Full wwPDB X-ray Structure Validation Report

Aug 18, 2026 – 09:35 pm BST

PDB ID	:	6GIX / pdb_00006gix
Title	:	Water-soluble Chlorophyll Protein (WSCP) from Lepidium virginicum (Mutation L91P) with Chlorophyll-b
Authors	:	Palm, D.M.; Agostini, A.; Averesch, V.; Girr, P.; Werwie, M.; Takahashi, S.; Satoh, H.; Jaenicke, E.; Paulsen, H.
Deposited on	:	2018-05-15
Resolution	:	2.80 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:

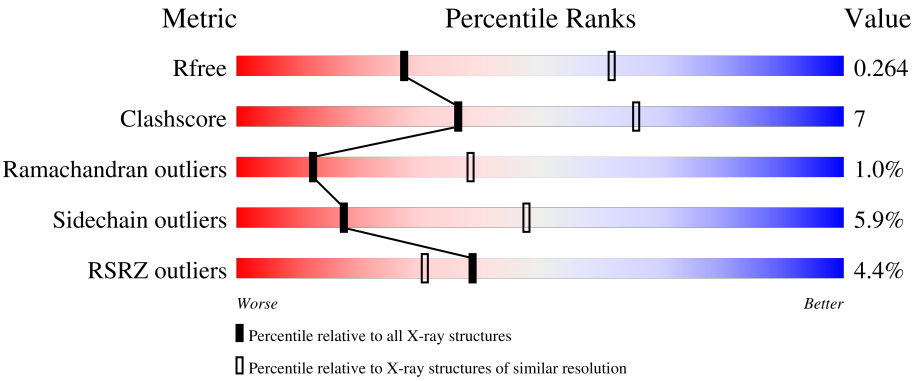
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	180	3% 68% 19% • 13%
1	B	180	4% 69% 17% • 12%
1	C	180	4% 72% 16% • 11%
1	D	180	4% 72% 18% • 9%

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
2	CHL	A	1001	X	-	-	-
2	CHL	B	1001	X	-	-	-
2	CHL	C	1001	X	-	-	-
2	CHL	D	1001	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5231 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.

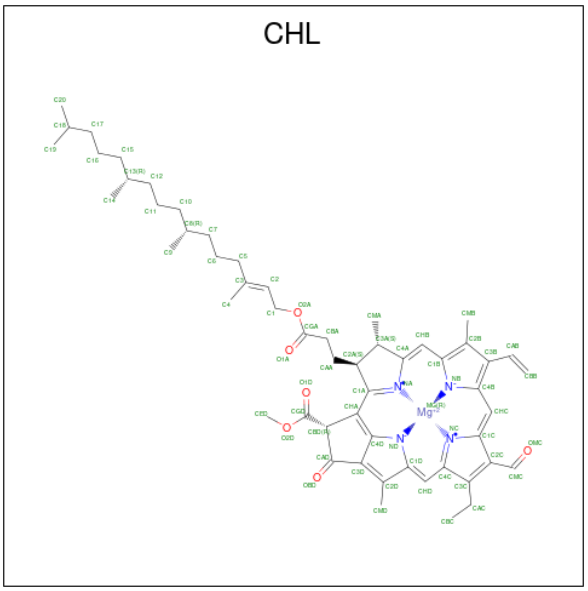
- Molecule 1 is a protein called Water-soluble chlorophyll protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1209	775	199	233	2			
1	B	158	Total	C	N	O	S	0	0	0
			1211	773	198	238	2			
1	C	161	Total	C	N	O	S	0	0	0
			1242	792	204	244	2			
1	D	163	Total	C	N	O	S	0	0	0
			1255	798	206	249	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	PRO	LEU	engineered mutation	UNP O04797
B	91	PRO	LEU	engineered mutation	UNP O04797
C	91	PRO	LEU	engineered mutation	UNP O04797
D	91	PRO	LEU	engineered mutation	UNP O04797

- Molecule 2 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



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

- Molecule 3 is water.

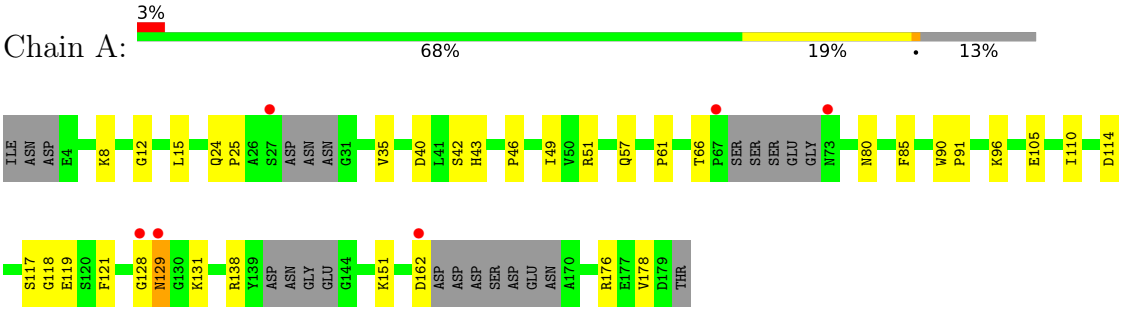
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	10	Total	O	0	0
			10	10		
3	C	11	Total	O	0	0
			11	11		
3	D	14	Total	O	0	0
			14	14		

3 Residue-property plots (i)

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.

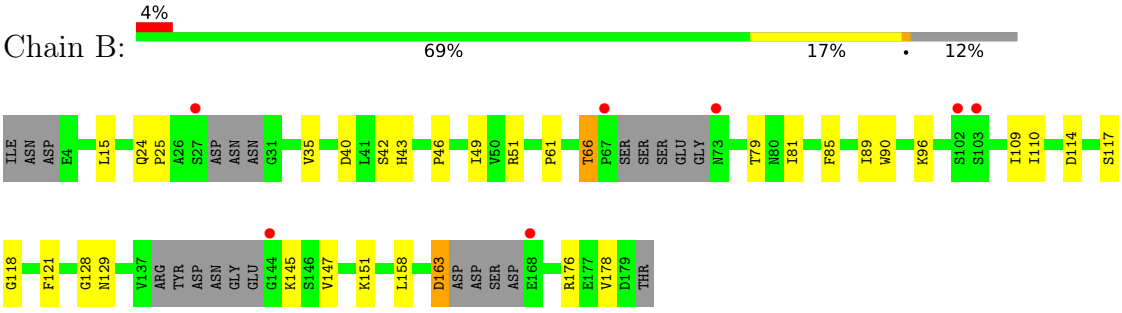
• Molecule 1: Water-soluble chlorophyll protein

Chain A:



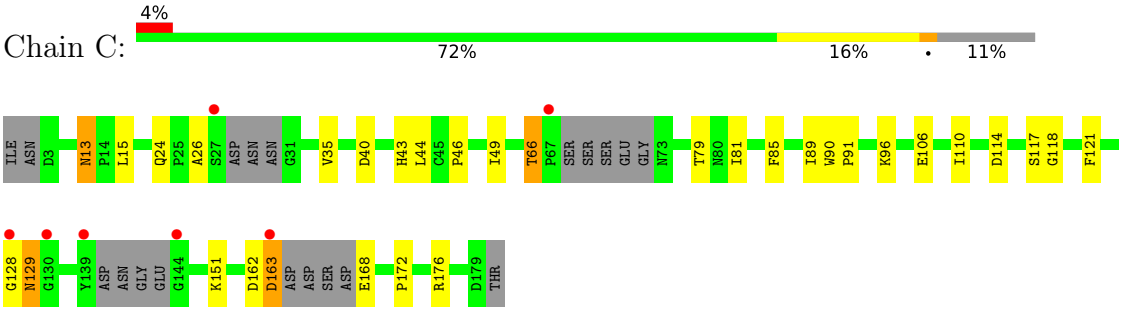
• Molecule 1: Water-soluble chlorophyll protein

Chain B:



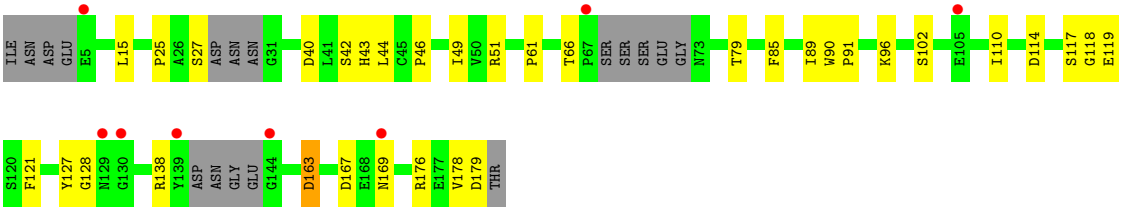
• Molecule 1: Water-soluble chlorophyll protein

Chain C:



• Molecule 1: Water-soluble chlorophyll protein

Chain D:


ILE ASN ASP GLU E5 L15 P25 A26 S27 ASP ASN ASN G31 D40 L41 S42 H43 L44 C45 P46 I49 V50 R51 P61 T66 P67 SER SER SER GLU GLY N73 T79 F85 I89 W90 P91 K96 S102 E105 I110 D114 S117 G118 E119
S120 F121 Y127 G128 N129 G130 R138 Y139 ASP ASN GLY GLU G144 D163 D167 E168 N169 R176 E177 V178 D179 THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.86Å 82.13Å 122.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.80 19.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.73-2.80) 98.9 (19.73-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.28 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.214 , 0.259 0.225 , 0.264	Depositor DCC
R_{free} test set	925 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5231	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL

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	0.62	0/1238	0.95	4/1684 (0.2%)
1	B	0.60	0/1239	0.91	2/1686 (0.1%)
1	C	0.61	0/1271	0.93	4/1729 (0.2%)
1	D	0.62	0/1285	0.93	3/1750 (0.2%)
All	All	0.61	0/5033	0.93	13/6849 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	TRP	CA-C-N	6.68	126.38	119.56
1	A	90	TRP	C-N-CA	6.68	126.38	119.56
1	C	90	TRP	CA-C-N	6.39	126.08	119.56
1	C	90	TRP	C-N-CA	6.39	126.08	119.56
1	D	90	TRP	CA-C-N	5.99	125.67	119.56
1	D	90	TRP	C-N-CA	5.99	125.67	119.56
1	B	90	TRP	CA-C-N	5.96	125.64	119.56
1	B	90	TRP	C-N-CA	5.96	125.64	119.56
1	C	162	ASP	N-CA-C	5.62	117.49	111.36
1	C	129	ASN	N-CA-C	5.52	118.35	110.24
1	A	66	THR	CA-CB-CG2	5.43	119.73	110.50
1	D	163	ASP	N-CA-C	5.38	122.26	110.80
1	A	129	ASN	N-CA-C	5.02	121.49	110.80

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	A	1209	0	1196	16	1
1	B	1211	0	1190	19	0
1	C	1242	0	1216	16	1
1	D	1255	0	1224	12	0
2	A	66	0	70	7	0
2	B	66	0	70	9	0
2	C	66	0	70	5	0
2	D	66	0	70	4	0
3	A	15	0	0	1	0
3	B	10	0	0	0	0
3	C	11	0	0	0	0
3	D	14	0	0	0	0
All	All	5231	0	5106	74	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.

All (74) 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:B:109:ILE:HD12	1:B:158:LEU:HB3	1.38	1.06
1:B:109:ILE:CD1	1:B:158:LEU:HB3	1.96	0.94
2:C:1001:CHL:H191	2:D:1001:CHL:H91	1.56	0.88
1:B:109:ILE:HD12	1:B:158:LEU:CB	2.03	0.87
2:B:1001:CHL:HBB2	1:C:44:LEU:HD11	1.58	0.85
2:B:1001:CHL:HBB1	2:B:1001:CHL:HHC	1.65	0.79
1:B:109:ILE:HD11	1:B:147:VAL:HG13	1.66	0.78
2:D:1001:CHL:HBB1	2:D:1001:CHL:HMB3	1.70	0.74
2:B:1001:CHL:HBB2	1:C:44:LEU:CD1	2.21	0.71
1:A:91:PRO:HG2	2:B:1001:CHL:H61	1.73	0.70
2:C:1001:CHL:H122	2:C:1001:CHL:H62	1.73	0.69
2:C:1001:CHL:HBB1	2:C:1001:CHL:HMB3	1.76	0.68
1:A:114:ASP:HB3	1:A:117:SER:HB3	1.82	0.61
1:D:114:ASP:HB3	1:D:117:SER:HB3	1.83	0.61
1:C:114:ASP:HB3	1:C:117:SER:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ASP:HB3	1:B:117:SER:HB3	1.83	0.60
2:A:1001:CHL:H18	2:C:1001:CHL:H102	1.85	0.58
1:D:119:GLU:HA	1:D:138:ARG:HH22	1.69	0.57
1:A:80:ASN:HD22	1:A:121:PHE:HB3	1.70	0.57
1:A:119:GLU:HA	1:A:138:ARG:HH22	1.69	0.57
1:D:127:TYR:CE2	1:D:167:ASP:HB3	2.39	0.57
1:A:8:LYS:HD3	1:A:12:GLY:O	2.06	0.55
2:A:1001:CHL:HBB1	2:A:1001:CHL:HMB3	1.89	0.55
2:B:1001:CHL:HBB1	2:B:1001:CHL:CHC	2.36	0.54
1:C:91:PRO:HG2	2:D:1001:CHL:H72	1.89	0.54
1:A:57:GLN:HB3	3:A:1107:HOH:O	2.11	0.50
1:B:66:THR:HG23	1:B:81:ILE:HG22	1.95	0.49
1:B:42:SER:O	1:C:91:PRO:HA	2.12	0.49
1:C:66:THR:HG23	1:C:81:ILE:HG22	1.93	0.48
1:C:13:ASN:HD22	1:C:13:ASN:N	2.12	0.48
1:C:46:PRO:HG2	1:C:110:ILE:HD12	1.94	0.48
1:B:25:PRO:HG2	1:B:51:ARG:HG3	1.95	0.47
1:B:118:GLY:HA2	1:B:121:PHE:CD2	2.50	0.47
1:C:118:GLY:HA2	1:C:121:PHE:CD2	2.50	0.47
2:A:1001:CHL:HBB2	1:D:44:LEU:HD11	1.96	0.46
1:A:25:PRO:HG2	1:A:51:ARG:HG3	1.97	0.46
1:C:85:PHE:HB2	1:C:96:LYS:HB3	1.97	0.46
1:A:118:GLY:HA2	1:A:121:PHE:CD2	2.50	0.46
1:D:118:GLY:HA2	1:D:121:PHE:CD2	2.50	0.46
1:A:40:ASP:OD1	1:A:43:HIS:HD2	1.99	0.46
1:A:46:PRO:HG2	1:A:110:ILE:HD12	1.98	0.46
1:C:40:ASP:OD1	1:C:43:HIS:HD2	2.00	0.45
1:B:40:ASP:OD1	1:B:43:HIS:HD2	1.99	0.45
1:A:85:PHE:HB2	1:A:96:LYS:HB3	1.99	0.45
1:B:46:PRO:HG2	1:B:110:ILE:HD12	1.98	0.45
1:B:109:ILE:HD12	1:B:158:LEU:C	2.42	0.45
1:D:46:PRO:HG2	1:D:110:ILE:HD12	1.97	0.45
2:A:1001:CHL:H62	2:A:1001:CHL:H41	1.59	0.44
1:B:85:PHE:HB2	1:B:96:LYS:HB3	1.99	0.44
2:B:1001:CHL:H41	2:B:1001:CHL:H62	1.71	0.44
2:B:1001:CHL:H71	2:B:1001:CHL:H111	1.78	0.44
1:D:40:ASP:OD1	1:D:43:HIS:HD2	2.00	0.44
2:A:1001:CHL:H41	2:A:1001:CHL:H93	1.99	0.44
1:D:85:PHE:HB2	1:D:96:LYS:HB3	1.98	0.44
1:B:109:ILE:HD11	1:B:147:VAL:CG1	2.39	0.44
1:A:42:SER:O	1:D:91:PRO:HA	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:HE2	1:B:163:ASP:HA	2.00	0.43
1:C:35:VAL:HG11	2:C:1001:CHL:CAD	2.48	0.43
1:C:163:ASP:OD1	1:C:163:ASP:N	2.51	0.43
1:A:91:PRO:HA	1:D:42:SER:O	2.19	0.43
1:B:35:VAL:HG11	2:B:1001:CHL:CAD	2.49	0.43
1:B:61:PRO:HB3	1:B:178:VAL:HG21	2.02	0.42
2:A:1001:CHL:H62	2:A:1001:CHL:H93	1.90	0.41
1:B:163:ASP:OD1	1:B:163:ASP:N	2.54	0.41
1:A:24:GLN:HE22	1:A:176:ARG:HD2	1.86	0.41
1:C:24:GLN:HE22	1:C:176:ARG:HD2	1.86	0.41
1:B:24:GLN:HE22	1:B:176:ARG:HD2	1.86	0.41
1:C:91:PRO:HG2	2:D:1001:CHL:C7	2.49	0.41
1:A:61:PRO:HB3	1:A:178:VAL:HG21	2.03	0.41
1:D:61:PRO:HB3	1:D:178:VAL:HG21	2.03	0.41
1:A:35:VAL:HG11	2:A:1001:CHL:CAD	2.51	0.40
2:B:1001:CHL:HHC	2:B:1001:CHL:CBB	2.44	0.40
1:D:25:PRO:HG2	1:D:51:ARG:HG3	2.03	0.40
1:C:26:ALA:HB3	1:C:172:PRO:HB2	2.03	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)
1:A:129:ASN:ND2	1:C:106:GLU:O[4_547]	2.15	0.05

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	147/180 (82%)	143 (97%)	3 (2%)	1 (1%)	18 47
1	B	148/180 (82%)	144 (97%)	2 (1%)	2 (1%)	9 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	151/180 (84%)	147 (97%)	3 (2%)	1 (1%)	18 47
1	D	155/180 (86%)	150 (97%)	3 (2%)	2 (1%)	9 31
All	All	601/720 (84%)	584 (97%)	11 (2%)	6 (1%)	12 38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	ASP
1	A	128	GLY
1	C	128	GLY
1	B	128	GLY
1	B	129	ASN
1	D	128	GLY

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	A	137/158 (87%)	131 (96%)	6 (4%)	25 59
1	B	138/158 (87%)	131 (95%)	7 (5%)	21 54
1	C	141/158 (89%)	131 (93%)	10 (7%)	13 39
1	D	143/158 (90%)	133 (93%)	10 (7%)	14 40
All	All	559/632 (88%)	526 (94%)	33 (6%)	18 48

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	49	ILE
1	A	105	GLU
1	A	131	LYS
1	A	151	LYS
1	A	162	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	15	LEU
1	B	49	ILE
1	B	66	THR
1	B	79	THR
1	B	89	ILE
1	B	151	LYS
1	B	163	ASP
1	C	13	ASN
1	C	15	LEU
1	C	49	ILE
1	C	66	THR
1	C	79	THR
1	C	89	ILE
1	C	129	ASN
1	C	151	LYS
1	C	163	ASP
1	C	168	GLU
1	D	15	LEU
1	D	27	SER
1	D	49	ILE
1	D	66	THR
1	D	79	THR
1	D	89	ILE
1	D	102	SER
1	D	169	ASN
1	D	176	ARG
1	D	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	57	GLN
1	A	80	ASN
1	B	43	HIS
1	B	57	GLN
1	B	73	ASN
1	C	11	ASN
1	C	13	ASN
1	C	43	HIS
1	C	57	GLN
1	D	43	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	57	GLN
1	D	73	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 oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	CHL	A	1001	1	70,74,74	1.84	15 (21%)	80,114,114	2.28	21 (26%)
2	CHL	C	1001	1	70,74,74	1.90	13 (18%)	80,114,114	2.29	22 (27%)
2	CHL	B	1001	1	70,74,74	1.79	12 (17%)	80,114,114	2.24	26 (32%)
2	CHL	D	1001	1	70,74,74	1.82	15 (21%)	80,114,114	2.24	21 (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
2	CHL	A	1001	1	1/1/15/21	19/41/117/117	-
2	CHL	C	1001	1	1/1/15/21	15/41/117/117	-
2	CHL	B	1001	1	1/1/15/21	22/41/117/117	-
2	CHL	D	1001	1	1/1/15/21	13/41/117/117	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	CHL	O2D-CGD	5.74	1.47	1.33
2	C	1001	CHL	CHD-C1D	5.28	1.48	1.38
2	D	1001	CHL	CHD-C1D	5.26	1.48	1.38
2	B	1001	CHL	CHD-C1D	5.14	1.48	1.38
2	C	1001	CHL	CHC-C1C	5.02	1.48	1.38
2	B	1001	CHL	O2D-CGD	4.96	1.45	1.33
2	A	1001	CHL	O2D-CGD	4.87	1.45	1.33
2	C	1001	CHL	C3D-C4D	-4.87	1.33	1.44
2	D	1001	CHL	O2D-CGD	4.84	1.45	1.33
2	D	1001	CHL	CHD-C4C	4.77	1.50	1.39
2	B	1001	CHL	CHC-C1C	4.72	1.48	1.38
2	A	1001	CHL	CHD-C1D	4.72	1.47	1.38
2	D	1001	CHL	C3D-C4D	-4.59	1.33	1.44
2	D	1001	CHL	CHC-C1C	4.54	1.47	1.38
2	A	1001	CHL	CHD-C4C	4.50	1.49	1.39
2	A	1001	CHL	C3D-C4D	-4.47	1.34	1.44
2	C	1001	CHL	CHD-C4C	4.35	1.49	1.39
2	C	1001	CHL	O2A-CGA	4.31	1.45	1.33
2	B	1001	CHL	CHD-C4C	4.27	1.49	1.39
2	C	1001	CHL	CHC-C4B	4.26	1.49	1.39
2	A	1001	CHL	CHC-C1C	4.25	1.47	1.38
2	A	1001	CHL	O2A-CGA	4.21	1.45	1.33
2	B	1001	CHL	C3D-C4D	-4.18	1.34	1.44
2	B	1001	CHL	CHC-C4B	4.17	1.48	1.39
2	B	1001	CHL	OBD-CAD	4.06	1.29	1.22
2	D	1001	CHL	O2A-CGA	3.96	1.44	1.33
2	B	1001	CHL	O2A-CGA	3.95	1.44	1.33
2	D	1001	CHL	CHC-C4B	3.76	1.47	1.39
2	C	1001	CHL	OBD-CAD	3.70	1.28	1.22
2	A	1001	CHL	CHC-C4B	3.70	1.47	1.39
2	D	1001	CHL	CHB-C1B	3.63	1.47	1.39
2	A	1001	CHL	C1B-NB	-3.62	1.33	1.37
2	A	1001	CHL	OBD-CAD	3.48	1.28	1.22
2	C	1001	CHL	CHB-C1B	3.43	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CHL	CHB-C1B	3.39	1.47	1.39
2	B	1001	CHL	CHB-C1B	3.22	1.46	1.39
2	C	1001	CHL	C1B-NB	-3.13	1.33	1.37
2	A	1001	CHL	C4B-NB	-2.99	1.34	1.37
2	D	1001	CHL	C4C-C3C	-2.76	1.40	1.45
2	B	1001	CHL	C4C-C3C	-2.74	1.40	1.45
2	D	1001	CHL	C2C-C1C	-2.74	1.39	1.44
2	D	1001	CHL	C1C-NC	-2.67	1.33	1.37
2	D	1001	CHL	OBD-CAD	2.60	1.27	1.22
2	A	1001	CHL	C1C-NC	-2.59	1.33	1.37
2	A	1001	CHL	CMC-C2C	2.51	1.50	1.45
2	D	1001	CHL	CMC-C2C	2.47	1.50	1.45
2	B	1001	CHL	C2C-C1C	-2.36	1.40	1.44
2	C	1001	CHL	CMC-C2C	2.35	1.50	1.45
2	D	1001	CHL	C1B-NB	-2.25	1.35	1.37
2	C	1001	CHL	C4C-C3C	-2.25	1.41	1.45
2	B	1001	CHL	C1C-NC	-2.19	1.34	1.37
2	A	1001	CHL	C4C-C3C	-2.18	1.41	1.45
2	D	1001	CHL	C4B-NB	-2.15	1.35	1.37
2	A	1001	CHL	C1D-C2D	-2.14	1.41	1.45
2	C	1001	CHL	C4B-NB	-2.05	1.35	1.37

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	CHL	C2B-C1B-NB	8.33	115.81	110.23
2	A	1001	CHL	C2B-C1B-NB	8.13	115.68	110.23
2	D	1001	CHL	C2B-C1B-NB	7.99	115.59	110.23
2	C	1001	CHL	CMD-C2D-C1D	7.33	137.64	124.71
2	B	1001	CHL	C2B-C1B-NB	7.18	115.05	110.23
2	B	1001	CHL	CMD-C2D-C1D	6.81	136.72	124.71
2	D	1001	CHL	CMD-C2D-C1D	6.79	136.68	124.71
2	A	1001	CHL	O2D-CGD-CBD	6.19	122.26	111.27
2	D	1001	CHL	O2D-CGD-CBD	6.06	122.03	111.27
2	A	1001	CHL	CMD-C2D-C1D	5.73	134.81	124.71
2	A	1001	CHL	CHD-C1D-ND	-5.40	119.49	124.45
2	C	1001	CHL	CHD-C1D-ND	-5.31	119.57	124.45
2	C	1001	CHL	O2D-CGD-CBD	5.30	120.68	111.27
2	C	1001	CHL	C2C-C3C-C4C	-5.29	102.72	106.49
2	B	1001	CHL	C2C-C3C-C4C	-5.19	102.79	106.49
2	B	1001	CHL	O2D-CGD-CBD	5.07	120.28	111.27
2	B	1001	CHL	CHD-C1D-ND	-5.03	119.83	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	CHL	C2C-C3C-C4C	-4.87	103.02	106.49
2	D	1001	CHL	CHB-C1B-NB	-4.73	119.25	124.26
2	D	1001	CHL	CHD-C1D-ND	-4.57	120.26	124.45
2	C	1001	CHL	C1D-ND-C4D	-4.47	103.16	106.33
2	A	1001	CHL	C2C-C3C-C4C	-4.47	103.30	106.49
2	A	1001	CHL	C4-C3-C5	4.41	122.70	115.27
2	A	1001	CHL	C1D-ND-C4D	-4.32	103.26	106.33
2	D	1001	CHL	C3B-C2B-C1B	-4.24	102.05	107.16
2	B	1001	CHL	CMB-C2B-C1B	4.23	131.81	125.37
2	A	1001	CHL	CHB-C1B-NB	-4.23	119.78	124.26
2	B	1001	CHL	C1D-ND-C4D	-4.12	103.41	106.33
2	A	1001	CHL	C3B-C2B-C1B	-4.10	102.22	107.16
2	C	1001	CHL	CAC-C3C-C4C	4.02	130.03	124.81
2	B	1001	CHL	C3B-C2B-C1B	-3.92	102.42	107.16
2	D	1001	CHL	C1D-ND-C4D	-3.85	103.60	106.33
2	C	1001	CHL	C3C-C4C-NC	3.84	114.88	110.57
2	A	1001	CHL	CAC-C3C-C4C	3.78	129.71	124.81
2	A	1001	CHL	C3B-C4B-NB	3.73	113.98	110.52
2	A	1001	CHL	C3C-C4C-NC	3.71	114.73	110.57
2	C	1001	CHL	C3B-C2B-C1B	-3.71	102.68	107.16
2	C	1001	CHL	CHB-C1B-NB	-3.67	120.37	124.26
2	A	1001	CHL	C2D-C1D-ND	3.53	112.71	110.10
2	C	1001	CHL	C4-C3-C5	3.47	121.12	115.27
2	A	1001	CHL	O2D-CGD-O1D	-3.41	117.17	123.84
2	B	1001	CHL	C2D-C1D-ND	3.41	112.61	110.10
2	C	1001	CHL	C2D-C1D-ND	3.39	112.60	110.10
2	D	1001	CHL	CAC-C3C-C4C	3.37	129.18	124.81
2	D	1001	CHL	C3C-C4C-NC	3.31	114.28	110.57
2	B	1001	CHL	C4-C3-C2	-3.29	115.23	123.68
2	B	1001	CHL	C3C-C4C-NC	3.29	114.26	110.57
2	B	1001	CHL	CHB-C1B-NB	-3.28	120.78	124.26
2	B	1001	CHL	CHB-C4A-NA	3.18	128.90	124.51
2	C	1001	CHL	CMD-C2D-C3D	-3.12	120.44	127.61
2	B	1001	CHL	C4-C3-C5	3.07	120.43	115.27
2	D	1001	CHL	C3B-C4B-NB	3.06	113.35	110.52
2	B	1001	CHL	C1-O2A-CGA	3.04	124.41	116.44
2	D	1001	CHL	C6-C5-C3	-3.01	105.56	113.45
2	D	1001	CHL	C2D-C1D-ND	2.94	112.27	110.10
2	D	1001	CHL	O2D-CGD-O1D	-2.91	118.16	123.84
2	B	1001	CHL	CMD-C2D-C3D	-2.90	120.95	127.61
2	C	1001	CHL	C3D-C2D-C1D	-2.87	101.92	105.83
2	A	1001	CHL	C4-C3-C2	-2.84	116.40	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	CHL	C3D-C2D-C1D	-2.82	101.98	105.83
2	D	1001	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
2	A	1001	CHL	CED-O2D-CGD	2.56	121.73	115.94
2	B	1001	CHL	C3D-C2D-C1D	-2.56	102.33	105.83
2	C	1001	CHL	C4A-NA-C1A	-2.52	105.57	106.71
2	A	1001	CHL	CHC-C1C-NC	-2.49	120.43	124.20
2	C	1001	CHL	C3B-C4B-NB	2.48	112.82	110.52
2	B	1001	CHL	CAC-C3C-C4C	2.48	128.03	124.81
2	D	1001	CHL	C1-O2A-CGA	2.46	122.89	116.44
2	B	1001	CHL	O2A-CGA-CBA	2.45	119.61	111.91
2	D	1001	CHL	CHB-C4A-NA	2.44	127.89	124.51
2	C	1001	CHL	C5-C3-C2	-2.42	116.22	121.12
2	C	1001	CHL	O1D-CGD-CBD	-2.41	119.56	124.48
2	A	1001	CHL	C1-O2A-CGA	2.35	122.61	116.44
2	A	1001	CHL	CMD-C2D-C3D	-2.35	122.21	127.61
2	C	1001	CHL	CED-O2D-CGD	2.34	121.22	115.94
2	B	1001	CHL	CHD-C4C-C3C	-2.31	121.44	124.84
2	D	1001	CHL	O1D-CGD-CBD	-2.28	119.82	124.48
2	B	1001	CHL	CHC-C4B-NB	-2.28	121.85	124.26
2	B	1001	CHL	O2A-C1-C2	-2.26	102.69	108.64
2	C	1001	CHL	C1-O2A-CGA	2.26	122.38	116.44
2	B	1001	CHL	CED-O2D-CGD	2.24	121.00	115.94
2	B	1001	CHL	O1D-CGD-CBD	-2.23	119.92	124.48
2	C	1001	CHL	CHC-C1C-NC	-2.14	120.96	124.20
2	A	1001	CHL	C3D-C2D-C1D	-2.09	102.98	105.83
2	C	1001	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
2	A	1001	CHL	C4D-CHA-C1A	-2.07	118.72	121.25
2	B	1001	CHL	O2D-CGD-O1D	-2.07	119.80	123.84
2	D	1001	CHL	C4A-NA-C1A	-2.06	105.78	106.71
2	D	1001	CHL	CMB-C2B-C1B	2.03	128.46	125.37
2	B	1001	CHL	CHC-C1C-NC	-2.03	121.13	124.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	CHL	C8
2	B	1001	CHL	C8
2	C	1001	CHL	C8
2	D	1001	CHL	C8

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	CHL	CBD-CGD-O2D-CED
2	A	1001	CHL	C4-C3-C5-C6
2	B	1001	CHL	C2-C3-C5-C6
2	B	1001	CHL	C4-C3-C5-C6
2	D	1001	CHL	CBD-CGD-O2D-CED
2	D	1001	CHL	O1D-CGD-O2D-CED
2	B	1001	CHL	CBD-CGD-O2D-CED
2	C	1001	CHL	CBD-CGD-O2D-CED
2	A	1001	CHL	O1D-CGD-O2D-CED
2	A	1001	CHL	C3-C5-C6-C7
2	B	1001	CHL	C3-C5-C6-C7
2	A	1001	CHL	C2-C3-C5-C6
2	C	1001	CHL	C3-C5-C6-C7
2	A	1001	CHL	C15-C16-C17-C18
2	A	1001	CHL	C6-C7-C8-C9
2	A	1001	CHL	C11-C12-C13-C14
2	D	1001	CHL	C14-C13-C15-C16
2	C	1001	CHL	O1D-CGD-O2D-CED
2	C	1001	CHL	C10-C11-C12-C13
2	D	1001	CHL	C5-C6-C7-C8
2	D	1001	CHL	C15-C16-C17-C18
2	B	1001	CHL	C11-C10-C8-C7
2	B	1001	CHL	C11-C12-C13-C15
2	B	1001	CHL	O1D-CGD-O2D-CED
2	B	1001	CHL	C13-C15-C16-C17
2	A	1001	CHL	C5-C6-C7-C8
2	A	1001	CHL	C8-C10-C11-C12
2	A	1001	CHL	C13-C15-C16-C17
2	B	1001	CHL	C16-C17-C18-C20
2	B	1001	CHL	C6-C7-C8-C10
2	C	1001	CHL	C11-C10-C8-C7
2	C	1001	CHL	C12-C13-C15-C16
2	B	1001	CHL	C11-C10-C8-C9
2	B	1001	CHL	C11-C12-C13-C14
2	B	1001	CHL	C14-C13-C15-C16
2	C	1001	CHL	C11-C10-C8-C9
2	C	1001	CHL	C14-C13-C15-C16
2	B	1001	CHL	C16-C17-C18-C19
2	B	1001	CHL	C12-C13-C15-C16
2	D	1001	CHL	C12-C13-C15-C16
2	B	1001	CHL	C6-C7-C8-C9
2	D	1001	CHL	C6-C7-C8-C9
2	A	1001	CHL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1001	CHL	C15-C16-C17-C18
2	A	1001	CHL	C2-C1-O2A-CGA
2	D	1001	CHL	C6-C7-C8-C10
2	B	1001	CHL	CAD-CBD-CGD-O1D
2	A	1001	CHL	C16-C17-C18-C19
2	C	1001	CHL	C8-C10-C11-C12
2	A	1001	CHL	C16-C17-C18-C20
2	B	1001	CHL	C2-C1-O2A-CGA
2	B	1001	CHL	C8-C10-C11-C12
2	C	1001	CHL	C6-C7-C8-C9
2	D	1001	CHL	C4-C3-C5-C6
2	C	1001	CHL	CAA-CBA-CGA-O2A
2	A	1001	CHL	CAA-CBA-CGA-O2A
2	B	1001	CHL	CAA-CBA-CGA-O2A
2	D	1001	CHL	C2-C3-C5-C6
2	D	1001	CHL	CAA-CBA-CGA-O2A
2	B	1001	CHL	CAA-CBA-CGA-O1A
2	C	1001	CHL	CAA-CBA-CGA-O1A
2	A	1001	CHL	CAA-CBA-CGA-O1A
2	B	1001	CHL	C15-C16-C17-C18
2	A	1001	CHL	CAD-CBD-CGD-O1D
2	C	1001	CHL	CAD-CBD-CGD-O1D
2	D	1001	CHL	CAD-CBD-CGD-O1D
2	D	1001	CHL	CAA-CBA-CGA-O1A
2	A	1001	CHL	C6-C7-C8-C10
2	C	1001	CHL	C6-C7-C8-C10

There are no ring outliers.

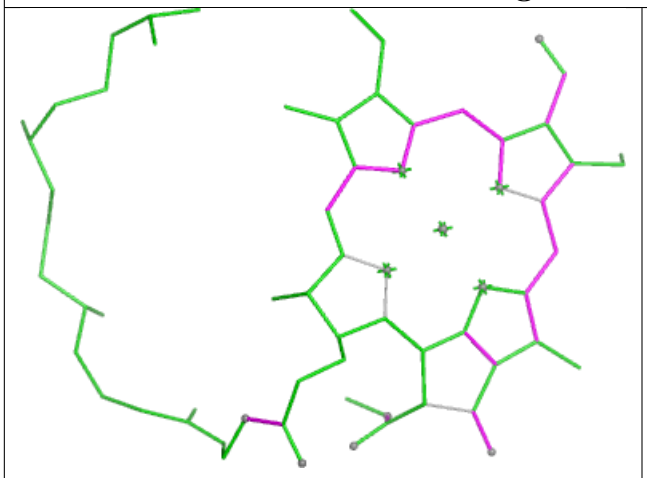
4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	CHL	7	0
2	C	1001	CHL	5	0
2	B	1001	CHL	9	0
2	D	1001	CHL	4	0

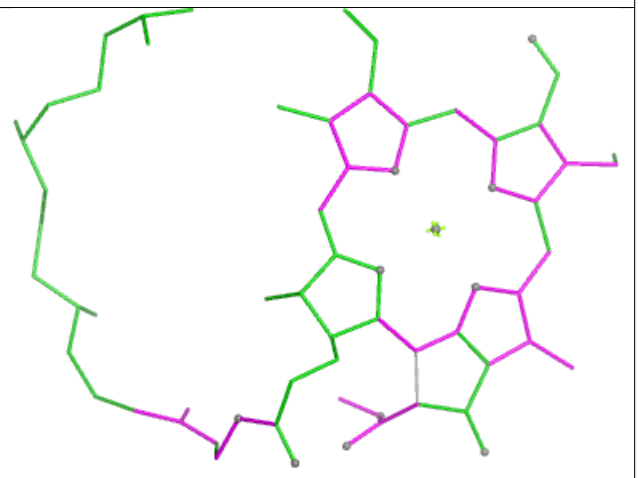
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

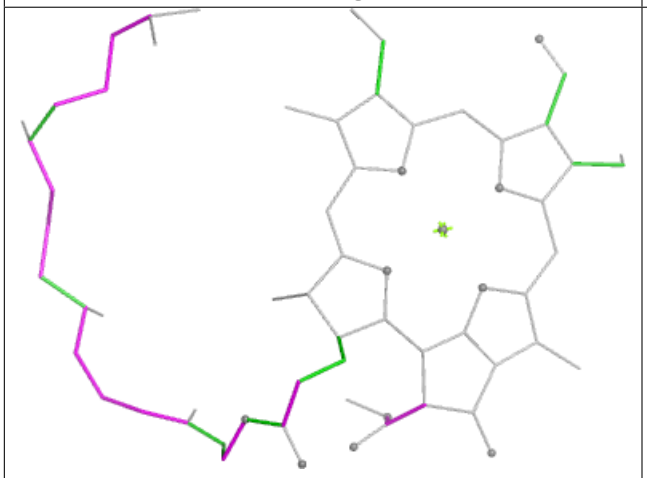
Ligand CHL A 1001



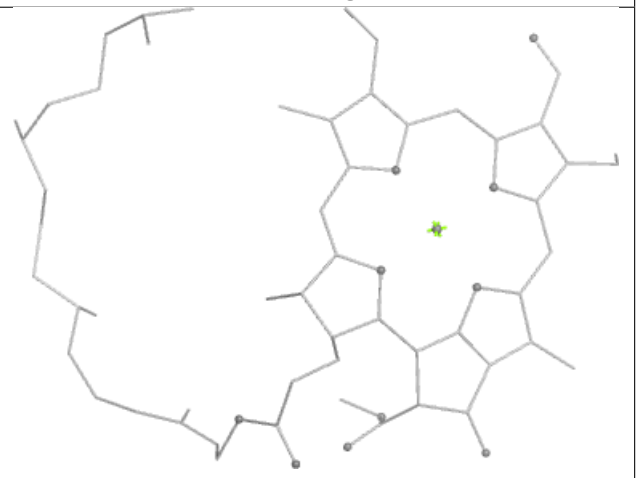
Bond lengths



Bond angles

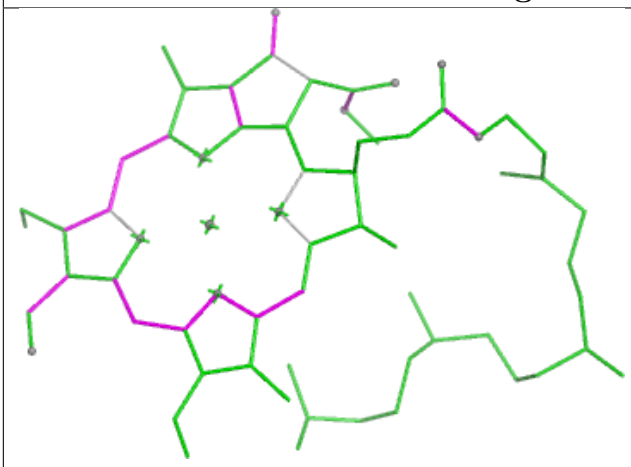


Torsions

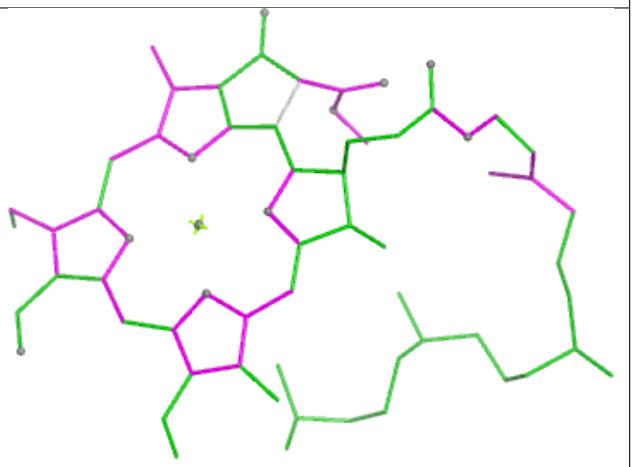


Rings

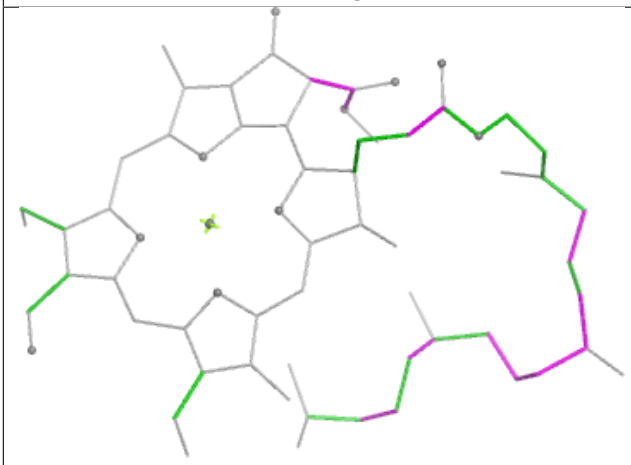
Ligand CHL C 1001



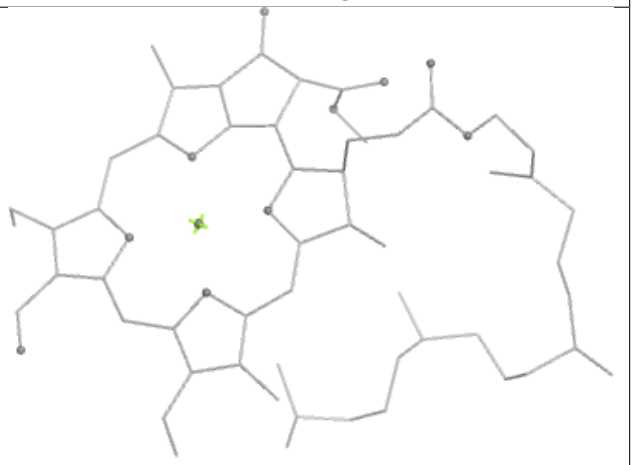
Bond lengths



Bond angles

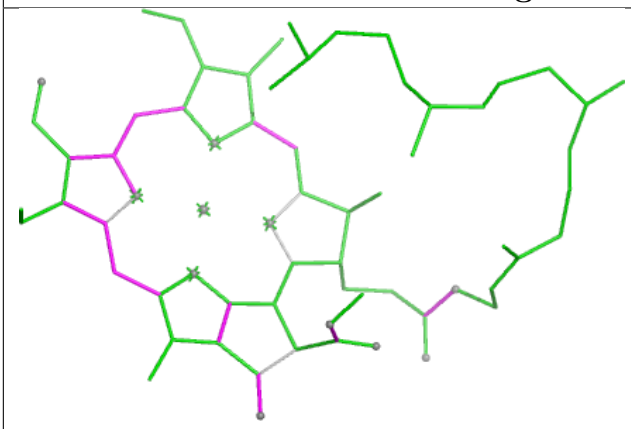


Torsions

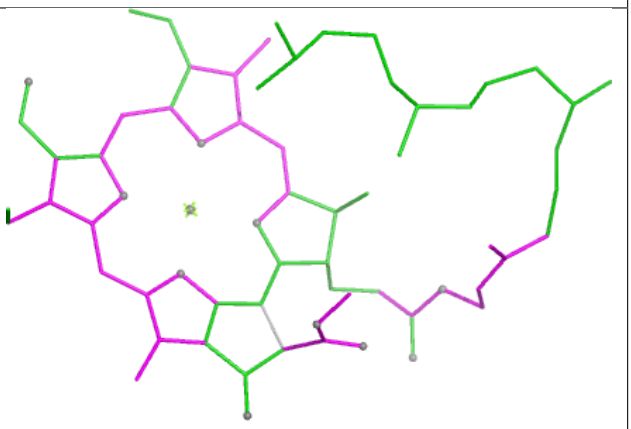


Rings

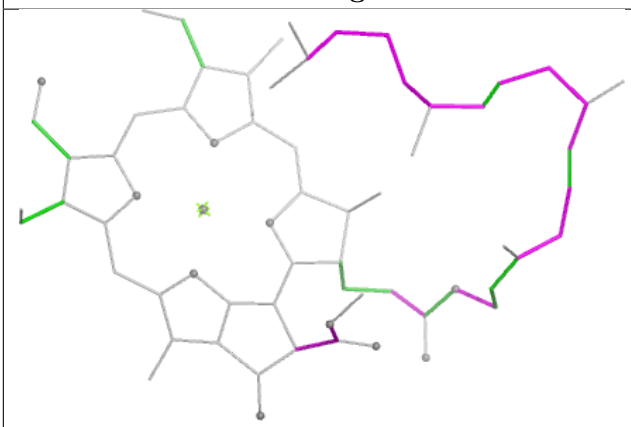
Ligand CHL B 1001



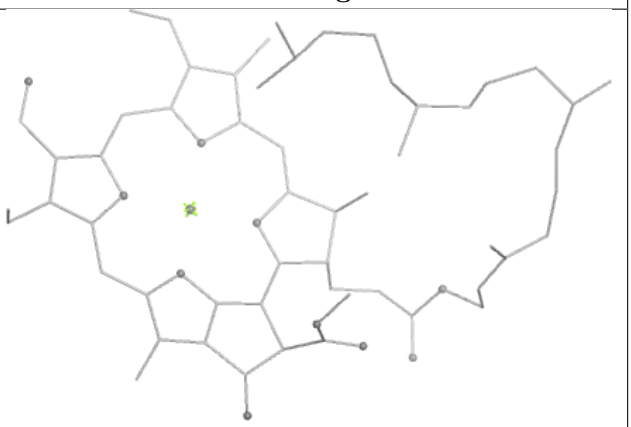
Bond lengths



Bond angles

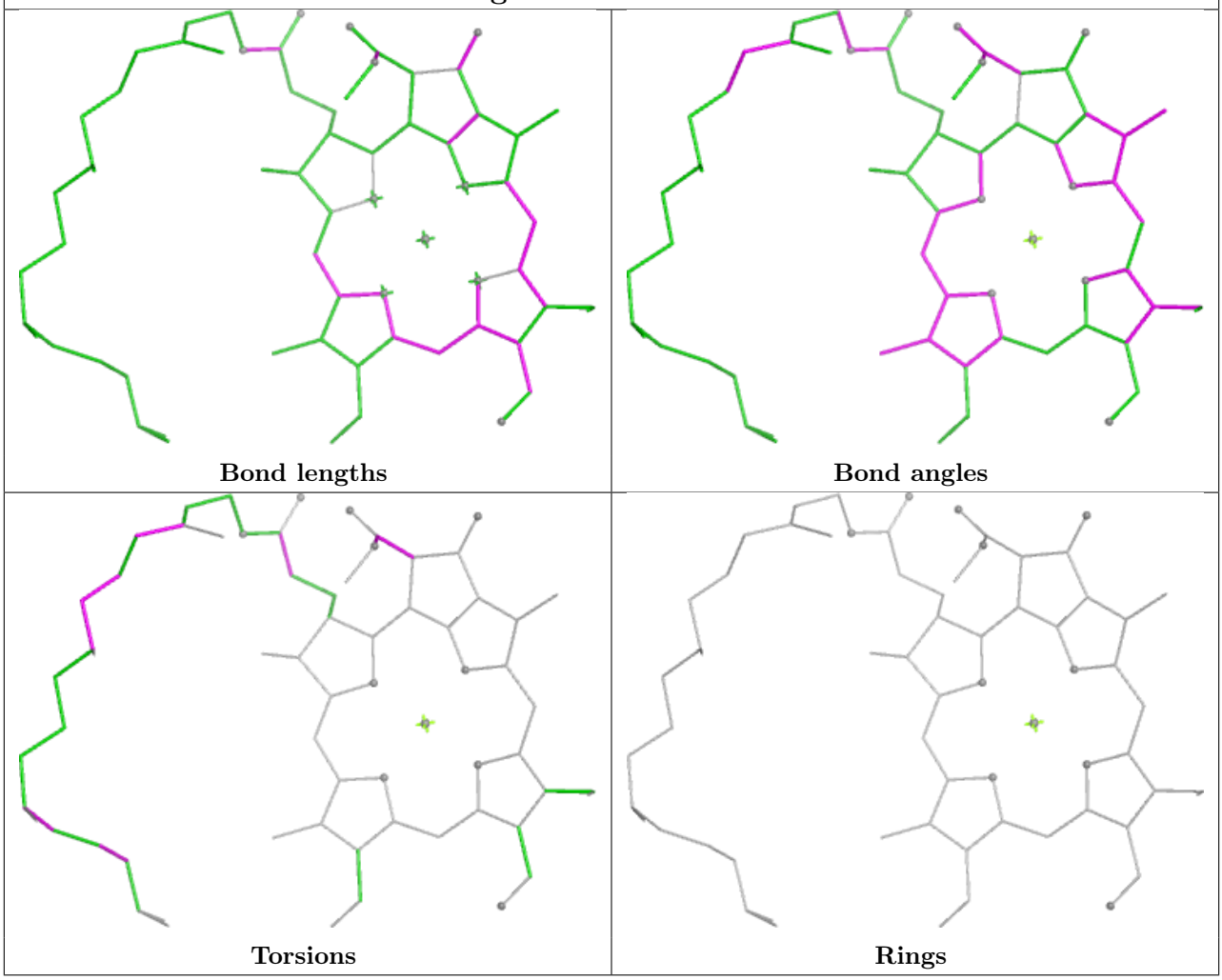


Torsions



Rings

Ligand CHL D 1001



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, 95^{th} 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	157/180 (87%)	-0.01	6 (3%)	44	35	23, 37, 70, 90	0
1	B	158/180 (87%)	0.26	7 (4%)	39	31	26, 44, 83, 117	0
1	C	161/180 (89%)	-0.01	7 (4%)	40	31	23, 39, 78, 104	0
1	D	163/180 (90%)	0.10	8 (4%)	35	27	21, 42, 71, 93	0
All	All	639/720 (88%)	0.09	28 (4%)	39	31	21, 41, 79, 117	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	PRO	4.8
1	D	144	GLY	3.9
1	A	129	ASN	3.7
1	C	144	GLY	3.5
1	D	5	GLU	3.2
1	C	27	SER	3.1
1	C	163	ASP	3.0
1	B	73	ASN	2.9
1	D	129	ASN	2.7
1	B	67	PRO	2.6
1	A	27	SER	2.5
1	C	67	PRO	2.5
1	D	169	ASN	2.5
1	A	162	ASP	2.4
1	B	144	GLY	2.4
1	B	27	SER	2.4
1	D	67	PRO	2.4
1	B	168	GLU	2.3
1	D	139	TYR	2.2
1	B	102	SER	2.2
1	C	139	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	105	GLU	2.2
1	A	128	GLY	2.1
1	C	130	GLY	2.1
1	D	130	GLY	2.1
1	C	128	GLY	2.1
1	A	73	ASN	2.0
1	B	103	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

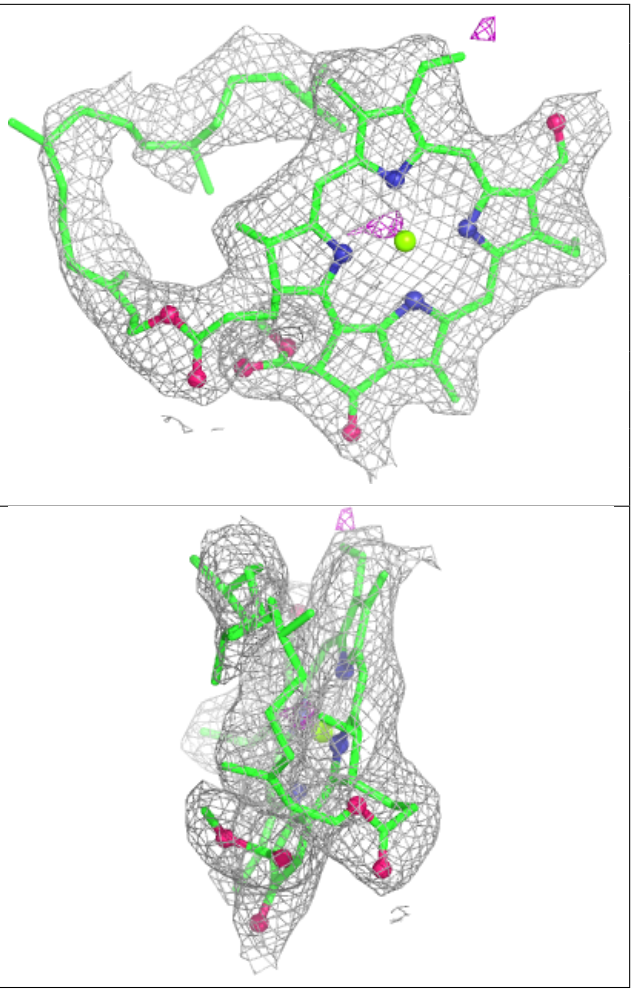
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	CHL	B	1001	66/66	0.92	0.10	26,30,77,79	0
2	CHL	D	1001	66/66	0.92	0.10	21,24,54,59	0
2	CHL	A	1001	66/66	0.93	0.09	24,29,71,74	0
2	CHL	C	1001	66/66	0.94	0.09	23,26,65,69	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.

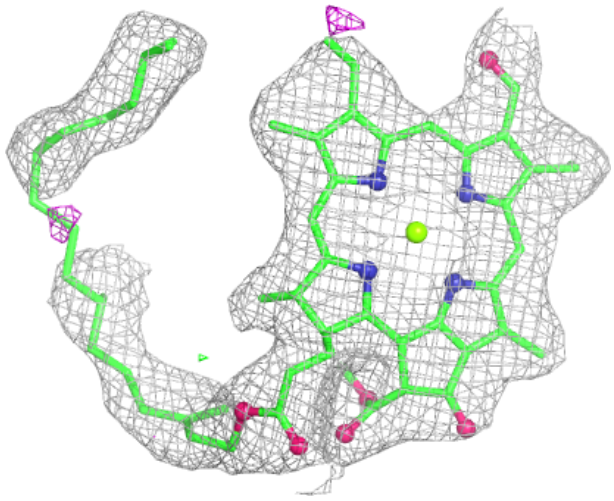
Electron density around CHL B 1001:

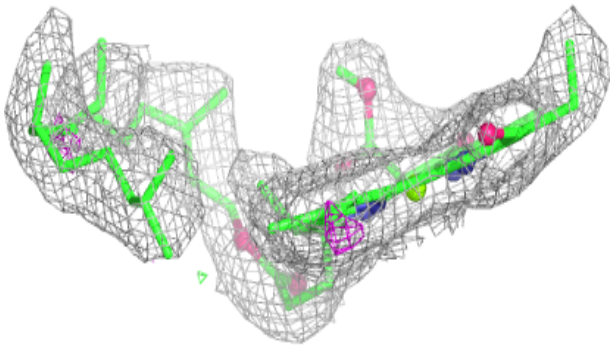
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CHL D 1001:

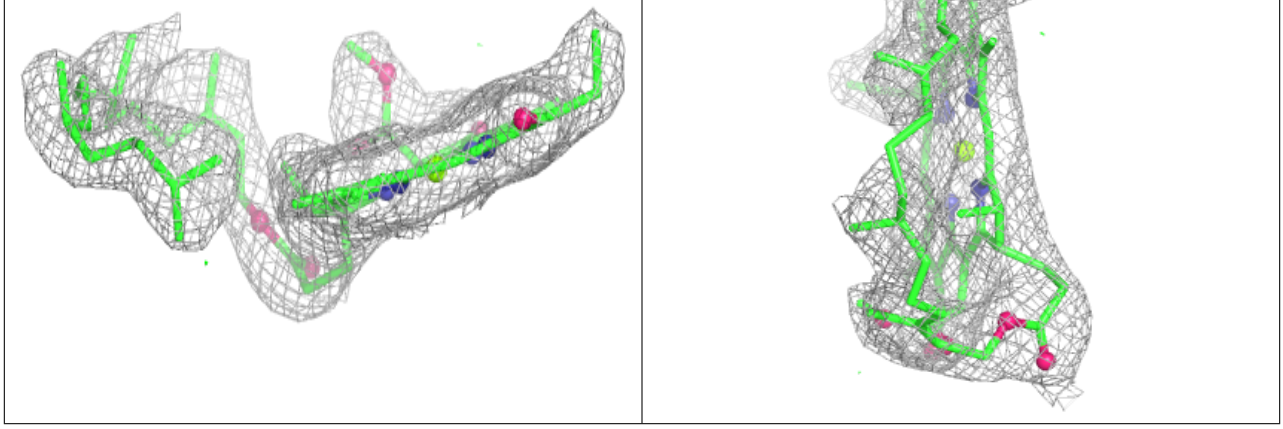
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





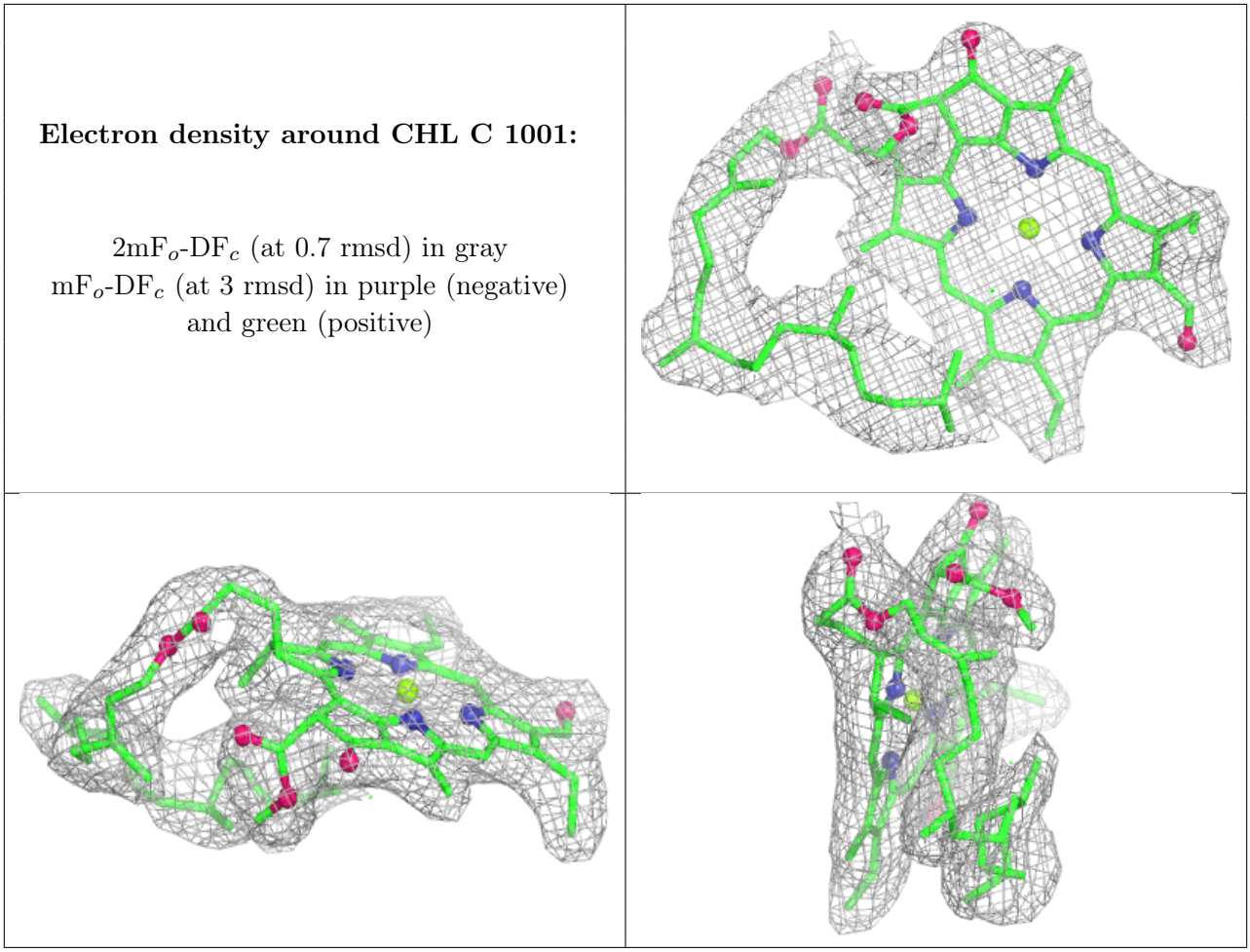
Electron density around CHL A 1001:

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



Electron density around CHL C 1001:

$2mF_o$-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.