



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

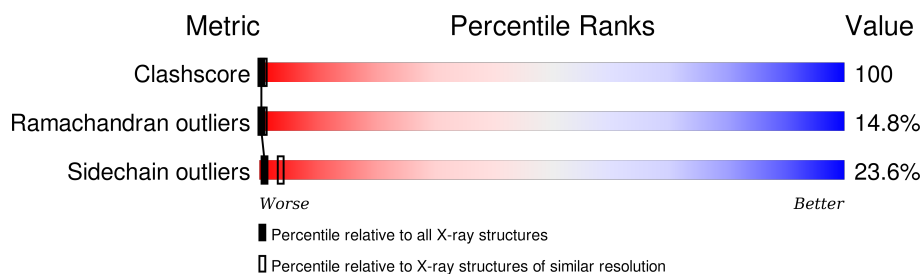
1 Overall quality at a glance

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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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
5	BCL	L	350	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	450	-	-	X	-
5	BCL	M	400	-	-	X	-
5	BCL	M	601	-	-	X	-
6	BPH	M	500	-	-	X	-
7	UQ	L	800	-	-	X	-
7	UQ	M	750	-	-	X	-

2 Entry composition

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
1	L	278	Total	C	N	O	S	0	0	0
			2203	1491	349	355	8			

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

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

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

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

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

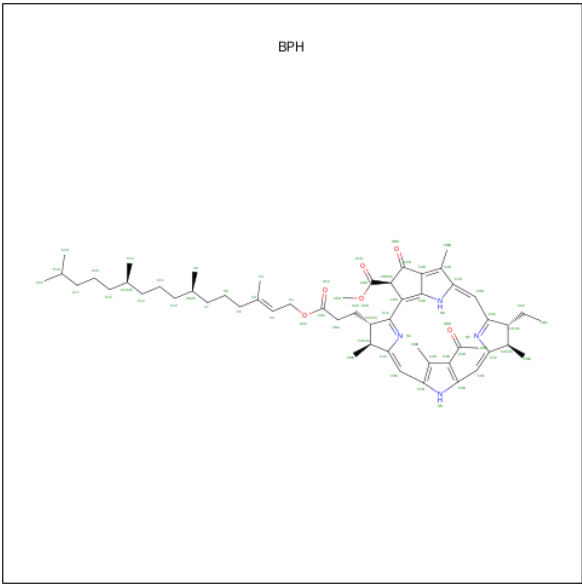
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



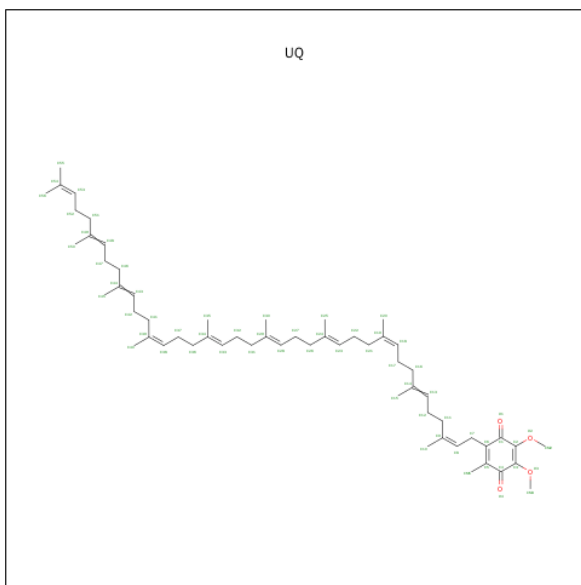
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	7	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	3	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	6	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



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

- Molecule 7 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



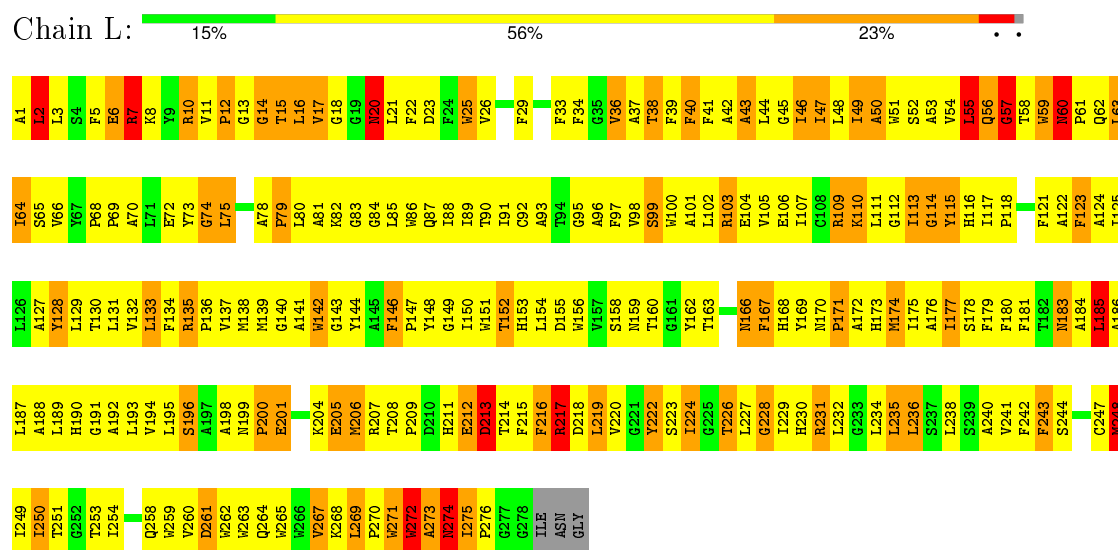
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	16	0
			48	44	4		
7	L	1	Total	C	O	16	0
			48	44	4		

3 Residue-property plots

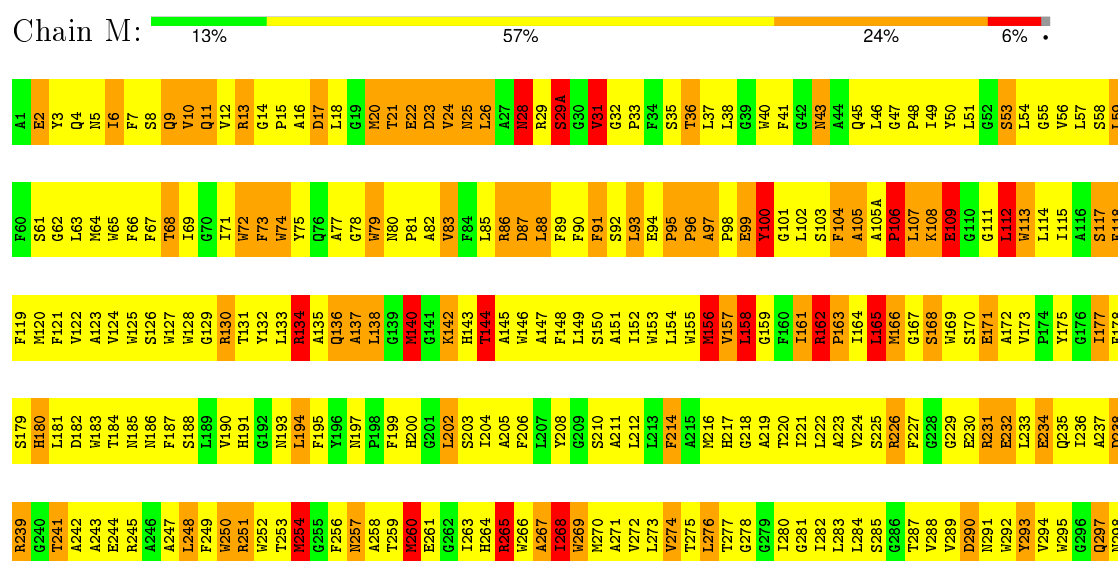
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

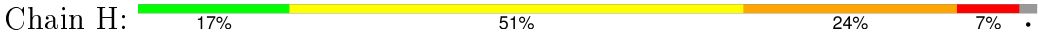


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)



H299
G300
P301
A302
P303
LEU
ASN

● Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



H1	H2	G3	V4	T5	A6	F7	G8	H9	F10	D11	L12	A13	S14	L15	A16	I17	F20	W21	I22	F23	L24	A25	G26	L27	I28	Y29	Y30	L31	Q32	T33	E34	N35	M36	R37	E38	G39	Y40	P41	E45	T48	P49	N52	Q53	G54	P55	F56	P57	L58	P59	K60	P61	K62	T63	F64	I65
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L66	P67	H68	G69	R70	G71	T72	L73	T74	V75	P76	G77	P78	E79	S80	E81	D82	R83	P84	L87	A88	R89	T90	A91	V92	S93	E94	G95	F96	P97	H98	A99	P100	D103	P104	M105	K106	D107	G108	V109	G110	P111	A112	S113	W114	V115	A116	R117	R118	D119	L120	P121	E122	L123	D124	H128	N129
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K130	I131	K132	P133	M134	K135	F140	H141	V142	S143	A144	G145	K146	M147	P148	S149	G150	L151	P152	V153	R154	G155	G156	D157	L158	E159	I160	A161	G162	K163	V164	V165	D166	I167	W168	V169	D170	I171	P172	E173	Q174	M175	A176	R177	F178	L179	E180	V181	E182	L183	K184	D185	G186	S187	T188	R189	L190	L191	P192
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K193	Q194	M195	V196	K197	V198	Q199	S200	N201	R202	V203	H204	V205	R206	A207	L208	S209	S210	D211	L212	F213	A214	G215	I216	P217	T218	I219	K220	S221	P222	T223	E224	V225	T226	L227	L228	E229	E230	D231	K232	I233	C234	G235	Y236	V237	A238	G239	G240	L241	M242	Y243	A244	A245	R248	K249	S250	V251	V252	A253
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A254
H255
LEU
ALA
GLU
TVR
ALA

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	1.00	2/2291 (0.1%)	1.47	24/3137 (0.8%)
2	M	1.21	6/2521 (0.2%)	1.57	36/3442 (1.0%)
3	H	0.96	4/1977 (0.2%)	1.52	23/2689 (0.9%)
All	All	1.07	12/6789 (0.2%)	1.52	83/9268 (0.9%)

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

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

All (12) bond length outliers are listed below:

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

All (83) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 100.

All (1373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:750:UQ:C13	7:M:750:UQ:C12	1.84	1.50
1:L:183:ASN:ND2	1:L:236:LEU:HB2	1.24	1.48
2:M:96:PRO:HG2	2:M:170:SER:CA	1.57	1.33
1:L:183:ASN:HD22	1:L:236:LEU:CB	1.44	1.30
2:M:96:PRO:CG	2:M:170:SER:HA	1.75	1.17
1:L:229:ILE:HD13	7:L:800:UQ:HM53	1.24	1.16
3:H:33:THR:HG22	3:H:34:GLU:H	1.08	1.16
1:L:185:LEU:CD2	7:L:800:UQ:H153	1.75	1.16
1:L:187:LEU:HD21	2:M:267:ALA:CB	1.77	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:102:LEU:HA	2:M:169:TRP:HD1	1.04	1.15
1:L:172:ALA:HB3	1:L:247:CYS:HB2	1.16	1.15
1:L:114:GLY:HA3	2:M:223:ALA:HB1	1.17	1.15
3:H:182:GLU:HG3	3:H:187:SER:HA	1.15	1.13
1:L:193:LEU:HD11	1:L:216:PHE:CE1	1.84	1.12
1:L:183:ASN:ND2	1:L:236:LEU:CB	2.05	1.12
5:L:350:BCL:HBD	5:L:450:BCL:HBC1	1.16	1.12
2:M:69:ILE:HA	2:M:93:LEU:HD11	1.23	1.11
3:H:168:TRP:HZ3	3:H:180:GLU:HB2	1.16	1.11
1:L:187:LEU:CD2	2:M:267:ALA:HB1	1.80	1.11
5:M:400:BCL:HBA1	5:M:400:BCL:HBD	1.14	1.10
5:L:350:BCL:HBD	5:L:450:BCL:CBC	1.81	1.10
2:M:254:MET:HE1	7:M:750:UQ:H112	1.27	1.10
2:M:102:LEU:HA	2:M:169:TRP:CD1	1.86	1.10
2:M:69:ILE:HA	2:M:93:LEU:CD1	1.80	1.10
2:M:162:ARG:HG3	2:M:282:ILE:HG22	1.34	1.09
1:L:117:ILE:HD13	2:M:249:PHE:CD2	1.86	1.08
1:L:58:THR:HG22	1:L:59:TRP:H	1.12	1.06
2:M:99:GLU:O	2:M:100:TYR:HB2	1.52	1.06
3:H:61:PRO:HA	3:H:76:PRO:HG3	1.07	1.06
1:L:74:GLY:HA2	1:L:141:ALA:HB2	1.38	1.06
1:L:37:ALA:O	1:L:40:PHE:HB2	1.53	1.05
3:H:245:ALA:HB3	3:H:248:ARG:HG3	1.37	1.05
1:L:117:ILE:HD13	2:M:249:PHE:CE2	1.91	1.05
1:L:218:ASP:OD2	2:M:50:TYR:HE1	1.37	1.04
1:L:185:LEU:HD21	7:L:800:UQ:H153	1.33	1.03
2:M:101:GLY:HA2	2:M:168:SER:HA	1.40	1.03
2:M:162:ARG:HB3	2:M:163:PRO:HD3	1.39	1.03
2:M:274:VAL:HG12	2:M:275:THR:N	1.68	1.03
1:L:218:ASP:OD2	2:M:50:TYR:CE1	2.12	1.01
1:L:195:LEU:HD13	2:M:265:ARG:HH11	1.19	1.01
1:L:3:LEU:HB3	1:L:6:GLU:HB2	1.39	1.01
5:M:601:BCL:C1	6:M:500:BPH:HMB2	1.89	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
5:M:601:BCL:H11	6:M:500:BPH:CMB	1.93	0.99
2:M:96:PRO:HG2	2:M:170:SER:HA	1.00	0.99
2:M:204:ILE:HG23	5:M:400:BCL:HMB3	1.41	0.99
1:L:231:ARG:NE	2:M:6:ILE:H	1.59	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:350:BCL:H152	6: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
3:H:33:THR:HG22	3:H:34:GLU:N	1.79	0.96
2:M:97:ALA:HB3	2:M:98:PRO:HD3	1.48	0.95
1:L:180:PHE:CE1	1:L:240:ALA:HB1	2.02	0.95
3:H:130:LYS:HG3	3:H:172:PRO:HG2	1.49	0.95
2:M:16:ALA:HB1	2:M:45:GLN:HE22	1.28	0.95
3:H:151:LEU:HD21	3:H:203:VAL:CG2	1.96	0.94
2:M:183:TRP:CZ3	5:M:601:BCL:HMC1	2.02	0.94
5:M:601:BCL:H11	6:M:500:BPH:HMB2	0.97	0.94
2:M:96:PRO:HG2	2:M:170:SER:N	1.83	0.94
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.32	0.94
1:L:231:ARG:HE	2:M:6:ILE:H	0.98	0.93
2:M:186:ASN:O	2:M:190:VAL:HG23	1.67	0.93
1:L:231:ARG:HE	2:M:6:ILE:N	1.67	0.93
2:M:31:VAL:CG2	2:M:33:PRO:HD3	1.97	0.93
1:L:218:ASP:HB3	2:M:50:TYR:CE1	2.02	0.93
3:H:164:VAL:O	3:H:165:VAL:HG23	1.66	0.93
2:M:69:ILE:CA	2:M:93:LEU:HD11	2.00	0.92
3:H:160:ILE:HG23	3:H:160:ILE:O	1.67	0.92
2:M:78:GLY:O	2:M:79:TRP:HB2	1.70	0.92
2:M:157:VAL:HA	2:M:161:ILE:HG22	1.50	0.92
1:L:114:GLY:HA3	2:M:223:ALA:CB	1.98	0.92
1:L:229:ILE:CD1	7:L:800:UQ:HM53	1.99	0.92
3:H:168:TRP:CZ3	3:H:180:GLU:HB2	2.05	0.92
3:H:111:PRO:HD2	3:H:243:TYR:CE2	2.04	0.91
3:H:56:PHE:H	3:H:57:PRO:HD2	1.34	0.91
1:L:58:THR:CG2	1:L:59:TRP:H	1.83	0.91
2:M:254:MET:CE	7:M:750:UQ:H112	1.99	0.91
1:L:195:LEU:HD11	2:M:265:ARG:HG3	1.50	0.91
3:H:182:GLU:HG3	3:H:187:SER:CA	2.00	0.91
3:H:170:ASP:OD2	3:H:173:GLU:HB3	1.70	0.91
3:H:103:ASP:O	3:H:107:ASP:HB2	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:ALA:HB2	1:L:7:ARG:HG2	1.53	0.90
2:M:106:PRO:C	2:M:108:LYS:H	1.74	0.90
1:L:183:ASN:HD22	1:L:236:LEU:CG	1.83	0.90
1:L:37:ALA:O	1:L:40:PHE:CB	2.20	0.90
1:L:58:THR:HG22	1:L:59:TRP:N	1.87	0.90
3:H:207:ALA:O	3:H:240:GLY:HA3	1.72	0.89
2:M:113:TRP:CZ3	2:M:169:TRP:HE3	1.91	0.89
2:M:254:MET:HE1	7:M:750:UQ:C11	2.03	0.88
2:M:101:GLY:CA	2:M:168:SER:HA	2.03	0.88
1:L:1:ALA:O	1:L:2:LEU:HB2	1.70	0.88
2:M:128:TRP:HE1	2:M:145:ALA:HB1	1.36	0.88
3:H:131:ILE:HG22	3:H:168:TRP:HD1	1.37	0.88
3:H:164:VAL:O	3:H:165:VAL:CG2	2.21	0.88
2:M:258:ALA:HA	3:H:35:ASN:HB3	1.54	0.88
2:M:95:PRO:HB2	2:M:96:PRO:HD2	1.55	0.87
3:H:182:GLU:CG	3:H:187:SER:HA	2.01	0.87
5:L:350:BCL:H72	5:L:450:BCL:CBB	2.03	0.87
1:L:264:GLN:HA	1:L:267:VAL:HG23	1.56	0.87
3:H:5:THR:HA	3:H:11:ASP:HA	1.57	0.87
2:M:158:LEU:HD21	2:M:183:TRP:CZ3	2.10	0.87
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
5:M:400:BCL:HBA1	5:M:400:BCL:CB D	2.03	0.86
1:L:53:ALA:HB2	1:L:64:ILE:CD1	2.05	0.86
1:L:37:ALA:C	1:L:40:PHE:HB2	1.94	0.86
1:L:230:HIS:CE1	2:M:221:ILE:HG21	2.09	0.86
2:M:157:VAL:CG1	2:M:162:ARG:HB2	2.06	0.86
2:M:103:SER:C	2:M:105:ALA:N	2.28	0.85
2:M:227:PHE:HE2	3:H:235:GLY:HA2	1.41	0.85
1:L:121:PHE:O	1:L:124:ALA:HB3	1.76	0.85
2:M:20:MET:HG3	2:M:21:THR:H	1.40	0.85
2:M:128:TRP:NE1	2:M:145:ALA:HB1	1.91	0.85
3:H:157:ASP:O	3:H:158:LEU:HB2	1.75	0.85
3:H:191:LEU:HD11	3:H:213:PHE:CE2	2.12	0.85
3:H:56:PHE:H	3:H:57:PRO:CD	1.90	0.84
1:L:130:THR:HB	1:L:249:ILE:HD11	1.60	0.84
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.58	0.84
2:M:274:VAL:HG12	2:M:275:THR:H	1.40	0.84
2:M:54:LEU:H	2:M:54:LEU:HD12	1.43	0.84
3:H:81:GLU:O	3:H:82:ASP:HB2	1.77	0.83
2:M:250:TRP:O	2:M:254:MET:HG3	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:8:GLY:O	3:H:9:ASN:HB2	1.78	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
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
2:M:13:ARG:HG2	2:M:14:GLY:H	1.44	0.82
1:L:183:ASN:HD22	1:L:236:LEU:CD1	1.91	0.82
2:M:113:TRP:HZ3	2:M:169:TRP:HE3	1.24	0.82
1:L:227:LEU:HD21	1:L:231:ARG:NH2	1.95	0.82
2:M:97:ALA:C	2:M:99:GLU:H	1.80	0.82
5:M:400:BCL:H43	6:M:500:BPH:CAB	2.09	0.82
3:H:17:ILE:HG23	3:H:21:TRP:CD1	2.14	0.82
1:L:149:GLY:HA3	1:L:152:THR:CG2	2.09	0.82
1:L:229:ILE:HB	7:L:800:UQ:CM5	2.10	0.82
1:L:264:GLN:OE1	1:L:267:VAL:HG21	1.78	0.82
3:H:252:VAL:HG12	3:H:253:ALA:N	1.93	0.81
2:M:153:TRP:CZ2	2:M:283:LEU:HD12	2.14	0.81
1:L:104:GLU:HA	1:L:107:ILE:HD12	1.63	0.81
1:L:230:HIS:ND1	2:M:221:ILE:HG21	1.95	0.81
1:L:212:GLU:N	2:M:140:MET:HE3	1.94	0.81
1:L:169:TYR:CG	1:L:260:VAL:HG22	2.15	0.81
1:L:5:PHE:HB2	2:M:244:GLU:OE1	1.79	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:HH11	2:M:251:ARG:HG3	1.45	0.81
1:L:150:ILE:HG12	6:L:550:BPH:H193	1.61	0.81
3:H:173:GLU:O	3:H:174:GLN:HB2	1.81	0.81
2:M:89:PHE:HB3	2:M:178:PHE:CD1	2.15	0.81
2:M: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
5:L:350:BCL:HAA2	5:L:450:BCL:HBC1	1.64	0.80
2:M:250:TRP:HE1	7:M:750:UQ:HM53	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:M:183:TRP:HZ3	5:M:601:BCL:HMC1	1.43	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
5:M:400:BCL:CBB	5:M:400:BCL:HMB1	2.12	0.79
3:H:164:VAL:C	3:H:165:VAL:HG23	2.03	0.79
2:M:105(A):ALA:HB3	2:M:109:GLU:HG2	1.64	0.79
3:H:66:LEU:HB3	3:H:67:PRO:HD2	1.64	0.79
1:L:117:ILE:CD1	2:M:249:PHE:CD2	2.65	0.79
1:L:74:GLY:HA2	1:L:141:ALA:CB	2.12	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:HB	7:L:800:UQ:HM52	1.63	0.78
2:M:113:TRP:HZ2	2:M:172:ALA:HB1	1.47	0.78
1:L:229:ILE:HG13	2:M:214:PHE:HZ	1.47	0.78
3:H:161:ALA:HA	3:H:210:SER:HB3	1.65	0.78
3:H:28:ILE:HG22	3:H:29:TYR:N	1.98	0.78
2:M:103:SER:O	2:M:105:ALA:N	2.17	0.77
2:M:202:LEU:O	2:M:205:ALA:HB3	1.83	0.77
2:M:102:LEU:O	2:M:102:LEU:HD12	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
5:L:350:BCL:H72	5: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:219:ILE:HG12	3:H:221:SER:O	1.83	0.77
2:M:288:VAL:O	3:H:4:VAL:HG11	1.84	0.77
5:M:601:BCL:HMA1	5:M:400:BCL:H202	1.65	0.77
2:M:202:LEU:HD23	3:H:20:PHE:HE2	1.49	0.77
1:L:198:ALA:HB2	2:M:233:LEU:HD13	1.66	0.77
2:M:162:ARG:HB3	2:M:163:PRO:CD	2.15	0.77
2:M:32:GLY:HA2	2:M:46:LEU:O	1.84	0.77
2:M:226:ARG:HH21	3:H:238:ALA:HB1	1.51	0.77
2:M:224:VAL:HG12	2:M:242:ALA:HB1	1.67	0.76
5:M:400:BCL:C14	6:M:500:BPH:H2	2.15	0.76
1:L:41:PHE:CD2	1:L:92:CYS:HA	2.21	0.76
2:M:154:LEU:HD13	2:M:275:THR:HG22	1.66	0.76
3:H:128:HIS:CD2	3:H:129:ASN:H	2.03	0.76
1:L:150:ILE:HG12	6:L:550:BPH:C19	2.15	0.76
1:L:218:ASP:CG	2:M:50:TYR:HE1	1.87	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
5:M:601:BCL:HBC1	5:M:400:BCL:HBD	1.68	0.76
3:H:131:ILE:HG22	3:H:168:TRP:CD1	2.20	0.76
3:H:33:THR:CG2	3:H:34:GLU:H	1.91	0.76
1:L:128:TYR:CE2	5:L:450:BCL:HBB1	2.20	0.76
2:M:216:MET:HG2	2:M:250:TRP:HZ2	1.50	0.76
3:H:130:LYS:HG3	3:H:172:PRO:CG	2.16	0.76
1:L:274:ASN:O	1:L:275:ILE:HB	1.83	0.76
5:L:350:BCL:HMB1	5:L:350:BCL:HBB3	1.66	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
2:M:157:VAL:HG12	2:M:162:ARG:HB2	1.67	0.75
1:L:128:TYR:HE1	1:L:132:VAL:HG21	1.51	0.75
2:M:16:ALA:HB1	2:M:45:GLN:NE2	2.00	0.75
3:H:67:PRO:CG	3:H:123:LEU:HD21	2.17	0.75
1:L:231:ARG:HD3	2:M:6:ILE:HD13	1.69	0.75
1:L:70:ALA:HB3	1:L:73:TYR:CD2	2.22	0.75
3:H:27:LEU:HG	3:H:28:ILE:N	2.02	0.74
1:L:271:TRP:HB2	1:L:274:ASN:HD22	1.52	0.74
1:L:218:ASP:CB	2:M:50:TYR:CE1	2.71	0.74
1:L:20:ASN:C	1:L:22:PHE:H	1.90	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:259:THR:C	2:M:261:GLU:H	1.88	0.74
1:L:13:GLY:H	1:L:110:LYS:HE2	1.53	0.74
1:L:212:GLU:HB3	7:L:800:UQ:O2	1.86	0.74
1:L:198:ALA:HB2	2:M:233:LEU:CD1	2.18	0.74
2:M:274:VAL:CG1	2:M:275:THR:N	2.39	0.74
2:M:130:ARG:O	2:M:134:ARG:HB2	1.88	0.74
2:M:161:ILE:HG23	2:M:283:LEU:HD21	1.69	0.74
3:H:5:THR:HG23	3:H:10:PHE:H	1.51	0.74
5:L:350:BCL:H52	5:L:450:BCL:OBB	1.88	0.73
1:L:75:LEU:HG	1:L:140:GLY:O	1.87	0.73
2:M:87:ASP:HB3	2:M:90:PHE:HB2	1.69	0.73
3:H:240:GLY:O	3:H:244:ALA:HB3	1.87	0.73
1:L:158:SER:O	1:L:162:TYR:HD2	1.69	0.73
2:M:111:GLY:O	2:M:114:LEU:HB2	1.88	0.73
3:H:192:PRO:CG	3:H:237:VAL:HG21	2.17	0.73
3:H:135:LYS:NZ	3:H:165:VAL:CG1	2.51	0.73
1:L:70:ALA:HB3	1:L:73:TYR:HD2	1.54	0.73
3:H:122:GLU:O	3:H:123:LEU:HG	1.88	0.73
2:M:22:GLU:HB3	2:M:137:ALA:HA	1.69	0.73
1:L:176:ALA:O	1:L:180:PHE:HD1	1.72	0.73
2:M:204:ILE:CG2	5:M:400:BCL:HMB3	2.18	0.73
1:L:162:TYR:CE2	5: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:226:ARG:NH2	3:H:238:ALA:HB1	2.05	0.72
2:M:24:VAL:CG1	2:M:26:LEU:HB2	2.20	0.72
2:M:142:LYS:HG2	2:M:142:LYS:O	1.88	0.72
1:L:183:ASN:OD1	2:M:214:PHE:HD2	1.73	0.72
1:L:211:HIS:C	2:M:140:MET:HE3	2.09	0.72
2:M:162:ARG:NH2	2:M:187:PHE:CE1	2.58	0.72
2:M:96:PRO:CD	2:M:170:SER:HA	2.20	0.72
1:L:10:ARG:HG3	1:L:25:TRP:CH2	2.24	0.72
1:L:211:HIS:CD2	2:M:138:LEU:O	2.42	0.72
1:L:166:ASN:OD1	2:M:185:ASN:ND2	2.22	0.72
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:106:PRO:C	2:M:108:LYS:N	2.43	0.72
3:H:111:PRO:HG3	3:H:242:MET:SD	2.30	0.72
2:M:35:SER:HB3	2:M:38:LEU:HB3	1.70	0.72
3:H:148:PRO:HA	3:H:151:LEU:HB3	1.70	0.72
2:M:80:ASN:HB3	2:M:81:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:TYR:HD1	1:L:223:SER:N	1.88	0.71
5:L:350:BCL:HBA2	2:M:208:TYR:HE1	1.55	0.71
1:L:212:GLU:HA	7:L:800:UQ:HM21	1.71	0.71
1:L:86:TRP:O	1:L:90:THR:HG22	1.90	0.71
2:M:144:THR:O	2:M:147:ALA:HB3	1.88	0.71
2:M:113:TRP:CZ2	2:M:172:ALA:HB3	2.25	0.71
5:L:450:BCL:HMB1	5:L:450:BCL:HBB2	1.70	0.71
1:L:185:LEU:CA	6:M:500:BPH:HMC2	2.20	0.71
3:H:37:ARG:HB3	3:H:75:VAL:CG1	2.20	0.71
2:M:165:LEU:H	2:M:165:LEU:HD23	1.53	0.71
2:M:115:ILE:CG2	2:M:119:PHE:HE2	2.02	0.71
1:L:54:VAL:C	1:L:55:LEU:O	2.24	0.71
3:H:245:ALA:CB	3:H:248:ARG:HG3	2.17	0.71
2:M:235:GLN:HE21	2:M:260:MET:CE	2.03	0.71
1:L:217:ARG:NH2	2:M:17:ASP:OD2	2.24	0.71
1:L:222:TYR:CE2	2:M:38:LEU:HD21	2.26	0.71
2:M:195:PHE:CE2	5:M:400:BCL:HMC2	2.26	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
2:M:288:VAL:HB	3:H:4:VAL:HG13	1.72	0.70
5:M:400:BCL:H42	6:M:500:BPH:CHC	2.21	0.70
1:L:20:ASN:ND2	1:L:23:ASP:HB3	2.06	0.70
1:L:187:LEU:HD23	1:L:187:LEU:C	2.12	0.70
5:L:350:BCL:C7	5:L:450:BCL:CBB	2.69	0.70
1:L:274:ASN:O	1:L:275:ILE:CB	2.39	0.70
2:M:13:ARG:CG	2:M:14:GLY:H	2.01	0.70
2:M:87:ASP:HB2	2:M:91:PHE:CE2	2.27	0.70
2:M:256:PHE:HE1	7:M:750:UQ:H252	1.55	0.70
1:L:168:HIS:NE2	5:M:601:BCL:HMD3	2.07	0.70
5: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	7:L:800:UQ:H153	1.69	0.70
2:M:117:SER:HA	2:M:175:TYR:OH	1.92	0.70
2:M:182:ASP:O	2:M:185:ASN:HB3	1.90	0.70
1:L:264:GLN:HA	1:L:267:VAL:CG2	2.21	0.70
2:M:68:THR:O	2:M:72:TRP:HB2	1.92	0.70
3:H:167:ILE:HG23	3:H:179:LEU:HD12	1.74	0.70
2:M:171:GLU:O	2:M:172:ALA:HB3	1.90	0.69
1:L:68:PRO:HD3	1:L:147:PRO:HA	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:450:BCL:HMD2	5:M:400:BCL:HBB3	1.73	0.69
5:M:400:BCL:HBD	5: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
5:M:400:BCL:H43	6: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
7:L:800:UQ:C25	2:M:127:TRP:CZ2	2.76	0.69
2:M:250:TRP:HE1	7:M:750:UQ:CM5	2.05	0.69
2:M:24:VAL:HG11	2:M:26:LEU:HB2	1.74	0.69
1:L:1:ALA:CB	1:L:7:ARG:HG2	2.21	0.69
1:L:65:SER:OG	1:L:66:VAL:N	2.26	0.69
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
3:H:134:MET:HE1	3:H:142:VAL:HG22	1.75	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
5:L:450:BCL:CBB	5:L:450:BCL:HMB1	2.23	0.68
2:M:153:TRP:CH2	2:M:283:LEU:CD1	2.76	0.68
3:H:135:LYS:HG3	3:H:166:ASP:OD2	1.94	0.68
1:L:187:LEU:HD23	1:L:187:LEU:O	1.94	0.68
2:M:97:ALA:C	2:M:99:GLU:N	2.47	0.68
1:L:212:GLU:CA	7: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
1:L:168:HIS:CE1	5:L:350:BCL:HMC2	2.29	0.68
3:H:27:LEU:HD21	3:H:32:GLN:NE2	2.09	0.68
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.75	0.68
2:M:95:PRO:CB	2:M:96:PRO:HD2	2.24	0.68
1:L:180:PHE:CD1	1:L:240:ALA:HB1	2.28	0.67
2:M:216:MET:HG2	2:M:250:TRP:CZ2	2.29	0.67
2:M:72:TRP:CE3	2:M:72:TRP:HA	2.28	0.67
1:L:214:THR:O	1:L:218:ASP:HB2	1.93	0.67
2:M:50:TYR:C	2:M:51:LEU:HG	2.13	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
3:H:104:PRO:HB3	3:H:243:TYR:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:400:BCL:C4	6:M:500:BPH:CAB	2.73	0.67
1:L:59:TRP:O	1:L:60:ASN:HB2	1.95	0.67
5:L:350:BCL:C2	6:L:550:BPH:HBB3	2.25	0.66
3:H:63:THR:HA	3:H:74:THR:HG23	1.77	0.66
5:M:400:BCL:H142	6:M:500:BPH:H2	1.75	0.66
1:L:185:LEU:CD2	7:L:800:UQ:C15	2.64	0.66
1:L:80:LEU:CD1	1:L:85:LEU:HD21	2.26	0.66
2:M:29:ARG:HG2	2:M:29:ARG:HH11	1.61	0.66
2:M:101:GLY:C	2:M:168:SER:HA	2.15	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
2:M:72:TRP:CD1	2:M:112:LEU:HB3	2.30	0.66
2:M:235:GLN:HB2	2:M:260:MET:HE2	1.76	0.66
2:M:54:LEU:HD22	2:M:129:GLY:HA3	1.77	0.66
2:M:102:LEU:CA	2:M:169:TRP:CD1	2.71	0.66
2:M:72:TRP:HZ3	2:M:75:TYR:HB2	1.61	0.66
1:L:172:ALA:HB1	1:L:243:PHE:O	1.96	0.66
5:L:450:BCL:HMD2	5:M:400:BCL:CBB	2.26	0.66
2:M:4:GLN:HG3	3:H:193:MET:C	2.16	0.66
1:L:183:ASN:CG	1:L:236:LEU:HB2	2.13	0.65
2:M:265:ARG:O	2:M:269:TRP:CD1	2.49	0.65
2:M:58:SER:OG	6:M:500:BPH:H4C2	1.96	0.65
1:L:117:ILE:HD13	2:M:249:PHE:HE2	1.57	0.65
1:L:213:ASP:O	1:L:217:ARG:HB2	1.95	0.65
2:M:239:ARG:HD3	3:H:38:GLU:OE1	1.96	0.65
3:H:244:ALA:O	3:H:245:ALA:C	2.32	0.65
1:L:127:ALA:O	1:L:131:LEU:HG	1.96	0.65
3:H:88:ALA:O	3:H:98:HIS:HB3	1.97	0.65
5:L:450:BCL:HMD3	2:M:195:PHE:HE1	1.61	0.65
1:L:218:ASP:CG	2:M:50:TYR:CE1	2.68	0.65
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
1:L:193:LEU:HD21	1:L:215:PHE:CE2	2.32	0.65
3:H:209:SER:C	3:H:211:ASP:H	1.98	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
1:L:20:ASN:HD22	1:L:23:ASP:HB3	1.62	0.64
2:M:158:LEU:HD21	2:M:183:TRP:CH2	2.32	0.64
2:M:254:MET:CE	7:M:750:UQ:C11	2.67	0.64
2:M:265:ARG:O	2:M:269:TRP:HD1	1.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:74:GLY:O	1:L:75:LEU:HB2	1.96	0.64
2:M:157:VAL:HG13	2:M:162:ARG:HB2	1.77	0.64
3:H:216:ILE:HG12	3:H:236:TYR:CE1	2.32	0.64
3:H:115:VAL:HG12	3:H:116:ALA:H	1.62	0.64
2:M:204:ILE:HG12	5: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	5:M:400:BCL:H2	1.80	0.64
1:L:86:TRP:HZ3	1:L:142:TRP:HB3	1.63	0.63
2:M:81:PRO:C	2:M:85:LEU:HD12	2.19	0.63
3:H:5:THR:HG23	3:H:10:PHE:N	2.13	0.63
2:M:199:PHE:CE1	2:M:280:ILE:HG22	2.33	0.63
2:M:31:VAL:HG23	2:M:33:PRO:HD3	1.81	0.63
1:L:43:ALA:O	1:L:47:ILE:HB	1.98	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:141:ALA:C	1:L:143:GLY:H	2.02	0.63
1:L:41:PHE:HD2	1:L:92:CYS:HA	1.63	0.63
2:M:72:TRP:HE3	2:M:72:TRP:HA	1.64	0.63
7:M:750:UQ:C25	7:M:750:UQ:H211	2.28	0.63
1:L:218:ASP:CB	2:M:50:TYR:HE1	2.08	0.63
3:H:118:ARG:NH2	3:H:120:LEU:HD21	2.13	0.63
1:L:218:ASP:HB3	2:M:50:TYR:HE1	1.62	0.63
3:H:152:PRO:HG2	3:H:201:ASN:O	1.98	0.63
1:L:172:ALA:O	1:L:175:ILE:N	2.32	0.63
5:L:350:BCL:CBB	5:L:350:BCL:HMB1	2.29	0.63
1:L:156:TRP:CH2	1:L:248:MET:HE3	2.34	0.63
2:M:264:HIS:O	2:M:267:ALA:HB3	1.99	0.63
1:L:175:ILE:HG21	1:L:243:PHE:CD2	2.33	0.62
2:M:113:TRP:CZ3	2:M:169:TRP:CE3	2.82	0.62
1:L:185:LEU:HA	6:M:500:BPH:HMC2	1.79	0.62
2:M:108:LYS:HG2	2:M:108:LYS:O	1.97	0.62
2:M:45:GLN:HG2	2:M:47:GLY:O	1.99	0.62
3:H:36:MET:O	3:H:40:TYR:HB2	1.99	0.62
2:M:234:GLU:OE2	3:H:123:LEU:HD11	1.99	0.62
5:L:350:BCL:C2	6:L:550:BPH:CBB	2.76	0.62
3:H:149:ILE:C	3:H:164:VAL:HB	2.20	0.62
1:L:44:LEU:HA	1:L:47:ILE:CG2	2.29	0.62
1:L:193:LEU:HD11	1:L:216:PHE:CD1	2.33	0.62
1:L:269:LEU:HG	1:L:270:PRO:HD2	1.81	0.62
1:L:112:GLY:O	2:M:226:ARG:NH2	2.33	0.62
2:M:199:PHE:HB3	2:M:277:THR:O	1.99	0.62

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:THR:O	3:H:34:GLU:HB2	1.99	0.61
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: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
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
2:M:29(A):SER:OG	2:M:51:LEU:HD11	2.01	0.61
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.83	0.61
7:M:750:UQ:C12	7:M:750:UQ:C14	2.71	0.61
3:H:63:THR:CA	3:H:74:THR:HG23	2.30	0.61
3:H:56:PHE:N	3:H:57:PRO:CD	2.63	0.61
2:M:113:TRP:HZ3	2:M:169:TRP:CE3	2.13	0.60
1:L:200:PRO:HG2	1:L:205:GLU:O	2.01	0.60
3:H:123:LEU:O	3:H:124:ASP:HB2	2.00	0.60
2:M:278:GLY:O	2:M:282:ILE:HG12	2.01	0.60
3:H:165:VAL:O	3:H:166:ASP:HB2	2.00	0.60
2:M:4:GLN:CD	3:H:193:MET:HG3	2.22	0.60
2:M:164:ILE:C	2:M:166:MET:H	2.04	0.60
5:M:400:BCL:HMB1	5:M:400:BCL:HBB2	1.82	0.60
2:M:256:PHE:CE1	7: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
1:L:17:VAL:HG22	1:L:33:PHE:HB2	1.82	0.60
2:M:96:PRO:CG	2:M:170:SER:N	2.63	0.60
1:L:44:LEU:HA	1:L:47:ILE:HB	1.83	0.60
5:M:601:BCL:HBC1	5:M:400:BCL:HBA1	1.82	0.60
3:H:87:LEU:HG	3:H:109:VAL:HG11	1.82	0.60
2:M:157:VAL:HA	2:M:161:ILE:CG2	2.30	0.60
2:M:95:PRO:CB	2:M:96:PRO:CD	2.79	0.60
1:L:133:LEU:O	1:L:137:VAL:HG23	2.01	0.60
2:M:204:ILE:HG12	5:M:400:BCL:C1B	2.32	0.60
1:L:194:VAL:O	1:L:195:LEU:C	2.39	0.60
1:L:227:LEU:CD2	1:L:231:ARG:NH2	2.63	0.60
5:M:400:BCL:H43	6:M:500:BPH:HBB2	1.83	0.60
1:L:274:ASN:O	1:L:275:ILE:HG12	2.01	0.60
2:M:4:GLN:CG	3:H:193:MET:O	2.43	0.60
1:L:127:ALA:HB3	5:L:350:BCL:C4	2.31	0.60
2:M:251:ARG:NH1	2:M:251:ARG:HG3	2.16	0.60
3:H:70:ARG:HG2	3:H:70:ARG:HH11	1.67	0.60
2:M:21:THR:HG23	2:M:50:TYR:OH	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:128:TRP:HE1	2:M:145:ALA:CB	2.11	0.59
2:M:244:GLU:O	2:M:247:ALA:N	2.36	0.59
1:L:97:PHE:O	1:L:100:TRP:HB3	2.02	0.59
1:L:152:THR:HA	2:M:303:PRO:HB3	1.85	0.59
2:M:71:ILE:O	2:M:74:TRP:HB3	2.02	0.59
1:L:1:ALA:HB2	1:L:7:ARG:CG	2.28	0.59
1:L:53:ALA:CB	1:L:64:ILE:HG13	2.33	0.59
2:M:235:GLN:NE2	2:M:260:MET:CE	2.64	0.59
1:L:104:GLU:HA	1:L:107:ILE:CD1	2.32	0.59
2:M:158:LEU:HD23	2:M:173:VAL:CG2	2.32	0.59
7:M:750:UQ:H252	7:M:750:UQ:H211	1.83	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	5:M:400:BCL:HED1	1.85	0.59
3:H:37:ARG:HB3	3:H:75:VAL:HG11	1.83	0.59
3:H:111:PRO:HD2	3:H:243:TYR:CZ	2.37	0.59
1:L:86:TRP:CZ3	1:L:142:TRP:HB3	2.37	0.59
2:M:154:LEU:CD1	2:M:275:THR:HG22	2.31	0.59
2:M:59:LEU:O	2:M:63:LEU:HB2	2.03	0.59
3:H:237:VAL:O	3:H:239:GLY:N	2.36	0.59
1:L:185:LEU:CG	1:L:186:ALA:N	2.62	0.58
1:L:51:TRP:CZ2	1:L:80:LEU:HD21	2.39	0.58
3:H:66:LEU:HB2	3:H:71:GLY:HA2	1.85	0.58
2:M:158:LEU:HD23	2:M:173:VAL:HG21	1.85	0.58
3:H:170:ASP:CG	3:H:173:GLU:HB3	2.23	0.58
2:M:193:ASN:C	2:M:195:PHE:H	2.07	0.58
1:L:116:HIS:HB2	2:M:223:ALA:HB2	1.85	0.58
2:M:259:THR:O	2:M:261:GLU:N	2.36	0.58
1:L:231:ARG:NE	2:M:6:ILE:N	2.37	0.58
1:L:55:LEU:HG	1:L:56:GLN:N	2.17	0.58
3:H:65:ILE:O	3:H:66:LEU:O	2.22	0.58
1:L:185:LEU:HD23	1:L:186:ALA:N	2.18	0.58
2:M:92:SER:HA	2:M:175:TYR:O	2.04	0.58
1:L:185:LEU:HD22	7:L:800:UQ:C15	2.31	0.58
2:M:97:ALA:CB	2:M:98:PRO:CD	2.82	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
2:M:218:GLY:O	2:M:222:LEU:HD12	2.03	0.57
2:M:165:LEU:N	2:M:165:LEU:CD2	2.64	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:114:TRP:CG	3:H:232:LYS:HG3	2.39	0.57
3:H:207:ALA:HB3	3:H:237:VAL:HG12	1.85	0.57
1:L:229:ILE:HB	7:L:800:UQ:HM53	1.86	0.57
2:M:113:TRP:CZ2	2:M:172:ALA:HB1	2.30	0.57
2:M:97:ALA:CB	2:M:98:PRO:HD3	2.31	0.57
1:L:3:LEU:CB	1:L:6:GLU:HB2	2.24	0.57
2:M:259:THR:C	2:M:261:GLU:N	2.57	0.57
3:H:122:GLU:HA	3:H:227:LEU:HD21	1.86	0.57
3:H:111:PRO:HD2	3:H:243:TYR:HE2	1.60	0.57
3:H:67:PRO:HG2	3:H:123:LEU:CD2	2.28	0.57
5:L:350:BCL:CAA	5:L:450:BCL:HBC1	2.34	0.57
5:L:350:BCL:CBD	5:L:450:BCL:HBC1	2.11	0.57
2:M:148:PHE:CZ	2:M:152:ILE:HD11	2.40	0.57
2:M:238:ASP:OD2	3:H:117:ARG:HG3	2.04	0.57
1:L:13:GLY:HA3	3:H:242:MET:HE1	1.86	0.57
2:M:124:VAL:CG1	2:M:152:ILE:HD12	2.34	0.57
2:M:97:ALA:O	2:M:99:GLU:N	2.38	0.57
1:L:169:TYR:CD2	1:L:260:VAL:HG22	2.38	0.57
2:M:217:HIS:HD1	2:M:263:ILE:HG12	1.70	0.57
2:M:278:GLY:CA	5:M:400:BCL:HED3	2.33	0.57
2:M:106:PRO:O	2:M:108:LYS:N	2.38	0.57
1:L:206:MET:HE1	2:M:237:ALA:HB2	1.85	0.57
3:H:121:PRO:O	3:H:122:GLU:C	2.43	0.57
2:M:216:MET:CG	2:M:250:TRP:CZ2	2.88	0.57
3:H:131:ILE:HD13	3:H:131:ILE:N	2.20	0.57
1:L:11:VAL:HG21	3:H:111:PRO:HD3	1.87	0.57
2:M:87:ASP:O	2:M:88:LEU:HB3	2.03	0.57
1:L:169:TYR:CD1	1:L:260:VAL:HG22	2.40	0.57
3:H:141:HIS:HE1	3:H:143:SER:HB2	1.69	0.57
3:H:5:THR:HG21	3:H:9:ASN:HA	1.86	0.57
1:L:156:TRP:CH2	1:L:248:MET:CE	2.87	0.57
2:M:164:ILE:O	2:M:166:MET:N	2.38	0.57
2:M:79:TRP:HB3	2:M:80:ASN:OD1	2.05	0.57
3:H:208:LEU:HD13	3:H:216:ILE:HD11	1.86	0.57
3:H:124:ASP:HB3	3:H:128:HIS:O	2.05	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:250:TRP:NE1	7:M:750:UQ:HM53	2.17	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:149:ILE:H	3:H:164:VAL:HG11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:134:MET:CE	3:H:142:VAL:HG22	2.33	0.56
2:M:164:ILE:C	2:M:166:MET:N	2.56	0.56
2:M:274:VAL:CG1	2:M:275:THR:H	2.06	0.56
2:M:25:ASN:N	2:M:25:ASN:ND2	2.54	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
1:L:13:GLY:N	1:L:110:LYS:HE2	2.20	0.56
2:M:184:THR:CG2	2:M:185:ASN:N	2.68	0.56
2:M:221:ILE:O	2:M:225:SER:OG	2.21	0.56
2:M:272:VAL:C	2:M:274:VAL:N	2.59	0.56
2:M:202:LEU:HD23	3:H:20:PHE:CE2	2.36	0.56
3:H:205:VAL:HG12	3:H:206:ASN:N	2.20	0.56
1:L:10:ARG:HG3	1:L:25:TRP:CZ3	2.39	0.56
2:M:250:TRP:NE1	7:M:750:UQ:CM5	2.67	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
2:M:254:MET:SD	7:M:750:UQ:H203	2.45	0.56
3:H:159:GLU:CG	3:H:160:ILE:H	2.19	0.56
1:L:260:VAL:O	1:L:263:TRP:HB2	2.04	0.56
2:M:272:VAL:C	2:M:274:VAL:H	2.09	0.56
3:H:83:ARG:HB3	3:H:84:PRO:HD2	1.88	0.56
6:L:550:BPH:HBB2	6:L:550:BPH:HHC	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
6:M:500:BPH:O1A	6:M:500:BPH:H3A	2.06	0.56
1:L:122:ALA:O	1:L:123:PHE:C	2.44	0.56
1:L:61:PRO:HA	1:L:64:ILE:HG22	1.87	0.56
2:M:99:GLU:O	2:M:100:TYR:CB	2.37	0.56
3:H:1:MET:CG	3:H:2:VAL:H	2.19	0.56
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
2:M:74:TRP:C	2:M:74:TRP:CD1	2.80	0.55
2:M:15:PRO:HD2	3:H:140:PHE:CD1	2.42	0.55
1:L:60:ASN:C	1:L:62:GLN:H	2.08	0.55
2:M:96:PRO:CG	2:M:170:SER:CA	2.50	0.55
1:L:25:TRP:HB3	1:L:29:PHE:O	2.06	0.55
1:L:111:LEU:HB2	1:L:113:ILE:CG1	2.36	0.55

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:294:VAL:O	2:M:298:ASN:N	2.41	0.54
3:H:192:PRO:HG3	3:H:237:VAL:HG21	1.87	0.54
3:H:75:VAL:C	3:H:77:GLY:H	2.11	0.54
1:L:141:ALA:C	1:L:143:GLY:N	2.61	0.54
3:H:36:MET:HG2	3:H:40:TYR:CE2	2.42	0.54
3:H:189:ARG:HH21	3:H:218:THR:CG2	2.21	0.54
2:M:92:SER:O	2:M:93:LEU:HD23	2.08	0.53
1:L:190:HIS:CG	1:L:229:ILE:HG12	2.43	0.53
1:L:190:HIS:O	1:L:194:VAL:HG23	2.08	0.53
1:L:107:ILE:HD13	2:M:253:THR:OG1	2.09	0.53
1:L:37:ALA:CA	1:L:40:PHE:HB2	2.37	0.53
3:H:151:LEU:CD2	3:H:203:VAL:HG21	2.37	0.53
1:L:20:ASN:CG	1:L:21:LEU:H	2.12	0.53
2:M:179:SER:C	2:M:181:LEU:N	2.61	0.53
2:M:96:PRO:HD2	2:M:170:SER:HA	1.91	0.53
1:L:174:MET:CE	5:M:601:BCL:HED2	2.38	0.53
3:H:105:MET:CE	3:H:212:LEU:HD22	2.37	0.53
5:L:350:BCL:H152	6:L:550:BPH:O2A	2.06	0.53
2:M:216:MET:CG	2:M:250:TRP:HZ2	2.21	0.53
2:M:25:ASN:HD22	2:M:25:ASN:H	1.56	0.53
1:L:54:VAL:O	1:L:55:LEU:O	2.26	0.53
3:H:105:MET:HE1	3:H:212:LEU:HD13	1.90	0.53
1:L:175:ILE:HG22	1:L:179:PHE:CE1	2.44	0.53
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.90	0.53
3:H:28:ILE:HG22	3:H:29:TYR:H	1.73	0.53
3:H:83:ARG:HB3	3:H:84:PRO:CD	2.38	0.53
3:H:66:LEU:HB2	3:H:71:GLY:CA	2.38	0.53
1:L:41:PHE:HB2	1:L:96:ALA:HB2	1.89	0.53
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:174:GLN:O	3:H:175:MET:HB2	2.09	0.53
1:L:169:TYR:CD2	1:L:260:VAL:HG13	2.44	0.53
1:L:103:ARG:O	1:L:107:ILE:HG13	2.09	0.52
1:L:158:SER:O	1:L:162:TYR:CD2	2.58	0.52
1:L:241:VAL:HA	1:L:244:SER:HB3	1.89	0.52
2:M:187:PHE:HD2	5:M:400:BCL:HMD3	1.75	0.52
2:M:119:PHE:HA	2:M:122:VAL:HG23	1.91	0.52
1:L:12:PRO:HD3	3:H:97:PRO:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:TYR:O	1:L:163:THR:C	2.48	0.52
1:L:62:GLN:HA	1:L:150:ILE:HB	1.90	0.52
2:M:216:MET:HE3	7:M:750:UQ:H13	1.92	0.52
3:H:30:TYR:O	3:H:33:THR:HB	2.09	0.52
1:L:177:ILE:HD13	5:L:350:BCL:HMB3	1.92	0.52
2:M:158:LEU:CD2	2:M:183:TRP:CH2	2.92	0.52
3:H:27:LEU:CG	3:H:32:GLN:HB2	2.39	0.52
3:H:13:ALA:O	3:H:16:ALA:HB3	2.10	0.52
3:H:66:LEU:HB3	3:H:67:PRO:CD	2.37	0.52
1:L:93:ALA:HB1	1:L:97:PHE:CE2	2.45	0.52
2:M:66:PHE:CD2	6:M:500:BPH:H111	2.45	0.52
1:L:48:LEU:O	1:L:51:TRP:HB3	2.09	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:153:TRP:CH2	2:M:283:LEU:HD12	2.45	0.52
2:M:72:TRP:CB	2:M:93:LEU:HD13	2.39	0.52
2:M:12:VAL:HG21	3:H:169:VAL:HG11	1.92	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
3:H:6:ALA:HB3	3:H:10:PHE:O	2.10	0.52
1:L:172:ALA:O	1:L:173:HIS:C	2.47	0.52
1:L:242:PHE:C	1:L:242:PHE:CD1	2.83	0.52
7:L:800:UQ:H251	2:M:127:TRP:CZ2	2.45	0.52
2:M:162:ARG:HD2	2:M:163:PRO:N	2.25	0.52
2:M:179:SER:O	2:M:180:HIS:C	2.45	0.52
2:M:250:TRP:HB3	2:M:254:MET:HG3	1.91	0.52
3:H:61:PRO:CB	3:H:76:PRO:HG3	2.39	0.52
2:M:4:GLN:CB	3:H:194:GLN:HA	2.40	0.51
1:L:183:ASN:HA	1:L:186:ALA:HB3	1.92	0.51
7: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
1:L:274:ASN:O	1:L:275:ILE:CG1	2.58	0.51
1:L:176:ALA:O	1:L:180:PHE:CD1	2.60	0.51
2:M:113:TRP:CH2	2:M:172:ALA:HB3	2.44	0.51
2:M:291:ASN:OD1	2:M:294:VAL:HG23	2.10	0.51
3:H:27:LEU:O	3:H:28:ILE:O	2.27	0.51

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:400:BCL:C4	6:M:500:BPH:CHC	2.89	0.50
3:H:61:PRO:HB2	3:H:74:THR:HG21	1.92	0.50
3:H:242:MET:HG2	3:H:249:LYS:HB3	1.94	0.50
2:M:179:SER:O	2:M:181:LEU:N	2.45	0.50
2:M:72:TRP:HB3	2:M:93:LEU:HD22	1.93	0.50
1:L:47:ILE:HG22	1:L:48:LEU:HG	1.93	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:56:VAL:HG13	2:M:57:LEU:N	2.25	0.50
2:M:244:GLU:O	2:M:247:ALA:HB3	2.12	0.50
1:L:271:TRP:HB2	1:L:274:ASN:ND2	2.25	0.50
2:M:101:GLY:O	2:M:169:TRP:N	2.40	0.50
5:M:400:BCL:HBB3	5:M:400:BCL:HMB1	1.91	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
2:M:77:ALA:O	2:M:83:VAL:HG11	2.12	0.50
3:H:91:ALA:HB3	3:H:96:PHE:CG	2.47	0.50
1:L:100:TRP:CZ2	1:L:103:ARG:NH2	2.80	0.50
1:L:116:HIS:C	1:L:118:PRO:HD2	2.31	0.50
1:L:122:ALA:C	1:L:124:ALA:N	2.64	0.50
1:L:208:THR:HB	1:L:209:PRO:HD2	1.92	0.50
1:L:230:HIS:O	2:M:222:LEU:HD11	2.12	0.50
2:M:263:ILE:HG23	2:M:264:HIS:N	2.27	0.50
2:M:271:ALA:O	2:M:274:VAL:CB	2.57	0.50
2:M:69:ILE:CG1	2:M:93:LEU:HD12	2.38	0.50
3:H:170:ASP:HB2	3:H:175:MET:O	2.11	0.49
3:H:8:GLY:O	3:H:9:ASN:CB	2.57	0.49
1:L:118:PRO:O	1:L:121:PHE:HB3	2.12	0.49
5:M:601:BCL:HAC1	5:M:400:BCL:C3D	2.42	0.49
5:M:601:BCL:HMA1	5:M:400:BCL:C20	2.41	0.49
3:H:91:ALA:HB3	3:H:96:PHE:HB3	1.93	0.49
2:M:8:SER:O	2:M:9:GLN:CB	2.58	0.49
1:L:13:GLY:H	1:L:110:LYS:CE	2.21	0.49
1:L:152:THR:O	1:L:154:LEU:N	2.45	0.49
1:L:181:PHE:CE1	5:M:400:BCL:HAA1	2.47	0.49
5:L:350:BCL:H122	6:L:550:BPH:HBA1	1.93	0.49
1:L:93:ALA:O	1:L:96:ALA:HB3	2.12	0.49
2:M:184:THR:HG23	2:M:185:ASN:N	2.27	0.49
2:M:266:TRP:HE1	3:H:35:ASN:HD21	1.59	0.49
1:L:218:ASP:CB	2:M:50:TYR:CD1	2.95	0.49
3:H:36:MET:HG2	3:H:40:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:12:VAL:HG11	3:H:169:VAL:HG21	1.94	0.49
1:L:158:SER:C	1:L:162:TYR:HD2	2.16	0.49
5:L:350:BCL:H71	5:L:450:BCL:HBB2	1.93	0.49
3:H:135:LYS:HZ1	3:H:165:VAL:CG1	2.25	0.49
3:H:134:MET:SD	3:H:142:VAL:HG22	2.52	0.49
1:L:234:LEU:O	1:L:238:LEU:HB2	2.12	0.49
2:M:72:TRP:HB3	2:M:93:LEU:CD2	2.42	0.49
1:L:275:ILE:C	1:L:276:PRO:O	2.50	0.49
3:H:190:LEU:H	3:H:190:LEU:HD23	1.76	0.49
2:M:37:LEU:HA	2:M:40:TRP:CD1	2.48	0.49
3:H:110:GLY:C	3:H:112:ALA:H	2.15	0.49
3:H:67:PRO:HB2	3:H:68:HIS:CE1	2.47	0.49
3:H:160:ILE:C	3:H:162:GLY:N	2.64	0.49
2:M:54:LEU:CD2	2:M:129:GLY:HA3	2.43	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:13:GLY:O	1:L:14:GLY:C	2.50	0.49
1:L:128:TYR:CD2	5: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: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
3:H:171:ILE:CB	3:H:172:PRO:CD	2.91	0.49
1:L:128:TYR:HD1	1:L:128:TYR:C	2.16	0.49
1:L:131:LEU:HD23	1:L:131:LEU:N	2.28	0.49
2:M:178:PHE:O	2:M:181:LEU:HB2	2.13	0.49
2:M:73:PHE:CG	2:M:91:PHE:HB3	2.48	0.49
3:H:149:ILE:N	3:H:164:VAL:HB	2.28	0.49
2:M:56:VAL:CG1	2:M:57:LEU:N	2.76	0.49
2:M:208:TYR:O	2:M:211:ALA:HB3	2.13	0.48
3:H:209:SER:C	3:H:211:ASP:N	2.66	0.48
3:H:1:MET:HG2	3:H:2:VAL:H	1.77	0.48
1:L:97:PHE:CE1	5:L:350:BCL:H112	2.48	0.48
2:M:284:LEU:O	2:M:288:VAL:HG22	2.12	0.48
2:M:69:ILE:O	2:M:73:PHE:N	2.45	0.48
1:L:43:ALA:C	1:L:45:GLY:N	2.66	0.48
1:L:150:ILE:HG12	6:L:550:BPH:H191	1.95	0.48
1:L:212:GLU:HA	2:M:140:MET:CE	2.44	0.48
2:M:235:GLN:NE2	2:M:260:MET:HE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:250:TRP:CD1	7:M:750:UQ:HM51	2.48	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
5:L:450:BCL:HMD3	2:M:195:PHE:CE1	2.45	0.48
2:M:212:LEU:HD23	2:M:212:LEU:C	2.33	0.48
2:M:4:GLN:OE1	3:H:193:MET:HG3	2.12	0.48
2:M:157:VAL:HA	2:M:162:ARG:H	1.77	0.48
1:L:141:ALA:O	1:L:143:GLY:N	2.32	0.48
1:L:80:LEU:HD12	1:L:85:LEU:CD2	2.44	0.48
2:M:161:ILE:HG22	2:M:162:ARG:H	1.79	0.48
2:M:113:TRP:CH2	2:M:172:ALA:CB	2.96	0.48
2:M:136:GLN:O	2:M:137:ALA:HB2	2.13	0.48
3:H:208:LEU:CD1	3:H:216:ILE:HD11	2.44	0.48
3:H:24:LEU:C	3:H:26:GLY:N	2.66	0.48
1:L:61:PRO:O	1:L:150:ILE:HD12	2.14	0.48
1:L:168:HIS:CD2	5:M:601:BCL:HMD3	2.48	0.48
6:M:500:BPH:H1C2	6:M:500:BPH:HAA2	1.95	0.48
1:L:85:LEU:O	1:L:89:ILE:HD12	2.12	0.48
2:M:83:VAL:HG22	2:M:86:ARG:NH1	2.26	0.48
3:H:80:SER:OG	3:H:81:GLU:N	2.45	0.48
1:L:155:ASP:O	1:L:159:ASN:HB2	2.13	0.48
1:L:212:GLU:HB3	7:L:800:UQ:CM2	2.44	0.48
6:M:500:BPH:H13	6:M:500:BPH:H101	1.69	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
3:H:177:ARG:O	3:H:193:MET:CB	2.61	0.48
1:L:13:GLY:HA2	3:H:242:MET:HE3	1.95	0.48
1:L:212:GLU:CB	7:L:800:UQ:HM21	2.44	0.48
1:L:86:TRP:CZ3	1:L:142:TRP:HE3	2.32	0.48
2:M:148:PHE:O	2:M:152:ILE:HG12	2.14	0.48
2:M:151:ALA:O	5:M:400:BCL:H52	2.13	0.48
1:L:74:GLY:CA	1:L:141:ALA:HB2	2.26	0.48
2:M:74:TRP:O	2:M:77:ALA:N	2.47	0.48
1:L:212:GLU:CA	2:M:140:MET:HE3	2.44	0.48
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.13	0.48
2:M:188:SER:CB	2:M:194:LEU:HB2	2.43	0.48
1:L:128:TYR:C	1:L:128:TYR:CD1	2.87	0.47
1:L:151:TRP:O	2:M:303:PRO:CB	2.58	0.47
2:M: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:195:MET:CE	3:H:238:ALA:HB2	2.45	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
1:L:56:GLN:C	1:L:57:GLY:O	2.52	0.46
2:M:68:THR:HG23	2:M:112:LEU:CD1	2.39	0.46
3:H:154:ARG:NH1	3:H:158:LEU:CD1	2.78	0.46
3:H:5:THR:CG2	3:H:10:PHE:H	2.23	0.46
1:L:185:LEU:HG	1:L:186:ALA:N	2.22	0.46
2:M:265:ARG:O	2:M:268:ILE:HG23	2.15	0.46
2:M:269:TRP:HA	2:M:269:TRP:CE3	2.49	0.46
1:L:231:ARG:CZ	2:M:6:ILE:H	2.24	0.46
1:L:141:ALA:H	1:L:144:TYR:HE1	1.64	0.46
3:H:170:ASP:OD2	3:H:173:GLU:CB	2.55	0.46
1:L:132:VAL:HG22	1:L:146:PHE:CE1	2.50	0.46
1:L:171:PRO:O	1:L:174:MET:HB3	2.15	0.46
1:L:215:PHE:HD1	2:M:138:LEU:CD2	2.27	0.46
2:M:130:ARG:C	2:M:132:TYR:H	2.19	0.46
1:L:84:GLY:O	1:L:87:GLN:HB2	2.16	0.46
5:L:450:BCL:HBA1	5:L:450:BCL:H3A	1.73	0.46
2:M:148:PHE:HB2	6:M:500:BPH:C2D	2.46	0.46
2:M:278:GLY:O	5:M:400:BCL:HED3	2.15	0.46
2:M:65:TRP:CD2	2:M:66:PHE:N	2.83	0.46
1:L:49:ILE:HG22	1:L:50:ALA:N	2.31	0.46
1:L:117:ILE:HG21	2:M:250:TRP:CH2	2.50	0.46
1:L:226:THR:O	1:L:229:ILE:HG22	2.16	0.46
2:M:204:ILE:HG12	5:M:400:BCL:C2B	2.46	0.46
2:M:32:GLY:N	2:M:33:PRO:CD	2.78	0.46
1:L:177:ILE:HD12	5:M:601:BCL:CMD	2.46	0.46
7:M:750:UQ:HM23	7:M:750:UQ:O3	2.16	0.46
2:M:81:PRO:O	2:M:82:ALA:C	2.54	0.46
3:H:27:LEU:HD23	3:H:28:ILE:H	1.81	0.46
2:M:191:HIS:HA	2:M:290:ASP:O	2.16	0.46
1:L:181:PHE:HZ	5:M:400:BCL:HAA2	1.80	0.46
2:M:162:ARG:CB	2:M:163:PRO:CD	2.88	0.46
2:M:199:PHE:HA	2:M:277:THR:HG22	1.98	0.46
5:M:400:BCL:H62	5:M:400:BCL:H41	1.39	0.46
2:M:104:PHE:CD2	2:M:114:LEU:HD21	2.50	0.46
2:M:14:GLY:HA3	2:M:15:PRO:HD2	1.72	0.46
3:H:111:PRO:CD	3:H:243:TYR:CE2	2.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:LEU:O	1:L:193:LEU:CB	2.64	0.46
2:M:224:VAL:HG11	2:M:242:ALA:O	2.15	0.46
1:L:74:GLY:O	1:L:75:LEU:CB	2.64	0.46
3:H:164:VAL:O	3:H:165:VAL:HG22	2.10	0.46
1:L:250:ILE:HA	1:L:254:ILE:HB	1.97	0.46
3:H:67:PRO:CG	3:H:123:LEU:CD2	2.89	0.46
3:H:7:PHE:HB3	3:H:8:GLY:H	1.61	0.46
1:L:100:TRP:CH2	1:L:103:ARG:NH2	2.84	0.46
3:H:182:GLU:HG3	3:H:187:SER:C	2.36	0.46
3:H:118:ARG:HG3	3:H:227:LEU:HD12	1.98	0.45
2:M:148:PHE:CD1	6:M:500:BPH:C4D	2.99	0.45
2:M:162:ARG:HD3	2:M:166:MET:HE3	1.98	0.45
2:M:221:ILE:HD11	7:M:750:UQ:HM31	1.98	0.45
2:M:241:THR:HB	3:H:115:VAL:HG23	1.98	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
1:L:44:LEU:HA	1:L:47:ILE:CB	2.45	0.45
3:H:78:PRO:HG2	3:H:79:GLU:H	1.81	0.45
2:M:237:ALA:O	3:H:73:LEU:HD22	2.15	0.45
1:L:185:LEU:CD2	1:L:186:ALA:N	2.79	0.45
1:L:150:ILE:HA	6:L:550:BPH:H193	1.99	0.45
2:M:212:LEU:CD1	7:M:750:UQ:H161	2.47	0.45
3:H:154:ARG:NH1	3:H:158:LEU:HD11	2.31	0.45
3:H:183:LEU:N	3:H:186:GLY:O	2.50	0.45
3:H:79:GLU:O	3:H:80:SER:HB3	2.16	0.45
3:H:188:THR:O	3:H:189:ARG:CD	2.64	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
1:L:25:TRP:NE1	2:M:252:TRP:CD2	2.80	0.45
3:H:177:ARG:O	3:H:193:MET:HB3	2.16	0.45
3:H:111:PRO:CG	3:H:242:MET:SD	3.01	0.45
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
1:L:190:HIS:HE1	2:M:232:GLU:OE2	2.00	0.45
1:L:86:TRP:O	1:L:90:THR:CG2	2.64	0.45
2:M:212:LEU:HD21	7:M:750:UQ:C16	2.45	0.45
3:H:200:SER:O	3:H:201:ASN:HB3	2.17	0.45
2:M:227:PHE:CE2	3:H:235:GLY:HA2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:GLY:O	1:L:15:THR:HG23	2.16	0.45
5:M:601:BCL:O2D	5:M:601:BCL:H2A	2.17	0.45
2:M:67:PHE:O	2:M:69:ILE:N	2.50	0.45
2:M:88:LEU:HG	2:M:89:PHE:N	2.31	0.45
3:H:148:PRO:C	3:H:149:ILE:CG1	2.80	0.45
3:H:103:ASP:O	3:H:107:ASP:N	2.48	0.45
3:H:79:GLU:HB3	3:H:80:SER:H	1.43	0.45
3:H:27:LEU:HD11	3:H:32:GLN:HB2	1.97	0.45
2:M:28:ASN:ND2	2:M:29:ARG:H	2.15	0.45
1:L:251:THR:HG22	1:L:259:TRP:CZ2	2.52	0.45
1:L:193:LEU:HD11	1:L:216:PHE:HE1	1.66	0.45
1:L:240:ALA:O	1:L:244:SER:HB2	2.17	0.45
1:L:53:ALA:HB2	1:L:64:ILE:HG13	1.97	0.45
2:M:225:SER:HA	2:M:229:GLY:H	1.82	0.45
3:H:130:LYS:HE3	3:H:172:PRO:HG2	1.99	0.45
1:L:216:PHE:O	1:L:219:LEU:HB2	2.17	0.45
2:M:282:ILE:CG1	5:M:400:BCL:HED1	2.46	0.45
2:M:118:PHE:O	2:M:121:PHE:HB3	2.17	0.45
3:H:134:MET:SD	3:H:142:VAL:CG2	3.04	0.45
3:H:105:MET:CE	3:H:212:LEU:HD13	2.47	0.45
2:M:12:VAL:HG21	3:H:169:VAL:CG1	2.46	0.45
1:L:228:GLY:C	1:L:232:LEU:HD13	2.38	0.45
1:L:58:THR:HG21	1:L:63:LEU:HD11	1.99	0.45
2:M:66:PHE:HD1	2:M:67:PHE:HD1	1.65	0.45
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
2:M:74:TRP:O	2:M:77:ALA:CB	2.63	0.45
1:L:275:ILE:N	1:L:276:PRO:CD	2.80	0.45
1:L:26:VAL:O	1:L:26:VAL:HG13	2.17	0.45
2:M:216:MET:HE2	2:M:216:MET:HB3	1.86	0.44
3:H:149:ILE:H	3:H:164:VAL:CG1	2.29	0.44
1:L:261:ASP:O	1:L:264:GLN:N	2.43	0.44
1:L:185:LEU:HD23	1:L:186:ALA:CA	2.47	0.44
1:L:188:ALA:HB2	2:M:271:ALA:HB1	1.96	0.44
2:M:248:LEU:HD21	2:M:252:TRP:CZ2	2.51	0.44
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.99	0.44
1:L:106:GLU:O	1:L:109:ARG:HB2	2.17	0.44
2:M:153:TRP:CH2	2:M:283:LEU:HD11	2.53	0.44
5:M:400:BCL:C4	6:M:500:BPH:C4B	2.96	0.44
2:M:87:ASP:HB2	2:M:91:PHE:CD2	2.52	0.44
1:L:48:LEU:O	1:L:49:ILE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:107:ILE:O	1:L:111:LEU:HD12	2.18	0.44
1:L:86:TRP:HZ3	1:L:142:TRP:HE3	1.64	0.44
1:L:226:THR:CG2	2:M:230:GLU:HB2	2.47	0.44
2:M:276:LEU:HD23	2:M:276:LEU:HA	1.76	0.44
2:M:67:PHE:C	2:M:69:ILE:N	2.68	0.44
2:M:24:VAL:HG12	2:M:26:LEU:HB2	1.97	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: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
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
3:H:195:MET:HE1	3:H:238:ALA:HB2	2.00	0.44
1:L:117:ILE:CG2	2:M:250:TRP:CH2	3.00	0.44
2:M: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
2:M:13:ARG:O	3:H:140:PHE:CD2	2.71	0.44
2:M:130:ARG:C	2:M:132:TYR:N	2.71	0.44
1:L:206:MET:HE2	2:M:237:ALA:HB2	1.97	0.44
1:L:152:THR:HA	2:M:303:PRO:CB	2.47	0.44
1:L:168:HIS:HE1	5:L:350:BCL:HMC2	1.80	0.44
1:L:69:PRO:HD2	1:L:142:TRP:O	2.18	0.44
2:M:152:ILE:O	2:M:156:MET:N	2.46	0.44
1:L:5:PHE:HB2	2:M:244:GLU:CD	2.38	0.44
1:L:192:ALA:HB1	2:M:143:HIS:HB3	1.99	0.44
1:L:149:GLY:HA3	1:L:152:THR:HG23	1.93	0.44
2:M:24:VAL:HG12	2:M:25:ASN:N	2.33	0.44
2:M:16:ALA:CB	2:M:45:GLN:HE22	2.15	0.44
3:H:103:ASP:CB	3:H:106:LYS:HB3	2.48	0.44
2:M:29:ARG:HG2	2:M:29:ARG:NH1	2.29	0.44
3:H:245:ALA:HB3	3:H:248:ARG:CD	2.48	0.43
1:L:100:TRP:O	1:L:103:ARG:HB3	2.18	0.43
1:L:189:LEU:HD13	6:M:500:BPH:HED1	2.00	0.43
1:L:224:ILE:HG22	7:L:800:UQ:H103	1.99	0.43
1:L:230:HIS:ND1	2:M:221:ILE:CG2	2.76	0.43
2:M:158:LEU:HG	2:M:183:TRP:HH2	1.83	0.43
1:L:226:THR:HG22	2:M:230:GLU:HB2	1.99	0.43
1:L:226:THR:HG21	2:M:231:ARG:H	1.83	0.43
2:M:250:TRP:CD1	7:M:750:UQ:CM5	3.01	0.43
3:H:135:LYS:HZ3	3:H:165:VAL:HG12	1.72	0.43
2:M:121:PHE:O	2:M:125:TRP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:28:ILE:CG2	3:H:29:TYR:N	2.64	0.43
2:M:134:ARG:HA	2:M:134:ARG:HD3	1.36	0.43
3:H:237:VAL:O	3:H:238:ALA:C	2.57	0.43
3:H:239:GLY:O	3:H:243:TYR:HB2	2.17	0.43
1:L:172:ALA:O	1:L:175:ILE:HB	2.18	0.43
2:M:235:GLN:HE22	2:M:243:ALA:N	2.16	0.43
2:M:65:TRP:O	2:M:66:PHE:C	2.57	0.43
3:H:103:ASP:HB3	3:H:106:LYS:CB	2.48	0.43
2:M:162:ARG:NH2	2:M:187:PHE:CD1	2.86	0.43
1:L:75:LEU:CG	1:L:140:GLY:O	2.61	0.43
3:H:183:LEU:C	3:H:185:ASP:H	2.20	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
3:H:118:ARG:CG	3:H:227:LEU:HD12	2.48	0.43
2:M:234:GLU:HG2	3:H:123:LEU:HD12	1.99	0.43
2:M:193:ASN:C	2:M:195:PHE:N	2.70	0.43
2:M:230:GLU:O	2:M:231:ARG:C	2.55	0.43
2:M:35:SER:CB	2:M:38:LEU:HB3	2.43	0.43
3:H:181:VAL:CB	3:H:189:ARG:O	2.67	0.43
3:H:207:ALA:CB	3:H:237:VAL:HG12	2.48	0.43
3:H:240:GLY:O	3:H:244:ALA:CB	2.62	0.43
1:L:13:GLY:CA	3:H:242:MET:CE	2.96	0.43
1:L:215:PHE:CB	2:M:138:LEU:HD22	2.48	0.43
1:L:130:THR:CB	1:L:249:ILE:HD11	2.40	0.43
2:M:195:PHE:CE2	5:M:400:BCL:CMC	3.01	0.43
2:M:282:ILE:O	2:M:284:LEU:N	2.52	0.43
2:M:216:MET:HE1	7:M:750:UQ:H13	1.99	0.43
2:M:108:LYS:O	2:M:109:GLU:HB3	2.16	0.43
1:L:189:LEU:CD1	6:M:500:BPH:HED1	2.48	0.43
6:L:550:BPH:H2	6:L:550:BPH:H6C1	1.72	0.43
2:M:166:MET:SD	2:M:171:GLU:OE2	2.76	0.43
2:M:218:GLY:O	2:M:222:LEU:CD1	2.66	0.43
2:M:217:HIS:HE1	2:M:264:HIS:CE1	2.36	0.43
2:M:61:SER:O	2:M:62:GLY:C	2.57	0.43
1:L:12:PRO:HG3	3:H:97:PRO:HB2	2.01	0.43
3:H:212:LEU:C	3:H:214:ALA:N	2.72	0.43
1:L:113:ILE:HG21	2:M:224:VAL:HG22	1.99	0.43
1:L:61:PRO:HA	1:L:64:ILE:CG2	2.48	0.43
2:M:216:MET:O	2:M:220:THR:HG23	2.19	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:ILE:HG22	1:L:179:PHE:CD1	2.54	0.43
2:M:235:GLN:HE21	2:M:243:ALA:HB2	1.80	0.43
1:L:166:ASN:O	1:L:168:HIS:N	2.51	0.43
1:L:187:LEU:C	1:L:187:LEU:CD2	2.82	0.43
1:L:235:LEU:O	1:L:238:LEU:N	2.51	0.43
1:L:41:PHE:HD2	1:L:92:CYS:CA	2.30	0.43
2:M:127:TRP:CD1	6:M:500:BPH:HAA1	2.54	0.43
1:L:230:HIS:NE2	2:M:217:HIS:CD2	2.86	0.43
2:M:227:PHE:HE2	3:H:235:GLY:CA	2.20	0.43
2:M:263:ILE:HG23	2:M:264:HIS:ND1	2.33	0.43
2:M:62:GLY:O	2:M:65:TRP:HB3	2.19	0.43
3:H:27:LEU:HD11	3:H:32:GLN:CD	2.39	0.43
2:M:142:LYS:O	2:M:143:HIS:C	2.53	0.43
3:H:39:GLY:O	3:H:40:TYR:CD1	2.71	0.43
3:H:130:LYS:O	3:H:171:ILE:HB	2.18	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:46:ILE:O	1:L:46:ILE:HG13	2.17	0.43
7:M:750:UQ:H222	7:M:750:UQ:H201	1.64	0.43
1:L:36:VAL:HA	1:L:39:PHE:HB3	2.00	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
3:H:237:VAL:C	3:H:239:GLY:N	2.71	0.42
2:M:250:TRP:NE1	7:M:750:UQ:HM51	2.34	0.42
3:H:20:PHE:CD2	3:H:21:TRP:CD1	3.07	0.42
3:H:33:THR:C	3:H:35:ASN:H	2.21	0.42
2:M:104:PHE:HD2	2:M:114:LEU:HD21	1.83	0.42
2:M:202:LEU:O	2:M:206:PHE:N	2.48	0.42
1:L:123:PHE:CZ	1:L:242:PHE:HD2	2.37	0.42
2:M:243:ALA:O	7:M:750:UQ:CM2	2.67	0.42
2:M:282:ILE:C	2:M:284:LEU:N	2.72	0.42
2:M:24:VAL:HG11	2:M:26:LEU:CD1	2.44	0.42
3:H:135:LYS:HZ1	3:H:165:VAL:HG12	1.82	0.42
3:H:60:LYS:HG2	3:H:60:LYS:H	1.63	0.42
1:L:11:VAL:CG2	3:H:111:PRO:HD3	2.50	0.42
1:L:125:ILE:HG21	1:L:125:ILE:HD13	1.83	0.42
1:L:190:HIS:HB2	1:L:229:ILE:CD1	2.50	0.42
1:L:121:PHE:HD1	6:L:550:BPH:C4D	2.32	0.42
6:L:550:BPH:HBA1	6:L:550:BPH:H3A	1.22	0.42
2:M:199:PHE:HB3	2:M:277:THR:HG22	2.01	0.42
5:M:601:BCL:CAA	5:M:601:BCL:HBD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:29(A):SER:HB2	2:M:49:ILE:O	2.19	0.42
2:M:4:GLN:HG3	3:H:194:GLN:HA	2.00	0.42
1:L:185:LEU:HD12	6:M:500:BPH:NC	2.35	0.42
2:M:66:PHE:O	2:M:69:ILE:HB	2.19	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:251:THR:CG2	1:L:259:TRP:HE1	2.32	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:163:PRO:HB3	2:M:171:GLU:HB2	2.01	0.42
2:M:170:SER:C	2:M:171:GLU:O	2.58	0.42
2:M:148:PHE:HB2	6:M:500:BPH:HMD3	2.02	0.42
2:M:212:LEU:CD2	7:M:750:UQ:C16	2.97	0.42
2:M:105:ALA:HB1	2:M:105(A):ALA:H	1.43	0.42
1:L:80:LEU:C	1:L:82:LYS:N	2.72	0.42
1:L:211:HIS:O	1:L:215:PHE:CB	2.68	0.42
1:L:240:ALA:O	1:L:244:SER:CB	2.68	0.42
2:M:219:ALA:C	2:M:221:ILE:H	2.23	0.42
2:M:263:ILE:HG21	7:M:750:UQ:HM33	2.00	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
1:L:232:LEU:HD12	2:M:41:PHE:CE2	2.55	0.42
3:H:104:PRO:CB	3:H:243:TYR:CD1	3.03	0.42
2:M:204:ILE:HG12	5:M:400:BCL:HMB3	2.00	0.42
1:L:43:ALA:O	1:L:47:ILE:N	2.52	0.42
1:L:261:ASP:O	1:L:262:TRP:C	2.56	0.42
2:M:241:THR:HG22	3:H:231:ASP:OD1	2.20	0.42
1:L:88:ILE:HA	1:L:88:ILE:HD13	1.88	0.42
2:M:186:ASN:O	2:M:190:VAL:CG2	2.54	0.42
2:M:129:GLY:O	2:M:133:LEU:HB2	2.20	0.42
1:L:181:PHE:CZ	5:M:400:BCL:HAA2	2.54	0.42
6:M:500:BPH:H9C1	6:M:500:BPH:H112	1.69	0.42
3:H:104:PRO:CB	3:H:243:TYR:CE1	3.00	0.41
2:M:102:LEU:O	2:M:102:LEU:CD1	2.63	0.41
2:M:197:ASN:OD1	2:M:199:PHE:HD2	2.03	0.41
1:L:195:LEU:CD1	2:M:265:ARG:HG3	2.34	0.41
1:L:181:PHE:CE1	5:M:400:BCL:O1A	2.73	0.41
2:M:69:ILE:O	2:M:93:LEU:HD11	2.20	0.41
1:L:273:ALA:CB	2:M:82:ALA:O	2.68	0.41
1:L:201:GLU:HB2	1:L:204:LYS:HB2	2.02	0.41
1:L:111:LEU:CB	1:L:113:ILE:HG12	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:235:LEU:O	1:L:236:LEU:C	2.59	0.41
2:M:150:SER:OG	2:M:276:LEU:HD23	2.20	0.41
3:H:32:GLN:O	3:H:32:GLN:HG3	2.20	0.41
3:H:31:LEU:HD12	3:H:31:LEU:HA	1.90	0.41
1:L:17:VAL:HG22	1:L:33:PHE:HB3	1.99	0.41
2:M:65:TRP:CG	2:M:66:PHE:N	2.88	0.41
1:L:34:PHE:O	1:L:38:THR:HB	2.19	0.41
1:L:275:ILE:O	1:L:275:ILE:CG2	2.56	0.41
3:H:216:ILE:CG2	3:H:217:PRO:HD2	2.48	0.41
1:L:78:ALA:HB1	1:L:79:PRO:CD	2.51	0.41
1:L:227:LEU:HD23	1:L:231:ARG:NH1	2.36	0.41
1:L:53:ALA:CB	1:L:64:ILE:CD1	2.90	0.41
1:L:193:LEU:HD22	7:L:800:UQ:HM23	2.03	0.41
3:H:183:LEU:HD11	3:H:213:PHE:O	2.20	0.41
3:H:36:MET:HA	3:H:40:TYR:CD1	2.56	0.41
1:L:200:PRO:HB2	1:L:201:GLU:H	1.35	0.41
1:L:16:LEU:HD11	1:L:105:VAL:CG1	2.50	0.41
2:M:149:LEU:HA	2:M:149:LEU:HD12	1.84	0.41
1:L:104:GLU:HG2	2:M:249:PHE:CZ	2.54	0.41
1:L:166:ASN:C	1:L:168:HIS:N	2.73	0.41
1:L:183:ASN:HB2	1:L:236:LEU:HB3	2.01	0.41
7:L:800:UQ:C8	7:L:800:UQ:HM51	2.50	0.41
2:M:69:ILE:C	2:M:93:LEU:HD11	2.38	0.41
2:M:251:ARG:CG	2:M:251:ARG:NH1	2.81	0.41
3:H:93:SER:HB3	3:H:96:PHE:HD2	1.84	0.41
2:M:231:ARG:NH1	3:H:122:GLU:OE1	2.54	0.41
3:H:124:ASP:HB2	3:H:129:ASN:O	2.21	0.41
3:H:173:GLU:O	3:H:173:GLU:CG	2.69	0.41
1:L:158:SER:OG	1:L:162:TYR:HE2	1.99	0.41
1:L:215:PHE:CD1	2:M:138:LEU:CD2	3.04	0.41
2:M:288:VAL:HB	3:H:4:VAL:CG1	2.45	0.41
2:M:6:ILE:HA	2:M:6:ILE:HD13	1.94	0.41
3:H:148:PRO:O	3:H:149:ILE:CB	2.68	0.41
3:H:2:VAL:CG1	3:H:2:VAL:O	2.68	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
5:L:350:BCL:H93	5:L:350:BCL:H62	1.76	0.41
2:M:74:TRP:CD1	2:M:79:TRP:CD1	3.08	0.41
3:H:17:ILE:CG2	3:H:21:TRP:CD1	2.95	0.41
3:H:206:ASN:HD22	3:H:206:ASN:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:115:VAL:HG12	3:H:116:ALA:N	2.34	0.41
1:L:129:LEU:HB3	1:L:134:PHE:CE2	2.56	0.41
2:M:158:LEU:CG	2:M:183:TRP:HH2	2.34	0.41
2:M:224:VAL:C	2:M:226:ARG:N	2.74	0.41
2:M:21:THR:CG2	2:M:50:TYR:OH	2.67	0.41
1:L:80:LEU:O	1:L:83:GLY:N	2.54	0.41
3:H:209:SER:O	3:H:213:PHE:CD1	2.72	0.41
6:L:550:BPH:H203	6:L:550:BPH:H152	2.02	0.41
2:M:162:ARG:O	2:M:164:ILE:N	2.54	0.41
2:M:267:ALA:O	2:M:268:ILE:C	2.58	0.41
1:L:177:ILE:CD1	5:L:350:BCL:HMB3	2.51	0.41
1:L:42:ALA:CB	6:L:550:BPH:H5C1	2.50	0.41
1:L:234:LEU:HD13	2:M:222:LEU:CD1	2.50	0.41
2:M:65:TRP:CE3	2:M:66:PHE:N	2.89	0.41
3:H:182:GLU:C	3:H:184:LYS:H	2.24	0.41
1:L:36:VAL:O	1:L:40:PHE:HD1	2.04	0.41
2:M:105(A):ALA:HB1	2:M:109:GLU:OE1	2.21	0.41
3:H:167:ILE:CG2	3:H:179:LEU:HD12	2.46	0.41
1:L:16:LEU:HD11	1:L:105:VAL:HG12	2.03	0.41
1:L:128:TYR:O	1:L:132:VAL:HG23	2.21	0.41
1:L:215:PHE:CD1	2:M:138:LEU:HD21	2.56	0.41
2:M:216:MET:O	2:M:219:ALA:HB3	2.21	0.41
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
2:M:43:ASN:HA	2:M:43:ASN:HD22	1.68	0.41
1:L:222:TYR:HD2	2:M:46:LEU:HD21	1.86	0.40
1:L:113:ILE:CG2	2:M:224:VAL:HG22	2.50	0.40
2:M:243:ALA:O	7:M:750:UQ:HM22	2.21	0.40
2:M:105(A):ALA:O	2:M:106:PRO:C	2.47	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
3:H:12:LEU:HD13	3:H:12:LEU:HA	1.86	0.40
5:L:450:BCL:OBD	5:L:450:BCL:O2D	2.39	0.40
2:M:25:ASN:O	2:M:26:LEU:C	2.59	0.40
3:H:170:ASP:OD2	3:H:177:ARG:NH2	2.54	0.40
3:H:177:ARG:O	3:H:193:MET:HB2	2.21	0.40
3:H:66:LEU:CB	3:H:67:PRO:CD	2.99	0.40
1:L:175:ILE:C	1:L:177:ILE:N	2.74	0.40
1:L:248:MET:HE3	5:L:350:BCL:HMD1	2.03	0.40
2:M:131:THR:HG21	6:M:500:BPH:OBD	2.21	0.40
2:M:217:HIS:ND1	2:M:263:ILE:HG12	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:282:ILE:C	2:M:284:LEU:H	2.24	0.40
1:L:93:ALA:HB1	1:L:97:PHE:HE2	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
2:M:55:GLY:HA3	2:M:130:ARG:HH11	1.87	0.40
1:L:11:VAL:HG12	3:H:98:HIS:O	2.22	0.40
5:L:450:BCL:H13	5:L:450:BCL:H102	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
3:H:212:LEU:C	3:H:214:ALA:H	2.25	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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	1

All (123) Ramachandran outliers are listed below:

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

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

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Mol	Chain	Res	Type
2	M	231	ARG
3	H	59	PRO
3	H	95	GLY
3	H	174	GLN
3	H	175	MET
3	H	199	GLN
3	H	205	VAL
3	H	237	VAL
1	L	57	GLY
1	L	142	TRP
1	L	258	GLN
2	M	105	ALA
2	M	144	THR
2	M	267	ALA
2	M	273	LEU
1	L	6	GLU
1	L	15	THR
1	L	43	ALA
1	L	171	PRO
1	L	267	VAL
2	M	91	PHE
2	M	99	GLU
2	M	163	PRO
3	H	183	LEU
3	H	222	PRO
3	H	26	GLY
3	H	145	GLY
1	L	12	PRO
2	M	268	ILE
2	M	300	GLY
3	H	67	PRO
1	L	228	GLY
2	M	302	ALA
2	M	83	VAL
3	H	160	ILE
1	L	114	GLY
3	H	133	PRO
3	H	97	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	216/220 (98%)	169 (78%)	47 (22%)	1	5
2	M	238/240 (99%)	179 (75%)	59 (25%)	1	3
3	H	203/208 (98%)	154 (76%)	49 (24%)	1	3
All	All	657/668 (98%)	502 (76%)	155 (24%)	1	3

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

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

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

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

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

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

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

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

5.3.3 RNA [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 carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	BCL	L	350	-	53,74,74	1.10	4 (7%)	57,115,115	1.36	9 (15%)
5	BCL	L	450	-	53,74,74	1.19	5 (9%)	57,115,115	1.32	7 (12%)
6	BPH	L	550	-	64,70,70	1.06	5 (7%)	73,101,101	1.23	8 (10%)
7	UQ	L	800	-	48,48,63	2.34	14 (29%)	58,61,79	2.60	26 (44%)
5	BCL	M	400	2	53,74,74	1.11	5 (9%)	57,115,115	1.31	9 (15%)
6	BPH	M	500	-	64,70,70	1.19	6 (9%)	73,101,101	1.15	6 (8%)
5	BCL	M	601	2	53,74,74	1.12	5 (9%)	57,115,115	1.29	8 (14%)
7	UQ	M	750	-	48,48,63	2.37	11 (22%)	58,61,79	2.20	18 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	350	-	-	0/37/137/137	0/0/9/9
5	BCL	L	450	-	-	0/37/137/137	0/0/9/9
6	BPH	L	550	-	-	0/54/105/105	0/1/6/6
7	UQ	L	800	-	-	0/45/69/87	0/1/1/1
5	BCL	M	400	2	-	0/37/137/137	0/0/9/9
6	BPH	M	500	-	-	0/54/105/105	0/1/6/6
5	BCL	M	601	2	-	0/37/137/137	0/0/9/9
7	UQ	M	750	-	-	1/45/69/87	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	800	UQ	C16-C17	-8.59	1.24	1.53
5	L	350	BCL	C3C-C4C	-3.81	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	400	BCL	C3C-C4C	-3.79	1.46	1.51
6	L	550	BPH	C2C-C1C	-3.54	1.45	1.52
7	L	800	UQ	C18-C19	-3.41	1.26	1.33
6	M	500	BPH	C2C-C1C	-3.39	1.46	1.52
5	L	450	BCL	C3C-C4C	-3.36	1.47	1.51
5	M	601	BCL	C3C-C4C	-3.17	1.47	1.51
5	L	450	BCL	C2C-C3C	-3.04	1.45	1.54
6	M	500	BPH	C2A-C1A	-3.04	1.46	1.51
6	L	550	BPH	C2C-C3C	-3.02	1.45	1.54
5	M	400	BCL	C2C-C3C	-2.96	1.45	1.54
5	M	601	BCL	C2C-C3C	-2.92	1.45	1.54
6	M	500	BPH	C3D-C4D	-2.89	1.37	1.41
5	L	350	BCL	C2C-C3C	-2.84	1.46	1.54
6	M	500	BPH	C2C-C3C	-2.82	1.46	1.54
5	L	450	BCL	C3B-C2B	-2.76	1.33	1.40
6	L	550	BPH	C2A-C1A	-2.75	1.46	1.51
5	M	601	BCL	C2A-C1A	-2.72	1.46	1.52
5	L	450	BCL	C2A-C1A	-2.71	1.46	1.52
5	M	400	BCL	C2A-C1A	-2.71	1.46	1.52
7	M	750	UQ	C18-C19	-2.42	1.28	1.33
5	L	350	BCL	C2A-C1A	-2.36	1.47	1.52
5	L	350	BCL	C3B-C2B	-2.35	1.34	1.40
5	M	601	BCL	C3B-C2B	-2.33	1.34	1.40
7	L	800	UQ	O3-C3	-2.28	1.31	1.37
5	L	450	BCL	C2C-C1C	-2.08	1.45	1.51
5	M	400	BCL	C3B-C2B	-2.00	1.35	1.40
5	M	400	BCL	CBB-CAB	2.03	1.55	1.49
5	M	601	BCL	CBB-CAB	2.03	1.55	1.49
7	M	750	UQ	C37-C38	2.20	1.56	1.50
7	L	800	UQ	C32-C33	2.32	1.57	1.50
7	M	750	UQ	C31-C29	2.39	1.56	1.51
7	L	800	UQ	C40-C39	2.42	1.57	1.50
7	M	750	UQ	C7-C6	2.43	1.55	1.51
6	L	550	BPH	CBB-CAB	2.48	1.55	1.50
7	L	800	UQ	C22-C23	2.50	1.57	1.50
7	M	750	UQ	C35-C34	2.55	1.56	1.50
7	M	750	UQ	C16-C14	2.62	1.57	1.51
7	M	750	UQ	C30-C29	2.62	1.57	1.50
7	L	800	UQ	C33-C34	2.64	1.38	1.33
6	M	500	BPH	CBB-CAB	2.65	1.55	1.50
6	L	550	BPH	CHC-C1C	2.72	1.41	1.36
7	M	750	UQ	C11-C9	2.74	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	750	UQ	C27-C28	2.84	1.58	1.50
7	L	800	UQ	C36-C34	2.88	1.57	1.51
7	L	800	UQ	C16-C14	2.93	1.57	1.51
7	L	800	UQ	C11-C9	2.95	1.58	1.51
6	M	500	BPH	CHC-C1C	3.54	1.43	1.36
7	L	800	UQ	C31-C29	3.56	1.59	1.51
7	L	800	UQ	C26-C24	3.80	1.59	1.51
7	L	800	UQ	C35-C34	3.88	1.60	1.50
7	M	750	UQ	C7-C8	4.38	1.57	1.50
7	L	800	UQ	C7-C8	6.25	1.60	1.50
7	M	750	UQ	C12-C13	11.88	1.84	1.50

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	800	UQ	C30-C29-C28	-5.85	112.01	123.50
7	L	800	UQ	C25-C24-C23	-5.18	113.34	123.50
7	M	750	UQ	C12-C13-C14	-5.12	116.63	127.76
7	M	750	UQ	C10-C9-C8	-4.75	114.17	123.50
7	L	800	UQ	C20-C19-C18	-4.16	115.33	123.50
5	L	350	BCL	OBD-CAD-CBD	-4.00	119.89	125.94
7	L	800	UQ	C37-C36-C34	-3.92	99.93	112.71
7	L	800	UQ	C17-C18-C19	-3.84	119.41	127.76
7	L	800	UQ	C37-C38-C39	-3.79	113.13	127.73
5	L	450	BCL	OBD-CAD-CBD	-3.62	120.48	125.94
7	M	750	UQ	C5-C6-C1	-3.53	116.10	120.12
5	M	400	BCL	OBD-CAD-CBD	-3.46	120.72	125.94
6	L	550	BPH	OBD-CAD-CBD	-3.43	120.77	125.94
7	M	750	UQ	C22-C21-C19	-3.32	101.91	112.71
7	L	800	UQ	C15-C14-C13	-3.22	117.17	123.50
7	M	750	UQ	O1-C1-C6	-3.09	115.87	121.68
5	M	601	BCL	OBD-CAD-CBD	-3.09	121.28	125.94
7	L	800	UQ	C11-C9-C8	-3.06	115.24	121.05
5	M	400	BCL	OBB-CAB-CBB	-3.01	112.91	120.13
5	M	601	BCL	OBB-CAB-CBB	-2.95	113.06	120.13
7	M	750	UQ	C26-C24-C23	-2.87	115.61	121.05
5	L	450	BCL	OBB-CAB-CBB	-2.80	113.42	120.13
5	L	350	BCL	OBB-CAB-CBB	-2.80	113.43	120.13
6	L	550	BPH	OBB-CAB-CBB	-2.78	113.17	119.69
6	M	500	BPH	OBB-CAB-CBB	-2.73	113.27	119.69
7	M	750	UQ	C36-C34-C33	-2.65	116.02	121.05
7	L	800	UQ	O1-C1-C6	-2.59	116.81	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	800	UQ	C6-C5-C4	-2.55	117.74	120.42
6	L	550	BPH	C1C-NC-C4C	-2.45	107.93	110.44
6	M	500	BPH	OBD-CAD-CBD	-2.41	122.30	125.94
7	L	800	UQ	CM3-O3-C3	-2.39	108.13	116.61
7	M	750	UQ	C15-C14-C13	-2.35	118.88	123.50
5	L	350	BCL	CMB-C2B-C1B	-2.29	124.57	128.36
7	L	800	UQ	CM5-C5-C6	-2.28	119.21	124.10
5	M	601	BCL	CMB-C2B-C1B	-2.28	124.59	128.36
6	M	500	BPH	C1C-NC-C4C	-2.27	108.11	110.44
6	L	550	BPH	CGD-CBD-CAD	-2.27	102.94	110.62
7	M	750	UQ	C20-C19-C18	-2.25	119.08	123.50
7	M	750	UQ	C32-C33-C34	-2.25	122.88	127.76
7	L	800	UQ	C12-C13-C14	-2.22	122.94	127.76
5	L	450	BCL	CMB-C2B-C1B	-2.17	124.78	128.36
5	L	350	BCL	CHA-C1A-NA	-2.12	120.85	126.06
5	L	450	BCL	O2D-CGD-CBD	-2.10	108.41	111.30
7	L	800	UQ	O4-C4-C3	-2.05	116.34	120.79
5	M	400	BCL	CMB-C2B-C1B	-2.05	124.98	128.36
5	M	400	BCL	CHA-C1A-NA	-2.04	121.03	126.06
5	M	601	BCL	C4-C3-C2	-2.00	119.57	123.50
6	M	500	BPH	OBD-CAD-C3D	2.00	132.44	128.35
7	L	800	UQ	CM2-O2-C2	2.15	124.25	116.61
5	M	400	BCL	C2A-C1A-CHA	2.17	127.88	123.89
5	M	400	BCL	C4-C3-C5	2.29	118.90	115.41
5	L	350	BCL	C2A-C1A-CHA	2.31	128.15	123.89
6	L	550	BPH	CMD-C2D-C3D	2.37	129.73	125.09
7	M	750	UQ	C35-C34-C36	2.38	119.04	115.41
7	L	800	UQ	C27-C26-C24	2.46	120.71	112.71
5	M	601	BCL	CMD-C2D-C3D	2.52	130.01	125.09
5	L	350	BCL	C2C-C3C-C4C	2.52	105.77	101.50
5	M	601	BCL	C4A-NA-C1A	2.53	109.63	106.36
7	L	800	UQ	O2-C2-C1	2.56	124.57	116.41
6	L	550	BPH	CBD-CHA-C1A	2.58	132.44	126.36
7	M	750	UQ	C21-C22-C23	2.59	118.46	111.69
5	M	601	BCL	C2C-C3C-C4C	2.65	105.99	101.50
7	L	800	UQ	C26-C24-C23	2.69	126.15	121.05
7	M	750	UQ	C25-C24-C26	2.70	119.53	115.41
5	L	350	BCL	C4A-NA-C1A	2.72	109.88	106.36
7	M	750	UQ	O2-C2-C1	2.74	125.14	116.41
5	L	350	BCL	CMD-C2D-C3D	2.75	130.47	125.09
6	M	500	BPH	C2C-C3C-C4C	2.78	106.22	101.50
5	L	450	BCL	CMD-C2D-C3D	2.80	130.56	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	450	BCL	C2C-C3C-C4C	2.81	106.27	101.50
5	M	400	BCL	C2C-C3C-C4C	2.84	106.32	101.50
5	M	400	BCL	CMD-C2D-C3D	2.90	130.76	125.09
6	L	550	BPH	C4-C3-C5	2.93	119.88	115.41
7	L	800	UQ	C30-C29-C31	2.98	119.95	115.41
6	L	550	BPH	C2C-C3C-C4C	3.01	106.60	101.50
5	L	450	BCL	C4-C3-C5	3.01	120.00	115.41
5	M	400	BCL	C4A-NA-C1A	3.03	110.28	106.36
7	L	800	UQ	C41-C39-C40	3.04	122.11	114.64
7	M	750	UQ	C20-C19-C21	3.14	120.21	115.41
5	L	350	BCL	C4-C3-C5	3.18	120.27	115.41
7	L	800	UQ	C25-C24-C26	3.33	120.49	115.41
5	M	601	BCL	C4-C3-C5	3.34	120.52	115.41
6	M	500	BPH	C4-C3-C5	3.42	120.63	115.41
7	L	800	UQ	C31-C29-C28	3.68	128.03	121.05
7	L	800	UQ	C15-C14-C16	4.38	122.09	115.41
7	L	800	UQ	C8-C7-C6	4.88	126.29	111.64
7	M	750	UQ	C7-C8-C9	4.96	135.09	126.70
7	M	750	UQ	C11-C9-C8	5.20	130.91	121.05
7	L	800	UQ	C10-C9-C11	5.62	123.99	115.41
7	L	800	UQ	C20-C19-C21	5.88	124.39	115.41
7	M	750	UQ	C11-C12-C13	6.64	129.08	111.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	750	UQ	C24-C23-C22-C21

There are no ring outliers.

8 monomers are involved in 190 short contacts:

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.