



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:46 am BST

PDB ID : 1UYO  
Title : Translocator domain of autotransporter NalP from *Neisseria meningitidis*  
Authors : Oomen, C.J.; Van Ulsen, P.; Van Gelder, P.; Feijen, M.; Tommassen, J.; Gros, P.  
Deposited on : 2004-03-02  
Resolution : 3.20 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.

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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 : 2.11  
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) : 2.11

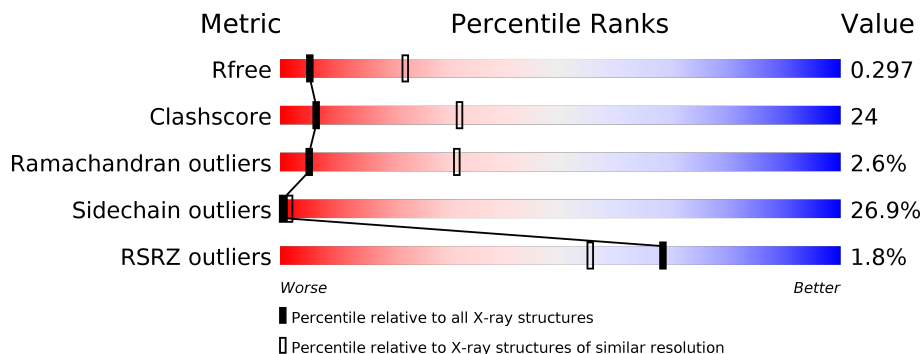
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	X	308	

## 2 Entry composition [i](#)

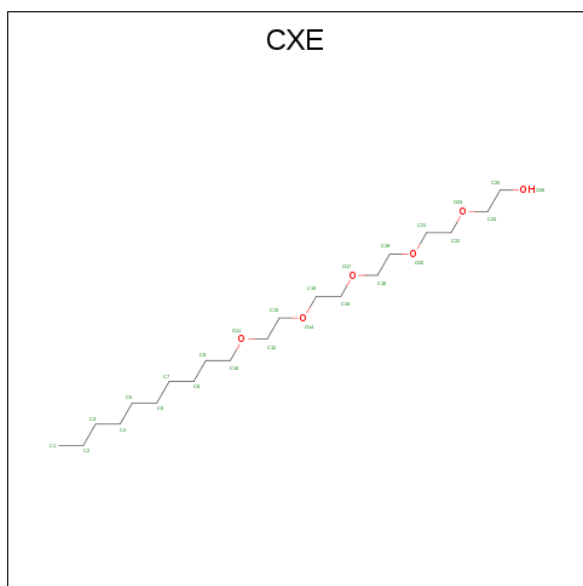
There are 2 unique types of molecules in this entry. The entry contains 1968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NALP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	X	277	1958	1200	363	390	5	0	0	0

- Molecule 2 is PENTAETHYLENE GLYCOL MONODECYL ETHER (three-letter code: CXE) (formula: C<sub>20</sub>H<sub>42</sub>O<sub>6</sub>).

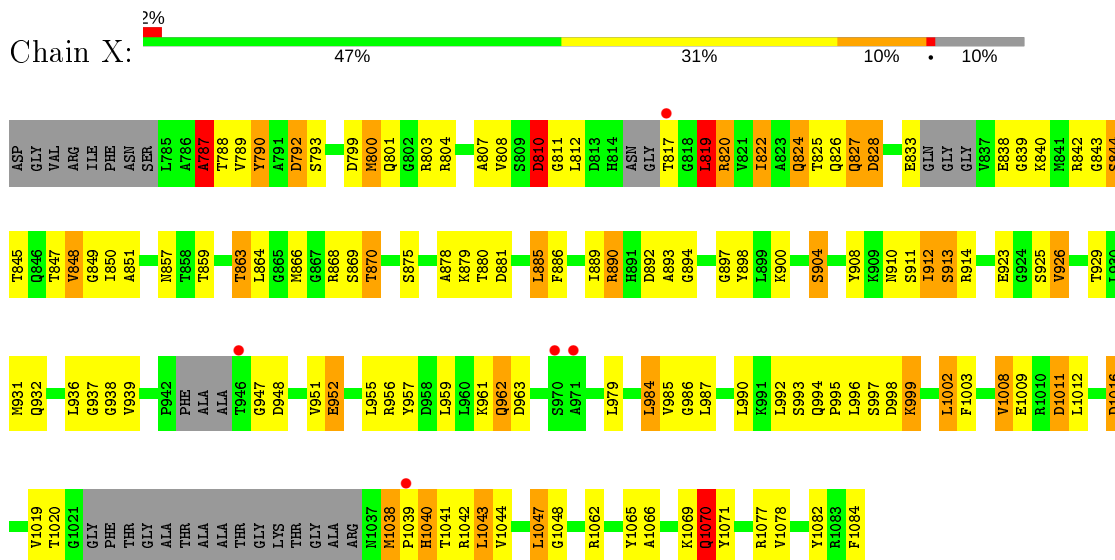


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	X	1	10	8	2	0	0

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

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

- Molecule 1: NALP



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.43Å 84.89Å 122.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 19.57 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.2 (30.00-3.20) 90.5 (19.57-3.20)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 3.22Å)	Xtrriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.215 , 0.298 0.221 , 0.297	Depositor DCC
$R_{free}$ test set	208 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtrriage
Anisotropy	0.233	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 81.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	1968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% 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: CXE

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	X	0.74	0/1975	1.06	10/2654 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	828	ASP	CB-CG-OD2	7.28	124.85	118.30
1	X	1047	LEU	CA-CB-CG	7.03	131.47	115.30
1	X	787	ALA	N-CA-C	-6.23	94.17	111.00
1	X	963	ASP	CB-CG-OD2	5.99	123.69	118.30
1	X	792	ASP	CB-CG-OD2	5.95	123.66	118.30
1	X	810	ASP	CB-CG-OD2	5.84	123.56	118.30
1	X	799	ASP	CB-CG-OD2	5.66	123.39	118.30
1	X	998	ASP	CB-CG-OD2	5.32	123.08	118.30
1	X	848	VAL	CB-CA-C	-5.09	101.72	111.40
1	X	948	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	819	LEU	Peptide

## 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	X	1958	0	1852	92	0
2	X	10	0	12	0	0
All	All	1968	0	1864	92	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 24.

All (92) 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:X:931:MSE:CE	1:X:931:MSE:SE	2.17	1.42
1:X:985:VAL:HG22	1:X:1011:ASP:OD1	1.74	0.88
1:X:959:LEU:HD21	1:X:961:LYS:HE3	1.55	0.87
1:X:827:GLN:OE1	1:X:844:SER:HB2	1.76	0.85
1:X:807:ALA:O	1:X:810:ASP:HB2	1.81	0.80
1:X:822:ILE:CD1	1:X:824:GLN:NE2	2.45	0.79
1:X:931:MSE:CE	1:X:931:MSE:HB3	2.13	0.78
1:X:822:ILE:HD11	1:X:824:GLN:NE2	2.01	0.75
1:X:824:GLN:OE1	1:X:1077:ARG:HD2	1.86	0.75
1:X:904:SER:OG	1:X:932:GLN:HB2	1.88	0.73
1:X:845:THR:HB	1:X:866:MSE:O	1.90	0.71
1:X:959:LEU:CD2	1:X:961:LYS:HE3	2.20	0.71
1:X:979:LEU:HD12	1:X:1019:VAL:HG12	1.73	0.70
1:X:931:MSE:HB3	1:X:931:MSE:HE2	1.75	0.69
1:X:908:TYR:OH	1:X:962:GLN:HG3	1.92	0.69
1:X:817:THR:HG22	1:X:1084:PHE:OXT	1.95	0.67
1:X:822:ILE:HD12	1:X:824:GLN:NE2	2.08	0.67
1:X:801:GLN:HA	1:X:804:ARG:HD2	1.77	0.66
1:X:1044:VAL:HG22	1:X:1066:ALA:HA	1.79	0.65
1:X:1003:PHE:HZ	1:X:1062:ARG:CZ	2.11	0.64
1:X:827:GLN:HG2	1:X:842:ARG:HH21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:804:ARG:HE	1:X:845:THR:HG21	1.64	0.62
1:X:822:ILE:CD1	1:X:824:GLN:HE21	2.11	0.62
1:X:849:GLY:HA3	1:X:863:THR:OG1	2.00	0.62
1:X:885:LEU:HD12	1:X:885:LEU:C	2.20	0.61
1:X:936:LEU:HD21	1:X:952:GLU:OE2	2.01	0.61
1:X:959:LEU:HD21	1:X:961:LYS:CE	2.30	0.60
1:X:804:ARG:HA	1:X:826:GLN:HE22	1.67	0.58
1:X:828:ASP:O	1:X:842:ARG:HD2	2.04	0.58
1:X:897:GLY:HA3	1:X:938:GLY:O	2.03	0.57
1:X:947:GLY:HA2	1:X:995:PRO:HD3	1.88	0.55
1:X:1008:VAL:HG22	1:X:1042:ARG:O	2.06	0.55
1:X:955:LEU:HA	1:X:985:VAL:O	2.08	0.53
1:X:822:ILE:HD11	1:X:824:GLN:HE22	1.70	0.52
1:X:910:ASN:HB2	1:X:926:VAL:HG13	1.90	0.52
1:X:822:ILE:CD1	1:X:824:GLN:HE22	2.22	0.52
1:X:803:ARG:NE	1:X:828:ASP:OD1	2.37	0.51
1:X:1016:ASP:C	1:X:1016:ASP:OD1	2.47	0.51
1:X:956:ARG:O	1:X:984:LEU:HD12	2.11	0.51
1:X:787:ALA:HA	1:X:790:TYR:HD2	1.76	0.50
1:X:1069:LYS:O	1:X:1070:GLN:HB2	2.13	0.49
1:X:820:ARG:HG2	1:X:851:ALA:HB3	1.93	0.49
1:X:819:LEU:H	1:X:819:LEU:HD23	1.77	0.49
1:X:789:VAL:O	1:X:793:SER:N	2.35	0.49
1:X:857:ASN:HB3	1:X:892:ASP:HB2	1.94	0.49
1:X:1044:VAL:CG2	1:X:1066:ALA:HA	2.43	0.49
1:X:987:LEU:CD2	1:X:1009:GLU:OE1	2.62	0.48
1:X:820:ARG:HA	1:X:1082:TYR:O	2.14	0.48
1:X:833:GLU:CB	1:X:838:GLU:HA	2.44	0.47
1:X:1044:VAL:HG22	1:X:1066:ALA:CA	2.42	0.47
1:X:898:TYR:O	1:X:937:GLY:HA2	2.14	0.47
1:X:893:ALA:O	1:X:894:GLY:C	2.52	0.47
1:X:957:TYR:HB2	1:X:984:LEU:HD13	1.95	0.47
1:X:1040:HIS:HB3	1:X:1041:THR:H	1.34	0.46
1:X:822:ILE:HD12	1:X:824:GLN:HE21	1.75	0.46
1:X:800:MSE:HE2	1:X:804:ARG:NH2	2.31	0.45
1:X:881:ASP:O	1:X:908:TYR:HA	2.15	0.45
1:X:936:LEU:CD2	1:X:952:GLU:OE2	2.65	0.45
1:X:1008:VAL:HG23	1:X:1043:LEU:HD22	1.97	0.45
1:X:1044:VAL:HA	1:X:1065:TYR:O	2.17	0.45
1:X:800:MSE:HE1	1:X:869:SER:HB2	1.98	0.45
1:X:900:LYS:HB2	1:X:936:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:955:LEU:HD23	1:X:985:VAL:O	2.17	0.44
1:X:984:LEU:HD12	1:X:984:LEU:HA	1.54	0.44
1:X:1003:PHE:CE1	1:X:1048:GLY:HA3	2.53	0.44
1:X:951:VAL:HG22	1:X:990:LEU:CD1	2.48	0.44
1:X:839:GLY:O	1:X:840:LYS:HG2	2.17	0.44
1:X:1038:MSE:HA	1:X:1039:PRO:HD3	1.68	0.44
1:X:801:GLN:HA	1:X:804:ARG:CD	2.44	0.44
1:X:908:TYR:C	1:X:908:TYR:CD1	2.91	0.43
1:X:1016:ASP:O	1:X:1016:ASP:OD1	2.35	0.43
1:X:842:ARG:HG2	1:X:842:ARG:HH11	1.83	0.43
1:X:788:THR:HG22	1:X:792:ASP:OD2	2.18	0.43
1:X:996:LEU:HD22	1:X:1002:LEU:HD12	2.01	0.43
1:X:955:LEU:HD23	1:X:986:GLY:HA2	2.01	0.43
1:X:804:ARG:NE	1:X:845:THR:HG21	2.33	0.43
1:X:850:ILE:HD13	1:X:850:ILE:HG21	1.72	0.43
1:X:869:SER:O	1:X:880:THR:N	2.52	0.43
1:X:897:GLY:CA	1:X:938:GLY:O	2.66	0.43
1:X:1008:VAL:HG13	1:X:1009:GLU:N	2.34	0.42
1:X:869:SER:HB3	1:X:880:THR:HB	2.01	0.42
1:X:826:GLN:HB2	1:X:1077:ARG:HG3	2.00	0.42
1:X:889:ILE:HG23	1:X:889:ILE:O	2.21	0.41
1:X:931:MSE:CB	1:X:931:MSE:CE	2.94	0.41
1:X:812:LEU:HD13	1:X:890:ARG:HB2	2.02	0.41
1:X:984:LEU:HG	1:X:1012:LEU:HD12	2.02	0.41
1:X:800:MSE:CE	1:X:843:GLY:HA3	2.51	0.41
1:X:870:THR:HA	1:X:878:ALA:O	2.21	0.41
1:X:1070:GLN:HB3	1:X:1070:GLN:HE21	1.73	0.41
1:X:808:VAL:HG21	1:X:886:PHE:CB	2.51	0.41
1:X:912:ILE:CG2	1:X:913:SER:N	2.83	0.41
1:X:788:THR:O	1:X:792:ASP:N	2.42	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	X	267/308 (87%)	234 (88%)	26 (10%)	7 (3%)	5 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	787	ALA
1	X	1071	TYR
1	X	819	LEU
1	X	999	LYS
1	X	1070	GLN
1	X	811	GLY
1	X	790	TYR

### 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	X	182/214 (85%)	133 (73%)	49 (27%)	0 2

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	800	MSE
1	X	810	ASP
1	X	819	LEU
1	X	820	ARG
1	X	822	ILE
1	X	824	GLN
1	X	825	THR
1	X	827	GLN
1	X	844	SER
1	X	847	THR
1	X	848	VAL
1	X	859	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	X	863	THR
1	X	864	LEU
1	X	868	ARG
1	X	870	THR
1	X	875	SER
1	X	879	LYS
1	X	885	LEU
1	X	890	ARG
1	X	904	SER
1	X	911	SER
1	X	912	ILE
1	X	913	SER
1	X	914	ARG
1	X	923	GLU
1	X	925	SER
1	X	926	VAL
1	X	929	THR
1	X	939	VAL
1	X	952	GLU
1	X	962	GLN
1	X	984	LEU
1	X	992	LEU
1	X	993	SER
1	X	994	GLN
1	X	997	SER
1	X	999	LYS
1	X	1002	LEU
1	X	1008	VAL
1	X	1011	ASP
1	X	1016	ASP
1	X	1020	THR
1	X	1038	MSE
1	X	1040	HIS
1	X	1043	LEU
1	X	1047	LEU
1	X	1070	GLN
1	X	1078	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	X	826	GLN

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Mol	Chain	Res	Type
1	X	910	ASN
1	X	927	ASN
1	X	1070	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is 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	CXE	X	2085	-	9,9,25	0.33	0	8,8,24	0.34	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	CXE	X	2085	-	-	5/7/7/23	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

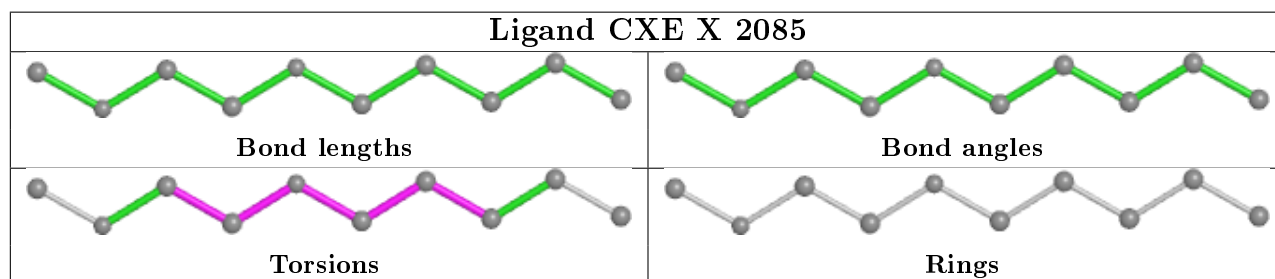
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	2085	CXE	C9-C10-O11-C12
2	X	2085	CXE	O11-C12-C13-O14
2	X	2085	CXE	O11-C10-C9-C8
2	X	2085	CXE	C7-C8-C9-C10
2	X	2085	CXE	C13-C12-O11-C10

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	X	272/308 (88%)	-0.49	5 (1%) 68 55	2, 19, 42, 63	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	817	THR	2.9
1	X	1039	PRO	2.6
1	X	971	ALA	2.4
1	X	946	THR	2.2
1	X	970	SER	2.1

### 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.

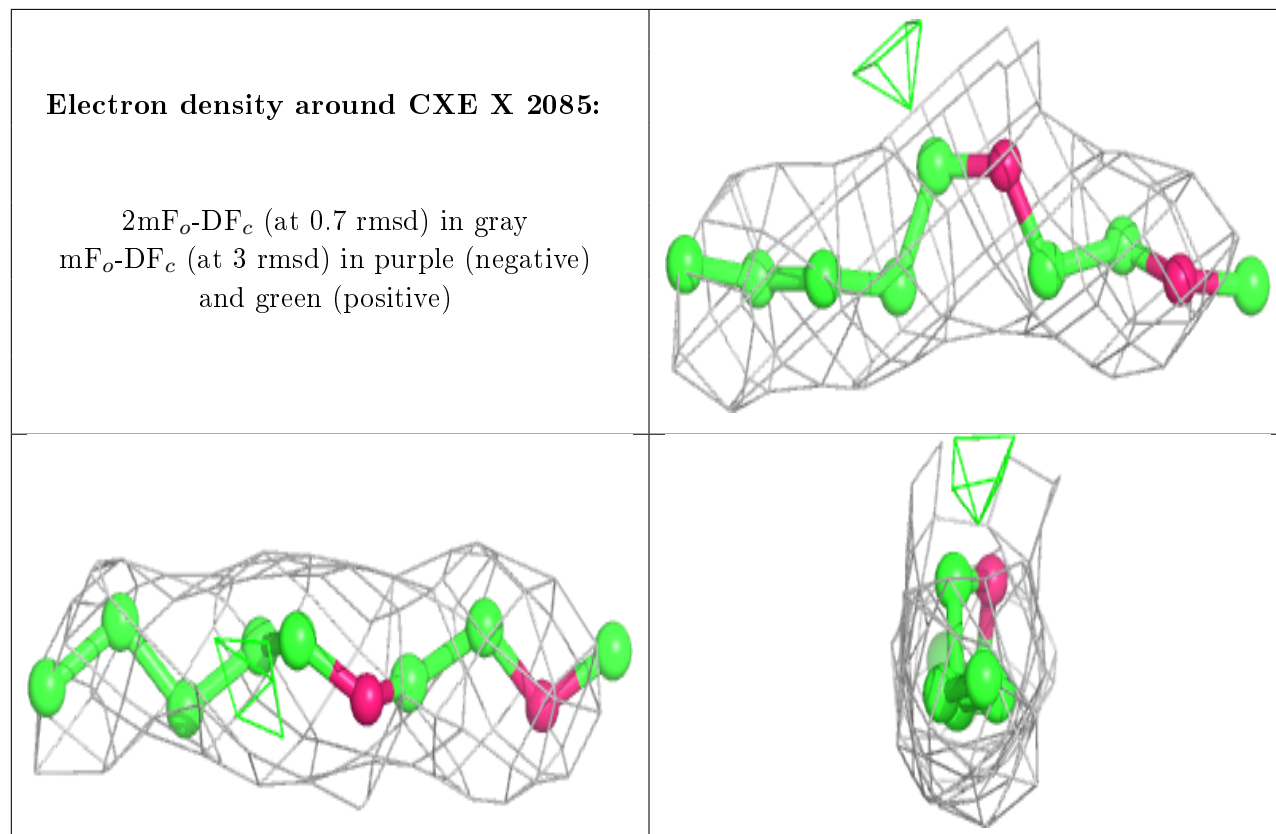
### 6.4 Ligands [i](#)

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. 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	CXE	X	2085	10/26	0.90	0.23	68,71,76,78	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.