



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1PPR  
Title : PERIDININ-CHLOROPHYLL-PROTEIN OF AMPHIDINIUM CARTERAE  
Authors : Hofmann, E.; Welte, W.; Diederichs, K.  
Deposited on : 1996-03-06  
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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

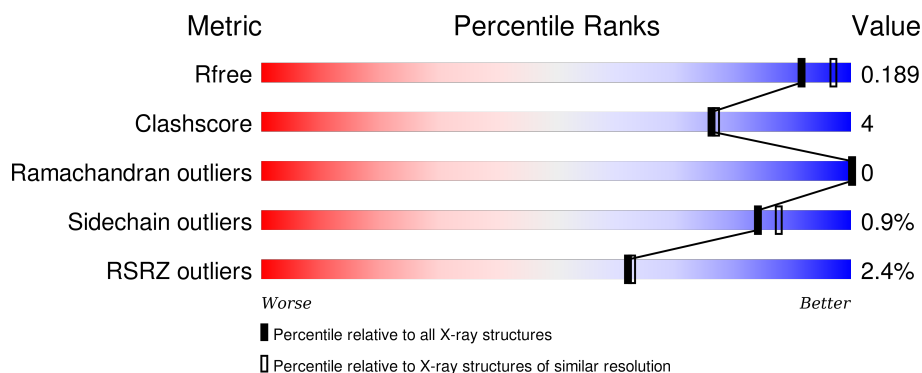
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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	312	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
1	N	312	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
1	O	312	<div> <div>2%</div> <div>95%</div> <div>5%</div> </div>

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	M	601	X	-	-	X
2	CLA	M	602	X	-	-	-
2	CLA	N	601	X	-	-	X
2	CLA	N	602	X	-	-	X
2	CLA	O	601	X	-	-	X
2	CLA	O	602	X	-	-	-
3	PID	M	612	-	-	-	X
3	PID	M	613	X	-	-	X
3	PID	N	612	-	-	-	X
3	PID	N	613	X	-	-	X
3	PID	N	622	-	-	-	X
3	PID	N	623	-	-	-	X
3	PID	O	612	-	-	-	X
3	PID	O	613	X	-	-	-
4	DGD	M	615	X	-	-	X
4	DGD	N	615	X	-	-	X
4	DGD	O	615	X	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9152 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.

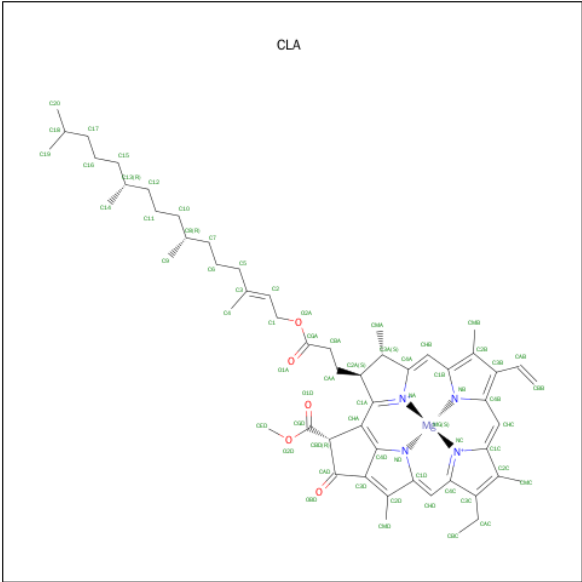
- Molecule 1 is a protein called PERIDININ-CHLOROPHYLL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	312	Total	C	N	O	S	0	0	0
			2282	1445	382	444	11			
1	N	312	Total	C	N	O	S	0	0	0
			2282	1445	382	444	11			
1	O	312	Total	C	N	O	S	0	0	0
			2282	1445	382	444	11			

There are 9 discrepancies between the modelled and reference sequences:

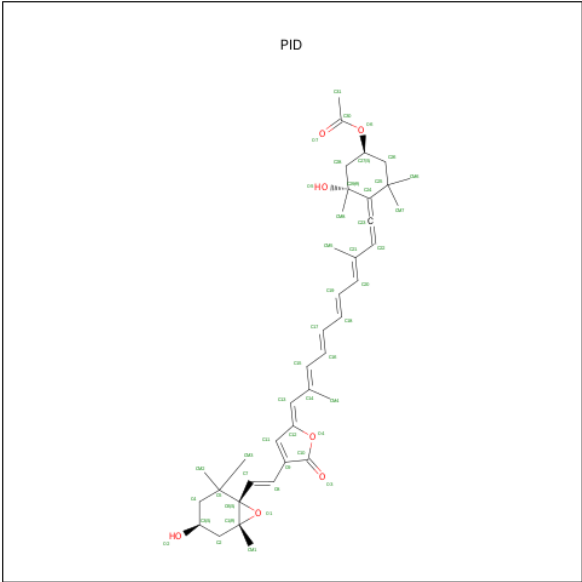
Chain	Residue	Modelled	Actual	Comment	Reference
M	73	ILE	VAL	CONFLICT	UNP P80484
M	128	ASN	SER	CONFLICT	UNP P80484
M	276	VAL	ALA	CONFLICT	UNP P80484
N	73	ILE	VAL	CONFLICT	UNP P80484
N	128	ASN	SER	CONFLICT	UNP P80484
N	276	VAL	ALA	CONFLICT	UNP P80484
O	73	ILE	VAL	CONFLICT	UNP P80484
O	128	ASN	SER	CONFLICT	UNP P80484
O	276	VAL	ALA	CONFLICT	UNP P80484

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

- Molecule 3 is PERIDININ (three-letter code: PID) (formula: C<sub>39</sub>H<sub>50</sub>O<sub>7</sub>).



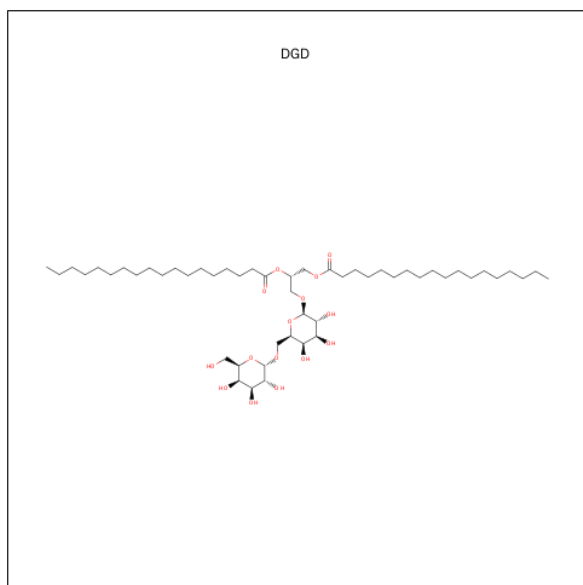
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	M	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	N	1	Total	C	O	0	0
			46	39	7		
3	N	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		
3	O	1	Total	C	O	0	0
			46	39	7		

- 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	0	0
			66	51	15		

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

- Molecule 5 is water.

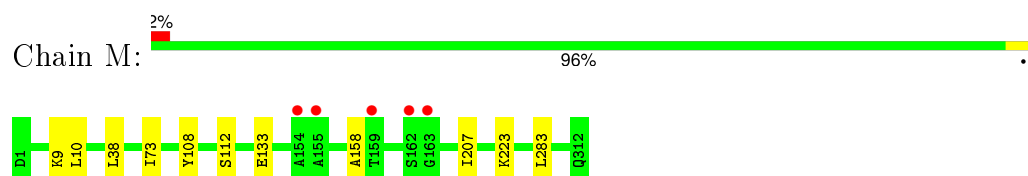
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	139	Total	O	0	0
			139	139		
5	N	137	Total	O	0	0
			137	137		
5	O	140	Total	O	0	0
			140	140		



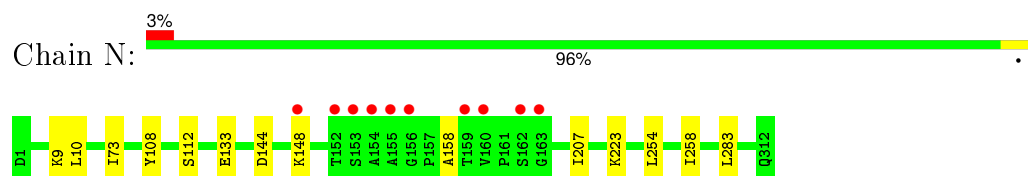
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

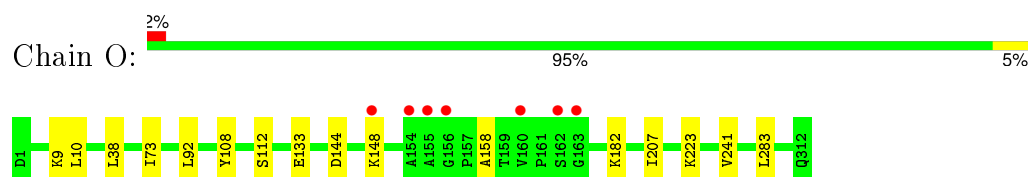
- Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN



- Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN



- Molecule 1: PERIDININ-CHLOROPHYLL PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.43 Å   116.30 Å   67.03 Å 90.00°   94.89°   90.00°	Depositor
Resolution (Å)	40.00 – 2.00 33.84 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.5 (40.00-2.00) 89.5 (33.84-1.99)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.77 (at 2.00 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.179   ,   0.201 0.168   ,   0.189	Depositor DCC
$R_{free}$ test set	2325 reflections (2.59%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 96045 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PID, CLA, DGD

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	0.58	0/2323	0.60	0/3154
1	N	0.56	0/2323	0.58	0/3154
1	O	0.59	0/2323	0.60	0/3154
All	All	0.58	0/6969	0.59	0/9462

There are no bond length outliers.

There are no bond angle outliers.

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	2282	0	2300	9	0
1	N	2282	0	2300	10	0
1	O	2282	0	2300	12	0
2	M	130	0	144	3	0
2	N	130	0	144	2	0
2	O	130	0	144	4	0
3	M	368	0	400	9	0
3	N	368	0	400	9	0
3	O	368	0	400	9	0
4	M	132	0	192	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	132	0	192	10	0
4	O	132	0	192	11	0
5	M	139	0	0	0	0
5	N	137	0	0	0	0
5	O	140	0	0	0	0
All	All	9152	0	9108	67	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 4.

All (67) 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:O:73:ILE:HD11	3:O:614:PID:HM72	1.27	1.15
1:M:73:ILE:HD11	3:M:614:PID:HM72	1.30	1.07
1:N:73:ILE:HD11	3:N:614:PID:HM72	1.31	1.06
1:O:73:ILE:HD11	3:O:614:PID:CM7	2.12	0.75
2:M:602:CLA:HBB1	2:M:602:CLA:HHC	1.71	0.72
2:O:602:CLA:HBB1	2:O:602:CLA:HHC	1.74	0.69
2:N:602:CLA:HHC	2:N:602:CLA:HBB1	1.76	0.68
2:N:601:CLA:HHC	2:N:601:CLA:HBB1	1.78	0.66
2:O:601:CLA:HHC	2:O:601:CLA:HBB1	1.78	0.66
1:M:73:ILE:HD11	3:M:614:PID:CM7	2.17	0.65
2:M:601:CLA:HBB1	2:M:601:CLA:HHC	1.78	0.65
1:O:112:SER:HA	4:O:615:DGD:HB51	1.80	0.63
1:N:73:ILE:HD11	3:N:614:PID:CM7	2.19	0.63
1:N:112:SER:HA	4:N:615:DGD:HB51	1.81	0.62
1:M:112:SER:HA	4:M:615:DGD:HB51	1.82	0.62
3:N:611:PID:H3	4:N:615:DGD:HD61	1.85	0.59
3:M:611:PID:H3	4:M:615:DGD:HD61	1.85	0.59
3:O:611:PID:H3	4:O:615:DGD:HD61	1.85	0.59
4:N:615:DGD:HB62	4:N:615:DGD:HA22	1.88	0.55
4:M:615:DGD:HB62	4:M:615:DGD:HA22	1.88	0.54
1:O:9:LYS:N	1:O:9:LYS:HD2	2.24	0.52
1:M:9:LYS:N	1:M:9:LYS:HD2	2.25	0.52
1:N:9:LYS:N	1:N:9:LYS:HD2	2.25	0.51
1:M:108:TYR:CD1	4:M:615:DGD:HB82	2.47	0.50
1:O:108:TYR:CD1	4:O:615:DGD:HB82	2.47	0.49
1:N:207:ILE:HD12	3:N:611:PID:H261	1.94	0.49
1:N:108:TYR:CD1	4:N:615:DGD:HB82	2.48	0.49
1:O:207:ILE:HD12	3:O:611:PID:H261	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:158:ALA:HB2	1:O:223:LYS:HD3	1.94	0.47
4:O:615:DGD:HA22	4:O:615:DGD:HB62	1.96	0.47
4:O:615:DGD:HBN2	4:O:615:DGD:HBG3	1.73	0.47
1:M:207:ILE:HD12	3:M:611:PID:H261	1.97	0.46
4:M:615:DGD:HBN2	4:M:615:DGD:HBG3	1.72	0.45
1:M:158:ALA:HB2	1:M:223:LYS:HD3	2.00	0.44
3:O:622:PID:H312	4:O:615:DGD:HBG2	2.00	0.44
4:M:625:DGD:O1A	3:N:621:PID:H11	2.17	0.44
4:O:615:DGD:HD2	4:O:615:DGD:HG31	1.73	0.43
3:M:622:PID:H312	4:M:615:DGD:HBG2	2.00	0.43
4:M:615:DGD:HD2	4:M:615:DGD:HG31	1.75	0.43
4:M:615:DGD:HA21	4:M:615:DGD:HB91	2.01	0.43
1:O:144:ASP:O	1:O:148:LYS:HG2	2.19	0.42
1:N:133:GLU:HG2	4:N:615:DGD:O5E	2.19	0.42
3:M:623:PID:H16	4:O:625:DGD:HBT1	2.01	0.42
1:O:133:GLU:HG2	4:O:615:DGD:O5E	2.19	0.42
3:M:611:PID:H11	4:M:615:DGD:O1A	2.20	0.42
1:O:38:LEU:HD23	1:O:38:LEU:HA	1.84	0.42
4:N:615:DGD:HBG3	4:N:615:DGD:HBN2	1.73	0.42
1:O:92:LEU:HD22	2:O:601:CLA:HMD3	2.01	0.42
1:O:182:LYS:HG2	1:O:241:VAL:HG11	2.01	0.42
1:N:158:ALA:HB2	1:N:223:LYS:HD3	2.00	0.42
4:N:625:DGD:O1A	3:O:621:PID:H11	2.20	0.42
2:M:602:CLA:H161	2:M:602:CLA:H203	1.83	0.41
3:O:611:PID:H11	4:O:615:DGD:O1A	2.21	0.41
1:M:133:GLU:HG2	4:M:615:DGD:O5E	2.19	0.41
3:N:612:PID:HM52	4:N:615:DGD:HAH1	2.02	0.41
3:N:622:PID:H312	4:N:615:DGD:HBG2	2.02	0.41
3:O:621:PID:HM41	3:O:621:PID:H16	1.93	0.41
3:M:612:PID:HM52	4:M:615:DGD:HAH1	2.00	0.41
3:O:613:PID:H16	3:O:613:PID:HM41	1.93	0.41
4:N:615:DGD:HA21	4:N:615:DGD:HB91	2.03	0.41
3:N:624:PID:HM41	3:N:624:PID:H16	1.86	0.41
3:N:612:PID:HM41	3:N:612:PID:H16	1.91	0.40
3:M:621:PID:H11	4:O:625:DGD:O1A	2.20	0.40
1:M:38:LEU:HA	1:M:38:LEU:HD23	1.84	0.40
1:N:144:ASP:O	1:N:148:LYS:HG2	2.22	0.40
2:O:602:CLA:H161	2:O:602:CLA:H203	1.85	0.40
1:N:254:LEU:O	1:N:258:ILE:HG12	2.22	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	M	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
1	N	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
1	O	310/312 (99%)	307 (99%)	3 (1%)	0	100	100
All	All	930/936 (99%)	921 (99%)	9 (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	233/233 (100%)	231 (99%)	2 (1%)	84	88
1	N	233/233 (100%)	231 (99%)	2 (1%)	84	88
1	O	233/233 (100%)	231 (99%)	2 (1%)	84	88
All	All	699/699 (100%)	693 (99%)	6 (1%)	84	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	10	LEU
1	M	283	LEU
1	N	10	LEU
1	N	283	LEU
1	O	10	LEU

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Mol	Chain	Res	Type
1	O	283	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	216	GLN
1	N	216	GLN
1	O	216	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

36 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	M	601	5	55,73,73	1.24	7 (12%)	61,113,113	1.44	11 (18%)
2	CLA	M	602	5	55,73,73	1.08	6 (10%)	61,113,113	1.62	10 (16%)
3	PID	M	611	-	42,49,49	1.92	12 (28%)	49,76,76	1.94	12 (24%)
3	PID	M	612	-	42,49,49	1.97	11 (26%)	49,76,76	2.05	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PID	M	613	-	42,49,49	1.84	12 (28%)	49,76,76	1.95	14 (28%)
3	PID	M	614	-	42,49,49	2.00	11 (26%)	49,76,76	1.91	11 (22%)
4	DGD	M	615	-	67,67,67	0.82	1 (1%)	81,81,81	1.39	8 (9%)
3	PID	M	621	-	42,49,49	1.89	12 (28%)	49,76,76	1.77	12 (24%)
3	PID	M	622	-	42,49,49	1.88	12 (28%)	49,76,76	2.06	15 (30%)
3	PID	M	623	-	42,49,49	1.84	12 (28%)	49,76,76	1.91	13 (26%)
3	PID	M	624	-	42,49,49	1.77	10 (23%)	49,76,76	1.76	11 (22%)
4	DGD	M	625	-	67,67,67	0.71	0	81,81,81	0.89	4 (4%)
2	CLA	N	601	5	55,73,73	1.20	8 (14%)	61,113,113	1.49	10 (16%)
2	CLA	N	602	5	55,73,73	1.07	5 (9%)	61,113,113	1.63	11 (18%)
3	PID	N	611	-	42,49,49	1.89	11 (26%)	49,76,76	1.95	15 (30%)
3	PID	N	612	-	42,49,49	1.92	13 (30%)	49,76,76	2.05	18 (36%)
3	PID	N	613	-	42,49,49	1.91	12 (28%)	49,76,76	1.90	15 (30%)
3	PID	N	614	-	42,49,49	1.99	13 (30%)	49,76,76	1.99	13 (26%)
4	DGD	N	615	-	67,67,67	0.75	1 (1%)	81,81,81	1.39	8 (9%)
3	PID	N	621	-	42,49,49	1.81	11 (26%)	49,76,76	1.85	13 (26%)
3	PID	N	622	-	42,49,49	2.01	13 (30%)	49,76,76	1.99	13 (26%)
3	PID	N	623	-	42,49,49	1.95	9 (21%)	49,76,76	1.93	13 (26%)
3	PID	N	624	-	42,49,49	1.90	12 (28%)	49,76,76	1.92	15 (30%)
4	DGD	N	625	-	67,67,67	0.76	1 (1%)	81,81,81	0.98	6 (7%)
2	CLA	O	601	5	55,73,73	1.22	8 (14%)	61,113,113	1.50	12 (19%)
2	CLA	O	602	5	55,73,73	1.07	4 (7%)	61,113,113	1.62	13 (21%)
3	PID	O	611	-	42,49,49	1.79	9 (21%)	49,76,76	1.87	15 (30%)
3	PID	O	612	-	42,49,49	1.82	12 (28%)	49,76,76	2.05	16 (32%)
3	PID	O	613	-	42,49,49	1.76	9 (21%)	49,76,76	1.98	13 (26%)
3	PID	O	614	-	42,49,49	1.92	10 (23%)	49,76,76	1.85	12 (24%)
4	DGD	O	615	-	67,67,67	0.83	1 (1%)	81,81,81	1.39	9 (11%)
3	PID	O	621	-	42,49,49	1.67	9 (21%)	49,76,76	1.70	13 (26%)
3	PID	O	622	-	42,49,49	1.94	11 (26%)	49,76,76	2.05	13 (26%)
3	PID	O	623	-	42,49,49	1.80	7 (16%)	49,76,76	1.78	13 (26%)
3	PID	O	624	-	42,49,49	1.77	11 (26%)	49,76,76	1.80	13 (26%)
4	DGD	O	625	-	67,67,67	0.75	1 (1%)	81,81,81	0.98	5 (6%)

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	M	601	5	4/4/20/25	0/37/135/135	0/0/9/9
2	CLA	M	602	5	3/3/20/25	0/37/135/135	0/0/9/9
3	PID	M	611	-	-	0/24/93/93	0/3/4/4
3	PID	M	612	-	-	0/24/93/93	0/3/4/4
3	PID	M	613	-	1/1/14/25	0/24/93/93	0/3/4/4
3	PID	M	614	-	-	0/24/93/93	0/3/4/4
4	DGD	M	615	-	3/3/13/13	0/55/95/95	0/2/2/2
3	PID	M	621	-	-	0/24/93/93	0/3/4/4
3	PID	M	622	-	-	0/24/93/93	0/3/4/4
3	PID	M	623	-	-	0/24/93/93	0/3/4/4
3	PID	M	624	-	-	0/24/93/93	0/3/4/4
4	DGD	M	625	-	-	0/55/95/95	0/2/2/2
2	CLA	N	601	5	4/4/20/25	0/37/135/135	0/0/9/9
2	CLA	N	602	5	3/3/20/25	0/37/135/135	0/0/9/9
3	PID	N	611	-	-	0/24/93/93	0/3/4/4
3	PID	N	612	-	-	0/24/93/93	0/3/4/4
3	PID	N	613	-	1/1/14/25	0/24/93/93	0/3/4/4
3	PID	N	614	-	-	0/24/93/93	0/3/4/4
4	DGD	N	615	-	3/3/13/13	0/55/95/95	0/2/2/2
3	PID	N	621	-	-	0/24/93/93	0/3/4/4
3	PID	N	622	-	-	0/24/93/93	0/3/4/4
3	PID	N	623	-	-	0/24/93/93	0/3/4/4
3	PID	N	624	-	-	0/24/93/93	0/3/4/4
4	DGD	N	625	-	-	0/55/95/95	0/2/2/2
2	CLA	O	601	5	4/4/20/25	0/37/135/135	0/0/9/9
2	CLA	O	602	5	3/3/20/25	0/37/135/135	0/0/9/9
3	PID	O	611	-	-	0/24/93/93	0/3/4/4
3	PID	O	612	-	-	0/24/93/93	0/3/4/4
3	PID	O	613	-	1/1/14/25	0/24/93/93	0/3/4/4
3	PID	O	614	-	-	0/24/93/93	0/3/4/4
4	DGD	O	615	-	3/3/13/13	0/55/95/95	0/2/2/2
3	PID	O	621	-	-	0/24/93/93	0/3/4/4
3	PID	O	622	-	-	0/24/93/93	0/3/4/4
3	PID	O	623	-	-	0/24/93/93	0/3/4/4
3	PID	O	624	-	-	0/24/93/93	0/3/4/4
4	DGD	O	625	-	-	0/55/95/95	0/2/2/2

All (307) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	623	PID	C6-C7	-4.96	1.42	1.50
3	M	614	PID	C6-C7	-4.50	1.43	1.50
3	N	614	PID	C6-C7	-4.35	1.43	1.50
3	O	623	PID	C6-C7	-4.31	1.43	1.50
3	N	622	PID	C6-C7	-3.96	1.44	1.50
3	O	613	PID	C6-C7	-3.92	1.44	1.50
3	O	614	PID	C6-C7	-3.85	1.44	1.50
3	M	623	PID	C6-C7	-3.85	1.44	1.50
3	N	613	PID	C6-C7	-3.80	1.44	1.50
3	M	613	PID	C6-C7	-3.73	1.44	1.50
3	M	612	PID	O4-C10	-3.53	1.32	1.39
2	O	602	CLA	C3B-C2B	-3.43	1.35	1.40
3	O	622	PID	O4-C10	-3.41	1.32	1.39
2	N	601	CLA	C3B-C2B	-3.31	1.36	1.40
3	M	622	PID	C6-C7	-3.28	1.45	1.50
2	M	601	CLA	C3B-C2B	-3.26	1.36	1.40
3	N	612	PID	C6-C7	-3.17	1.45	1.50
3	N	624	PID	C6-C7	-3.16	1.45	1.50
3	M	612	PID	C6-C7	-3.16	1.45	1.50
3	M	623	PID	O4-C10	-3.13	1.33	1.39
3	M	613	PID	O4-C10	-3.09	1.33	1.39
3	O	624	PID	O4-C10	-3.05	1.33	1.39
3	O	622	PID	C6-C7	-3.03	1.45	1.50
3	N	623	PID	O4-C10	-3.03	1.33	1.39
3	O	612	PID	C6-C7	-3.02	1.45	1.50
3	M	624	PID	C6-C7	-3.01	1.45	1.50
3	N	612	PID	O4-C10	-2.96	1.33	1.39
3	N	611	PID	C6-C7	-2.84	1.46	1.50
3	N	624	PID	O4-C10	-2.83	1.33	1.39
3	M	611	PID	C6-C7	-2.83	1.46	1.50
3	O	624	PID	C6-C7	-2.81	1.46	1.50
3	M	621	PID	C6-C7	-2.80	1.46	1.50
3	N	621	PID	C6-C7	-2.80	1.46	1.50
2	N	601	CLA	O2D-CED	-2.79	1.38	1.45
3	O	621	PID	C6-C7	-2.77	1.46	1.50
3	O	623	PID	O4-C10	-2.75	1.33	1.39
3	O	614	PID	O4-C10	-2.72	1.33	1.39
2	O	601	CLA	C3B-C2B	-2.69	1.36	1.40
3	O	612	PID	O4-C10	-2.62	1.34	1.39
3	O	612	PID	O6-C30	-2.61	1.29	1.35
3	O	613	PID	O4-C10	-2.61	1.34	1.39
3	N	614	PID	O4-C10	-2.60	1.34	1.39
3	M	624	PID	O4-C10	-2.54	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	614	PID	O4-C10	-2.52	1.34	1.39
3	N	613	PID	O4-C10	-2.52	1.34	1.39
3	O	613	PID	C8-C9	-2.51	1.40	1.46
3	M	622	PID	O4-C10	-2.50	1.34	1.39
3	M	612	PID	O6-C30	-2.47	1.29	1.35
3	N	612	PID	O6-C30	-2.46	1.29	1.35
3	M	621	PID	O4-C10	-2.40	1.34	1.39
3	N	611	PID	O4-C10	-2.40	1.34	1.39
3	M	611	PID	C13-C14	-2.39	1.41	1.46
3	N	613	PID	C8-C9	-2.37	1.40	1.46
3	N	613	PID	C11-C12	-2.36	1.40	1.44
2	N	601	CLA	C3B-CAB	-2.36	1.42	1.47
2	N	602	CLA	C3B-C2B	-2.35	1.37	1.40
3	N	621	PID	O4-C10	-2.35	1.34	1.39
3	N	611	PID	C13-C14	-2.32	1.41	1.46
3	M	622	PID	O6-C30	-2.29	1.29	1.35
3	N	624	PID	C8-C9	-2.29	1.40	1.46
3	M	613	PID	C8-C9	-2.28	1.40	1.46
3	O	621	PID	O4-C10	-2.27	1.34	1.39
3	N	622	PID	O4-C10	-2.23	1.35	1.39
2	N	602	CLA	C3B-CAB	-2.21	1.43	1.47
3	M	611	PID	O4-C10	-2.20	1.35	1.39
3	O	614	PID	C8-C9	-2.19	1.41	1.46
3	N	614	PID	C8-C9	-2.16	1.41	1.46
3	M	613	PID	O6-C30	-2.15	1.30	1.35
2	M	602	CLA	C3B-C2B	-2.14	1.37	1.40
2	O	601	CLA	O2D-CED	-2.10	1.40	1.45
3	O	611	PID	O4-C10	-2.10	1.35	1.39
3	N	613	PID	C13-C14	-2.09	1.41	1.46
3	M	622	PID	C13-C14	-2.06	1.41	1.46
3	O	622	PID	C13-C14	-2.05	1.41	1.46
3	M	613	PID	C11-C12	-2.04	1.41	1.44
3	O	613	PID	C13-C14	-2.04	1.41	1.46
3	M	622	PID	C13-C12	2.00	1.41	1.36
3	M	623	PID	O4-C12	2.00	1.41	1.38
3	N	613	PID	C17-C16	2.03	1.41	1.35
3	O	621	PID	CM8-C29	2.03	1.55	1.52
2	M	601	CLA	O2A-CGA	2.04	1.39	1.33
4	O	625	DGD	C4D-C5D	2.04	1.57	1.53
3	N	621	PID	O4-C12	2.04	1.42	1.38
3	N	612	PID	C25-C24	2.05	1.58	1.54
3	N	614	PID	CM4-C14	2.06	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	612	PID	CM4-C14	2.06	1.55	1.50
2	O	601	CLA	CHC-C1C	2.06	1.41	1.35
3	M	613	PID	O4-C12	2.07	1.42	1.38
3	M	623	PID	C19-C18	2.07	1.41	1.35
3	M	624	PID	C19-C18	2.08	1.41	1.35
2	M	602	CLA	C4-C3	2.09	1.55	1.50
3	M	611	PID	C2-C1	2.09	1.55	1.52
3	O	622	PID	C25-C24	2.09	1.58	1.54
3	M	623	PID	CM5-C21	2.09	1.55	1.50
3	M	612	PID	O4-C12	2.10	1.42	1.38
3	O	612	PID	C17-C16	2.10	1.41	1.35
3	N	612	PID	O4-C12	2.11	1.42	1.38
3	M	611	PID	CM5-C21	2.11	1.55	1.50
3	N	612	PID	C13-C12	2.11	1.41	1.36
2	N	601	CLA	CMC-C2C	2.12	1.55	1.50
3	M	614	PID	C19-C18	2.13	1.41	1.35
3	M	611	PID	O4-C12	2.13	1.42	1.38
3	M	623	PID	C13-C12	2.14	1.41	1.36
3	O	612	PID	O4-C12	2.14	1.42	1.38
2	M	601	CLA	CHC-C1C	2.14	1.42	1.35
3	N	622	PID	O1-C1	2.14	1.49	1.46
3	N	614	PID	C17-C16	2.14	1.41	1.35
3	O	622	PID	CM4-C14	2.16	1.55	1.50
3	N	624	PID	CM5-C21	2.16	1.55	1.50
2	N	602	CLA	O2D-CGD	2.16	1.38	1.33
3	N	621	PID	C13-C12	2.16	1.41	1.36
3	O	611	PID	C28-C27	2.17	1.55	1.51
3	M	622	PID	O4-C12	2.17	1.42	1.38
3	N	624	PID	CM4-C14	2.20	1.55	1.50
3	N	614	PID	O1-C1	2.20	1.49	1.46
3	N	611	PID	CM4-C14	2.20	1.55	1.50
3	O	624	PID	O1-C1	2.20	1.49	1.46
3	N	622	PID	CM5-C21	2.20	1.55	1.50
3	O	624	PID	C19-C18	2.21	1.41	1.35
3	M	624	PID	C15-C14	2.21	1.38	1.35
2	M	602	CLA	CMD-C2D	2.21	1.56	1.51
2	O	602	CLA	C4-C3	2.21	1.56	1.50
3	N	621	PID	CM4-C14	2.21	1.55	1.50
3	M	614	PID	O1-C1	2.22	1.49	1.46
3	N	613	PID	O1-C1	2.22	1.49	1.46
2	N	601	CLA	O1D-CGD	2.22	1.26	1.21
3	O	621	PID	C17-C16	2.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	611	PID	C19-C18	2.24	1.41	1.35
3	M	621	PID	O1-C1	2.25	1.49	1.46
3	N	612	PID	O1-C1	2.25	1.49	1.46
3	M	613	PID	C17-C16	2.25	1.41	1.35
3	O	612	PID	CM4-C14	2.25	1.55	1.50
3	N	622	PID	CM4-C14	2.27	1.55	1.50
3	O	622	PID	C13-C12	2.28	1.41	1.36
3	N	611	PID	O4-C12	2.28	1.42	1.38
3	N	622	PID	C13-C12	2.28	1.42	1.36
3	O	624	PID	CM1-C1	2.29	1.55	1.51
4	N	625	DGD	O5D-C1E	2.29	1.44	1.40
4	N	615	DGD	O5D-C1E	2.31	1.44	1.40
3	O	621	PID	C25-C24	2.31	1.58	1.54
3	N	611	PID	C17-C16	2.32	1.42	1.35
3	N	622	PID	C2-C1	2.32	1.55	1.52
3	N	612	PID	C19-C18	2.33	1.42	1.35
3	N	624	PID	C19-C18	2.33	1.42	1.35
2	N	601	CLA	C2-C3	2.34	1.37	1.33
3	N	614	PID	CM5-C21	2.34	1.55	1.50
3	O	611	PID	C17-C16	2.35	1.42	1.35
2	O	601	CLA	CAC-C3C	2.35	1.57	1.51
3	M	612	PID	C17-C16	2.36	1.42	1.35
2	O	602	CLA	CMA-C3A	2.36	1.58	1.53
4	O	615	DGD	O5D-C1E	2.37	1.44	1.40
3	M	614	PID	C17-C16	2.37	1.42	1.35
3	O	612	PID	C25-C24	2.37	1.58	1.54
3	N	623	PID	O1-C1	2.38	1.50	1.46
3	O	612	PID	C19-C18	2.38	1.42	1.35
2	M	602	CLA	CMC-C2C	2.38	1.55	1.50
3	O	614	PID	C17-C16	2.39	1.42	1.35
3	N	614	PID	C19-C18	2.40	1.42	1.35
3	O	624	PID	CM4-C14	2.40	1.56	1.50
3	N	614	PID	O4-C12	2.41	1.42	1.38
2	O	601	CLA	O1D-CGD	2.41	1.27	1.21
4	M	615	DGD	O5D-C1E	2.42	1.44	1.40
3	N	622	PID	C19-C18	2.42	1.42	1.35
3	M	611	PID	O1-C1	2.43	1.50	1.46
3	M	612	PID	C25-C24	2.45	1.58	1.54
2	M	602	CLA	CHC-C1C	2.46	1.43	1.35
3	O	624	PID	CM5-C21	2.46	1.56	1.50
3	O	622	PID	CM5-C21	2.46	1.56	1.50
3	N	613	PID	O4-C12	2.48	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	621	PID	C19-C18	2.51	1.42	1.35
3	M	622	PID	C2-C1	2.52	1.55	1.52
3	O	613	PID	O4-C12	2.52	1.42	1.38
3	M	612	PID	O1-C1	2.54	1.50	1.46
3	N	623	PID	O4-C12	2.55	1.43	1.38
3	N	621	PID	C19-C18	2.56	1.42	1.35
3	M	623	PID	C17-C16	2.57	1.42	1.35
2	O	601	CLA	CMC-C2C	2.57	1.56	1.50
2	M	601	CLA	C2-C3	2.58	1.38	1.33
3	M	624	PID	CM4-C14	2.58	1.56	1.50
3	O	624	PID	C15-C14	2.59	1.39	1.35
3	M	614	PID	O4-C12	2.59	1.43	1.38
3	M	621	PID	O4-C12	2.60	1.43	1.38
2	N	602	CLA	C4-C3	2.63	1.57	1.50
3	O	623	PID	C17-C16	2.63	1.42	1.35
3	M	624	PID	CM5-C21	2.64	1.56	1.50
3	O	611	PID	CM4-C14	2.69	1.56	1.50
2	N	601	CLA	O2A-CGA	2.70	1.41	1.33
3	M	614	PID	CM5-C21	2.70	1.56	1.50
3	O	614	PID	C20-C21	2.70	1.39	1.35
3	M	611	PID	C19-C18	2.71	1.43	1.35
3	N	622	PID	C25-C24	2.72	1.59	1.54
3	M	613	PID	O1-C1	2.72	1.50	1.46
3	O	621	PID	C20-C21	2.73	1.39	1.35
2	M	601	CLA	O1D-CGD	2.74	1.28	1.21
3	O	623	PID	C20-C21	2.75	1.39	1.35
3	M	622	PID	CM5-C21	2.75	1.56	1.50
2	M	601	CLA	CMC-C2C	2.76	1.56	1.50
3	O	611	PID	O4-C12	2.77	1.43	1.38
3	O	612	PID	C23-C22	2.79	1.37	1.32
3	O	614	PID	O4-C12	2.81	1.43	1.38
3	O	621	PID	C15-C14	2.83	1.39	1.35
3	N	612	PID	C23-C22	2.84	1.37	1.32
3	N	624	PID	CM1-C1	2.85	1.56	1.51
3	N	623	PID	C17-C16	2.85	1.43	1.35
3	M	623	PID	CM4-C14	2.85	1.57	1.50
3	N	624	PID	C20-C21	2.86	1.39	1.35
3	N	621	PID	CM8-C29	2.86	1.57	1.52
2	O	601	CLA	C2-C3	2.88	1.38	1.33
3	O	613	PID	C20-C21	2.89	1.39	1.35
3	M	614	PID	C20-C21	2.91	1.39	1.35
3	O	614	PID	CM5-C21	2.91	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	621	PID	CM4-C14	2.94	1.57	1.50
3	M	611	PID	C20-C21	2.94	1.39	1.35
3	N	624	PID	O1-C1	3.07	1.51	1.46
3	N	624	PID	C15-C14	3.07	1.39	1.35
3	N	623	PID	C23-C22	3.07	1.37	1.32
3	O	623	PID	C23-C22	3.10	1.37	1.32
2	N	601	CLA	O2D-CGD	3.15	1.41	1.33
3	M	622	PID	C23-C22	3.15	1.38	1.32
3	M	624	PID	C20-C21	3.15	1.39	1.35
3	N	621	PID	C20-C21	3.16	1.39	1.35
3	O	614	PID	C23-C22	3.16	1.38	1.32
3	M	623	PID	C20-C21	3.18	1.40	1.35
3	N	622	PID	C15-C14	3.20	1.40	1.35
3	M	612	PID	C23-C22	3.20	1.38	1.32
2	N	602	CLA	C2-C3	3.22	1.39	1.33
3	O	611	PID	C23-C22	3.23	1.38	1.32
3	M	623	PID	C23-C22	3.23	1.38	1.32
3	O	612	PID	C20-C21	3.27	1.40	1.35
3	N	614	PID	C23-C22	3.31	1.38	1.32
3	O	613	PID	C23-C22	3.31	1.38	1.32
3	M	621	PID	C15-C14	3.33	1.40	1.35
3	O	624	PID	C23-C22	3.34	1.38	1.32
3	M	621	PID	C25-C24	3.35	1.60	1.54
3	M	621	PID	CM8-C29	3.38	1.57	1.52
3	N	613	PID	C20-C21	3.38	1.40	1.35
3	N	612	PID	C15-C14	3.41	1.40	1.35
3	O	613	PID	C15-C14	3.48	1.40	1.35
3	M	613	PID	C23-C22	3.48	1.38	1.32
3	N	614	PID	C20-C21	3.49	1.40	1.35
3	N	611	PID	C20-C21	3.50	1.40	1.35
3	N	611	PID	C23-C22	3.50	1.38	1.32
3	M	621	PID	C23-C22	3.51	1.38	1.32
3	O	612	PID	C15-C14	3.51	1.40	1.35
3	O	624	PID	C20-C21	3.56	1.40	1.35
3	O	611	PID	C20-C21	3.57	1.40	1.35
2	M	602	CLA	C2-C3	3.59	1.40	1.33
3	M	621	PID	C20-C21	3.65	1.40	1.35
2	O	602	CLA	C2-C3	3.65	1.40	1.33
3	M	624	PID	O1-C1	3.67	1.52	1.46
3	M	612	PID	C20-C21	3.68	1.40	1.35
3	O	622	PID	C15-C14	3.73	1.40	1.35
3	M	613	PID	C20-C21	3.73	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	623	PID	C20-C21	3.75	1.40	1.35
3	O	621	PID	C23-C22	3.76	1.39	1.32
3	M	613	PID	C15-C14	3.77	1.40	1.35
3	N	621	PID	C15-C14	3.82	1.40	1.35
3	N	612	PID	C20-C21	3.85	1.40	1.35
3	O	613	PID	C8-C7	3.86	1.39	1.32
3	O	622	PID	C20-C21	3.90	1.40	1.35
3	O	622	PID	C23-C22	3.90	1.39	1.32
3	M	612	PID	C15-C14	3.91	1.40	1.35
3	M	623	PID	C15-C14	3.96	1.41	1.35
3	N	621	PID	C23-C22	3.97	1.39	1.32
3	O	624	PID	C8-C7	3.99	1.40	1.32
3	N	613	PID	C15-C14	4.06	1.41	1.35
3	M	624	PID	C23-C22	4.06	1.39	1.32
3	M	622	PID	C15-C14	4.11	1.41	1.35
3	N	623	PID	C15-C14	4.12	1.41	1.35
3	M	613	PID	C8-C7	4.12	1.40	1.32
3	O	611	PID	C8-C7	4.16	1.40	1.32
3	M	614	PID	C23-C22	4.17	1.39	1.32
3	O	623	PID	C15-C14	4.21	1.41	1.35
3	N	622	PID	C23-C22	4.22	1.40	1.32
3	M	622	PID	C20-C21	4.24	1.41	1.35
2	M	601	CLA	O2D-CGD	4.24	1.44	1.33
3	N	624	PID	C23-C22	4.28	1.40	1.32
3	O	614	PID	C15-C14	4.28	1.41	1.35
3	O	611	PID	C15-C14	4.32	1.41	1.35
3	M	611	PID	C15-C14	4.33	1.41	1.35
3	M	611	PID	C23-C22	4.35	1.40	1.32
2	O	601	CLA	O2D-CGD	4.39	1.44	1.33
3	N	622	PID	C20-C21	4.46	1.41	1.35
3	N	613	PID	C8-C7	4.49	1.41	1.32
3	M	621	PID	C8-C7	4.56	1.41	1.32
3	N	614	PID	C15-C14	4.57	1.41	1.35
3	N	613	PID	C23-C22	4.61	1.40	1.32
3	N	611	PID	C15-C14	4.61	1.41	1.35
3	M	623	PID	C8-C7	4.62	1.41	1.32
3	O	623	PID	C8-C7	4.81	1.41	1.32
3	M	614	PID	C15-C14	4.83	1.42	1.35
3	M	624	PID	C8-C7	4.87	1.41	1.32
3	O	621	PID	C8-C7	4.91	1.42	1.32
3	O	612	PID	C8-C7	5.05	1.42	1.32
3	N	623	PID	C8-C7	5.06	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	622	PID	C8-C7	5.09	1.42	1.32
3	N	621	PID	C8-C7	5.10	1.42	1.32
3	O	614	PID	C8-C7	5.16	1.42	1.32
3	N	614	PID	C8-C7	5.23	1.42	1.32
3	M	614	PID	C8-C7	5.29	1.42	1.32
3	M	611	PID	C8-C7	5.30	1.42	1.32
3	O	622	PID	C8-C7	5.37	1.42	1.32
3	N	611	PID	C8-C7	5.42	1.43	1.32
3	N	622	PID	C8-C7	5.46	1.43	1.32
3	N	624	PID	C8-C7	5.53	1.43	1.32
3	M	612	PID	C8-C7	5.68	1.43	1.32
3	N	612	PID	C8-C7	5.96	1.44	1.32

All (435) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	613	PID	O3-C10-C9	-5.24	120.89	130.70
3	O	613	PID	O3-C10-C9	-4.89	121.54	130.70
3	O	614	PID	O3-C10-C9	-4.80	121.71	130.70
3	M	613	PID	O3-C10-C9	-4.79	121.73	130.70
3	M	614	PID	C12-O4-C10	-4.52	104.84	107.68
3	N	614	PID	C12-O4-C10	-4.51	104.85	107.68
3	M	614	PID	O3-C10-C9	-4.43	122.42	130.70
3	N	623	PID	C12-O4-C10	-4.42	104.91	107.68
3	N	614	PID	O3-C10-C9	-4.39	122.49	130.70
3	N	611	PID	C12-O4-C10	-4.27	105.00	107.68
3	M	623	PID	C12-O4-C10	-4.14	105.08	107.68
3	N	621	PID	C12-O4-C10	-4.04	105.15	107.68
3	N	624	PID	C12-O4-C10	-4.01	105.16	107.68
3	N	622	PID	O3-C10-C9	-3.97	123.27	130.70
3	N	612	PID	C19-C20-C21	-3.90	121.57	127.20
3	O	614	PID	C12-O4-C10	-3.90	105.23	107.68
3	M	611	PID	O3-C10-C9	-3.88	123.43	130.70
3	O	611	PID	O3-C10-C9	-3.84	123.51	130.70
3	M	622	PID	C19-C20-C21	-3.81	121.70	127.20
3	N	611	PID	O3-C10-C9	-3.80	123.58	130.70
3	O	611	PID	C12-O4-C10	-3.80	105.29	107.68
3	N	622	PID	C12-O4-C10	-3.80	105.30	107.68
3	M	611	PID	C12-O4-C10	-3.80	105.30	107.68
3	O	612	PID	C19-C20-C21	-3.78	121.74	127.20
3	O	622	PID	C19-C20-C21	-3.78	121.74	127.20
3	M	612	PID	C19-C20-C21	-3.78	121.74	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	623	PID	O3-C10-C9	-3.74	123.70	130.70
3	O	612	PID	O3-C10-C9	-3.72	123.75	130.70
3	N	622	PID	C19-C20-C21	-3.66	121.91	127.20
3	N	624	PID	O3-C10-C9	-3.64	123.88	130.70
2	O	602	CLA	CMB-C2B-C1B	-3.64	122.35	128.36
3	O	622	PID	O3-C10-C9	-3.62	123.93	130.70
3	O	622	PID	C12-O4-C10	-3.58	105.43	107.68
3	M	622	PID	C12-O4-C10	-3.55	105.45	107.68
3	O	612	PID	C12-O4-C10	-3.55	105.46	107.68
3	M	622	PID	O3-C10-C9	-3.54	124.07	130.70
3	M	621	PID	O3-C10-C9	-3.51	124.13	130.70
3	M	621	PID	C12-O4-C10	-3.51	105.48	107.68
4	N	625	DGD	C1D-O6D-C5D	-3.50	106.96	113.75
3	O	613	PID	C12-O4-C10	-3.48	105.50	107.68
2	O	602	CLA	C3B-CAB-CBB	-3.47	119.21	126.32
3	O	623	PID	O3-C10-C9	-3.44	124.26	130.70
3	N	623	PID	O3-C10-C9	-3.44	124.27	130.70
3	N	622	PID	C17-C16-C15	-3.43	115.81	123.39
3	N	614	PID	C16-C15-C14	-3.38	122.31	127.20
2	N	602	CLA	CMB-C2B-C1B	-3.38	122.77	128.36
2	O	601	CLA	CMB-C2B-C1B	-3.37	122.79	128.36
3	M	612	PID	O3-C10-C9	-3.36	124.41	130.70
3	M	622	PID	C17-C16-C15	-3.35	115.98	123.39
3	N	612	PID	O3-C10-C9	-3.34	124.45	130.70
2	M	602	CLA	CMB-C2B-C1B	-3.32	122.87	128.36
3	M	622	PID	C17-C18-C19	-3.30	117.30	124.94
3	M	612	PID	C12-O4-C10	-3.29	105.62	107.68
4	O	625	DGD	O3G-C1D-C2D	-3.28	103.90	108.04
2	N	602	CLA	C3B-CAB-CBB	-3.26	119.65	126.32
3	O	624	PID	C16-C15-C14	-3.25	122.50	127.20
2	M	602	CLA	C3B-CAB-CBB	-3.24	119.69	126.32
3	N	624	PID	C16-C15-C14	-3.23	122.53	127.20
3	O	622	PID	C17-C16-C15	-3.22	116.28	123.39
3	O	624	PID	C9-C11-C12	-3.20	105.49	110.42
3	O	622	PID	C17-C18-C19	-3.19	117.56	124.94
3	N	612	PID	CM3-C5-C4	-3.19	103.25	108.94
4	N	615	DGD	C3G-O3G-C1D	-3.18	107.13	113.82
3	N	623	PID	C9-C11-C12	-3.18	105.52	110.42
3	M	622	PID	C27-O6-C30	-3.18	111.92	117.92
3	N	613	PID	C19-C20-C21	-3.16	122.64	127.20
3	N	621	PID	O3-C10-C9	-3.15	124.80	130.70
3	O	621	PID	C18-C19-C20	-3.14	116.44	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	614	PID	C9-C11-C12	-3.14	105.57	110.42
3	M	614	PID	C9-C11-C12	-3.14	105.58	110.42
3	N	614	PID	C27-O6-C30	-3.13	112.01	117.92
3	M	612	PID	CM3-C5-C4	-3.13	103.35	108.94
3	M	612	PID	C9-C11-C12	-3.12	105.61	110.42
3	M	611	PID	C16-C15-C14	-3.12	122.69	127.20
2	N	601	CLA	O1D-CGD-CBD	-3.12	120.16	124.62
3	M	624	PID	C16-C15-C14	-3.11	122.70	127.20
3	N	612	PID	C12-O4-C10	-3.10	105.73	107.68
3	O	622	PID	C9-C11-C12	-3.10	105.64	110.42
2	N	602	CLA	O1D-CGD-CBD	-3.08	120.20	124.62
3	N	611	PID	C8-C9-C11	-3.08	122.08	127.17
3	M	621	PID	C18-C19-C20	-3.08	116.59	123.39
3	M	624	PID	C9-C11-C12	-3.06	105.71	110.42
3	N	624	PID	C9-C11-C12	-3.05	105.72	110.42
3	O	611	PID	C8-C9-C11	-3.04	122.15	127.17
3	M	622	PID	C9-C11-C12	-3.03	105.74	110.42
3	O	611	PID	C18-C19-C20	-3.03	116.70	123.39
3	N	614	PID	C9-C11-C12	-3.03	105.75	110.42
3	M	613	PID	C9-C11-C12	-3.01	105.77	110.42
3	O	612	PID	CM3-C5-C4	-3.01	103.56	108.94
3	O	613	PID	C19-C20-C21	-3.01	122.85	127.20
2	M	602	CLA	O1D-CGD-CBD	-3.01	120.31	124.62
3	O	621	PID	O3-C10-C9	-2.99	125.10	130.70
3	M	611	PID	C8-C9-C11	-2.99	122.23	127.17
3	M	623	PID	C9-C11-C12	-2.99	105.81	110.42
2	N	602	CLA	OBD-CAD-CBD	-2.99	121.43	125.94
4	M	615	DGD	C3G-O3G-C1D	-2.98	107.55	113.82
3	O	624	PID	O3-C10-C9	-2.98	125.12	130.70
2	O	602	CLA	C2C-C1C-NC	-2.98	108.02	110.24
3	N	612	PID	C9-C11-C12	-2.98	105.82	110.42
3	O	623	PID	C9-C11-C12	-2.97	105.84	110.42
3	M	614	PID	C16-C15-C14	-2.94	122.94	127.20
3	O	613	PID	C9-C11-C12	-2.94	105.88	110.42
3	M	613	PID	C19-C20-C21	-2.94	122.95	127.20
4	O	615	DGD	C3G-O3G-C1D	-2.91	107.70	113.82
3	M	613	PID	C8-C9-C11	-2.91	122.36	127.17
3	N	622	PID	C27-O6-C30	-2.91	112.44	117.92
3	O	622	PID	C27-O6-C30	-2.90	112.45	117.92
3	N	622	PID	C17-C18-C19	-2.89	118.25	124.94
3	O	613	PID	C8-C9-C11	-2.89	122.40	127.17
4	O	625	DGD	C1D-O6D-C5D	-2.88	108.15	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	602	CLA	OBD-CAD-CBD	-2.86	121.62	125.94
3	N	623	PID	C19-C20-C21	-2.86	123.07	127.20
2	M	601	CLA	O1D-CGD-CBD	-2.85	120.53	124.62
3	N	613	PID	C8-C9-C11	-2.83	122.49	127.17
4	O	625	DGD	O2G-C2G-C1G	-2.83	98.39	108.36
3	N	622	PID	C9-C11-C12	-2.82	106.07	110.42
3	O	621	PID	C17-C16-C15	-2.81	117.17	123.39
3	M	624	PID	O3-C10-C9	-2.81	125.45	130.70
3	M	624	PID	C12-O4-C10	-2.79	105.93	107.68
3	O	623	PID	C19-C20-C21	-2.79	123.17	127.20
3	M	623	PID	C19-C20-C21	-2.78	123.18	127.20
3	M	611	PID	C18-C19-C20	-2.76	117.28	123.39
2	O	601	CLA	C3B-CAB-CBB	-2.75	120.68	126.32
3	N	613	PID	C9-C11-C12	-2.74	106.19	110.42
3	O	614	PID	C16-C15-C14	-2.74	123.24	127.20
3	N	611	PID	C16-C15-C14	-2.74	123.25	127.20
2	N	601	CLA	OBD-CAD-CBD	-2.73	121.83	125.94
2	O	601	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
3	N	611	PID	C18-C19-C20	-2.72	117.37	123.39
3	O	623	PID	C27-O6-C30	-2.71	112.80	117.92
3	N	623	PID	C27-O6-C30	-2.70	112.82	117.92
3	N	611	PID	C9-C11-C12	-2.70	106.25	110.42
3	M	612	PID	C17-C16-C15	-2.69	117.44	123.39
2	N	601	CLA	C3B-CAB-CBB	-2.69	120.82	126.32
3	N	614	PID	C19-C20-C21	-2.68	123.32	127.20
3	O	612	PID	C9-C11-C12	-2.68	106.29	110.42
3	N	621	PID	C16-C15-C14	-2.68	123.33	127.20
2	O	602	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
3	N	621	PID	C18-C19-C20	-2.66	117.50	123.39
2	M	601	CLA	OBD-CAD-CBD	-2.65	121.94	125.94
3	M	621	PID	C9-C11-C12	-2.65	106.33	110.42
3	O	623	PID	C17-C16-C15	-2.65	117.53	123.39
2	M	601	CLA	C3B-CAB-CBB	-2.65	120.90	126.32
3	M	611	PID	C9-C11-C12	-2.65	106.34	110.42
3	O	624	PID	C12-O4-C10	-2.64	106.02	107.68
2	M	601	CLA	C2C-C1C-NC	-2.63	108.28	110.24
3	N	624	PID	C19-C20-C21	-2.61	123.43	127.20
4	N	625	DGD	O6D-C1D-O3G	-2.61	103.78	110.05
4	O	625	DGD	O6D-C1D-O3G	-2.60	103.78	110.05
3	O	621	PID	C12-O4-C10	-2.60	106.05	107.68
3	O	623	PID	C18-C19-C20	-2.60	117.65	123.39
3	O	614	PID	C18-C19-C20	-2.60	117.65	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	602	CLA	O1D-CGD-CBD	-2.59	120.91	124.62
3	M	614	PID	C19-C20-C21	-2.58	123.47	127.20
3	M	613	PID	C16-C15-C14	-2.57	123.48	127.20
3	M	612	PID	C16-C15-C14	-2.57	123.49	127.20
3	N	621	PID	C8-C9-C11	-2.56	122.93	127.17
3	O	624	PID	C19-C20-C21	-2.56	123.50	127.20
2	O	601	CLA	O1D-CGD-CBD	-2.56	120.96	124.62
3	N	612	PID	C16-C15-C14	-2.55	123.51	127.20
3	N	623	PID	C8-C9-C11	-2.55	122.95	127.17
3	O	612	PID	C8-C9-C11	-2.54	122.96	127.17
3	O	613	PID	C16-C15-C14	-2.54	123.52	127.20
3	O	614	PID	C27-O6-C30	-2.54	113.13	117.92
2	M	602	CLA	C2C-C1C-NC	-2.53	108.36	110.24
4	M	625	DGD	C1D-O6D-C5D	-2.53	108.83	113.75
3	N	613	PID	C16-C15-C14	-2.53	123.55	127.20
3	O	621	PID	C16-C15-C14	-2.53	123.55	127.20
3	M	613	PID	C12-O4-C10	-2.52	106.10	107.68
3	M	624	PID	C8-C9-C11	-2.52	123.00	127.17
3	M	623	PID	C27-O6-C30	-2.51	113.17	117.92
3	N	613	PID	C12-O4-C10	-2.51	106.10	107.68
3	N	611	PID	C26-C25-C24	-2.50	106.89	109.24
3	N	612	PID	C8-C9-C11	-2.50	123.04	127.17
3	O	621	PID	C9-C11-C12	-2.49	106.58	110.42
3	M	612	PID	C27-O6-C30	-2.48	113.24	117.92
2	M	601	CLA	CMB-C2B-C1B	-2.47	124.27	128.36
3	M	614	PID	C8-C9-C11	-2.47	123.09	127.17
3	O	624	PID	C18-C19-C20	-2.46	117.94	123.39
3	N	614	PID	C8-C9-C11	-2.46	123.10	127.17
3	N	624	PID	C27-O6-C30	-2.46	113.27	117.92
3	M	621	PID	C8-C9-C11	-2.46	123.11	127.17
2	N	601	CLA	CMB-C2B-C1B	-2.43	124.34	128.36
3	N	623	PID	C17-C16-C15	-2.43	118.01	123.39
4	M	625	DGD	O6D-C1D-O3G	-2.43	104.20	110.05
3	O	611	PID	C16-C15-C14	-2.42	123.70	127.20
3	O	621	PID	C8-C9-C11	-2.42	123.17	127.17
3	O	612	PID	C17-C16-C15	-2.42	118.04	123.39
3	N	621	PID	C27-O6-C30	-2.42	113.36	117.92
3	O	623	PID	C12-O4-C10	-2.41	106.17	107.68
3	M	624	PID	C18-C19-C20	-2.41	118.06	123.39
3	M	621	PID	C17-C16-C15	-2.40	118.08	123.39
3	O	623	PID	C8-C9-C11	-2.40	123.20	127.17
3	N	621	PID	C9-C11-C12	-2.40	106.72	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	614	PID	C18-C19-C20	-2.38	118.12	123.39
3	O	614	PID	C8-C9-C11	-2.38	123.23	127.17
2	N	602	CLA	C2C-C1C-NC	-2.37	108.48	110.24
3	N	612	PID	C17-C16-C15	-2.37	118.15	123.39
3	M	614	PID	C18-C19-C20	-2.37	118.15	123.39
3	O	624	PID	C8-C9-C11	-2.37	123.25	127.17
3	O	624	PID	C17-C16-C15	-2.37	118.16	123.39
3	O	612	PID	C16-C15-C14	-2.37	123.78	127.20
3	N	612	PID	C27-O6-C30	-2.36	113.46	117.92
2	O	602	CLA	O2D-CGD-O1D	-2.36	118.91	123.79
3	O	611	PID	C19-C20-C21	-2.36	123.79	127.20
3	M	623	PID	C17-C16-C15	-2.36	118.18	123.39
2	O	601	CLA	C2C-C1C-NC	-2.35	108.50	110.24
3	M	623	PID	C8-C9-C11	-2.35	123.29	127.17
2	N	602	CLA	O2A-CGA-O1A	-2.34	117.44	123.49
3	N	612	PID	C17-C18-C19	-2.34	119.52	124.94
3	M	612	PID	C8-C9-C11	-2.34	123.30	127.17
3	M	612	PID	O6-C30-O7	-2.33	118.27	122.92
3	O	611	PID	C18-C17-C16	-2.33	119.56	124.94
3	M	623	PID	C16-C15-C14	-2.32	123.84	127.20
3	M	622	PID	C8-C9-C11	-2.32	123.33	127.17
3	O	614	PID	C19-C20-C21	-2.30	123.87	127.20
3	M	624	PID	C17-C16-C15	-2.30	118.31	123.39
3	M	614	PID	C27-O6-C30	-2.30	113.58	117.92
3	O	621	PID	C27-O6-C30	-2.28	113.62	117.92
2	N	601	CLA	C2C-C1C-NC	-2.28	108.55	110.24
3	O	612	PID	C17-C18-C19	-2.27	119.68	124.94
3	N	611	PID	C18-C17-C16	-2.26	119.70	124.94
3	O	611	PID	C9-C11-C12	-2.26	106.94	110.42
3	N	622	PID	C8-C9-C11	-2.25	123.44	127.17
3	N	611	PID	C19-C20-C21	-2.24	123.96	127.20
3	N	612	PID	CM4-C14-C15	-2.24	119.60	122.90
3	O	613	PID	C17-C16-C15	-2.23	118.45	123.39
3	M	612	PID	C17-C18-C19	-2.23	119.77	124.94
4	N	625	DGD	O2G-C2G-C1G	-2.23	100.51	108.36
3	M	623	PID	C18-C19-C20	-2.22	118.48	123.39
3	M	613	PID	C11-C12-C13	-2.21	121.18	130.47
4	M	625	DGD	O2G-C2G-C1G	-2.21	100.59	108.36
3	M	611	PID	C18-C17-C16	-2.20	119.85	124.94
3	N	623	PID	C18-C19-C20	-2.20	118.53	123.39
3	N	624	PID	CM4-C14-C15	-2.19	119.67	122.90
3	N	613	PID	C11-C12-C13	-2.19	121.29	130.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	611	PID	C11-C12-C13	-2.19	121.29	130.47
3	O	613	PID	C11-C12-C13	-2.18	121.31	130.47
3	N	621	PID	C17-C16-C15	-2.18	118.58	123.39
3	N	624	PID	C8-C9-C11	-2.17	123.58	127.17
3	N	611	PID	C27-O6-C30	-2.17	113.82	117.92
4	N	625	DGD	O3G-C3G-C2G	-2.16	105.84	110.99
3	N	614	PID	CM7-C25-C24	-2.16	108.54	110.48
2	M	602	CLA	O2D-CGD-O1D	-2.15	119.34	123.79
3	O	614	PID	CM7-C25-C24	-2.15	108.54	110.48
4	N	625	DGD	O3G-C1D-C2D	-2.15	105.32	108.04
3	O	622	PID	C8-C9-C11	-2.14	123.62	127.17
3	O	611	PID	C26-C25-C24	-2.14	107.23	109.24
3	M	611	PID	C11-C12-C13	-2.14	121.51	130.47
3	N	614	PID	C11-C12-C13	-2.13	121.55	130.47
3	N	621	PID	C11-C12-C13	-2.13	121.55	130.47
3	O	611	PID	C17-C16-C15	-2.12	118.69	123.39
3	O	624	PID	C26-C25-C24	-2.12	107.25	109.24
3	O	611	PID	C11-C12-C13	-2.12	121.58	130.47
3	M	613	PID	C17-C18-C19	-2.11	120.05	124.94
3	O	612	PID	C26-C25-C24	-2.11	107.26	109.24
3	O	621	PID	C18-C17-C16	-2.10	120.08	124.94
2	N	601	CLA	O2A-CGA-O1A	-2.10	118.08	123.49
2	O	601	CLA	O2A-CGA-O1A	-2.09	118.09	123.49
3	M	622	PID	C16-C15-C14	-2.09	124.18	127.20
3	N	624	PID	C17-C16-C15	-2.07	118.81	123.39
3	N	613	PID	C27-O6-C30	-2.07	114.01	117.92
3	N	613	PID	C17-C18-C19	-2.07	120.15	124.94
2	M	601	CLA	O2A-CGA-O1A	-2.07	118.15	123.49
3	M	621	PID	C16-C15-C14	-2.07	124.21	127.20
3	M	613	PID	C17-C16-C15	-2.06	118.83	123.39
3	M	614	PID	C11-C12-C13	-2.06	121.83	130.47
3	O	614	PID	C17-C16-C15	-2.05	118.86	123.39
3	N	613	PID	C17-C16-C15	-2.05	118.87	123.39
3	M	621	PID	C11-C12-C13	-2.04	121.92	130.47
3	M	612	PID	CM4-C14-C15	-2.04	119.89	122.90
2	N	602	CLA	O2D-CGD-O1D	-2.03	119.59	123.79
3	N	624	PID	C18-C19-C20	-2.03	118.90	123.39
3	N	614	PID	CM4-C14-C15	-2.02	119.91	122.90
2	O	602	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
4	O	615	DGD	C1D-O6D-C5D	-2.01	109.84	113.75
2	O	602	CLA	C3A-C2A-C1A	2.00	104.89	101.50
3	N	624	PID	C25-C26-C27	2.00	118.22	113.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	624	PID	O4-C10-O3	2.00	123.46	120.12
3	M	624	PID	O4-C10-O3	2.01	123.47	120.12
3	N	612	PID	C25-C26-C27	2.01	118.23	113.52
3	N	612	PID	O4-C10-C9	2.03	109.87	108.10
2	M	601	CLA	CED-O2D-CGD	2.04	120.76	115.99
2	M	601	CLA	C1D-CHD-C4C	2.04	125.69	122.60
3	N	623	PID	C25-C26-C27	2.06	118.34	113.52
4	M	615	DGD	O3G-C1D-C2D	2.12	110.72	108.04
2	O	601	CLA	C1D-CHD-C4C	2.14	125.83	122.60
3	N	613	PID	C5-C4-C3	2.16	118.66	115.02
2	M	602	CLA	CMB-C2B-C3B	2.17	129.32	125.09
2	N	602	CLA	CMB-C2B-C3B	2.18	129.35	125.09
3	M	622	PID	C25-C26-C27	2.18	118.64	113.52
4	N	615	DGD	O5D-C6D-C5D	2.18	113.03	109.08
3	O	623	PID	O4-C10-C9	2.18	110.01	108.10
4	O	615	DGD	O5D-C6D-C5D	2.19	113.06	109.08
2	O	601	CLA	CMB-C2B-C3B	2.20	129.39	125.09
3	O	611	PID	C5-C4-C3	2.22	118.77	115.02
3	M	613	PID	C25-C26-C27	2.24	118.78	113.52
3	O	613	PID	C5-C4-C3	2.25	118.81	115.02
3	O	623	PID	C25-C26-C27	2.25	118.80	113.52
3	M	622	PID	O4-C10-C9	2.25	110.07	108.10
3	N	612	PID	CM2-C5-C4	2.25	112.95	108.94
3	M	613	PID	C5-C4-C3	2.26	118.83	115.02
3	N	621	PID	O4-C10-O3	2.26	123.89	120.12
3	N	623	PID	C5-C4-C3	2.28	118.87	115.02
2	O	602	CLA	CED-O2D-CGD	2.29	121.37	115.99
3	O	613	PID	C25-C26-C27	2.30	118.92	113.52
3	O	612	PID	C25-C26-C27	2.31	118.95	113.52
2	O	602	CLA	CMB-C2B-C3B	2.32	129.62	125.09
3	O	621	PID	O4-C10-O3	2.32	123.99	120.12
4	M	615	DGD	O5D-C6D-C5D	2.33	113.31	109.08
2	N	601	CLA	CED-O2D-CGD	2.33	121.46	115.99
3	M	623	PID	C5-C4-C3	2.34	118.96	115.02
3	O	624	PID	O4-C10-C9	2.36	110.16	108.10
3	N	611	PID	C5-C4-C3	2.36	119.01	115.02
4	O	615	DGD	O3G-C1D-C2D	2.39	111.05	108.04
3	O	612	PID	O6-C30-C31	2.40	115.62	111.10
4	O	615	DGD	C1E-O6E-C5E	2.40	118.40	113.75
4	M	625	DGD	O2G-C1B-C2B	2.41	116.76	111.53
3	M	621	PID	O4-C10-O3	2.41	124.14	120.12
4	M	615	DGD	C1E-O6E-C5E	2.43	118.45	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	612	PID	O4-C10-C9	2.43	110.22	108.10
3	N	624	PID	O4-C10-O3	2.47	124.25	120.12
4	O	625	DGD	O2G-C1B-C2B	2.51	116.99	111.53
4	N	625	DGD	O2G-C1B-C2B	2.55	117.07	111.53
3	N	622	PID	O4-C10-C9	2.55	110.33	108.10
3	M	611	PID	C5-C4-C3	2.56	119.33	115.02
3	M	612	PID	O6-C30-C31	2.56	115.93	111.10
4	N	615	DGD	O3G-C1D-C2D	2.60	111.32	108.04
4	N	615	DGD	C1E-O6E-C5E	2.60	118.79	113.75
4	M	615	DGD	O6D-C1D-C2D	2.60	115.61	110.28
3	M	624	PID	O4-C10-C9	2.61	110.38	108.10
4	N	615	DGD	O6D-C1D-C2D	2.63	115.67	110.28
3	N	612	PID	O6-C30-C31	2.67	116.13	111.10
3	O	623	PID	C5-C4-C3	2.68	119.55	115.02
3	O	612	PID	O4-C10-C9	2.76	110.51	108.10
3	O	622	PID	O4-C10-C9	2.79	110.54	108.10
2	O	601	CLA	CED-O2D-CGD	2.81	122.58	115.99
3	N	613	PID	C25-C26-C27	2.81	120.12	113.52
3	N	622	PID	C5-C4-C3	2.85	119.84	115.02
4	O	615	DGD	O6D-C1D-C2D	2.88	116.19	110.28
3	M	623	PID	O4-C10-C9	2.97	110.70	108.10
2	N	601	CLA	C4A-NA-C1A	2.99	110.22	106.36
4	N	615	DGD	O2G-C1B-C2B	3.02	118.09	111.53
4	O	615	DGD	O2G-C1B-C2B	3.09	118.25	111.53
3	O	621	PID	O4-C10-C9	3.09	110.80	108.10
4	M	615	DGD	O2G-C1B-C2B	3.13	118.32	111.53
2	O	601	CLA	C4A-NA-C1A	3.16	110.44	106.36
2	O	602	CLA	C4A-NA-C1A	3.17	110.46	106.36
2	O	602	CLA	O2A-CGA-CBA	3.18	121.58	111.90
3	M	611	PID	O6-C30-C31	3.19	117.11	111.10
2	M	602	CLA	O2A-CGA-CBA	3.19	121.62	111.90
3	N	623	PID	O4-C10-C9	3.20	110.90	108.10
3	N	624	PID	O4-C10-C9	3.26	110.95	108.10
3	M	622	PID	O6-C30-C31	3.27	117.26	111.10
3	N	622	PID	O6-C30-C31	3.30	117.32	111.10
3	O	622	PID	C5-C4-C3	3.33	120.64	115.02
3	O	624	PID	O6-C30-C31	3.35	117.42	111.10
3	M	624	PID	O6-C30-C31	3.35	117.42	111.10
3	M	621	PID	O4-C10-C9	3.35	111.03	108.10
3	O	612	PID	C1-C2-C3	3.37	118.50	113.03
2	N	602	CLA	O2A-CGA-CBA	3.39	122.23	111.90
3	N	621	PID	O4-C10-C9	3.40	111.07	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	601	CLA	O2A-CGA-CBA	3.41	122.29	111.90
3	O	611	PID	O6-C30-C31	3.42	117.56	111.10
3	O	622	PID	O6-C30-C31	3.43	117.56	111.10
2	M	601	CLA	O2A-CGA-CBA	3.45	122.42	111.90
3	O	613	PID	O6-C30-C31	3.47	117.64	111.10
3	N	611	PID	O6-C30-C31	3.47	117.65	111.10
3	M	623	PID	O6-C30-C31	3.49	117.69	111.10
3	N	613	PID	O6-C30-C31	3.52	117.74	111.10
3	N	611	PID	C1-C2-C3	3.53	118.76	113.03
3	O	621	PID	O6-C30-C31	3.53	117.76	111.10
2	N	601	CLA	O2A-CGA-CBA	3.53	122.67	111.90
2	M	601	CLA	C4A-NA-C1A	3.54	110.94	106.36
3	N	624	PID	O6-C30-C31	3.54	117.78	111.10
3	M	612	PID	C1-C2-C3	3.60	118.87	113.03
2	N	602	CLA	C4A-NA-C1A	3.65	111.08	106.36
2	M	602	CLA	C4A-NA-C1A	3.66	111.09	106.36
3	M	614	PID	O6-C30-C31	3.68	118.04	111.10
3	M	622	PID	C5-C4-C3	3.70	121.25	115.02
3	O	614	PID	O6-C30-C31	3.71	118.09	111.10
3	N	612	PID	C1-C2-C3	3.72	119.07	113.03
3	M	613	PID	O6-C30-C31	3.75	118.18	111.10
3	O	611	PID	C1-C2-C3	3.76	119.13	113.03
3	N	623	PID	O6-C30-C31	3.77	118.21	111.10
3	N	614	PID	O6-C30-C31	3.85	118.36	111.10
3	O	623	PID	O6-C30-C31	3.86	118.39	111.10
3	M	611	PID	C1-C2-C3	3.90	119.36	113.03
3	N	621	PID	O6-C30-C31	3.99	118.63	111.10
3	M	621	PID	O6-C30-C31	4.05	118.74	111.10
3	O	621	PID	O4-C12-C11	4.06	110.01	107.50
3	N	612	PID	C5-C4-C3	4.11	121.95	115.02
3	O	612	PID	C5-C4-C3	4.39	122.43	115.02
3	M	612	PID	C5-C4-C3	4.43	122.49	115.02
3	M	621	PID	O4-C12-C11	4.44	110.25	107.50
3	N	622	PID	C1-C2-C3	4.44	120.23	113.03
4	M	615	DGD	O6D-C5D-C6D	4.47	115.74	106.61
2	M	601	CLA	O2D-CGD-CBD	4.53	117.51	111.30
4	N	615	DGD	O6D-C5D-C6D	4.56	115.92	106.61
3	O	622	PID	C1-C2-C3	4.56	120.43	113.03
4	O	615	DGD	O6D-C5D-C6D	4.58	115.97	106.61
2	O	601	CLA	O2D-CGD-CBD	4.62	117.64	111.30
3	N	613	PID	O4-C12-C11	4.66	110.38	107.50
3	M	622	PID	C1-C2-C3	4.70	120.65	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	611	PID	O4-C12-C11	4.86	110.51	107.50
3	O	623	PID	O4-C12-C11	4.92	110.54	107.50
3	N	621	PID	O4-C12-C11	5.10	110.65	107.50
3	O	612	PID	O4-C12-C11	5.11	110.66	107.50
3	N	613	PID	C1-C2-C3	5.14	121.36	113.03
3	O	613	PID	O4-C12-C11	5.24	110.74	107.50
3	M	613	PID	C1-C2-C3	5.24	121.54	113.03
3	N	622	PID	O4-C12-C11	5.33	110.80	107.50
3	O	613	PID	C1-C2-C3	5.38	121.76	113.03
3	M	612	PID	O4-C12-C11	5.44	110.86	107.50
3	M	613	PID	O4-C12-C11	5.53	110.92	107.50
3	M	622	PID	O4-C12-C11	5.57	110.94	107.50
3	M	623	PID	O4-C12-C11	5.58	110.95	107.50
3	O	622	PID	O4-C12-C11	5.58	110.95	107.50
2	N	601	CLA	O2D-CGD-CBD	5.59	118.97	111.30
3	N	611	PID	O4-C12-C11	5.63	110.98	107.50
3	N	612	PID	O4-C12-C11	5.67	111.01	107.50
3	M	611	PID	O4-C12-C11	5.67	111.01	107.50
3	O	614	PID	O4-C12-C11	5.69	111.02	107.50
3	N	624	PID	O4-C12-C11	5.81	111.09	107.50
3	M	624	PID	O4-C12-C11	5.82	111.10	107.50
3	O	624	PID	O4-C12-C11	5.88	111.14	107.50
3	N	623	PID	O4-C12-C11	6.17	111.32	107.50
2	N	602	CLA	O2D-CGD-CBD	6.38	120.06	111.30
2	O	602	CLA	O2D-CGD-CBD	6.40	120.08	111.30
3	N	614	PID	O4-C12-C11	6.44	111.48	107.50
3	M	614	PID	O4-C12-C11	6.46	111.50	107.50
2	M	602	CLA	O2D-CGD-CBD	6.53	120.25	111.30
4	N	615	DGD	O6E-C5E-C4E	7.25	123.28	109.68
4	O	615	DGD	O6E-C5E-C4E	7.32	123.43	109.68
4	M	615	DGD	O6E-C5E-C4E	7.33	123.44	109.68

All (33) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	N	613	PID	C3
2	M	602	CLA	NC
2	M	602	CLA	ND
2	M	602	CLA	NA
2	M	601	CLA	C8
2	M	601	CLA	NC
2	M	601	CLA	ND

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Mol	Chain	Res	Type	Atom
2	M	601	CLA	NA
4	N	615	DGD	C2D
4	N	615	DGD	C5D
4	N	615	DGD	C5E
4	M	615	DGD	C2D
4	M	615	DGD	C5D
4	M	615	DGD	C5E
2	O	601	CLA	C8
2	O	601	CLA	NC
2	O	601	CLA	ND
2	O	601	CLA	NA
3	M	613	PID	C3
3	O	613	PID	C3
2	N	602	CLA	NC
2	N	602	CLA	ND
2	N	602	CLA	NA
2	O	602	CLA	NC
2	O	602	CLA	ND
2	O	602	CLA	NA
2	N	601	CLA	C8
2	N	601	CLA	NC
2	N	601	CLA	ND
2	N	601	CLA	NA
4	O	615	DGD	C2D
4	O	615	DGD	C5D
4	O	615	DGD	C5E

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	601	CLA	1	0
2	M	602	CLA	2	0
3	M	611	PID	3	0
3	M	612	PID	1	0
3	M	614	PID	2	0
4	M	615	DGD	11	0
3	M	621	PID	1	0
3	M	622	PID	1	0
3	M	623	PID	1	0
4	M	625	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	601	CLA	1	0
2	N	602	CLA	1	0
3	N	611	PID	2	0
3	N	612	PID	2	0
3	N	614	PID	2	0
4	N	615	DGD	9	0
3	N	621	PID	1	0
3	N	622	PID	1	0
3	N	624	PID	1	0
4	N	625	DGD	1	0
2	O	601	CLA	2	0
2	O	602	CLA	2	0
3	O	611	PID	3	0
3	O	613	PID	1	0
3	O	614	PID	2	0
4	O	615	DGD	9	0
3	O	621	PID	2	0
3	O	622	PID	1	0
4	O	625	DGD	2	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	312/312 (100%)	-0.63	5 (1%) 74 75	20, 31, 53, 63	0
1	N	312/312 (100%)	-0.48	10 (3%) 51 52	22, 34, 57, 66	0
1	O	312/312 (100%)	-0.65	7 (2%) 65 66	21, 29, 51, 64	0
All	All	936/936 (100%)	-0.58	22 (2%) 62 63	20, 31, 53, 66	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	159	THR	3.8
1	M	162	SER	3.6
1	N	163	GLY	3.4
1	O	163	GLY	3.4
1	N	153	SER	3.3
1	M	163	GLY	3.1
1	N	162	SER	3.0
1	N	154	ALA	3.0
1	N	155	ALA	2.8
1	O	156	GLY	2.8
1	O	162	SER	2.8
1	M	159	THR	2.8
1	O	154	ALA	2.7
1	N	152	THR	2.7
1	N	148	LYS	2.7
1	O	148	LYS	2.4
1	O	160	VAL	2.3
1	O	155	ALA	2.2
1	N	160	VAL	2.2
1	M	154	ALA	2.1
1	M	155	ALA	2.1
1	N	156	GLY	2.1

## 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, 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
4	DGD	O	615	66/66	0.64	0.25	4.46	37,49,104,104	0
2	CLA	O	601	65/65	0.96	0.14	3.51	21,26,43,45	0
4	DGD	M	615	66/66	0.66	0.24	3.39	38,50,105,105	0
4	DGD	N	615	66/66	0.61	0.25	3.38	42,51,105,106	0
3	PID	N	622	46/46	0.96	0.11	3.13	21,26,33,37	0
3	PID	M	613	46/46	0.89	0.15	2.75	25,36,56,61	0
2	CLA	N	601	65/65	0.96	0.15	2.67	26,32,46,47	0
2	CLA	M	601	65/65	0.96	0.14	2.41	22,29,43,46	0
2	CLA	N	602	65/65	0.97	0.11	2.38	19,26,34,37	0
3	PID	O	612	46/46	0.93	0.14	2.32	20,25,35,48	0
3	PID	N	623	46/46	0.93	0.13	2.27	22,30,38,42	0
3	PID	M	612	46/46	0.92	0.13	2.24	24,27,37,47	0
3	PID	N	612	46/46	0.91	0.14	2.11	26,29,40,51	0
3	PID	N	613	46/46	0.86	0.15	2.05	30,40,57,61	0
3	PID	M	622	46/46	0.95	0.12	1.94	18,25,29,33	0
3	PID	O	611	46/46	0.92	0.12	1.53	19,26,36,43	0
2	CLA	M	602	65/65	0.97	0.11	1.51	19,23,33,35	0
3	PID	O	613	46/46	0.89	0.13	1.46	23,34,54,60	0
3	PID	O	623	46/46	0.94	0.12	1.33	18,24,34,42	0
2	CLA	O	602	65/65	0.98	0.11	1.32	18,22,31,34	0
3	PID	N	621	46/46	0.98	0.08	1.29	20,22,28,29	0
4	DGD	O	625	66/66	0.96	0.10	1.27	19,24,39,41	0
3	PID	M	611	46/46	0.93	0.12	1.22	20,28,39,41	0
4	DGD	N	625	66/66	0.95	0.11	1.22	19,24,38,41	0
3	PID	M	623	46/46	0.95	0.11	1.19	18,26,33,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PID	O	622	46/46	0.96	0.11	1.18	18,24,29,32	0
4	DGD	M	625	66/66	0.96	0.11	1.12	22,25,41,43	0
3	PID	O	624	46/46	0.97	0.08	1.02	19,23,28,32	0
3	PID	M	621	46/46	0.98	0.09	0.99	17,21,26,28	0
3	PID	N	624	46/46	0.97	0.08	0.70	22,26,31,35	0
3	PID	O	614	46/46	0.95	0.10	0.58	20,30,38,41	0
3	PID	O	621	46/46	0.97	0.09	0.58	17,21,25,26	0
3	PID	N	611	46/46	0.92	0.11	0.54	21,30,41,45	0
3	PID	M	624	46/46	0.97	0.08	0.37	19,22,26,34	0
3	PID	M	614	46/46	0.94	0.10	0.23	24,34,41,44	0
3	PID	N	614	46/46	0.94	0.10	-0.02	25,38,44,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.