WORLDWIDE

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:19 pm GMT

PDB ID	:	2X20
Title	:	STRUCTURE OF PERIDININ-CHLOROPHYLL-PROTEIN RECONSTITUTED WITH CHL-B
Authors	:	Schulte, T.; Hiller, R.G.; Hofmann, E.
Deposited on	:	2010-01-09
Resolution	:	1.95 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.194
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		1.8%
RSRZ outliers		0.7%

Worse　　　　　　　　　　　　　　　　　　　　　Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
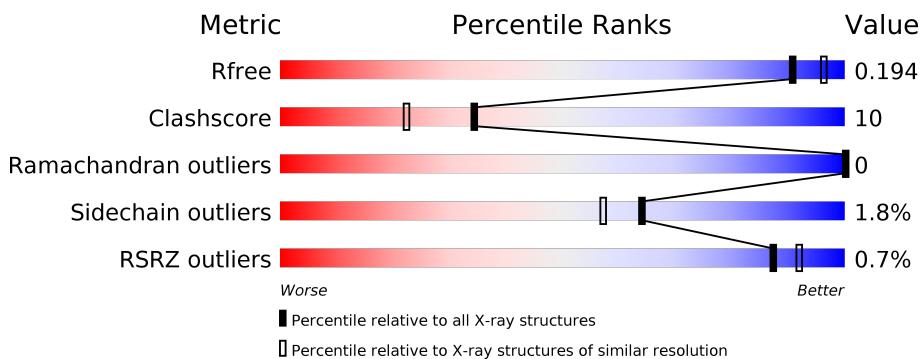
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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. 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	M	151	85%　　　　　　　　　　　　　　　14%　　•
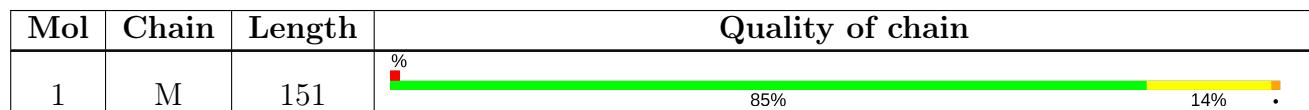
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	PEG	M	1162	-	-	-	X

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 1689 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 PERIDININ-CHLOROPHYLL A-BINDING PROTEIN, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	151	Total 1149	C 726	N 192	O 225	S 6	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	87	SER	ASN	CONFLICT	UNP P80484
M	128	ASN	SER	CONFLICT	UNP P80484

- Molecule 2 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).
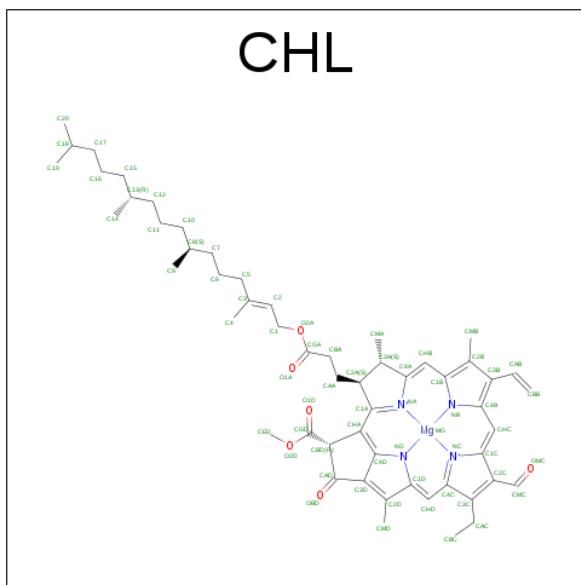
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total 69	C 58	Mg 1	N 4	O 6	0	1

- Molecule 3 is PERIDININ (three-letter code: PID) (formula: $C_{39}H_{50}O_7$).
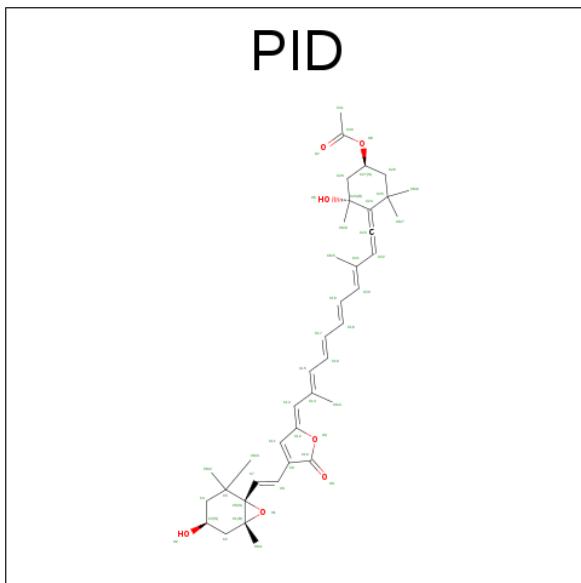
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total 46	C 39	O 7	0	0
3	M	1	Total 51	C 42	O 9	0	1
3	M	1	Total 46	C 39	O 7	0	0
3	M	1	Total 46	C 39	O 7	0	0

- Molecule 4 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).
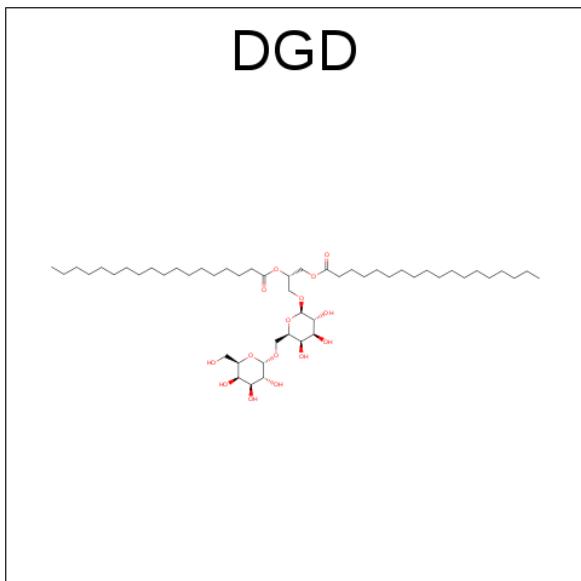
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total C O 66 51 15			0	0

- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	6	Total Cd 8 8		0	2

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	3	Total Cl 3 3		0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total K 1 1		0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

C4

OH O4

O2

O

C3

C1

C2

HO

O1
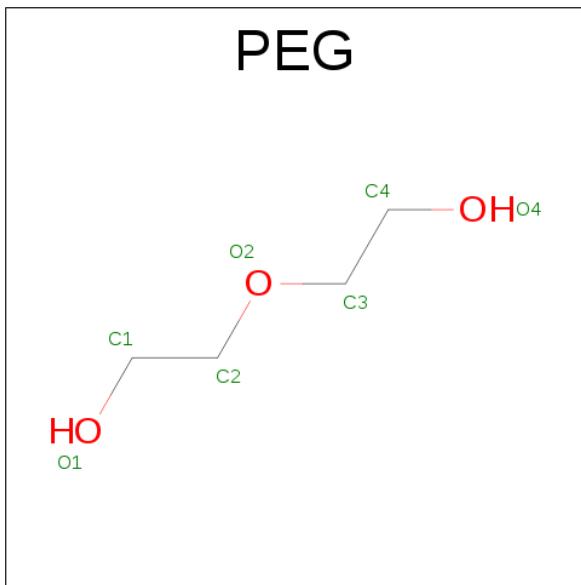
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total 7	C 4	O 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	196	Total 196	O 196	0	0

3   Residue-property plots ⓘ

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: PERIDININ-CHLOROPHYLL A-BINDING PROTEIN, CHLOROPLASTIC
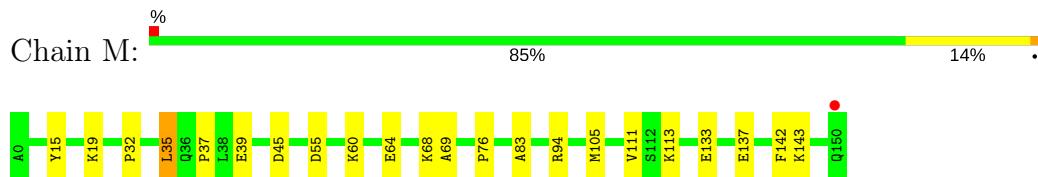
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	68.57Å 82.00Å 75.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 1.95 41.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.15-1.95) 99.3 (41.00-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.155 , 0.196 0.155 , 0.194	Depositor DCC
R_{free} test set	787 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	12.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	1689	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, CL, NA, K, CHL, CD, PEG, PID

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	M	1.19	4/1169 (0.3%)	0.90	6/1578 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	83	ALA	CA-CB	6.81	1.66	1.52
1	M	69	ALA	CA-CB	6.00	1.65	1.52
1	M	142	PHE	CE2-CZ	5.85	1.48	1.37
1	M	15	TYR	CD1-CE1	5.29	1.47	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	55	ASP	CB-CG-OD1	8.46	125.91	118.30
1	M	55	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	M	94	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	M	19	LYS	CD-CE-NZ	-5.23	99.67	111.70
1	M	94	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	M	45	ASP	CB-CG-OD1	5.18	122.97	118.30

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	M	1149	0	1151	14	0
2	M	69	0	6	3	0
3	M	189	0	166	2	0
4	M	66	0	96	11	0
5	M	8	0	0	1	0
6	M	3	0	0	1	0
7	M	1	0	0	0	0
8	M	1	0	0	0	0
9	M	7	0	10	1	0
10	M	196	0	0	6	0
All	All	1689	0	1429	26	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 10.

All (26) 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)
9:M:1162:PEG:H21	10:M:2192:HOH:O	1.34	1.21
1:M:68:LYS:HE3	10:M:2119:HOH:O	1.80	0.82
4:M:615:DGD:HAW1	4:M:615:DGD:HBN1	1.65	0.78
1:M:105[B]:MET:SD	10:M:2070:HOH:O	2.43	0.76
1:M:133:GLU:HG2	4:M:615:DGD:O5E	1.86	0.75
1:M:105[B]:MET:CE	10:M:2070:HOH:O	2.36	0.73
4:M:615:DGD:HAW1	4:M:615:DGD:CFB	2.19	0.72
5:M:1154[A]:CD:CD	6:M:1159:CL:CL	1.96	0.71
1:M:137:GLU:OE2	4:M:615:DGD:HE61	1.99	0.62
4:M:615:DGD:HBS1	4:M:615:DGD:HBW2	1.81	0.62
1:M:39:GLU:HG2	1:M:113:LYS:HZ2	1.65	0.61
1:M:111:VAL:HG21	4:M:615:DGD:HBH2	1.83	0.59
4:M:615:DGD:HBN1	4:M:615:DGD:CCA	2.33	0.58
1:M:39:GLU:HG2	1:M:113:LYS:NZ	2.19	0.58
4:M:615:DGD:CCB	4:M:615:DGD:HBS1	2.34	0.57
1:M:68:LYS:NZ	10:M:2104:HOH:O	2.19	0.57
1:M:60:LYS:O	1:M:64[A]:GLU:HG3	2.06	0.55
1:M:32:PRO:HG3	4:M:615:DGD:HA92	1.89	0.53
3:M:611:PID:H11	4:M:615:DGD:O1A	2.13	0.47
1:M:76:PRO:O	10:M:2112:HOH:O	2.21	0.43
3:M:613:PID:H22	4:M:615:DGD:HBG3	2.00	0.43
1:M:35:LEU:HD12	1:M:37:PRO:HD3	2.00	0.42
1:M:113:LYS:HG2	1:M:113:LYS:HZ2	1.76	0.41

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	M	153/151 (101%)	152 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	M	118/114 (104%)	116 (98%)	2 (2%)	66	60

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	35	LEU
1	M	143	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	36	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 13 are monoatomic - leaving 9 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	PEG	M	1162	-	6,6,6	0.65	0	5,5,5	0.49	0
2	CHL	M	601[A]	-	64,74,74	4.26	24 (37%)	51,114,114	2.43	15 (29%)
2	CHL	M	601[B]	-	64,74,74	4.26	24 (37%)	51,114,114	2.43	16 (31%)
3	PID	M	611	-	41,49,49	1.62	7 (17%)	49,76,76	3.80	19 (38%)
3	PID	M	612[A]	-	41,49,49	1.63	7 (17%)	49,76,76	3.97	19 (38%)
3	PID	M	612[B]	-	41,49,49	1.62	7 (17%)	49,76,76	3.99	22 (44%)
3	PID	M	613	-	41,49,49	1.40	3 (7%)	49,76,76	4.30	16 (32%)
3	PID	M	614	-	41,49,49	1.48	7 (17%)	49,76,76	3.70	16 (32%)
4	DGD	M	615	-	67,67,67	0.93	3 (4%)	81,81,81	1.50	12 (14%)

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
9	PEG	M	1162	-	-	0/4/4/4	0/0/0/0
2	CHL	M	601[A]	-	-	0/41/177/177	0/0/9/9
2	CHL	M	601[B]	-	-	0/41/177/177	0/0/9/9
3	PID	M	611	-	-	0/24/93/93	0/3/4/4
3	PID	M	612[A]	-	-	0/24/93/93	0/3/4/4
3	PID	M	612[B]	-	-	0/24/93/93	0/3/4/4
3	PID	M	613	-	-	0/24/93/93	0/3/4/4
3	PID	M	614	-	-	0/24/93/93	0/3/4/4
4	DGD	M	615	-	-	0/55/95/95	0/2/2/2

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	601[A]	CHL	C3D-C4D	-17.34	1.34	1.54
2	M	601[B]	CHL	C3D-C4D	-17.34	1.34	1.54
2	M	601[B]	CHL	C3B-C2B	-15.50	1.36	1.55
2	M	601[A]	CHL	C3B-C4B	-14.28	1.38	1.54
2	M	601[A]	CHL	C3B-C2B	-13.91	1.38	1.55
2	M	601[B]	CHL	C3B-C4B	-12.60	1.40	1.54
2	M	601[A]	CHL	C2B-C1B	-6.41	1.40	1.53
2	M	601[B]	CHL	C2B-C1B	-6.41	1.40	1.53
2	M	601[A]	CHL	C1B-NB	-6.39	1.36	1.50
2	M	601[B]	CHL	C1B-NB	-6.39	1.36	1.50
2	M	601[A]	CHL	C1D-ND	-5.94	1.37	1.50
2	M	601[B]	CHL	C1D-ND	-5.94	1.37	1.50
2	M	601[A]	CHL	CHB-C4A	-5.92	1.38	1.52
2	M	601[B]	CHL	CHB-C4A	-5.92	1.38	1.52
2	M	601[A]	CHL	C2D-C1D	-5.75	1.42	1.53
2	M	601[B]	CHL	C2D-C1D	-5.75	1.42	1.53
2	M	601[A]	CHL	C4B-NB	-5.74	1.38	1.50
2	M	601[B]	CHL	C4B-NB	-5.74	1.38	1.50
2	M	601[A]	CHL	C4D-ND	-5.43	1.38	1.50
2	M	601[B]	CHL	C4D-ND	-5.43	1.38	1.50
2	M	601[A]	CHL	C3D-C2D	-4.99	1.42	1.55
2	M	601[B]	CHL	C3D-C2D	-4.99	1.42	1.55
2	M	601[A]	CHL	CHD-C1D	-4.95	1.45	1.53
2	M	601[B]	CHL	CHD-C1D	-4.95	1.45	1.53
2	M	601[A]	CHL	C1A-CHA	-4.72	1.46	1.53
2	M	601[B]	CHL	C1A-CHA	-4.72	1.46	1.53
2	M	601[A]	CHL	CHC-C4B	-4.16	1.47	1.53
2	M	601[B]	CHL	CHC-C4B	-4.16	1.47	1.53
2	M	601[A]	CHL	CHA-CBD	-3.17	1.45	1.53
2	M	601[B]	CHL	CHA-CBD	-3.17	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	601[A]	CHL	C4C-C3C	-2.71	1.42	1.50
2	M	601[B]	CHL	C4C-C3C	-2.71	1.42	1.50
2	M	601[A]	CHL	CHB-C1B	-2.51	1.49	1.53
2	M	601[B]	CHL	CHB-C1B	-2.51	1.49	1.53
3	M	614	PID	CM1-C1	-2.36	1.48	1.51
3	M	614	PID	C23-C22	-2.15	1.28	1.32
3	M	612[A]	PID	C23-C22	-2.10	1.28	1.32
3	M	612[B]	PID	C23-C22	-2.10	1.28	1.32
2	M	601[A]	CHL	CHC-C1C	-2.09	1.49	1.53
2	M	601[B]	CHL	CHC-C1C	-2.09	1.49	1.53
2	M	601[A]	CHL	CHD-C4C	-2.06	1.49	1.53
2	M	601[B]	CHL	CHD-C4C	-2.06	1.49	1.53
3	M	611	PID	C8-C7	2.01	1.36	1.32
3	M	612[A]	PID	C13-C14	2.04	1.50	1.46
3	M	612[B]	PID	C13-C14	2.04	1.50	1.46
3	M	614	PID	C19-C20	2.06	1.49	1.43
3	M	614	PID	C20-C21	2.19	1.38	1.35
3	M	612[A]	PID	CM4-C14	2.19	1.55	1.50
3	M	612[B]	PID	CM4-C14	2.19	1.55	1.50
3	M	612[A]	PID	CM1-C1	2.21	1.55	1.51
3	M	612[B]	PID	CM1-C1	2.21	1.55	1.51
3	M	611	PID	C20-C21	2.24	1.38	1.35
3	M	614	PID	C2-C1	2.33	1.55	1.52
3	M	613	PID	C18-C17	2.39	1.51	1.44
3	M	611	PID	CM1-C1	2.42	1.55	1.51
4	M	615	DGD	O5D-C1E	2.44	1.44	1.40
3	M	613	PID	O6-C30	2.60	1.41	1.35
3	M	611	PID	C25-C24	2.72	1.59	1.54
3	M	614	PID	O6-C30	2.84	1.41	1.35
4	M	615	DGD	O1G-C1A	2.88	1.41	1.33
3	M	611	PID	O3-C10	2.89	1.27	1.21
2	M	601[A]	CHL	CMC-C2C	2.95	1.50	1.45
2	M	601[B]	CHL	CMC-C2C	2.95	1.50	1.45
3	M	612[B]	PID	O6-C30	3.43	1.43	1.35
3	M	611	PID	O6-C30	3.51	1.43	1.35
3	M	612[A]	PID	O3-C10	3.62	1.29	1.21
3	M	612[B]	PID	O3-C10	3.62	1.29	1.21
3	M	612[A]	PID	O6-C30	3.63	1.43	1.35
2	M	601[A]	CHL	O2A-CGA	3.69	1.44	1.33
2	M	601[B]	CHL	O2A-CGA	3.69	1.44	1.33
2	M	601[A]	CHL	O2D-CGD	3.85	1.42	1.33
2	M	601[B]	CHL	O2D-CGD	3.85	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	601[A]	CHL	C3C-C2C	4.00	1.39	1.34
2	M	601[B]	CHL	C3C-C2C	4.00	1.39	1.34
3	M	614	PID	C13-C12	4.32	1.46	1.36
2	M	601[A]	CHL	OBD-CAD	4.32	1.28	1.21
2	M	601[B]	CHL	OBD-CAD	4.32	1.28	1.21
4	M	615	DGD	O2G-C1B	4.39	1.47	1.34
3	M	611	PID	C13-C12	5.27	1.48	1.36
3	M	613	PID	C13-C12	5.36	1.48	1.36
3	M	612[A]	PID	C13-C12	5.91	1.49	1.36
3	M	612[B]	PID	C13-C12	5.91	1.49	1.36

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	613	PID	C12-O4-C10	-14.34	99.86	107.64
3	M	614	PID	C12-O4-C10	-11.84	101.21	107.64
3	M	611	PID	C12-O4-C10	-10.65	101.86	107.64
3	M	612[A]	PID	C12-O4-C10	-7.59	103.52	107.64
3	M	612[B]	PID	C12-O4-C10	-7.59	103.52	107.64
3	M	612[A]	PID	CM1-C1-C6	-7.16	110.20	122.31
3	M	612[B]	PID	CM1-C1-C6	-7.16	110.20	122.31
3	M	613	PID	C6-C7-C8	-6.22	112.85	125.99
2	M	601[A]	CHL	OMC-CMC-C2C	-5.00	117.91	124.29
2	M	601[B]	CHL	OMC-CMC-C2C	-5.00	117.91	124.29
3	M	613	PID	C9-C11-C12	-4.66	101.44	110.24
3	M	612[A]	PID	C9-C11-C12	-4.65	101.45	110.24
3	M	612[B]	PID	C9-C11-C12	-4.65	101.45	110.24
3	M	612[B]	PID	O6-C27-C28	-4.57	96.20	107.61
3	M	612[A]	PID	C17-C16-C15	-4.48	113.90	123.46
3	M	612[B]	PID	C17-C16-C15	-4.48	113.90	123.46
4	M	615	DGD	O1G-C1A-O1A	-4.31	112.86	123.55
3	M	614	PID	CM1-C1-C6	-4.24	115.14	122.31
2	M	601[A]	CHL	C1C-C2C-C3C	-4.23	107.31	111.52
2	M	601[B]	CHL	C1C-C2C-C3C	-4.23	107.31	111.52
3	M	611	PID	C18-C17-C16	-4.17	115.49	124.88
3	M	611	PID	C6-C7-C8	-4.16	117.19	125.99
3	M	614	PID	C9-C11-C12	-4.14	102.41	110.24
3	M	611	PID	C9-C11-C12	-4.01	102.66	110.24
3	M	613	PID	O3-C10-C9	-3.77	124.44	130.74
3	M	613	PID	O5-C29-CM8	-3.67	103.07	109.51
2	M	601[A]	CHL	O2D-CGD-O1D	-3.66	116.47	123.82
2	M	601[B]	CHL	O2D-CGD-O1D	-3.66	116.47	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	612[A]	PID	O1-C1-C2	-3.47	110.82	113.33
3	M	612[B]	PID	O1-C1-C2	-3.47	110.82	113.33
3	M	614	PID	C18-C17-C16	-3.40	117.23	124.88
3	M	611	PID	CM1-C1-C2	-3.35	110.44	114.28
3	M	612[A]	PID	O6-C30-O7	-3.33	116.21	122.94
4	M	615	DGD	CAB-C9B-C8B	-3.27	97.60	114.45
3	M	612[A]	PID	O1-C1-C6	-3.17	56.28	58.94
3	M	612[B]	PID	O1-C1-C6	-3.17	56.28	58.94
3	M	613	PID	CM1-C1-C6	-3.15	116.98	122.31
3	M	614	PID	O6-C30-O7	-3.12	116.62	122.94
4	M	615	DGD	O3G-C3G-C2G	-3.10	103.60	110.99
2	M	601[A]	CHL	CBA-CAA-C2A	-3.05	111.55	115.76
2	M	601[B]	CHL	CBA-CAA-C2A	-3.05	111.55	115.76
3	M	612[A]	PID	C19-C20-C21	-2.95	123.09	127.31
3	M	612[B]	PID	C19-C20-C21	-2.95	123.09	127.31
3	M	612[A]	PID	O2-C3-C2	-2.88	104.02	109.86
3	M	612[B]	PID	O2-C3-C2	-2.88	104.02	109.86
3	M	613	PID	O6-C30-O7	-2.88	117.11	122.94
3	M	614	PID	C8-C9-C11	-2.81	121.59	127.29
3	M	611	PID	C17-C18-C19	-2.80	118.59	124.88
3	M	612[A]	PID	C8-C9-C11	-2.79	121.62	127.29
3	M	612[B]	PID	C8-C9-C11	-2.79	121.62	127.29
3	M	611	PID	O6-C30-O7	-2.78	117.31	122.94
3	M	614	PID	O3-C10-C9	-2.73	126.17	130.74
3	M	611	PID	C8-C9-C11	-2.71	121.78	127.29
3	M	613	PID	C19-C20-C21	-2.66	123.51	127.31
3	M	612[B]	PID	C27-O6-C30	-2.64	112.83	117.94
4	M	615	DGD	C3B-C2B-C1B	-2.54	104.32	113.58
2	M	601[B]	CHL	C3B-CAB-CBB	-2.51	119.55	125.20
3	M	612[A]	PID	C29-C24-C25	-2.50	117.22	119.70
3	M	612[B]	PID	C29-C24-C25	-2.50	117.22	119.70
3	M	614	PID	C18-C19-C20	-2.48	118.17	123.46
3	M	611	PID	O1-C1-C6	-2.47	56.87	58.94
4	M	615	DGD	O5D-C1E-C2E	-2.40	104.32	108.23
3	M	613	PID	O1-C1-C6	-2.39	56.93	58.94
3	M	612[A]	PID	C6-C7-C8	-2.38	120.97	125.99
3	M	612[B]	PID	C6-C7-C8	-2.38	120.97	125.99
3	M	614	PID	CM3-C5-CM2	-2.36	103.78	107.34
3	M	611	PID	C1-C2-C3	-2.33	108.17	112.64
3	M	611	PID	CM3-C5-C6	-2.31	103.80	110.05
3	M	612[B]	PID	O6-C30-O7	-2.24	118.41	122.94
4	M	615	DGD	CCB-CBB-CAB	-2.19	103.16	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	612[A]	PID	O3-C10-C9	-2.13	127.17	130.74
3	M	612[B]	PID	O3-C10-C9	-2.13	127.17	130.74
2	M	601[A]	CHL	C4-C3-C2	-2.10	118.08	123.69
2	M	601[B]	CHL	C4-C3-C2	-2.10	118.08	123.69
3	M	611	PID	C18-C19-C20	-2.05	119.09	123.46
4	M	615	DGD	C9B-C8B-C7B	-2.00	104.14	114.45
3	M	611	PID	C26-C25-C24	2.14	111.29	109.21
3	M	612[B]	PID	O6-C30-C31	2.18	115.19	111.10
3	M	612[A]	PID	CM3-C5-CM2	2.23	110.70	107.34
3	M	612[B]	PID	CM3-C5-CM2	2.23	110.70	107.34
4	M	615	DGD	O3G-C1D-C2D	2.31	112.01	108.23
3	M	614	PID	CM6-C25-C24	2.33	112.56	110.47
2	M	601[A]	CHL	C1-O2A-CGA	2.39	122.50	116.77
2	M	601[B]	CHL	C1-O2A-CGA	2.39	122.50	116.77
3	M	614	PID	CM7-C25-C24	2.50	112.71	110.47
2	M	601[A]	CHL	CHB-C1B-C2B	2.55	124.04	116.99
2	M	601[B]	CHL	CHB-C1B-C2B	2.55	124.04	116.99
3	M	612[A]	PID	CM7-C25-C24	2.56	112.76	110.47
3	M	612[B]	PID	CM7-C25-C24	2.56	112.76	110.47
3	M	612[B]	PID	O6-C27-C26	2.59	114.08	107.61
3	M	611	PID	CM6-C25-C24	2.61	112.81	110.47
4	M	615	DGD	O6D-C5D-C6D	2.78	112.19	106.64
3	M	613	PID	CM1-C1-C2	2.83	117.52	114.28
4	M	615	DGD	O1G-C1A-C2A	2.83	120.13	111.90
3	M	614	PID	O6-C30-C31	2.91	116.56	111.10
3	M	612[A]	PID	CM6-C25-C24	2.98	113.14	110.47
3	M	612[B]	PID	CM6-C25-C24	2.98	113.14	110.47
3	M	613	PID	C27-O6-C30	3.06	123.84	117.94
4	M	615	DGD	O6D-C1D-C2D	3.16	116.40	110.30
2	M	601[A]	CHL	CHD-C1D-C2D	3.27	126.05	116.99
2	M	601[B]	CHL	CHD-C1D-C2D	3.27	126.05	116.99
2	M	601[A]	CHL	O2D-CGD-CBD	3.64	120.07	111.20
2	M	601[B]	CHL	O2D-CGD-CBD	3.64	120.07	111.20
3	M	613	PID	O6-C30-C31	3.65	117.96	111.10
3	M	614	PID	O1-C1-C2	3.72	116.03	113.33
3	M	613	PID	CM7-C25-C24	3.73	113.81	110.47
4	M	615	DGD	O6E-C5E-C6E	3.81	115.54	106.41
3	M	611	PID	O6-C30-C31	3.95	118.52	111.10
3	M	611	PID	O4-C10-C9	4.17	111.67	108.11
3	M	612[A]	PID	O6-C30-C31	4.21	119.00	111.10
2	M	601[A]	CHL	C4-C3-C5	4.29	122.74	115.29
2	M	601[B]	CHL	C4-C3-C5	4.29	122.74	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	614	PID	O4-C10-C9	4.56	112.00	108.11
2	M	601[B]	CHL	C3B-C4B-NB	4.62	111.60	103.55
3	M	614	PID	CM1-C1-C2	4.73	119.70	114.28
2	M	601[A]	CHL	C1D-CHD-C4C	4.90	122.81	112.37
2	M	601[B]	CHL	C1D-CHD-C4C	4.90	122.81	112.37
2	M	601[A]	CHL	CMD-C2D-C3D	4.90	126.67	114.27
2	M	601[B]	CHL	CMD-C2D-C3D	4.90	126.67	114.27
2	M	601[A]	CHL	C3B-C4B-NB	4.97	112.21	103.55
2	M	601[B]	CHL	CMB-C2B-C3B	5.65	126.84	113.69
2	M	601[A]	CHL	CMB-C2B-C3B	5.89	127.39	113.69
2	M	601[A]	CHL	C4B-CHC-C1C	5.99	125.13	112.37
2	M	601[B]	CHL	C4B-CHC-C1C	5.99	125.13	112.37
3	M	613	PID	O4-C10-C9	6.20	113.41	108.11
3	M	613	PID	O1-C1-C2	6.61	118.13	113.33
3	M	611	PID	O1-C1-CM1	6.76	123.47	115.02
3	M	611	PID	O1-C1-C2	8.65	119.61	113.33
3	M	612[A]	PID	O1-C1-CM1	12.76	130.99	115.02
3	M	612[B]	PID	O1-C1-CM1	12.76	130.99	115.02
3	M	611	PID	O4-C12-C11	16.79	116.93	107.41
3	M	612[A]	PID	O4-C12-C11	17.69	117.43	107.41
3	M	612[B]	PID	O4-C12-C11	17.69	117.43	107.41
3	M	614	PID	O4-C12-C11	18.34	117.81	107.41
3	M	613	PID	O4-C12-C11	20.42	118.98	107.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	1162	PEG	1	0
2	M	601[A]	CHL	1	0
2	M	601[B]	CHL	2	0
3	M	611	PID	1	0
3	M	613	PID	1	0
4	M	615	DGD	11	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	M	151/151 (100%)	-0.48	1 (0%)	87	92	4, 9, 20, 27	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	150	GLN	2.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
9	PEG	M	1162	7/7	0.68	0.17	7.71	42,44,44,45	0
4	DGD	M	615	66/66	0.92	0.14	1.70	15,27,37,44	0
3	PID	M	613	46/46	0.96	0.11	1.63	4,8,14,23	0
2	CHL	M	601[A]	66/66	0.98	0.10	1.53	2,6,12,13	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	CHL	M	601[B]	66/66	0.98	0.10	1.53	2,6,12,13	3
3	PID	M	612[A]	46/46	0.93	0.12	1.06	5,9,30,38	5
3	PID	M	612[B]	46/46	0.93	0.12	1.06	5,9,30,38	5
3	PID	M	611	46/46	0.96	0.09	0.35	2,7,13,22	0
3	PID	M	614	46/46	0.98	0.09	-0.05	2,6,9,14	0
5	CD	M	1154[B]	1/1	1.00	0.06	-1.84	10,10,10,10	1
5	CD	M	1151[B]	1/1	1.00	0.05	-	19,19,19,19	1
5	CD	M	1153	1/1	0.99	0.07	-	14,14,14,14	1
5	CD	M	1152	1/1	1.00	0.05	-	9,9,9,9	0
6	CL	M	1158	1/1	0.93	0.07	-	34,34,34,34	0
6	CL	M	1159	1/1	0.99	0.08	-	8,8,8,8	1
8	NA	M	1161	1/1	0.81	0.15	-	27,27,27,27	0
7	K	M	1160	1/1	0.95	0.07	-	38,38,38,38	0
6	CL	M	1157	1/1	1.00	0.06	-	9,9,9,9	0
5	CD	M	1155	1/1	0.99	0.05	-	16,16,16,16	1
5	CD	M	1156	1/1	0.99	0.04	-	32,32,32,32	1
5	CD	M	1151[A]	1/1	1.00	0.05	-	13,13,13,13	1
5	CD	M	1154[A]	1/1	1.00	0.06	-	6,6,6,6	1

6.5 Other polymers ⓘ

There are no such residues in this entry.