



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:25 AM UTC

PDB ID : 5FOK / pdb_00005fok
Title : Crystal structure of the siderophore receptor PiuA from *Pseudomonas aeruginosa*
Authors : Moynie, L.; Naismith, J.H.
Deposited on : 2015-11-23
Resolution : 1.90 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

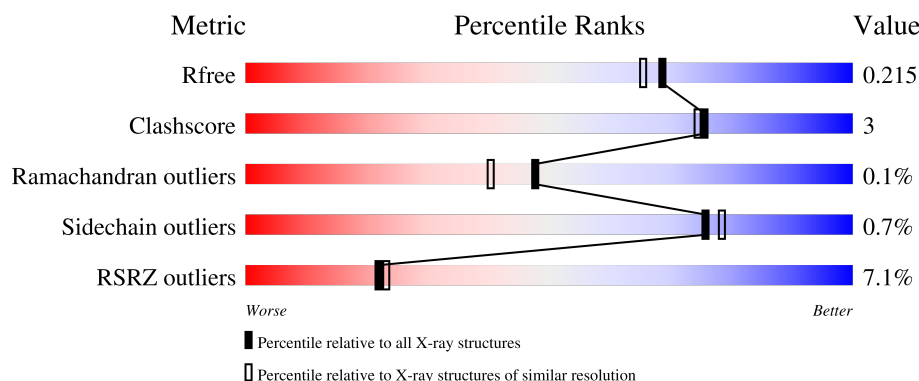
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	730	
1	B	730	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11048 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 IRON TRANSPORT OUTER MEMBRANE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	4	0
			5166	3219	906	1030	11			
1	B	651	Total	C	N	O	S	0	5	0
			5124	3194	897	1022	11			

There are 26 discrepancies between the modelled and reference sequences:

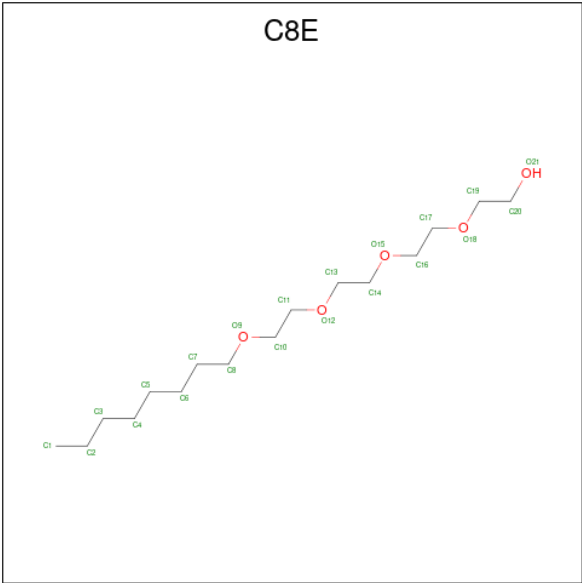
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP G3XCY8
A	1	ASN	-	expression tag	UNP G3XCY8
A	719	SER	-	expression tag	UNP G3XCY8
A	720	ALA	-	expression tag	UNP G3XCY8
A	721	ALA	-	expression tag	UNP G3XCY8
A	722	LEU	-	expression tag	UNP G3XCY8
A	723	GLU	-	expression tag	UNP G3XCY8
A	724	HIS	-	expression tag	UNP G3XCY8
A	725	HIS	-	expression tag	UNP G3XCY8
A	726	HIS	-	expression tag	UNP G3XCY8
A	727	HIS	-	expression tag	UNP G3XCY8
A	728	HIS	-	expression tag	UNP G3XCY8
A	729	HIS	-	expression tag	UNP G3XCY8
B	0	MET	-	expression tag	UNP G3XCY8
B	1	ASN	-	expression tag	UNP G3XCY8
B	719	SER	-	expression tag	UNP G3XCY8
B	720	ALA	-	expression tag	UNP G3XCY8
B	721	ALA	-	expression tag	UNP G3XCY8
B	722	LEU	-	expression tag	UNP G3XCY8
B	723	GLU	-	expression tag	UNP G3XCY8
B	724	HIS	-	expression tag	UNP G3XCY8
B	725	HIS	-	expression tag	UNP G3XCY8
B	726	HIS	-	expression tag	UNP G3XCY8
B	727	HIS	-	expression tag	UNP G3XCY8
B	728	HIS	-	expression tag	UNP G3XCY8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	729	HIS	-	expression tag	UNP G3XCY8

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			15	12	3		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			9	8	1		
2	B	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

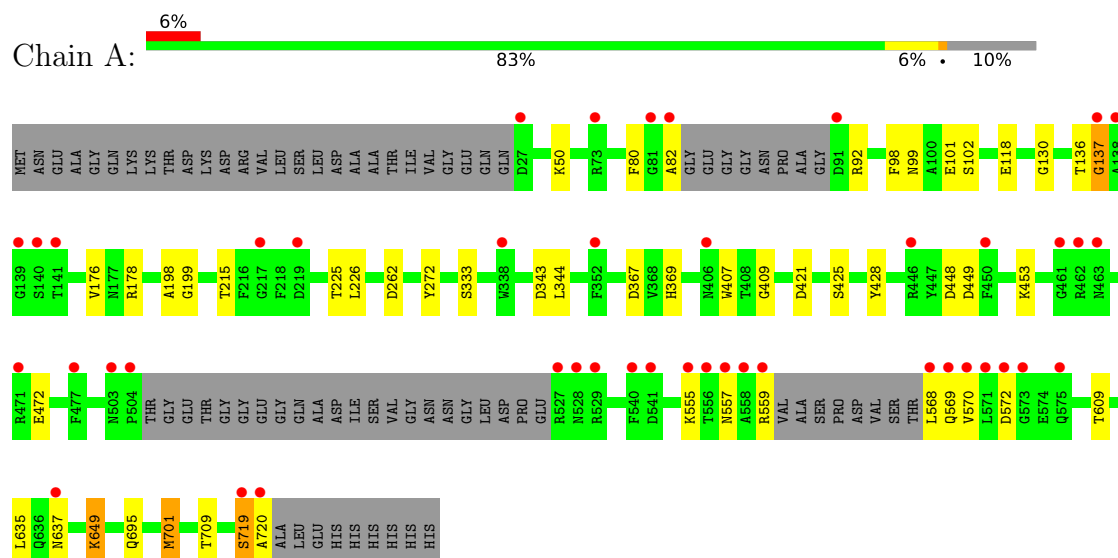
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	325	Total	O	0	0
			325	325		
5	B	270	Total	O	0	0
			270	270		

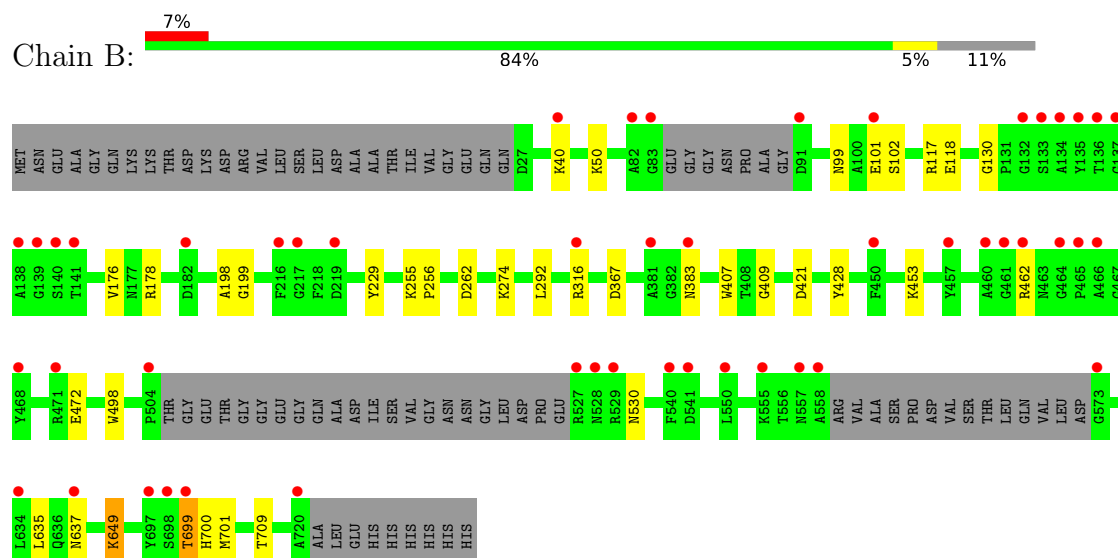
3 Residue-property plots [i](#)

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: IRON TRANSPORT OUTER MEMBRANE RECEPTOR



• Molecule 1: IRON TRANSPORT OUTER MEMBRANE RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.01Å 132.97Å 73.59Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	71.93 – 1.90 71.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.93-1.90) 99.7 (71.93-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.188 , 0.211 0.194 , 0.215	Depositor DCC
R_{free} test set	7166 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11048	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, C8E, NA

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	0.72	0/5281	0.73	1/7174 (0.0%)
1	B	0.66	0/5242	0.72	1/7121 (0.0%)
All	All	0.69	0/10523	0.73	2/14295 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	699	THR	N-CA-C	-5.15	101.96	108.45
1	A	701	MET	N-CA-C	5.14	116.11	108.60

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	5166	0	4930	33	0
1	B	5124	0	4889	24	0
2	A	99	0	160	6	0
2	B	51	0	85	3	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	325	0	0	2	0
5	B	270	0	0	0	0
All	All	11048	0	10064	61	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 3.

All (61) 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:453:LYS:HG2	1:A:472:GLU:HG2	1.54	0.90
1:B:453:LYS:HG2	1:B:472:GLU:HG2	1.64	0.78
1:B:50:LYS:HB2	1:B:130:GLY:HA3	1.69	0.73
1:A:50:LYS:HB2	1:A:130:GLY:HA3	1.72	0.71
1:A:719:SER:O	1:A:720:ALA:C	2.39	0.64
2:A:1725:C8E:H72	5:A:2086:HOH:O	1.96	0.64
1:A:101:GLU:HG3	1:A:102:SER:N	2.14	0.62
1:A:136:THR:O	1:A:137:GLY:C	2.43	0.61
2:A:1722:C8E:H42	5:A:2127:HOH:O	2.01	0.61
1:A:453:LYS:HG2	1:A:472:GLU:CG	2.29	0.60
1:B:101:GLU:HG3	1:B:102:SER:N	2.16	0.60
1:A:225:THR:C	1:A:226:LEU:HD12	2.30	0.56
1:B:40:LYS:HE3	1:B:428:TYR:CZ	2.43	0.52
1:B:198:ALA:HB2	1:B:709:THR:HG22	1.91	0.52
1:A:198:ALA:HB2	1:A:709:THR:HG22	1.92	0.51
1:A:559:ARG:HA	1:A:569:GLN:O	2.09	0.51
1:B:407:TRP:CZ2	1:B:409:GLY:HA3	2.46	0.51
1:A:572:ASP:OD2	1:B:462:ARG:HG3	2.10	0.51
1:A:198:ALA:CB	1:A:709:THR:HG22	2.42	0.49
1:A:425:SER:HB2	1:A:449:ASP:OD1	2.12	0.49
1:A:215:THR:OG1	1:A:225:THR:HG22	2.12	0.49
1:A:635:LEU:C	1:A:637:ASN:H	2.20	0.49
1:B:198:ALA:CB	1:B:709:THR:HG22	2.43	0.49
1:A:449:ASP:OD1	1:A:449:ASP:C	2.57	0.48
1:A:226:LEU:HD12	1:A:226:LEU:N	2.29	0.47
1:B:274:LYS:NZ	2:B:1723:C8E:H61	2.29	0.47
1:A:99:ASN:HD21	1:A:101:GLU:HG2	1.80	0.47
1:B:274:LYS:HZ2	2:B:1723:C8E:H61	1.80	0.47
1:A:649:LYS:HE3	1:A:649:LYS:HB3	1.52	0.46
2:A:1721:C8E:H13	2:A:1724:C8E:H81	1.96	0.46
1:B:649:LYS:HB3	1:B:649:LYS:HE3	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:LEU:C	1:B:637:ASN:H	2.23	0.46
1:B:117:ARG:HD3	1:B:229:TYR:CZ	2.52	0.45
1:B:699:THR:O	1:B:700:HIS:HB2	2.16	0.45
2:A:1721:C8E:H13	2:A:1724:C8E:C8	2.46	0.45
1:A:80:PHE:O	1:A:695:GLN:HG3	2.16	0.45
1:A:272:TYR:CD1	2:A:1725:C8E:H62	2.52	0.44
1:B:176:VAL:HG23	1:B:178:ARG:NH1	2.33	0.44
1:B:316:ARG:HD3	1:B:383:ASN:HB3	1.99	0.43
1:A:344:LEU:C	1:A:344:LEU:HD23	2.44	0.43
1:B:99:ASN:HD21	1:B:101:GLU:HG2	1.83	0.43
2:A:1725:C8E:H101	2:A:1725:C8E:H71	1.81	0.43
1:B:274:LYS:HD2	2:B:1723:C8E:H32	2.00	0.42
1:A:82:ALA:HB3	1:A:92:ARG:HD2	2.00	0.42
1:A:92:ARG:NH1	1:A:568:LEU:HG	2.35	0.42
1:B:367:ASP:OD2	1:B:421:ASP:OD1	2.37	0.42
1:A:343:ASP:CG	1:A:428:TYR:HH	2.27	0.42
1:A:199:GLY:O	1:A:262:ASP:HA	2.20	0.42
1:B:498:TRP:HA	1:B:530:ASN:O	2.19	0.42
1:B:40:LYS:HE3	1:B:428:TYR:CE1	2.54	0.41
1:A:572:ASP:HB2	1:A:609:THR:HG23	2.02	0.41
1:A:98:PHE:CD1	1:A:555:LYS:HE2	2.55	0.41
1:A:407:TRP:CZ2	1:A:409:GLY:HA3	2.56	0.41
1:A:557:ASN:HB3	1:A:570:VAL:CG1	2.50	0.41
1:B:255:LYS:HB2	1:B:256:PRO:CD	2.51	0.41
1:A:176:VAL:HG23	1:A:178:ARG:NH1	2.35	0.41
1:A:333:SER:HA	1:A:369:HIS:O	2.21	0.41
1:B:199:GLY:O	1:B:262:ASP:HA	2.19	0.41
1:A:136:THR:O	1:A:448:ASP:OD1	2.39	0.40
1:A:367:ASP:OD2	1:A:421:ASP:OD1	2.39	0.40
1:B:635:LEU:C	1:B:637:ASN:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	652/730 (89%)	639 (98%)	12 (2%)	1 (0%)	43	36
1	B	648/730 (89%)	635 (98%)	13 (2%)	0	100	100
All	All	1300/1460 (89%)	1274 (98%)	25 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/610 (92%)	555 (99%)	4 (1%)	76	78
1	B	554/610 (91%)	550 (99%)	4 (1%)	76	78
All	All	1113/1220 (91%)	1105 (99%)	8 (1%)	76	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLU
1	A	649	LYS
1	A	701	MET
1	A	719	SER
1	B	118	GLU
1	B	292	LEU
1	B	649	LYS
1	B	701	MET

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	154	GLN
1	A	341	GLN
1	A	481	GLN
1	A	557	ASN
1	A	715	ASN
1	B	121	ASN
1	B	183	ASN
1	B	291	ASN
1	B	341	GLN
1	B	347	ASN
1	B	481	GLN
1	B	677	ASN
1	B	715	ASN
1	B	717	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z > 2$
2	C8E	B	1721	3	20,20,20	0.44	0	19,19,19	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C8E	A	1722	-	14,14,20	0.39	0	13,13,19	0.41	0
2	C8E	B	1723	-	20,20,20	0.43	0	19,19,19	0.36	0
4	SO4	A	1728	-	4,4,4	0.51	0	6,6,6	0.31	0
2	C8E	A	1724	-	20,20,20	0.43	0	19,19,19	0.30	0
2	C8E	A	1721	-	20,20,20	0.35	0	19,19,19	0.43	0
4	SO4	A	1727	-	4,4,4	0.50	0	6,6,6	0.26	0
2	C8E	A	1723	-	20,20,20	0.37	0	19,19,19	0.70	0
2	C8E	A	1725	3	20,20,20	0.48	0	19,19,19	0.53	0
2	C8E	B	1722	-	8,8,20	0.20	0	7,7,19	0.53	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	B	1721	3	-	6/18/18/18	-
2	C8E	A	1722	-	-	6/12/12/18	-
2	C8E	B	1723	-	-	7/18/18/18	-
2	C8E	A	1724	-	-	12/18/18/18	-
2	C8E	A	1721	-	-	8/18/18/18	-
2	C8E	A	1723	-	-	5/18/18/18	-
2	C8E	A	1725	3	-	5/18/18/18	-
2	C8E	B	1722	-	-	4/6/6/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1725	C8E	C7-C8-O9-C10
2	A	1721	C8E	O15-C16-C17-O18
2	A	1721	C8E	O9-C10-C11-O12
2	A	1724	C8E	O9-C10-C11-O12
2	A	1722	C8E	O9-C10-C11-O12
2	A	1725	C8E	C6-C7-C8-O9
2	A	1721	C8E	C6-C7-C8-O9
2	A	1724	C8E	C6-C7-C8-O9

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Mol	Chain	Res	Type	Atoms
2	B	1723	C8E	C5-C6-C7-C8
2	A	1721	C8E	O12-C13-C14-O15
2	B	1721	C8E	C3-C4-C5-C6
2	B	1723	C8E	C3-C4-C5-C6
2	B	1722	C8E	C3-C4-C5-C6
2	A	1722	C8E	C4-C5-C6-C7
2	A	1723	C8E	C2-C3-C4-C5
2	B	1723	C8E	C7-C8-O9-C10
2	B	1722	C8E	C5-C6-C7-C8
2	A	1721	C8E	C5-C6-C7-C8
2	A	1721	C8E	O18-C19-C20-O21
2	A	1723	C8E	O18-C19-C20-O21
2	B	1722	C8E	C6-C7-C8-O9
2	B	1721	C8E	C4-C5-C6-C7
2	B	1723	C8E	C2-C3-C4-C5
2	A	1722	C8E	C6-C7-C8-O9
2	A	1722	C8E	C1-C2-C3-C4
2	B	1721	C8E	C1-C2-C3-C4
2	A	1724	C8E	O12-C13-C14-O15
2	A	1721	C8E	C2-C3-C4-C5
2	A	1724	C8E	C4-C5-C6-C7
2	A	1724	C8E	C1-C2-C3-C4
2	B	1721	C8E	C2-C3-C4-C5
2	A	1724	C8E	C14-C13-O12-C11
2	B	1722	C8E	C1-C2-C3-C4
2	A	1724	C8E	C10-C11-O12-C13
2	A	1724	C8E	C20-C19-O18-C17
2	A	1725	C8E	C4-C5-C6-C7
2	A	1722	C8E	C7-C8-O9-C10
2	A	1725	C8E	O18-C19-C20-O21
2	A	1721	C8E	C20-C19-O18-C17
2	B	1721	C8E	O9-C10-C11-O12
2	B	1723	C8E	C20-C19-O18-C17
2	A	1722	C8E	O12-C13-C14-O15
2	A	1724	C8E	C7-C8-O9-C10
2	A	1724	C8E	O15-C16-C17-O18
2	B	1723	C8E	O18-C19-C20-O21
2	A	1724	C8E	C2-C3-C4-C5
2	A	1725	C8E	O12-C13-C14-O15
2	B	1723	C8E	O12-C13-C14-O15
2	A	1723	C8E	O12-C13-C14-O15
2	A	1723	C8E	O15-C16-C17-O18

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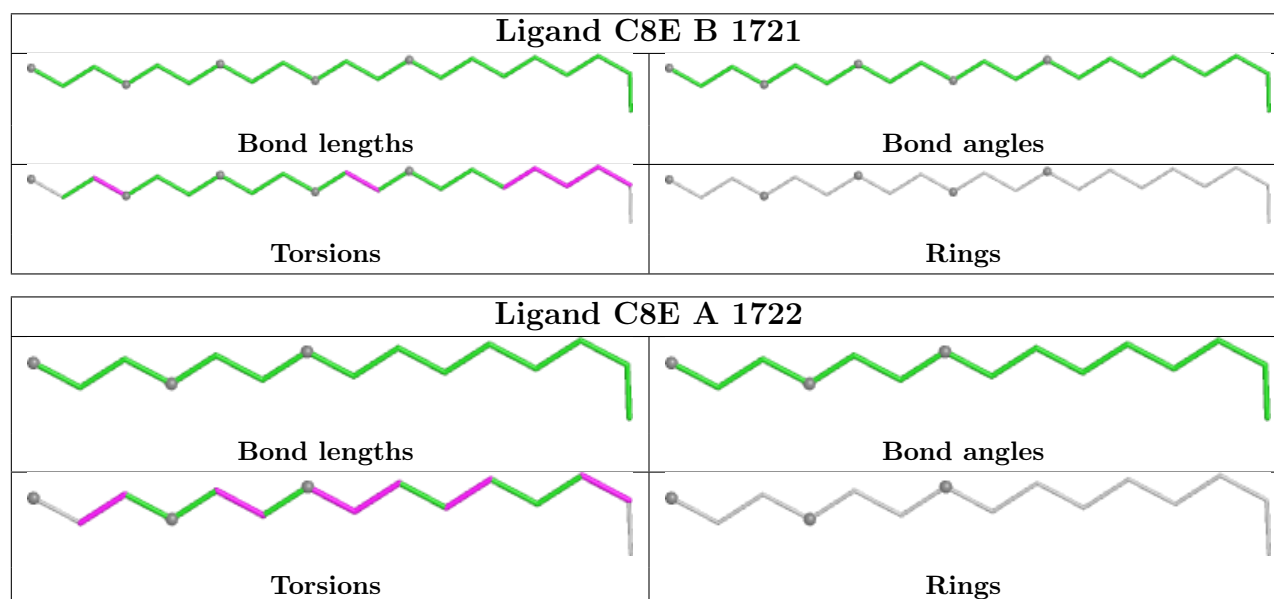
Mol	Chain	Res	Type	Atoms
2	A	1723	C8E	C10-C11-O12-C13
2	A	1724	C8E	O18-C19-C20-O21
2	B	1721	C8E	C20-C19-O18-C17

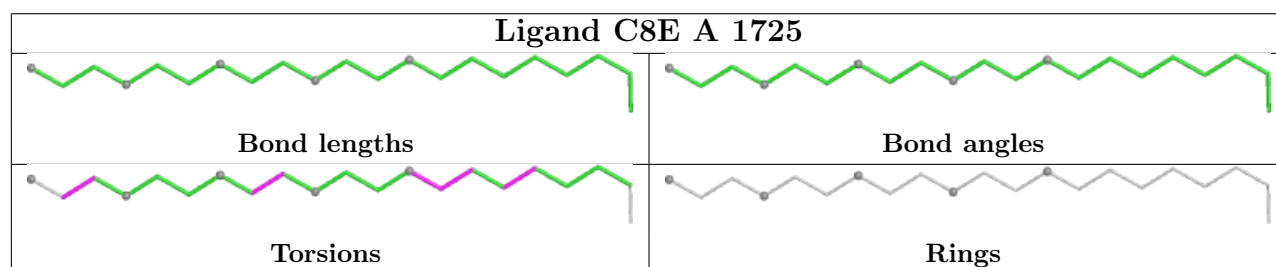
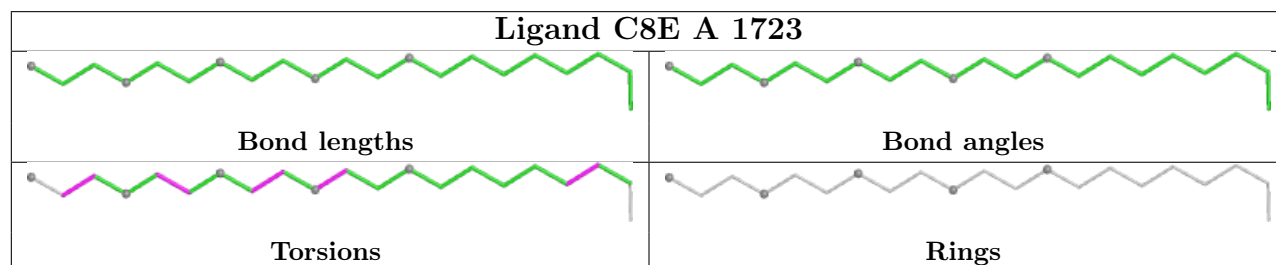
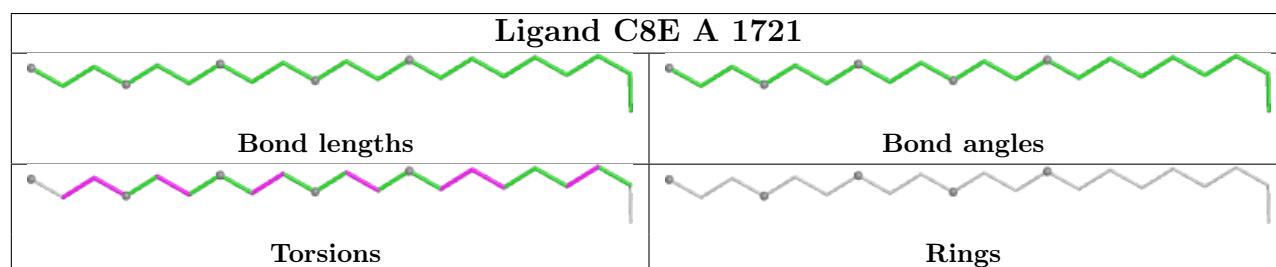
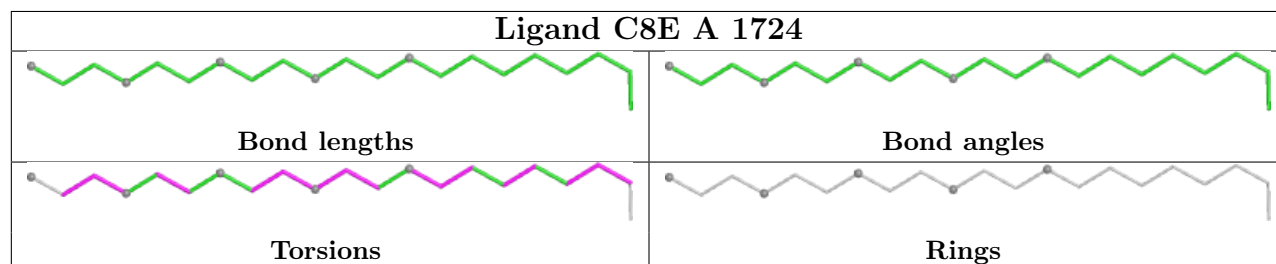
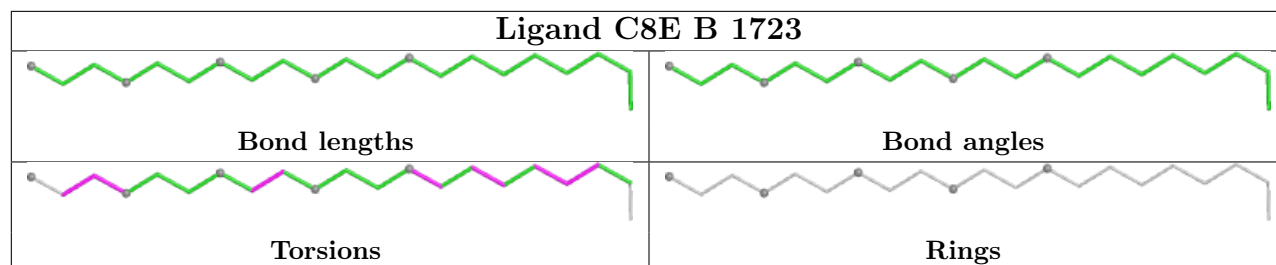
There are no ring outliers.

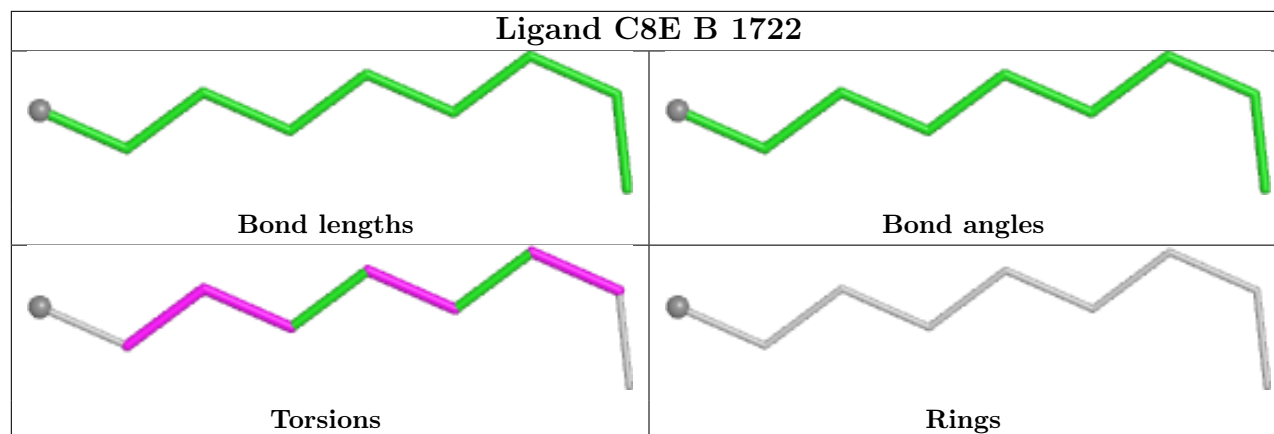
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1722	C8E	1	0
2	B	1723	C8E	3	0
2	A	1724	C8E	2	0
2	A	1721	C8E	2	0
2	A	1725	C8E	3	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	656/730 (89%)	0.28	44 (6%) 24 25	11, 26, 53, 100	4 (0%)
1	B	651/730 (89%)	0.43	49 (7%) 20 21	12, 28, 54, 113	5 (0%)
All	All	1307/1460 (89%)	0.36	93 (7%) 22 23	11, 27, 54, 113	9 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	LEU	6.0
1	B	138	ALA	6.0
1	A	82	ALA	6.0
1	A	450	PHE	5.6
1	B	83	GLY	5.4
1	A	720	ALA	4.6
1	B	82	ALA	4.4
1	A	571	LEU	4.3
1	A	572	ASP	4.2
1	B	462	ARG	4.1
1	A	352	PHE	4.1
1	B	134	ALA	4.1
1	B	573	GLY	4.1
1	B	139	GLY	4.0
1	B	558	ALA	4.0
1	B	217	GLY	4.0
1	B	637	ASN	3.9
1	A	570	VAL	3.9
1	A	573	GLY	3.8
1	B	504	PRO	3.7
1	B	720	ALA	3.6
1	A	558	ALA	3.6
1	B	697	TYR	3.5
1	B	136	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	527	ARG	3.5
1	B	141	THR	3.4
1	B	140	SER	3.3
1	B	527	ARG	3.3
1	A	406	ASN	3.3
1	A	141	THR	3.2
1	B	698	SER	3.2
1	A	504	PRO	3.2
1	B	137	GLY	3.2
1	B	464	GLY	3.2
1	A	462	ARG	3.2
1	A	503	ASN	3.1
1	B	132	GLY	3.1
1	B	540	PHE	3.1
1	A	471	ARG	3.1
1	A	140	SER	3.1
1	B	383	ASN	3.0
1	B	182	ASP	3.0
1	A	81	GLY	2.9
1	A	556	THR	2.9
1	B	381	ALA	2.8
1	A	338	TRP	2.8
1	A	461	GLY	2.8
1	B	465	PRO	2.8
1	A	719	SER	2.8
1	B	450	PHE	2.7
1	A	219	ASP	2.7
1	B	541	ASP	2.7
1	B	529	ARG	2.7
1	B	135	TYR	2.7
1	A	575	GLN	2.7
1	B	471	ARG	2.7
1	B	555	LYS	2.7
1	A	91	ASP	2.6
1	B	466	ALA	2.6
1	B	557	ASN	2.6
1	A	559	ARG	2.6
1	A	446	ARG	2.5
1	B	468	TYR	2.5
1	A	463	ASN	2.5
1	A	637	ASN	2.5
1	B	457	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	217	GLY	2.5
1	A	557	ASN	2.4
1	B	91	ASP	2.4
1	B	40	LYS	2.4
1	B	699	THR	2.4
1	A	73	ARG	2.3
1	B	219	ASP	2.3
1	A	541	ASP	2.3
1	B	528	ASN	2.3
1	A	529	ARG	2.2
1	B	216	PHE	2.2
1	B	460	ALA	2.2
1	A	27	ASP	2.2
1	B	101	GLU	2.2
1	A	138	ALA	2.2
1	A	137	GLY	2.2
1	B	461	GLY	2.2
1	B	550	LEU	2.2
1	A	528	ASN	2.1
1	B	634	LEU	2.1
1	A	569	GLN	2.1
1	B	133	SER	2.1
1	B	316	ARG	2.1
1	A	139	GLY	2.1
1	A	477	PHE	2.0
1	A	540	PHE	2.0
1	A	555	LYS	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 oligosaccharides in this entry.

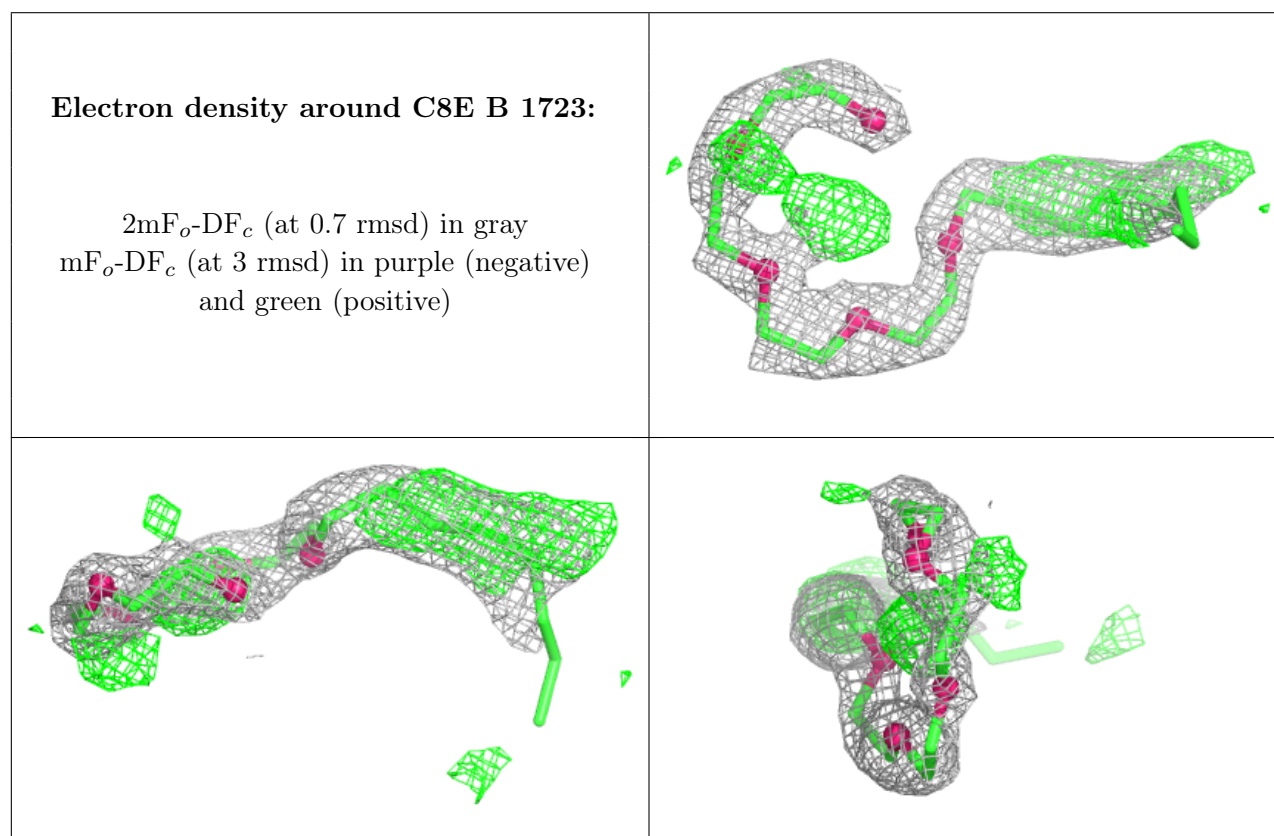
6.4 Ligands [i](#)

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.

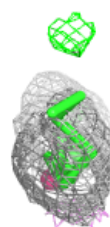
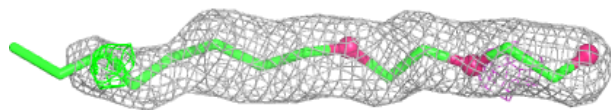
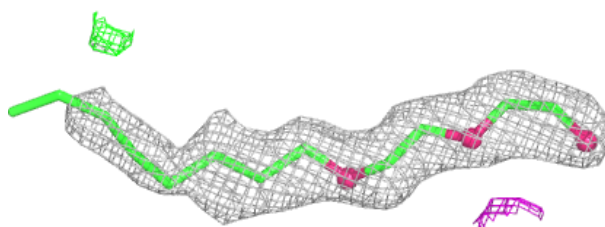
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	1725	1/1	0.78	0.20	51,51,51,51	0
2	C8E	B	1723	21/21	0.84	0.28	21,29,38,38	21
2	C8E	A	1722	15/21	0.85	0.19	35,50,64,68	0
2	C8E	A	1724	21/21	0.85	0.16	40,50,56,59	0
2	C8E	A	1721	21/21	0.86	0.17	36,51,79,80	0
4	SO4	A	1728	5/5	0.87	0.11	44,45,57,59	0
2	C8E	B	1721	21/21	0.88	0.14	29,38,49,51	0
2	C8E	B	1722	9/21	0.89	0.16	43,49,53,57	0
2	C8E	A	1725	21/21	0.92	0.12	24,30,41,50	0
2	C8E	A	1723	21/21	0.92	0.13	22,33,51,56	0
3	NA	B	1724	1/1	0.93	0.14	41,41,41,41	0
4	SO4	A	1727	5/5	0.96	0.08	34,36,39,41	5
3	NA	A	1726	1/1	0.97	0.12	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.

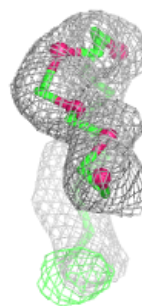
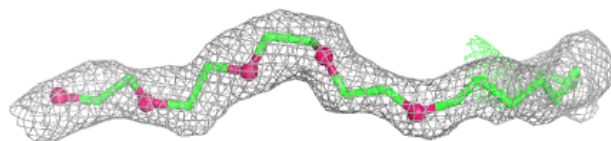
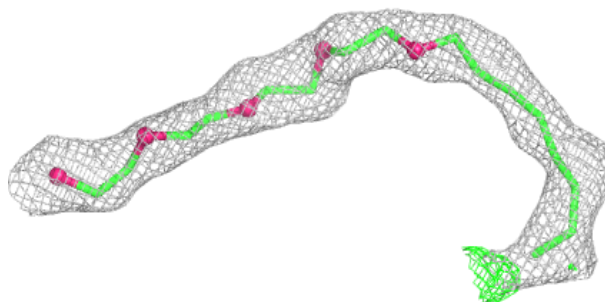


Electron density around C8E A 1722:

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

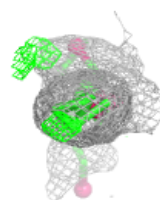
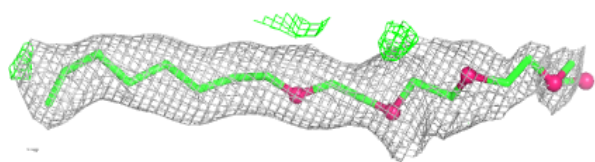
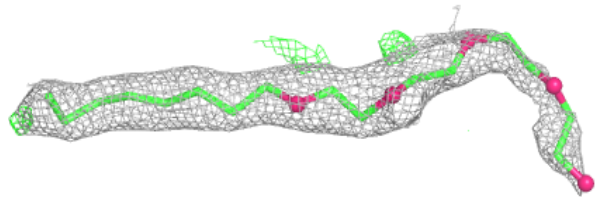
**Electron density around C8E A 1724:**

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



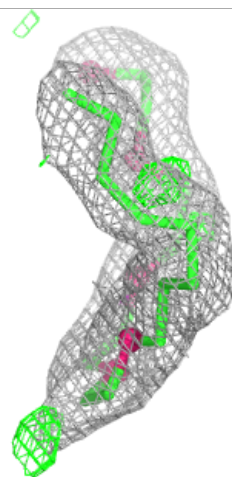
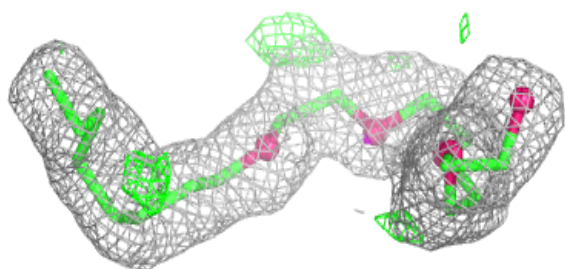
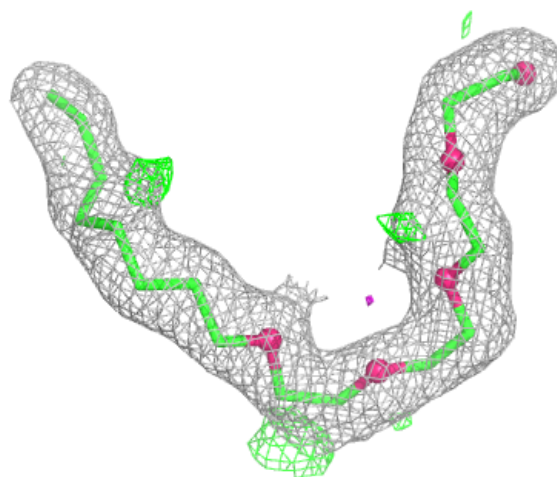
Electron density around C8E A 1721:

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



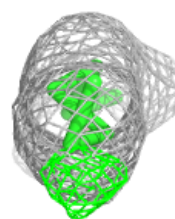
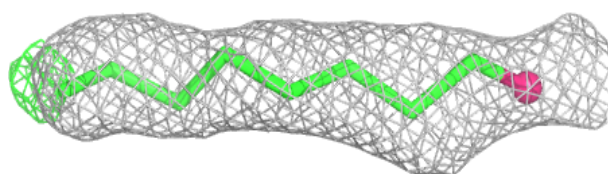
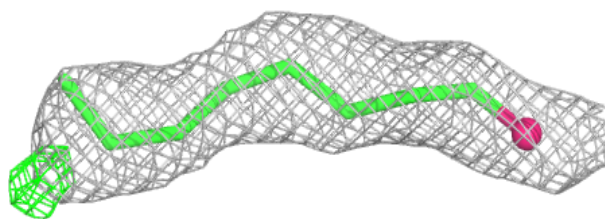
Electron density around C8E B 1721:

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

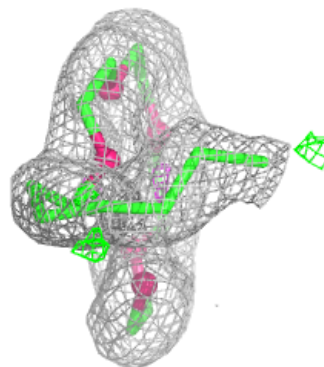
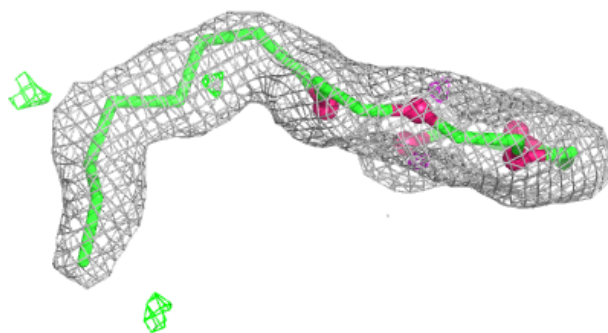
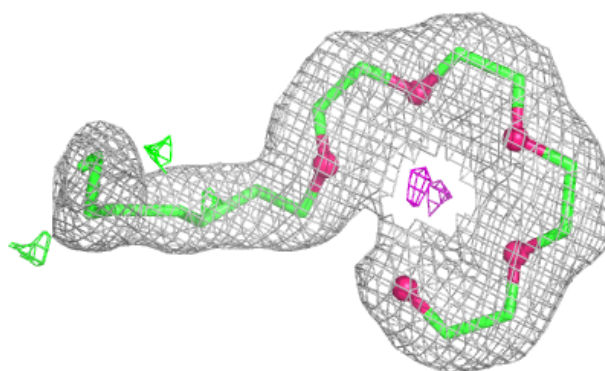


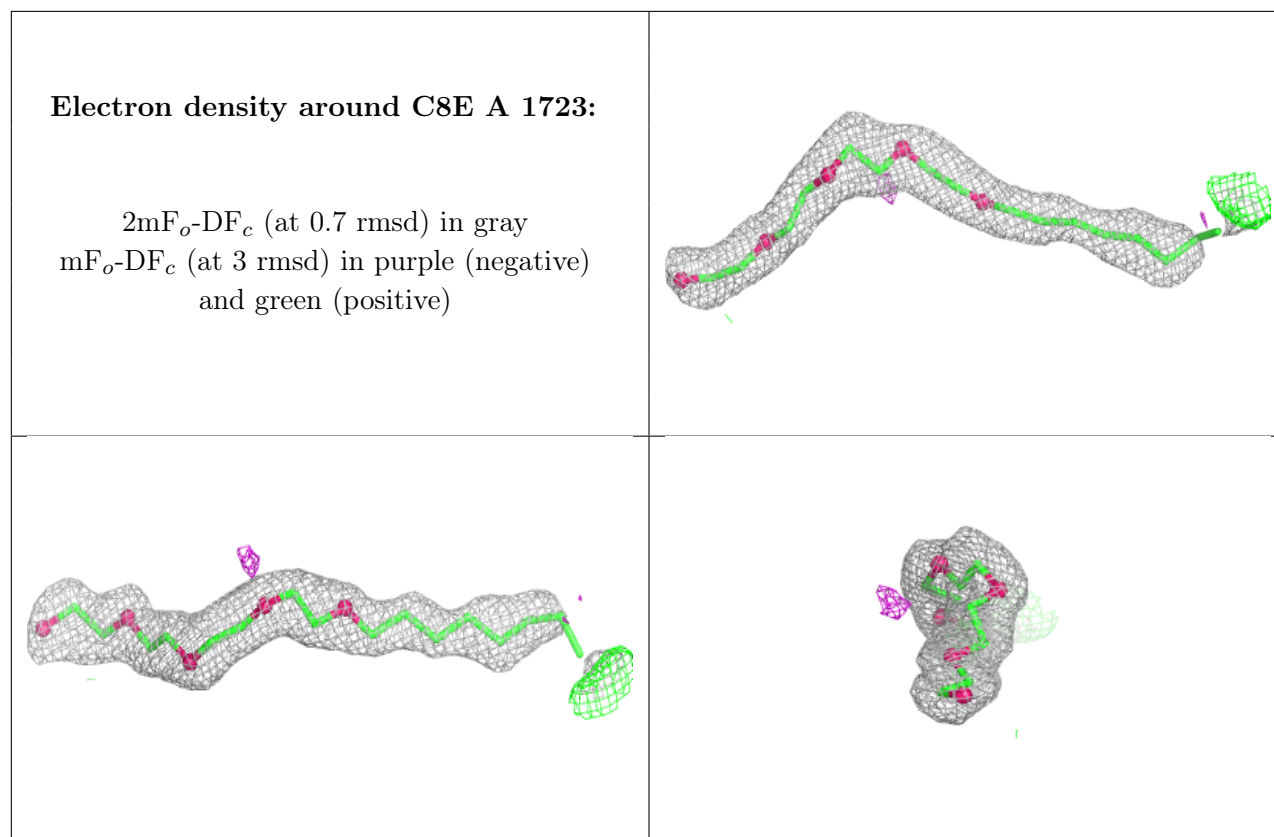
Electron density around C8E B 1722:

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

**Electron density around C8E A 1725:**

$2mF_o-DF_c$ (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.