



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:34 PM UTC

PDB ID : 1Z9J / pdb_00001z9j
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides
Authors : Thielges, M.; Uyeda, G.; Camara-Artigas, A.; Kalman, L.; Williams, J.C.; Allen, J.P.
Deposited on : 2005-04-02
Resolution : 4.50 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

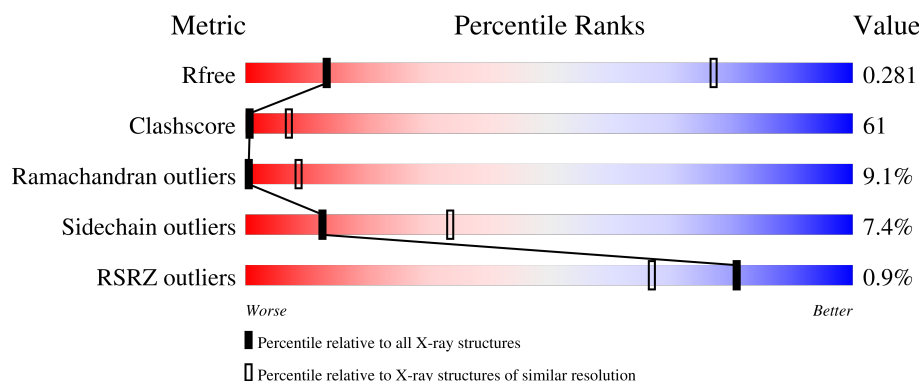
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	% 22% 56% 20% •
2	B	307	% 22% 56% 20% ••
3	C	260	32% 48% 10% • 8%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6957 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
			2234	1507	357	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	HIS	LEU	engineered mutation	UNP P0C0Y8

- 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
			2415	1609	395	402	9			

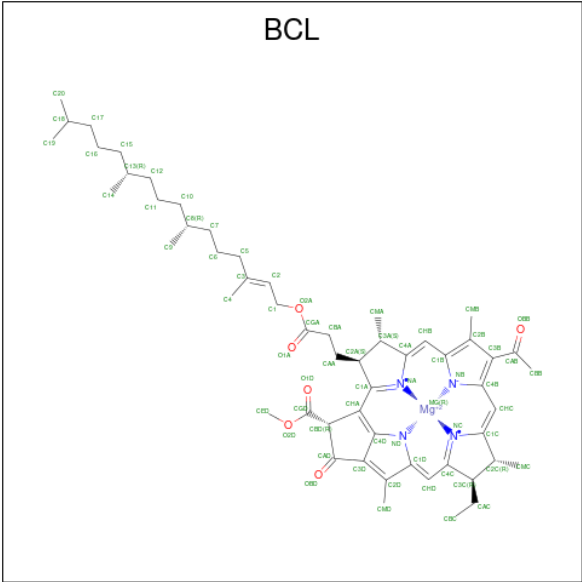
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	LEU	engineered mutation	UNP P0C0Y9
B	164	TYR	ARG	engineered mutation	UNP P0C0Y9
B	168	GLU	MET	engineered mutation	UNP P0C0Y9
B	197	HIS	PHE	engineered mutation	UNP P0C0Y9
B	288	ASP	GLY	engineered mutation	UNP P0C0Y9

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

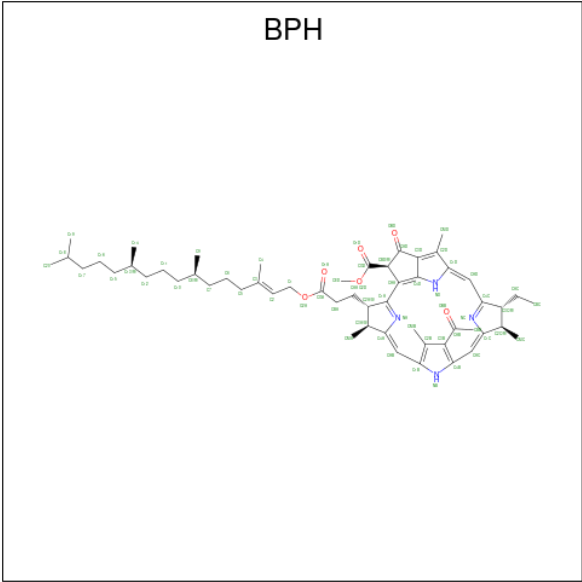
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	9			

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



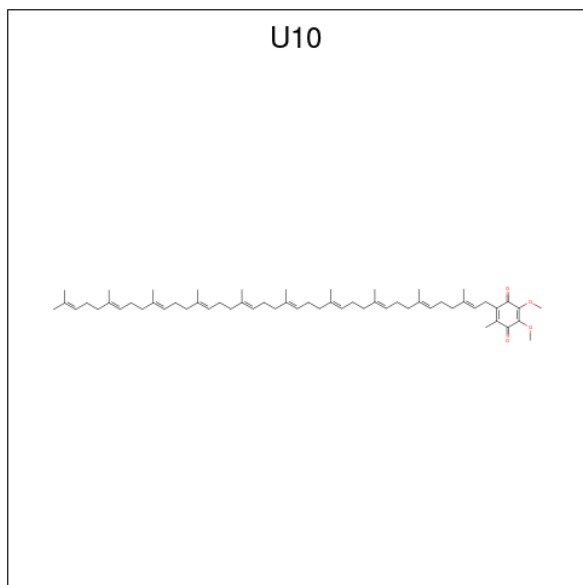
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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	B	1	Total	Mn	0	0
			1	1		

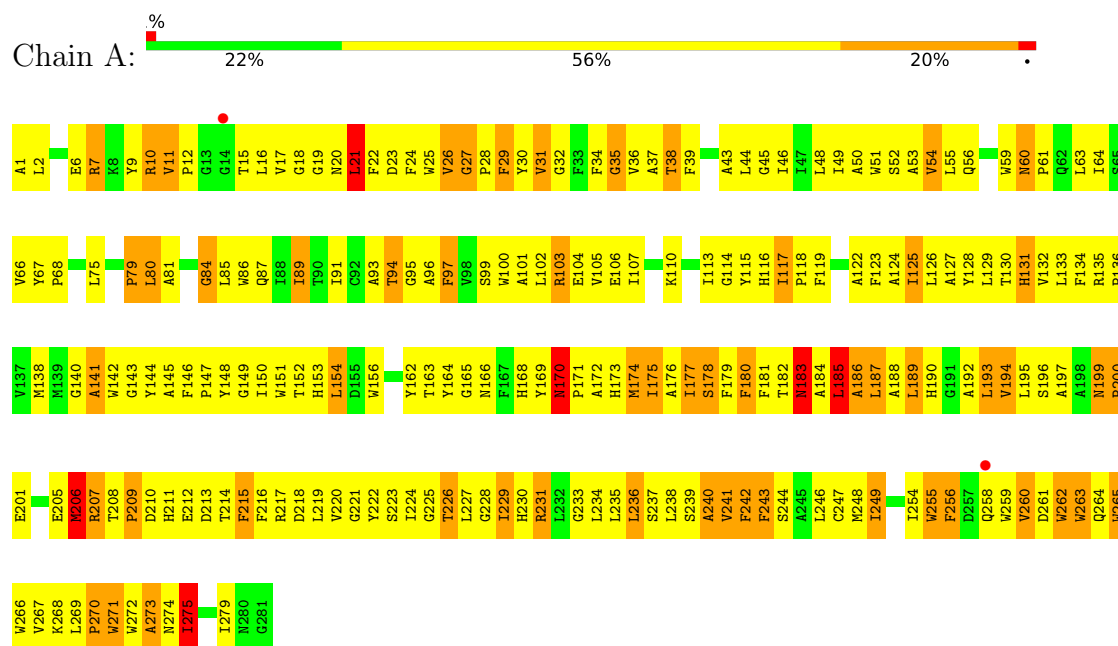
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	O	0	0
			2	2		

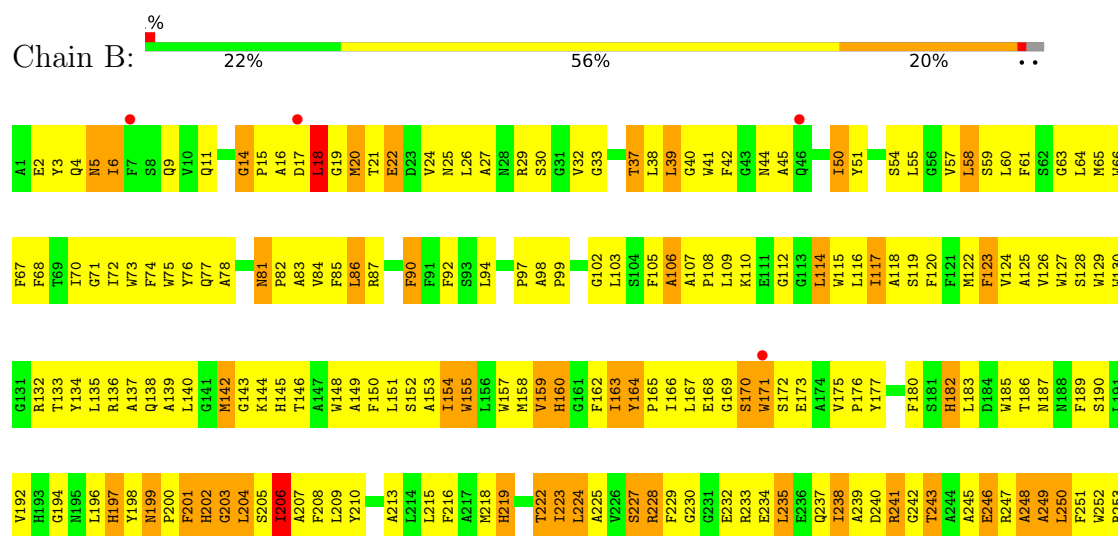
3 Residue-property plots

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

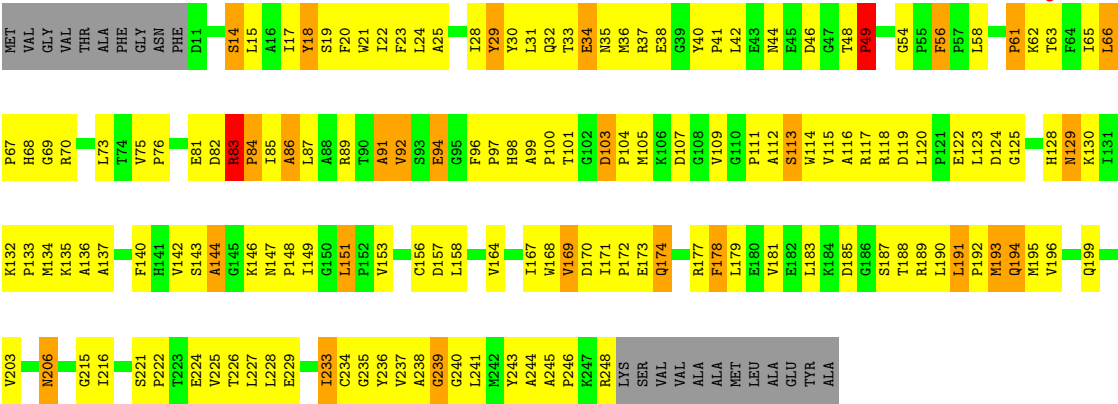


• Molecule 2: Reaction center protein M chain





• 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	203.84Å 203.84Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 4.50 19.96 – 4.50	Depositor EDS
% Data completeness (in resolution range)	79.9 (19.96-4.50) 78.8 (19.96-4.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 4.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.299 , 0.338 0.224 , 0.281	Depositor DCC
R_{free} test set	712 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	145.2	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 1.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6957	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 2.91% 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, BCL, MN, U10, BPH

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	0.77	0/2323	1.23	31/3179 (1.0%)
2	B	0.76	2/2509 (0.1%)	1.20	36/3428 (1.1%)
3	C	0.74	1/1862 (0.1%)	1.29	27/2534 (1.1%)
All	All	0.76	3/6694 (0.0%)	1.24	94/9141 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	206	ILE	CA-CB	6.46	1.61	1.54
3	C	22	ILE	CA-CB	5.08	1.60	1.54
2	B	167	LEU	CA-C	5.01	1.59	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ILE	N-CA-C	-9.70	101.30	110.42
1	A	54	VAL	N-CA-C	-9.48	102.63	111.45
3	C	83	ARG	CA-C-N	8.92	130.21	120.13
3	C	83	ARG	C-N-CA	8.92	130.21	120.13
3	C	103	ASP	CA-C-N	8.44	129.26	119.47
3	C	103	ASP	C-N-CA	8.44	129.26	119.47
1	A	174	MET	N-CA-C	-8.41	99.92	112.04
1	A	131	HIS	N-CA-C	8.11	120.84	111.11
2	B	6	ILE	N-CA-C	-8.11	102.95	110.82
3	C	56	PHE	CA-C-N	8.04	128.19	120.31
3	C	56	PHE	C-N-CA	8.04	128.19	120.31
2	B	2	GLU	N-CA-C	7.47	120.44	109.69
2	B	37	THR	N-CA-C	-7.34	104.06	113.16
2	B	199	ASN	CA-C-N	7.32	126.95	119.19
2	B	199	ASN	C-N-CA	7.32	126.95	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	SER	N-CA-C	-7.28	102.95	111.03
1	A	231	ARG	N-CA-C	-7.27	103.01	112.68
2	B	263	GLU	N-CA-C	-7.23	103.00	111.03
2	B	170	SER	N-CA-C	7.23	121.11	108.75
2	B	81	ASN	CA-C-N	7.20	128.84	119.84
2	B	81	ASN	C-N-CA	7.20	128.84	119.84
1	A	60	ASN	N-CA-C	-7.06	100.75	109.65
1	A	141	ALA	N-CA-C	7.06	119.90	107.61
3	C	54	GLY	CA-C-N	7.04	128.65	119.84
3	C	54	GLY	C-N-CA	7.04	128.65	119.84
3	C	92	VAL	N-CA-C	6.97	117.11	110.42
2	B	98	ALA	CA-C-N	6.84	128.39	119.84
2	B	98	ALA	C-N-CA	6.84	128.39	119.84
2	B	203	GLY	N-CA-C	-6.82	104.55	112.73
1	A	185	LEU	N-CA-C	-6.55	104.14	111.28
1	A	7	ARG	N-CA-C	6.53	118.47	111.36
2	B	164	TYR	CA-C-N	6.52	126.45	119.28
2	B	164	TYR	C-N-CA	6.52	126.45	119.28
3	C	91	ALA	CA-C-N	6.46	128.70	120.56
3	C	91	ALA	C-N-CA	6.46	128.70	120.56
1	A	67	TYR	N-CA-C	6.45	119.62	110.40
3	C	63	THR	N-CA-C	6.41	119.34	108.90
1	A	97	PHE	N-CA-C	-6.39	103.57	112.45
1	A	197	ALA	N-CA-C	-6.30	105.24	113.12
1	A	163	THR	N-CA-C	-6.30	104.86	112.54
3	C	178	PHE	N-CA-C	6.22	118.52	109.07
1	A	199	ASN	CA-C-N	6.21	127.61	119.84
1	A	199	ASN	C-N-CA	6.21	127.61	119.84
2	B	301	HIS	N-CA-C	-6.20	102.69	111.56
2	B	237	GLN	N-CA-C	-6.18	103.86	112.45
1	A	243	PHE	N-CA-C	6.13	117.63	111.07
3	C	151	LEU	CA-C-N	6.12	126.33	119.90
3	C	151	LEU	C-N-CA	6.12	126.33	119.90
2	B	159	VAL	N-CA-C	-6.10	105.19	110.74
2	B	227	SER	N-CA-C	-6.04	104.27	111.69
2	B	243	THR	N-CA-C	-5.95	105.98	113.18
3	C	191	LEU	CA-C-N	5.94	127.27	119.84
3	C	191	LEU	C-N-CA	5.94	127.27	119.84
1	A	201	GLU	N-CA-C	-5.91	102.72	110.53
1	A	27	GLY	N-CA-C	-5.86	100.38	112.34
2	B	45	ALA	N-CA-C	-5.85	105.98	114.12
2	B	197	HIS	N-CA-C	-5.81	105.29	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASN	N-CA-C	-5.79	99.45	109.58
2	B	224	LEU	N-CA-C	5.79	117.67	111.36
2	B	142	MET	N-CA-C	5.75	118.97	110.46
2	B	254	TRP	N-CA-C	-5.72	105.96	113.17
1	A	209	PRO	N-CA-C	-5.71	106.62	113.98
1	A	103	ARG	N-CA-C	-5.68	104.29	111.11
2	B	106	ALA	N-CA-C	-5.66	107.02	114.04
2	B	14	GLY	N-CA-C	-5.66	100.80	112.34
1	A	110	LYS	N-CA-C	-5.62	104.78	111.69
1	A	255	TRP	N-CA-C	-5.58	99.32	108.76
2	B	248	ALA	N-CA-C	-5.51	104.50	111.11
1	A	189	LEU	N-CA-C	5.47	117.10	111.03
3	C	84	PRO	N-CA-C	5.45	119.43	110.55
1	A	177	ILE	N-CA-C	5.41	116.14	110.62
2	B	114	LEU	N-CA-C	-5.40	106.53	113.23
1	A	224	ILE	N-CA-C	-5.38	106.61	113.22
1	A	226	THR	N-CA-C	5.37	122.24	110.80
3	C	94	GLU	N-CA-C	5.36	117.80	109.60
2	B	201	PHE	N-CA-C	-5.35	106.59	113.01
1	A	29	PHE	N-CA-C	5.29	117.36	108.96
3	C	203	VAL	N-CA-C	-5.29	100.84	108.71
2	B	98	ALA	N-CA-C	5.28	116.48	109.93
3	C	132	LYS	CA-C-N	5.26	126.41	119.84
3	C	132	LYS	C-N-CA	5.26	126.41	119.84
1	A	115	TYR	N-CA-C	-5.25	106.73	112.72
1	A	242	PHE	N-CA-C	-5.21	105.29	110.97
2	B	235	LEU	N-CA-C	5.17	116.60	111.07
2	B	246	GLU	N-CA-C	-5.17	105.56	111.14
3	C	18	TYR	N-CA-C	-5.15	103.06	111.04
2	B	256	MET	N-CA-C	5.15	119.13	111.87
2	B	202	HIS	N-CA-C	-5.11	106.73	113.12
2	B	206	ILE	N-CA-C	-5.11	104.92	110.23
2	B	54	SER	N-CA-C	-5.08	105.83	111.36
1	A	35	GLY	N-CA-C	-5.08	101.15	113.18
3	C	91	ALA	N-CA-C	5.03	116.49	108.79
3	C	124	ASP	N-CA-C	-5.02	100.10	110.80
3	C	129	ASN	N-CA-C	5.01	118.05	110.64

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	2234	0	2183	349	0
2	B	2415	0	2309	386	0
3	C	1814	0	1818	203	1
4	A	132	0	148	17	0
4	B	132	0	148	17	0
5	A	65	0	76	13	0
5	B	65	0	76	11	0
6	A	48	0	63	6	0
6	B	48	0	63	16	0
7	B	1	0	0	0	0
8	B	1	0	0	0	0
9	B	2	0	0	1	0
All	All	6957	0	6884	850	1

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 61.

All (850) 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:64:LEU:HD21	5:B:854:BPH:H112	1.32	1.10
2:B:267:ARG:O	2:B:270:ILE:HG22	1.65	0.96
1:A:171:PRO:HA	1:A:174:MET:HG3	1.48	0.95
2:B:242:GLY:HA2	3:C:117:ARG:HD2	1.49	0.94
1:A:114:GLY:H	2:B:225:ALA:HB1	1.32	0.93
2:B:287:SER:CB	2:B:294:TRP:HE1	1.82	0.92
5:A:855:BPH:HBB2	4:B:853:BCL:H11	1.49	0.91
1:A:271:TRP:CD1	1:A:271:TRP:H	1.85	0.91
3:C:87:LEU:HD22	3:C:98:HIS:O	1.72	0.90
1:A:22:PHE:HA	1:A:24:PHE:CE2	2.06	0.90
3:C:61:PRO:HA	3:C:76:PRO:HD2	1.54	0.89
1:A:146:PHE:HA	1:A:156:TRP:CD1	2.08	0.87
2:B:299:GLN:HE21	2:B:299:GLN:HA	1.38	0.87
3:C:86:ALA:HB1	3:C:101:THR:OG1	1.75	0.87
1:A:9:TYR:O	1:A:11:VAL:HG13	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PHE:O	1:A:38:THR:HG23	1.76	0.86
1:A:229:ILE:HD12	6:A:857:U10:H3M2	1.55	0.86
3:C:233:ILE:O	3:C:237:VAL:HG23	1.75	0.86
2:B:202:HIS:CE1	2:B:206:ILE:HD11	2.10	0.86
1:A:227:LEU:HD21	2:B:5:ASN:ND2	1.90	0.85
1:A:116:HIS:CD2	2:B:224:LEU:HB3	2.12	0.85
3:C:117:ARG:O	3:C:228:LEU:HB2	1.75	0.85
2:B:227:SER:C	2:B:229:PHE:H	1.85	0.83
1:A:38:THR:HG22	1:A:99:SER:CB	2.08	0.83
1:A:227:LEU:HD21	2:B:5:ASN:HD21	1.44	0.83
1:A:60:ASN:O	1:A:64:ILE:HG12	1.79	0.82
1:A:229:ILE:CG2	1:A:230:HIS:N	2.42	0.82
2:B:299:GLN:HA	2:B:299:GLN:NE2	1.94	0.82
1:A:114:GLY:N	2:B:225:ALA:HB1	1.94	0.81
2:B:97:PRO:HB3	2:B:112:GLY:HA3	1.60	0.81
2:B:64:LEU:CD2	5:B:854:BPH:H112	2.09	0.81
2:B:271:TRP:O	2:B:273:ALA:N	2.13	0.81
1:A:185:LEU:O	1:A:188:ALA:HB3	1.80	0.81
2:B:245:ALA:HB2	2:B:262:MET:HE2	1.63	0.81
1:A:38:THR:HG22	1:A:99:SER:HB3	1.62	0.79
2:B:180:PHE:O	2:B:183:LEU:HB2	1.82	0.79
3:C:83:ARG:HB2	3:C:84:PRO:HD2	1.64	0.79
3:C:189:ARG:HD2	3:C:216:ILE:HB	1.62	0.79
3:C:87:LEU:HD23	3:C:100:PRO:HA	1.65	0.79
1:A:173:HIS:CE1	1:A:177:ILE:HD11	2.17	0.79
2:B:247:ARG:NH2	3:C:111:PRO:O	2.15	0.78
2:B:241:ARG:HD3	3:C:38:GLU:OE1	1.84	0.78
2:B:26:LEU:HD22	2:B:29:ARG:HD2	1.65	0.78
1:A:177:ILE:HD12	4:A:850:BCL:OBD	1.84	0.77
1:A:193:LEU:O	1:A:196:SER:N	2.16	0.77
1:A:219:LEU:HD12	2:B:132:ARG:NH1	1.99	0.77
1:A:124:ALA:HB1	4:A:851:BCL:H62	1.67	0.76
1:A:12:PRO:HG3	3:C:97:PRO:HB2	1.65	0.76
1:A:150:ILE:HG22	1:A:151:TRP:CD1	2.21	0.76
3:C:89:ARG:HD3	3:C:91:ALA:O	1.85	0.76
2:B:74:PHE:CE2	2:B:92:PHE:HB2	2.20	0.76
1:A:12:PRO:HG3	3:C:97:PRO:CB	2.16	0.76
1:A:241:VAL:HG21	5:A:855:BPH:HAC2	1.68	0.76
2:B:14:GLY:HA3	3:C:140:PHE:CE1	2.20	0.76
1:A:239:SER:O	1:A:242:PHE:N	2.19	0.76
2:B:281:GLY:O	2:B:285:LEU:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:MET:HE3	3:C:193:MET:HA	1.67	0.76
2:B:102:GLY:HA2	2:B:170:SER:CB	2.16	0.75
1:A:173:HIS:HE1	1:A:177:ILE:HD11	1.51	0.75
2:B:103:LEU:HG	2:B:169:GLY:O	1.87	0.75
2:B:153:ALA:HB1	4:B:852:BCL:H62	1.67	0.75
2:B:207:ALA:HA	4:B:853:BCL:O1A	1.86	0.75
1:A:183:ASN:O	1:A:186:ALA:HB3	1.86	0.74
3:C:29:TYR:HD1	3:C:56:PHE:HE1	1.32	0.74
1:A:22:PHE:HA	1:A:24:PHE:HE2	1.50	0.74
1:A:190:HIS:HA	6:A:857:U10:H4M1	1.70	0.74
1:A:16:LEU:HD12	1:A:106:GLU:HG2	1.69	0.74
1:A:229:ILE:HG22	1:A:230:HIS:H	1.53	0.74
2:B:3:TYR:CD2	3:C:194:GLN:HA	2.22	0.73
1:A:173:HIS:O	1:A:173:HIS:ND1	2.21	0.73
1:A:39:PHE:HB2	6:B:856:U10:H352	1.70	0.73
2:B:164:TYR:HB3	2:B:165:PRO:HD3	1.71	0.73
2:B:280:GLY:O	2:B:282:ILE:N	2.21	0.73
1:A:182:THR:O	1:A:185:LEU:N	2.21	0.73
3:C:140:PHE:CD2	3:C:169:VAL:HG21	2.24	0.73
2:B:253:ARG:HH11	2:B:259:ASN:ND2	1.87	0.72
2:B:103:LEU:HD22	2:B:166:ILE:HD13	1.70	0.72
3:C:14:SER:O	3:C:17:ILE:HG22	1.89	0.72
1:A:35:GLY:HA2	1:A:103:ARG:HD2	1.71	0.72
4:B:852:BCL:H201	5:B:854:BPH:H9C2	1.71	0.72
2:B:19:GLY:O	2:B:20:MET:O	2.08	0.72
3:C:115:VAL:HG12	3:C:116:ALA:N	2.04	0.72
1:A:9:TYR:O	1:A:11:VAL:N	2.22	0.72
1:A:145:ALA:O	1:A:156:TRP:NE1	2.23	0.72
2:B:63:GLY:HA3	5:B:854:BPH:H5C1	1.72	0.72
2:B:3:TYR:CE2	3:C:194:GLN:HA	2.25	0.71
2:B:242:GLY:CA	3:C:117:ARG:HD2	2.19	0.71
1:A:229:ILE:HG23	1:A:230:HIS:N	2.06	0.71
3:C:173:GLU:O	3:C:174:GLN:C	2.33	0.71
1:A:46:ILE:HG12	4:B:853:BCL:H191	1.72	0.71
2:B:18:LEU:HD22	2:B:18:LEU:H	1.55	0.71
3:C:75:VAL:HA	3:C:76:PRO:C	2.16	0.71
1:A:28:PRO:HB3	2:B:253:ARG:HE	1.56	0.70
1:A:100:TRP:HZ3	6:B:856:U10:H321	1.54	0.70
1:A:135:ARG:HB3	1:A:136:PRO:HD3	1.72	0.70
1:A:51:TRP:O	1:A:54:VAL:HG22	1.92	0.70
2:B:38:LEU:O	2:B:40:GLY:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:MET:O	3:C:196:VAL:HG22	1.91	0.70
1:A:271:TRP:CD1	1:A:271:TRP:N	2.59	0.70
3:C:192:PRO:O	3:C:195:MET:N	2.24	0.70
1:A:183:ASN:HA	1:A:236:LEU:HD12	1.73	0.69
1:A:187:LEU:HB2	2:B:216:PHE:CD2	2.27	0.69
2:B:182:HIS:ND1	2:B:183:LEU:N	2.40	0.69
3:C:61:PRO:CA	3:C:76:PRO:HD2	2.21	0.69
1:A:217:ARG:HH21	2:B:44:ASN:HD22	1.39	0.69
1:A:20:ASN:HA	1:A:23:ASP:HB2	1.74	0.69
1:A:180:PHE:O	2:B:209:LEU:HD11	1.93	0.69
2:B:168:GLU:HG2	2:B:173:GLU:HG3	1.75	0.69
1:A:96:ALA:HB1	5:A:855:BPH:H4C2	1.74	0.69
3:C:133:PRO:HB3	3:C:168:TRP:CE2	2.28	0.69
3:C:18:TYR:O	3:C:21:TRP:N	2.26	0.68
4:A:850:BCL:H11	5:B:854:BPH:HBB3	1.74	0.68
2:B:26:LEU:CD2	2:B:29:ARG:HD2	2.23	0.68
2:B:90:PHE:N	2:B:90:PHE:HD1	1.91	0.68
2:B:287:SER:OG	2:B:294:TRP:NE1	2.26	0.68
1:A:183:ASN:HD22	1:A:184:ALA:N	1.92	0.68
1:A:193:LEU:O	1:A:194:VAL:C	2.35	0.68
3:C:148:PRO:HA	3:C:151:LEU:HD12	1.74	0.68
3:C:170:ASP:OD1	3:C:172:PRO:HG2	1.94	0.68
1:A:267:VAL:HG23	2:B:87:ARG:HD2	1.76	0.68
2:B:153:ALA:O	2:B:155:TRP:N	2.27	0.67
4:A:850:BCL:HBC1	4:B:852:BCL:HBD	1.74	0.67
1:A:189:LEU:O	1:A:192:ALA:N	2.27	0.67
1:A:186:ALA:O	1:A:189:LEU:N	2.27	0.67
3:C:37:ARG:CZ	3:C:62:LYS:HD2	2.25	0.67
2:B:270:ILE:HD13	2:B:270:ILE:O	1.94	0.67
1:A:16:LEU:HD12	1:A:106:GLU:CG	2.25	0.66
2:B:123:PHE:HA	2:B:157:TRP:HH2	1.60	0.66
1:A:261:ASP:O	1:A:263:TRP:N	2.28	0.66
1:A:97:PHE:HB3	1:A:125:ILE:CD1	2.26	0.66
2:B:102:GLY:HA2	2:B:170:SER:HB3	1.77	0.66
1:A:229:ILE:CG2	1:A:230:HIS:H	2.07	0.66
3:C:29:TYR:CD1	3:C:56:PHE:HE1	2.13	0.66
3:C:37:ARG:NH1	3:C:62:LYS:HG2	2.11	0.66
1:A:114:GLY:CA	2:B:225:ALA:HB1	2.25	0.66
2:B:202:HIS:CE1	2:B:206:ILE:CD1	2.78	0.66
2:B:227:SER:O	2:B:229:PHE:N	2.27	0.66
3:C:142:VAL:HG21	3:C:147:ASN:ND2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:HIS:O	1:A:177:ILE:HG13	1.95	0.66
2:B:227:SER:C	2:B:229:PHE:N	2.54	0.66
2:B:32:VAL:HG12	2:B:33:GLY:O	1.96	0.65
3:C:36:MET:HG2	3:C:40:TYR:CE1	2.31	0.65
2:B:153:ALA:C	2:B:155:TRP:N	2.54	0.65
3:C:68:HIS:CD2	3:C:123:LEU:HD12	2.30	0.65
1:A:222:TYR:CZ	2:B:39:LEU:HD13	2.32	0.65
2:B:149:ALA:O	2:B:152:SER:HB3	1.96	0.65
2:B:275:LEU:O	2:B:279:THR:HG23	1.95	0.65
2:B:268:TRP:O	2:B:269:ALA:C	2.40	0.65
2:B:243:THR:O	2:B:247:ARG:HG3	1.97	0.65
1:A:221:GLY:CA	2:B:50:ILE:HG12	2.27	0.65
3:C:221:SER:HB3	3:C:224:GLU:HG3	1.79	0.65
3:C:179:LEU:O	3:C:181:VAL:HG23	1.97	0.64
3:C:193:MET:HE3	3:C:196:VAL:CG2	2.27	0.64
2:B:287:SER:HB3	2:B:294:TRP:HE1	1.60	0.64
3:C:226:THR:OG1	3:C:229:GLU:HG3	1.97	0.64
2:B:260:ALA:C	6:B:856:U10:H4M3	2.21	0.64
1:A:233:GLY:HA3	2:B:216:PHE:CE1	2.33	0.64
2:B:140:LEU:O	2:B:142:MET:HG3	1.98	0.64
2:B:18:LEU:HD22	2:B:18:LEU:N	2.13	0.64
2:B:222:THR:HG22	2:B:223:ILE:N	2.11	0.63
1:A:194:VAL:HG11	2:B:266:HIS:CD2	2.33	0.63
2:B:90:PHE:N	2:B:90:PHE:CD1	2.62	0.63
3:C:70:ARG:NH2	3:C:120:LEU:HD22	2.13	0.63
1:A:174:MET:HB3	4:A:850:BCL:O1D	1.97	0.63
3:C:61:PRO:HG3	3:C:76:PRO:HG2	1.81	0.63
1:A:146:PHE:HB2	1:A:147:PRO:HD2	1.81	0.63
1:A:182:THR:O	1:A:183:ASN:C	2.39	0.63
1:A:53:ALA:HB1	1:A:64:ILE:HD12	1.80	0.63
2:B:187:ASN:O	2:B:190:SER:HB3	1.98	0.63
3:C:41:PRO:HG3	3:C:58:LEU:HD11	1.79	0.63
3:C:65:ILE:HD12	3:C:65:ILE:H	1.64	0.63
1:A:219:LEU:HD12	2:B:132:ARG:HH12	1.63	0.63
1:A:269:LEU:HB2	1:A:272:TRP:NE1	2.13	0.63
2:B:287:SER:O	2:B:288:ASP:HB3	1.98	0.63
1:A:194:VAL:HG21	2:B:266:HIS:CD2	2.33	0.63
1:A:216:PHE:O	1:A:219:LEU:N	2.31	0.63
1:A:168:HIS:HB3	2:B:183:LEU:HD13	1.81	0.63
2:B:271:TRP:C	2:B:273:ALA:N	2.56	0.63
3:C:115:VAL:CG1	3:C:116:ALA:N	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PRO:HD2	1:A:259:TRP:CZ3	2.34	0.62
2:B:267:ARG:O	2:B:268:TRP:C	2.41	0.62
3:C:153:VAL:HG21	3:C:181:VAL:HG13	1.81	0.62
2:B:233:ARG:NE	3:C:122:GLU:OE1	2.30	0.62
3:C:192:PRO:O	3:C:193:MET:C	2.43	0.62
2:B:66:TRP:CD1	2:B:122:MET:HB2	2.33	0.62
2:B:175:VAL:HG22	2:B:185:TRP:CE2	2.34	0.62
1:A:38:THR:HG22	1:A:99:SER:HB2	1.79	0.62
3:C:96:PHE:HB3	3:C:97:PRO:CD	2.30	0.62
1:A:45:GLY:HA3	5:A:855:BPH:H9C1	1.79	0.62
1:A:269:LEU:HB2	1:A:272:TRP:HE1	1.64	0.62
2:B:153:ALA:O	2:B:154:ILE:C	2.43	0.62
3:C:83:ARG:HD2	3:C:114:TRP:CH2	2.35	0.62
3:C:134:MET:O	3:C:136:ALA:N	2.33	0.62
2:B:199:ASN:HA	2:B:294:TRP:CE3	2.35	0.61
2:B:270:ILE:HG23	2:B:271:TRP:N	2.13	0.61
2:B:76:TYR:OH	2:B:110:LYS:NZ	2.33	0.61
2:B:223:ILE:HD11	2:B:234:GLU:OE2	2.00	0.61
1:A:1:ALA:O	1:A:2:LEU:HD23	1.99	0.61
1:A:172:ALA:HB3	1:A:247:CYS:CB	2.31	0.61
2:B:82:PRO:O	2:B:86:LEU:HD23	2.00	0.61
1:A:180:PHE:CD2	1:A:240:ALA:HB1	2.35	0.61
2:B:102:GLY:HA2	2:B:170:SER:HB2	1.83	0.61
1:A:138:MET:SD	1:A:249:ILE:HD11	2.41	0.61
2:B:64:LEU:O	2:B:65:MET:C	2.44	0.61
1:A:52:SER:O	1:A:56:GLN:HB2	2.02	0.60
2:B:11:GLN:HB2	3:C:144:ALA:HB3	1.83	0.60
2:B:97:PRO:CB	2:B:112:GLY:HA3	2.31	0.60
3:C:143:SER:O	3:C:144:ALA:HB2	2.01	0.60
1:A:192:ALA:HB1	2:B:146:THR:HA	1.82	0.60
2:B:64:LEU:HD21	5:B:854:BPH:C11	2.21	0.60
3:C:238:ALA:O	3:C:240:GLY:N	2.34	0.60
3:C:111:PRO:HD2	3:C:243:TYR:OH	2.02	0.60
4:A:851:BCL:CAA	4:B:853:BCL:HBC1	2.31	0.60
2:B:125:ALA:O	5:B:854:BPH:H1C2	2.02	0.60
1:A:147:PRO:HD3	1:A:156:TRP:CD1	2.36	0.60
1:A:183:ASN:ND2	1:A:184:ALA:N	2.48	0.60
1:A:265:TRP:CH2	1:A:266:TRP:HE3	2.19	0.60
2:B:280:GLY:C	2:B:282:ILE:N	2.59	0.60
2:B:287:SER:O	2:B:288:ASP:CB	2.48	0.60
1:A:186:ALA:O	1:A:188:ALA:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:SER:O	1:A:241:VAL:N	2.35	0.60
2:B:198:TYR:O	2:B:199:ASN:C	2.44	0.60
2:B:288:ASP:OD2	9:B:911:HOH:O	2.17	0.60
2:B:18:LEU:H	2:B:18:LEU:CD2	2.14	0.59
2:B:159:VAL:HA	2:B:163:ILE:HB	1.83	0.59
3:C:94:GLU:O	3:C:96:PHE:HD1	1.85	0.59
3:C:227:LEU:O	3:C:228:LEU:C	2.45	0.59
1:A:261:ASP:O	1:A:262:TRP:C	2.45	0.59
2:B:82:PRO:O	2:B:85:PHE:HB3	2.01	0.59
2:B:129:TRP:O	2:B:130:TRP:C	2.44	0.59
2:B:143:GLY:C	2:B:145:HIS:H	2.09	0.59
2:B:238:ILE:HG22	2:B:239:ALA:N	2.16	0.59
2:B:251:PHE:C	2:B:251:PHE:CD1	2.80	0.59
1:A:9:TYR:OH	2:B:246:GLU:OE1	2.11	0.59
2:B:229:PHE:CZ	2:B:247:ARG:NH1	2.71	0.59
2:B:175:VAL:HG13	2:B:176:PRO:HD2	1.83	0.59
2:B:267:ARG:O	2:B:268:TRP:O	2.21	0.59
3:C:151:LEU:O	3:C:164:VAL:HG23	2.03	0.59
1:A:46:ILE:HG12	4:B:853:BCL:C19	2.33	0.59
3:C:68:HIS:HD2	3:C:123:LEU:HD12	1.68	0.59
1:A:208:THR:OG1	1:A:210:ASP:HB2	2.03	0.58
3:C:156:CYS:SG	3:C:248:ARG:HB2	2.42	0.58
1:A:175:ILE:O	1:A:176:ALA:C	2.46	0.58
1:A:189:LEU:O	1:A:190:HIS:C	2.46	0.58
2:B:227:SER:O	2:B:230:GLY:N	2.35	0.58
1:A:164:TYR:CE1	1:A:256:PHE:O	2.57	0.58
3:C:112:ALA:O	3:C:113:SER:C	2.46	0.58
1:A:129:LEU:O	1:A:130:THR:C	2.47	0.58
1:A:175:ILE:HG21	1:A:243:PHE:CD2	2.39	0.58
2:B:222:THR:O	2:B:223:ILE:C	2.45	0.58
2:B:279:THR:O	2:B:282:ILE:HB	2.04	0.58
2:B:38:LEU:C	2:B:40:GLY:N	2.62	0.57
1:A:39:PHE:HB2	6:B:856:U10:C35	2.34	0.57
1:A:164:TYR:HE1	1:A:256:PHE:O	1.87	0.57
2:B:287:SER:HG	2:B:294:TRP:NE1	2.02	0.57
1:A:101:ALA:O	1:A:104:GLU:HB2	2.04	0.57
1:A:193:LEU:HD21	1:A:212:GLU:HB3	1.85	0.57
1:A:239:SER:O	1:A:240:ALA:C	2.47	0.57
4:B:852:BCL:CBB	4:B:853:BCL:HMD1	2.34	0.57
1:A:185:LEU:O	1:A:185:LEU:HD23	2.04	0.57
1:A:187:LEU:H	2:B:216:PHE:HE2	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:TRP:CE2	2:B:122:MET:HE3	2.39	0.57
3:C:193:MET:CE	3:C:196:VAL:CG2	2.83	0.57
2:B:97:PRO:HG2	2:B:171:TRP:HB2	1.86	0.57
2:B:204:LEU:O	2:B:207:ALA:HB3	2.04	0.57
1:A:187:LEU:HD13	2:B:216:PHE:CG	2.39	0.57
1:A:179:PHE:HB3	1:A:240:ALA:HB2	1.86	0.57
2:B:270:ILE:CG2	2:B:271:TRP:N	2.68	0.57
3:C:29:TYR:CD1	3:C:56:PHE:CE1	2.93	0.57
1:A:87:GLN:O	1:A:91:ILE:HG12	2.05	0.57
1:A:179:PHE:O	1:A:181:PHE:N	2.37	0.57
1:A:193:LEU:HD22	6:A:857:U10:H4M2	1.86	0.57
1:A:272:TRP:CZ3	2:B:86:LEU:CB	2.88	0.57
3:C:112:ALA:O	3:C:113:SER:O	2.23	0.57
3:C:133:PRO:HB3	3:C:168:TRP:CD2	2.40	0.57
2:B:242:GLY:O	2:B:246:GLU:HG3	2.05	0.57
2:B:246:GLU:O	2:B:249:ALA:HB3	2.05	0.56
2:B:182:HIS:O	2:B:183:LEU:C	2.49	0.56
3:C:195:MET:HA	3:C:195:MET:HE2	1.87	0.56
1:A:170:ASN:HA	1:A:259:TRP:CD2	2.40	0.56
1:A:272:TRP:HB3	2:B:83:ALA:HB1	1.86	0.56
2:B:271:TRP:O	2:B:272:MET:C	2.47	0.56
1:A:255:TRP:HZ2	1:A:258:GLN:O	1.88	0.56
3:C:89:ARG:NH1	3:C:92:VAL:O	2.38	0.56
1:A:75:LEU:HD21	1:A:140:GLY:C	2.31	0.56
3:C:233:ILE:C	3:C:237:VAL:HG23	2.30	0.56
1:A:35:GLY:O	6:B:856:U10:C35	2.54	0.56
1:A:54:VAL:HG12	1:A:59:TRP:HZ2	1.70	0.56
2:B:3:TYR:CE2	2:B:5:ASN:OD1	2.58	0.56
1:A:30:TYR:CG	1:A:31:VAL:N	2.74	0.56
1:A:130:THR:HA	1:A:134:PHE:HB2	1.86	0.56
1:A:228:GLY:O	1:A:229:ILE:C	2.48	0.56
1:A:97:PHE:HB3	1:A:125:ILE:HD11	1.86	0.56
1:A:205:GLU:O	1:A:206:MET:C	2.49	0.56
1:A:97:PHE:CE1	4:A:851:BCL:H101	2.40	0.55
1:A:153:HIS:O	1:A:156:TRP:HB3	2.06	0.55
1:A:186:ALA:O	1:A:187:LEU:C	2.48	0.55
2:B:270:ILE:HD13	2:B:270:ILE:C	2.31	0.55
2:B:228:ARG:HH12	3:C:241:LEU:HD11	1.72	0.55
3:C:46:ASP:OD1	3:C:48:THR:HG23	2.06	0.55
3:C:193:MET:O	3:C:195:MET:N	2.40	0.55
3:C:226:THR:O	3:C:229:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:O	1:A:97:PHE:CD2	2.60	0.55
2:B:280:GLY:HA2	4:B:852:BCL:HED2	1.88	0.55
2:B:168:GLU:O	2:B:168:GLU:HG3	2.06	0.55
1:A:118:PRO:O	1:A:119:PHE:C	2.50	0.55
1:A:194:VAL:HG11	2:B:266:HIS:CG	2.42	0.55
1:A:244:SER:OG	4:A:851:BCL:HMA1	2.07	0.55
3:C:33:THR:O	3:C:35:ASN:N	2.40	0.55
1:A:223:SER:HA	6:A:857:U10:O2	2.06	0.55
5:A:855:BPH:CBB	2:B:210:TYR:HB3	2.37	0.55
2:B:68:PHE:O	2:B:71:GLY:N	2.40	0.55
3:C:229:GLU:O	3:C:233:ILE:HG13	2.07	0.55
1:A:6:GLU:OE2	1:A:10:ARG:NH2	2.40	0.54
4:A:850:BCL:HAA2	4:A:850:BCL:HBD	1.88	0.54
3:C:37:ARG:NH2	3:C:62:LYS:HD2	2.22	0.54
2:B:269:ALA:O	2:B:271:TRP:N	2.40	0.54
1:A:149:GLY:HA3	1:A:152:THR:OG1	2.08	0.54
2:B:282:ILE:O	2:B:285:LEU:N	2.41	0.54
1:A:12:PRO:HG3	3:C:97:PRO:HB3	1.88	0.54
3:C:86:ALA:HB1	3:C:101:THR:HG1	1.70	0.54
1:A:20:ASN:O	1:A:21:LEU:C	2.50	0.54
1:A:230:HIS:CD2	2:B:223:ILE:HG13	2.42	0.54
2:B:299:GLN:NE2	2:B:299:GLN:CA	2.61	0.54
1:A:192:ALA:HB1	2:B:146:THR:CA	2.37	0.54
3:C:193:MET:C	3:C:195:MET:H	2.15	0.54
1:A:20:ASN:HA	1:A:23:ASP:CB	2.38	0.54
2:B:37:THR:HG22	2:B:37:THR:O	2.07	0.54
2:B:171:TRP:HE3	2:B:171:TRP:HA	1.73	0.54
3:C:111:PRO:HG2	3:C:243:TYR:HE2	1.73	0.54
1:A:272:TRP:CZ3	2:B:86:LEU:HB3	2.43	0.54
1:A:27:GLY:C	1:A:29:PHE:H	2.16	0.53
5:A:855:BPH:HBB1	2:B:210:TYR:CG	2.43	0.53
2:B:130:TRP:HD1	2:B:150:PHE:CD2	2.26	0.53
3:C:146:LYS:HE3	3:C:151:LEU:HD11	1.90	0.53
3:C:226:THR:O	3:C:227:LEU:C	2.50	0.53
1:A:16:LEU:CD1	1:A:106:GLU:HG2	2.36	0.53
1:A:125:ILE:O	1:A:128:TYR:HB3	2.08	0.53
1:A:196:SER:HB2	2:B:143:GLY:O	2.07	0.53
1:A:267:VAL:HG23	2:B:87:ARG:CD	2.38	0.53
2:B:269:ALA:O	2:B:270:ILE:C	2.50	0.53
3:C:215:GLY:O	3:C:216:ILE:C	2.49	0.53
1:A:254:ILE:C	1:A:254:ILE:HD12	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:HA	1:A:259:TRP:CE3	2.43	0.53
1:A:235:LEU:O	1:A:236:LEU:C	2.49	0.53
1:A:80:LEU:HA	1:A:84:GLY:HA3	1.89	0.53
2:B:37:THR:O	2:B:41:TRP:NE1	2.41	0.53
3:C:17:ILE:O	3:C:21:TRP:CD1	2.62	0.53
1:A:170:ASN:ND2	1:A:259:TRP:CZ2	2.76	0.53
1:A:239:SER:C	1:A:241:VAL:N	2.65	0.53
2:B:171:TRP:HA	2:B:171:TRP:CE3	2.44	0.53
2:B:286:LEU:HD22	2:B:290:VAL:HB	1.89	0.53
1:A:35:GLY:O	6:B:856:U10:H353	2.08	0.53
3:C:111:PRO:HG2	3:C:243:TYR:CE2	2.44	0.53
1:A:179:PHE:C	1:A:181:PHE:N	2.66	0.53
2:B:229:PHE:CE1	3:C:238:ALA:HB2	2.44	0.53
2:B:253:ARG:HH11	2:B:259:ASN:HD21	1.57	0.53
1:A:60:ASN:HB3	1:A:63:LEU:HD12	1.91	0.53
4:A:851:BCL:HAA2	4:B:853:BCL:HBC1	1.91	0.52
2:B:192:VAL:HG12	2:B:192:VAL:O	2.09	0.52
1:A:54:VAL:HG23	1:A:55:LEU:N	2.24	0.52
1:A:141:ALA:HB3	1:A:144:TYR:CE2	2.45	0.52
4:A:850:BCL:H191	2:B:70:ILE:HG21	1.91	0.52
2:B:277:THR:HG21	5:B:854:BPH:HAC2	1.91	0.52
3:C:118:ARG:C	3:C:120:LEU:H	2.18	0.52
1:A:172:ALA:HB3	1:A:247:CYS:HB3	1.91	0.52
1:A:272:TRP:CZ3	2:B:86:LEU:HB2	2.44	0.52
3:C:178:PHE:HD1	3:C:191:LEU:O	1.92	0.52
2:B:4:GLN:O	2:B:6:ILE:N	2.43	0.52
3:C:193:MET:HE3	3:C:196:VAL:HG22	1.91	0.52
3:C:140:PHE:HD2	3:C:169:VAL:HG21	1.75	0.52
1:A:79:PRO:O	1:A:80:LEU:C	2.53	0.52
1:A:207:ARG:HG3	1:A:211:HIS:CG	2.45	0.52
1:A:272:TRP:O	1:A:275:ILE:HG12	2.09	0.52
3:C:234:CYS:O	3:C:237:VAL:HB	2.10	0.52
1:A:215:PHE:O	1:A:218:ASP:N	2.43	0.52
2:B:261:THR:HG23	3:C:35:ASN:HA	1.92	0.52
2:B:265:ILE:HG22	2:B:266:HIS:ND1	2.25	0.52
3:C:23:PHE:C	3:C:23:PHE:CD2	2.88	0.52
1:A:116:HIS:CD2	2:B:224:LEU:CB	2.89	0.51
1:A:243:PHE:O	1:A:244:SER:C	2.50	0.51
1:A:211:HIS:O	1:A:212:GLU:C	2.53	0.51
2:B:72:ILE:O	2:B:75:TRP:HB2	2.10	0.51
2:B:155:TRP:HA	2:B:155:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:TRP:HA	2:B:155:TRP:HE3	1.75	0.51
3:C:17:ILE:O	3:C:21:TRP:HD1	1.94	0.51
2:B:228:ARG:NH1	3:C:241:LEU:HD11	2.26	0.51
1:A:144:TYR:O	1:A:156:TRP:HZ2	1.93	0.51
1:A:179:PHE:C	1:A:181:PHE:H	2.18	0.51
1:A:187:LEU:N	2:B:216:PHE:CE2	2.78	0.51
4:A:850:BCL:HMC2	2:B:160:HIS:CD2	2.46	0.51
2:B:183:LEU:O	2:B:186:THR:HB	2.09	0.51
2:B:203:GLY:O	2:B:206:ILE:HB	2.10	0.51
2:B:208:PHE:CE2	2:B:275:LEU:HB3	2.46	0.51
1:A:267:VAL:HG23	2:B:87:ARG:CG	2.41	0.51
2:B:3:TYR:CE1	2:B:9:GLN:CG	2.93	0.51
2:B:164:TYR:OH	2:B:288:ASP:CB	2.58	0.51
3:C:18:TYR:O	3:C:21:TRP:HB2	2.11	0.51
3:C:181:VAL:O	3:C:188:THR:HA	2.11	0.51
1:A:54:VAL:HG12	1:A:59:TRP:CZ2	2.46	0.51
2:B:106:ALA:O	2:B:107:ALA:C	2.53	0.51
2:B:255:THR:HG22	2:B:256:MET:N	2.26	0.51
3:C:189:ARG:HG2	3:C:189:ARG:HH11	1.76	0.51
1:A:172:ALA:CB	1:A:247:CYS:HB3	2.40	0.51
3:C:156:CYS:HB3	3:C:206:ASN:O	2.11	0.51
1:A:15:THR:HG21	1:A:19:GLY:O	2.11	0.51
1:A:36:VAL:O	1:A:39:PHE:HB3	2.11	0.51
2:B:74:PHE:CZ	2:B:92:PHE:HB2	2.45	0.51
2:B:175:VAL:CG1	2:B:176:PRO:HD2	2.40	0.51
1:A:2:LEU:HB3	1:A:6:GLU:HB3	1.93	0.51
1:A:25:TRP:HZ2	2:B:254:TRP:CZ3	2.28	0.51
1:A:36:VAL:O	1:A:39:PHE:N	2.39	0.51
1:A:49:ILE:CD1	1:A:89:ILE:HD13	2.40	0.51
2:B:57:VAL:O	2:B:58:LEU:C	2.54	0.51
3:C:29:TYR:HD1	3:C:56:PHE:CE1	2.20	0.51
2:B:24:VAL:HG22	2:B:139:ALA:HB1	1.92	0.50
2:B:239:ALA:HA	3:C:73:LEU:CD2	2.41	0.50
2:B:299:GLN:HE21	2:B:299:GLN:CA	2.08	0.50
3:C:33:THR:O	3:C:34:GLU:C	2.55	0.50
1:A:52:SER:OG	1:A:66:VAL:HG22	2.11	0.50
1:A:126:LEU:O	1:A:127:ALA:C	2.54	0.50
1:A:123:PHE:CG	1:A:238:LEU:HD22	2.46	0.50
1:A:212:GLU:O	1:A:213:ASP:C	2.55	0.50
2:B:260:ALA:CB	2:B:265:ILE:HD13	2.41	0.50
2:B:287:SER:HG	2:B:294:TRP:HE1	1.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:SER:O	3:C:15:LEU:C	2.54	0.50
3:C:115:VAL:CG1	3:C:116:ALA:H	2.24	0.50
3:C:233:ILE:O	3:C:234:CYS:C	2.53	0.50
1:A:186:ALA:CB	2:B:216:PHE:HE2	2.25	0.50
2:B:280:GLY:O	2:B:281:GLY:C	2.53	0.50
5:A:855:BPH:HAA2	5:A:855:BPH:HBD	1.94	0.50
1:A:214:THR:O	1:A:215:PHE:O	2.29	0.50
1:A:244:SER:HB3	4:A:851:BCL:O1D	2.12	0.50
2:B:250:LEU:HD22	2:B:254:TRP:NE1	2.26	0.50
1:A:18:GLY:O	1:A:21:LEU:HB2	2.11	0.50
2:B:116:LEU:O	2:B:117:ILE:C	2.55	0.50
1:A:206:MET:CE	2:B:235:LEU:HD22	2.42	0.49
2:B:16:ALA:O	2:B:18:LEU:HD22	2.12	0.49
1:A:187:LEU:N	2:B:216:PHE:HE2	2.09	0.49
2:B:66:TRP:CZ2	2:B:122:MET:HE3	2.47	0.49
2:B:235:LEU:O	2:B:238:ILE:HB	2.12	0.49
2:B:264:GLY:C	2:B:266:HIS:N	2.69	0.49
1:A:175:ILE:HG22	1:A:176:ALA:N	2.27	0.49
1:A:186:ALA:C	1:A:188:ALA:N	2.70	0.49
2:B:117:ILE:O	2:B:120:PHE:HB3	2.13	0.49
2:B:185:TRP:CE3	2:B:185:TRP:C	2.90	0.49
2:B:264:GLY:O	2:B:265:ILE:C	2.55	0.49
3:C:83:ARG:CB	3:C:84:PRO:HD2	2.38	0.49
1:A:102:LEU:O	1:A:105:VAL:HB	2.12	0.49
2:B:108:PRO:O	2:B:109:LEU:C	2.55	0.49
2:B:240:ASP:O	2:B:241:ARG:C	2.55	0.49
1:A:2:LEU:HA	1:A:6:GLU:OE1	2.13	0.49
1:A:79:PRO:O	1:A:80:LEU:O	2.29	0.49
1:A:89:ILE:HG22	1:A:148:TYR:HE2	1.77	0.49
2:B:4:GLN:O	2:B:6:ILE:HD13	2.11	0.49
2:B:270:ILE:C	2:B:270:ILE:CD1	2.86	0.49
2:B:273:ALA:C	2:B:275:LEU:N	2.70	0.49
1:A:30:TYR:CD1	1:A:31:VAL:N	2.78	0.49
1:A:96:ALA:HB1	5:A:855:BPH:C4	2.39	0.49
2:B:20:MET:HE1	3:C:125:GLY:HA3	1.93	0.49
2:B:94:LEU:HD11	2:B:114:LEU:HB3	1.94	0.49
2:B:122:MET:HE2	4:B:852:BCL:H142	1.94	0.49
3:C:70:ARG:CZ	3:C:120:LEU:HD13	2.43	0.49
1:A:206:MET:HE2	2:B:235:LEU:HD22	1.94	0.49
1:A:208:THR:HG23	1:A:211:HIS:CE1	2.47	0.49
2:B:3:TYR:HD2	3:C:194:GLN:HA	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:PRO:HG3	2:B:172:SER:OG	2.12	0.49
2:B:152:SER:HB2	2:B:274:VAL:HG13	1.95	0.49
2:B:152:SER:O	2:B:155:TRP:HB3	2.12	0.49
2:B:258:PHE:O	2:B:259:ASN:HB3	2.11	0.49
2:B:280:GLY:C	2:B:282:ILE:H	2.21	0.49
3:C:18:TYR:O	3:C:20:PHE:N	2.46	0.49
1:A:186:ALA:HB3	2:B:216:PHE:HE2	1.77	0.49
2:B:4:GLN:O	2:B:5:ASN:C	2.55	0.49
1:A:26:VAL:C	1:A:27:GLY:O	2.52	0.49
1:A:105:VAL:O	1:A:106:GLU:C	2.55	0.49
2:B:38:LEU:O	2:B:39:LEU:C	2.54	0.49
2:B:38:LEU:C	2:B:40:GLY:H	2.20	0.49
2:B:140:LEU:HB3	2:B:142:MET:HG3	1.94	0.49
2:B:192:VAL:O	2:B:192:VAL:CG1	2.61	0.49
2:B:239:ALA:HA	3:C:73:LEU:HD22	1.94	0.49
2:B:300:ASN:C	2:B:301:HIS:ND1	2.71	0.49
1:A:230:HIS:CE1	2:B:234:GLU:CD	2.91	0.49
1:A:243:PHE:O	1:A:246:LEU:HB3	2.12	0.49
2:B:151:LEU:HD12	2:B:151:LEU:HA	1.62	0.49
2:B:201:PHE:HB2	2:B:283:GLY:HA2	1.95	0.49
2:B:229:PHE:HE1	3:C:238:ALA:HB2	1.76	0.49
1:A:85:LEU:O	1:A:86:TRP:C	2.54	0.48
1:A:208:THR:C	1:A:210:ASP:N	2.64	0.48
2:B:168:GLU:CG	2:B:173:GLU:HG3	2.42	0.48
2:B:222:THR:O	2:B:224:LEU:N	2.46	0.48
3:C:183:LEU:HD11	3:C:189:ARG:HG3	1.95	0.48
1:A:179:PHE:CB	1:A:240:ALA:HB2	2.43	0.48
1:A:237:SER:O	1:A:238:LEU:C	2.55	0.48
2:B:58:LEU:O	2:B:61:PHE:N	2.46	0.48
2:B:189:PHE:O	2:B:189:PHE:CD1	2.66	0.48
2:B:208:PHE:O	2:B:209:LEU:C	2.53	0.48
3:C:40:TYR:HB3	3:C:58:LEU:HD21	1.94	0.48
3:C:189:ARG:HG2	3:C:189:ARG:NH1	2.28	0.48
1:A:187:LEU:HB2	2:B:216:PHE:HD2	1.78	0.48
1:A:217:ARG:HH21	2:B:44:ASN:ND2	2.09	0.48
1:A:249:ILE:O	1:A:249:ILE:CD1	2.62	0.48
2:B:17:ASP:C	2:B:19:GLY:H	2.22	0.48
2:B:273:ALA:O	2:B:274:VAL:C	2.52	0.48
2:B:282:ILE:O	2:B:283:GLY:C	2.56	0.48
1:A:169:TYR:O	1:A:170:ASN:C	2.52	0.48
1:A:178:SER:O	1:A:181:PHE:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TRP:C	2:B:273:ALA:H	2.20	0.48
3:C:193:MET:HE3	3:C:196:VAL:HG21	1.94	0.48
1:A:53:ALA:CB	1:A:64:ILE:HD12	2.43	0.48
2:B:228:ARG:O	2:B:229:PHE:CD1	2.67	0.48
3:C:238:ALA:O	3:C:239:GLY:C	2.57	0.48
1:A:100:TRP:CZ3	6:B:856:U10:H321	2.42	0.48
1:A:146:PHE:HA	1:A:156:TRP:NE1	2.29	0.48
1:A:181:PHE:CD2	5:B:854:BPH:HBB1	2.49	0.48
1:A:30:TYR:HB2	2:B:254:TRP:HB3	1.96	0.48
1:A:114:GLY:HA3	2:B:225:ALA:CB	2.44	0.48
2:B:148:TRP:HA	2:B:148:TRP:CE3	2.49	0.48
2:B:263:GLU:O	2:B:266:HIS:HB2	2.12	0.48
3:C:81:GLU:OE2	3:C:81:GLU:HA	2.12	0.48
3:C:83:ARG:HB2	3:C:84:PRO:CD	2.41	0.48
1:A:173:HIS:O	1:A:173:HIS:CG	2.66	0.48
1:A:217:ARG:NH2	2:B:44:ASN:HD22	2.10	0.48
2:B:199:ASN:HB2	2:B:294:TRP:CD2	2.49	0.48
1:A:25:TRP:O	1:A:26:VAL:HG23	2.14	0.48
1:A:219:LEU:HD11	2:B:133:THR:HG22	1.96	0.48
1:A:229:ILE:HD11	6:A:857:U10:O4	2.14	0.48
3:C:82:ASP:O	3:C:83:ARG:HB3	2.14	0.48
1:A:89:ILE:HG22	1:A:148:TYR:CE2	2.49	0.47
2:B:164:TYR:OH	2:B:288:ASP:HB3	2.13	0.47
2:B:235:LEU:HA	2:B:235:LEU:HD23	1.67	0.47
1:A:28:PRO:CB	2:B:253:ARG:HE	2.26	0.47
1:A:228:GLY:O	1:A:231:ARG:HB2	2.14	0.47
3:C:83:ARG:NH2	3:C:107:ASP:O	2.47	0.47
3:C:134:MET:C	3:C:136:ALA:N	2.71	0.47
3:C:170:ASP:C	3:C:172:PRO:HD2	2.39	0.47
1:A:16:LEU:C	1:A:17:VAL:CG2	2.87	0.47
1:A:173:HIS:HB2	1:A:247:CYS:SG	2.54	0.47
2:B:123:PHE:HA	2:B:157:TRP:CH2	2.46	0.47
2:B:260:ALA:O	6:B:856:U10:H4M3	2.14	0.47
3:C:20:PHE:O	3:C:21:TRP:C	2.57	0.47
3:C:111:PRO:CG	3:C:243:TYR:CE2	2.97	0.47
3:C:177:ARG:HH11	3:C:177:ARG:HG2	1.79	0.47
2:B:20:MET:HE1	3:C:125:GLY:C	2.39	0.47
2:B:73:TRP:O	2:B:77:GLN:HG3	2.15	0.47
2:B:134:TYR:O	2:B:137:ALA:N	2.48	0.47
3:C:134:MET:C	3:C:136:ALA:H	2.22	0.47
3:C:148:PRO:HA	3:C:151:LEU:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:THR:O	3:C:229:GLU:HB2	2.14	0.47
1:A:26:VAL:O	1:A:29:PHE:HB2	2.14	0.47
1:A:28:PRO:O	2:B:253:ARG:O	2.33	0.47
1:A:54:VAL:CG2	1:A:55:LEU:N	2.78	0.47
1:A:68:PRO:HB2	1:A:143:GLY:HA2	1.97	0.47
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.74	0.47
1:A:210:ASP:HB3	2:B:20:MET:SD	2.55	0.47
1:A:215:PHE:O	1:A:216:PHE:C	2.56	0.47
2:B:205:SER:OG	4:B:852:BCL:HMA1	2.15	0.47
2:B:215:LEU:O	2:B:218:MET:HB2	2.15	0.47
2:B:218:MET:HE3	2:B:252:TRP:CH2	2.50	0.47
2:B:241:ARG:O	3:C:117:ARG:HG2	2.14	0.47
4:B:852:BCL:HBB3	4:B:853:BCL:HMD1	1.97	0.47
1:A:187:LEU:HD13	2:B:216:PHE:CB	2.45	0.47
1:A:207:ARG:HG3	1:A:211:HIS:CD2	2.48	0.47
2:B:30:SER:OG	2:B:50:ILE:HG22	2.13	0.47
3:C:240:GLY:O	3:C:244:ALA:HB3	2.14	0.47
1:A:52:SER:HB2	1:A:85:LEU:HD12	1.97	0.47
1:A:141:ALA:O	1:A:142:TRP:C	2.57	0.47
1:A:185:LEU:HG	5:B:854:BPH:NC	2.30	0.47
5:A:855:BPH:HBB1	2:B:210:TYR:CD2	2.50	0.47
2:B:261:THR:CG2	3:C:35:ASN:HA	2.45	0.47
2:B:271:TRP:O	2:B:274:VAL:N	2.47	0.47
2:B:240:ASP:O	3:C:117:ARG:NE	2.46	0.46
3:C:66:LEU:HD13	3:C:118:ARG:HH12	1.79	0.46
1:A:131:HIS:HB3	1:A:146:PHE:HE2	1.79	0.46
2:B:143:GLY:C	2:B:145:HIS:N	2.72	0.46
2:B:150:PHE:O	2:B:151:LEU:C	2.57	0.46
3:C:153:VAL:HG21	3:C:181:VAL:CG1	2.45	0.46
1:A:190:HIS:CE1	1:A:230:HIS:CE1	3.03	0.46
2:B:293:ASN:OD1	2:B:295:TYR:N	2.45	0.46
3:C:171:ILE:N	3:C:171:ILE:HD13	2.30	0.46
3:C:185:ASP:OD1	3:C:187:SER:OG	2.32	0.46
1:A:244:SER:C	1:A:246:LEU:N	2.73	0.46
2:B:64:LEU:O	2:B:68:PHE:N	2.40	0.46
2:B:134:TYR:O	2:B:135:LEU:C	2.59	0.46
3:C:170:ASP:OD1	3:C:172:PRO:CG	2.63	0.46
3:C:96:PHE:HB3	3:C:97:PRO:HD2	1.96	0.46
2:B:19:GLY:C	2:B:20:MET:O	2.56	0.46
2:B:24:VAL:CG2	2:B:139:ALA:HB1	2.45	0.46
2:B:97:PRO:HG2	2:B:171:TRP:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH2	2:B:44:ASN:ND2	2.63	0.46
1:A:217:ARG:O	1:A:221:GLY:HA2	2.16	0.46
1:A:274:ASN:O	1:A:275:ILE:C	2.58	0.46
3:C:44:ASN:ND2	3:C:49:PRO:O	2.48	0.46
3:C:147:ASN:OD1	3:C:149:ILE:HG13	2.15	0.46
2:B:256:MET:O	2:B:256:MET:HG3	2.15	0.46
3:C:61:PRO:HG3	3:C:76:PRO:CG	2.44	0.46
3:C:193:MET:CE	3:C:196:VAL:HG21	2.44	0.46
1:A:31:VAL:HG12	1:A:32:GLY:N	2.31	0.46
1:A:50:ALA:O	1:A:54:VAL:HG13	2.16	0.46
1:A:279:ILE:HG22	1:A:279:ILE:O	2.15	0.46
2:B:64:LEU:O	2:B:67:PHE:N	2.49	0.46
2:B:285:LEU:O	2:B:285:LEU:HG	2.16	0.46
3:C:24:LEU:O	3:C:28:ILE:HG12	2.15	0.46
3:C:100:PRO:O	3:C:101:THR:C	2.59	0.46
1:A:151:TRP:O	1:A:154:LEU:HB2	2.16	0.45
2:B:59:SER:OG	2:B:129:TRP:HB2	2.16	0.45
2:B:182:HIS:O	2:B:185:TRP:HB3	2.16	0.45
1:A:125:ILE:O	1:A:126:LEU:C	2.58	0.45
2:B:199:ASN:O	2:B:202:HIS:HB3	2.16	0.45
2:B:215:LEU:HD23	2:B:269:ALA:HA	1.98	0.45
3:C:37:ARG:HH11	3:C:37:ARG:HG2	1.81	0.45
1:A:183:ASN:O	1:A:186:ALA:CB	2.60	0.45
1:A:230:HIS:HE1	2:B:234:GLU:OE1	1.99	0.45
2:B:253:ARG:HA	2:B:258:PHE:O	2.16	0.45
3:C:146:LYS:HG2	3:C:199:GLN:O	2.17	0.45
1:A:148:TYR:CD2	5:A:855:BPH:H143	2.51	0.45
2:B:206:ILE:CG2	2:B:210:TYR:CE2	2.99	0.45
2:B:218:MET:O	2:B:219:HIS:C	2.58	0.45
1:A:28:PRO:CB	2:B:253:ARG:NE	2.79	0.45
1:A:213:ASP:O	1:A:214:THR:C	2.57	0.45
5:A:855:BPH:CMC	2:B:213:ALA:HB3	2.47	0.45
2:B:81:ASN:HB3	2:B:84:VAL:CG2	2.45	0.45
2:B:206:ILE:HG21	4:B:853:BCL:CAD	2.46	0.45
1:A:114:GLY:CA	2:B:225:ALA:CB	2.94	0.45
1:A:146:PHE:HB2	1:A:147:PRO:CD	2.47	0.45
3:C:134:MET:HB2	3:C:167:ILE:O	2.17	0.45
1:A:54:VAL:CG1	1:A:59:TRP:HZ2	2.29	0.45
1:A:174:MET:HE1	2:B:180:PHE:HE1	1.82	0.45
1:A:205:GLU:C	1:A:206:MET:O	2.58	0.45
1:A:267:VAL:HG23	2:B:87:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ALA:HB2	2:B:92:PHE:CZ	2.52	0.45
2:B:290:VAL:HG12	2:B:290:VAL:O	2.16	0.45
3:C:37:ARG:CZ	3:C:62:LYS:CD	2.93	0.45
3:C:37:ARG:HB3	3:C:75:VAL:HB	1.99	0.45
1:A:166:ASN:HB3	1:A:169:TYR:CD2	2.52	0.45
1:A:208:THR:C	1:A:210:ASP:H	2.25	0.45
2:B:144:LYS:O	2:B:145:HIS:C	2.58	0.45
2:B:190:SER:O	2:B:194:GLY:O	2.35	0.45
2:B:247:ARG:O	2:B:248:ALA:C	2.56	0.45
2:B:290:VAL:C	2:B:291:VAL:HG23	2.42	0.45
3:C:48:THR:O	3:C:49:PRO:C	2.60	0.45
3:C:65:ILE:HD12	3:C:65:ILE:N	2.29	0.45
1:A:187:LEU:HG	2:B:269:ALA:HB1	1.98	0.45
1:A:214:THR:O	1:A:215:PHE:C	2.60	0.45
1:A:233:GLY:O	1:A:234:LEU:C	2.58	0.45
2:B:3:TYR:CE1	2:B:9:GLN:HG3	2.51	0.45
1:A:178:SER:HA	4:A:850:BCL:O1A	2.16	0.45
1:A:267:VAL:HA	2:B:87:ARG:HG3	1.98	0.45
2:B:163:ILE:O	2:B:164:TYR:C	2.60	0.45
3:C:122:GLU:OE2	3:C:130:LYS:HE2	2.17	0.45
2:B:209:LEU:O	2:B:210:TYR:C	2.59	0.44
4:B:853:BCL:HAA2	4:B:853:BCL:HBD	1.99	0.44
3:C:37:ARG:NH1	3:C:37:ARG:HG2	2.32	0.44
1:A:43:ALA:O	1:A:44:LEU:C	2.59	0.44
1:A:279:ILE:O	1:A:279:ILE:CG2	2.65	0.44
2:B:215:LEU:O	2:B:218:MET:N	2.46	0.44
3:C:29:TYR:HB3	3:C:30:TYR:H	1.62	0.44
1:A:100:TRP:CZ2	6:B:856:U10:H253	2.52	0.44
1:A:123:PHE:CD2	1:A:238:LEU:HD22	2.52	0.44
1:A:199:ASN:O	1:A:200:PRO:O	2.36	0.44
1:A:183:ASN:HB2	1:A:236:LEU:HB3	2.00	0.44
2:B:115:TRP:CZ3	2:B:116:LEU:HD23	2.52	0.44
2:B:222:THR:O	2:B:225:ALA:N	2.48	0.44
3:C:36:MET:C	3:C:38:GLU:H	2.25	0.44
1:A:162:TYR:HA	1:A:165:GLY:O	2.18	0.44
1:A:175:ILE:CG2	1:A:243:PHE:CD2	3.00	0.44
2:B:135:LEU:N	2:B:135:LEU:HD23	2.32	0.44
3:C:120:LEU:O	3:C:227:LEU:N	2.43	0.44
1:A:170:ASN:C	1:A:170:ASN:OD1	2.59	0.44
2:B:97:PRO:HD2	2:B:171:TRP:HB3	1.99	0.44
3:C:89:ARG:HG3	3:C:98:HIS:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLY:O	6:B:856:U10:H351	2.18	0.44
1:A:49:ILE:HD13	1:A:89:ILE:HD13	2.00	0.44
3:C:99:ALA:HA	3:C:100:PRO:HD3	1.78	0.44
3:C:238:ALA:C	3:C:240:GLY:N	2.74	0.44
1:A:216:PHE:O	1:A:220:VAL:N	2.44	0.44
2:B:153:ALA:C	2:B:155:TRP:H	2.26	0.44
1:A:127:ALA:HB1	4:A:851:BCL:H12	1.99	0.44
2:B:21:THR:O	2:B:22:GLU:C	2.61	0.44
3:C:133:PRO:HA	3:C:168:TRP:HA	2.00	0.44
3:C:193:MET:HE3	3:C:193:MET:CA	2.45	0.44
1:A:94:THR:HG22	1:A:95:GLY:N	2.32	0.43
1:A:122:ALA:O	1:A:125:ILE:HB	2.18	0.43
1:A:148:TYR:HA	5:A:855:BPH:H193	2.00	0.43
1:A:156:TRP:CE3	1:A:156:TRP:C	2.96	0.43
1:A:222:TYR:CG	1:A:223:SER:N	2.85	0.43
2:B:264:GLY:O	2:B:267:ARG:N	2.37	0.43
1:A:16:LEU:O	1:A:17:VAL:HG22	2.18	0.43
1:A:256:PHE:CD1	1:A:256:PHE:N	2.87	0.43
3:C:235:GLY:O	3:C:236:TYR:C	2.61	0.43
2:B:25:ASN:OD1	2:B:27:ALA:HB3	2.19	0.43
1:A:34:PHE:CZ	1:A:102:LEU:HD13	2.53	0.43
2:B:268:TRP:CE3	3:C:31:LEU:HD13	2.53	0.43
3:C:87:LEU:HA	3:C:99:ALA:O	2.19	0.43
1:A:16:LEU:C	1:A:17:VAL:HG23	2.44	0.43
2:B:200:PRO:HD2	2:B:294:TRP:CZ3	2.53	0.43
2:B:227:SER:HB2	2:B:232:GLU:OE1	2.18	0.43
2:B:97:PRO:CA	2:B:112:GLY:HA3	2.49	0.43
2:B:127:TRP:O	2:B:128:SER:C	2.61	0.43
2:B:205:SER:O	2:B:206:ILE:C	2.61	0.43
2:B:228:ARG:O	3:C:234:CYS:HB3	2.18	0.43
2:B:296:VAL:O	2:B:299:GLN:N	2.41	0.43
3:C:33:THR:C	3:C:35:ASN:N	2.77	0.43
3:C:183:LEU:HD11	3:C:189:ARG:CG	2.48	0.43
1:A:48:LEU:C	1:A:89:ILE:HD11	2.43	0.43
1:A:63:LEU:O	1:A:64:ILE:C	2.60	0.43
1:A:193:LEU:HB3	1:A:194:VAL:H	1.69	0.43
2:B:3:TYR:HE2	3:C:194:GLN:HA	1.80	0.43
2:B:4:GLN:O	2:B:6:ILE:CD1	2.66	0.43
2:B:176:PRO:HD3	2:B:185:TRP:CD1	2.53	0.43
2:B:199:ASN:HB2	2:B:294:TRP:CG	2.54	0.43
1:A:249:ILE:O	1:A:249:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:HA	1:A:268:LYS:HD3	1.82	0.43
2:B:59:SER:HB2	2:B:128:SER:OG	2.18	0.43
3:C:134:MET:O	3:C:137:ALA:N	2.38	0.43
1:A:183:ASN:HA	1:A:236:LEU:CD1	2.45	0.43
1:A:244:SER:O	1:A:246:LEU:N	2.52	0.43
2:B:159:VAL:HG13	2:B:285:LEU:HD12	2.01	0.43
1:A:28:PRO:HB3	2:B:253:ARG:NE	2.28	0.43
1:A:48:LEU:O	1:A:89:ILE:HD11	2.18	0.43
1:A:117:ILE:O	1:A:118:PRO:C	2.60	0.43
1:A:183:ASN:O	1:A:186:ALA:N	2.52	0.43
2:B:32:VAL:HG12	2:B:33:GLY:N	2.33	0.43
2:B:240:ASP:O	2:B:241:ARG:O	2.36	0.43
1:A:169:TYR:CD2	1:A:260:VAL:HB	2.53	0.42
2:B:81:ASN:O	2:B:84:VAL:HB	2.19	0.42
1:A:208:THR:HB	1:A:209:PRO:HD2	2.01	0.42
2:B:273:ALA:O	2:B:275:LEU:N	2.53	0.42
3:C:119:ASP:C	3:C:226:THR:HB	2.45	0.42
3:C:129:ASN:ND2	3:C:224:GLU:HB3	2.35	0.42
3:C:157:ASP:O	3:C:158:LEU:HB2	2.18	0.42
1:A:181:PHE:CE1	4:B:852:BCL:O1A	2.71	0.42
1:A:272:TRP:HZ3	2:B:86:LEU:CB	2.33	0.42
2:B:123:PHE:O	2:B:126:VAL:N	2.43	0.42
2:B:286:LEU:HD23	2:B:286:LEU:HA	1.79	0.42
2:B:296:VAL:HG12	2:B:297:TRP:N	2.33	0.42
1:A:25:TRP:C	1:A:26:VAL:HG23	2.45	0.42
1:A:107:ILE:HG21	2:B:251:PHE:CD2	2.54	0.42
1:A:259:TRP:C	1:A:261:ASP:N	2.77	0.42
2:B:204:LEU:O	2:B:205:SER:C	2.62	0.42
6:B:856:U10:H122	6:B:856:U10:H101	1.90	0.42
3:C:85:ILE:O	3:C:87:LEU:N	2.48	0.42
1:A:264:GLN:O	1:A:266:TRP:N	2.52	0.42
2:B:189:PHE:CD1	2:B:189:PHE:C	2.98	0.42
2:B:208:PHE:CE2	2:B:279:THR:HG21	2.54	0.42
3:C:25:ALA:O	3:C:28:ILE:HB	2.20	0.42
1:A:166:ASN:HB3	1:A:169:TYR:HD2	1.85	0.42
3:C:48:THR:O	3:C:49:PRO:O	2.37	0.42
3:C:168:TRP:NE1	3:C:190:LEU:HD21	2.33	0.42
1:A:262:TRP:HE3	1:A:263:TRP:CD1	2.38	0.42
2:B:58:LEU:O	2:B:59:SER:C	2.62	0.42
2:B:132:ARG:C	2:B:134:TYR:N	2.78	0.42
3:C:245:ALA:N	3:C:246:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:CZ	1:A:132:VAL:HG21	2.55	0.42
2:B:282:ILE:HG22	2:B:283:GLY:N	2.35	0.42
3:C:112:ALA:HB2	3:C:239:GLY:HA3	2.00	0.42
1:A:215:PHE:HB3	1:A:216:PHE:H	1.59	0.42
2:B:253:ARG:O	2:B:253:ARG:HG2	2.19	0.42
1:A:61:PRO:HA	1:A:64:ILE:HG12	2.02	0.42
1:A:193:LEU:O	1:A:195:LEU:N	2.52	0.42
1:A:216:PHE:O	1:A:217:ARG:C	2.62	0.42
2:B:81:ASN:HA	2:B:82:PRO:HD3	1.77	0.42
2:B:293:ASN:OD1	2:B:294:TRP:N	2.53	0.42
2:B:140:LEU:C	2:B:142:MET:N	2.77	0.41
1:A:194:VAL:HG21	2:B:266:HIS:NE2	2.35	0.41
2:B:51:TYR:CE2	2:B:136:ARG:CZ	3.03	0.41
2:B:200:PRO:C	2:B:202:HIS:N	2.76	0.41
2:B:222:THR:C	2:B:224:LEU:N	2.75	0.41
1:A:116:HIS:NE2	2:B:224:LEU:HB3	2.35	0.41
1:A:217:ARG:HA	1:A:222:TYR:N	2.35	0.41
2:B:239:ALA:O	3:C:73:LEU:HD22	2.20	0.41
1:A:35:GLY:CA	1:A:103:ARG:HD2	2.45	0.41
1:A:221:GLY:HA3	2:B:50:ILE:HG12	2.02	0.41
2:B:38:LEU:HD12	2:B:38:LEU:HA	1.80	0.41
2:B:66:TRP:HD1	2:B:118:ALA:O	2.03	0.41
1:A:59:TRP:HA	1:A:64:ILE:HD11	2.02	0.41
1:A:144:TYR:O	1:A:156:TRP:CZ2	2.73	0.41
1:A:192:ALA:HB1	2:B:146:THR:N	2.36	0.41
2:B:199:ASN:HA	2:B:200:PRO:HD2	1.90	0.41
2:B:264:GLY:O	2:B:266:HIS:N	2.54	0.41
3:C:32:GLN:OE1	3:C:32:GLN:HA	2.20	0.41
1:A:264:GLN:O	1:A:265:TRP:C	2.63	0.41
1:A:272:TRP:O	1:A:273:ALA:C	2.63	0.41
3:C:36:MET:C	3:C:38:GLU:N	2.79	0.41
3:C:82:ASP:O	3:C:83:ARG:CB	2.69	0.41
3:C:171:ILE:N	3:C:172:PRO:HD2	2.35	0.41
2:B:9:GLN:NE2	3:C:193:MET:HE2	2.35	0.41
2:B:148:TRP:HA	2:B:148:TRP:HE3	1.84	0.41
2:B:260:ALA:C	6:B:856:U10:C4M	2.92	0.41
2:B:280:GLY:O	2:B:283:GLY:N	2.53	0.41
3:C:18:TYR:C	3:C:20:PHE:N	2.79	0.41
1:A:107:ILE:CG2	2:B:251:PHE:CD2	3.04	0.41
1:A:170:ASN:HB2	1:A:259:TRP:CE2	2.56	0.41
1:A:229:ILE:CD1	6:A:857:U10:O4	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:THR:O	2:B:37:THR:CG2	2.67	0.41
2:B:84:VAL:O	2:B:87:ARG:N	2.51	0.41
2:B:119:SER:O	2:B:120:PHE:C	2.64	0.41
1:A:2:LEU:O	3:C:42:LEU:HA	2.21	0.41
1:A:43:ALA:C	1:A:45:GLY:N	2.77	0.41
1:A:85:LEU:C	1:A:87:GLN:N	2.79	0.41
1:A:97:PHE:CZ	4:A:851:BCL:H91	2.55	0.41
1:A:185:LEU:O	1:A:185:LEU:CD2	2.69	0.41
1:A:216:PHE:HB3	1:A:222:TYR:O	2.20	0.41
2:B:70:ILE:HD11	2:B:177:TYR:CD2	2.56	0.41
2:B:136:ARG:HA	2:B:136:ARG:NE	2.32	0.41
2:B:155:TRP:O	2:B:158:MET:N	2.54	0.41
2:B:247:ARG:CZ	3:C:111:PRO:O	2.68	0.41
2:B:248:ALA:HB1	6:B:856:U10:O3	2.20	0.41
2:B:250:LEU:HD22	2:B:254:TRP:HE1	1.84	0.41
3:C:33:THR:O	3:C:36:MET:N	2.54	0.41
3:C:103:ASP:HA	3:C:104:PRO:HD2	1.66	0.41
3:C:120:LEU:N	3:C:226:THR:HB	2.35	0.41
1:A:37:ALA:C	1:A:39:PHE:N	2.78	0.41
2:B:4:GLN:C	2:B:6:ILE:N	2.77	0.41
2:B:218:MET:HE3	2:B:252:TRP:CZ3	2.55	0.41
1:A:27:GLY:C	1:A:29:PHE:N	2.79	0.40
1:A:96:ALA:CB	5:A:855:BPH:H4C2	2.48	0.40
1:A:227:LEU:O	1:A:227:LEU:HD12	2.21	0.40
2:B:14:GLY:HA3	3:C:140:PHE:CD1	2.55	0.40
2:B:135:LEU:O	2:B:138:GLN:N	2.54	0.40
2:B:260:ALA:O	6:B:856:U10:C4M	2.70	0.40
3:C:112:ALA:C	3:C:113:SER:O	2.64	0.40
3:C:191:LEU:HD23	3:C:192:PRO:HD3	2.03	0.40
1:A:16:LEU:HD12	1:A:106:GLU:HG3	2.00	0.40
1:A:259:TRP:O	1:A:261:ASP:N	2.54	0.40
2:B:206:ILE:CG2	2:B:210:TYR:CD2	3.05	0.40
1:A:246:LEU:C	1:A:248:MET:H	2.30	0.40
1:A:248:MET:HG3	4:A:851:BCL:OBD	2.22	0.40
2:B:60:LEU:HD12	2:B:60:LEU:HA	1.89	0.40
2:B:140:LEU:CB	2:B:142:MET:HG3	2.51	0.40
2:B:239:ALA:HB1	3:C:66:LEU:HD21	2.03	0.40
2:B:297:TRP:O	2:B:297:TRP:CE3	2.74	0.40
3:C:104:PRO:HA	3:C:109:VAL:HG22	2.03	0.40
3:C:173:GLU:O	3:C:174:GLN:O	2.39	0.40
1:A:86:TRP:C	1:A:86:TRP:CE3	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:O	1:A:133:LEU:N	2.54	0.40
2:B:18:LEU:N	2:B:18:LEU:CD2	2.79	0.40
2:B:105:PHE:CD2	2:B:116:LEU:HD13	2.57	0.40
2:B:260:ALA:HB2	6:B:856:U10:H103	2.03	0.40
2:B:265:ILE:HD12	2:B:265:ILE:HA	1.72	0.40
5:B:854:BPH:HMB1	5:B:854:BPH:HHB	1.94	0.40
3:C:34:GLU:CD	3:C:37:ARG:HH21	2.29	0.40
3:C:170:ASP:O	3:C:171:ILE:C	2.64	0.40
3:C:248:ARG:O	3:C:248:ARG:HG2	2.20	0.40
1:A:134:PHE:O	1:A:135:ARG:C	2.65	0.40
1:A:138:MET:C	1:A:140:GLY:H	2.27	0.40
1:A:185:LEU:CD2	1:A:185:LEU:C	2.93	0.40
1:A:260:VAL:O	1:A:260:VAL:HG22	2.21	0.40
6:B:856:U10:H201	6:B:856:U10:H222	1.66	0.40
3:C:17:ILE:O	3:C:17:ILE:HG13	2.21	0.40

All (1) 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)
3:C:128:HIS:NE2	3:C:128:HIS:NE2[5_656]	2.18	0.02

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%)	199 (71%)	51 (18%)	29 (10%)	0	6
2	B	300/307 (98%)	202 (67%)	69 (23%)	29 (10%)	0	8
3	C	236/260 (91%)	175 (74%)	45 (19%)	16 (7%)	1	12
All	All	815/848 (96%)	576 (71%)	165 (20%)	74 (9%)	0	9

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	80	LEU
1	A	186	ALA
1	A	200	PRO
1	A	215	PHE
1	A	262	TRP
2	B	5	ASN
2	B	20	MET
2	B	39	LEU
2	B	228	ARG
2	B	269	ALA
2	B	270	ILE
2	B	272	MET
3	C	113	SER
1	A	26	VAL
1	A	187	LEU
1	A	194	VAL
1	A	226	THR
1	A	240	ALA
1	A	273	ALA
2	B	58	LEU
2	B	123	PHE
2	B	154	ILE
2	B	155	TRP
2	B	162	PHE
2	B	163	ILE
2	B	241	ARG
2	B	249	ALA
2	B	268	TRP
2	B	281	GLY
2	B	288	ASP
3	C	19	SER
3	C	29	TYR
3	C	34	GLU
3	C	135	LYS
3	C	194	GLN
3	C	233	ILE
3	C	239	GLY
1	A	180	PHE
1	A	263	TRP
1	A	265	TRP
1	A	270	PRO

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Mol	Chain	Res	Type
2	B	15	PRO
2	B	18	LEU
2	B	124	VAL
2	B	222	THR
3	C	49	PRO
3	C	69	GLY
3	C	86	ALA
3	C	174	GLN
1	A	81	ALA
2	B	219	HIS
2	B	223	ILE
2	B	250	LEU
3	C	193	MET
1	A	21	LEU
1	A	175	ILE
1	A	183	ASN
1	A	193	LEU
1	A	206	MET
1	A	275	ILE
2	B	22	GLU
3	C	144	ALA
2	B	117	ILE
2	B	283	GLY
2	B	296	VAL
3	C	83	ARG
1	A	260	VAL
1	A	84	GLY
1	A	225	GLY
3	C	66	LEU
1	A	31	VAL
1	A	113	ILE
1	A	117	ILE

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%)	198 (90%)	22 (10%)	7	24
2	B	237/241 (98%)	219 (92%)	18 (8%)	12	33
3	C	193/208 (93%)	185 (96%)	8 (4%)	27	49
All	All	650/669 (97%)	602 (93%)	48 (7%)	13	34

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	11	VAL
1	A	21	LEU
1	A	38	THR
1	A	79	PRO
1	A	89	ILE
1	A	94	THR
1	A	154	LEU
1	A	170	ASN
1	A	178	SER
1	A	183	ASN
1	A	185	LEU
1	A	206	MET
1	A	207	ARG
1	A	229	ILE
1	A	236	LEU
1	A	241	VAL
1	A	249	ILE
1	A	256	PHE
1	A	270	PRO
1	A	271	TRP
1	A	275	ILE
2	B	18	LEU
2	B	42	PHE
2	B	50	ILE
2	B	55	LEU
2	B	86	LEU
2	B	90	PHE
2	B	160	HIS
2	B	171	TRP
2	B	182	HIS
2	B	196	LEU
2	B	197	HIS
2	B	204	LEU

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Mol	Chain	Res	Type
2	B	206	ILE
2	B	238	ILE
2	B	255	THR
2	B	258	PHE
2	B	265	ILE
2	B	270	ILE
3	C	49	PRO
3	C	61	PRO
3	C	67	PRO
3	C	105	MET
3	C	169	VAL
3	C	206	ASN
3	C	222	PRO
3	C	225	VAL

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	60	ASN
1	A	62	GLN
1	A	87	GLN
1	A	116	HIS
1	A	168	HIS
2	B	5	ASN
2	B	160	HIS
2	B	188	ASN
2	B	202	HIS
2	B	259	ASN
2	B	299	GLN
3	C	68	HIS
3	C	129	ASN
3	C	204	HIS
3	C	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	A	851	1	69,74,74	1.50	12 (17%)	79,115,115	1.63	14 (17%)
6	U10	A	857	-	48,48,63	2.74	16 (33%)	60,61,79	2.04	18 (30%)
4	BCL	B	852	2	69,74,74	1.53	11 (15%)	79,115,115	1.78	18 (22%)
4	BCL	A	850	-	69,74,74	1.56	12 (17%)	79,115,115	1.82	21 (26%)
5	BPH	B	854	-	59,70,70	2.00	17 (28%)	59,101,101	2.40	18 (30%)
4	BCL	B	853	1	69,74,74	1.46	13 (18%)	79,115,115	2.03	24 (30%)
5	BPH	A	855	-	59,70,70	1.74	11 (18%)	59,101,101	2.26	17 (28%)
6	U10	B	856	-	48,48,63	2.47	15 (31%)	60,61,79	2.03	19 (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
4	BCL	A	851	1	-	6/41/137/137	-
6	U10	A	857	-	-	12/45/69/87	0/1/1/1
4	BCL	B	852	2	-	11/41/137/137	-
4	BCL	A	850	-	-	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	B	854	-	-	7/37/105/105	0/5/6/6
4	BCL	B	853	1	-	7/41/137/137	-
5	BPH	A	855	-	-	7/37/105/105	0/5/6/6
6	U10	B	856	-	-	12/45/69/87	0/1/1/1

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	856	U10	C6-C1	10.61	1.54	1.35
6	A	857	U10	C6-C1	10.27	1.53	1.35
5	B	854	BPH	C2C-C3C	-6.04	1.49	1.54
5	B	854	BPH	C3A-C2A	-5.84	1.49	1.54
5	A	855	BPH	C3A-C2A	-5.81	1.49	1.54
5	A	855	BPH	CBD-CGD	5.25	1.59	1.52
6	A	857	U10	C28-C29	5.14	1.44	1.33
6	A	857	U10	C33-C34	5.09	1.44	1.33
6	B	856	U10	C28-C29	4.90	1.44	1.33
5	A	855	BPH	C3B-C2B	4.88	1.48	1.39
5	A	855	BPH	C3D-C2D	4.77	1.47	1.39
5	B	854	BPH	C3B-C2B	4.75	1.47	1.39
5	B	854	BPH	C3D-CAD	-4.69	1.38	1.47
6	A	857	U10	C18-C19	4.55	1.43	1.33
4	B	852	BCL	C1D-C2D	-4.52	1.36	1.45
6	B	856	U10	C4-C3	4.24	1.51	1.36
4	A	851	BCL	C1D-C2D	-4.21	1.37	1.45
6	A	857	U10	C13-C14	4.20	1.42	1.33
5	B	854	BPH	C2-C3	4.16	1.42	1.33
4	A	850	BCL	C3B-CAB	4.07	1.59	1.46
6	A	857	U10	C4-C3	4.02	1.50	1.36
4	A	850	BCL	C1D-C2D	-3.90	1.37	1.45
6	B	856	U10	C33-C34	3.88	1.42	1.33
6	A	857	U10	C38-C39	3.87	1.44	1.32
4	A	851	BCL	C1B-NB	-3.79	1.32	1.37
4	A	851	BCL	C3D-C2D	3.77	1.49	1.39
6	A	857	U10	C7-C8	-3.76	1.44	1.50
4	B	852	BCL	C1B-NB	-3.74	1.32	1.37
4	B	852	BCL	C3D-C2D	3.74	1.49	1.39
6	A	857	U10	C26-C24	3.72	1.59	1.51
6	A	857	U10	C7-C6	3.70	1.58	1.51
6	B	856	U10	C18-C19	3.68	1.41	1.33
6	A	857	U10	C23-C24	3.63	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	852	BCL	C2-C3	3.47	1.41	1.33
6	B	856	U10	C7-C6	3.45	1.57	1.51
6	A	857	U10	C36-C34	3.33	1.58	1.51
4	A	851	BCL	C2-C3	3.31	1.40	1.33
4	B	853	BCL	C1D-C2D	-3.28	1.38	1.45
4	B	853	BCL	C2-C3	3.25	1.40	1.33
4	B	853	BCL	C3B-CAB	3.22	1.56	1.46
4	B	852	BCL	CMB-C2B	3.14	1.57	1.50
4	B	852	BCL	CBB-CAB	3.13	1.56	1.50
4	A	851	BCL	CBB-CAB	3.12	1.56	1.50
6	B	856	U10	C7-C8	-3.10	1.45	1.50
5	B	854	BPH	O2A-CGA	-3.10	1.24	1.33
6	B	856	U10	C6-C5	3.10	1.55	1.46
4	B	853	BCL	C3C-C4C	-3.06	1.47	1.51
4	A	850	BCL	C3C-C4C	-3.05	1.47	1.51
5	B	854	BPH	CMB-C2B	3.03	1.57	1.51
4	B	853	BCL	CBB-CAB	3.03	1.56	1.50
5	B	854	BPH	C5-C3	3.00	1.57	1.51
4	A	850	BCL	CBB-CAB	2.99	1.56	1.50
4	A	850	BCL	O2D-CGD	-2.98	1.25	1.33
6	B	856	U10	C23-C24	2.98	1.39	1.33
6	A	857	U10	C6-C5	2.95	1.54	1.46
4	B	852	BCL	CMD-C2D	2.94	1.56	1.50
4	B	853	BCL	C1D-ND	-2.89	1.34	1.37
4	B	853	BCL	CMB-C2B	2.88	1.56	1.50
4	A	851	BCL	C3B-CAB	2.88	1.55	1.46
4	A	850	BCL	CMB-C2B	2.84	1.56	1.50
4	B	853	BCL	C3D-C2D	2.80	1.46	1.39
6	A	857	U10	C8-C9	2.79	1.39	1.33
4	A	850	BCL	C3B-C4B	2.75	1.46	1.41
4	A	850	BCL	C1B-NB	-2.73	1.34	1.37
4	B	852	BCL	MG-ND	-2.72	2.00	2.05
5	A	855	BPH	CMB-C2B	2.71	1.57	1.51
4	A	850	BCL	O2A-CGA	-2.69	1.25	1.33
4	A	850	BCL	C3D-C2D	2.68	1.46	1.39
4	B	852	BCL	C3C-C4C	-2.67	1.48	1.51
4	A	851	BCL	C3A-C2A	-2.67	1.47	1.54
5	A	855	BPH	C2-C3	2.65	1.39	1.33
6	A	857	U10	C16-C14	2.59	1.56	1.51
4	A	850	BCL	C3A-C2A	-2.58	1.47	1.54
6	B	856	U10	C26-C24	2.57	1.56	1.51
4	B	853	BCL	C1B-NB	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	850	BCL	MG-ND	-2.53	2.00	2.05
6	B	856	U10	C38-C39	2.51	1.40	1.32
5	A	855	BPH	O2A-CGA	-2.49	1.26	1.33
5	B	854	BPH	C3D-C2D	2.48	1.43	1.39
5	A	855	BPH	C2C-C3C	-2.48	1.52	1.54
4	A	851	BCL	CMB-C2B	2.47	1.55	1.50
4	A	851	BCL	O2D-CGD	-2.46	1.27	1.33
6	B	856	U10	C13-C14	2.44	1.38	1.33
5	B	854	BPH	C3B-CAB	2.42	1.55	1.49
5	A	855	BPH	C3D-CAD	-2.39	1.43	1.47
6	A	857	U10	C31-C29	2.36	1.56	1.51
4	B	853	BCL	C3A-C2A	-2.36	1.48	1.54
4	A	851	BCL	CMD-C2D	2.33	1.55	1.50
4	B	853	BCL	O2A-CGA	-2.33	1.26	1.33
4	B	853	BCL	C3B-C4B	2.30	1.45	1.41
4	B	852	BCL	C3B-CAB	2.28	1.53	1.46
4	A	851	BCL	MG-ND	-2.26	2.01	2.05
4	B	853	BCL	MG-ND	-2.22	2.01	2.05
5	B	854	BPH	C4D-ND	-2.22	1.35	1.38
4	A	851	BCL	O2A-CGA	-2.20	1.26	1.33
5	B	854	BPH	CMD-C2D	2.13	1.55	1.51
6	B	856	U10	C22-C23	-2.13	1.44	1.50
5	A	855	BPH	CHA-CBD	2.11	1.54	1.51
5	B	854	BPH	C6-C5	2.11	1.59	1.52
6	B	856	U10	C8-C9	2.10	1.37	1.33
5	A	855	BPH	CMD-C2D	2.08	1.55	1.51
5	B	854	BPH	C1D-C2D	-2.07	1.37	1.39
5	B	854	BPH	C4-C3	2.07	1.55	1.50
4	B	852	BCL	O2A-CGA	-2.06	1.27	1.33
6	B	856	U10	O3-C3	2.05	1.41	1.36
5	B	854	BPH	C1B-NB	-2.04	1.34	1.38
5	B	854	BPH	C4C-C3C	-2.01	1.48	1.51

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	855	BPH	C4D-CHA-CBD	-7.13	105.03	108.45
5	B	854	BPH	C4D-CHA-CBD	-6.75	105.22	108.45
4	B	853	BCL	CAA-C2A-C1A	-6.68	90.10	111.97
5	A	855	BPH	C1-O2A-CGA	6.00	131.17	116.65
5	B	854	BPH	C3D-C4D-ND	5.89	115.26	107.71
6	A	857	U10	C7-C6-C5	5.67	125.10	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	854	BPH	C1-O2A-CGA	5.54	130.06	116.65
5	A	855	BPH	C3D-C4D-ND	5.50	114.76	107.71
4	A	850	BCL	CAA-C2A-C1A	-5.15	95.11	111.97
5	B	854	BPH	CMB-C2B-C3B	5.10	134.88	124.68
6	B	856	U10	C7-C6-C5	5.07	124.40	118.52
4	B	853	BCL	CMB-C2B-C1B	-4.95	117.88	125.42
5	A	855	BPH	CMB-C2B-C3B	4.95	134.58	124.68
6	A	857	U10	C15-C14-C16	4.87	123.67	115.23
6	B	856	U10	C15-C14-C16	4.82	123.60	115.23
4	B	853	BCL	CHC-C4B-NB	-4.81	116.84	124.05
5	A	855	BPH	O2D-CGD-CBD	4.80	116.22	110.95
4	A	850	BCL	CMB-C2B-C1B	-4.77	118.16	125.42
4	A	851	BCL	CMB-C2B-C1B	-4.71	118.25	125.42
4	B	852	BCL	C6-C5-C3	4.52	124.47	113.47
4	B	853	BCL	CBA-CAA-C2A	4.51	127.20	113.79
4	A	850	BCL	CHC-C4B-NB	-4.49	117.31	124.05
4	A	851	BCL	C4D-CHA-C1A	4.49	126.59	121.24
4	B	852	BCL	CMB-C2B-C1B	-4.47	118.61	125.42
4	B	853	BCL	CED-O2D-CGD	4.45	126.00	115.92
5	B	854	BPH	C4D-ND-C1D	-4.43	103.57	108.87
5	B	854	BPH	C2B-C1B-NB	4.42	112.62	109.43
6	B	856	U10	C25-C24-C23	-4.37	112.39	123.63
6	B	856	U10	C15-C14-C13	-4.29	112.60	123.63
4	B	852	BCL	CED-O2D-CGD	4.29	125.64	115.92
5	B	854	BPH	C4-C3-C5	4.23	122.57	115.23
4	B	852	BCL	CHC-C4B-NB	-4.15	117.83	124.05
6	A	857	U10	C15-C14-C13	-4.11	113.07	123.63
6	A	857	U10	C7-C6-C1	-4.10	117.85	124.89
5	A	855	BPH	C4-C3-C5	4.08	122.30	115.23
4	A	851	BCL	CHC-C4B-NB	-4.07	117.94	124.05
4	B	853	BCL	C4A-NA-C1A	4.02	108.51	106.68
4	B	852	BCL	C4D-CHA-C1A	3.95	125.95	121.24
4	A	850	BCL	CED-O2D-CGD	3.93	124.83	115.92
6	B	856	U10	C10-C9-C8	-3.92	113.55	123.63
4	A	851	BCL	CED-O2D-CGD	3.87	124.70	115.92
6	A	857	U10	C25-C24-C23	-3.82	113.81	123.63
5	B	854	BPH	O1D-CGD-CBD	-3.81	118.95	124.72
6	B	856	U10	C7-C6-C1	-3.77	118.42	124.89
4	B	853	BCL	C3D-C4D-ND	3.77	116.11	109.99
4	B	852	BCL	C2A-C1A-CHA	3.71	130.31	123.87
6	A	857	U10	C10-C9-C8	-3.68	114.18	123.63
4	B	852	BCL	CGD-CBD-CAD	-3.62	99.11	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	854	BPH	C3B-C4B-NB	3.62	113.31	108.05
5	A	855	BPH	C4D-ND-C1D	-3.61	104.54	108.87
4	B	853	BCL	CMD-C2D-C1D	3.58	131.03	124.73
4	B	853	BCL	C4D-CHA-C1A	3.58	125.51	121.24
5	B	854	BPH	C6-C5-C3	3.56	122.15	113.47
4	B	852	BCL	CHA-C1A-NA	-3.49	118.48	126.39
4	A	850	BCL	CBA-CAA-C2A	3.48	124.15	113.79
5	A	855	BPH	O1D-CGD-CBD	-3.46	119.48	124.72
4	A	851	BCL	C2A-C1A-CHA	3.39	129.75	123.87
5	B	854	BPH	C7-C6-C5	3.37	122.24	113.26
6	A	857	U10	C25-C24-C26	3.34	121.03	115.23
4	A	850	BCL	C4A-NA-C1A	3.28	108.18	106.68
5	B	854	BPH	CED-O2D-CGD	3.27	123.32	115.92
4	A	851	BCL	CHA-C1A-NA	-3.24	119.05	126.39
4	A	850	BCL	C4D-CHA-C1A	3.23	125.09	121.24
6	A	857	U10	C21-C19-C18	3.21	128.37	121.17
5	B	854	BPH	C2D-C1D-ND	3.19	111.74	109.43
5	B	854	BPH	C3D-CAD-CBD	3.19	111.81	107.61
6	A	857	U10	C35-C34-C33	-3.18	115.46	123.63
4	A	850	BCL	C6-C5-C3	3.16	121.17	113.47
4	A	850	BCL	C3D-C4D-ND	3.15	115.10	109.99
4	A	851	BCL	C2A-C3A-C4A	3.13	106.93	101.87
5	A	855	BPH	C3D-CAD-CBD	3.12	111.71	107.61
4	A	850	BCL	C2A-C3A-C4A	3.11	106.89	101.87
4	B	853	BCL	CMD-C2D-C3D	-3.10	120.57	127.69
5	B	854	BPH	O2D-CGD-CBD	3.06	114.31	110.95
4	B	852	BCL	C2A-C3A-C4A	3.06	106.82	101.87
6	B	856	U10	C35-C34-C33	-3.05	115.80	123.63
4	B	852	BCL	OBD-CAD-C3D	-2.94	121.55	128.42
6	B	856	U10	C7-C8-C9	2.93	131.87	126.83
5	A	855	BPH	CED-O2D-CGD	2.92	122.53	115.92
4	B	852	BCL	C4A-NA-C1A	2.91	108.00	106.68
6	B	856	U10	C26-C24-C23	2.89	127.66	121.17
4	A	850	BCL	C3D-C2D-C1D	2.88	109.76	105.83
4	A	851	BCL	C4D-C3D-CAD	-2.87	104.99	108.11
4	A	851	BCL	C3D-C4D-ND	2.86	114.63	109.99
4	A	850	BCL	OBD-CAD-C3D	-2.82	121.81	128.42
5	B	854	BPH	C4A-C3A-C2A	2.82	105.52	102.84
5	A	855	BPH	C3B-C4B-NB	2.81	112.14	108.05
6	A	857	U10	C20-C19-C18	-2.80	116.43	123.63
4	A	851	BCL	C6-C5-C3	2.80	120.29	113.47
5	A	855	BPH	C4A-C3A-C2A	2.80	105.50	102.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	852	BCL	C3D-C4D-ND	2.76	114.48	109.99
4	B	853	BCL	C2A-C3A-C4A	2.72	106.26	101.87
6	B	856	U10	C25-C24-C26	2.72	119.95	115.23
6	B	856	U10	C11-C9-C8	2.70	127.24	121.17
4	B	852	BCL	C4D-C3D-CAD	-2.67	105.21	108.11
6	B	856	U10	C20-C19-C18	-2.65	116.81	123.63
6	A	857	U10	C1-C6-C5	-2.65	117.04	119.62
4	B	853	BCL	CMB-C2B-C3B	2.65	134.03	125.67
4	A	850	BCL	CMD-C2D-C3D	-2.65	121.62	127.69
4	A	851	BCL	C4A-NA-C1A	2.64	107.88	106.68
4	A	850	BCL	C1-O2A-CGA	2.60	122.94	116.65
4	B	853	BCL	C2A-C1A-CHA	2.59	128.37	123.87
4	B	853	BCL	OBD-CAD-C3D	-2.58	122.39	128.42
4	A	851	BCL	CMB-C2B-C3B	2.56	133.74	125.67
4	A	850	BCL	C4D-C3D-CAD	-2.53	105.36	108.11
6	B	856	U10	C1-C6-C5	-2.51	117.18	119.62
4	B	852	BCL	CMB-C2B-C3B	2.49	133.52	125.67
4	B	853	BCL	CHA-C1A-NA	-2.48	120.78	126.39
4	A	850	BCL	CMB-C2B-C3B	2.48	133.49	125.67
4	A	850	BCL	O2D-CGD-CBD	2.46	115.53	111.23
6	B	856	U10	O5-C5-C4	-2.43	115.88	121.03
6	A	857	U10	C11-C9-C8	2.40	126.56	121.17
5	B	854	BPH	OBD-CAD-C3D	-2.40	124.15	127.89
4	B	853	BCL	C1D-ND-C4D	-2.39	104.63	106.31
4	A	851	BCL	OBD-CAD-C3D	-2.38	122.85	128.42
6	A	857	U10	C30-C29-C28	-2.38	117.51	123.63
4	B	853	BCL	C1-O2A-CGA	2.35	122.34	116.65
4	B	853	BCL	CAA-C2A-C3A	-2.34	106.67	113.00
6	A	857	U10	O5-C5-C4	-2.34	116.07	121.03
6	A	857	U10	C10-C9-C11	2.32	119.25	115.23
5	A	855	BPH	C2D-C1D-ND	2.31	111.10	109.43
4	A	850	BCL	CHA-C1A-NA	-2.30	121.17	126.39
6	B	856	U10	C10-C9-C11	2.29	119.21	115.23
4	B	853	BCL	O1D-CGD-CBD	-2.28	120.02	124.52
4	B	853	BCL	C1C-NC-C4C	2.28	107.72	106.68
4	B	852	BCL	CBC-CAC-C3C	2.27	118.23	113.41
5	A	855	BPH	CBB-CAB-C3B	-2.27	113.55	120.34
5	A	855	BPH	C2B-C1B-NB	2.26	111.06	109.43
5	B	854	BPH	O2A-C1-C2	-2.26	99.43	108.11
6	B	856	U10	C36-C34-C33	2.25	126.22	121.17
5	A	855	BPH	C6-C5-C3	2.25	118.95	113.47
4	B	852	BCL	C15-C13-C12	-2.25	100.68	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	853	BCL	O2D-CGD-CBD	2.24	115.14	111.23
4	A	850	BCL	CMD-C2D-C1D	2.21	128.62	124.73
6	B	856	U10	C1M-C1-C6	-2.20	120.83	124.45
4	B	852	BCL	CMD-C2D-C1D	2.19	128.59	124.73
4	A	851	BCL	CMD-C2D-C1D	2.17	128.55	124.73
4	B	852	BCL	O2A-CGA-CBA	2.16	118.42	111.83
6	A	857	U10	C36-C34-C33	2.14	125.97	121.17
4	A	850	BCL	O1D-CGD-CBD	-2.14	120.30	124.52
4	B	853	BCL	C15-C13-C12	-2.13	101.27	112.07
6	A	857	U10	C1M-C1-C6	-2.12	120.96	124.45
6	B	856	U10	C8-C7-C6	-2.12	106.87	112.08
4	B	853	BCL	C2C-C3C-C4C	2.09	104.47	101.34
5	A	855	BPH	CMC-C2C-C1C	-2.08	110.12	114.61
6	A	857	U10	C17-C16-C14	2.05	119.98	113.19
4	B	853	BCL	C3B-C4B-NB	2.04	112.45	109.76
4	A	850	BCL	CAB-C3B-C2B	2.03	131.95	127.74
6	B	856	U10	C6-C1-C2	2.02	120.77	119.17

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	850	BCL	C2C-C3C-CAC-CBC
4	A	850	BCL	C4C-C3C-CAC-CBC
4	B	852	BCL	C2C-C3C-CAC-CBC
4	B	852	BCL	C4C-C3C-CAC-CBC
5	A	855	BPH	C4C-C3C-CAC-CBC
6	A	857	U10	C34-C36-C37-C38
6	B	856	U10	C20-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
4	B	852	BCL	C2-C3-C5-C6
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
6	B	856	U10	C13-C14-C16-C17
6	B	856	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
6	A	857	U10	C29-C31-C32-C33
6	B	856	U10	C19-C21-C22-C23
4	B	852	BCL	C4-C3-C5-C6
6	B	856	U10	C18-C19-C21-C22
6	B	856	U10	C29-C31-C32-C33
4	B	853	BCL	C5-C6-C7-C8
5	A	855	BPH	C2A-CAA-CBA-CGA
4	A	850	BCL	C3-C5-C6-C7
4	A	851	BCL	C15-C16-C17-C18
4	A	851	BCL	C2A-CAA-CBA-CGA
6	B	856	U10	C12-C11-C9-C10
5	B	854	BPH	C8-C10-C11-C12
4	A	851	BCL	C5-C6-C7-C8
4	A	850	BCL	C5-C6-C7-C8
6	B	856	U10	C12-C11-C9-C8
4	B	853	BCL	C3-C5-C6-C7
5	A	855	BPH	C2C-C3C-CAC-CBC
5	B	854	BPH	C2C-C3C-CAC-CBC
4	A	851	BCL	C11-C10-C8-C7
4	B	852	BCL	C3-C5-C6-C7
4	A	851	BCL	C11-C10-C8-C9
5	B	854	BPH	C2A-CAA-CBA-CGA
6	B	856	U10	C14-C16-C17-C18
4	A	850	BCL	C15-C16-C17-C18
4	B	852	BCL	C5-C6-C7-C8
5	B	854	BPH	C4C-C3C-CAC-CBC
4	A	850	BCL	CHA-CBD-CGD-O1D
4	B	852	BCL	CHA-CBD-CGD-O1D
4	B	852	BCL	CHA-CBD-CGD-O2D
6	A	857	U10	C3-C4-O4-C4M
6	A	857	U10	C26-C27-C28-C29
6	A	857	U10	C5-C4-O4-C4M
6	A	857	U10	C20-C19-C21-C22
4	B	852	BCL	C12-C13-C15-C16
4	A	850	BCL	C4-C3-C5-C6
6	B	856	U10	C30-C29-C31-C32
4	A	850	BCL	C2-C3-C5-C6
6	A	857	U10	C18-C19-C21-C22
5	A	855	BPH	CHA-CBD-CGD-O2D
4	B	852	BCL	C14-C13-C15-C16
4	B	853	BCL	O2A-C1-C2-C3
4	B	853	BCL	C15-C16-C17-C18

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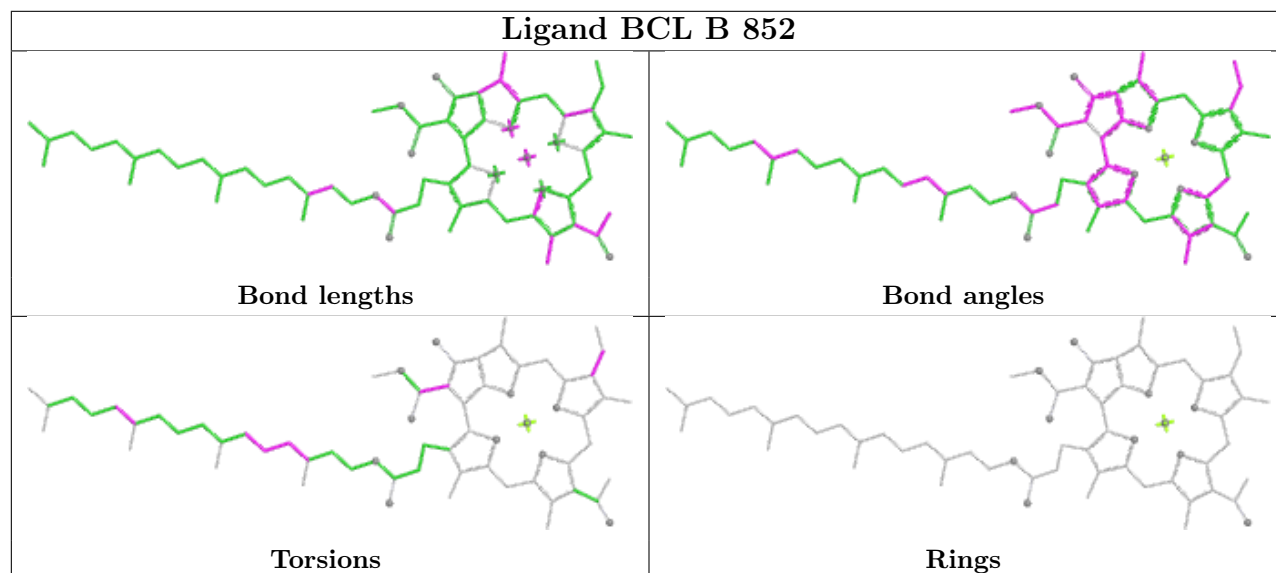
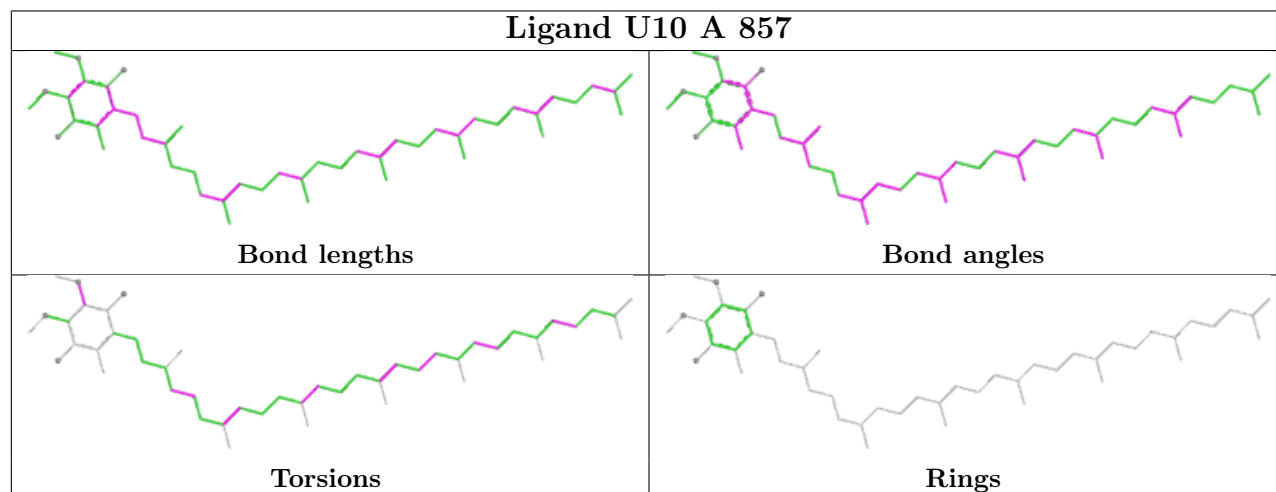
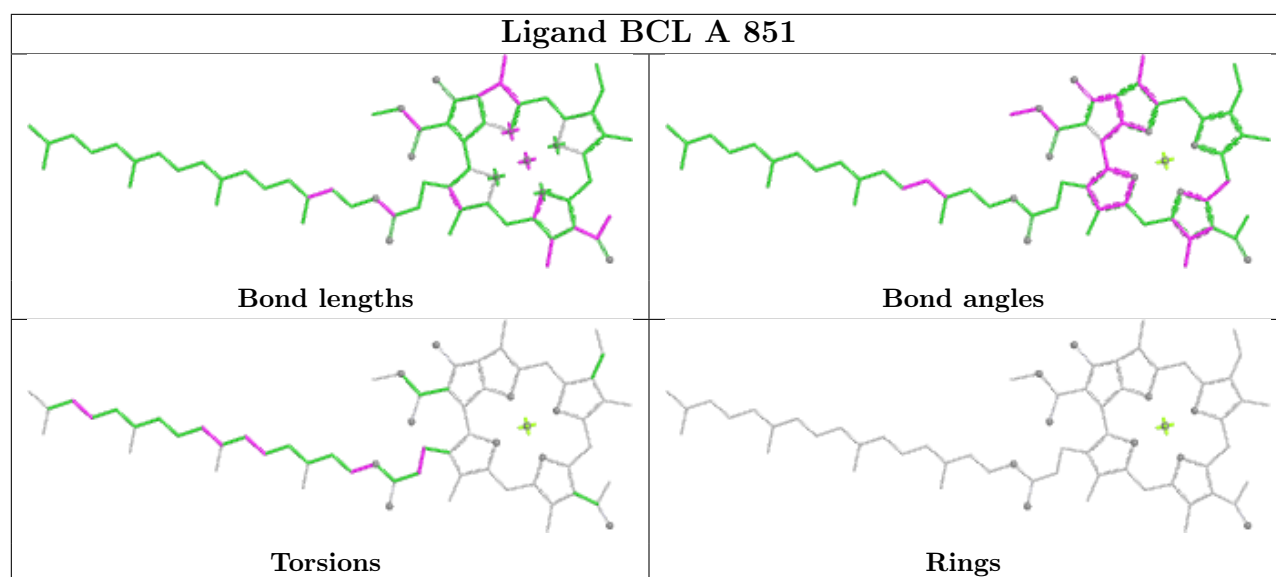
Mol	Chain	Res	Type	Atoms
4	B	853	BCL	CAA-CBA-CGA-O2A
5	A	855	BPH	C8-C10-C11-C12
4	B	853	BCL	CAA-CBA-CGA-O1A
4	B	853	BCL	C2A-CAA-CBA-CGA
6	A	857	U10	C9-C11-C12-C13
5	B	854	BPH	C10-C11-C12-C13
4	B	852	BCL	CAD-CBD-CGD-O2D
4	A	851	BCL	C2-C1-O2A-CGA

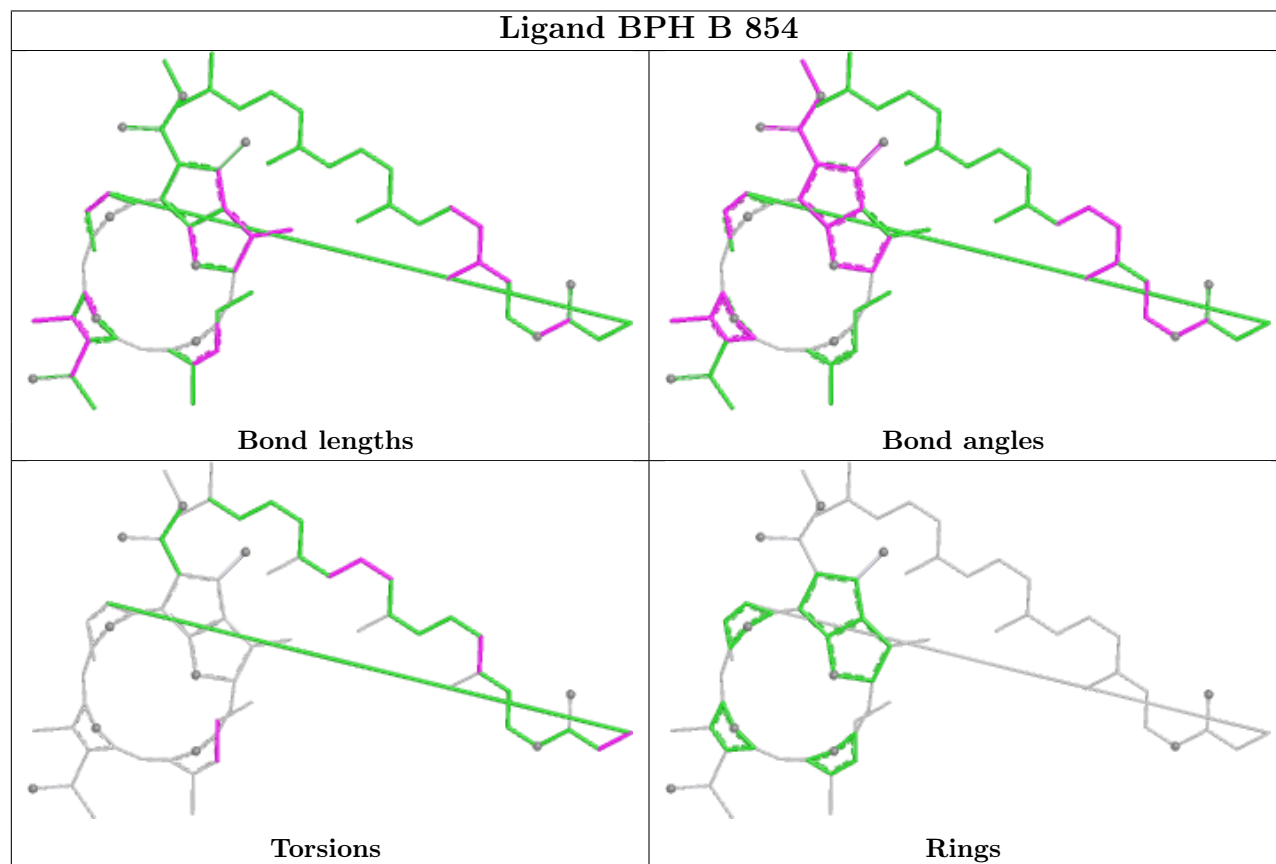
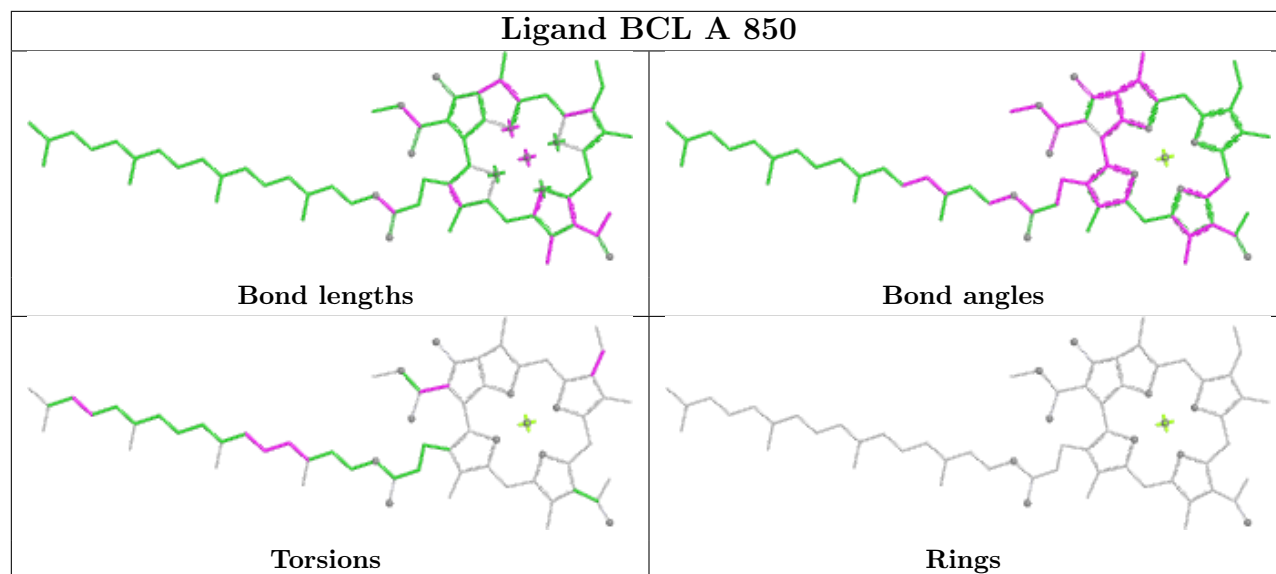
There are no ring outliers.

8 monomers are involved in 74 short contacts:

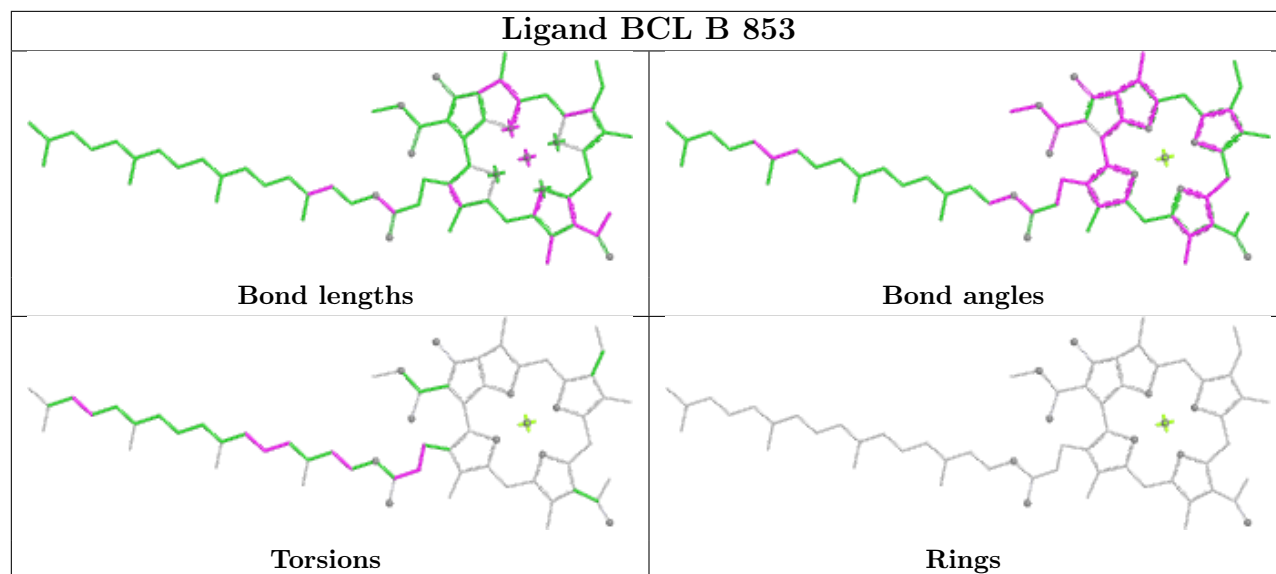
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	851	BCL	9	0
6	A	857	U10	6	0
4	B	852	BCL	9	0
4	A	850	BCL	8	0
5	B	854	BPH	11	0
4	B	853	BCL	10	0
5	A	855	BPH	13	0
6	B	856	U10	16	0

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

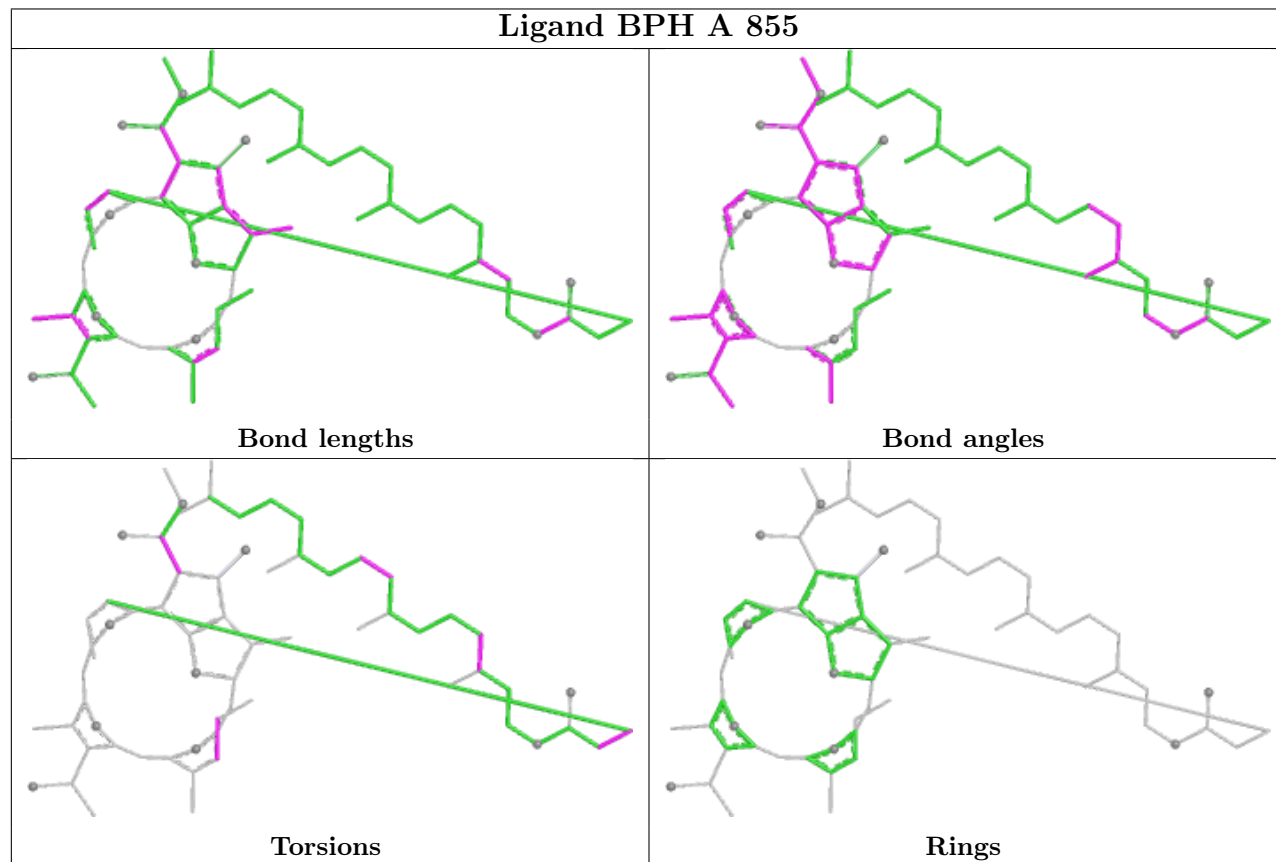


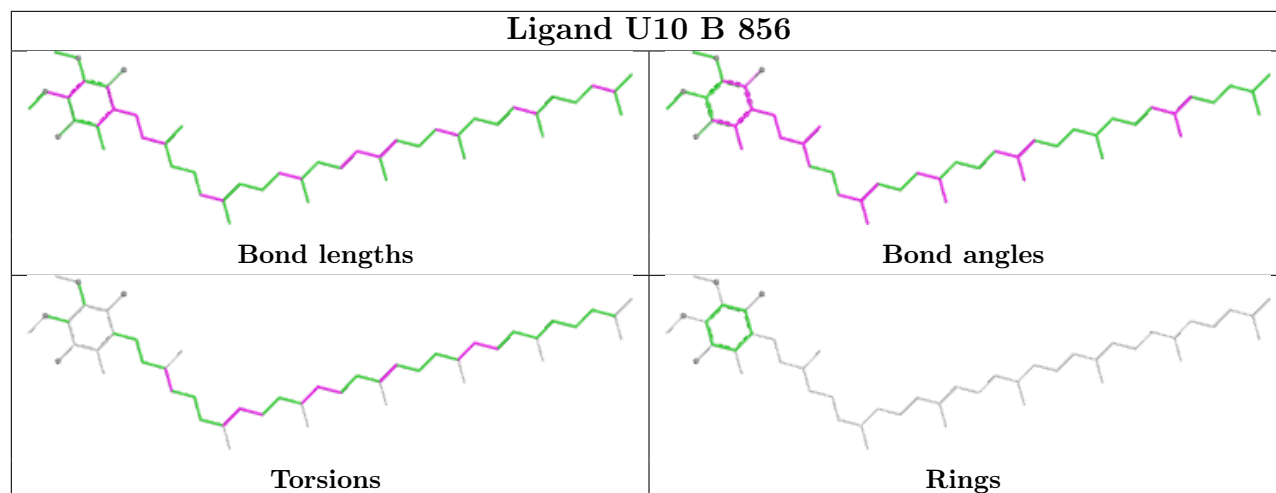


Ligand BCL B 853



Ligand BPH A 855





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 [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%)	-0.30	2 (0%) 84 71	90, 90, 90, 90	0
2	B	302/307 (98%)	-0.11	4 (1%) 75 60	82, 90, 90, 90	0
3	C	238/260 (91%)	-0.14	1 (0%) 88 77	90, 90, 90, 90	0
All	All	821/848 (96%)	-0.18	7 (0%) 81 67	82, 90, 90, 90	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	171	TRP	4.0
2	B	17	ASP	3.3
2	B	7	PHE	2.5
2	B	46	GLN	2.2
1	A	14	GLY	2.1
1	A	258	GLN	2.1
3	C	63	THR	2.1

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,

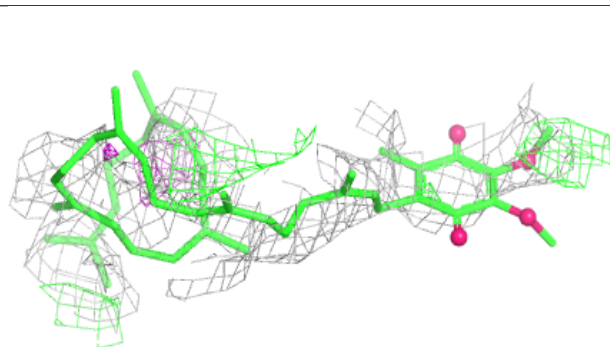
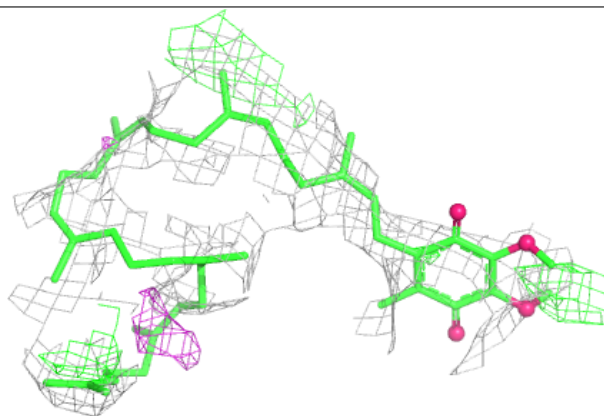
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U10	A	857	48/63	0.81	0.19	90,90,90,90	13
8	MN	B	900	1/1	0.87	0.24	90,90,90,90	0
6	U10	B	856	48/63	0.91	0.13	90,90,90,90	0
4	BCL	A	850	66/66	0.93	0.15	90,90,90,90	0
5	BPH	B	854	65/65	0.95	0.13	90,90,90,90	0
4	BCL	B	852	66/66	0.96	0.14	90,90,90,90	0
4	BCL	B	853	66/66	0.96	0.12	90,90,90,90	0
4	BCL	A	851	66/66	0.96	0.15	90,90,90,90	0
5	BPH	A	855	65/65	0.97	0.14	90,90,90,90	0
7	FE	B	858	1/1	1.00	0.02	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.

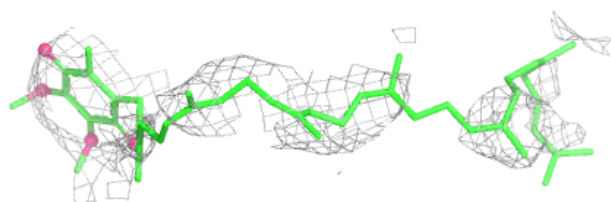
Electron density around U10 A 857:

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



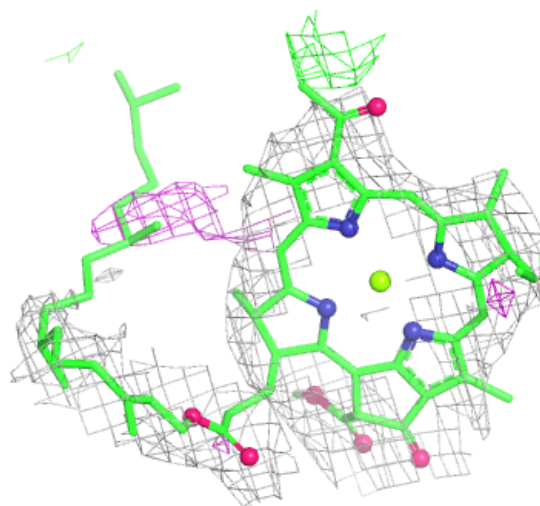
Electron density around U10 B 856:

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



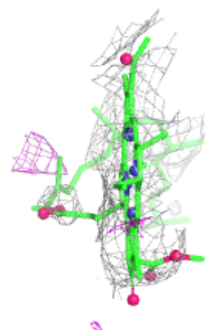
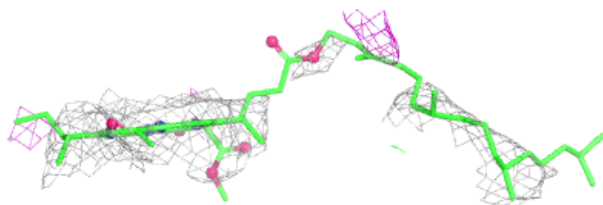
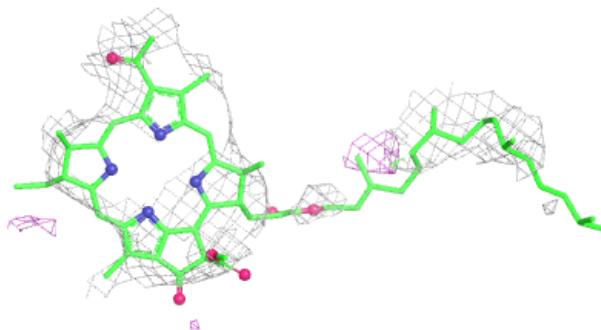
Electron density around BCL A 850:

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

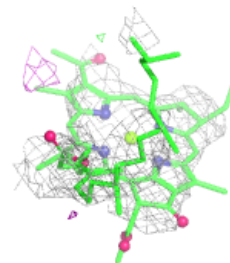
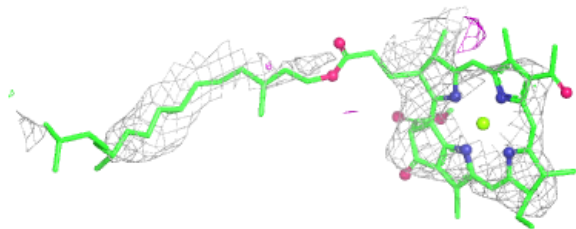
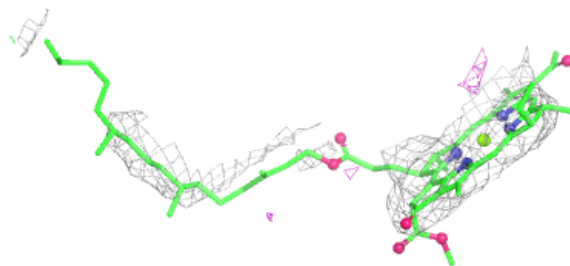


Electron density around BPH B 854:

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

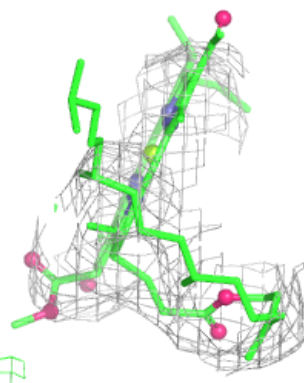
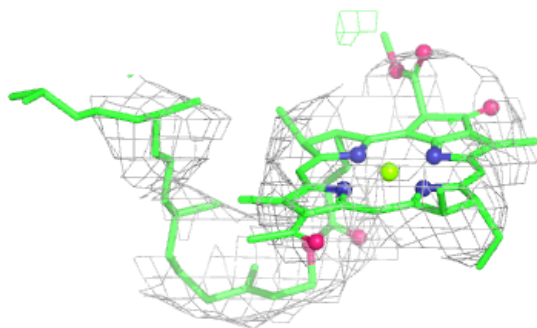
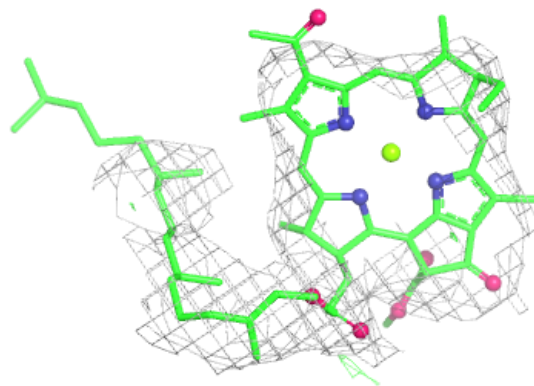
**Electron density around BCL B 852:**

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

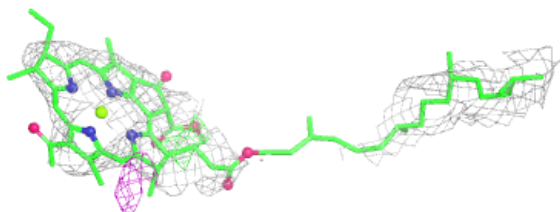
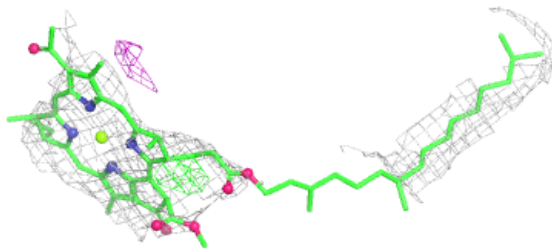


Electron density around BCL B 853:

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

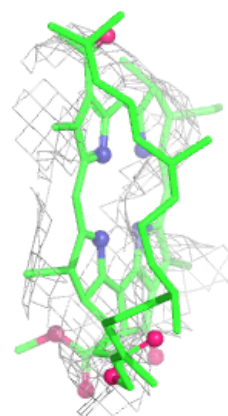
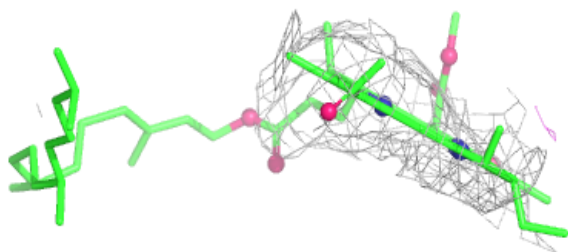
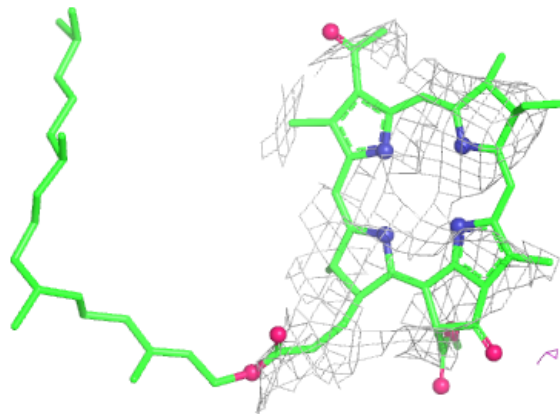
**Electron density around BCL A 851:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.