Full wwPDB X-ray Structure Validation 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

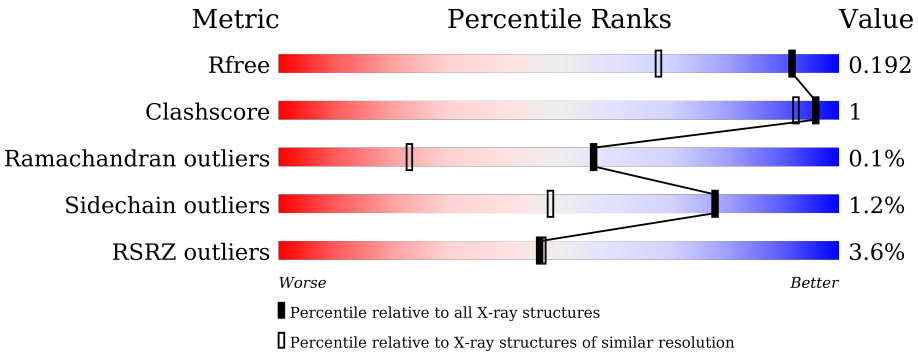
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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 <=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	4% 97% .
1	B	342	4% 95% 5%
1	C	342	2% 96% .
1	D	342	6% 96% .
1	E	342	4% 97% .
1	F	342	% 98% .

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

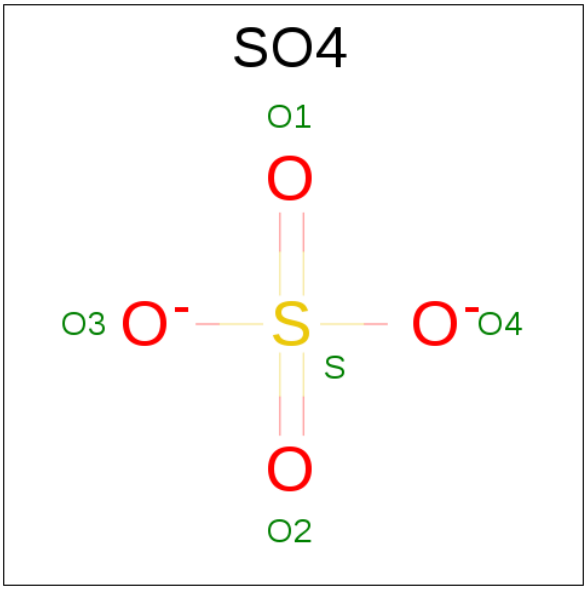
There are 13 unique types of molecules in this entry. The entry contains 19668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

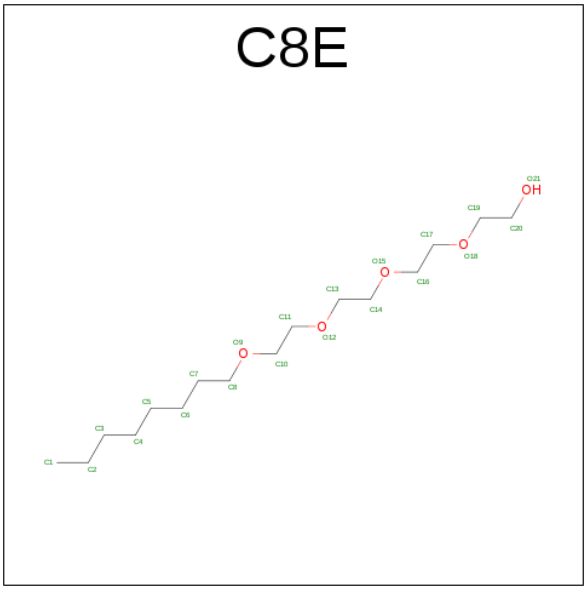
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	4	8	0
			2722	1704	455	560	3			
1	B	342	Total	C	N	O	S	0	4	0
			2700	1685	451	561	3			
1	C	342	Total	C	N	O	S	0	5	0
			2704	1691	451	559	3			
1	D	342	Total	C	N	O	S	0	6	0
			2710	1693	452	562	3			
1	E	342	Total	C	N	O	S	0	6	0
			2708	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: O_4S).



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: $C_{16}H_{34}O_5$).



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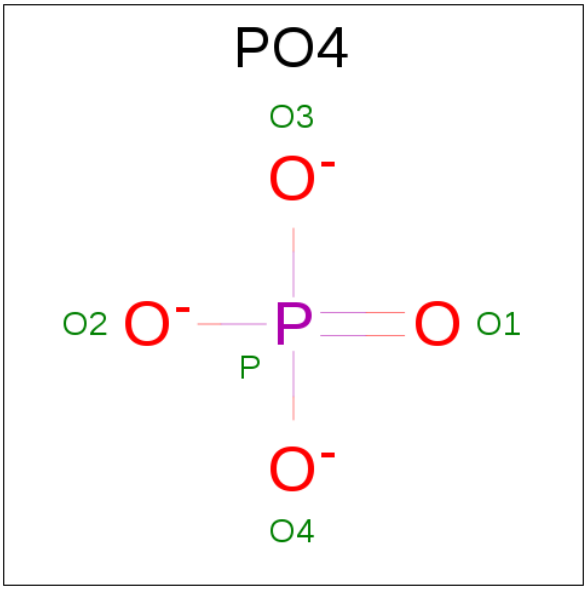
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 11 10 1	0	0
3	D	1	Total C O 4 3 1	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 6 6	0	0
3	F	1	Total C 3 3	0	0
3	F	1	Total C 4 4	0	0
3	F	1	Total C 8 8	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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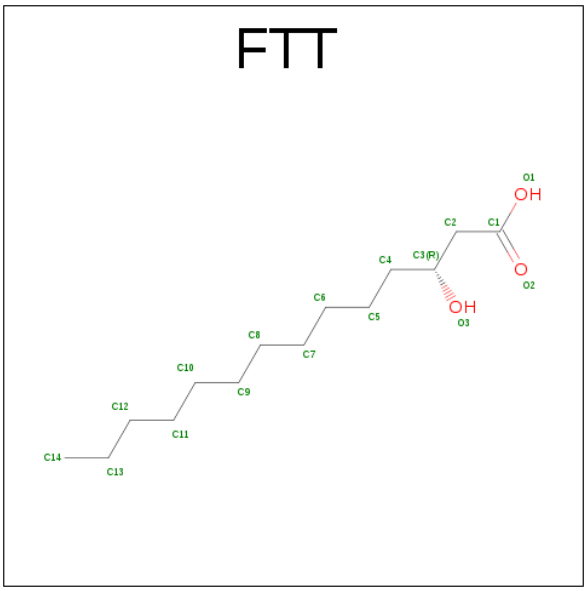
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

- 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 14 12 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C O 13 11 2	0	0
5	A	1	Total C O 16 14 2	0	0
5	B	1	Total C O 15 13 2	0	0
5	B	1	Total C O 13 11 2	0	0
5	B	1	Total C O 16 14 2	0	0
5	B	1	Total C O 14 12 2	0	0
5	C	1	Total C O 16 14 2	0	0

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

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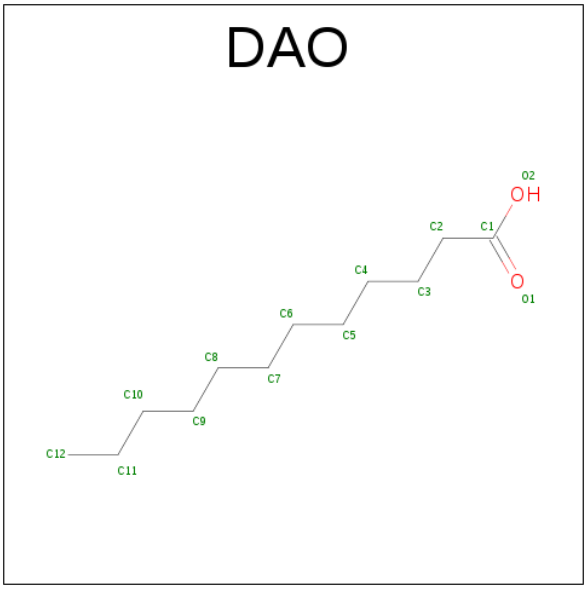
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 12 10 2	0	0
5	F	1	Total C O 16 14 2	0	0
5	F	1	Total C O 14 12 2	0	0
5	F	1	Total C O 11 9 2	0	0
5	F	1	Total C O 16 14 2	0	0
5	F	1	Total C O 14 12 2	0	0

- 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 8 7 1	0	0
6	A	1	Total C O 5 4 1	0	0
6	B	1	Total C O 5 4 1	0	0
6	C	1	Total C O 13 12 1	0	0
6	C	1	Total C O 10 9 1	0	0

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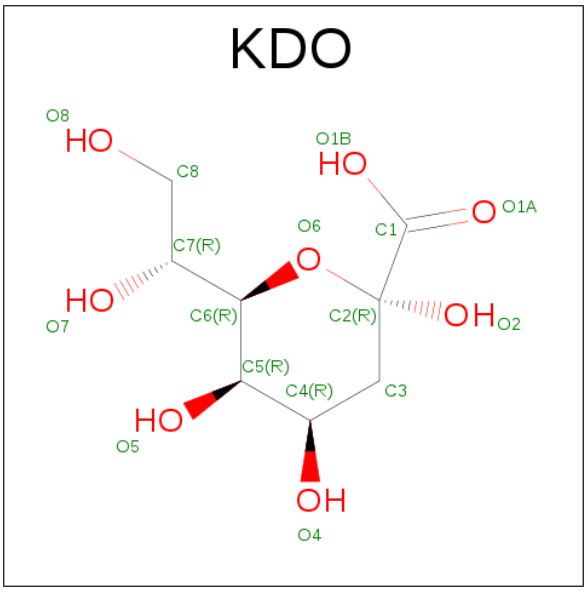
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 8 7 1	0	0
6	C	1	Total C O 5 4 1	0	0
6	D	1	Total C O 3 2 1	0	0
6	D	1	Total C O 6 5 1	0	0
6	D	1	Total C O 5 4 1	0	0
6	E	1	Total C O 5 4 1	0	0
6	E	1	Total C O 5 4 1	0	0
6	F	1	Total C O 5 4 1	0	0
6	F	1	Total C O 5 4 1	0	0
6	F	1	Total C O 8 7 1	0	0

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

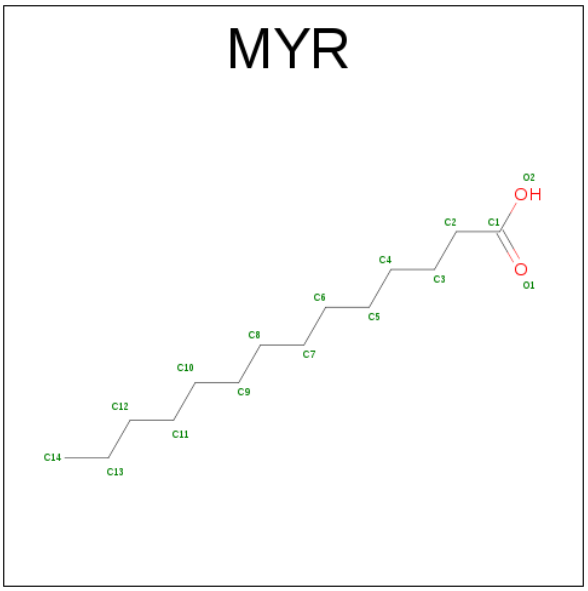
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total C N O P 46 20 2 22 2	0	0
7	D	3	Total C N O P 45 20 2 21 2	0	0
7	D	3	Total C N O P 46 20 2 22 2	0	0
7	E	3	Total C N O P 46 20 2 22 2	0	0
7	F	3	Total C N O P 46 20 2 22 2	0	0

- Molecule 8 is SUGAR (3-DEOXY-D-MANNO-OCT-2-ULOSONIC ACID) (three-letter code: KDO) (formula: $C_8H_{14}O_8$).



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

- Molecule 9 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

- 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 59 27 2 28 2	0	0
10	C	4	Total C N O P 59 27 2 28 2	0	0
10	F	4	Total C N O P 59 27 2 28 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total Ca 1 1	0	0
11	F	1	Total Ca 1 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 C N O P 61 28 2 29 2	0	0

- Molecule 13 is water.

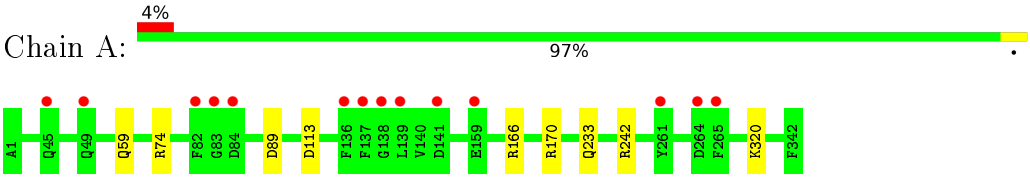
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	320	Total O 320 320	0	0
13	B	315	Total O 315 315	0	0
13	C	324	Total O 324 324	0	0
13	D	295	Total O 295 295	0	0
13	E	306	Total O 306 306	0	0
13	F	350	Total O 350 350	0	0

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.

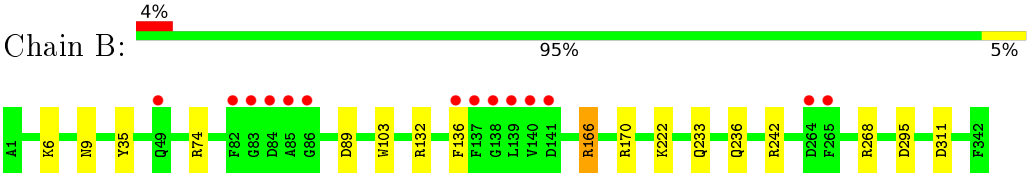
- Molecule 1: OMPC PORIN

Chain A:



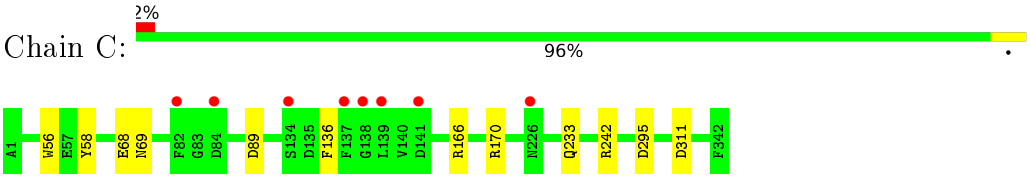
- Molecule 1: OMPC PORIN

Chain B:



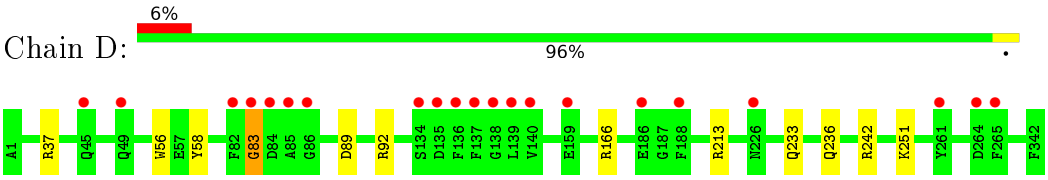
- Molecule 1: OMPC PORIN

Chain C:



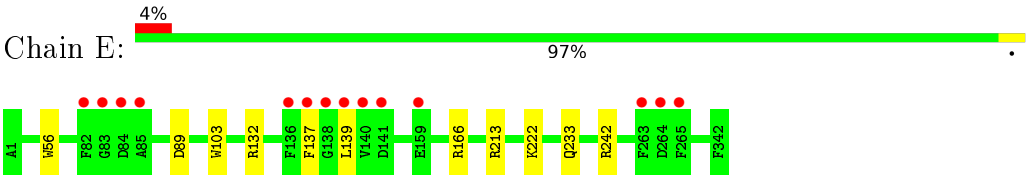
- Molecule 1: OMPC PORIN

Chain D:



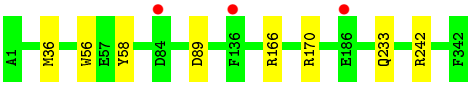
- Molecule 1: OMPC PORIN

Chain E:



- Molecule 1: OMPC PORIN

Chain F:


A1
M36
W56
E57
Y58
D84
D89
F136
R166
R170
E186
Q233
R242
F342

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	A	242	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	E	242	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	B	242	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	170	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	F	242	ARG	NE-CZ-NH1	-7.45	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	242	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	C	242	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	B	132	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	74	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	F	170	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	E	132	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	B	268	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	170	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	213	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	242	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	74	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	170	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	170	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	92	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	F	170	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	170	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	37	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	E	213	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	B	166	ARG	NE-CZ-NH2	-5.07	117.77	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2722	0	2520	2	0
1	B	2700	0	2475	8	0
1	C	2704	0	2491	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:D:251:LYS:HG3	13:D:710:HOH:O	1.73	0.86
10:C:415:KDO:HO4	8:C:417:KDO:C2	1.90	0.81
3:F:401:C8E:H11	5:F:411:FTT:C10	2.11	0.80
1:D:236:GLN:HG3	13:D:710:HOH:O	1.87	0.74
1:C:69:ASN:H	3:C:405:C8E:H13	1.55	0.72
7:F:420:KDO:HO4	8:F:421:KDO:C2	2.09	0.65
10:F:408:KDO:C4	8:F:410:KDO:C2	2.75	0.62
1:D:236:GLN:CG	13:D:710:HOH:O	2.45	0.60
12:C:427:KDO:C4	12:C:428:KDO:C2	2.76	0.59
7:E:407:KDO:C4	8:E:408:KDO:C2	2.79	0.58
3:D:409:C8E:H81	13:D:596:HOH:O	2.04	0.58
10:C:415:KDO:C4	8:C:417:KDO:C2	2.79	0.57
1:B:236:GLN:HG3	13:B:815:HOH:O	2.06	0.56
1:B:236:GLN:CG	13:B:815:HOH:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLU:HB2	3:C:405:C8E:C1	2.37	0.55
1:C:68:GLU:HA	3:C:405:C8E:H22	1.87	0.55
10:B:409:KDO:C4	8:B:411:KDO:C2	2.83	0.54
7:D:425:KDO:C4	8:D:426:KDO:C2	2.86	0.52
1:A:59:GLN:HE22	3:A:408:C8E:H132	1.76	0.51
7:F:420:KDO:C4	8:F:421:KDO:C2	2.82	0.51
10:C:415:KDO:O4	10:C:416:GMH:H1	2.11	0.51
3:B:403:C8E:H101	13:B:628:HOH:O	2.11	0.51
10:C:415:KDO:O4	8:C:417:KDO:C1	2.55	0.49
1:C:68:GLU:HB2	3:C:405:C8E:H11	1.94	0.48
1:B:103:TRP:CE2	1:B:222:LYS:HE2	2.48	0.48
1:E:137:PHE:HB2	1:E:139:LEU:HD13	1.97	0.47
1:B:35:TYR:CD1	3:B:403:C8E:H102	2.53	0.44
1:B:236:GLN:HG2	13:B:815:HOH:O	2.17	0.43
1:B:9:ASN:HB3	13:C:594:HOH:O	2.18	0.43
7:A:416:KDO:C4	8:A:417:KDO:C2	2.89	0.43
3:F:403:C8E:H13	5:F:427:FTT:H22	2.01	0.43
1:E:103:TRP:CE2	1:E:222:LYS:HE2	2.54	0.43
1:B:295:ASP:OD1	1:B:311:ASP:OD1	2.37	0.42
12:C:427:KDO:O4	12:C:428:KDO:C1	2.55	0.42
7:E:407:KDO:O4	8:E:408:KDO:C3	2.63	0.42
1:D:56:TRP:CZ2	1:D:58:TYR:HB2	2.55	0.42
1:F:56:TRP:CZ2	1:F:58:TYR:HB2	2.56	0.41
1:B:6:LYS:HE2	13:B:558:HOH:O	2.20	0.41
1:C:56:TRP:CZ2	1:C:58:TYR:HB2	2.55	0.41
1:A:113:ASP:OD2	3:A:407:C8E:H102	2.21	0.41
1:C:295:ASP:OD1	1:C:311:ASP:OD1	2.40	0.40
1:E:56:TRP:CD1	1:F:36:MET:HG2	2.57	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	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

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

Mol	Chain	Res	Type
1	A	89	ASP
1	A	166	ARG

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	320	LYS
1	B	89	ASP
1	B	166	ARG
1	B	233	GLN
1	C	89	ASP
1	C	166	ARG
1	C	233	GLN
1	D	89	ASP
1	D	166	ARG
1	D	233	GLN
1	E	89	ASP
1	E	166	ARG
1	E	233	GLN
1	F	89	ASP
1	F	166	ARG
1	F	233	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
10	F	408	KDO	C6-C5-C4	-3.50	105.09	111.24
7	F	418	L1L	O1-P-O2	-3.45	99.24	107.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	428	KDO	O4-C4-C3	-3.30	101.96	110.02
7	D	414	KDO	C5-C6-C7	-3.29	108.58	113.49
12	C	427	KDO	C4-C5-C6	-3.06	104.22	110.56
7	A	416	KDO	C4-C5-C6	-3.00	104.35	110.56
7	F	420	KDO	C4-C5-C6	-2.78	104.81	110.56
10	F	406	L1L	O3-C3-C2	-2.75	105.34	110.28
7	D	425	KDO	C4-C5-C6	-2.73	104.91	110.56
10	C	416	GMH	O5-C1-C2	-2.72	105.25	110.00
7	E	405	L1L	O1-P-O2	-2.57	101.35	107.48
7	E	407	KDO	C4-C5-C6	-2.49	105.41	110.56
12	C	425	L1L	O3-C3-C4	-2.42	104.89	110.36
10	C	416	GMH	C1-C2-C3	-2.29	106.93	110.68
7	D	425	KDO	O4-C4-C5	-2.19	105.78	110.19
10	B	409	KDO	O6-C6-C5	-2.17	107.94	109.75
7	F	418	L1L	O3-C3-C4	-2.14	105.53	110.36
7	D	412	L1L	O5-C1-O1	-2.14	108.55	111.36
7	D	424	Z9M	C3-C2-N1	-2.02	107.15	110.66
7	E	406	Z9M	O7-P1-O4	2.02	112.65	106.62
10	C	414	Z9M	O4-C4-C5	2.04	112.68	108.53
10	B	409	KDO	C6-O6-C2	2.08	116.34	112.17
7	D	413	Z9M	C1-C2-C3	2.11	112.59	109.21
12	C	428	KDO	O4-C4-C5	2.17	114.56	110.19
10	C	416	GMH	O5-C5-C4	2.23	112.03	108.22
10	F	407	Z9M	O8-P1-O4	2.23	113.28	106.62
7	A	415	Z9M	O4-C4-C5	2.26	113.14	108.53
7	A	416	KDO	O5-C5-C6	2.27	115.26	109.89
7	A	415	Z9M	C1-C2-C3	2.27	112.85	109.21
10	C	415	KDO	C5-C4-C3	2.28	114.88	110.82
7	A	414	L1L	O8-P-O1	2.30	113.51	106.62
7	E	406	Z9M	P1-O4-C4	2.34	127.54	121.56
10	F	409	GMH	O5-C1-C2	2.36	114.13	110.00
10	C	413	L1L	O1-C1-C2	2.37	112.78	108.42
7	D	424	Z9M	O4-C4-C5	2.37	113.36	108.53
10	C	414	Z9M	O8-P1-O4	2.41	113.82	106.62
7	D	425	KDO	C3-C4-C5	2.41	113.76	110.54
7	E	405	L1L	O1-C1-C2	2.44	112.91	108.42
10	F	409	GMH	O5-C5-C4	2.44	112.40	108.22
7	D	413	Z9M	C1-O5-C5	2.50	115.81	112.14
7	D	423	L1L	O1-C1-C2	2.50	113.02	108.42
7	F	418	L1L	O8-P-O1	2.61	114.41	106.62
10	C	416	GMH	O1-C1-C2	2.62	116.30	109.05
7	E	407	KDO	C3-C4-C5	2.64	114.07	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	414	Z9M	C1-O5-C5	2.65	116.03	112.14
7	A	415	Z9M	O7-P1-O4	2.75	114.84	106.62
7	D	412	L1L	O1-C1-C2	2.82	113.60	108.42
12	C	428	KDO	O6-C2-C3	2.83	115.32	109.77
10	F	408	KDO	C6-O6-C2	2.88	117.94	112.17
7	D	423	L1L	O1-P-O2	2.90	114.40	107.48
10	C	413	L1L	O9-P-O1	3.17	116.09	106.62
10	F	407	Z9M	C1-O5-C5	3.22	116.87	112.14
7	F	419	Z9M	P1-O4-C4	3.29	129.99	121.56
12	C	425	L1L	O1-C1-C2	3.30	114.50	108.42
7	D	412	L1L	O9-P-O1	3.33	116.57	106.62
7	E	405	L1L	O9-P-O1	3.45	116.94	106.62
10	B	408	Z9M	P1-O4-C4	3.56	130.67	121.56
7	A	415	Z9M	P1-O4-C4	3.56	130.67	121.56
12	C	426	Z9M	P1-O4-C4	3.56	130.69	121.56
7	D	424	Z9M	P1-O4-C4	3.75	131.18	121.56
12	C	425	L1L	O8-P-O1	4.16	119.06	106.62
7	F	418	L1L	O1-C1-C2	4.46	116.62	108.42
7	D	412	L1L	O8-P-O1	4.48	120.00	106.62
7	D	414	KDO	C6-O6-C2	5.16	122.50	112.17
10	C	414	Z9M	P1-O4-C4	5.75	136.28	121.56
10	F	407	Z9M	P1-O4-C4	6.11	137.22	121.56
10	B	407	L1L	O8-P-O1	7.26	128.34	106.62
7	D	414	KDO	O6-C6-C5	9.61	117.80	109.75

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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
5	D	416	FTT	O2-C1-C2	-3.11	114.03	125.28
5	C	430	FTT	O2-C1-C2	-2.89	114.84	125.28
5	A	419	FTT	O2-C1-C2	-2.85	114.97	125.28
5	B	417	FTT	O2-C1-C2	-2.74	115.39	125.28
5	E	403	FTT	O2-C1-C2	-2.63	115.76	125.28
5	F	427	FTT	O2-C1-C2	-2.62	115.83	125.28
6	E	404	DAO	O1-C1-C2	-2.55	115.37	125.44
5	C	421	FTT	O2-C1-C2	-2.39	116.64	125.28
5	D	418	FTT	O2-C1-C2	-2.35	116.79	125.28
6	A	422	DAO	O1-C1-C2	-2.34	116.17	125.44
5	C	419	FTT	O2-C1-C2	-2.29	117.02	125.28
6	A	413	DAO	O1-C1-C2	-2.28	116.41	125.44
5	F	411	FTT	O2-C1-C2	-2.27	117.07	125.28
5	E	410	FTT	O2-C1-C2	-2.20	117.34	125.28
5	C	429	FTT	C11-C10-C9	-2.16	103.31	114.54
5	D	428	FTT	O2-C1-C2	-2.16	117.47	125.28
5	F	412	FTT	O2-C1-C2	-2.14	117.54	125.28
5	E	411	FTT	C10-C9-C8	-2.11	103.57	114.54
9	D	420	MYR	O1-C1-C2	-2.11	117.09	125.44
5	C	429	FTT	C7-C6-C5	-2.07	103.80	114.54
8	C	417	KDO	O8-C8-C7	-2.03	106.57	111.07
5	C	420	FTT	C3-C2-C1	2.06	115.71	111.90
5	E	403	FTT	O3-C3-C2	2.09	114.10	108.98
5	F	413	FTT	C3-C2-C1	2.16	115.91	111.90
5	B	413	FTT	C3-C2-C1	2.37	116.28	111.90
5	F	414	FTT	O3-C3-C2	2.37	114.78	108.98
8	F	410	KDO	O6-C2-C3	2.49	114.65	109.77
5	E	410	FTT	C3-C2-C1	2.61	116.74	111.90
8	A	417	KDO	O6-C2-C3	3.18	115.99	109.77
8	F	421	KDO	O6-C2-C3	3.46	116.56	109.77
8	C	417	KDO	O6-C2-C3	3.47	116.57	109.77
8	B	411	KDO	O6-C2-C3	3.48	116.58	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	426	KDO	O6-C2-C3	3.75	117.12	109.77
8	E	408	KDO	O6-C2-C3	3.96	117.53	109.77
5	C	434	FTT	O3-C3-C4	11.09	141.07	109.36

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
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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)

All (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
1	D	84	ASP	6.1
1	B	137	PHE	6.1
1	D	138	GLY	5.7
1	A	138	GLY	5.6
1	A	82	PHE	5.6
1	B	136	PHE	5.2
1	C	138	GLY	5.1
1	D	136	PHE	5.1
1	D	139	LEU	5.1
1	A	137	PHE	5.0
1	D	265	PHE	5.0
1	B	84	ASP	4.9
1	B	138	GLY	4.9
1	D	134	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	82	PHE	4.7
1	E	82	PHE	4.4
1	B	83	GLY	4.3
1	E	137	PHE	4.3
1	E	138	GLY	4.2
1	E	265	PHE	4.1
1	B	140	VAL	3.8
1	D	82	PHE	3.6
1	D	49	GLN	3.6
1	D	85	ALA	3.6
1	D	159	GLU	3.6
1	A	159	GLU	3.5
1	E	84	ASP	3.2
1	A	83	GLY	3.2
1	E	85	ALA	3.2
1	E	141	ASP	3.1
1	E	264	ASP	3.1
1	A	84	ASP	2.9
1	B	265	PHE	2.9
1	C	226	ASN	2.9
1	B	85	ALA	2.8
1	C	137	PHE	2.8
1	D	135	ASP	2.8
1	C	139	LEU	2.7
1	F	186	GLU	2.7
1	C	84	ASP	2.7
1	A	136	PHE	2.7
1	F	84	ASP	2.6
1	B	264[A]	ASP	2.6
1	A	264	ASP	2.6
1	C	82	PHE	2.6
1	D	261	TYR	2.5
1	B	49	GLN	2.5
1	D	86	GLY	2.5
1	A	265	PHE	2.5
1	E	140	VAL	2.5
1	E	83	GLY	2.4
1	E	136	PHE	2.4
1	B	86	GLY	2.4
1	A	141	ASP	2.4
1	D	140	VAL	2.3
1	F	136	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	141	ASP	2.3
1	D	264[A]	ASP	2.3
1	A	49	GLN	2.3
1	D	186	GLU	2.3
1	D	45	GLN	2.3
1	D	188	PHE	2.2
1	E	159	GLU	2.2
1	E	263	PHE	2.1
1	A	261	TYR	2.1
1	B	141	ASP	2.1
1	A	45	GLN	2.0
1	C	134	SER	2.0
1	D	226	ASN	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)

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, 95^{th} 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(Å^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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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, 95^{th} 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(Å^2)	Q<0.9
3	C8E	A	407	5/21	0.71	0.24	43.31	18,20,26,28	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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.