



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:44 AM UTC

PDB ID : 2XE5 / pdb_00002xe5
Title : Molecular insights into clinically isolated OmpC mutants and their role in multi-drug resistance (OmpC26)
Authors : Bamford, V.A.; Naismith, J.H.
Deposited on : 2010-05-11
Resolution : 2.28 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

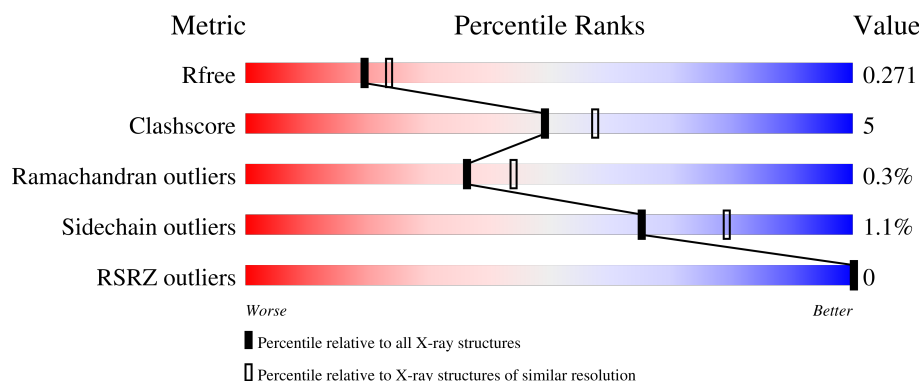
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	343	88% 11%
1	B	343	90% 10%
1	C	343	91% 9%
1	D	343	90% 9%
1	E	343	90% 10%

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Mol	Chain	Length	Quality of chain
1	F	343	 90%9%

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
6	SO4	A	1348	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17072 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.

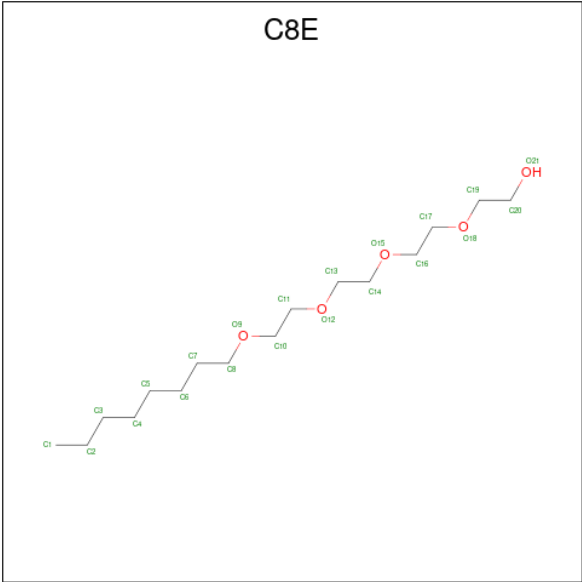
- Molecule 1 is a protein called OUTER MEMBRANE PORIN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2710	1699	452	555	4			
1	B	343	Total	C	N	O	S	0	0	0
			2710	1699	452	555	4			
1	C	343	Total	C	N	O	S	0	0	0
			2710	1699	452	555	4			
1	D	343	Total	C	N	O	S	0	0	0
			2710	1699	452	555	4			
1	E	343	Total	C	N	O	S	0	0	0
			2710	1699	452	555	4			
1	F	343	Total	C	N	O	S	0	0	0
			2710	1699	452	555	4			

There are 6 discrepancies between the modelled and reference sequences:

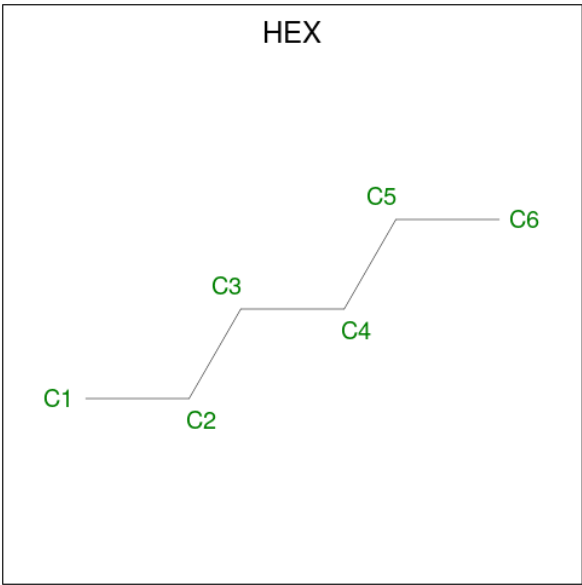
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
B	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
C	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
D	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
E	18	GLU	ASP	SEE REMARK 999	UNP Q9K597
F	18	GLU	ASP	SEE REMARK 999	UNP Q9K597

- 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	B	1	Total	C	O	0	0
			21	16	5		
2	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



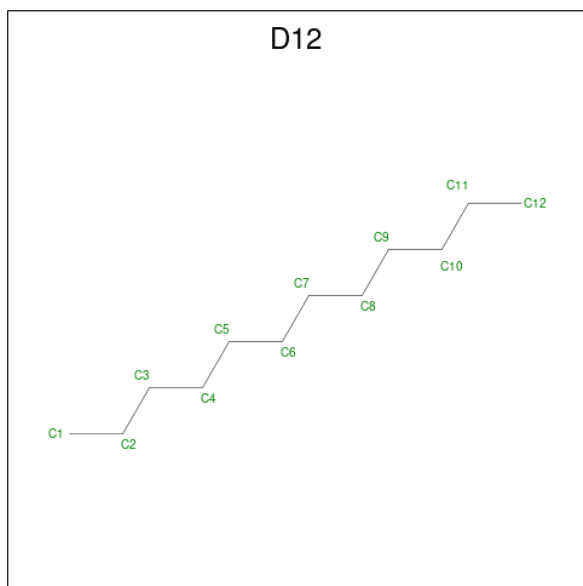
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 6 6	0	0
3	E	1	Total C 6 6	0	0
3	F	1	Total C 6 6	0	0

- Molecule 4 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



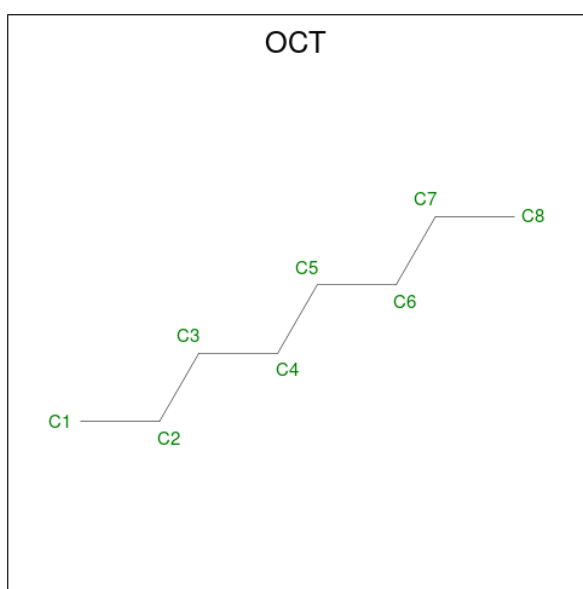
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 12 12	0	0
4	C	1	Total C 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C 12 12	0	0
4	E	1	Total C 12 12	0	0
4	E	1	Total C 11 11	0	0
4	F	1	Total C 12 12	0	0

- Molecule 5 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



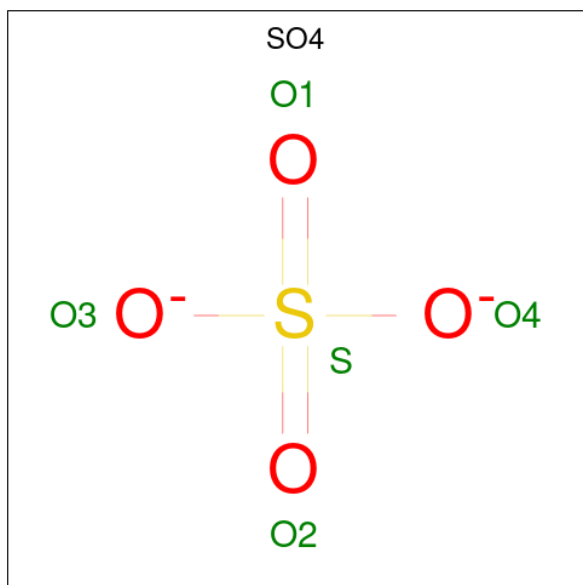
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	C	1	Total C 8 8	0	0
5	D	1	Total C 8 8	0	0

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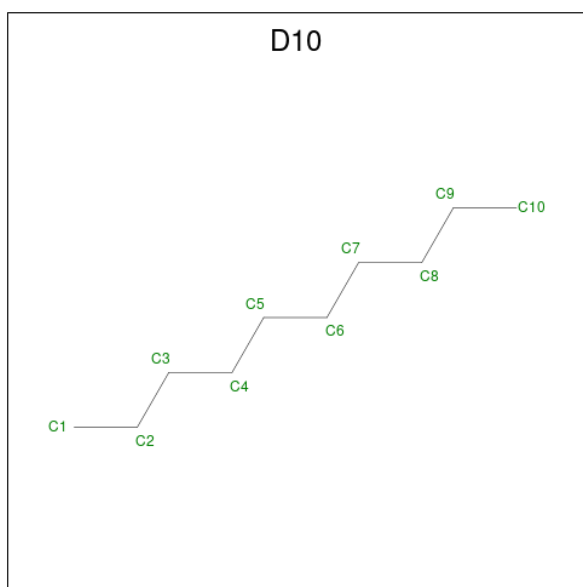
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C 8 8	0	0
5	E	1	Total C 8 8	0	0
5	F	1	Total C 8 8	0	0

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



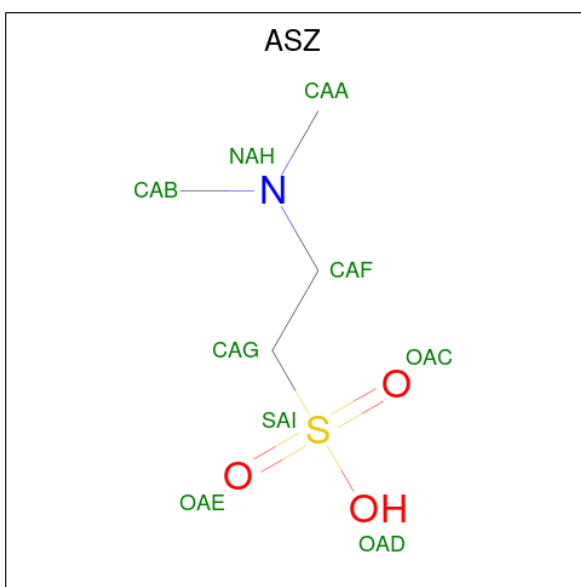
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0

- Molecule 7 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



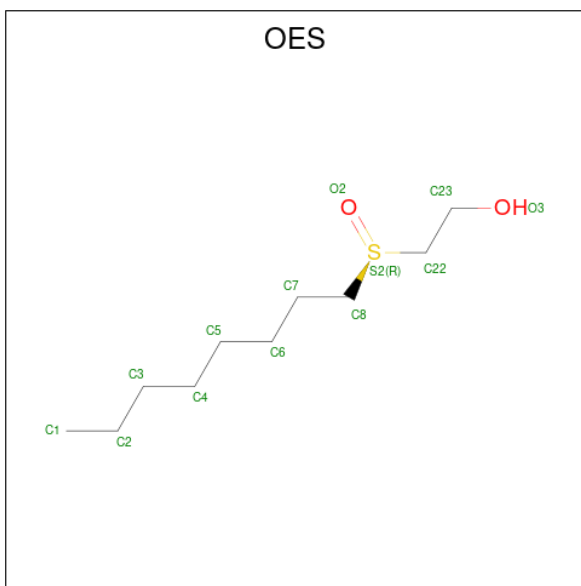
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C 10 10	0	0
7	B	1	Total C 10 10	0	0
7	B	1	Total C 10 10	0	0
7	B	1	Total C 10 10	0	0
7	B	1	Total C 10 10	0	0
7	B	1	Total C 10 10	0	0

- Molecule 8 is 2-(DIMETHYLAMINO)ETHANESULFONIC ACID (CCD ID: ASZ) (formula: $C_4H_{11}NO_3S$).



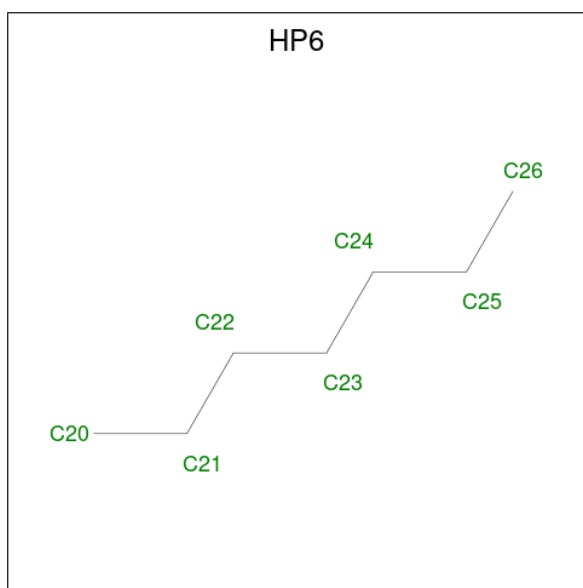
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			9	4	1	3	1		

- Molecule 9 is N-OCTYL-2-HYDROXYETHYL SULFOXIDE (CCD ID: OES) (formula: $C_{10}H_{22}O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	S	0	0
			13	10	2	1		
9	D	1	Total	C	O	S	0	0
			13	10	2	1		

- Molecule 10 is HEPTANE (CCD ID: HP6) (formula: C_7H_{16}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 7 7	0	0
10	D	1	Total C 7 7	0	0
10	F	1	Total C 7 7	0	0

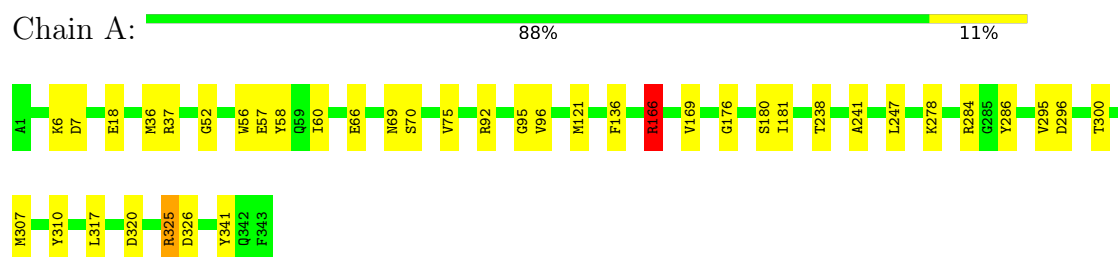
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	88	Total O 88 88	0	0
11	B	40	Total O 40 40	0	0
11	C	64	Total O 64 64	0	0
11	D	70	Total O 70 70	0	0
11	E	78	Total O 78 78	0	0
11	F	52	Total O 52 52	0	0

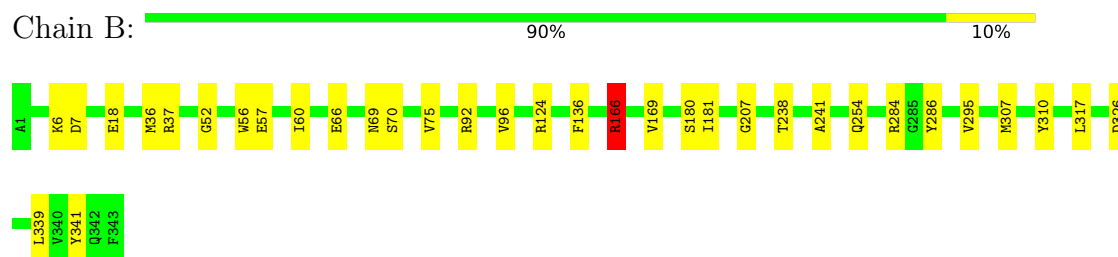
3 Residue-property plots

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.

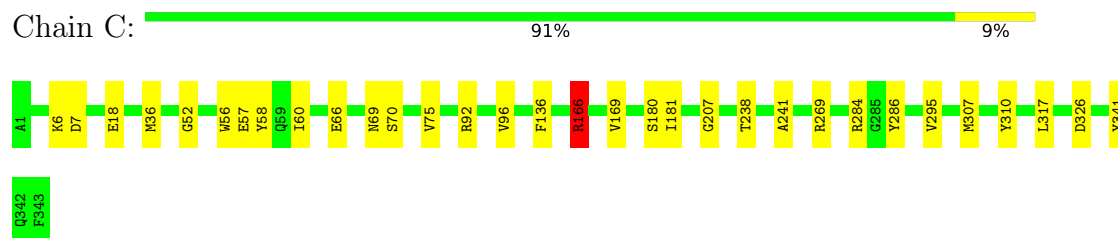
• Molecule 1: OUTER MEMBRANE PORIN C



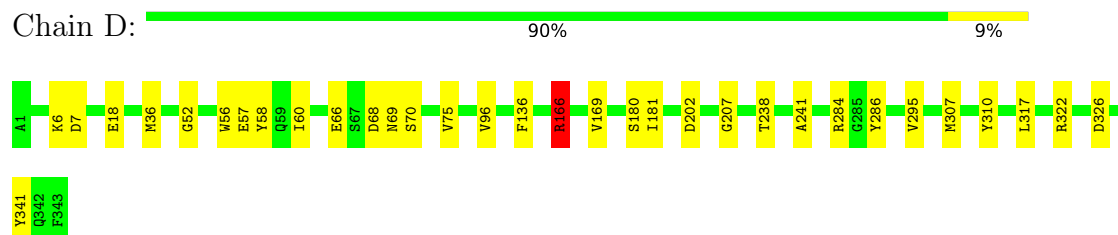
• Molecule 1: OUTER MEMBRANE PORIN C



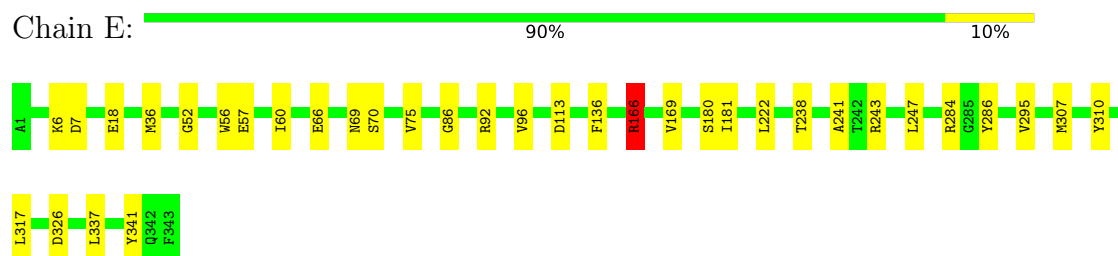
• Molecule 1: OUTER MEMBRANE PORIN C



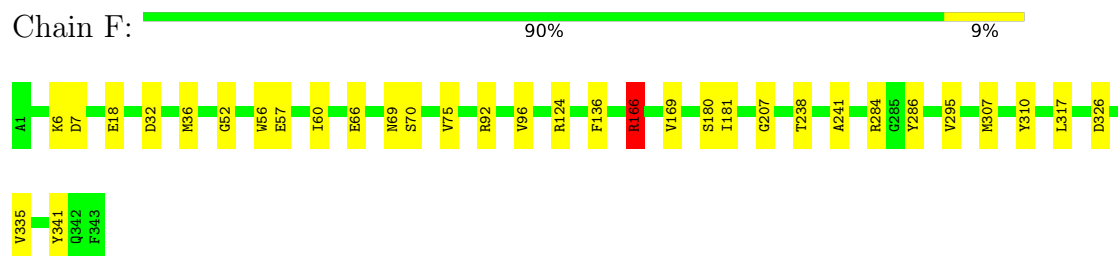
• Molecule 1: OUTER MEMBRANE PORIN C



● Molecule 1: OUTER MEMBRANE PORIN C



● Molecule 1: OUTER MEMBRANE PORIN C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.18Å 93.68Å 115.91Å 98.74° 108.79° 109.71°	Depositor
Resolution (Å)	29.41 – 2.28 29.41 – 2.28	Depositor EDS
% Data completeness (in resolution range)	79.1 (29.41-2.28) 79.1 (29.41-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0060	Depositor
R, R_{free}	0.226 , 0.267 0.233 , 0.271	Depositor DCC
R_{free} test set	4815 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 24.3	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	0.93	EDS
Total number of atoms	17072	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: D12, HP6, D10, C8E, OES, SO4, HEX, ASZ, OCT

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	0.75	0/2771	0.80	1/3749 (0.0%)
1	B	0.71	0/2771	0.79	1/3749 (0.0%)
1	C	0.73	0/2771	0.79	1/3749 (0.0%)
1	D	0.73	0/2771	0.79	1/3749 (0.0%)
1	E	0.74	0/2771	0.80	1/3749 (0.0%)
1	F	0.72	0/2771	0.79	1/3749 (0.0%)
All	All	0.73	0/16626	0.79	6/22494 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	CG-CD-NE	-5.88	99.06	112.00
1	E	166	ARG	CG-CD-NE	-5.80	99.23	112.00
1	D	166	ARG	CG-CD-NE	-5.75	99.35	112.00
1	B	166	ARG	CG-CD-NE	-5.74	99.37	112.00
1	F	166	ARG	CG-CD-NE	-5.69	99.49	112.00
1	C	166	ARG	CG-CD-NE	-5.66	99.55	112.00

There are no chirality outliers.

There are no planarity outliers.

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	2710	0	2481	38	0
1	B	2710	0	2481	34	0
1	C	2710	0	2481	28	0
1	D	2710	0	2481	29	0
1	E	2710	0	2481	32	0
1	F	2710	0	2481	30	0
2	A	21	0	34	0	0
2	B	21	0	34	0	0
2	D	21	0	34	0	0
3	A	12	0	28	0	0
3	B	12	0	28	3	0
3	C	24	0	56	0	0
3	E	6	0	14	0	0
3	F	6	0	14	0	0
4	A	12	0	26	0	0
4	C	12	0	26	2	0
4	E	35	0	73	1	0
4	F	12	0	26	0	0
5	A	16	0	36	0	0
5	B	24	0	54	1	0
5	C	8	0	18	0	0
5	D	16	0	36	0	0
5	E	8	0	18	1	0
5	F	8	0	18	1	0
6	A	10	0	0	2	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	F	10	0	0	1	0
7	B	60	0	132	2	0
8	B	9	0	11	2	0
9	B	13	0	22	0	0
9	D	13	0	22	0	0
10	B	7	0	16	1	0
10	D	7	0	16	0	0
10	F	7	0	16	0	0
11	A	88	0	0	6	0
11	B	40	0	0	0	0
11	C	64	0	0	2	0
11	D	70	0	0	2	0
11	E	78	0	0	2	0
11	F	52	0	0	3	0
All	All	17072	0	15694	174	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 5.

All (174) 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:307:MET:HE1	1:A:341:TYR:HD1	1.43	0.83
1:E:307:MET:HE1	1:E:341:TYR:HD1	1.44	0.82
1:F:307:MET:HE1	1:F:341:TYR:HD1	1.44	0.82
1:B:307:MET:HE1	1:B:341:TYR:HD1	1.44	0.82
1:E:36:MET:HE1	1:E:60:ILE:HD12	1.63	0.81
1:D:307:MET:HE1	1:D:341:TYR:HD1	1.44	0.81
1:A:36:MET:HE1	1:A:60:ILE:HD12	1.63	0.81
1:C:307:MET:HE1	1:C:341:TYR:HD1	1.44	0.81
1:B:36:MET:HE1	1:B:60:ILE:HD12	1.61	0.80
1:D:36:MET:HE1	1:D:60:ILE:HD12	1.63	0.80
1:F:36:MET:HE1	1:F:60:ILE:HD12	1.62	0.80
1:B:36:MET:CE	1:B:60:ILE:HD12	2.12	0.79
1:C:36:MET:HE1	1:C:60:ILE:HD12	1.64	0.78
1:D:307:MET:CE	1:D:341:TYR:HD1	1.97	0.78
1:C:307:MET:CE	1:C:341:TYR:HD1	1.97	0.78
1:E:36:MET:CE	1:E:60:ILE:HD12	2.13	0.78
1:D:36:MET:CE	1:D:60:ILE:HD12	2.14	0.78
1:A:307:MET:CE	1:A:341:TYR:HD1	1.96	0.78
1:F:36:MET:CE	1:F:60:ILE:HD12	2.13	0.78
1:A:36:MET:CE	1:A:60:ILE:HD12	2.13	0.78
1:B:307:MET:CE	1:B:341:TYR:HD1	1.97	0.77
1:F:307:MET:CE	1:F:341:TYR:HD1	1.97	0.77
1:E:307:MET:CE	1:E:341:TYR:HD1	1.97	0.77
1:C:36:MET:CE	1:C:60:ILE:HD12	2.15	0.77
1:A:300:THR:OG1	11:A:2076:HOH:O	2.07	0.72
1:A:307:MET:HE1	1:A:341:TYR:CD1	2.25	0.72
1:E:307:MET:HE1	1:E:341:TYR:CD1	2.25	0.71
1:B:307:MET:HE1	1:B:341:TYR:CD1	2.25	0.71
1:F:307:MET:HE1	1:F:341:TYR:CD1	2.25	0.71
1:D:36:MET:HE3	1:D:60:ILE:HB	1.74	0.69
1:C:36:MET:HE3	1:C:60:ILE:HB	1.74	0.69
1:D:307:MET:HE1	1:D:341:TYR:CD1	2.26	0.68
1:A:284:ARG:NH1	11:A:2069:HOH:O	2.26	0.68
1:C:307:MET:HE1	1:C:341:TYR:CD1	2.26	0.68
1:E:36:MET:HE3	1:E:60:ILE:HB	1.75	0.68
1:A:36:MET:HE3	1:A:60:ILE:HB	1.75	0.68
1:B:36:MET:HE3	1:B:60:ILE:HB	1.75	0.68
1:F:36:MET:HE3	1:F:60:ILE:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1346:D12:H122	4:C:1346:D12:H82	1.77	0.66
4:C:1346:D12:H122	4:C:1346:D12:C8	2.24	0.65
1:F:66:GLU:OE1	11:F:2013:HOH:O	2.16	0.62
1:A:176:GLY:O	11:A:2046:HOH:O	2.16	0.62
1:A:36:MET:HE2	1:B:56:TRP:CE2	2.36	0.61
1:F:335:VAL:HG21	5:F:1347:OCT:H41	1.82	0.61
1:D:36:MET:HE2	1:E:56:TRP:CE2	2.36	0.60
1:D:68:ASP:OD1	11:D:2010:HOH:O	2.17	0.60
1:B:124:ARG:HH12	8:B:1350:ASZ:HAA2	1.66	0.59
1:A:56:TRP:CE2	1:C:36:MET:HE2	2.38	0.58
1:B:254:GLN:HE22	3:B:1353:HEX:H62	1.68	0.58
1:E:36:MET:HE2	1:F:56:TRP:CE2	2.40	0.57
1:E:243:ARG:NH2	11:E:2058:HOH:O	2.37	0.56
1:B:36:MET:HE1	1:B:60:ILE:CD1	2.34	0.56
1:D:52:GLY:HA3	1:F:307:MET:HE3	1.88	0.56
1:D:56:TRP:CE2	1:F:36:MET:HE2	2.40	0.56
1:E:222:LEU:HB3	4:E:1346:D12:H12	1.88	0.56
1:B:254:GLN:NE2	3:B:1353:HEX:H62	2.21	0.56
1:F:36:MET:HE1	1:F:60:ILE:CD1	2.35	0.56
1:E:36:MET:HE1	1:E:60:ILE:CD1	2.35	0.55
1:A:36:MET:HE1	1:A:60:ILE:CD1	2.35	0.55
1:A:37:ARG:NH1	6:A:1348:SO4:O1	2.40	0.55
1:F:18:GLU:OE2	1:F:310:TYR:OH	2.20	0.55
1:D:295:VAL:HG23	1:D:317:LEU:HD11	1.89	0.54
1:B:36:MET:HE2	1:C:56:TRP:CE2	2.42	0.54
1:A:325:ARG:NH2	1:D:322:ARG:HD3	2.23	0.54
1:C:295:VAL:HG23	1:C:317:LEU:HD11	1.90	0.54
1:C:269:ARG:HD2	11:C:2049:HOH:O	2.08	0.54
1:B:18:GLU:OE2	1:B:310:TYR:OH	2.19	0.53
1:E:295:VAL:HG23	1:E:317:LEU:HD11	1.89	0.53
1:A:295:VAL:HG23	1:A:317:LEU:HD11	1.89	0.53
1:E:307:MET:HE3	1:F:52:GLY:HA3	1.91	0.53
1:F:295:VAL:HG23	1:F:317:LEU:HD11	1.90	0.53
1:B:295:VAL:HG23	1:B:317:LEU:HD11	1.90	0.53
1:A:66:GLU:HG3	1:B:92:ARG:NH2	2.24	0.53
1:A:52:GLY:HA3	1:C:307:MET:HE3	1.91	0.52
1:A:92:ARG:NH2	1:C:66:GLU:HG3	2.24	0.52
1:A:307:MET:HE3	1:B:52:GLY:HA3	1.92	0.52
1:F:286:TYR:OH	1:F:326:ASP:OD2	2.28	0.52
1:B:317:LEU:HD13	5:B:1358:OCT:H71	1.92	0.52
1:A:247:LEU:HD22	1:A:284:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:MET:HE1	1:D:60:ILE:CD1	2.35	0.51
1:B:286:TYR:OH	1:B:326:ASP:OD2	2.28	0.51
1:D:66:GLU:HG3	1:E:92:ARG:NH2	2.25	0.51
1:C:286:TYR:OH	1:C:326:ASP:OD2	2.28	0.51
1:C:36:MET:HE1	1:C:60:ILE:CD1	2.36	0.51
1:C:18:GLU:OE2	1:C:310:TYR:OH	2.19	0.51
1:D:286:TYR:OH	1:D:326:ASP:OD2	2.28	0.51
1:B:307:MET:HE3	1:C:52:GLY:HA3	1.94	0.50
1:E:247:LEU:HD22	1:E:284:ARG:NH1	2.27	0.50
1:A:166:ARG:CD	1:A:166:ARG:N	2.75	0.50
1:B:166:ARG:N	1:B:166:ARG:CD	2.75	0.50
1:E:166:ARG:N	1:E:166:ARG:CD	2.75	0.50
1:A:278:LYS:HE2	7:B:1348:D10:H102	1.93	0.50
1:F:166:ARG:N	1:F:166:ARG:CD	2.75	0.50
1:D:18:GLU:OE2	1:D:310:TYR:OH	2.19	0.49
1:D:238:THR:HB	1:D:241:ALA:HB3	1.94	0.49
1:D:307:MET:HE3	1:E:52:GLY:HA3	1.94	0.49
1:E:337:LEU:HD21	5:E:1348:OCT:H72	1.94	0.49
1:C:238:THR:HB	1:C:241:ALA:HB3	1.94	0.49
1:E:238:THR:HB	1:E:241:ALA:HB3	1.95	0.49
1:F:238:THR:HB	1:F:241:ALA:HB3	1.94	0.49
1:B:207:GLY:O	1:B:284:ARG:NH2	2.46	0.49
1:A:238:THR:HB	1:A:241:ALA:HB3	1.95	0.49
1:F:207:GLY:O	1:F:284:ARG:NH2	2.46	0.49
1:C:166:ARG:N	1:C:166:ARG:CD	2.75	0.49
1:D:166:ARG:CD	1:D:166:ARG:N	2.75	0.49
1:A:320:ASP:OD2	1:A:325:ARG:NH1	2.46	0.49
1:B:238:THR:HB	1:B:241:ALA:HB3	1.95	0.48
1:A:37:ARG:NH2	6:A:1348:SO4:O3	2.43	0.48
1:B:254:GLN:HE22	3:B:1353:HEX:C6	2.26	0.47
1:C:69:ASN:HD22	1:C:70:SER:N	2.13	0.47
1:C:207:GLY:O	1:C:284:ARG:NH2	2.48	0.47
1:C:96:VAL:HG22	1:C:180:SER:HB3	1.97	0.47
1:D:96:VAL:HG22	1:D:180:SER:HB3	1.97	0.47
1:E:96:VAL:HG22	1:E:180:SER:HB3	1.97	0.46
1:B:37:ARG:HH22	8:B:1350:ASZ:HAG2	1.79	0.46
1:A:96:VAL:HG22	1:A:180:SER:HB3	1.97	0.46
1:B:69:ASN:HD22	1:B:70:SER:N	2.14	0.46
1:E:69:ASN:HD22	1:E:70:SER:N	2.12	0.46
1:B:57:GLU:HB3	1:B:75:VAL:HG22	1.98	0.46
1:C:36:MET:HE3	1:C:36:MET:HB3	1.86	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:VAL:HG22	1:F:180:SER:HB3	1.98	0.46
1:D:207:GLY:O	1:D:284:ARG:NH2	2.48	0.46
1:B:96:VAL:HG22	1:B:180:SER:HB3	1.98	0.46
1:D:69:ASN:HD22	1:D:70:SER:N	2.14	0.46
1:F:69:ASN:HD22	1:F:70:SER:N	2.14	0.46
1:F:57:GLU:HB3	1:F:75:VAL:HG22	1.98	0.46
1:B:66:GLU:HG3	1:C:92:ARG:NH2	2.30	0.45
1:B:339:LEU:HB2	10:B:1354:HP6:H261	1.97	0.45
1:D:57:GLU:HB3	1:D:75:VAL:HG22	1.97	0.45
1:E:57:GLU:HB3	1:E:75:VAL:HG22	1.99	0.45
1:A:57:GLU:HB3	1:A:75:VAL:HG22	1.99	0.45
1:A:69:ASN:HD22	1:A:70:SER:N	2.13	0.45
1:C:57:GLU:HB3	1:C:75:VAL:HG22	1.98	0.45
1:C:69:ASN:HD22	1:C:70:SER:H	1.65	0.45
1:D:36:MET:HE3	1:D:36:MET:HB3	1.87	0.45
1:E:66:GLU:HG3	1:F:92:ARG:NH2	2.32	0.45
11:A:2080:HOH:O	1:D:284:ARG:HD3	2.16	0.44
1:E:86:GLY:HA2	11:E:2037:HOH:O	2.17	0.44
1:E:18:GLU:OE2	1:E:310:TYR:OH	2.20	0.44
1:A:296:ASP:OD2	11:A:2074:HOH:O	2.21	0.44
1:E:69:ASN:HD22	1:E:70:SER:H	1.65	0.44
1:D:69:ASN:HD22	1:D:70:SER:H	1.66	0.43
1:D:202:ASP:HB2	11:D:2039:HOH:O	2.18	0.43
1:A:18:GLU:OE2	1:A:310:TYR:OH	2.20	0.43
1:E:286:TYR:OH	1:E:326:ASP:OD2	2.29	0.43
1:A:69:ASN:HD22	1:A:70:SER:H	1.65	0.43
1:F:69:ASN:HD22	1:F:70:SER:H	1.66	0.43
1:B:69:ASN:HD22	1:B:70:SER:H	1.66	0.42
1:E:307:MET:HE3	1:F:52:GLY:C	2.45	0.42
1:F:124:ARG:NH1	6:F:1348:SO4:O2	2.49	0.42
1:F:32:ASP:OD2	11:F:2005:HOH:O	2.21	0.42
1:B:36:MET:HE3	1:B:36:MET:HB3	1.87	0.42
1:A:307:MET:HE3	1:B:52:GLY:C	2.46	0.41
1:E:36:MET:CE	1:E:60:ILE:CD1	2.93	0.41
1:F:36:MET:HE3	1:F:36:MET:HB3	1.87	0.41
1:A:36:MET:CE	1:A:60:ILE:CD1	2.94	0.41
1:F:166:ARG:NH2	11:F:2033:HOH:O	2.53	0.41
1:A:6:LYS:O	1:A:7:ASP:C	2.64	0.41
1:E:6:LYS:O	1:E:7:ASP:C	2.64	0.41
1:B:6:LYS:O	1:B:7:ASP:C	2.63	0.41
1:D:6:LYS:O	1:D:7:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TRP:CZ2	1:A:58:TYR:HB2	2.56	0.40
1:C:6:LYS:O	1:C:7:ASP:C	2.64	0.40
1:A:307:MET:CE	1:A:341:TYR:CD1	2.88	0.40
11:A:2064:HOH:O	7:B:1348:D10:H82	2.20	0.40
1:B:310:TYR:CD1	1:B:310:TYR:C	3.00	0.40
1:A:286:TYR:OH	1:A:326:ASP:OD2	2.29	0.40
1:C:56:TRP:CZ2	1:C:58:TYR:HB2	2.56	0.40
1:C:269:ARG:NH1	11:C:2049:HOH:O	2.54	0.40
1:E:113:ASP:N	1:E:113:ASP:OD1	2.55	0.40
1:E:307:MET:CE	1:E:341:TYR:CD1	2.89	0.40
1:F:6:LYS:O	1:F:7:ASP:C	2.64	0.40
1:A:95:GLY:HA3	1:A:121:MET:O	2.22	0.40
1:D:56:TRP:CZ2	1:D:58:TYR:HB2	2.56	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	341/343 (99%)	323 (95%)	17 (5%)	1 (0%)	36	44
1	B	341/343 (99%)	323 (95%)	17 (5%)	1 (0%)	36	44
1	C	341/343 (99%)	323 (95%)	17 (5%)	1 (0%)	36	44
1	D	341/343 (99%)	323 (95%)	17 (5%)	1 (0%)	36	44
1	E	341/343 (99%)	323 (95%)	17 (5%)	1 (0%)	36	44
1	F	341/343 (99%)	323 (95%)	17 (5%)	1 (0%)	36	44
All	All	2046/2058 (99%)	1938 (95%)	102 (5%)	6 (0%)	36	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	PHE
1	B	136	PHE
1	C	136	PHE
1	D	136	PHE
1	E	136	PHE
1	F	136	PHE

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	277/277 (100%)	273 (99%)	4 (1%)	59	74
1	B	277/277 (100%)	274 (99%)	3 (1%)	65	79
1	C	277/277 (100%)	274 (99%)	3 (1%)	65	79
1	D	277/277 (100%)	274 (99%)	3 (1%)	65	79
1	E	277/277 (100%)	274 (99%)	3 (1%)	65	79
1	F	277/277 (100%)	274 (99%)	3 (1%)	65	79
All	All	1662/1662 (100%)	1643 (99%)	19 (1%)	65	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	ARG
1	A	169	VAL
1	A	181	ILE
1	A	325	ARG
1	B	166	ARG
1	B	169	VAL
1	B	181	ILE
1	C	166	ARG
1	C	169	VAL
1	C	181	ILE
1	D	166	ARG
1	D	169	VAL
1	D	181	ILE

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Mol	Chain	Res	Type
1	E	166	ARG
1	E	169	VAL
1	E	181	ILE
1	F	166	ARG
1	F	169	VAL
1	F	181	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	122	GLN
1	A	227	ASN
1	B	9	ASN
1	B	122	GLN
1	B	227	ASN
1	B	254	GLN
1	C	9	ASN
1	C	122	GLN
1	C	227	ASN
1	D	9	ASN
1	D	122	GLN
1	D	227	ASN
1	E	9	ASN
1	E	122	GLN
1	E	150	GLN
1	E	227	ASN
1	F	9	ASN
1	F	122	GLN
1	F	227	ASN

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](#)

47 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	HEX	C	1345	-	5,5,5	0.35	0	4,4,4	0.24	0
3	HEX	A	1345	-	5,5,5	0.27	0	4,4,4	0.38	0
9	OES	D	1345	-	12,12,12	1.02	1 (8%)	11,12,12	2.36	1 (9%)
5	OCT	D	1346	-	7,7,7	0.38	0	6,6,6	0.23	0
4	D12	E	1345	-	11,11,11	0.21	0	10,10,10	0.66	0
3	HEX	B	1355	-	5,5,5	0.39	0	4,4,4	0.21	0
8	ASZ	B	1350	-	8,8,8	2.36	1 (12%)	10,11,11	1.74	3 (30%)
7	D10	B	1349	-	9,9,9	0.28	0	8,8,8	0.56	0
4	D12	E	1347	-	10,10,11	0.35	0	9,9,10	0.25	0
5	OCT	A	1351	-	7,7,7	0.43	0	6,6,6	0.28	0
5	OCT	C	1347	-	7,7,7	0.46	0	6,6,6	0.34	0
3	HEX	C	1349	-	5,5,5	0.36	0	4,4,4	0.24	0
5	OCT	D	1347	-	7,7,7	0.39	0	6,6,6	0.36	0
6	SO4	D	1348	-	4,4,4	0.27	0	6,6,6	0.36	0
6	SO4	C	1348	-	4,4,4	0.27	0	6,6,6	0.38	0
7	D10	B	1346	-	9,9,9	0.37	0	8,8,8	0.36	0
2	C8E	D	1344	-	20,20,20	0.48	0	19,19,19	0.46	0
6	SO4	A	1348	-	4,4,4	0.25	0	6,6,6	0.65	0
4	D12	F	1346	-	11,11,11	0.40	0	10,10,10	0.49	0
6	SO4	F	1348	-	4,4,4	0.22	0	6,6,6	0.42	0
10	HP6	B	1354	-	6,6,6	0.22	0	5,5,5	0.61	0
10	HP6	F	1345	-	6,6,6	0.23	0	5,5,5	0.72	0
2	C8E	A	1344	-	20,20,20	0.47	0	19,19,19	0.66	0
4	D12	C	1346	-	11,11,11	0.31	0	10,10,10	0.35	0
10	HP6	D	1349	-	6,6,6	0.21	0	5,5,5	0.60	0
5	OCT	B	1356	-	7,7,7	0.47	0	6,6,6	0.33	0
5	OCT	E	1348	-	7,7,7	0.31	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	F	1349	-	4,4,4	0.38	0	6,6,6	0.21	0
7	D10	B	1347	-	9,9,9	0.39	0	8,8,8	0.45	0
2	C8E	B	1351	-	20,20,20	0.51	0	19,19,19	0.32	0
5	OCT	A	1347	-	7,7,7	0.32	0	6,6,6	0.37	0
6	SO4	A	1349	-	4,4,4	0.25	0	6,6,6	0.31	0
5	OCT	B	1358	-	7,7,7	0.28	0	6,6,6	0.49	0
3	HEX	B	1353	-	5,5,5	0.34	0	4,4,4	0.17	0
7	D10	B	1348	-	9,9,9	0.21	0	8,8,8	1.03	0
4	D12	E	1346	-	11,11,11	0.40	0	10,10,10	0.34	0
3	HEX	F	1344	-	5,5,5	0.36	0	4,4,4	0.19	0
4	D12	A	1346	-	11,11,11	0.51	0	10,10,10	0.26	0
3	HEX	C	1350	-	5,5,5	0.31	0	4,4,4	0.30	0
3	HEX	A	1350	-	5,5,5	0.30	0	4,4,4	0.29	0
7	D10	B	1344	-	9,9,9	0.49	0	8,8,8	0.18	0
9	OES	B	1352	-	12,12,12	0.86	0	11,12,12	2.66	2 (18%)
5	OCT	B	1357	-	7,7,7	0.41	0	6,6,6	0.20	0
3	HEX	C	1344	-	5,5,5	0.35	0	4,4,4	0.27	0
7	D10	B	1345	-	9,9,9	0.47	0	8,8,8	0.31	0
5	OCT	F	1347	-	7,7,7	0.25	0	6,6,6	0.40	0
3	HEX	E	1344	-	5,5,5	0.34	0	4,4,4	0.30	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	HEX	C	1345	-	-	2/3/3/3	-
3	HEX	A	1345	-	-	0/3/3/3	-
9	OES	D	1345	-	-	9/11/11/11	-
5	OCT	D	1346	-	-	1/5/5/5	-
4	D12	E	1345	-	-	5/9/9/9	-
3	HEX	B	1355	-	-	2/3/3/3	-
8	ASZ	B	1350	-	-	5/6/6/6	-
7	D10	B	1349	-	-	0/7/7/7	-
4	D12	E	1347	-	-	5/8/8/9	-
5	OCT	A	1351	-	-	2/5/5/5	-
5	OCT	C	1347	-	-	2/5/5/5	-
3	HEX	C	1349	-	-	2/3/3/3	-
5	OCT	D	1347	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	D10	B	1346	-	-	3/7/7/7	-
2	C8E	D	1344	-	-	11/18/18/18	-
4	D12	F	1346	-	-	5/9/9/9	-
10	HP6	B	1354	-	-	0/4/4/4	-
10	HP6	F	1345	-	-	0/4/4/4	-
2	C8E	A	1344	-	-	10/18/18/18	-
4	D12	C	1346	-	-	5/9/9/9	-
10	HP6	D	1349	-	-	1/4/4/4	-
5	OCT	B	1356	-	-	3/5/5/5	-
5	OCT	E	1348	-	-	4/5/5/5	-
7	D10	B	1347	-	-	4/7/7/7	-
2	C8E	B	1351	-	-	9/18/18/18	-
5	OCT	A	1347	-	-	3/5/5/5	-
7	D10	B	1348	-	-	0/7/7/7	-
5	OCT	B	1358	-	-	2/5/5/5	-
3	HEX	B	1353	-	-	3/3/3/3	-
4	D12	E	1346	-	-	5/9/9/9	-
3	HEX	F	1344	-	-	2/3/3/3	-
4	D12	A	1346	-	-	5/9/9/9	-
3	HEX	C	1350	-	-	0/3/3/3	-
3	HEX	A	1350	-	-	1/3/3/3	-
7	D10	B	1344	-	-	6/7/7/7	-
9	OES	B	1352	-	-	4/11/11/11	-
5	OCT	B	1357	-	-	2/5/5/5	-
3	HEX	C	1344	-	-	0/3/3/3	-
7	D10	B	1345	-	-	3/7/7/7	-
5	OCT	F	1347	-	-	3/5/5/5	-
3	HEX	E	1344	-	-	1/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1350	ASZ	CAG-SAI	-6.07	1.69	1.77
9	D	1345	OES	C22-S2	-2.07	1.70	1.80

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1352	OES	C22-S2-C8	7.84	113.60	97.40
9	D	1345	OES	C22-S2-C8	7.56	113.04	97.40
9	B	1352	OES	O2-S2-C8	3.68	113.88	105.73
8	B	1350	ASZ	OAD-SAI-CAG	3.26	112.38	106.00
8	B	1350	ASZ	OAE-SAI-CAG	2.95	111.19	106.73
8	B	1350	ASZ	OAE-SAI-OAC	-2.30	106.34	113.82

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1350	ASZ	CAF-CAG-SAI-OAC
8	B	1350	ASZ	CAF-CAG-SAI-OAD
8	B	1350	ASZ	CAG-CAF-NAH-CAB
8	B	1350	ASZ	CAG-CAF-NAH-CAA
9	B	1352	OES	C6-C7-C8-S2
9	B	1352	OES	C7-C8-S2-C22
9	B	1352	OES	C7-C8-S2-O2
9	D	1345	OES	C7-C8-S2-C22
9	D	1345	OES	C23-C22-S2-O2
2	A	1344	C8E	O12-C13-C14-O15
2	B	1351	C8E	O9-C10-C11-O12
2	B	1351	C8E	O15-C16-C17-O18
2	D	1344	C8E	O15-C16-C17-O18
4	C	1346	D12	C11-C10-C9-C8
2	B	1351	C8E	O18-C19-C20-O21
2	D	1344	C8E	C6-C7-C8-O9
5	E	1348	OCT	C2-C3-C4-C5
2	D	1344	C8E	C3-C4-C5-C6
4	E	1346	D12	C6-C7-C8-C9
4	E	1347	D12	C3-C4-C5-C6
5	A	1347	OCT	C2-C3-C4-C5
2	B	1351	C8E	C4-C5-C6-C7
2	D	1344	C8E	C5-C6-C7-C8
5	A	1347	OCT	C4-C5-C6-C7
7	B	1344	D10	C5-C6-C7-C8
5	A	1351	OCT	C4-C5-C6-C7
5	D	1347	OCT	C3-C4-C5-C6
4	E	1346	D12	C11-C10-C9-C8
4	A	1346	D12	C3-C4-C5-C6
7	B	1346	D10	C6-C7-C8-C9
4	A	1346	D12	C4-C5-C6-C7
4	E	1345	D12	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	A	1346	D12	C11-C10-C9-C8
3	B	1353	HEX	C2-C3-C4-C5
9	D	1345	OES	C6-C7-C8-S2
4	E	1346	D12	C4-C5-C6-C7
7	B	1345	D10	C3-C4-C5-C6
7	B	1347	D10	C5-C6-C7-C8
9	D	1345	OES	C4-C5-C6-C7
3	A	1350	HEX	C2-C3-C4-C5
4	A	1346	D12	C7-C8-C9-C10
10	D	1349	HP6	C20-C21-C22-C23
4	E	1345	D12	C3-C4-C5-C6
2	D	1344	C8E	C4-C5-C6-C7
3	C	1349	HEX	C2-C3-C4-C5
4	E	1345	D12	C2-C3-C4-C5
7	B	1344	D10	C3-C4-C5-C6
4	A	1346	D12	C6-C7-C8-C9
9	D	1345	OES	C3-C4-C5-C6
2	B	1351	C8E	C5-C6-C7-C8
4	F	1346	D12	C2-C3-C4-C5
2	D	1344	C8E	O9-C10-C11-O12
3	B	1355	HEX	C1-C2-C3-C4
5	B	1357	OCT	C2-C3-C4-C5
5	F	1347	OCT	C1-C2-C3-C4
3	F	1344	HEX	C2-C3-C4-C5
3	F	1344	HEX	C1-C2-C3-C4
4	E	1345	D12	C9-C10-C11-C12
4	E	1346	D12	C1-C2-C3-C4
3	B	1353	HEX	C1-C2-C3-C4
5	E	1348	OCT	C1-C2-C3-C4
5	A	1347	OCT	C3-C4-C5-C6
4	F	1346	D12	C11-C10-C9-C8
7	B	1347	D10	C2-C3-C4-C5
3	C	1345	HEX	C2-C3-C4-C5
5	F	1347	OCT	C2-C3-C4-C5
3	C	1349	HEX	C1-C2-C3-C4
4	E	1347	D12	C11-C10-C9-C8
2	B	1351	C8E	C1-C2-C3-C4
5	E	1348	OCT	C5-C6-C7-C8
3	B	1355	HEX	C3-C4-C5-C6
5	D	1346	OCT	C2-C3-C4-C5
7	B	1345	D10	C4-C5-C6-C7
7	B	1344	D10	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	B	1347	D10	C1-C2-C3-C4
4	F	1346	D12	C6-C7-C8-C9
9	B	1352	OES	C4-C5-C6-C7
4	C	1346	D12	C7-C8-C9-C10
5	B	1356	OCT	C5-C6-C7-C8
7	B	1344	D10	C6-C7-C8-C9
7	B	1346	D10	C7-C8-C9-C10
8	B	1350	ASZ	CAF-CAG-SAI-OAE
2	A	1344	C8E	C13-C14-O15-C16
4	E	1346	D12	C3-C4-C5-C6
2	D	1344	C8E	C13-C14-O15-C16
4	E	1347	D12	C5-C6-C7-C8
7	B	1347	D10	C7-C8-C9-C10
2	A	1344	C8E	C11-C10-O9-C8
2	A	1344	C8E	C16-C17-O18-C19
2	B	1351	C8E	C17-C16-O15-C14
5	B	1358	OCT	C2-C3-C4-C5
7	B	1345	D10	C6-C7-C8-C9
7	B	1344	D10	C4-C5-C6-C7
5	B	1356	OCT	C4-C5-C6-C7
7	B	1346	D10	C5-C6-C7-C8
5	B	1357	OCT	C4-C5-C6-C7
5	D	1347	OCT	C4-C5-C6-C7
2	A	1344	C8E	C7-C8-O9-C10
4	C	1346	D12	C9-C10-C11-C12
3	C	1345	HEX	C1-C2-C3-C4
3	B	1353	HEX	C3-C4-C5-C6
2	A	1344	C8E	C20-C19-O18-C17
9	D	1345	OES	S2-C22-C23-O3
2	A	1344	C8E	O9-C10-C11-O12
2	A	1344	C8E	C17-C16-O15-C14
5	B	1356	OCT	C2-C3-C4-C5
5	C	1347	OCT	C1-C2-C3-C4
4	C	1346	D12	C3-C4-C5-C6
7	B	1344	D10	C1-C2-C3-C4
5	C	1347	OCT	C5-C6-C7-C8
5	A	1351	OCT	C5-C6-C7-C8
2	B	1351	C8E	C2-C3-C4-C5
4	E	1347	D12	C4-C5-C6-C7
2	D	1344	C8E	O18-C19-C20-O21
4	F	1346	D12	C4-C5-C6-C7
2	D	1344	C8E	C11-C10-O9-C8

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Mol	Chain	Res	Type	Atoms
3	E	1344	HEX	C2-C3-C4-C5
4	F	1346	D12	C5-C6-C7-C8
5	E	1348	OCT	C3-C4-C5-C6
9	D	1345	OES	C2-C3-C4-C5
2	D	1344	C8E	C2-C3-C4-C5
9	D	1345	OES	C1-C2-C3-C4
4	E	1345	D12	C1-C2-C3-C4
5	B	1358	OCT	C5-C6-C7-C8
4	E	1347	D12	C2-C3-C4-C5
5	F	1347	OCT	C5-C6-C7-C8
9	D	1345	OES	C23-C22-S2-C8
2	A	1344	C8E	C10-C11-O12-C13
4	C	1346	D12	C4-C5-C6-C7
2	A	1344	C8E	O15-C16-C17-O18
2	B	1351	C8E	O12-C13-C14-O15
2	D	1344	C8E	C14-C13-O12-C11

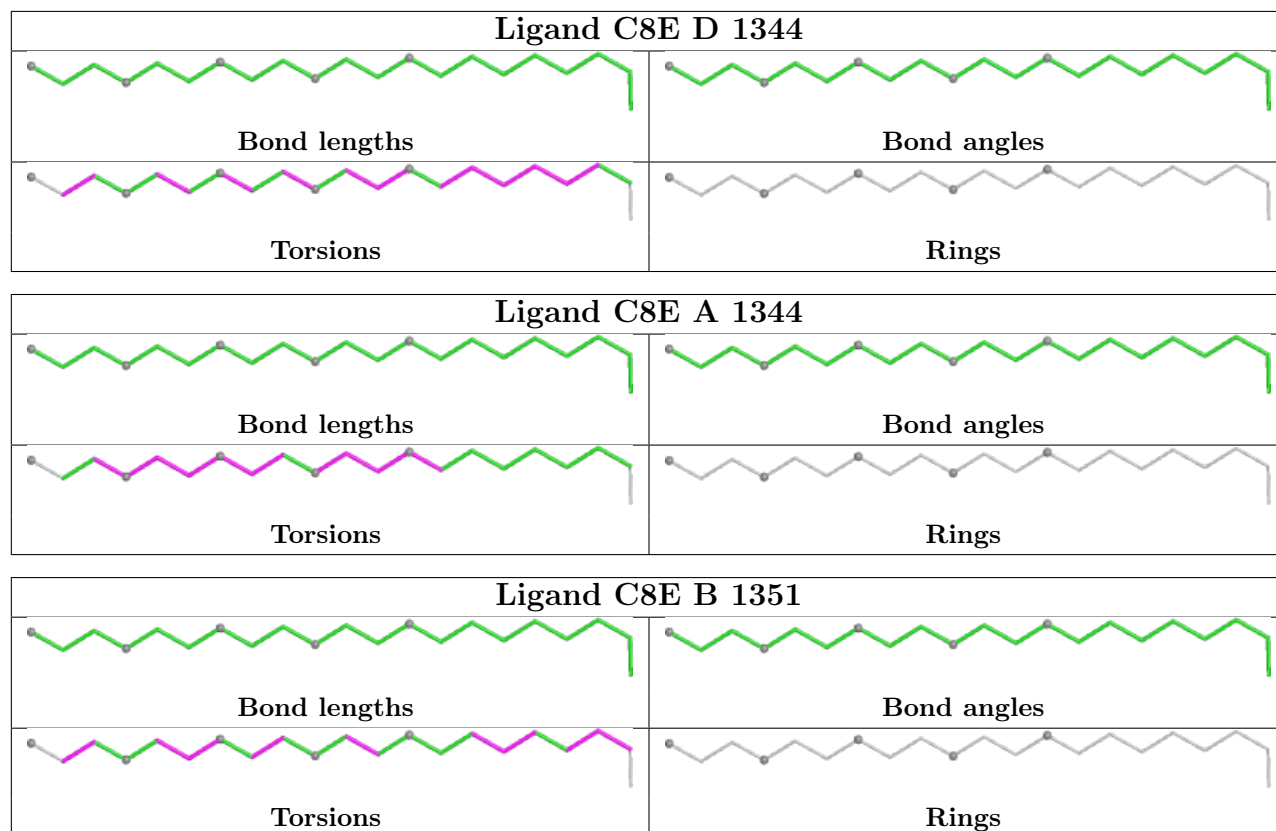
There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1350	ASZ	2	0
6	A	1348	SO4	2	0
6	F	1348	SO4	1	0
10	B	1354	HP6	1	0
4	C	1346	D12	2	0
5	E	1348	OCT	1	0
5	B	1358	OCT	1	0
3	B	1353	HEX	3	0
7	B	1348	D10	2	0
4	E	1346	D12	1	0
5	F	1347	OCT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	343/343 (100%)	-1.18	0 100 100	34, 51, 74, 103	0
1	B	343/343 (100%)	-1.13	0 100 100	36, 58, 95, 120	0
1	C	343/343 (100%)	-1.17	0 100 100	34, 54, 84, 116	0
1	D	343/343 (100%)	-1.20	0 100 100	32, 53, 85, 109	0
1	E	343/343 (100%)	-1.18	0 100 100	37, 50, 75, 94	0
1	F	343/343 (100%)	-1.20	0 100 100	33, 57, 90, 108	0
All	All	2058/2058 (100%)	-1.18	0 100 100	32, 54, 85, 120	0

There are no RSRZ outliers to report.

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
3	HEX	B	1353	6/6	0.96	0.07	57,70,79,82	0

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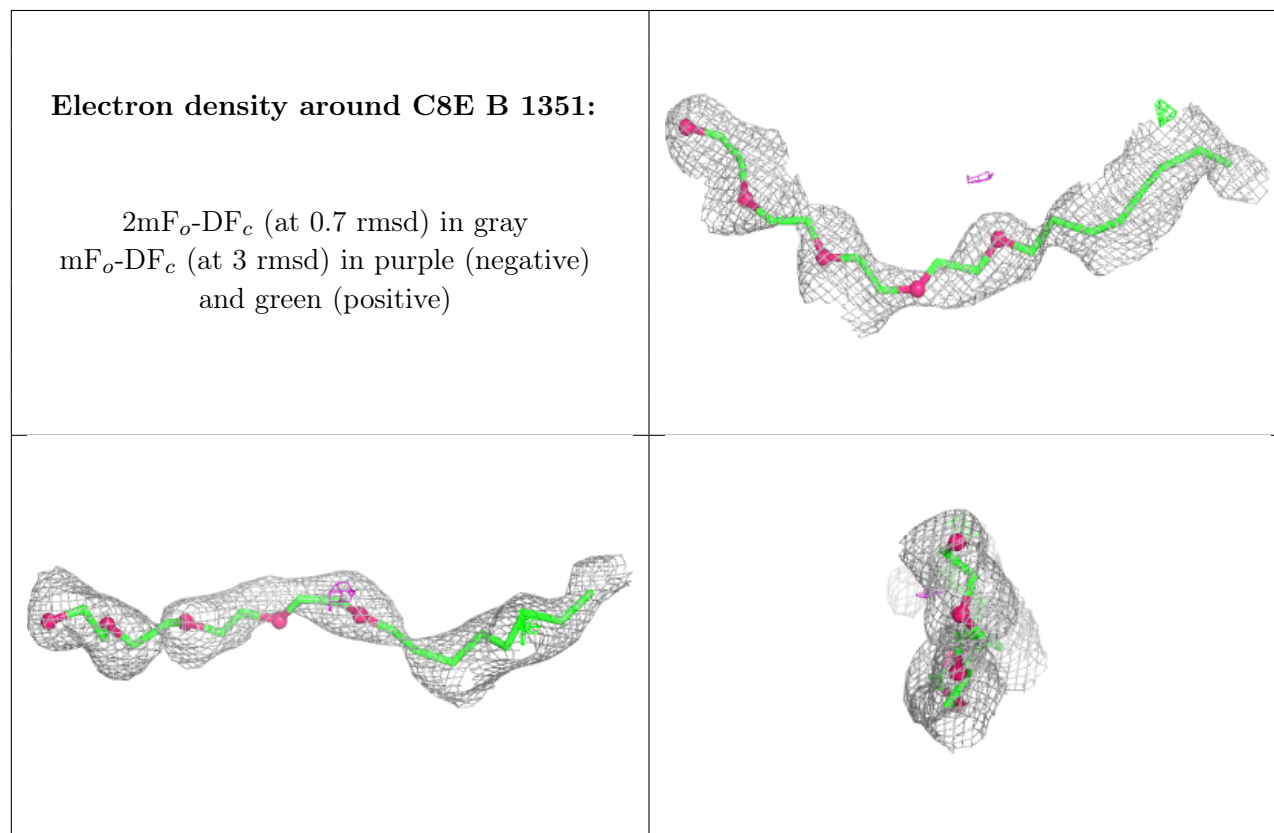
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OCT	B	1358	8/8	0.96	0.06	55,58,64,65	0
5	OCT	B	1357	8/8	0.96	0.06	72,78,85,85	0
3	HEX	C	1350	6/6	0.97	0.08	84,86,89,91	0
4	D12	A	1346	12/12	0.97	0.07	59,63,70,72	0
4	D12	F	1346	12/12	0.97	0.07	41,61,72,72	0
2	C8E	B	1351	21/21	0.97	0.06	65,90,110,115	0
5	OCT	B	1356	8/8	0.97	0.05	52,66,68,70	0
3	HEX	C	1344	6/6	0.97	0.07	45,54,59,61	0
5	OCT	C	1347	8/8	0.97	0.07	55,59,67,72	0
5	OCT	D	1346	8/8	0.97	0.06	40,49,64,67	0
5	OCT	E	1348	8/8	0.97	0.06	56,62,74,74	0
5	OCT	F	1347	8/8	0.97	0.06	51,55,61,61	0
6	SO4	C	1348	5/5	0.97	0.04	59,76,84,89	0
6	SO4	D	1348	5/5	0.97	0.06	68,71,78,80	0
8	ASZ	B	1350	9/9	0.97	0.07	66,76,99,101	0
3	HEX	C	1345	6/6	0.98	0.07	59,65,69,69	0
3	HEX	C	1349	6/6	0.98	0.07	51,55,57,62	0
3	HEX	A	1345	6/6	0.98	0.05	47,54,55,57	0
3	HEX	F	1344	6/6	0.98	0.07	47,54,57,59	0
3	HEX	B	1355	6/6	0.98	0.05	62,65,70,71	0
4	D12	E	1345	12/12	0.98	0.04	48,56,68,74	0
4	D12	E	1346	12/12	0.98	0.04	49,54,61,61	0
6	SO4	A	1349	5/5	0.98	0.04	70,90,98,103	0
4	D12	E	1347	11/12	0.98	0.06	43,67,88,89	0
3	HEX	A	1350	6/6	0.98	0.07	50,55,60,62	0
7	D10	B	1345	10/10	0.98	0.05	47,59,65,68	0
7	D10	B	1347	10/10	0.98	0.05	61,67,73,73	0
7	D10	B	1348	10/10	0.98	0.04	28,35,51,56	0
7	D10	B	1349	10/10	0.98	0.05	62,71,82,86	0
5	OCT	A	1351	8/8	0.98	0.06	57,70,75,80	0
9	OES	D	1345	13/13	0.98	0.05	62,68,80,85	0
10	HP6	F	1345	7/7	0.98	0.06	55,61,69,75	0
6	SO4	F	1348	5/5	0.99	0.04	68,69,78,82	0
6	SO4	F	1349	5/5	0.99	0.04	63,73,77,96	0
7	D10	B	1344	10/10	0.99	0.05	51,61,67,68	0
5	OCT	D	1347	8/8	0.99	0.04	49,60,64,68	0
7	D10	B	1346	10/10	0.99	0.04	57,70,75,76	0
2	C8E	A	1344	21/21	0.99	0.04	38,54,77,85	0
2	C8E	D	1344	21/21	0.99	0.05	56,71,89,94	0
6	SO4	A	1348	5/5	0.99	0.05	58,65,90,99	0
4	D12	C	1346	12/12	0.99	0.04	47,63,68,72	0
9	OES	B	1352	13/13	0.99	0.04	48,65,84,98	0

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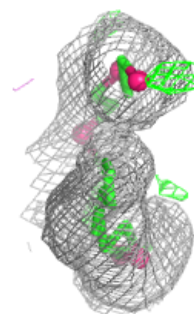
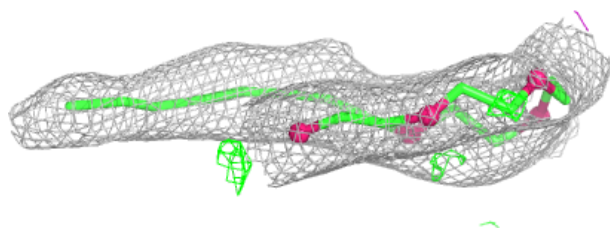
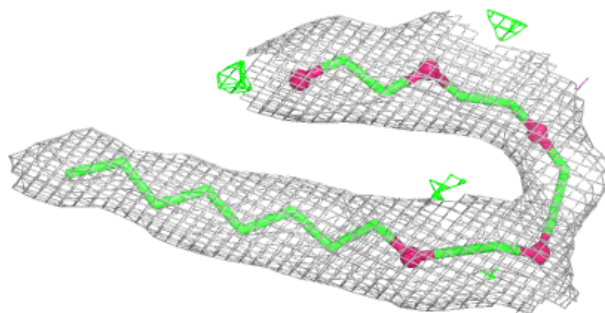
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OCT	A	1347	8/8	0.99	0.04	49,56,80,84	0
10	HP6	B	1354	7/7	0.99	0.05	47,48,51,56	0
10	HP6	D	1349	7/7	0.99	0.05	49,52,66,69	0
3	HEX	E	1344	6/6	0.99	0.05	67,84,88,89	0

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.

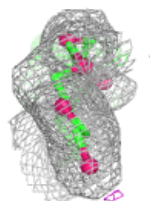
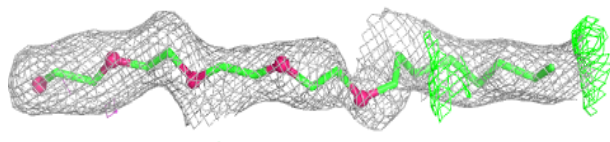
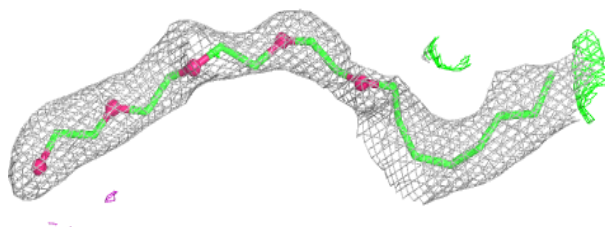


Electron density around C8E A 1344:

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

**Electron density around C8E D 1344:**

$2mF_o-DF_c$ (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.