



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:27 PM EDT

PDB ID : 2DRE / pdb_00002dre
Title : Crystal structure of Water-soluble chlorophyll protein from lepidium virginicum at 2.00 angstrom resolution
Authors : Horigome, D.; Satoh, H.; Itoh, N.; Mitsunaga, K.; Oonishi, I.; Nakagawa, A.; Uchida, A.
Deposited on : 2006-06-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

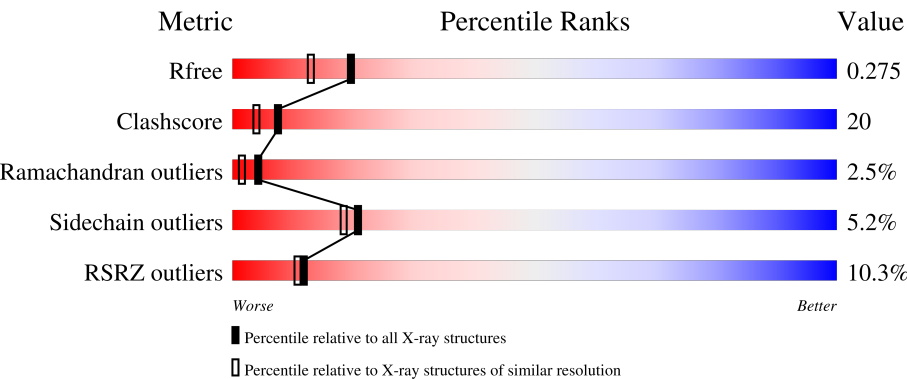
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	180	6% 58% 27% 9% • •
1	B	180	16% 56% 34% 6% • •
1	C	180	9% 71% 26% • •
1	D	180	9% 65% 30% • •

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

2 Entry composition [i](#)

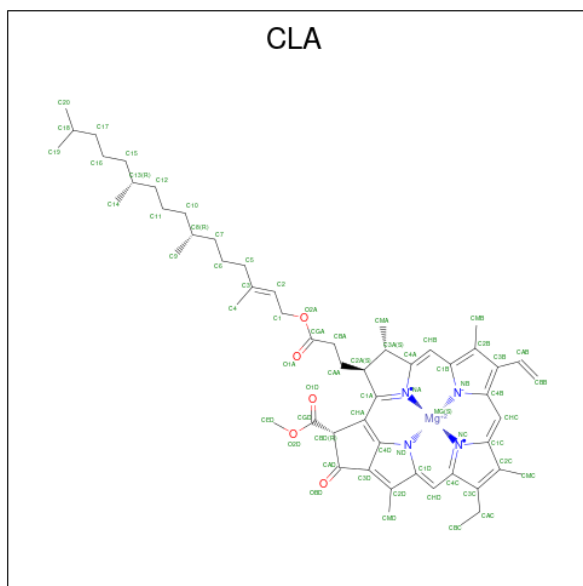
There are 3 unique types of molecules in this entry. The entry contains 6168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	172	Total	C	N	O	S	0	0	0
			1318	831	219	266	2			
1	B	173	Total	C	N	O	S	0	0	0
			1321	830	218	271	2			
1	C	177	Total	C	N	O	S	0	0	0
			1357	851	223	281	2			
1	D	177	Total	C	N	O	S	0	0	0
			1357	851	223	281	2			

- Molecule 2 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

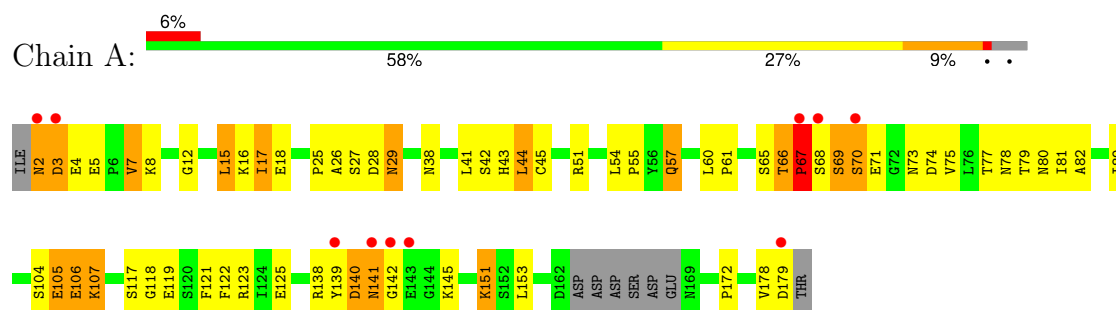
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		
3	B	156	Total	O	0	0
			156	156		
3	C	139	Total	O	0	0
			139	139		
3	D	110	Total	O	0	0
			110	110		

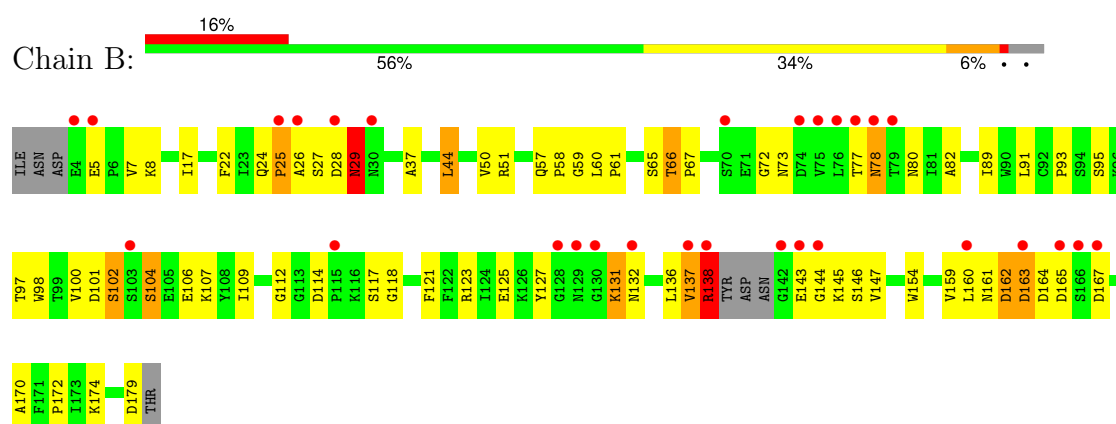
3 Residue-property plots [i](#)

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.

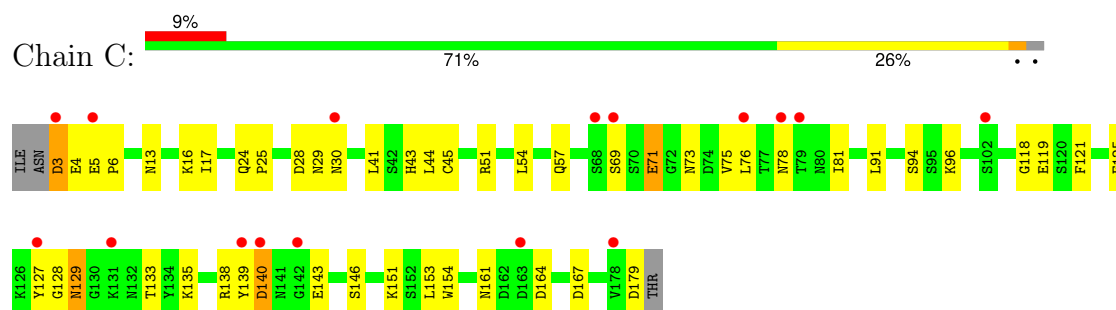
• Molecule 1: Water-soluble chlorophyll protein



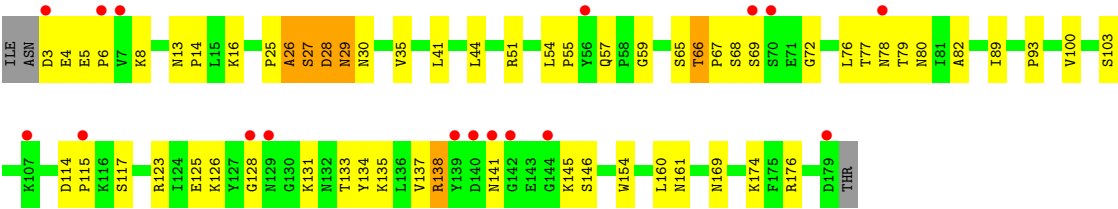
• Molecule 1: Water-soluble chlorophyll protein



• Molecule 1: Water-soluble chlorophyll protein



• Molecule 1: Water-soluble chlorophyll protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.06Å 82.73Å 121.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.00 28.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.99-2.00) 99.5 (28.99-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.280 0.238 , 0.275	Depositor DCC
R_{free} test set	2489 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/1349 (0.1%)	1.16	15/1838 (0.8%)
1	B	0.57	0/1351	1.27	18/1840 (1.0%)
1	C	0.39	0/1389	1.03	11/1894 (0.6%)
1	D	0.41	0/1389	1.08	15/1894 (0.8%)
All	All	0.50	1/5478 (0.0%)	1.14	59/7466 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	PRO	N-CD	-11.56	1.31	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	SER	N-CA-C	9.20	130.38	110.80
1	B	138	ARG	N-CA-C	9.12	136.55	111.00
1	B	66	THR	CA-C-N	8.94	129.12	119.28
1	B	66	THR	C-N-CA	8.94	129.12	119.28
1	B	59	GLY	N-CA-C	-8.72	103.14	112.04
1	B	28	ASP	CA-C-N	8.49	137.76	121.54
1	B	28	ASP	C-N-CA	8.49	137.76	121.54
1	B	24	GLN	CA-C-N	8.24	130.14	119.84
1	B	24	GLN	C-N-CA	8.24	130.14	119.84
1	A	66	THR	CA-C-N	7.62	129.36	119.84
1	A	66	THR	C-N-CA	7.62	129.36	119.84
1	B	29	ASN	N-CA-C	7.54	126.86	110.80
1	B	44	LEU	N-CA-C	-7.49	104.66	113.88
1	C	29	ASN	N-CA-C	-7.43	102.46	112.94
1	D	54	LEU	CA-C-N	7.36	127.72	119.32
1	D	54	LEU	C-N-CA	7.36	127.72	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASN	O-C-N	6.93	131.81	122.59
1	A	57	GLN	CA-C-N	6.81	126.50	119.56
1	A	57	GLN	C-N-CA	6.81	126.50	119.56
1	A	141	ASN	CA-C-N	6.60	134.34	121.41
1	A	141	ASN	C-N-CA	6.60	134.34	121.41
1	C	57	GLN	CA-C-N	6.57	126.19	119.56
1	C	57	GLN	C-N-CA	6.57	126.19	119.56
1	D	26	ALA	N-CA-C	-6.53	104.00	112.23
1	D	103	SER	CA-C-N	-6.33	112.45	121.50
1	D	103	SER	C-N-CA	-6.33	112.45	121.50
1	C	5	GLU	CA-C-N	6.27	126.19	119.85
1	C	5	GLU	C-N-CA	6.27	126.19	119.85
1	B	57	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	D	68	SER	N-CA-C	5.92	118.06	108.41
1	D	59	GLY	N-CA-C	-5.92	106.00	112.04
1	D	57	GLN	CA-C-N	5.90	125.52	119.56
1	D	57	GLN	C-N-CA	5.90	125.52	119.56
1	A	142	GLY	CA-C-N	5.83	130.71	122.09
1	A	142	GLY	C-N-CA	5.83	130.71	122.09
1	B	24	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	B	109	ILE	N-CA-C	-5.68	101.40	108.89
1	B	7	VAL	N-CA-C	-5.64	101.54	109.21
1	D	103	SER	N-CA-C	-5.59	105.95	112.89
1	C	5	GLU	N-CA-C	5.53	116.66	109.64
1	B	137	VAL	CA-C-O	-5.50	116.06	121.67
1	B	28	ASP	CB-CA-C	5.47	118.46	110.26
1	C	54	LEU	CA-C-N	5.42	125.50	119.32
1	C	54	LEU	C-N-CA	5.42	125.50	119.32
1	C	94	SER	N-CA-C	5.37	117.25	110.33
1	A	55	PRO	N-CA-C	5.36	120.89	113.65
1	B	57	GLN	CB-CA-C	5.36	116.24	110.08
1	D	66	THR	CA-C-N	5.33	124.52	118.97
1	D	66	THR	C-N-CA	5.33	124.52	118.97
1	D	5	GLU	CA-C-N	5.21	125.22	119.90
1	D	5	GLU	C-N-CA	5.21	125.22	119.90
1	C	164	ASP	N-CA-C	-5.14	105.29	112.03
1	A	44	LEU	N-CA-C	-5.10	107.19	113.41
1	A	2	ASN	CA-C-N	5.09	131.27	121.54
1	A	2	ASN	C-N-CA	5.09	131.27	121.54
1	A	7	VAL	N-CA-C	-5.09	102.29	109.21
1	D	55	PRO	N-CA-C	5.05	121.28	113.75
1	C	28	ASP	N-CA-C	5.04	116.34	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASP	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1318	0	1278	52	0
1	B	1321	0	1276	66	0
1	C	1357	0	1300	48	0
1	D	1357	0	1300	58	0
2	A	65	0	72	4	0
2	B	65	0	72	10	0
2	C	65	0	72	6	0
2	D	65	0	72	7	0
3	A	150	0	0	3	0
3	B	156	0	0	9	0
3	C	139	0	0	7	0
3	D	110	0	0	13	0
All	All	6168	0	5442	224	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 20.

All (224) 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:C:151:LYS:H	1:C:151:LYS:HD2	1.10	1.11
1:B:29:ASN:O	1:B:29:ASN:ND2	1.97	0.97
1:D:29:ASN:N	1:D:29:ASN:HD22	1.61	0.97
1:D:29:ASN:ND2	1:D:29:ASN:H	1.62	0.92
1:D:29:ASN:HD22	1:D:29:ASN:H	0.89	0.85
1:B:123:ARG:HB2	1:B:137:VAL:HG23	1.58	0.85
1:A:2:ASN:HB2	3:A:1151:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HD2	1:C:151:LYS:N	1.90	0.82
1:B:131:LYS:HG2	3:B:1155:HOH:O	1.80	0.82
1:B:26:ALA:HB2	1:B:174:LYS:HG3	1.63	0.81
1:C:127:TYR:CE1	1:C:167:ASP:HB3	2.16	0.80
1:D:25:PRO:HG2	1:D:51:ARG:HE	1.47	0.80
1:A:138:ARG:HG3	1:A:138:ARG:HH11	1.46	0.80
1:B:100:VAL:HG21	1:B:138:ARG:HD3	1.63	0.79
1:C:3:ASP:HB2	1:C:78:ASN:HD22	1.48	0.78
1:B:123:ARG:HB2	1:B:137:VAL:CG2	2.14	0.76
1:B:8:LYS:HE2	1:B:132:ASN:ND2	2.00	0.76
1:C:179:ASP:HA	3:C:1095:HOH:O	1.87	0.75
1:B:29:ASN:O	1:B:29:ASN:CG	2.32	0.73
1:C:6:PRO:HA	1:C:76:LEU:HD23	1.71	0.72
1:C:96:LYS:HE3	3:C:1037:HOH:O	1.90	0.72
1:D:65:SER:OG	1:D:82:ALA:HB3	1.89	0.71
1:D:131:LYS:HG2	3:D:1085:HOH:O	1.90	0.71
1:B:131:LYS:H	1:B:131:LYS:HD2	1.55	0.70
1:D:65:SER:HG	1:D:82:ALA:HB3	1.57	0.69
1:A:44:LEU:HD12	2:D:1001:CLA:HBB2	1.75	0.68
1:A:66:THR:O	1:A:66:THR:HG23	1.93	0.68
1:B:114:ASP:HB3	1:B:117:SER:HB3	1.75	0.68
1:A:153:LEU:HD12	1:C:41:LEU:HD11	1.75	0.67
1:D:114:ASP:HB3	1:D:117:SER:HB3	1.74	0.67
1:B:101:ASP:HB3	3:B:1017:HOH:O	1.94	0.66
1:B:131:LYS:HD2	1:B:131:LYS:N	2.11	0.66
1:A:17:ILE:HG12	1:A:18:GLU:HG2	1.78	0.65
1:B:78:ASN:N	1:B:78:ASN:HD22	1.94	0.65
1:A:153:LEU:CD1	1:C:41:LEU:HD11	2.27	0.64
1:A:65:SER:OG	1:A:82:ALA:HB3	1.98	0.64
1:B:106:GLU:O	1:B:159:VAL:HB	1.98	0.63
1:D:126:LYS:HD3	3:D:1102:HOH:O	1.98	0.63
1:B:60:LEU:HD12	1:B:61:PRO:HD3	1.79	0.62
1:D:26:ALA:HB1	1:D:174:LYS:HE3	1.81	0.62
1:A:38:ASN:HD21	1:A:153:LEU:HD23	1.64	0.62
1:B:78:ASN:HD22	1:B:78:ASN:H	1.48	0.62
1:B:104:SER:HB3	3:B:1017:HOH:O	1.98	0.62
1:C:4:GLU:HG3	3:C:1133:HOH:O	2.00	0.62
1:A:42:SER:HB3	3:A:1111:HOH:O	1.99	0.61
1:D:114:ASP:HB3	1:D:117:SER:CB	2.31	0.60
1:B:8:LYS:HE2	1:B:132:ASN:HD21	1.66	0.60
1:D:77:THR:HG21	3:D:1060:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ASN:ND2	3:D:1073:HOH:O	2.35	0.60
2:A:1001:CLA:HMB2	2:B:1001:CLA:H121	1.82	0.59
1:A:44:LEU:HD13	1:D:44:LEU:HD13	1.84	0.59
1:C:151:LYS:H	1:C:151:LYS:CD	1.97	0.59
1:D:8:LYS:HE3	3:D:1111:HOH:O	2.01	0.59
1:A:178:VAL:O	1:A:179:ASP:HB2	2.02	0.59
1:B:26:ALA:CB	1:B:174:LYS:HG3	2.32	0.59
2:A:1001:CLA:H11	1:B:89:ILE:HD11	1.84	0.59
1:B:167:ASP:O	1:B:167:ASP:OD2	2.21	0.59
1:D:6:PRO:HA	1:D:76:LEU:HD13	1.85	0.59
1:A:89:ILE:HD12	2:B:1001:CLA:H43	1.85	0.59
2:D:1001:CLA:HHC	2:D:1001:CLA:HBB1	1.86	0.58
2:A:1001:CLA:HBB2	1:D:44:LEU:HD12	1.85	0.58
1:D:25:PRO:HG2	1:D:51:ARG:NE	2.17	0.58
1:D:28:ASP:O	1:D:51:ARG:NH2	2.35	0.58
1:B:137:VAL:HA	1:B:145:LYS:O	2.04	0.57
1:D:25:PRO:HG2	1:D:51:ARG:HG3	1.87	0.57
1:D:29:ASN:N	1:D:29:ASN:ND2	2.35	0.57
1:B:72:GLY:C	1:B:73:ASN:HD22	2.13	0.56
1:C:129:ASN:C	1:C:129:ASN:HD22	2.13	0.56
1:A:67:PRO:HB3	1:A:121:PHE:CZ	2.39	0.56
1:A:138:ARG:HH11	1:A:138:ARG:CG	2.17	0.56
1:B:37:ALA:HB3	1:B:50:VAL:CG2	2.36	0.56
1:B:44:LEU:HD12	2:C:1001:CLA:HBB2	1.86	0.56
2:B:1001:CLA:HBB2	1:C:44:LEU:HD12	1.87	0.55
1:D:6:PRO:CA	1:D:76:LEU:HD13	2.36	0.55
1:D:78:ASN:OD1	1:D:125:GLU:HG2	2.05	0.55
1:A:123:ARG:HD2	1:A:139:TYR:CE1	2.41	0.55
1:A:2:ASN:OD1	1:A:2:ASN:C	2.49	0.54
1:A:106:GLU:CD	1:A:106:GLU:N	2.66	0.54
2:B:1001:CLA:H171	2:D:1001:CLA:H18	1.90	0.54
1:C:3:ASP:N	1:C:78:ASN:HB2	2.22	0.54
1:C:25:PRO:HG2	1:C:51:ARG:HG2	1.89	0.54
1:A:7:VAL:HG22	1:A:77:THR:HG22	1.89	0.54
1:C:17:ILE:HD11	1:C:73:ASN:OD1	2.08	0.54
1:D:125:GLU:OE1	1:D:135:LYS:HE3	2.08	0.54
1:D:66:THR:HG23	3:D:1078:HOH:O	2.07	0.54
1:B:78:ASN:N	1:B:78:ASN:ND2	2.54	0.53
2:B:1001:CLA:H201	1:D:154:TRP:HZ2	1.72	0.53
1:A:138:ARG:HG3	1:A:138:ARG:NH1	2.19	0.53
1:A:8:LYS:HD3	1:A:12:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLY:HA2	1:B:121:PHE:CD1	2.44	0.53
1:C:71:GLU:HB3	3:C:1091:HOH:O	2.09	0.53
2:C:1001:CLA:HMB2	2:D:1001:CLA:H121	1.90	0.53
1:D:27:SER:OG	1:D:28:ASP:N	2.42	0.53
1:B:44:LEU:HG	1:C:91:LEU:HB3	1.91	0.53
1:A:151:LYS:NZ	3:A:1022:HOH:O	2.41	0.53
1:B:127:TYR:CZ	1:B:172:PRO:HG3	2.44	0.53
1:A:67:PRO:HD2	1:A:80:ASN:O	2.09	0.52
1:A:15:LEU:HB3	1:A:75:VAL:HB	1.91	0.52
1:A:16:LYS:HA	1:A:73:ASN:O	2.09	0.52
1:C:140:ASP:C	1:C:140:ASP:OD1	2.51	0.52
1:A:107:LYS:HD3	1:A:107:LYS:N	2.24	0.52
1:C:154:TRP:HH2	2:C:1001:CLA:H202	1.73	0.52
1:D:26:ALA:CB	1:D:174:LYS:HE3	2.39	0.52
1:D:138:ARG:HG2	1:D:160:LEU:HD11	1.91	0.52
1:B:179:ASP:HA	3:B:1002:HOH:O	2.09	0.52
1:A:38:ASN:ND2	1:A:153:LEU:HD23	2.26	0.51
1:D:25:PRO:HG2	1:D:51:ARG:CG	2.41	0.51
1:A:66:THR:O	1:A:66:THR:CG2	2.59	0.51
1:D:16:LYS:NZ	3:D:1057:HOH:O	2.35	0.50
1:A:104:SER:O	1:A:107:LYS:HD3	2.12	0.50
1:B:165:ASP:O	1:B:165:ASP:OD2	2.29	0.50
1:D:100:VAL:HG21	1:D:138:ARG:HD2	1.93	0.50
1:A:119:GLU:HA	1:A:138:ARG:NH2	2.27	0.50
1:A:67:PRO:HB3	1:A:121:PHE:CE2	2.47	0.49
1:C:4:GLU:O	1:C:76:LEU:HD22	2.11	0.49
1:B:8:LYS:HE3	3:B:1067:HOH:O	2.12	0.49
1:B:25:PRO:HG2	1:B:51:ARG:HD2	1.95	0.49
1:B:162:ASP:O	1:B:164:ASP:N	2.39	0.49
1:A:41:LEU:HA	2:C:1001:CLA:H191	1.95	0.49
1:B:37:ALA:HB3	1:B:50:VAL:HG21	1.94	0.49
1:C:6:PRO:CA	1:C:76:LEU:HD23	2.42	0.49
1:A:16:LYS:NZ	1:A:74:ASP:OD1	2.40	0.48
1:D:8:LYS:CD	3:D:1086:HOH:O	2.61	0.48
2:B:1001:CLA:HHC	2:B:1001:CLA:HBB1	1.95	0.48
1:C:127:TYR:HB3	1:C:133:THR:HG22	1.96	0.48
1:B:8:LYS:HB2	1:B:132:ASN:ND2	2.28	0.48
1:B:60:LEU:HD12	1:B:61:PRO:CD	2.44	0.47
1:A:25:PRO:HG2	1:A:51:ARG:HG3	1.96	0.47
1:B:29:ASN:HA	1:B:51:ARG:HH22	1.79	0.47
1:A:117:SER:HB3	1:A:119:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:GLY:HA2	1:C:121:PHE:CD1	2.50	0.47
1:A:81:ILE:HG13	1:A:122:PHE:O	2.15	0.47
1:B:93:PRO:HG3	1:C:45:CYS:O	2.14	0.47
1:C:129:ASN:O	1:C:129:ASN:ND2	2.46	0.47
1:D:27:SER:HB3	3:D:1105:HOH:O	2.14	0.47
1:B:29:ASN:ND2	1:B:29:ASN:C	2.71	0.47
1:B:138:ARG:HG2	1:B:160:LEU:CD2	2.45	0.47
1:C:16:LYS:HA	1:C:73:ASN:O	2.15	0.47
1:B:138:ARG:HG2	1:B:160:LEU:HD21	1.96	0.46
2:D:1001:CLA:HED2	2:D:1001:CLA:H61	1.96	0.46
1:B:127:TYR:CE1	1:B:167:ASP:HB2	2.50	0.46
1:D:3:ASP:HA	1:D:78:ASN:HB2	1.97	0.46
1:A:27:SER:C	1:A:29:ASN:H	2.23	0.46
1:A:138:ARG:CG	1:A:138:ARG:NH1	2.74	0.46
1:B:22:PHE:CE2	1:B:58:PRO:HB2	2.49	0.46
1:A:78:ASN:OD1	1:A:125:GLU:HG2	2.15	0.46
1:B:17:ILE:O	1:B:17:ILE:HD12	2.15	0.46
1:B:17:ILE:HD12	1:B:17:ILE:C	2.41	0.46
1:A:26:ALA:HB2	1:A:172:PRO:HB2	1.97	0.46
1:B:65:SER:OG	1:B:82:ALA:HB3	2.15	0.46
1:A:77:THR:O	1:A:79:THR:HG23	2.17	0.45
1:A:118:GLY:HA2	1:A:121:PHE:CD1	2.50	0.45
2:A:1001:CLA:H201	1:C:153:LEU:HD21	1.98	0.45
1:B:145:LYS:HD3	1:B:160:LEU:HD21	1.99	0.45
1:B:131:LYS:O	3:B:1155:HOH:O	2.21	0.45
2:B:1001:CLA:H193	1:D:41:LEU:CD2	2.46	0.45
1:A:45:CYS:O	1:D:93:PRO:HD3	2.16	0.45
1:C:154:TRP:CH2	2:C:1001:CLA:H202	2.52	0.45
1:B:66:THR:HA	1:B:67:PRO:HD3	1.49	0.45
1:D:79:THR:O	1:D:123:ARG:HG2	2.17	0.44
1:B:101:ASP:O	1:B:102:SER:C	2.60	0.44
1:A:89:ILE:HD11	2:B:1001:CLA:H11	2.00	0.44
1:C:17:ILE:HG12	1:C:73:ASN:HA	1.99	0.44
1:D:135:LYS:NZ	3:D:1009:HOH:O	2.51	0.44
1:B:136:LEU:HB2	1:B:147:VAL:CG2	2.48	0.44
1:A:105:GLU:H	1:A:105:GLU:HG3	1.43	0.44
1:D:25:PRO:CG	1:D:51:ARG:HG3	2.47	0.44
1:D:128:GLY:CA	3:D:1107:HOH:O	2.65	0.44
1:A:121:PHE:O	1:A:138:ARG:NH1	2.51	0.44
1:C:129:ASN:C	1:C:129:ASN:ND2	2.75	0.44
1:B:114:ASP:HB3	1:B:117:SER:CB	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ALA:HB2	1:D:174:LYS:HG3	2.00	0.43
1:B:80:ASN:N	1:B:123:ARG:HH11	2.17	0.43
1:D:115:PRO:HG3	3:D:1050:HOH:O	2.18	0.43
1:C:135:LYS:NZ	1:C:167:ASP:OD1	2.40	0.43
1:C:138:ARG:HG2	1:C:139:TYR:N	2.33	0.43
1:D:79:THR:HG22	1:D:80:ASN:N	2.34	0.43
1:D:137:VAL:HG13	1:D:145:LYS:O	2.18	0.43
1:B:107:LYS:HA	3:B:1017:HOH:O	2.18	0.43
1:C:78:ASN:OD1	1:C:125:GLU:HG2	2.18	0.43
1:B:97:THR:HG22	1:B:98:TRP:O	2.19	0.43
1:C:138:ARG:HG2	1:C:139:TYR:H	1.83	0.43
1:D:13:ASN:HB3	1:D:14:PRO:HD2	2.01	0.43
1:B:146:SER:HB2	1:B:165:ASP:HA	2.00	0.43
2:B:1001:CLA:C20	1:D:154:TRP:HZ2	2.31	0.43
1:C:17:ILE:HG12	1:C:73:ASN:HB3	2.00	0.42
1:C:81:ILE:HD12	1:C:81:ILE:C	2.44	0.42
1:D:4:GLU:O	1:D:76:LEU:HD12	2.19	0.42
1:B:170:ALA:O	1:B:172:PRO:HD3	2.19	0.42
1:D:145:LYS:HB3	1:D:161:ASN:O	2.19	0.42
1:A:17:ILE:N	1:A:17:ILE:HD13	2.35	0.42
1:C:3:ASP:HB3	3:C:1127:HOH:O	2.19	0.42
1:C:24:GLN:HA	1:C:25:PRO:HD3	1.80	0.42
1:C:75:VAL:HA	3:C:1118:HOH:O	2.19	0.42
1:A:60:LEU:HD12	1:A:61:PRO:HD2	2.02	0.42
1:C:81:ILE:HD12	1:C:81:ILE:O	2.19	0.42
1:D:66:THR:HA	1:D:67:PRO:HD3	1.93	0.42
1:A:54:LEU:HB2	1:A:57:GLN:HG2	2.01	0.42
1:B:161:ASN:HB3	3:B:1144:HOH:O	2.20	0.42
2:C:1001:CLA:H43	1:D:89:ILE:HG21	2.01	0.42
1:B:125:GLU:HB3	3:B:1092:HOH:O	2.20	0.41
1:D:8:LYS:HD2	3:D:1086:HOH:O	2.20	0.41
1:B:5:GLU:O	1:B:77:THR:HG23	2.20	0.41
1:B:95:SER:N	1:B:112:GLY:HA2	2.36	0.41
1:D:146:SER:O	1:D:161:ASN:ND2	2.53	0.41
2:B:1001:CLA:H93	2:B:1001:CLA:HED1	2.02	0.41
1:D:77:THR:O	1:D:78:ASN:C	2.63	0.41
1:A:4:GLU:CD	1:A:79:THR:HG22	2.45	0.41
1:B:25:PRO:CG	1:B:51:ARG:HD2	2.50	0.41
1:B:91:LEU:HB3	1:C:44:LEU:HG	2.02	0.41
1:C:30:ASN:C	1:C:30:ASN:HD22	2.28	0.41
1:B:154:TRP:CZ2	2:D:1001:CLA:H191	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:N	1:C:151:LYS:CD	2.67	0.41
1:D:35:VAL:HG11	2:D:1001:CLA:CAD	2.50	0.41
1:B:118:GLY:HA2	1:B:121:PHE:CE1	2.56	0.41
1:C:13:ASN:N	1:C:13:ASN:HD22	2.19	0.41
1:C:13:ASN:N	1:C:13:ASN:ND2	2.69	0.41
1:A:140:ASP:OD2	1:A:145:LYS:HD2	2.21	0.41
1:D:66:THR:HG23	1:D:66:THR:O	2.20	0.41
1:C:146:SER:O	1:C:161:ASN:HB2	2.20	0.40
1:D:141:ASN:OD1	1:D:141:ASN:O	2.39	0.40
1:A:106:GLU:CD	1:A:106:GLU:H	2.30	0.40
1:C:3:ASP:N	3:C:1131:HOH:O	2.55	0.40
1:D:133:THR:C	1:D:134:TYR:CD1	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	168/180 (93%)	153 (91%)	9 (5%)	6 (4%)	2	1
1	B	169/180 (94%)	149 (88%)	14 (8%)	6 (4%)	2	1
1	C	175/180 (97%)	164 (94%)	10 (6%)	1 (1%)	21	17
1	D	175/180 (97%)	160 (91%)	11 (6%)	4 (2%)	5	2
All	All	687/720 (95%)	626 (91%)	44 (6%)	17 (2%)	4	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	104	SER
1	B	163	ASP

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Mol	Chain	Res	Type
1	C	128	GLY
1	D	27	SER
1	A	67	PRO
1	A	141	ASN
1	B	102	SER
1	B	144	GLY
1	D	69	SER
1	A	28	ASP
1	A	70	SER
1	B	162	ASP
1	D	28	ASP
1	D	72	GLY
1	B	25	PRO
1	A	3	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/158 (95%)	136 (91%)	14 (9%)	8	5
1	B	151/158 (96%)	145 (96%)	6 (4%)	28	27
1	C	155/158 (98%)	147 (95%)	8 (5%)	21	18
1	D	155/158 (98%)	151 (97%)	4 (3%)	40	44
All	All	611/632 (97%)	579 (95%)	32 (5%)	21	18

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	5	GLU
1	A	15	LEU
1	A	17	ILE
1	A	43	HIS
1	A	68	SER
1	A	69	SER

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Mol	Chain	Res	Type
1	A	70	SER
1	A	71	GLU
1	A	105	GLU
1	A	106	GLU
1	A	107	LYS
1	A	140	ASP
1	A	151	LYS
1	B	27	SER
1	B	29	ASN
1	B	78	ASN
1	B	131	LYS
1	B	138	ARG
1	B	143	GLU
1	C	3	ASP
1	C	43	HIS
1	C	69	SER
1	C	71	GLU
1	C	119	GLU
1	C	129	ASN
1	C	140	ASP
1	C	143	GLU
1	D	29	ASN
1	D	30	ASN
1	D	138	ARG
1	D	176	ARG

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

Mol	Chain	Res	Type
1	A	80	ASN
1	A	169	ASN
1	B	29	ASN
1	B	43	HIS
1	B	73	ASN
1	B	78	ASN
1	B	129	ASN
1	B	132	ASN
1	C	13	ASN
1	C	30	ASN
1	C	78	ASN
1	C	129	ASN
1	D	29	ASN

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Mol	Chain	Res	Type
1	D	73	ASN
1	D	169	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	CLA	B	1001	1	69,73,73	1.57	8 (11%)	82,113,113	1.87	10 (12%)
2	CLA	A	1001	1	69,73,73	1.90	10 (14%)	82,113,113	1.78	10 (12%)
2	CLA	C	1001	1	69,73,73	1.73	10 (14%)	82,113,113	1.76	10 (12%)
2	CLA	D	1001	1	69,73,73	1.66	10 (14%)	82,113,113	1.93	10 (12%)

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	CLA	B	1001	1	1/1/15/20	8/39/115/115	-
2	CLA	A	1001	1	1/1/15/20	11/39/115/115	-
2	CLA	C	1001	1	1/1/15/20	12/39/115/115	-
2	CLA	D	1001	1	1/1/15/20	8/39/115/115	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CLA	MG-NB	8.50	2.22	2.05
2	D	1001	CLA	MG-NA	7.17	2.23	2.06
2	A	1001	CLA	MG-NA	6.87	2.22	2.06
2	C	1001	CLA	MG-NB	6.64	2.18	2.05
2	B	1001	CLA	MG-NC	6.20	2.21	2.06
2	C	1001	CLA	MG-NA	5.64	2.19	2.06
2	C	1001	CLA	MG-NC	4.92	2.18	2.06
2	A	1001	CLA	MG-NC	4.72	2.17	2.06
2	D	1001	CLA	MG-NC	4.44	2.16	2.06
2	B	1001	CLA	MG-ND	4.37	2.14	2.05
2	A	1001	CLA	O2D-CGD	4.34	1.43	1.33
2	C	1001	CLA	O2D-CGD	4.32	1.43	1.33
2	B	1001	CLA	O2D-CGD	4.26	1.43	1.33
2	D	1001	CLA	MG-ND	3.82	2.13	2.05
2	D	1001	CLA	O2D-CGD	3.80	1.42	1.33
2	B	1001	CLA	MG-NA	3.77	2.15	2.06
2	D	1001	CLA	CMC-C2C	3.66	1.58	1.50
2	C	1001	CLA	C2-C3	3.60	1.41	1.33
2	C	1001	CLA	CMC-C2C	3.20	1.57	1.50
2	A	1001	CLA	CMC-C2C	3.14	1.57	1.50
2	A	1001	CLA	O2A-CGA	3.13	1.42	1.33
2	D	1001	CLA	MG-NB	2.99	2.11	2.05
2	D	1001	CLA	O1D-CGD	2.98	1.28	1.21
2	A	1001	CLA	O1D-CGD	2.93	1.28	1.21
2	B	1001	CLA	O1D-CGD	2.89	1.28	1.21
2	A	1001	CLA	CMD-C2D	2.83	1.56	1.50
2	C	1001	CLA	O1D-CGD	2.74	1.28	1.21
2	B	1001	CLA	C2-C3	2.56	1.39	1.33
2	C	1001	CLA	CBB-CAB	2.48	1.42	1.30
2	A	1001	CLA	C2-C3	2.47	1.38	1.33
2	D	1001	CLA	O2A-CGA	2.39	1.40	1.33
2	D	1001	CLA	C2-C3	2.30	1.38	1.33
2	C	1001	CLA	CMD-C2D	2.30	1.55	1.50
2	D	1001	CLA	CBB-CAB	2.20	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	CLA	CMC-C2C	2.16	1.55	1.50
2	B	1001	CLA	O2A-CGA	2.13	1.39	1.33
2	C	1001	CLA	C3B-C4B	2.08	1.48	1.42
2	A	1001	CLA	CHD-C1D	2.07	1.42	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	CLA	C4A-NA-C1A	12.21	112.25	106.68
2	A	1001	CLA	C4A-NA-C1A	11.73	112.03	106.68
2	C	1001	CLA	C4A-NA-C1A	11.55	111.95	106.68
2	D	1001	CLA	C4A-NA-C1A	11.18	111.78	106.68
2	D	1001	CLA	CBC-CAC-C3C	-6.26	95.45	112.42
2	D	1001	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
2	B	1001	CLA	O2D-CGD-CBD	3.50	117.35	111.23
2	B	1001	CLA	C6-C5-C3	-3.38	105.23	113.47
2	A	1001	CLA	O2A-CGA-CBA	3.37	122.11	111.83
2	D	1001	CLA	C1-C2-C3	3.28	131.57	126.20
2	A	1001	CLA	O2D-CGD-CBD	3.24	116.90	111.23
2	D	1001	CLA	O2A-CGA-CBA	3.23	121.69	111.83
2	B	1001	CLA	O2A-CGA-CBA	3.23	121.68	111.83
2	D	1001	CLA	O2D-CGD-CBD	3.16	116.75	111.23
2	C	1001	CLA	O2A-CGA-CBA	3.12	121.36	111.83
2	C	1001	CLA	O2D-CGD-CBD	3.08	116.62	111.23
2	B	1001	CLA	C3B-C4B-NB	-3.05	107.81	110.53
2	D	1001	CLA	C3C-C4C-NC	-3.00	106.59	110.43
2	C	1001	CLA	CMA-C3A-C2A	-2.66	103.71	113.98
2	B	1001	CLA	C1-C2-C3	2.58	130.42	126.20
2	C	1001	CLA	C3B-C4B-NB	-2.57	108.23	110.53
2	D	1001	CLA	C3B-C4B-NB	-2.55	108.25	110.53
2	A	1001	CLA	C3C-C4C-NC	-2.51	107.21	110.43
2	B	1001	CLA	C3C-C4C-NC	-2.50	107.23	110.43
2	C	1001	CLA	C4D-CHA-C1A	2.49	124.22	121.24
2	A	1001	CLA	C3B-C4B-NB	-2.40	108.39	110.53
2	A	1001	CLA	CED-O2D-CGD	2.32	121.17	115.92
2	B	1001	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
2	C	1001	CLA	CED-O2D-CGD	2.29	121.12	115.92
2	A	1001	CLA	C1-C2-C3	2.29	129.95	126.20
2	C	1001	CLA	C3C-C4C-NC	-2.29	107.50	110.43
2	D	1001	CLA	CED-O2D-CGD	2.28	121.08	115.92
2	A	1001	CLA	CMD-C2D-C3D	2.24	132.82	127.69
2	A	1001	CLA	O2A-CGA-O1A	-2.21	118.11	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	CLA	C4D-CHA-C1A	2.14	123.80	121.24
2	B	1001	CLA	CED-O2D-CGD	2.11	120.71	115.92
2	C	1001	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
2	C	1001	CLA	C2A-C1A-CHA	2.09	127.49	123.87
2	D	1001	CLA	C2A-C1A-CHA	2.02	127.37	123.87
2	B	1001	CLA	CMD-C2D-C1D	2.01	128.27	124.73

All (4) chirality outliers are listed below:

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

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1001	CLA	C14-C13-C15-C16
2	A	1001	CLA	C3-C5-C6-C7
2	B	1001	CLA	C3-C5-C6-C7
2	C	1001	CLA	C3-C5-C6-C7
2	A	1001	CLA	C13-C15-C16-C17
2	C	1001	CLA	C10-C11-C12-C13
2	A	1001	CLA	C10-C11-C12-C13
2	B	1001	CLA	C13-C15-C16-C17
2	D	1001	CLA	C11-C12-C13-C15
2	D	1001	CLA	C13-C15-C16-C17
2	A	1001	CLA	C11-C12-C13-C14
2	B	1001	CLA	O2A-C1-C2-C3
2	C	1001	CLA	C11-C12-C13-C14
2	A	1001	CLA	C11-C12-C13-C15
2	D	1001	CLA	C12-C13-C15-C16
2	D	1001	CLA	C6-C7-C8-C9
2	C	1001	CLA	C11-C12-C13-C15
2	D	1001	CLA	C6-C7-C8-C10
2	D	1001	CLA	C11-C12-C13-C14
2	B	1001	CLA	CBA-CGA-O2A-C1
2	C	1001	CLA	C13-C15-C16-C17
2	B	1001	CLA	O1A-CGA-O2A-C1
2	C	1001	CLA	C4-C3-C5-C6
2	A	1001	CLA	C4-C3-C5-C6

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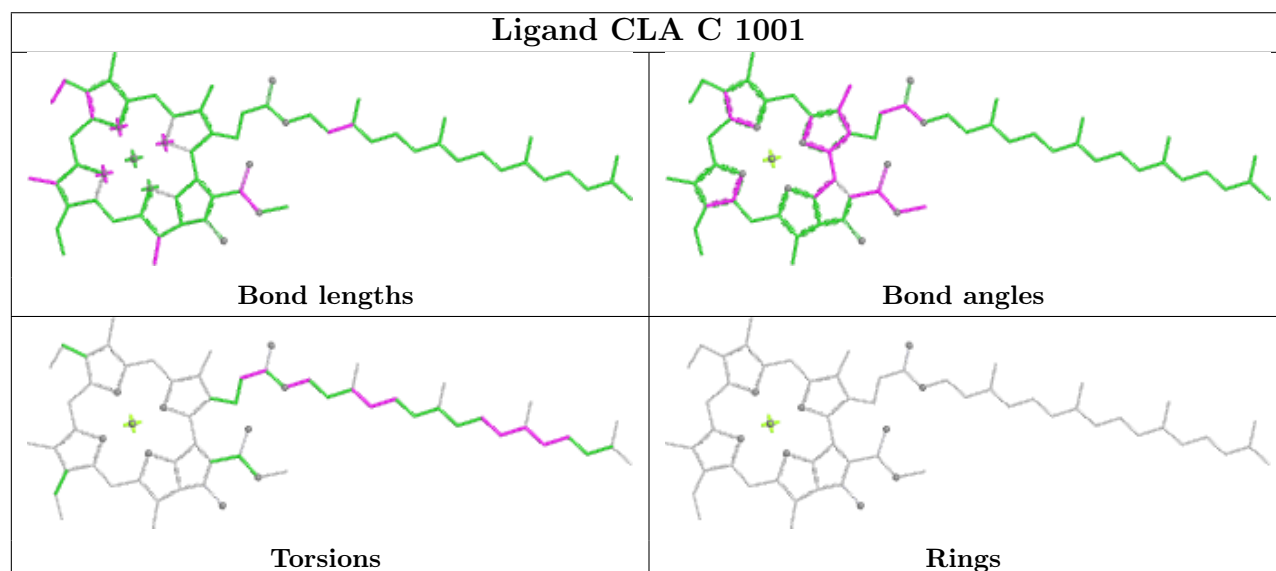
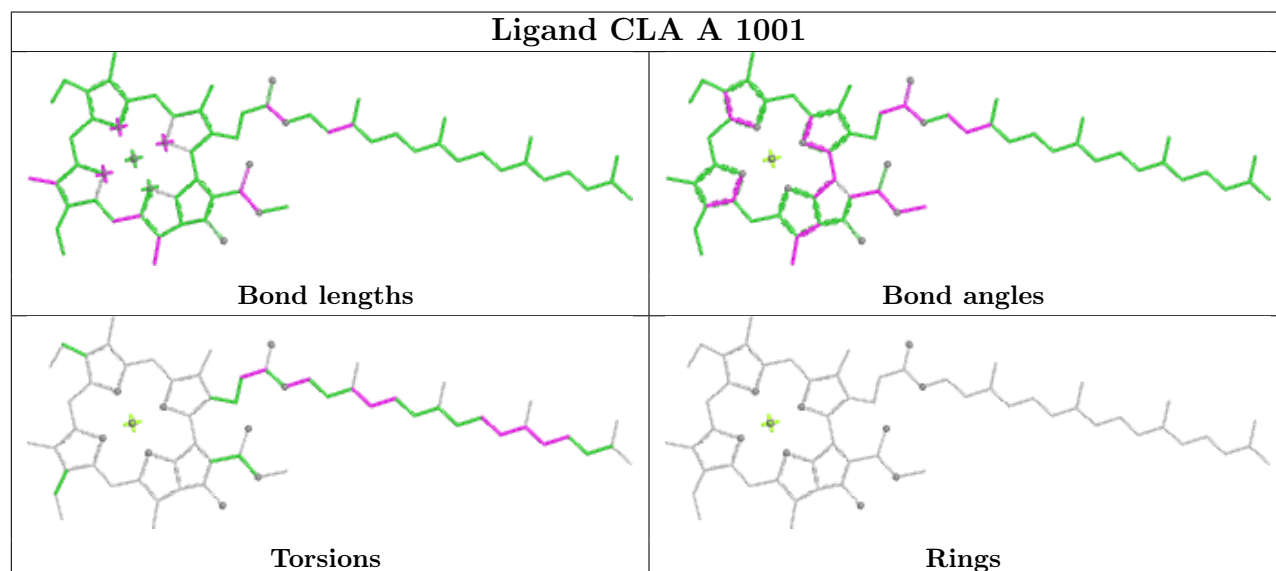
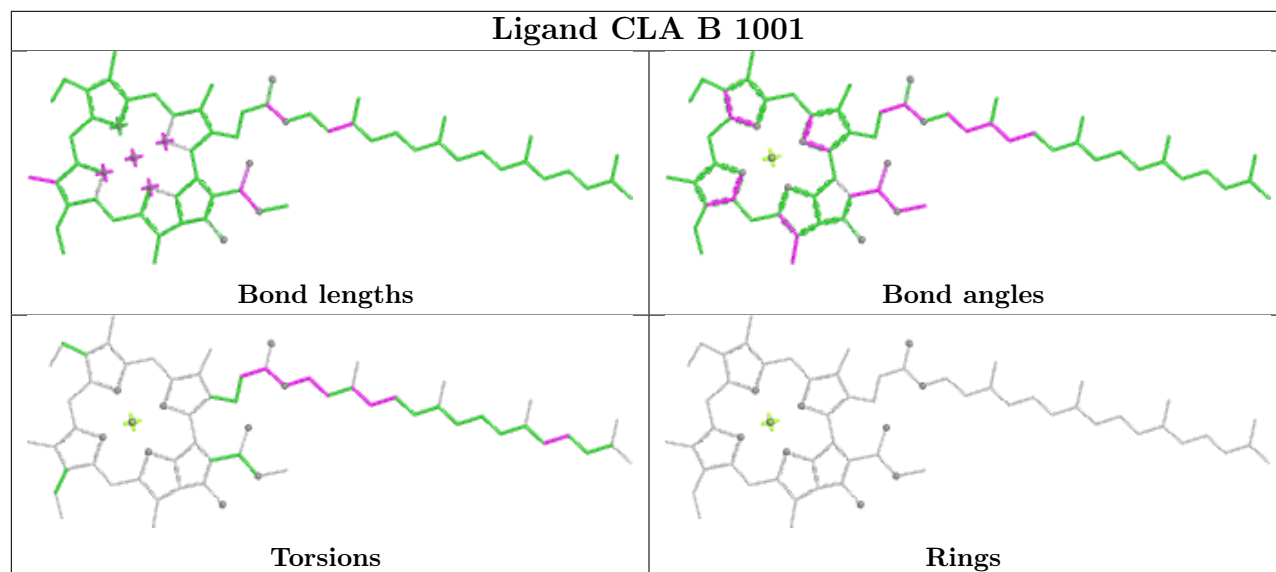
Mol	Chain	Res	Type	Atoms
2	C	1001	CLA	C2-C3-C5-C6
2	A	1001	CLA	C2-C3-C5-C6
2	C	1001	CLA	C14-C13-C15-C16
2	A	1001	CLA	C14-C13-C15-C16
2	C	1001	CLA	C2-C1-O2A-CGA
2	B	1001	CLA	C4-C3-C5-C6
2	A	1001	CLA	C12-C13-C15-C16
2	C	1001	CLA	C12-C13-C15-C16
2	A	1001	CLA	C2-C1-O2A-CGA
2	D	1001	CLA	C4-C3-C5-C6
2	B	1001	CLA	C2-C1-O2A-CGA
2	C	1001	CLA	CAA-CBA-CGA-O2A
2	A	1001	CLA	CAA-CBA-CGA-O2A
2	B	1001	CLA	CAA-CBA-CGA-O2A
2	C	1001	CLA	CAA-CBA-CGA-O1A

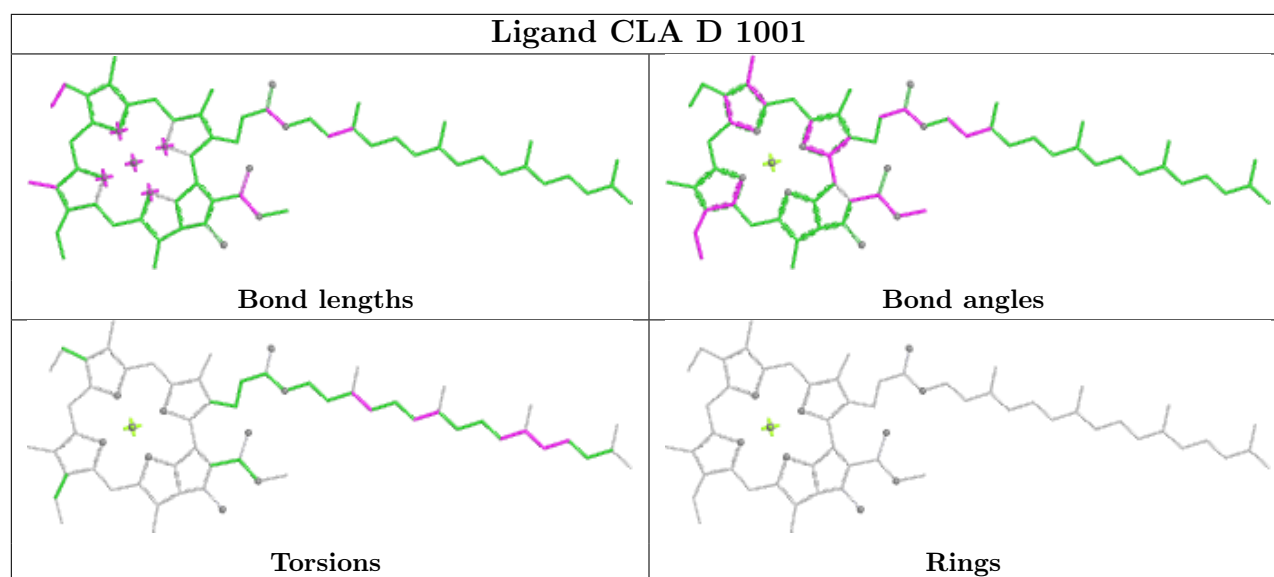
There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	CLA	10	0
2	A	1001	CLA	4	0
2	C	1001	CLA	6	0
2	D	1001	CLA	7	0

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





5.7 Other polymers [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	A	172/180 (95%)	0.52	10 (5%) 29 27	18, 34, 72, 84	0
1	B	173/180 (96%)	1.03	29 (16%) 4 4	25, 43, 77, 88	0
1	C	177/180 (98%)	0.66	16 (9%) 15 14	16, 38, 72, 86	0
1	D	177/180 (98%)	0.78	17 (9%) 13 12	19, 42, 71, 91	0
All	All	699/720 (97%)	0.75	72 (10%) 12 11	16, 40, 74, 91	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	TYR	4.0
1	B	142	GLY	3.9
1	A	70	SER	3.7
1	A	67	PRO	3.7
1	D	144	GLY	3.7
1	B	103	SER	3.5
1	D	129	ASN	3.5
1	D	3	ASP	3.5
1	B	76	LEU	3.4
1	B	143	GLU	3.2
1	B	166	SER	3.1
1	A	139	TYR	3.0
1	B	115	PRO	3.0
1	C	163	ASP	3.0
1	A	2	ASN	2.9
1	A	142	GLY	2.9
1	B	75	VAL	2.9
1	D	70	SER	2.9
1	B	167	ASP	2.7
1	C	140	ASP	2.7
1	B	78	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	2.7
1	B	26	ALA	2.7
1	D	140	ASP	2.6
1	C	30	ASN	2.6
1	B	70	SER	2.6
1	C	3	ASP	2.6
1	B	79	THR	2.6
1	D	6	PRO	2.6
1	B	132	ASN	2.6
1	C	79	THR	2.6
1	C	5	GLU	2.5
1	C	142	GLY	2.5
1	B	77	THR	2.5
1	D	69	SER	2.5
1	A	143	GLU	2.5
1	D	115	PRO	2.4
1	D	7	VAL	2.4
1	A	141	ASN	2.4
1	B	129	ASN	2.3
1	B	138	ARG	2.3
1	C	69	SER	2.3
1	B	160	LEU	2.3
1	A	179	ASP	2.3
1	B	28	ASP	2.3
1	B	165	ASP	2.3
1	C	102	SER	2.3
1	C	178	VAL	2.3
1	B	30	ASN	2.3
1	B	130	GLY	2.3
1	B	137	VAL	2.3
1	D	179	ASP	2.3
1	C	127	TYR	2.3
1	C	139	TYR	2.3
1	A	68	SER	2.2
1	C	78	ASN	2.2
1	B	163	ASP	2.2
1	B	144	GLY	2.2
1	C	76	LEU	2.2
1	D	78	ASN	2.2
1	B	25	PRO	2.1
1	B	128	GLY	2.1
1	D	128	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	131	LYS	2.1
1	B	4	GLU	2.1
1	B	74	ASP	2.1
1	C	68	SER	2.1
1	B	5	GLU	2.1
1	D	107	LYS	2.1
1	D	141	ASN	2.0
1	D	56	TYR	2.0
1	D	142	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

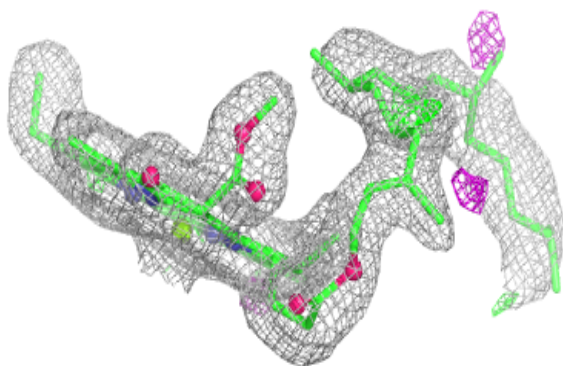
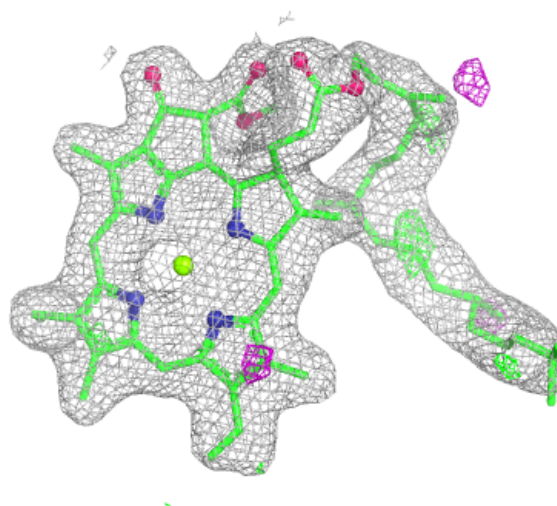
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CLA	B	1001	65/65	0.91	0.11	22,28,60,63	0
2	CLA	A	1001	65/65	0.93	0.10	20,26,67,70	0
2	CLA	D	1001	65/65	0.94	0.09	15,24,57,61	0
2	CLA	C	1001	65/65	0.95	0.09	15,22,64,69	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.

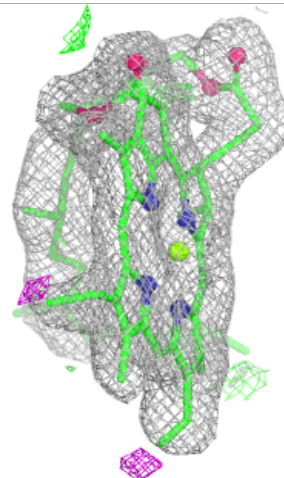
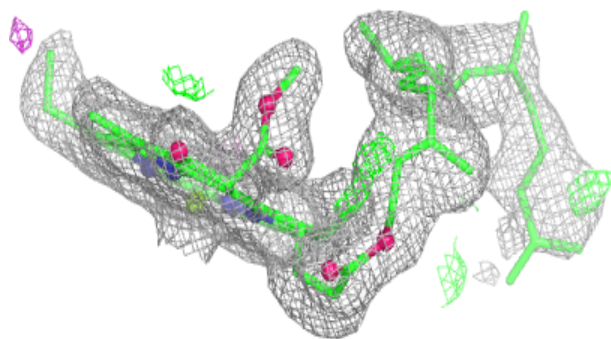
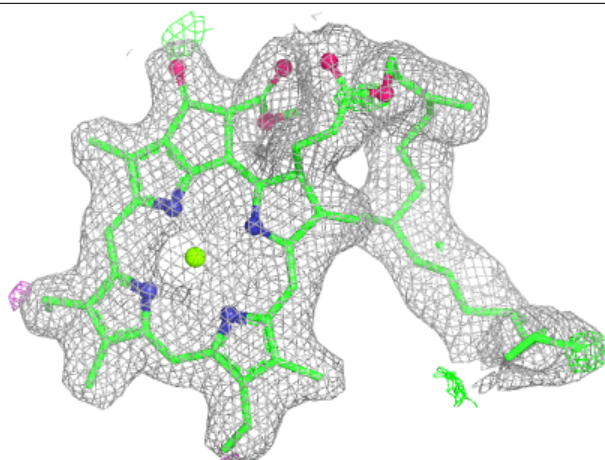
Electron density around CLA B 1001:

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



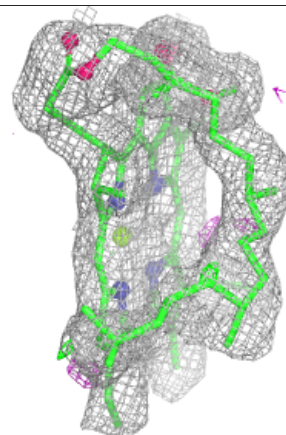
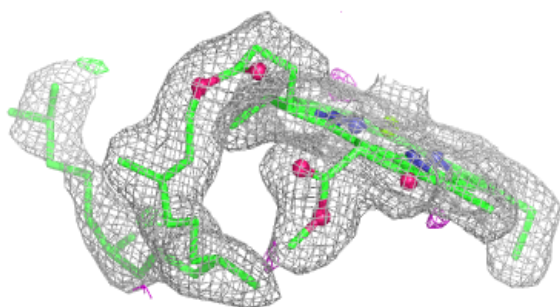
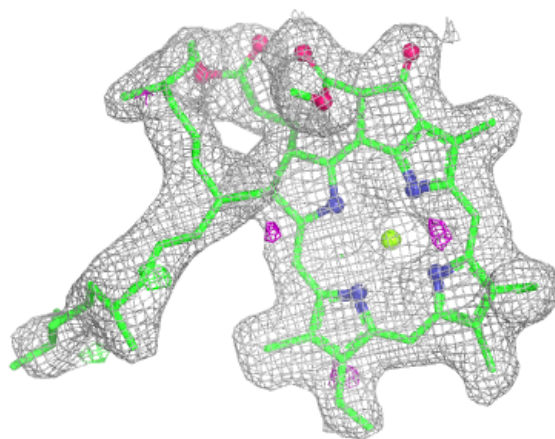
Electron density around CLA A 1001:

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



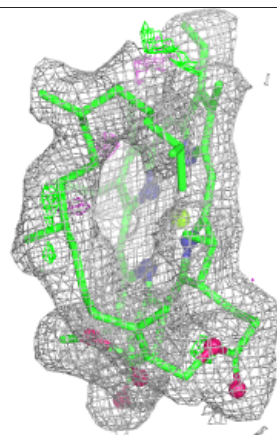
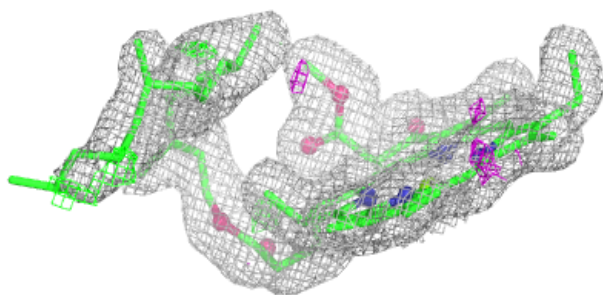
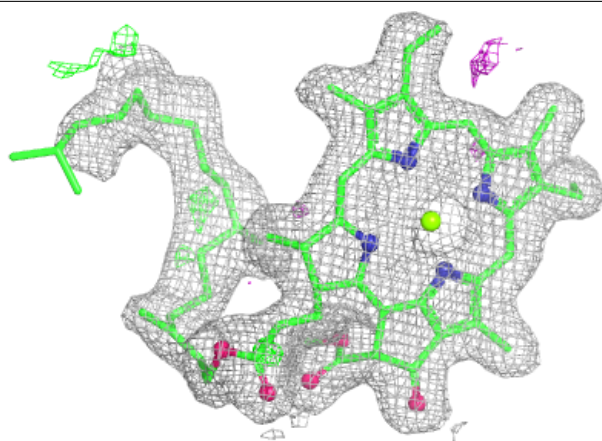
Electron density around CLA D 1001:

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



Electron density around CLA 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 [i](#)

There are no such residues in this entry.