



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:08 AM EDT

PDB ID : 1Z9K / pdb_00001z9k
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides
Authors : Camara-Artigas, A.; Allen, J.P.
Deposited on : 2005-04-02
Resolution : 4.60 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

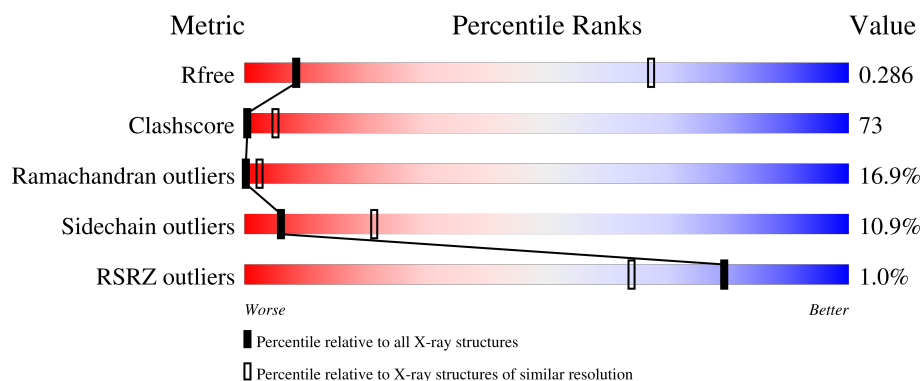
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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))
R_{free}	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	281	2% 17% 59% 21% .
2	B	307	% 20% 49% 26% ..
3	C	260	24% 48% 17% 8% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6946 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

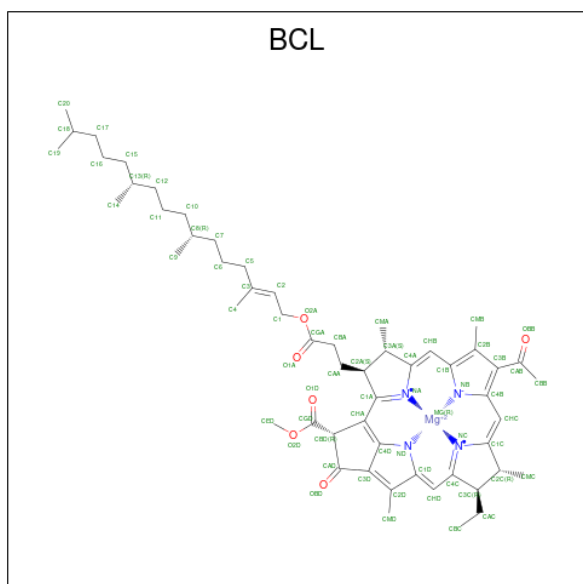
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

- Molecule 3 is a protein called Reaction center protein H chain.

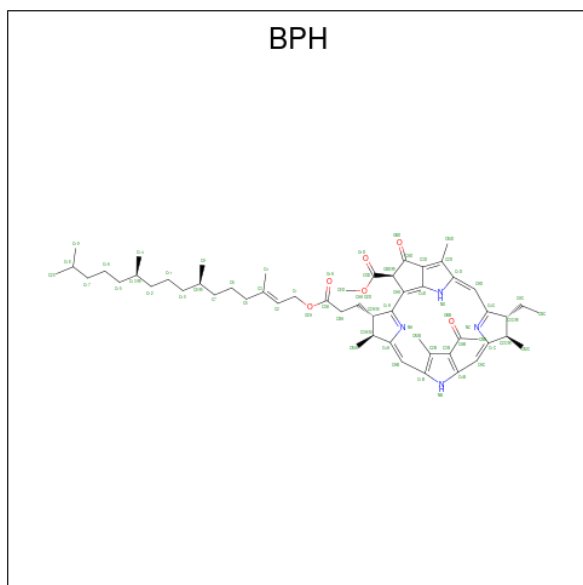
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



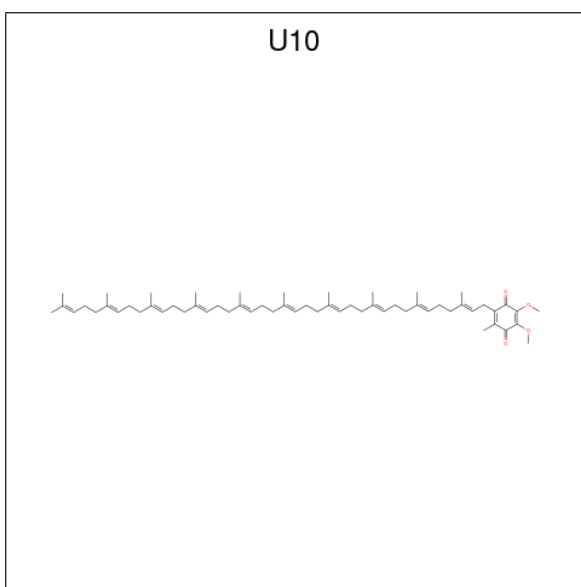
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			65	55	4	6		
5	B	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			48	44	4		
6	B	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

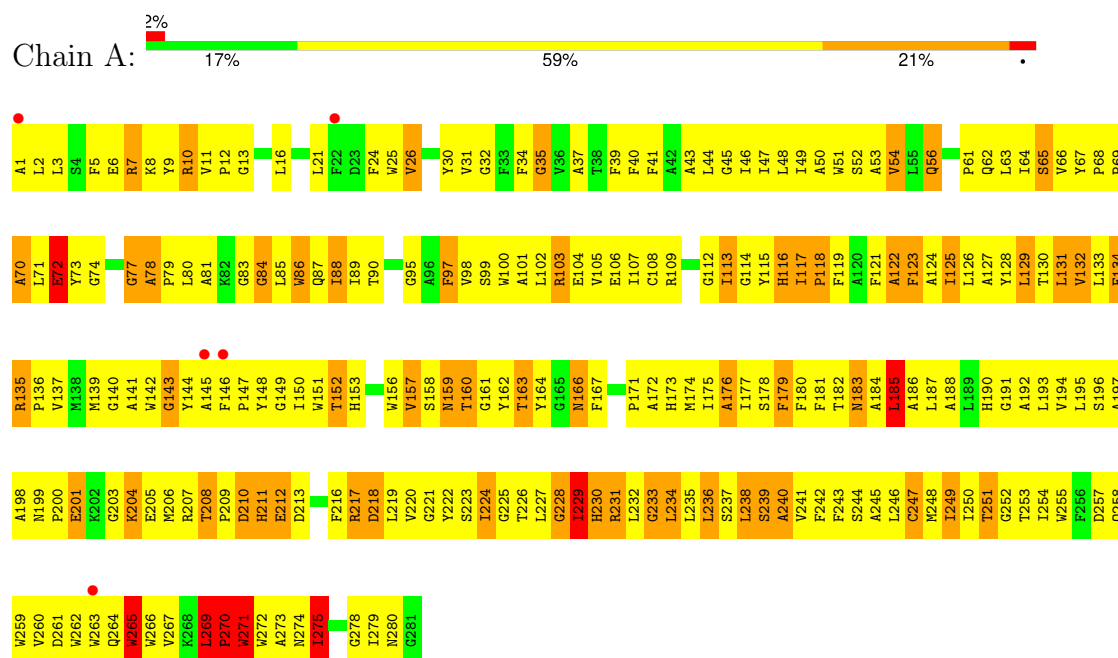
- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mn	0	0
			1	1		

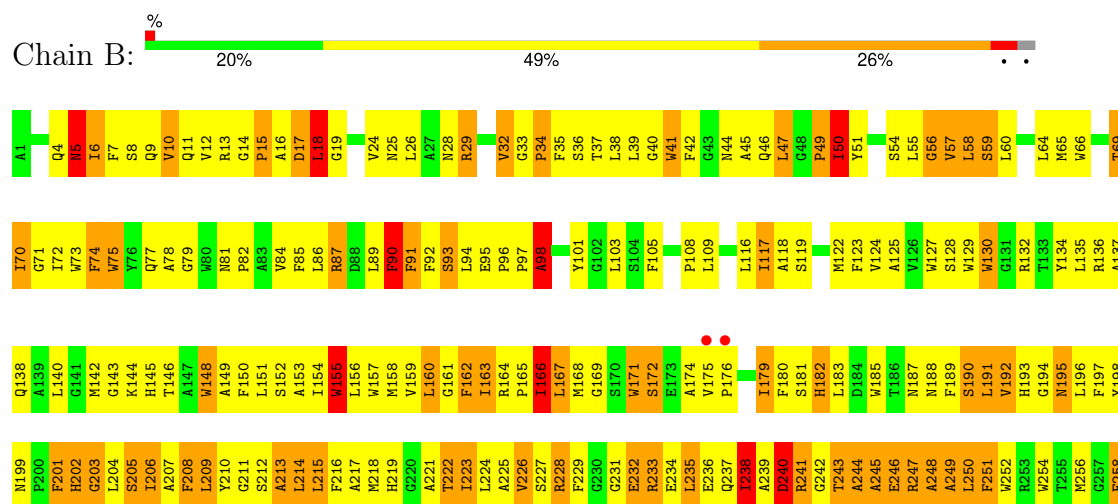
3 Residue-property plots

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 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.

• Molecule 1: Reaction center protein L chain

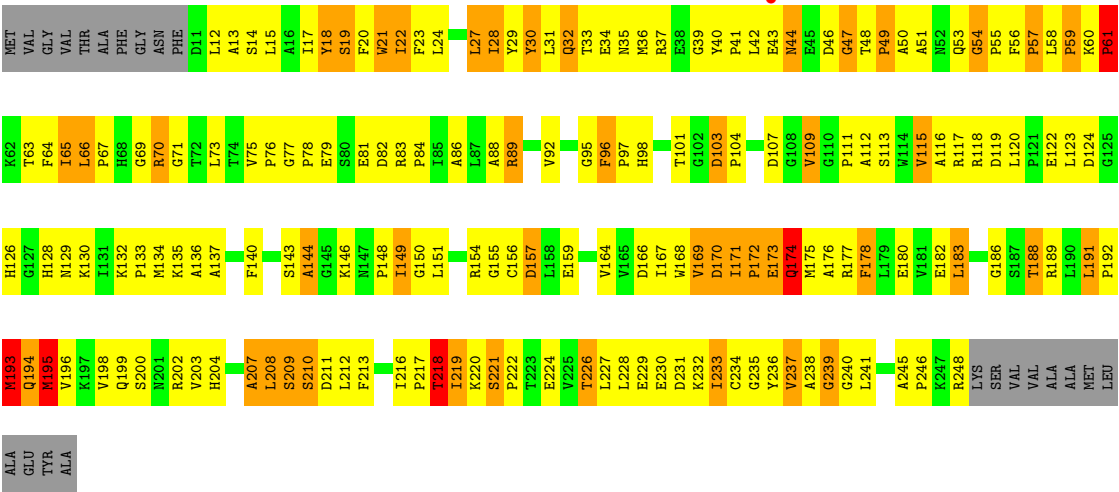
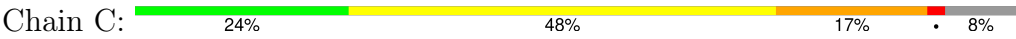


• Molecule 2: Reaction center protein M chain





● Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	207.80Å 207.80Å 107.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 4.60 25.00 – 4.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-4.60) 92.6 (25.00-4.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.330 , 0.330 0.256 , 0.286	Depositor DCC
R_{free} test set	2066 reflections (8.55%)	wwPDB-VP
Wilson B-factor (Å ²)	174.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6946	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, BPH, MN, U10, BCL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	0/2320	1.08	23/3175 (0.7%)
2	B	0.58	0/2500	1.13	30/3413 (0.9%)
3	C	0.70	0/1862	1.25	24/2534 (0.9%)
All	All	0.62	0/6682	1.15	77/9122 (0.8%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	VAL	N-CA-C	11.18	121.42	111.81
3	C	115	VAL	N-CA-C	10.35	123.66	108.96
3	C	21	TRP	N-CA-C	-10.12	100.95	113.20
2	B	70	ILE	N-CA-C	-9.45	101.86	111.88
1	A	265	TRP	N-CA-C	-9.32	100.99	111.71
3	C	191	LEU	CA-C-N	8.90	130.97	119.84
3	C	191	LEU	C-N-CA	8.90	130.97	119.84
2	B	202	HIS	N-CA-C	-8.62	101.40	114.16
1	A	176	ALA	N-CA-C	-8.19	102.74	112.89
1	A	124	ALA	N-CA-C	-8.15	101.67	111.69
1	A	98	VAL	N-CA-C	-8.09	102.46	110.30
2	B	128	SER	N-CA-C	-8.07	102.91	114.12
2	B	54	SER	N-CA-C	-7.94	101.72	111.33
2	B	197	PHE	N-CA-C	-7.85	102.33	112.23
1	A	275	ILE	CA-C-N	7.74	128.34	119.99
1	A	275	ILE	C-N-CA	7.74	128.34	119.99
3	C	103	ASP	CA-C-N	7.73	127.63	119.05
3	C	103	ASP	C-N-CA	7.73	127.63	119.05
1	A	35	GLY	N-CA-C	-7.57	105.28	114.66
2	B	166	ILE	N-CA-C	-7.40	106.68	113.71
2	B	201	PHE	N-CA-C	-7.35	103.28	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	205	SER	N-CA-C	-7.28	102.53	111.33
1	A	198	ALA	N-CA-C	-7.15	106.47	114.62
2	B	238	ILE	N-CA-C	-7.10	103.60	110.42
1	A	108	CYS	N-CA-C	-6.94	104.69	113.72
1	A	208	THR	N-CA-C	6.83	119.20	108.55
2	B	167	LEU	N-CA-C	-6.72	104.70	113.17
2	B	45	ALA	N-CA-C	-6.72	105.24	113.50
2	B	295	TYR	N-CA-C	-6.62	105.07	113.01
2	B	243	THR	N-CA-C	-6.58	103.79	112.34
2	B	294	TRP	N-CA-C	6.48	121.47	113.50
1	A	217	ARG	N-CA-C	-6.40	104.35	111.71
2	B	190	SER	N-CA-C	-6.37	104.61	112.38
3	C	208	LEU	N-CA-C	6.37	119.50	110.14
1	A	231	ARG	N-CA-C	-6.33	97.31	110.80
3	C	170	ASP	N-CA-C	-6.30	99.42	109.76
3	C	207	ALA	N-CA-C	6.28	118.00	111.03
2	B	56	GLY	N-CA-C	-6.24	105.09	112.64
2	B	10	VAL	N-CA-C	6.21	118.87	108.81
3	C	178	PHE	N-CA-C	6.20	118.19	108.96
1	A	271	TRP	N-CA-C	6.18	121.90	113.37
3	C	218	THR	N-CA-C	6.17	118.79	109.41
1	A	106	GLU	N-CA-C	-6.17	104.86	112.38
3	C	188	THR	N-CA-C	6.10	119.46	109.76
3	C	109	VAL	N-CA-C	6.06	115.93	108.53
2	B	130	TRP	N-CA-C	-6.02	103.88	111.11
2	B	75	TRP	N-CA-C	-6.02	104.32	112.26
3	C	132	LYS	CA-C-N	5.96	127.28	119.84
3	C	132	LYS	C-N-CA	5.96	127.28	119.84
3	C	173	GLU	N-CA-C	-5.89	103.34	110.88
1	A	56	GLN	N-CA-C	-5.88	106.24	113.41
2	B	262	MET	N-CA-C	-5.87	102.58	111.56
3	C	88	ALA	N-CA-C	5.68	117.87	108.49
1	A	97	PHE	N-CA-C	-5.57	105.60	112.90
2	B	29	ARG	N-CA-C	-5.51	100.70	109.96
3	C	27	LEU	N-CA-C	-5.48	106.65	113.55
2	B	93	SER	N-CA-C	5.43	117.48	108.13
2	B	226	VAL	N-CA-C	5.33	116.66	111.91
3	C	213	PHE	N-CA-C	-5.33	106.28	112.89
3	C	209	SER	N-CA-C	5.32	118.25	109.85
1	A	269	LEU	CA-C-N	5.29	126.45	119.84
1	A	269	LEU	C-N-CA	5.29	126.45	119.84
1	A	166	ASN	N-CA-C	-5.28	103.51	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	ASN	N-CA-C	-5.24	100.49	109.24
2	B	191	LEU	N-CA-C	5.20	119.59	112.68
3	C	63	THR	N-CA-C	5.20	117.08	108.20
2	B	105	PHE	N-CA-C	-5.17	105.44	112.26
1	A	5	PHE	N-CA-C	5.14	118.86	112.59
2	B	203	GLY	N-CA-C	-5.12	101.05	113.18
2	B	208	PHE	N-CA-C	5.11	116.93	111.36
1	A	273	ALA	N-CA-C	5.09	116.52	110.97
3	C	137	ALA	N-CA-C	-5.09	103.81	110.53
2	B	213	ALA	N-CA-C	-5.08	106.18	112.93
3	C	18	TYR	N-CA-C	-5.07	107.16	113.55
1	A	103	ARG	N-CA-C	-5.07	105.85	112.23
1	A	185	LEU	N-CA-C	-5.04	105.29	111.75
2	B	98	ALA	N-CA-C	5.03	120.92	109.81

There are no chirality outliers.

There are no planarity outliers.

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	A	2232	0	2187	395	0
2	B	2408	0	2321	457	0
3	C	1814	0	1818	243	0
4	A	132	0	148	18	0
4	B	132	0	148	13	0
5	A	65	0	76	9	0
5	B	65	0	76	9	0
6	A	48	0	63	4	0
6	B	48	0	63	13	0
7	B	1	0	0	0	0
8	C	1	0	0	0	0
All	All	6946	0	6900	1006	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 73.

All (1006) 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)
2:B:50:ILE:HD13	2:B:51:TYR:H	1.08	1.08
1:A:187:LEU:HD21	2:B:269:ALA:HB1	1.31	1.06
1:A:179:PHE:O	1:A:240:ALA:HB2	1.57	1.05
3:C:170:ASP:HB2	3:C:177:ARG:HE	1.22	1.03
2:B:159:VAL:HA	2:B:163:ILE:HB	1.36	1.03
1:A:52:SER:HB2	1:A:85:LEU:HD13	1.43	1.00
1:A:227:LEU:HD13	2:B:232:GLU:HB3	1.42	1.00
3:C:156:CYS:HB2	3:C:248:ARG:HD3	1.41	1.00
1:A:180:PHE:CD2	1:A:240:ALA:HB1	1.97	0.99
2:B:32:VAL:HG12	2:B:33:GLY:H	1.27	0.97
3:C:195:MET:HA	3:C:195:MET:HE2	1.46	0.97
2:B:50:ILE:HD13	2:B:51:TYR:N	1.78	0.97
2:B:265:ILE:O	2:B:268:TRP:HB2	1.65	0.96
2:B:90:PHE:HA	2:B:179:ILE:HD12	1.46	0.94
1:A:149:GLY:HA3	1:A:152:THR:HG1	1.30	0.94
1:A:269:LEU:HD13	1:A:270:PRO:HD2	1.49	0.93
1:A:264:GLN:HA	1:A:267:VAL:HG12	1.49	0.93
2:B:208:PHE:HB3	2:B:276:VAL:HG22	1.49	0.92
3:C:86:ALA:HB1	3:C:101:THR:OG1	1.72	0.89
1:A:16:LEU:HD21	1:A:109:ARG:HD2	1.53	0.89
3:C:148:PRO:HA	3:C:151:LEU:HG	1.53	0.89
2:B:155:TRP:CD1	2:B:278:LEU:HD12	2.08	0.89
2:B:4:GLN:O	2:B:6:ILE:HG12	1.72	0.88
3:C:18:TYR:C	3:C:20:PHE:H	1.79	0.88
2:B:95:GLU:HA	2:B:176:PRO:HB3	1.54	0.87
3:C:70:ARG:NH2	3:C:120:LEU:HD13	1.89	0.87
3:C:115:VAL:HG12	3:C:116:ALA:N	1.90	0.87
1:A:44:LEU:HA	1:A:47:ILE:HD12	1.57	0.86
1:A:149:GLY:HA3	1:A:152:THR:OG1	1.73	0.86
1:A:100:TRP:O	1:A:104:GLU:HG3	1.74	0.85
3:C:170:ASP:HB2	3:C:177:ARG:NE	1.90	0.85
2:B:193:HIS:CD2	2:B:287:SER:HB3	2.12	0.85
1:A:185:LEU:O	1:A:188:ALA:HB3	1.76	0.85
4:A:850:BCL:H2	4:A:850:BCL:H71	1.59	0.84
2:B:155:TRP:HD1	2:B:278:LEU:HA	1.43	0.83
4:A:850:BCL:HED1	2:B:183:LEU:HD11	1.59	0.82
1:A:12:PRO:HG3	3:C:97:PRO:HB3	1.60	0.82
1:A:244:SER:C	1:A:246:LEU:H	1.85	0.81
2:B:36:SER:HB3	2:B:39:LEU:HD12	1.63	0.80
1:A:122:ALA:HA	1:A:125:ILE:HB	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ALA:O	2:B:217:ALA:HB3	1.81	0.80
1:A:271:TRP:CD1	1:A:271:TRP:H	2.00	0.79
1:A:196:SER:HB3	2:B:145:HIS:HB2	1.63	0.79
2:B:154:ILE:HG22	2:B:158:MET:HG2	1.63	0.79
1:A:187:LEU:HD13	2:B:216:PHE:HB2	1.62	0.79
1:A:239:SER:O	1:A:241:VAL:N	2.16	0.78
2:B:159:VAL:HG21	2:B:281:GLY:O	1.84	0.78
2:B:12:VAL:HG12	2:B:13:ARG:H	1.48	0.78
2:B:93:SER:HB2	2:B:181:SER:HB3	1.66	0.78
2:B:243:THR:N	3:C:115:VAL:HG21	1.99	0.78
3:C:29:TYR:O	3:C:31:LEU:N	2.17	0.78
1:A:173:HIS:ND1	1:A:177:ILE:HD11	1.99	0.77
3:C:170:ASP:CB	3:C:177:ARG:HE	1.97	0.77
2:B:90:PHE:CA	2:B:179:ILE:HD12	2.14	0.77
2:B:208:PHE:CB	2:B:276:VAL:HG22	2.15	0.77
2:B:228:ARG:HG3	2:B:229:PHE:CE1	2.20	0.77
3:C:220:LYS:O	3:C:221:SER:HB2	1.84	0.77
3:C:57:PRO:O	3:C:58:LEU:HD23	1.83	0.77
2:B:36:SER:H	2:B:47:LEU:HD11	1.49	0.76
2:B:273:ALA:O	2:B:276:VAL:HG23	1.85	0.76
3:C:75:VAL:HA	3:C:76:PRO:O	1.84	0.76
3:C:115:VAL:HG12	3:C:116:ALA:H	1.48	0.76
2:B:95:GLU:HB3	2:B:96:PRO:HD2	1.66	0.76
2:B:149:ALA:O	2:B:152:SER:HB3	1.85	0.76
3:C:83:ARG:HB2	3:C:84:PRO:HD2	1.66	0.76
1:A:224:ILE:O	1:A:228:GLY:HA3	1.86	0.75
2:B:14:GLY:HA3	3:C:140:PHE:CE1	2.20	0.75
1:A:116:HIS:HB2	2:B:221:ALA:O	1.86	0.75
2:B:46:GLN:O	2:B:47:LEU:HD23	1.86	0.75
3:C:171:ILE:HB	3:C:172:PRO:CD	2.17	0.75
1:A:50:ALA:O	1:A:54:VAL:HG22	1.86	0.75
1:A:117:ILE:C	1:A:119:PHE:H	1.95	0.75
1:A:177:ILE:O	1:A:180:PHE:HB2	1.87	0.74
1:A:223:SER:C	1:A:225:GLY:H	1.94	0.74
1:A:12:PRO:HG3	3:C:97:PRO:CB	2.17	0.74
1:A:222:TYR:CG	1:A:223:SER:N	2.56	0.73
1:A:172:ALA:C	1:A:247:CYS:HB3	2.13	0.73
1:A:177:ILE:HG22	1:A:181:PHE:CE2	2.24	0.72
1:A:210:ASP:OD1	3:C:172:PRO:HG3	1.89	0.72
3:C:156:CYS:CB	3:C:248:ARG:HD3	2.17	0.72
2:B:32:VAL:HG12	2:B:33:GLY:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:THR:OG1	2:B:262:MET:N	2.20	0.72
1:A:113:ILE:CG2	2:B:226:VAL:HG12	2.20	0.72
2:B:25:ASN:HD22	2:B:28:ASN:HD22	1.37	0.72
3:C:148:PRO:HB2	3:C:164:VAL:HG21	1.72	0.72
2:B:38:LEU:C	2:B:40:GLY:H	1.97	0.72
2:B:229:PHE:CZ	3:C:238:ALA:HB2	2.25	0.71
1:A:248:MET:C	1:A:250:ILE:H	1.96	0.71
2:B:26:LEU:C	2:B:28:ASN:H	1.98	0.71
1:A:35:GLY:HA2	1:A:103:ARG:HD2	1.72	0.71
3:C:115:VAL:CG1	3:C:116:ALA:H	2.02	0.71
3:C:18:TYR:C	3:C:20:PHE:N	2.49	0.70
1:A:173:HIS:HD1	1:A:177:ILE:HD11	1.55	0.70
2:B:214:LEU:HD11	2:B:218:MET:SD	2.31	0.70
3:C:70:ARG:HH22	3:C:120:LEU:HD13	1.55	0.70
1:A:219:LEU:HD11	2:B:129:TRP:CZ2	2.26	0.70
1:A:160:THR:O	1:A:163:THR:HB	1.92	0.70
2:B:103:LEU:HD21	2:B:169:GLY:HA2	1.74	0.70
2:B:175:VAL:CG1	2:B:182:HIS:HB2	2.21	0.70
1:A:187:LEU:HD13	2:B:216:PHE:CB	2.21	0.70
2:B:90:PHE:HA	2:B:179:ILE:CD1	2.21	0.70
2:B:215:LEU:O	2:B:218:MET:HB2	1.91	0.69
1:A:254:ILE:HD12	1:A:255:TRP:HB2	1.74	0.69
1:A:173:HIS:O	1:A:177:ILE:HG13	1.91	0.69
1:A:246:LEU:C	1:A:248:MET:H	2.00	0.69
1:A:183:ASN:O	1:A:186:ALA:HB3	1.92	0.69
2:B:36:SER:CB	2:B:39:LEU:HD12	2.22	0.69
2:B:264:GLY:HA3	3:C:35:ASN:OD1	1.92	0.69
2:B:293:ASN:OD1	2:B:296:VAL:HG23	1.93	0.69
3:C:115:VAL:CG1	3:C:116:ALA:N	2.56	0.69
2:B:268:TRP:HE1	6:B:856:U10:C10	2.05	0.69
3:C:14:SER:O	3:C:17:ILE:HG22	1.92	0.69
2:B:16:ALA:O	2:B:18:LEU:N	2.25	0.68
2:B:256:MET:HE2	2:B:258:PHE:CE2	2.29	0.68
1:A:1:ALA:O	1:A:2:LEU:HG	1.93	0.68
2:B:82:PRO:O	2:B:86:LEU:HD23	1.94	0.68
2:B:229:PHE:O	2:B:244:ALA:HB2	1.93	0.68
2:B:134:TYR:CE2	2:B:144:LYS:HD2	2.27	0.68
3:C:195:MET:HA	3:C:195:MET:CE	2.20	0.68
2:B:17:ASP:O	2:B:19:GLY:N	2.26	0.68
3:C:22:ILE:HG22	3:C:23:PHE:N	2.08	0.67
1:A:236:LEU:O	1:A:236:LEU:HD23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ILE:HG21	6:B:856:U10:H3M2	1.75	0.67
3:C:29:TYR:OH	3:C:57:PRO:HG3	1.94	0.67
2:B:41:TRP:H	2:B:41:TRP:CD1	2.13	0.67
1:A:254:ILE:HD12	1:A:254:ILE:C	2.19	0.67
2:B:237:GLN:O	2:B:241:ARG:N	2.28	0.67
2:B:211:GLY:O	2:B:215:LEU:N	2.27	0.67
1:A:72:GLU:O	1:A:74:GLY:N	2.28	0.67
2:B:247:ARG:NH2	3:C:111:PRO:O	2.27	0.66
1:A:190:HIS:CE1	1:A:194:VAL:HG21	2.29	0.66
1:A:220:VAL:HG23	1:A:221:GLY:N	2.11	0.66
2:B:258:PHE:HD1	3:C:32:GLN:HE22	1.43	0.66
3:C:178:PHE:HD1	3:C:191:LEU:O	1.78	0.66
1:A:190:HIS:CE1	1:A:230:HIS:HE1	2.14	0.66
2:B:215:LEU:CD2	2:B:269:ALA:HB2	2.25	0.66
1:A:230:HIS:CD2	2:B:223:ILE:HG13	2.30	0.65
2:B:269:ALA:HA	2:B:272:MET:HB3	1.77	0.65
3:C:86:ALA:C	3:C:101:THR:HG23	2.22	0.65
2:B:266:HIS:C	2:B:268:TRP:N	2.54	0.65
1:A:248:MET:C	1:A:250:ILE:N	2.54	0.65
2:B:213:ALA:O	2:B:217:ALA:CB	2.45	0.65
1:A:43:ALA:C	1:A:45:GLY:H	2.04	0.65
2:B:159:VAL:HG12	2:B:160:LEU:HD23	1.78	0.65
1:A:217:ARG:HH21	2:B:44:ASN:ND2	1.95	0.65
1:A:250:ILE:HG13	1:A:251:THR:N	2.11	0.65
2:B:90:PHE:HD1	2:B:90:PHE:H	1.44	0.65
2:B:214:LEU:HD12	2:B:214:LEU:C	2.22	0.65
2:B:215:LEU:O	2:B:216:PHE:C	2.40	0.65
1:A:172:ALA:CB	1:A:247:CYS:HB3	2.27	0.65
1:A:178:SER:C	1:A:180:PHE:H	2.04	0.65
1:A:135:ARG:HB3	1:A:136:PRO:HD3	1.79	0.65
1:A:177:ILE:HD12	4:A:850:BCL:OBD	1.97	0.65
1:A:116:HIS:ND1	2:B:225:ALA:HA	2.11	0.65
3:C:171:ILE:HB	3:C:172:PRO:HD2	1.77	0.65
1:A:239:SER:O	1:A:240:ALA:C	2.40	0.64
2:B:268:TRP:HE1	6:B:856:U10:H101	1.60	0.64
2:B:152:SER:OG	2:B:274:VAL:HG13	1.98	0.64
1:A:9:TYR:O	1:A:11:VAL:HG13	1.97	0.64
1:A:187:LEU:CD2	2:B:269:ALA:HB1	2.17	0.64
1:A:224:ILE:HG23	1:A:229:ILE:H	1.63	0.64
2:B:5:ASN:C	2:B:6:ILE:HD13	2.22	0.64
2:B:64:LEU:C	2:B:66:TRP:H	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:GLY:C	2:B:213:ALA:H	2.02	0.64
1:A:196:SER:CB	2:B:145:HIS:HB2	2.26	0.64
2:B:208:PHE:C	2:B:210:TYR:H	2.06	0.64
1:A:52:SER:OG	1:A:66:VAL:HG22	1.98	0.64
4:A:850:BCL:HMD3	4:A:851:BCL:HBB3	1.80	0.64
2:B:232:GLU:O	2:B:233:ARG:C	2.41	0.64
1:A:100:TRP:HE1	5:A:855:BPH:HBD	1.63	0.63
3:C:89:ARG:HG3	3:C:98:HIS:CE1	2.33	0.63
3:C:192:PRO:O	3:C:193:MET:C	2.40	0.63
1:A:139:MET:HE3	1:A:252:GLY:HA3	1.80	0.63
1:A:232:LEU:O	1:A:236:LEU:HB2	1.99	0.63
1:A:142:TRP:H	1:A:142:TRP:CD1	2.14	0.63
3:C:64:PHE:HB2	3:C:73:LEU:O	1.98	0.63
2:B:218:MET:HE3	2:B:252:TRP:CH2	2.34	0.63
1:A:231:ARG:NH2	2:B:5:ASN:HD21	1.96	0.63
3:C:112:ALA:HB2	3:C:239:GLY:HA3	1.79	0.63
1:A:265:TRP:CD1	1:A:266:TRP:N	2.67	0.63
2:B:243:THR:O	2:B:247:ARG:HG3	1.99	0.63
1:A:233:GLY:HA3	2:B:216:PHE:CE1	2.34	0.63
3:C:61:PRO:HG3	3:C:76:PRO:HD2	1.81	0.63
3:C:182:GLU:CG	3:C:186:GLY:HA2	2.29	0.63
1:A:246:LEU:O	1:A:250:ILE:HG23	1.99	0.62
3:C:54:GLY:C	3:C:56:PHE:H	2.07	0.62
3:C:61:PRO:HG3	3:C:76:PRO:HG2	1.81	0.62
1:A:247:CYS:HA	1:A:250:ILE:CD1	2.29	0.62
2:B:228:ARG:HG3	2:B:229:PHE:CZ	2.34	0.62
3:C:77:GLY:O	3:C:79:GLU:HG3	1.98	0.62
1:A:43:ALA:C	1:A:45:GLY:N	2.51	0.62
2:B:270:ILE:HG23	2:B:271:TRP:N	2.13	0.62
3:C:156:CYS:HB2	3:C:248:ARG:CD	2.24	0.62
1:A:163:THR:HG22	1:A:163:THR:O	1.98	0.62
2:B:164:ARG:HB3	2:B:165:PRO:HD3	1.80	0.62
3:C:219:ILE:HD12	3:C:222:PRO:HB3	1.81	0.62
2:B:201:PHE:O	2:B:205:SER:CB	2.48	0.62
3:C:81:GLU:O	3:C:83:ARG:N	2.27	0.62
1:A:114:GLY:HA3	2:B:225:ALA:HA	1.82	0.62
5:A:855:BPH:C1D	2:B:214:LEU:HD13	2.29	0.62
2:B:214:LEU:CD1	2:B:218:MET:SD	2.88	0.62
2:B:271:TRP:O	2:B:275:LEU:HG	1.99	0.62
1:A:114:GLY:N	2:B:225:ALA:O	2.33	0.62
1:A:176:ALA:CB	1:A:243:PHE:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ALA:HA	2:B:277:THR:HG21	1.82	0.61
2:B:10:VAL:HG12	2:B:11:GLN:N	2.15	0.61
3:C:148:PRO:HA	3:C:151:LEU:CG	2.28	0.61
2:B:127:TRP:CZ2	2:B:154:ILE:HG21	2.35	0.61
2:B:199:ASN:HA	2:B:294:TRP:CZ3	2.36	0.61
2:B:116:LEU:C	2:B:118:ALA:H	2.09	0.61
2:B:242:GLY:C	2:B:244:ALA:N	2.50	0.61
3:C:59:PRO:O	3:C:61:PRO:HD3	2.01	0.61
1:A:146:PHE:HA	1:A:156:TRP:CD1	2.35	0.61
3:C:41:PRO:HG3	3:C:58:LEU:HD11	1.82	0.61
2:B:134:TYR:O	2:B:137:ALA:N	2.33	0.61
2:B:152:SER:CB	2:B:274:VAL:HG13	2.30	0.61
1:A:54:VAL:C	1:A:56:GLN:H	2.07	0.61
2:B:89:LEU:HA	2:B:92:PHE:CE2	2.36	0.61
3:C:27:LEU:C	3:C:29:TYR:N	2.56	0.61
2:B:37:THR:HG22	2:B:37:THR:O	2.01	0.61
2:B:199:ASN:OD1	2:B:201:PHE:HB2	2.00	0.61
2:B:214:LEU:HD12	2:B:214:LEU:O	2.00	0.61
3:C:146:LYS:HE2	3:C:200:SER:O	2.00	0.61
1:A:3:LEU:HD22	3:C:39:GLY:C	2.26	0.60
1:A:173:HIS:C	1:A:177:ILE:HG13	2.26	0.60
3:C:148:PRO:CA	3:C:151:LEU:HG	2.28	0.60
1:A:278:GLY:O	1:A:279:ILE:HD13	2.01	0.60
2:B:164:ARG:O	2:B:168:MET:HG2	2.02	0.60
2:B:211:GLY:C	2:B:213:ALA:N	2.59	0.60
1:A:77:GLY:O	1:A:78:ALA:HB2	2.02	0.60
1:A:222:TYR:OH	1:A:224:ILE:HA	2.01	0.60
2:B:218:MET:HE3	2:B:252:TRP:CZ3	2.36	0.60
2:B:264:GLY:O	2:B:266:HIS:N	2.34	0.60
3:C:29:TYR:C	3:C:31:LEU:N	2.59	0.60
2:B:124:VAL:HG12	2:B:124:VAL:O	2.00	0.60
2:B:270:ILE:HD13	2:B:270:ILE:O	2.02	0.60
2:B:193:HIS:HD2	2:B:287:SER:HB3	1.66	0.60
2:B:216:PHE:HD1	2:B:216:PHE:O	1.85	0.60
2:B:101:TYR:CZ	2:B:108:PRO:HD2	2.37	0.60
1:A:117:ILE:H	1:A:118:PRO:HD2	1.66	0.60
2:B:46:GLN:C	2:B:47:LEU:HG	2.27	0.60
1:A:184:ALA:HB3	5:B:854:BPH:CMC	2.32	0.59
1:A:244:SER:O	1:A:246:LEU:N	2.34	0.59
4:A:850:BCL:H52	6:A:857:U10:H302	1.84	0.59
1:A:231:ARG:HH21	2:B:5:ASN:HD21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:MET:O	3:C:196:VAL:HG22	2.02	0.59
1:A:179:PHE:C	1:A:240:ALA:HB2	2.27	0.59
2:B:239:ALA:O	2:B:240:ASP:HB2	2.01	0.59
2:B:273:ALA:O	2:B:275:LEU:N	2.36	0.59
3:C:143:SER:O	3:C:144:ALA:HB3	2.02	0.59
1:A:185:LEU:HG	5:B:854:BPH:NC	2.16	0.59
1:A:247:CYS:HA	1:A:250:ILE:HD11	1.84	0.59
2:B:211:GLY:HA3	2:B:272:MET:CE	2.32	0.59
1:A:219:LEU:HD12	2:B:132:ARG:HH12	1.67	0.59
2:B:12:VAL:HG12	2:B:13:ARG:N	2.17	0.59
2:B:26:LEU:C	2:B:28:ASN:N	2.55	0.59
2:B:262:MET:O	2:B:265:ILE:HG22	2.01	0.59
3:C:69:GLY:C	3:C:71:GLY:H	2.10	0.59
1:A:126:LEU:HD12	1:A:129:LEU:HD12	1.83	0.59
3:C:168:TRP:HB2	3:C:178:PHE:HB2	1.84	0.59
1:A:37:ALA:C	1:A:39:PHE:H	2.11	0.59
2:B:215:LEU:O	2:B:218:MET:N	2.35	0.59
1:A:174:MET:HA	1:A:177:ILE:HD12	1.83	0.59
5:A:855:BPH:HED3	2:B:252:TRP:HZ3	1.67	0.59
2:B:77:GLN:C	2:B:79:GLY:H	2.10	0.59
1:A:89:ILE:HG23	1:A:90:THR:N	2.17	0.59
2:B:280:GLY:HA2	4:B:852:BCL:HED2	1.83	0.59
2:B:266:HIS:O	2:B:268:TRP:N	2.36	0.59
3:C:36:MET:HG2	3:C:40:TYR:CE1	2.38	0.59
1:A:62:GLN:HG2	1:A:151:TRP:CD1	2.38	0.58
2:B:85:PHE:O	2:B:89:LEU:HB2	2.03	0.58
2:B:156:LEU:O	2:B:160:LEU:HG	2.03	0.58
1:A:52:SER:HB2	1:A:85:LEU:CD1	2.27	0.58
2:B:122:MET:SD	2:B:157:TRP:HZ2	2.25	0.58
2:B:229:PHE:CE1	3:C:238:ALA:HB2	2.38	0.58
1:A:30:TYR:CG	1:A:31:VAL:N	2.71	0.58
2:B:50:ILE:CD1	2:B:51:TYR:N	2.61	0.58
2:B:207:ALA:O	2:B:210:TYR:HB2	2.04	0.58
1:A:142:TRP:O	1:A:144:TYR:N	2.35	0.58
2:B:49:PRO:O	2:B:50:ILE:HB	2.02	0.58
2:B:265:ILE:HG23	2:B:266:HIS:N	2.17	0.58
1:A:216:PHE:HB3	1:A:220:VAL:HG22	1.85	0.58
1:A:235:LEU:O	1:A:236:LEU:C	2.46	0.58
2:B:191:LEU:C	2:B:193:HIS:H	2.11	0.58
2:B:205:SER:HA	2:B:279:THR:OG1	2.02	0.58
2:B:152:SER:HB2	2:B:274:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:TYR:O	3:C:20:PHE:N	2.36	0.58
3:C:32:GLN:HG2	3:C:56:PHE:CE2	2.38	0.58
3:C:178:PHE:CE1	3:C:192:PRO:HA	2.38	0.58
1:A:176:ALA:HB2	1:A:243:PHE:HB3	1.86	0.58
4:A:850:BCL:HAA2	4:A:850:BCL:HBD	1.85	0.58
4:A:850:BCL:CMD	4:A:851:BCL:HBB3	2.33	0.58
2:B:55:LEU:HD23	2:B:132:ARG:HB2	1.84	0.58
3:C:35:ASN:O	3:C:36:MET:HG3	2.04	0.58
1:A:239:SER:O	1:A:242:PHE:N	2.37	0.58
1:A:266:TRP:HE1	2:B:87:ARG:HA	1.69	0.58
2:B:40:GLY:C	2:B:42:PHE:H	2.12	0.58
2:B:245:ALA:O	2:B:248:ALA:HB3	2.04	0.58
2:B:129:TRP:HD1	2:B:150:PHE:HE2	1.51	0.57
2:B:201:PHE:O	2:B:205:SER:HB3	2.04	0.57
2:B:243:THR:H	3:C:115:VAL:HG21	1.67	0.57
1:A:190:HIS:NE2	2:B:266:HIS:NE2	2.50	0.57
1:A:191:GLY:O	1:A:195:LEU:HB2	2.03	0.57
2:B:234:GLU:O	2:B:237:GLN:HB2	2.05	0.57
2:B:265:ILE:C	2:B:268:TRP:HB2	2.29	0.57
1:A:97:PHE:HB3	1:A:125:ILE:HD11	1.87	0.57
2:B:74:PHE:N	2:B:74:PHE:HD1	2.03	0.57
2:B:78:ALA:HB2	2:B:92:PHE:CZ	2.39	0.57
2:B:91:PHE:O	2:B:92:PHE:C	2.47	0.57
2:B:180:PHE:HD1	2:B:183:LEU:HD12	1.70	0.57
2:B:266:HIS:C	2:B:268:TRP:H	2.11	0.57
2:B:38:LEU:C	2:B:40:GLY:N	2.56	0.57
2:B:166:ILE:HG22	2:B:167:LEU:HD23	1.86	0.57
1:A:185:LEU:C	1:A:188:ALA:HB3	2.29	0.57
1:A:187:LEU:HB2	2:B:216:PHE:HD2	1.68	0.57
2:B:73:TRP:CD1	2:B:94:LEU:HB2	2.40	0.57
2:B:163:ILE:HG22	2:B:285:LEU:HD13	1.86	0.57
1:A:174:MET:HG3	1:A:175:ILE:N	2.19	0.57
1:A:210:ASP:O	1:A:211:HIS:C	2.46	0.57
1:A:226:THR:C	1:A:228:GLY:N	2.61	0.57
2:B:246:GLU:O	2:B:247:ARG:C	2.48	0.57
2:B:261:THR:HG23	3:C:35:ASN:HA	1.85	0.57
3:C:31:LEU:O	3:C:33:THR:N	2.38	0.57
1:A:211:HIS:O	1:A:212:GLU:C	2.47	0.57
1:A:244:SER:HA	1:A:247:CYS:SG	2.44	0.57
3:C:54:GLY:O	3:C:56:PHE:N	2.36	0.57
3:C:17:ILE:O	3:C:21:TRP:HD1	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLY:C	2:B:145:HIS:H	2.12	0.56
2:B:269:ALA:O	2:B:272:MET:HB3	2.04	0.56
2:B:192:VAL:HG12	2:B:192:VAL:O	2.05	0.56
2:B:237:GLN:NE2	3:C:117:ARG:NH2	2.52	0.56
2:B:258:PHE:HD1	3:C:32:GLN:NE2	2.04	0.56
3:C:219:ILE:CD1	3:C:222:PRO:HB3	2.35	0.56
2:B:64:LEU:C	2:B:66:TRP:N	2.62	0.56
2:B:270:ILE:CG2	2:B:271:TRP:N	2.68	0.56
3:C:65:ILE:HD12	3:C:65:ILE:N	2.21	0.56
1:A:180:PHE:CE2	1:A:240:ALA:HB1	2.39	0.56
2:B:69:THR:C	2:B:70:ILE:HD13	2.30	0.56
2:B:215:LEU:HD23	2:B:269:ALA:HB2	1.86	0.56
3:C:134:MET:C	3:C:136:ALA:H	2.13	0.56
6:A:857:U10:H122	6:A:857:U10:H303	1.87	0.56
2:B:74:PHE:N	2:B:74:PHE:CD1	2.73	0.56
2:B:90:PHE:CD1	2:B:90:PHE:N	2.72	0.56
2:B:242:GLY:C	2:B:244:ALA:H	2.12	0.56
6:B:856:U10:H3M3	6:B:856:U10:H4M2	1.88	0.56
1:A:117:ILE:O	1:A:119:PHE:N	2.39	0.56
3:C:119:ASP:OD1	3:C:228:LEU:HD23	2.05	0.56
3:C:208:LEU:CD2	3:C:240:GLY:HA3	2.35	0.56
2:B:155:TRP:CD1	2:B:278:LEU:HA	2.33	0.56
1:A:171:PRO:HD2	1:A:259:TRP:CZ3	2.41	0.56
2:B:55:LEU:O	2:B:56:GLY:C	2.48	0.56
3:C:32:GLN:O	3:C:32:GLN:HG3	2.06	0.56
3:C:104:PRO:O	3:C:109:VAL:HG22	2.05	0.56
3:C:236:TYR:O	3:C:237:VAL:C	2.49	0.56
1:A:241:VAL:HG12	1:A:242:PHE:N	2.21	0.55
3:C:31:LEU:C	3:C:33:THR:H	2.15	0.55
1:A:113:ILE:HG21	2:B:226:VAL:HG12	1.87	0.55
1:A:166:ASN:ND2	2:B:187:ASN:HB2	2.20	0.55
2:B:273:ALA:O	2:B:276:VAL:N	2.36	0.55
2:B:243:THR:OG1	2:B:247:ARG:NE	2.39	0.55
3:C:61:PRO:HG3	3:C:76:PRO:CG	2.36	0.55
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.72	0.55
2:B:77:GLN:C	2:B:79:GLY:N	2.65	0.55
3:C:29:TYR:C	3:C:31:LEU:H	2.15	0.55
1:A:244:SER:C	1:A:246:LEU:N	2.52	0.55
3:C:31:LEU:C	3:C:33:THR:N	2.64	0.55
3:C:43:GLU:O	3:C:44:ASN:O	2.25	0.55
1:A:107:ILE:HG22	1:A:107:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:HD21	2:B:187:ASN:HB2	1.73	0.54
2:B:4:GLN:O	2:B:6:ILE:N	2.40	0.54
2:B:237:GLN:NE2	3:C:117:ARG:HH22	2.05	0.54
2:B:246:GLU:O	2:B:248:ALA:N	2.40	0.54
3:C:148:PRO:O	3:C:164:VAL:HB	2.08	0.54
1:A:16:LEU:CD2	1:A:109:ARG:HD2	2.32	0.54
1:A:237:SER:O	1:A:238:LEU:C	2.49	0.54
2:B:243:THR:N	3:C:115:VAL:CG2	2.68	0.54
3:C:61:PRO:HG3	3:C:76:PRO:CD	2.37	0.54
3:C:238:ALA:O	3:C:240:GLY:N	2.41	0.54
1:A:65:SER:OG	1:A:149:GLY:HA3	2.08	0.54
1:A:117:ILE:C	1:A:119:PHE:N	2.63	0.54
1:A:233:GLY:O	1:A:234:LEU:C	2.50	0.54
2:B:174:ALA:O	2:B:185:TRP:NE1	2.40	0.54
2:B:201:PHE:O	2:B:205:SER:HB2	2.07	0.54
3:C:15:LEU:CD1	3:C:19:SER:HB3	2.37	0.54
3:C:148:PRO:O	3:C:150:GLY:N	2.40	0.54
3:C:170:ASP:HB2	3:C:177:ARG:CD	2.38	0.54
3:C:217:PRO:HD3	3:C:236:TYR:CD2	2.43	0.54
3:C:233:ILE:O	3:C:234:CYS:C	2.51	0.54
1:A:9:TYR:CE1	3:C:113:SER:HB2	2.43	0.54
1:A:65:SER:CB	1:A:149:GLY:HA3	2.38	0.54
1:A:226:THR:OG1	1:A:227:LEU:N	2.37	0.54
3:C:95:GLY:O	3:C:96:PHE:O	2.26	0.54
1:A:147:PRO:CD	1:A:156:TRP:HB2	2.37	0.54
1:A:200:PRO:O	1:A:201:GLU:C	2.50	0.54
1:A:208:THR:C	1:A:210:ASP:H	2.15	0.54
2:B:40:GLY:C	2:B:42:PHE:N	2.65	0.54
2:B:150:PHE:O	2:B:151:LEU:C	2.50	0.54
2:B:275:LEU:O	2:B:279:THR:HG23	2.08	0.54
1:A:41:PHE:CD2	1:A:95:GLY:HA3	2.42	0.54
1:A:183:ASN:HB2	1:A:236:LEU:HD22	1.90	0.54
3:C:178:PHE:CD1	3:C:191:LEU:O	2.61	0.54
1:A:39:PHE:O	1:A:40:PHE:C	2.51	0.53
1:A:116:HIS:CD2	2:B:224:LEU:HB2	2.43	0.53
1:A:223:SER:C	1:A:225:GLY:N	2.63	0.53
1:A:241:VAL:O	1:A:244:SER:N	2.37	0.53
2:B:270:ILE:HD13	2:B:270:ILE:C	2.32	0.53
3:C:189:ARG:HD2	3:C:216:ILE:HB	1.90	0.53
1:A:156:TRP:HE3	1:A:157:VAL:HG23	1.74	0.53
2:B:116:LEU:O	2:B:118:ALA:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:GLY:O	2:B:265:ILE:C	2.49	0.53
3:C:203:VAL:HG12	3:C:204:HIS:H	1.72	0.53
1:A:43:ALA:O	1:A:47:ILE:HG13	2.09	0.53
1:A:83:GLY:O	1:A:85:LEU:N	2.41	0.53
2:B:90:PHE:CG	2:B:179:ILE:HD12	2.44	0.53
3:C:171:ILE:CB	3:C:172:PRO:CD	2.84	0.53
1:A:128:TYR:O	1:A:129:LEU:C	2.51	0.53
3:C:43:GLU:HB3	3:C:47:GLY:HA2	1.91	0.53
3:C:129:ASN:ND2	3:C:224:GLU:HB2	2.24	0.53
3:C:169:VAL:HG23	3:C:170:ASP:N	2.24	0.53
1:A:231:ARG:O	1:A:232:LEU:C	2.52	0.53
3:C:83:ARG:HB2	3:C:84:PRO:CD	2.36	0.53
1:A:186:ALA:O	1:A:187:LEU:C	2.52	0.53
1:A:192:ALA:O	1:A:196:SER:HB3	2.08	0.53
1:A:230:HIS:CD2	2:B:223:ILE:HG21	2.44	0.53
1:A:255:TRP:CZ2	1:A:262:TRP:HB2	2.44	0.53
2:B:271:TRP:O	2:B:272:MET:C	2.52	0.53
4:A:851:BCL:HAA2	4:A:851:BCL:HBD	1.91	0.53
2:B:89:LEU:HA	2:B:92:PHE:CD2	2.44	0.53
3:C:171:ILE:O	3:C:173:GLU:N	2.41	0.53
1:A:130:THR:HA	1:A:134:PHE:HB2	1.91	0.53
2:B:25:ASN:ND2	2:B:28:ASN:HD22	2.06	0.53
2:B:204:LEU:O	2:B:205:SER:C	2.51	0.53
3:C:182:GLU:HG3	3:C:186:GLY:HA2	1.90	0.53
1:A:250:ILE:HG13	1:A:251:THR:H	1.74	0.52
2:B:246:GLU:C	2:B:248:ALA:N	2.66	0.52
1:A:217:ARG:NH2	2:B:44:ASN:ND2	2.57	0.52
1:A:220:VAL:CG2	1:A:221:GLY:N	2.73	0.52
1:A:246:LEU:C	1:A:248:MET:N	2.65	0.52
2:B:212:SER:OG	2:B:272:MET:HG3	2.08	0.52
1:A:182:THR:O	1:A:185:LEU:N	2.42	0.52
1:A:263:TRP:CE3	2:B:180:PHE:HZ	2.26	0.52
3:C:66:LEU:HD22	3:C:67:PRO:HD2	1.92	0.52
3:C:134:MET:C	3:C:136:ALA:N	2.68	0.52
3:C:156:CYS:SG	3:C:209:SER:HB3	2.48	0.52
1:A:86:TRP:O	1:A:90:THR:OG1	2.25	0.52
2:B:66:TRP:CD1	2:B:122:MET:HB2	2.43	0.52
1:A:208:THR:C	1:A:210:ASP:N	2.66	0.52
1:A:208:THR:OG1	1:A:210:ASP:HB2	2.09	0.52
2:B:103:LEU:CD2	2:B:169:GLY:HA2	2.40	0.52
2:B:46:GLN:HG2	2:B:47:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:TRP:O	2:B:156:LEU:C	2.52	0.52
2:B:210:TYR:HD2	4:B:853:BCL:H11	1.75	0.52
3:C:22:ILE:C	3:C:24:LEU:H	2.17	0.52
1:A:85:LEU:O	1:A:87:GLN:N	2.43	0.52
1:A:113:ILE:HB	2:B:226:VAL:HG12	1.91	0.52
1:A:116:HIS:CD2	2:B:224:LEU:CB	2.92	0.52
2:B:116:LEU:C	2:B:118:ALA:N	2.68	0.52
2:B:155:TRP:HA	2:B:155:TRP:CE3	2.45	0.52
2:B:260:ALA:HB1	3:C:35:ASN:OD1	2.09	0.52
3:C:169:VAL:HG23	3:C:170:ASP:C	2.35	0.52
2:B:5:ASN:C	2:B:5:ASN:HD22	2.18	0.52
4:B:853:BCL:HAA2	4:B:853:BCL:HBD	1.91	0.52
3:C:207:ALA:HA	3:C:241:LEU:HD23	1.92	0.52
1:A:141:ALA:O	1:A:142:TRP:C	2.53	0.52
1:A:159:ASN:O	1:A:161:GLY:N	2.43	0.52
3:C:135:LYS:HZ2	3:C:166:ASP:CG	2.18	0.52
2:B:60:LEU:HD12	5:B:854:BPH:H5C2	1.92	0.52
2:B:78:ALA:HB2	2:B:92:PHE:HZ	1.75	0.52
2:B:243:THR:H	3:C:115:VAL:CG2	2.24	0.51
1:A:190:HIS:CE1	1:A:230:HIS:CE1	2.98	0.51
2:B:26:LEU:HD22	2:B:29:ARG:CD	2.40	0.51
3:C:75:VAL:HA	3:C:76:PRO:C	2.30	0.51
1:A:237:SER:O	1:A:239:SER:N	2.43	0.51
2:B:153:ALA:O	2:B:154:ILE:C	2.52	0.51
2:B:251:PHE:C	2:B:251:PHE:CD1	2.88	0.51
1:A:44:LEU:O	1:A:48:LEU:HG	2.10	0.51
2:B:36:SER:C	2:B:38:LEU:H	2.18	0.51
3:C:122:GLU:O	3:C:123:LEU:HD23	2.10	0.51
1:A:54:VAL:C	1:A:56:GLN:N	2.68	0.51
2:B:154:ILE:CG2	2:B:158:MET:HG2	2.39	0.51
2:B:155:TRP:HA	2:B:155:TRP:HE3	1.76	0.51
2:B:187:ASN:O	2:B:191:LEU:HG	2.09	0.51
1:A:184:ALA:HB3	5:B:854:BPH:HMC3	1.92	0.51
1:A:217:ARG:O	2:B:50:ILE:HA	2.10	0.51
2:B:34:PRO:C	2:B:47:LEU:HD12	2.36	0.51
1:A:51:TRP:HD1	1:A:51:TRP:O	1.94	0.51
1:A:87:GLN:O	1:A:90:THR:N	2.44	0.51
1:A:89:ILE:CG2	1:A:90:THR:N	2.74	0.51
1:A:166:ASN:OD1	1:A:167:PHE:N	2.44	0.51
1:A:226:THR:O	1:A:228:GLY:N	2.44	0.51
1:A:235:LEU:O	1:A:237:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:O	2:B:66:TRP:N	2.44	0.51
3:C:159:GLU:HB3	3:C:210:SER:HB3	1.92	0.51
1:A:216:PHE:HA	1:A:219:LEU:HB3	1.94	0.50
2:B:265:ILE:CG2	2:B:266:HIS:N	2.74	0.50
2:B:265:ILE:HD12	2:B:268:TRP:HD1	1.76	0.50
3:C:23:PHE:O	3:C:27:LEU:HB2	2.11	0.50
3:C:86:ALA:O	3:C:101:THR:HG23	2.11	0.50
1:A:173:HIS:O	1:A:176:ALA:N	2.44	0.50
2:B:95:GLU:HA	2:B:176:PRO:CB	2.34	0.50
2:B:280:GLY:O	2:B:281:GLY:C	2.54	0.50
3:C:235:GLY:O	3:C:236:TYR:C	2.53	0.50
1:A:61:PRO:HB3	1:A:150:ILE:HD12	1.93	0.50
2:B:78:ALA:O	2:B:81:ASN:HB3	2.12	0.50
3:C:22:ILE:C	3:C:24:LEU:N	2.70	0.50
1:A:56:GLN:HE22	1:A:64:ILE:HA	1.76	0.50
1:A:123:PHE:CG	1:A:238:LEU:HD22	2.46	0.50
1:A:218:ASP:OD2	2:B:29:ARG:NH2	2.44	0.50
2:B:10:VAL:CG1	2:B:11:GLN:N	2.74	0.50
2:B:93:SER:CB	2:B:181:SER:HB3	2.39	0.50
2:B:273:ALA:C	2:B:275:LEU:N	2.68	0.50
3:C:220:LYS:O	3:C:220:LYS:HG3	2.12	0.50
1:A:176:ALA:O	1:A:180:PHE:HD2	1.95	0.50
2:B:40:GLY:O	2:B:42:PHE:N	2.44	0.50
1:A:51:TRP:CD1	1:A:51:TRP:C	2.90	0.50
1:A:65:SER:HB2	1:A:149:GLY:HA3	1.92	0.50
1:A:116:HIS:HB3	2:B:221:ALA:HA	1.92	0.50
1:A:132:VAL:HG23	1:A:133:LEU:N	2.27	0.50
5:A:855:BPH:HED3	2:B:252:TRP:CZ3	2.46	0.50
3:C:173:GLU:O	3:C:174:GLN:C	2.55	0.50
1:A:216:PHE:O	1:A:220:VAL:N	2.44	0.50
1:A:229:ILE:C	1:A:231:ARG:H	2.20	0.50
2:B:267:ARG:O	2:B:270:ILE:HG22	2.12	0.50
3:C:148:PRO:HG2	3:C:164:VAL:HG11	1.94	0.50
1:A:34:PHE:CZ	1:A:102:LEU:HD13	2.47	0.49
1:A:121:PHE:C	1:A:123:PHE:H	2.20	0.49
1:A:190:HIS:CG	1:A:229:ILE:HD11	2.47	0.49
1:A:269:LEU:CD1	1:A:270:PRO:HD2	2.33	0.49
2:B:190:SER:O	2:B:194:GLY:O	2.29	0.49
2:B:231:GLY:O	2:B:232:GLU:O	2.29	0.49
3:C:169:VAL:HG23	3:C:170:ASP:O	2.12	0.49
1:A:162:TYR:C	1:A:164:TYR:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:850:BCL:H3A	4:A:850:BCL:H152	1.95	0.49
1:A:126:LEU:C	1:A:128:TYR:N	2.68	0.49
1:A:193:LEU:HD22	1:A:216:PHE:HE2	1.77	0.49
4:A:850:BCL:H171	4:A:850:BCL:CHB	2.42	0.49
1:A:101:ALA:O	1:A:104:GLU:N	2.45	0.49
1:A:190:HIS:CE1	2:B:266:HIS:HE2	2.30	0.49
2:B:265:ILE:HG21	6:B:856:U10:C3M	2.41	0.49
3:C:20:PHE:C	3:C:22:ILE:H	2.18	0.49
3:C:180:GLU:OE2	3:C:188:THR:HG21	2.12	0.49
1:A:157:VAL:O	1:A:158:SER:C	2.55	0.49
2:B:96:PRO:CG	2:B:172:SER:HA	2.42	0.49
2:B:242:GLY:CA	3:C:117:ARG:HD2	2.43	0.49
2:B:259:ASN:HA	6:B:856:U10:H8	1.95	0.49
1:A:266:TRP:CD1	1:A:266:TRP:C	2.89	0.49
2:B:265:ILE:HD12	2:B:268:TRP:CD1	2.48	0.49
1:A:139:MET:HE3	1:A:252:GLY:CA	2.43	0.49
3:C:27:LEU:O	3:C:28:ILE:C	2.54	0.49
3:C:183:LEU:HD11	3:C:189:ARG:HG3	1.94	0.49
3:C:192:PRO:O	3:C:194:GLN:N	2.45	0.49
1:A:85:LEU:O	1:A:86:TRP:C	2.55	0.49
1:A:173:HIS:CE1	1:A:177:ILE:HD11	2.48	0.49
2:B:210:TYR:O	2:B:213:ALA:HB3	2.13	0.49
3:C:53:GLN:O	3:C:54:GLY:O	2.30	0.49
2:B:248:ALA:C	2:B:250:LEU:N	2.70	0.49
1:A:69:PRO:HG2	1:A:87:GLN:HE21	1.78	0.49
1:A:83:GLY:O	1:A:84:GLY:C	2.56	0.49
1:A:209:PRO:CA	2:B:235:LEU:HD12	2.43	0.49
1:A:229:ILE:HD12	6:A:857:U10:H4M1	1.95	0.49
1:A:250:ILE:O	1:A:252:GLY:N	2.46	0.49
4:A:850:BCL:H71	4:A:850:BCL:C2	2.33	0.49
2:B:204:LEU:O	2:B:207:ALA:HB3	2.13	0.49
1:A:2:LEU:HD22	1:A:6:GLU:HB3	1.95	0.48
2:B:239:ALA:O	2:B:240:ASP:CB	2.61	0.48
2:B:265:ILE:O	2:B:268:TRP:CB	2.49	0.48
1:A:44:LEU:HA	1:A:47:ILE:CD1	2.38	0.48
1:A:157:VAL:C	1:A:159:ASN:N	2.71	0.48
1:A:264:GLN:C	1:A:266:TRP:N	2.66	0.48
1:A:187:LEU:HB2	2:B:216:PHE:CD2	2.46	0.48
2:B:266:HIS:O	2:B:267:ARG:C	2.55	0.48
1:A:172:ALA:HB3	1:A:247:CYS:HB3	1.94	0.48
2:B:14:GLY:O	2:B:15:PRO:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:TYR:CD1	3:C:56:PHE:HE1	2.31	0.48
3:C:245:ALA:N	3:C:246:PRO:CD	2.76	0.48
1:A:37:ALA:C	1:A:39:PHE:N	2.71	0.48
2:B:159:VAL:HA	2:B:163:ILE:CB	2.26	0.48
2:B:222:THR:O	2:B:223:ILE:C	2.57	0.48
2:B:240:ASP:O	2:B:241:ARG:C	2.55	0.48
2:B:57:VAL:O	2:B:58:LEU:C	2.56	0.48
2:B:175:VAL:HG22	2:B:185:TRP:CD2	2.49	0.48
2:B:202:HIS:O	2:B:206:ILE:HD12	2.14	0.48
1:A:41:PHE:HD2	1:A:95:GLY:C	2.22	0.48
2:B:282:ILE:O	2:B:283:GLY:C	2.57	0.48
1:A:34:PHE:HA	1:A:37:ALA:HB3	1.95	0.48
1:A:131:LEU:O	1:A:132:VAL:HG13	2.14	0.48
2:B:127:TRP:HZ2	2:B:154:ILE:HG21	1.78	0.48
2:B:159:VAL:CA	2:B:163:ILE:HB	2.25	0.48
2:B:273:ALA:O	2:B:274:VAL:C	2.57	0.48
3:C:29:TYR:O	3:C:30:TYR:C	2.57	0.48
1:A:142:TRP:O	1:A:143:GLY:C	2.56	0.48
1:A:234:LEU:O	1:A:237:SER:HB2	2.14	0.48
1:A:235:LEU:C	1:A:237:SER:N	2.69	0.48
2:B:226:VAL:O	2:B:227:SER:C	2.56	0.48
4:B:852:BCL:HBB3	4:B:853:BCL:HMD2	1.96	0.48
3:C:120:LEU:N	3:C:226:THR:HB	2.29	0.48
1:A:67:TYR:O	1:A:86:TRP:HB2	2.14	0.48
1:A:224:ILE:HG23	1:A:229:ILE:N	2.26	0.48
2:B:71:GLY:O	2:B:75:TRP:HD1	1.97	0.48
2:B:195:ASN:HB3	2:B:198:TYR:HD2	1.78	0.47
2:B:198:TYR:O	2:B:294:TRP:HE3	1.97	0.47
3:C:111:PRO:HB2	3:C:239:GLY:HA2	1.95	0.47
1:A:236:LEU:HD23	1:A:236:LEU:C	2.39	0.47
2:B:4:GLN:OE1	2:B:4:GLN:HA	2.14	0.47
2:B:123:PHE:HE2	2:B:158:MET:HE1	1.78	0.47
1:A:209:PRO:N	2:B:235:LEU:HD12	2.29	0.47
2:B:17:ASP:CG	3:C:126:HIS:HE1	2.22	0.47
2:B:90:PHE:CB	2:B:179:ILE:HD12	2.44	0.47
2:B:161:GLY:O	2:B:162:PHE:HB2	2.14	0.47
2:B:228:ARG:HG3	2:B:229:PHE:CD1	2.48	0.47
3:C:65:ILE:HD12	3:C:65:ILE:H	1.80	0.47
3:C:69:GLY:C	3:C:71:GLY:N	2.73	0.47
1:A:25:TRP:HE1	2:B:254:TRP:CD1	2.32	0.47
1:A:227:LEU:HD23	3:C:175:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:GLY:C	3:C:115:VAL:HG21	2.39	0.47
2:B:248:ALA:O	2:B:250:LEU:N	2.47	0.47
3:C:65:ILE:O	3:C:66:LEU:O	2.33	0.47
3:C:103:ASP:O	3:C:107:ASP:OD2	2.31	0.47
1:A:46:ILE:HA	1:A:49:ILE:HB	1.96	0.47
1:A:163:THR:O	1:A:163:THR:CG2	2.61	0.47
1:A:172:ALA:O	1:A:247:CYS:HB3	2.13	0.47
2:B:242:GLY:O	2:B:244:ALA:N	2.47	0.47
1:A:208:THR:HB	1:A:209:PRO:HD2	1.96	0.47
2:B:199:ASN:HA	2:B:294:TRP:HZ3	1.80	0.47
3:C:104:PRO:HA	3:C:109:VAL:HG22	1.97	0.47
1:A:127:ALA:HB1	4:A:851:BCL:H12	1.96	0.47
1:A:187:LEU:HD13	2:B:216:PHE:CG	2.49	0.47
1:A:193:LEU:O	1:A:194:VAL:C	2.57	0.47
2:B:32:VAL:CG1	2:B:33:GLY:H	2.11	0.47
2:B:90:PHE:O	2:B:92:PHE:N	2.47	0.47
2:B:256:MET:CE	2:B:258:PHE:HE2	2.28	0.47
2:B:269:ALA:HA	2:B:272:MET:CB	2.44	0.47
3:C:17:ILE:HG23	3:C:18:TYR:CD1	2.50	0.47
3:C:37:ARG:HG2	3:C:76:PRO:HD3	1.96	0.47
3:C:66:LEU:HB3	3:C:67:PRO:HD2	1.96	0.47
3:C:143:SER:O	3:C:144:ALA:CB	2.63	0.47
3:C:171:ILE:C	3:C:173:GLU:H	2.22	0.47
1:A:100:TRP:NE1	5:A:855:BPH:HAA2	2.30	0.47
1:A:123:PHE:CE2	1:A:238:LEU:HB3	2.49	0.47
1:A:279:ILE:HG22	1:A:279:ILE:O	2.15	0.47
2:B:171:TRP:HA	2:B:171:TRP:CE3	2.50	0.47
1:A:99:SER:O	1:A:100:TRP:C	2.58	0.47
1:A:117:ILE:HG12	2:B:221:ALA:HB1	1.96	0.47
1:A:195:LEU:HD11	2:B:267:ARG:N	2.29	0.47
1:A:41:PHE:CE2	1:A:95:GLY:HA3	2.50	0.47
1:A:226:THR:C	1:A:228:GLY:H	2.23	0.47
2:B:216:PHE:C	2:B:216:PHE:CD1	2.93	0.47
2:B:291:VAL:HG12	2:B:293:ASN:O	2.15	0.47
3:C:245:ALA:N	3:C:246:PRO:HD3	2.30	0.47
1:A:12:PRO:HG3	3:C:97:PRO:HB2	1.96	0.46
1:A:79:PRO:C	1:A:81:ALA:H	2.24	0.46
2:B:268:TRP:CE3	2:B:268:TRP:HA	2.50	0.46
2:B:280:GLY:HA2	4:B:852:BCL:CED	2.45	0.46
2:B:282:ILE:O	2:B:284:ILE:N	2.48	0.46
1:A:185:LEU:N	5:B:854:BPH:HMC2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG23	2:B:87:ARG:HG2	1.97	0.46
1:A:271:TRP:H	1:A:271:TRP:HD1	1.56	0.46
2:B:25:ASN:ND2	2:B:28:ASN:ND2	2.64	0.46
3:C:156:CYS:SG	3:C:248:ARG:NH1	2.88	0.46
1:A:70:ALA:O	1:A:72:GLU:N	2.48	0.46
1:A:187:LEU:N	2:B:216:PHE:CE2	2.83	0.46
3:C:203:VAL:HG12	3:C:204:HIS:N	2.30	0.46
1:A:137:VAL:HG12	1:A:137:VAL:O	2.15	0.46
1:A:156:TRP:CE3	1:A:157:VAL:HG23	2.50	0.46
1:A:209:PRO:HG2	3:C:130:LYS:HE2	1.97	0.46
2:B:38:LEU:HD12	2:B:41:TRP:CD1	2.51	0.46
2:B:90:PHE:HA	2:B:179:ILE:CG1	2.44	0.46
2:B:129:TRP:HD1	2:B:150:PHE:CE2	2.31	0.46
2:B:190:SER:CB	4:B:852:BCL:HBC3	2.45	0.46
2:B:211:GLY:HA3	2:B:272:MET:HE3	1.97	0.46
2:B:229:PHE:HB3	2:B:243:THR:CG2	2.45	0.46
2:B:237:GLN:HE22	3:C:117:ARG:NH1	2.13	0.46
2:B:242:GLY:HA2	3:C:117:ARG:HD2	1.97	0.46
1:A:159:ASN:O	1:A:160:THR:C	2.59	0.46
1:A:175:ILE:HG22	1:A:243:PHE:CD1	2.51	0.46
2:B:34:PRO:O	2:B:47:LEU:HD12	2.15	0.46
3:C:37:ARG:HG2	3:C:37:ARG:HH11	1.79	0.46
2:B:125:ALA:O	5:B:854:BPH:H1C2	2.15	0.46
2:B:256:MET:HE2	2:B:258:PHE:HE2	1.79	0.46
3:C:36:MET:HG2	3:C:40:TYR:CD1	2.51	0.46
3:C:233:ILE:O	3:C:237:VAL:HG23	2.15	0.46
1:A:113:ILE:CB	2:B:226:VAL:HG12	2.44	0.46
1:A:171:PRO:HD2	1:A:259:TRP:CE3	2.51	0.46
1:A:178:SER:HA	1:A:181:PHE:HD2	1.79	0.46
2:B:268:TRP:NE1	6:B:856:U10:H101	2.29	0.46
3:C:173:GLU:O	3:C:175:MET:N	2.48	0.46
1:A:147:PRO:C	1:A:149:GLY:H	2.24	0.46
1:A:226:THR:O	1:A:229:ILE:HG23	2.15	0.46
1:A:246:LEU:O	1:A:248:MET:N	2.48	0.46
3:C:182:GLU:CD	3:C:186:GLY:HA2	2.41	0.46
3:C:198:VAL:HG12	3:C:199:GLN:N	2.31	0.46
1:A:239:SER:C	1:A:241:VAL:N	2.74	0.46
2:B:122:MET:SD	2:B:157:TRP:CZ2	3.07	0.46
2:B:171:TRP:HA	2:B:171:TRP:HE3	1.80	0.46
2:B:208:PHE:C	2:B:210:TYR:N	2.68	0.46
2:B:219:HIS:NE2	2:B:223:ILE:HG13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:ASN:HD22	3:C:224:GLU:HB2	1.80	0.46
1:A:125:ILE:HG22	1:A:126:LEU:HD12	1.98	0.46
1:A:56:GLN:NE2	1:A:64:ILE:HA	2.31	0.45
1:A:184:ALA:CB	5:B:854:BPH:HMC3	2.45	0.45
1:A:34:PHE:CE2	1:A:102:LEU:HB3	2.51	0.45
1:A:212:GLU:O	1:A:213:ASP:C	2.59	0.45
1:A:255:TRP:NE1	1:A:257:ASP:O	2.50	0.45
2:B:258:PHE:N	2:B:258:PHE:CD2	2.83	0.45
3:C:238:ALA:O	3:C:239:GLY:C	2.60	0.45
1:A:85:LEU:C	1:A:87:GLN:N	2.72	0.45
2:B:189:PHE:C	2:B:191:LEU:N	2.72	0.45
2:B:216:PHE:C	2:B:216:PHE:HD1	2.24	0.45
4:B:852:BCL:HAA2	4:B:852:BCL:HBD	1.98	0.45
3:C:17:ILE:O	3:C:17:ILE:HG13	2.14	0.45
1:A:2:LEU:HD21	1:A:10:ARG:CZ	2.46	0.45
1:A:175:ILE:HG22	1:A:243:PHE:CE1	2.51	0.45
1:A:230:HIS:HD2	2:B:223:ILE:HG13	1.81	0.45
1:A:271:TRP:CD1	1:A:271:TRP:N	2.79	0.45
2:B:203:GLY:HA2	4:B:853:BCL:O1D	2.17	0.45
2:B:242:GLY:HA2	3:C:115:VAL:HG21	1.98	0.45
1:A:24:PHE:C	1:A:24:PHE:CD1	2.94	0.45
1:A:90:THR:HG23	1:A:148:TYR:OH	2.16	0.45
5:A:855:BPH:H112	5:A:855:BPH:H7C1	1.77	0.45
2:B:190:SER:HB3	4:B:852:BCL:HBC3	1.99	0.45
2:B:216:PHE:C	2:B:218:MET:H	2.25	0.45
3:C:37:ARG:HG2	3:C:37:ARG:NH1	2.32	0.45
1:A:116:HIS:CB	2:B:221:ALA:O	2.61	0.45
1:A:226:THR:O	1:A:227:LEU:C	2.60	0.45
5:A:855:BPH:HHC	5:A:855:BPH:HBB2	1.98	0.45
2:B:55:LEU:HB3	2:B:132:ARG:HD2	1.99	0.45
2:B:60:LEU:HD12	5:B:854:BPH:C5	2.46	0.45
2:B:187:ASN:C	2:B:189:PHE:H	2.25	0.45
2:B:240:ASP:O	2:B:241:ARG:O	2.34	0.45
2:B:91:PHE:H	2:B:91:PHE:HD1	1.60	0.45
2:B:182:HIS:O	2:B:185:TRP:HB3	2.16	0.45
2:B:260:ALA:O	6:B:856:U10:H4M3	2.15	0.45
2:B:264:GLY:O	2:B:267:ARG:N	2.50	0.45
2:B:293:ASN:OD1	2:B:293:ASN:C	2.59	0.45
3:C:189:ARG:HD3	3:C:218:THR:HG23	1.98	0.45
1:A:113:ILE:HG22	2:B:229:PHE:HE2	1.82	0.45
1:A:172:ALA:HB3	1:A:247:CYS:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:CG1	1:A:251:THR:N	2.78	0.45
1:A:274:ASN:O	1:A:275:ILE:O	2.35	0.45
2:B:17:ASP:OD2	3:C:172:PRO:HB3	2.17	0.45
1:A:26:VAL:O	1:A:26:VAL:HG12	2.16	0.45
1:A:117:ILE:N	1:A:118:PRO:HD2	2.31	0.45
2:B:256:MET:HE1	6:B:856:U10:H121	1.99	0.45
2:B:265:ILE:HG12	6:B:856:U10:C2	2.47	0.45
1:A:116:HIS:CE1	2:B:225:ALA:HA	2.52	0.45
2:B:215:LEU:HD23	2:B:269:ALA:CB	2.47	0.45
6:B:856:U10:H222	6:B:856:U10:H201	1.64	0.45
3:C:44:ASN:ND2	3:C:50:ALA:HA	2.32	0.45
3:C:191:LEU:HA	3:C:192:PRO:HD3	1.57	0.45
3:C:14:SER:O	3:C:17:ILE:CG2	2.63	0.44
3:C:27:LEU:O	3:C:29:TYR:N	2.50	0.44
3:C:115:VAL:CG1	3:C:117:ARG:HG3	2.47	0.44
3:C:128:HIS:O	3:C:129:ASN:C	2.60	0.44
1:A:199:ASN:N	1:A:200:PRO:CD	2.80	0.44
2:B:46:GLN:C	2:B:47:LEU:CG	2.90	0.44
1:A:63:LEU:O	1:A:64:ILE:C	2.60	0.44
1:A:69:PRO:HG3	1:A:83:GLY:HA3	1.98	0.44
1:A:139:MET:HG3	1:A:253:THR:HG22	1.99	0.44
1:A:174:MET:HB2	4:A:850:BCL:CGD	2.48	0.44
1:A:203:GLY:O	1:A:204:LYS:O	2.36	0.44
1:A:244:SER:HB3	4:A:851:BCL:O1D	2.16	0.44
2:B:130:TRP:CD1	2:B:154:ILE:HD11	2.52	0.44
2:B:290:VAL:HG12	2:B:290:VAL:O	2.18	0.44
3:C:37:ARG:HA	3:C:76:PRO:HB3	1.99	0.44
3:C:122:GLU:N	3:C:227:LEU:HD21	2.33	0.44
2:B:191:LEU:C	2:B:193:HIS:N	2.72	0.44
2:B:242:GLY:O	2:B:243:THR:C	2.60	0.44
3:C:69:GLY:O	3:C:71:GLY:N	2.45	0.44
3:C:171:ILE:O	3:C:174:GLN:N	2.51	0.44
1:A:61:PRO:O	1:A:150:ILE:HD12	2.18	0.44
1:A:128:TYR:O	1:A:131:LEU:N	2.51	0.44
2:B:258:PHE:O	2:B:259:ASN:HB3	2.18	0.44
2:B:229:PHE:HZ	3:C:238:ALA:HB2	1.75	0.44
2:B:256:MET:CE	2:B:258:PHE:CE2	3.00	0.44
3:C:212:LEU:HD23	3:C:212:LEU:N	2.33	0.44
1:A:139:MET:CE	1:A:252:GLY:HA3	2.46	0.44
1:A:185:LEU:HA	1:A:188:ALA:HB3	2.00	0.44
1:A:190:HIS:NE2	1:A:230:HIS:HE1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLN:HB3	2:B:6:ILE:HD11	1.99	0.44
2:B:8:SER:C	2:B:10:VAL:N	2.73	0.44
2:B:90:PHE:O	2:B:91:PHE:C	2.60	0.44
2:B:97:PRO:O	2:B:98:ALA:O	2.36	0.44
2:B:132:ARG:C	2:B:134:TYR:N	2.74	0.44
1:A:116:HIS:CD2	2:B:224:LEU:HB3	2.52	0.44
1:A:126:LEU:O	1:A:127:ALA:C	2.60	0.44
1:A:134:PHE:O	1:A:135:ARG:C	2.61	0.44
1:A:249:ILE:HD13	1:A:249:ILE:O	2.18	0.44
4:A:850:BCL:HMD3	4:A:851:BCL:CBB	2.47	0.44
2:B:38:LEU:O	2:B:40:GLY:N	2.50	0.44
2:B:119:SER:O	2:B:122:MET:HB3	2.17	0.44
1:A:153:HIS:O	1:A:156:TRP:HB3	2.18	0.43
1:A:174:MET:HB2	4:A:850:BCL:O1D	2.18	0.43
2:B:143:GLY:C	2:B:145:HIS:N	2.76	0.43
2:B:232:GLU:HG3	3:C:177:ARG:HH12	1.82	0.43
3:C:115:VAL:CG2	3:C:231:ASP:OD2	2.66	0.43
3:C:175:MET:HE3	3:C:176:ALA:O	2.18	0.43
1:A:112:GLY:O	1:A:113:ILE:O	2.35	0.43
1:A:115:TYR:O	1:A:118:PRO:HD2	2.18	0.43
1:A:146:PHE:HB2	1:A:147:PRO:HD2	2.00	0.43
1:A:187:LEU:N	2:B:216:PHE:HE2	2.16	0.43
3:C:27:LEU:C	3:C:29:TYR:H	2.25	0.43
3:C:66:LEU:HD13	3:C:118:ARG:HH12	1.83	0.43
1:A:2:LEU:HD23	1:A:6:GLU:OE2	2.17	0.43
1:A:122:ALA:CA	1:A:125:ILE:HB	2.41	0.43
1:A:267:VAL:HG23	2:B:87:ARG:CG	2.48	0.43
2:B:204:LEU:C	2:B:206:ILE:N	2.72	0.43
2:B:227:SER:O	2:B:229:PHE:N	2.51	0.43
3:C:227:LEU:O	3:C:230:GLU:HB2	2.17	0.43
1:A:34:PHE:CE1	1:A:102:LEU:HD13	2.53	0.43
1:A:195:LEU:C	1:A:197:ALA:N	2.75	0.43
1:A:209:PRO:CG	3:C:130:LYS:HE2	2.49	0.43
2:B:142:MET:O	2:B:143:GLY:C	2.62	0.43
2:B:209:LEU:HD12	2:B:209:LEU:O	2.19	0.43
3:C:235:GLY:O	3:C:238:ALA:HB3	2.18	0.43
1:A:196:SER:HB2	2:B:143:GLY:O	2.19	0.43
4:A:850:BCL:HBC1	4:B:852:BCL:HAA2	1.99	0.43
2:B:17:ASP:C	2:B:19:GLY:N	2.73	0.43
2:B:206:ILE:HD12	4:B:853:BCL:OBD	2.18	0.43
2:B:291:VAL:CG1	2:B:293:ASN:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:O	3:C:42:LEU:HA	2.19	0.43
2:B:268:TRP:CE2	6:B:856:U10:H122	2.54	0.43
3:C:120:LEU:O	3:C:227:LEU:HG	2.19	0.43
3:C:154:ARG:HG2	3:C:155:GLY:N	2.33	0.43
3:C:192:PRO:HG2	3:C:237:VAL:HG21	2.00	0.43
3:C:229:GLU:O	3:C:233:ILE:HG13	2.19	0.43
1:A:83:GLY:C	1:A:85:LEU:N	2.77	0.43
1:A:86:TRP:C	1:A:89:ILE:HG22	2.44	0.43
3:C:245:ALA:H	3:C:246:PRO:HD3	1.82	0.43
1:A:219:LEU:HG	1:A:220:VAL:N	2.34	0.43
2:B:268:TRP:CZ2	6:B:856:U10:H122	2.53	0.43
2:B:293:ASN:OD1	2:B:294:TRP:N	2.52	0.43
3:C:133:PRO:HG2	3:C:136:ALA:HB3	1.99	0.43
3:C:230:GLU:O	3:C:234:CYS:SG	2.75	0.43
1:A:61:PRO:HB3	1:A:150:ILE:CD1	2.49	0.43
1:A:116:HIS:O	2:B:221:ALA:HB1	2.19	0.43
2:B:26:LEU:HD22	2:B:29:ARG:HG3	2.00	0.43
2:B:294:TRP:C	2:B:296:VAL:N	2.76	0.43
3:C:66:LEU:HB2	3:C:71:GLY:O	2.19	0.43
3:C:178:PHE:HD1	3:C:191:LEU:C	2.26	0.43
1:A:65:SER:HB2	1:A:149:GLY:CA	2.49	0.43
1:A:255:TRP:CH2	1:A:262:TRP:HD1	2.37	0.43
1:A:255:TRP:CZ3	1:A:262:TRP:HD1	2.36	0.43
2:B:73:TRP:C	2:B:74:PHE:HD1	2.25	0.43
2:B:138:GLN:C	2:B:140:LEU:N	2.74	0.43
2:B:210:TYR:CD2	4:B:853:BCL:H11	2.54	0.43
2:B:240:ASP:O	3:C:117:ARG:HG2	2.18	0.43
1:A:49:ILE:O	1:A:53:ALA:HB2	2.19	0.42
1:A:68:PRO:HA	1:A:86:TRP:CG	2.54	0.42
1:A:265:TRP:CD1	1:A:265:TRP:C	2.96	0.42
2:B:25:ASN:HD22	2:B:28:ASN:ND2	2.09	0.42
2:B:204:LEU:O	2:B:207:ALA:N	2.52	0.42
3:C:60:LYS:O	3:C:61:PRO:C	2.62	0.42
2:B:7:PHE:HD1	2:B:41:TRP:HB3	1.84	0.42
2:B:136:ARG:HD3	2:B:136:ARG:HA	1.85	0.42
3:C:202:ARG:HH11	3:C:202:ARG:HG2	1.84	0.42
3:C:231:ASP:O	3:C:232:LYS:C	2.62	0.42
1:A:114:GLY:H	2:B:225:ALA:C	2.26	0.42
1:A:51:TRP:O	1:A:54:VAL:HG23	2.19	0.42
1:A:87:GLN:O	1:A:88:ILE:C	2.61	0.42
1:A:231:ARG:NH1	2:B:41:TRP:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:SER:C	2:B:229:PHE:N	2.78	0.42
3:C:134:MET:HE2	3:C:149:ILE:HD11	2.01	0.42
1:A:219:LEU:CD1	2:B:132:ARG:HH12	2.30	0.42
2:B:78:ALA:HA	2:B:84:VAL:HG11	2.01	0.42
3:C:96:PHE:HD2	3:C:97:PRO:HD2	1.84	0.42
3:C:148:PRO:O	3:C:149:ILE:C	2.62	0.42
1:A:171:PRO:HA	1:A:174:MET:HG2	2.00	0.42
1:A:219:LEU:HD12	2:B:132:ARG:NH1	2.35	0.42
2:B:148:TRP:HE3	2:B:148:TRP:HA	1.85	0.42
2:B:206:ILE:HG21	4:B:853:BCL:CAD	2.50	0.42
2:B:238:ILE:HG22	2:B:239:ALA:N	2.33	0.42
3:C:122:GLU:HB2	3:C:227:LEU:HD21	2.01	0.42
2:B:206:ILE:O	2:B:207:ALA:C	2.62	0.42
3:C:224:GLU:O	3:C:224:GLU:HG3	2.19	0.42
1:A:49:ILE:O	1:A:49:ILE:CG2	2.67	0.42
1:A:64:ILE:O	1:A:65:SER:HB2	2.19	0.42
1:A:114:GLY:HA3	2:B:225:ALA:CA	2.48	0.42
1:A:187:LEU:HD11	2:B:269:ALA:CB	2.50	0.42
1:A:217:ARG:HH21	2:B:44:ASN:HD22	1.66	0.42
1:A:228:GLY:O	1:A:229:ILE:C	2.61	0.42
1:A:267:VAL:HA	2:B:87:ARG:HG3	2.01	0.42
2:B:38:LEU:O	2:B:41:TRP:HD1	2.03	0.42
2:B:148:TRP:HA	2:B:148:TRP:CE3	2.55	0.42
2:B:228:ARG:NH1	3:C:195:MET:HE3	2.35	0.42
3:C:33:THR:OG1	3:C:34:GLU:N	2.52	0.42
3:C:146:LYS:HG2	3:C:199:GLN:O	2.19	0.42
1:A:65:SER:CB	1:A:149:GLY:CA	2.98	0.42
1:A:105:VAL:C	1:A:107:ILE:N	2.70	0.42
1:A:115:TYR:O	1:A:117:ILE:N	2.53	0.42
2:B:268:TRP:CE3	3:C:31:LEU:HD13	2.55	0.42
2:B:269:ALA:O	2:B:270:ILE:C	2.62	0.42
3:C:189:ARG:HG2	3:C:189:ARG:HH11	1.84	0.42
1:A:2:LEU:HD23	1:A:6:GLU:CD	2.45	0.42
1:A:43:ALA:O	1:A:45:GLY:N	2.52	0.42
1:A:47:ILE:HG22	1:A:48:LEU:HD23	2.02	0.42
2:B:248:ALA:O	2:B:249:ALA:C	2.61	0.42
1:A:174:MET:HA	1:A:177:ILE:CD1	2.50	0.41
1:A:229:ILE:O	1:A:232:LEU:HB3	2.20	0.41
2:B:211:GLY:O	2:B:213:ALA:N	2.52	0.41
2:B:224:LEU:O	2:B:225:ALA:C	2.61	0.41
2:B:233:ARG:H	2:B:233:ARG:HG3	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:TRP:HB3	2:B:269:ALA:H	1.59	0.41
2:B:280:GLY:O	2:B:282:ILE:N	2.53	0.41
3:C:103:ASP:HA	3:C:104:PRO:HD2	1.80	0.41
3:C:174:GLN:H	3:C:174:GLN:HG2	1.56	0.41
3:C:236:TYR:C	3:C:236:TYR:CD1	2.98	0.41
1:A:7:ARG:O	1:A:9:TYR:N	2.47	0.41
1:A:56:GLN:HE22	1:A:65:SER:N	2.18	0.41
1:A:162:TYR:C	1:A:164:TYR:N	2.76	0.41
1:A:229:ILE:O	1:A:231:ARG:N	2.54	0.41
2:B:41:TRP:CD1	2:B:41:TRP:N	2.84	0.41
3:C:70:ARG:HE	3:C:123:LEU:HD11	1.84	0.41
3:C:157:ASP:OD1	3:C:209:SER:HB2	2.20	0.41
1:A:9:TYR:CE1	3:C:113:SER:CB	3.03	0.41
1:A:9:TYR:HE1	3:C:113:SER:HB2	1.84	0.41
1:A:87:GLN:C	1:A:89:ILE:N	2.77	0.41
1:A:185:LEU:CA	1:A:188:ALA:HB3	2.50	0.41
1:A:263:TRP:HZ3	2:B:90:PHE:CE2	2.37	0.41
1:A:265:TRP:CD1	1:A:266:TRP:HB2	2.55	0.41
2:B:13:ARG:HG2	2:B:14:GLY:N	2.35	0.41
2:B:24:VAL:HG12	2:B:25:ASN:N	2.34	0.41
2:B:123:PHE:C	2:B:125:ALA:H	2.29	0.41
2:B:153:ALA:C	2:B:155:TRP:N	2.76	0.41
3:C:20:PHE:C	3:C:22:ILE:N	2.72	0.41
1:A:220:VAL:HG23	1:A:222:TYR:N	2.34	0.41
2:B:59:SER:OG	2:B:129:TRP:HE3	2.03	0.41
2:B:163:ILE:HG22	2:B:164:ARG:N	2.35	0.41
3:C:175:MET:O	3:C:177:ARG:HG3	2.20	0.41
1:A:87:GLN:O	1:A:89:ILE:N	2.54	0.41
1:A:184:ALA:O	1:A:185:LEU:C	2.64	0.41
1:A:196:SER:CA	2:B:145:HIS:HB2	2.50	0.41
5:A:855:BPH:ND	2:B:214:LEU:HD13	2.35	0.41
2:B:46:GLN:HG2	2:B:47:LEU:H	1.85	0.41
2:B:94:LEU:O	2:B:94:LEU:HG	2.21	0.41
2:B:154:ILE:HG22	2:B:158:MET:CG	2.42	0.41
2:B:232:GLU:HG2	2:B:233:ARG:HG3	2.02	0.41
2:B:239:ALA:HB1	3:C:66:LEU:HD21	2.02	0.41
2:B:258:PHE:N	2:B:258:PHE:HD2	2.18	0.41
3:C:176:ALA:HB1	3:C:193:MET:SD	2.60	0.41
1:A:147:PRO:O	1:A:153:HIS:HB3	2.20	0.41
1:A:180:PHE:CG	1:A:240:ALA:HB1	2.51	0.41
1:A:227:LEU:HD13	2:B:232:GLU:CB	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:VAL:HG22	2:B:185:TRP:CE2	2.55	0.41
2:B:229:PHE:CZ	3:C:238:ALA:CB	2.98	0.41
3:C:66:LEU:HD13	3:C:118:ARG:HH22	1.85	0.41
1:A:147:PRO:O	1:A:149:GLY:N	2.46	0.41
2:B:8:SER:O	2:B:10:VAL:N	2.54	0.41
2:B:158:MET:O	2:B:163:ILE:HG12	2.21	0.41
2:B:208:PHE:HB3	2:B:276:VAL:CG2	2.35	0.41
3:C:17:ILE:O	3:C:17:ILE:CG1	2.68	0.41
1:A:62:GLN:HG2	1:A:151:TRP:NE1	2.36	0.41
1:A:182:THR:O	1:A:183:ASN:C	2.62	0.41
1:A:254:ILE:HD12	1:A:255:TRP:N	2.36	0.41
4:A:850:BCL:H11	5:B:854:BPH:HBB2	2.03	0.41
2:B:84:VAL:C	2:B:86:LEU:N	2.78	0.41
2:B:229:PHE:HZ	3:C:238:ALA:CB	2.34	0.41
2:B:285:LEU:HD12	2:B:285:LEU:O	2.21	0.41
3:C:124:ASP:N	3:C:130:LYS:HB2	2.36	0.41
1:A:34:PHE:HB2	1:A:103:ARG:HB2	2.02	0.41
1:A:153:HIS:C	1:A:156:TRP:H	2.26	0.41
1:A:173:HIS:O	1:A:177:ILE:N	2.51	0.41
1:A:192:ALA:HB1	2:B:146:THR:HA	2.01	0.41
2:B:57:VAL:O	2:B:59:SER:N	2.54	0.41
2:B:134:TYR:O	2:B:135:LEU:C	2.64	0.41
2:B:238:ILE:HD11	2:B:263:GLU:HA	2.02	0.41
3:C:70:ARG:HE	3:C:123:LEU:CD1	2.34	0.41
3:C:96:PHE:CD2	3:C:97:PRO:HD2	2.56	0.41
1:A:100:TRP:CG	5:A:855:BPH:O1A	2.74	0.41
1:A:147:PRO:HD2	1:A:156:TRP:HB2	2.02	0.41
1:A:164:TYR:CE2	1:A:251:THR:HG22	2.56	0.41
1:A:208:THR:OG1	1:A:210:ASP:CB	2.69	0.41
2:B:13:ARG:CG	2:B:14:GLY:N	2.83	0.41
3:C:135:LYS:NZ	3:C:166:ASP:CB	2.84	0.41
3:C:166:ASP:CG	3:C:167:ILE:N	2.79	0.41
1:A:31:VAL:HG12	1:A:32:GLY:O	2.21	0.40
2:B:13:ARG:HD3	2:B:35:PHE:CD2	2.56	0.40
3:C:13:ALA:O	3:C:14:SER:C	2.63	0.40
3:C:48:THR:O	3:C:49:PRO:C	2.64	0.40
1:A:231:ARG:C	1:A:233:GLY:N	2.72	0.40
2:B:6:ILE:HD13	2:B:6:ILE:N	2.36	0.40
2:B:17:ASP:C	2:B:19:GLY:H	2.29	0.40
1:A:181:PHE:O	1:A:182:THR:C	2.65	0.40
1:A:193:LEU:C	1:A:195:LEU:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PHE:CD2	2:B:179:ILE:HD13	2.57	0.40
2:B:101:TYR:OH	2:B:108:PRO:HD2	2.21	0.40
1:A:64:ILE:HA	1:A:64:ILE:HD13	1.95	0.40
1:A:86:TRP:O	1:A:89:ILE:HG22	2.21	0.40
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.34	0.40
1:A:117:ILE:HA	2:B:221:ALA:HB1	2.03	0.40
1:A:121:PHE:O	1:A:123:PHE:N	2.55	0.40
1:A:133:LEU:O	1:A:137:VAL:HG23	2.21	0.40
1:A:195:LEU:O	1:A:197:ALA:N	2.55	0.40
1:A:205:GLU:O	1:A:206:MET:C	2.64	0.40
2:B:66:TRP:NE1	2:B:122:MET:HB2	2.37	0.40
2:B:151:LEU:HA	2:B:154:ILE:HD12	2.04	0.40
2:B:164:ARG:CZ	2:B:168:MET:HE2	2.51	0.40
2:B:264:GLY:C	2:B:266:HIS:N	2.78	0.40
2:B:291:VAL:C	2:B:293:ASN:H	2.28	0.40
1:A:190:HIS:CG	1:A:229:ILE:CD1	3.04	0.40
1:A:213:ASP:OD1	1:A:213:ASP:N	2.46	0.40
1:A:223:SER:OG	6:A:857:U10:H3M3	2.22	0.40
2:B:153:ALA:O	2:B:155:TRP:N	2.55	0.40
2:B:201:PHE:HB3	2:B:283:GLY:HA3	2.04	0.40
2:B:235:LEU:HA	2:B:235:LEU:HD23	1.79	0.40
2:B:293:ASN:CG	2:B:296:VAL:HG23	2.46	0.40
3:C:148:PRO:O	3:C:151:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	279/281 (99%)	149 (53%)	76 (27%)	54 (19%)	0 2
2	B	300/307 (98%)	164 (55%)	84 (28%)	52 (17%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	236/260 (91%)	144 (61%)	60 (25%)	32 (14%)	0	3
All	All	815/848 (96%)	457 (56%)	220 (27%)	138 (17%)	0	2

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	21	LEU
1	A	73	TYR
1	A	113	ILE
1	A	143	GLY
1	A	145	ALA
1	A	160	THR
1	A	204	LYS
1	A	212	GLU
1	A	239	SER
1	A	240	ALA
1	A	251	THR
1	A	275	ILE
2	B	5	ASN
2	B	15	PRO
2	B	17	ASP
2	B	18	LEU
2	B	49	PRO
2	B	57	VAL
2	B	98	ALA
2	B	109	LEU
2	B	223	ILE
2	B	232	GLU
2	B	240	ASP
2	B	241	ARG
2	B	244	ALA
2	B	248	ALA
2	B	268	TRP
3	C	30	TYR
3	C	44	ASN
3	C	51	ALA
3	C	54	GLY
3	C	59	PRO
3	C	66	LEU
3	C	78	PRO
3	C	82	ASP

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Mol	Chain	Res	Type
3	C	89	ARG
3	C	96	PHE
3	C	149	ILE
3	C	171	ILE
3	C	219	ILE
3	C	221	SER
1	A	10	ARG
1	A	65	SER
1	A	71	LEU
1	A	72	GLU
1	A	80	LEU
1	A	84	GLY
1	A	86	TRP
1	A	116	HIS
1	A	159	ASN
1	A	230	HIS
1	A	238	LEU
1	A	245	ALA
1	A	247	CYS
1	A	280	ASN
2	B	32	VAL
2	B	50	ILE
2	B	58	LEU
2	B	59	SER
2	B	87	ARG
2	B	91	PHE
2	B	117	ILE
2	B	155	TRP
2	B	162	PHE
2	B	163	ILE
2	B	215	LEU
2	B	228	ARG
2	B	265	ILE
2	B	274	VAL
2	B	283	GLY
3	C	19	SER
3	C	144	ALA
3	C	174	GLN
3	C	193	MET
3	C	239	GLY
1	A	26	VAL
1	A	77	GLY

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Mol	Chain	Res	Type
1	A	122	ALA
1	A	131	LEU
1	A	132	VAL
1	A	233	GLY
2	B	34	PRO
2	B	65	MET
2	B	69	THR
2	B	90	PHE
2	B	247	ARG
2	B	297	TRP
3	C	12	LEU
3	C	32	GLN
3	C	55	PRO
3	C	61	PRO
3	C	70	ARG
3	C	172	PRO
3	C	195	MET
1	A	118	PRO
1	A	129	LEU
1	A	179	PHE
1	A	201	GLU
1	A	234	LEU
1	A	272	TRP
2	B	41	TRP
2	B	222	THR
2	B	235	LEU
2	B	246	GLU
2	B	249	ALA
2	B	267	ARG
2	B	287	SER
3	C	194	GLN
1	A	70	ALA
1	A	134	PHE
1	A	163	THR
1	A	236	LEU
1	A	270	PRO
2	B	9	GLN
2	B	179	ILE
2	B	245	ALA
2	B	259	ASN
2	B	296	VAL
3	C	47	GLY

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Mol	Chain	Res	Type
3	C	183	LEU
1	A	117	ILE
1	A	211	HIS
1	A	224	ILE
2	B	272	MET
3	C	57	PRO
3	C	210	SER
1	A	13	GLY
1	A	140	GLY
1	A	228	GLY
1	A	229	ILE
1	A	78	ALA
1	A	88	ILE
2	B	291	VAL
3	C	237	VAL
2	B	192	VAL
2	B	281	GLY
1	A	135	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/220 (100%)	199 (90%)	21 (10%)	8	25
2	B	236/240 (98%)	201 (85%)	35 (15%)	3	14
3	C	193/208 (93%)	178 (92%)	15 (8%)	11	32
All	All	649/668 (97%)	578 (89%)	71 (11%)	6	21

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	54	VAL
1	A	72	GLU
1	A	123	PHE

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Mol	Chain	Res	Type
1	A	125	ILE
1	A	152	THR
1	A	157	VAL
1	A	183	ASN
1	A	185	LEU
1	A	207	ARG
1	A	210	ASP
1	A	218	ASP
1	A	229	ILE
1	A	249	ILE
1	A	258	GLN
1	A	260	VAL
1	A	261	ASP
1	A	265	TRP
1	A	269	LEU
1	A	270	PRO
1	A	271	TRP
2	B	5	ASN
2	B	6	ILE
2	B	18	LEU
2	B	47	LEU
2	B	50	ILE
2	B	72	ILE
2	B	74	PHE
2	B	90	PHE
2	B	117	ILE
2	B	148	TRP
2	B	155	TRP
2	B	160	LEU
2	B	166	ILE
2	B	171	TRP
2	B	172	SER
2	B	182	HIS
2	B	188	ASN
2	B	196	LEU
2	B	206	ILE
2	B	209	LEU
2	B	214	LEU
2	B	233	ARG
2	B	236	GLU
2	B	238	ILE
2	B	240	ASP

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Mol	Chain	Res	Type
2	B	250	LEU
2	B	251	PHE
2	B	258	PHE
2	B	261	THR
2	B	263	GLU
2	B	268	TRP
2	B	270	ILE
2	B	289	THR
2	B	292	ASP
2	B	297	TRP
3	C	22	ILE
3	C	28	ILE
3	C	46	ASP
3	C	49	PRO
3	C	61	PRO
3	C	65	ILE
3	C	157	ASP
3	C	169	VAL
3	C	174	GLN
3	C	193	MET
3	C	195	MET
3	C	211	ASP
3	C	218	THR
3	C	226	THR
3	C	233	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	87	GLN
2	B	5	ASN
2	B	25	ASN
2	B	28	ASN
2	B	44	ASN
2	B	77	GLN
2	B	145	HIS
2	B	188	ASN
2	B	193	HIS
2	B	195	ASN
2	B	237	GLN
3	C	126	HIS

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Mol	Chain	Res	Type
3	C	204	HIS
3	C	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 10 ligands modelled in this entry, 2 are 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	B	853	-	69,74,74	1.45	10 (14%)	79,115,115	1.87	21 (26%)
6	U10	B	856	-	48,48,63	2.35	13 (27%)	60,61,79	2.00	20 (33%)
5	BPH	A	855	-	59,70,70	1.78	9 (15%)	59,101,101	2.40	16 (27%)
4	BCL	A	850	2	69,74,74	1.73	13 (18%)	79,115,115	2.13	27 (34%)
6	U10	A	857	-	48,48,63	2.79	19 (39%)	60,61,79	1.79	19 (31%)
4	BCL	B	852	2	69,74,74	1.40	9 (13%)	79,115,115	1.72	17 (21%)
5	BPH	B	854	-	59,70,70	1.84	11 (18%)	59,101,101	2.37	17 (28%)
4	BCL	A	851	1	69,74,74	1.41	10 (14%)	79,115,115	1.70	18 (22%)

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	B	853	-	-	7/41/137/137	-
6	U10	B	856	-	-	14/45/69/87	0/1/1/1
5	BPH	A	855	-	-	9/37/105/105	0/5/6/6
4	BCL	A	850	2	-	5/41/137/137	-
6	U10	A	857	-	-	16/45/69/87	0/1/1/1
4	BCL	B	852	2	-	11/41/137/137	-
5	BPH	B	854	-	-	10/37/105/105	0/5/6/6
4	BCL	A	851	1	-	7/41/137/137	-

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	857	U10	C6-C1	11.94	1.56	1.35
6	B	856	U10	C6-C1	9.43	1.52	1.35
4	A	850	BCL	C2-C3	5.37	1.45	1.33
5	A	855	BPH	C3A-C2A	-5.32	1.50	1.54
5	B	854	BPH	C3D-C2D	5.04	1.48	1.39
5	B	854	BPH	C3A-C2A	-4.95	1.50	1.54
5	B	854	BPH	C3B-C2B	4.93	1.48	1.39
6	A	857	U10	C4-C3	4.88	1.53	1.36
6	A	857	U10	C7-C6	4.68	1.60	1.51
4	A	850	BCL	C5-C3	4.53	1.60	1.51
6	A	857	U10	C28-C29	4.51	1.43	1.33
5	A	855	BPH	C3B-C2B	4.45	1.47	1.39
6	B	856	U10	C4-C3	4.37	1.52	1.36
4	A	850	BCL	CAA-C2A	4.36	1.62	1.54
5	A	855	BPH	C3D-C2D	4.14	1.46	1.39
6	B	856	U10	C28-C29	4.11	1.42	1.33
6	A	857	U10	C18-C19	4.02	1.42	1.33
5	A	855	BPH	C3B-C4B	4.02	1.47	1.41
5	A	855	BPH	C2C-C3C	-3.98	1.51	1.54
5	B	854	BPH	C2-C3	3.93	1.42	1.33
6	B	856	U10	C7-C8	-3.91	1.44	1.50
4	B	852	BCL	C3D-C2D	3.91	1.49	1.39
4	B	852	BCL	C2-C3	3.82	1.41	1.33
4	A	851	BCL	C2-C3	3.80	1.41	1.33
6	A	857	U10	C13-C14	3.78	1.41	1.33
4	A	851	BCL	C3B-CAB	3.69	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	852	BCL	C1D-C2D	-3.67	1.38	1.45
4	B	853	BCL	C3B-CAB	3.64	1.58	1.46
4	A	851	BCL	C1D-C2D	-3.63	1.38	1.45
6	A	857	U10	C23-C24	3.63	1.41	1.33
4	A	850	BCL	C3B-CAB	3.59	1.57	1.46
6	B	856	U10	C33-C34	3.52	1.41	1.33
5	A	855	BPH	CMB-C2B	3.51	1.58	1.51
4	A	850	BCL	C3B-C4B	3.51	1.48	1.41
5	A	855	BPH	C3D-CAD	-3.47	1.41	1.47
5	B	854	BPH	C3B-C4B	3.46	1.47	1.41
6	A	857	U10	C6-C5	3.36	1.56	1.46
4	A	851	BCL	C3D-C2D	3.36	1.48	1.39
6	A	857	U10	C33-C34	3.34	1.40	1.33
6	B	856	U10	C7-C6	3.30	1.57	1.51
5	A	855	BPH	C2-C3	3.29	1.40	1.33
6	A	857	U10	C38-C39	3.28	1.42	1.32
6	A	857	U10	O4-C4	3.25	1.44	1.36
4	B	853	BCL	C1D-C2D	-3.24	1.38	1.45
4	A	850	BCL	CMB-C2B	3.24	1.57	1.50
4	A	851	BCL	CMD-C2D	3.20	1.57	1.50
5	B	854	BPH	C2C-C3C	-3.17	1.52	1.54
4	B	853	BCL	CMB-C2B	3.13	1.57	1.50
6	B	856	U10	C23-C24	3.10	1.40	1.33
5	B	854	BPH	C3D-CAD	-3.10	1.41	1.47
6	B	856	U10	C6-C5	3.10	1.55	1.46
6	B	856	U10	C18-C19	3.08	1.40	1.33
4	B	852	BCL	C1B-NB	-3.03	1.33	1.37
4	B	853	BCL	C3D-C2D	3.01	1.47	1.39
4	A	851	BCL	CBB-CAB	3.00	1.56	1.50
4	A	850	BCL	C1B-NB	-2.99	1.33	1.37
4	A	851	BCL	CMB-C2B	2.94	1.56	1.50
4	B	853	BCL	C2-C3	2.94	1.39	1.33
4	B	852	BCL	CMB-C2B	2.91	1.56	1.50
4	B	853	BCL	C1B-NB	-2.91	1.34	1.37
5	B	854	BPH	CMB-C2B	2.89	1.57	1.51
4	A	850	BCL	CBA-CGA	2.88	1.59	1.50
6	A	857	U10	C8-C9	2.82	1.39	1.33
4	A	850	BCL	CBB-CAB	2.81	1.55	1.50
4	A	851	BCL	C1B-NB	-2.81	1.34	1.37
6	B	856	U10	O4-C4	2.80	1.43	1.36
6	B	856	U10	C38-C39	2.77	1.40	1.32
4	B	852	BCL	CBB-CAB	2.71	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	856	U10	C13-C14	2.70	1.39	1.33
4	B	853	BCL	CBB-CAB	2.59	1.55	1.50
6	A	857	U10	C1M-C1	2.54	1.56	1.50
4	A	850	BCL	O2D-CGD	-2.52	1.27	1.33
5	A	855	BPH	CMD-C2D	2.49	1.56	1.51
4	A	850	BCL	C3D-C2D	2.49	1.45	1.39
4	B	853	BCL	C3C-C4C	-2.47	1.48	1.51
6	A	857	U10	C7-C8	-2.44	1.46	1.50
4	B	852	BCL	CMD-C2D	2.43	1.55	1.50
5	B	854	BPH	C1B-C2B	2.40	1.42	1.39
4	B	853	BCL	O2D-CGD	-2.35	1.27	1.33
4	B	852	BCL	C3B-CAB	2.32	1.54	1.46
6	A	857	U10	O3-C3	2.30	1.42	1.36
4	B	853	BCL	MG-ND	-2.29	2.01	2.05
5	B	854	BPH	C3B-CAB	2.22	1.55	1.49
6	A	857	U10	C16-C14	2.19	1.55	1.51
4	A	851	BCL	O2D-CGD	-2.16	1.27	1.33
5	B	854	BPH	C5-C3	2.11	1.55	1.51
6	A	857	U10	C31-C29	2.11	1.55	1.51
4	B	852	BCL	MG-ND	-2.08	2.01	2.05
6	B	856	U10	C36-C34	2.08	1.55	1.51
4	A	850	BCL	MG-NB	2.04	2.09	2.05
6	A	857	U10	C26-C24	2.04	1.55	1.51
4	A	851	BCL	OBD-CAD	2.04	1.26	1.22
4	A	850	BCL	C1D-C2D	-2.03	1.41	1.45
6	A	857	U10	C30-C29	2.00	1.55	1.50

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	854	BPH	C4D-CHA-CBD	-8.58	104.34	108.45
5	A	855	BPH	C4D-CHA-CBD	-8.06	104.59	108.45
5	A	855	BPH	C1-O2A-CGA	6.28	131.86	116.65
5	B	854	BPH	C1-O2A-CGA	6.04	131.27	116.65
5	A	855	BPH	C3D-C4D-ND	5.82	115.16	107.71
5	B	854	BPH	C3D-C4D-ND	5.58	114.87	107.71
6	B	856	U10	C7-C6-C5	5.52	124.92	118.52
4	B	853	BCL	CAA-C2A-C1A	-5.44	94.15	111.97
4	A	850	BCL	C6-C5-C3	5.37	126.55	113.47
4	A	850	BCL	CHC-C4B-NB	-5.02	116.52	124.05
5	B	854	BPH	O2D-CGD-CBD	5.02	116.46	110.95
4	B	853	BCL	CMB-C2B-C1B	-4.94	117.90	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	851	BCL	CMB-C2B-C1B	-4.76	118.17	125.42
6	B	856	U10	C15-C14-C16	4.76	123.49	115.23
4	B	852	BCL	C4D-CHA-C1A	4.73	126.88	121.24
5	B	854	BPH	CMB-C2B-C3B	4.65	133.98	124.68
5	A	855	BPH	C4-C3-C5	4.63	123.26	115.23
5	A	855	BPH	CMB-C2B-C3B	4.62	133.92	124.68
4	B	852	BCL	CMB-C2B-C1B	-4.49	118.58	125.42
4	A	850	BCL	C6-C7-C8	4.43	130.69	115.97
4	A	850	BCL	CAA-C2A-C1A	-4.42	97.50	111.97
4	B	853	BCL	CHC-C4B-NB	-4.42	117.42	124.05
5	A	855	BPH	O2D-CGD-CBD	4.41	115.79	110.95
4	A	850	BCL	CMB-C2B-C1B	-4.33	118.83	125.42
6	B	856	U10	C7-C6-C1	-4.32	117.48	124.89
6	A	857	U10	C15-C14-C16	4.32	122.72	115.23
4	B	853	BCL	C4A-NA-C1A	4.25	108.62	106.68
6	A	857	U10	C15-C14-C13	-4.21	112.83	123.63
4	A	850	BCL	CMD-C2D-C1D	4.17	132.07	124.73
4	B	852	BCL	CHC-C4B-NB	-4.13	117.86	124.05
5	B	854	BPH	O1D-CGD-CBD	-4.09	118.51	124.72
4	B	852	BCL	CED-O2D-CGD	4.07	125.14	115.92
6	B	856	U10	C10-C9-C8	-4.03	113.27	123.63
4	A	850	BCL	CBA-CAA-C2A	3.97	125.60	113.79
4	A	851	BCL	CED-O2D-CGD	3.95	124.86	115.92
5	A	855	BPH	C2B-C1B-NB	3.93	112.27	109.43
5	A	855	BPH	C4D-ND-C1D	-3.93	104.17	108.87
4	B	853	BCL	CBA-CAA-C2A	3.90	125.40	113.79
4	A	851	BCL	C4D-CHA-C1A	3.90	125.89	121.24
6	B	856	U10	C15-C14-C13	-3.87	113.68	123.63
4	A	851	BCL	CHC-C4B-NB	-3.86	118.25	124.05
4	A	851	BCL	C4D-C3D-CAD	-3.86	103.92	108.11
4	B	852	BCL	C6-C5-C3	3.83	122.80	113.47
4	A	850	BCL	C2A-C3A-C4A	3.81	108.03	101.87
5	A	855	BPH	O1D-CGD-CBD	-3.81	118.95	124.72
4	A	850	BCL	CMD-C2D-C3D	-3.80	118.97	127.69
5	B	854	BPH	C4-C3-C5	3.74	121.72	115.23
5	B	854	BPH	C4D-ND-C1D	-3.68	104.47	108.87
4	B	853	BCL	CED-O2D-CGD	3.63	124.16	115.92
6	A	857	U10	C10-C9-C8	-3.63	114.31	123.63
4	A	851	BCL	C6-C5-C3	3.62	122.28	113.47
4	A	850	BCL	CED-O2D-CGD	3.60	124.08	115.92
4	A	850	BCL	C3D-C4D-ND	3.60	115.84	109.99
4	A	850	BCL	C1-O2A-CGA	3.52	125.18	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	850	BCL	C4D-CHA-C1A	3.52	125.44	121.24
5	A	855	BPH	C6-C5-C3	3.51	122.03	113.47
4	A	851	BCL	C2A-C3A-C4A	3.50	107.52	101.87
4	A	850	BCL	C10-C8-C7	-3.41	94.80	112.07
6	B	856	U10	C25-C24-C23	-3.40	114.90	123.63
4	B	853	BCL	C3D-C4D-ND	3.39	115.50	109.99
4	B	852	BCL	C2A-C3A-C4A	3.34	107.27	101.87
6	A	857	U10	C35-C34-C33	-3.32	115.10	123.63
4	A	851	BCL	OBD-CAD-C3D	-3.31	120.69	128.42
5	B	854	BPH	C6-C5-C3	3.29	121.48	113.47
4	B	853	BCL	CMD-C2D-C1D	3.21	130.38	124.73
4	B	853	BCL	C4D-CHA-C1A	3.21	125.07	121.24
5	A	855	BPH	C2D-C1D-ND	3.18	111.73	109.43
6	B	856	U10	C35-C34-C33	-3.17	115.48	123.63
6	A	857	U10	C25-C24-C26	3.16	120.71	115.23
6	A	857	U10	C25-C24-C23	-3.14	115.57	123.63
4	B	852	BCL	C3D-C4D-ND	3.10	115.03	109.99
4	B	852	BCL	CHA-C1A-NA	-3.04	119.51	126.39
4	A	851	BCL	CHA-C1A-NA	-3.03	119.52	126.39
6	A	857	U10	C7-C6-C5	3.02	122.02	118.52
4	B	852	BCL	C4D-C3D-CAD	-3.00	104.85	108.11
6	B	856	U10	C25-C24-C26	3.00	120.43	115.23
5	B	854	BPH	C2B-C1B-NB	2.96	111.57	109.43
4	B	853	BCL	C2A-C3A-C4A	2.95	106.64	101.87
5	A	855	BPH	CED-O2D-CGD	2.91	122.51	115.92
4	A	850	BCL	C7-C6-C5	-2.85	105.67	113.26
6	B	856	U10	C11-C9-C8	2.84	127.54	121.17
5	B	854	BPH	C3B-C4B-NB	2.80	112.12	108.05
4	B	853	BCL	CMB-C2B-C3B	2.80	134.49	125.67
5	B	854	BPH	C2D-C1D-ND	2.79	111.45	109.43
5	A	855	BPH	C4A-C3A-C2A	2.77	105.47	102.84
4	A	850	BCL	C1-C2-C3	2.76	130.71	126.20
5	A	855	BPH	C3D-CAD-CBD	2.73	111.20	107.61
4	B	852	BCL	OBD-CAD-C3D	-2.73	122.04	128.42
4	A	850	BCL	OBD-CAD-C3D	-2.72	122.05	128.42
6	A	857	U10	C20-C19-C18	-2.71	116.68	123.63
4	B	852	BCL	C4A-NA-C1A	2.70	107.91	106.68
5	A	855	BPH	C5-C3-C2	-2.69	115.13	121.17
5	B	854	BPH	CED-O2D-CGD	2.68	121.99	115.92
6	B	856	U10	C4M-O4-C4	2.68	125.87	116.47
4	A	851	BCL	C3D-C2D-C1D	2.66	109.47	105.83
5	A	855	BPH	C3B-C4B-NB	2.66	111.93	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	851	BCL	C3B-C4B-NB	2.63	113.23	109.76
4	A	851	BCL	C3D-C4D-ND	2.62	114.25	109.99
6	A	857	U10	C4M-O4-C4	2.62	125.68	116.47
4	A	850	BCL	C4A-NA-C1A	2.61	107.87	106.68
4	A	850	BCL	CHA-C1A-NA	-2.60	120.51	126.39
6	A	857	U10	C30-C29-C31	2.59	119.73	115.23
4	B	853	BCL	OBD-CAD-C3D	-2.59	122.37	128.42
4	A	851	BCL	CAB-C3B-C2B	2.57	133.09	127.74
4	B	853	BCL	C3B-C4B-NB	2.57	113.15	109.76
4	A	851	BCL	CMB-C2B-C3B	2.56	133.76	125.67
6	A	857	U10	C1-C6-C5	-2.55	117.14	119.62
5	B	854	BPH	C3D-CAD-CBD	2.55	110.96	107.61
4	B	852	BCL	CMB-C2B-C3B	2.55	133.70	125.67
4	A	851	BCL	C4A-NA-C1A	2.54	107.84	106.68
4	B	853	BCL	C2A-C1A-CHA	2.53	128.26	123.87
4	B	853	BCL	CAB-C3B-C2B	2.52	132.98	127.74
6	B	856	U10	C20-C19-C18	-2.50	117.21	123.63
4	B	853	BCL	O2D-CGD-CBD	2.49	115.59	111.23
6	A	857	U10	C11-C9-C8	2.48	126.74	121.17
6	B	856	U10	C7-C8-C9	2.48	131.11	126.83
4	B	852	BCL	CMD-C2D-C1D	2.48	129.09	124.73
4	B	853	BCL	CHA-C1A-NA	-2.48	120.78	126.39
4	B	853	BCL	CMD-C2D-C3D	-2.46	122.05	127.69
5	B	854	BPH	C4A-C3A-C2A	2.46	105.18	102.84
4	A	850	BCL	C12-C11-C10	-2.45	102.32	113.28
4	B	852	BCL	O2A-CGA-CBA	2.40	119.16	111.83
4	A	850	BCL	C15-C13-C12	-2.39	99.95	112.07
6	A	857	U10	C7-C6-C1	-2.37	120.83	124.89
6	B	856	U10	C1M-C1-C6	-2.35	120.58	124.45
6	A	857	U10	C21-C19-C18	2.35	126.44	121.17
4	A	850	BCL	CMB-C2B-C3B	2.32	132.98	125.67
4	B	852	BCL	C2A-C1A-CHA	2.31	127.88	123.87
4	B	853	BCL	C6-C5-C3	2.29	119.06	113.47
4	A	850	BCL	C3D-C2D-C1D	2.29	108.96	105.83
6	B	856	U10	C10-C9-C11	2.28	119.19	115.23
6	B	856	U10	O5-C5-C4	-2.25	116.25	121.03
5	B	854	BPH	O2A-C1-C2	-2.23	99.52	108.11
4	A	851	BCL	CMD-C2D-C3D	-2.21	122.62	127.69
6	A	857	U10	C30-C29-C28	-2.21	117.95	123.63
6	B	856	U10	C30-C29-C31	2.21	119.06	115.23
6	A	857	U10	O5-C5-C4	-2.21	116.36	121.03
6	B	856	U10	C35-C34-C36	2.21	119.06	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	857	U10	C35-C34-C36	2.20	119.05	115.23
4	A	850	BCL	C1D-ND-C4D	-2.19	104.77	106.31
4	A	851	BCL	C2A-C1A-CHA	2.16	127.62	123.87
4	A	851	BCL	O2A-CGA-CBA	2.15	118.39	111.83
6	A	857	U10	C10-C9-C11	2.15	118.95	115.23
6	B	856	U10	C8-C7-C6	-2.14	106.81	112.08
4	A	850	BCL	C2C-C3C-C4C	2.12	104.51	101.34
4	B	853	BCL	C1D-ND-C4D	-2.11	104.83	106.31
6	A	857	U10	C36-C34-C33	2.09	125.85	121.17
6	B	856	U10	C1-C6-C5	-2.08	117.59	119.62
4	A	850	BCL	C3B-C4B-NB	2.08	112.51	109.76
4	A	850	BCL	O1D-CGD-CBD	-2.06	120.46	124.52
4	B	852	BCL	C3B-C4B-NB	2.05	112.46	109.76
4	B	852	BCL	CAB-C3B-C2B	2.02	131.95	127.74
4	B	853	BCL	O2A-CGA-CBA	2.02	117.99	111.83
6	B	856	U10	C30-C29-C28	-2.01	118.47	123.63
5	B	854	BPH	CBB-CAB-C3B	-2.01	114.33	120.34

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	853	BCL	CHA-CBD-CGD-O1D
4	B	853	BCL	CHA-CBD-CGD-O2D
5	A	855	BPH	C4C-C3C-CAC-CBC
5	A	855	BPH	C2C-C3C-CAC-CBC
5	A	855	BPH	C6-C7-C8-C9
5	B	854	BPH	C4C-C3C-CAC-CBC
5	B	854	BPH	C2C-C3C-CAC-CBC
4	B	852	BCL	C4-C3-C5-C6
6	B	856	U10	C20-C19-C21-C22
6	B	856	U10	C18-C19-C21-C22
5	A	855	BPH	C4-C3-C5-C6
5	B	854	BPH	C4-C3-C5-C6
6	A	857	U10	C15-C14-C16-C17
6	A	857	U10	C25-C24-C26-C27
6	B	856	U10	C15-C14-C16-C17
6	B	856	U10	C25-C24-C26-C27
5	A	855	BPH	C2-C3-C5-C6
5	B	854	BPH	C2-C3-C5-C6
6	A	857	U10	C13-C14-C16-C17
6	A	857	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
6	B	856	U10	C13-C14-C16-C17
6	B	856	U10	C23-C24-C26-C27
6	A	857	U10	C19-C21-C22-C23
6	A	857	U10	C34-C36-C37-C38
6	B	856	U10	C14-C16-C17-C18
6	B	856	U10	C29-C31-C32-C33
6	B	856	U10	C34-C36-C37-C38
6	A	857	U10	C30-C29-C31-C32
4	B	852	BCL	C2-C3-C5-C6
5	B	854	BPH	C6-C7-C8-C9
4	A	851	BCL	C2A-CAA-CBA-CGA
5	A	855	BPH	C11-C10-C8-C7
6	B	856	U10	C19-C21-C22-C23
4	A	851	BCL	C5-C6-C7-C8
4	A	850	BCL	C15-C16-C17-C18
4	B	853	BCL	C5-C6-C7-C8
5	A	855	BPH	C8-C10-C11-C12
4	B	852	BCL	C3-C5-C6-C7
4	B	852	BCL	C15-C16-C17-C18
6	A	857	U10	C28-C29-C31-C32
5	B	854	BPH	C3-C5-C6-C7
6	A	857	U10	C5-C6-C7-C8
4	A	851	BCL	C11-C10-C8-C7
5	A	855	BPH	C6-C7-C8-C10
4	B	852	BCL	C14-C13-C15-C16
6	A	857	U10	C29-C31-C32-C33
5	B	854	BPH	C8-C10-C11-C12
4	A	850	BCL	C4-C3-C5-C6
4	A	851	BCL	C11-C10-C8-C9
4	A	851	BCL	C14-C13-C15-C16
4	A	851	BCL	C12-C13-C15-C16
4	B	852	BCL	C11-C10-C8-C7
4	B	852	BCL	C12-C13-C15-C16
5	B	854	BPH	C11-C10-C8-C7
4	A	850	BCL	C2-C3-C5-C6
4	B	853	BCL	C15-C16-C17-C18
6	A	857	U10	C24-C26-C27-C28
5	B	854	BPH	C11-C10-C8-C9
6	B	856	U10	C12-C11-C9-C10
4	A	851	BCL	C15-C16-C17-C18
4	A	850	BCL	C11-C10-C8-C7
4	B	852	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	855	BPH	C11-C10-C8-C9
6	B	856	U10	C5-C4-O4-C4M
6	A	857	U10	C2-C3-O3-C3M
6	A	857	U10	C5-C4-O4-C4M
6	A	857	U10	C14-C16-C17-C18
4	B	853	BCL	C12-C13-C15-C16
4	A	850	BCL	C11-C10-C8-C9
4	B	853	BCL	C14-C13-C15-C16
6	B	856	U10	C3-C4-O4-C4M
6	B	856	U10	C12-C11-C9-C8
4	B	853	BCL	C2A-CAA-CBA-CGA
4	B	852	BCL	C2-C1-O2A-CGA
4	B	852	BCL	CAA-CBA-CGA-O2A
6	A	857	U10	C4-C3-O3-C3M
6	A	857	U10	C1-C6-C7-C8
5	B	854	BPH	CAD-CBD-CGD-O2D
4	B	852	BCL	CAA-CBA-CGA-O1A

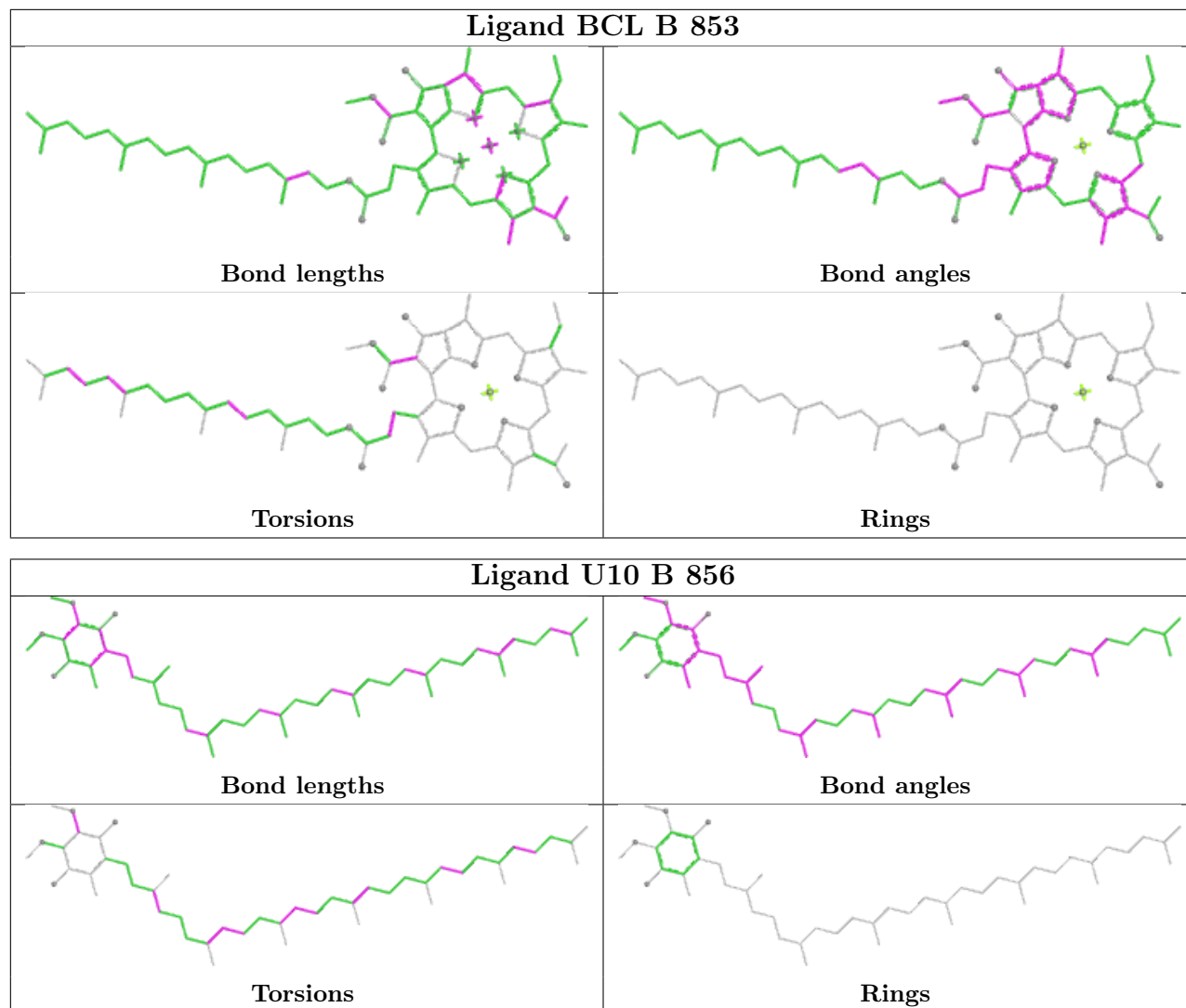
There are no ring outliers.

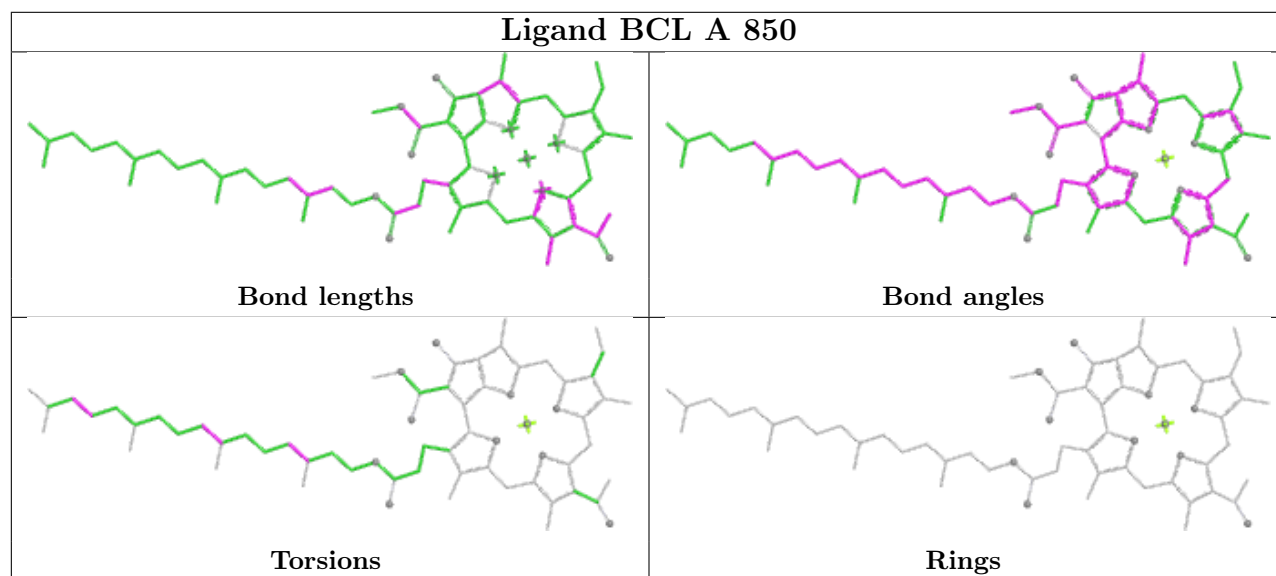
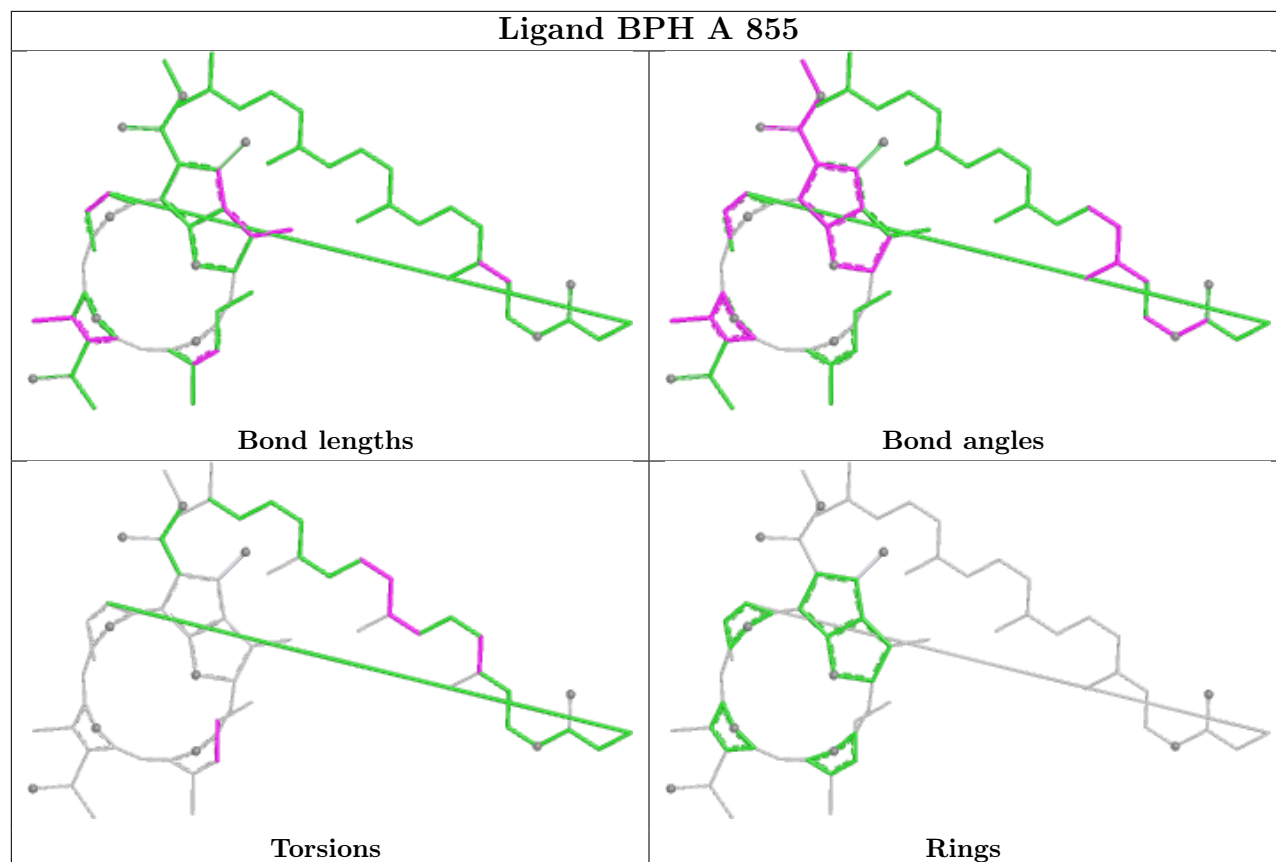
8 monomers are involved in 63 short contacts:

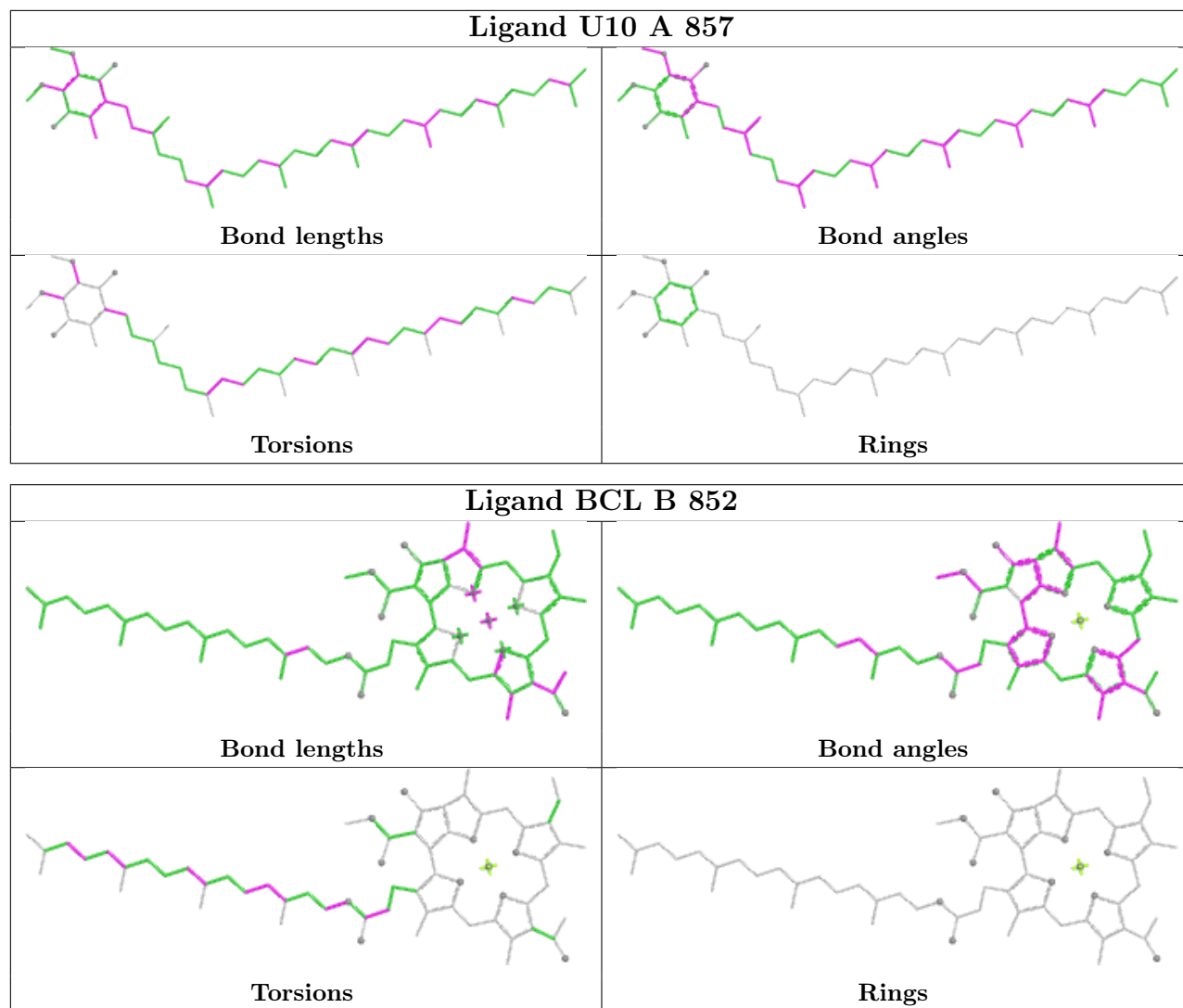
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	853	BCL	7	0
6	B	856	U10	13	0
5	A	855	BPH	9	0
4	A	850	BCL	15	0
6	A	857	U10	4	0
4	B	852	BCL	7	0
5	B	854	BPH	9	0
4	A	851	BCL	6	0

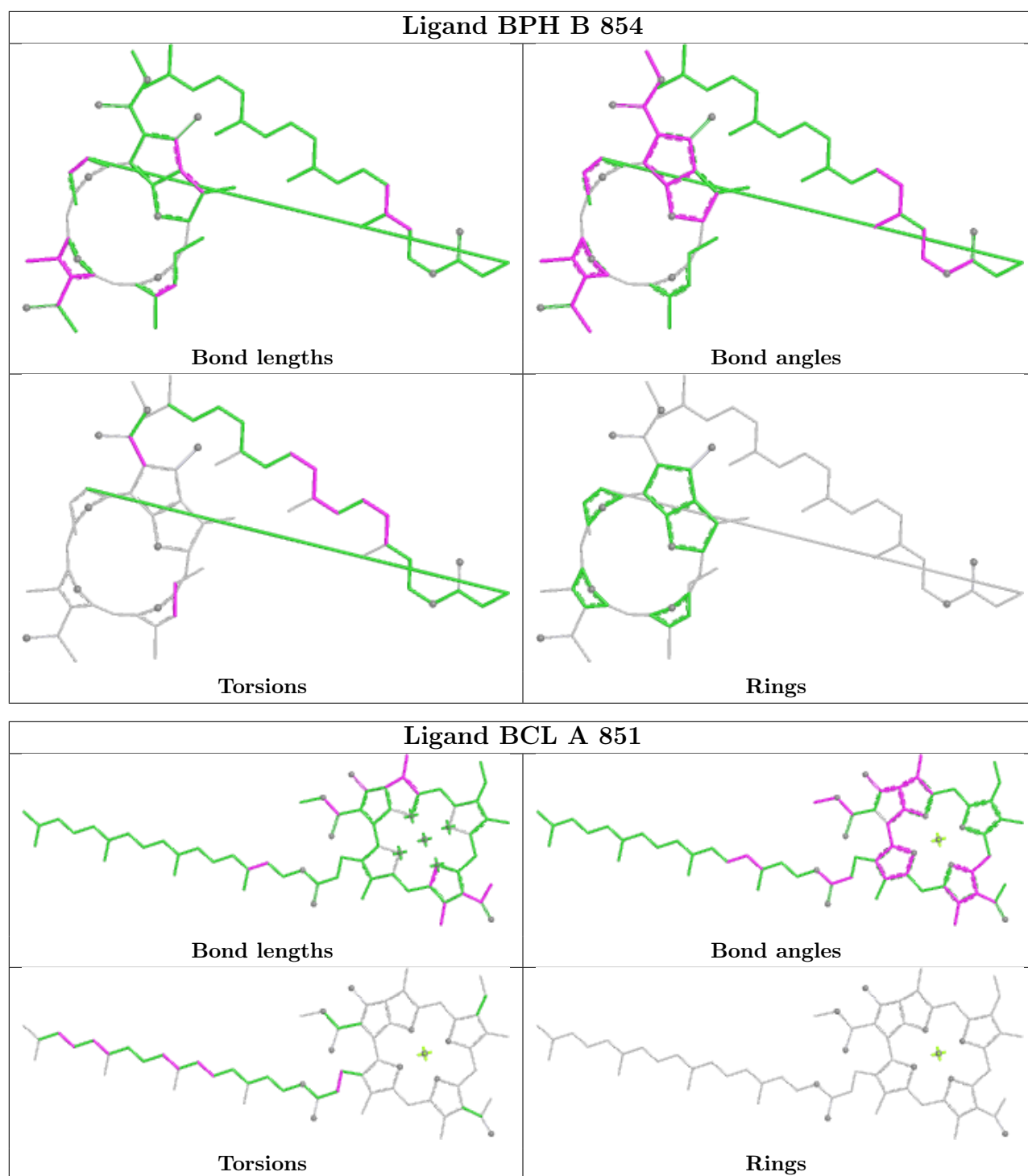
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/281 (100%)	-0.23	5 (1%) 67 54	90, 90, 90, 90	0
2	B	302/307 (98%)	-0.16	2 (0%) 84 70	90, 90, 90, 90	0
3	C	238/260 (91%)	-0.34	1 (0%) 88 77	90, 90, 90, 90	0
All	All	821/848 (96%)	-0.24	8 (0%) 79 64	90, 90, 90, 90	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	4.0
2	B	176	PRO	4.0
2	B	175	VAL	3.3
1	A	22	PHE	3.2
1	A	146	PHE	3.1
3	C	43	GLU	2.1
1	A	145	ALA	2.1
1	A	263	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

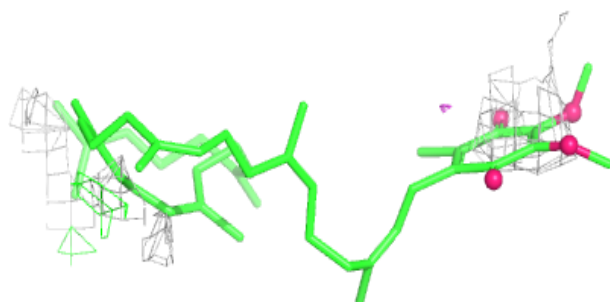
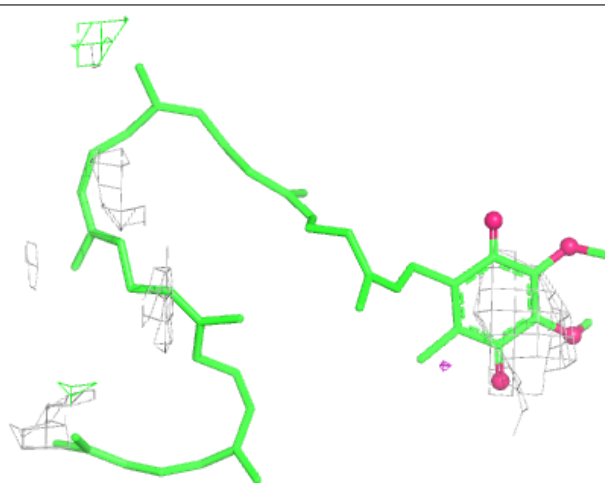
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U10	A	857	48/63	0.74	0.21	90,90,90,90	0
8	MN	C	860	1/1	0.84	0.20	181,181,181,181	1
5	BPH	B	854	65/65	0.86	0.19	90,90,90,90	0
4	BCL	A	850	66/66	0.87	0.19	90,90,90,90	0
6	U10	B	856	48/63	0.91	0.16	90,90,90,90	0
4	BCL	B	852	66/66	0.95	0.18	90,90,90,90	0
5	BPH	A	855	65/65	0.95	0.15	90,90,90,90	0
4	BCL	A	851	66/66	0.96	0.20	90,90,90,90	0
4	BCL	B	853	66/66	0.97	0.13	90,90,90,90	0
7	FE	B	858	1/1	0.99	0.08	90,90,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

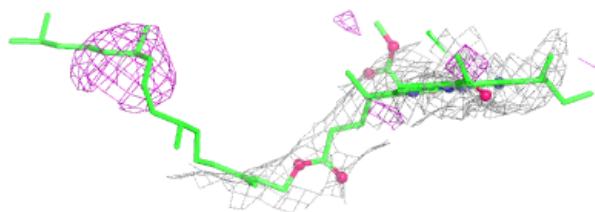
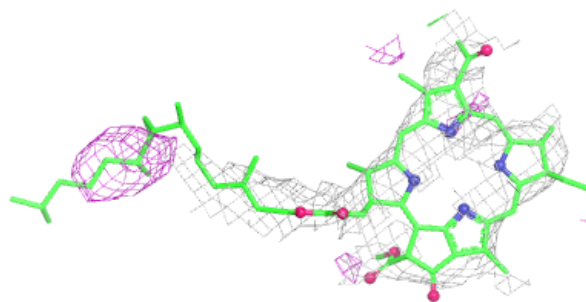
Electron density around U10 A 857:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



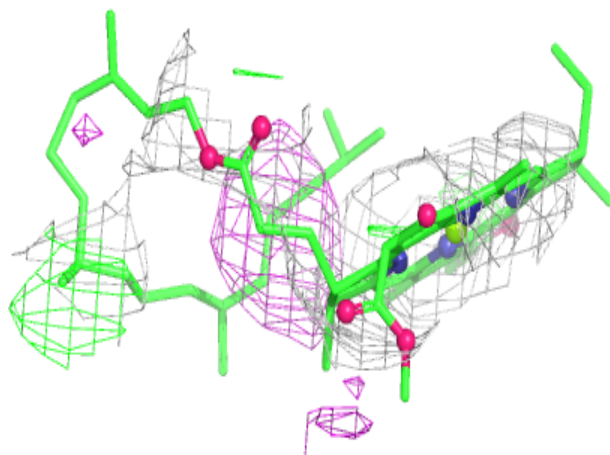
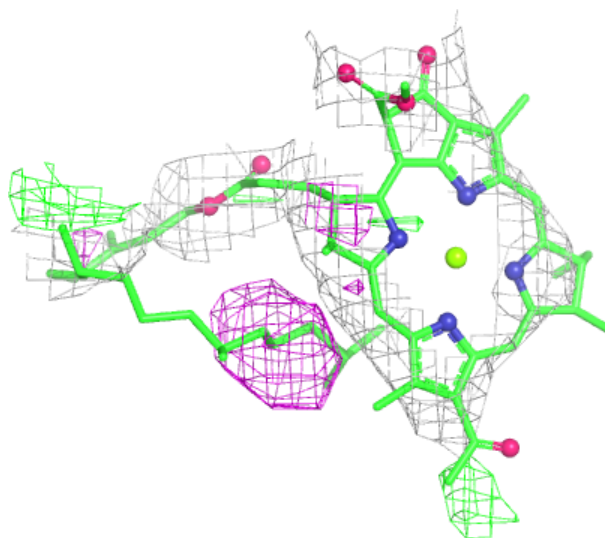
Electron density around BPH B 854:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



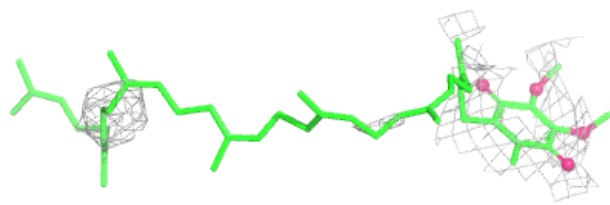
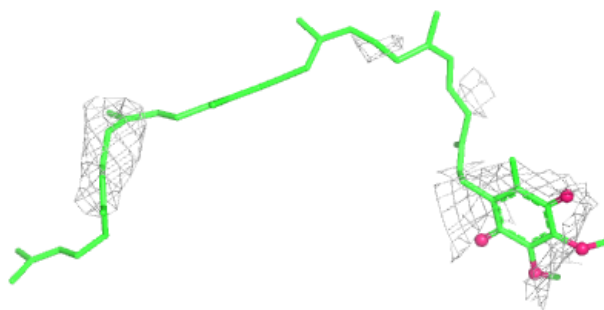
Electron density around BCL A 850:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

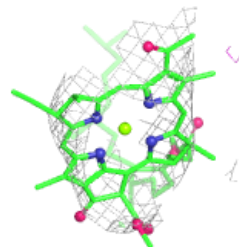
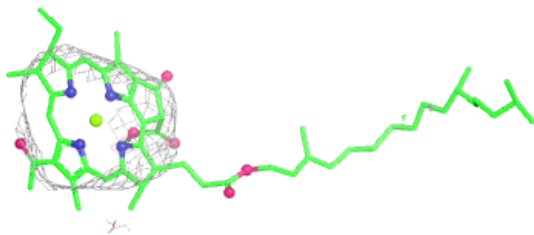
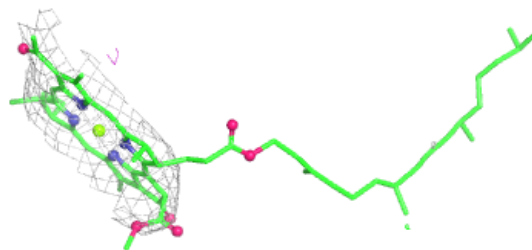


Electron density around U10 B 856:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

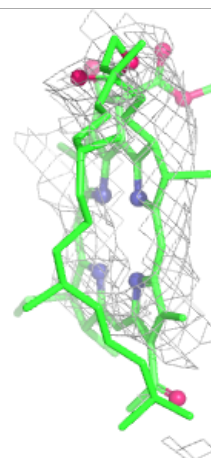
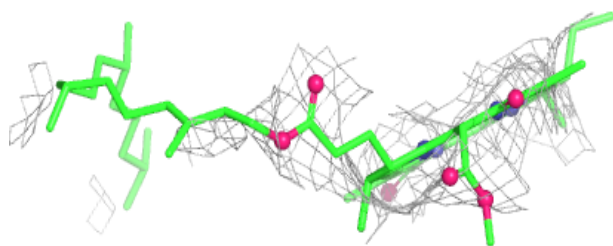
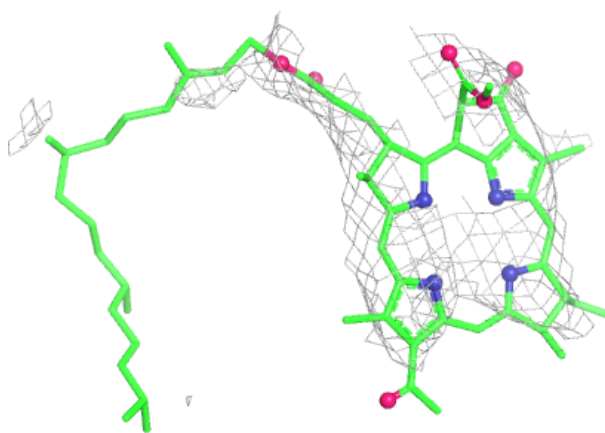
**Electron density around BCL B 852:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



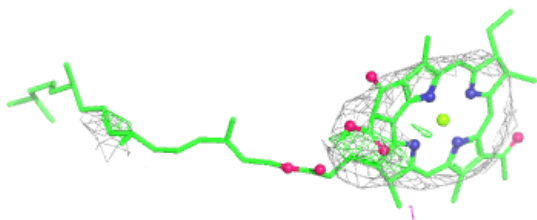
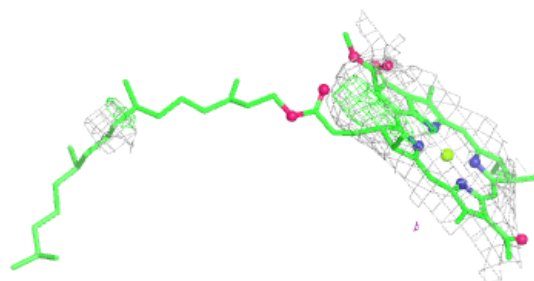
Electron density around BPH A 855:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

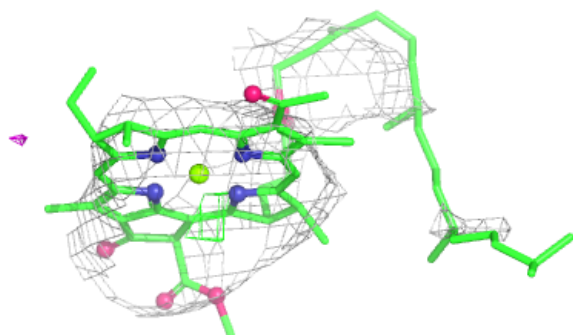
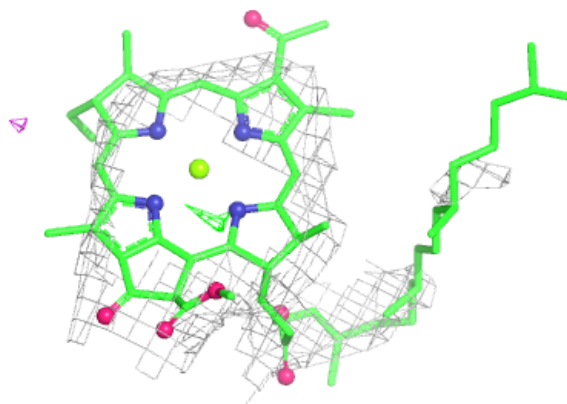


Electron density around BCL A 851:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCL B 853:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.