



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 6QGY / pdb_00006qgy
Title : Crystal structure of E.coli BamA beta-barrel in complex with nanobody B12
Authors : Hartmann, J.-B.; Kaur, H.; Jakob, R.P.; Zahn, M.; Zimmermann, I.; Seeger, M.; Maier, T.; Hiller, S.
Deposited on : 2019-01-14
Resolution : 2.51 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

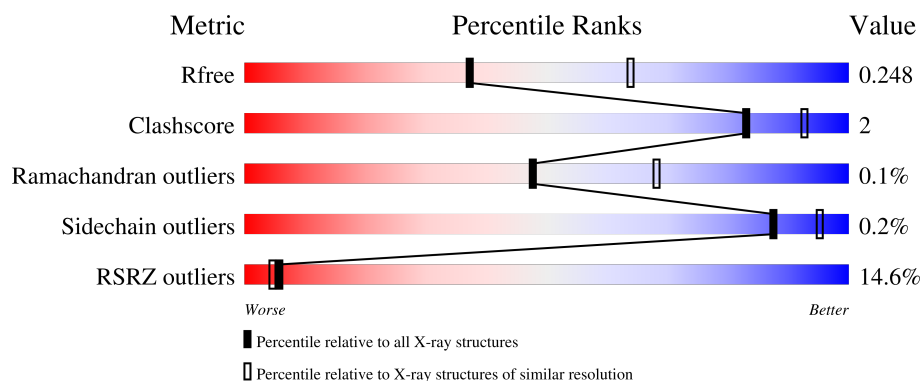
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

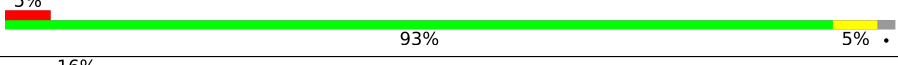
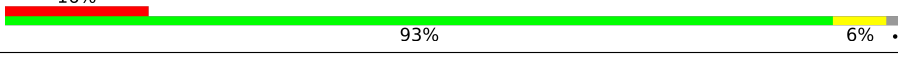
The reported resolution of this entry is 2.51 Å.

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	411	
1	C	411	
2	B	124	
2	D	124	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15487 atoms, of which 7334 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	H	N	O	S	0	0	0
			5585	1859	2667	471	580	8			
1	C	370	Total	C	H	N	O	S	0	0	0
			5607	1865	2680	473	581	8			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	MET	-	initiating methionine	UNP P0A942
A	401	GLY	-	expression tag	UNP P0A942
A	402	SER	-	expression tag	UNP P0A942
A	403	SER	-	expression tag	UNP P0A942
A	404	HIS	-	expression tag	UNP P0A942
A	405	HIS	-	expression tag	UNP P0A942
A	406	HIS	-	expression tag	UNP P0A942
A	407	HIS	-	expression tag	UNP P0A942
A	408	HIS	-	expression tag	UNP P0A942
A	409	HIS	-	expression tag	UNP P0A942
A	410	SER	-	expression tag	UNP P0A942
A	411	SER	-	expression tag	UNP P0A942
A	412	GLY	-	expression tag	UNP P0A942
A	413	GLU	-	expression tag	UNP P0A942
A	414	ASN	-	expression tag	UNP P0A942
A	415	LEU	-	expression tag	UNP P0A942
A	416	TYR	-	expression tag	UNP P0A942
A	417	PHE	-	expression tag	UNP P0A942
A	418	GLN	-	expression tag	UNP P0A942
A	419	HIS	-	expression tag	UNP P0A942
A	420	MET	-	expression tag	UNP P0A942
A	690	SER	CYS	engineered mutation	UNP P0A942
A	700	SER	CYS	engineered mutation	UNP P0A942
C	400	MET	-	initiating methionine	UNP P0A942
C	401	GLY	-	expression tag	UNP P0A942

Continued on next page...

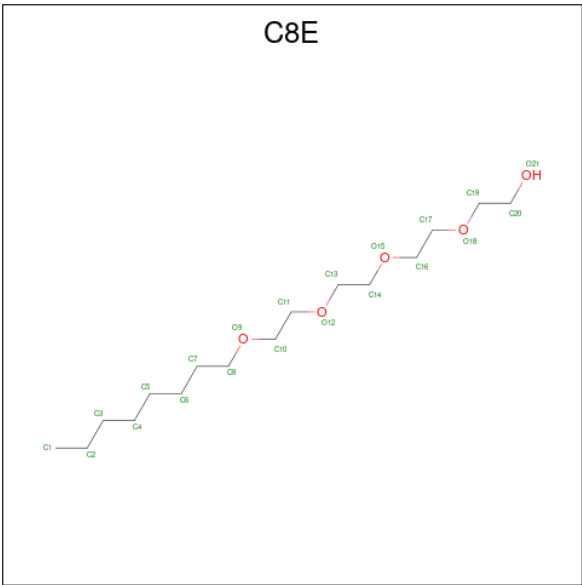
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	402	SER	-	expression tag	UNP P0A942
C	403	SER	-	expression tag	UNP P0A942
C	404	HIS	-	expression tag	UNP P0A942
C	405	HIS	-	expression tag	UNP P0A942
C	406	HIS	-	expression tag	UNP P0A942
C	407	HIS	-	expression tag	UNP P0A942
C	408	HIS	-	expression tag	UNP P0A942
C	409	HIS	-	expression tag	UNP P0A942
C	410	SER	-	expression tag	UNP P0A942
C	411	SER	-	expression tag	UNP P0A942
C	412	GLY	-	expression tag	UNP P0A942
C	413	GLU	-	expression tag	UNP P0A942
C	414	ASN	-	expression tag	UNP P0A942
C	415	LEU	-	expression tag	UNP P0A942
C	416	TYR	-	expression tag	UNP P0A942
C	417	PHE	-	expression tag	UNP P0A942
C	418	GLN	-	expression tag	UNP P0A942
C	419	HIS	-	expression tag	UNP P0A942
C	420	MET	-	expression tag	UNP P0A942
C	690	SER	CYS	engineered mutation	UNP P0A942
C	700	SER	CYS	engineered mutation	UNP P0A942

- Molecule 2 is a protein called NanoB12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	121	Total	C	H	N	O	S	0	0	0
			1833	585	893	169	181	5			
2	D	122	Total	C	H	N	O	S	0	0	0
			1840	587	896	170	182	5			

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 29 9 19 1	0	0
3	A	1	Total C H O 29 9 19 1	0	0
3	A	1	Total C H 22 7 15	0	0
3	A	1	Total C H O 29 9 19 1	0	0
3	A	1	Total C H O 39 12 25 2	0	0
3	C	1	Total C H O 47 14 29 4	0	0
3	C	1	Total C H 22 7 15	0	0
3	C	1	Total C H O 40 12 25 3	0	0
3	C	1	Total C H O 26 8 17 1	0	0
3	C	1	Total C H 22 7 15	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	134	Total O 134 134	0	0
4	B	31	Total O 31 31	0	0

Continued on next page...

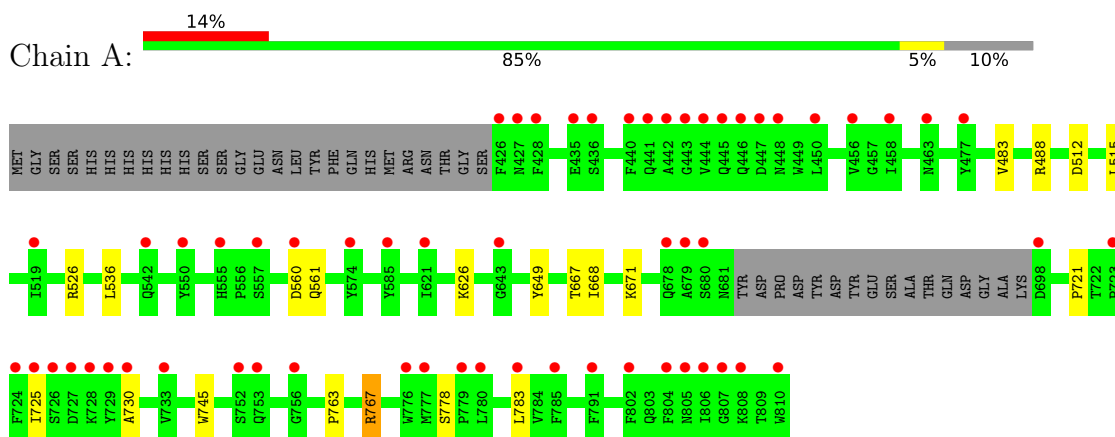
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	122	Total 122	O 122	0	0
4	D	30	Total 30	O 30	0	0

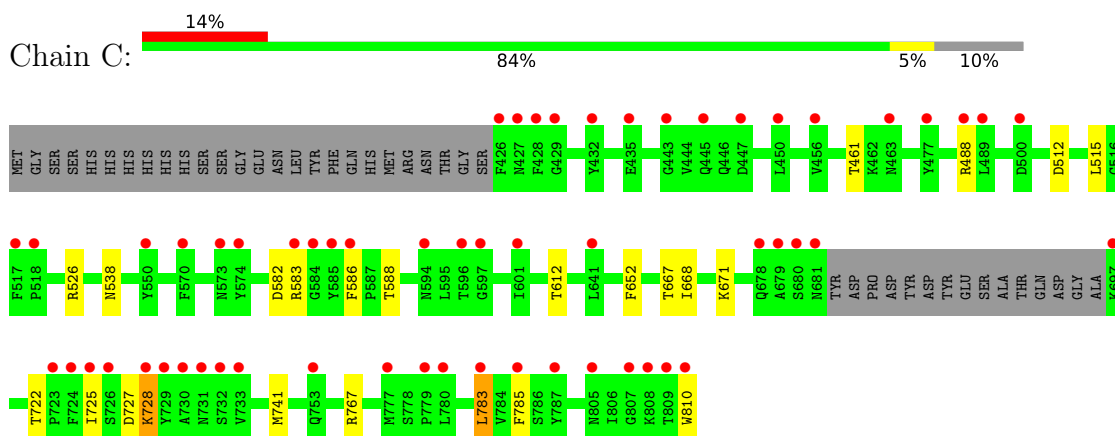
3 Residue-property plots [i](#)

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.

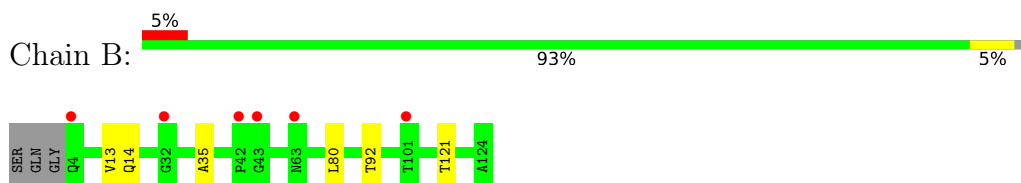
- Molecule 1: Outer membrane protein assembly factor BamA



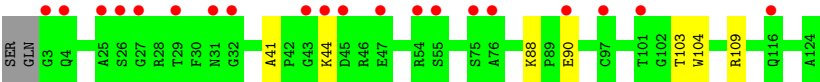
- Molecule 1: Outer membrane protein assembly factor BamA



- Molecule 2: NanoB12



- Molecule 2: NanoB12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.71Å 86.66Å 125.03Å 90.00° 105.26° 90.00°	Depositor
Resolution (Å)	48.48 – 2.51 48.48 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.48-2.51) 98.4 (48.48-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.222 , 0.244 0.228 , 0.248	Depositor DCC
R_{free} test set	3567 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15487	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.19	0/3008	0.34	0/4094
1	C	0.20	0/3017	0.36	0/4105
2	B	0.19	0/961	0.33	0/1298
2	D	0.21	0/965	0.38	0/1303
All	All	0.20	0/7951	0.35	0/10800

There are no bond length outliers.

There are no bond angle outliers.

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	2918	2667	2667	12	0
1	C	2927	2680	2680	19	0
2	B	940	893	893	3	0
2	D	944	896	896	4	0
3	A	51	97	87	1	0
3	C	56	101	97	0	0
4	A	134	0	0	0	0
4	B	31	0	0	0	0
4	C	122	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	30	0	0	0	0
All	All	8153	7334	7320	37	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 2.

All (37) 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:C:783:LEU:HD21	1:C:785:PHE:CE2	2.21	0.74
1:C:488:ARG:NH2	1:C:512:ASP:OD2	2.25	0.69
1:A:725:ILE:O	1:A:730:ALA:HB2	1.94	0.66
1:C:538:ASN:OD1	2:D:109:ARG:NH1	2.28	0.66
1:A:667:THR:O	1:A:671:LYS:NZ	2.29	0.64
1:C:667:THR:O	1:C:671:LYS:NZ	2.31	0.63
1:A:488:ARG:NH2	1:A:512:ASP:OD2	2.31	0.62
2:D:41:ALA:HB3	2:D:44:LYS:HD2	1.81	0.62
1:C:783:LEU:HD21	1:C:785:PHE:CD2	2.36	0.61
1:A:483:VAL:HG21	3:A:904:C8E:H82	1.91	0.53
1:C:722:THR:O	1:C:725:ILE:HG22	2.09	0.52
1:C:727:ASP:O	1:C:728:LYS:HB2	2.12	0.50
1:C:582:ASP:OD2	1:C:588:THR:OG1	2.29	0.50
2:D:88:LYS:HD2	2:D:90:GLU:OE2	2.11	0.50
1:C:668:ILE:HG23	1:C:767:ARG:CD	2.42	0.50
1:C:783:LEU:C	1:C:783:LEU:HD23	2.38	0.49
1:C:668:ILE:HG23	1:C:767:ARG:HD3	1.95	0.49
1:A:536:LEU:HD11	1:A:649:TYR:CE1	2.50	0.47
1:A:626:LYS:HB3	1:A:721:PRO:HG3	1.97	0.46
1:C:612:THR:HG22	1:C:652:PHE:HE1	1.81	0.45
1:A:515:LEU:O	1:A:526:ARG:HA	2.17	0.44
1:C:583:ARG:NH2	1:C:586:PHE:HB2	2.32	0.44
1:A:560:ASP:OD1	1:A:561:GLN:N	2.50	0.44
1:C:741:MET:HA	1:C:767:ARG:O	2.18	0.44
1:A:778:SER:OG	1:A:783:LEU:HD13	2.17	0.44
1:C:461:THR:HG23	1:C:810:TRP:NE1	2.33	0.43
1:C:461:THR:HG23	1:C:810:TRP:CE2	2.54	0.43
1:A:725:ILE:O	1:A:725:ILE:HG13	2.20	0.42
1:A:668:ILE:HG23	1:A:767:ARG:HD2	2.01	0.42
2:D:103:THR:HG22	2:D:104:TRP:N	2.35	0.42
1:C:612:THR:HG22	1:C:652:PHE:CE1	2.54	0.41
2:B:13:VAL:HG12	2:B:14:GLN:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ALA:HB1	2:B:80:LEU:HD22	2.02	0.41
1:C:461:THR:HG23	1:C:810:TRP:CZ2	2.55	0.41
1:C:515:LEU:O	1:C:526:ARG:HA	2.21	0.40
1:A:745:TRP:CE2	1:A:763:PRO:HB3	2.56	0.40
2:B:92:THR:HG23	2:B:121:THR:HA	2.04	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	365/411 (89%)	353 (97%)	12 (3%)	0	100	100
1	C	366/411 (89%)	353 (96%)	12 (3%)	1 (0%)	36	55
2	B	119/124 (96%)	119 (100%)	0	0	100	100
2	D	120/124 (97%)	119 (99%)	1 (1%)	0	100	100
All	All	970/1070 (91%)	944 (97%)	25 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	728	LYS

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	309/345 (90%)	308 (100%)	1 (0%)	86	94
1	C	310/345 (90%)	309 (100%)	1 (0%)	86	94
2	B	94/96 (98%)	94 (100%)	0	100	100
2	D	94/96 (98%)	94 (100%)	0	100	100
All	All	807/882 (92%)	805 (100%)	2 (0%)	87	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	767	ARG
1	C	783	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	466	GLN
1	A	540	GLN
1	A	606	ASN
1	A	666	ASN
1	A	677	HIS
1	A	789	GLN
1	A	801	GLN
1	C	466	GLN
1	C	492	ASN
1	C	506	ASN
1	C	534	ASN
1	C	540	GLN
1	C	606	ASN
1	C	664	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
3	C8E	A	902	-	9,9,20	0.28	0	8,8,19	0.50	0
3	C8E	A	903	-	6,6,20	0.30	0	5,5,19	0.43	0
3	C8E	A	905	-	13,13,20	0.41	0	12,12,19	0.46	0
3	C8E	A	904	-	9,9,20	0.27	0	8,8,19	0.52	0
3	C8E	C	902	-	6,6,20	0.30	0	5,5,19	0.47	0
3	C8E	C	904	-	8,8,20	0.27	0	7,7,19	0.60	0
3	C8E	C	905	-	6,6,20	0.29	0	5,5,19	0.42	0
3	C8E	C	903	-	14,14,20	0.39	0	13,13,19	0.41	0
3	C8E	A	901	-	9,9,20	0.28	0	8,8,19	0.52	0
3	C8E	C	901	-	17,17,20	0.40	0	16,16,19	0.60	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
3	C8E	A	902	-	-	2/7/7/18	-
3	C8E	A	903	-	-	0/4/4/18	-
3	C8E	A	905	-	-	3/11/11/18	-
3	C8E	A	904	-	-	2/7/7/18	-
3	C8E	C	902	-	-	1/4/4/18	-
3	C8E	C	904	-	-	1/6/6/18	-
3	C8E	C	905	-	-	3/4/4/18	-
3	C8E	C	903	-	-	2/12/12/18	-
3	C8E	A	901	-	-	1/7/7/18	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	C	901	-	-	5/15/15/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	903	C8E	O9-C10-C11-O12
3	A	904	C8E	C7-C8-O9-C10
3	C	901	C8E	O9-C10-C11-O12
3	C	901	C8E	C4-C5-C6-C7
3	C	905	C8E	C3-C4-C5-C6
3	A	902	C8E	C4-C5-C6-C7
3	A	902	C8E	C7-C8-O9-C10
3	A	905	C8E	C14-C13-O12-C11
3	A	904	C8E	C3-C4-C5-C6
3	C	901	C8E	O12-C13-C14-O15
3	C	902	C8E	C4-C5-C6-C7
3	C	904	C8E	C3-C4-C5-C6
3	C	901	C8E	C6-C7-C8-O9
3	C	905	C8E	C2-C3-C4-C5
3	A	901	C8E	C6-C7-C8-O9
3	A	905	C8E	C2-C3-C4-C5
3	C	905	C8E	C1-C2-C3-C4
3	A	905	C8E	C10-C11-O12-C13
3	C	903	C8E	C14-C13-O12-C11
3	C	901	C8E	C11-C10-O9-C8

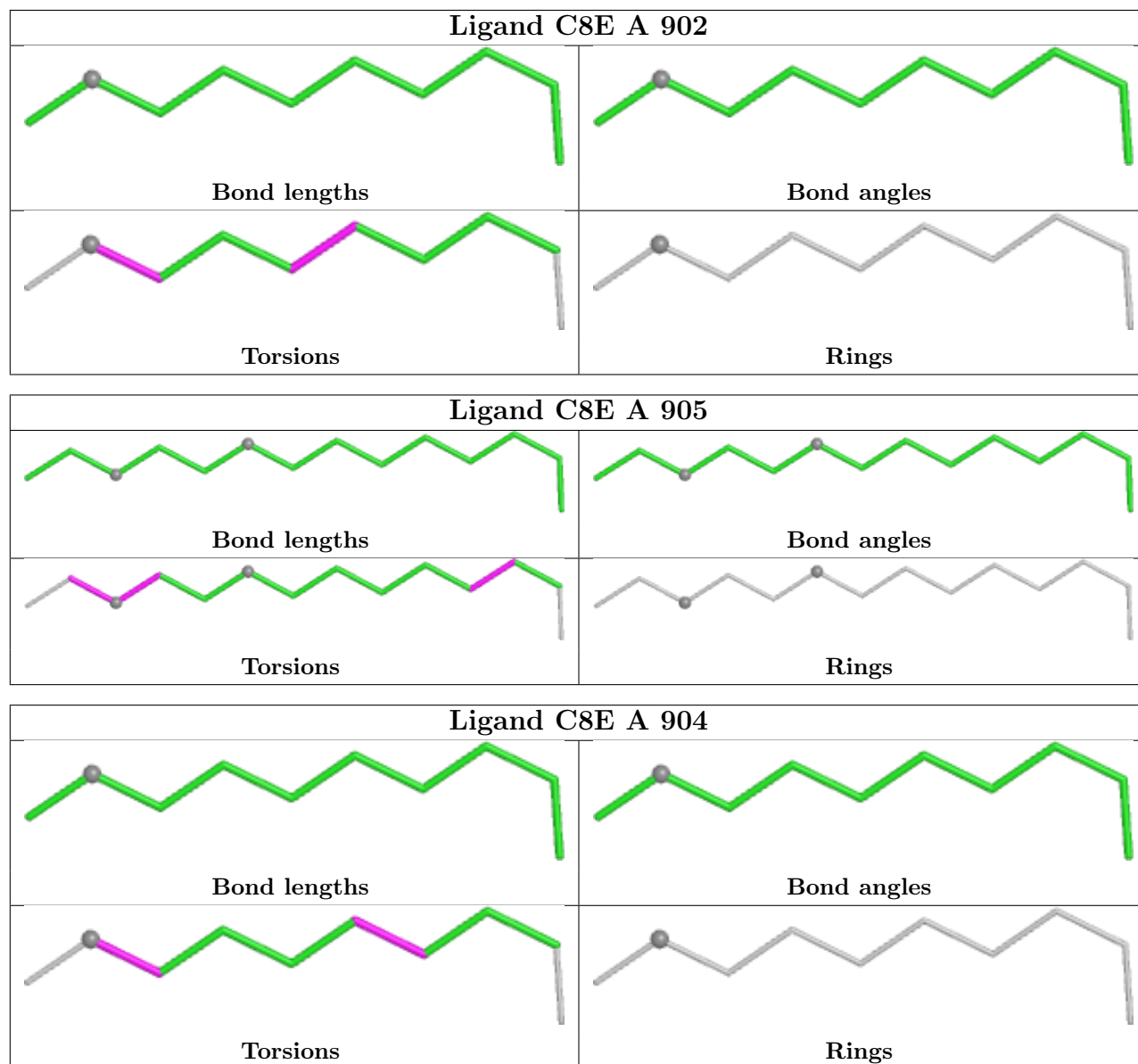
There are no ring outliers.

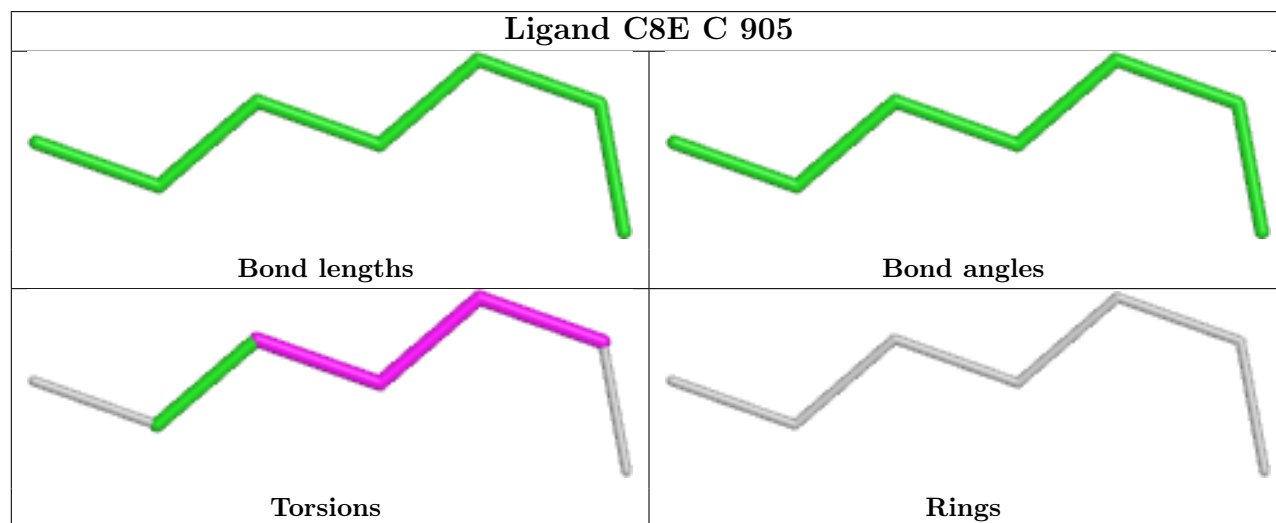
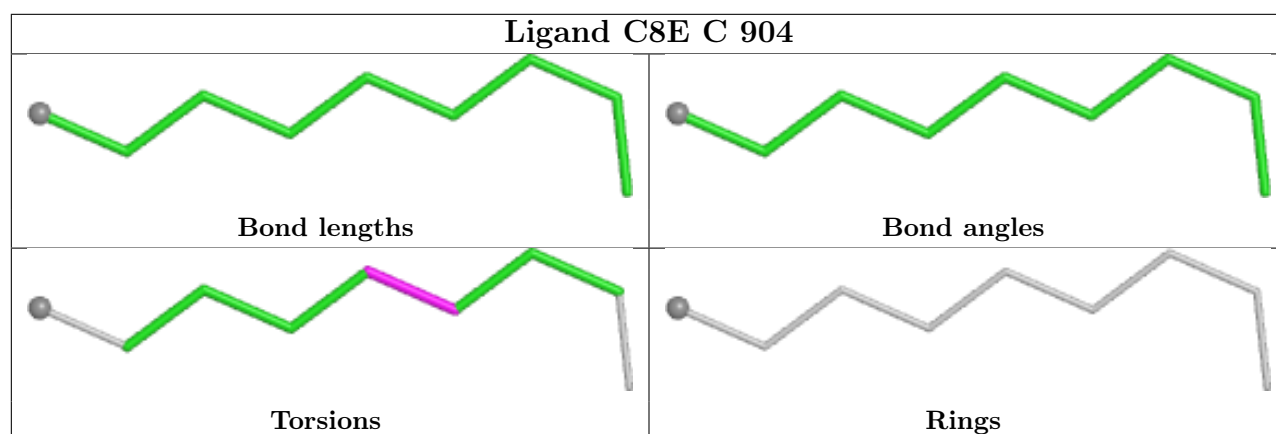
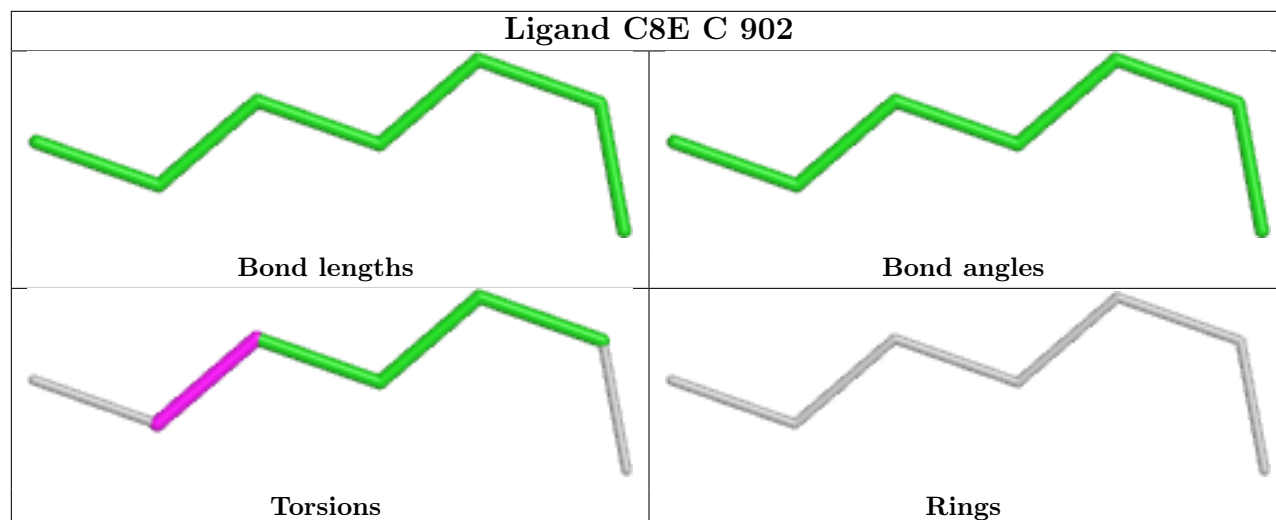
1 monomer is involved in 1 short contact:

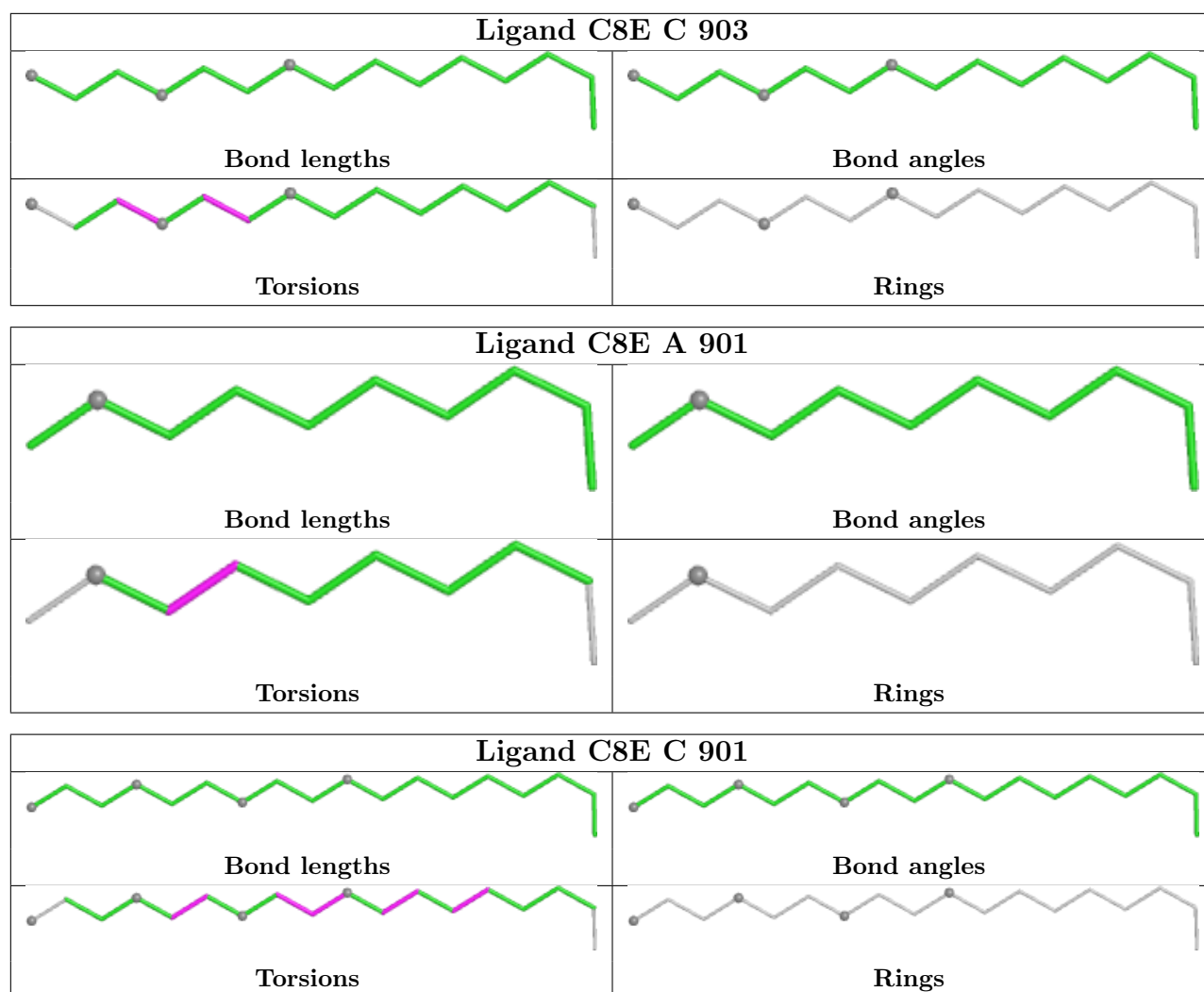
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	C8E	1	0

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, 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	369/411 (89%)	0.96	59 (15%) 5 4	54, 72, 126, 162	0
1	C	370/411 (90%)	0.96	58 (15%) 5 4	49, 72, 133, 187	0
2	B	121/124 (97%)	0.66	6 (4%) 34 30	55, 70, 108, 121	0
2	D	122/124 (98%)	0.92	20 (16%) 4 3	50, 66, 117, 153	0
All	All	982/1070 (91%)	0.92	143 (14%) 6 4	49, 71, 125, 187	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	810	TRP	9.4
1	C	585	TYR	6.9
1	A	426	PHE	6.7
1	C	426	PHE	6.4
1	A	729	TYR	6.3
1	C	729	TYR	5.4
1	C	574	TYR	5.3
2	D	3	GLY	4.9
1	C	780	LEU	4.8
2	D	31	ASN	4.8
1	A	574	TYR	4.7
1	A	585	TYR	4.6
1	A	802	PHE	4.5
1	A	730	ALA	4.5
1	C	730	ALA	4.5
1	C	428	PHE	4.5
1	C	681	ASN	4.4
1	C	679	ALA	4.4
1	C	724	PHE	4.3
2	D	26	SER	4.2
1	A	621	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	779	PRO	4.1
1	A	698	ASP	4.0
1	C	725	ILE	4.0
1	A	785	PHE	4.0
1	C	808	LYS	3.9
2	D	25	ALA	3.9
2	B	4	GLN	3.8
1	A	724	PHE	3.8
1	C	477	TYR	3.8
1	A	804	PHE	3.7
1	C	807	GLY	3.7
2	D	27	GLY	3.6
1	A	726	SER	3.6
1	C	723	PRO	3.6
2	D	116	GLN	3.6
1	A	779	PRO	3.6
2	D	90	GLU	3.5
1	C	463	ASN	3.5
1	A	550	TYR	3.5
1	A	807	GLY	3.4
1	A	728	LYS	3.4
1	A	428	PHE	3.4
1	A	463	ASN	3.3
1	A	808	LYS	3.3
1	C	809	THR	3.3
1	C	427	ASN	3.3
1	A	806	ILE	3.3
2	D	4	GLN	3.2
1	C	583	ARG	3.2
2	D	29	THR	3.2
1	A	680	SER	3.1
1	C	517	PHE	3.1
1	A	723	PRO	3.1
1	A	777	MET	3.1
1	C	805	ASN	3.1
1	C	680	SER	3.1
1	A	725	ILE	3.1
1	A	780	LEU	3.1
1	C	731	ASN	3.1
1	C	435	GLU	3.0
2	D	47	GLU	3.0
1	C	783	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	584	GLY	3.0
1	A	727	ASP	3.0
1	A	445	GLN	2.9
1	A	810	TRP	2.9
1	A	435	GLU	2.8
1	A	442	ALA	2.8
1	C	586	PHE	2.8
1	A	450	LEU	2.8
1	C	570	PHE	2.8
2	D	32	GLY	2.7
2	D	76	ALA	2.7
1	C	432	TYR	2.7
1	A	679	ALA	2.7
1	A	447	ASP	2.7
1	A	783	LEU	2.6
1	A	427	ASN	2.6
1	A	542	GLN	2.6
1	A	560	ASP	2.6
2	B	43	GLY	2.6
1	A	443	GLY	2.6
1	A	446	GLN	2.6
1	A	444	VAL	2.5
2	B	32	GLY	2.5
1	C	785	PHE	2.5
1	A	678	GLN	2.5
1	C	445	GLN	2.5
2	B	42	PRO	2.5
1	C	489	LEU	2.5
2	D	44	LYS	2.5
1	A	448	ASN	2.5
1	A	557	SER	2.5
1	A	441	GLN	2.4
2	D	101	THR	2.4
1	C	594	ASN	2.4
1	C	450	LEU	2.4
1	C	573	ASN	2.4
1	C	726	SER	2.4
1	C	697	LYS	2.4
1	C	601	ILE	2.3
1	A	733	VAL	2.3
1	A	440	PHE	2.3
1	A	643	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	756	GLY	2.3
2	D	43	GLY	2.3
2	B	101	THR	2.3
1	C	488	ARG	2.3
2	D	55	SER	2.2
2	D	97	CYS	2.2
1	A	776	TRP	2.2
1	C	518	PRO	2.2
1	A	477	TYR	2.2
1	C	550	TYR	2.2
1	A	456	VAL	2.2
1	A	805	ASN	2.2
1	C	753	GLN	2.2
1	C	429	GLY	2.2
1	A	519	ILE	2.2
2	D	54	ARG	2.2
1	A	753	GLN	2.1
1	A	791	PHE	2.1
1	C	777	MET	2.1
2	B	63	ASN	2.1
1	C	728	LYS	2.1
1	C	641	LEU	2.1
1	A	752	SER	2.1
1	C	597	GLY	2.1
2	D	45	ASP	2.1
1	C	732	SER	2.1
1	C	733	VAL	2.0
1	A	458	ILE	2.0
1	C	447	ASP	2.0
1	A	436	SER	2.0
2	D	75	SER	2.0
1	A	555	HIS	2.0
1	C	678	GLN	2.0
1	C	456	VAL	2.0
1	C	443	GLY	2.0
1	C	596	THR	2.0
1	C	500	ASP	2.0
1	C	787	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

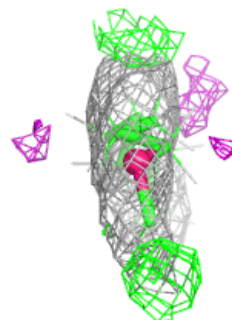
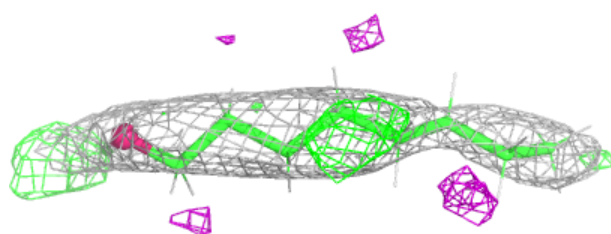
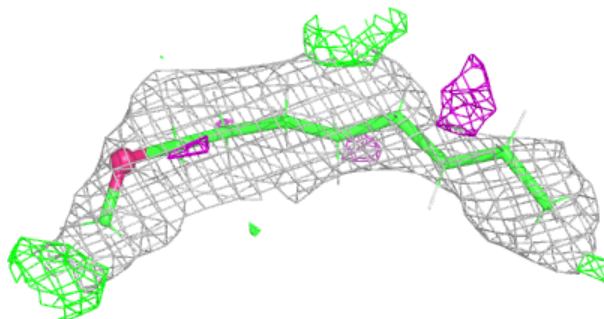
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C8E	A	903	7/21	0.70	0.31	75,94,108,120	0
3	C8E	A	904	10/21	0.77	0.31	73,91,103,110	0
3	C8E	A	902	10/21	0.78	0.32	77,105,126,132	0
3	C8E	C	902	7/21	0.81	0.24	66,83,93,100	0
3	C8E	A	901	10/21	0.85	0.20	67,84,91,99	0
3	C8E	C	904	9/21	0.87	0.21	73,89,101,102	0
3	C8E	C	905	7/21	0.87	0.27	69,87,99,99	0
3	C8E	C	901	18/21	0.88	0.19	57,80,114,123	0
3	C8E	C	903	15/21	0.88	0.19	66,89,127,128	0
3	C8E	A	905	14/21	0.92	0.19	72,91,111,116	0

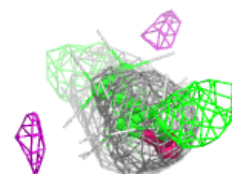
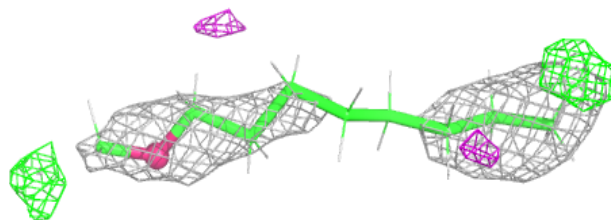
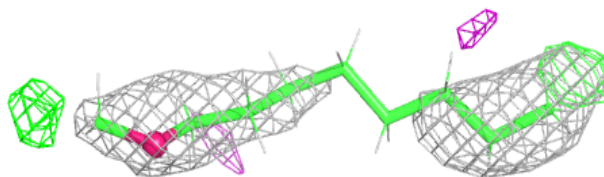
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 904:

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

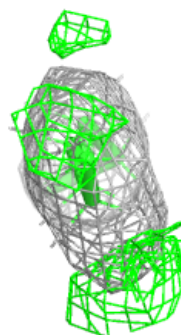
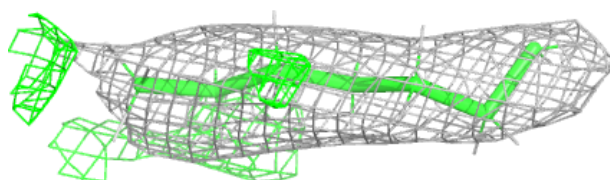
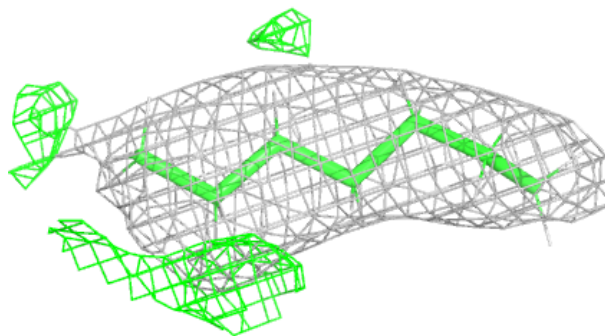
**Electron density around C8E A 902:**

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

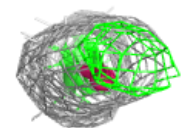
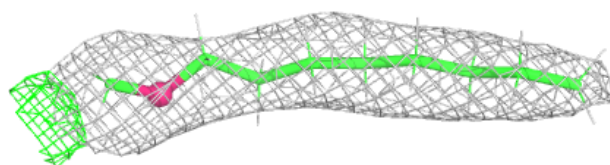
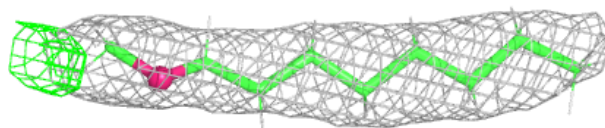


Electron density around C8E C 902:

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

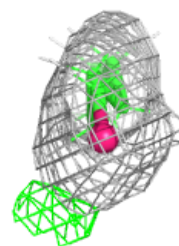
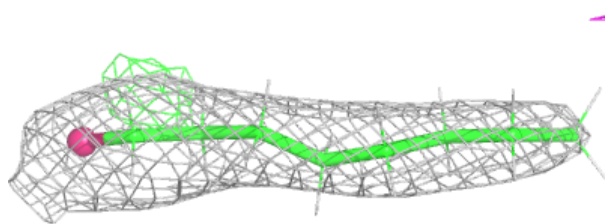
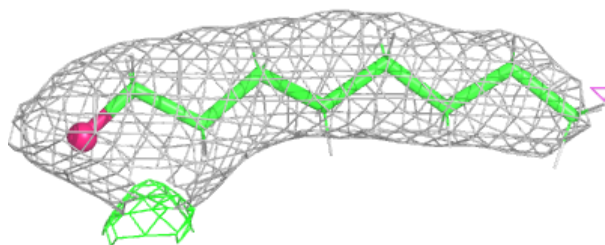
**Electron density around C8E A 901:**

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

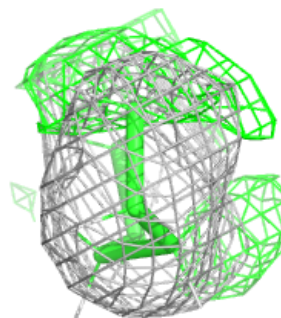
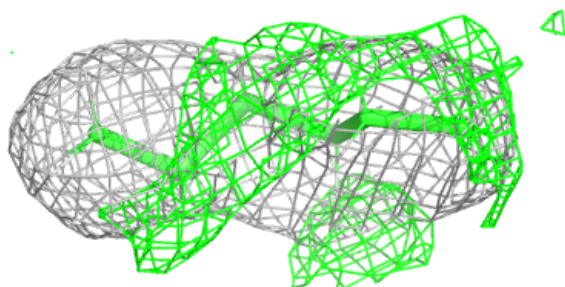
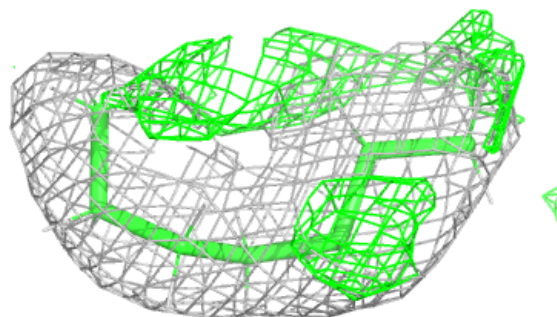


Electron density around C8E C 904:

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

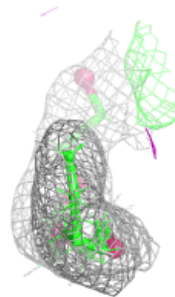
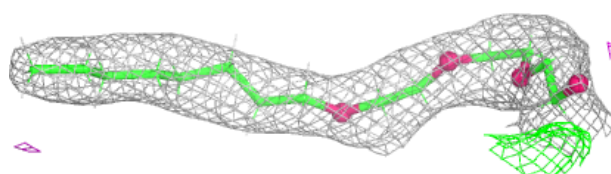
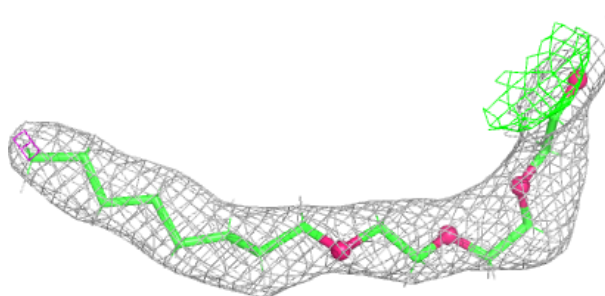
**Electron density around C8E C 905:**

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

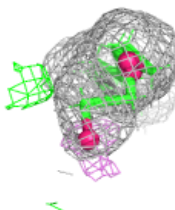
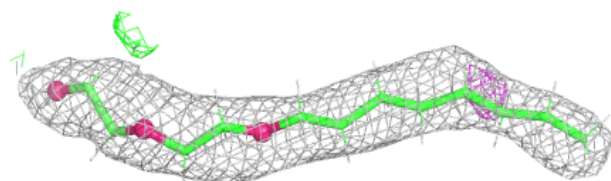
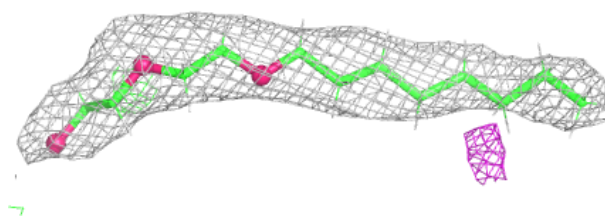


Electron density around C8E C 901:

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

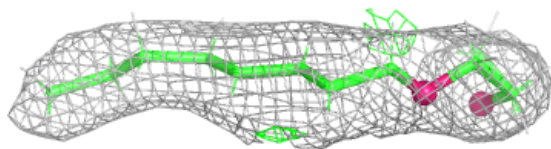
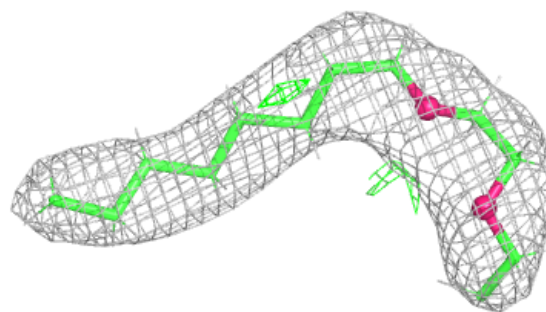
**Electron density around C8E C 903:**

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



Electron density around C8E A 905:

$2mF_o-DF_c$ (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.