Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 02:28 AM BST

PDB ID	:	5NEC
Title	:	Crystal structure of the siderophore receptor PiuD from Pseudomonas aeruginosa
Authors	:	Moynie, L.; Naismith, J.H.
Deposited on	:	2017-03-10
Resolution	:	2.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

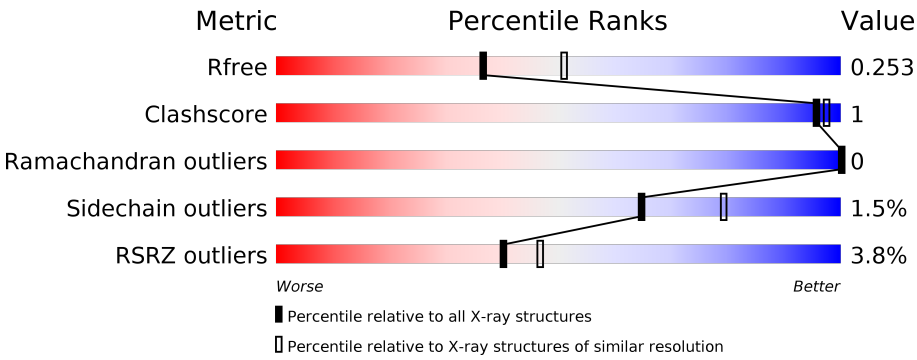
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 >=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 <=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	741	3% 82% • 14%
1	B	741	4% 83% • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10154 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.

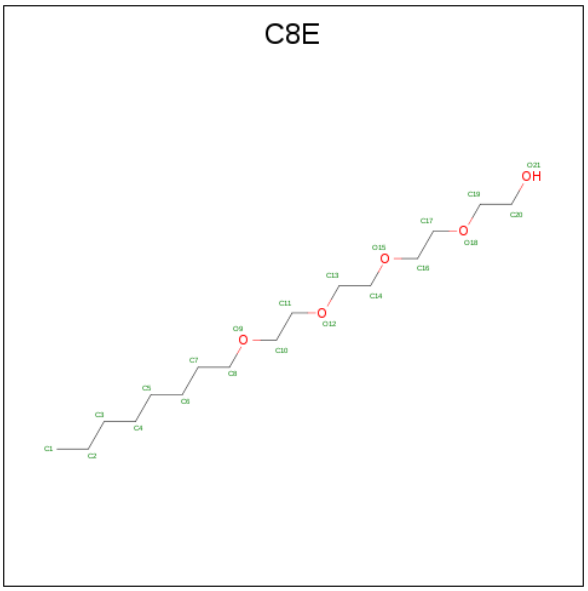
- Molecule 1 is a protein called TonB-dependent siderophore receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	637	5014	3145	868	997	4	0	0	0
1	B	646	5059	3169	878	1008	4	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP V6ALN4
A	0	MET	-	expression tag	UNP V6ALN4
A	1	ASN	ASP	conflict	UNP V6ALN4
A	732	LEU	-	expression tag	UNP V6ALN4
A	733	GLU	-	expression tag	UNP V6ALN4
A	734	HIS	-	expression tag	UNP V6ALN4
A	735	HIS	-	expression tag	UNP V6ALN4
A	736	HIS	-	expression tag	UNP V6ALN4
A	737	HIS	-	expression tag	UNP V6ALN4
A	738	HIS	-	expression tag	UNP V6ALN4
A	739	HIS	-	expression tag	UNP V6ALN4
B	-1	ALA	-	expression tag	UNP V6ALN4
B	0	MET	-	expression tag	UNP V6ALN4
B	1	ASN	ASP	conflict	UNP V6ALN4
B	732	LEU	-	expression tag	UNP V6ALN4
B	733	GLU	-	expression tag	UNP V6ALN4
B	734	HIS	-	expression tag	UNP V6ALN4
B	735	HIS	-	expression tag	UNP V6ALN4
B	736	HIS	-	expression tag	UNP V6ALN4
B	737	HIS	-	expression tag	UNP V6ALN4
B	738	HIS	-	expression tag	UNP V6ALN4
B	739	HIS	-	expression tag	UNP V6ALN4

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0

- Molecule 3 is water.

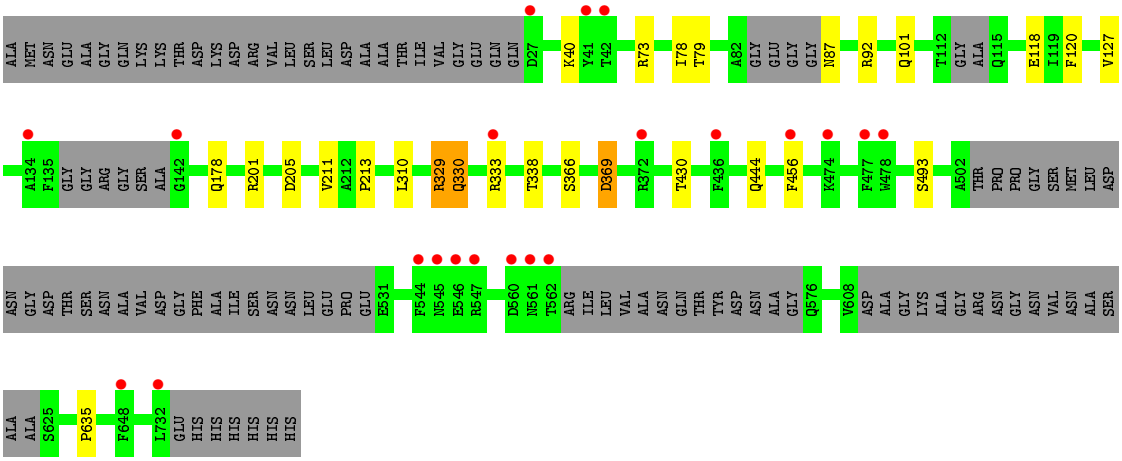
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	32	Total O 32 32	0	0

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.

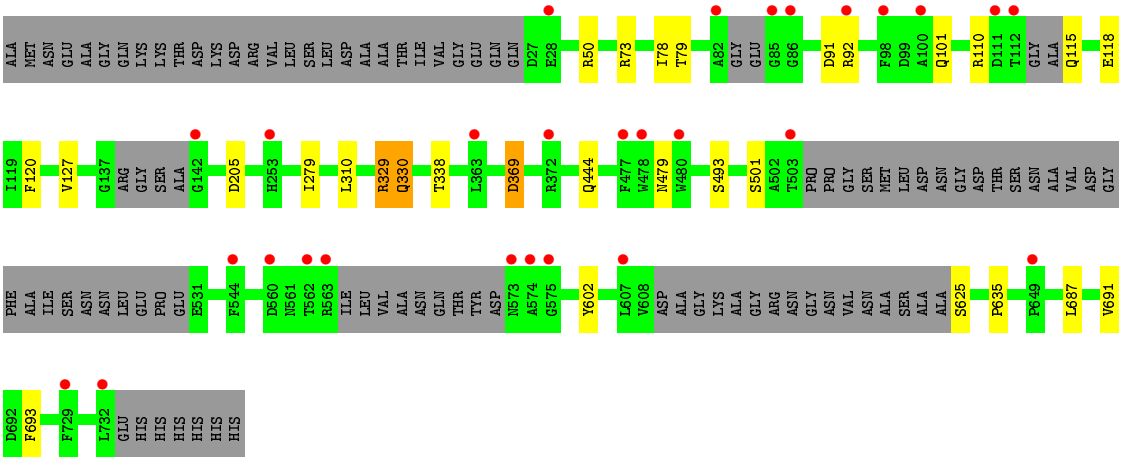
- Molecule 1: TonB-dependent siderophore receptor

Chain A:



- Molecule 1: TonB-dependent siderophore receptor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.52Å 136.45Å 118.95Å 90.00° 132.04° 90.00°	Depositor
Resolution (Å)	91.03 – 2.30 49.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (91.03-2.30) 98.5 (49.24-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.223 , 0.249 0.228 , 0.253	Depositor DCC
R_{free} test set	4250 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10154	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: C8E

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	0.53	0/5132	0.73	3/6972 (0.0%)
1	B	0.54	0/5177	0.74	5/7032 (0.1%)
All	All	0.54	0/10309	0.73	8/14004 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	B	329	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	B	73	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	A	73	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	205	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	205	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	50	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	201	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5014	0	4750	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5059	0	4785	10	1
2	A	16	0	30	0	0
3	A	33	0	0	0	0
3	B	32	0	0	0	0
All	All	10154	0	9565	22	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 1.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:SER:HG	1:A:430:THR:HG1	1.49	0.56
1:A:79:THR:HG21	1:A:635:PRO:HD3	1.87	0.56
1:B:79:THR:HG21	1:B:635:PRO:HD3	1.89	0.54
1:B:687:LEU:HD12	1:B:691:VAL:HG12	1.90	0.53
1:A:92:ARG:HG3	1:A:101:GLN:HB3	1.93	0.51
1:A:329:ARG:HD2	1:A:330:GLN:O	2.10	0.51
1:B:338:THR:HB	1:B:369:ASP:HB2	1.92	0.51
1:A:78:ILE:HD11	1:A:127:VAL:HG11	1.92	0.50
1:B:92:ARG:HG3	1:B:101:GLN:HB3	1.93	0.50
1:A:87:ASN:OD1	1:A:333:ARG:NH2	2.44	0.49
1:A:338:THR:HB	1:A:369:ASP:HB2	1.94	0.49
1:B:78:ILE:HD11	1:B:127:VAL:HG11	1.94	0.49
1:A:366:SER:OG	1:A:430:THR:OG1	2.22	0.46
1:A:310:LEU:HD11	1:A:330:GLN:HG2	2.00	0.44
1:A:430:THR:HG22	1:A:456:PHE:HD1	1.84	0.42
1:A:211:VAL:HG22	1:A:213:PRO:HD3	2.01	0.42
1:B:118:GLU:HG3	1:B:120:PHE:HD1	1.85	0.41
1:B:279:ILE:HD12	1:B:279:ILE:N	2.35	0.41
1:B:310:LEU:HD11	1:B:330:GLN:HG2	2.01	0.41
1:A:118:GLU:HG3	1:A:120:PHE:HD1	1.85	0.41
1:B:479:ASN:HD22	1:B:501:SER:HB3	1.85	0.41
1:B:687:LEU:HD11	1:B:693:PHE:HB2	2.02	0.40

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:B:602:TYR:OH	1:B:602:TYR:OH[2_656]	2.16	0.04

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	623/741 (84%)	611 (98%)	12 (2%)	0	100	100
1	B	632/741 (85%)	618 (98%)	14 (2%)	0	100	100
All	All	1255/1482 (85%)	1229 (98%)	26 (2%)	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	545/618 (88%)	538 (99%)	7 (1%)	69	82
1	B	547/618 (88%)	538 (98%)	9 (2%)	62	78
All	All	1092/1236 (88%)	1076 (98%)	16 (2%)	65	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	178	GLN
1	A	329	ARG
1	A	330	GLN
1	A	369	ASP
1	A	444	GLN
1	A	493	SER
1	B	91	ASP

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Mol	Chain	Res	Type
1	B	110	ARG
1	B	115	GLN
1	B	329	ARG
1	B	330	GLN
1	B	369	ASP
1	B	444	GLN
1	B	493	SER
1	B	625	SER

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	C8E	A	801	-	7,7,20	0.40	0	6,6,19	0.21	0
2	C8E	A	802	-	7,7,20	0.35	0	6,6,19	0.28	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	C8E	A	801	-	-	1/5/5/18	-
2	C8E	A	802	-	-	2/5/5/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

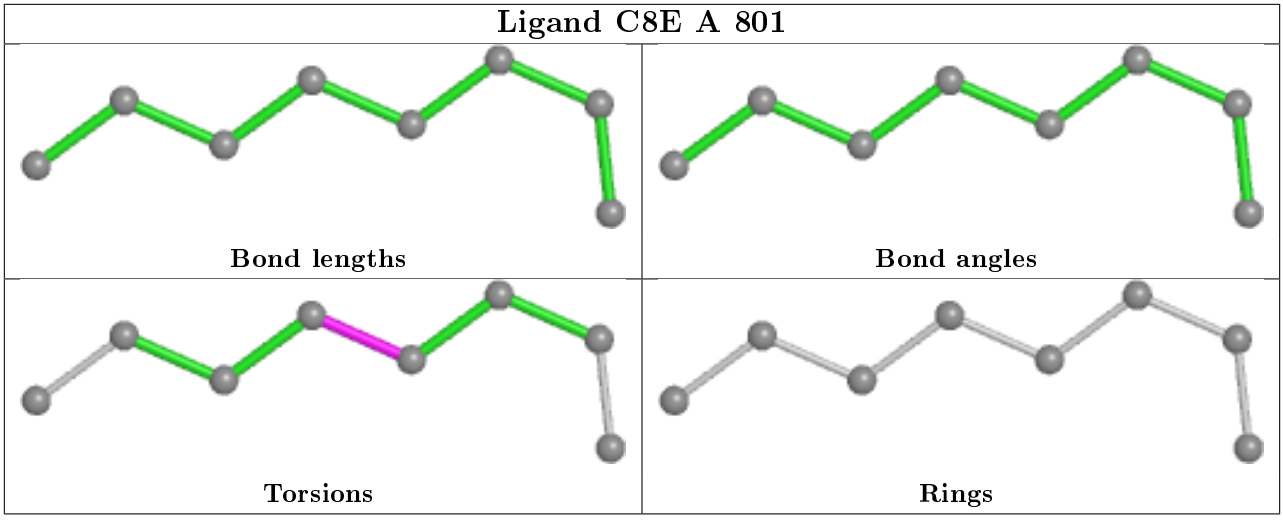
All (3) torsion outliers are listed below:

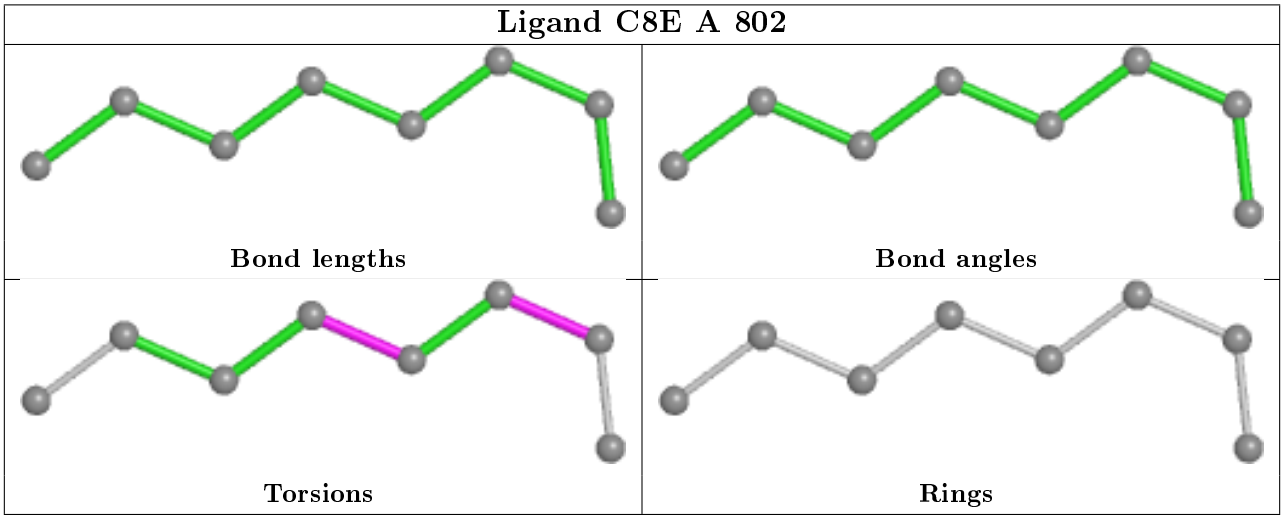
Mol	Chain	Res	Type	Atoms
2	A	801	C8E	C3-C4-C5-C6
2	A	802	C8E	C1-C2-C3-C4
2	A	802	C8E	C3-C4-C5-C6

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 then 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, 95th 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^2)	Q<0.9
1	A	637/741 (85%)	0.13	21 (3%)	46	53	34, 55, 82, 107	0
1	B	646/741 (87%)	0.18	28 (4%)	35	42	35, 53, 84, 107	0
All	All	1283/1482 (86%)	0.15	49 (3%)	40	47	34, 54, 83, 107	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	GLY	9.0
1	B	478	TRP	5.6
1	B	112	THR	4.5
1	A	478	TRP	3.8
1	B	111	ASP	3.6
1	A	544	PHE	3.4
1	A	27	ASP	3.4
1	A	142	GLY	3.3
1	B	574	ALA	3.3
1	A	41	TYR	3.3
1	A	561	ASN	3.2
1	B	100	ALA	3.2
1	A	547	ARG	3.1
1	A	456	PHE	3.1
1	A	474	LYS	3.0
1	A	477	PHE	3.0
1	B	575	GLY	3.0
1	A	436	PHE	2.9
1	B	729	PHE	2.9
1	A	134	ALA	2.9
1	B	142	GLY	2.9
1	A	562	THR	2.8
1	A	732	LEU	2.8
1	B	28	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	546	GLU	2.7
1	A	560	ASP	2.6
1	A	545	ASN	2.5
1	A	333	ARG	2.4
1	B	92	ARG	2.3
1	B	82	ALA	2.3
1	B	649	PRO	2.3
1	B	573	ASN	2.3
1	A	42	THR	2.3
1	B	607	LEU	2.2
1	B	560	ASP	2.2
1	B	480	TRP	2.2
1	B	98	PHE	2.2
1	A	372	ARG	2.1
1	B	563	ARG	2.1
1	B	253	HIS	2.1
1	B	372	ARG	2.1
1	B	732	LEU	2.1
1	B	544	PHE	2.1
1	B	86	GLY	2.1
1	B	363	LEU	2.0
1	A	648	PHE	2.0
1	B	477	PHE	2.0
1	B	503	THR	2.0
1	B	562	THR	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

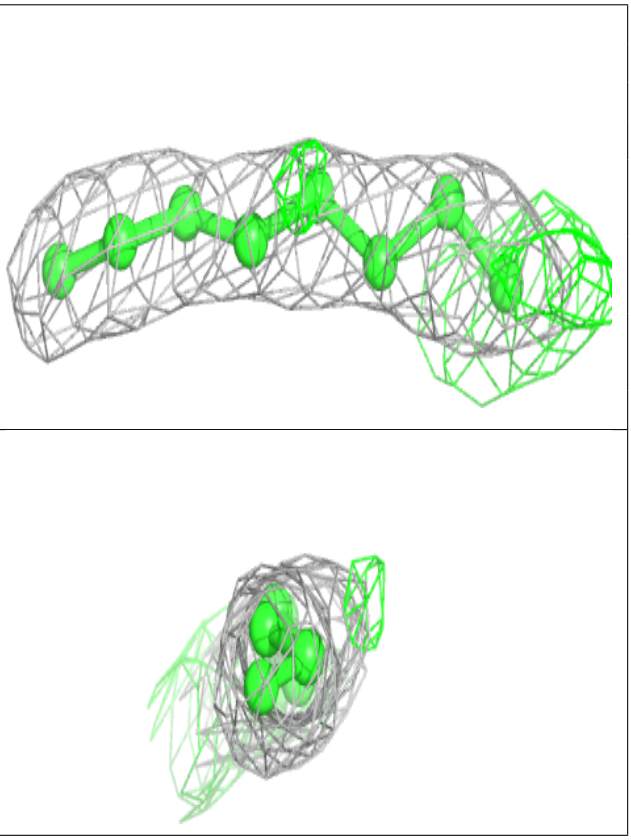
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	C8E	A	802	8/21	0.79	0.16	66,68,69,69	0
2	C8E	A	801	8/21	0.81	0.22	54,58,61,61	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.

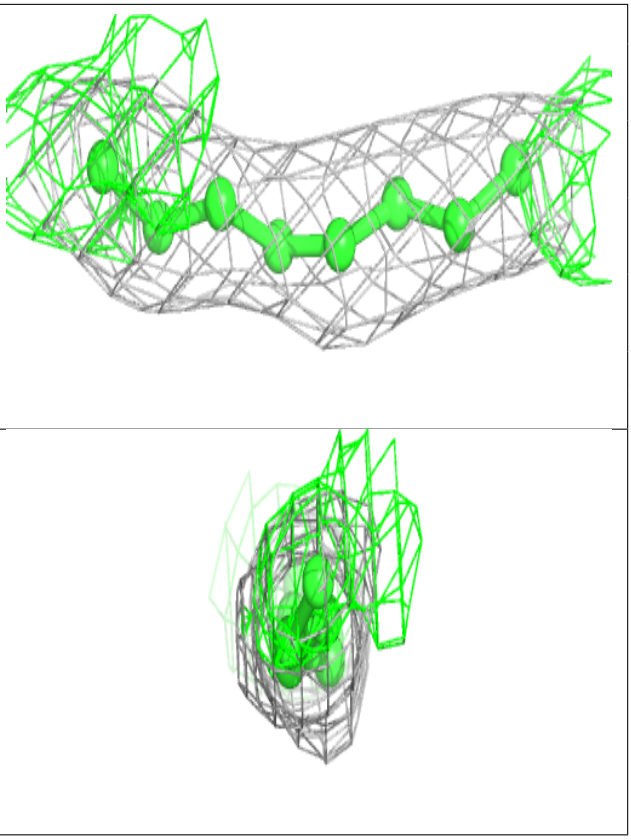
Electron density around C8E A 802:

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 C8E A 801:

$2mF_o$-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.