



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2017 – 01:00 PM EST

PDB ID : 2OBD  
Title : Crystal Structure of Cholesteryl Ester Transfer Protein  
Authors : Qiu, X.  
Deposited on : unknown  
Resolution : 2.10 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

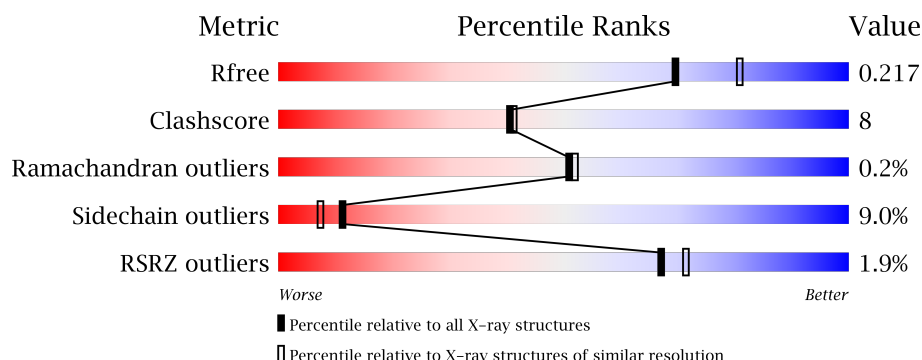
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PG4	A	492	-	-	-	X
7	PCW	A	487	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PCW	A	488	-	-	-	X
9	1PE	A	491	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4465 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.

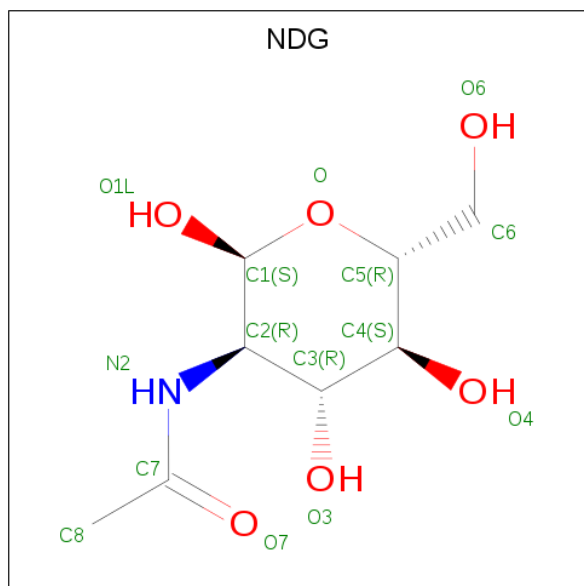
- Molecule 1 is a protein called Cholesteryl ester transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3748	2410	613	708	17	0	6	0

There are 6 discrepancies between the modelled and reference sequences:

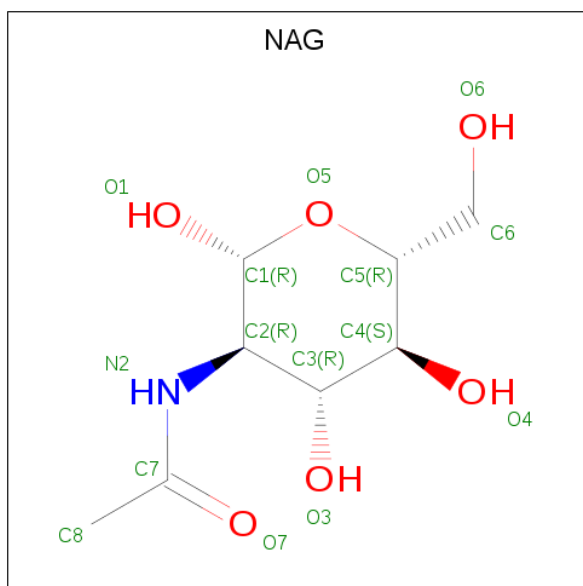
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	ENGINEERED	UNP P11597
A	88	ASP	ASN	ENGINEERED	UNP P11597
A	131	ALA	CYS	ENGINEERED	UNP P11597
A	240	ASP	ASN	ENGINEERED	UNP P11597
A	341	ASP	ASN	ENGINEERED	UNP P11597
A	405	ILE	VAL	ENGINEERED	UNP P11597

- Molecule 2 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



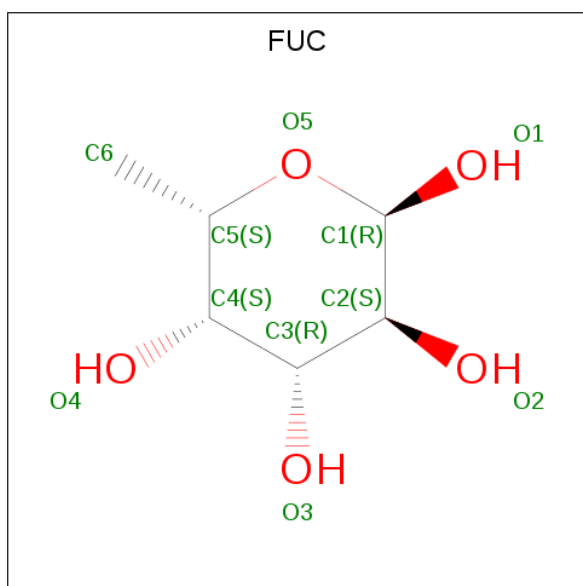
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).

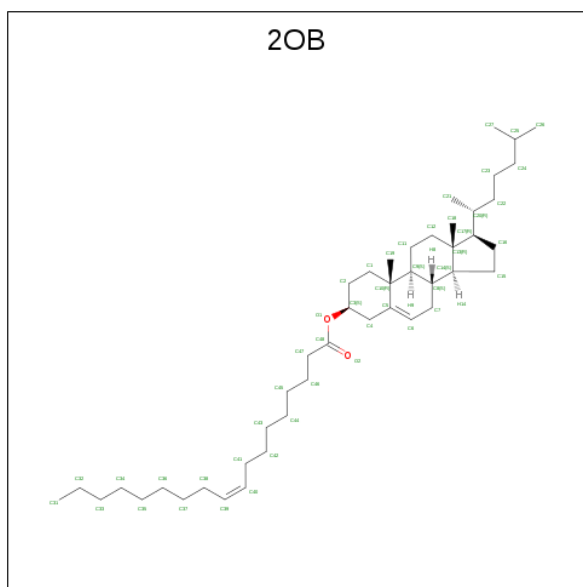


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

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

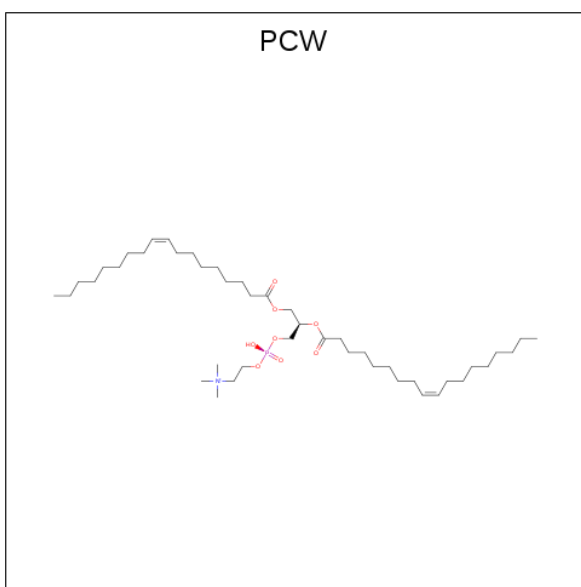
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Cl		0	0
			1	1			

- Molecule 6 is CHOLESTERYL OLEATE (three-letter code: 2OB) (formula: C<sub>45</sub>H<sub>78</sub>O<sub>2</sub>).



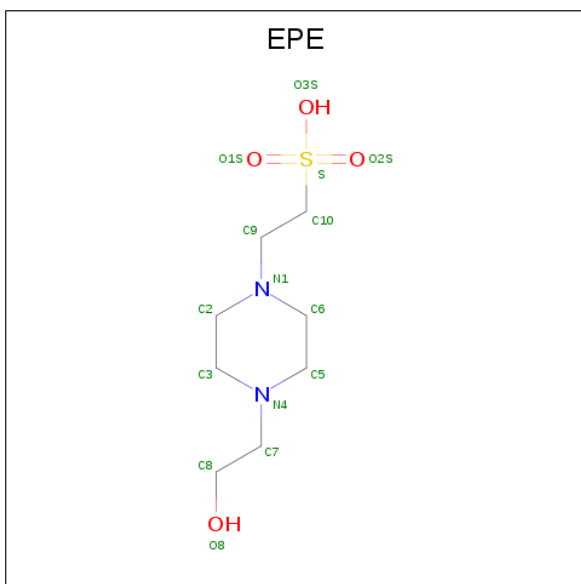
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			47	45	2		
6	A	1	Total	C	O	0	0
			47	45	2		

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



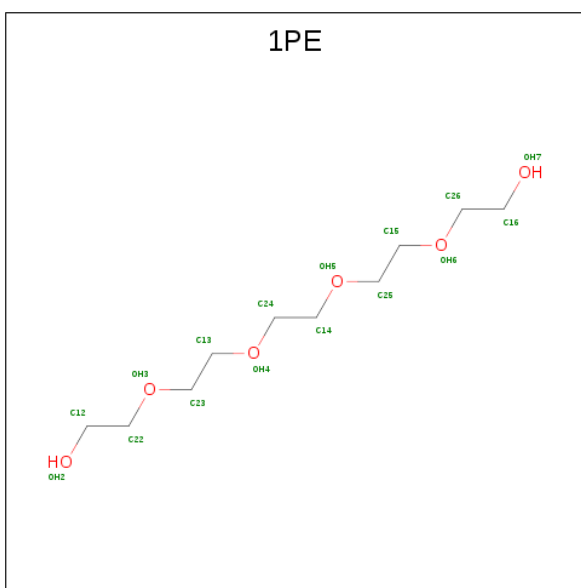
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
7	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



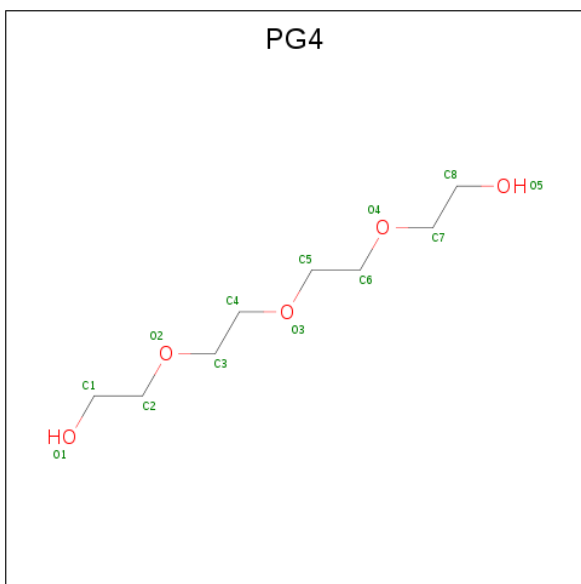
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			16	10	6		
9	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			13	8	5		



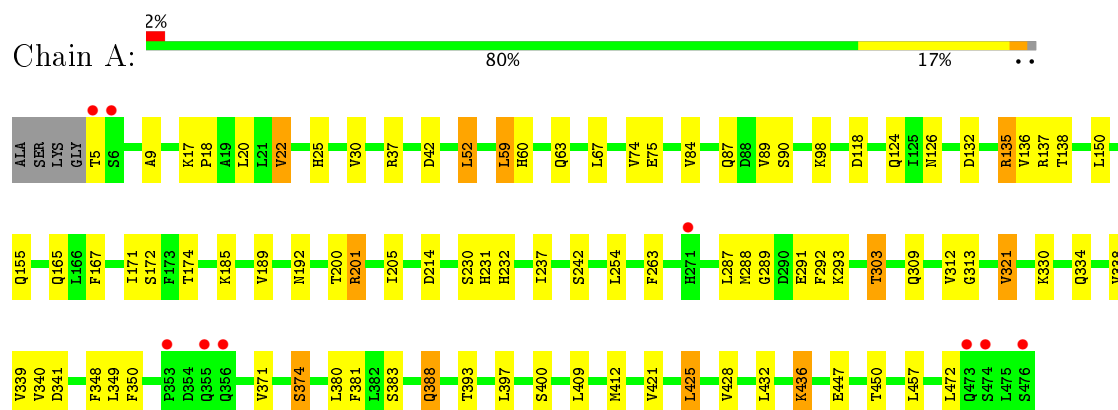
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	416	Total 416	O 416	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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cholesteryl ester transfer protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.78Å 70.32Å 187.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.88 – 2.10 46.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	82.0 (46.88-2.10) 82.0 (46.89-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.217 , 0.265 0.214 , 0.217	Depositor DCC
$R_{free}$ test set	2170 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, 2OB, PCW, NDG, 1PE, PG4, FUC, EPE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	0/3848	0.72	1/5216 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	52	LEU	CA-CB-CG	5.37	127.65	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3748	0	3754	63	0
2	A	14	0	13	0	0
3	A	14	0	11	0	0
4	A	10	0	10	0	0
5	A	1	0	0	0	0
6	A	94	0	156	5	0
7	A	108	0	168	18	0
8	A	15	0	18	0	0
9	A	32	0	44	2	0
10	A	13	0	18	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	416	0	0	9	0
All	All	4465	0	4192	68	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 8.

The worst 5 of 68 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLN:HE21	1:A:126:ASN:HD21	1.05	0.93
1:A:135:ARG:HH12	1:A:200[B]:THR:HG23	1.43	0.82
1:A:291[A]:GLU:HG3	11:A:690:HOH:O	1.85	0.76
1:A:201:ARG:HG2	7:A:487:PCW:H122	1.72	0.72
1:A:287:LEU:HD22	1:A:291[A]:GLU:HG2	1.73	0.71

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	476/476 (100%)	465 (98%)	10 (2%)	1 (0%)	51 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	428/424 (101%)	388 (91%)	40 (9%)	10 7

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165[B]	GLN
1	A	230	SER
1	A	409	LEU
1	A	189	VAL
1	A	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	GLN
1	A	334	GLN
1	A	388	GLN
1	A	192	ASN
1	A	357	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z  > 2$
2	NDG	A	481	3	14,14,15	0.79	1 (7%)	15,19,21	2.20	5 (33%)
3	NAG	A	482	1,2,4	14,14,15	0.59	0	15,19,21	1.57	2 (13%)
4	FUC	A	483	3	9,10,11	0.31	0	13,14,16	0.64	0
6	2OB	A	485	-	50,50,50	0.76	1 (2%)	68,68,68	1.13	5 (7%)
6	2OB	A	486	-	50,50,50	0.67	1 (2%)	68,68,68	1.31	9 (13%)
7	PCW	A	487	-	53,53,53	1.22	4 (7%)	58,61,61	0.93	3 (5%)
7	PCW	A	488	-	53,53,53	1.22	4 (7%)	58,61,61	1.16	6 (10%)
8	EPE	A	489	-	15,15,15	1.90	1 (6%)	18,20,20	1.44	2 (11%)
9	1PE	A	490	-	15,15,15	0.54	0	14,14,14	0.19	0
9	1PE	A	491	-	15,15,15	0.50	0	14,14,14	0.31	0
10	PG4	A	492	-	12,12,12	0.46	0	11,11,11	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	A	481	3	-	0/6/23/26	0/1/1/1
3	NAG	A	482	1,2,4	-	0/6/23/26	0/1/1/1
4	FUC	A	483	3	-	0/0/17/20	0/1/1/1
6	2OB	A	485	-	-	0/31/89/89	0/4/4/4
6	2OB	A	486	-	-	0/31/89/89	0/4/4/4
7	PCW	A	487	-	-	1/57/57/57	0/0/0/0
7	PCW	A	488	-	-	0/57/57/57	0/0/0/0
8	EPE	A	489	-	-	0/9/19/19	0/1/1/1
9	1PE	A	490	-	-	0/13/13/13	0/0/0/0
9	1PE	A	491	-	-	0/13/13/13	0/0/0/0
10	PG4	A	492	-	-	0/10/10/10	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	489	EPE	C10-S	-6.96	1.67	1.77
7	A	487	PCW	P-O2P	2.52	1.60	1.50
2	A	481	NDG	C1-C2	2.63	1.56	1.52
7	A	488	PCW	P-O2P	2.65	1.60	1.50
6	A	486	2OB	O1-C48	3.43	1.44	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	482	NAG	O5-C1-C2	-3.72	106.30	111.47
6	A	486	2OB	C21-C20-C22	-3.62	104.64	110.35
6	A	486	2OB	C4-C5-C6	-3.09	115.87	120.59
6	A	486	2OB	C8-C7-C6	-2.70	108.66	112.74
7	A	488	PCW	O3-C11-O11	-2.61	117.07	123.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	487	PCW	P-O3P-C1-C2

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	485	2OB	2	0
6	A	486	2OB	3	0
7	A	487	PCW	10	0
7	A	488	PCW	8	0
9	A	490	1PE	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	472/476 (99%)	-0.07	9 (1%) 67 71	29, 41, 58, 82	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	SER	6.4
1	A	5	THR	4.8
1	A	473	GLN	3.2
1	A	355	GLN	2.6
1	A	353	PRO	2.5

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	PG4	A	492	13/13	0.92	0.25	4.84	65,68,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PCW	A	487	54/54	0.76	0.21	3.35	42,70,99,99	0
7	PCW	A	488	54/54	0.75	0.26	3.23	53,62,85,86	0
9	1PE	A	491	16/16	0.80	0.17	2.24	62,75,78,79	0
6	2OB	A	485	47/47	0.93	0.18	1.91	42,51,59,63	0
6	2OB	A	486	47/47	0.92	0.18	1.57	32,41,50,55	0
4	FUC	A	483	10/11	0.96	0.13	1.49	60,61,63,63	0
8	EPE	A	489	15/15	0.94	0.15	0.39	75,79,82,82	0
5	CL	A	493	1/1	1.00	0.12	-0.66	35,35,35,35	0
9	1PE	A	490	16/16	0.87	0.11	-	66,71,75,75	0
2	NDG	A	481	14/15	0.76	0.32	-	72,73,75,75	0
3	NAG	A	482	14/15	0.86	0.15	-	58,60,65,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.