



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:19 pm GMT

PDB ID : 2X1Z  
Title : STRUCTURE OF PERIDININ-CHLOROPHYLL-PROTEIN RECONSTITUTED WITH CHL-D  
Authors : Schulte, T.; Hiller, R.G.; Hofmann, E.  
Deposited on : 2010-01-09  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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

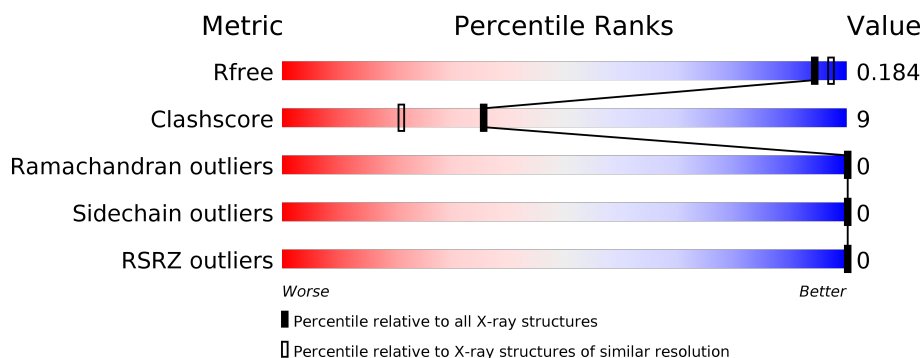
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	M	151	

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
3	CL7	M	1151	X	-	-	-
5	CL	M	1162	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PEG	M	1165	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 1758 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.

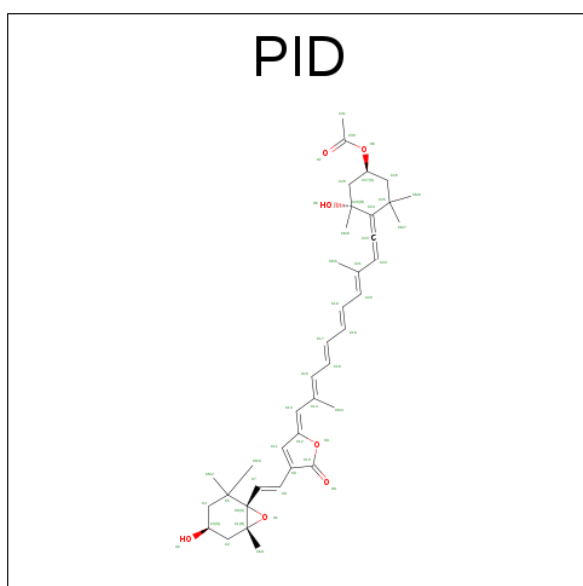
- Molecule 1 is a protein called PERIDININ-CHLOROPHYLL A-BINDING PROTEIN, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	151	Total	C	N	O	S	0	10	0
			1200	759	202	233	6			

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 PERIDININ (three-letter code: PID) (formula:  $C_{39}H_{50}O_7$ ).



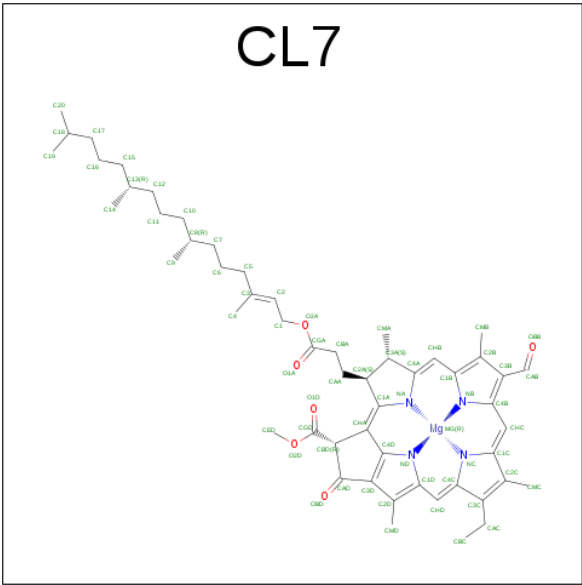
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total	C	O	0	1
			49	41	8		
2	M	1	Total	C	O	0	1
			51	42	9		

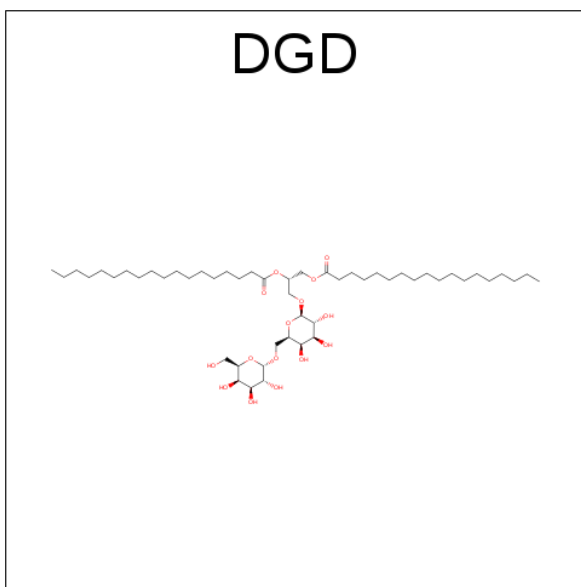
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total	C	O	0	0
			46	39	7		
2	M	1	Total	C	O	0	0
			46	39	7		

- Molecule 3 is CHLOROPHYLL D (three-letter code: CL7) (formula: C<sub>54</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			66	51	15		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	4	Total	Cl	0	0
			4	4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	2	Total	Na	0	0
			2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 8 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 9 is water.

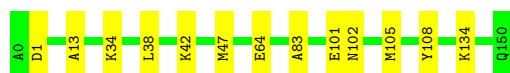
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	214	Total	O	0	0
			214	214		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PERIDININ-CHLOROPHYLL A-BINDING PROTEIN, CHLOROPLASTIC

Chain M:  91% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.58Å 81.99Å 75.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.11 – 1.80 43.11 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.11-1.80) 100.0 (43.11-1.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.67 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.141 , 0.183 0.141 , 0.184	Depositor DCC
$R_{free}$ test set	1002 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, DGD, CL, NA, PID, CD, CL7

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	1.16	2/1220 (0.2%)	0.92	1/1645 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	83	ALA	CA-CB	6.17	1.65	1.52
1	M	101	GLU	CG-CD	5.12	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1	ASP	CB-CG-OD1	5.40	123.16	118.30

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	M	1200	0	1206	23	0
2	M	192	0	134	0	0
3	M	65	0	69	0	0
4	M	66	0	96	9	0
5	M	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	2	0	0	0	0
7	M	7	0	10	0	0
8	M	8	0	0	1	0
9	M	214	0	0	10	1
All	All	1758	0	1515	27	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 9.

All (27) 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:M:38[B]:LEU:HD23	5:M:1162:CL:CL	2.00	0.98
5:M:1167:CL:CL	8:M:1174[A]:CD:CD	1.85	0.82
1:M:134[A]:LYS:HD3	9:M:2183:HOH:O	1.88	0.72
1:M:105:MET:SD	9:M:2149:HOH:O	2.47	0.72
1:M:38[B]:LEU:N	1:M:38[B]:LEU:HD22	2.07	0.69
1:M:64[B]:GLU:OE1	9:M:2112:HOH:O	2.15	0.65
4:M:1152:DGD:HBH1	4:M:1152:DGD:HBV2	1.79	0.64
1:M:38[B]:LEU:HD22	1:M:38[B]:LEU:H	1.63	0.64
1:M:134[B]:LYS:HD3	9:M:2177:HOH:O	1.99	0.61
1:M:42[A]:LYS:HE2	9:M:2085:HOH:O	2.02	0.58
1:M:134[A]:LYS:HE3	9:M:2018:HOH:O	2.03	0.58
1:M:47[B]:MET:HE1	4:M:1152:DGD:HBN1	1.86	0.58
1:M:38[B]:LEU:CD2	1:M:38[B]:LEU:H	2.18	0.56
1:M:108:TYR:HD1	4:M:1152:DGD:HB91	1.71	0.55
1:M:102[B]:ASN:ND2	9:M:2147:HOH:O	2.13	0.53
1:M:38[B]:LEU:N	1:M:38[B]:LEU:CD2	2.72	0.50
1:M:47[B]:MET:CE	4:M:1152:DGD:HBN1	2.44	0.47
4:M:1152:DGD:HA41	4:M:1152:DGD:HB62	1.97	0.46
1:M:108:TYR:CD1	4:M:1152:DGD:HB91	2.51	0.45
1:M:64[B]:GLU:CD	9:M:2112:HOH:O	2.53	0.45
1:M:134[A]:LYS:CD	9:M:2183:HOH:O	2.55	0.44
1:M:47[B]:MET:HE2	4:M:1152:DGD:HBH2	2.00	0.44
1:M:38[B]:LEU:CD2	5:M:1162:CL:CL	2.89	0.43
1:M:47[B]:MET:HE2	4:M:1152:DGD:CDB	2.49	0.42
4:M:1152:DGD:HA22	4:M:1152:DGD:HB62	2.02	0.41
1:M:34:LYS:NZ	9:M:2070:HOH:O	2.52	0.41
1:M:13:ALA:HA	1:M:134[A]:LYS:HE2	2.01	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:2070:HOH:O	9:M:2153:HOH:O[3_455]	1.97	0.23

## 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	M	159/151 (105%)	158 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	M	124/114 (109%)	124 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

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 23 ligands modelled in this entry, 14 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$
3	CL7	M	1151	9	53,73,73	1.67	9 (16%)	54,113,113	1.44	8 (14%)
4	DGD	M	1152	-	67,67,67	0.96	3 (4%)	81,81,81	1.36	11 (13%)
7	PEG	M	1165	-	6,6,6	0.65	0	5,5,5	0.38	0
2	PID	M	611[A]	-	41,49,49	1.90	11 (26%)	49,76,76	3.52	20 (40%)
2	PID	M	611[B]	-	41,49,49	1.83	9 (21%)	49,76,76	3.27	18 (36%)
2	PID	M	612[A]	-	41,49,49	1.64	6 (14%)	49,76,76	4.17	17 (34%)
2	PID	M	612[B]	-	41,49,49	1.58	6 (14%)	49,76,76	4.24	19 (38%)
2	PID	M	613	-	41,49,49	1.63	10 (24%)	49,76,76	4.63	22 (44%)
2	PID	M	614	-	41,49,49	1.51	5 (12%)	49,76,76	3.43	23 (46%)

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
3	CL7	M	1151	9	2/2/15/20	0/37/115/115	0/0/9/9
4	DGD	M	1152	-	-	0/55/95/95	0/2/2/2
7	PEG	M	1165	-	-	0/4/4/4	0/0/0/0
2	PID	M	611[A]	-	-	0/24/93/93	0/3/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PID	M	611[B]	-	-	0/24/93/93	0/3/4/4
2	PID	M	612[A]	-	-	0/24/93/93	0/3/4/4
2	PID	M	612[B]	-	-	0/24/93/93	0/3/4/4
2	PID	M	613	-	-	0/24/93/93	0/3/4/4
2	PID	M	614	-	-	0/24/93/93	0/3/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1151	CL7	C4D-CHA	-4.15	1.39	1.45
3	M	1151	CL7	C3D-C4D	-3.73	1.35	1.41
2	M	611[A]	PID	C23-C22	-3.17	1.26	1.32
2	M	611[B]	PID	C23-C22	-3.17	1.26	1.32
2	M	612[B]	PID	C11-C12	-2.24	1.41	1.44
2	M	612[A]	PID	C11-C12	-2.24	1.41	1.44
2	M	613	PID	C11-C12	-2.04	1.41	1.44
3	M	1151	CL7	C4B-CHC	2.04	1.45	1.40
2	M	614	PID	C19-C20	2.10	1.50	1.43
2	M	613	PID	O3-C10	2.10	1.26	1.21
2	M	613	PID	O1-C1	2.12	1.49	1.46
2	M	613	PID	O6-C30	2.16	1.40	1.35
2	M	611[A]	PID	C2-C1	2.17	1.55	1.52
2	M	613	PID	CM8-C29	2.18	1.56	1.52
2	M	611[A]	PID	C2-C3	2.19	1.55	1.52
2	M	614	PID	C26-C27	2.24	1.55	1.51
2	M	614	PID	O3-C10	2.32	1.26	1.21
2	M	612[B]	PID	C2-C1	2.35	1.55	1.52
2	M	612[A]	PID	C2-C1	2.35	1.55	1.52
2	M	611[A]	PID	C26-C27	2.38	1.56	1.51
2	M	611[B]	PID	C26-C27	2.38	1.56	1.51
2	M	614	PID	CM7-C25	2.40	1.58	1.53
2	M	613	PID	C26-C27	2.43	1.56	1.51
4	M	1152	DGD	O5D-C1E	2.58	1.44	1.40
2	M	611[A]	PID	C8-C9	2.62	1.51	1.45
2	M	611[B]	PID	C8-C9	2.62	1.51	1.45
2	M	613	PID	C18-C17	2.79	1.52	1.44
3	M	1151	CL7	OBD-CAD	2.84	1.26	1.22
2	M	611[A]	PID	C20-C21	2.94	1.39	1.35
2	M	611[B]	PID	C20-C21	2.94	1.39	1.35
2	M	613	PID	C20-C21	3.00	1.39	1.35
2	M	612[B]	PID	CM4-C14	3.03	1.57	1.50
2	M	612[A]	PID	CM4-C14	3.03	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	611[A]	PID	C15-C14	3.06	1.39	1.35
2	M	611[B]	PID	C15-C14	3.06	1.39	1.35
2	M	611[A]	PID	C28-C27	3.18	1.57	1.51
2	M	611[B]	PID	C28-C27	3.18	1.57	1.51
4	M	1152	DGD	O1G-C1A	3.21	1.42	1.33
3	M	1151	CL7	O2A-CGA	3.23	1.42	1.33
2	M	611[A]	PID	O3-C10	3.26	1.28	1.21
2	M	611[B]	PID	O3-C10	3.26	1.28	1.21
3	M	1151	CL7	C2A-C1A	3.26	1.56	1.50
2	M	613	PID	C2-C1	3.29	1.56	1.52
2	M	612[B]	PID	O6-C30	3.32	1.42	1.35
3	M	1151	CL7	O2D-CGD	3.40	1.41	1.33
2	M	611[A]	PID	O6-C30	3.58	1.43	1.35
2	M	611[B]	PID	O6-C30	3.58	1.43	1.35
3	M	1151	CL7	C1B-CHB	3.61	1.49	1.40
4	M	1152	DGD	O2G-C1B	3.98	1.45	1.34
2	M	612[A]	PID	O6-C30	4.13	1.44	1.35
2	M	612[B]	PID	O3-C10	4.48	1.31	1.21
2	M	612[A]	PID	O3-C10	4.48	1.31	1.21
2	M	612[B]	PID	C13-C12	4.80	1.47	1.36
2	M	612[A]	PID	C13-C12	4.80	1.47	1.36
3	M	1151	CL7	CHB-C4A	5.09	1.40	1.33
2	M	611[A]	PID	C13-C12	5.19	1.48	1.36
2	M	611[B]	PID	C13-C12	5.19	1.48	1.36
2	M	614	PID	C13-C12	5.37	1.48	1.36
2	M	613	PID	C13-C12	5.38	1.48	1.36

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	613	PID	C12-O4-C10	-16.53	98.66	107.64
2	M	611[A]	PID	C12-O4-C10	-9.38	102.55	107.64
2	M	611[B]	PID	C12-O4-C10	-9.38	102.55	107.64
2	M	612[B]	PID	C12-O4-C10	-9.14	102.68	107.64
2	M	612[A]	PID	C12-O4-C10	-9.14	102.68	107.64
2	M	614	PID	C12-O4-C10	-8.66	102.94	107.64
2	M	612[B]	PID	CM1-C1-C6	-5.91	112.31	122.31
2	M	612[A]	PID	CM1-C1-C6	-5.91	112.31	122.31
2	M	611[A]	PID	C18-C17-C16	-5.32	112.91	124.88
2	M	611[B]	PID	C18-C17-C16	-5.32	112.91	124.88
2	M	613	PID	C9-C11-C12	-4.90	100.98	110.24
2	M	612[B]	PID	C9-C11-C12	-4.82	101.13	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	612[A]	PID	C9-C11-C12	-4.82	101.13	110.24
2	M	612[B]	PID	C8-C9-C11	-4.65	117.84	127.29
2	M	612[A]	PID	C8-C9-C11	-4.65	117.84	127.29
2	M	614	PID	C18-C19-C20	-4.45	113.97	123.46
2	M	613	PID	C6-C7-C8	-4.37	116.76	125.99
2	M	613	PID	C18-C17-C16	-4.28	115.25	124.88
2	M	614	PID	C9-C11-C12	-4.28	102.15	110.24
2	M	611[A]	PID	C6-C7-C8	-4.18	117.16	125.99
2	M	611[B]	PID	C6-C7-C8	-4.18	117.16	125.99
2	M	614	PID	C18-C17-C16	-3.83	116.26	124.88
2	M	611[A]	PID	C9-C11-C12	-3.82	103.02	110.24
2	M	611[B]	PID	C9-C11-C12	-3.82	103.02	110.24
2	M	614	PID	C6-C7-C8	-3.80	117.96	125.99
2	M	612[B]	PID	O6-C27-C28	-3.80	98.13	107.61
4	M	1152	DGD	O5D-C6D-C5D	-3.78	102.62	108.94
2	M	611[A]	PID	O2-C3-C4	-3.73	102.28	109.86
3	M	1151	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
2	M	614	PID	CM1-C1-C6	-3.57	116.28	122.31
2	M	613	PID	CM7-C25-C24	-3.48	107.36	110.47
2	M	612[B]	PID	O1-C1-C6	-3.47	56.03	58.94
2	M	612[A]	PID	O1-C1-C6	-3.47	56.03	58.94
2	M	612[B]	PID	C17-C16-C15	-3.42	116.16	123.46
2	M	612[A]	PID	C17-C16-C15	-3.42	116.16	123.46
2	M	613	PID	C26-C25-C24	-3.38	105.92	109.21
2	M	613	PID	O1-C1-C6	-3.38	56.10	58.94
2	M	613	PID	O6-C30-O7	-3.26	116.35	122.94
2	M	611[A]	PID	C17-C18-C19	-3.23	117.62	124.88
2	M	611[B]	PID	C17-C18-C19	-3.23	117.62	124.88
2	M	611[A]	PID	C8-C9-C11	-3.18	120.82	127.29
2	M	611[B]	PID	C8-C9-C11	-3.18	120.82	127.29
2	M	614	PID	O6-C30-O7	-3.18	116.49	122.94
4	M	1152	DGD	O1G-C1A-O1A	-3.18	115.66	123.55
2	M	611[A]	PID	O3-C10-C9	-3.02	125.68	130.74
2	M	611[B]	PID	O3-C10-C9	-3.02	125.68	130.74
2	M	613	PID	CM1-C1-C6	-2.96	117.30	122.31
3	M	1151	CL7	C1B-CHB-C4A	-2.92	124.33	130.12
2	M	612[B]	PID	C17-C18-C19	-2.91	118.33	124.88
2	M	612[A]	PID	C17-C18-C19	-2.91	118.33	124.88
4	M	1152	DGD	CCB-CBB-CAB	-2.86	99.70	114.45
3	M	1151	CL7	C7-C6-C5	-2.75	105.46	113.11
2	M	614	PID	C29-C24-C25	-2.75	116.97	119.70
2	M	614	PID	CM3-C5-CM2	-2.70	103.27	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	611[B]	PID	O2-C3-C2	-2.68	104.41	109.86
2	M	614	PID	C17-C16-C15	-2.65	117.81	123.46
2	M	614	PID	C26-C25-C24	-2.60	106.69	109.21
2	M	614	PID	O2-C3-C4	-2.58	104.62	109.86
2	M	613	PID	O4-C12-C13	-2.58	117.22	122.88
2	M	614	PID	C17-C18-C19	-2.57	119.09	124.88
2	M	612[B]	PID	O6-C30-O7	-2.53	117.81	122.94
4	M	1152	DGD	CFB-CEB-CDB	-2.51	101.54	114.45
4	M	1152	DGD	O6D-C1D-O3G	-2.50	104.08	110.02
2	M	614	PID	CM5-C21-C22	-2.43	112.58	118.77
2	M	612[B]	PID	CM1-C1-C2	-2.39	111.54	114.28
2	M	612[A]	PID	CM1-C1-C2	-2.39	111.54	114.28
2	M	613	PID	O6-C27-C26	-2.38	101.67	107.61
2	M	612[B]	PID	CM3-C5-C4	-2.29	104.91	108.97
2	M	612[A]	PID	CM3-C5-C4	-2.29	104.91	108.97
4	M	1152	DGD	O1G-C1G-C2G	-2.29	102.91	108.66
2	M	611[A]	PID	CM2-C5-C6	-2.26	103.94	110.05
2	M	611[B]	PID	CM2-C5-C6	-2.26	103.94	110.05
2	M	613	PID	O6-C27-C28	-2.25	102.00	107.61
2	M	613	PID	O3-C10-C9	-2.25	126.98	130.74
2	M	611[A]	PID	C18-C19-C20	-2.21	118.75	123.46
2	M	611[B]	PID	C18-C19-C20	-2.21	118.75	123.46
2	M	613	PID	C8-C9-C11	-2.19	122.84	127.29
2	M	614	PID	O3-C10-C9	-2.18	127.10	130.74
2	M	612[A]	PID	O6-C27-C26	-2.17	102.18	107.61
2	M	614	PID	O2-C3-C2	-2.15	105.48	109.86
2	M	613	PID	O2-C3-C4	-2.14	105.51	109.86
2	M	612[B]	PID	C6-C7-C8	-2.13	121.49	125.99
2	M	612[A]	PID	C6-C7-C8	-2.13	121.49	125.99
4	M	1152	DGD	O4E-C4E-C3E	-2.11	105.77	110.36
3	M	1151	CL7	CAA-CBA-CGA	-2.09	107.06	113.35
2	M	614	PID	C8-C9-C11	-2.05	123.13	127.29
2	M	613	PID	O5-C29-CM8	-2.04	105.93	109.51
4	M	1152	DGD	C6E-C5E-C4E	2.04	117.77	113.00
4	M	1152	DGD	C4D-C3D-C2D	2.07	114.48	110.84
2	M	611[A]	PID	C4-C3-C2	2.08	114.91	110.68
2	M	612[B]	PID	C28-C27-C26	2.10	113.66	109.87
2	M	612[A]	PID	O6-C30-C31	2.13	115.11	111.10
2	M	613	PID	C27-O6-C30	2.22	122.23	117.94
2	M	611[B]	PID	C4-C3-C2	2.27	115.31	110.68
2	M	614	PID	CM5-C21-C20	2.28	126.11	122.92
3	M	1151	CL7	C4-C3-C5	2.29	119.26	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	614	PID	CM7-C25-C24	2.36	112.58	110.47
2	M	612[B]	PID	O1-C1-C2	2.43	115.09	113.33
2	M	612[A]	PID	O1-C1-C2	2.43	115.09	113.33
3	M	1151	CL7	CMD-C2D-C1D	2.47	132.25	128.46
4	M	1152	DGD	CBA-CAA-C9A	2.53	127.51	114.45
2	M	611[A]	PID	C29-C24-C25	2.57	122.25	119.70
2	M	611[B]	PID	C29-C24-C25	2.57	122.25	119.70
2	M	612[B]	PID	CM4-C14-C13	2.64	125.67	118.91
2	M	612[A]	PID	CM4-C14-C13	2.64	125.67	118.91
2	M	611[B]	PID	O1-C1-C2	2.66	115.26	113.33
3	M	1151	CL7	C3B-C4B-NB	2.87	112.92	109.21
2	M	611[A]	PID	O2-C3-C2	2.91	115.78	109.86
2	M	612[B]	PID	O6-C27-C26	2.94	114.97	107.61
2	M	611[A]	PID	C28-C27-C26	2.99	115.27	109.87
2	M	611[B]	PID	C28-C27-C26	2.99	115.27	109.87
2	M	614	PID	O1-C1-CM1	3.04	118.82	115.02
2	M	613	PID	O6-C30-C31	3.04	116.81	111.10
2	M	611[A]	PID	CM3-C5-CM2	3.06	111.95	107.34
2	M	611[B]	PID	CM3-C5-CM2	3.06	111.95	107.34
3	M	1151	CL7	O2D-CGD-CBD	3.10	116.83	111.30
2	M	614	PID	O4-C10-C9	3.52	111.11	108.11
4	M	1152	DGD	O1G-C1A-C2A	3.72	122.72	111.90
2	M	611[A]	PID	C1-C2-C3	3.86	120.05	112.64
2	M	611[A]	PID	O1-C1-CM1	3.93	119.94	115.02
2	M	611[B]	PID	O1-C1-CM1	3.93	119.94	115.02
2	M	613	PID	CM6-C25-C24	3.98	114.04	110.47
2	M	614	PID	CM1-C1-C2	4.15	119.03	114.28
2	M	613	PID	O1-C1-CM1	4.36	120.48	115.02
2	M	612[B]	PID	CM3-C5-CM2	4.67	114.38	107.34
2	M	612[A]	PID	CM3-C5-CM2	4.67	114.38	107.34
2	M	611[A]	PID	O4-C10-C9	4.67	112.09	108.11
2	M	611[B]	PID	O4-C10-C9	4.67	112.09	108.11
2	M	613	PID	O4-C10-C9	5.39	112.71	108.11
2	M	611[A]	PID	O1-C1-C2	7.70	118.92	113.33
2	M	612[B]	PID	O1-C1-CM1	12.68	130.89	115.02
2	M	612[A]	PID	O1-C1-CM1	12.68	130.89	115.02
2	M	611[A]	PID	O4-C12-C11	15.20	116.03	107.41
2	M	611[B]	PID	O4-C12-C11	15.20	116.03	107.41
2	M	614	PID	O4-C12-C11	16.50	116.76	107.41
2	M	612[B]	PID	O4-C12-C11	19.87	118.67	107.41
2	M	612[A]	PID	O4-C12-C11	19.87	118.67	107.41
2	M	613	PID	O4-C12-C11	22.79	120.33	107.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	1151	CL7	NC
3	M	1151	CL7	NA

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1152	DGD	9	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	M	151/151 (100%)	-0.73	0 100 100	5, 9, 20, 28	0

There are no RSRZ outliers to report.

### 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 carbohydrates 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	PEG	M	1165	7/7	0.86	0.17	3.96	35,38,42,42	0
4	DGD	M	1152	66/66	0.90	0.13	0.95	14,23,38,43	0
2	PID	M	613	46/46	0.97	0.07	0.88	3,7,15,26	0
2	PID	M	612[B]	46/46	0.96	0.10	0.77	2,9,28,32	5
2	PID	M	612[A]	46/46	0.96	0.10	0.77	5,10,28,32	5
8	CD	M	1175	1/1	0.99	0.10	0.60	12,12,12,12	1
3	CL7	M	1151	65/65	0.98	0.06	0.29	2,6,12,18	0
2	PID	M	611[B]	46/46	0.97	0.07	-0.10	3,7,12,16	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PID	M	611[A]	46/46	0.97	0.07	-0.10	3,7,13,16	3
2	PID	M	614	46/46	0.98	0.06	-0.36	2,5,9,15	0
5	CL	M	1166	1/1	0.92	0.07	-	41,41,41,41	0
6	NA	M	1164	1/1	0.96	0.07	-	19,19,19,19	0
5	CL	M	1161	1/1	0.99	0.05	-	10,10,10,10	0
8	CD	M	1173	1/1	0.98	0.04	-	25,25,25,25	1
5	CL	M	1162	1/1	0.97	0.05	-	31,31,31,31	0
8	CD	M	1176	1/1	0.99	0.07	-	22,22,22,22	1
5	CL	M	1167	1/1	0.98	0.15	-	11,11,11,11	1
8	CD	M	1172	1/1	1.00	0.06	-	8,8,8,8	0
8	CD	M	1174[A]	1/1	1.00	0.07	-	10,10,10,10	1
8	CD	M	1171[A]	1/1	1.00	0.05	-	10,10,10,10	1
8	CD	M	1171[B]	1/1	1.00	0.05	-	22,22,22,22	1
6	NA	M	1163	1/1	0.98	0.05	-	15,15,15,15	0
8	CD	M	1174[B]	1/1	1.00	0.07	-	8,8,8,8	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.