W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 03:18 pm BST

PDB ID	:	2J8C
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 8 in the neutral state
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2006-10-24
Resolution	:	1.87 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		2.6%
RSRZ outliers		2.8%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
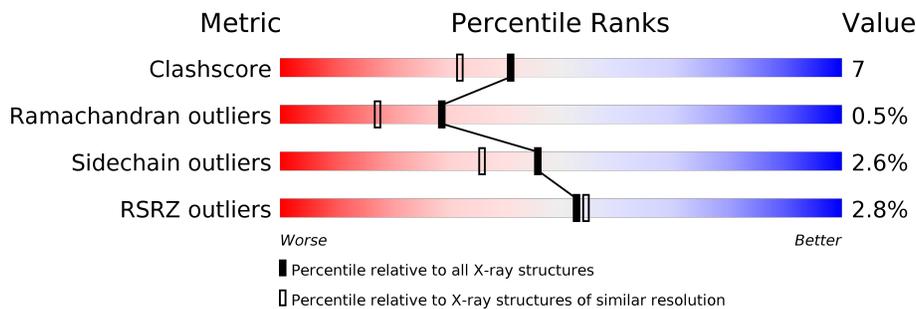
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	260	2% 82% 10% • 7%
2	L	281	2% 92% 7% •
3	M	307	3% 88% 10% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HTO	L	1291	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	PC1	M	1312	X	-	-	-
4	GOL	H	1251	-	-	X	-
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 7774 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	241	Total 1850	C 1183	N 321	O 337	S 9	0	5	1

- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total 2239	C 1513	N 355	O 363	S 8	0	2	0

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total 2411	C 1607	N 396	O 398	S 10	0	1	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
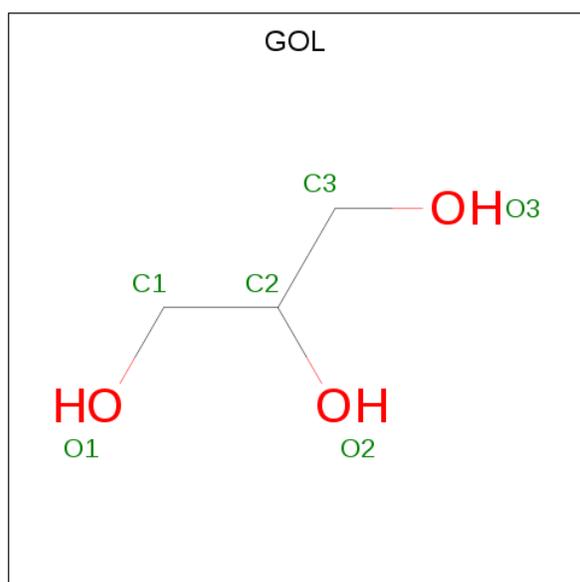
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	L	1	Total 6	C 3	O 3	0	0
4	L	1	Total 6	C 3	O 3	0	0
4	L	1	Total 6	C 3	O 3	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).

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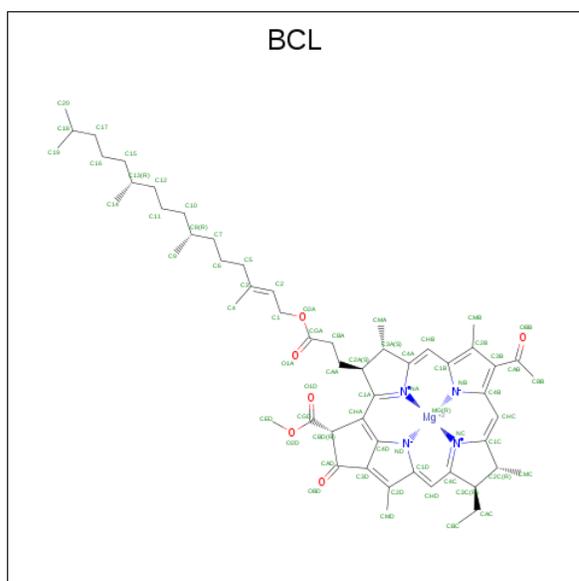
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

$C_{14}H_{31}NO$).
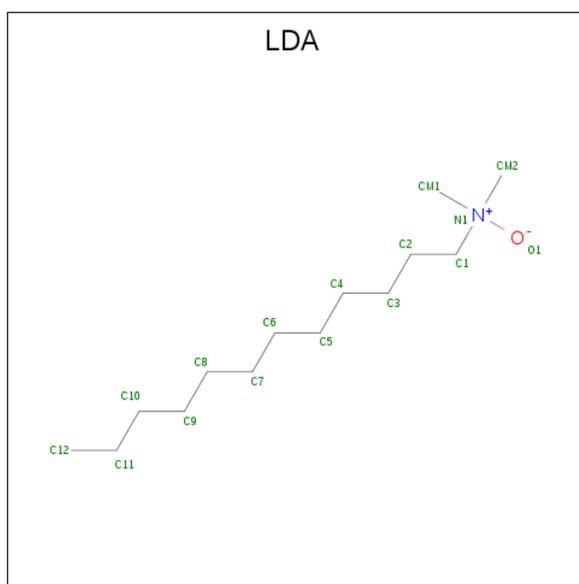
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).
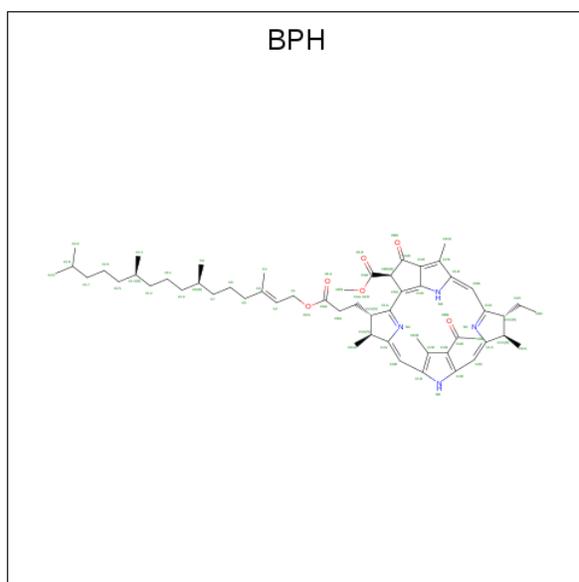
BPH

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

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).
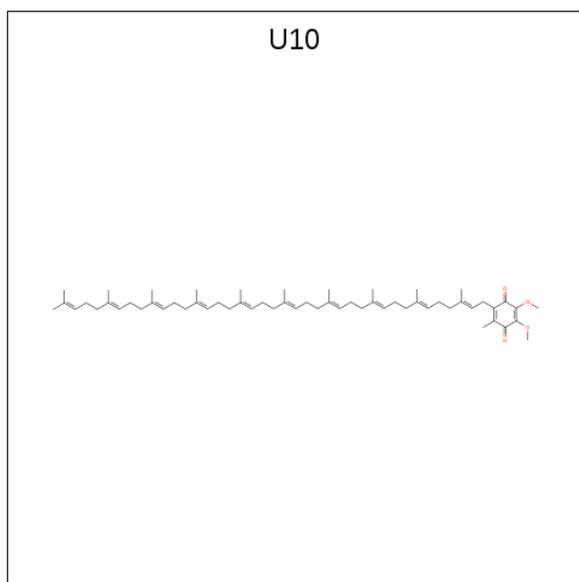
U10

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		
8	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
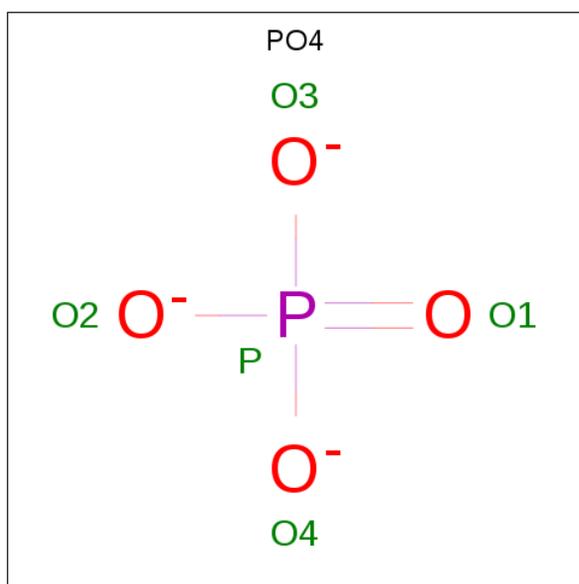
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total 5	O 4	P 1	0	0

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).
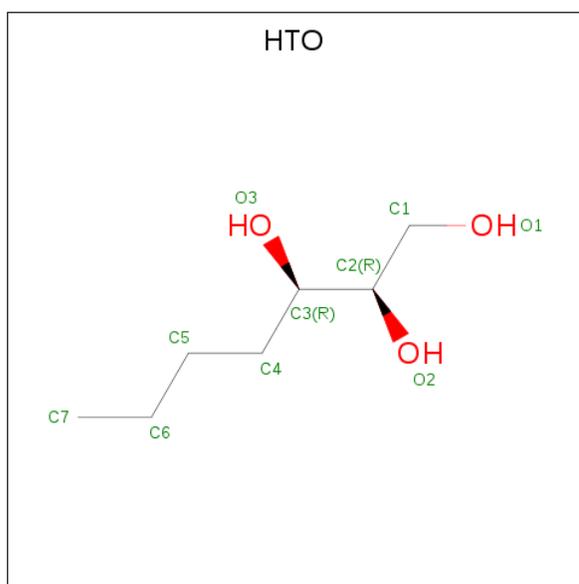
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total 10	C 7	O 3	0	0
10	L	1	Total 10	C 7	O 3	0	0

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).
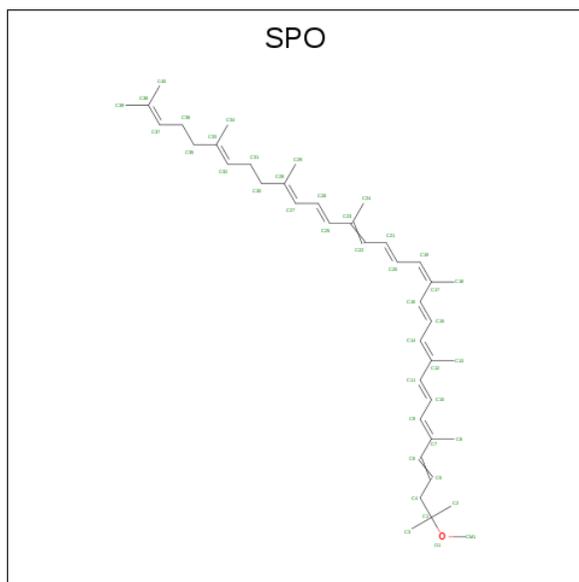
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total 42	C 41	O 1	0	0

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).
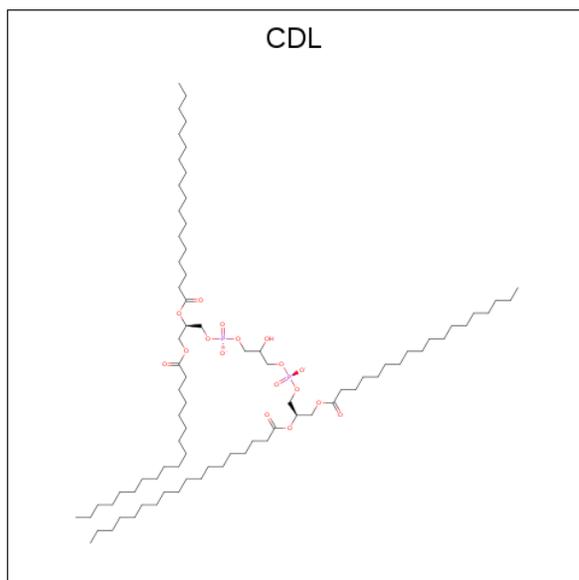
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
13	M	1	81	62	17	2	0	0

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).
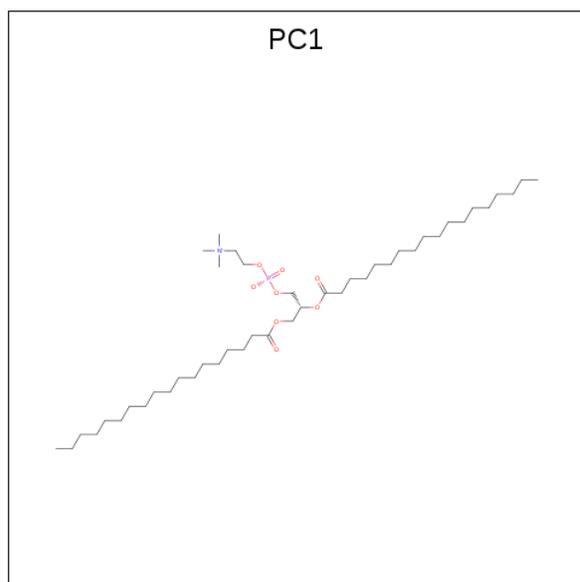
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	M	1	43	33	1	8	1	0	0

- Molecule 15 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY]-1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula: $C_{52}H_{94}O_{15}$).

GGD
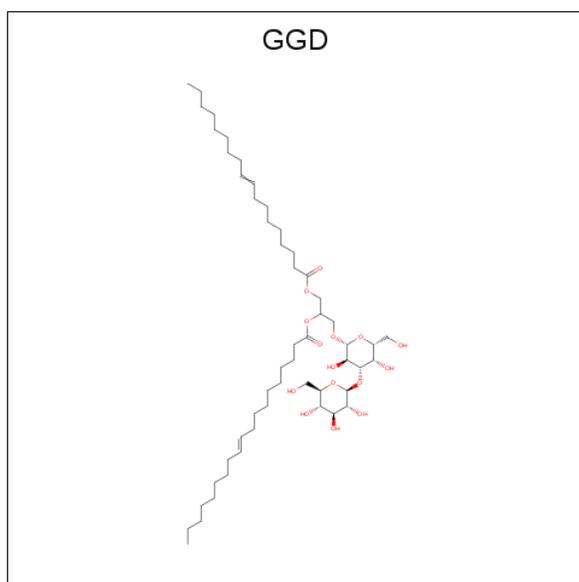
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total 57	C 42	O 15	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	172	Total 172	O 172	0	0
16	L	116	Total 116	O 116	0	0
16	M	127	Total 127	O 127	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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
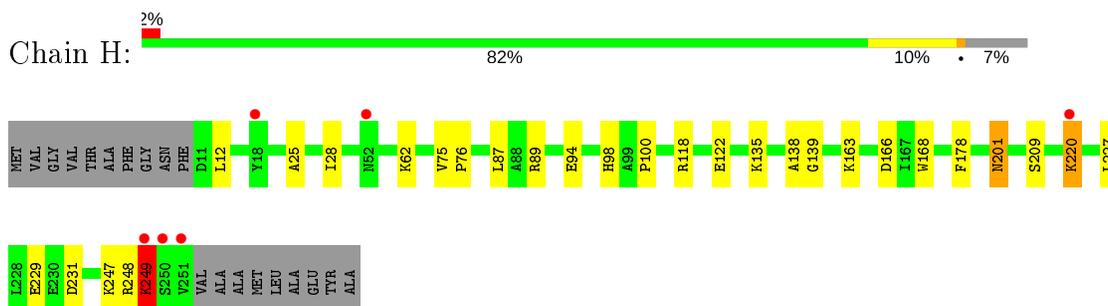
• Molecule 2: REACTION CENTER PROTEIN L CHAIN
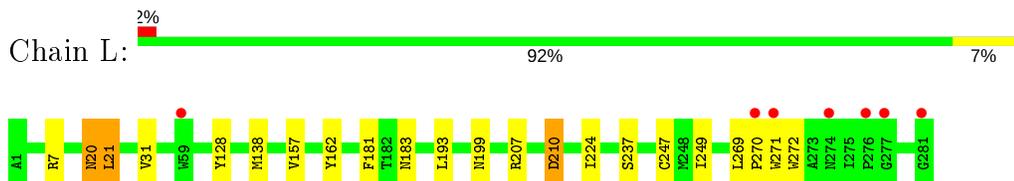
• Molecule 3: REACTION CENTER PROTEIN M CHAIN
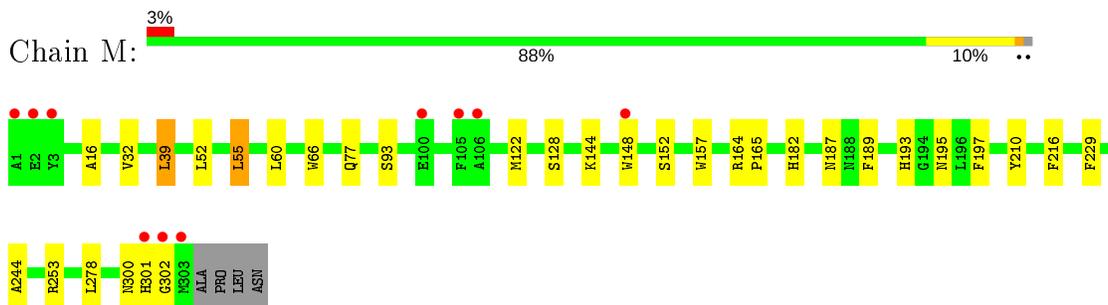
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.69Å 138.69Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 1.87 29.81 – 1.87	Depositor EDS
% Data completeness (in resolution range)	87.0 (119.52-1.87) 87.0 (29.81-1.87)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.196 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 70.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7774	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: BCL, GOL, LDA, GGD, CDL, BPH, PO4, PC1, HTO, FE, SPO, U10

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	0.63	0/1930	0.70	1/2621 (0.0%)
2	L	0.66	0/2339	0.61	1/3203 (0.0%)
3	M	0.65	0/2508	0.64	0/3424
All	All	0.65	0/6777	0.65	2/9248 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	139	GLY	N-CA-C	-5.27	99.92	113.10
2	L	210	ASP	CB-CG-OD1	5.25	123.03	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	138	ALA	Peptide

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	1850	0	1873	29	0
2	L	2239	0	2185	20	0
3	M	2411	0	2319	23	0
4	H	24	0	32	7	0
4	L	18	0	24	2	0
5	L	132	0	147	6	0
5	M	132	0	148	16	0
6	L	48	0	93	0	0
6	M	32	0	62	2	0
7	L	65	0	76	4	0
7	M	65	0	76	12	0
8	L	46	0	46	4	0
8	M	48	0	63	1	0
9	L	5	0	0	0	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	42	0	60	4	0
13	M	81	0	90	8	0
14	M	43	0	60	0	0
15	M	57	0	67	2	0
16	H	172	0	0	4	1
16	L	116	0	0	1	0
16	M	127	0	0	1	0
All	All	7774	0	7453	105	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 7.

The worst 5 of 105 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:248:ARG:HA	1:H:249[A]:LYS:HB2	1.33	1.06
7:M:1308:BPH:HBB3	7:M:1308:BPH:HHC	1.39	1.01
4:H:1251:GOL:H32	16:H:2002:HOH:O	1.67	0.93
7:L:1286:BPH:HBB3	7:L:1286:BPH:HHC	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1282:BCL:HHC	5:L:1282:BCL:HBB2	1.59	0.85

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)
16:H:2039:HOH:O	16:H:2039:HOH:O[4_555]	1.66	0.54

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	245/260 (94%)	241 (98%)	2 (1%)	2 (1%)	19	9
2	L	281/281 (100%)	275 (98%)	5 (2%)	1 (0%)	34	22
3	M	302/307 (98%)	293 (97%)	7 (2%)	2 (1%)	22	11
All	All	828/848 (98%)	809 (98%)	14 (2%)	5 (1%)	29	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	301	HIS
3	M	195	ASN
2	L	31	VAL

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	200/208 (96%)	190 (95%)	10 (5%)	24	13
2	L	221/220 (100%)	215 (97%)	6 (3%)	44	34
3	M	237/240 (99%)	232 (98%)	5 (2%)	53	45
All	All	658/668 (98%)	637 (97%)	21 (3%)	46	27

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	249[B]	LYS
2	L	21	LEU
3	M	52	LEU
1	H	249[A]	LYS
3	M	55	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
2	L	264	GLN
3	M	77	GLN
2	L	159	ASN
3	M	4	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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
9	PO4	L	1289	-	4,4,4	1.04	0	6,6,6	0.75	0
5	BCL	M	1304	3	58,74,74	2.19	9 (15%)	69,115,115	2.02	19 (27%)
4	GOL	L	1292	-	5,5,5	0.46	0	5,5,5	0.86	0
5	BCL	L	1282	2	58,74,74	2.06	10 (17%)	69,115,115	2.08	20 (28%)
5	BCL	M	1303	3	58,74,74	2.06	9 (15%)	69,115,115	1.82	11 (15%)
12	SPO	M	1310	-	40,41,41	3.83	12 (30%)	47,50,50	2.27	20 (42%)
10	HTO	L	1290	-	9,9,9	0.29	0	10,10,10	0.79	1 (10%)
14	PC1	M	1312	-	42,42,53	1.74	8 (19%)	48,50,61	1.32	6 (12%)
4	GOL	L	1293	-	5,5,5	0.41	0	5,5,5	0.27	0
6	LDA	M	1306	-	12,15,15	2.01	1 (8%)	14,17,17	0.54	0
8	U10	L	1287[B]	-	23,23,63	2.70	8 (34%)	28,31,79	1.27	3 (10%)
8	U10	M	1309	-	48,48,63	2.54	11 (22%)	58,61,79	1.59	11 (18%)
8	U10	L	1287[A]	-	23,23,63	2.49	8 (34%)	28,31,79	1.89	7 (25%)
4	GOL	H	1252	-	5,5,5	0.43	0	5,5,5	0.39	0
6	LDA	M	1305	-	12,15,15	2.03	1 (8%)	14,17,17	0.48	0
6	LDA	L	1283	-	12,15,15	2.02	1 (8%)	14,17,17	0.45	0
5	BCL	L	1288	2	58,74,74	2.05	8 (13%)	69,115,115	2.04	19 (27%)
7	BPH	L	1286	-	64,70,70	2.71	16 (25%)	76,101,101	1.62	16 (21%)
10	HTO	L	1291	-	9,9,9	0.33	0	10,10,10	0.87	1 (10%)
13	CDL	M	1311	-	79,79,99	1.89	16 (20%)	84,90,111	2.71	14 (16%)
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.25	0
6	LDA	L	1285	-	12,15,15	2.07	1 (8%)	14,17,17	0.58	0
4	GOL	H	1251	-	5,5,5	0.48	0	5,5,5	0.81	0
7	BPH	M	1308	-	64,70,70	2.84	16 (25%)	76,101,101	1.70	13 (17%)
4	GOL	H	1253	-	5,5,5	0.36	0	5,5,5	0.19	0
6	LDA	L	1284	-	12,15,15	2.03	1 (8%)	14,17,17	0.45	0
15	GGD	M	1313	-	58,58,68	2.14	12 (20%)	72,72,82	1.79	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GOL	L	1294	-	5,5,5	0.36	0	5,5,5	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	M	1304	3	2/2/21/25	10/37/137/137	-
4	GOL	L	1292	-	-	2/4/4/4	-
5	BCL	L	1282	2	2/2/21/25	9/37/137/137	-
5	BCL	M	1303	3	2/2/21/25	18/37/137/137	-
12	SPO	M	1310	-	-	6/47/47/47	-
10	HTO	L	1290	-	-	10/10/10/10	-
14	PC1	M	1312	-	1/1/5/5	25/46/46/57	-
4	GOL	L	1293	-	-	2/4/4/4	-
6	LDA	M	1306	-	-	7/13/13/13	-
8	U10	L	1287[B]	-	-	8/15/39/87	0/1/1/1
8	U10	M	1309	-	-	6/45/69/87	0/1/1/1
8	U10	L	1287[A]	-	-	7/15/39/87	0/1/1/1
4	GOL	H	1252	-	-	2/4/4/4	-
6	LDA	M	1305	-	-	5/13/13/13	-
6	LDA	L	1283	-	-	7/13/13/13	-
5	BCL	L	1288	2	2/2/21/25	10/37/137/137	-
7	BPH	L	1286	-	-	6/54/105/105	0/5/6/6
10	HTO	L	1291	-	-	9/10/10/10	-
13	CDL	M	1311	-	-	50/88/88/110	-
4	GOL	H	1254	-	-	0/4/4/4	-
6	LDA	L	1285	-	-	10/13/13/13	-
4	GOL	H	1251	-	-	2/4/4/4	-
7	BPH	M	1308	-	-	19/54/105/105	0/5/6/6
4	GOL	H	1253	-	-	2/4/4/4	-
6	LDA	L	1284	-	-	7/13/13/13	-
15	GGD	M	1313	-	-	19/47/87/97	0/2/2/2
4	GOL	L	1294	-	-	1/4/4/4	-

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1310	SPO	C27-C28	12.95	1.47	1.34
7	M	1308	BPH	OBD-CAD	11.84	1.38	1.22
5	L	1282	BCL	OBD-CAD	11.49	1.38	1.22
5	M	1304	BCL	OBD-CAD	11.34	1.38	1.22
5	M	1303	BCL	OBD-CAD	11.02	1.37	1.22

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1311	CDL	C13-C12-C11	12.96	159.78	113.19
13	M	1311	CDL	C17-C16-C15	11.70	173.84	114.42
13	M	1311	CDL	C20-C19-C18	9.40	162.17	114.42
13	M	1311	CDL	C12-C11-CA5	7.55	141.08	113.62
7	M	1308	BPH	O2D-CGD-CBD	7.15	123.98	111.27

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1303	BCL	C8

5 of 259 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1292	GOL	C1-C2-C3-O3
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
10	L	1290	HTO	O1-C1-C2-O2
10	L	1290	HTO	O1-C1-C2-C3

There are no ring outliers.

17 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1304	BCL	11	0
4	L	1292	GOL	1	0
5	L	1282	BCL	4	0
5	M	1303	BCL	7	0
12	M	1310	SPO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1306	LDA	1	0
8	M	1309	U10	1	0
8	L	1287[A]	U10	4	0
4	H	1252	GOL	1	0
6	M	1305	LDA	1	0
5	L	1288	BCL	2	0
7	L	1286	BPH	4	0
13	M	1311	CDL	8	0
4	H	1251	GOL	6	0
7	M	1308	BPH	12	0
15	M	1313	GGD	2	0
4	L	1294	GOL	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 BCL M 1304

Bond lengths | Bond angles

Torsions | Rings

Ligand BCL L 1282

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand SPO M 1310

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 M 1312

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 L 1287 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 M 1309

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 L 1287 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 1288

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH L 1286

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL M 1311

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH M 1308

Bond lengths

Bond angles

Torsions

Rings

Ligand GGD M 1313

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	H	241/260 (92%)	-0.33	6 (2%)	57	59	17, 24, 33, 61	3 (1%)
2	L	281/281 (100%)	-0.49	7 (2%)	57	59	16, 21, 37, 50	0
3	M	303/307 (98%)	-0.24	10 (3%)	46	47	14, 25, 42, 56	6 (1%)
All	All	825/848 (97%)	-0.35	23 (2%)	53	54	14, 23, 41, 61	9 (1%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	9.9
1	H	250	SER	8.3
3	M	1	ALA	5.6
3	M	301	HIS	5.3
2	L	281	GLY	4.7

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 carbohydrates 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(Å²)	Q<0.9
14	PC1	M	1312	43/54	0.33	0.36	66,82,95,96	0
10	HTO	L	1291	10/10	0.35	0.56	78,80,81,82	0
6	LDA	L	1284	16/16	0.43	0.34	72,73,77,77	0
15	GGD	M	1313	57/67	0.43	0.36	47,73,90,90	0
6	LDA	L	1283	16/16	0.56	0.30	41,64,73,74	0
6	LDA	L	1285	16/16	0.56	0.34	72,76,80,81	0
4	GOL	H	1253	6/6	0.59	0.28	65,66,67,68	0
4	GOL	L	1294	6/6	0.60	0.18	80,81,81,81	0
4	GOL	L	1292	6/6	0.64	0.21	29,42,44,45	0
8	U10	L	1287[A]	23/63	0.70	0.34	24,40,48,49	23
8	U10	L	1287[B]	23/63	0.70	0.34	34,42,44,44	23
13	CDL	M	1311	81/100	0.71	0.38	42,69,83,83	0
10	HTO	L	1290	10/10	0.72	0.28	60,62,63,64	0
6	LDA	M	1306	16/16	0.79	0.23	54,58,63,64	0
4	GOL	H	1251	6/6	0.79	0.27	32,46,47,49	0
4	GOL	H	1254	6/6	0.79	0.19	63,64,64,65	0
4	GOL	H	1252	6/6	0.80	0.26	63,63,63,64	0
6	LDA	M	1305	16/16	0.80	0.20	31,45,51,51	0
12	SPO	M	1310	42/42	0.88	0.15	21,26,48,51	0
8	U10	M	1309	48/63	0.92	0.13	15,25,45,48	0
4	GOL	L	1293	6/6	0.93	0.15	66,68,68,69	0
7	BPH	M	1308	65/65	0.94	0.12	17,22,69,71	0
5	BCL	M	1303	66/66	0.96	0.12	16,21,58,58	0
5	BCL	M	1304	66/66	0.96	0.11	12,19,38,46	0
5	BCL	L	1282	66/66	0.97	0.11	13,18,41,43	0
5	BCL	L	1288	66/66	0.97	0.10	14,17,31,37	0
7	BPH	L	1286	65/65	0.98	0.08	10,16,26,28	0
9	PO4	L	1289	5/5	0.99	0.13	33,35,36,36	0
11	FE	M	1307	1/1	1.00	0.04	15,15,15,15	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 PC1 M 1312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
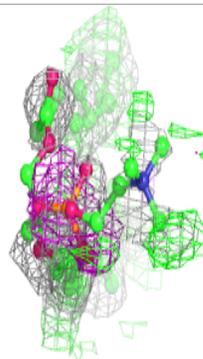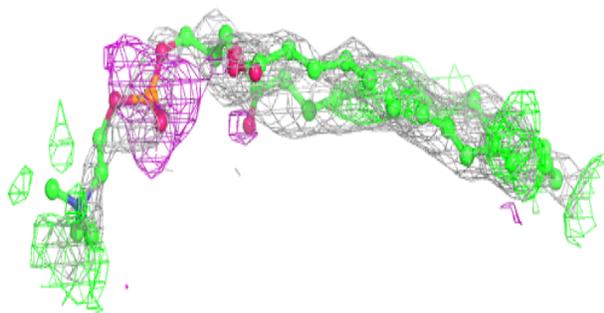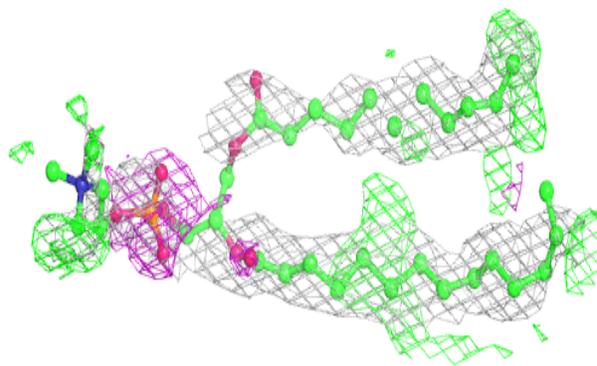
Electron density around GGD M 1313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
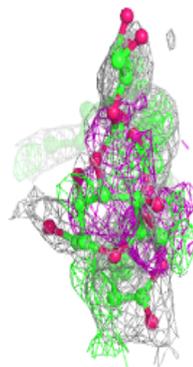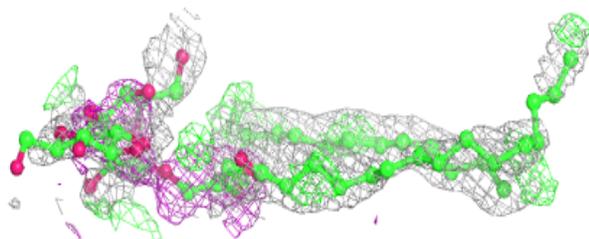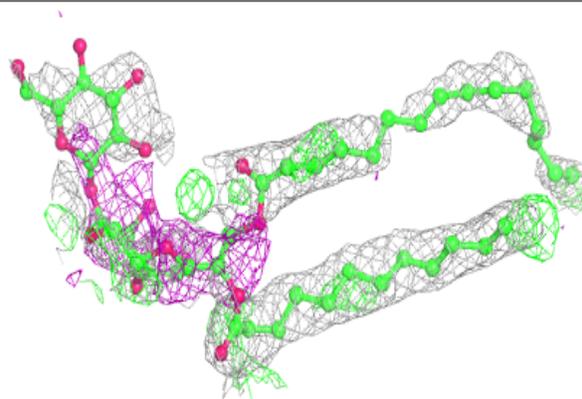
Electron density around U10 L 1287 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
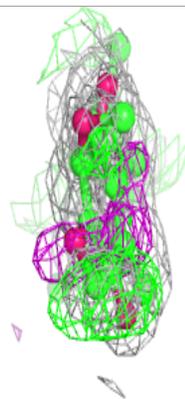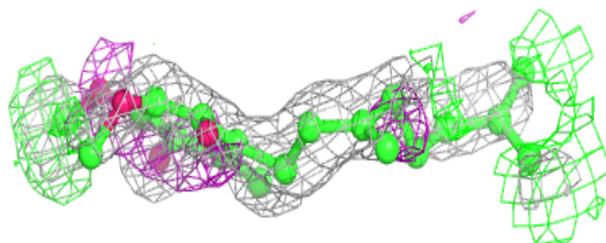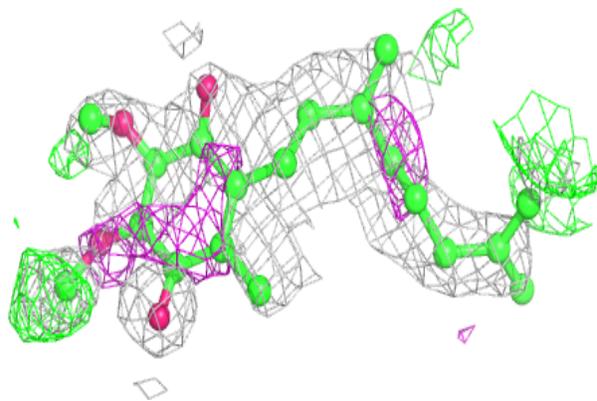
Electron density around U10 L 1287 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
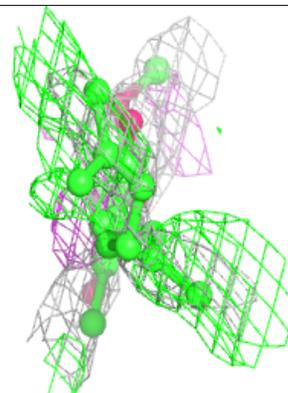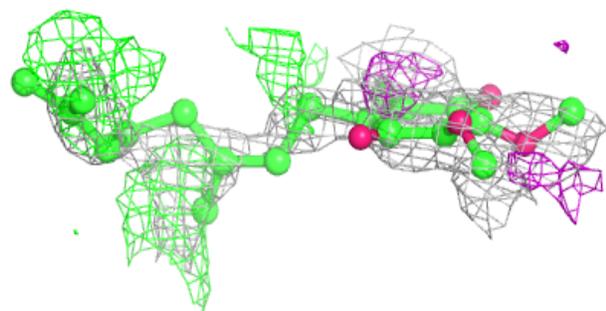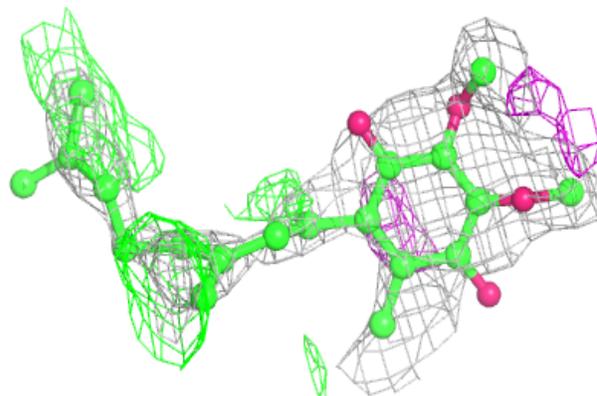
Electron density around CDL M 1311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
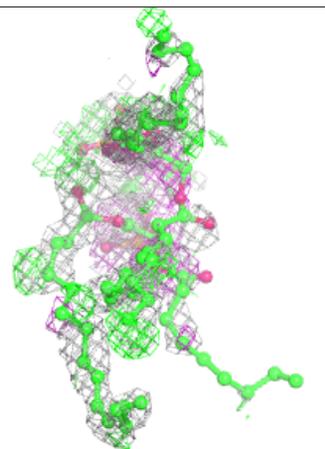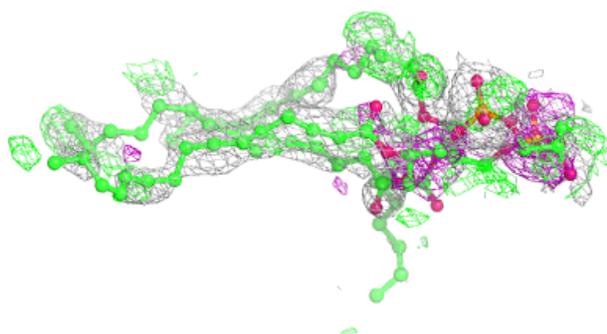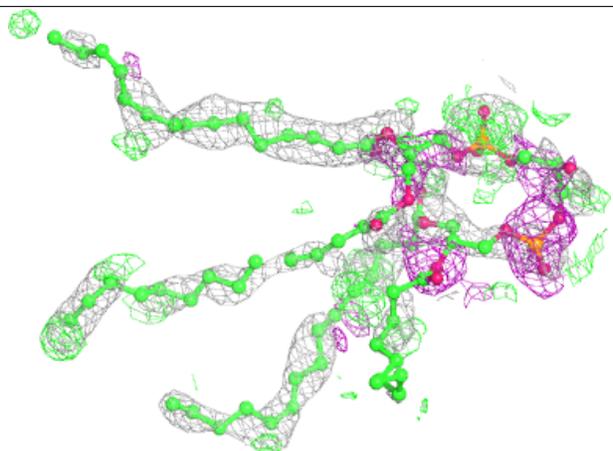
Electron density around SPO M 1310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
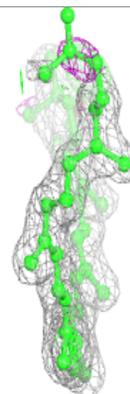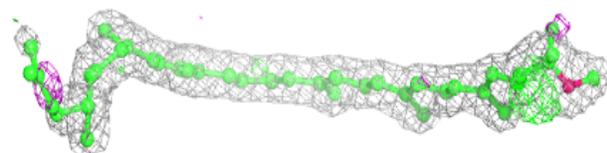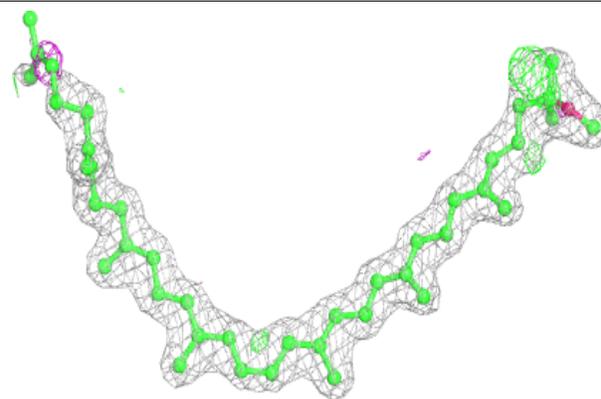
Electron density around U10 M 1309:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
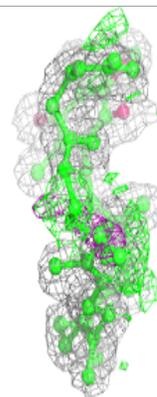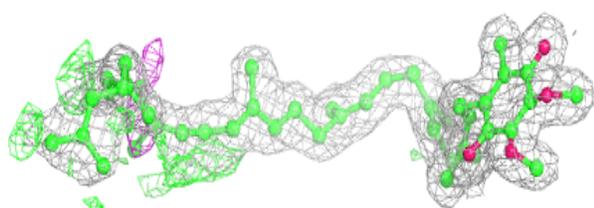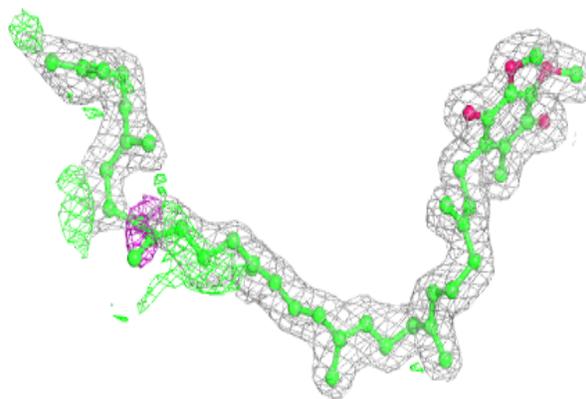
Electron density around BPH M 1308:

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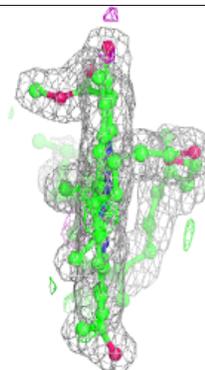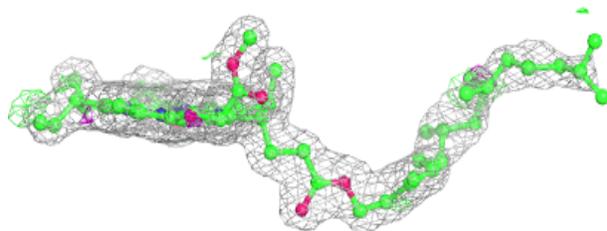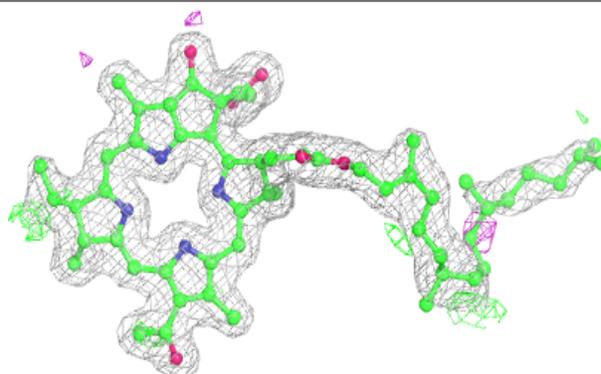
Electron density around BCL M 1303:

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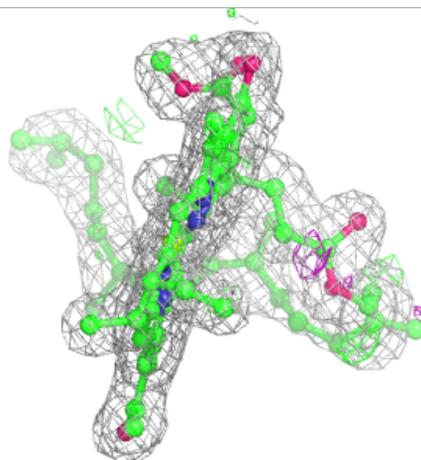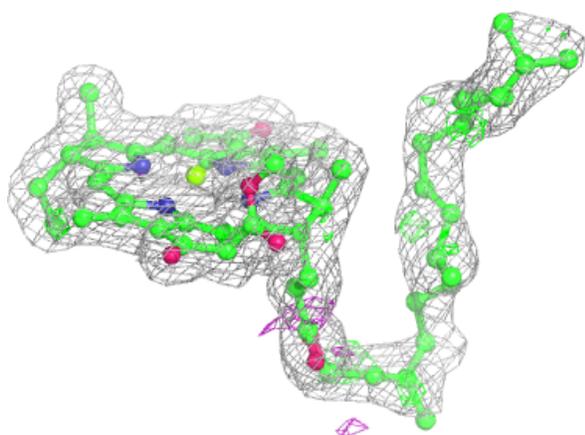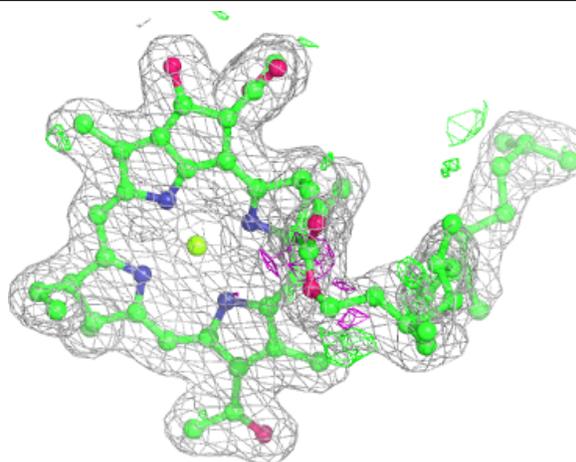
Electron density around BCL M 1304:

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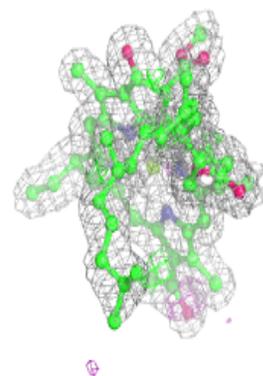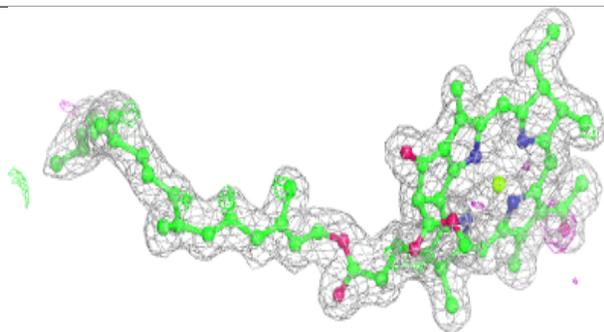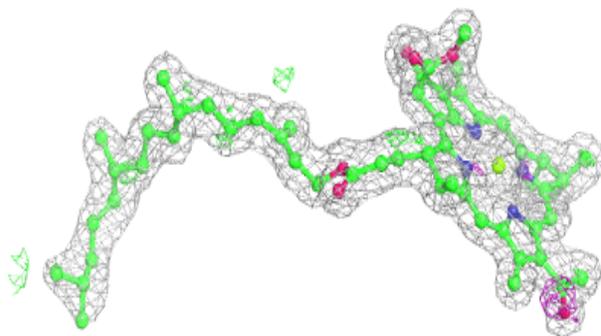
Electron density around BCL L 1282:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
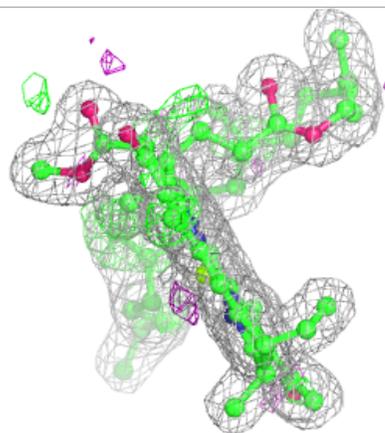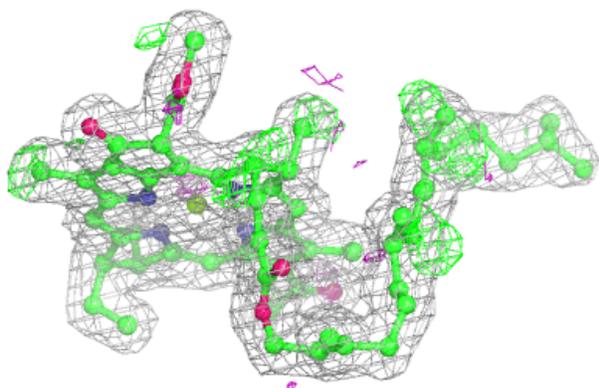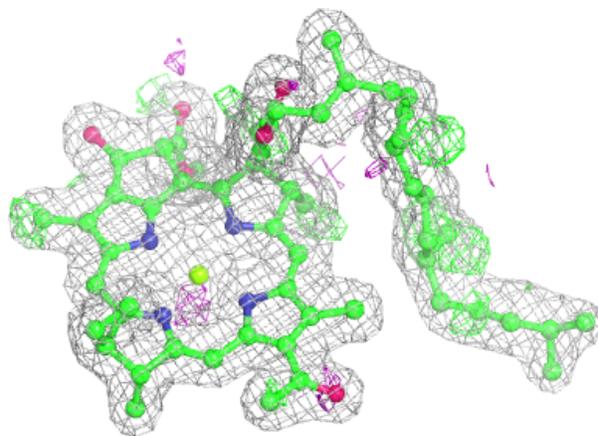
Electron density around BCL L 1288:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
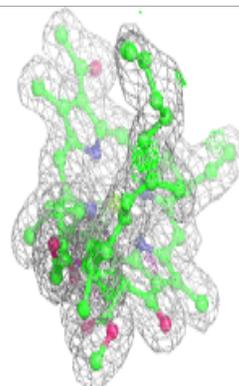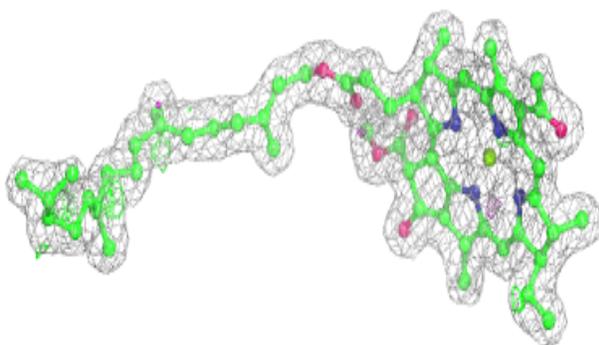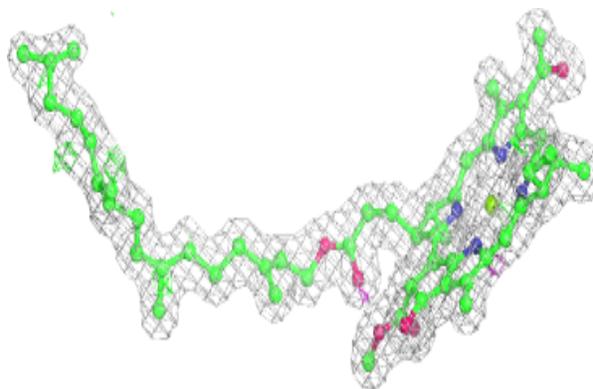
Electron density around BPH L 1286:

$2mF_o$-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.