Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 05:14 am GMT

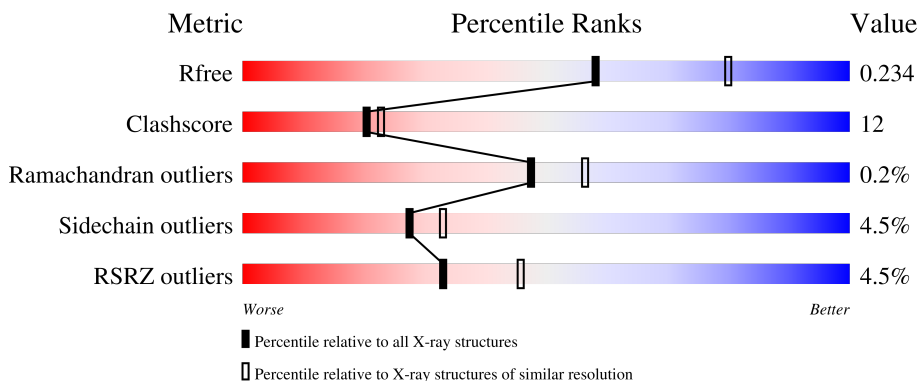|		
PDB ID	:	1OGV
Title	:	Lipidic cubic phase crystal structure of the photosynthetic reaction centre from Rhodobacter sphaeroides
Authors	:	Katona, G.; Andreasson, U.; Landau, E.M.; Andreasson, L.-E.; Neutze, R.
Deposited on	:	2003-05-13
Resolution	:	2.35 Å(reported)

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 2.35 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		12
Ramachandran outliers		0.2%
Sidechain outliers		4.5%
RSRZ outliers		4.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	H	250	4% 69% 25% · 5%
2	L	281	5% 75% 23% ··
3	M	307	5% 79% 19% ··

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 7051 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	237	Total	C	N	O	S	31	0	0
			1803	1154	307	333	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	4	0	0
			2232	1507	355	362	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	19	0	1
			2405	1605	394	396	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).
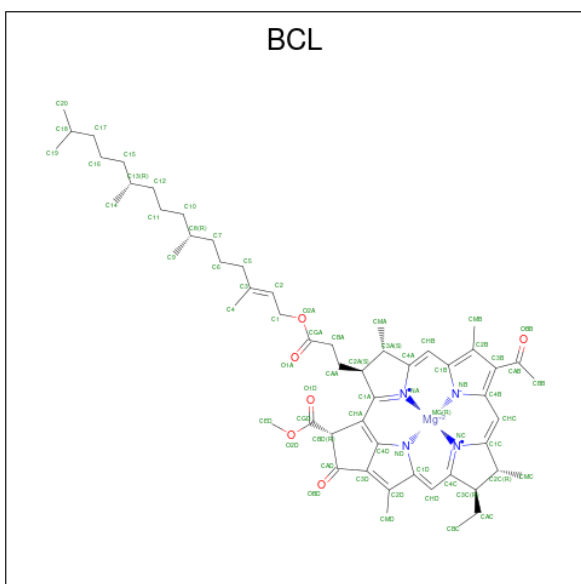
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).
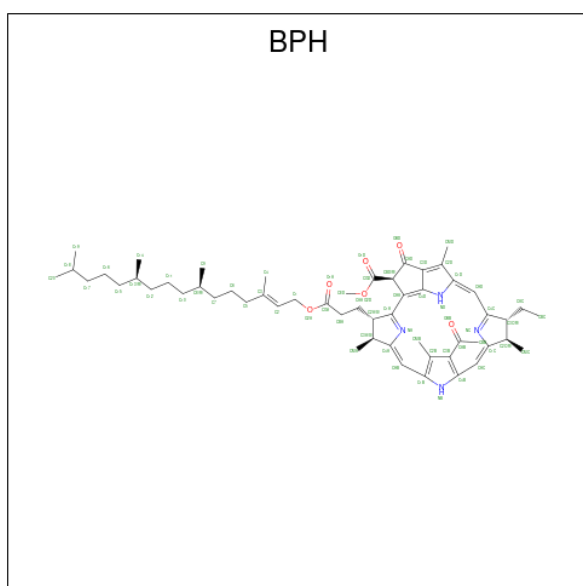
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			51	41	4	6		

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

U10
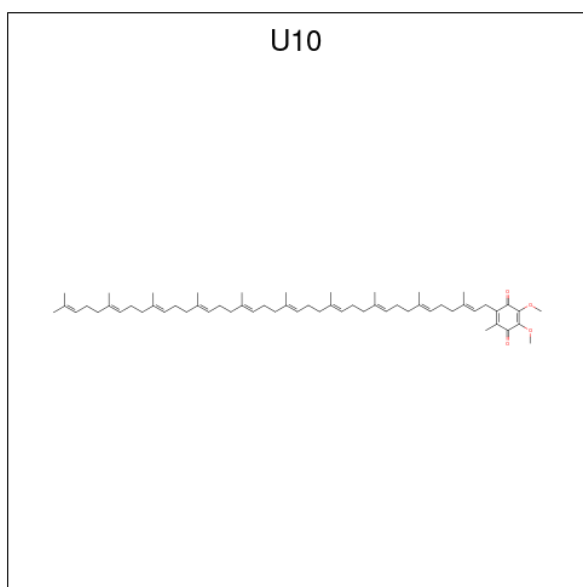
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	M	1	38	34	4	0	0

- Molecule 7 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

CDL
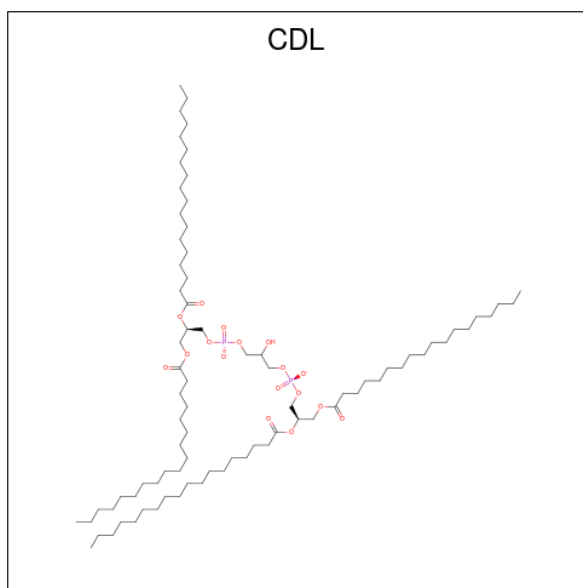
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
7	M	1	70	52	16	2	0	0

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total 1	Cl 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	49	Total 49	O 49	0	0
10	L	46	Total 46	O 46	0	0
10	M	41	Total 41	O 41	0	0

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 H chain
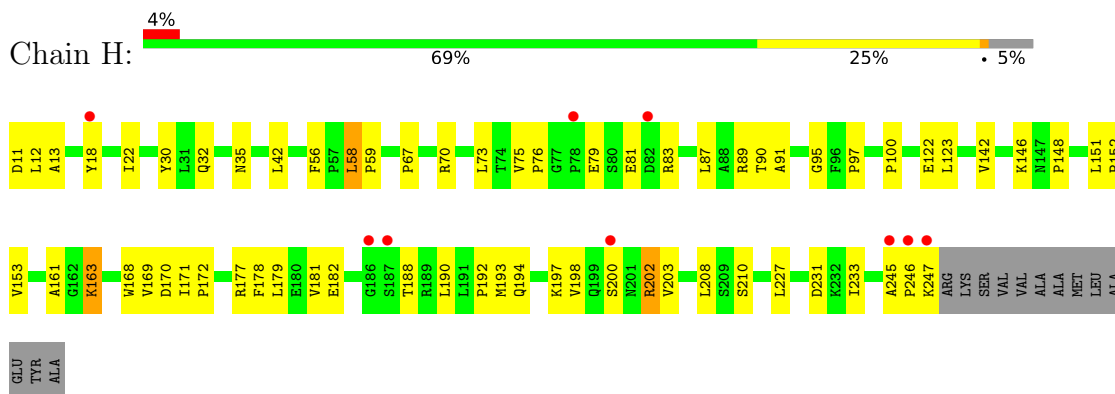
- Molecule 2: Reaction center protein L chain
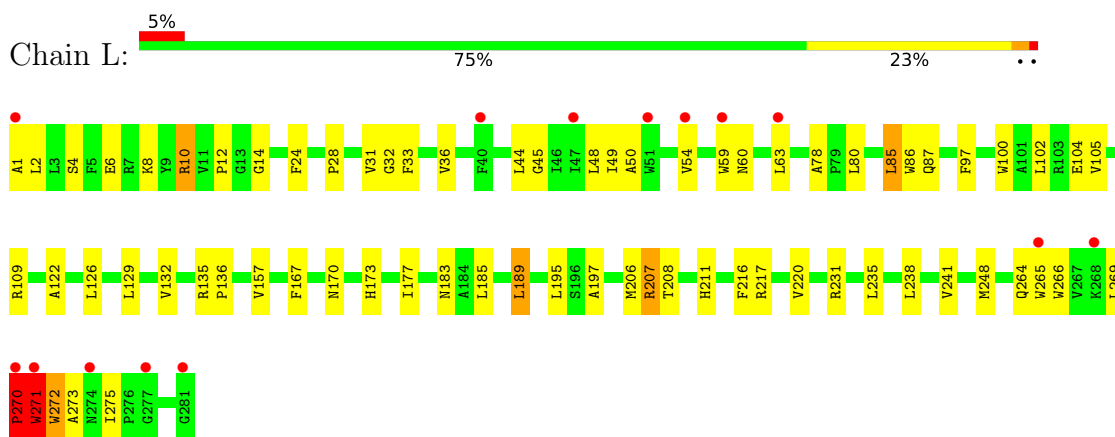
- Molecule 3: Reaction center protein M chain

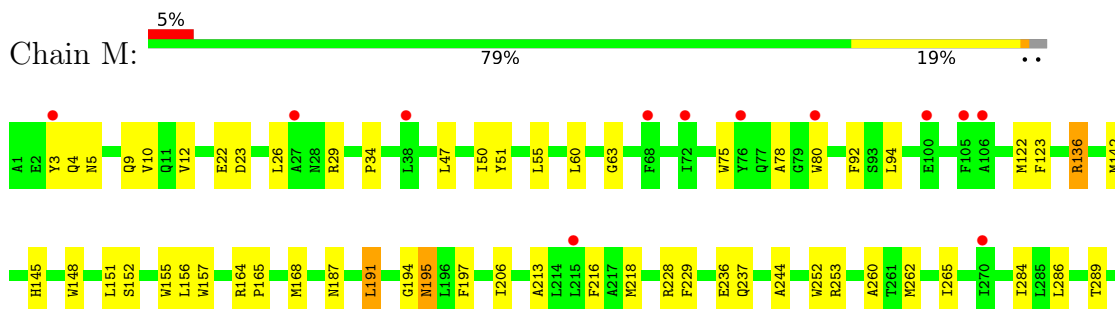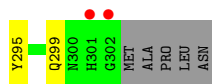# 4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.97Å 99.97Å 237.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.25 – 2.35 42.25 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.8 (42.25-2.35) 95.9 (42.25-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.244 0.204 , 0.234	Depositor DCC
R_{free} test set	2451 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.6	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7051	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, BPH, CDL, BCL, U10, FE2

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	H	0.32	0/1851	0.58	0/2520
2	L	0.39	0/2320	0.55	0/3175
3	M	0.40	0/2497	0.54	0/3410
All	All	0.38	0/6668	0.55	0/9105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1803	0	1805	66	0
2	L	2232	0	2187	62	0
3	M	2405	0	2318	59	0
4	L	132	0	148	8	0
4	M	117	0	115	10	0
5	L	65	0	74	5	0
5	M	51	0	45	3	0
6	M	38	0	47	1	0
7	M	70	0	90	3	0
8	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	1	0	0	0	0
10	H	49	0	0	1	0
10	L	46	0	0	0	0
10	M	41	0	0	1	0
All	All	7051	0	6829	168	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 12.

All (168) 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)
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.55	0.88
3:M:63:GLY:HA3	5:M:1304:BPH:H5C2	1.65	0.78
3:M:136:ARG:NE	3:M:136:ARG:HA	1.99	0.78
1:H:197:LYS:HA	3:M:9:GLN:HE22	1.49	0.76
2:L:208:THR:H	2:L:211:HIS:HD2	1.34	0.76
3:M:122:MET:HE3	3:M:157:TRP:HE1	1.51	0.75
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.71	0.72
1:H:194:GLN:CG	3:M:228:ARG:HA	2.20	0.72
2:L:60:ASN:HB3	2:L:63:LEU:HD23	1.75	0.67
2:L:241:VAL:HG21	5:L:1284:BPH:HAC1	1.75	0.66
1:H:198:VAL:H	3:M:9:GLN:NE2	1.91	0.66
3:M:168:MET:HE3	3:M:289:THR:HA	1.79	0.65
2:L:231:ARG:HD2	3:M:5:ASN:O	1.97	0.65
2:L:208:THR:H	2:L:211:HIS:CD2	2.14	0.64
2:L:272:TRP:HA	2:L:275:ILE:HG13	1.79	0.64
1:H:194:GLN:HG2	3:M:228:ARG:HA	1.80	0.64
3:M:197:PHE:HZ	4:M:1303:BCL:HBB2	1.61	0.63
3:M:197:PHE:CZ	4:M:1303:BCL:HBB2	2.33	0.63
2:L:78:ALA:H	2:L:87:GLN:HE22	1.45	0.63
1:H:122:GLU:HG3	3:M:236:GLU:HG3	1.80	0.62
2:L:33:PHE:O	2:L:36:VAL:HG22	1.98	0.62
3:M:34:PRO:O	3:M:47:LEU:HB2	1.98	0.62
3:M:122:MET:CE	3:M:157:TRP:HE1	2.13	0.62
2:L:217:ARG:HD2	10:M:2007:HOH:O	2.00	0.61
2:L:157:VAL:HG11	4:M:1303:BCL:HBB1	1.81	0.61
1:H:163:LYS:HB2	1:H:163:LYS:NZ	2.15	0.61
2:L:105:VAL:O	2:L:109:ARG:HG3	2.01	0.61
1:H:194:GLN:H	1:H:194:GLN:CD	2.04	0.60
2:L:177:ILE:HG12	4:L:1282:BCL:HMB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:187:ASN:O	3:M:191:LEU:HD22	2.02	0.60
1:H:79:GLU:HG2	2:L:4:SER:OG	2.02	0.59
3:M:157:TRP:HB2	4:M:1303:BCL:H62	1.84	0.59
1:H:122:GLU:CD	3:M:236:GLU:HG3	2.23	0.58
1:H:12:LEU:HD12	3:M:286:LEU:HD21	1.83	0.58
1:H:198:VAL:H	3:M:9:GLN:HE22	1.50	0.58
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.85	0.57
1:H:70:ARG:HH22	1:H:123:LEU:HD13	1.69	0.57
2:L:264:GLN:C	2:L:266:TRP:H	2.06	0.57
7:M:1306:CDL:HB4	7:M:1306:CDL:HB22	1.87	0.57
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.88	0.56
2:L:269:LEU:O	2:L:273:ALA:HB2	2.05	0.56
1:H:12:LEU:HD12	3:M:286:LEU:CD2	2.35	0.56
1:H:146:LYS:NZ	1:H:200:SER:O	2.39	0.56
1:H:87:LEU:CD1	2:L:8:LYS:HA	2.37	0.55
1:H:182:GLU:HA	1:H:188:THR:HG22	1.89	0.55
2:L:269:LEU:HG	2:L:271:TRP:CZ2	2.42	0.55
1:H:122:GLU:CG	3:M:236:GLU:HG3	2.37	0.55
3:M:122:MET:HE3	3:M:157:TRP:NE1	2.21	0.54
1:H:90:THR:HB	1:H:97:PRO:O	2.06	0.54
2:L:80:LEU:HD22	2:L:85:LEU:HD13	1.90	0.54
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.90	0.54
2:L:97:PHE:CE1	4:L:1282:BCL:H121	2.42	0.53
3:M:78:ALA:HB2	3:M:92:PHE:CZ	2.44	0.53
2:L:264:GLN:C	2:L:266:TRP:N	2.61	0.53
2:L:189:LEU:HD13	5:M:1304:BPH:HMD2	1.92	0.51
2:L:197:ALA:O	2:L:207:ARG:HB2	2.11	0.51
4:L:1283:BCL:H121	4:L:1283:BCL:HMA1	1.92	0.51
1:H:58:LEU:CD2	1:H:59:PRO:HD2	2.41	0.51
2:L:135:ARG:HD2	2:L:248:MET:O	2.11	0.51
1:H:192:PRO:HB3	1:H:194:GLN:HE21	1.75	0.51
4:L:1282:BCL:H122	5:L:1284:BPH:H3A	1.92	0.51
1:H:161:ALA:HB2	1:H:210:SER:HA	1.93	0.51
1:H:73:LEU:HD11	1:H:75:VAL:HG13	1.93	0.50
1:H:194:GLN:HG3	3:M:228:ARG:HA	1.90	0.50
2:L:185:LEU:CD2	4:M:1302:BCL:H43	2.40	0.50
2:L:185:LEU:HD12	2:L:189:LEU:HD22	1.93	0.50
2:L:14:GLY:O	2:L:109:ARG:HD3	2.12	0.50
3:M:284:ILE:HG12	4:M:1303:BCL:HED3	1.93	0.50
1:H:42:LEU:HB3	2:L:1:ALA:HB1	1.94	0.50
2:L:1:ALA:O	2:L:2:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:270:PRO:HB2	2:L:271:TRP:CE3	2.46	0.49
3:M:168:MET:HA	3:M:168:MET:CE	2.43	0.49
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.95	0.49
4:L:1282:BCL:NC	4:M:1303:BCL:HBB3	2.28	0.49
4:L:1283:BCL:HBB3	5:L:1284:BPH:H141	1.95	0.49
3:M:136:ARG:NE	3:M:136:ARG:CA	2.74	0.49
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.48	0.48
2:L:44:LEU:O	2:L:48:LEU:HG	2.13	0.48
1:H:198:VAL:N	3:M:9:GLN:HE22	2.11	0.48
1:H:59:PRO:HG2	1:H:76:PRO:CG	2.44	0.48
2:L:207:ARG:HG2	3:M:142:MET:HG2	1.95	0.48
3:M:237:GLN:HB2	3:M:262:MET:HG2	1.96	0.48
1:H:73:LEU:CD1	1:H:75:VAL:HG13	2.44	0.47
3:M:50:ILE:HG12	3:M:51:TYR:N	2.29	0.47
2:L:28:PRO:HB3	3:M:253:ARG:CZ	2.44	0.47
3:M:123:PHE:HA	3:M:157:TRP:HH2	1.77	0.47
1:H:89:ARG:HG2	1:H:91:ALA:O	2.15	0.47
1:H:90:THR:HG23	10:H:2019:HOH:O	2.15	0.47
2:L:86:TRP:CZ2	2:L:132:VAL:HG22	2.49	0.47
3:M:145:HIS:CD2	7:M:1306:CDL:HB62	2.50	0.47
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.79	0.47
2:L:63:LEU:N	2:L:63:LEU:HD22	2.30	0.46
5:L:1284:BPH:HMC2	3:M:213:ALA:HB3	1.97	0.46
4:M:1302:BCL:HBC1	4:M:1303:BCL:HAA2	1.97	0.46
1:H:12:LEU:HD13	1:H:12:LEU:O	2.15	0.46
1:H:58:LEU:HD22	1:H:59:PRO:HD2	1.97	0.46
1:H:97:PRO:HB2	2:L:12:PRO:HG3	1.98	0.46
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.96	0.46
2:L:50:ALA:O	2:L:54:VAL:HG23	2.16	0.46
1:H:152:PRO:HG2	1:H:202:ARG:HB2	1.97	0.46
2:L:31:VAL:HG12	2:L:32:GLY:N	2.31	0.46
2:L:60:ASN:CB	2:L:63:LEU:HD23	2.43	0.46
2:L:264:GLN:O	2:L:266:TRP:N	2.49	0.46
1:H:148:PRO:O	1:H:151:LEU:HB2	2.16	0.45
1:H:67:PRO:HG3	2:L:206:MET:O	2.17	0.45
3:M:55:LEU:HD12	3:M:55:LEU:HA	1.82	0.45
2:L:122:ALA:O	2:L:126:LEU:HD13	2.17	0.45
1:H:87:LEU:HD12	2:L:8:LYS:HA	1.99	0.45
1:H:177:ARG:HG2	1:H:177:ARG:NH1	2.32	0.45
1:H:177:ARG:HG2	1:H:177:ARG:HH11	1.83	0.44
2:L:6:GLU:OE2	2:L:10:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:269:LEU:HD12	2:L:269:LEU:HA	1.86	0.44
3:M:3:TYR:CE1	3:M:9:GLN:HG3	2.53	0.44
1:H:11:ASP:OD1	1:H:13:ALA:HB3	2.18	0.44
2:L:45:GLY:HA3	5:L:1284:BPH:H9C3	1.99	0.44
2:L:45:GLY:O	2:L:49:ILE:HG13	2.17	0.44
3:M:75:TRP:HB3	3:M:80:TRP:CE3	2.53	0.44
1:H:32:GLN:HG2	1:H:56:PHE:CD2	2.52	0.44
1:H:153:VAL:HG21	1:H:181:VAL:CG2	2.48	0.44
1:H:163:LYS:HB2	1:H:163:LYS:HZ2	1.81	0.44
2:L:220:VAL:O	2:L:220:VAL:HG22	2.17	0.44
1:H:35:ASN:OD1	3:M:260:ALA:HB1	2.17	0.44
1:H:245:ALA:N	1:H:246:PRO:CD	2.80	0.44
3:M:148:TRP:CE3	3:M:151:LEU:HD12	2.52	0.44
1:H:198:VAL:N	3:M:9:GLN:NE2	2.64	0.44
2:L:185:LEU:HD23	4:M:1302:BCL:H43	1.99	0.44
3:M:195:ASN:ND2	3:M:197:PHE:H	2.15	0.44
2:L:207:ARG:HA	2:L:207:ARG:HD2	1.79	0.43
4:L:1283:BCL:H193	4:L:1283:BCL:H162	1.80	0.43
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.01	0.43
2:L:183:ASN:ND2	3:M:213:ALA:HA	2.34	0.43
3:M:168:MET:HE3	3:M:289:THR:CA	2.46	0.43
1:H:202:ARG:HG2	1:H:203:VAL:N	2.34	0.43
1:H:87:LEU:HD11	2:L:8:LYS:HA	2.01	0.43
1:H:12:LEU:HD13	1:H:12:LEU:C	2.38	0.43
1:H:169:VAL:HG11	3:M:12:VAL:HG11	2.01	0.42
4:L:1283:BCL:HMD1	3:M:206:ILE:HD13	1.99	0.42
2:L:185:LEU:CD1	2:L:189:LEU:HD22	2.50	0.42
3:M:22:GLU:HB3	3:M:23:ASP:H	1.61	0.42
2:L:170:ASN:HB3	2:L:173:HIS:HB2	2.02	0.42
1:H:170:ASP:OD1	1:H:172:PRO:HD2	2.19	0.42
2:L:185:LEU:HD13	5:M:1304:BPH:ND	2.34	0.42
3:M:194:GLY:O	3:M:195:ASN:HB3	2.20	0.42
2:L:59:TRP:HA	2:L:59:TRP:CE3	2.54	0.41
2:L:100:TRP:O	2:L:104:GLU:HG3	2.20	0.41
3:M:218:MET:HG2	3:M:252:TRP:CH2	2.55	0.41
6:M:1305:U10:H4M2	6:M:1305:U10:H3M3	2.02	0.41
1:H:59:PRO:HG2	1:H:76:PRO:HG3	2.01	0.41
1:H:70:ARG:NH2	1:H:123:LEU:HD13	2.34	0.41
1:H:75:VAL:HA	1:H:76:PRO:C	2.41	0.41
3:M:4:GLN:NE2	3:M:4:GLN:HA	2.34	0.41
1:H:18:TYR:O	1:H:22:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:TYR:CE2	7:M:1306:CDL:H112	2.56	0.41
2:L:170:ASN:HB3	2:L:173:HIS:CB	2.50	0.41
2:L:265:TRP:O	2:L:269:LEU:HD13	2.20	0.41
3:M:168:MET:CE	3:M:289:THR:HG22	2.51	0.41
2:L:207:ARG:HG3	2:L:211:HIS:CG	2.55	0.41
1:H:73:LEU:HD11	1:H:75:VAL:CG1	2.51	0.41
4:M:1302:BCL:HHC	4:M:1302:BCL:HBB3	2.03	0.41
2:L:86:TRP:HZ2	2:L:132:VAL:HG22	1.84	0.41
3:M:295:TYR:O	3:M:299:GLN:HG2	2.21	0.41
1:H:190:LEU:HB2	1:H:233:ILE:HD13	2.03	0.40
3:M:152:SER:O	3:M:155:TRP:HB3	2.21	0.40
1:H:142:VAL:HG13	3:M:10:VAL:HG23	2.03	0.40
1:H:81:GLU:O	1:H:83:ARG:N	2.53	0.40
1:H:179:LEU:HG	1:H:193:MET:SD	2.62	0.40
1:H:95:GLY:O	2:L:24:PHE:HB2	2.21	0.40
3:M:265:ILE:HD12	3:M:265:ILE:HA	1.93	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	H	235/250 (94%)	226 (96%)	9 (4%)	0	100	100
2	L	279/281 (99%)	265 (95%)	12 (4%)	2 (1%)	22	23
3	M	300/307 (98%)	288 (96%)	12 (4%)	0	100	100
All	All	814/838 (97%)	779 (96%)	33 (4%)	2 (0%)	47	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	271	TRP

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Mol	Chain	Res	Type
2	L	270	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	192/201 (96%)	186 (97%)	6 (3%)	40	48
2	L	220/220 (100%)	206 (94%)	14 (6%)	17	18
3	M	236/240 (98%)	227 (96%)	9 (4%)	33	41
All	All	648/661 (98%)	619 (96%)	29 (4%)	27	33

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	58	LEU
1	H	163	LYS
1	H	202	ARG
1	H	208	LEU
1	H	231	ASP
1	H	247	LYS
2	L	10	ARG
2	L	85	LEU
2	L	102	LEU
2	L	129	LEU
2	L	167	PHE
2	L	189	LEU
2	L	195	LEU
2	L	207	ARG
2	L	216	PHE
2	L	235	LEU
2	L	238	LEU
2	L	270	PRO
2	L	271	TRP
2	L	272	TRP
3	M	26	LEU

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Mol	Chain	Res	Type
3	M	29	ARG
3	M	60	LEU
3	M	94	LEU
3	M	136	ARG
3	M	156	LEU
3	M	191	LEU
3	M	195	ASN
3	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	194	GLN
2	L	87	GLN
2	L	183	ASN
2	L	211	HIS
3	M	4	GLN
3	M	9	GLN
3	M	195	ASN
3	M	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
7	CDL	M	1306	-	69,69,99	1.20	3 (4%)	74,80,111	1.05	3 (4%)
4	BCL	L	1283	2	64,74,74	1.57	12 (18%)	78,115,115	1.84	20 (25%)
4	BCL	M	1302	3	49,59,74	1.66	11 (22%)	60,97,115	1.80	13 (21%)
5	BPH	M	1304	-	37,56,70	2.11	12 (32%)	35,84,101	3.21	18 (51%)
4	BCL	M	1303	3	64,74,74	1.52	11 (17%)	78,115,115	1.88	24 (30%)
5	BPH	L	1284	-	51,70,70	1.89	11 (21%)	52,101,101	2.73	22 (42%)
4	BCL	L	1282	2	64,74,74	1.46	9 (14%)	78,115,115	1.91	22 (28%)
6	U10	M	1305	-	38,38,63	1.96	13 (34%)	46,49,79	1.90	12 (26%)

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
7	CDL	M	1306	-	-	25/78/78/110	-
4	BCL	L	1283	2	-	14/37/137/137	-
4	BCL	M	1302	3	-	2/19/119/137	-
5	BPH	M	1304	-	-	6/21/89/105	0/5/6/6
4	BCL	M	1303	3	-	13/37/137/137	-
5	BPH	L	1284	-	-	14/37/105/105	0/5/6/6
4	BCL	L	1282	2	-	6/37/137/137	-
6	U10	M	1305	-	-	2/33/57/87	0/1/1/1

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BPH	C2C-C3C	-7.51	1.47	1.54
5	L	1284	BPH	C2C-C3C	-7.20	1.48	1.54
5	L	1284	BPH	C11-C10	-5.51	1.28	1.52
4	L	1282	BCL	MG-ND	5.47	2.16	2.05
7	M	1306	CDL	OA8-CA7	5.31	1.48	1.33
4	M	1303	BCL	MG-ND	5.28	2.16	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1283	BCL	MG-ND	5.15	2.16	2.05
4	M	1302	BCL	MG-ND	5.06	2.15	2.05
7	M	1306	CDL	OA6-CA5	4.96	1.48	1.34
6	M	1305	U10	O4-C4	4.90	1.48	1.36
7	M	1306	CDL	OB8-CB7	4.75	1.47	1.33
5	L	1284	BPH	O2D-CGD	4.41	1.44	1.33
5	L	1284	BPH	O2A-CGA	4.07	1.45	1.33
5	M	1304	BPH	O2A-CGA	4.03	1.45	1.33
5	M	1304	BPH	O2D-CGD	4.01	1.43	1.33
4	M	1303	BCL	C4D-ND	-3.54	1.32	1.37
6	M	1305	U10	C13-C14	3.54	1.41	1.33
4	L	1283	BCL	MG-NA	3.51	2.14	2.06
6	M	1305	U10	C7-C8	-3.37	1.45	1.50
4	M	1302	BCL	C4D-ND	-3.34	1.33	1.37
4	M	1303	BCL	MG-NA	3.33	2.14	2.06
6	M	1305	U10	C23-C24	3.33	1.41	1.33
5	M	1304	BPH	C3A-C2A	-3.29	1.51	1.54
4	L	1282	BCL	MG-NA	3.29	2.14	2.06
4	M	1302	BCL	MG-NA	3.27	2.14	2.06
4	L	1282	BCL	CHD-C1D	3.24	1.44	1.38
4	L	1283	BCL	C1B-NB	3.23	1.38	1.35
4	L	1283	BCL	C4D-ND	-3.19	1.33	1.37
4	M	1303	BCL	C1B-NB	3.13	1.38	1.35
6	M	1305	U10	C6-C1	3.10	1.40	1.35
6	M	1305	U10	O3-C3M	-3.05	1.38	1.45
4	L	1282	BCL	C1B-NB	3.04	1.37	1.35
6	M	1305	U10	O3-C3	2.98	1.44	1.36
4	M	1302	BCL	C3D-C4D	-2.95	1.37	1.44
5	M	1304	BPH	C2-C3	2.84	1.39	1.33
4	M	1303	BCL	C3D-C4D	-2.78	1.37	1.44
4	L	1283	BCL	C3D-C4D	-2.75	1.38	1.44
5	M	1304	BPH	CAA-C2A	2.71	1.60	1.54
6	M	1305	U10	C18-C19	2.69	1.39	1.33
5	M	1304	BPH	C1A-C2A	2.67	1.55	1.51
5	L	1284	BPH	C2-C3	2.64	1.39	1.33
5	L	1284	BPH	O2D-CED	-2.64	1.39	1.45
4	L	1282	BCL	C3D-C4D	-2.61	1.38	1.44
4	M	1303	BCL	CHD-C1D	2.59	1.43	1.38
6	M	1305	U10	C8-C9	2.58	1.39	1.33
4	L	1283	BCL	MG-NC	-2.57	2.00	2.06
4	M	1302	BCL	C1-C2	2.53	1.56	1.49
5	L	1284	BPH	C3A-C2A	-2.50	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1302	BCL	C1D-C2D	-2.50	1.40	1.45
5	M	1304	BPH	O2D-CED	-2.45	1.39	1.45
4	L	1283	BCL	CAA-CBA	2.45	1.60	1.52
4	M	1303	BCL	C3C-C4C	-2.42	1.48	1.51
4	M	1303	BCL	MG-NC	-2.42	2.00	2.06
4	L	1283	BCL	CAA-C2A	2.41	1.58	1.54
4	M	1303	BCL	CMD-C2D	2.40	1.55	1.50
4	L	1282	BCL	C4-C3	2.39	1.56	1.50
4	L	1283	BCL	CHD-C1D	2.39	1.43	1.38
5	M	1304	BPH	CHA-CBD	2.38	1.55	1.52
4	L	1282	BCL	C4D-ND	-2.37	1.34	1.37
5	L	1284	BPH	O1D-CGD	2.35	1.27	1.21
4	L	1282	BCL	CBB-CAB	2.33	1.56	1.49
5	L	1284	BPH	CHA-CBD	2.33	1.55	1.52
4	L	1282	BCL	CMD-C2D	2.31	1.55	1.50
4	M	1302	BCL	C1B-NB	2.29	1.37	1.35
4	L	1283	BCL	C1D-C2D	-2.25	1.40	1.45
4	M	1302	BCL	CAA-CBA	2.25	1.59	1.52
5	M	1304	BPH	O1D-CGD	2.25	1.26	1.21
4	M	1302	BCL	CAA-C2A	2.22	1.58	1.54
5	L	1284	BPH	CAA-C2A	2.19	1.58	1.54
4	M	1303	BCL	C4-C3	2.19	1.56	1.50
6	M	1305	U10	C15-C14	2.17	1.56	1.50
4	M	1302	BCL	CHD-C1D	2.12	1.42	1.38
4	L	1283	BCL	C4-C3	2.11	1.56	1.50
4	M	1303	BCL	C1-C2	2.10	1.55	1.49
4	M	1302	BCL	CBB-CAB	2.09	1.55	1.49
5	L	1284	BPH	C3D-C2D	-2.05	1.35	1.39
5	M	1304	BPH	CMA-C3A	2.04	1.57	1.53
6	M	1305	U10	C27-C28	-2.04	1.43	1.50
6	M	1305	U10	C28-C29	2.02	1.38	1.32
4	L	1283	BCL	C3C-C4C	-2.01	1.49	1.51
5	M	1304	BPH	C3D-C2D	-2.01	1.35	1.39
6	M	1305	U10	C20-C19	2.00	1.55	1.50

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1304	BPH	O2D-CGD-CBD	11.83	125.98	111.00
5	L	1284	BPH	O2D-CGD-CBD	11.22	125.22	111.00
4	L	1282	BCL	C4A-NA-C1A	-6.60	103.74	106.71
6	M	1305	U10	C3M-O3-C3	6.25	138.62	116.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BPH	C1-C2-C3	5.78	136.04	126.04
5	L	1284	BPH	C1-C2-C3	5.67	135.85	126.04
4	L	1283	BCL	C4A-NA-C1A	-5.65	104.17	106.71
4	M	1302	BCL	C4A-NA-C1A	-5.30	104.32	106.71
4	M	1303	BCL	C4A-NA-C1A	-5.04	104.44	106.71
5	L	1284	BPH	CBC-CAC-C3C	4.73	123.30	113.77
5	M	1304	BPH	O1D-CGD-CBD	-4.57	117.13	124.74
6	M	1305	U10	C27-C28-C29	4.50	143.12	127.75
4	L	1283	BCL	C1D-ND-C4D	4.36	109.43	106.33
5	M	1304	BPH	CMA-C3A-C4A	-4.32	104.92	114.38
4	M	1302	BCL	C1D-ND-C4D	4.30	109.39	106.33
5	L	1284	BPH	O1D-CGD-CBD	-4.30	117.58	124.74
4	L	1282	BCL	C1D-ND-C4D	4.28	109.38	106.33
4	M	1303	BCL	C1D-ND-C4D	4.26	109.36	106.33
5	L	1284	BPH	CED-O2D-CGD	4.24	125.53	115.94
5	M	1304	BPH	CED-O2D-CGD	4.24	125.52	115.94
4	M	1302	BCL	OBB-CAB-CBB	-4.09	110.96	120.17
4	L	1283	BCL	OBB-CAB-CBB	-4.06	111.03	120.17
4	L	1282	BCL	OBB-CAB-CBB	-4.00	111.16	120.17
5	L	1284	BPH	CMA-C3A-C4A	-3.98	105.67	114.38
5	M	1304	BPH	CBC-CAC-C3C	3.91	121.65	113.77
4	M	1303	BCL	OBB-CAB-CBB	-3.80	111.63	120.17
4	L	1282	BCL	CHD-C1D-ND	-3.69	121.06	124.45
6	M	1305	U10	O5-C5-C6	-3.66	115.13	121.55
4	L	1283	BCL	CHD-C1D-ND	-3.61	121.14	124.45
5	L	1284	BPH	C11-C10-C8	3.59	127.52	115.92
5	M	1304	BPH	O2D-CGD-O1D	-3.56	116.88	123.84
4	L	1283	BCL	C11-C12-C13	-3.55	104.45	115.92
4	M	1303	BCL	CHD-C1D-ND	-3.54	121.20	124.45
5	M	1304	BPH	C1C-C2C-C3C	3.53	106.20	102.84
4	M	1303	BCL	C4D-CHA-C1A	3.53	125.54	121.25
7	M	1306	CDL	OA6-CA5-C11	3.48	119.01	111.50
4	M	1302	BCL	C4D-CHA-C1A	3.48	125.49	121.25
5	L	1284	BPH	C6-C5-C3	3.48	122.58	113.45
5	L	1284	BPH	O2D-CGD-O1D	-3.40	117.18	123.84
5	L	1284	BPH	CAC-C3C-C4C	3.39	121.31	113.73
5	L	1284	BPH	C1C-C2C-C3C	3.38	106.05	102.84
4	M	1303	BCL	C11-C12-C13	-3.37	105.02	115.92
4	L	1283	BCL	C4D-CHA-C1A	3.35	125.33	121.25
5	L	1284	BPH	C4C-C3C-C2C	3.33	106.01	102.84
4	M	1302	BCL	CHD-C1D-ND	-3.32	121.40	124.45
5	M	1304	BPH	CAA-C2A-C3A	-3.29	103.78	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	1282	BCL	CAC-C3C-C4C	-3.29	105.29	112.58
4	L	1282	BCL	CMB-C2B-C3B	3.27	130.80	124.68
4	L	1283	BCL	CMB-C2B-C3B	3.23	130.71	124.68
4	L	1283	BCL	C2C-C3C-C4C	3.16	106.07	101.34
4	L	1282	BCL	C7-C6-C5	-3.10	104.94	113.36
6	M	1305	U10	O2-C2-C3	-3.09	114.38	120.93
4	L	1283	BCL	CAA-C2A-C3A	-3.05	104.43	112.78
6	M	1305	U10	C20-C19-C21	-3.04	110.16	115.27
4	L	1282	BCL	C4D-CHA-C1A	3.04	124.95	121.25
4	M	1302	BCL	C2C-C3C-C4C	3.00	105.84	101.34
5	M	1304	BPH	C4C-C3C-C2C	3.00	105.69	102.84
4	L	1283	BCL	C7-C6-C5	-2.95	105.34	113.36
5	L	1284	BPH	CAA-C2A-C3A	-2.95	104.71	112.78
4	M	1303	BCL	CAC-C3C-C4C	-2.94	106.06	112.58
4	M	1302	BCL	CHA-C1A-NA	-2.93	119.68	126.40
5	L	1284	BPH	CMB-C2B-C3B	2.93	130.15	124.68
4	M	1303	BCL	CMB-C2B-C3B	2.89	130.09	124.68
4	M	1303	BCL	CHA-C1A-NA	-2.89	119.78	126.40
5	M	1304	BPH	CMA-C3A-C2A	-2.86	102.47	113.99
4	M	1303	BCL	CBC-CAC-C3C	-2.84	107.14	113.47
5	M	1304	BPH	CMB-C2B-C3B	2.84	129.99	124.68
4	L	1283	BCL	CHA-C1A-NA	-2.83	119.91	126.40
4	L	1282	BCL	CAA-C2A-C3A	-2.82	105.06	112.78
5	M	1304	BPH	C4-C3-C5	2.80	119.19	115.98
4	M	1303	BCL	CAC-C3C-C2C	-2.80	107.27	114.26
7	M	1306	CDL	OA8-CA7-C31	2.78	120.63	111.91
4	M	1302	BCL	CMB-C2B-C3B	2.77	129.87	124.68
4	L	1282	BCL	CMB-C2B-C1B	-2.77	124.21	128.46
4	L	1283	BCL	CMB-C2B-C1B	-2.77	124.21	128.46
4	M	1302	BCL	CAA-C2A-C3A	-2.76	105.23	112.78
4	L	1282	BCL	CHA-C1A-NA	-2.71	120.20	126.40
4	L	1282	BCL	C11-C12-C13	-2.70	107.19	115.92
4	L	1282	BCL	O1D-CGD-CBD	2.65	129.91	124.48
5	L	1284	BPH	CMA-C3A-C2A	-2.63	103.41	113.99
4	L	1282	BCL	CAC-C3C-C2C	-2.61	107.73	114.26
6	M	1305	U10	C1-C6-C5	-2.53	117.20	119.58
6	M	1305	U10	C21-C19-C18	2.50	126.18	121.12
4	M	1303	BCL	C7-C6-C5	-2.50	106.57	113.36
6	M	1305	U10	C16-C14-C13	2.49	126.16	121.12
4	M	1303	BCL	CMB-C2B-C1B	-2.46	124.68	128.46
4	L	1283	BCL	CBB-CAB-C3B	2.46	127.65	120.34
4	M	1302	BCL	CMB-C2B-C1B	-2.41	124.75	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1284	BPH	C6-C7-C8	-2.41	108.11	115.92
4	M	1303	BCL	C2C-C3C-C4C	2.40	104.93	101.34
4	M	1303	BCL	C4-C3-C5	2.40	119.30	115.27
4	L	1282	BCL	O2D-CGD-CBD	-2.39	107.02	111.27
4	L	1283	BCL	C1-C2-C3	-2.38	121.92	126.04
6	M	1305	U10	C6-C1-C2	2.38	121.06	119.18
6	M	1305	U10	C31-C29-C30	-2.37	109.36	114.60
7	M	1306	CDL	OB8-CB7-C71	2.37	119.34	111.91
4	M	1302	BCL	CBB-CAB-C3B	2.36	127.36	120.34
6	M	1305	U10	C7-C8-C9	2.36	130.72	126.79
5	L	1284	BPH	CMD-C2D-C3D	2.36	129.10	124.68
4	M	1303	BCL	C15-C13-C12	2.34	124.44	112.13
5	L	1284	BPH	OBD-CAD-CBD	-2.33	122.41	125.82
4	M	1303	BCL	O1D-CGD-CBD	2.33	129.24	124.48
5	L	1284	BPH	O2A-C1-C2	-2.31	102.58	108.64
4	L	1283	BCL	CAC-C3C-C4C	-2.30	107.49	112.58
4	L	1282	BCL	C12-C11-C10	-2.29	102.72	113.24
5	L	1284	BPH	O2A-CGA-O1A	-2.29	117.83	123.59
4	L	1282	BCL	C2C-C3C-C4C	2.28	104.75	101.34
4	L	1283	BCL	C12-C11-C10	-2.27	102.83	113.24
5	L	1284	BPH	C5-C3-C2	-2.26	116.53	121.12
4	M	1303	BCL	CBB-CAB-C3B	2.24	127.00	120.34
4	M	1303	BCL	C4D-C3D-CAD	-2.24	105.46	108.10
4	L	1282	BCL	C16-C15-C13	-2.23	108.70	115.92
4	L	1283	BCL	C16-C15-C13	-2.23	108.72	115.92
4	L	1282	BCL	CHD-C1D-C2D	2.20	130.10	125.48
4	L	1282	BCL	CBC-CAC-C3C	-2.20	108.56	113.47
5	M	1304	BPH	O2A-CGA-O1A	-2.19	118.07	123.59
5	M	1304	BPH	O2A-C1-C2	-2.18	102.91	108.64
4	M	1302	BCL	CMD-C2D-C3D	2.18	132.62	127.61
5	M	1304	BPH	CMD-C2D-C3D	2.16	128.72	124.68
4	L	1282	BCL	C4D-C3D-CAD	-2.14	105.58	108.10
4	M	1303	BCL	CED-O2D-CGD	2.14	120.77	115.94
4	L	1283	BCL	C4D-C3D-CAD	-2.11	105.61	108.10
4	L	1283	BCL	CHD-C1D-C2D	2.11	129.90	125.48
5	M	1304	BPH	OBD-CAD-CBD	-2.10	122.73	125.82
4	M	1303	BCL	CGD-CBD-CAD	-2.10	103.92	110.73
5	L	1284	BPH	C7-C6-C5	-2.09	107.68	113.36
6	M	1305	U10	C7-C6-C5	-2.09	115.97	118.48
5	M	1304	BPH	C4A-C3A-C2A	2.07	104.81	102.84
4	M	1302	BCL	C4D-C3D-CAD	-2.07	105.66	108.10
4	M	1303	BCL	CAA-C2A-C1A	2.06	118.72	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1303	BCL	CMD-C2D-C3D	2.06	132.34	127.61
4	M	1303	BCL	CHD-C1D-C2D	2.03	129.75	125.48
4	L	1282	BCL	CBB-CAB-C3B	2.03	126.37	120.34
4	L	1283	BCL	CMD-C2D-C3D	2.02	132.27	127.61

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1283	BCL	C2C-C3C-CAC-CBC
5	M	1304	BPH	C4C-C3C-CAC-CBC
5	M	1304	BPH	C2C-C3C-CAC-CBC
7	M	1306	CDL	CA2-OA2-PA1-OA3
7	M	1306	CDL	OB6-CB4-CB6-OB8
4	M	1303	BCL	C3-C5-C6-C7
7	M	1306	CDL	O1-C1-CB2-OB2
7	M	1306	CDL	CA2-C1-CB2-OB2
7	M	1306	CDL	CB3-CB4-CB6-OB8
4	M	1303	BCL	C15-C16-C17-C18
4	M	1303	BCL	C12-C13-C15-C16
5	L	1284	BPH	C8-C10-C11-C12
7	M	1306	CDL	CA2-OA2-PA1-OA5
4	L	1283	BCL	C16-C17-C18-C20
7	M	1306	CDL	C78-C79-C80-C81
4	M	1303	BCL	C16-C17-C18-C19
7	M	1306	CDL	C11-C12-C13-C14
7	M	1306	CDL	C31-C32-C33-C34
7	M	1306	CDL	C34-C35-C36-C37
4	M	1303	BCL	C16-C17-C18-C20
5	L	1284	BPH	O2A-C1-C2-C3
7	M	1306	CDL	C17-C18-C19-C20
4	L	1282	BCL	C11-C10-C8-C7
4	L	1282	BCL	C2A-CAA-CBA-CGA
4	M	1303	BCL	C4-C3-C5-C6
4	M	1303	BCL	C14-C13-C15-C16
5	L	1284	BPH	C11-C12-C13-C14
4	L	1283	BCL	C1A-C2A-CAA-CBA
4	L	1283	BCL	C15-C16-C17-C18
7	M	1306	CDL	OA5-CA3-CA4-CA6
4	L	1283	BCL	C11-C12-C13-C15
4	M	1303	BCL	C11-C10-C8-C7
5	L	1284	BPH	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
5	L	1284	BPH	C11-C12-C13-C15
7	M	1306	CDL	C39-C40-C41-C42
4	L	1283	BCL	C16-C17-C18-C19
4	M	1303	BCL	C11-C10-C8-C9
5	M	1304	BPH	C4-C3-C5-C6
7	M	1306	CDL	C40-C41-C42-C43
5	L	1284	BPH	C12-C13-C15-C16
5	L	1284	BPH	C15-C16-C17-C18
4	L	1282	BCL	CAD-CBD-CGD-O2D
4	M	1302	BCL	CAD-CBD-CGD-O2D
5	L	1284	BPH	CAD-CBD-CGD-O2D
4	M	1303	BCL	C13-C15-C16-C17
6	M	1305	U10	C5-C4-O4-C4M
7	M	1306	CDL	CA3-CA4-CA6-OA8
4	M	1303	BCL	C6-C7-C8-C9
7	M	1306	CDL	CA2-OA2-PA1-OA4
5	M	1304	BPH	C2-C3-C5-C6
4	L	1282	BCL	C3-C5-C6-C7
4	L	1282	BCL	C12-C13-C15-C16
4	M	1303	BCL	C6-C7-C8-C10
7	M	1306	CDL	C16-C17-C18-C19
7	M	1306	CDL	C77-C78-C79-C80
4	M	1303	BCL	C2-C3-C5-C6
4	L	1283	BCL	C11-C10-C8-C9
5	L	1284	BPH	C6-C7-C8-C9
5	L	1284	BPH	C14-C13-C15-C16
7	M	1306	CDL	OA5-CA3-CA4-OA6
7	M	1306	CDL	CB2-OB2-PB2-OB5
5	M	1304	BPH	O2A-C1-C2-C3
5	L	1284	BPH	C2C-C3C-CAC-CBC
7	M	1306	CDL	CA5-C11-C12-C13
4	L	1283	BCL	C11-C10-C8-C7
4	L	1283	BCL	C4C-C3C-CAC-CBC
5	L	1284	BPH	C2-C3-C5-C6
4	L	1283	BCL	C13-C15-C16-C17
7	M	1306	CDL	C80-C81-C82-C83
7	M	1306	CDL	C71-C72-C73-C74
4	L	1283	BCL	C11-C12-C13-C14
5	M	1304	BPH	CAD-CBD-CGD-O2D
4	L	1283	BCL	CHA-CBD-CGD-O1D
4	L	1283	BCL	CHA-CBD-CGD-O2D
4	L	1282	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
4	L	1283	BCL	C2A-CAA-CBA-CGA
7	M	1306	CDL	C32-C33-C34-C35
7	M	1306	CDL	C12-C11-CA5-OA6
5	L	1284	BPH	C4-C3-C5-C6
4	M	1302	BCL	C2C-C3C-CAC-CBC
5	L	1284	BPH	C11-C10-C8-C7
6	M	1305	U10	C3-C4-O4-C4M

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1306	CDL	3	0
4	L	1283	BCL	4	0
4	M	1302	BCL	4	0
5	M	1304	BPH	3	0
4	M	1303	BCL	7	0
5	L	1284	BPH	5	0
4	L	1282	BCL	4	0
6	M	1305	U10	1	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 then 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 CDL M 1306

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 1283

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH M 1304

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH L 1284

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 1282

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 M 1305

Bond lengths

Bond angles

Torsions

Rings

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	H	237/250 (94%)	0.11	9 (3%)	40	53	28, 43, 58, 90	8 (3%)
2	L	281/281 (100%)	0.07	14 (4%)	28	41	24, 36, 64, 79	1 (0%)
3	M	301/307 (98%)	0.11	14 (4%)	31	44	23, 36, 58, 85	4 (1%)
All	All	819/838 (97%)	0.10	37 (4%)	33	46	23, 39, 59, 90	13 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	281	GLY	5.5
1	H	245	ALA	5.1
2	L	270	PRO	4.9
2	L	51	TRP	4.6
2	L	59	TRP	4.4
1	H	247	LYS	4.3
1	H	246	PRO	4.3
3	M	38	LEU	3.9
3	M	302	GLY	3.7
3	M	68	PHE	3.6
2	L	277	GLY	3.4
2	L	265	TRP	3.3
3	M	3	TYR	3.2
3	M	301	HIS	3.0
2	L	268	LYS	2.7
2	L	54	VAL	2.6
3	M	100	GLU	2.6
3	M	27	ALA	2.6
2	L	47	ILE	2.5
1	H	82	ASP	2.4
2	L	274	ASN	2.4
1	H	78	PRO	2.4
2	L	63	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	186	GLY	2.4
1	H	18	TYR	2.3
2	L	271	TRP	2.3
3	M	106	ALA	2.2
2	L	40	PHE	2.2
1	H	200	SER	2.2
3	M	72	ILE	2.1
3	M	270	ILE	2.1
3	M	80	TRP	2.1
3	M	215	LEU	2.1
3	M	76	TYR	2.1
2	L	1	ALA	2.1
1	H	187	SER	2.1
3	M	105	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
7	CDL	M	1306	70/100	0.79	0.33	41,70,80,83	0
4	BCL	L	1282	66/66	0.92	0.16	25,32,45,56	0
4	BCL	M	1303	66/66	0.93	0.16	26,31,53,57	0
9	CL	M	1308	1/1	0.93	0.26	48,48,48,48	0
5	BPH	L	1284	65/65	0.94	0.19	24,29,47,50	0
5	BPH	M	1304	51/65	0.94	0.15	27,33,52,56	0
6	U10	M	1305	38/63	0.94	0.21	28,34,62,64	0
4	BCL	M	1302	51/66	0.94	0.15	27,32,47,51	0
4	BCL	L	1283	66/66	0.94	0.15	26,32,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FE2	M	1307	1/1	1.00	0.12	28,28,28,28	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 CDL M 1306:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
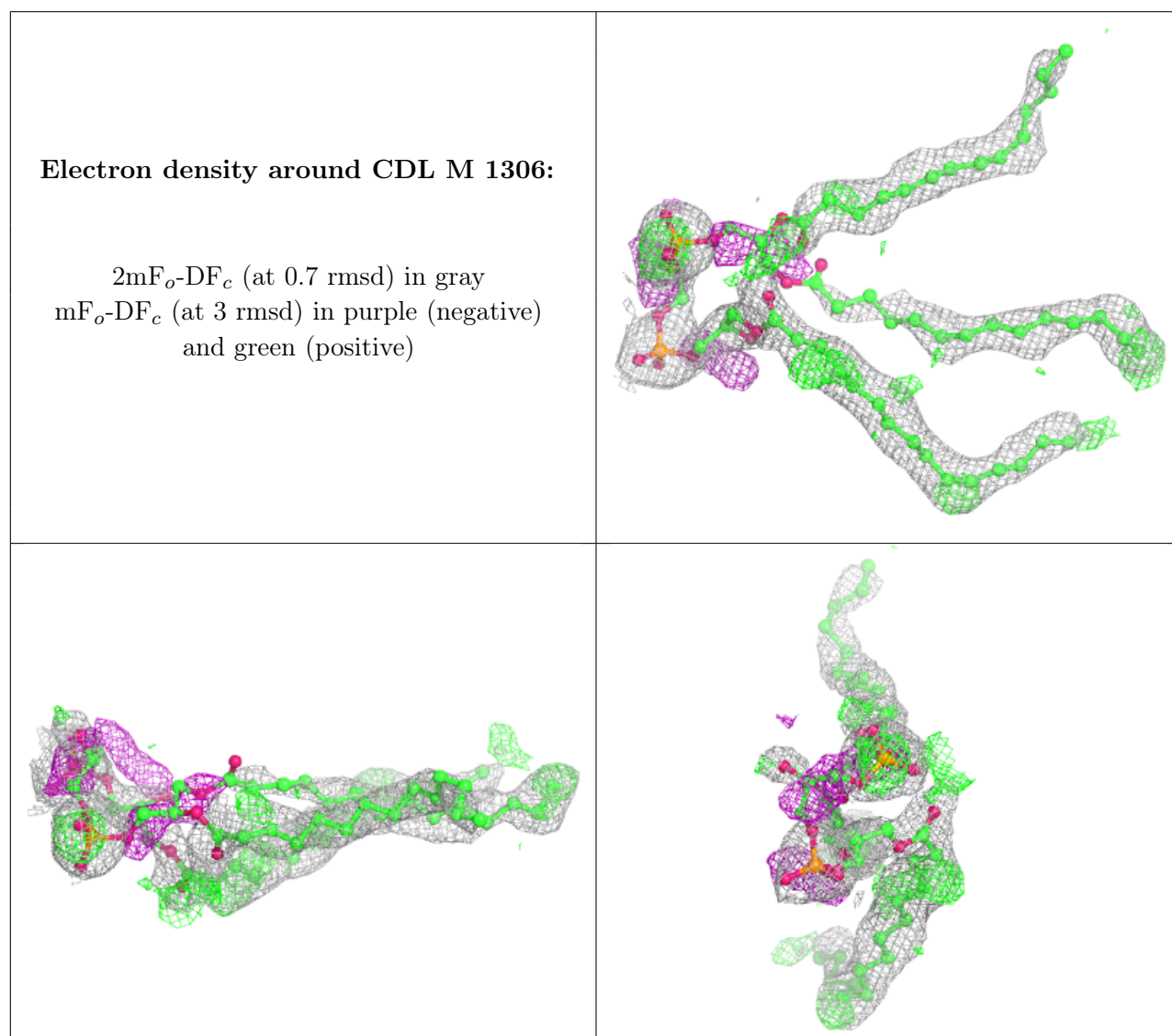
Electron density around BCL L 1282:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
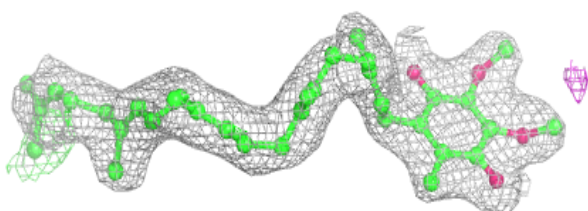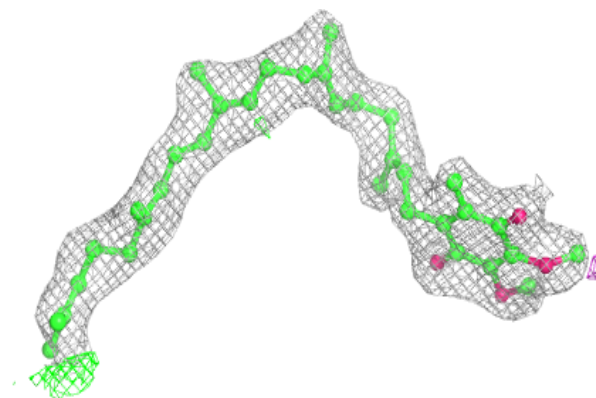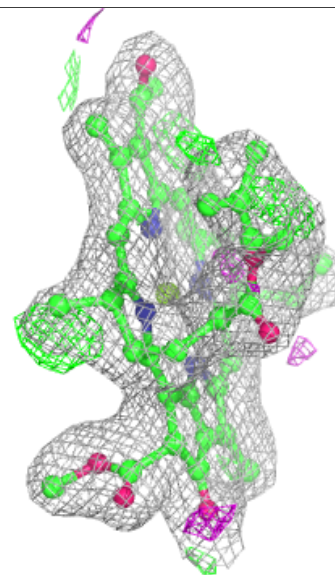mF_o-DF_c (at 3 rmsd) in purple (negative)
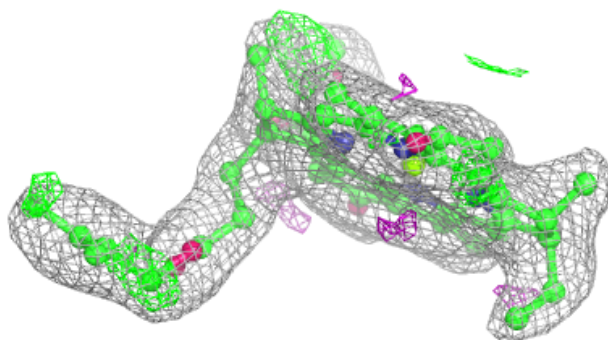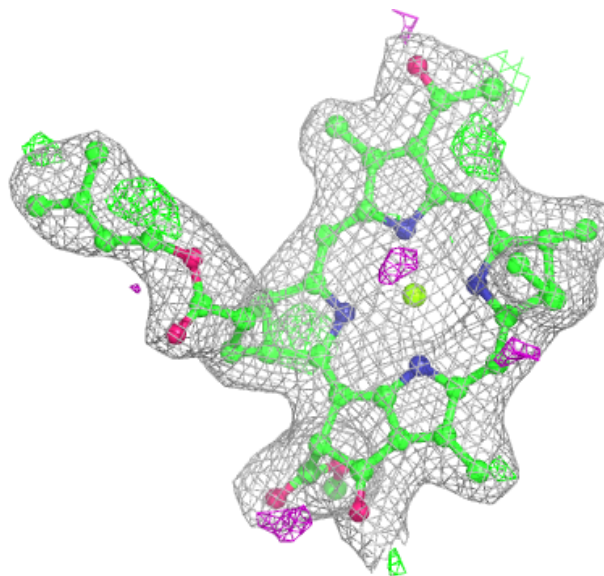and green (positive)
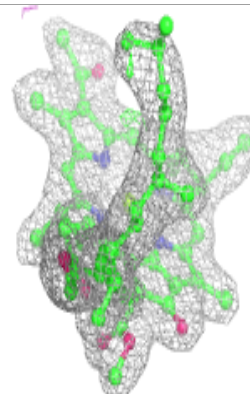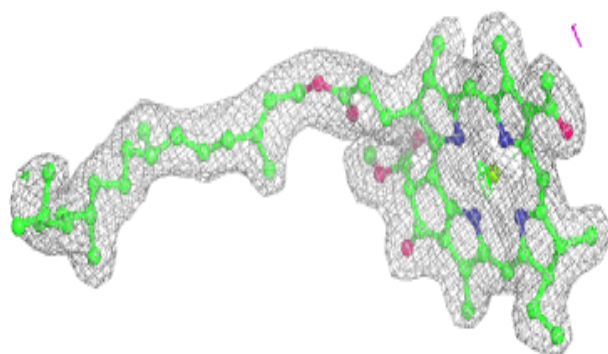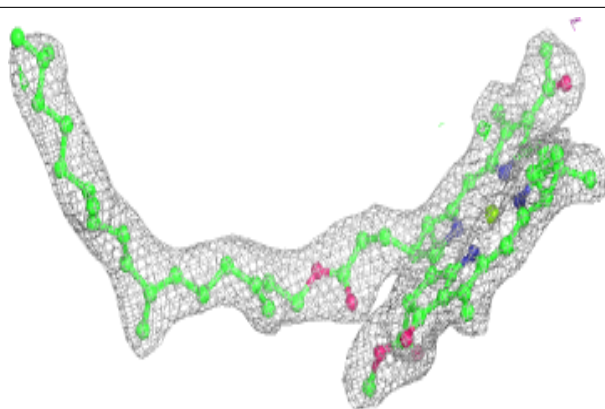
Electron density around BCL M 1303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
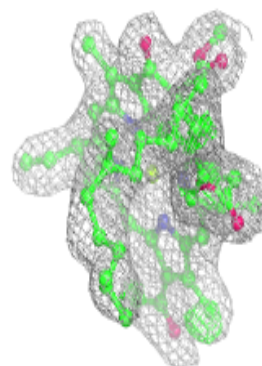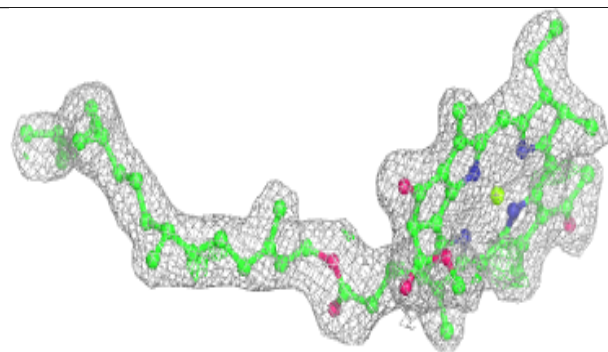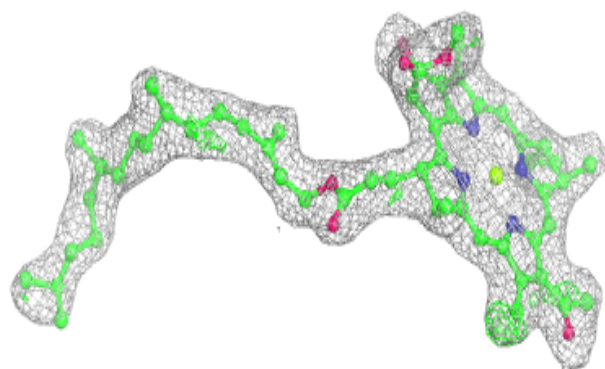
Electron density around BPH L 1284:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
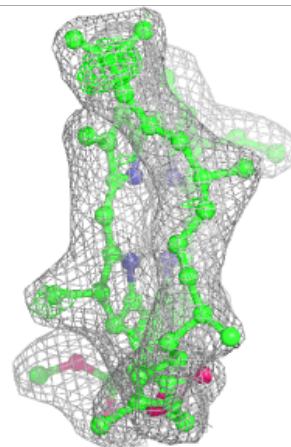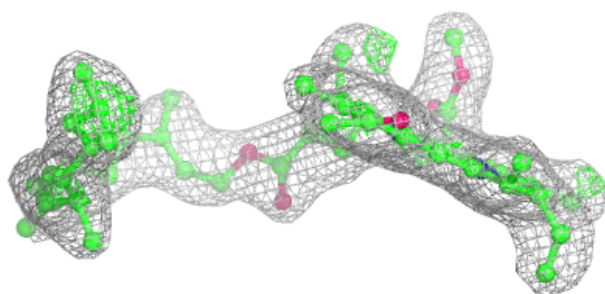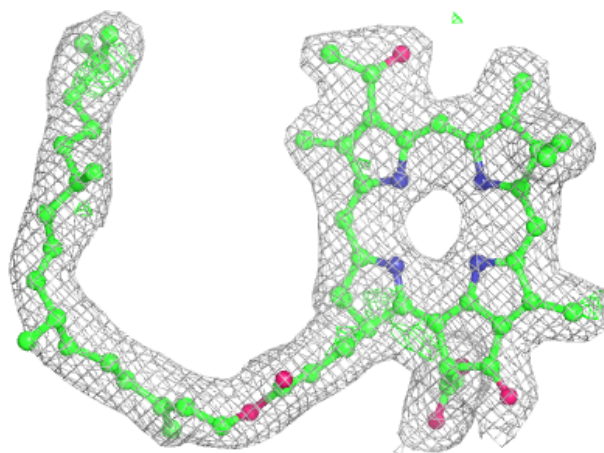
Electron density around BPH M 1304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
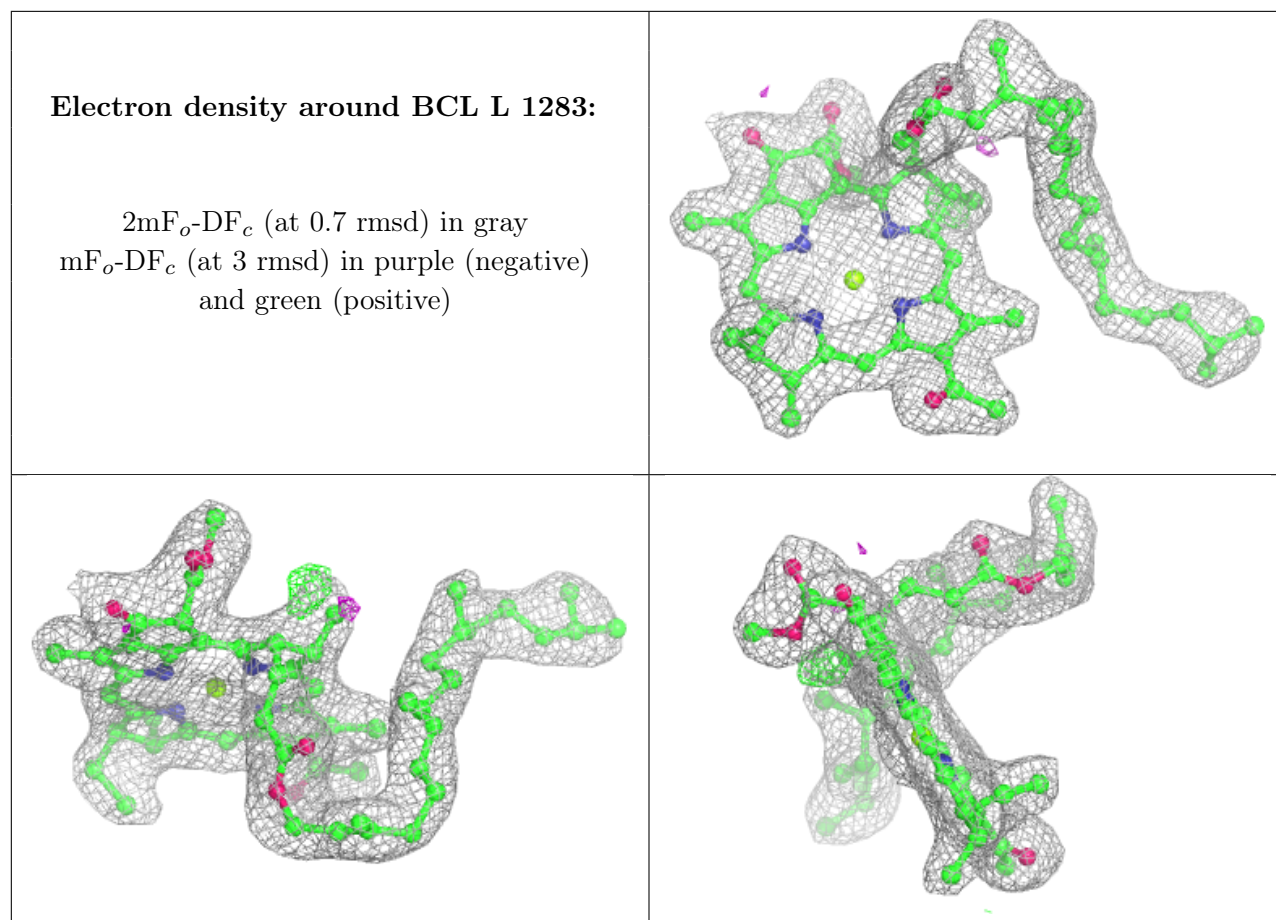and green (positive)
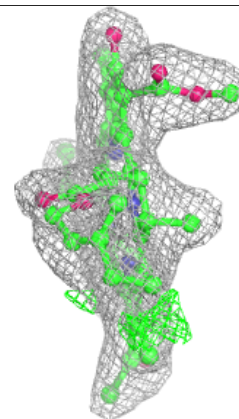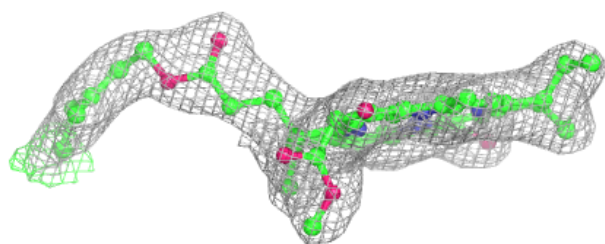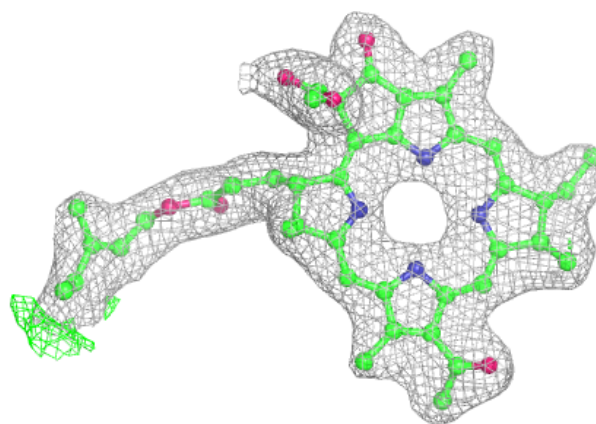
Electron density around U10 M 1305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
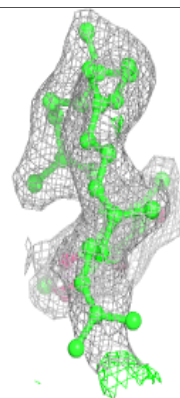
Electron density around BCL M 1302:

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 L 1283:

$2mF_o$-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 ⓘ

There are no such residues in this entry.