Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:43 PM GMT

PDB ID	:	1C51
Title	:	PHOTOSYNTHETIC REACTION CENTER AND CORE ANTENNA SYSTEM (TRIMERIC), ALPHA CARBON ONLY
Authors	:	Klukas, O.; Schubert, W.D.; Jordan, P.; Krauss, N.; Fromme, P.; Witt, H.T.; Saenger, W.
Deposited on	:	1999-10-21
Resolution	:	4.00 Å(reported)

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

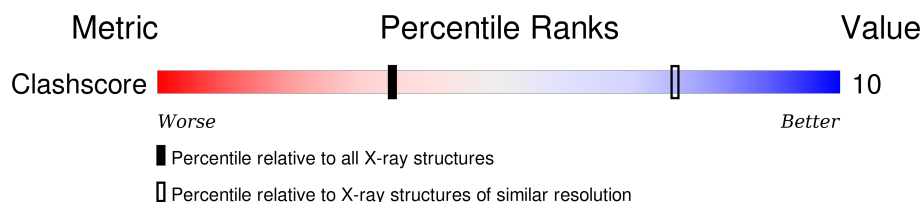|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	Percentile Ranks	Value
Clashscore		10

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))
Clashscore	102246	1052 (4.40-3.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	597	99% ⋅
2	B	619	100%
3	C	77	95% 5%
4	D	125	97% ⋅
5	E	75	97% ⋅
6	F	153	100%
7	K	78	100%
8	L	120	96% ⋅

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CLA	A	598	X	-	-	-
9	CLA	A	599	X	-	-	-
9	CLA	A	600	X	-	-	-
9	CLA	A	603	X	-	-	-
9	CLA	A	604	X	-	-	-
9	CLA	A	605	X	-	-	-
9	CLA	A	606	X	-	-	-
9	CLA	A	607	X	-	-	-
9	CLA	A	608	X	-	-	-
9	CLA	A	609	X	-	-	-
9	CLA	A	610	X	-	-	-
9	CLA	A	611	X	-	-	-
9	CLA	A	612	X	-	-	-
9	CLA	A	613	X	-	-	-
9	CLA	A	616	X	-	-	-
9	CLA	A	619	X	-	-	-
9	CLA	A	620	X	-	-	-
9	CLA	A	621	X	-	-	-
9	CLA	A	622	X	-	-	-
9	CLA	A	623	X	-	-	-
9	CLA	A	624	X	-	-	-
9	CLA	A	625	X	-	-	-
9	CLA	A	626	X	-	-	-
9	CLA	A	627	X	-	-	-
9	CLA	A	628	X	-	-	-
9	CLA	A	629	X	-	-	-
9	CLA	B	620	X	-	-	-
9	CLA	B	621	X	-	-	-
9	CLA	B	622	X	-	-	-
9	CLA	B	624	X	-	-	-
9	CLA	B	625	X	-	-	-
9	CLA	B	626	X	-	-	-
9	CLA	B	627	X	-	-	-
9	CLA	B	628	X	-	-	-
9	CLA	B	629	X	-	-	-
9	CLA	B	630	X	-	-	-
9	CLA	B	631	X	-	-	-
9	CLA	B	632	X	-	-	-
9	CLA	B	633	X	-	-	-
9	CLA	B	634	X	-	-	-
9	CLA	B	635	X	-	-	-
9	CLA	B	636	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CLA	B	637	X	-	-	-
9	CLA	B	638	X	-	-	-
9	CLA	B	639	X	-	-	-
9	CLA	B	640	X	-	-	-
9	CLA	B	641	X	-	-	-
9	CLA	B	642	X	-	-	-
9	CLA	B	643	X	-	-	-
9	CLA	B	644	X	-	-	-
9	CLA	B	645	X	-	-	-
9	CLA	B	646	X	-	-	-
9	CLA	B	647	X	-	-	-
9	CLA	B	648	X	-	-	-
9	CLA	B	649	X	-	-	-
9	CLA	B	650	X	-	-	-
9	CLA	B	651	X	-	-	-
9	CLA	B	652	X	-	-	-
9	CLA	B	653	X	-	-	-
9	CLA	F	154	X	-	-	-
9	CLA	F	155	X	-	-	-
9	CLA	F	156	X	-	-	-
9	CLA	F	157	X	-	-	-
9	CLA	K	135	X	-	-	-
9	CLA	L	147	X	-	-	-
9	CLA	L	149	X	-	-	-
9	CLA	L	163	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 3672 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 PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAA).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	597	Total C 597 597		0	0	597

- Molecule 2 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAB).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	619	Total C 619 619		0	0	619

- Molecule 3 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAC).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	77	Total C 77 77		0	0	77

- Molecule 4 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAD).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	125	Total C 125 125		0	0	125

- Molecule 5 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAE).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	E	75	Total C 75 75		0	0	75

- Molecule 6 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAF).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	F	153	Total 153	C 153	0	0	153

- Molecule 7 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAK).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	K	78	Total 78	C 78	0	0	78

- Molecule 8 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAL).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	L	120	Total 120	C 120	0	0	120

- Molecule 9 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).
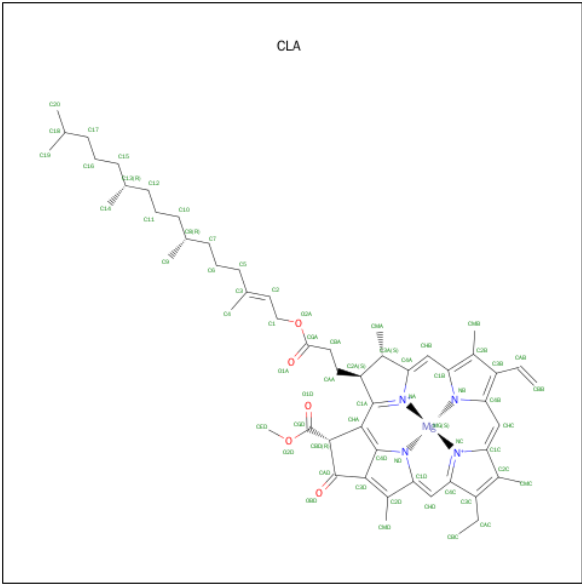
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	F	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	K	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	F	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	F	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	L	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	L	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	F	1	Total 25	C 20	Mg 1	N 4	0	0
9	A	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0
9	B	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 10 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).
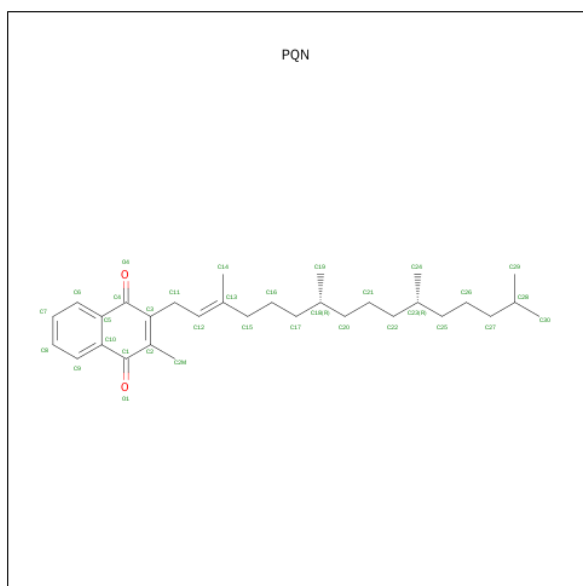
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	C	0	0
			2	2		
10	B	1	Total	C	0	0
			2	2		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
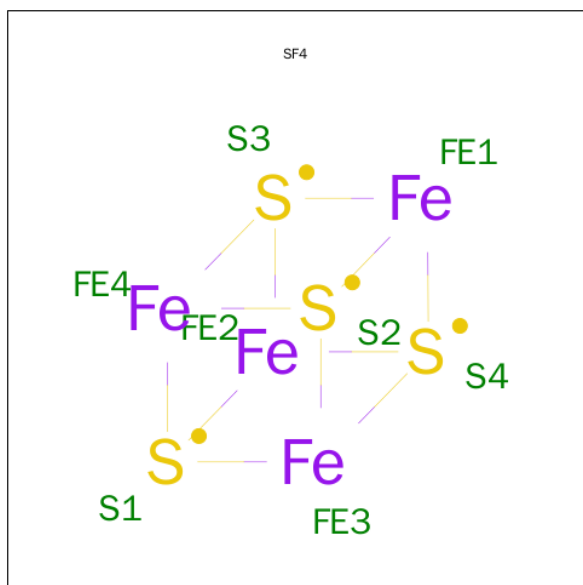
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total 8	Fe 4	S 4	0	0
11	C	1	Total 8	Fe 4	S 4	0	0
11	C	1	Total 8	Fe 4	S 4	0	0

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.
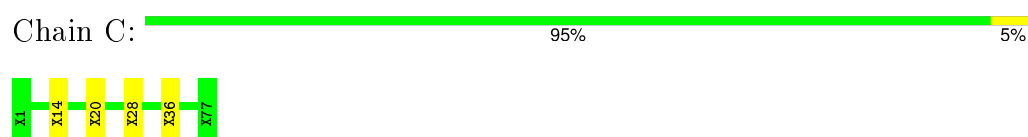
Note EDS was not executed.

- Molecule 1: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAA)
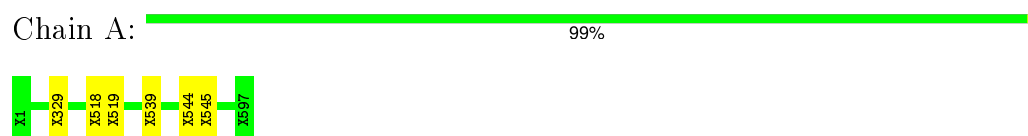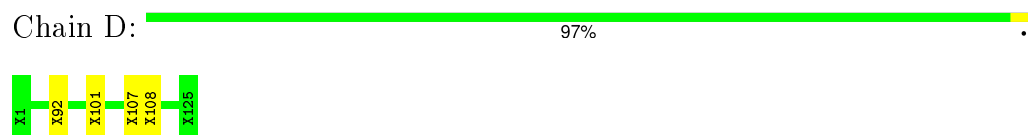
Chain A:

- Molecule 2: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAB)

Chain B:

- Molecule 3: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAC)

Chain C:

- Molecule 4: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAD)

Chain D:

- Molecule 5: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAE)
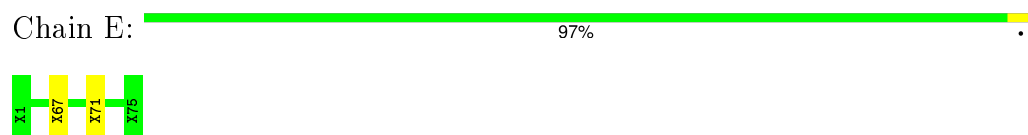
Chain E:

- Molecule 6: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAF)

Chain F:

100%

There are no outlier residues recorded for this chain.

• Molecule 7: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAK)

Chain K:

100%

There are no outlier residues recorded for this chain.

• Molecule 8: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAL)

Chain L:

96%

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	286.00Å 286.00Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 − 4.00	Depositor
% Data completeness (in resolution range)	(Not available) (60.00-4.00)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3672	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

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: SF4, CLA, PQN

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	597	0	0	4	0
2	B	619	0	0	6	0
3	C	77	0	0	3	0
4	D	125	0	0	2	0
5	E	75	0	0	1	0
6	F	153	0	0	0	0
7	K	78	0	0	0	0
8	L	120	0	0	0	4
9	A	750	0	90	8	0
9	B	825	0	99	22	0
9	F	125	0	15	0	0
9	K	25	0	3	13	0
9	L	75	0	9	0	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
11	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	16	0	0	2	0
All	All	3672	0	216	39	4

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 (39) 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:A:628:CLA:HHD	9:A:629:CLA:C2D	1.46	1.44
2:B:358:UNK:CA	9:B:627:CLA:C1A	2.28	1.10
9:A:628:CLA:C3C	9:A:629:CLA:C3D	2.33	1.06
9:A:628:CLA:CHD	9:A:629:CLA:C2D	2.33	1.06
9:B:641:CLA:HHC	9:K:135:CLA:C3D	1.95	0.95
3:C:20:UNK:CA	11:C:78:SF4:S1	2.56	0.94
3:C:28:UNK:CA	3:C:36:UNK:CA	2.47	0.93
9:A:628:CLA:HHD	9:A:629:CLA:C3D	1.99	0.93
2:B:358:UNK:CA	9:B:627:CLA:C2A	2.47	0.92
9:B:641:CLA:HHC	9:K:135:CLA:C2D	2.06	0.85
9:B:641:CLA:CHC	9:K:135:CLA:C2D	2.57	0.82
9:B:641:CLA:CHC	9:K:135:CLA:C3D	2.58	0.81
9:A:628:CLA:CHD	9:A:629:CLA:C3D	2.60	0.78
9:B:629:CLA:C3B	9:B:636:CLA:C3A	2.62	0.78
4:D:107:UNK:CA	4:D:108:UNK:CA	2.64	0.75
2:B:358:UNK:CA	9:B:627:CLA:NA	2.51	0.73
9:B:641:CLA:C2C	9:K:135:CLA:C2D	2.66	0.73
9:B:629:CLA:C3B	9:B:636:CLA:C2A	2.66	0.73
9:B:641:CLA:C2C	9:K:135:CLA:CHD	2.68	0.71
3:C:14:UNK:CA	11:C:79:SF4:S2	2.82	0.68
2:B:358:UNK:CA	9:B:627:CLA:C4A	2.73	0.67
2:B:358:UNK:CA	9:B:627:CLA:C3A	2.74	0.66
9:A:628:CLA:C4C	9:A:629:CLA:C3D	2.75	0.65
2:B:455:UNK:CA	2:B:456:UNK:CA	2.75	0.65
1:A:544:UNK:CA	1:A:545:UNK:CA	2.74	0.65
9:B:641:CLA:C2C	9:K:135:CLA:C1D	2.78	0.61
9:B:641:CLA:C1C	9:K:135:CLA:C1D	2.79	0.60
9:B:641:CLA:C1C	9:K:135:CLA:C2D	2.81	0.59
9:B:641:CLA:C2C	9:K:135:CLA:HHD	2.35	0.57
9:B:629:CLA:C3B	9:B:636:CLA:C4A	2.84	0.56
1:A:329:UNK:CA	9:A:612:CLA:C2D	2.88	0.51
9:B:629:CLA:C3B	9:B:636:CLA:C1A	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:UNK:CA	1:A:519:UNK:CA	2.91	0.49
5:E:67:UNK:CA	5:E:71:UNK:CA	2.91	0.47
9:B:641:CLA:CHC	9:K:135:CLA:C1D	2.91	0.47
9:B:641:CLA:CHC	9:K:135:CLA:C4D	2.94	0.45
4:D:92:UNK:CA	4:D:101:UNK:CA	2.96	0.43
9:B:641:CLA:C3C	9:K:135:CLA:CHD	2.97	0.42
1:A:539:UNK:CA	9:A:600:CLA:C3A	2.99	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:42:UNK:CA	8:L:85:UNK:CA[3_665]	1.93	0.27
8:L:42:UNK:CA	8:L:84:UNK:CA[3_665]	2.08	0.12
8:L:41:UNK:CA	8:L:85:UNK:CA[3_665]	2.08	0.12
8:L:43:UNK:CA	8:L:84:UNK:CA[3_665]	2.09	0.11

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

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)

77 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	#$|Z| > 2$
9	CLA	A	598	-	16,32,73	2.32	5 (31%)	21,54,113	1.01	0
9	CLA	A	599	-	16,32,73	2.34	5 (31%)	21,54,113	1.10	2 (9%)
9	CLA	A	600	-	16,32,73	2.33	4 (25%)	21,54,113	0.96	0
10	PQN	A	601	-	0,0,34	0.00	-	0,0,45	0.00	-
11	SF4	A	602	1	0,12,12	0.00	-	0,24,24	0.00	-
9	CLA	A	603	-	16,32,73	2.12	5 (31%)	21,54,113	1.07	0
9	CLA	A	604	-	16,32,73	2.26	5 (31%)	21,54,113	1.11	1 (4%)
9	CLA	A	605	-	16,32,73	2.21	5 (31%)	21,54,113	1.21	2 (9%)
9	CLA	A	606	-	16,32,73	2.13	5 (31%)	21,54,113	1.02	0
9	CLA	A	607	-	16,32,73	2.13	5 (31%)	21,54,113	1.09	1 (4%)
9	CLA	A	608	-	16,32,73	2.24	5 (31%)	21,54,113	1.07	1 (4%)
9	CLA	A	609	-	16,32,73	2.15	5 (31%)	21,54,113	1.14	2 (9%)
9	CLA	A	610	-	16,32,73	2.15	4 (25%)	21,54,113	1.10	2 (9%)
9	CLA	A	611	-	16,32,73	2.16	5 (31%)	21,54,113	1.06	2 (9%)
9	CLA	A	612	-	16,32,73	1.76	4 (25%)	21,54,113	2.37	7 (33%)
9	CLA	A	613	-	16,32,73	2.07	3 (18%)	21,54,113	1.04	0
9	CLA	A	614	-	16,32,73	2.60	7 (43%)	21,54,113	2.23	5 (23%)
9	CLA	A	615	-	16,32,73	2.60	7 (43%)	21,54,113	2.22	5 (23%)
9	CLA	A	616	-	16,32,73	2.18	5 (31%)	21,54,113	1.02	0
9	CLA	A	617	-	16,32,73	2.60	7 (43%)	21,54,113	2.23	5 (23%)
9	CLA	A	618	-	16,32,73	2.61	7 (43%)	21,54,113	2.23	5 (23%)
9	CLA	A	619	-	16,32,73	2.13	5 (31%)	21,54,113	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z|>2	Counts	RMSZ	#|Z|>2
9	CLA	A	620	-	16,32,73	2.20	5 (31%)	21,54,113	1.07	2 (9%)
9	CLA	A	621	-	16,32,73	2.14	5 (31%)	21,54,113	0.98	0
9	CLA	A	622	-	16,32,73	2.12	4 (25%)	21,54,113	1.12	3 (14%)
9	CLA	A	623	-	16,32,73	2.22	4 (25%)	21,54,113	1.04	1 (4%)
9	CLA	A	624	-	16,32,73	2.21	5 (31%)	21,54,113	1.06	0
9	CLA	A	625	-	16,32,73	2.23	5 (31%)	21,54,113	1.12	2 (9%)
9	CLA	A	626	-	16,32,73	2.11	5 (31%)	21,54,113	1.09	2 (9%)
9	CLA	A	627	-	16,32,73	2.14	5 (31%)	21,54,113	1.03	1 (4%)
9	CLA	A	628	-	16,32,73	2.19	5 (31%)	21,54,113	1.14	2 (9%)
9	CLA	A	629	-	16,32,73	2.13	5 (31%)	21,54,113	1.14	3 (14%)
9	CLA	B	620	-	16,32,73	2.49	5 (31%)	21,54,113	1.16	2 (9%)
9	CLA	B	621	-	16,32,73	2.28	5 (31%)	21,54,113	1.02	1 (4%)
9	CLA	B	622	-	16,32,73	2.29	4 (25%)	21,54,113	1.06	1 (4%)
10	PQN	B	623	-	0,0,34	0.00	-	0,0,45	0.00	-
9	CLA	B	624	-	16,32,73	2.13	5 (31%)	21,54,113	1.08	1 (4%)
9	CLA	B	625	-	16,32,73	2.11	5 (31%)	21,54,113	1.12	2 (9%)
9	CLA	B	626	-	16,32,73	2.16	5 (31%)	21,54,113	1.09	1 (4%)
9	CLA	B	627	-	16,32,73	2.17	5 (31%)	21,54,113	1.06	0
9	CLA	B	628	-	16,32,73	2.14	5 (31%)	21,54,113	1.15	2 (9%)
9	CLA	B	629	-	16,32,73	2.11	4 (25%)	21,54,113	1.08	1 (4%)
9	CLA	B	630	-	16,32,73	2.17	5 (31%)	21,54,113	1.06	3 (14%)
9	CLA	B	631	-	16,32,73	2.10	5 (31%)	21,54,113	1.03	1 (4%)
9	CLA	B	632	-	16,32,73	2.20	5 (31%)	21,54,113	1.10	1 (4%)
9	CLA	B	633	-	16,32,73	2.17	5 (31%)	21,54,113	1.06	1 (4%)
9	CLA	B	634	-	16,32,73	2.17	3 (18%)	21,54,113	0.94	0
9	CLA	B	635	-	16,32,73	1.69	4 (25%)	21,54,113	2.38	6 (28%)
9	CLA	B	636	-	16,32,73	2.15	5 (31%)	21,54,113	1.19	2 (9%)
9	CLA	B	637	-	16,32,73	2.17	5 (31%)	21,54,113	1.10	3 (14%)
9	CLA	B	638	-	16,32,73	2.18	4 (25%)	21,54,113	0.97	0
9	CLA	B	639	-	16,32,73	2.22	5 (31%)	21,54,113	1.05	2 (9%)
9	CLA	B	640	-	16,32,73	1.63	4 (25%)	21,54,113	2.16	6 (28%)
9	CLA	B	641	-	16,32,73	2.27	5 (31%)	21,54,113	1.19	2 (9%)
9	CLA	B	642	-	16,32,73	2.16	5 (31%)	21,54,113	1.12	2 (9%)
9	CLA	B	643	-	16,32,73	2.10	5 (31%)	21,54,113	1.06	1 (4%)
9	CLA	B	644	-	16,32,73	2.15	4 (25%)	21,54,113	0.97	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	CLA	B	645	-	16,32,73	2.21	5 (31%)	21,54,113	1.13	2 (9%)
9	CLA	B	646	-	16,32,73	2.22	5 (31%)	21,54,113	1.08	1 (4%)
9	CLA	B	647	-	16,32,73	2.12	5 (31%)	21,54,113	1.07	0
9	CLA	B	648	-	16,32,73	2.12	5 (31%)	21,54,113	1.03	1 (4%)
9	CLA	B	649	-	16,32,73	2.16	5 (31%)	21,54,113	1.05	1 (4%)
9	CLA	B	650	-	16,32,73	2.14	5 (31%)	21,54,113	1.01	0
9	CLA	B	651	-	16,32,73	2.09	5 (31%)	21,54,113	1.10	2 (9%)
9	CLA	B	652	-	16,32,73	2.05	5 (31%)	21,54,113	1.12	2 (9%)
9	CLA	B	653	-	16,32,73	2.13	3 (18%)	21,54,113	1.04	2 (9%)
11	SF4	C	78	-	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	C	79	-	0,12,12	0.00	-	0,24,24	0.00	-
9	CLA	F	154	-	16,32,73	2.23	5 (31%)	21,54,113	1.11	0
9	CLA	F	155	-	16,32,73	2.12	4 (25%)	21,54,113	1.02	1 (4%)
9	CLA	F	156	-	16,32,73	2.22	5 (31%)	21,54,113	1.16	3 (14%)
9	CLA	F	157	-	16,32,73	2.16	5 (31%)	21,54,113	1.08	0
9	CLA	F	158	-	16,32,73	2.61	7 (43%)	21,54,113	2.21	5 (23%)
9	CLA	K	135	-	16,32,73	2.27	6 (37%)	21,54,113	1.17	1 (4%)
9	CLA	L	147	-	16,32,73	2.12	5 (31%)	21,54,113	1.06	1 (4%)
9	CLA	L	149	-	16,32,73	2.08	5 (31%)	21,54,113	1.20	3 (14%)
9	CLA	L	163	-	16,32,73	2.13	3 (18%)	21,54,113	1.10	2 (9%)

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	CLA	A	598	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	599	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	600	-	3/3/7/25	0/0/66/135	0/0/8/9
10	PQN	A	601	-	-	0/0/0/43	0/0/0/2
11	SF4	A	602	1	-	0/0/48/48	0/6/5/5
9	CLA	A	603	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	604	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	605	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	606	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	607	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	608	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	609	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	610	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	611	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	612	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	613	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	614	-	-	0/0/66/135	0/0/8/9
9	CLA	A	615	-	-	0/0/66/135	0/0/8/9
9	CLA	A	616	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	617	-	-	0/0/66/135	0/0/8/9
9	CLA	A	618	-	-	0/0/66/135	0/0/8/9
9	CLA	A	619	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	620	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	621	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	622	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	623	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	624	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	625	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	626	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	627	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	628	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	A	629	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	620	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	621	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	622	-	3/3/7/25	0/0/66/135	0/0/8/9
10	PQN	B	623	-	-	0/0/0/43	0/0/0/2
9	CLA	B	624	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	625	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	626	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	627	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	628	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	629	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	630	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	631	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	632	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	633	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	634	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	635	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	636	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	637	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	638	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	639	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	640	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	641	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	642	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	643	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	644	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	645	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	646	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	647	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	648	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	649	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	650	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	651	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	652	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	B	653	-	3/3/7/25	0/0/66/135	0/0/8/9
11	SF4	C	78	-	-	0/0/48/48	0/6/5/5
11	SF4	C	79	-	-	0/0/48/48	0/6/5/5
9	CLA	F	154	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	F	155	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	F	156	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	F	157	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	F	158	-	-	0/0/66/135	0/0/8/9
9	CLA	K	135	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	L	147	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	L	149	-	3/3/7/25	0/0/66/135	0/0/8/9
9	CLA	L	163	-	3/3/7/25	0/0/66/135	0/0/8/9

All (351) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	620	CLA	C3A-C2A	-7.14	1.33	1.52
9	A	600	CLA	C3A-C2A	-7.01	1.34	1.52
9	A	599	CLA	C3A-C2A	-6.88	1.34	1.52
9	A	598	CLA	C3A-C2A	-6.79	1.34	1.52
9	B	622	CLA	C3A-C2A	-6.70	1.35	1.52
9	B	621	CLA	C3A-C2A	-6.55	1.35	1.52
9	A	604	CLA	C3A-C2A	-6.44	1.35	1.52
9	A	624	CLA	C3A-C2A	-6.41	1.35	1.52
9	B	646	CLA	C3A-C2A	-6.39	1.35	1.52
9	K	135	CLA	C3A-C2A	-6.38	1.35	1.52
9	A	625	CLA	C3A-C2A	-6.36	1.35	1.52
9	F	158	CLA	C3A-C2A	-6.36	1.35	1.52
9	A	617	CLA	C3A-C2A	-6.35	1.36	1.52
9	A	614	CLA	C3A-C2A	-6.34	1.36	1.52
9	B	626	CLA	C3A-C2A	-6.33	1.36	1.52
9	F	156	CLA	C3A-C2A	-6.32	1.36	1.52
9	A	610	CLA	C3A-C2A	-6.32	1.36	1.52
9	A	615	CLA	C3A-C2A	-6.32	1.36	1.52
9	A	616	CLA	C3A-C2A	-6.31	1.36	1.52
9	F	154	CLA	C3A-C2A	-6.30	1.36	1.52
9	B	641	CLA	C3A-C2A	-6.29	1.36	1.52
9	A	608	CLA	C3A-C2A	-6.29	1.36	1.52
9	A	618	CLA	C3A-C2A	-6.28	1.36	1.52
9	B	634	CLA	C3A-C2A	-6.27	1.36	1.52
9	B	632	CLA	C3A-C2A	-6.27	1.36	1.52
9	B	653	CLA	C3A-C2A	-6.25	1.36	1.52
9	A	619	CLA	C3A-C2A	-6.23	1.36	1.52
9	B	639	CLA	C3A-C2A	-6.22	1.36	1.52
9	A	627	CLA	C3A-C2A	-6.22	1.36	1.52
9	B	624	CLA	C3A-C2A	-6.22	1.36	1.52
9	B	645	CLA	C3A-C2A	-6.21	1.36	1.52
9	A	607	CLA	C3A-C2A	-6.20	1.36	1.52
9	B	644	CLA	C3A-C2A	-6.19	1.36	1.52
9	A	621	CLA	C3A-C2A	-6.19	1.36	1.52
9	A	611	CLA	C3A-C2A	-6.19	1.36	1.52
9	B	638	CLA	C3A-C2A	-6.18	1.36	1.52
9	F	157	CLA	C3A-C2A	-6.18	1.36	1.52
9	A	620	CLA	C3A-C2A	-6.17	1.36	1.52
9	A	609	CLA	C3A-C2A	-6.17	1.36	1.52
9	B	627	CLA	C3A-C2A	-6.17	1.36	1.52
9	B	637	CLA	C3A-C2A	-6.15	1.36	1.52
9	A	622	CLA	C3A-C2A	-6.14	1.36	1.52
9	L	149	CLA	C3A-C2A	-6.13	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	629	CLA	C3A-C2A	-6.13	1.36	1.52
9	B	631	CLA	C3A-C2A	-6.12	1.36	1.52
9	B	649	CLA	C3A-C2A	-6.12	1.36	1.52
9	B	636	CLA	C3A-C2A	-6.12	1.36	1.52
9	B	650	CLA	C3A-C2A	-6.11	1.36	1.52
9	B	642	CLA	C3A-C2A	-6.11	1.36	1.52
9	B	633	CLA	C3A-C2A	-6.10	1.36	1.52
9	A	623	CLA	C3A-C2A	-6.08	1.36	1.52
9	F	155	CLA	C3A-C2A	-6.08	1.36	1.52
9	B	625	CLA	C3A-C2A	-6.06	1.36	1.52
9	A	605	CLA	C3A-C2A	-6.03	1.36	1.52
9	A	603	CLA	C3A-C2A	-6.03	1.36	1.52
9	B	648	CLA	C3A-C2A	-6.02	1.36	1.52
9	A	626	CLA	C3A-C2A	-6.01	1.36	1.52
9	L	163	CLA	C3A-C2A	-6.00	1.36	1.52
9	B	643	CLA	C3A-C2A	-6.00	1.36	1.52
9	B	652	CLA	C3A-C2A	-6.00	1.36	1.52
9	B	628	CLA	C3A-C2A	-5.98	1.36	1.52
9	A	628	CLA	C3A-C2A	-5.97	1.37	1.52
9	L	147	CLA	C3A-C2A	-5.96	1.37	1.52
9	B	651	CLA	C3A-C2A	-5.95	1.37	1.52
9	A	629	CLA	C3A-C2A	-5.93	1.37	1.52
9	A	606	CLA	C3A-C2A	-5.91	1.37	1.52
9	B	647	CLA	C3A-C2A	-5.89	1.37	1.52
9	B	630	CLA	C3A-C2A	-5.87	1.37	1.52
9	A	613	CLA	C3A-C2A	-5.83	1.37	1.52
9	L	163	CLA	C1B-CHB	-3.71	1.35	1.43
9	B	620	CLA	C1B-CHB	-3.64	1.36	1.43
9	A	611	CLA	C1B-CHB	-3.59	1.36	1.43
9	B	640	CLA	C4B-CHC	-3.54	1.36	1.43
9	B	634	CLA	C4B-CHC	-3.50	1.36	1.43
9	B	629	CLA	C1B-CHB	-3.47	1.36	1.43
9	A	613	CLA	C4B-CHC	-3.45	1.36	1.43
9	A	622	CLA	C1B-CHB	-3.45	1.36	1.43
9	B	651	CLA	C4B-CHC	-3.38	1.36	1.43
9	A	606	CLA	C1B-CHB	-3.36	1.36	1.43
9	F	155	CLA	C4B-CHC	-3.31	1.36	1.43
9	B	644	CLA	C4B-CHC	-3.28	1.36	1.43
9	K	135	CLA	C4B-CHC	-3.28	1.36	1.43
9	B	638	CLA	C1B-CHB	-3.28	1.36	1.43
9	B	637	CLA	C4B-CHC	-3.28	1.36	1.43
9	A	620	CLA	C1B-CHB	-3.26	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	627	CLA	C1B-CHB	-3.26	1.36	1.43
9	B	647	CLA	C1B-CHB	-3.22	1.36	1.43
9	A	628	CLA	C1B-CHB	-3.21	1.37	1.43
9	B	622	CLA	C1B-CHB	-3.20	1.37	1.43
9	A	598	CLA	C1B-CHB	-3.17	1.37	1.43
9	A	604	CLA	C4B-CHC	-3.13	1.37	1.43
9	B	653	CLA	C1B-CHB	-3.13	1.37	1.43
9	A	604	CLA	C1B-CHB	-3.09	1.37	1.43
9	B	642	CLA	C4B-CHC	-3.09	1.37	1.43
9	B	648	CLA	C1B-CHB	-3.08	1.37	1.43
9	B	638	CLA	C4B-CHC	-3.08	1.37	1.43
9	A	613	CLA	C1B-CHB	-3.07	1.37	1.43
9	B	624	CLA	C1B-CHB	-3.06	1.37	1.43
9	B	635	CLA	C1B-CHB	-3.06	1.37	1.43
9	A	612	CLA	C4B-CHC	-3.03	1.37	1.43
9	A	625	CLA	C4B-CHC	-3.02	1.37	1.43
9	B	621	CLA	C1B-CHB	-3.02	1.37	1.43
9	B	632	CLA	C4B-CHC	-3.01	1.37	1.43
9	B	636	CLA	C1B-CHB	-2.99	1.37	1.43
9	B	641	CLA	C1B-CHB	-2.98	1.37	1.43
9	A	609	CLA	C4B-CHC	-2.97	1.37	1.43
9	A	607	CLA	C4B-CHC	-2.96	1.37	1.43
9	A	621	CLA	C4B-CHC	-2.95	1.37	1.43
9	B	653	CLA	C4B-CHC	-2.95	1.37	1.43
9	B	626	CLA	C1B-CHB	-2.92	1.37	1.43
9	F	154	CLA	C4B-CHC	-2.92	1.37	1.43
9	A	623	CLA	C4B-CHC	-2.90	1.37	1.43
9	L	163	CLA	C4B-CHC	-2.90	1.37	1.43
9	A	603	CLA	C4B-CHC	-2.90	1.37	1.43
9	B	626	CLA	C4B-CHC	-2.90	1.37	1.43
9	B	649	CLA	C4B-CHC	-2.89	1.37	1.43
9	B	633	CLA	C4B-CHC	-2.87	1.37	1.43
9	B	646	CLA	C4B-CHC	-2.87	1.37	1.43
9	B	631	CLA	C1B-CHB	-2.85	1.37	1.43
9	A	608	CLA	C4B-CHC	-2.85	1.37	1.43
9	A	619	CLA	C4B-CHC	-2.84	1.37	1.43
9	A	619	CLA	C1B-CHB	-2.84	1.37	1.43
9	B	627	CLA	C4B-CHC	-2.83	1.37	1.43
9	A	616	CLA	C4B-CHC	-2.82	1.37	1.43
9	B	629	CLA	C4B-CHC	-2.81	1.37	1.43
9	A	609	CLA	C1B-CHB	-2.81	1.37	1.43
9	B	647	CLA	C4B-CHC	-2.80	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	634	CLA	C1B-CHB	-2.80	1.37	1.43
9	A	624	CLA	C1B-CHB	-2.79	1.37	1.43
9	A	610	CLA	C1B-CHB	-2.79	1.37	1.43
9	A	605	CLA	C1B-CHB	-2.79	1.37	1.43
9	A	626	CLA	C4B-CHC	-2.78	1.37	1.43
9	B	640	CLA	C1B-CHB	-2.78	1.37	1.43
9	A	626	CLA	C1B-CHB	-2.78	1.37	1.43
9	B	643	CLA	C4B-CHC	-2.78	1.37	1.43
9	A	610	CLA	C4B-CHC	-2.78	1.37	1.43
9	B	621	CLA	C4B-CHC	-2.77	1.37	1.43
9	A	608	CLA	C1B-CHB	-2.77	1.37	1.43
9	B	646	CLA	C1B-CHB	-2.75	1.37	1.43
9	A	612	CLA	C1B-CHB	-2.75	1.37	1.43
9	A	603	CLA	C1B-CHB	-2.74	1.37	1.43
9	A	605	CLA	C4B-CHC	-2.73	1.38	1.43
9	B	650	CLA	C4B-CHC	-2.72	1.38	1.43
9	B	639	CLA	C1B-CHB	-2.70	1.38	1.43
9	B	643	CLA	C1B-CHB	-2.69	1.38	1.43
9	A	625	CLA	C1B-CHB	-2.69	1.38	1.43
9	B	630	CLA	C1B-CHB	-2.68	1.38	1.43
9	B	645	CLA	C4B-CHC	-2.68	1.38	1.43
9	A	628	CLA	C4B-CHC	-2.67	1.38	1.43
9	B	652	CLA	C4B-CHC	-2.66	1.38	1.43
9	L	147	CLA	C4B-CHC	-2.65	1.38	1.43
9	A	629	CLA	C1B-CHB	-2.65	1.38	1.43
9	B	631	CLA	C4B-CHC	-2.64	1.38	1.43
9	A	621	CLA	C1B-CHB	-2.64	1.38	1.43
9	B	627	CLA	C1B-CHB	-2.62	1.38	1.43
9	B	645	CLA	C1B-CHB	-2.62	1.38	1.43
9	B	632	CLA	C1B-CHB	-2.62	1.38	1.43
9	A	616	CLA	C1B-CHB	-2.61	1.38	1.43
9	A	599	CLA	C1B-CHB	-2.60	1.38	1.43
9	B	651	CLA	C1B-CHB	-2.60	1.38	1.43
9	A	606	CLA	C4B-CHC	-2.59	1.38	1.43
9	B	642	CLA	C1B-CHB	-2.58	1.38	1.43
9	F	156	CLA	C1B-CHB	-2.57	1.38	1.43
9	A	624	CLA	C4B-CHC	-2.56	1.38	1.43
9	A	622	CLA	C4B-CHC	-2.56	1.38	1.43
9	B	650	CLA	C1B-CHB	-2.56	1.38	1.43
9	B	625	CLA	C1B-CHB	-2.55	1.38	1.43
9	L	149	CLA	C4B-CHC	-2.55	1.38	1.43
9	B	652	CLA	C1B-CHB	-2.54	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	649	CLA	C1B-CHB	-2.54	1.38	1.43
9	F	155	CLA	C1B-CHB	-2.54	1.38	1.43
9	A	598	CLA	C4B-CHC	-2.53	1.38	1.43
9	F	156	CLA	C4B-CHC	-2.53	1.38	1.43
9	B	640	CLA	CHD-C4C	-2.52	1.35	1.41
9	F	157	CLA	C1B-CHB	-2.51	1.38	1.43
9	A	620	CLA	C4B-CHC	-2.47	1.38	1.43
9	A	615	CLA	C4B-CHC	-2.44	1.38	1.43
9	B	636	CLA	C4B-CHC	-2.43	1.38	1.43
9	F	154	CLA	C1B-CHB	-2.43	1.38	1.43
9	A	614	CLA	C4B-CHC	-2.42	1.38	1.43
9	A	617	CLA	C4B-CHC	-2.42	1.38	1.43
9	B	644	CLA	C1B-CHB	-2.42	1.38	1.43
9	A	618	CLA	C4B-CHC	-2.42	1.38	1.43
9	L	147	CLA	C1B-CHB	-2.41	1.38	1.43
9	B	633	CLA	C1B-CHB	-2.40	1.38	1.43
9	A	629	CLA	C4B-CHC	-2.40	1.38	1.43
9	F	158	CLA	C4C-NC	-2.39	1.33	1.37
9	A	618	CLA	C4C-NC	-2.39	1.33	1.37
9	F	158	CLA	C4B-CHC	-2.38	1.38	1.43
9	A	617	CLA	C4C-NC	-2.38	1.33	1.37
9	B	628	CLA	C4B-CHC	-2.37	1.38	1.43
9	A	614	CLA	C4C-NC	-2.37	1.33	1.37
9	B	648	CLA	C4B-CHC	-2.37	1.38	1.43
9	A	627	CLA	C4B-CHC	-2.37	1.38	1.43
9	A	611	CLA	C4B-CHC	-2.37	1.38	1.43
9	A	615	CLA	C4C-NC	-2.36	1.33	1.37
9	B	641	CLA	C4B-CHC	-2.34	1.38	1.43
9	B	628	CLA	C1B-CHB	-2.33	1.38	1.43
9	F	157	CLA	C4B-CHC	-2.32	1.38	1.43
9	K	135	CLA	C1B-CHB	-2.31	1.38	1.43
9	B	630	CLA	C4B-CHC	-2.29	1.38	1.43
9	B	624	CLA	C4B-CHC	-2.26	1.38	1.43
9	L	149	CLA	C1B-CHB	-2.26	1.38	1.43
9	B	639	CLA	C4B-CHC	-2.26	1.38	1.43
9	B	620	CLA	C4B-CHC	-2.24	1.39	1.43
9	A	607	CLA	C1B-CHB	-2.23	1.39	1.43
9	K	135	CLA	CHD-C4C	-2.23	1.35	1.41
9	B	635	CLA	C4B-CHC	-2.16	1.39	1.43
9	B	637	CLA	C1B-CHB	-2.15	1.39	1.43
9	A	599	CLA	C4B-CHC	-2.09	1.39	1.43
9	A	600	CLA	C4B-CHC	-2.02	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	625	CLA	C4B-CHC	-2.01	1.39	1.43
9	A	627	CLA	C2B-C1B	2.02	1.43	1.40
9	B	644	CLA	C2B-C1B	2.03	1.43	1.40
9	L	149	CLA	C3B-C4B	2.03	1.43	1.40
9	A	606	CLA	C2B-C1B	2.04	1.43	1.40
9	B	629	CLA	C3B-C4B	2.06	1.43	1.40
9	A	611	CLA	C2B-C1B	2.07	1.43	1.40
9	B	631	CLA	C2B-C1B	2.09	1.43	1.40
9	B	652	CLA	C2B-C1B	2.11	1.43	1.40
9	A	603	CLA	C3B-C4B	2.12	1.43	1.40
9	A	619	CLA	C2B-C1B	2.13	1.43	1.40
9	B	626	CLA	C2B-C1B	2.14	1.43	1.40
9	B	638	CLA	C2B-C1B	2.15	1.43	1.40
9	B	651	CLA	C3B-C4B	2.15	1.43	1.40
9	B	637	CLA	C3B-C4B	2.16	1.43	1.40
9	B	621	CLA	C3B-C4B	2.17	1.43	1.40
9	B	626	CLA	C3B-C4B	2.18	1.43	1.40
9	B	624	CLA	C2B-C1B	2.18	1.43	1.40
9	A	619	CLA	C3B-C4B	2.19	1.43	1.40
9	B	651	CLA	C2B-C1B	2.21	1.43	1.40
9	A	627	CLA	C3B-C4B	2.21	1.43	1.40
9	A	604	CLA	C2B-C1B	2.21	1.43	1.40
9	A	621	CLA	C3B-C4B	2.21	1.43	1.40
9	B	652	CLA	C3B-C4B	2.23	1.43	1.40
9	B	620	CLA	C2B-C1B	2.24	1.43	1.40
9	B	648	CLA	C2B-C1B	2.24	1.43	1.40
9	A	622	CLA	C3B-C4B	2.26	1.43	1.40
9	A	621	CLA	C2B-C1B	2.26	1.43	1.40
9	A	609	CLA	C2B-C1B	2.26	1.43	1.40
9	A	610	CLA	C2B-C1B	2.27	1.44	1.40
9	A	609	CLA	C3B-C4B	2.28	1.44	1.40
9	B	643	CLA	C2B-C1B	2.29	1.44	1.40
9	B	642	CLA	C3B-C4B	2.32	1.44	1.40
9	F	155	CLA	C2B-C1B	2.35	1.44	1.40
9	B	632	CLA	C3B-C4B	2.35	1.44	1.40
9	K	135	CLA	C3B-C4B	2.36	1.44	1.40
9	B	625	CLA	C2B-C1B	2.36	1.44	1.40
9	B	631	CLA	C3B-C4B	2.37	1.44	1.40
9	B	647	CLA	C2B-C1B	2.37	1.44	1.40
9	B	643	CLA	C3B-C4B	2.39	1.44	1.40
9	B	624	CLA	C3B-C4B	2.40	1.44	1.40
9	B	647	CLA	C3B-C4B	2.40	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	604	CLA	C3B-C4B	2.41	1.44	1.40
9	B	636	CLA	C2B-C1B	2.42	1.44	1.40
9	A	607	CLA	C3B-C4B	2.43	1.44	1.40
9	A	626	CLA	C3B-C4B	2.46	1.44	1.40
9	A	603	CLA	C2B-C1B	2.47	1.44	1.40
9	B	627	CLA	C3B-C4B	2.48	1.44	1.40
9	A	598	CLA	C2B-C1B	2.48	1.44	1.40
9	B	649	CLA	C3B-C4B	2.49	1.44	1.40
9	F	156	CLA	C3B-C4B	2.49	1.44	1.40
9	A	620	CLA	C2B-C1B	2.49	1.44	1.40
9	B	645	CLA	C2B-C1B	2.50	1.44	1.40
9	A	616	CLA	C2B-C1B	2.51	1.44	1.40
9	L	147	CLA	C3B-C4B	2.52	1.44	1.40
9	A	628	CLA	C2B-C1B	2.52	1.44	1.40
9	B	628	CLA	C2B-C1B	2.53	1.44	1.40
9	A	608	CLA	C3B-C4B	2.53	1.44	1.40
9	B	636	CLA	C3B-C4B	2.53	1.44	1.40
9	B	646	CLA	C3B-C4B	2.54	1.44	1.40
9	B	650	CLA	C2B-C1B	2.54	1.44	1.40
9	B	650	CLA	C3B-C4B	2.55	1.44	1.40
9	A	629	CLA	C2B-C1B	2.57	1.44	1.40
9	B	648	CLA	C3B-C4B	2.58	1.44	1.40
9	L	149	CLA	C2B-C1B	2.60	1.44	1.40
9	A	624	CLA	C2B-C1B	2.61	1.44	1.40
9	A	625	CLA	C3B-C4B	2.64	1.44	1.40
9	F	157	CLA	C2B-C1B	2.65	1.44	1.40
9	B	637	CLA	C2B-C1B	2.66	1.44	1.40
9	B	633	CLA	C3B-C4B	2.66	1.44	1.40
9	A	624	CLA	C3B-C4B	2.68	1.44	1.40
9	A	626	CLA	C2B-C1B	2.69	1.44	1.40
9	F	157	CLA	C3B-C4B	2.70	1.44	1.40
9	B	625	CLA	C3B-C4B	2.70	1.44	1.40
9	B	628	CLA	C3B-C4B	2.70	1.44	1.40
9	A	607	CLA	C2B-C1B	2.71	1.44	1.40
9	B	649	CLA	C2B-C1B	2.74	1.44	1.40
9	B	627	CLA	C2B-C1B	2.74	1.44	1.40
9	L	147	CLA	C2B-C1B	2.75	1.44	1.40
9	A	606	CLA	C3B-C4B	2.76	1.44	1.40
9	B	646	CLA	C2B-C1B	2.77	1.44	1.40
9	A	611	CLA	C3B-C4B	2.78	1.44	1.40
9	F	154	CLA	C3B-C4B	2.78	1.44	1.40
9	B	642	CLA	C2B-C1B	2.78	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	598	CLA	C3B-C4B	2.81	1.44	1.40
9	K	135	CLA	C2B-C1B	2.81	1.44	1.40
9	A	616	CLA	C3B-C4B	2.81	1.44	1.40
9	B	645	CLA	C3B-C4B	2.82	1.44	1.40
9	A	605	CLA	C2B-C1B	2.84	1.45	1.40
9	B	632	CLA	C2B-C1B	2.85	1.45	1.40
9	F	154	CLA	C2B-C1B	2.87	1.45	1.40
9	A	628	CLA	C3B-C4B	2.87	1.45	1.40
9	A	620	CLA	C3B-C4B	2.88	1.45	1.40
9	A	625	CLA	C2B-C1B	2.88	1.45	1.40
9	A	629	CLA	C3B-C4B	2.89	1.45	1.40
9	B	639	CLA	C2B-C1B	2.92	1.45	1.40
9	A	599	CLA	C3B-C4B	2.92	1.45	1.40
9	B	622	CLA	C2B-C1B	2.92	1.45	1.40
9	A	623	CLA	C3B-C4B	2.96	1.45	1.40
9	A	608	CLA	C2B-C1B	2.96	1.45	1.40
9	B	622	CLA	C3B-C4B	2.96	1.45	1.40
9	B	641	CLA	C2B-C1B	2.96	1.45	1.40
9	F	156	CLA	C2B-C1B	2.96	1.45	1.40
9	B	621	CLA	C2B-C1B	2.97	1.45	1.40
9	A	600	CLA	C3B-C4B	2.97	1.45	1.40
9	B	640	CLA	C2B-C1B	3.03	1.45	1.40
9	A	605	CLA	C3B-C4B	3.06	1.45	1.40
9	B	639	CLA	C3B-C4B	3.10	1.45	1.40
9	B	633	CLA	C2B-C1B	3.15	1.45	1.40
9	A	599	CLA	C2B-C1B	3.15	1.45	1.40
9	A	600	CLA	C2B-C1B	3.17	1.45	1.40
9	F	158	CLA	C3D-C2D	3.18	1.55	1.39
9	A	618	CLA	C3D-C2D	3.19	1.55	1.39
9	A	614	CLA	C3D-C2D	3.20	1.55	1.39
9	A	615	CLA	C3D-C2D	3.20	1.55	1.39
9	A	617	CLA	C3D-C2D	3.20	1.55	1.39
9	A	617	CLA	C3C-C2C	3.26	1.42	1.35
9	B	641	CLA	C3B-C4B	3.29	1.45	1.40
9	A	614	CLA	C3C-C2C	3.29	1.42	1.35
9	A	618	CLA	C3C-C2C	3.29	1.42	1.35
9	A	614	CLA	C3B-C4B	3.30	1.45	1.40
9	A	617	CLA	C3B-C4B	3.30	1.45	1.40
9	F	158	CLA	C3C-C2C	3.31	1.42	1.35
9	A	615	CLA	C3C-C2C	3.31	1.42	1.35
9	B	630	CLA	C3B-C4B	3.32	1.45	1.40
9	A	615	CLA	C3B-C4B	3.33	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	630	CLA	C2B-C1B	3.34	1.45	1.40
9	F	158	CLA	C3B-C4B	3.40	1.45	1.40
9	B	620	CLA	C3B-C4B	3.41	1.45	1.40
9	B	635	CLA	C2B-C1B	3.48	1.46	1.40
9	A	618	CLA	C3B-C4B	3.50	1.46	1.40
9	A	623	CLA	C2B-C1B	3.52	1.46	1.40
9	A	612	CLA	C2B-C1B	3.55	1.46	1.40
9	B	635	CLA	C3B-C4B	3.56	1.46	1.40
9	A	612	CLA	C3B-C4B	3.65	1.46	1.40
9	A	615	CLA	C2B-C1B	4.10	1.47	1.40
9	A	614	CLA	C2B-C1B	4.12	1.47	1.40
9	F	158	CLA	C2B-C1B	4.13	1.47	1.40
9	A	617	CLA	C2B-C1B	4.13	1.47	1.40
9	A	618	CLA	C2B-C1B	4.14	1.47	1.40

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	158	CLA	C3C-C4C-CHD	-6.61	114.45	125.32
9	A	615	CLA	C3C-C4C-CHD	-6.59	114.47	125.32
9	A	617	CLA	C3C-C4C-CHD	-6.58	114.50	125.32
9	A	614	CLA	C3C-C4C-CHD	-6.57	114.52	125.32
9	A	618	CLA	C3C-C4C-CHD	-6.53	114.57	125.32
9	B	635	CLA	C1C-NC-C4C	-4.23	101.22	106.07
9	A	617	CLA	C2D-C3D-C4D	-3.94	102.83	106.30
9	A	618	CLA	C2D-C3D-C4D	-3.92	102.85	106.30
9	A	614	CLA	C2D-C3D-C4D	-3.92	102.85	106.30
9	A	615	CLA	C2D-C3D-C4D	-3.86	102.90	106.30
9	F	158	CLA	C2D-C3D-C4D	-3.80	102.95	106.30
9	B	640	CLA	C1C-NC-C4C	-3.70	101.83	106.07
9	A	612	CLA	C1C-NC-C4C	-3.68	101.85	106.07
9	A	614	CLA	C3D-C2D-C1D	-3.65	103.09	106.30
9	A	615	CLA	C3D-C2D-C1D	-3.63	103.10	106.30
9	A	617	CLA	C3D-C2D-C1D	-3.63	103.11	106.30
9	A	618	CLA	C3D-C2D-C1D	-3.62	103.11	106.30
9	F	158	CLA	C3D-C2D-C1D	-3.60	103.13	106.30
9	A	612	CLA	C3A-C4A-CHB	-3.18	120.84	124.06
9	B	635	CLA	C3A-C4A-CHB	-2.97	121.06	124.06
9	A	618	CLA	C3C-C2C-C1C	-2.83	104.05	107.23
9	A	614	CLA	C3C-C2C-C1C	-2.76	104.12	107.23
9	F	158	CLA	C3C-C2C-C1C	-2.73	104.16	107.23
9	A	615	CLA	C3C-C2C-C1C	-2.72	104.17	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	617	CLA	C3C-C2C-C1C	-2.70	104.19	107.23
9	B	628	CLA	C1C-NC-C4C	-2.57	103.12	106.07
9	B	652	CLA	C1C-NC-C4C	-2.43	103.28	106.07
9	B	640	CLA	C3D-C2D-C1D	-2.43	104.16	106.30
9	A	607	CLA	C1C-NC-C4C	-2.39	103.34	106.07
9	A	599	CLA	C1C-NC-C4C	-2.34	103.39	106.07
9	A	622	CLA	C1C-NC-C4C	-2.34	103.39	106.07
9	L	149	CLA	C1C-NC-C4C	-2.26	103.48	106.07
9	A	610	CLA	C1C-NC-C4C	-2.24	103.51	106.07
9	B	637	CLA	C1C-NC-C4C	-2.20	103.55	106.07
9	B	625	CLA	C1C-NC-C4C	-2.16	103.60	106.07
9	B	622	CLA	C1C-NC-C4C	-2.13	103.63	106.07
9	B	636	CLA	C1C-NC-C4C	-2.13	103.63	106.07
9	A	626	CLA	C1C-NC-C4C	-2.10	103.66	106.07
9	A	627	CLA	C1C-NC-C4C	-2.07	103.70	106.07
9	B	646	CLA	C1C-NC-C4C	-2.06	103.71	106.07
9	B	653	CLA	C1C-NC-C4C	-2.05	103.73	106.07
9	B	651	CLA	C1C-NC-C4C	-2.02	103.76	106.07
9	B	630	CLA	C1C-NC-C4C	-2.01	103.77	106.07
9	B	639	CLA	C2B-C1B-NB	2.00	111.89	110.09
9	A	622	CLA	C2B-C1B-NB	2.01	111.89	110.09
9	B	630	CLA	C2B-C1B-NB	2.01	111.89	110.09
9	B	621	CLA	C3D-C4D-ND	2.01	111.91	110.13
9	B	653	CLA	C3D-C4D-ND	2.02	111.92	110.13
9	B	629	CLA	C3D-C4D-ND	2.02	111.92	110.13
9	B	620	CLA	C2D-C1D-ND	2.02	111.92	110.13
9	B	630	CLA	C3B-C4B-NB	2.02	111.91	110.09
9	B	637	CLA	C3C-C4C-NC	2.03	111.88	110.09
9	B	644	CLA	C3C-C4C-NC	2.03	111.88	110.09
9	B	649	CLA	C3B-C4B-NB	2.03	111.91	110.09
9	B	639	CLA	C3C-C4C-NC	2.03	111.88	110.09
9	F	156	CLA	C3B-C4B-NB	2.03	111.92	110.09
9	B	637	CLA	C3B-C4B-NB	2.04	111.92	110.09
9	A	609	CLA	C2B-C1B-NB	2.05	111.93	110.09
9	A	626	CLA	C2D-C1D-ND	2.05	111.95	110.13
9	B	631	CLA	C3C-C4C-NC	2.07	111.91	110.09
9	F	155	CLA	C3B-C4B-NB	2.08	111.96	110.09
9	A	625	CLA	C3D-C4D-ND	2.08	111.98	110.13
9	A	629	CLA	C3D-C4D-ND	2.09	111.98	110.13
9	B	648	CLA	C3D-C4D-ND	2.09	111.98	110.13
9	A	625	CLA	C3B-C4B-NB	2.09	111.97	110.09
9	B	642	CLA	C2D-C1D-ND	2.10	111.99	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	643	CLA	C3C-C4C-NC	2.10	111.94	110.09
9	A	620	CLA	C3D-C4D-ND	2.10	111.99	110.13
9	L	147	CLA	C2D-C1D-ND	2.10	112.00	110.13
9	A	622	CLA	C3C-C4C-NC	2.11	111.95	110.09
9	A	623	CLA	C3B-C4B-NB	2.12	112.00	110.09
9	A	629	CLA	C2B-C1B-NB	2.12	112.00	110.09
9	F	156	CLA	C3D-C4D-ND	2.13	112.02	110.13
9	B	624	CLA	C2D-C1D-ND	2.13	112.02	110.13
9	F	156	CLA	C2D-C1D-ND	2.15	112.03	110.13
9	B	642	CLA	C3B-C4B-NB	2.15	112.02	110.09
9	A	608	CLA	C3B-C4B-NB	2.16	112.03	110.09
9	B	633	CLA	C3B-C4B-NB	2.19	112.05	110.09
9	A	605	CLA	C3B-C4B-NB	2.19	112.06	110.09
9	B	645	CLA	C3C-C4C-NC	2.19	112.02	110.09
9	A	604	CLA	C2B-C1B-NB	2.20	112.06	110.09
9	A	620	CLA	C2B-C1B-NB	2.20	112.06	110.09
9	A	611	CLA	C2B-C1B-NB	2.21	112.07	110.09
9	B	635	CLA	C2B-C1B-NB	2.21	112.07	110.09
9	L	163	CLA	C2D-C1D-ND	2.22	112.10	110.13
9	B	632	CLA	C3B-C4B-NB	2.25	112.11	110.09
9	B	640	CLA	C3B-C4B-NB	2.26	112.11	110.09
9	A	599	CLA	C3C-C4C-NC	2.26	112.08	110.09
9	B	641	CLA	C2B-C1B-NB	2.26	112.12	110.09
9	B	651	CLA	C2D-C1D-ND	2.26	112.14	110.13
9	A	609	CLA	C2D-C1D-ND	2.28	112.15	110.13
9	L	163	CLA	C3D-C4D-ND	2.28	112.15	110.13
9	L	149	CLA	C3C-C4C-NC	2.28	112.10	110.09
9	A	629	CLA	C3C-C4C-NC	2.28	112.10	110.09
9	L	149	CLA	C2D-C1D-ND	2.32	112.18	110.13
9	A	611	CLA	C3D-C4D-ND	2.32	112.19	110.13
9	A	610	CLA	C3C-C4C-NC	2.36	112.16	110.09
9	B	625	CLA	C3C-C4C-NC	2.40	112.20	110.09
9	A	628	CLA	C2B-C1B-NB	2.41	112.26	110.09
9	B	620	CLA	C2B-C1B-NB	2.45	112.29	110.09
9	B	645	CLA	C2B-C1B-NB	2.45	112.29	110.09
9	A	612	CLA	C2D-C1D-ND	2.45	112.31	110.13
9	K	135	CLA	C2D-C1D-ND	2.48	112.33	110.13
9	A	628	CLA	C2D-C1D-ND	2.54	112.38	110.13
9	A	618	CLA	C2A-C1A-CHA	2.56	127.11	122.58
9	A	614	CLA	C2A-C1A-CHA	2.59	127.16	122.58
9	B	641	CLA	C3D-C4D-ND	2.59	112.43	110.13
9	F	158	CLA	C2A-C1A-CHA	2.60	127.18	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	626	CLA	C3D-C4D-ND	2.61	112.44	110.13
9	A	615	CLA	C2A-C1A-CHA	2.61	127.20	122.58
9	A	617	CLA	C2A-C1A-CHA	2.62	127.22	122.58
9	B	636	CLA	C3C-C4C-NC	2.63	112.40	110.09
9	A	605	CLA	C2B-C1B-NB	2.70	112.51	110.09
9	B	652	CLA	C3C-C4C-NC	2.73	112.50	110.09
9	B	635	CLA	C2D-C1D-ND	2.77	112.58	110.13
9	B	628	CLA	C3C-C4C-NC	2.83	112.58	110.09
9	A	612	CLA	C2B-C1B-NB	2.90	112.70	110.09
9	B	640	CLA	C2D-C1D-ND	3.16	112.93	110.13
9	A	612	CLA	C3C-C4C-NC	3.19	112.90	110.09
9	A	612	CLA	C3B-C4B-NB	3.47	113.20	110.09
9	B	640	CLA	C3C-C4C-NC	3.50	113.17	110.09
9	B	635	CLA	C3C-C4C-NC	4.57	114.11	110.09
9	B	635	CLA	C3D-C4D-ND	5.77	115.25	110.13
9	A	612	CLA	C3D-C4D-ND	5.90	115.37	110.13
9	B	640	CLA	C3D-C4D-ND	5.96	115.42	110.13

All (201) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	635	CLA	NC
9	B	635	CLA	ND
9	B	635	CLA	NA
9	F	154	CLA	NC
9	F	154	CLA	ND
9	F	154	CLA	NA
9	B	652	CLA	NC
9	B	652	CLA	ND
9	B	652	CLA	NA
9	B	625	CLA	NC
9	B	625	CLA	ND
9	B	625	CLA	NA
9	B	641	CLA	NC
9	B	641	CLA	ND
9	B	641	CLA	NA
9	B	624	CLA	NC
9	B	624	CLA	ND
9	B	624	CLA	NA
9	A	598	CLA	NC
9	A	598	CLA	ND
9	A	598	CLA	NA

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Mol	Chain	Res	Type	Atom
9	B	648	CLA	NC
9	B	648	CLA	ND
9	B	648	CLA	NA
9	A	620	CLA	NC
9	A	620	CLA	ND
9	A	620	CLA	NA
9	A	599	CLA	NC
9	A	599	CLA	ND
9	A	599	CLA	NA
9	A	623	CLA	NC
9	A	623	CLA	ND
9	A	623	CLA	NA
9	B	644	CLA	NC
9	B	644	CLA	ND
9	B	644	CLA	NA
9	A	627	CLA	NC
9	A	627	CLA	ND
9	A	627	CLA	NA
9	A	621	CLA	NC
9	A	621	CLA	ND
9	A	621	CLA	NA
9	L	149	CLA	NC
9	L	149	CLA	ND
9	L	149	CLA	NA
9	F	155	CLA	NC
9	F	155	CLA	ND
9	F	155	CLA	NA
9	B	651	CLA	NC
9	B	651	CLA	ND
9	B	651	CLA	NA
9	B	643	CLA	NC
9	B	643	CLA	ND
9	B	643	CLA	NA
9	B	642	CLA	NC
9	B	642	CLA	ND
9	B	642	CLA	NA
9	A	600	CLA	NC
9	A	600	CLA	ND
9	A	600	CLA	NA
9	B	646	CLA	NC
9	B	646	CLA	ND
9	B	646	CLA	NA

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Mol	Chain	Res	Type	Atom
9	B	631	CLA	NC
9	B	631	CLA	ND
9	B	631	CLA	NA
9	A	616	CLA	NC
9	A	616	CLA	ND
9	A	616	CLA	NA
9	K	135	CLA	NC
9	K	135	CLA	ND
9	K	135	CLA	NA
9	F	157	CLA	NC
9	F	157	CLA	ND
9	F	157	CLA	NA
9	A	619	CLA	NC
9	A	619	CLA	ND
9	A	619	CLA	NA
9	F	156	CLA	NC
9	F	156	CLA	ND
9	F	156	CLA	NA
9	A	613	CLA	NC
9	A	613	CLA	ND
9	A	613	CLA	NA
9	A	608	CLA	NC
9	A	608	CLA	ND
9	A	608	CLA	NA
9	A	606	CLA	NC
9	A	606	CLA	ND
9	A	606	CLA	NA
9	B	640	CLA	NC
9	B	640	CLA	ND
9	B	640	CLA	NA
9	B	634	CLA	NC
9	B	634	CLA	ND
9	B	634	CLA	NA
9	B	630	CLA	NC
9	B	630	CLA	ND
9	B	630	CLA	NA
9	B	639	CLA	NC
9	B	639	CLA	ND
9	B	639	CLA	NA
9	B	645	CLA	NC
9	B	645	CLA	ND
9	B	645	CLA	NA

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Mol	Chain	Res	Type	Atom
9	B	626	CLA	NC
9	B	626	CLA	ND
9	B	626	CLA	NA
9	B	649	CLA	NC
9	B	649	CLA	ND
9	B	649	CLA	NA
9	A	609	CLA	NC
9	A	609	CLA	ND
9	A	609	CLA	NA
9	A	612	CLA	NC
9	A	612	CLA	ND
9	A	612	CLA	NA
9	B	636	CLA	NC
9	B	636	CLA	ND
9	B	636	CLA	NA
9	B	621	CLA	NC
9	B	621	CLA	ND
9	B	621	CLA	NA
9	B	637	CLA	NC
9	B	637	CLA	ND
9	B	637	CLA	NA
9	B	632	CLA	NC
9	B	632	CLA	ND
9	B	632	CLA	NA
9	B	633	CLA	NC
9	B	633	CLA	ND
9	B	633	CLA	NA
9	B	653	CLA	NC
9	B	653	CLA	ND
9	B	653	CLA	NA
9	A	624	CLA	NC
9	A	624	CLA	ND
9	A	624	CLA	NA
9	A	625	CLA	NC
9	A	625	CLA	ND
9	A	625	CLA	NA
9	B	647	CLA	NC
9	B	647	CLA	ND
9	B	647	CLA	NA
9	B	629	CLA	NC
9	B	629	CLA	ND
9	B	629	CLA	NA

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Mol	Chain	Res	Type	Atom
9	B	620	CLA	NC
9	B	620	CLA	ND
9	B	620	CLA	NA
9	A	611	CLA	NC
9	A	611	CLA	ND
9	A	611	CLA	NA
9	A	610	CLA	NC
9	A	610	CLA	ND
9	A	610	CLA	NA
9	L	147	CLA	NC
9	L	147	CLA	ND
9	L	147	CLA	NA
9	A	604	CLA	NC
9	A	604	CLA	ND
9	A	604	CLA	NA
9	B	622	CLA	NC
9	B	622	CLA	ND
9	B	622	CLA	NA
9	B	650	CLA	NC
9	B	650	CLA	ND
9	B	650	CLA	NA
9	B	628	CLA	NC
9	B	628	CLA	ND
9	B	628	CLA	NA
9	A	605	CLA	NC
9	A	605	CLA	ND
9	A	605	CLA	NA
9	A	622	CLA	NC
9	A	622	CLA	ND
9	A	622	CLA	NA
9	B	638	CLA	NC
9	B	638	CLA	ND
9	B	638	CLA	NA
9	L	163	CLA	NC
9	L	163	CLA	ND
9	L	163	CLA	NA
9	B	627	CLA	NC
9	B	627	CLA	ND
9	B	627	CLA	NA
9	A	603	CLA	NC
9	A	603	CLA	ND
9	A	603	CLA	NA

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Mol	Chain	Res	Type	Atom
9	A	628	CLA	NC
9	A	628	CLA	ND
9	A	628	CLA	NA
9	A	626	CLA	NC
9	A	626	CLA	ND
9	A	626	CLA	NA
9	A	607	CLA	NC
9	A	607	CLA	ND
9	A	607	CLA	NA
9	A	629	CLA	NC
9	A	629	CLA	ND
9	A	629	CLA	NA

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	600	CLA	1	0
9	A	612	CLA	1	0
9	A	628	CLA	6	0
9	A	629	CLA	6	0
9	B	627	CLA	5	0
9	B	629	CLA	4	0
9	B	636	CLA	4	0
9	B	641	CLA	13	0
11	C	78	SF4	1	0
11	C	79	SF4	1	0
9	K	135	CLA	13	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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.