLN:HB2	2.11	0.50
2:M:226:ARG:CB	3:H:195:MET:HE2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:ARG:HH21	3:H:62:LYS:CG	2.22	0.50
3:H:148:PRO:C	3:H:149:ILE:CG1	2.80	0.50
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:61:PRO:HB2	3:H:74:THR:HG21	1.92	0.50
1:L:47:ILE:HG22	1:L:48:LEU:HG	1.93	0.50
1:L:272:TRP:O	1:L:273:ALA:HB3	2.11	0.50
2:M:72:TRP:HB3	2:M:93:LEU:HD22	1.93	0.50
2:M:179:SER:O	2:M:181:LEU:N	2.45	0.50
3:H:242:MET:HG2	3:H:249:LYS:HB3	1.94	0.50
1:L:271:TRP:HB2	1:L:274:ASN:ND2	2.25	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
2:M:244:GLU:O	2:M:247:ALA:HB3	2.12	0.50
2:M:77:ALA:O	2:M:83:VAL:HG11	2.12	0.50
2:M:101:GLY:O	2:M:169:TRP:N	2.40	0.50
3:H:91:ALA:HB3	3:H:96:PHE:CG	2.47	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
1:L:100:TRP:CZ2	1:L:103:ARG:NH2	2.80	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:69:ILE:CG1	2:M:93:LEU:HD12	2.38	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
1:L:20:ASN:C	1:L:22:PHE:N	2.60	0.49
1:L:118:PRO:O	1:L:121:PHE:HB3	2.12	0.49
2:M:8:SER:O	2:M:9:GLN:CB	2.58	0.49
4:M:601:BCL:HAC1	4:M:400:BCL:C3D	2.42	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
3:H:170:ASP:HB2	3:H:175:MET:O	2.11	0.49
1:L:13:GLY:H	1:L:110:LYS:CE	2.21	0.49
1:L:93:ALA:O	1:L:96:ALA:HB3	2.12	0.49
1:L:152:THR:O	1:L:154:LEU:N	2.45	0.49
1:L:181:PHE:CE1	4:M:400:BCL:HAA1	2.47	0.49
1:L:187:LEU:CD2	1:L:187:LEU:C	2.82	0.49
1:L:218:ASP:CB	2:M:50:TYR:CD1	2.95	0.49
4:L:350:BCL:H122	5:L:550:BPH:HBA1	1.93	0.49
2:M:12:VAL:HG11	3:H:169:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:36:MET:HG2	3:H:40:TYR:CE1	2.47	0.49
1:L:228:GLY:C	1:L:232:LEU:HD13	2.38	0.49
4:L:350:BCL:H71	4:L:450:BCL:HBB2	1.93	0.49
3:H:134:MET:SD	3:H:142:VAL:HG22	2.52	0.49
3:H:135:LYS:HZ1	3:H:165:VAL:CG1	2.25	0.49
1:L:234:LEU:O	1:L:238:LEU:HB2	2.12	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:190:LEU:H	3:H:190:LEU:HD23	1.76	0.49
2:M:54:LEU:CD2	2:M:129:GLY:HA3	2.43	0.49
3:H:67:PRO:HB2	3:H:68:HIS:CE1	2.47	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
3:H:188:THR:HG21	3:H:219:ILE:HG22	1.93	0.49
1:L:48:LEU:O	1:L:49:ILE:C	2.55	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
1:L:42:ALA:O	1:L:46:ILE:HG23	2.13	0.49
2:M:67:PHE:C	2:M:69:ILE:N	2.68	0.49
2:M:69:ILE:HD11	2:M:175:TYR:CG	2.48	0.49
3:H:70:ARG:HG2	3:H:70:ARG:O	2.13	0.49
2:M:202:LEU:HD12	2:M:205:ALA:HB3	1.95	0.49
1:L:131:LEU:N	1:L:131:LEU:HD23	2.28	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
2:M:178:PHE:O	2:M:181:LEU:HB2	2.13	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
4:L:450:BCL:HBB2	4:L:450:BCL:HMB1	1.95	0.48
2:M:208:TYR:O	2:M:211:ALA:HB3	2.13	0.48
3:H:1:MET:HG2	3:H:2:VAL:H	1.77	0.48
1:L:5:PHE:HB2	2:M:244:GLU:CD	2.38	0.48
1:L:97:PHE:CE1	4:L:350:BCL:H112	2.48	0.48
2:M:69:ILE:O	2:M:73:PHE:N	2.45	0.48
2:M:69:ILE:C	2:M:93:LEU:HD11	2.38	0.48
2:M:284:LEU:O	2:M:288:VAL:HG22	2.12	0.48
1:L:150:ILE:HG12	5:L:550:BPH:H191	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:LEU:HD12	1:L:85:LEU:CD2	2.44	0.48
1:L:141:ALA:O	1:L:143:GLY:N	2.32	0.48
2:M:4:GLN:OE1	3:H:193:MET:HG3	2.12	0.48
2:M:65:TRP:O	2:M:66:PHE:C	2.57	0.48
2:M:157:VAL:HA	2:M:162:ARG:H	1.77	0.48
3:H:237:VAL:O	3:H:238:ALA:C	2.57	0.48
2:M:113:TRP:CH2	2:M:172:ALA:CB	2.96	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:230:GLU:O	2:M:231:ARG:C	2.55	0.48
3:H:183:LEU:C	3:H:185:ASP:H	2.20	0.48
3:H:208:LEU:CD1	3:H:216:ILE:HD11	2.44	0.48
1:L:61:PRO:O	1:L:150:ILE:HD12	2.14	0.48
1:L:85:LEU:O	1:L:89:ILE:HD12	2.12	0.48
1:L:155:ASP:O	1:L:159:ASN:HB2	2.13	0.48
2:M:83:VAL:HG22	2:M:86:ARG:NH1	2.26	0.48
5:M:500:BPH:H1C2	5:M:500:BPH:HAA2	1.95	0.48
1:L:44:LEU:O	1:L:48:LEU:HD12	2.14	0.48
1:L:105:VAL:HG13	1:L:115:TYR:CZ	2.48	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
1:L:74:GLY:CA	1:L:141:ALA:HB2	2.26	0.48
1:L:86:TRP:CZ3	1:L:142:TRP:HE3	2.32	0.48
1:L:212:GLU:CB	6:L:800:UQ:HM21	2.44	0.48
2:M:61:SER:O	2:M:62:GLY:C	2.57	0.48
2:M:74:TRP:O	2:M:77:ALA:N	2.47	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
3:H:177:ARG:O	3:H:193:MET:CB	2.61	0.48
2:M:188:SER:CB	2:M:194:LEU:HB2	2.43	0.48
3:H:209:SER:C	3:H:211:ASP:N	2.66	0.48
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.13	0.48
1:L:151:TRP:O	2:M:303:PRO:CB	2.58	0.47
2:M:89:PHE:CD2	2:M:177:ILE:HG21	2.49	0.47
2:M:114:LEU:O	2:M:118:PHE:CD2	2.67	0.47
3:H:22:ILE:CG2	3:H:23:PHE:N	2.77	0.47
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
2:M:130:ARG:C	2:M:132:TYR:N	2.71	0.47
2:M:142:LYS:O	2:M:143:HIS:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:LEU:HD11	3:H:32:GLN:CD	2.39	0.47
2:M:13:ARG:CG	2:M:14:GLY:N	2.74	0.47
3:H:96:PHE:HA	3:H:97:PRO:HD2	1.67	0.47
3:H:230:GLU:O	3:H:234:CYS:SG	2.71	0.47
1:L:14:GLY:HA2	1:L:109:ARG:HB2	1.97	0.47
2:M:53:SER:HB3	2:M:54:LEU:HD12	1.97	0.47
2:M:153:TRP:CZ2	2:M:283:LEU:CD1	2.88	0.47
3:H:146:LYS:O	3:H:148:PRO:HD3	2.13	0.47
1:L:37:ALA:O	1:L:40:PHE:HB3	2.10	0.47
2:M:24:VAL:CG1	2:M:26:LEU:HD13	2.41	0.47
2:M:55:GLY:CA	2:M:130:ARG:HH11	2.27	0.47
2:M:247:ALA:HB1	2:M:257:ASN:HD22	1.80	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
1:L:92:CYS:O	1:L:96:ALA:HB2	2.15	0.47
1:L:169:TYR:CE2	1:L:260:VAL:HG13	2.50	0.47
1:L:209:PRO:HA	1:L:212:GLU:OE1	2.15	0.47
2:M:10:VAL:HG13	2:M:11:GLN:N	2.29	0.47
2:M:193:ASN:C	2:M:195:PHE:N	2.70	0.47
2:M:282:ILE:C	2:M:284:LEU:N	2.72	0.47
3:H:33:THR:C	3:H:35:ASN:H	2.21	0.47
3:H:99:ALA:HB1	3:H:100:PRO:HD2	1.97	0.47
3:H:117:ARG:HG2	3:H:227:LEU:HB3	1.95	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
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.97	0.47
1:L:80:LEU:C	1:L:82:LYS:N	2.72	0.47
1:L:193:LEU:HD21	1:L:215:PHE:HE2	1.77	0.47
1:L:206:MET:CE	2:M:237:ALA:HB2	2.29	0.47
2:M:135:ALA:HA	2:M:138:LEU:HD11	1.97	0.47
2:M:234:GLU:OE2	3:H:123:LEU:CD1	2.62	0.47
2:M:254:MET:HB3	6:M:750:UQ:H203	1.95	0.47
2:M:293:TYR:OH	2:M:297:GLN:NE2	2.46	0.47
3:H:171:ILE:HB	3:H:172:PRO:CD	2.43	0.47
1:L:261:ASP:O	1:L:262:TRP:C	2.56	0.47
2:M:2:GLU:CG	2:M:3:TYR:H	2.28	0.47
2:M:227:PHE:HD2	3:H:234:CYS:HB3	1.78	0.47
3:H:195:MET:HE1	3:H:238:ALA:CB	2.36	0.47
3:H:237:VAL:C	3:H:239:GLY:N	2.71	0.47
1:L:58:THR:CG2	1:L:59:TRP:N	2.53	0.47
1:L:97:PHE:CE1	4:L:350:BCL:H121	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:152:THR:C	1:L:154:LEU:N	2.67	0.47
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.79	0.47
3:H:170:ASP:N	3:H:175:MET:O	2.43	0.47
2:M:169:TRP:O	2:M:171:GLU:O	2.33	0.46
3:H:40:TYR:HA	3:H:41:PRO:O	2.15	0.46
1:L:167:PHE:O	1:L:170:ASN:N	2.48	0.46
3:H:62:LYS:N	3:H:74:THR:HG22	2.30	0.46
2:M:68:THR:HG23	2:M:112:LEU:CD1	2.39	0.46
3:H:24:LEU:C	3:H:26:GLY:N	2.66	0.46
3:H:154:ARG:NH1	3:H:158:LEU:CD1	2.78	0.46
1:L:141:ALA:H	1:L:144:TYR:HE1	1.64	0.46
1:L:231:ARG:CZ	2:M:6:ILE:H	2.24	0.46
1:L:235:LEU:O	1:L:236:LEU:C	2.59	0.46
2:M:219:ALA:C	2:M:221:ILE:H	2.23	0.46
2:M:265:ARG:O	2:M:268:ILE:HG23	2.15	0.46
2:M:269:TRP:CE3	2:M:269:TRP:HA	2.49	0.46
3:H:5:THR:CG2	3:H:10:PHE:H	2.23	0.46
1:L:84:GLY:O	1:L:87:GLN:HB2	2.16	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:215:PHE:HD1	2:M:138:LEU:CD2	2.27	0.46
3:H:170:ASP:OD2	3:H:173:GLU:CB	2.55	0.46
1:L:49:ILE:HG22	1:L:50:ALA:N	2.31	0.46
4:L:450:BCL:HBA1	4:L:450:BCL:H3A	1.73	0.46
2:M:65:TRP:CD2	2:M:66:PHE:N	2.83	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
1:L:117:ILE:HG21	2:M:250:TRP:CH2	2.50	0.46
1:L:177:ILE:HD12	4:M:601:BCL:CMD	2.46	0.46
1:L:226:THR:O	1:L:229:ILE:HG22	2.16	0.46
2:M:32:GLY:N	2:M:33:PRO:CD	2.78	0.46
2:M:191:HIS:HA	2:M:290:ASP:O	2.16	0.46
2:M:204:ILE:HG12	4:M:400:BCL:C2B	2.46	0.46
6:M:750:UQ:HM23	6:M:750:UQ:O3	2.16	0.46
3:H:27:LEU:HD23	3:H:28:ILE:H	1.81	0.46
3:H:105:MET:HE1	3:H:212:LEU:HD13	1.98	0.46
1:L:166:ASN:C	1:L:168:HIS:N	2.73	0.46
1:L:181:PHE:HZ	4:M:400:BCL:HAA2	1.80	0.46
2:M:14:GLY:HA3	2:M:15:PRO:HD2	1.72	0.46
2:M:104:PHE:CD2	2:M:114:LEU:HD21	2.50	0.46
2:M:162:ARG:CB	2:M:163:PRO:CD	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:GLY:O	1:L:75:LEU:CB	2.64	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
2:M:224:VAL:HG11	2:M:242:ALA:O	2.15	0.46
3:H:111:PRO:CD	3:H:243:TYR:CE2	2.90	0.46
3:H:164:VAL:O	3:H:165:VAL:HG22	2.10	0.46
1:L:100:TRP:CH2	1:L:103:ARG:NH2	2.84	0.46
2:M:224:VAL:C	2:M:226:ARG:N	2.74	0.46
3:H:7:PHE:HB3	3:H:8:GLY:H	1.61	0.46
3:H:67:PRO:CG	3:H:123:LEU:CD2	2.89	0.46
3:H:80:SER:OG	3:H:81:GLU:N	2.45	0.46
2:M:148:PHE:CD1	5:M:500:BPH:C4D	2.99	0.45
2:M:221:ILE:HD11	6:M:750:UQ:HM31	1.98	0.45
2:M:241:THR:HB	3:H:115:VAL:HG23	1.98	0.45
2:M:267:ALA:O	2:M:268:ILE:C	2.58	0.45
3:H:118:ARG:HG3	3:H:227:LEU:HD12	1.98	0.45
1:L:44:LEU:HA	1:L:47:ILE:CB	2.45	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
2:M:24:VAL:HG12	2:M:26:LEU:N	2.10	0.45
2:M:170:SER:C	2:M:171:GLU:O	2.58	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
3:H:182:GLU:C	3:H:184:LYS:H	2.24	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:79:GLU:O	3:H:80:SER:HB3	2.16	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
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:27:LEU:HD21	3:H:32:GLN:HE21	1.82	0.45
3:H:188:THR:O	3:H:189:ARG:CD	2.64	0.45
2:M:25:ASN:O	2:M:26:LEU:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:111:PRO:CG	3:H:242:MET:SD	3.01	0.45
3:H:177:ARG:O	3:H:193:MET:HB3	2.16	0.45
1:L:86:TRP:O	1:L:90:THR:CG2	2.64	0.45
1:L:175:ILE:C	1:L:177:ILE:N	2.74	0.45
1:L:190:HIS:HE1	2:M:232:GLU:OE2	2.00	0.45
2:M:212:LEU:HD21	6:M:750:UQ:C16	2.45	0.45
3:H:200:SER:O	3:H:201:ASN:HB3	2.17	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
2:M:67:PHE:O	2:M:69:ILE:N	2.50	0.45
2:M:227:PHE:CE2	3:H:235:GLY:HA2	2.33	0.45
4:M:601:BCL:H2A	4:M:601:BCL:O2D	2.17	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
3:H:103:ASP:O	3:H:107:ASP:N	2.48	0.45
1:L:53:ALA:HB2	1:L:64:ILE:HG13	1.97	0.45
1:L:193:LEU:HD11	1:L:216:PHE:HE1	1.66	0.45
1:L:209:PRO:C	1:L:211:HIS:N	2.73	0.45
1:L:240:ALA:O	1:L:244:SER:HB2	2.17	0.45
2:M:225:SER:HA	2:M:229:GLY:H	1.82	0.45
3:H:212:LEU:C	3:H:214:ALA:H	2.25	0.45
1:L:54:VAL:O	1:L:55:LEU:C	2.60	0.45
1:L:216:PHE:O	1:L:219:LEU:HB2	2.17	0.45
2:M:12:VAL:HG21	3:H:169:VAL:CG1	2.46	0.45
2:M:118:PHE:O	2:M:121:PHE:HB3	2.17	0.45
2:M:282:ILE:CG1	4:M:400:BCL:HED1	2.46	0.45
3:H:105:MET:CE	3:H:212:LEU:HD13	2.47	0.45
3:H:130:LYS:HE3	3:H:172:PRO:HG2	1.99	0.45
3:H:134:MET:SD	3:H:142:VAL:CG2	3.04	0.45
1:L:26:VAL:HG13	1:L:26:VAL:O	2.17	0.45
1:L:58:THR:HG21	1:L:63:LEU:HD11	1.99	0.45
1:L:168:HIS:NE2	4:M:601:BCL:HMD3	2.32	0.45
1:L:262:TRP:C	1:L:264:GLN:H	2.25	0.45
1:L:275:ILE:N	1:L:276:PRO:CD	2.80	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
2:M:156:MET:O	2:M:157:VAL:C	2.60	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:261:ASP:O	1:L:264:GLN:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:149:ILE:H	3:H:164:VAL:CG1	2.29	0.44
3:H:212:LEU:C	3:H:214:ALA:N	2.72	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
1:L:106:GLU:O	1:L:109:ARG:HB2	2.17	0.44
2:M:87:ASP:HB2	2:M:91:PHE:CD2	2.52	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
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.99	0.44
1:L:86:TRP:HZ3	1:L:142:TRP:HE3	1.64	0.44
1:L:107:ILE:O	1:L:111:LEU:HD12	2.18	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
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
2:M:88:LEU:HG	2:M:89:PHE:N	2.31	0.44
2:M:282:ILE:C	2:M:284:LEU:H	2.24	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:81:PRO:O	2:M:85:LEU:HD12	2.18	0.44
2:M:251:ARG:HB2	2:M:257:ASN:HB3	2.00	0.44
3:H:209:SER:C	3:H:213:PHE:CD1	2.95	0.44
1:L:117:ILE:CG2	2:M:250:TRP:CH2	3.00	0.44
1:L:168:HIS:NE2	4:M:601:BCL:CMD	2.81	0.44
2:M:13:ARG:O	3:H:140:PHE:CD2	2.71	0.44
2:M:35:SER:HB3	2:M:38:LEU:CD2	2.48	0.44
2:M:121:PHE:O	2:M:125:TRP:HD1	2.01	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
2:M:152:ILE:O	2:M:156:MET:N	2.46	0.44
2:M:292:TRP:O	2:M:293:TYR:C	2.60	0.44
4:M:400:BCL:CBB	4:M:400:BCL:CMB	2.95	0.44
1:L:149:GLY:HA3	1:L:152:THR:HG23	1.93	0.44
2:M:16:ALA:CB	2:M:45:GLN:HE22	2.15	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
3:H:103:ASP:CB	3:H:106:LYS:HB3	2.48	0.44
1:L:100:TRP:O	1:L:103:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:LEU:HD13	5:M:500:BPH:HED1	2.00	0.43
1:L:224:ILE:HG22	6:L:800:UQ:H103	1.99	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
2:M:121:PHE:O	2:M:125:TRP:HB2	2.18	0.43
2:M:121:PHE:CE1	2:M:156:MET:HE2	2.53	0.43
2:M:134:ARG:HA	2:M:134:ARG:HD3	1.36	0.43
2:M:158:LEU:HG	2:M:183:TRP:HH2	1.83	0.43
3:H:28:ILE:CG2	3:H:29:TYR:N	2.64	0.43
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
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
3:H:103:ASP:HB3	3:H:106:LYS:CB	2.48	0.43
3:H:157:ASP:CG	3:H:209:SER:OG	2.61	0.43
3:H:239:GLY:O	3:H:243:TYR:HB2	2.17	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:64:MET:SD	2:M:119:PHE:CE1	3.11	0.43
2:M:162:ARG:NH2	2:M:187:PHE:CD1	2.86	0.43
2:M:244:GLU:O	2:M:245:ARG:C	2.60	0.43
1:L:174:MET:CE	4:M:601:BCL:HED2	2.38	0.43
2:M:35:SER:CB	2:M:38:LEU:HB3	2.43	0.43
2:M:77:ALA:C	2:M:79:TRP:H	2.26	0.43
2:M:234:GLU:HG2	3:H:123:LEU:HD12	1.99	0.43
3:H:118:ARG:CG	3:H:227:LEU:HD12	2.48	0.43
3:H:181:VAL:CB	3:H:189:ARG:O	2.67	0.43
1:L:130:THR:CB	1:L:249:ILE:HD11	2.40	0.43
1:L:215:PHE:CB	2:M:138:LEU:HD22	2.48	0.43
2:M:108:LYS:O	2:M:109:GLU:HB3	2.16	0.43
2:M:195:PHE:CE2	4:M:400:BCL:CMC	3.01	0.43
2:M:282:ILE:O	2:M:284:LEU:N	2.52	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: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:H6C1	5:L:550:BPH:H2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:PRO:HA	1:L:64:ILE:CG2	2.48	0.43
1:L:113:ILE:HG21	2:M:224:VAL:HG22	1.99	0.43
2:M:216:MET:O	2:M:220:THR:HG23	2.19	0.43
3:H:179:LEU:O	3:H:190:LEU:HA	2.18	0.43
1:L:14:GLY:HA2	1:L:109:ARG:CB	2.49	0.43
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
2:M:294:VAL:C	2:M:298:ASN:HB2	2.37	0.43
1:L:13:GLY:CA	3:H:242:MET:CE	2.96	0.43
1:L:41:PHE:HD2	1:L:92:CYS:CA	2.30	0.43
1:L:166:ASN:O	1:L:168:HIS:N	2.51	0.43
1:L:185:LEU:CB	5:M:500:BPH:HMC2	2.48	0.43
1:L:230:HIS:NE2	2:M:217:HIS:CD2	2.86	0.43
1:L:235:LEU:O	1:L:238:LEU:N	2.51	0.43
2:M:62:GLY:O	2:M:65:TRP:HB3	2.19	0.43
2:M:127:TRP:CD1	5:M:500:BPH:HAA1	2.54	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
3:H:39:GLY:O	3:H:40:TYR:CD1	2.71	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
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
2:M:285:SER:HB2	2:M:292:TRP:HE1	1.83	0.43
6:M:750:UQ:H201	6:M:750:UQ:H222	1.64	0.43
3:H:130:LYS:O	3:H:171:ILE:HB	2.18	0.43
3:H:160:ILE:O	3:H:161:ALA:C	2.62	0.43
2:M:238:ASP:CG	3:H:118:ARG:HD2	2.44	0.42
3:H:20:PHE:CD2	3:H:21:TRP:CD1	3.07	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
1:L:123:PHE:CZ	1:L:242:PHE:HD2	2.37	0.42
2:M:24:VAL:HG11	2:M:26:LEU:CD1	2.44	0.42
2:M:243:ALA:O	6:M:750:UQ:CM2	2.67	0.42
3:H:60:LYS:H	3:H:60:LYS:HG2	1.63	0.42
3:H:95:GLY:O	3:H:96:PHE:C	2.62	0.42
3:H:135:LYS:HZ1	3:H:165:VAL:HG12	1.82	0.42
3:H:148:PRO:C	3:H:150:GLY:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:125:ILE:HD13	1:L:125:ILE:HG21	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:29(A):SER:HB2	2:M:49:ILE:O	2.19	0.42
2:M:121:PHE:HE1	2:M:156:MET:HE2	1.84	0.42
2:M:199:PHE:HB3	2:M:277:THR:HG22	2.01	0.42
4:M:601:BCL:HBD	4:M:601:BCL:CAA	2.49	0.42
3:H:62:LYS:C	3:H:74:THR:HG22	2.44	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
1:L:185:LEU:HD12	5:M:500:BPH:NC	2.35	0.42
1:L:251:THR:CG2	1:L:259:TRP:HE1	2.32	0.42
2:M:4:GLN:HG3	3:H:194:GLN:HA	2.00	0.42
2:M:66:PHE:O	2:M:69:ILE:HB	2.19	0.42
3:H:226:THR:O	3:H:227:LEU:C	2.62	0.42
1:L:60:ASN:C	1:L:62:GLN:N	2.73	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
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:212:LEU:CD2	6:M:750:UQ:C16	2.97	0.42
1:L:211:HIS:O	1:L:215:PHE:CB	2.68	0.42
1:L:232:LEU:HD12	2:M:41:PHE:CE2	2.55	0.42
1:L:240:ALA:O	1:L:244:SER:CB	2.68	0.42
2:M:72:TRP:CD1	2:M:112:LEU:CB	3.01	0.42
2:M:115:ILE:CG2	2:M:119:PHE:CE2	2.92	0.42
2:M:263:ILE:HG21	6:M:750:UQ:HM33	2.00	0.42
3:H:31:LEU:C	3:H:33:THR:N	2.78	0.42
3:H:134:MET:HE3	3:H:169:VAL:CG1	2.50	0.42
1:L:43:ALA:O	1:L:47:ILE:N	2.52	0.42
1:L:88:ILE:HD13	1:L:88:ILE:HA	1.88	0.42
2:M:241:THR:HG22	3:H:231:ASP:OD1	2.20	0.42
3:H:75:VAL:C	3:H:77:GLY:N	2.77	0.42
3:H:104:PRO:CB	3:H:243:TYR:CD1	3.03	0.42
1:L:194:VAL:C	1:L:196:SER:N	2.78	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
2:M:67:PHE:C	2:M:69:ILE:H	2.28	0.42
5:M:500:BPH:H9C1	5:M:500:BPH:H112	1.69	0.42
3:H:120:LEU:C	3:H:226:THR:HG22	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:PHE:CE1	4:M:400:BCL:O1A	2.73	0.41
1:L:195:LEU:CD1	2:M:265:ARG:HG3	2.34	0.41
1:L:201:GLU:HB2	1:L:204:LYS:HB2	2.02	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
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
3:H:104:PRO:CB	3:H:243:TYR:CE1	3.00	0.41
1:L:111:LEU:CB	1:L:113:ILE:HG12	2.42	0.41
1:L:275:ILE:O	1:L:276:PRO:C	2.62	0.41
2:M:150:SER:OG	2:M:276:LEU:HD23	2.20	0.41
3:H:31:LEU:HD12	3:H:31:LEU:HA	1.90	0.41
3:H:32:GLN:O	3:H:32:GLN:HG3	2.20	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
1:L:275:ILE:O	1:L:275:ILE:CG2	2.56	0.41
2:M:65:TRP:CG	2:M:66:PHE:N	2.88	0.41
3:H:110:GLY:C	3:H:112:ALA:N	2.78	0.41
3:H:216:ILE:CG2	3:H:217:PRO:HD2	2.48	0.41
1:L:16:LEU:HD11	1:L:105:VAL:CG1	2.50	0.41
1:L:53:ALA:CB	1:L:64:ILE:CD1	2.90	0.41
1:L:185:LEU:HA	5:M:500:BPH:CMC	2.50	0.41
1:L:193:LEU:HD22	6:L:800:UQ:HM23	2.03	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
2:M:149:LEU:HD12	2:M:149:LEU:HA	1.84	0.41
2:M:250:TRP:CD1	6:M:750:UQ:CM5	3.01	0.41
4:M:601:BCL:CMA	4:M:400:BCL:H202	2.51	0.41
3:H:36:MET:HA	3:H:40:TYR:CD1	2.56	0.41
3:H:183:LEU:HD11	3:H:213:PHE:O	2.20	0.41
1:L:104:GLU:HG2	2:M:249:PHE:CZ	2.54	0.41
1:L:183:ASN:HB2	1:L:236:LEU:HB3	2.01	0.41
2:M:102:LEU:HD12	2:M:102:LEU:C	2.45	0.41
2:M:251:ARG:NH1	2:M:251:ARG:CG	2.81	0.41
3:H:33:THR:C	3:H:35:ASN:N	2.78	0.41
3:H:93:SER:HB3	3:H:96:PHE:HD2	1.84	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:6:ILE:HD13	2:M:6:ILE:HA	1.94	0.41
2:M:231:ARG:NH1	3:H:122:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:288:VAL:HB	3:H:4:VAL:CG1	2.45	0.41
3:H:2:VAL:O	3:H:2:VAL:CG1	2.68	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
1:L:51:TRP:C	1:L:53:ALA:H	2.28	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
1:L:229:ILE:CD1	6:L:800:UQ:CM5	2.90	0.41
1:L:232:LEU:O	1:L:233:GLY:C	2.63	0.41
4:L:350:BCL:H93	4:L:350:BCL:H62	1.76	0.41
2:M:74:TRP:CD1	2:M:79:TRP:CD1	3.08	0.41
2:M:183:TRP:O	2:M:184:THR:C	2.64	0.41
3:H:17:ILE:CG2	3:H:21:TRP:CD1	2.95	0.41
3:H:115:VAL:HG12	3:H:116:ALA:N	2.34	0.41
3:H:164:VAL:C	3:H:165:VAL:CG2	2.69	0.41
3:H:206:ASN:HD22	3:H:206:ASN:HA	1.71	0.41
1:L:80:LEU:O	1:L:83:GLY:N	2.54	0.41
1:L:129:LEU:HB3	1:L:134:PHE:CE2	2.56	0.41
1:L:177:ILE:HD13	4:L:350:BCL:HMB1	2.02	0.41
2:M:21:THR:CG2	2:M:50:TYR:OH	2.67	0.41
2:M:158:LEU:CG	2:M:183:TRP:HH2	2.34	0.41
3:H:209:SER:O	3:H:213:PHE:CD1	2.72	0.41
1:L:16:LEU:HD11	1:L:105:VAL:HG12	2.03	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
1:L:151:TRP:C	2:M:303:PRO:HB3	2.45	0.41
1:L:234:LEU:HD13	2:M:222:LEU:CD1	2.50	0.41
5:L:550:BPH:H152	5:L:550:BPH:H203	2.02	0.41
2:M:65:TRP:CE3	2:M:66:PHE:N	2.89	0.41
2:M:105(A):ALA:HB1	2:M:109:GLU:OE1	2.21	0.41
2:M:162:ARG:O	2:M:164:ILE:N	2.54	0.41
3:H:167:ILE:CG2	3:H:179:LEU:HD12	2.46	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:43:ASN:HD22	2:M:43:ASN:HA	1.68	0.41
2:M:216:MET:O	2:M:219:ALA:HB3	2.21	0.41
3:H:63:THR:N	3:H:74:THR:HG23	2.35	0.41
3:H:156:CYS:O	3:H:157:ASP:O	2.38	0.41
1:L:43:ALA:C	1:L:45:GLY:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:113:ILE:CG2	2:M:224:VAL:HG22	2.50	0.40
1:L:222:TYR:HD2	2:M:46:LEU:HD21	1.86	0.40
2:M:80:ASN:HB3	2:M:81:PRO:CD	2.44	0.40
2:M:202:LEU:HA	2:M:205:ALA:HB3	2.04	0.40
2:M:230:GLU:C	2:M:232:GLU:N	2.79	0.40
2:M:243:ALA:O	6:M:750:UQ:HM22	2.21	0.40
3:H:12:LEU:HD13	3:H:12:LEU:HA	1.86	0.40
1:L:44:LEU:C	1:L:47:ILE:HB	2.47	0.40
1:L:115:TYR:C	1:L:118:PRO:HD2	2.47	0.40
4:L:450:BCL:HMD1	2:M:195:PHE:CE1	2.57	0.40
4:L:450:BCL:OBD	4:L:450:BCL:O2D	2.39	0.40
2:M:88:LEU:HD12	2:M:88:LEU:C	2.46	0.40
4:M:601:BCL:HMA1	4:M:400:BCL:H202	2.02	0.40
3:H:105:MET:HE1	3:H:208:LEU:HD22	2.01	0.40
2:M:131:THR:HG21	5:M:500:BPH:OBD	2.21	0.40
2:M:217:HIS:ND1	2:M:263:ILE:HG12	2.34	0.40
3:H:66:LEU:CB	3:H:67:PRO:CD	2.99	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
1:L:93:ALA:HB1	1:L:97:PHE:HE2	1.87	0.40
1:L:168:HIS:CE1	4:L:350:BCL:HMC2	2.56	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:2:VAL:C	3:H:4:VAL:N	2.79	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:96:PRO:HG2	2:M:170:SER:CB	2.40	0.40
2:M:121:PHE:O	2:M:125:TRP:CD1	2.74	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	216/220 (98%)	170 (79%)	46 (21%)	1	5
2	M	238/240 (99%)	179 (75%)	59 (25%)	1	2
3	H	203/208 (98%)	151 (74%)	52 (26%)	0	2
All	All	657/668 (98%)	500 (76%)	157 (24%)	1	3

All (157) 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	36	VAL
1	L	38	THR
1	L	40	PHE
1	L	46	ILE

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Mol	Chain	Res	Type
1	L	47	ILE
1	L	54	VAL
1	L	55	LEU
1	L	56	GLN
1	L	60	ASN
1	L	63	LEU
1	L	64	ILE
1	L	88	ILE
1	L	91	ILE
1	L	99	SER
1	L	102	LEU
1	L	110	LYS
1	L	113	ILE
1	L	123	PHE
1	L	131	LEU
1	L	133	LEU
1	L	138	MET
1	L	146	PHE
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	224	ILE
1	L	226	THR
1	L	234	LEU
1	L	248	MET
1	L	250	ILE
1	L	253	THR
1	L	254	ILE
1	L	261	ASP
1	L	269	LEU
1	L	274	ASN
2	M	2	GLU
2	M	10	VAL
2	M	11	GLN

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Mol	Chain	Res	Type
2	M	17	ASP
2	M	22	GLU
2	M	23	ASP
2	M	24	VAL
2	M	25	ASN
2	M	26	LEU
2	M	31	VAL
2	M	36	THR
2	M	37	LEU
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
2	M	126	SER
2	M	134	ARG
2	M	138	LEU
2	M	142	LYS
2	M	144	THR
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	232	GLU
2	M	233	LEU
2	M	234	GLU
2	M	236	ILE
2	M	238	ASP

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Mol	Chain	Res	Type
2	M	241	THR
2	M	248	LEU
2	M	251	ARG
2	M	254	MET
2	M	257	ASN
2	M	260	MET
2	M	263	ILE
2	M	268	ILE
2	M	270	MET
2	M	276	LEU
2	M	287	THR
2	M	289	VAL
2	M	295	TRP
2	M	297	GLN
3	H	2	VAL
3	H	9	ASN
3	H	11	ASP
3	H	12	LEU
3	H	14	SER
3	H	15	LEU
3	H	22	ILE
3	H	27	LEU
3	H	32	GLN
3	H	33	THR
3	H	45	GLU
3	H	48	THR
3	H	52	ASN
3	H	58	LEU
3	H	68	HIS
3	H	73	LEU
3	H	74	THR
3	H	79	GLU
3	H	82	ASP
3	H	85	ILE
3	H	89	ARG
3	H	92	VAL
3	H	109	VAL
3	H	122	GLU
3	H	131	ILE
3	H	147	ASN
3	H	149	ILE
3	H	151	LEU

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Mol	Chain	Res	Type
3	H	158	LEU
3	H	159	GLU
3	H	160	ILE
3	H	164	VAL
3	H	167	ILE
3	H	171	ILE
3	H	179	LEU
3	H	183	LEU
3	H	188	THR
3	H	189	ARG
3	H	194	GLN
3	H	200	SER
3	H	203	VAL
3	H	206	ASN
3	H	210	SER
3	H	211	ASP
3	H	221	SER
3	H	223	THR
3	H	225	VAL
3	H	229	GLU
3	H	237	VAL
3	H	241	LEU
3	H	251	VAL
3	H	252	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	62	GLN
1	L	173	HIS
1	L	183	ASN
1	L	211	HIS
1	L	274	ASN
2	M	5	ASN
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

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Mol	Chain	Res	Type
2	M	257	ASN
2	M	297	GLN
3	H	9	ASN
3	H	68	HIS
3	H	129	ASN
3	H	141	HIS
3	H	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	BCL	M	400	2	69,74,74	1.65	12 (17%)	79,115,115	1.63	13 (16%)
6	UQ	M	750	-	48,48,63	2.31	11 (22%)	60,61,79	1.92	18 (30%)
4	BCL	M	601	2	69,74,74	1.35	11 (15%)	79,115,115	1.63	10 (12%)
4	BCL	L	350	-	69,74,74	1.53	11 (15%)	79,115,115	1.79	13 (16%)
4	BCL	L	450	1	69,74,74	1.31	12 (17%)	79,115,115	1.40	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	UQ	L	800	-	48,48,63	2.41	15 (31%)	60,61,79	2.38	25 (41%)
5	BPH	M	500	-	59,70,70	2.04	13 (22%)	59,101,101	1.75	12 (20%)
5	BPH	L	550	-	59,70,70	2.06	11 (18%)	59,101,101	1.80	14 (23%)

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
4	BCL	M	400	2	-	24/41/137/137	-
6	UQ	M	750	-	-	19/45/69/87	0/1/1/1
4	BCL	M	601	2	-	20/41/137/137	-
4	BCL	L	350	-	-	20/41/137/137	-
4	BCL	L	450	1	-	14/41/137/137	-
6	UQ	L	800	-	-	14/45/69/87	0/1/1/1
5	BPH	M	500	-	-	15/37/105/105	0/5/6/6
5	BPH	L	550	-	-	13/37/105/105	0/5/6/6

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	750	UQ	C12-C13	11.08	1.84	1.50
5	L	550	BPH	C2C-C3C	-10.60	1.45	1.54
5	M	500	BPH	C2C-C3C	-9.91	1.46	1.54
6	L	800	UQ	C16-C17	-8.98	1.24	1.53
4	M	400	BCL	MG-NA	8.79	2.27	2.06
6	L	800	UQ	C7-C8	6.33	1.60	1.50
5	L	550	BPH	C1B-C2B	6.19	1.46	1.39
5	M	500	BPH	C1B-C2B	5.20	1.45	1.39
4	L	350	BCL	MG-NC	5.00	2.18	2.06
6	M	750	UQ	C7-C8	4.48	1.57	1.50
6	L	800	UQ	C26-C24	4.15	1.59	1.51
4	L	350	BCL	MG-NA	4.08	2.16	2.06
6	L	800	UQ	C31-C29	3.89	1.59	1.51
4	L	350	BCL	C3C-C4C	-3.89	1.46	1.51
4	M	400	BCL	C3C-C4C	-3.88	1.46	1.51
6	L	800	UQ	C35-C34	3.85	1.60	1.50
5	M	500	BPH	C3B-C4B	3.57	1.47	1.41
4	L	350	BCL	C3B-C4B	3.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	601	BCL	MG-ND	-3.44	1.99	2.05
4	L	450	BCL	C3C-C4C	-3.44	1.47	1.51
4	L	350	BCL	C1D-ND	3.43	1.42	1.37
5	M	500	BPH	C1A-C2A	-3.41	1.46	1.51
5	M	500	BPH	C4D-ND	-3.34	1.33	1.38
4	L	450	BCL	C2C-C3C	-3.34	1.45	1.54
4	L	350	BCL	MG-ND	-3.32	1.99	2.05
4	M	400	BCL	C2C-C3C	-3.25	1.45	1.54
4	M	601	BCL	C3C-C4C	-3.24	1.47	1.51
6	L	800	UQ	C11-C9	3.23	1.58	1.51
6	L	800	UQ	C16-C14	3.21	1.57	1.51
4	M	601	BCL	C2C-C3C	-3.20	1.45	1.54
4	M	400	BCL	C3B-C4B	3.18	1.47	1.41
4	M	601	BCL	MG-NC	3.16	2.13	2.06
6	L	800	UQ	C36-C34	3.15	1.57	1.51
4	L	350	BCL	C2C-C3C	-3.11	1.46	1.54
5	L	550	BPH	C1C-C2C	-3.10	1.45	1.51
5	L	550	BPH	C1A-C2A	-3.06	1.46	1.51
5	L	550	BPH	C4C-C3C	-3.03	1.46	1.51
4	L	450	BCL	C1D-ND	3.01	1.41	1.37
6	M	750	UQ	C11-C9	3.00	1.57	1.51
6	L	800	UQ	C18-C19	-2.96	1.26	1.33
5	M	500	BPH	C1C-C2C	-2.95	1.46	1.51
4	M	601	BCL	CBB-CAB	2.89	1.55	1.50
5	M	500	BPH	C4A-C3A	-2.89	1.46	1.51
4	M	400	BCL	CBB-CAB	2.88	1.55	1.50
6	M	750	UQ	C16-C14	2.86	1.57	1.51
5	L	550	BPH	CHA-CBD	2.86	1.55	1.51
5	L	550	BPH	C4A-C3A	-2.82	1.46	1.51
5	M	500	BPH	C1D-C2D	2.80	1.42	1.39
5	M	500	BPH	C4C-C3C	-2.74	1.46	1.51
5	M	500	BPH	C3B-C2B	-2.72	1.35	1.39
6	M	750	UQ	C27-C28	2.67	1.58	1.50
4	L	450	BCL	C3B-C2B	-2.67	1.33	1.42
5	L	550	BPH	C3B-C4B	2.66	1.45	1.41
6	L	800	UQ	C40-C39	2.63	1.57	1.50
6	M	750	UQ	C31-C29	2.62	1.56	1.51
4	L	450	BCL	CBB-CAB	2.61	1.55	1.50
5	M	500	BPH	C3D-C4D	-2.61	1.37	1.41
6	M	750	UQ	C30-C29	2.61	1.57	1.50
4	M	601	BCL	MG-NA	2.59	2.12	2.06
4	L	350	BCL	CBB-CAB	2.57	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	750	UQ	C35-C34	2.54	1.56	1.50
5	M	500	BPH	C3D-CAD	-2.53	1.42	1.47
5	L	550	BPH	C3B-C2B	-2.52	1.35	1.39
4	L	350	BCL	CHC-C1C	2.47	1.43	1.37
4	M	601	BCL	CHD-C1D	2.46	1.43	1.38
4	M	400	BCL	MG-ND	-2.45	2.00	2.05
4	M	601	BCL	C2A-C1A	-2.43	1.46	1.52
4	L	450	BCL	C2A-C1A	-2.42	1.46	1.52
4	M	400	BCL	C2A-C1A	-2.42	1.46	1.52
4	M	601	BCL	C3B-C4B	2.40	1.45	1.41
5	L	550	BPH	C3D-CAD	-2.39	1.43	1.47
6	L	800	UQ	O3-C3	-2.39	1.31	1.36
6	M	750	UQ	C7-C6	2.38	1.55	1.51
4	L	350	BCL	C3B-C2B	-2.38	1.34	1.42
4	M	601	BCL	C3B-C2B	-2.36	1.34	1.42
6	L	800	UQ	C22-C23	2.36	1.57	1.50
4	M	400	BCL	CHC-C1C	2.34	1.43	1.37
4	L	450	BCL	MG-ND	-2.32	2.01	2.05
4	L	450	BCL	C3B-C4B	2.32	1.45	1.41
4	L	450	BCL	MG-NC	2.30	2.11	2.06
6	L	800	UQ	C33-C34	2.21	1.38	1.33
4	M	400	BCL	C1D-ND	2.19	1.40	1.37
6	L	800	UQ	C32-C33	2.18	1.57	1.50
6	L	800	UQ	C21-C19	2.18	1.55	1.51
4	M	601	BCL	C1D-ND	2.17	1.40	1.37
4	M	400	BCL	C1-C2	2.13	1.55	1.49
4	M	400	BCL	C3B-C2B	-2.13	1.35	1.42
4	L	450	BCL	CHD-C1D	2.13	1.42	1.38
5	M	500	BPH	CBB-CAB	2.12	1.55	1.49
6	M	750	UQ	C18-C19	-2.12	1.28	1.33
4	L	450	BCL	CHB-C1B	-2.10	1.34	1.39
4	L	350	BCL	C2A-C1A	-2.09	1.47	1.52
4	M	400	BCL	C1D-C2D	-2.08	1.41	1.45
4	L	450	BCL	C2C-C1C	-2.08	1.45	1.51
6	M	750	UQ	C37-C38	2.07	1.56	1.50
5	L	550	BPH	C1D-C2D	2.01	1.41	1.39

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	400	BCL	C4A-NA-C1A	7.89	110.28	106.68
5	L	550	BPH	C4D-CHA-CBD	-7.22	104.99	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	350	BCL	C4A-NA-C1A	7.01	109.88	106.68
4	L	350	BCL	C4D-CHA-C1A	6.98	129.57	121.24
4	M	601	BCL	C4A-NA-C1A	6.46	109.63	106.68
4	M	601	BCL	C4D-CHA-C1A	5.93	128.32	121.24
6	L	800	UQ	C8-C7-C6	5.77	126.29	112.08
5	M	500	BPH	C4D-CHA-CBD	-5.75	105.70	108.45
6	L	800	UQ	C20-C19-C21	5.28	124.39	115.23
6	L	800	UQ	C10-C9-C11	5.05	123.99	115.23
6	M	750	UQ	C12-C13-C14	-4.80	116.63	127.62
6	M	750	UQ	C7-C8-C9	4.80	135.09	126.83
6	L	800	UQ	C30-C29-C28	-4.52	112.01	123.63
6	L	800	UQ	C37-C38-C39	-4.35	113.13	127.64
6	M	750	UQ	C11-C9-C8	4.34	130.91	121.17
5	M	500	BPH	C3D-C4D-ND	4.23	113.13	107.71
4	L	350	BCL	C1-C2-C3	-4.19	119.33	126.20
4	M	601	BCL	C1-C2-C3	-4.18	119.35	126.20
4	L	450	BCL	C4A-NA-C1A	4.01	108.51	106.68
6	L	800	UQ	C25-C24-C23	-4.01	113.34	123.63
6	L	800	UQ	C37-C36-C34	-4.00	99.93	113.19
6	L	800	UQ	C15-C14-C16	3.95	122.09	115.23
5	L	550	BPH	C4C-C3C-C2C	3.95	106.60	102.84
4	M	400	BCL	C1-C2-C3	-3.75	120.06	126.20
5	L	550	BPH	C1-C2-C3	-3.73	120.08	126.20
4	M	400	BCL	C4D-CHA-C1A	3.70	125.66	121.24
6	M	750	UQ	C10-C9-C8	-3.68	114.17	123.63
6	M	750	UQ	C5-C6-C1	-3.62	116.10	119.62
6	L	800	UQ	C17-C18-C19	-3.59	119.41	127.62
4	L	450	BCL	C4D-CHA-C1A	3.58	125.51	121.24
5	M	500	BPH	C4C-C3C-C2C	3.55	106.22	102.84
4	L	450	BCL	C1-C2-C3	-3.52	120.44	126.20
6	M	750	UQ	C11-C12-C13	3.45	129.08	112.02
5	L	550	BPH	OBD-CAD-CBD	-3.44	120.77	125.82
4	L	350	BCL	C1C-NC-C4C	3.43	108.24	106.68
6	M	750	UQ	C22-C21-C19	-3.40	101.91	113.19
5	M	500	BPH	C1-C2-C3	-3.37	120.67	126.20
4	M	400	BCL	C2C-C3C-C4C	3.33	106.32	101.34
5	L	550	BPH	OBB-CAB-CBB	-3.29	113.17	120.19
4	L	450	BCL	C2C-C3C-C4C	3.29	106.27	101.34
6	L	800	UQ	C41-C39-C40	3.27	122.11	114.59
5	M	500	BPH	OBB-CAB-CBB	-3.25	113.27	120.19
6	L	800	UQ	C20-C19-C18	-3.23	115.33	123.63
4	L	350	BCL	C1D-ND-C4D	3.20	108.56	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	800	UQ	CM5-C5-C6	-3.18	119.21	124.45
4	M	400	BCL	C1C-NC-C4C	3.17	108.12	106.68
4	M	601	BCL	C1D-ND-C4D	3.16	108.53	106.31
5	M	500	BPH	C4-C3-C5	3.11	120.63	115.23
4	M	601	BCL	C2C-C3C-C4C	3.11	105.99	101.34
4	M	400	BCL	OBb-CAB-CBB	-3.06	112.91	119.77
6	M	750	UQ	O1-C1-C6	-3.06	115.87	121.79
6	L	800	UQ	C31-C29-C28	3.06	128.03	121.17
4	M	601	BCL	C4-C3-C5	3.05	120.52	115.23
6	L	800	UQ	C25-C24-C26	3.03	120.49	115.23
5	M	500	BPH	C4D-ND-C1D	-3.01	105.27	108.87
4	M	601	BCL	OBb-CAB-CBB	-3.00	113.06	119.77
4	L	350	BCL	C2C-C3C-C4C	2.96	105.77	101.34
5	M	500	BPH	OBd-CAD-C3D	2.92	132.44	127.89
4	L	350	BCL	C4-C3-C5	2.90	120.27	115.23
6	M	750	UQ	C20-C19-C21	2.87	120.21	115.23
4	L	450	BCL	OBb-CAB-CBB	-2.84	113.42	119.77
4	L	350	BCL	OBb-CAB-CBB	-2.83	113.43	119.77
4	L	450	BCL	C4-C3-C5	2.75	120.00	115.23
5	L	550	BPH	C4D-ND-C1D	-2.74	105.59	108.87
6	L	800	UQ	C30-C29-C31	2.72	119.95	115.23
6	M	750	UQ	C3-C2-C1	-2.68	115.77	120.69
5	L	550	BPH	C4-C3-C5	2.68	119.88	115.23
6	L	800	UQ	C11-C9-C8	-2.64	115.24	121.17
4	M	400	BCL	CHd-C1D-ND	-2.62	121.12	124.80
4	L	450	BCL	CHd-C1D-ND	-2.61	121.13	124.80
6	L	800	UQ	O1-C1-C6	-2.57	116.81	121.79
4	M	400	BCL	C2B-C1B-NB	-2.56	107.67	110.33
4	L	350	BCL	C4D-C3D-CAD	-2.55	105.34	108.11
5	M	500	BPH	C1C-C2C-C3C	2.54	105.25	102.84
5	L	550	BPH	CMD-C2D-C3D	2.53	129.73	124.68
6	M	750	UQ	O2-C2-C1	2.52	125.14	116.64
6	L	800	UQ	C15-C14-C13	-2.51	117.17	123.63
5	L	550	BPH	OBd-CAD-C3D	2.50	131.79	127.89
6	M	750	UQ	C25-C24-C26	2.48	119.53	115.23
6	M	750	UQ	C26-C24-C23	-2.47	115.61	121.17
4	L	350	BCL	C2A-C1A-CHA	2.47	128.15	123.87
4	L	350	BCL	CHA-C1A-NA	-2.45	120.85	126.39
5	L	550	BPH	CGD-CBD-CAD	-2.44	102.94	110.85
5	M	500	BPH	OBd-CAD-CBD	-2.40	122.30	125.82
4	M	601	BCL	C1C-NC-C4C	2.39	107.77	106.68
6	L	800	UQ	CM3-O3-C3	-2.37	108.13	116.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	400	BCL	CHA-C1A-NA	-2.37	121.03	126.39
6	L	800	UQ	O2-C2-C1	2.35	124.57	116.64
4	M	400	BCL	C2A-C1A-CHA	2.31	127.88	123.87
6	M	750	UQ	C36-C34-C33	-2.29	116.02	121.17
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
6	L	800	UQ	C27-C26-C24	2.27	120.71	113.19
4	L	450	BCL	CHA-C1A-NA	-2.23	121.34	126.39
6	L	800	UQ	C26-C24-C23	2.22	126.15	121.17
6	L	800	UQ	CM2-O2-C2	2.21	124.25	116.47
6	L	800	UQ	O4-C4-C3	-2.21	116.34	121.03
4	M	601	BCL	CHA-C1A-NA	-2.21	121.38	126.39
6	M	750	UQ	C35-C34-C36	2.19	119.04	115.23
5	L	550	BPH	C2B-C1B-NB	-2.19	107.85	109.43
4	L	350	BCL	CBB-CAB-C3B	2.18	125.00	120.40
4	M	601	BCL	CHD-C1D-ND	-2.14	121.79	124.80
6	M	750	UQ	C3-C4-C5	2.13	122.31	118.10
5	L	550	BPH	CMC-C2C-C1C	-2.12	110.05	114.61
5	L	550	BPH	C3D-C4D-ND	2.12	110.42	107.71
4	M	400	BCL	C4-C3-C5	2.12	118.90	115.23
6	M	750	UQ	C6-C5-C4	2.10	120.82	119.17
5	L	550	BPH	C2D-C1D-ND	2.09	110.94	109.43
4	L	450	BCL	C4D-C3D-CAD	-2.09	105.84	108.11
6	M	750	UQ	C32-C33-C34	-2.07	122.88	127.62
4	M	400	BCL	CBB-CAB-C3B	2.07	124.77	120.40
4	L	450	BCL	C1D-ND-C4D	2.05	107.75	106.31
6	L	800	UQ	C12-C13-C14	-2.04	122.94	127.62
5	M	500	BPH	CMD-C2D-C3D	2.03	128.74	124.68
5	M	500	BPH	CMC-C2C-C1C	-2.02	110.25	114.61
4	L	450	BCL	CBB-CAB-C3B	2.02	124.66	120.40
4	L	450	BCL	C1C-NC-C4C	2.02	107.60	106.68

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	350	BCL	C6-C7-C8-C9
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	M	601	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	M	601	BCL	C3A-C2A-CAA-CBA
4	M	601	BCL	C2B-C3B-CAB-OBB
4	M	601	BCL	C2B-C3B-CAB-CBB
4	M	601	BCL	C2C-C3C-CAC-CBC
4	M	400	BCL	C1A-C2A-CAA-CBA
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	L	550	BPH	C2C-C3C-CAC-CBC
5	L	550	BPH	C3A-C2A-CAA-CBA
5	L	550	BPH	C1A-C2A-CAA-CBA
5	M	500	BPH	C4C-C3C-CAC-CBC
5	M	500	BPH	C2C-C3C-CAC-CBC
6	M	750	UQ	C21-C22-C23-C24
6	M	750	UQ	C24-C26-C27-C28
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
4	L	350	BCL	C4-C3-C5-C6
6	L	800	UQ	C20-C19-C21-C22
6	L	800	UQ	C30-C29-C31-C32
6	L	800	UQ	C35-C34-C36-C37
6	M	750	UQ	C30-C29-C31-C32
4	L	350	BCL	C2-C3-C5-C6
6	L	800	UQ	C18-C19-C21-C22
6	M	750	UQ	C28-C29-C31-C32
4	M	601	BCL	C2A-CAA-CBA-CGA
5	L	550	BPH	C2A-CAA-CBA-CGA
4	L	450	BCL	O1A-CGA-O2A-C1
5	M	500	BPH	O1A-CGA-O2A-C1
4	M	400	BCL	O1D-CGD-O2D-CED
5	M	500	BPH	CBA-CGA-O2A-C1
4	L	450	BCL	CBA-CGA-O2A-C1
4	M	400	BCL	C4-C3-C5-C6
4	M	400	BCL	C2-C3-C5-C6
6	L	800	UQ	C12-C11-C9-C8
6	L	800	UQ	C28-C29-C31-C32
6	L	800	UQ	C14-C16-C17-C18
6	L	800	UQ	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
6	M	750	UQ	C34-C36-C37-C38
6	M	750	UQ	C12-C13-C14-C15
6	L	800	UQ	C12-C11-C9-C10
4	M	400	BCL	C6-C7-C8-C9
4	M	601	BCL	C2-C1-O2A-CGA
4	L	350	BCL	C10-C11-C12-C13
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	601	BCL	C5-C6-C7-C8
4	L	350	BCL	C2A-CAA-CBA-CGA
5	M	500	BPH	C8-C10-C11-C12
6	M	750	UQ	C12-C13-C14-C16
4	M	400	BCL	C13-C15-C16-C17
4	M	400	BCL	C10-C11-C12-C13
5	M	500	BPH	C5-C6-C7-C8
6	L	800	UQ	C33-C34-C36-C37
6	L	800	UQ	C19-C21-C22-C23
4	M	400	BCL	C16-C17-C18-C19
5	M	500	BPH	C10-C11-C12-C13
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
5	M	500	BPH	C16-C17-C18-C20
4	L	350	BCL	C6-C7-C8-C10
4	L	450	BCL	C11-C10-C8-C7
4	L	450	BCL	C11-C12-C13-C15
4	M	400	BCL	C6-C7-C8-C10
4	M	400	BCL	C11-C10-C8-C7
5	L	550	BPH	C11-C10-C8-C7
4	M	601	BCL	C4B-C3B-CAB-OBB
4	M	601	BCL	C4B-C3B-CAB-CBB
4	L	450	BCL	C11-C10-C8-C9
4	L	450	BCL	C11-C12-C13-C14
4	M	400	BCL	C8-C10-C11-C12
4	M	601	BCL	CBA-CGA-O2A-C1
4	L	450	BCL	C4-C3-C5-C6
4	M	400	BCL	C11-C10-C8-C9
5	L	550	BPH	C11-C10-C8-C9
5	M	500	BPH	C14-C13-C15-C16
4	M	400	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
5	M	500	BPH	C12-C13-C15-C16
5	L	550	BPH	C3-C5-C6-C7
6	M	750	UQ	C25-C24-C26-C27
4	L	450	BCL	C2-C3-C5-C6
5	L	550	BPH	C16-C17-C18-C20
4	M	601	BCL	C11-C12-C13-C14
4	M	601	BCL	O1A-CGA-O2A-C1
4	L	350	BCL	C12-C13-C15-C16
6	M	750	UQ	C7-C8-C9-C10
5	M	500	BPH	C2A-CAA-CBA-CGA
5	L	550	BPH	C16-C17-C18-C19
6	M	750	UQ	C1-C2-O2-CM2
6	L	800	UQ	C1-C6-C7-C8
6	M	750	UQ	C20-C19-C21-C22
6	M	750	UQ	C23-C24-C26-C27
4	M	601	BCL	C11-C10-C8-C7
4	M	400	BCL	CBA-CGA-O2A-C1
4	L	350	BCL	C14-C13-C15-C16
4	M	400	BCL	O1A-CGA-O2A-C1
4	L	350	BCL	CAD-CBD-CGD-O2D
4	L	350	BCL	CAD-CBD-CGD-O1D
4	M	601	BCL	C3-C5-C6-C7
4	L	350	BCL	C11-C10-C8-C9
4	L	350	BCL	C11-C10-C8-C7
4	M	601	BCL	C10-C11-C12-C13
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
6	M	750	UQ	C7-C8-C9-C11
5	L	550	BPH	O1A-CGA-O2A-C1
4	M	601	BCL	C4C-C3C-CAC-CBC
6	M	750	UQ	C12-C11-C9-C10
5	L	550	BPH	C15-C16-C17-C18
5	L	550	BPH	C2-C1-O2A-CGA
4	L	450	BCL	C3-C5-C6-C7
6	M	750	UQ	C14-C16-C17-C18
4	L	350	BCL	CAA-CBA-CGA-O2A
5	M	500	BPH	CAA-CBA-CGA-O2A
4	M	400	BCL	C14-C13-C15-C16
4	M	601	BCL	CAA-CBA-CGA-O2A
6	M	750	UQ	C18-C19-C21-C22

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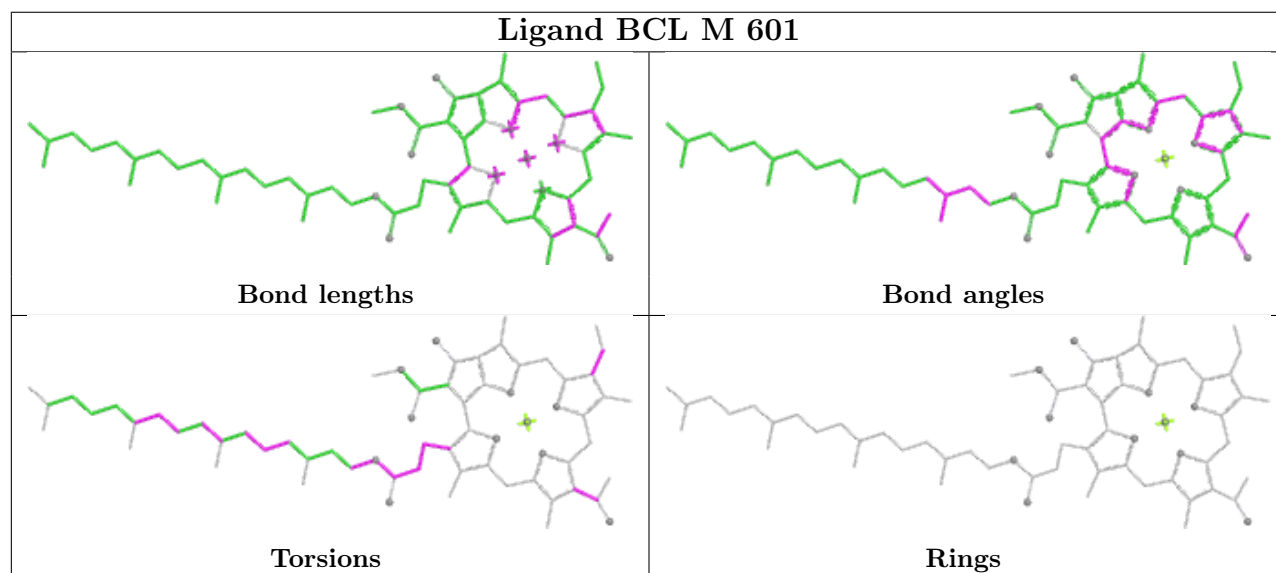
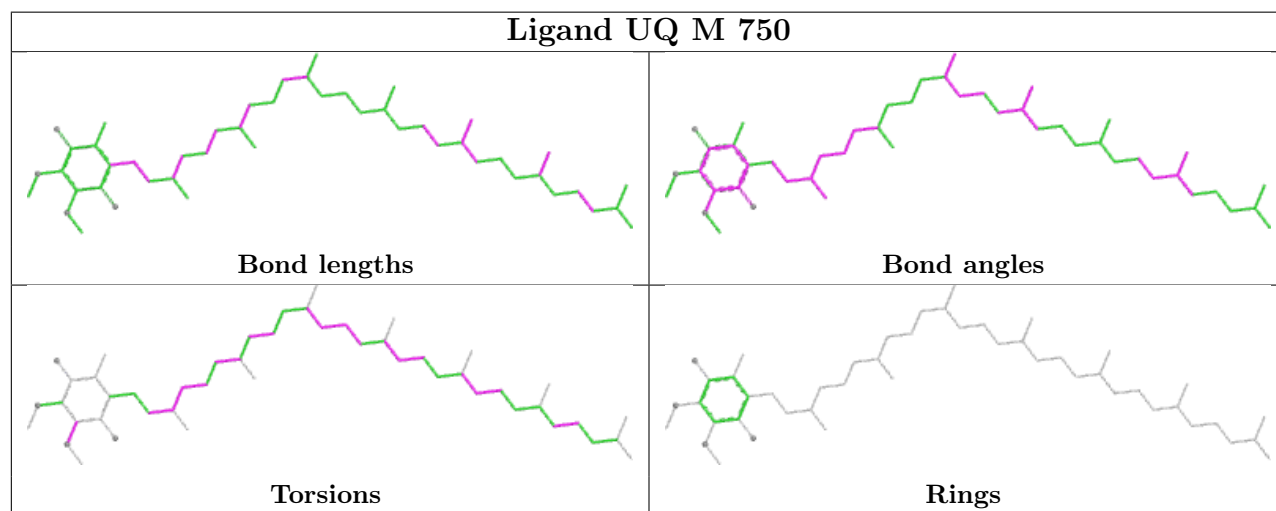
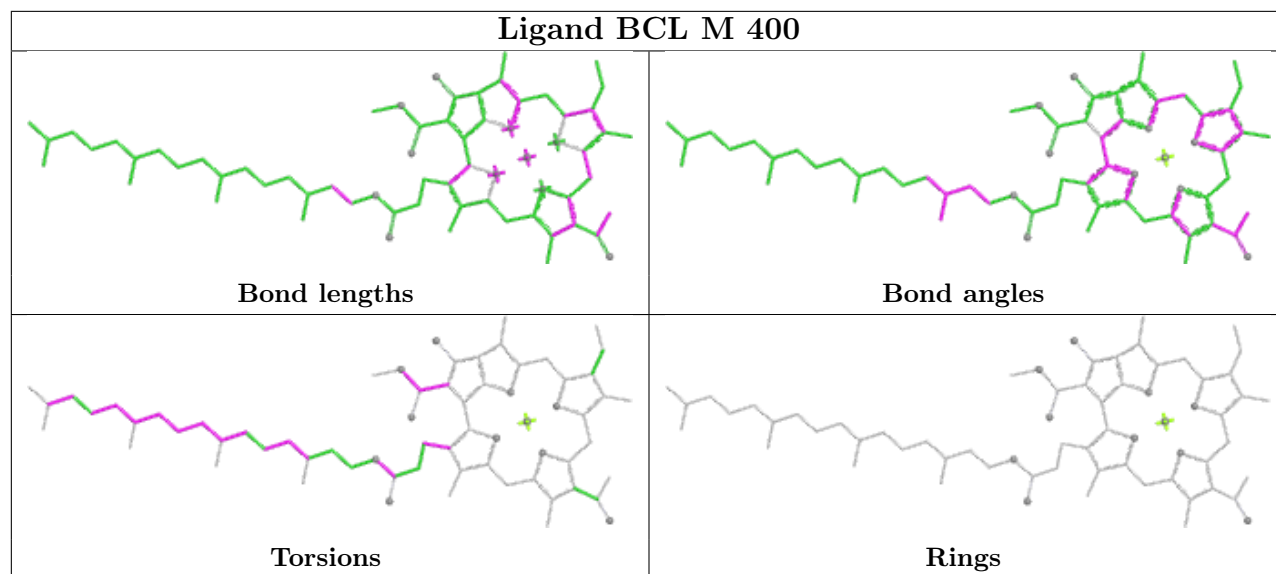
Mol	Chain	Res	Type	Atoms
6	L	800	UQ	C2-C3-O3-CM3
4	M	400	BCL	C3A-C2A-CAA-CBA
6	L	800	UQ	C4-C3-O3-CM3
4	L	350	BCL	CAA-CBA-CGA-O1A
5	M	500	BPH	CAA-CBA-CGA-O1A
4	M	601	BCL	CAA-CBA-CGA-O1A
4	L	350	BCL	C13-C15-C16-C17

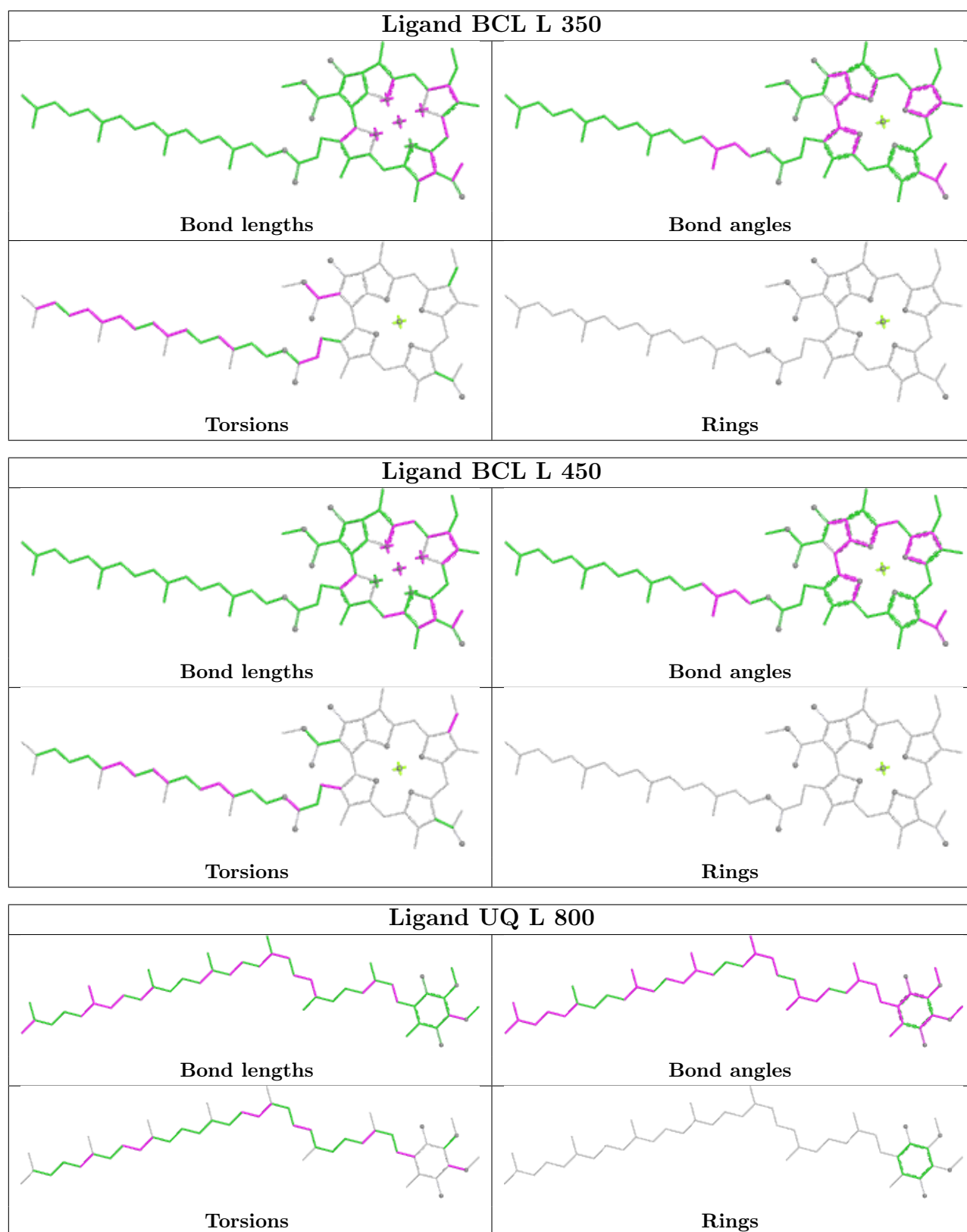
There are no ring outliers.

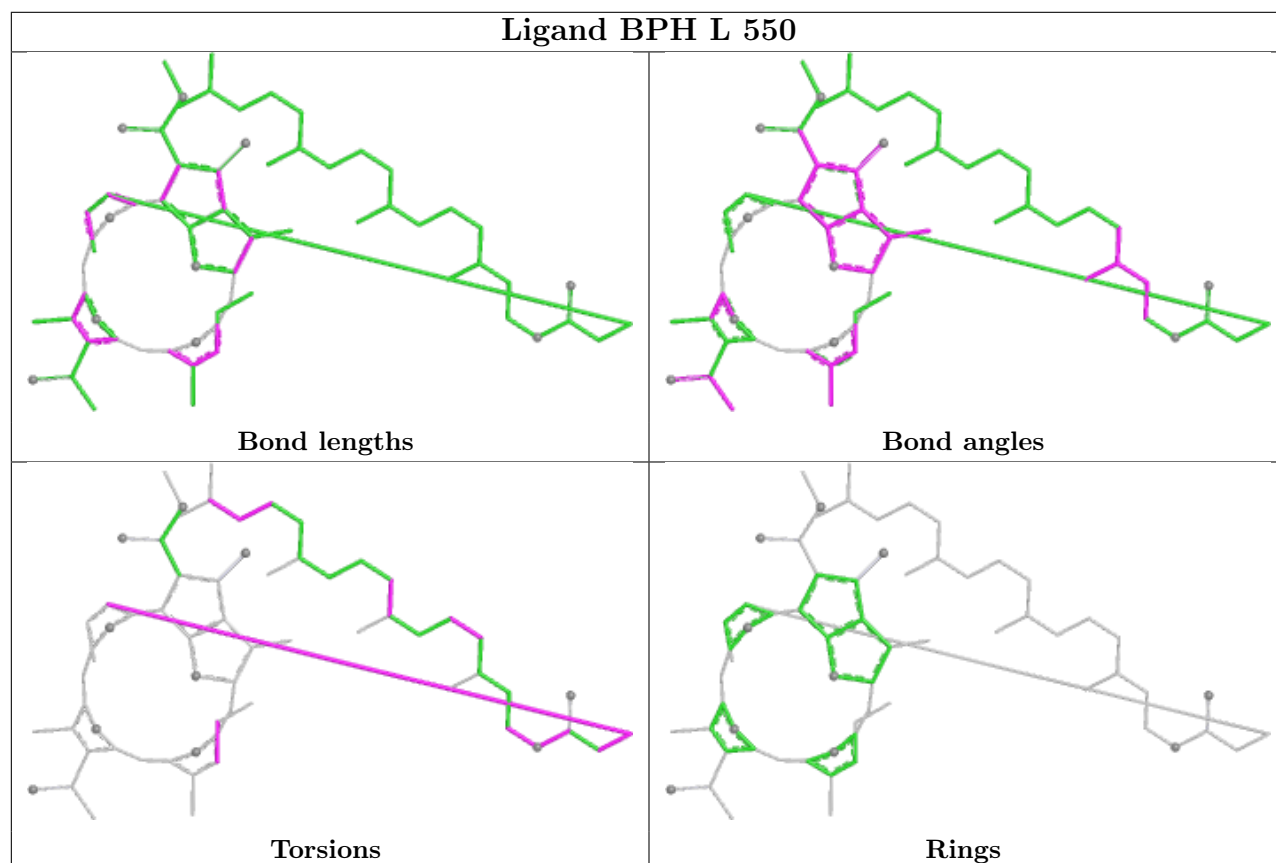
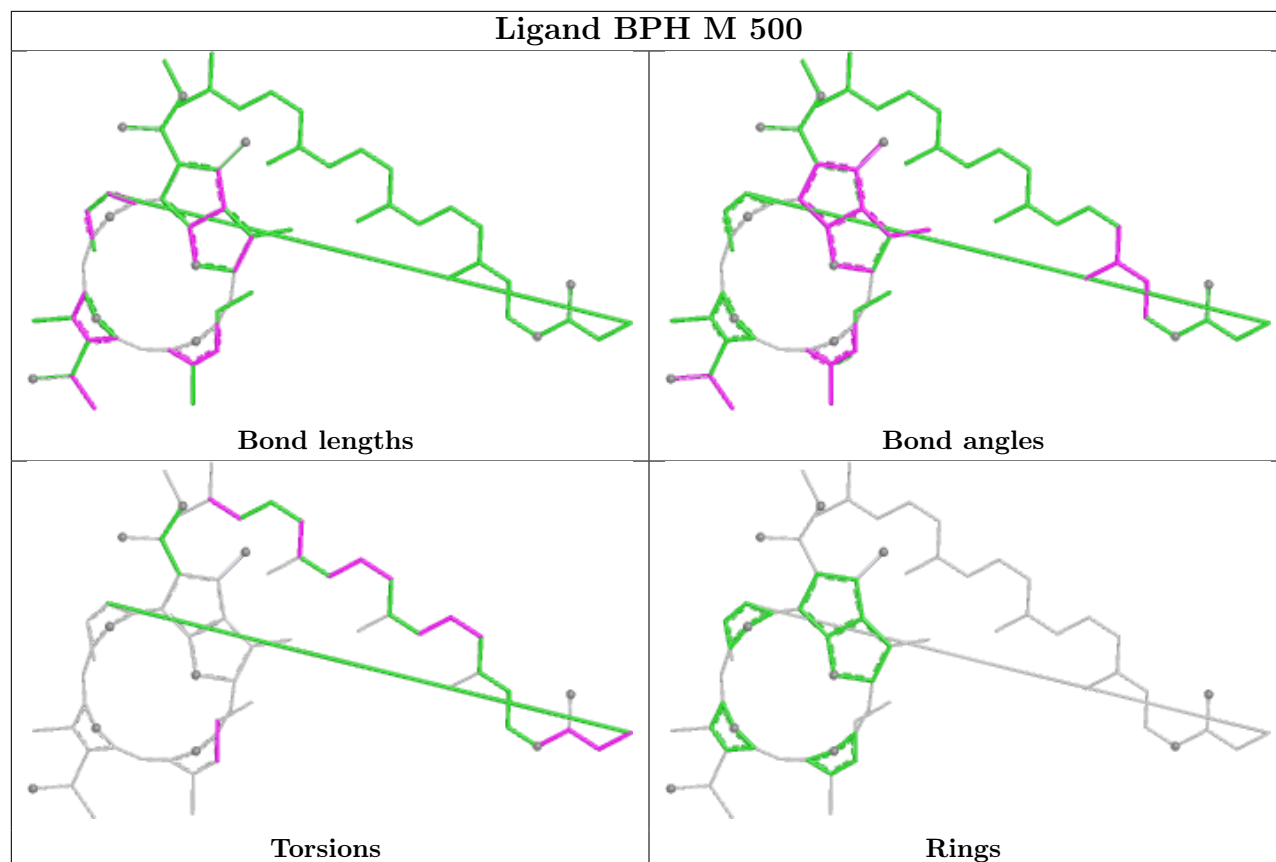
8 monomers are involved in 183 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	400	BCL	44	0
6	M	750	UQ	33	0
4	M	601	BCL	25	0
4	L	350	BCL	30	0
4	L	450	BCL	20	0
6	L	800	UQ	22	0
5	M	500	BPH	31	0
5	L	550	BPH	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [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.