wwPDB X-ray Structure Validation Summary 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)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

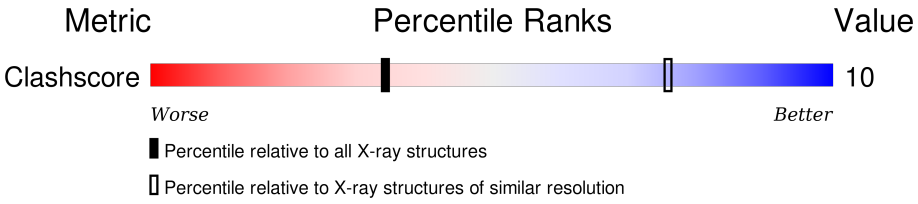
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

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 C 153 153	0	0	153

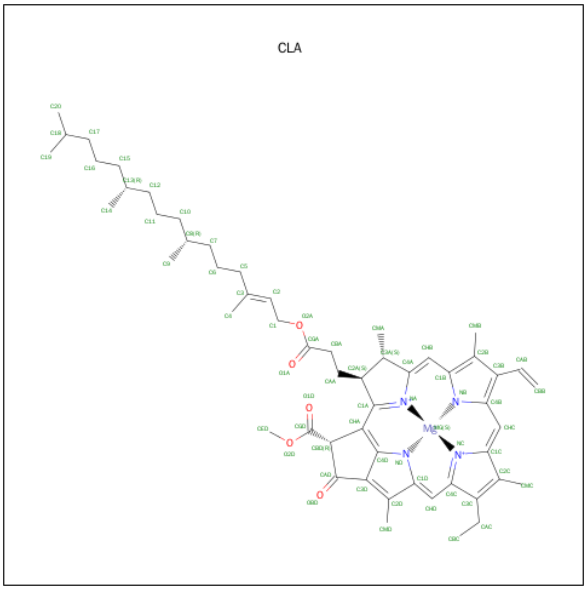
- Molecule 7 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAK).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	K	78	Total C 78 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 C 120 120	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 C Mg N 25 20 1 4	0	0
9	A	1	Total C Mg N 25 20 1 4	0	0
9	B	1	Total C Mg N 25 20 1 4	0	0
9	B	1	Total C Mg N 25 20 1 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	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	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	F	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	K	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	F	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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	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	L	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	L	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	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	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		
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		

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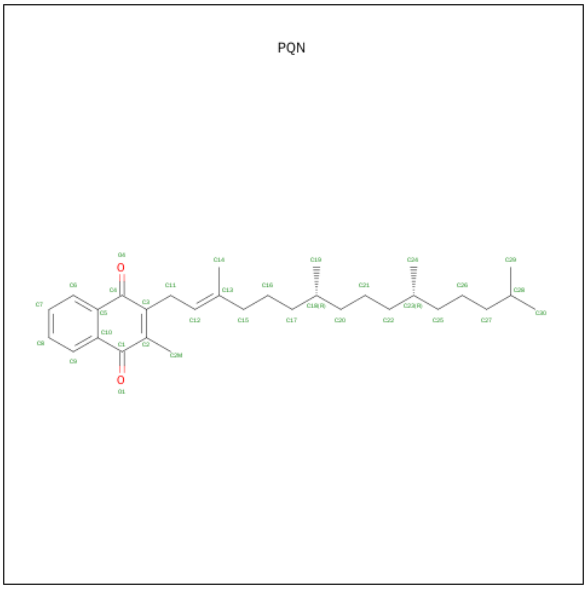
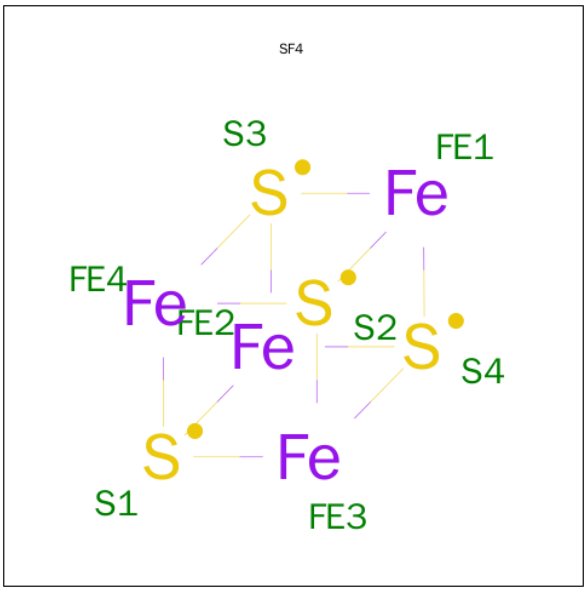
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C Mg N 25 20 1 4	0	0
9	L	1	Total C Mg N 25 20 1 4	0	0
9	B	1	Total C Mg N 25 20 1 4	0	0
9	A	1	Total C Mg N 25 20 1 4	0	0
9	A	1	Total C Mg N 25 20 1 4	0	0

- 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 2 2	0	0
10	B	1	Total C 2 2	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Fe S 8 4 4	0	0
11	C	1	Total Fe S 8 4 4	0	0
11	C	1	Total Fe S 8 4 4	0	0

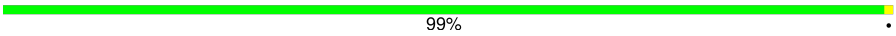
3 Residue-property plots (i)

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.

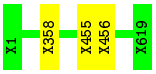
- Molecule 1: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAA)

Chain A:



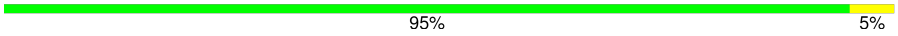
- Molecule 2: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAB)

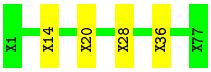
Chain B:



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

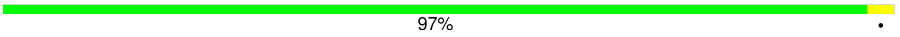
Chain C:





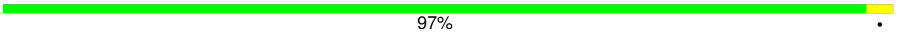
- Molecule 4: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAD)

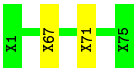
Chain D:



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

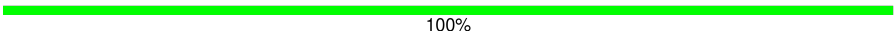
Chain E:





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

Chain F:



There are no outlier residues recorded for this chain.

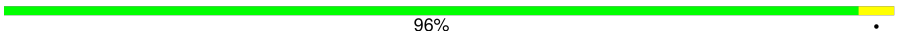
• Molecule 7: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAK)

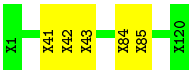
Chain K:

There are no outlier residues recorded for this chain.

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

Chain L:





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

5.1 Standard geometry

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

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.

The worst 5 of 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

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

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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

5.3.3 RNA

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	L	163	-	3/3/7/25	0/0/66/135	0/0/8/9

The worst 5 of 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

The worst 5 of 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

5 of 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

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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