



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 03:27 AM UTC

PDB ID : 6I98 / pdb_00006i98
Title : Structure of the ferrioxamine B transporter FoxA from *Pseudomonas aeruginosa*, apo state
Authors : Josts, I.; Tidow, H.
Deposited on : 2018-11-22
Resolution : 2.80 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

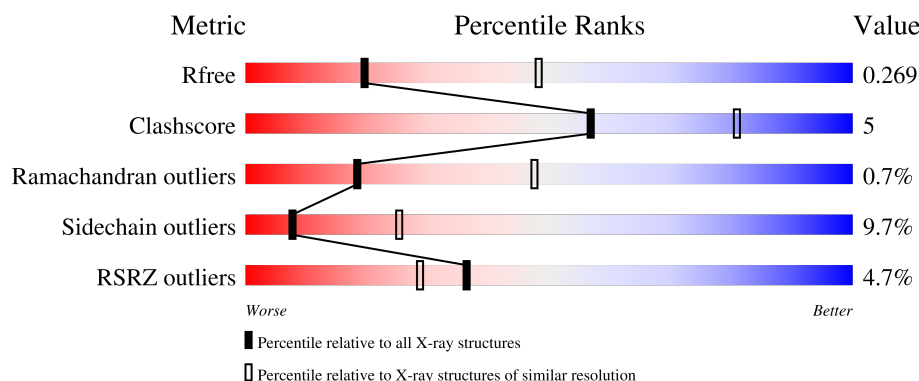
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	677	5% 79% 16% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FTT	A	911	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5532 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.

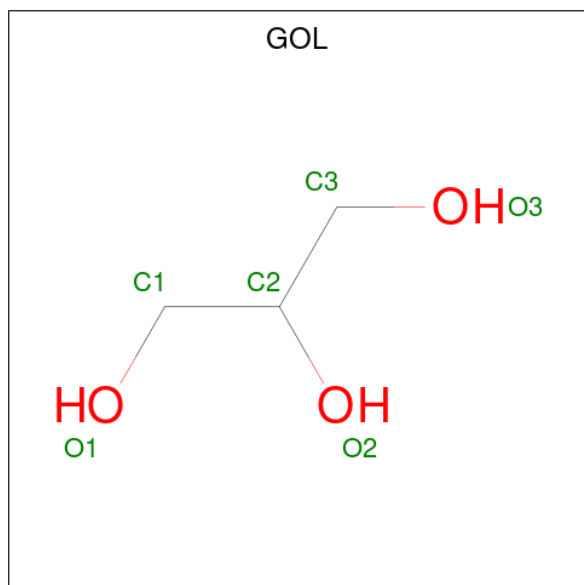
- Molecule 1 is a protein called Metal-pseudopaline receptor CntO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5325	3345	910	1059	11			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



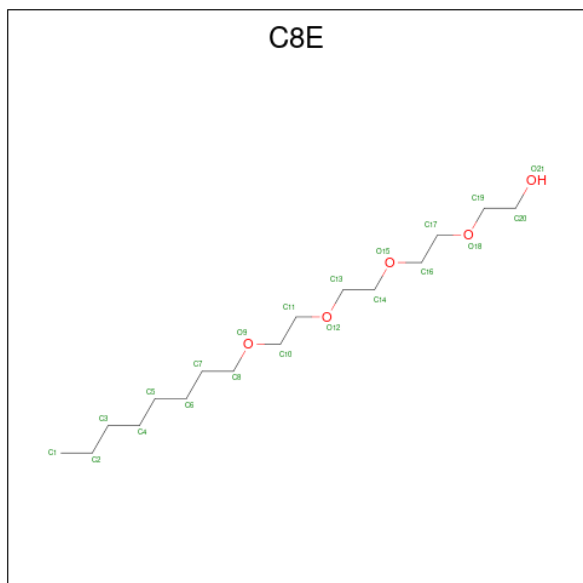
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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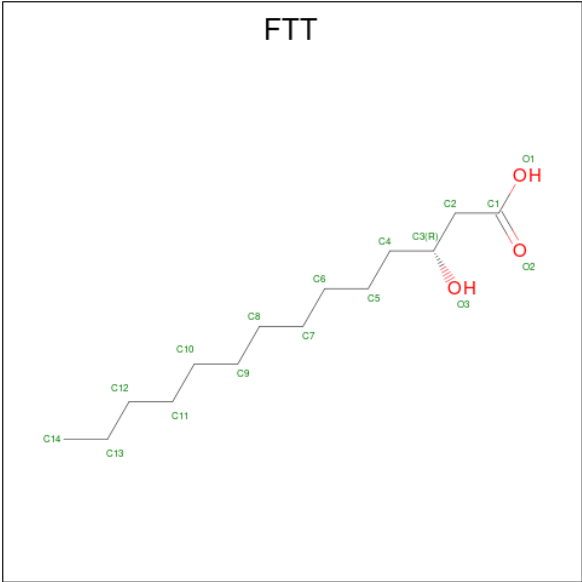
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: $C_{16}H_{34}O_5$).



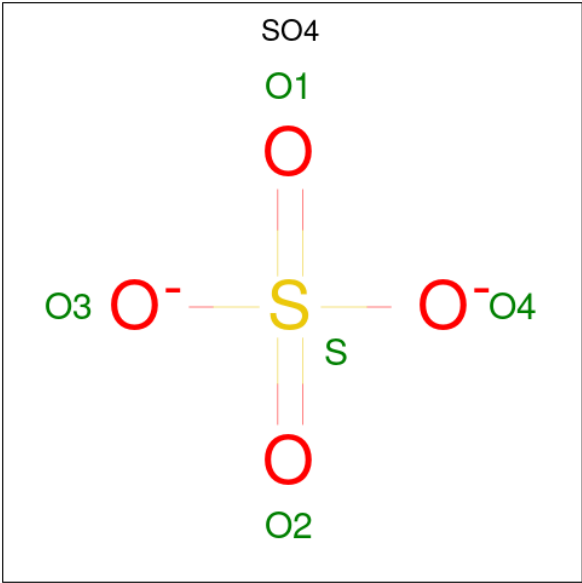
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	10	2		
4	A	1	Total	C	O	0	0
			12	10	2		
4	A	1	Total	C	O	0	0
			10	9	1		
4	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 5 is 3-HYDROXY-TETRADECANOIC ACID (CCD ID: FTT) (formula: $C_{14}H_{28}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	14	3		
5	A	1	Total	C	O	0	0
			17	14	3		
5	A	1	Total	C	O	0	0
			17	14	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

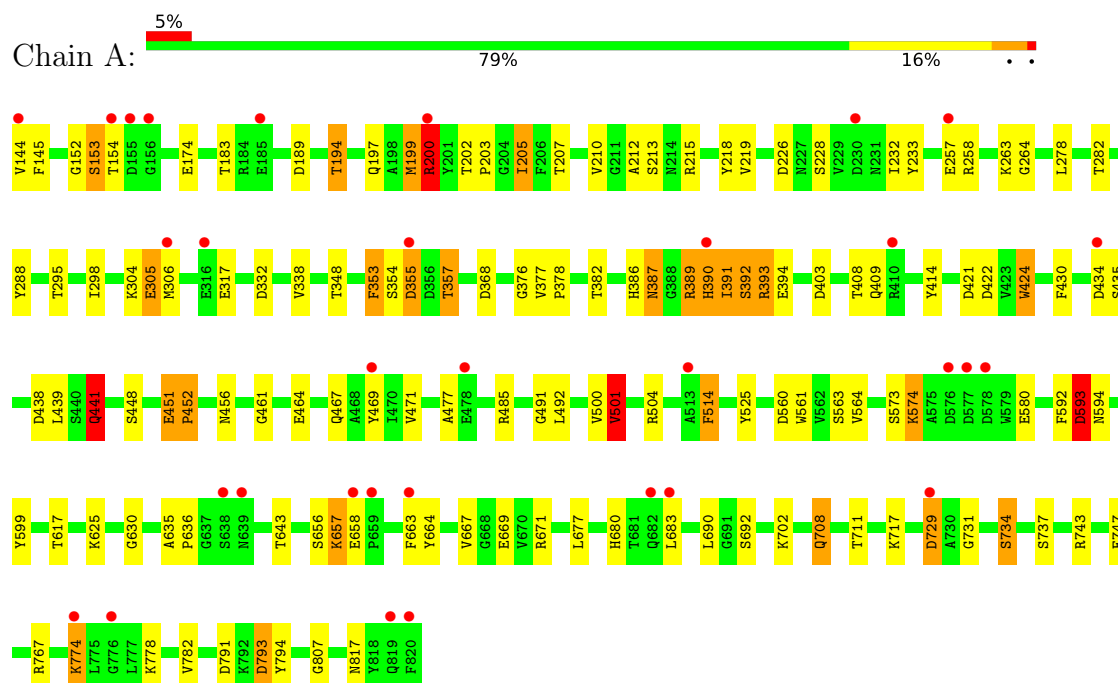
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	14	Total	O	0	0
			14	14		

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: Metal-pseudopaline receptor CntO



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.55Å 174.55Å 180.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.53 – 2.80 48.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.53-2.80) 99.8 (48.53-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.260 0.225 , 0.269	Depositor DCC
R_{free} test set	2029 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5532	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, C8E, GOL, NI, NA, FTT

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	1.44	25/5451 (0.5%)	1.30	46/7397 (0.6%)

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	A	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	593	ASP	CB-CG	9.09	1.74	1.52
1	A	205	ILE	C-O	-7.02	1.17	1.24
1	A	574	LYS	C-O	-6.88	1.16	1.23
1	A	391	ILE	N-CA	6.63	1.54	1.46
1	A	390	HIS	CA-C	-6.34	1.43	1.52
1	A	500	VAL	C-O	-6.19	1.17	1.24
1	A	564	VAL	C-O	-5.86	1.18	1.24
1	A	394	GLU	CA-C	5.82	1.60	1.52
1	A	152	GLY	C-O	-5.81	1.16	1.23
1	A	671	ARG	CZ-NH1	5.79	1.40	1.32
1	A	213	SER	C-O	-5.76	1.16	1.23
1	A	467	GLN	C-O	-5.75	1.17	1.24
1	A	817	ASN	N-CA	5.66	1.52	1.46
1	A	368	ASP	C-O	-5.64	1.19	1.24
1	A	357	THR	C-O	-5.59	1.17	1.23
1	A	403	ASP	C-O	-5.54	1.17	1.23
1	A	461	GLY	C-O	-5.50	1.16	1.23
1	A	408	THR	CA-C	-5.42	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	GLU	C-O	-5.27	1.17	1.23
1	A	174	GLU	CA-C	5.16	1.60	1.52
1	A	492	LEU	N-CA	-5.11	1.40	1.46
1	A	232	ILE	C-O	-5.09	1.18	1.24
1	A	471	VAL	C-O	-5.07	1.19	1.24
1	A	376	GLY	C-O	-5.04	1.17	1.23
1	A	491	GLY	CA-C	-5.02	1.46	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	ILE	N-CA-C	12.23	134.78	109.34
1	A	391	ILE	CB-CA-C	-11.33	92.71	111.29
1	A	332	ASP	N-CA-C	-8.37	99.25	110.55
1	A	387	ASN	N-CA-C	-8.13	95.96	108.31
1	A	451	GLU	N-CA-C	-7.71	97.07	109.40
1	A	592	PHE	CA-C-N	7.38	130.17	120.28
1	A	592	PHE	C-N-CA	7.38	130.17	120.28
1	A	390	HIS	CA-C-O	-6.94	110.71	118.69
1	A	278	LEU	N-CA-C	6.84	119.47	109.07
1	A	441	GLN	N-CA-C	6.76	119.60	108.99
1	A	731	GLY	CA-C-N	6.59	126.37	119.05
1	A	731	GLY	C-N-CA	6.59	126.37	119.05
1	A	658	GLU	N-CA-C	-6.53	99.91	109.50
1	A	451	GLU	CB-CA-C	6.51	118.20	109.42
1	A	469	TYR	N-CA-C	6.49	119.29	109.23
1	A	421	ASP	CB-CA-C	-6.43	96.64	111.95
1	A	226	ASP	CA-C-N	-6.43	111.77	123.34
1	A	226	ASP	C-N-CA	-6.43	111.77	123.34
1	A	353	PHE	CA-C-N	-6.35	114.02	121.64
1	A	353	PHE	C-N-CA	-6.35	114.02	121.64
1	A	264	GLY	CA-C-N	6.06	126.41	119.93
1	A	264	GLY	C-N-CA	6.06	126.41	119.93
1	A	514	PHE	N-CA-C	-5.97	98.34	108.26
1	A	793	ASP	CB-CA-C	-5.94	99.49	109.53
1	A	456	ASN	N-CA-C	-5.89	101.56	110.28
1	A	389	ARG	N-CA-C	5.87	118.40	109.95
1	A	332	ASP	CA-C-N	-5.85	110.37	121.54
1	A	332	ASP	C-N-CA	-5.85	110.37	121.54
1	A	153	SER	N-CA-C	-5.72	99.73	108.76
1	A	594	ASN	N-CA-C	5.58	119.96	113.20
1	A	202	THR	CB-CA-C	5.55	116.02	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ARG	N-CA-C	-5.53	101.57	110.14
1	A	711	THR	N-CA-C	-5.43	102.82	110.31
1	A	708	GLN	N-CA-C	5.31	119.47	113.15
1	A	424	TRP	N-CA-C	5.29	118.35	109.95
1	A	593	ASP	N-CA-C	-5.27	105.54	111.28
1	A	501	VAL	N-CA-CB	-5.24	104.24	111.99
1	A	200	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	232	ILE	N-CA-C	5.20	116.19	108.23
1	A	183	THR	N-CA-C	5.18	117.36	110.53
1	A	617	THR	N-CA-C	5.14	116.36	109.83
1	A	635	ALA	CA-C-N	5.14	126.26	119.84
1	A	635	ALA	C-N-CA	5.14	126.26	119.84
1	A	671	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	288	TYR	CB-CA-C	5.10	118.61	110.09
1	A	504	ARG	CA-CB-CG	5.10	124.30	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	GLU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5325	0	5038	47	1
2	A	1	0	0	0	0
3	A	24	0	32	0	0
4	A	55	0	93	0	0
5	A	51	0	81	2	0
6	A	60	0	0	1	0
7	A	2	0	0	0	0
8	A	14	0	0	0	0
All	All	5532	0	5244	49	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 5.

All (49) 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:593:ASP:CB	1:A:593:ASP:CG	1.74	1.60
1:A:391:ILE:HG22	1:A:391:ILE:O	1.58	0.97
1:A:734:SER:HB3	1:A:774:LYS:HD2	1.70	0.73
1:A:729:ASP:OD2	1:A:729:ASP:N	2.22	0.71
1:A:561:TRP:CD1	1:A:580:GLU:HG2	2.27	0.70
1:A:355:ASP:N	1:A:355:ASP:OD1	2.30	0.65
1:A:194:THR:HG22	1:A:197:GLN:H	1.62	0.64
1:A:200:ARG:HD2	1:A:743:ARG:HH11	1.66	0.60
1:A:207:THR:HG22	1:A:207:THR:O	2.07	0.55
1:A:794:TYR:CZ	1:A:807:GLY:HA3	2.42	0.55
1:A:207:THR:O	1:A:207:THR:CG2	2.55	0.54
5:A:910:FTT:H52	5:A:911:FTT:O2	2.08	0.54
1:A:464:GLU:HG2	1:A:501:VAL:HG22	1.91	0.52
1:A:199:MET:HG2	1:A:205:ILE:HD13	1.91	0.52
1:A:386:HIS:O	1:A:387:ASN:C	2.54	0.51
1:A:200:ARG:HD2	1:A:743:ARG:NH1	2.27	0.49
1:A:215:ARG:HH12	1:A:441:GLN:NE2	2.10	0.48
1:A:210:VAL:HG21	1:A:218:TYR:CE2	2.49	0.48
1:A:377:VAL:HB	1:A:378:PRO:CD	2.45	0.47
1:A:680:HIS:CE1	1:A:690:LEU:HD22	2.50	0.47
1:A:353:PHE:HB2	1:A:357:THR:HB	1.98	0.45
1:A:669:GLU:HB2	1:A:702:LYS:HB2	1.99	0.44
1:A:391:ILE:O	1:A:391:ILE:CG2	2.24	0.44
1:A:599:TYR:CE1	1:A:630:GLY:HA3	2.53	0.44
1:A:200:ARG:NE	1:A:207:THR:HB	2.33	0.43
1:A:393:ARG:NH1	1:A:791:ASP:OD1	2.51	0.43
1:A:389:ARG:NH2	1:A:389:ARG:HG2	2.32	0.43
1:A:561:TRP:NE1	1:A:580:GLU:OE2	2.52	0.43
1:A:424:TRP:CZ3	1:A:477:ALA:HB2	2.54	0.43
1:A:664:TYR:CD1	1:A:664:TYR:N	2.86	0.43
1:A:215:ARG:HH22	1:A:441:GLN:HE22	1.67	0.42
1:A:525:TYR:OH	6:A:915:SO4:O4	2.32	0.42
1:A:391:ILE:HD13	1:A:391:ILE:HG21	1.64	0.42
1:A:657:LYS:HB3	1:A:657:LYS:HE3	1.42	0.42
1:A:377:VAL:HB	1:A:378:PRO:HD2	2.01	0.42
1:A:233:TYR:CD1	1:A:233:TYR:N	2.88	0.41
1:A:203:PRO:HB3	1:A:692:SER:HB2	2.03	0.41
1:A:257:GLU:O	1:A:257:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HD12	1:A:298:ILE:HA	1.94	0.41
1:A:430:PHE:CD1	1:A:430:PHE:C	2.99	0.41
1:A:593:ASP:CG	1:A:593:ASP:H	2.28	0.41
1:A:199:MET:HE3	1:A:219:VAL:HG11	2.03	0.41
1:A:200:ARG:HG2	1:A:207:THR:CB	2.50	0.40
1:A:424:TRP:CH2	1:A:477:ALA:HB2	2.55	0.40
1:A:663:PHE:CD1	1:A:663:PHE:C	2.99	0.40
5:A:910:FTT:H51	5:A:910:FTT:O1	2.22	0.40
1:A:391:ILE:O	1:A:392:SER:C	2.65	0.40
1:A:414:TYR:CD1	1:A:414:TYR:C	2.99	0.40
1:A:189:ASP:O	1:A:767:ARG:HD2	2.22	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:A:434:ASP:OD2	1:A:580:GLU:OE2[2_445]	1.74	0.46

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	675/677 (100%)	640 (95%)	30 (4%)	5 (1%)	18 47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	SER
1	A	145	PHE
1	A	636	PRO
1	A	212	ALA
1	A	452	PRO

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	566/566 (100%)	511 (90%)	55 (10%)	8 25

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	153	SER
1	A	154	THR
1	A	194	THR
1	A	199	MET
1	A	200	ARG
1	A	228	SER
1	A	258	ARG
1	A	263	LYS
1	A	282	THR
1	A	295	THR
1	A	304	LYS
1	A	305	GLU
1	A	306	MET
1	A	317	GLU
1	A	338	VAL
1	A	348	THR
1	A	354	SER
1	A	355	ASP
1	A	382	THR
1	A	390	HIS
1	A	393	ARG
1	A	409	GLN
1	A	422	ASP
1	A	435	SER
1	A	438	ASP
1	A	439	LEU
1	A	441	GLN
1	A	448	SER
1	A	452	PRO

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Mol	Chain	Res	Type
1	A	485	ARG
1	A	501	VAL
1	A	514	PHE
1	A	560	ASP
1	A	563	SER
1	A	573	SER
1	A	574	LYS
1	A	593	ASP
1	A	625	LYS
1	A	643	THR
1	A	656	SER
1	A	657	LYS
1	A	667	VAL
1	A	677	LEU
1	A	683	LEU
1	A	708	GLN
1	A	717	LYS
1	A	729	ASP
1	A	734	SER
1	A	737	SER
1	A	747	GLU
1	A	774	LYS
1	A	778	LYS
1	A	782	VAL
1	A	793	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	441	GLN
1	A	515	ASN
1	A	559	GLN
1	A	639	ASN
1	A	686	ASN

5.3.3 RNA ⓘ

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 26 ligands modelled in this entry, 3 are monoatomic - leaving 23 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	$\# Z > 2$
6	SO4	A	919	-	4,4,4	0.52	0	6,6,6	0.46	0
6	SO4	A	914	-	4,4,4	0.52	0	6,6,6	0.53	0
6	SO4	A	918	-	4,4,4	0.25	0	6,6,6	0.25	0
6	SO4	A	915	-	4,4,4	0.57	0	6,6,6	0.41	0
3	GOL	A	903	-	5,5,5	0.34	0	5,5,5	1.15	1 (20%)
3	GOL	A	904	-	5,5,5	0.58	0	5,5,5	0.91	0
3	GOL	A	902	-	5,5,5	0.18	0	5,5,5	0.63	0
5	FTT	A	912	-	16,16,16	0.62	0	16,17,17	1.24	1 (6%)
4	C8E	A	906	-	11,11,20	0.63	0	10,10,19	0.62	0
6	SO4	A	916	-	4,4,4	0.52	0	6,6,6	0.31	0
6	SO4	A	917	-	4,4,4	0.48	0	6,6,6	0.56	0
4	C8E	A	908	-	9,9,20	0.48	0	8,8,19	0.36	0
5	FTT	A	911	-	16,16,16	0.69	0	16,17,17	0.86	1 (6%)
6	SO4	A	921	-	4,4,4	0.49	0	6,6,6	0.22	0
6	SO4	A	923	-	4,4,4	0.46	0	6,6,6	0.19	0
6	SO4	A	924	-	4,4,4	0.46	0	6,6,6	0.21	0
6	SO4	A	920	-	4,4,4	0.50	0	6,6,6	0.23	0
6	SO4	A	913	-	4,4,4	0.47	0	6,6,6	0.32	0
4	C8E	A	907	-	11,11,20	0.58	0	10,10,19	0.39	0
5	FTT	A	910	-	16,16,16	0.41	0	16,17,17	1.57	3 (18%)
3	GOL	A	905	-	5,5,5	0.51	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	C8E	A	909	-	20,20,20	0.66	0	19,19,19	0.77	0
6	SO4	A	922	-	4,4,4	0.55	0	6,6,6	0.31	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
4	C8E	A	907	-	-	1/9/9/18	-
4	C8E	A	909	-	-	11/18/18/18	-
3	GOL	A	905	-	-	4/4/4/4	-
5	FTT	A	910	-	-	4/15/15/15	-
4	C8E	A	908	-	-	3/7/7/18	-
3	GOL	A	904	-	-	3/4/4/4	-
5	FTT	A	911	-	-	5/15/15/15	-
5	FTT	A	912	-	-	8/15/15/15	-
3	GOL	A	903	-	-	4/4/4/4	-
3	GOL	A	902	-	-	2/4/4/4	-
4	C8E	A	906	-	-	3/9/9/18	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	910	FTT	O1-C1-C2	4.23	127.14	114.00
5	A	912	FTT	O1-C1-C2	3.01	123.36	114.00
5	A	910	FTT	O2-C1-C2	-2.99	113.67	122.84
5	A	910	FTT	C4-C3-C2	-2.23	105.37	112.88
3	A	903	GOL	O2-C2-C1	2.11	117.91	109.18
5	A	911	FTT	O1-C1-C2	2.07	120.45	114.00

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	GOL	C1-C2-C3-O3
3	A	903	GOL	O2-C2-C3-O3
3	A	904	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	905	GOL	O1-C1-C2-C3
5	A	910	FTT	C2-C3-C4-C5
5	A	912	FTT	C1-C2-C3-C4
5	A	912	FTT	C1-C2-C3-O3
4	A	909	C8E	C17-C16-O15-C14
4	A	909	C8E	O12-C13-C14-O15
4	A	909	C8E	O9-C10-C11-O12
5	A	910	FTT	O3-C3-C4-C5
4	A	909	C8E	O15-C16-C17-O18
3	A	903	GOL	O1-C1-C2-C3
3	A	903	GOL	C1-C2-C3-O3
3	A	905	GOL	C1-C2-C3-O3
5	A	912	FTT	O3-C3-C4-C5
3	A	902	GOL	O2-C2-C3-O3
5	A	910	FTT	C5-C6-C7-C8
4	A	908	C8E	C7-C8-O9-C10
5	A	912	FTT	C10-C11-C12-C13
5	A	911	FTT	C10-C11-C12-C13
5	A	911	FTT	C11-C10-C9-C8
4	A	906	C8E	C5-C6-C7-C8
5	A	912	FTT	C11-C10-C9-C8
3	A	903	GOL	O1-C1-C2-O2
3	A	905	GOL	O1-C1-C2-O2
5	A	911	FTT	C5-C6-C7-C8
3	A	904	GOL	O2-C2-C3-O3
4	A	909	C8E	C2-C3-C4-C5
5	A	911	FTT	C11-C12-C13-C14
4	A	908	C8E	C2-C3-C4-C5
5	A	912	FTT	C5-C6-C7-C8
4	A	906	C8E	C2-C3-C4-C5
4	A	908	C8E	C5-C6-C7-C8
4	A	909	C8E	O18-C19-C20-O21
4	A	909	C8E	C10-C11-O12-C13
4	A	909	C8E	C11-C10-O9-C8
4	A	907	C8E	O9-C10-C11-O12
4	A	909	C8E	C5-C6-C7-C8
3	A	904	GOL	O1-C1-C2-O2
4	A	906	C8E	O9-C10-C11-O12
5	A	910	FTT	C4-C5-C6-C7
4	A	909	C8E	C20-C19-O18-C17
5	A	911	FTT	C3-C4-C5-C6
5	A	912	FTT	C11-C12-C13-C14

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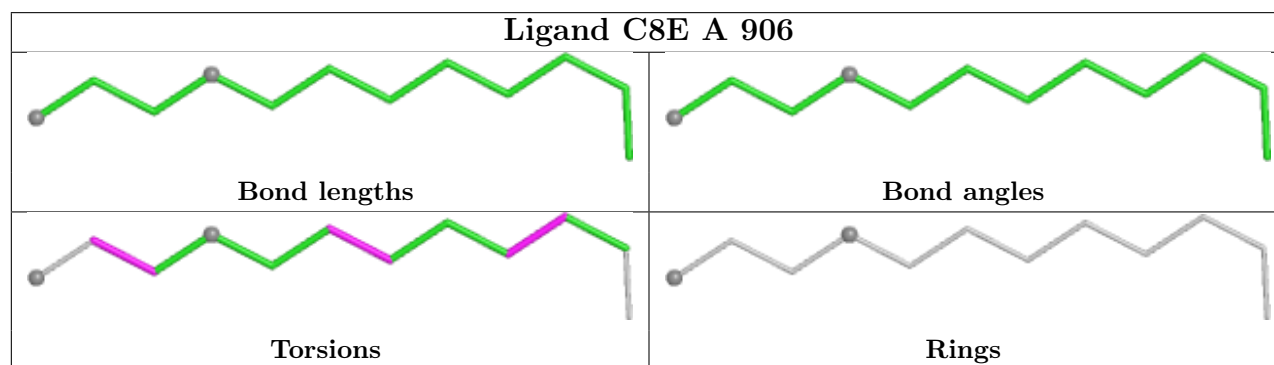
Mol	Chain	Res	Type	Atoms
3	A	905	GOL	O2-C2-C3-O3
4	A	909	C8E	C14-C13-O12-C11
5	A	912	FTT	C6-C7-C8-C9

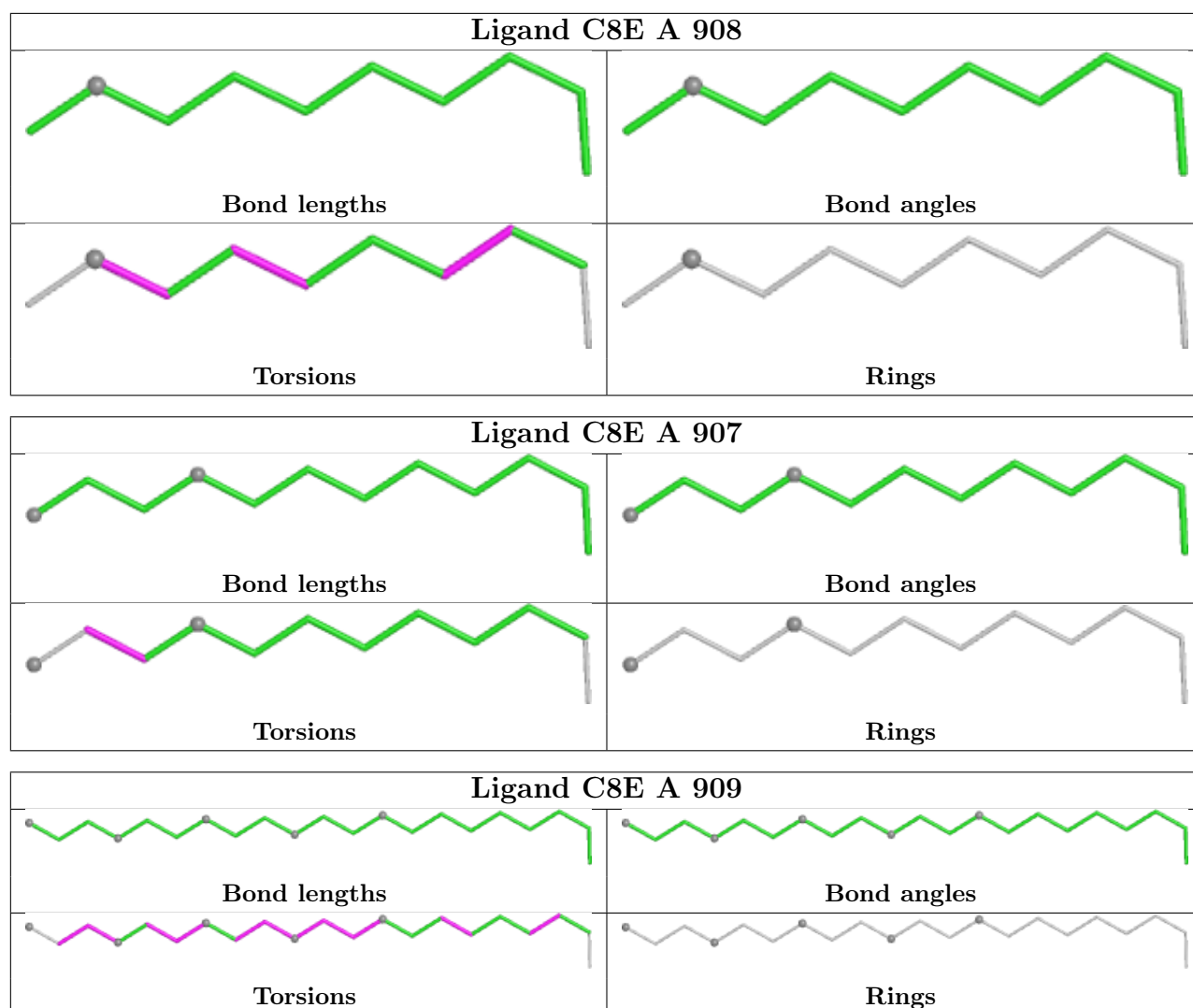
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	915	SO4	1	0
5	A	911	FTT	1	0
5	A	910	FTT	2	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	677/677 (100%)	0.12	32 (4%)	36 29	30, 56, 79, 109	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	820	PHE	7.1
1	A	155	ASP	6.7
1	A	639	ASN	4.0
1	A	682	GLN	3.6
1	A	156	GLY	3.6
1	A	819	GLN	3.5
1	A	200	ARG	3.3
1	A	410	ARG	3.3
1	A	154	THR	3.1
1	A	683	LEU	3.0
1	A	658	GLU	2.9
1	A	434	ASP	2.9
1	A	355	ASP	2.8
1	A	478	GLU	2.8
1	A	390	HIS	2.7
1	A	306	MET	2.6
1	A	185	GLU	2.6
1	A	659	PRO	2.4
1	A	776	GLY	2.4
1	A	576	ASP	2.4
1	A	638	SER	2.4
1	A	230	ASP	2.4
1	A	578	ASP	2.2
1	A	663	PHE	2.2
1	A	729	ASP	2.2
1	A	774	LYS	2.2
1	A	577	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	144	VAL	2.1
1	A	469	TYR	2.1
1	A	513	ALA	2.0
1	A	257	GLU	2.0
1	A	316	GLU	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(Å ²)	Q<0.9
6	SO4	A	922	5/5	0.35	0.14	124,124,133,136	0
5	FTT	A	911	17/17	0.64	0.50	88,101,111,111	0
3	GOL	A	904	6/6	0.68	0.26	74,78,83,83	0
6	SO4	A	915	5/5	0.77	0.12	111,112,131,137	0
6	SO4	A	924	5/5	0.78	0.12	130,135,137,138	0
6	SO4	A	921	5/5	0.79	0.09	124,131,138,141	0
6	SO4	A	916	5/5	0.82	0.25	91,94,101,103	0
5	FTT	A	912	17/17	0.84	0.28	68,78,108,114	0
6	SO4	A	923	5/5	0.84	0.14	115,125,133,135	0
3	GOL	A	905	6/6	0.84	0.26	89,103,104,107	0
6	SO4	A	919	5/5	0.85	0.17	108,113,131,132	0
4	C8E	A	909	21/21	0.86	0.27	65,82,115,122	0
4	C8E	A	908	10/21	0.87	0.23	63,69,81,81	0
6	SO4	A	917	5/5	0.88	0.10	90,101,104,105	0
6	SO4	A	920	5/5	0.88	0.10	121,121,133,136	0
5	FTT	A	910	17/17	0.90	0.20	43,51,65,76	0
6	SO4	A	913	5/5	0.90	0.10	80,81,94,95	0
6	SO4	A	914	5/5	0.90	0.26	93,100,113,121	0

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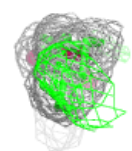
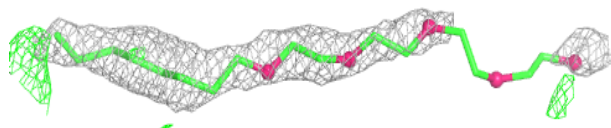
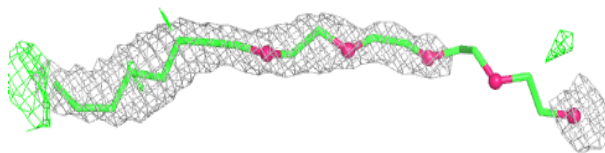
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	C8E	A	906	12/21	0.90	0.21	61,76,85,86	0
4	C8E	A	907	12/21	0.91	0.25	72,89,102,106	0
3	GOL	A	903	6/6	0.92	0.12	63,65,67,68	0
6	SO4	A	918	5/5	0.93	0.18	89,93,100,105	0
7	NA	A	926	1/1	0.94	0.12	69,69,69,69	0
2	NI	A	901	1/1	0.95	0.06	99,99,99,99	0
3	GOL	A	902	6/6	0.97	0.10	65,70,72,78	0
7	NA	A	925	1/1	0.99	0.30	54,54,54,54	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.

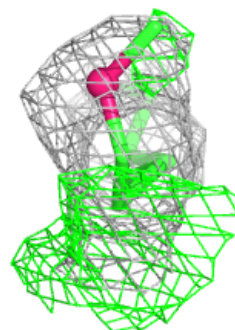
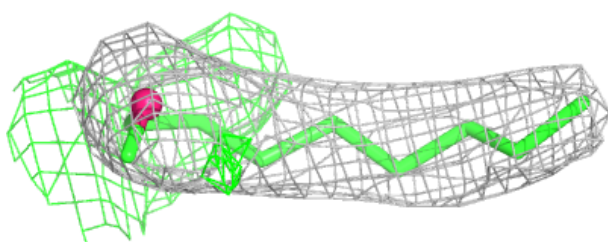
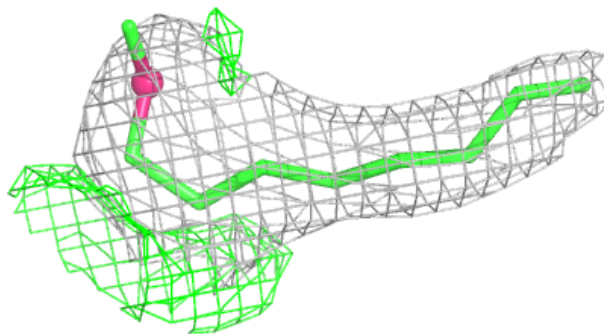
Electron density around C8E A 909:

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

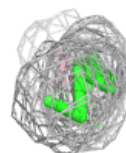
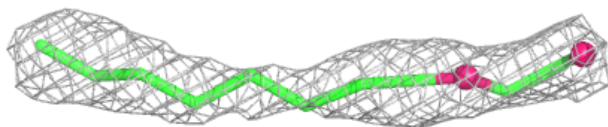
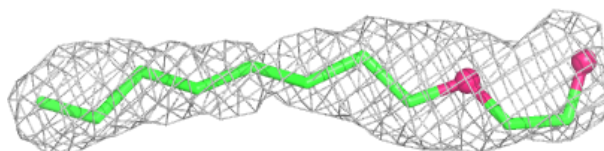


Electron density around C8E A 908:

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

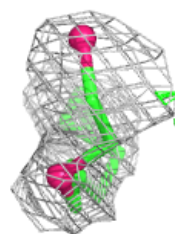
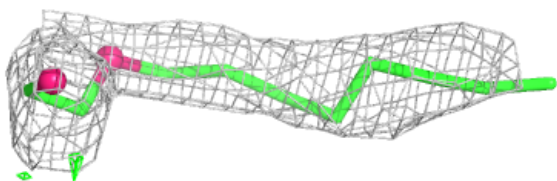
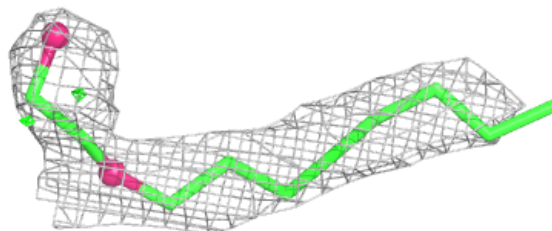
**Electron density around C8E A 906:**

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



Electron density around C8E A 907:

$2mF_o-DF_c$ (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.