



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:45 AM GMT

PDB ID : 3FXI
Title : Crystal structure of the human TLR4-human MD-2-E.coli LPS Ra complex
Authors : Park, B.S.; Song, D.H.; Kim, H.M.; Lee, J.-O.
Deposited on : 2009-01-21
Resolution : 3.10 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

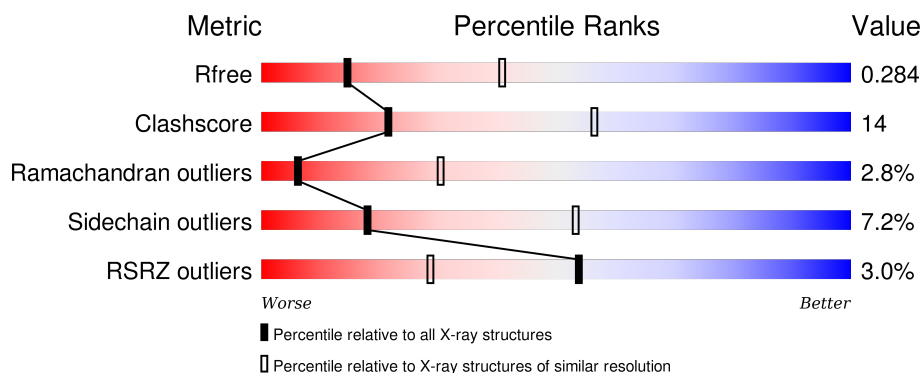
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	605	<div> <div>2%</div> <div>68% 26% 5%</div> </div>
1	B	605	<div> <div>5%</div> <div>68% 25% 5%</div> </div>
2	C	142	<div> <div>58% 34% 7%</div> </div>
2	D	142	<div> <div>% 61% 31% 7%</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	PA1	A	1001	X	-	-	-
4	FTT	A	1003	-	-	-	X
4	FTT	A	1004	-	-	-	X
4	FTT	A	1005	-	-	-	X
4	FTT	A	1006	-	-	-	X
4	FTT	B	1003	-	-	-	X
4	FTT	B	1004	-	-	-	X
4	FTT	B	1005	-	-	-	X
4	FTT	B	1006	-	-	-	X
5	DAO	A	1007	-	-	-	X
5	DAO	B	1007	-	-	-	X
6	MYR	A	1008	-	-	-	X
6	MYR	B	1008	-	-	-	X
9	NAG	A	761	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12500 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 Toll-like receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4803	3075	790	911	27			
1	B	601	Total	C	N	O	S	0	0	0
			4803	3075	790	911	27			

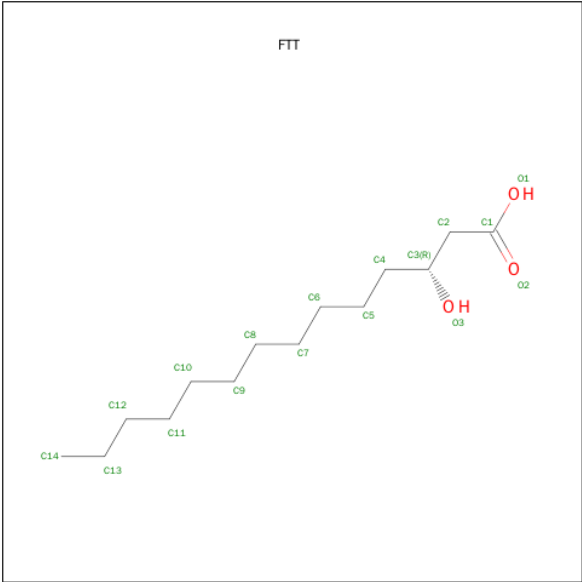
- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			
2	D	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			

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

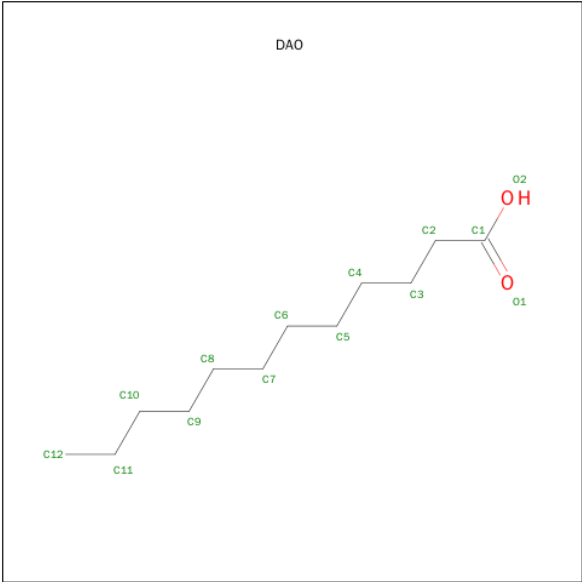
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			92	49	2	41		

- Molecule 4 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: C₁₄H₂₈O₃).



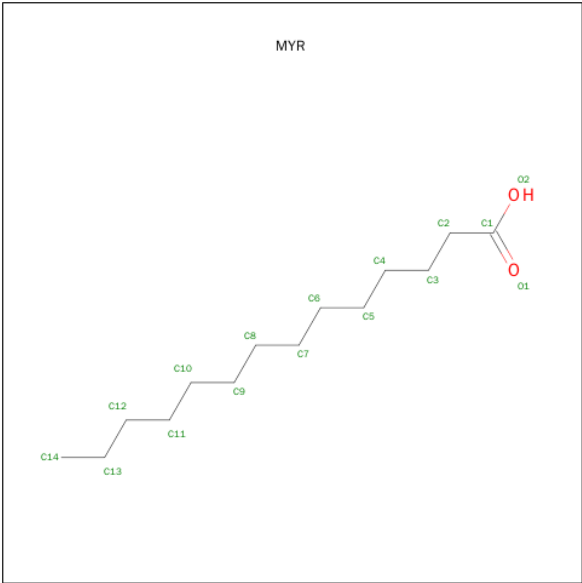
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			16	14	2		
4	B	1	Total	C	O	0	0
			16	14	2		
4	B	1	Total	C	O	0	0
			16	14	2		
4	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 5 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



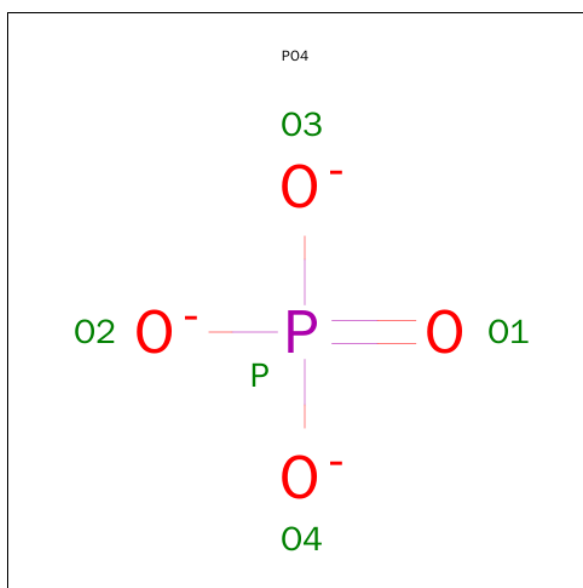
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	12	1		
5	B	1	Total	C	O	0	0
			13	12	1		

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



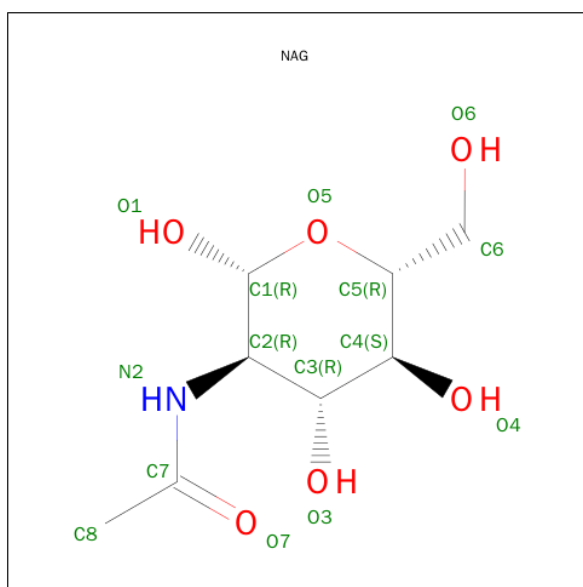
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	14	1		
6	B	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			4	3	1		
7	A	1	Total	O	P	0	0
			4	3	1		
7	A	1	Total	O	P	0	0
			4	3	1		
7	A	1	Total	O	P	0	0
			4	3	1		
7	B	1	Total	O	P	0	0
			4	3	1		
7	B	1	Total	O	P	0	0
			4	3	1		
7	B	1	Total	O	P	0	0
			4	3	1		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	2	Total	C	N	O	0	0
			28	16	2	10		
9	A	2	Total	C	N	O	0	0
			28	16	2	10		
9	B	2	Total	C	N	O	0	0
			28	16	2	10		
9	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Mg	0	0
			1	1		
10	A	1	Total	Mg	0	0
			1	1		

- Molecule 11 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	7	Total	C	N	O	0	0
			92	49	2	41		

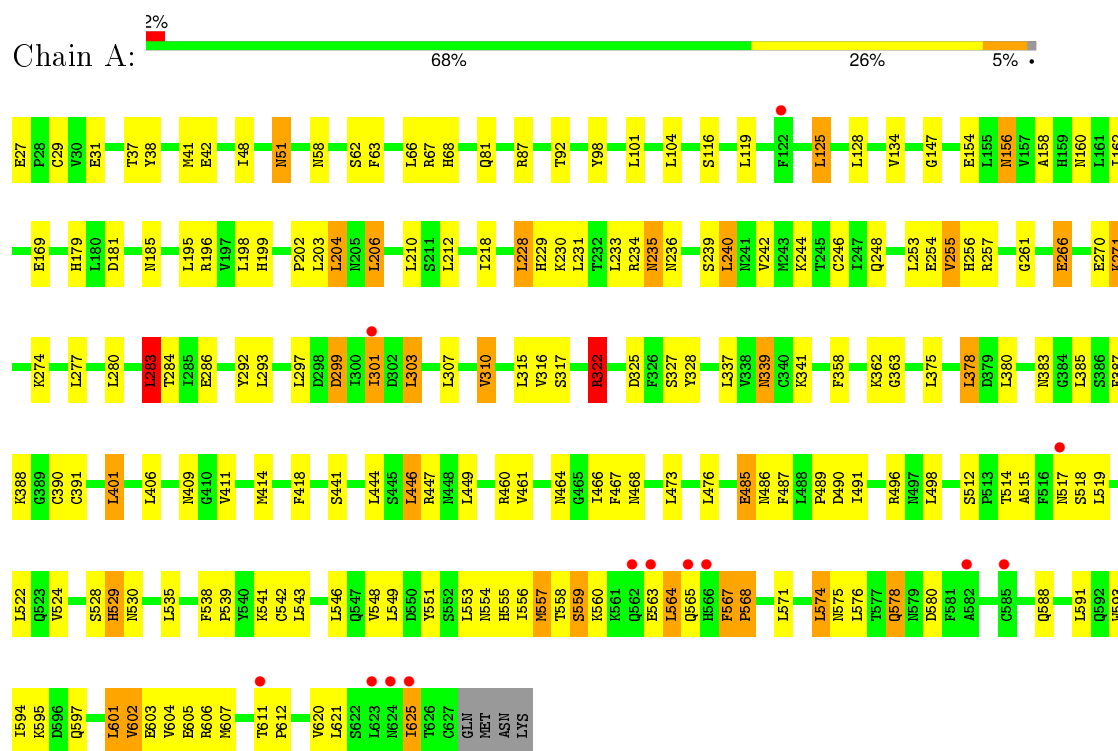
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	O	0	0
			1	1		
12	B	1	Total	O	0	0
			1	1		

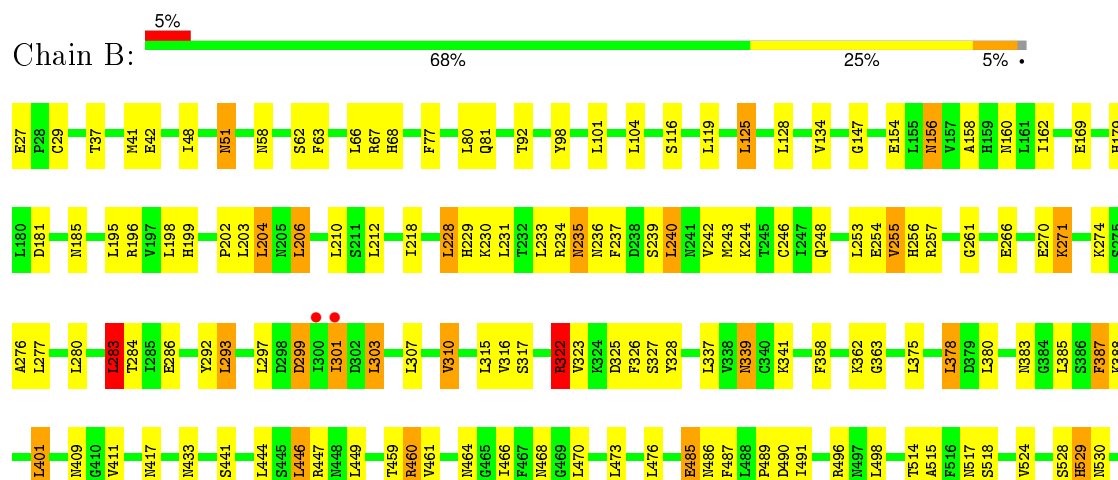
3 Residue-property plots

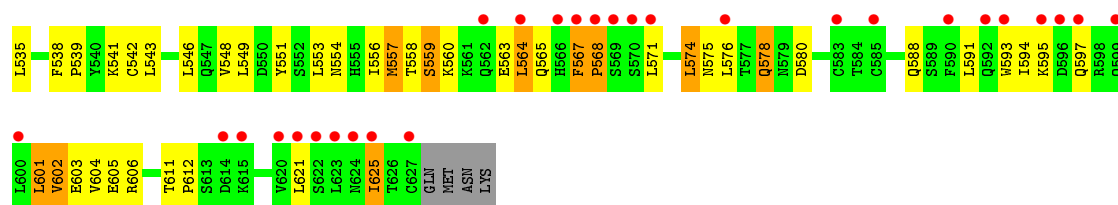
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Toll-like receptor 4



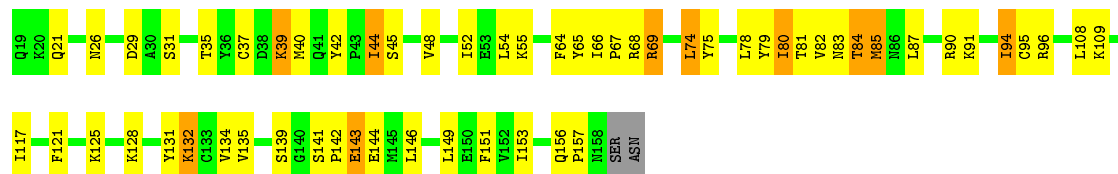
• Molecule 1: Toll-like receptor 4





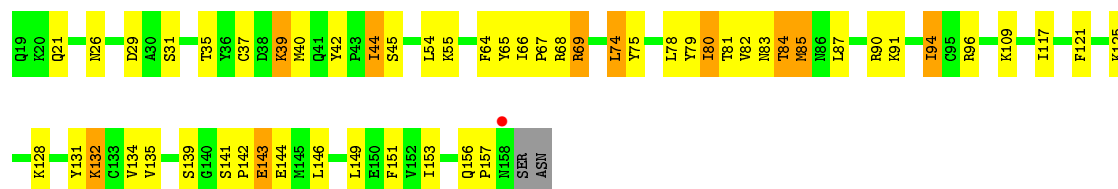
• Molecule 2: Lymphocyte antigen 96

Chain C: 58% 34% 7%



• Molecule 2: Lymphocyte antigen 96

Chain D: 61% 31% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.16Å 103.50Å 251.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.87 – 3.10 47.86 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.87-3.10) 93.9 (47.86-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.281 0.252 , 0.284	Depositor DCC
R_{free} test set	2068 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44108 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12500	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PA1, MG, GMH, NAG, PO4, MYR, DAO, GCS, KDO, FTT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/4903	0.70	4/6639 (0.1%)
1	B	0.45	0/4903	0.70	5/6639 (0.1%)
2	C	0.45	0/1159	0.75	1/1562 (0.1%)
2	D	0.47	0/1159	0.75	1/1562 (0.1%)
All	All	0.45	0/12124	0.71	11/16402 (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
3	A	1	0

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	CB-CA-C	-6.93	96.54	110.40
1	A	67	ARG	CB-CA-C	-6.91	96.57	110.40
1	B	68	HIS	N-CA-CB	6.24	121.84	110.60
1	A	68	HIS	N-CA-CB	6.12	121.61	110.60
1	B	66	LEU	CB-CA-C	5.80	121.21	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1001	PA1	C1

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4803	0	4743	130	0
1	B	4803	0	4743	128	0
2	C	1133	0	1129	48	0
2	D	1133	0	1129	45	0
3	A	92	0	68	0	0
4	A	64	0	106	5	0
4	B	64	0	106	4	0
5	A	13	0	23	1	0
5	B	13	0	23	1	0
6	A	15	0	27	0	0
6	B	15	0	27	0	0
7	A	16	0	0	0	0
7	B	16	0	0	0	0
8	A	42	0	39	1	0
8	B	42	0	39	0	0
8	C	14	0	13	1	0
8	D	14	0	13	0	0
9	A	56	0	50	2	0
9	B	56	0	50	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	92	0	68	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
All	All	12500	0	12396	351	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 14.

The worst 5 of 351 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:LEU:HD21	1:B:476:LEU:HD23	1.52	0.90
1:A:473:LEU:HD21	1:A:476:LEU:HD23	1.52	0.90
2:D:80:ILE:H	2:D:80:ILE:HD12	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:H	1:B:48:ILE:HD12	1.42	0.85
1:A:375:LEU:HD21	1:A:378:LEU:HG	1.58	0.84

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	599/605 (99%)	482 (80%)	98 (16%)	19 (3%)	5	26
1	B	599/605 (99%)	484 (81%)	96 (16%)	19 (3%)	5	26
2	C	138/142 (97%)	126 (91%)	10 (7%)	2 (1%)	14	48
2	D	138/142 (97%)	125 (91%)	11 (8%)	2 (1%)	14	48
All	All	1474/1494 (99%)	1217 (83%)	215 (15%)	42 (3%)	6	30

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	ALA
1	A	529	HIS
1	B	515	ALA
1	B	529	HIS
2	C	143	GLU

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	559/563 (99%)	525 (94%)	34 (6%)	23	59
1	B	559/563 (99%)	522 (93%)	37 (7%)	21	56
2	C	130/132 (98%)	116 (89%)	14 (11%)	8	30
2	D	130/132 (98%)	116 (89%)	14 (11%)	8	30
All	All	1378/1390 (99%)	1279 (93%)	99 (7%)	18	53

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	LYS
1	B	387	PHE
2	D	69	ARG
1	B	293	LEU
1	B	310	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	592	GLN
1	B	200	GLN
1	B	597	GLN
1	B	51	ASN
1	B	129	GLN

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](#)

22 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
3	PA1	A	1001	3,4,7	11,11,12	0.71	0	13,15,17	2.85	4 (30%)
3	PA1	A	1002	3,4,7	12,12,12	1.11	1 (8%)	15,17,17	2.25	6 (40%)
3	KDO	A	1012	3	12,15,16	1.40	2 (16%)	12,21,24	1.29	1 (8%)
3	KDO	A	1013	3	12,15,16	0.77	0	12,21,24	0.81	1 (8%)
3	GMH	A	1014	3,7	13,13,14	0.71	0	17,18,20	2.05	2 (11%)
3	GMH	A	1015	3,7	13,13,14	1.02	1 (7%)	17,18,20	2.28	3 (17%)
3	GMH	A	1016	3	13,13,14	0.85	1 (7%)	17,18,20	2.27	4 (23%)
9	NAG	A	731	1,9	14,14,15	0.79	0	15,19,21	0.84	1 (6%)
9	NAG	A	732	9	14,14,15	1.16	1 (7%)	15,19,21	0.99	1 (6%)
9	NAG	A	761	1,9	14,14,15	0.92	0	15,19,21	0.88	1 (6%)
9	NAG	A	762	9	14,14,15	0.89	1 (7%)	15,19,21	0.84	0
11	GCS	B	1001	11,4,7	11,11,12	0.73	0	13,15,17	2.80	4 (30%)
11	PA1	B	1002	11,4,7	12,12,12	0.94	1 (8%)	15,17,17	2.25	5 (33%)
11	KDO	B	1012	11	12,15,16	1.39	2 (16%)	12,21,24	1.27	1 (8%)
11	KDO	B	1013	11	12,15,16	0.84	1 (8%)	12,21,24	0.78	0
11	GMH	B	1014	11,7	13,13,14	0.76	0	17,18,20	2.09	2 (11%)
11	GMH	B	1015	11,7	13,13,14	0.96	0	17,18,20	2.31	4 (23%)
11	GMH	B	1016	11	13,13,14	0.77	0	17,18,20	2.30	5 (29%)
9	NAG	B	831	1,9	14,14,15	0.59	0	15,19,21	0.92	1 (6%)
9	NAG	B	832	9	14,14,15	0.70	0	15,19,21	1.05	2 (13%)
9	NAG	B	861	1,9	14,14,15	0.70	0	15,19,21	1.01	1 (6%)
9	NAG	B	862	9	14,14,15	0.78	0	15,19,21	0.84	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PA1	A	1001	3,4,7	1/1/4/5	0/2/19/22	0/1/1/1
3	PA1	A	1002	3,4,7	-	0/2/22/22	0/1/1/1
3	KDO	A	1012	3	-	0/6/26/30	0/1/1/1
3	KDO	A	1013	3	-	0/6/26/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GMH	A	1014	3,7	-	0/6/23/26	0/1/1/1
3	GMH	A	1015	3,7	-	0/6/23/26	0/1/1/1
3	GMH	A	1016	3	-	0/6/23/26	0/1/1/1
9	NAG	A	731	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	732	9	-	0/6/23/26	0/1/1/1
9	NAG	A	761	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	762	9	-	0/6/23/26	0/1/1/1
11	GCS	B	1001	11,4,7	-	0/2/19/22	0/1/1/1
11	PA1	B	1002	11,4,7	-	0/2/22/22	0/1/1/1
11	KDO	B	1012	11	-	0/6/26/30	0/1/1/1
11	KDO	B	1013	11	-	0/6/26/30	0/1/1/1
11	GMH	B	1014	11,7	-	0/6/23/26	0/1/1/1
11	GMH	B	1015	11,7	-	0/6/23/26	0/1/1/1
11	GMH	B	1016	11	-	0/6/23/26	0/1/1/1
9	NAG	B	831	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	832	9	-	1/6/23/26	0/1/1/1
9	NAG	B	861	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	862	9	-	0/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1015	GMH	O5-C5	2.02	1.45	1.43
11	B	1012	KDO	C5-C6	2.03	1.58	1.52
11	B	1013	KDO	C4-C5	2.06	1.55	1.52
3	A	1016	GMH	O5-C5	2.08	1.46	1.43
3	A	1012	KDO	C5-C6	2.09	1.58	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PA1	C4-C3-C2	-5.62	103.81	111.39
11	B	1001	GCS	C4-C3-C2	-5.42	104.07	111.39
3	A	1002	PA1	O5-C1-C2	-5.20	103.51	109.62
11	B	1002	PA1	O5-C1-C2	-5.19	103.51	109.62
11	B	1001	GCS	C1-C2-N2	-3.72	102.53	111.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1001	PA1	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	832	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	761	NAG	2	0
9	A	762	NAG	1	0
9	B	832	NAG	1	0
9	B	862	NAG	1	0

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\# Z > 2$
4	FTT	A	1003	3	14,15,16	0.53	0	15,15,17	1.12	2 (13%)
4	FTT	A	1004	3	14,15,16	0.36	0	15,15,17	2.78	4 (26%)
4	FTT	A	1005	3,5	14,15,16	0.47	0	15,15,17	1.70	4 (26%)
4	FTT	A	1006	3,6	14,15,16	0.48	0	15,15,17	1.69	2 (13%)
5	DAO	A	1007	4	12,12,13	0.39	0	10,11,13	1.59	2 (20%)
6	MYR	A	1008	4	14,14,15	0.36	0	12,13,15	1.02	1 (8%)
7	PO4	A	1010	3	0,3,4	0.00	-	0,3,6	0.00	-
7	PO4	A	1011	3	0,3,4	0.00	-	0,3,6	0.00	-
7	PO4	A	1017	3	0,3,4	0.00	-	0,3,6	0.00	-
7	PO4	A	1018	3	0,3,4	0.00	-	0,3,6	0.00	-
8	NAG	A	711	1	14,14,15	0.98	1 (7%)	15,19,21	0.73	0
8	NAG	A	721	1	14,14,15	0.76	0	15,19,21	1.00	1 (6%)
8	NAG	A	741	1	14,14,15	0.91	1 (7%)	15,19,21	0.67	0
4	FTT	B	1003	11	14,15,16	0.62	0	15,15,17	1.12	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FTT	B	1004	11	14,15,16	0.32	0	15,15,17	2.79	4 (26%)
4	FTT	B	1005	11,5	14,15,16	0.41	0	15,15,17	1.71	3 (20%)
4	FTT	B	1006	11,6	14,15,16	0.49	0	15,15,17	1.69	2 (13%)
5	DAO	B	1007	4	12,12,13	0.31	0	10,11,13	1.59	2 (20%)
6	MYR	B	1008	4	14,14,15	0.28	0	12,13,15	1.03	1 (8%)
7	PO4	B	1010	11	0,3,4	0.00	-	0,3,6	0.00	-
7	PO4	B	1011	11	0,3,4	0.00	-	0,3,6	0.00	-
7	PO4	B	1017	11	0,3,4	0.00	-	0,3,6	0.00	-
7	PO4	B	1018	11	0,3,4	0.00	-	0,3,6	0.00	-
8	NAG	B	811	1	14,14,15	0.85	1 (7%)	15,19,21	0.77	1 (6%)
8	NAG	B	821	1	14,14,15	0.79	0	15,19,21	0.74	0
8	NAG	B	841	1	14,14,15	0.71	0	15,19,21	1.01	1 (6%)
8	NAG	C	751	2	14,14,15	0.80	1 (7%)	15,19,21	0.93	1 (6%)
8	NAG	D	851	2	14,14,15	0.71	0	15,19,21	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FTT	A	1003	3	-	0/14/14/15	0/0/0/0
4	FTT	A	1004	3	-	0/14/14/15	0/0/0/0
4	FTT	A	1005	3,5	-	0/14/14/15	0/0/0/0
4	FTT	A	1006	3,6	-	0/14/14/15	0/0/0/0
5	DAO	A	1007	4	-	0/9/10/11	0/0/0/0
6	MYR	A	1008	4	-	0/11/12/13	0/0/0/0
7	PO4	A	1010	3	-	0/0/0/0	0/0/0/0
7	PO4	A	1011	3	-	0/0/0/0	0/0/0/0
7	PO4	A	1017	3	-	0/0/0/0	0/0/0/0
7	PO4	A	1018	3	-	0/0/0/0	0/0/0/0
8	NAG	A	711	1	-	0/6/23/26	0/1/1/1
8	NAG	A	721	1	-	0/6/23/26	0/1/1/1
8	NAG	A	741	1	-	0/6/23/26	0/1/1/1
4	FTT	B	1003	11	-	0/14/14/15	0/0/0/0
4	FTT	B	1004	11	-	0/14/14/15	0/0/0/0
4	FTT	B	1005	11,5	-	0/14/14/15	0/0/0/0
4	FTT	B	1006	11,6	-	0/14/14/15	0/0/0/0
5	DAO	B	1007	4	-	0/9/10/11	0/0/0/0
6	MYR	B	1008	4	-	0/11/12/13	0/0/0/0
7	PO4	B	1010	11	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PO4	B	1011	11	-	0/0/0/0	0/0/0/0
7	PO4	B	1017	11	-	0/0/0/0	0/0/0/0
7	PO4	B	1018	11	-	0/0/0/0	0/0/0/0
8	NAG	B	811	1	-	0/6/23/26	0/1/1/1
8	NAG	B	821	1	-	0/6/23/26	0/1/1/1
8	NAG	B	841	1	-	0/6/23/26	0/1/1/1
8	NAG	C	751	2	-	0/6/23/26	0/1/1/1
8	NAG	D	851	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	751	NAG	C1-C2	2.20	1.55	1.52
8	A	711	NAG	C1-C2	2.34	1.55	1.52
8	B	811	NAG	C1-C2	2.37	1.55	1.52
8	A	741	NAG	C1-C2	2.37	1.55	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1004	FTT	C10-C9-C8	-3.46	96.64	114.53
4	B	1004	FTT	C10-C9-C8	-3.43	96.82	114.53
5	A	1007	DAO	C10-C9-C8	-3.39	97.02	114.53
4	B	1006	FTT	O3-C3-C4	-3.37	99.67	109.29
5	B	1007	DAO	C10-C9-C8	-3.37	97.15	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	FTT	3	0
4	A	1005	FTT	1	0
4	A	1006	FTT	2	0
5	A	1007	DAO	1	0
8	A	741	NAG	1	0
4	B	1004	FTT	2	0
4	B	1005	FTT	1	0
4	B	1006	FTT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1007	DAO	1	0
8	C	751	NAG	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	601/605 (99%)	0.01	13 (2%) 65 42	39, 74, 157, 178	0
1	B	601/605 (99%)	0.06	30 (4%) 32 13	40, 74, 158, 178	0
2	C	140/142 (98%)	-0.26	0 100 100	52, 70, 93, 110	0
2	D	140/142 (98%)	-0.21	1 (0%) 89 78	52, 71, 93, 110	0
All	All	1482/1494 (99%)	-0.01	44 (2%) 54 29	39, 73, 152, 178	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	614	ASP	4.8
1	A	563	GLU	4.5
1	A	582	ALA	4.4
1	A	562	GLN	4.4
1	B	569	SER	3.8

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
9	NAG	A	761	14/15	0.86	0.42	2.48	108,110,113,115	0
9	NAG	A	731	14/15	0.94	0.23	0.29	75,77,82,84	0
9	NAG	B	861	14/15	0.84	0.29	-0.14	102,107,111,113	0
9	NAG	B	831	14/15	0.95	0.19	-1.08	78,80,84,86	0
3	GMH	A	1014	13/14	0.89	0.25	-	116,123,127,127	0
11	KDO	B	1013	15/16	0.86	0.27	-	109,110,112,112	0
3	KDO	A	1013	15/16	0.85	0.26	-	109,110,112,113	0
11	GMH	B	1014	13/14	0.90	0.24	-	116,123,126,127	0
9	NAG	A	732	14/15	0.80	0.19	-	83,85,87,87	0
3	GMH	A	1015	13/14	0.77	0.24	-	128,130,131,131	0
3	PA1	A	1001	11/12	0.96	0.22	-	67,69,78,87	0
11	GMH	B	1015	13/14	0.72	0.32	-	128,130,131,131	0
9	NAG	B	832	14/15	0.87	0.19	-	91,95,99,99	0
3	PA1	A	1002	12/12	0.95	0.18	-	69,78,82,84	0
3	KDO	A	1012	15/16	0.92	0.22	-	93,96,104,107	0
11	GCS	B	1001	11/12	0.95	0.20	-	67,70,79,88	0
11	GMH	B	1016	13/14	0.82	0.29	-	132,133,134,134	0
9	NAG	A	762	14/15	0.77	0.27	-	116,118,118,119	0
11	KDO	B	1012	15/16	0.91	0.22	-	94,97,105,107	0
9	NAG	B	862	14/15	0.78	0.35	-	109,111,111,112	0
11	PA1	B	1002	12/12	0.98	0.20	-	71,77,81,83	0
3	GMH	A	1016	13/14	0.80	0.30	-	132,133,134,134	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
5	DAO	B	1007	13/14	0.84	0.54	13.48	70,71,76,77	0
4	FTT	B	1004	16/17	0.87	0.51	9.17	75,77,84,85	0
6	MYR	A	1008	15/16	0.93	0.59	8.03	66,74,79,79	0
4	FTT	A	1003	16/17	0.81	0.53	7.64	86,95,110,110	0
6	MYR	B	1008	15/16	0.89	0.41	6.86	65,73,78,78	0
4	FTT	B	1003	16/17	0.76	0.56	6.84	85,93,111,111	0
4	FTT	B	1005	16/17	0.93	0.36	5.97	68,70,81,83	0
4	FTT	A	1004	16/17	0.86	0.56	5.93	77,78,83,84	0
5	DAO	A	1007	13/14	0.90	0.47	4.47	70,72,75,76	0
4	FTT	A	1006	16/17	0.93	0.36	4.24	55,59,69,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	FTT	A	1005	16/17	0.90	0.43	4.21	68,70,81,83	0
4	FTT	B	1006	16/17	0.94	0.30	3.36	56,61,68,72	0
8	NAG	B	811	14/15	0.74	0.23	-	108,109,111,111	0
10	MG	B	2001	1/1	0.36	0.59	-	83,83,83,83	0
8	NAG	A	721	14/15	0.78	0.29	-	98,101,103,103	0
7	PO4	A	1018	4/5	0.88	0.34	-	126,126,126,127	0
8	NAG	B	841	14/15	0.90	0.13	-	87,89,91,91	0
7	PO4	A	1011	4/5	0.96	0.20	-	81,82,82,84	0
7	PO4	B	1011	4/5	0.97	0.24	-	81,82,83,83	0
7	PO4	B	1010	4/5	0.96	0.22	-	69,69,69,73	0
8	NAG	C	751	14/15	0.81	0.27	-	91,95,96,96	0
10	MG	A	2001	1/1	0.82	0.66	-	72,72,72,72	0
7	PO4	A	1010	4/5	0.99	0.24	-	66,66,67,68	0
8	NAG	A	711	14/15	0.72	0.18	-	111,113,114,115	0
8	NAG	A	741	14/15	0.78	0.21	-	99,102,103,104	0
8	NAG	D	851	14/15	0.84	0.22	-	84,90,93,94	0
7	PO4	B	1017	4/5	0.93	0.33	-	129,129,130,130	0
7	PO4	B	1018	4/5	0.90	0.41	-	125,125,126,126	0
7	PO4	A	1017	4/5	0.87	0.39	-	129,130,131,131	0
8	NAG	B	821	14/15	0.82	0.22	-	92,95,98,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.