



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:54 am GMT

PDB ID : 2PPS  
Title : PHOTOSYNTHETIC REACTION CENTER AND CORE ANTENNA SYSTEM (TRIMERIC), ALPHA CARBON ONLY  
Authors : Krauss, N.; Schubert, W.-D.; Klukas, O.; Fromme, P.; Witt, H.T.; Saenger, W.  
Deposited on : 1997-05-27  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

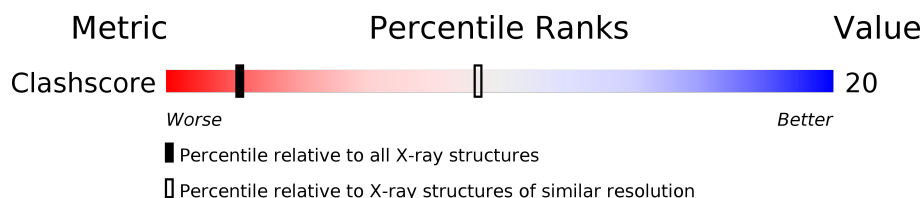
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

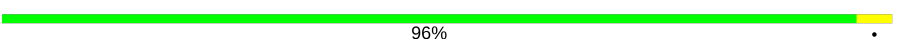
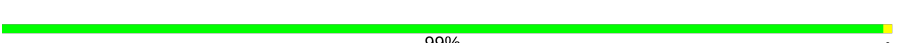

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1187 (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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	 96% .
2	B	503	 96% .
3	L	111	 100%
4	K	64	 95% 5%
5	F	130	 99% .
6	C	80	 93% 8%

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
7	CLA	A	2001	X	-	-	-
7	CLA	A	2006	X	-	-	-
7	CLA	A	2502	X	-	-	-
7	CLA	A	3005	X	-	-	-
7	CLA	A	3007	X	-	-	-
7	CLA	A	3009	X	-	-	-
7	CLA	A	3013	X	-	-	-
7	CLA	A	3016	X	-	-	-
7	CLA	A	3017	X	-	-	-
7	CLA	A	3018	X	-	-	-
7	CLA	A	3021	X	-	-	-
7	CLA	A	3024	X	-	-	-
7	CLA	A	3026	X	-	-	-
7	CLA	A	3027	X	-	-	-
7	CLA	A	3029	X	-	-	-
7	CLA	A	3030	X	-	-	-
7	CLA	A	3032	X	-	-	-
7	CLA	A	3039	X	-	-	-
7	CLA	A	3040	X	-	-	-
7	CLA	A	3041	X	-	-	-
7	CLA	A	3043	X	-	-	-
7	CLA	A	3045	X	-	-	-
7	CLA	A	3047	X	-	-	-
7	CLA	A	3048	X	-	-	-
7	CLA	A	3052	X	-	-	-
7	CLA	A	3053	X	-	-	-
7	CLA	A	3056	X	-	-	-
7	CLA	A	3057	X	-	-	-
7	CLA	A	3058	X	-	-	-
7	CLA	A	3062	X	-	-	-
7	CLA	A	3065	X	-	-	-
7	CLA	A	3067	X	-	-	-
7	CLA	A	3068	X	-	-	-
7	CLA	A	3071	X	-	-	-
7	CLA	A	3072	X	-	-	-
7	CLA	A	3073	X	-	-	-
7	CLA	A	3077	X	-	-	-
7	CLA	A	3078	X	-	-	-
7	CLA	A	3079	X	-	-	-
7	CLA	B	2002	X	-	-	-
7	CLA	B	2003	X	-	-	-
7	CLA	B	2004	X	-	-	-
7	CLA	B	2005	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CLA	B	2501	X	-	-	-
7	CLA	B	3001	X	-	-	-
7	CLA	B	3003	X	-	-	-
7	CLA	B	3006	X	-	-	-
7	CLA	B	3008	X	-	-	-
7	CLA	B	3010	X	-	-	-
7	CLA	B	3011	X	-	-	-
7	CLA	B	3015	X	-	-	-
7	CLA	B	3019	X	-	-	-
7	CLA	B	3020	X	-	-	-
7	CLA	B	3023	X	-	-	-
7	CLA	B	3025	X	-	-	-
7	CLA	B	3028	X	-	-	-
7	CLA	B	3034	X	-	-	-
7	CLA	B	3035	X	-	-	-
7	CLA	B	3037	X	-	-	-
7	CLA	B	3042	X	-	-	-
7	CLA	B	3044	X	-	-	-
7	CLA	B	3046	X	-	-	-
7	CLA	B	3055	X	-	-	-
7	CLA	B	3060	X	-	-	-
7	CLA	B	3063	X	-	-	-
7	CLA	B	3066	X	-	-	-
7	CLA	B	3069	X	-	-	-
7	CLA	B	3070	X	-	-	-
7	CLA	B	3074	X	-	-	-
7	CLA	B	3075	X	-	-	-
7	CLA	B	3076	X	-	-	-
7	CLA	B	3080	X	-	-	-
7	CLA	B	3081	X	-	-	-
7	CLA	F	3002	X	-	-	-
7	CLA	F	3004	X	-	-	-
7	CLA	F	3012	X	-	-	-
7	CLA	F	3022	X	-	-	-
7	CLA	F	3031	X	-	-	-
7	CLA	F	3033	X	-	-	-
7	CLA	F	3054	X	-	-	-
7	CLA	F	3059	X	-	-	-
7	CLA	F	3061	X	-	-	-
7	CLA	K	3050	X	-	-	-
7	CLA	K	3051	X	-	-	-
7	CLA	L	3036	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CLA	L	3038	X	-	-	-
7	CLA	L	3049	X	-	-	-
9	SF4	B	2008	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3616 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 PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	478	Total C 478 478	0	0	478

- Molecule 2 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	503	Total C 503 503	0	0	503

- Molecule 3 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	L	111	Total C 111 111	0	0	111

- Molecule 4 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	K	64	Total C 64 64	0	0	64

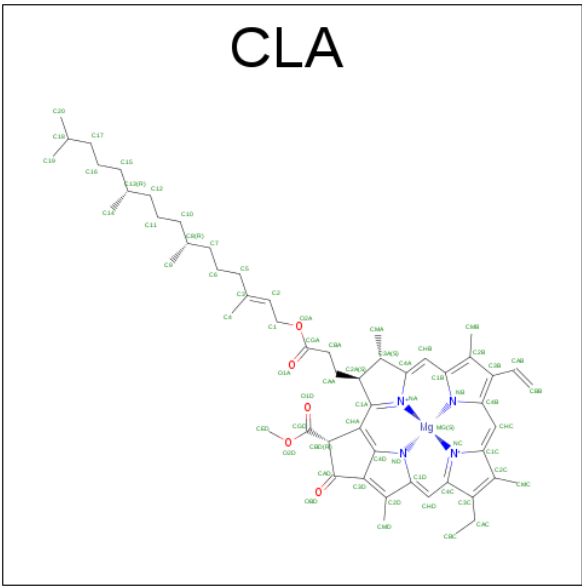
- Molecule 5 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	130	Total C 130 130	0	0	130

- Molecule 6 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	C	80	Total C 80 80	0	0	80

- Molecule 7 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
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
	B	1	Total	C	Mg	N		
			25	20	1	4		
	B	1	Total	C	Mg	N		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
	B	1	Total	C	Mg	N		
			25	20	1	4		
	B	1	Total	C	Mg	N		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
	B	1	Total	C	Mg	N		
			25	20	1	4		
	B	1	Total	C	Mg	N		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
	B	1	Total	C	Mg	N		
			25	20	1	4		
	B	1	Total	C	Mg	N		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
	B	1	Total	C	Mg	N		
			25	20	1	4		
	B	1	Total	C	Mg	N		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
	A	1	Total	C	Mg	N		
			25	20	1	4		
	A	1	Total	C	Mg	N		

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

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

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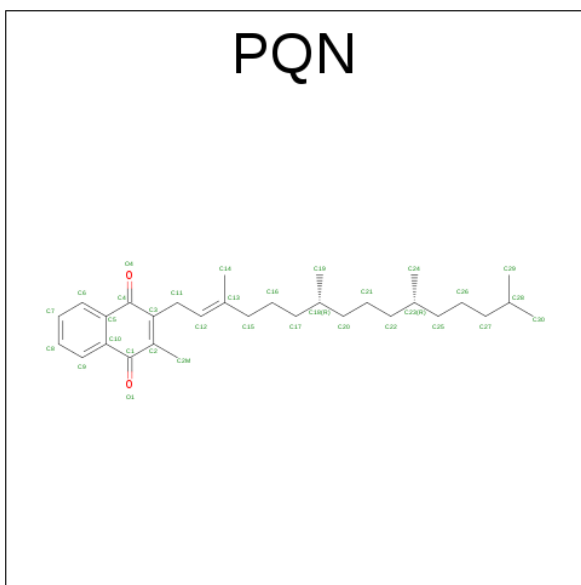
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 25	C 20	Mg 1	N 4	0	0
7	L	1	Total 25	C 20	Mg 1	N 4	0	0
7	K	1	Total 25	C 20	Mg 1	N 4	0	0
7	K	1	Total 25	C 20	Mg 1	N 4	0	0
7	A	1	Total 25	C 20	Mg 1	N 4	0	0
7	A	1	Total 25	C 20	Mg 1	N 4	0	0
7	F	1	Total 25	C 20	Mg 1	N 4	0	0
7	B	1	Total 25	C 20	Mg 1	N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

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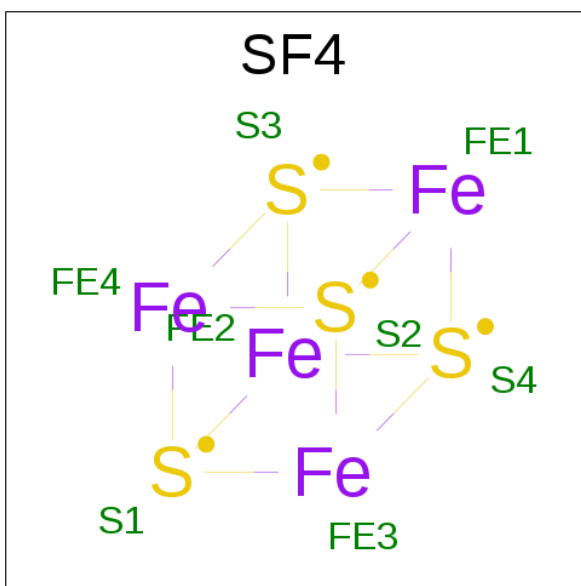
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25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

- Molecule 8 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 1 1	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



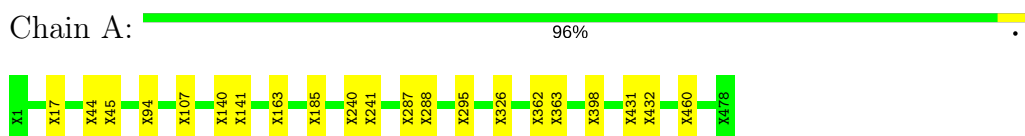
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0

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

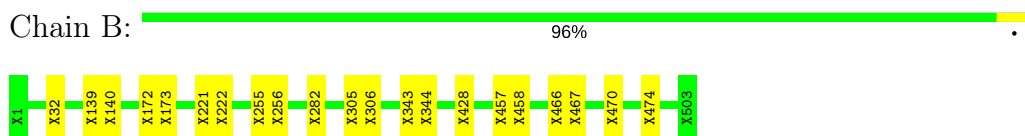
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: PHOTOSYSTEM I



- Molecule 2: PHOTOSYSTEM I

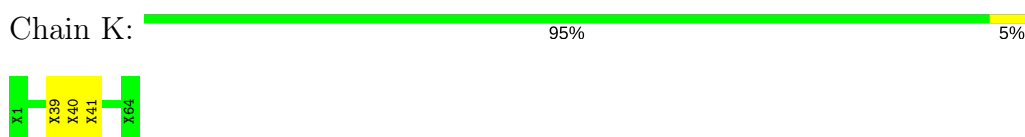


- Molecule 3: PHOTOSYSTEM I

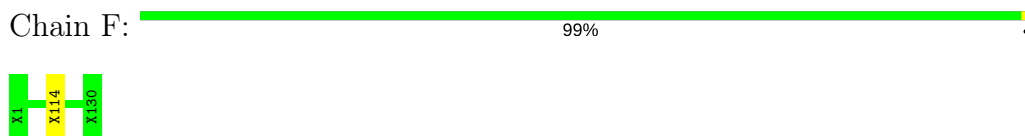


There are no outlier residues recorded for this chain.

- Molecule 4: PHOTOSYSTEM I



- Molecule 5: PHOTOSYSTEM I



- Molecule 6: PHOTOSYSTEM I



X4	X6	X7	X8	X9	X67	X68	X80
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.00Å 286.00Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	?	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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	478	0	0	16	0
2	B	503	0	0	16	0
3	L	111	0	0	0	0
4	K	64	0	0	2	0
5	F	130	0	0	1	0
6	C	80	0	0	4	0
7	A	1000	0	120	41	0
7	B	850	0	102	12	0
7	F	225	0	27	8	0
7	K	50	0	6	0	0
7	L	100	0	12	0	0
8	B	1	0	0	0	0
9	B	8	0	0	3	0
9	C	16	0	0	0	0
All	All	3616	0	267	78	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 20.

The worst 5 of 78 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)
7:A:3014:CLA:HHC	7:A:3029:CLA:C3D	1.61	1.31
1:A:94:UNK:CA	1:A:107:UNK:CA	2.11	1.29
2:B:470:UNK:CA	2:B:474:UNK:CA	2.12	1.27
1:A:295:UNK:CA	7:A:3016:CLA:C3C	2.19	1.20
2:B:428:UNK:CA	7:B:2005:CLA:C3A	2.20	1.20

There are no symmetry-related clashes.

## 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

Of 93 ligands modelled in this entry, 1 is modelled with single atom - leaving 92 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLA	A	2001	-	17,32,73	3.21	7 (41%)	24,54,113	2.39	8 (33%)
7	CLA	A	2006	-	17,32,73	3.19	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	A	2502	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3005	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3007	-	17,32,73	3.21	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	A	3009	-	17,32,73	3.17	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	A	3013	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3014	-	17,32,73	2.52	7 (41%)	24,54,113	2.72	8 (33%)
7	CLA	A	3016	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3017	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3018	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3021	-	17,32,73	3.19	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3024	-	17,32,73	3.19	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	A	3026	-	17,32,73	3.20	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	A	3027	-	17,32,73	3.19	7 (41%)	24,54,113	2.43	8 (33%)
7	CLA	A	3029	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3030	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3032	-	17,32,73	3.19	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3039	-	17,32,73	3.21	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3040	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3041	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3043	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3045	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3047	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3048	-	17,32,73	3.22	7 (41%)	24,54,113	2.41	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLA	A	3052	-	17,32,73	3.20	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	A	3053	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3056	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3057	-	17,32,73	3.21	7 (41%)	24,54,113	2.39	8 (33%)
7	CLA	A	3058	-	17,32,73	3.21	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3062	-	17,32,73	3.21	7 (41%)	24,54,113	2.39	8 (33%)
7	CLA	A	3065	-	17,32,73	3.21	7 (41%)	24,54,113	2.39	8 (33%)
7	CLA	A	3067	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3068	-	17,32,73	3.19	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3071	-	17,32,73	3.22	7 (41%)	24,54,113	2.39	8 (33%)
7	CLA	A	3072	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	A	3073	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3077	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3078	-	17,32,73	3.19	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	A	3079	-	17,32,73	3.22	7 (41%)	24,54,113	2.39	8 (33%)
7	CLA	B	2002	-	17,32,73	3.19	7 (41%)	24,54,113	2.43	8 (33%)
7	CLA	B	2003	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	2004	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	2005	-	17,32,73	3.20	7 (41%)	24,54,113	2.42	8 (33%)
9	SF4	B	2008	-	0,12,12	0.00	-	0,24,24	0.00	-
7	CLA	B	2501	-	17,32,73	3.22	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3001	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3003	-	17,32,73	3.20	7 (41%)	24,54,113	2.39	8 (33%)
7	CLA	B	3006	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3008	-	17,32,73	3.18	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	3010	-	17,32,73	3.22	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	3011	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3015	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3019	-	17,32,73	3.21	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	B	3020	-	17,32,73	3.21	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	3023	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	3025	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3028	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3034	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3035	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLA	B	3037	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3042	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3044	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3046	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3055	-	17,32,73	3.19	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	B	3060	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3063	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	3066	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3069	-	17,32,73	3.19	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	3070	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	B	3074	-	17,32,73	3.21	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3075	-	17,32,73	3.18	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3076	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3080	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	B	3081	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
9	SF4	C	2009	-	0,12,12	0.00	-	0,24,24	0.00	-
9	SF4	C	2010	-	0,12,12	0.00	-	0,24,24	0.00	-
7	CLA	F	3002	-	17,32,73	3.22	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	F	3004	-	17,32,73	3.21	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	F	3012	-	17,32,73	3.18	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	F	3022	-	17,32,73	3.20	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	F	3031	-	17,32,73	3.17	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	F	3033	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	F	3054	-	17,32,73	3.23	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	F	3059	-	17,32,73	3.21	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	F	3061	-	17,32,73	3.21	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	K	3050	-	17,32,73	3.20	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	K	3051	-	17,32,73	3.19	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	L	3036	-	17,32,73	3.20	7 (41%)	24,54,113	2.41	8 (33%)
7	CLA	L	3038	-	17,32,73	3.17	7 (41%)	24,54,113	2.40	8 (33%)
7	CLA	L	3049	-	17,32,73	3.17	7 (41%)	24,54,113	2.42	8 (33%)
7	CLA	L	3064	-	17,32,73	2.53	7 (41%)	24,54,113	2.71	8 (33%)

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. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	A	2001	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	2006	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	2502	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3005	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3007	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3009	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3013	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3014	-	-	0/0/66/135	0/0/8/9
7	CLA	A	3016	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3017	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3018	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3021	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3024	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3026	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3027	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3029	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3030	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3032	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3039	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3040	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3041	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3043	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3045	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3047	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3048	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3052	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3053	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3056	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3057	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3058	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3062	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3065	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3067	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3068	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	A	3071	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3072	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3073	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3077	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3078	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	A	3079	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	2002	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	2003	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	2004	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	2005	-	3/3/7/25	0/0/66/135	0/0/8/9
9	SF4	B	2008	-	-	0/0/48/48	0/6/5/5
7	CLA	B	2501	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3003	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3006	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3008	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3010	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3011	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3015	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3019	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3020	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3023	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3025	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3028	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3034	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3035	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3037	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3042	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3044	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3046	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3055	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3060	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3063	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3066	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	B	3069	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3070	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3074	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3075	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3076	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3080	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	B	3081	-	3/3/7/25	0/0/66/135	0/0/8/9
9	SF4	C	2009	-	-	0/0/48/48	0/6/5/5
9	SF4	C	2010	-	-	0/0/48/48	0/6/5/5
7	CLA	F	3002	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3004	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3012	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3022	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3031	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3033	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3054	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3059	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	F	3061	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	K	3050	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	K	3051	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	L	3036	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	L	3038	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	L	3049	-	3/3/7/25	0/0/66/135	0/0/8/9
7	CLA	L	3064	-	-	0/0/66/135	0/0/8/9

The worst 5 of 623 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2501	CLA	C3A-C2A	-6.29	1.35	1.52
7	A	3041	CLA	C3A-C2A	-6.28	1.35	1.52
7	A	3062	CLA	C3A-C2A	-6.27	1.35	1.52
7	F	3059	CLA	C3A-C2A	-6.27	1.35	1.52
7	F	3022	CLA	C3A-C2A	-6.27	1.36	1.52

The worst 5 of 712 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3014	CLA	C3C-C4C-CHD	-6.16	114.48	125.03
7	L	3064	CLA	C3C-C4C-CHD	-6.14	114.53	125.03
7	A	3009	CLA	C2C-C1C-CHC	-5.47	114.40	125.47
7	F	3033	CLA	C2C-C1C-CHC	-5.46	114.42	125.47
7	F	3002	CLA	C2C-C1C-CHC	-5.46	114.43	125.47

5 of 261 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	2003	CLA	NC
7	B	2003	CLA	ND
7	B	2003	CLA	NA
7	B	3044	CLA	NA
7	B	3044	CLA	NC

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3005	CLA	3	0
7	A	3007	CLA	5	0
7	A	3014	CLA	8	0
7	A	3016	CLA	6	0
7	A	3017	CLA	1	0
7	A	3018	CLA	1	0
7	A	3024	CLA	9	0
7	A	3026	CLA	1	0
7	A	3027	CLA	10	0
7	A	3029	CLA	10	0
7	A	3030	CLA	1	0
7	A	3039	CLA	3	0
7	A	3056	CLA	3	0
7	A	3057	CLA	3	0
7	A	3071	CLA	4	0
7	A	3079	CLA	1	0
7	B	2005	CLA	4	0
9	B	2008	SF4	3	0
7	B	3001	CLA	2	0
7	B	3003	CLA	2	0
7	B	3006	CLA	2	0
7	B	3011	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3020	CLA	1	0
7	B	3034	CLA	2	0
7	B	3069	CLA	1	0
7	F	3002	CLA	5	0
7	F	3012	CLA	2	0
7	F	3031	CLA	1	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.