



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 22, 2016 – 12:40 PM EDT

PDB ID : 5FVN
Title : X-ray crystal structure of Enterobacter cloacae OmpE36 porin
Authors : Arunmanee, W.; Pathania, M.; Soloyova, A.; Brun, A.; Ridley, H.; Basle, A.; vandenBerg, B.; Lakey, J.H.
Deposited on : 2016-02-09
Resolution : 1.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

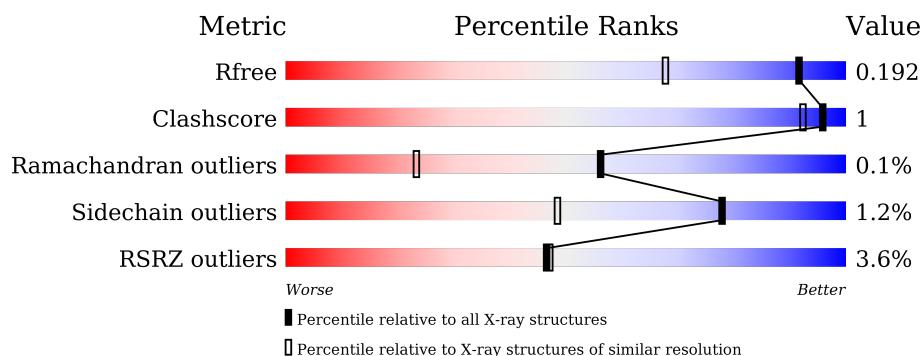
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	342	<div> <div>4%</div> <div>97%</div> <div>.</div> </div>
1	B	342	<div> <div>4%</div> <div>95%</div> <div>5%</div> </div>
1	C	342	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
1	D	342	<div> <div>6%</div> <div>96%</div> <div>.</div> </div>
1	E	342	<div> <div>4%</div> <div>97%</div> <div>.</div> </div>
1	F	342	<div> <div>%</div> <div>98%</div> <div>.</div> </div>

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
3	C8E	A	407	-	-	-	X
3	C8E	A	408	-	-	-	X
3	C8E	A	409	-	-	-	X
3	C8E	B	401	-	-	-	X
3	C8E	B	403	-	-	-	X
3	C8E	C	401	-	-	-	X
3	C8E	C	402	-	-	-	X
3	C8E	C	404	-	-	-	X
3	C8E	C	406	-	-	-	X
3	C8E	C	407	-	-	-	X
3	C8E	C	408	-	-	-	X
3	C8E	C	409	-	-	-	X
3	C8E	C	410	-	-	-	X
3	C8E	D	402	-	-	-	X
3	C8E	D	404	-	-	-	X
3	C8E	D	405	-	-	-	X
3	C8E	D	406	-	-	-	X
3	C8E	D	407	-	-	-	X
3	C8E	D	409	-	-	-	X
3	C8E	E	401	-	-	-	X
4	PO4	A	411	-	-	-	X
4	PO4	B	406	-	-	-	X
4	PO4	C	411	-	-	-	X
4	PO4	D	411	-	-	-	X
4	PO4	E	402	-	-	-	X
4	PO4	F	404	-	-	-	X
5	FTT	A	418	-	-	-	X
5	FTT	A	420	-	-	-	X
5	FTT	B	414	-	-	-	X
5	FTT	C	418	-	-	-	X
5	FTT	D	415	-	-	-	X
5	FTT	D	427	-	-	-	X
5	FTT	D	429	-	-	-	X
5	FTT	E	409	-	-	-	X
5	FTT	E	411	-	-	-	X
5	FTT	F	414	-	-	-	X
5	FTT	F	424	-	-	-	X
8	KDO	C	417	-	-	-	X
8	KDO	F	410	-	-	-	X
9	MYR	F	415	-	-	-	X

2 Entry composition [i](#)

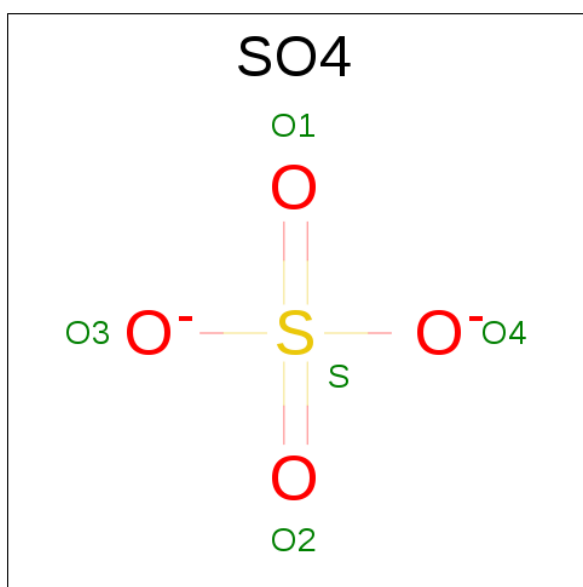
There are 13 unique types of molecules in this entry. The entry contains 19668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OMPC PORIN.

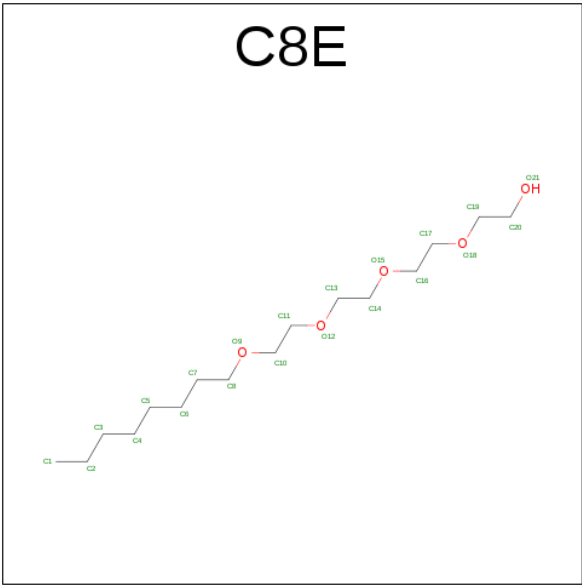
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	4	8	0
			2722	1704	455	560	3			
1	B	342	Total	C	N	O	S	0	4	0
			2700	1685	451	561	3			
1	C	342	Total	C	N	O	S	0	5	0
			2704	1691	451	559	3			
1	D	342	Total	C	N	O	S	0	6	0
			2710	1693	452	562	3			
1	E	342	Total	C	N	O	S	0	6	0
			2708	1694	451	560	3			
1	F	342	Total	C	N	O	S	0	4	0
			2701	1689	452	557	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 2 1	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C O 5 4 1	0	0
3	A	1	Total C O 8 5 3	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 7 7	0	0

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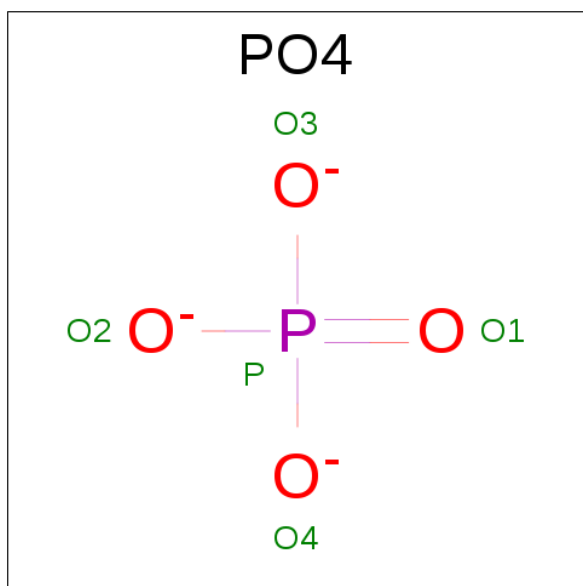
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 9 8 1	0	0
3	B	1	Total C 3 3	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 8 8	0	0
3	C	1	Total C 3 3	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 3 3	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 3 3	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C O 11 10 1	0	0
3	C	1	Total C O 11 10 1	0	0
3	C	1	Total C O 10 9 1	0	0
3	C	1	Total C 7 7	0	0
3	D	1	Total C 4 4	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 11 10 1	0	0
3	D	1	Total C O 4 3 1	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 6 6	0	0
3	F	1	Total C 3 3	0	0
3	F	1	Total C 4 4	0	0
3	F	1	Total C 8 8	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



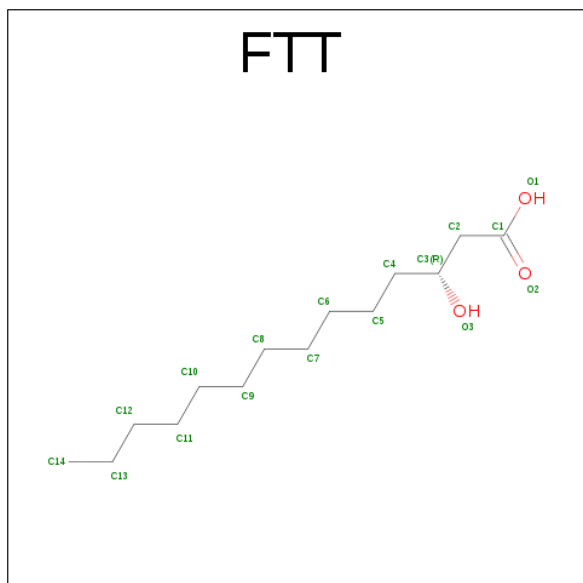
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	12	2		
5	A	1	Total	C	O	0	0
			15	13	2		
5	A	1	Total	C	O	0	0
			13	11	2		
5	A	1	Total	C	O	0	0
			16	14	2		
5	B	1	Total	C	O	0	0
			15	13	2		
5	B	1	Total	C	O	0	0
			13	11	2		
5	B	1	Total	C	O	0	0
			16	14	2		
5	B	1	Total	C	O	0	0
			14	12	2		
5	C	1	Total	C	O	0	0
			16	14	2		

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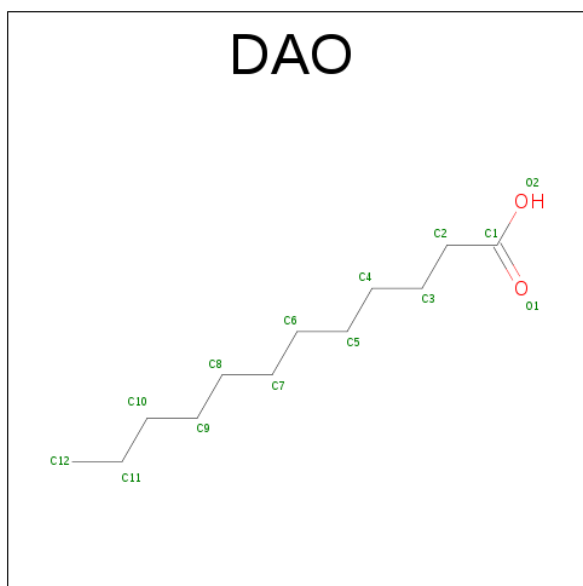
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	9	2		
5	C	1	Total	C	O	0	0
			16	14	2		
5	C	1	Total	C	O	0	0
			13	11	2		
5	C	1	Total	C	O	0	0
			16	14	2		
5	C	1	Total	C	O	0	0
			13	11	2		
5	C	1	Total	C	O	0	0
			16	14	2		
5	C	1	Total	C	O	0	0
			14	12	2		
5	D	1	Total	C	O	0	0
			14	12	2		
5	D	1	Total	C	O	0	0
			11	9	2		
5	D	1	Total	C	O	0	0
			13	11	2		
5	D	1	Total	C	O	0	0
			11	9	2		
5	D	1	Total	C	O	0	0
			14	12	2		
5	D	1	Total	C	O	0	0
			16	14	2		
5	D	1	Total	C	O	0	0
			13	11	2		
5	D	1	Total	C	O	0	0
			16	14	2		
5	E	1	Total	C	O	0	0
			14	12	2		
5	E	1	Total	C	O	0	0
			14	12	2		
5	E	1	Total	C	O	0	0
			12	10	2		
5	E	1	Total	C	O	0	0
			15	13	2		
5	F	1	Total	C	O	0	0
			12	10	2		
5	F	1	Total	C	O	0	0
			13	11	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			12	10	2		
5	F	1	Total	C	O	0	0
			16	14	2		
5	F	1	Total	C	O	0	0
			14	12	2		
5	F	1	Total	C	O	0	0
			11	9	2		
5	F	1	Total	C	O	0	0
			16	14	2		
5	F	1	Total	C	O	0	0
			14	12	2		

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	7	1		
6	A	1	Total	C	O	0	0
			5	4	1		
6	B	1	Total	C	O	0	0
			5	4	1		
6	C	1	Total	C	O	0	0
			13	12	1		
6	C	1	Total	C	O	0	0
			10	9	1		

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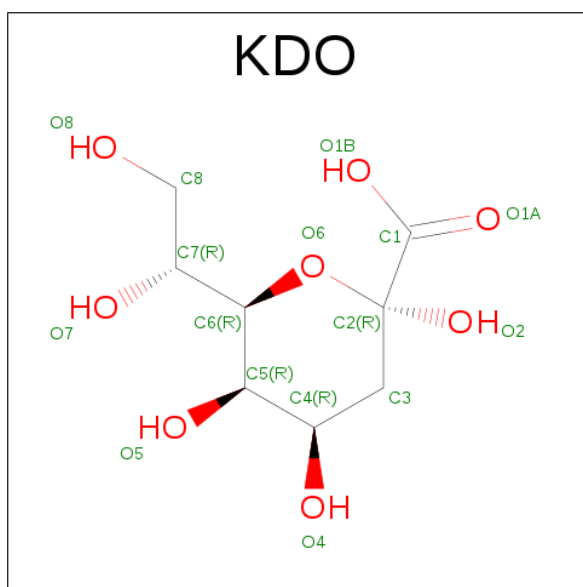
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			8	7	1		
6	C	1	Total	C	O	0	0
			5	4	1		
6	D	1	Total	C	O	0	0
			3	2	1		
6	D	1	Total	C	O	0	0
			6	5	1		
6	D	1	Total	C	O	0	0
			5	4	1		
6	E	1	Total	C	O	0	0
			5	4	1		
6	E	1	Total	C	O	0	0
			5	4	1		
6	F	1	Total	C	O	0	0
			5	4	1		
6	F	1	Total	C	O	0	0
			5	4	1		
6	F	1	Total	C	O	0	0
			8	7	1		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

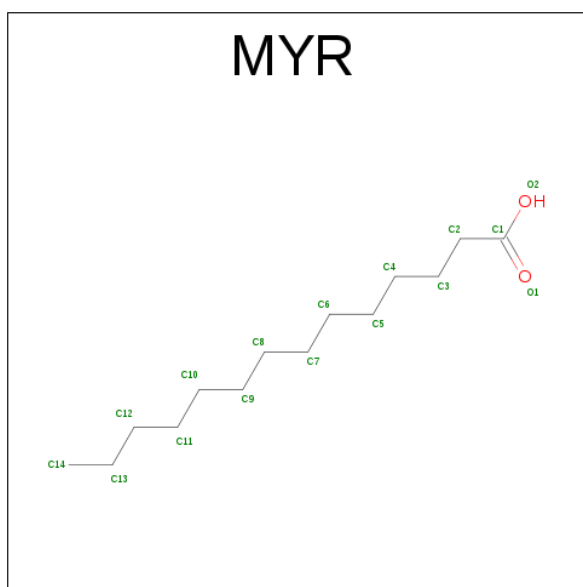
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	3	Total	C	N	O	P	0	0
			46	20	2	22	2		
7	D	3	Total	C	N	O	P	0	0
			45	20	2	21	2		
7	D	3	Total	C	N	O	P	0	0
			46	20	2	22	2		
7	E	3	Total	C	N	O	P	0	0
			46	20	2	22	2		
7	F	3	Total	C	N	O	P	0	0
			46	20	2	22	2		

- Molecule 8 is SUGAR (3-DEOXY-D-MANNO-OCT-2-ULOSONIC ACID) (three-letter code: KDO) (formula: C₈H₁₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			15	8	7		
8	B	1	Total	C	O	0	0
			15	8	7		
8	C	1	Total	C	O	0	0
			15	8	7		
8	D	1	Total	C	O	0	0
			15	8	7		
8	E	1	Total	C	O	0	0
			15	8	7		
8	F	1	Total	C	O	0	0
			15	8	7		
8	F	1	Total	C	O	0	0
			15	8	7		

- Molecule 9 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	5	1		
9	B	1	Total	C	O	0	0
			6	5	1		
9	C	1	Total	C	O	0	0
			8	7	1		
9	C	1	Total	C	O	0	0
			9	8	1		
9	D	1	Total	C	O	0	0
			5	4	1		
9	D	1	Total	C	O	0	0
			6	5	1		
9	E	1	Total	C	O	0	0
			6	5	1		
9	F	1	Total	C	O	0	0
			11	10	1		
9	F	1	Total	C	O	0	0
			12	11	1		

- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	4	Total	C	N	O	P	0	0
			59	27	2	28	2		
10	C	4	Total	C	N	O	P	0	0
			59	27	2	28	2		
10	F	4	Total	C	N	O	P	0	0
			59	27	2	28	2		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total 1	Ca 1	0	0
11	F	1	Total 1	Ca 1	0	0

- Molecule 12 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	4	Total 61	C 28	N 2	O 29	P 2	0	0

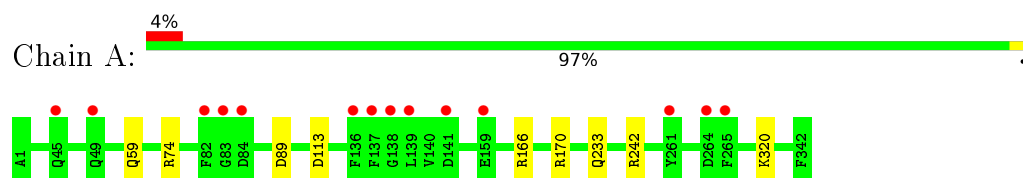
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	320	Total 320	O 320	0	0
13	B	315	Total 315	O 315	0	0
13	C	324	Total 324	O 324	0	0
13	D	295	Total 295	O 295	0	0
13	E	306	Total 306	O 306	0	0
13	F	350	Total 350	O 350	0	0

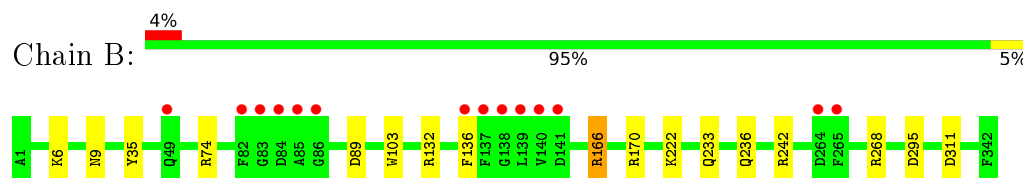
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

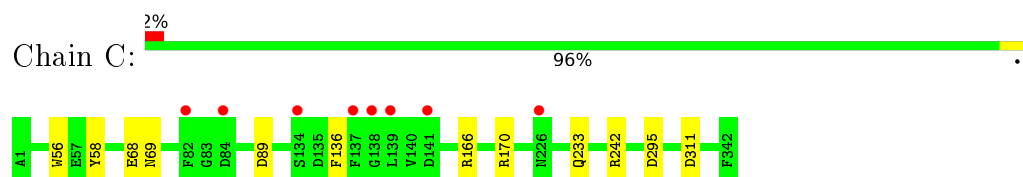
- Molecule 1: OMPC PORIN



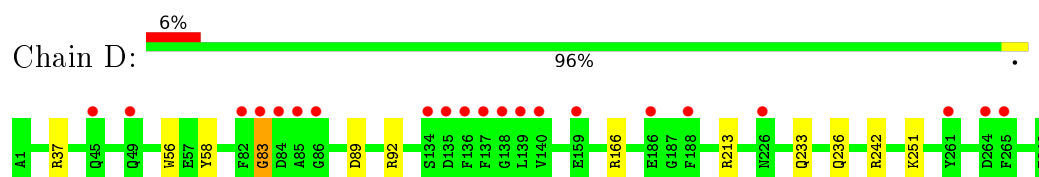
- Molecule 1: OMPC PORIN



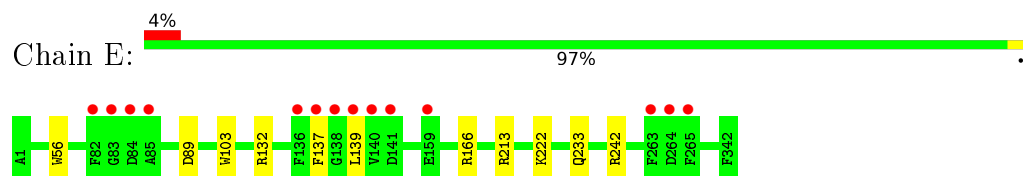
- Molecule 1: OMPC PORIN



- Molecule 1: OMPC PORIN

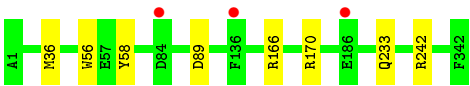


- Molecule 1: OMPC PORIN



- Molecule 1: OMPC PORIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.75Å 123.26Å 116.01Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	115.99 – 1.45 48.60 – 1.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (115.99-1.45) 99.9 (48.60-1.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.155 , 0.183 0.167 , 0.192	Depositor DCC
R_{free} test set	13912 reflections (2.63%)	DCC
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19668	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.10% 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: KDO, FTT, PO4, MYR, DAO, L1L, GMH, C8E, CA, Z9M, SO4

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	0.54	0/2799	0.83	4/3785 (0.1%)
1	B	0.52	0/2768	0.82	8/3743 (0.2%)
1	C	0.51	0/2775	0.81	4/3753 (0.1%)
1	D	0.52	0/2784	0.86	5/3765 (0.1%)
1	E	0.53	0/2782	0.82	4/3763 (0.1%)
1	F	0.49	0/2769	0.77	4/3745 (0.1%)
All	All	0.52	0/16677	0.82	29/22554 (0.1%)

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	D	1	1

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ARG	NE-CZ-NH1	-14.26	113.17	120.30
1	D	242	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	A	242	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	F	242	ARG	NE-CZ-NH2	9.71	125.15	120.30
1	C	242	ARG	NE-CZ-NH2	9.45	125.03	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	84	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	83	GLY	Peptide

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	2722	0	2520	2	0
1	B	2700	0	2475	8	0
1	C	2704	0	2491	6	0
1	D	2710	0	2492	4	0
1	E	2708	0	2498	3	0
1	F	2701	0	2488	2	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0
3	A	50	0	76	3	0
3	B	33	0	56	2	0
3	C	69	0	122	4	0
3	D	59	0	102	1	0
3	E	6	0	11	0	0
3	F	15	0	27	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	58	0	84	0	0
5	B	58	0	85	0	0
5	C	115	0	172	0	0
5	D	108	0	154	0	0
5	E	55	0	75	0	0
5	F	108	0	153	2	0
6	A	13	0	14	0	0
6	B	5	0	4	0	0
6	C	36	0	51	0	0
6	D	14	0	10	0	0
6	E	10	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	18	0	18	0	0
7	A	46	0	18	2	0
7	D	91	0	34	2	0
7	E	46	0	18	3	0
7	F	46	0	18	2	0
8	A	15	0	12	2	0
8	B	15	0	12	1	0
8	C	15	0	10	3	0
8	D	15	0	12	2	0
8	E	15	0	12	3	0
8	F	30	0	22	3	0
9	A	6	0	6	0	0
9	B	6	0	6	0	0
9	C	17	0	22	0	0
9	D	11	0	10	0	0
9	E	6	0	6	0	0
9	F	23	0	34	0	0
10	B	59	0	29	1	0
10	C	59	0	29	4	0
10	F	59	0	28	1	0
11	C	1	0	0	0	0
11	F	1	0	0	0	0
12	C	61	0	29	2	0
13	A	320	0	0	1	0
13	B	315	0	0	5	0
13	C	324	0	0	1	0
13	D	295	0	0	4	0
13	E	306	0	0	0	0
13	F	350	0	0	0	0
All	All	19668	0	16553	46	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 1.

The worst 5 of 46 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)
7:E:407:KDO:O4	8:E:408:KDO:C2	1.81	1.29
7:D:425:KDO:O4	8:D:426:KDO:C2	1.84	1.24
7:A:416:KDO:O4	8:A:417:KDO:C2	1.85	1.24
3:A:408:C8E:H112	13:A:581:HOH:O	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LYS:HG3	13:D:710:HOH:O	1.73	0.86

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	348/342 (102%)	332 (95%)	16 (5%)	0	100	100
1	B	344/342 (101%)	329 (96%)	14 (4%)	1 (0%)	46	17
1	C	345/342 (101%)	330 (96%)	14 (4%)	1 (0%)	46	17
1	D	346/342 (101%)	329 (95%)	16 (5%)	1 (0%)	46	17
1	E	346/342 (101%)	330 (95%)	16 (5%)	0	100	100
1	F	344/342 (101%)	332 (96%)	12 (4%)	0	100	100
All	All	2073/2052 (101%)	1982 (96%)	88 (4%)	3 (0%)	56	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	PHE
1	C	136	PHE
1	D	83	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/275 (103%)	279 (99%)	4 (1%)	74	42
1	B	279/275 (102%)	276 (99%)	3 (1%)	80	52
1	C	280/275 (102%)	277 (99%)	3 (1%)	80	52
1	D	281/275 (102%)	278 (99%)	3 (1%)	80	52
1	E	281/275 (102%)	278 (99%)	3 (1%)	80	52
1	F	279/275 (102%)	276 (99%)	3 (1%)	80	52
All	All	1683/1650 (102%)	1664 (99%)	19 (1%)	78	52

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	ARG
1	D	89	ASP
1	E	233	GLN
1	C	89	ASP
1	F	89	ASP

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

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 ⓘ

31 carbohydrates 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
7	L1L	A	414	5,7	15,16,16	0.57	0	22,24,24	1.10	1 (4%)
7	Z9M	A	415	5,7	14,15,16	0.51	0	20,22,24	1.47	4 (20%)
7	KDO	A	416	7	12,15,16	0.56	0	12,21,24	1.46	2 (16%)
10	L1L	B	407	10,5	15,16,16	0.56	0	22,24,24	2.24	2 (9%)
10	Z9M	B	408	10,5	14,15,16	0.55	0	20,22,24	1.30	1 (5%)
10	KDO	B	409	10,8	11,14,16	0.21	0	11,19,24	1.65	3 (27%)
10	GMH	B	410	10	14,14,14	0.55	0	17,20,20	0.88	0
10	L1L	C	413	10,5	15,16,16	0.75	0	22,24,24	1.20	2 (9%)
10	Z9M	C	414	10,5	14,15,16	0.66	0	20,22,24	1.80	4 (20%)
10	KDO	C	415	10,8	11,14,16	0.28	0	11,19,24	1.56	2 (18%)
10	GMH	C	416	10	14,14,14	0.83	0	17,20,20	1.50	4 (23%)
12	L1L	C	425	12,5	15,16,16	0.45	0	22,24,24	1.67	4 (18%)
12	Z9M	C	426	12,5	14,15,16	0.58	0	20,22,24	1.18	1 (5%)
12	KDO	C	427	12	12,15,16	0.57	0	12,21,24	1.28	1 (8%)
12	KDO	C	428	12	12,15,16	0.67	0	12,21,24	1.57	3 (25%)
7	L1L	D	412	5,7	15,16,16	0.59	0	22,24,24	2.26	5 (22%)
7	Z9M	D	413	5,7	14,15,16	0.53	0	20,22,24	1.18	2 (10%)
7	KDO	D	414	7	11,14,16	0.57	0	11,19,24	3.51	3 (27%)
7	L1L	D	423	5,7	15,16,16	0.57	0	22,24,24	1.06	2 (9%)
7	Z9M	D	424	5,7	14,15,16	0.59	0	20,22,24	1.32	3 (15%)
7	KDO	D	425	7	12,15,16	0.38	0	12,21,24	1.56	3 (25%)
7	L1L	E	405	5,7	15,16,16	0.68	0	22,24,24	1.26	3 (13%)
7	Z9M	E	406	5,7	14,15,16	0.54	0	20,22,24	1.05	2 (10%)
7	KDO	E	407	7	12,15,16	0.37	0	12,21,24	1.39	2 (16%)
10	L1L	F	406	10,5	15,16,16	0.59	0	22,24,24	1.01	1 (4%)
10	Z9M	F	407	10,5	14,15,16	0.62	0	20,22,24	1.80	3 (15%)
10	KDO	F	408	10,8	11,14,16	0.39	0	11,19,24	1.66	2 (18%)
10	GMH	F	409	10	14,14,14	0.64	0	17,20,20	1.24	2 (11%)
7	L1L	F	418	5,7	15,16,16	0.58	0	22,24,24	1.68	4 (18%)
7	Z9M	F	419	5,7	14,15,16	0.59	0	20,22,24	1.04	1 (5%)
7	KDO	F	420	8,7	12,15,16	0.50	0	12,21,24	1.22	1 (8%)

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
7	L1L	A	414	5,7	-	0/6/27/27	0/1/1/1
7	Z9M	A	415	5,7	-	0/7/24/27	0/1/1/1
7	KDO	A	416	7	-	0/6/26/30	0/1/1/1
10	L1L	B	407	10,5	-	0/6/27/27	0/1/1/1
10	Z9M	B	408	10,5	-	0/7/24/27	0/1/1/1
10	KDO	B	409	10,8	-	0/6/22/30	0/1/1/1
10	GMH	B	410	10	-	0/6/26/26	0/1/1/1
10	L1L	C	413	10,5	-	0/6/27/27	0/1/1/1
10	Z9M	C	414	10,5	-	0/7/24/27	0/1/1/1
10	KDO	C	415	10,8	-	0/6/22/30	0/1/1/1
10	GMH	C	416	10	-	0/6/26/26	0/1/1/1
12	L1L	C	425	12,5	-	0/6/27/27	0/1/1/1
12	Z9M	C	426	12,5	-	0/7/24/27	0/1/1/1
12	KDO	C	427	12	-	0/6/26/30	0/1/1/1
12	KDO	C	428	12	-	0/6/26/30	0/1/1/1
7	L1L	D	412	5,7	-	0/6/27/27	0/1/1/1
7	Z9M	D	413	5,7	-	0/7/24/27	0/1/1/1
7	KDO	D	414	7	-	0/6/22/30	0/1/1/1
7	L1L	D	423	5,7	-	0/6/27/27	0/1/1/1
7	Z9M	D	424	5,7	-	0/7/24/27	0/1/1/1
7	KDO	D	425	7	-	0/6/26/30	0/1/1/1
7	L1L	E	405	5,7	-	0/6/27/27	0/1/1/1
7	Z9M	E	406	5,7	-	0/7/24/27	0/1/1/1
7	KDO	E	407	7	-	0/6/26/30	0/1/1/1
10	L1L	F	406	10,5	-	0/6/27/27	0/1/1/1
10	Z9M	F	407	10,5	-	0/7/24/27	0/1/1/1
10	KDO	F	408	10,8	-	0/6/22/30	0/1/1/1
10	GMH	F	409	10	-	0/6/26/26	0/1/1/1
7	L1L	F	418	5,7	-	0/6/27/27	0/1/1/1
7	Z9M	F	419	5,7	-	0/7/24/27	0/1/1/1
7	KDO	F	420	8,7	-	0/6/26/30	0/1/1/1

There are no bond length outliers.

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	412	L1L	O1-P-O2	-7.92	88.58	107.48
10	B	407	L1L	O1-P-O2	-6.04	93.07	107.48
12	C	425	L1L	O1-P-O2	-3.74	98.55	107.48
10	C	415	KDO	C6-C5-C4	-3.60	104.91	111.24
10	B	409	KDO	C6-C5-C4	-3.55	104.99	111.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	416	KDO	2	0
10	B	409	KDO	1	0
10	C	415	KDO	4	0
10	C	416	GMH	1	0
12	C	427	KDO	2	0
12	C	428	KDO	2	0
7	D	425	KDO	2	0
7	E	407	KDO	3	0
10	F	408	KDO	1	0
7	F	420	KDO	2	0

5.6 Ligand geometry [i](#)

Of 114 ligands modelled in this entry, 2 are monoatomic - leaving 112 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	SO4	A	401	-	4,4,4	0.25	0	6,6,6	0.41	0
3	C8E	A	402	-	2,2,20	0.45	0	1,1,19	0.13	0
3	C8E	A	403	-	3,3,20	0.54	0	2,2,19	0.82	0
3	C8E	A	404	-	5,5,20	0.30	0	4,4,19	0.26	0
3	C8E	A	405	-	3,3,20	0.52	0	2,2,19	0.84	0
3	C8E	A	406	-	4,4,20	0.34	0	3,3,19	0.33	0
3	C8E	A	407	-	4,4,20	0.50	0	3,3,19	0.27	0
3	C8E	A	408	-	7,7,20	0.49	0	6,6,19	0.45	0
3	C8E	A	409	-	7,7,20	0.28	0	6,6,19	0.50	0
3	C8E	A	410	-	6,6,20	0.26	0	5,5,19	0.48	0
4	PO4	A	411	-	4,4,4	0.60	0	6,6,6	0.31	0
5	FTT	A	412	12,6	12,13,16	0.52	0	13,13,17	1.21	1 (7%)
6	DAO	A	413	5	7,7,13	0.50	0	6,6,13	1.07	1 (16%)
8	KDO	A	417	-	12,15,16	0.28	0	12,21,24	0.99	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FTT	A	418	7	13,14,16	0.37	0	14,14,17	0.74	0
5	FTT	A	419	7,6	11,12,16	0.50	0	12,12,17	1.31	1 (8%)
5	FTT	A	420	9,7	14,15,16	0.36	0	15,15,17	0.84	0
9	MYR	A	421	5	5,5,15	0.71	0	4,4,15	0.88	0
6	DAO	A	422	5	4,4,13	0.68	0	3,3,13	1.40	1 (33%)
3	C8E	B	401	-	8,8,20	0.39	0	7,7,19	0.57	0
3	C8E	B	402	-	2,2,20	0.47	0	0,1,19	0.00	-
3	C8E	B	403	-	4,4,20	0.31	0	3,3,19	0.27	0
3	C8E	B	404	-	7,7,20	0.29	0	6,6,19	0.35	0
3	C8E	B	405	-	7,7,20	0.30	0	6,6,19	0.65	0
4	PO4	B	406	-	4,4,4	0.69	0	6,6,6	0.25	0
8	KDO	B	411	10	12,15,16	0.33	0	12,21,24	1.07	1 (8%)
5	FTT	B	412	10	13,14,16	0.38	0	14,14,17	0.68	0
5	FTT	B	413	10,6	11,12,16	0.55	0	12,12,17	1.06	1 (8%)
5	FTT	B	414	9,10	14,15,16	0.41	0	15,15,17	0.81	0
9	MYR	B	415	5	5,5,15	0.64	0	4,4,15	1.03	0
6	DAO	B	416	5	4,4,13	0.68	0	3,3,13	0.94	0
5	FTT	B	417	7	12,13,16	0.48	0	13,13,17	0.90	1 (7%)
3	C8E	C	401	-	2,2,20	0.35	0	0,1,19	0.00	-
3	C8E	C	402	-	6,6,20	0.52	0	5,5,19	0.81	0
3	C8E	C	403	-	2,2,20	0.33	0	0,1,19	0.00	-
3	C8E	C	404	-	5,5,20	0.24	0	4,4,19	0.32	0
3	C8E	C	405	-	2,2,20	0.10	0	0,1,19	0.00	-
3	C8E	C	406	-	7,7,20	0.30	0	6,6,19	0.41	0
3	C8E	C	407	-	10,10,20	0.34	0	9,9,19	0.45	0
3	C8E	C	408	-	10,10,20	0.35	0	9,9,19	0.39	0
3	C8E	C	409	-	9,9,20	0.35	0	8,8,19	0.43	0
3	C8E	C	410	-	6,6,20	0.32	0	5,5,19	0.47	0
4	PO4	C	411	-	4,4,4	0.59	0	6,6,6	0.28	0
8	KDO	C	417	11,10	12,15,16	0.35	0	12,21,24	1.43	2 (16%)
5	FTT	C	418	10	14,15,16	0.46	0	15,15,17	1.06	0
5	FTT	C	419	9,10	9,10,16	0.65	0	10,10,17	1.00	1 (10%)
5	FTT	C	420	10,6	14,15,16	0.37	0	15,15,17	0.84	1 (6%)
5	FTT	C	421	10,6	11,12,16	0.56	0	12,12,17	0.85	1 (8%)
9	MYR	C	422	5	7,7,15	0.69	0	6,6,15	0.61	0
6	DAO	C	423	5	12,12,13	0.45	0	11,11,13	0.63	0
6	DAO	C	424	5	9,9,13	0.57	0	8,8,13	0.48	0
5	FTT	C	429	12	14,15,16	0.28	0	15,15,17	1.35	2 (13%)
5	FTT	C	430	12,6	11,12,16	0.53	0	12,12,17	1.02	1 (8%)
5	FTT	C	431	9,12	14,15,16	0.22	0	15,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MYR	C	432	5	8,8,15	0.44	0	7,7,15	0.75	0
6	DAO	C	433	5	7,7,13	0.57	0	6,6,13	0.86	0
5	FTT	C	434	10,6	12,13,16	20.41	2 (16%)	13,13,17	10.10	3 (23%)
6	DAO	C	435	5	4,4,13	0.69	0	3,3,13	0.72	0
2	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.31	0
3	C8E	D	402	-	3,3,20	0.50	0	2,2,19	0.86	0
3	C8E	D	403	-	5,5,20	0.32	0	4,4,19	0.32	0
3	C8E	D	404	-	5,5,20	0.28	0	4,4,19	0.33	0
3	C8E	D	405	-	5,5,20	0.28	0	4,4,19	0.34	0
3	C8E	D	406	-	7,7,20	0.33	0	6,6,19	0.46	0
3	C8E	D	407	-	7,7,20	0.30	0	6,6,19	0.29	0
3	C8E	D	408	-	10,10,20	0.39	0	9,9,19	0.26	0
3	C8E	D	409	-	3,3,20	0.55	0	2,2,19	0.34	0
3	C8E	D	410	-	5,5,20	0.26	0	4,4,19	0.34	0
4	PO4	D	411	-	4,4,4	0.58	0	6,6,6	0.26	0
5	FTT	D	415	7	12,13,16	0.51	0	13,13,17	0.64	0
5	FTT	D	416	7,6	9,10,16	0.52	0	10,10,17	1.19	1 (10%)
5	FTT	D	417	9,7	11,12,16	0.52	0	12,12,17	0.71	0
5	FTT	D	418	7	9,10,16	0.60	0	10,10,17	0.93	1 (10%)
6	DAO	D	419	5	2,2,13	0.96	0	0,1,13	0.00	-
9	MYR	D	420	5	4,4,15	0.86	0	3,3,15	1.24	1 (33%)
5	FTT	D	421	7	12,13,16	0.50	0	13,13,17	1.27	1 (7%)
6	DAO	D	422	-	5,5,13	0.53	0	4,4,13	1.07	0
8	KDO	D	426	-	12,15,16	0.31	0	12,21,24	1.15	1 (8%)
5	FTT	D	427	7	14,15,16	0.33	0	15,15,17	0.75	0
5	FTT	D	428	7,6	11,12,16	0.53	0	12,12,17	1.05	1 (8%)
5	FTT	D	429	9,7	14,15,16	0.35	0	15,15,17	0.76	0
9	MYR	D	430	5	5,5,15	0.63	0	4,4,15	0.91	0
6	DAO	D	431	5	4,4,13	0.66	0	3,3,13	0.81	0
3	C8E	E	401	-	5,5,20	0.29	0	4,4,19	0.34	0
4	PO4	E	402	-	4,4,4	0.74	0	6,6,6	0.26	0
5	FTT	E	403	7,6	12,13,16	0.56	0	13,13,17	1.22	2 (15%)
6	DAO	E	404	5	4,4,13	0.71	0	3,3,13	1.48	1 (33%)
8	KDO	E	408	-	12,15,16	0.34	0	12,21,24	1.24	1 (8%)
5	FTT	E	409	7	12,13,16	0.34	0	13,13,17	0.81	0
5	FTT	E	410	7,6	10,11,16	0.49	0	11,11,17	1.30	2 (18%)
5	FTT	E	411	9,7	13,14,16	0.51	0	14,14,17	0.94	1 (7%)
9	MYR	E	412	5	5,5,15	0.66	0	4,4,15	0.78	0
6	DAO	E	413	5	4,4,13	0.69	0	3,3,13	1.07	0
3	C8E	F	401	-	2,2,20	0.33	0	0,1,19	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	F	402	-	3,3,20	0.50	0	2,2,19	0.81	0
3	C8E	F	403	-	7,7,20	0.35	0	6,6,19	0.47	0
4	PO4	F	404	-	4,4,4	0.70	0	6,6,6	0.25	0
8	KDO	F	410	11,10	12,15,16	0.36	0	12,21,24	1.23	1 (8%)
5	FTT	F	411	10,6	10,11,16	0.68	0	11,11,17	1.13	1 (9%)
5	FTT	F	412	10,6	11,12,16	0.63	0	12,12,17	0.86	1 (8%)
5	FTT	F	413	9,10	10,11,16	0.47	0	11,11,17	0.94	1 (9%)
5	FTT	F	414	10	14,15,16	0.36	0	15,15,17	1.22	1 (6%)
9	MYR	F	415	5	10,10,15	0.44	0	9,9,15	0.68	0
6	DAO	F	416	5	4,4,13	0.63	0	3,3,13	0.77	0
6	DAO	F	417	5	4,4,13	0.71	0	3,3,13	0.58	0
8	KDO	F	421	7	12,15,16	0.32	0	12,21,24	1.15	1 (8%)
5	FTT	F	422	7	12,13,16	0.40	0	13,13,17	0.61	0
5	FTT	F	423	7,6	9,10,16	0.54	0	10,10,17	1.23	1 (10%)
5	FTT	F	424	9,7	14,15,16	0.28	0	15,15,17	0.79	0
9	MYR	F	425	5	11,11,15	0.45	0	10,10,15	0.71	0
6	DAO	F	426	5	7,7,13	0.59	0	6,6,13	0.73	0
5	FTT	F	427	7	12,13,16	0.49	0	13,13,17	0.89	1 (7%)

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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	C8E	A	402	-	-	0/0/0/18	0/0/0/0
3	C8E	A	403	-	-	0/1/1/18	0/0/0/0
3	C8E	A	404	-	-	0/3/3/18	0/0/0/0
3	C8E	A	405	-	-	0/1/1/18	0/0/0/0
3	C8E	A	406	-	-	0/2/2/18	0/0/0/0
3	C8E	A	407	-	-	0/2/2/18	0/0/0/0
3	C8E	A	408	-	-	0/5/5/18	0/0/0/0
3	C8E	A	409	-	-	0/5/5/18	0/0/0/0
3	C8E	A	410	-	-	0/4/4/18	0/0/0/0
4	PO4	A	411	-	-	0/0/0/0	0/0/0/0
5	FTT	A	412	12,6	-	0/12/12/15	0/0/0/0
6	DAO	A	413	5	-	0/4/5/11	0/0/0/0
8	KDO	A	417	-	-	0/6/26/30	0/1/1/1
5	FTT	A	418	7	-	0/13/13/15	0/0/0/0
5	FTT	A	419	7,6	-	0/11/11/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FTT	A	420	9,7	-	0/14/14/15	0/0/0/0
9	MYR	A	421	5	-	0/2/3/13	0/0/0/0
6	DAO	A	422	5	-	0/1/2/11	0/0/0/0
3	C8E	B	401	-	-	0/6/6/18	0/0/0/0
3	C8E	B	402	-	-	0/0/0/18	0/0/0/0
3	C8E	B	403	-	-	0/2/2/18	0/0/0/0
3	C8E	B	404	-	-	0/5/5/18	0/0/0/0
3	C8E	B	405	-	-	0/5/5/18	0/0/0/0
4	PO4	B	406	-	-	0/0/0/0	0/0/0/0
8	KDO	B	411	10	-	0/6/26/30	0/1/1/1
5	FTT	B	412	10	-	0/13/13/15	0/0/0/0
5	FTT	B	413	10,6	-	0/11/11/15	0/0/0/0
5	FTT	B	414	9,10	-	0/14/14/15	0/0/0/0
9	MYR	B	415	5	-	0/2/3/13	0/0/0/0
6	DAO	B	416	5	-	0/1/2/11	0/0/0/0
5	FTT	B	417	7	-	0/12/12/15	0/0/0/0
3	C8E	C	401	-	-	0/0/0/18	0/0/0/0
3	C8E	C	402	-	-	0/4/4/18	0/0/0/0
3	C8E	C	403	-	-	0/0/0/18	0/0/0/0
3	C8E	C	404	-	-	0/3/3/18	0/0/0/0
3	C8E	C	405	-	-	0/0/0/18	0/0/0/0
3	C8E	C	406	-	-	0/5/5/18	0/0/0/0
3	C8E	C	407	-	-	0/8/8/18	0/0/0/0
3	C8E	C	408	-	-	0/8/8/18	0/0/0/0
3	C8E	C	409	-	-	0/7/7/18	0/0/0/0
3	C8E	C	410	-	-	0/4/4/18	0/0/0/0
4	PO4	C	411	-	-	0/0/0/0	0/0/0/0
8	KDO	C	417	11,10	-	0/6/26/30	0/1/1/1
5	FTT	C	418	10	-	0/14/14/15	0/0/0/0
5	FTT	C	419	9,10	-	0/9/9/15	0/0/0/0
5	FTT	C	420	10,6	-	0/14/14/15	0/0/0/0
5	FTT	C	421	10,6	-	0/11/11/15	0/0/0/0
9	MYR	C	422	5	-	0/4/5/13	0/0/0/0
6	DAO	C	423	5	-	0/9/10/11	0/0/0/0
6	DAO	C	424	5	-	0/6/7/11	0/0/0/0
5	FTT	C	429	12	-	0/14/14/15	0/0/0/0
5	FTT	C	430	12,6	-	0/11/11/15	0/0/0/0
5	FTT	C	431	9,12	-	0/14/14/15	0/0/0/0
9	MYR	C	432	5	-	0/5/6/13	0/0/0/0
6	DAO	C	433	5	-	0/4/5/11	0/0/0/0
5	FTT	C	434	10,6	-	0/12/12/15	0/0/0/0
6	DAO	C	435	5	-	0/1/2/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
3	C8E	D	402	-	-	0/1/1/18	0/0/0/0
3	C8E	D	403	-	-	0/3/3/18	0/0/0/0
3	C8E	D	404	-	-	0/3/3/18	0/0/0/0
3	C8E	D	405	-	-	0/3/3/18	0/0/0/0
3	C8E	D	406	-	-	0/5/5/18	0/0/0/0
3	C8E	D	407	-	-	0/5/5/18	0/0/0/0
3	C8E	D	408	-	-	0/8/8/18	0/0/0/0
3	C8E	D	409	-	-	0/0/1/18	0/0/0/0
3	C8E	D	410	-	-	0/3/3/18	0/0/0/0
4	PO4	D	411	-	-	0/0/0/0	0/0/0/0
5	FTT	D	415	7	-	0/12/12/15	0/0/0/0
5	FTT	D	416	7,6	-	0/9/9/15	0/0/0/0
5	FTT	D	417	9,7	-	0/11/11/15	0/0/0/0
5	FTT	D	418	7	-	0/9/9/15	0/0/0/0
6	DAO	D	419	5	-	0/0/0/11	0/0/0/0
9	MYR	D	420	5	-	0/1/2/13	0/0/0/0
5	FTT	D	421	7	-	0/12/12/15	0/0/0/0
6	DAO	D	422	-	-	0/2/3/11	0/0/0/0
8	KDO	D	426	-	-	0/6/26/30	0/1/1/1
5	FTT	D	427	7	-	0/14/14/15	0/0/0/0
5	FTT	D	428	7,6	-	0/11/11/15	0/0/0/0
5	FTT	D	429	9,7	-	0/14/14/15	0/0/0/0
9	MYR	D	430	5	-	0/2/3/13	0/0/0/0
6	DAO	D	431	5	-	0/1/2/11	0/0/0/0
3	C8E	E	401	-	-	0/3/3/18	0/0/0/0
4	PO4	E	402	-	-	0/0/0/0	0/0/0/0
5	FTT	E	403	7,6	-	0/12/12/15	0/0/0/0
6	DAO	E	404	5	-	0/1/2/11	0/0/0/0
8	KDO	E	408	-	-	0/6/26/30	0/1/1/1
5	FTT	E	409	7	-	0/12/12/15	0/0/0/0
5	FTT	E	410	7,6	-	0/10/10/15	0/0/0/0
5	FTT	E	411	9,7	-	0/13/13/15	0/0/0/0
9	MYR	E	412	5	-	0/2/3/13	0/0/0/0
6	DAO	E	413	5	-	0/1/2/11	0/0/0/0
3	C8E	F	401	-	-	0/0/0/18	0/0/0/0
3	C8E	F	402	-	-	0/1/1/18	0/0/0/0
3	C8E	F	403	-	-	0/5/5/18	0/0/0/0
4	PO4	F	404	-	-	0/0/0/0	0/0/0/0
8	KDO	F	410	11,10	-	0/6/26/30	0/1/1/1
5	FTT	F	411	10,6	-	0/10/10/15	0/0/0/0
5	FTT	F	412	10,6	-	0/11/11/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FTT	F	413	9,10	-	0/10/10/15	0/0/0/0
5	FTT	F	414	10	-	0/14/14/15	0/0/0/0
9	MYR	F	415	5	-	0/7/8/13	0/0/0/0
6	DAO	F	416	5	-	0/1/2/11	0/0/0/0
6	DAO	F	417	5	-	0/1/2/11	0/0/0/0
8	KDO	F	421	7	-	0/6/26/30	0/1/1/1
5	FTT	F	422	7	-	0/12/12/15	0/0/0/0
5	FTT	F	423	7,6	-	0/9/9/15	0/0/0/0
5	FTT	F	424	9,7	-	0/14/14/15	0/0/0/0
9	MYR	F	425	5	-	0/8/9/13	0/0/0/0
6	DAO	F	426	5	-	0/4/5/11	0/0/0/0
5	FTT	F	427	7	-	0/12/12/15	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	434	FTT	O2-C1	28.87	3.00	1.19
5	C	434	FTT	O3-C3	64.52	3.32	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	434	FTT	O3-C3-C2	-28.82	38.59	108.98
5	C	434	FTT	O2-C1-C2	-19.20	55.93	125.28
5	A	412	FTT	O2-C1-C2	-3.83	111.43	125.28
5	D	421	FTT	O2-C1-C2	-3.49	112.67	125.28
5	F	423	FTT	O2-C1-C2	-3.35	113.19	125.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	C8E	1	0
3	A	408	C8E	2	0
8	A	417	KDO	2	0
3	B	403	C8E	2	0
8	B	411	KDO	1	0
3	C	405	C8E	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	417	KDO	3	0
3	D	409	C8E	1	0
8	D	426	KDO	2	0
8	E	408	KDO	3	0
3	F	401	C8E	1	0
3	F	403	C8E	1	0
8	F	410	KDO	1	0
5	F	411	FTT	1	0
8	F	421	KDO	2	0
5	F	427	FTT	1	0

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	342/342 (100%)	0.17	14 (4%) 41 41	9, 15, 28, 59	1 (0%)
1	B	342/342 (100%)	0.17	14 (4%) 41 41	9, 15, 31, 77	0
1	C	342/342 (100%)	0.09	8 (2%) 64 65	9, 14, 30, 54	0
1	D	342/342 (100%)	0.25	21 (6%) 25 24	10, 16, 31, 96	0
1	E	342/342 (100%)	0.16	14 (4%) 41 41	10, 15, 32, 58	0
1	F	342/342 (100%)	0.00	3 (0%) 85 87	9, 14, 25, 40	0
All	All	2052/2052 (100%)	0.14	74 (3%) 46 47	9, 15, 30, 96	1 (0%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	LEU	8.7
1	D	83	GLY	8.0
1	A	139	LEU	7.1
1	E	139	LEU	6.9
1	D	137	PHE	6.5

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
12	KDO	C	428	15/16	0.92	0.12	0.42	12,19,22,23	0
10	L1L	C	413	16/16	0.97	0.07	-1.28	17,19,33,35	0
10	Z9M	C	414	15/16	0.97	0.06	-2.19	18,21,41,41	0
12	Z9M	C	426	15/16	0.97	0.07	-	16,17,26,26	0
12	KDO	C	427	15/16	0.94	0.12	-	16,21,30,34	0
7	KDO	D	414	14/16	0.62	0.29	-	42,49,65,65	0
10	L1L	F	406	16/16	0.97	0.07	-	16,19,34,34	0
7	Z9M	E	406	15/16	0.96	0.20	-	21,21,26,27	0
12	L1L	C	425	16/16	0.95	0.08	-	17,19,44,44	0
10	GMH	C	416	14/14	0.79	0.20	-	27,45,58,69	0
7	L1L	A	414	16/16	0.93	0.21	-	22,27,48,52	0
10	KDO	B	409	14/16	0.90	0.20	-	22,26,33,41	0
10	Z9M	B	408	15/16	0.95	0.16	-	20,21,26,26	0
10	KDO	C	415	14/16	0.94	0.11	-	18,23,31,31	0
7	Z9M	A	415	15/16	0.94	0.22	-	22,24,31,34	0
10	Z9M	F	407	15/16	0.98	0.07	-	18,21,29,32	0
7	L1L	D	423	16/16	0.93	0.19	-	24,26,44,49	0
7	Z9M	F	419	15/16	0.97	0.06	-	17,18,24,27	0
10	L1L	B	407	16/16	0.94	0.14	-	22,24,50,51	0
7	Z9M	D	413	15/16	0.92	0.21	-	25,29,34,40	0
10	GMH	F	409	14/14	0.87	0.20	-	28,36,54,59	0
7	L1L	F	418	16/16	0.95	0.09	-	18,20,41,43	0
7	KDO	F	420	15/16	0.92	0.14	-	13,21,31,35	0
7	KDO	D	425	15/16	0.89	0.25	-	25,28,40,44	0
7	L1L	E	405	16/16	0.94	0.15	-	23,26,47,49	0
10	KDO	F	408	14/16	0.94	0.14	-	18,25,33,37	0
7	KDO	E	407	15/16	0.88	0.21	-	23,27,35,38	0
10	GMH	B	410	14/14	0.82	0.28	-	29,36,40,48	0
7	L1L	D	412	16/16	0.85	0.31	-	34,37,66,67	0
7	Z9M	D	424	15/16	0.95	0.17	-	23,24,30,30	0
7	KDO	A	416	15/16	0.89	0.28	-	24,29,40,48	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	C8E	A	407	5/21	0.71	0.24	43.31	18,20,26,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	C8E	D	409	4/21	0.88	0.29	34.38	21,23,30,39	0
3	C8E	C	401	3/21	0.89	0.20	19.55	45,45,50,51	0
4	PO4	A	411	5/5	0.91	0.20	17.94	36,36,41,47	0
4	PO4	D	411	5/5	0.88	0.24	15.15	32,37,40,47	0
3	C8E	D	405	6/21	0.77	0.13	14.04	30,37,41,42	0
3	C8E	C	410	7/21	0.81	0.26	13.99	23,24,39,43	0
4	PO4	C	411	5/5	0.94	0.23	12.37	32,35,44,44	0
4	PO4	E	402	5/5	0.88	0.25	12.08	34,35,41,44	0
5	FTT	E	411	15/17	0.86	0.23	11.24	25,31,40,41	0
4	PO4	B	406	5/5	0.92	0.18	10.99	31,33,40,44	0
5	FTT	A	420	16/17	0.70	0.25	10.83	27,39,59,66	0
5	FTT	B	414	16/17	0.84	0.20	10.82	23,30,36,39	0
5	FTT	D	415	14/17	0.72	0.18	9.94	36,47,53,54	0
3	C8E	C	402	7/21	0.86	0.27	9.62	25,32,38,43	0
3	C8E	C	408	11/21	0.83	0.21	8.48	36,39,45,49	0
5	FTT	D	429	16/17	0.87	0.18	8.16	28,36,41,43	0
4	PO4	F	404	5/5	0.92	0.19	8.15	31,36,45,45	0
3	C8E	A	408	8/21	0.88	0.22	7.98	19,29,52,66	0
3	C8E	A	409	8/21	0.80	0.18	7.45	29,34,38,38	0
3	C8E	B	403	5/21	0.83	0.20	7.29	30,32,33,41	0
9	MYR	F	415	11/16	0.81	0.12	6.80	26,31,36,36	0
3	C8E	C	406	8/21	0.80	0.18	6.78	30,33,33,35	0
5	FTT	A	418	15/17	0.85	0.13	6.10	15,22,26,38	0
3	C8E	E	401	6/21	0.78	0.19	6.05	44,52,63,65	0
3	C8E	D	402	4/21	0.84	0.18	5.73	32,33,34,39	0
3	C8E	D	406	8/21	0.77	0.16	5.58	48,52,54,58	0
5	FTT	F	424	16/17	0.85	0.16	5.28	21,32,42,45	0
3	C8E	D	407	8/21	0.81	0.17	5.17	25,41,44,48	0
3	C8E	C	409	10/21	0.82	0.13	4.52	35,38,50,54	0
5	FTT	D	427	16/17	0.85	0.14	4.50	17,23,28,30	0
5	FTT	F	414	16/17	0.86	0.13	4.42	28,33,39,41	0
3	C8E	C	404	6/21	0.84	0.15	3.62	28,41,49,51	0
3	C8E	B	401	9/21	0.85	0.15	2.76	31,43,63,64	0
3	C8E	D	404	6/21	0.80	0.13	2.49	32,41,41,43	0
3	C8E	C	407	11/21	0.89	0.17	2.47	33,35,43,47	0
5	FTT	E	409	14/17	0.90	0.10	2.46	18,21,25,26	0
5	FTT	C	418	16/17	0.90	0.13	2.26	23,32,37,38	0
8	KDO	C	417	15/16	0.95	0.09	2.19	14,15,19,24	0
8	KDO	F	410	15/16	0.94	0.12	2.14	15,16,20,29	0
5	FTT	C	429	16/17	0.93	0.10	1.85	15,20,27,31	0
5	FTT	B	412	15/17	0.93	0.09	1.28	19,21,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	KDO	A	417	15/16	0.89	0.24	1.27	18,23,30,30	0
6	DAO	C	423	13/14	0.93	0.09	1.21	22,27,31,33	0
3	C8E	B	405	8/21	0.81	0.11	1.20	38,39,41,41	0
3	C8E	A	404	6/21	0.83	0.13	0.81	39,46,50,51	0
8	KDO	D	426	15/16	0.88	0.20	0.80	14,22,27,27	0
8	KDO	E	408	15/16	0.91	0.16	0.78	19,21,26,27	0
3	C8E	F	401	3/21	0.93	0.10	0.73	21,21,30,37	0
8	KDO	B	411	15/16	0.92	0.14	0.64	18,20,25,27	0
5	FTT	F	422	14/17	0.94	0.09	0.61	16,18,24,27	0
8	KDO	F	421	15/16	0.93	0.12	0.50	17,18,21,24	0
3	C8E	D	408	11/21	0.82	0.23	0.46	27,41,43,43	0
5	FTT	C	431	16/17	0.94	0.10	0.36	18,30,41,41	0
2	SO4	D	401	5/5	0.99	0.10	0.34	18,21,25,29	0
5	FTT	C	420	16/17	0.96	0.08	-0.62	18,20,30,34	0
2	SO4	A	401	5/5	0.99	0.08	-1.47	17,19,22,27	0
9	MYR	D	430	6/16	0.75	0.18	-	43,47,49,50	0
5	FTT	B	413	13/17	0.85	0.16	-	21,26,42,44	0
5	FTT	E	410	12/17	0.82	0.14	-	26,29,36,39	0
5	FTT	A	412	14/17	0.81	0.18	-	39,44,66,68	0
6	DAO	C	435	5/14	0.62	0.19	-	49,50,63,63	0
5	FTT	D	417	13/17	0.88	0.16	-	29,43,53,54	0
6	DAO	E	413	5/14	0.70	0.36	-	49,54,55,56	0
6	DAO	D	422	6/14	0.86	0.10	-	44,48,51,57	0
6	DAO	C	424	10/14	0.90	0.12	-	25,30,32,33	0
6	DAO	B	416	5/14	0.68	0.61	-	39,48,59,60	0
9	MYR	C	432	9/16	0.88	0.15	-	33,55,63,71	0
5	FTT	C	430	13/17	0.89	0.11	-	20,22,34,39	0
6	DAO	C	433	8/14	0.84	0.19	-	37,62,72,73	0
3	C8E	A	403	4/21	0.83	0.12	-	62,71,76,79	0
5	FTT	D	418	11/17	0.63	0.26	-	46,51,67,67	0
3	C8E	F	402	4/21	0.85	0.16	-	41,44,47,47	0
3	C8E	C	405	3/21	0.93	0.17	-	26,26,28,35	0
6	DAO	D	431	5/14	0.63	0.50	-	47,58,58,73	0
9	MYR	B	415	6/16	0.75	0.24	-	43,60,68,68	0
5	FTT	F	427	14/17	0.66	0.18	-	38,42,47,48	0
9	MYR	F	425	12/16	0.87	0.12	-	29,32,44,50	0
3	C8E	A	402	3/21	0.74	0.30	-	33,33,41,41	0
5	FTT	F	411	12/17	0.91	0.12	-	19,24,43,48	0
3	C8E	A	405	4/21	0.87	0.12	-	77,80,84,87	0
5	FTT	B	417	14/17	0.62	0.18	-	35,40,55,61	0
3	C8E	D	410	6/21	0.84	0.21	-	40,43,45,45	0
3	C8E	D	403	6/21	0.84	0.20	-	39,44,51,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	C8E	B	404	8/21	0.76	0.14	-	41,46,47,47	0
6	DAO	D	419	3/14	0.68	0.42	-	51,51,52,53	0
9	MYR	D	420	5/16	0.79	0.27	-	16,25,37,38	0
6	DAO	F	416	5/14	0.93	0.10	-	26,27,35,40	0
5	FTT	C	421	13/17	0.95	0.13	-	19,26,52,55	0
6	DAO	A	413	8/14	0.72	0.17	-	40,41,44,57	0
6	DAO	F	426	8/14	0.87	0.18	-	34,49,64,66	0
5	FTT	C	419	11/17	0.92	0.10	-	18,20,24,30	0
3	C8E	B	402	3/21	0.82	0.10	-	46,46,50,55	0
5	FTT	F	413	12/17	0.91	0.11	-	21,26,34,38	0
11	CA	F	405	1/1	1.00	0.08	-	13,13,13,13	0
5	FTT	E	403	14/17	0.52	0.25	-	38,46,48,57	0
5	FTT	F	412	13/17	0.94	0.12	-	19,31,46,46	0
5	FTT	C	434	14/17	0.53	0.26	-	33,47,58,61	0
9	MYR	C	422	8/16	0.92	0.15	-	22,30,32,32	0
5	FTT	D	416	11/17	0.75	0.18	-	33,36,41,41	0
6	DAO	F	417	5/14	0.94	0.14	-	33,34,49,62	0
5	FTT	F	423	11/17	0.84	0.12	-	22,23,28,34	0
3	C8E	F	403	8/21	0.92	0.17	-	40,43,47,47	0
6	DAO	A	422	5/14	0.60	0.39	-	55,57,59,63	0
3	C8E	A	406	5/21	0.87	0.11	-	57,64,67,74	0
9	MYR	E	412	6/16	0.71	0.30	-	41,44,51,54	0
6	DAO	E	404	5/14	0.40	0.27	-	52,54,57,63	0
9	MYR	A	421	6/16	0.56	0.32	-	47,52,55,57	0
5	FTT	A	419	13/17	0.77	0.18	-	29,33,39,41	0
5	FTT	D	428	13/17	0.77	0.14	-	27,30,46,71	0
3	C8E	A	410	7/21	0.81	0.20	-	38,39,40,41	0
3	C8E	C	403	3/21	0.81	0.12	-	45,45,46,50	0
5	FTT	D	421	14/17	0.65	0.23	-	33,45,53,62	0
11	CA	C	412	1/1	1.00	0.08	-	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.