



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 10:16 AM EDT

PDB ID : 9OW2 / pdb\_00009ow2  
Title : Crystal Structure of the Surface Protein (CD630\_07380) from *Clostridium difficile* Strain 630  
Authors : Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Satchell, K.J.F.; Center for Structural Biology of Infectious Diseases (CSBID)  
Deposited on : 2025-06-02  
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

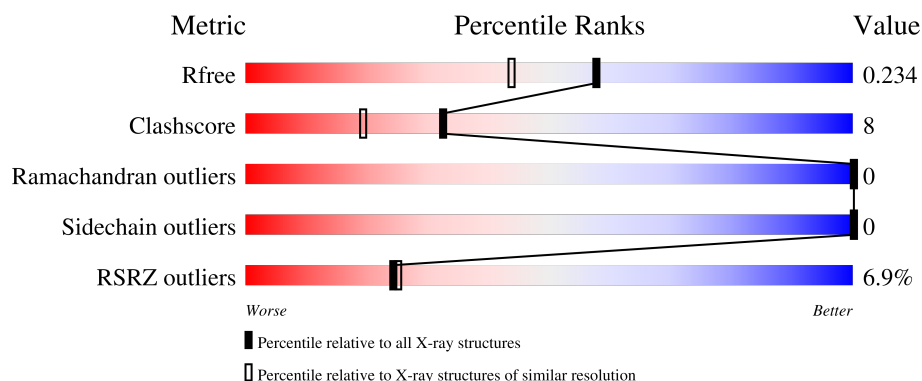
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	A	275	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>7%</div> </div> </div>
1	B	275	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4541 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 Exported protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			2141	1374	358	398	11			
1	B	252	Total	C	N	O	S	0	3	0
			2106	1350	354	392	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP Q189T6
A	294	HIS	-	expression tag	UNP Q189T6
A	295	HIS	-	expression tag	UNP Q189T6
A	296	HIS	-	expression tag	UNP Q189T6
A	297	HIS	-	expression tag	UNP Q189T6
A	298	HIS	-	expression tag	UNP Q189T6
A	299	HIS	-	expression tag	UNP Q189T6
A	300	HIS	-	expression tag	UNP Q189T6
A	301	HIS	-	expression tag	UNP Q189T6
B	27	MET	-	initiating methionine	UNP Q189T6
B	294	HIS	-	expression tag	UNP Q189T6
B	295	HIS	-	expression tag	UNP Q189T6
B	296	HIS	-	expression tag	UNP Q189T6
B	297	HIS	-	expression tag	UNP Q189T6
B	298	HIS	-	expression tag	UNP Q189T6
B	299	HIS	-	expression tag	UNP Q189T6
B	300	HIS	-	expression tag	UNP Q189T6
B	301	HIS	-	expression tag	UNP Q189T6

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

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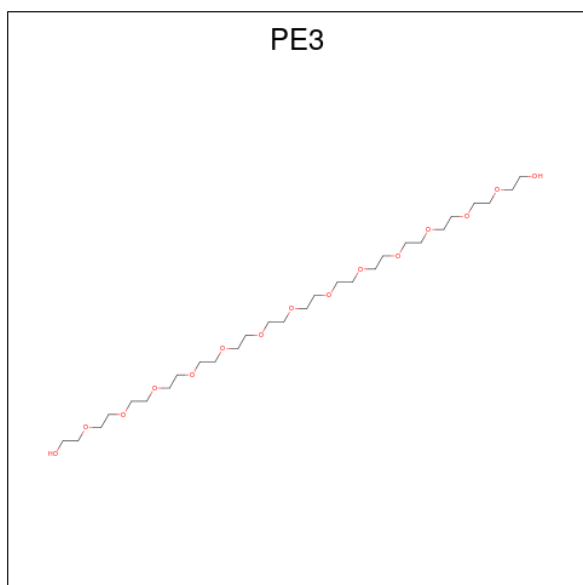
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Cl	0	0
			5	5		
3	B	3	Total	Cl	0	0
			3	3		

- Molecule 4 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAXAHENTETRACONTANE-1,41-DIOL (CCD ID: PE3) (formula: C<sub>28</sub>H<sub>58</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			43	28	15		
4	A	1	Total	C	O	0	0
			43	28	15		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

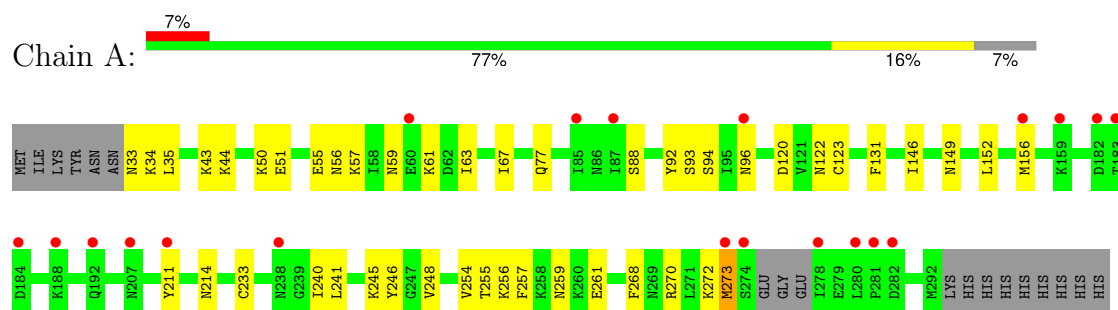
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	3
			93	93		
6	B	93	Total	O	0	0
			93	93		

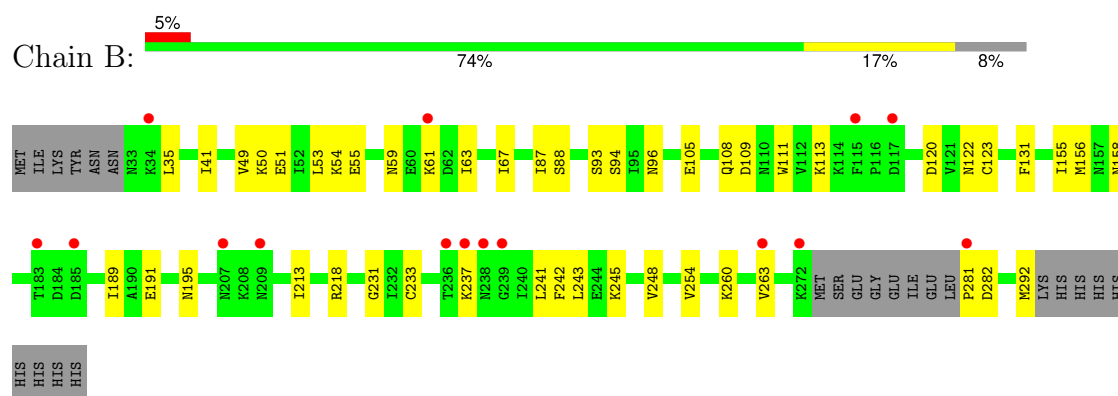
### 3 Residue-property plots [i](#)

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: Exported protein



#### • Molecule 1: Exported protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.08Å 94.87Å 57.09Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	28.55 – 1.85 28.55 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.55-1.85) 99.4 (28.55-1.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.179 , 0.224 0.192 , 0.234	Depositor DCC
$R_{free}$ test set	2156 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-l	Xtriage
Reported twinning fraction	0.664 for H, K, L 0.336 for -h,-k,l	Depositor
Outliers	1 of 37868 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.69% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CME, EDO, NA, PE3

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	0.45	0/2166	1.05	5/2903 (0.2%)
1	B	0.45	0/2131	1.05	4/2856 (0.1%)
All	All	0.45	0/4297	1.05	9/5759 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	120	ASP	CA-CB-CG	6.38	118.97	112.60
1	B	245	LYS	N-CA-C	-6.07	97.82	108.20
1	B	158	ASN	CB-CA-C	5.46	119.15	110.19
1	B	131	PHE	N-CA-CB	-5.28	102.94	110.80
1	A	245	LYS	N-CA-C	-5.12	99.45	108.20
1	A	77	GLN	CB-CA-C	-5.08	101.97	110.56
1	A	131	PHE	N-CA-CB	-5.04	103.29	110.80
1	A	273	MET	N-CA-C	-5.01	107.11	113.18

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	2141	0	2194	30	0
1	B	2106	0	2153	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	3	0	0	1	0
4	A	86	0	116	5	0
5	B	12	0	18	0	0
6	A	93	0	0	1	0
6	B	93	0	0	2	0
All	All	4541	0	4481	69	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.

All (69) 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:B:59:ASN:OD1	1:B:61:LYS:HB3	1.72	0.89
1:B:213:ILE:HD12	1:B:292:MET:HE3	1.66	0.78
1:B:233[A]:CYS:SG	1:B:260:LYS:NZ	2.60	0.74
1:A:88:SER:HB2	1:A:93:SER:OG	1.89	0.73
1:B:241:LEU:HD11	1:B:254:VAL:HG12	1.78	0.66
1:A:122:ASN:HB2	1:A:123:CME:HE2	1.76	0.66
1:B:213:ILE:HD12	1:B:292:MET:CE	2.26	0.64
1:A:43:LYS:NZ	1:B:109:ASP:OD1	2.28	0.63
4:A:407:PE3:H82	1:B:248:VAL:HG23	1.81	0.62
1:B:241:LEU:HD11	1:B:254:VAL:CG1	2.32	0.59
1:B:156:MET:HA	1:B:156:MET:HE2	1.85	0.59
1:B:51:GLU:O	1:B:55:GLU:HG3	2.03	0.59
1:A:146:ILE:HD12	1:A:149:ASN:ND2	2.18	0.58
1:B:122:ASN:HB2	1:B:123:CME:HE2	1.86	0.57
1:B:218:ARG:HD2	1:B:281:PRO:HB2	1.86	0.56
1:B:189:ILE:CD1	1:B:218:ARG:HE	2.19	0.56
1:A:246:TYR:O	1:A:270:ARG:NH1	2.39	0.55
1:B:61:LYS:HG2	6:B:535:HOH:O	2.05	0.55
1:A:241:LEU:HD11	1:A:254:VAL:HG12	1.88	0.55
1:A:233:CYS:SG	1:A:240:ILE:CG2	2.95	0.55
1:A:233:CYS:SG	1:A:240:ILE:HG21	2.48	0.54
1:B:233[B]:CYS:SG	1:B:263:VAL:HG11	2.49	0.53
1:B:189:ILE:HD11	1:B:218:ARG:HE	1.74	0.52
1:B:50:LYS:HG3	1:B:63:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:HB3	3:A:404:CL:CL	2.47	0.51
1:A:122:ASN:HB3	1:A:248:VAL:CG1	2.41	0.50
1:B:231:GLY:HA3	1:B:242:PHE:CZ	2.47	0.49
1:A:63:ILE:O	1:A:67:ILE:HG12	2.13	0.48
1:B:122:ASN:HB3	1:B:248:VAL:HG13	1.94	0.48
1:A:241:LEU:HD11	1:A:254:VAL:CG1	2.44	0.47
1:A:51:GLU:O	1:A:55:GLU:HG3	2.15	0.47
1:B:122:ASN:HB3	1:B:248:VAL:CG1	2.45	0.47
1:A:33:ASN:CG	1:A:34:LYS:H	2.23	0.46
1:A:122:ASN:HB3	1:A:248:VAL:HG13	1.98	0.46
1:B:35:LEU:O	1:B:94:SER:HA	2.15	0.46
1:B:237:LYS:C	1:B:237:LYS:HD3	2.41	0.46
1:B:218:ARG:NH1	1:B:282:ASP:O	2.48	0.46
4:A:407:PE3:H201	1:B:105:GLU:HA	1.98	0.46
1:B:41:ILE:HD11	1:B:87:ILE:CG2	2.46	0.46
1:A:59:ASN:OD1	1:A:61:LYS:HB3	2.16	0.45
1:B:41:ILE:HD11	1:B:87:ILE:HG21	1.98	0.45
1:B:191:GLU:OE1	1:B:195:ASN:OD1	2.34	0.45
1:A:50:LYS:HD3	1:A:67:ILE:HG13	1.98	0.44
1:A:255:THR:HG21	1:A:257:PHE:CZ	2.52	0.44
1:B:243:LEU:N	1:B:243:LEU:HD12	2.33	0.44
4:A:408:PE3:H202	4:A:408:PE3:H361	2.00	0.43
1:B:50:LYS:HE2	1:B:54:LYS:HE3	2.00	0.43
1:B:109:ASP:O	1:B:113:LYS:HG3	2.18	0.43
1:B:155:ILE:HG22	1:B:156:MET:HE3	1.99	0.43
1:A:211:TYR:CE2	1:A:233:CYS:SG	3.10	0.43
1:A:92:TYR:CZ	1:A:256:LYS:HE3	2.53	0.43
4:A:407:PE3:H111	1:B:108:GLN:NE2	2.33	0.43
1:A:56:ASN:O	1:A:57:LYS:HB2	2.17	0.43
1:B:96:ASN:OD1	3:B:404:CL:CL	2.74	0.43
1:B:213:ILE:HG13	1:B:233[B]:CYS:SG	2.59	0.42
1:A:259:ASN:OD1	1:A:261:GLU:HB3	2.19	0.42
1:A:268:PHE:CZ	1:A:272:LYS:HG3	2.54	0.42
1:B:63:ILE:O	1:B:67:ILE:HG12	2.19	0.42
1:A:270:ARG:HE	1:A:273:MET:HE2	1.84	0.42
1:A:214:ASN:ND2	6:A:504:HOH:O	2.44	0.41
1:B:111:TRP:CD1	1:B:111:TRP:C	2.96	0.41
1:A:35:LEU:O	1:A:94:SER:HA	2.20	0.41
1:B:49:VAL:O	1:B:53:LEU:HG	2.20	0.41
1:A:44:LYS:HE2	6:B:582:HOH:O	2.21	0.41
4:A:407:PE3:H111	1:B:108:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:HB2	1:B:93[A]:SER:OG	2.21	0.41
1:A:43:LYS:CE	1:B:109:ASP:OD1	2.69	0.41
1:A:152:LEU:O	1:A:156[B]:MET:HG2	2.20	0.41
1:A:59:ASN:OD1	1:A:61:LYS:N	2.52	0.40

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	254/275 (92%)	247 (97%)	7 (3%)	0	100	100
1	B	250/275 (91%)	240 (96%)	10 (4%)	0	100	100
All	All	504/550 (92%)	487 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	244/259 (94%)	244 (100%)	0	100	100
1	B	240/259 (93%)	240 (100%)	0	100	100
All	All	484/518 (93%)	484 (100%)	0	100	100

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

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 ⓘ

2 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	$\# Z  > 2$
1	CME	B	123	1	8,9,10	0.42	0	6,9,11	0.48	0
1	CME	A	123	1	8,9,10	0.41	0	6,9,11	0.50	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
1	CME	B	123	1	-	2/5/8/10	-
1	CME	A	123	1	-	0/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	123	CME	SD-CE-CZ-OH
1	B	123	CME	CA-CB-SG-SD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	123	CME	1	0
1	A	123	CME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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	$\# Z  > 2$
5	EDO	B	406	-	3,3,3	0.07	0	2,2,2	0.19	0
5	EDO	B	407	-	3,3,3	0.10	0	2,2,2	0.15	0
4	PE3	A	407	2	42,42,42	0.18	0	41,41,41	0.14	0
5	EDO	B	405	-	3,3,3	0.07	0	2,2,2	0.06	0
4	PE3	A	408	2	42,42,42	0.17	0	41,41,41	0.13	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
5	EDO	B	406	-	-	0/1/1/1	-
5	EDO	B	407	-	-	1/1/1/1	-
4	PE3	A	407	2	-	15/40/40/40	-
5	EDO	B	405	-	-	1/1/1/1	-
4	PE3	A	408	2	-	16/40/40/40	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

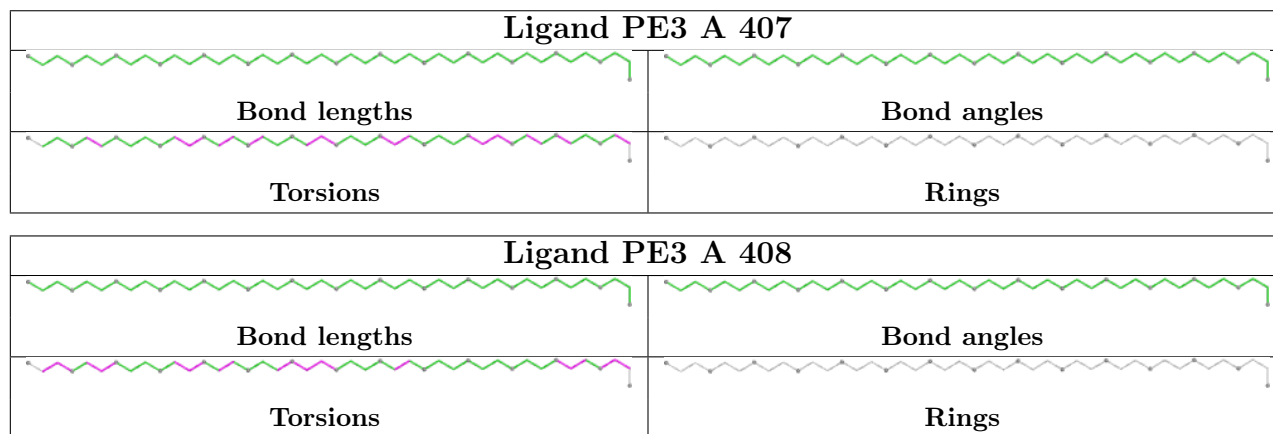
Mol	Chain	Res	Type	Atoms
4	A	408	PE3	O4-C5-C6-O7
4	A	407	PE3	O10-C11-C12-O13
4	A	408	PE3	O13-C14-C15-O16
4	A	408	PE3	O40-C41-C42-O43
4	A	407	PE3	O31-C32-C33-O34
4	A	407	PE3	O4-C5-C6-O7
4	A	407	PE3	O34-C35-C36-O37
4	A	407	PE3	O25-C26-C27-O28
4	A	407	PE3	O19-C20-C21-O22
4	A	407	PE3	O13-C14-C15-O16
4	A	408	PE3	O25-C26-C27-O28
4	A	408	PE3	O19-C20-C21-O22
4	A	408	PE3	O37-C38-C39-O40
4	A	407	PE3	C11-C12-O13-C14
4	A	408	PE3	C2-C3-O4-C5
4	A	407	PE3	C18-C17-O16-C15
4	A	407	PE3	C39-C38-O37-C36
4	A	408	PE3	C20-C21-O22-C23
4	A	408	PE3	C17-C18-O19-C20
4	A	407	PE3	C32-C33-O34-C35
4	A	408	PE3	C42-C41-O40-C39
4	A	408	PE3	C39-C38-O37-C36
4	A	407	PE3	C20-C21-O22-C23
5	B	405	EDO	O1-C1-C2-O2
4	A	408	PE3	C5-C6-O7-C8
4	A	408	PE3	O10-C11-C12-O13
5	B	407	EDO	O1-C1-C2-O2
4	A	407	PE3	C33-C32-O31-C30
4	A	407	PE3	O40-C41-C42-O43
4	A	408	PE3	C21-C20-O19-C18
4	A	408	PE3	O1-C2-C3-O4
4	A	407	PE3	C27-C26-O25-C24
4	A	408	PE3	C11-C12-O13-C14

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407	PE3	4	0
4	A	408	PE3	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.



## 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	A	256/275 (93%)	0.63	20 (7%)	20 21	13, 26, 51, 74	2 (0%)
1	B	251/275 (91%)	0.60	15 (5%)	29 31	12, 26, 48, 77	3 (1%)
All	All	507/550 (92%)	0.62	35 (6%)	24 25	12, 26, 48, 77	5 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	ILE	5.2
1	B	236	THR	3.6
1	B	207	ASN	3.5
1	B	237	LYS	3.2
1	A	274	SER	3.2
1	A	96	ASN	3.1
1	A	207	ASN	3.1
1	A	280	LEU	3.1
1	A	183	THR	3.0
1	B	281	PRO	3.0
1	B	117	ASP	2.9
1	B	183	THR	2.8
1	A	85	ILE	2.8
1	A	60	GLU	2.6
1	A	87	ILE	2.5
1	B	34	LYS	2.5
1	A	182	ASP	2.5
1	A	211	TYR	2.4
1	A	156[A]	MET	2.4
1	B	238	ASN	2.4
1	B	239	GLY	2.3
1	A	238	ASN	2.3
1	A	273	MET	2.2
1	A	192	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	2.2
1	A	159	LYS	2.2
1	A	188	LYS	2.2
1	B	209	ASN	2.2
1	B	115	PHE	2.2
1	B	185	ASP	2.1
1	A	184	ASP	2.1
1	A	281	PRO	2.0
1	B	61	LYS	2.0
1	A	282	ASP	2.0
1	B	272	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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
1	CME	A	123	10/11	0.91	0.11	13,17,29,36	0
1	CME	B	123	10/11	0.92	0.10	14,18,32,39	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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
5	EDO	B	405	4/4	0.79	0.13	41,42,43,44	0
4	PE3	A	408	43/43	0.83	0.14	28,37,44,49	0
4	PE3	A	407	43/43	0.84	0.13	30,39,52,57	0
5	EDO	B	406	4/4	0.85	0.15	42,43,43,49	0
3	CL	B	404	1/1	0.86	0.12	58,58,58,58	0

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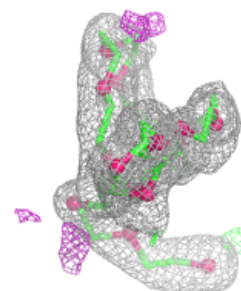
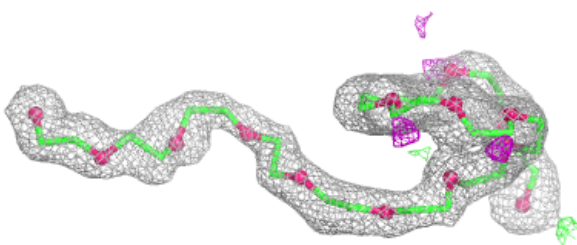
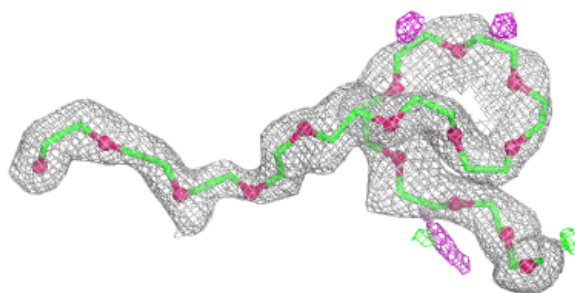
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	A	406	1/1	0.89	0.18	58,58,58,58	0
5	EDO	B	407	4/4	0.90	0.13	30,31,35,43	0
3	CL	A	404	1/1	0.95	0.07	43,43,43,43	0
3	CL	B	403	1/1	0.96	0.06	35,35,35,35	0
3	CL	A	405	1/1	0.97	0.05	34,34,34,34	0
3	CL	A	403	1/1	0.97	0.05	33,33,33,33	0
2	NA	A	401	1/1	0.97	0.06	26,26,26,26	0
3	CL	B	402	1/1	0.98	0.10	23,23,23,23	0
2	NA	B	401	1/1	0.99	0.05	19,19,19,19	0
3	CL	A	402	1/1	0.99	0.07	25,25,25,25	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.

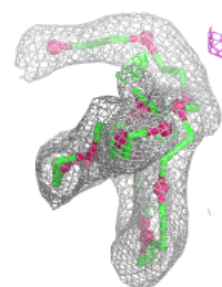
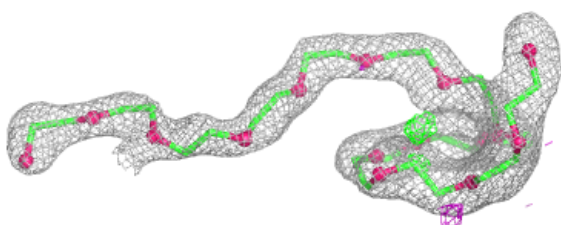
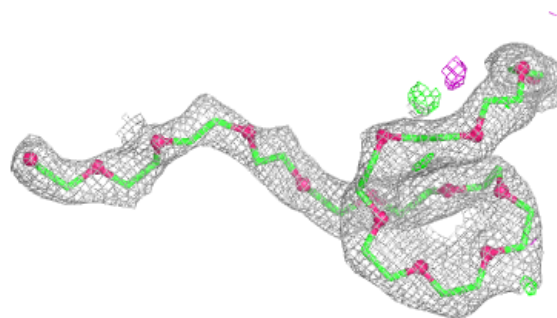
**Electron density around PE3 A 408:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PE3 A 407:**

$2mF_o-DF_c$  (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.