



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 6, 2021 – 11:36 am BST

PDB ID : 6YX8  
Title : The structure of allophycocyanin from cyanobacterium Nostoc sp. WR13, the C2221 crystal form.  
Authors : Patel, H.M.; Roszak, A.W.; Madamwar, D.; Cogdell, R.J.  
Deposited on : 2020-04-30  
Resolution : 1.83 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

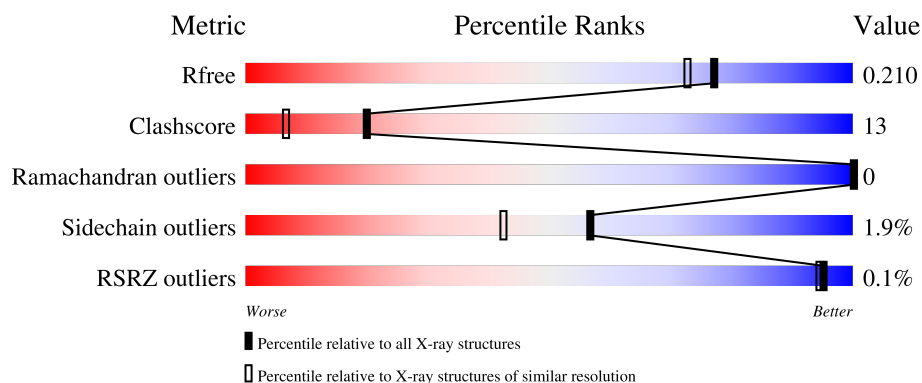
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	AAA	160	
1	CCC	160	
1	EEE	160	
2	BBB	161	
2	DDD	161	

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Mol	Chain	Length	Quality of chain
2	FFF	161	

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	DDD	207	-	-	-	X
10	PG4	EEE	201	-	-	-	X
4	MPD	BBB	204	-	-	-	X
4	MPD	DDD	204	-	-	-	X
4	MPD	FFF	203	-	-	X	-
4	MPD	FFF	204	-	-	-	X
6	1PE	BBB	217	-	-	-	X
7	PGE	EEE	219	-	-	X	-
7	PGE	FFF	210	-	-	-	X
8	PEG	AAA	206[B]	-	-	X	-
8	PEG	AAA	207	-	-	X	X
8	PEG	AAA	208	-	-	X	-
8	PEG	BBB	210	-	-	-	X
8	PEG	CCC	206	-	-	X	-
8	PEG	CCC	211	-	-	-	X
8	PEG	DDD	210	-	-	X	X
8	PEG	EEE	207	-	-	X	X
8	PEG	FFF	211	-	-	-	X
8	PEG	FFF	212	-	-	-	X
8	PEG	FFF	214	-	-	-	X
9	EDO	BBB	212	-	-	-	X
9	EDO	DDD	213	-	-	X	-
9	EDO	EEE	210	-	-	-	X
9	EDO	EEE	211	-	-	-	X
9	EDO	EEE	212	-	-	-	X
9	EDO	EEE	214	-	-	X	-
9	EDO	EEE	216	-	-	-	X
9	EDO	FFF	215	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9412 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.

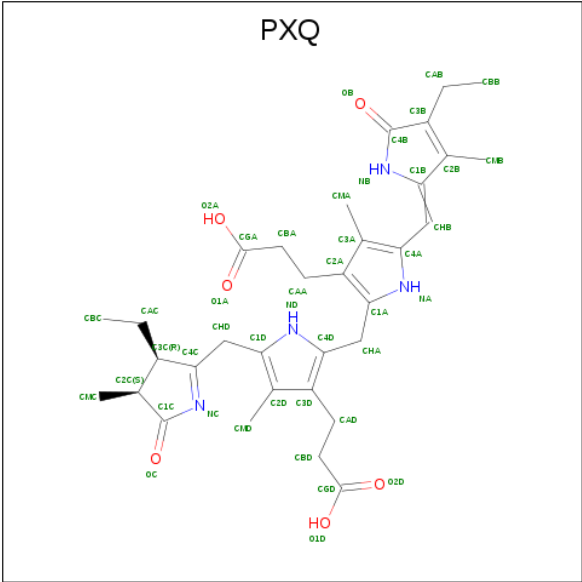
- Molecule 1 is a protein called ALPHA SUBUNIT OF CYANOBACTERIAL ALLOPHYCO-CYANIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	160	Total	C	N	O	S	0	9	0
			1248	784	217	241	6			
1	CCC	160	Total	C	N	O	S	0	8	0
			1243	781	215	241	6			
1	EEE	160	Total	C	N	O	S	0	10	0
			1254	791	220	237	6			

- Molecule 2 is a protein called BETA SUBUNIT OF CYANOBACTERIAL ALLOPHYCO-CYANIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	161	Total	C	N	O	S	0	3	0
			1239	784	208	241	6			
2	DDD	161	Total	C	N	O	S	0	6	0
			1254	793	212	243	6			
2	FFF	161	Total	C	N	O	S	0	13	0
			1280	812	208	254	6			

- Molecule 3 is 3-[5-[(3 {R},4 {R})-3-ethyl-4-methyl-5-oxidanylidene-3,4-dihydropyrrol-2-yl]methyl]-2-[[5-[( {Z})-(4-ethyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1 {H}-pyrrol-2-yl]methyl]-4-methyl-1 {H}-pyrrol-3-yl]propanoic acid (three-letter code: PXQ) (formula: C<sub>33</sub>H<sub>42</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



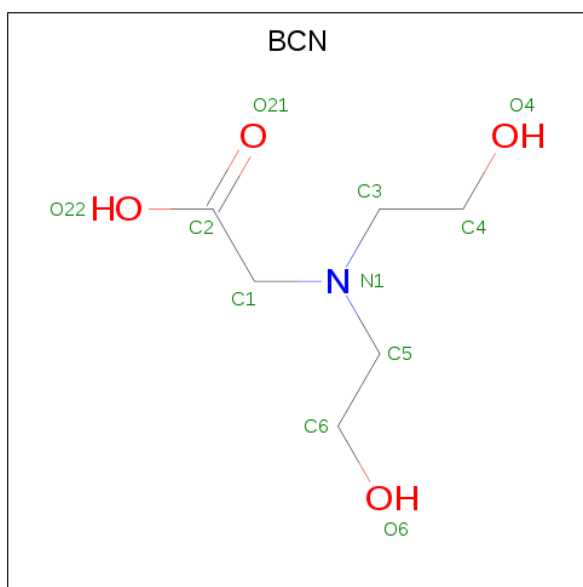
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			43	33	4	6		
3	BBB	1	Total	C	N	O	0	0
			43	33	4	6		
3	CCC	1	Total	C	N	O	0	0
			43	33	4	6		
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



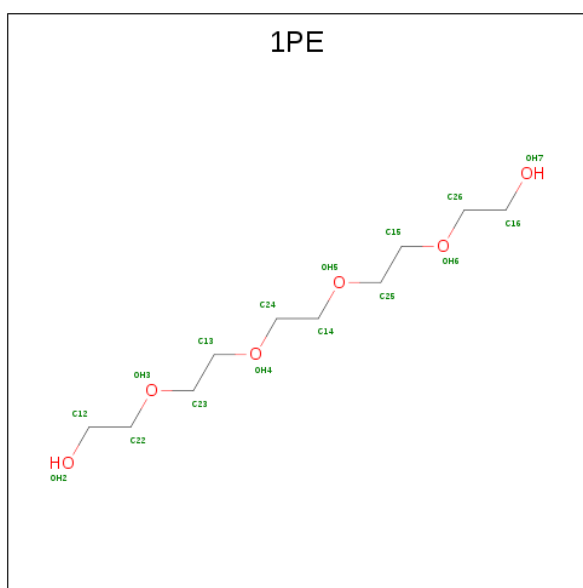
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			8	6	2		
4	BBB	1	Total	C	O	0	0
			8	6	2		
4	BBB	1	Total	C	O	0	0
			8	6	2		
4	BBB	1	Total	C	O	0	0
			8	6	2		
4	CCC	1	Total	C	O	0	0
			8	6	2		
4	DDD	1	Total	C	O	0	0
			8	6	2		
4	DDD	1	Total	C	O	0	0
			8	6	2		
4	DDD	1	Total	C	O	0	0
			8	6	2		
4	FFF	1	Total	C	O	0	0
			8	6	2		
4	FFF	1	Total	C	O	0	0
			8	6	2		
4	FFF	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is BICINE (three-letter code: BCN) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	0	0
			11	6	1	4		
5	DDD	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



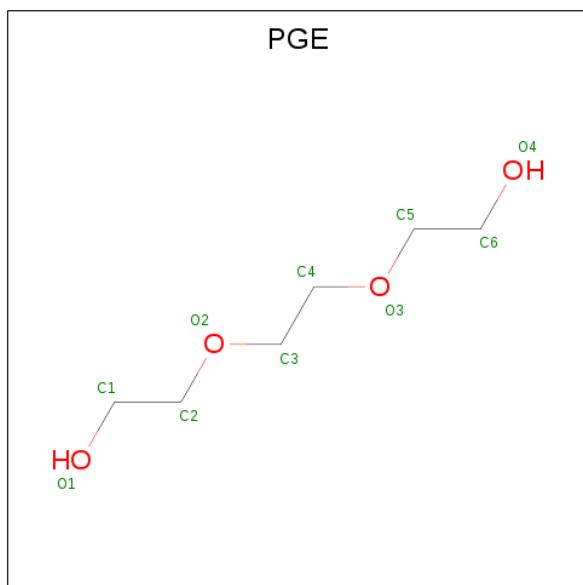
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			16	10	6		
6	BBB	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	C	O	0	0
			16	10	6		
6	BBB	1	Total	C	O	0	0
			16	10	6		
6	FFF	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			10	6	4		
7	AAA	1	Total	C	O	0	0
			10	6	4		
7	BBB	1	Total	C	O	0	0
			10	6	4		
7	BBB	1	Total	C	O	0	0
			10	6	4		
7	CCC	1	Total	C	O	0	0
			10	6	4		
7	EEE	1	Total	C	O	0	0
			10	6	4		
7	EEE	1	Total	C	O	0	0
			10	6	4		
7	FFF	1	Total	C	O	0	0
			10	6	4		

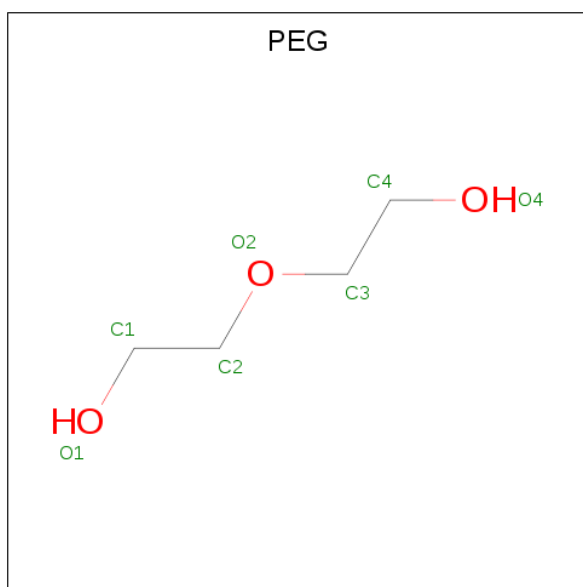
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	FFF	1	Total	C	O	0	0
			10	6	4		
7	FFF	1	Total	C	O	0	0
			10	6	4		
7	FFF	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



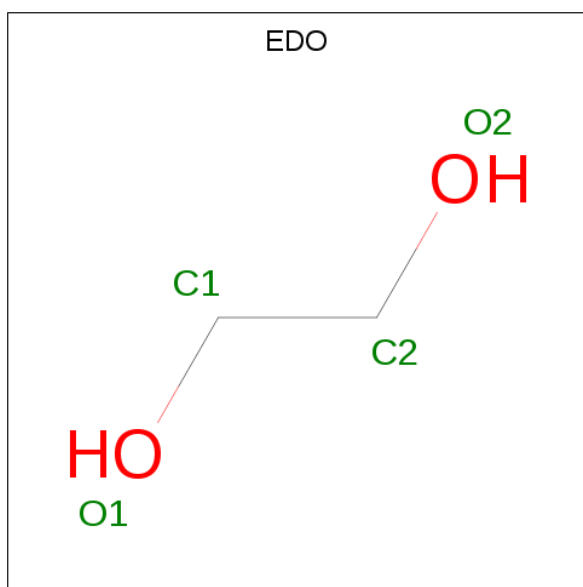
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	1
			14	8	6		
8	AAA	1	Total	C	O	0	0
			7	4	3		
8	AAA	1	Total	C	O	0	0
			7	4	3		
8	AAA	1	Total	C	O	0	0
			7	4	3		
8	BBB	1	Total	C	O	0	0
			7	4	3		
8	BBB	1	Total	C	O	0	0
			7	4	3		
8	BBB	1	Total	C	O	0	0
			7	4	3		
8	CCC	1	Total	C	O	0	1
			14	8	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	CCC	1	Total	C	O	0	0
			7	4	3		
8	CCC	1	Total	C	O	0	0
			7	4	3		
8	CCC	1	Total	C	O	0	0
			7	4	3		
8	CCC	1	Total	C	O	0	0
			7	4	3		
8	DDD	1	Total	C	O	0	0
			7	4	3		
8	DDD	1	Total	C	O	0	0
			7	4	3		
8	DDD	1	Total	C	O	0	0
			7	4	3		
8	EEE	1	Total	C	O	0	0
			7	4	3		
8	EEE	1	Total	C	O	0	0
			7	4	3		
8	EEE	1	Total	C	O	0	0
			7	4	3		
8	FFF	1	Total	C	O	0	0
			7	4	3		
8	FFF	1	Total	C	O	0	0
			7	4	3		
8	FFF	1	Total	C	O	0	0
			7	4	3		
8	FFF	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	AAA	1	Total	C	O	0	1
			8	4	4		
9	AAA	1	Total	C	O	0	0
			4	2	2		
9	AAA	1	Total	C	O	0	0
			4	2	2		
9	AAA	1	Total	C	O	0	0
			4	2	2		
9	AAA	1	Total	C	O	0	0
			4	2	2		
9	BBB	1	Total	C	O	0	0
			4	2	2		
9	BBB	1	Total	C	O	0	0
			4	2	2		
9	BBB	1	Total	C	O	0	0
			4	2	2		
9	BBB	1	Total	C	O	0	0
			4	2	2		
9	CCC	1	Total	C	O	0	0
			4	2	2		
9	CCC	1	Total	C	O	0	0
			4	2	2		
9	CCC	1	Total	C	O	0	0
			4	2	2		

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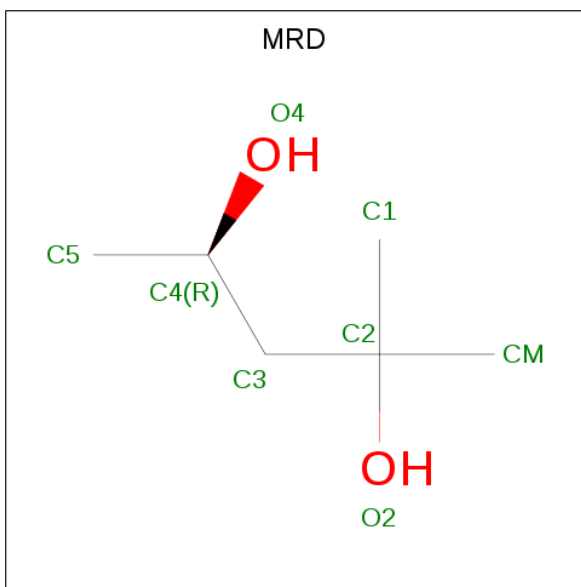
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	DDD	1	Total 4	C 2	O 2	0	0
9	DDD	1	Total 4	C 2	O 2	0	0
9	DDD	1	Total 4	C 2	O 2	0	0
9	DDD	1	Total 8	C 4	O 4	0	1
9	DDD	1	Total 4	C 2	O 2	0	0
9	DDD	1	Total 8	C 4	O 4	0	1
9	DDD	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 8	C 4	O 4	0	1
9	EEE	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 4	C 2	O 2	0	0
9	EEE	1	Total 4	C 2	O 2	0	0
9	FFF	1	Total 4	C 2	O 2	0	0
9	FFF	1	Total 4	C 2	O 2	0	0
9	FFF	1	Total 4	C 2	O 2	0	0
9	FFF	1	Total 4	C 2	O 2	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 11 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	EEE	1	Total	C	O	0	0
			8	6	2		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	AAA	161	Total	O	0	0
			161	161		
12	BBB	220	Total	O	0	0
			220	220		
12	CCC	121	Total	O	0	0
			121	121		
12	DDD	109	Total	O	0	0
			109	109		
12	EEE	155	Total	O	0	0
			155	155		
12	FFF	162	Total	O	0	0
			162	162		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

- Molecule 1: ALPHA SUBUNIT OF CYANOBACTERIAL ALLOPHYCOCYANIN PROTEIN

Chain AAA:  89% 10% .



- Molecule 1: ALPHA SUBUNIT OF CYANOBACTERIAL ALLOPHYCOCYANIN PROTEIN

Chain CCC:  88% 11% .



- Molecule 1: ALPHA SUBUNIT OF CYANOBACTERIAL ALLOPHYCOCYANIN PROTEIN

Chain EEE:  90% 9% .



- Molecule 2: BETA SUBUNIT OF CYANOBACTERIAL ALLOPHYCOCYANIN PROTEIN

Chain BBB:  92% 8% .



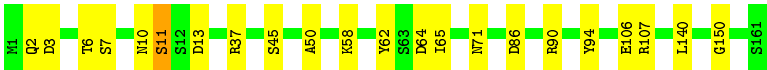
- Molecule 2: BETA SUBUNIT OF CYANOBACTERIAL ALLOPHYCOCYANIN PROTEIN

Chain DDD:  90% 8% .



- Molecule 2: BETA SUBUNIT OF CYANOBACTERIAL ALLOPHYCOCYANIN PROTEIN

Chain FFF:  86% 13% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.68Å 177.34Å 122.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.14 – 1.83 90.14 – 1.83	Depositor EDS
% Data completeness (in resolution range)	87.3 (90.14-1.83) 87.3 (90.14-1.83)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.160 , 0.198 0.174 , 0.210	Depositor DCC
$R_{free}$ test set	4339 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: 1PE, MRD, PGE, BCN, PEG, EDO, PXQ, MPD, PG4, MEN

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	AAA	0.79	0/1290	0.80	0/1741
1	CCC	0.74	0/1282	0.82	1/1731 (0.1%)
1	EEE	0.75	0/1299	0.84	1/1751 (0.1%)
2	BBB	0.77	0/1258	0.82	1/1699 (0.1%)
2	DDD	0.74	0/1279	0.94	4/1728 (0.2%)
2	FFF	0.74	0/1329	0.80	3/1799 (0.2%)
All	All	0.75	0/7737	0.84	10/10449 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	77[A]	ARG	NE-CZ-NH2	-10.23	115.19	120.30
2	DDD	77[B]	ARG	NE-CZ-NH2	-10.23	115.19	120.30
2	DDD	77[A]	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	DDD	77[B]	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	FFF	94	TYR	CB-CG-CD1	5.38	124.23	121.00

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	AAA	1248	0	1280	22	0
1	CCC	1243	0	1270	22	1
1	EEE	1254	0	1306	31	1
2	BBB	1239	0	1268	18	0
2	DDD	1254	0	1285	29	0
2	FFF	1280	0	1319	34	0
3	AAA	43	0	0	1	0
3	BBB	43	0	0	0	0
3	CCC	43	0	0	0	0
3	DDD	43	0	0	1	0
3	EEE	43	0	0	0	0
3	FFF	43	0	0	0	0
4	AAA	8	0	14	0	0
4	BBB	24	0	42	3	0
4	CCC	8	0	14	0	0
4	DDD	24	0	42	5	0
4	FFF	32	0	56	8	0
5	AAA	11	0	12	2	0
5	DDD	11	0	11	5	0
6	AAA	16	0	22	0	0
6	BBB	48	0	66	4	0
6	FFF	16	0	22	0	0
7	AAA	20	0	28	3	0
7	BBB	20	0	28	4	0
7	CCC	10	0	14	0	0
7	EEE	20	0	28	7	0
7	FFF	40	0	56	11	0
8	AAA	35	0	50	15	0
8	BBB	21	0	30	1	0
8	CCC	42	0	60	7	0
8	DDD	21	0	30	11	0
8	EEE	28	0	40	4	0
8	FFF	28	0	40	3	0
9	AAA	28	0	42	0	0
9	BBB	20	0	30	2	0
9	CCC	12	0	18	2	0
9	DDD	36	0	54	8	0
9	EEE	40	0	59	15	0
9	FFF	16	0	24	15	0
10	DDD	39	0	54	10	0
10	EEE	26	0	36	6	0
11	EEE	8	0	14	0	0
12	AAA	161	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	BBB	220	0	0	13	0
12	CCC	121	0	0	2	0
12	DDD	109	0	0	8	0
12	EEE	155	0	0	8	0
12	FFF	162	0	0	8	0
All	All	9412	0	8764	218	1

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 13.

The worst 5 of 218 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)
2:FFF:6[A]:THR:HG22	12:FFF:322:HOH:O	1.13	1.31
2:DDD:39[A]:ARG:NH2	8:DDD:210:PEG:H41	1.48	1.28
8:AAA:206[B]:PEG:H32	12:AAA:302:HOH:O	1.28	1.27
4:DDD:205:MPD:H52	4:DDD:205:MPD:CM	1.51	1.24
4:DDD:205:MPD:HM3	4:DDD:205:MPD:C5	1.56	1.24

All (1) 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)
1:CCC:23:ASP:OD2	1:EEE:24[B]:ARG:NH2[3_555]	2.02	0.18

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	167/160 (104%)	167 (100%)	0	0	100	100
1	CCC	166/160 (104%)	166 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EEE	168/160 (105%)	167 (99%)	1 (1%)	0	100	100
2	BBB	162/161 (101%)	159 (98%)	3 (2%)	0	100	100
2	DDD	164/161 (102%)	161 (98%)	3 (2%)	0	100	100
2	FFF	172/161 (107%)	171 (99%)	1 (1%)	0	100	100
All	All	999/963 (104%)	991 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	131/122 (107%)	130 (99%)	1 (1%)	81	75
1	CCC	130/122 (107%)	124 (95%)	6 (5%)	27	10
1	EEE	132/122 (108%)	129 (98%)	3 (2%)	50	34
2	BBB	129/125 (103%)	128 (99%)	1 (1%)	81	75
2	DDD	131/125 (105%)	125 (95%)	6 (5%)	27	10
2	FFF	139/125 (111%)	137 (99%)	2 (1%)	67	55
All	All	792/741 (107%)	773 (98%)	19 (2%)	57	32

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	24[A]	ARG
2	FFF	11[A]	SER
2	FFF	11[B]	SER
1	EEE	46	ARG
2	DDD	2	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MEN	DDD	71	2	7,8,9	1.73	1 (14%)	6,9,11	2.03	1 (16%)
2	MEN	BBB	71	2	7,8,9	0.58	0	6,9,11	0.47	0
2	MEN	FFF	71	2	7,8,9	0.80	0	6,9,11	1.11	1 (16%)

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	MEN	DDD	71	2	-	2/7/8/10	-
2	MEN	BBB	71	2	-	2/7/8/10	-
2	MEN	FFF	71	2	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	71	MEN	CB-CG	3.91	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	71	MEN	OD1-CG-CB	4.52	128.11	121.50
2	FFF	71	MEN	CB-CG-ND2	2.52	118.88	115.48

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	71	MEN	CA-CB-CG-OD1
2	FFF	71	MEN	CA-CB-CG-OD1
2	BBB	71	MEN	CA-CB-CG-ND2
2	DDD	71	MEN	CA-CB-CG-ND2
2	FFF	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	71	MEN	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

105 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	$\# Z  > 2$
7	PGE	CCC	204	-	9,9,9	0.14	0	8,8,8	0.09	0
9	EDO	FFF	215	-	3,3,3	0.51	0	2,2,2	0.36	0
9	EDO	BBB	215	-	3,3,3	0.11	0	2,2,2	0.22	0
9	EDO	FFF	218	-	3,3,3	0.39	0	2,2,2	0.69	0
6	1PE	FFF	206	-	15,15,15	0.40	0	14,14,14	0.45	0
8	PEG	BBB	210	-	6,6,6	0.11	0	5,5,5	0.07	0
9	EDO	EEE	217	-	3,3,3	0.11	0	2,2,2	0.23	0
8	PEG	AAA	206[B]	-	6,6,6	0.24	0	5,5,5	0.14	0
9	EDO	AAA	210[B]	-	3,3,3	0.10	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PEG	CCC	208	-	6,6,6	0.11	0	5,5,5	0.15	0
8	PEG	FFF	214	-	6,6,6	0.13	0	5,5,5	0.19	0
9	EDO	EEE	213	-	3,3,3	0.26	0	2,2,2	0.47	0
7	PGE	FFF	210	-	9,9,9	0.23	0	8,8,8	0.13	0
8	PEG	DDD	210	-	6,6,6	0.14	0	5,5,5	0.11	0
9	EDO	EEE	212	-	3,3,3	0.07	0	2,2,2	0.11	0
8	PEG	AAA	207	-	6,6,6	0.12	0	5,5,5	0.33	0
8	PEG	AAA	206[A]	-	6,6,6	0.19	0	5,5,5	0.11	0
4	MPD	AAA	202	-	7,7,7	0.33	0	9,10,10	0.49	0
9	EDO	EEE	218	-	3,3,3	0.06	0	2,2,2	0.23	0
9	EDO	BBB	214	-	3,3,3	0.13	0	2,2,2	0.26	0
10	PG4	EEE	204	-	12,12,12	0.27	0	11,11,11	0.20	0
8	PEG	CCC	206	-	6,6,6	0.14	0	5,5,5	0.07	0
3	PXQ	FFF	201	2	32,46,46	4.27	5 (15%)	34,67,67	1.32	4 (11%)
4	MPD	BBB	202	-	7,7,7	0.28	0	9,10,10	0.53	0
3	PXQ	BBB	201	2	32,46,46	4.40	4 (12%)	34,67,67	1.44	3 (8%)
8	PEG	EEE	209	-	6,6,6	0.14	0	5,5,5	0.08	0
9	EDO	EEE	215[B]	-	3,3,3	0.25	0	2,2,2	0.29	0
7	PGE	FFF	207	-	9,9,9	0.16	0	8,8,8	0.22	0
9	EDO	DDD	213	-	3,3,3	0.24	0	2,2,2	0.48	0
9	EDO	FFF	216	-	3,3,3	0.15	0	2,2,2	0.33	0
8	PEG	CCC	211	-	6,6,6	0.14	0	5,5,5	0.14	0
9	EDO	BBB	216	-	3,3,3	0.12	0	2,2,2	0.26	0
9	EDO	EEE	215[A]	-	3,3,3	0.35	0	2,2,2	0.61	0
9	EDO	CCC	209	-	3,3,3	0.09	0	2,2,2	0.22	0
4	MPD	CCC	203	-	7,7,7	0.27	0	9,10,10	0.45	0
7	PGE	FFF	208	-	9,9,9	0.12	0	8,8,8	0.12	0
3	PXQ	AAA	201	1	32,46,46	4.00	5 (15%)	34,67,67	1.59	6 (17%)
9	EDO	DDD	216	-	3,3,3	0.23	0	2,2,2	0.43	0
9	EDO	DDD	218	-	3,3,3	0.30	0	2,2,2	0.42	0
10	PG4	DDD	208	-	12,12,12	0.16	0	11,11,11	0.15	0
9	EDO	EEE	211	-	3,3,3	0.07	0	2,2,2	0.23	0
3	PXQ	CCC	202	1	32,46,46	4.63	7 (21%)	34,67,67	1.57	5 (14%)
8	PEG	AAA	208	-	6,6,6	0.23	0	5,5,5	0.23	0
9	EDO	AAA	213	-	3,3,3	0.08	0	2,2,2	0.17	0
8	PEG	FFF	211	-	6,6,6	0.16	0	5,5,5	0.10	0
10	PG4	DDD	209	-	12,12,12	0.24	0	11,11,11	0.22	0
4	MPD	BBB	203	-	7,7,7	0.23	0	9,10,10	0.50	0
11	MRD	EEE	203	-	7,7,7	0.30	0	9,10,10	0.59	0
7	PGE	EEE	219	-	9,9,9	0.22	0	8,8,8	0.16	0
9	EDO	DDD	214	-	3,3,3	0.19	0	2,2,2	0.24	0
6	1PE	BBB	205	-	15,15,15	0.42	0	14,14,14	0.60	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	EDO	AAA	211	-	3,3,3	0.40	0	2,2,2	0.47	0
9	EDO	DDD	215[A]	-	3,3,3	0.11	0	2,2,2	0.24	0
8	PEG	DDD	211	-	6,6,6	0.23	0	5,5,5	0.20	0
9	EDO	AAA	212	-	3,3,3	0.09	0	2,2,2	0.24	0
9	EDO	CCC	201	-	3,3,3	0.12	0	2,2,2	0.27	0
5	BCN	AAA	203	-	7,10,10	0.48	0	8,11,11	0.60	0
4	MPD	FFF	203	-	7,7,7	0.17	0	9,10,10	0.58	0
3	PXQ	EEE	202	1	32,46,46	4.19	6 (18%)	34,67,67	1.26	4 (11%)
6	1PE	AAA	204	-	15,15,15	0.51	0	14,14,14	0.60	0
8	PEG	EEE	208	-	6,6,6	0.17	0	5,5,5	0.17	0
8	PEG	AAA	209	-	6,6,6	0.15	0	5,5,5	0.06	0
9	EDO	CCC	210	-	3,3,3	0.10	0	2,2,2	0.41	0
8	PEG	FFF	213	-	6,6,6	0.16	0	5,5,5	0.08	0
8	PEG	DDD	212	-	6,6,6	0.09	0	5,5,5	0.30	0
9	EDO	DDD	217[A]	-	3,3,3	0.37	0	2,2,2	0.60	0
6	1PE	BBB	217	-	15,15,15	0.54	0	14,14,14	0.16	0
7	PGE	AAA	215	-	9,9,9	0.14	0	8,8,8	0.10	0
9	EDO	DDD	201	-	3,3,3	0.21	0	2,2,2	0.04	0
4	MPD	FFF	205	-	7,7,7	0.28	0	9,10,10	0.57	0
8	PEG	CCC	207	-	6,6,6	0.29	0	5,5,5	0.14	0
9	EDO	EEE	214	-	3,3,3	0.86	0	2,2,2	0.22	0
10	PG4	EEE	201	-	12,12,12	0.16	0	11,11,11	0.16	0
7	PGE	EEE	205	-	9,9,9	0.25	0	8,8,8	0.13	0
4	MPD	FFF	204	-	7,7,7	0.29	0	9,10,10	0.62	0
4	MPD	BBB	204	-	7,7,7	0.37	0	9,10,10	0.59	0
8	PEG	CCC	205[B]	-	6,6,6	0.22	0	5,5,5	0.11	0
9	EDO	DDD	215[B]	-	3,3,3	0.15	0	2,2,2	0.28	0
4	MPD	FFF	202	-	7,7,7	0.45	0	9,10,10	0.46	0
9	EDO	AAA	216	-	3,3,3	0.06	0	2,2,2	0.04	0
7	PGE	AAA	205	-	9,9,9	0.25	0	8,8,8	0.23	0
4	MPD	DDD	205	-	7,7,7	0.36	0	9,10,10	0.28	0
7	PGE	BBB	207	-	9,9,9	0.19	0	8,8,8	0.14	0
8	PEG	CCC	205[A]	-	6,6,6	0.21	0	5,5,5	0.17	0
4	MPD	DDD	204	-	7,7,7	0.15	0	9,10,10	0.44	0
9	EDO	FFF	217	-	3,3,3	0.22	0	2,2,2	0.38	0
8	PEG	FFF	212	-	6,6,6	0.32	0	5,5,5	0.35	0
7	PGE	BBB	208	-	9,9,9	0.37	0	8,8,8	0.30	0
10	PG4	DDD	207	-	12,12,12	0.16	0	11,11,11	0.21	0
6	1PE	BBB	206	-	15,15,15	0.50	0	14,14,14	0.68	0
7	PGE	FFF	209	-	9,9,9	0.21	0	8,8,8	0.22	0
9	EDO	DDD	217[B]	-	3,3,3	0.13	0	2,2,2	0.34	0
9	EDO	EEE	210	-	3,3,3	0.06	0	2,2,2	0.24	0
9	EDO	BBB	212	-	3,3,3	0.07	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PEG	EEE	207	-	6,6,6	0.23	0	5,5,5	0.17	0
9	EDO	AAA	210[A]	-	3,3,3	0.12	0	2,2,2	0.27	0
8	PEG	BBB	211	-	6,6,6	0.13	0	5,5,5	0.15	0
8	PEG	BBB	209	-	6,6,6	0.22	0	5,5,5	0.22	0
4	MPD	DDD	203	-	7,7,7	0.31	0	9,10,10	0.53	0
9	EDO	BBB	213	-	3,3,3	0.17	0	2,2,2	0.13	0
9	EDO	EEE	216	-	3,3,3	0.09	0	2,2,2	0.21	0
8	PEG	EEE	206	-	6,6,6	0.12	0	5,5,5	0.11	0
9	EDO	AAA	214	-	3,3,3	0.14	0	2,2,2	0.33	0
5	BCN	DDD	206	-	7,10,10	0.58	0	8,11,11	1.07	0
3	PXQ	DDD	202	2	32,46,46	4.43	4 (12%)	34,67,67	1.15	4 (11%)

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
7	PGE	CCC	204	-	-	4/7/7/7	-
9	EDO	FFF	215	-	-	0/1/1/1	-
9	EDO	BBB	215	-	-	1/1/1/1	-
9	EDO	FFF	218	-	-	1/1/1/1	-
6	1PE	FFF	206	-	-	6/13/13/13	-
8	PEG	BBB	210	-	-	2/4/4/4	-
9	EDO	EEE	217	-	-	0/1/1/1	-
8	PEG	AAA	206[B]	-	-	3/4/4/4	-
9	EDO	AAA	210[B]	-	-	1/1/1/1	-
8	PEG	CCC	208	-	-	2/4/4/4	-
8	PEG	FFF	214	-	-	4/4/4/4	-
9	EDO	EEE	213	-	-	0/1/1/1	-
7	PGE	FFF	210	-	-	3/7/7/7	-
8	PEG	DDD	210	-	-	0/4/4/4	-
9	EDO	EEE	212	-	-	0/1/1/1	-
8	PEG	AAA	207	-	-	3/4/4/4	-
8	PEG	AAA	206[A]	-	-	4/4/4/4	-
4	MPD	AAA	202	-	-	2/5/5/5	-
9	EDO	EEE	218	-	-	0/1/1/1	-
9	EDO	BBB	214	-	-	0/1/1/1	-
10	PG4	EEE	204	-	-	5/10/10/10	-
8	PEG	CCC	206	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PXQ	FFF	201	2	-	3/19/58/58	0/4/4/4
4	MPD	BBB	202	-	-	0/5/5/5	-
3	PXQ	BBB	201	2	-	4/19/58/58	0/4/4/4
8	PEG	EEE	209	-	-	2/4/4/4	-
9	EDO	EEE	215[B]	-	-	0/1/1/1	-
7	PGE	FFF	207	-	-	5/7/7/7	-
9	EDO	DDD	213	-	-	1/1/1/1	-
9	EDO	FFF	216	-	-	0/1/1/1	-
8	PEG	CCC	211	-	-	1/4/4/4	-
9	EDO	BBB	216	-	-	1/1/1/1	-
9	EDO	EEE	215[A]	-	-	1/1/1/1	-
9	EDO	CCC	209	-	-	1/1/1/1	-
4	MPD	CCC	203	-	-	0/5/5/5	-
7	PGE	FFF	208	-	-	4/7/7/7	-
3	PXQ	AAA	201	1	-	5/19/58/58	0/4/4/4
9	EDO	DDD	216	-	-	1/1/1/1	-
9	EDO	DDD	218	-	-	0/1/1/1	-
10	PG4	DDD	208	-	-	7/10/10/10	-
9	EDO	EEE	211	-	-	1/1/1/1	-
3	PXQ	CCC	202	1	-	5/19/58/58	0/4/4/4
8	PEG	AAA	208	-	-	3/4/4/4	-
9	EDO	AAA	213	-	-	0/1/1/1	-
8	PEG	FFF	211	-	-	0/4/4/4	-
10	PG4	DDD	209	-	-	7/10/10/10	-
4	MPD	BBB	203	-	-	2/5/5/5	-
11	MRD	EEE	203	-	-	0/5/5/5	-
7	PGE	EEE	219	-	-	4/7/7/7	-
9	EDO	DDD	214	-	-	1/1/1/1	-
6	1PE	BBB	205	-	-	9/13/13/13	-
9	EDO	AAA	211	-	-	1/1/1/1	-
9	EDO	DDD	215[A]	-	-	1/1/1/1	-
8	PEG	DDD	211	-	-	3/4/4/4	-
9	EDO	AAA	212	-	-	1/1/1/1	-
9	EDO	CCC	201	-	-	1/1/1/1	-
5	BCN	AAA	203	-	-	3/8/10/10	-
4	MPD	FFF	203	-	-	2/5/5/5	-
3	PXQ	EEE	202	1	-	5/19/58/58	0/4/4/4
6	1PE	AAA	204	-	-	2/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	EEE	208	-	-	3/4/4/4	-
8	PEG	AAA	209	-	-	2/4/4/4	-
9	EDO	CCC	210	-	-	1/1/1/1	-
8	PEG	FFF	213	-	-	2/4/4/4	-
8	PEG	DDD	212	-	-	2/4/4/4	-
9	EDO	DDD	217[A]	-	-	1/1/1/1	-
6	1PE	BBB	217	-	-	10/13/13/13	-
7	PGE	AAA	215	-	-	1/7/7/7	-
9	EDO	DDD	201	-	-	1/1/1/1	-
4	MPD	FFF	205	-	-	2/5/5/5	-
8	PEG	CCC	207	-	-	0/4/4/4	-
9	EDO	EEE	214	-	-	0/1/1/1	-
10	PG4	EEE	201	-	-	5/10/10/10	-
7	PGE	EEE	205	-	-	4/7/7/7	-
4	MPD	FFF	204	-	-	3/5/5/5	-
4	MPD	BBB	204	-	-	4/5/5/5	-
8	PEG	CCC	205[B]	-	-	3/4/4/4	-
9	EDO	DDD	215[B]	-	-	1/1/1/1	-
4	MPD	FFF	202	-	-	1/5/5/5	-
9	EDO	AAA	216	-	-	0/1/1/1	-
7	PGE	AAA	205	-	-	2/7/7/7	-
4	MPD	DDD	205	-	-	5/5/5/5	-
7	PGE	BBB	207	-	-	3/7/7/7	-
8	PEG	CCC	205[A]	-	-	3/4/4/4	-
4	MPD	DDD	204	-	-	1/5/5/5	-
9	EDO	FFF	217	-	-	1/1/1/1	-
8	PEG	FFF	212	-	-	0/4/4/4	-
7	PGE	BBB	208	-	-	5/7/7/7	-
10	PG4	DDD	207	-	-	6/10/10/10	-
6	1PE	BBB	206	-	-	6/13/13/13	-
7	PGE	FFF	209	-	-	5/7/7/7	-
9	EDO	DDD	217[B]	-	-	1/1/1/1	-
9	EDO	EEE	210	-	-	1/1/1/1	-
9	EDO	BBB	212	-	-	1/1/1/1	-
8	PEG	EEE	207	-	-	2/4/4/4	-
9	EDO	AAA	210[A]	-	-	1/1/1/1	-
8	PEG	BBB	211	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	BBB	209	-	-	3/4/4/4	-
4	MPD	DDD	203	-	-	0/5/5/5	-
9	EDO	BBB	213	-	-	1/1/1/1	-
9	EDO	EEE	216	-	-	1/1/1/1	-
8	PEG	EEE	206	-	-	1/4/4/4	-
9	EDO	AAA	214	-	-	0/1/1/1	-
5	BCN	DDD	206	-	-	2/8/10/10	-
3	PXQ	DDD	202	2	-	5/19/58/58	0/4/4/4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	202	PXQ	CHA-C1A	-15.86	1.39	1.51
3	CCC	202	PXQ	CHA-C4D	-15.47	1.39	1.51
3	CCC	202	PXQ	C4C-NC	15.21	1.40	1.29
3	BBB	201	PXQ	CHA-C4D	-15.19	1.40	1.51
3	DDD	202	PXQ	CHA-C4D	-15.18	1.40	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	201	PXQ	CAD-C3D-C4D	-5.26	123.60	127.30
3	CCC	202	PXQ	CAA-C2A-C1A	-5.22	123.63	127.30
3	BBB	201	PXQ	CAD-C3D-C4D	-4.96	123.81	127.30
3	FFF	201	PXQ	CAD-C3D-C4D	-4.40	124.21	127.30
3	CCC	202	PXQ	CAD-C3D-C4D	-3.98	124.50	127.30

There are no chirality outliers.

5 of 236 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	PXQ	C2A-C1A-CHA-C4D
3	AAA	201	PXQ	C3D-C4D-CHA-C1A
3	AAA	201	PXQ	NA-C4A-CHB-C1B
3	AAA	201	PXQ	C3A-C4A-CHB-C1B
3	AAA	201	PXQ	C2D-C1D-CHD-C4C

There are no ring outliers.

56 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	FFF	215	EDO	11	0
9	BBB	215	EDO	1	0
9	FFF	218	EDO	3	0
8	BBB	210	PEG	1	0
9	EEE	217	EDO	1	0
8	AAA	206[B]	PEG	4	0
8	FFF	214	PEG	1	0
9	EEE	213	EDO	3	0
7	FFF	210	PGE	5	0
8	DDD	210	PEG	9	0
9	EEE	212	EDO	1	0
8	AAA	207	PEG	4	0
8	AAA	206[A]	PEG	2	0
10	EEE	204	PG4	6	0
8	CCC	206	PEG	4	0
7	FFF	207	PGE	3	0
9	DDD	213	EDO	5	0
9	FFF	216	EDO	1	0
8	CCC	211	PEG	2	0
7	FFF	208	PGE	2	0
3	AAA	201	PXQ	1	0
9	DDD	216	EDO	1	0
10	DDD	208	PG4	6	0
8	AAA	208	PEG	4	0
8	FFF	211	PEG	1	0
4	BBB	203	MPD	2	0
7	EEE	219	PGE	6	0
8	DDD	211	PEG	1	0
9	CCC	201	EDO	1	0
5	AAA	203	BCN	2	0
4	FFF	203	MPD	7	0
8	AAA	209	PEG	1	0
9	CCC	210	EDO	1	0
8	FFF	213	PEG	1	0
8	DDD	212	PEG	1	0
9	DDD	217[A]	EDO	2	0
6	BBB	217	1PE	2	0
7	AAA	215	PGE	1	0
9	EEE	214	EDO	10	0
7	EEE	205	PGE	1	0
4	FFF	204	MPD	1	0
4	BBB	204	MPD	1	0
7	AAA	205	PGE	2	0

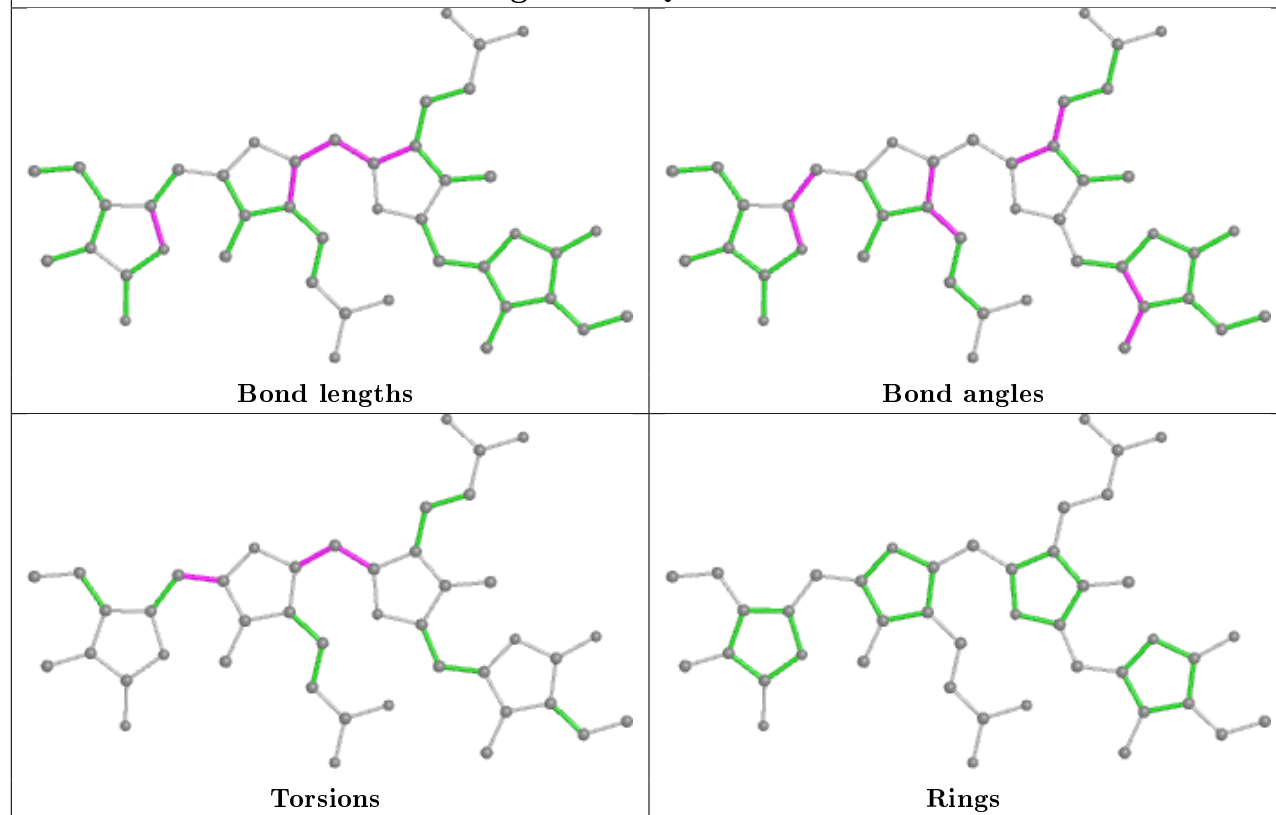
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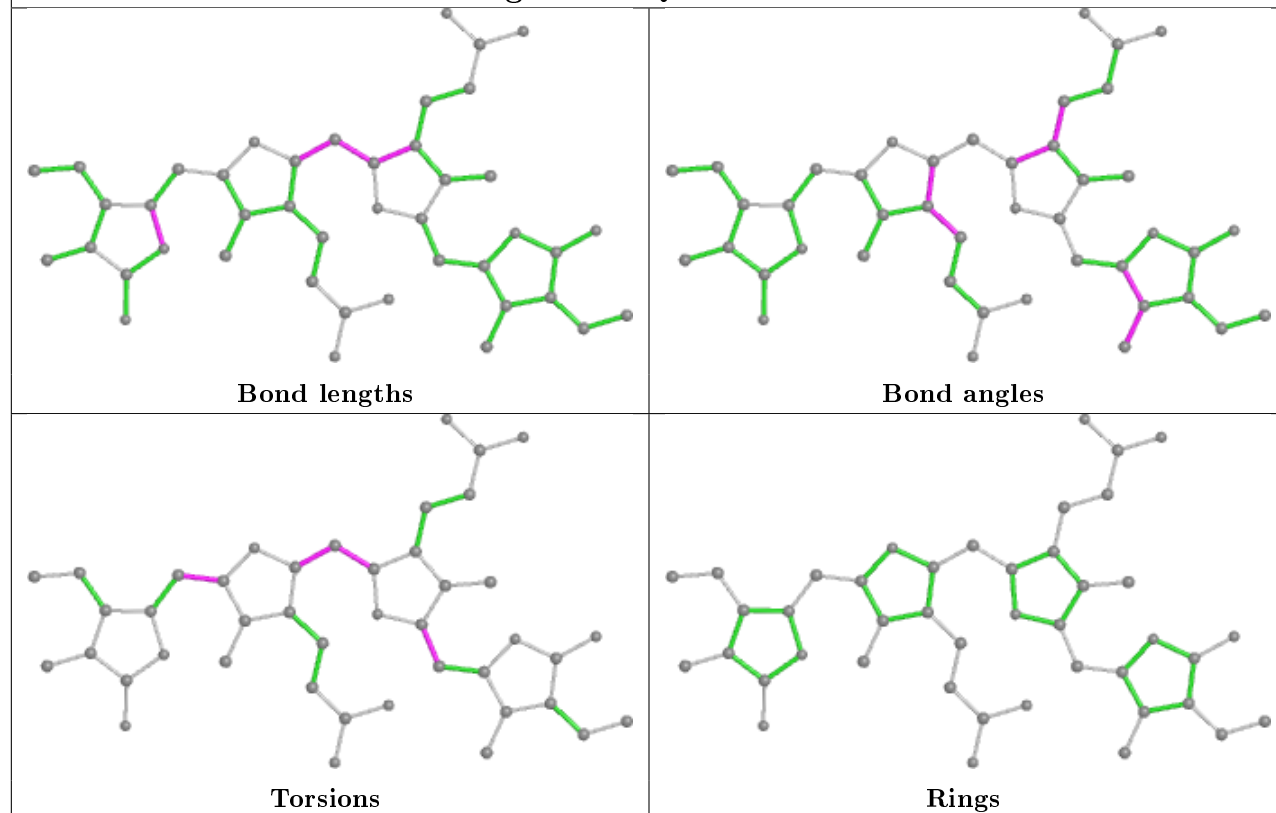
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	205	MPD	4	0
8	CCC	205[A]	PEG	1	0
8	FFF	212	PEG	1	0
7	BBB	208	PGE	4	0
10	DDD	207	PG4	4	0
6	BBB	206	1PE	2	0
7	FFF	209	PGE	1	0
9	EEE	210	EDO	1	0
9	BBB	212	EDO	1	0
8	EEE	207	PEG	4	0
4	DDD	203	MPD	1	0
5	DDD	206	BCN	5	0
3	DDD	202	PXQ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand PXQ FFF 201

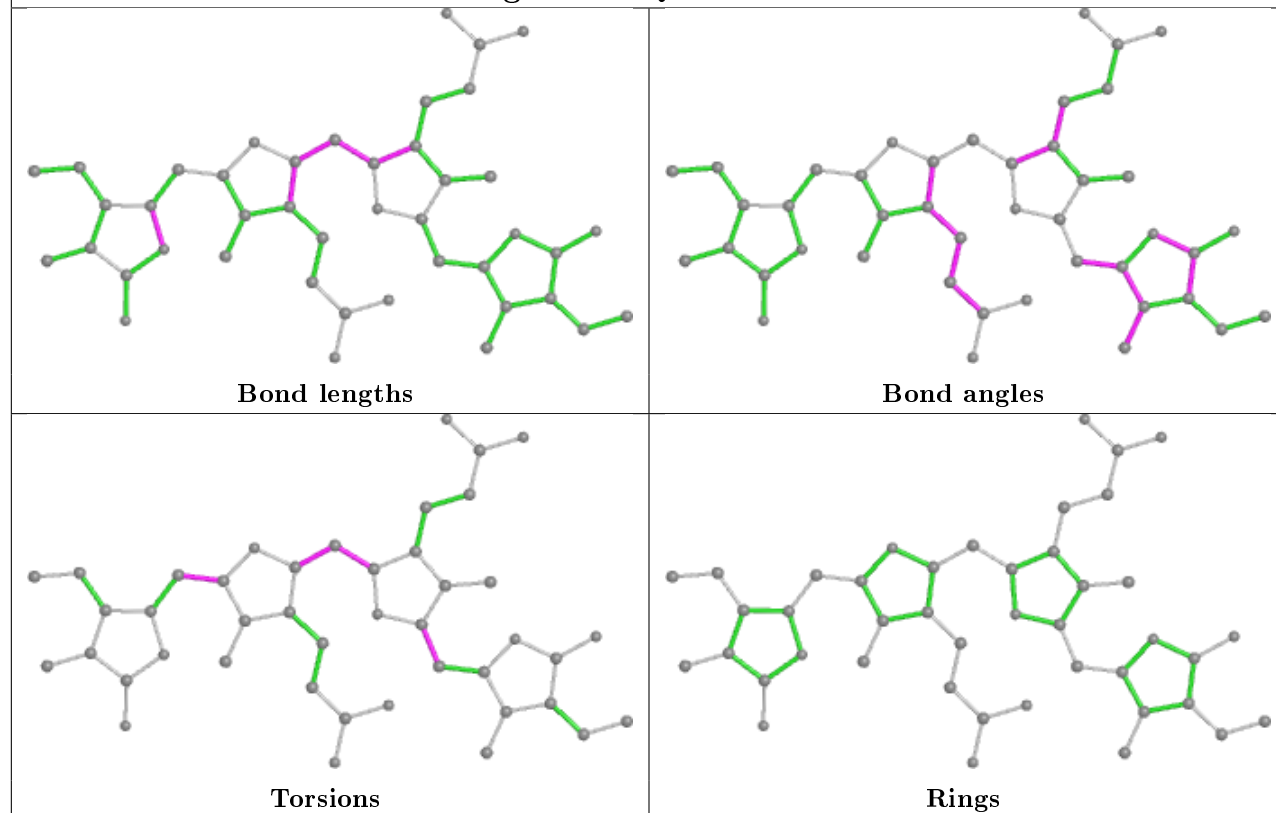


## Ligand PXQ BBB 201

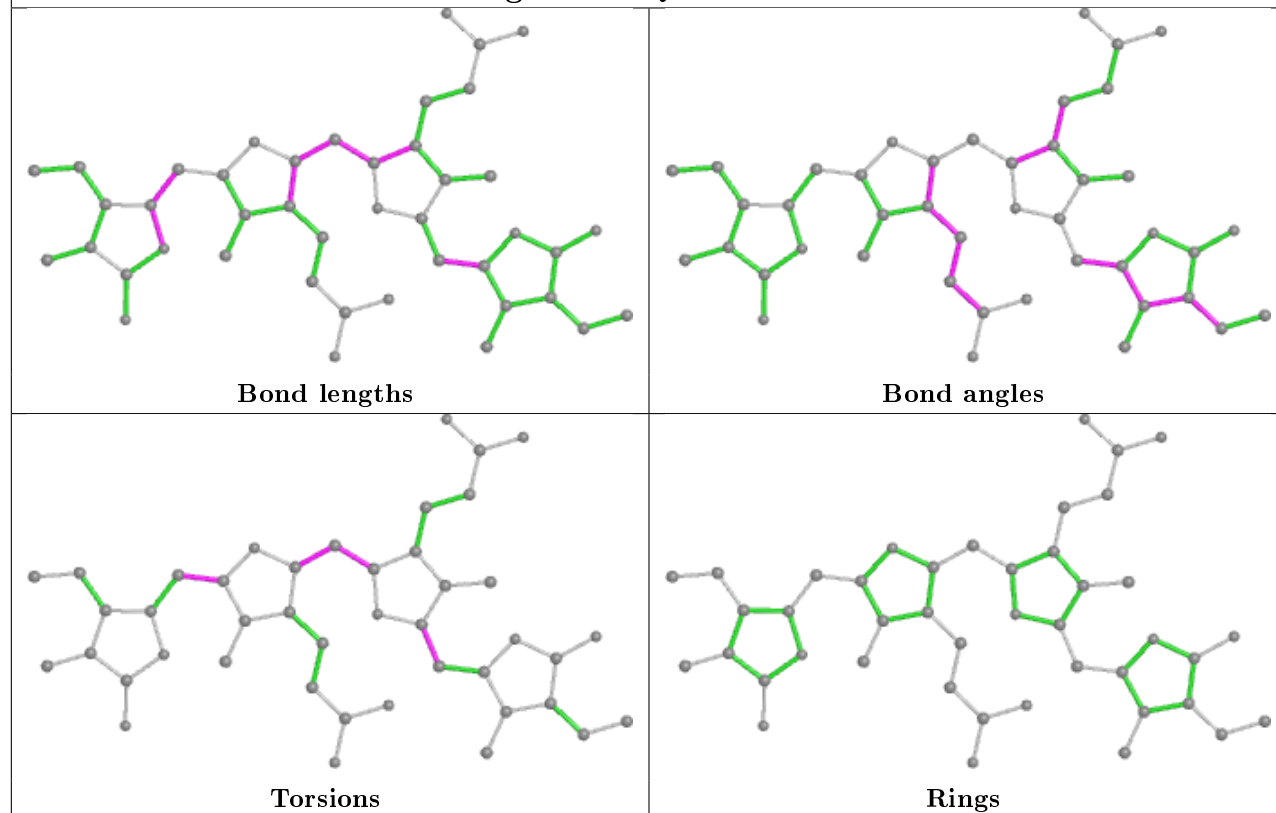




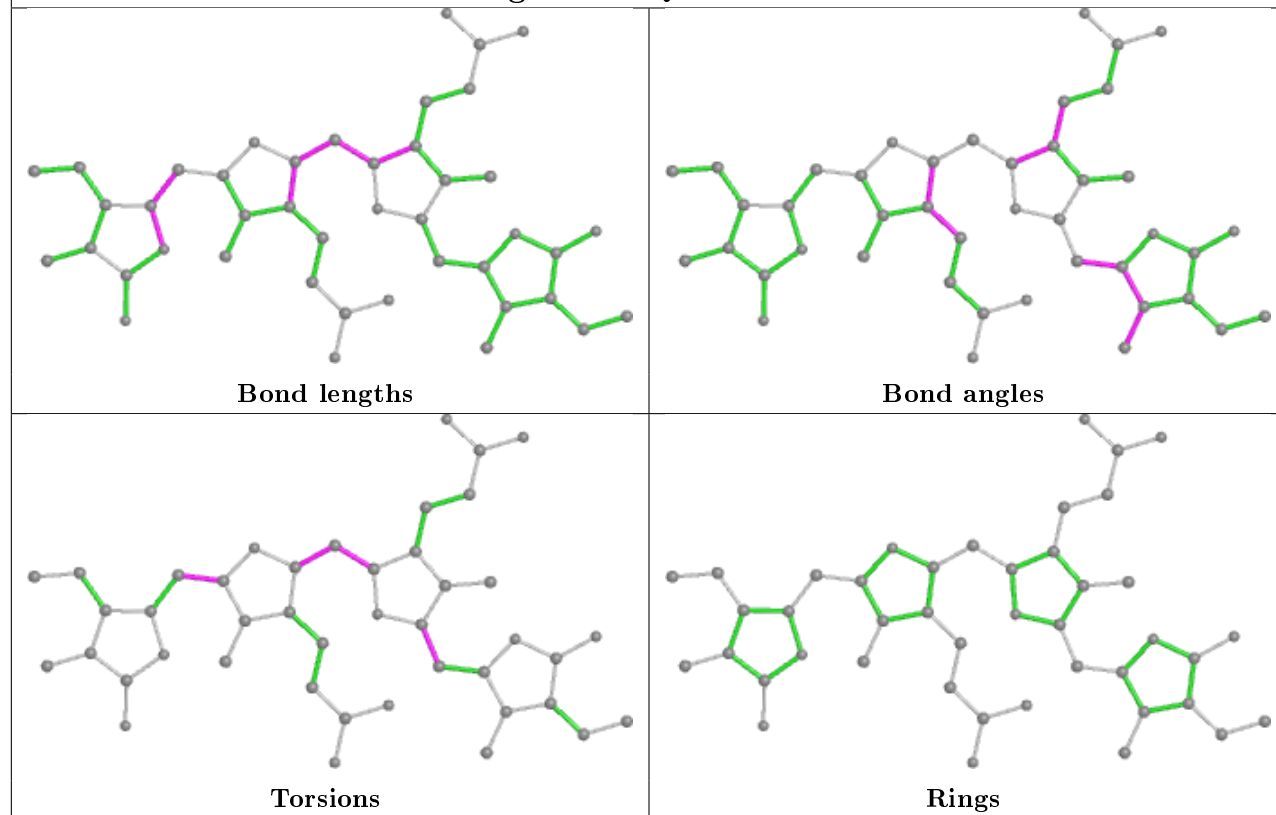
## Ligand PXQ AAA 201



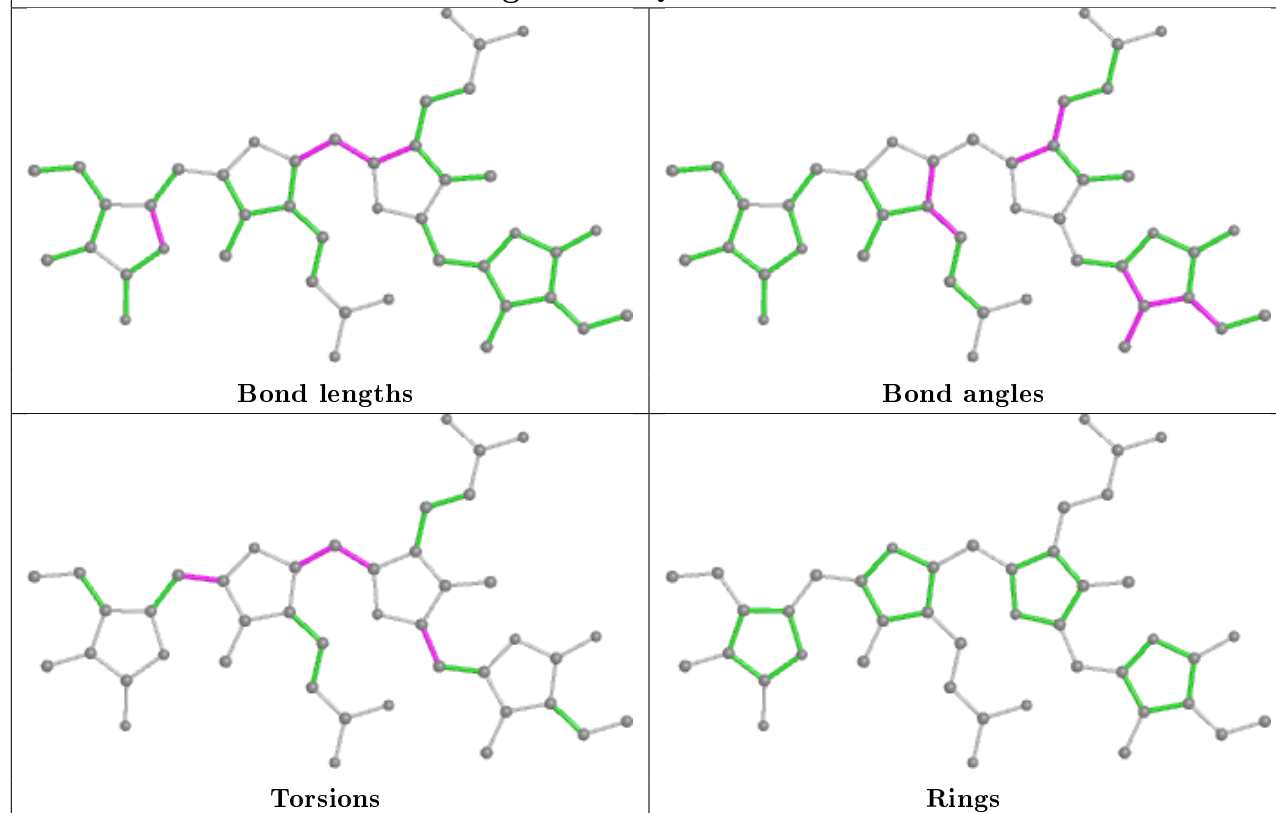
## Ligand PXQ CCC 202



## Ligand PXQ EEE 202



## Ligand PXQ DDD 202



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	160/160 (100%)	-0.58	0 100 100	21, 29, 42, 73	0
1	CCC	160/160 (100%)	-0.19	1 (0%) 89 89	23, 38, 60, 70	0
1	EEE	160/160 (100%)	-0.45	0 100 100	21, 31, 47, 58	0
2	BBB	160/161 (99%)	-0.60	0 100 100	22, 28, 38, 58	0
2	DDD	160/161 (99%)	-0.38	0 100 100	21, 33, 50, 70	0
2	FFF	160/161 (99%)	-0.52	0 100 100	25, 30, 43, 64	0
All	All	960/963 (99%)	-0.45	1 (0%) 95 94	21, 31, 49, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	12	ALA	2.1

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

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	MEN	DDD	71	9/10	0.96	0.08	23,25,29,31	0
2	MEN	BBB	71	9/10	0.97	0.06	22,23,24,25	0
2	MEN	FFF	71	9/10	0.97	0.07	25,28,32,34	0

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
9	EDO	FFF	217	4/4	0.44	0.37	44,46,47,48	4
7	PGE	FFF	210	10/10	0.47	0.48	42,47,48,48	10
9	EDO	BBB	215	4/4	0.48	0.32	43,46,47,50	4
9	EDO	CCC	201	4/4	0.54	0.32	43,44,46,46	4
9	EDO	DDD	214	4/4	0.56	0.40	46,47,48,48	4
8	PEG	CCC	207	7/7	0.56	0.33	46,47,48,49	7
9	EDO	EEE	211	4/4	0.60	0.41	43,43,43,44	4
8	PEG	BBB	210	7/7	0.60	0.76	47,48,50,50	7
8	PEG	AAA	208	7/7	0.61	0.29	43,44,45,46	7
8	PEG	CCC	206	7/7	0.62	0.34	47,48,50,50	7
9	EDO	DDD	218	4/4	0.62	0.31	40,42,42,42	4
8	PEG	AAA	209	7/7	0.65	0.29	42,43,46,47	7
6	1PE	BBB	217	16/16	0.65	0.51	42,46,46,47	16
9	EDO	DDD	215[B]	4/4	0.66	0.27	45,46,46,47	4
9	EDO	DDD	215[A]	4/4	0.66	0.27	45,45,46,47	4
8	PEG	BBB	209	7/7	0.68	0.25	36,42,47,48	7
8	PEG	DDD	211	7/7	0.68	0.35	46,47,48,49	7
8	PEG	AAA	207	7/7	0.69	0.46	38,39,43,43	7
4	MPD	DDD	204	8/8	0.69	0.49	44,46,47,48	8
8	PEG	EEE	207	7/7	0.69	0.50	41,44,47,47	7
8	PEG	FFF	211	7/7	0.69	0.43	43,43,46,48	7
8	PEG	FFF	214	7/7	0.70	0.41	45,46,47,48	7
9	EDO	CCC	209	4/4	0.70	0.35	43,43,43,45	4
10	PG4	DDD	207	13/13	0.70	0.44	41,42,45,45	13
5	BCN	AAA	203	11/11	0.71	0.28	45,46,51,53	11
10	PG4	DDD	209	13/13	0.71	0.31	43,47,49,49	13
7	PGE	EEE	205	10/10	0.72	0.22	36,43,46,46	10
9	EDO	AAA	216	4/4	0.73	0.34	43,46,46,50	4
7	PGE	CCC	204	10/10	0.73	0.40	45,46,48,49	10
7	PGE	AAA	215	10/10	0.73	0.26	41,54,56,57	10
6	1PE	BBB	205	16/16	0.74	0.40	32,38,50,52	16
8	PEG	CCC	211	7/7	0.74	0.46	43,44,45,46	7
8	PEG	DDD	210	7/7	0.74	0.50	51,51,51,52	7
7	PGE	AAA	205	10/10	0.74	0.30	35,41,46,46	10
8	PEG	DDD	212	7/7	0.74	0.30	39,44,48,48	7
7	PGE	FFF	209	10/10	0.75	0.34	44,46,47,49	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	EDO	EEE	212	4/4	0.75	0.72	45,45,46,46	4
10	PG4	DDD	208	13/13	0.75	0.35	40,46,49,49	13
9	EDO	EEE	218	4/4	0.75	0.36	43,44,44,45	4
9	EDO	EEE	216	4/4	0.76	0.50	44,44,44,46	4
9	EDO	AAA	210[A]	4/4	0.76	0.38	42,43,43,43	4
9	EDO	AAA	210[B]	4/4	0.76	0.38	57,57,58,58	4
10	PG4	EEE	201	13/13	0.76	0.46	41,44,50,50	13
10	PG4	EEE	204	13/13	0.76	0.21	31,51,72,72	13
11	MRD	EEE	203	8/8	0.76	0.18	42,43,46,48	8
4	MPD	BBB	204	8/8	0.77	0.57	40,41,42,44	8
9	EDO	EEE	217	4/4	0.77	0.26	46,47,48,48	4
8	PEG	BBB	211	7/7	0.77	0.24	42,45,47,48	7
7	PGE	EEE	219	10/10	0.77	0.31	39,47,48,49	10
7	PGE	BBB	207	10/10	0.77	0.32	41,43,44,46	10
9	EDO	DDD	217[A]	4/4	0.77	0.19	39,44,44,44	4
9	EDO	DDD	217[B]	4/4	0.77	0.19	43,44,44,45	4
9	EDO	BBB	212	4/4	0.77	0.46	43,44,45,47	4
4	MPD	AAA	202	8/8	0.77	0.36	37,39,40,41	8
8	PEG	FFF	212	7/7	0.77	0.40	28,36,45,47	7
4	MPD	BBB	203	8/8	0.78	0.35	42,46,48,52	8
4	MPD	FFF	204	8/8	0.78	0.61	45,46,51,52	8
9	EDO	CCC	210	4/4	0.78	0.24	43,44,44,44	4
5	BCN	DDD	206	11/11	0.79	0.21	35,40,53,55	11
9	EDO	EEE	210	4/4	0.80	0.56	46,46,46,46	4
4	MPD	FFF	205	8/8	0.80	0.20	37,44,47,49	8
9	EDO	FFF	215	4/4	0.80	0.25	36,40,40,43	4
8	PEG	CCC	208	7/7	0.80	0.49	44,45,47,48	7
6	1PE	BBB	206	16/16	0.80	0.21	38,44,48,48	16
8	PEG	EEE	208	7/7	0.82	0.48	45,46,47,47	7
8	PEG	EEE	209	7/7	0.82	0.30	41,44,45,48	7
4	MPD	FFF	203	8/8	0.82	0.49	38,40,41,41	8
9	EDO	BBB	214	4/4	0.82	0.72	44,47,47,48	4
9	EDO	EEE	215[B]	4/4	0.83	0.23	33,35,36,37	4
9	EDO	DDD	213	4/4	0.83	0.20	35,41,43,45	4
9	EDO	DDD	216	4/4	0.83	0.21	43,44,44,44	4
9	EDO	BBB	216	4/4	0.83	0.55	42,42,42,43	4
8	PEG	FFF	213	7/7	0.83	0.18	41,43,45,45	7
9	EDO	EEE	215[A]	4/4	0.83	0.23	37,37,38,39	4
7	PGE	BBB	208	10/10	0.84	0.17	38,41,44,45	10
4	MPD	DDD	205	8/8	0.84	0.38	41,43,44,45	8
9	EDO	EEE	213	4/4	0.84	0.21	47,47,49,50	4
9	EDO	DDD	201	4/4	0.84	0.35	40,42,42,44	4

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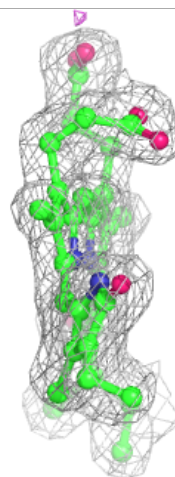
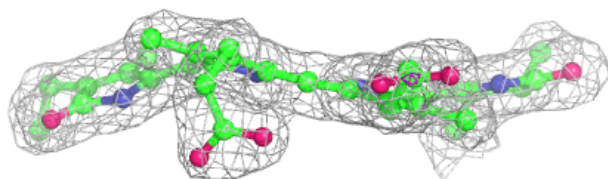
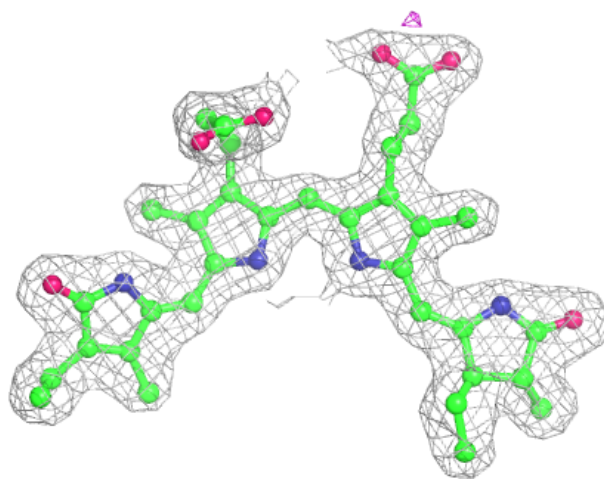
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	EDO	FFF	216	4/4	0.84	0.22	39,41,42,43	4
9	EDO	AAA	213	4/4	0.84	0.36	44,45,45,45	4
6	1PE	FFF	206	16/16	0.85	0.21	39,44,49,52	16
7	PGE	FFF	207	10/10	0.85	0.22	41,45,52,53	10
7	PGE	FFF	208	10/10	0.85	0.38	43,44,48,48	10
8	PEG	AAA	206[B]	7/7	0.86	0.16	27,35,42,42	7
8	PEG	AAA	206[A]	7/7	0.86	0.16	45,46,47,48	7
9	EDO	BBB	213	4/4	0.86	0.30	43,43,45,46	4
9	EDO	AAA	214	4/4	0.86	0.25	39,39,40,40	4
8	PEG	EEE	206	7/7	0.87	0.82	47,48,49,50	7
8	PEG	CCC	205[B]	7/7	0.87	0.21	42,43,44,44	7
8	PEG	CCC	205[A]	7/7	0.87	0.21	38,43,46,47	7
9	EDO	AAA	212	4/4	0.88	0.38	41,42,42,43	4
9	EDO	EEE	214	4/4	0.89	0.35	37,38,42,45	4
9	EDO	AAA	211	4/4	0.89	0.16	31,36,40,47	4
4	MPD	DDD	203	8/8	0.89	0.33	39,40,42,43	8
6	1PE	AAA	204	16/16	0.93	0.11	42,49,73,76	0
4	MPD	FFF	202	8/8	0.93	0.16	38,43,47,48	8
9	EDO	FFF	218	4/4	0.94	0.29	38,40,41,41	4
3	PXQ	FFF	201	43/43	0.95	0.08	28,35,41,49	0
3	PXQ	AAA	201	43/43	0.95	0.08	22,25,34,44	0
4	MPD	BBB	202	8/8	0.96	0.10	33,33,39,39	0
3	PXQ	EEE	202	43/43	0.97	0.07	19,22,27,33	0
3	PXQ	BBB	201	43/43	0.97	0.08	23,27,37,43	0
3	PXQ	CCC	202	43/43	0.97	0.07	22,26,30,35	0
3	PXQ	DDD	202	43/43	0.97	0.07	23,28,38,43	0
4	MPD	CCC	203	8/8	0.98	0.07	26,30,30,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around PXQ FFF 201:**

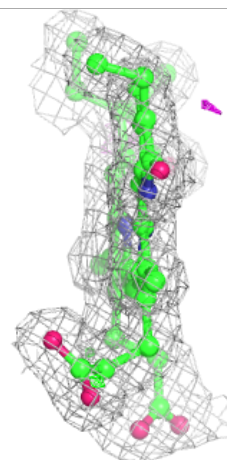
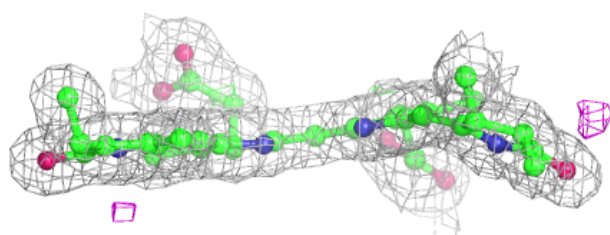
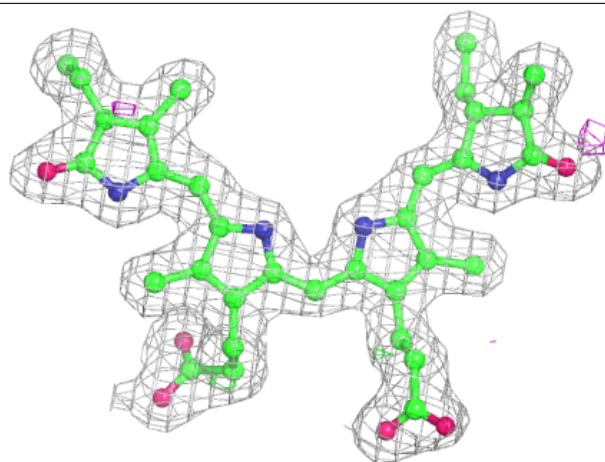
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





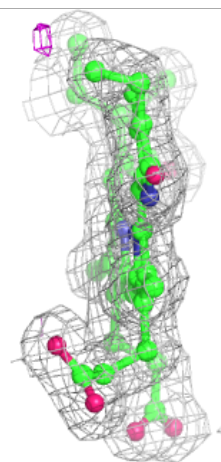
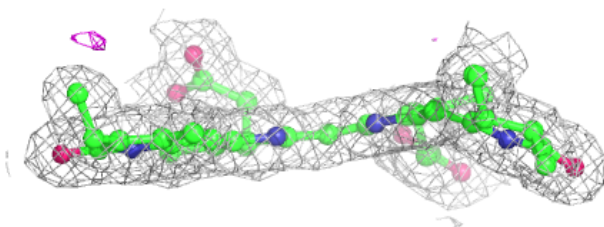
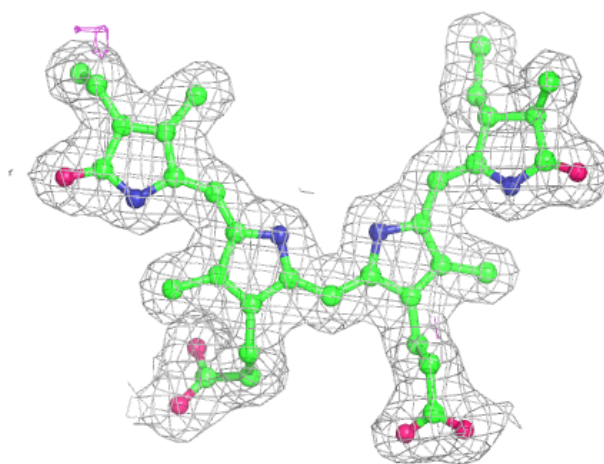
**Electron density around PXQ AAA 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



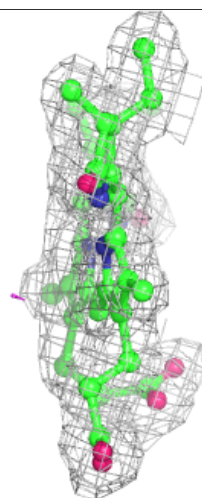
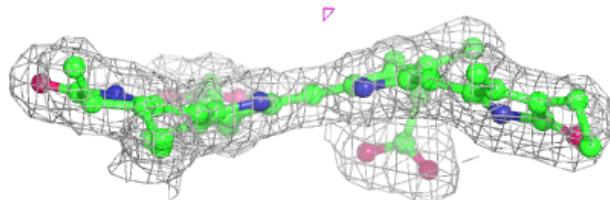
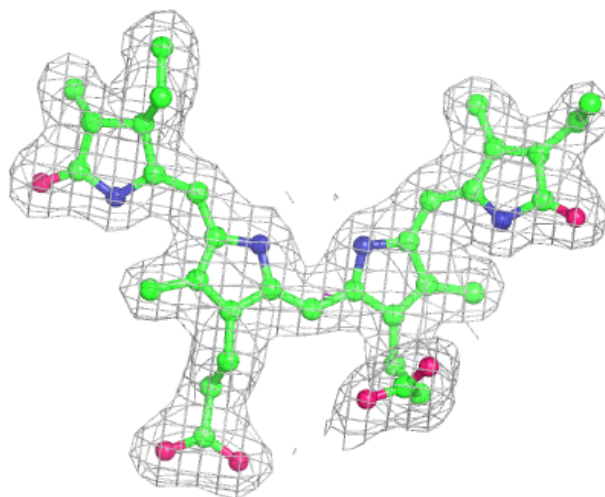
**Electron density around PXQ EEE 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



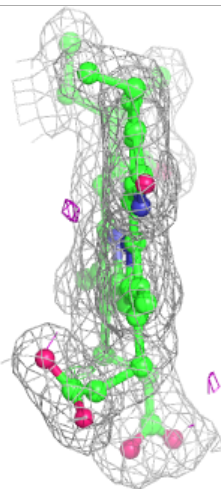
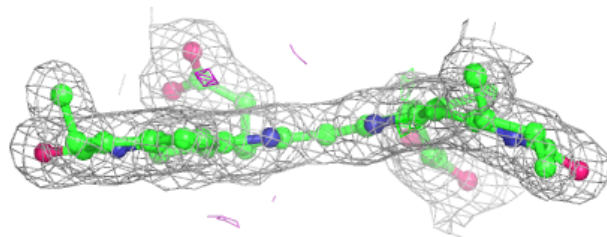
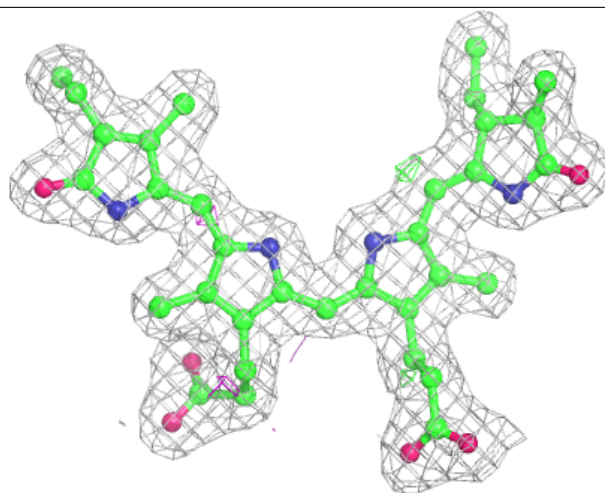
**Electron density around PXQ BBB 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



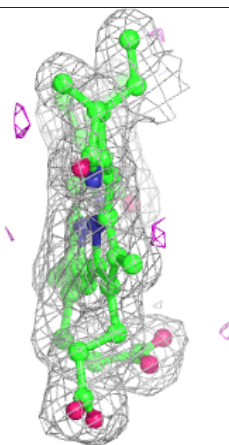
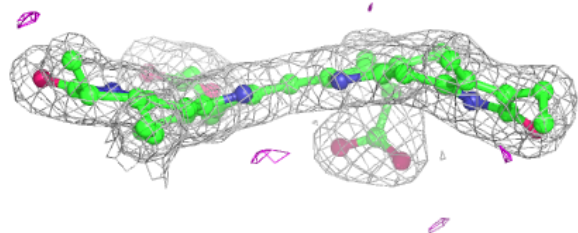
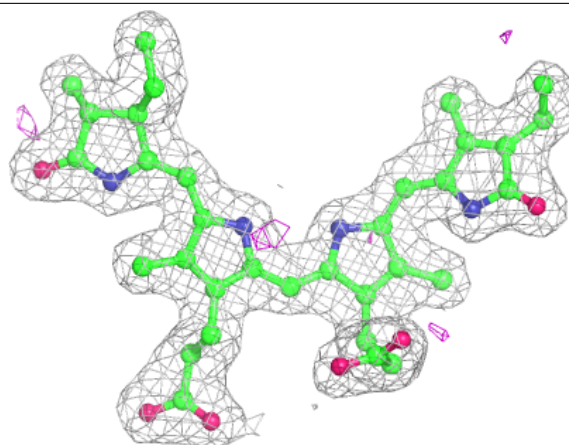
**Electron density around PXQ CCC 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PXQ DDD 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.