



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2016 – 03:20 PM EDT

PDB ID : 5IJJ
Title : The crystal structure of mouse TLR4/MD-2/lipid A complex
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Deposited on : 2016-03-01
Resolution : 2.70 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-20027257
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-20027257

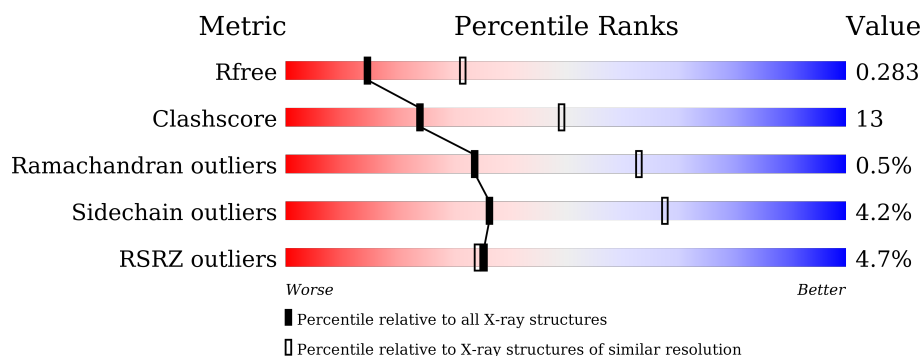
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	594	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>29%</div> <div>..</div> </div> </div>
1	B	594	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
2	C	150	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>.</div> <div>9%</div> </div> </div>
2	D	150	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>.</div> <div>9%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	702	X	-	-	-
3	NAG	A	704	-	-	-	X
3	NAG	B	703	X	-	-	X
3	NAG	B	704	X	-	-	-
3	NAG	B	705	X	-	-	-
3	NAG	B	707	X	-	-	-
3	NAG	C	202	X	-	-	-
3	NAG	D	802	X	-	-	-
6	DAO	C	206	-	-	-	X
7	MYR	C	207	-	-	-	X
7	MYR	D	807	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12385 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, Variable lymphocyte receptor B chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	1	0
			4708	3011	784	889	24			
1	B	592	Total	C	N	O	S	0	0	0
			4713	3014	783	891	25			

- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	137	Total	C	N	O	S	0	0	0
			1112	718	188	199	7			
2	D	137	Total	C	N	O	S	0	0	0
			1112	718	188	199	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	161	LYS	-	cloning artifact	UNP Q9JHF9
C	162	GLY	-	cloning artifact	UNP Q9JHF9
C	163	GLU	-	cloning artifact	UNP Q9JHF9
C	164	ASN	-	cloning artifact	UNP Q9JHF9
C	165	LEU	-	cloning artifact	UNP Q9JHF9
C	166	TYR	-	cloning artifact	UNP Q9JHF9
C	167	PHE	-	cloning artifact	UNP Q9JHF9
C	168	GLN	-	cloning artifact	UNP Q9JHF9
D	161	LYS	-	cloning artifact	UNP Q9JHF9
D	162	GLY	-	cloning artifact	UNP Q9JHF9
D	163	GLU	-	cloning artifact	UNP Q9JHF9
D	164	ASN	-	cloning artifact	UNP Q9JHF9
D	165	LEU	-	cloning artifact	UNP Q9JHF9
D	166	TYR	-	cloning artifact	UNP Q9JHF9
D	167	PHE	-	cloning artifact	UNP Q9JHF9
D	168	GLN	-	cloning artifact	UNP Q9JHF9

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



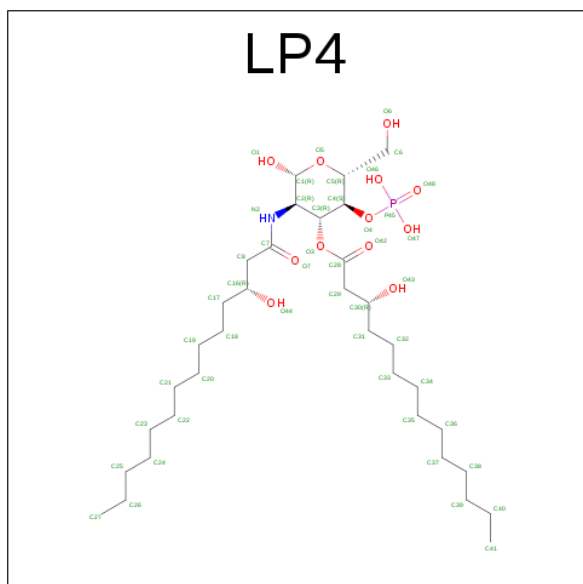
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

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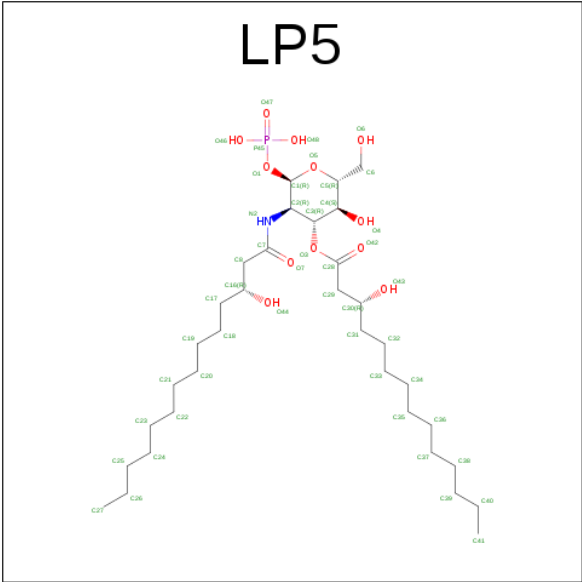
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-deoxy-3-O-[(3R)-3-hydroxytetradecanoyl]-2-[[[(3R)-3-hydroxytetradecanoyl]amino]-4-O-phosphono-beta-D-glucopyranose (three-letter code: LP4) (formula: C₃₄H₆₆NO₁₂P).



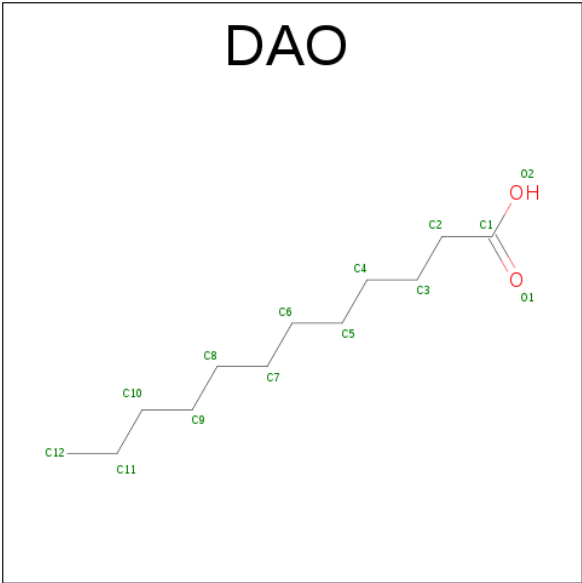
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			45	32	1	11	1		
4	D	1	Total	C	N	O	P	0	0
			45	32	1	11	1		

- Molecule 5 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOXY)TETRAHYDRO-2H-PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (three-letter code: LP5) (formula: C₃₄H₆₆NO₁₂P).



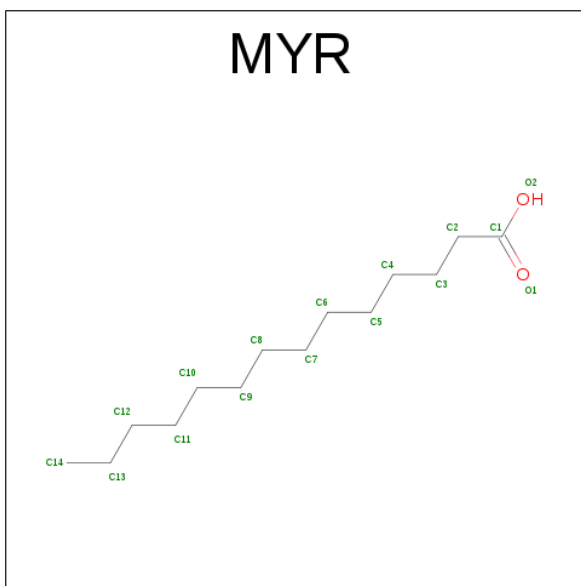
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			48	34	1	12	1		
5	D	1	Total	C	N	O	P	0	0
			48	34	1	12	1		

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	12	1		
6	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			15	14	1		
7	D	1	Total	C	O	0	0
			15	14	1		

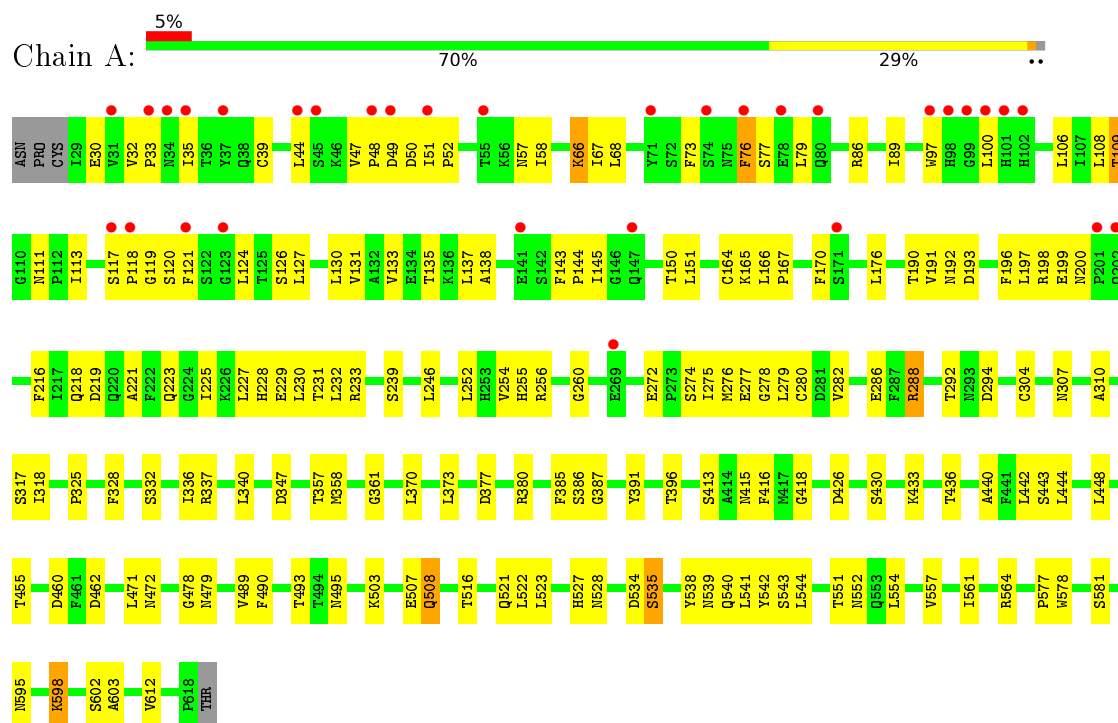
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	92	Total	O	0	0
			92	92		
8	C	29	Total	O	0	0
			29	29		
8	D	22	Total	O	0	0
			22	22		
8	B	89	Total	O	0	0
			89	89		

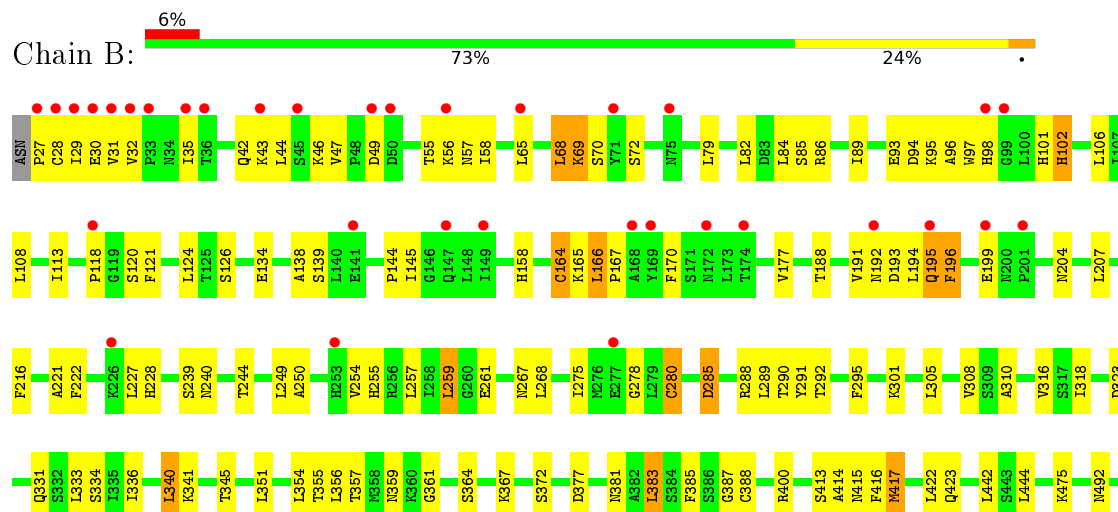
3 Residue-property plots

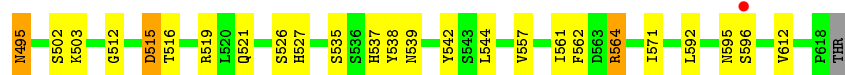
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

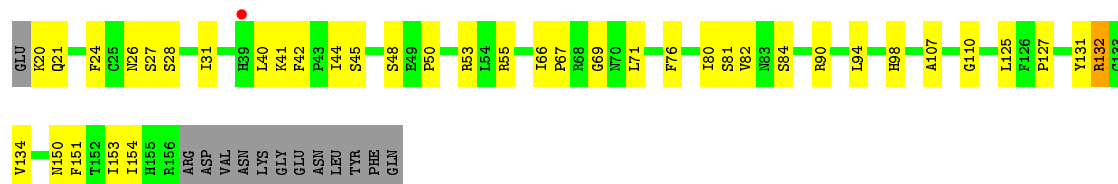


- Molecule 1: Toll-like receptor 4, Variable lymphocyte receptor B chimera

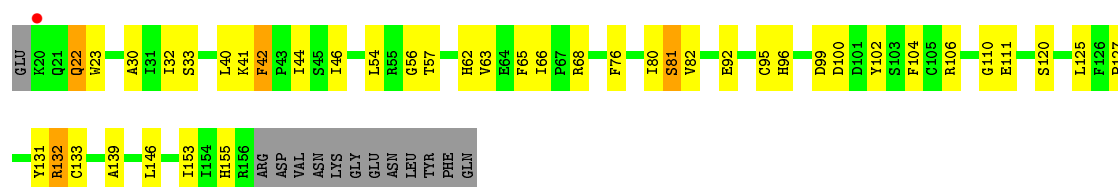




• Molecule 2: Lymphocyte antigen 96



• Molecule 2: Lymphocyte antigen 96



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.84Å 145.74Å 136.19Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	39.34 – 2.70 39.31 – 2.69	Depositor EDS
% Data completeness (in resolution range)	77.2 (39.34-2.70) 77.2 (39.31-2.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.215 , 0.285 0.217 , 0.283	Depositor DCC
R_{free} test set	1978 reflections (3.74%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12385	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LP4, LP5, MYR, NAG, DAO

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	0.67	0/4811	0.81	3/6519 (0.0%)
1	B	0.63	0/4814	0.81	3/6524 (0.0%)
2	C	0.69	0/1143	0.85	0/1544
2	D	0.69	0/1143	0.83	0/1544
All	All	0.66	0/11911	0.82	6/16131 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
2	C	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	VAL	N-CA-C	-8.56	87.90	111.00
1	A	288	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	426	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	383	LEU	CA-CB-CG	5.40	127.72	115.30
1	B	31	VAL	N-CA-C	5.36	125.47	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLY	Peptide
1	A	361	GLY	Peptide
1	B	361	GLY	Peptide
2	C	132	ARG	Sidechain

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	4708	0	4698	136	2
1	B	4713	0	4694	115	2
2	C	1112	0	1075	28	0
2	D	1112	0	1075	34	0
3	A	84	0	76	4	0
3	B	98	0	88	2	0
3	C	42	0	38	3	0
3	D	42	0	38	0	0
4	C	45	0	53	0	0
4	D	45	0	53	1	0
5	C	48	0	63	2	0
5	D	48	0	63	1	0
6	C	13	0	23	0	0
6	D	13	0	23	0	0
7	C	15	0	27	1	0
7	D	15	0	27	2	0
8	A	92	0	0	5	0
8	B	89	0	0	5	0
8	C	29	0	0	0	0
8	D	22	0	0	3	0
All	All	12385	0	12114	316	2

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 13.

The worst 5 of 316 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)
4:D:804:LP4:C1	5:D:805:LP5:O6	1.64	1.44
1:A:280:CYS:HG	1:A:304:CYS:HG	1.03	0.90
1:A:117:SER:O	1:A:119:GLY:N	2.04	0.90
1:A:191:VAL:HG12	1:A:221:ALA:HA	1.55	0.85
1:B:261:GLU:OE2	1:B:267:ASN:HB3	1.77	0.83

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ARG:NH1	1:B:542:TYR:CD1[1_655]	2.15	0.05
1:A:540:GLN:O	1:B:519:ARG:NH2[1_655]	2.18	0.02

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	589/594 (99%)	516 (88%)	72 (12%)	1 (0%)	52	80
1	B	590/594 (99%)	521 (88%)	64 (11%)	5 (1%)	24	51
2	C	135/150 (90%)	119 (88%)	16 (12%)	0	100	100
2	D	135/150 (90%)	114 (84%)	20 (15%)	1 (1%)	26	55
All	All	1449/1488 (97%)	1270 (88%)	172 (12%)	7 (0%)	34	63

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	PHE
1	B	195	GLN
1	A	118	PRO
1	B	515	ASP
1	B	93	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	548/551 (100%)	529 (96%)	19 (4%)	43	74
1	B	549/551 (100%)	522 (95%)	27 (5%)	31	61
2	C	124/136 (91%)	120 (97%)	4 (3%)	46	77
2	D	124/136 (91%)	118 (95%)	6 (5%)	31	62
All	All	1345/1374 (98%)	1289 (96%)	56 (4%)	36	68

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	81	SER
1	B	68	LEU
1	B	388	CYS
2	D	106	ARG
2	D	132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	21	GLN
2	C	98	HIS
2	C	130	HIS
1	B	57	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

19 non-standard protein/DNA/RNA residues 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	NAG	A	701	1,3	14,14,15	0.54	0	15,19,21	1.35	2 (13%)
3	NAG	A	702	3	14,14,15	0.47	0	15,19,21	1.61	3 (20%)
3	NAG	A	703	1	14,14,15	0.56	0	15,19,21	2.27	6 (40%)
3	NAG	A	704	1	14,14,15	0.69	0	15,19,21	2.13	5 (33%)
3	NAG	A	705	1,3	14,14,15	0.68	0	15,19,21	2.02	4 (26%)
3	NAG	A	706	3	14,14,15	0.59	0	15,19,21	1.09	1 (6%)
3	NAG	B	701	1,3	14,14,15	0.51	0	15,19,21	2.07	4 (26%)
3	NAG	B	702	3	14,14,15	0.75	1 (7%)	15,19,21	1.57	3 (20%)
3	NAG	B	703	1,3	14,14,15	0.77	0	15,19,21	1.92	4 (26%)
3	NAG	B	704	3	14,14,15	0.76	0	15,19,21	1.53	3 (20%)
3	NAG	B	705	1	14,14,15	1.27	3 (21%)	15,19,21	1.88	2 (13%)
3	NAG	B	706	1,3	14,14,15	0.93	1 (7%)	15,19,21	1.98	5 (33%)
3	NAG	B	707	3	14,14,15	0.70	0	15,19,21	1.51	3 (20%)
3	NAG	C	201	2	14,14,15	0.64	0	15,19,21	1.45	2 (13%)
3	NAG	C	202	3,2	14,14,15	0.69	0	15,19,21	2.13	5 (33%)
3	NAG	C	203	3	14,14,15	0.55	0	15,19,21	1.58	3 (20%)
3	NAG	D	801	3,2	14,14,15	0.74	0	15,19,21	2.91	6 (40%)
3	NAG	D	802	3	14,14,15	0.85	1 (7%)	15,19,21	1.72	2 (13%)
3	NAG	D	803	2	14,14,15	0.91	0	15,19,21	2.72	5 (33%)

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	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	704	1	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	706	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	704	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	705	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	706	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	707	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	201	2	-	0/6/23/26	0/1/1/1
3	NAG	C	202	3,2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	203	3	-	0/6/23/26	0/1/1/1
3	NAG	D	801	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	802	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	803	2	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	705	NAG	O5-C1	-2.27	1.40	1.43
3	D	802	NAG	C1-C2	2.18	1.55	1.52
3	B	702	NAG	C1-C2	2.28	1.55	1.52
3	B	705	NAG	C3-C2	2.39	1.57	1.52
3	B	706	NAG	C1-C2	2.76	1.56	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	NAG	C4-C3-C2	-5.74	102.42	111.34
3	B	705	NAG	O5-C5-C4	-4.81	102.17	110.13
3	A	704	NAG	C4-C3-C2	-4.39	104.53	111.34
3	D	802	NAG	O5-C5-C4	-4.31	103.00	110.13
3	A	702	NAG	C4-C3-C2	-4.16	104.88	111.34

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	702	NAG	C1
3	B	704	NAG	C1
3	B	705	NAG	C1
3	C	202	NAG	C1
3	D	802	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	1	0
3	A	704	NAG	3	0
3	B	705	NAG	1	0
3	B	706	NAG	1	0
3	C	202	NAG	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	701	1,3	14,14,15	0.54	0	15,19,21	1.35	2 (13%)
3	NAG	A	702	3	14,14,15	0.47	0	15,19,21	1.61	3 (20%)
3	NAG	A	703	1	14,14,15	0.56	0	15,19,21	2.27	6 (40%)
3	NAG	A	704	1	14,14,15	0.69	0	15,19,21	2.13	5 (33%)
3	NAG	A	705	1,3	14,14,15	0.68	0	15,19,21	2.02	4 (26%)
3	NAG	A	706	3	14,14,15	0.59	0	15,19,21	1.09	1 (6%)
3	NAG	B	701	1,3	14,14,15	0.51	0	15,19,21	2.07	4 (26%)
3	NAG	B	702	3	14,14,15	0.75	1 (7%)	15,19,21	1.57	3 (20%)
3	NAG	B	703	1,3	14,14,15	0.77	0	15,19,21	1.92	4 (26%)
3	NAG	B	704	3	14,14,15	0.76	0	15,19,21	1.53	3 (20%)
3	NAG	B	705	1	14,14,15	1.27	3 (21%)	15,19,21	1.88	2 (13%)
3	NAG	B	706	1,3	14,14,15	0.93	1 (7%)	15,19,21	1.98	5 (33%)
3	NAG	B	707	3	14,14,15	0.70	0	15,19,21	1.51	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	201	2	14,14,15	0.64	0	15,19,21	1.45	2 (13%)
3	NAG	C	202	3,2	14,14,15	0.69	0	15,19,21	2.13	5 (33%)
3	NAG	C	203	3	14,14,15	0.55	0	15,19,21	1.58	3 (20%)
4	LP4	C	204	-	44,45,48	0.77	2 (4%)	51,56,60	1.52	10 (19%)
5	LP5	C	205	-	47,48,48	0.73	2 (4%)	57,60,60	1.25	5 (8%)
6	DAO	C	206	-	12,12,13	0.50	0	11,11,13	1.14	1 (9%)
7	MYR	C	207	-	14,14,15	0.41	0	13,13,15	1.09	1 (7%)
3	NAG	D	801	3,2	14,14,15	0.74	0	15,19,21	2.91	6 (40%)
3	NAG	D	802	3	14,14,15	0.85	1 (7%)	15,19,21	1.72	2 (13%)
3	NAG	D	803	2	14,14,15	0.91	0	15,19,21	2.72	5 (33%)
4	LP4	D	804	-	44,45,48	0.85	2 (4%)	51,56,60	1.46	6 (11%)
5	LP5	D	805	-	47,48,48	0.71	2 (4%)	57,60,60	1.30	7 (12%)
6	DAO	D	806	-	12,12,13	0.53	0	11,11,13	0.71	0
7	MYR	D	807	-	14,14,15	0.36	0	13,13,15	1.28	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
3	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	704	1	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	706	3	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	704	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	705	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	706	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	707	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	201	2	-	0/6/23/26	0/1/1/1
3	NAG	C	202	3,2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	203	3	-	0/6/23/26	0/1/1/1
4	LP4	C	204	-	-	0/43/60/65	0/1/1/1
5	LP5	C	205	-	-	0/44/65/65	0/1/1/1
6	DAO	C	206	-	-	0/9/10/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MYR	C	207	-	-	0/11/12/13	0/0/0/0
3	NAG	D	801	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	802	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	803	2	-	0/6/23/26	0/1/1/1
4	LP4	D	804	-	-	0/43/60/65	0/1/1/1
5	LP5	D	805	-	-	0/44/65/65	0/1/1/1
6	DAO	D	806	-	-	0/9/10/11	0/0/0/0
7	MYR	D	807	-	-	0/11/12/13	0/0/0/0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	205	LP5	O3-C3	-2.66	1.40	1.44
4	D	804	LP4	O3-C3	-2.51	1.41	1.44
3	B	705	NAG	O5-C1	-2.27	1.40	1.43
5	D	805	LP5	O3-C3	-2.23	1.41	1.44
4	C	204	LP4	O3-C3	-2.22	1.41	1.44

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	NAG	C4-C3-C2	-5.74	102.42	111.34
3	B	705	NAG	O5-C5-C4	-4.81	102.17	110.13
3	A	704	NAG	C4-C3-C2	-4.39	104.53	111.34
3	D	802	NAG	O5-C5-C4	-4.31	103.00	110.13
3	A	702	NAG	C4-C3-C2	-4.16	104.88	111.34

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	702	NAG	C1
3	D	802	NAG	C1
3	B	704	NAG	C1
3	B	705	NAG	C1
3	C	202	NAG	C1

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	1	0
3	A	704	NAG	3	0
3	B	705	NAG	1	0
3	B	706	NAG	1	0
3	C	202	NAG	3	0
5	C	205	LP5	2	0
7	C	207	MYR	1	0
4	D	804	LP4	1	0
5	D	805	LP5	1	0
7	D	807	MYR	2	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	590/594 (99%)	-0.05	32 (5%) 29 28	9, 33, 95, 142	0
1	B	592/594 (99%)	0.09	35 (5%) 26 24	10, 43, 99, 132	0
2	C	137/150 (91%)	-0.27	1 (0%) 89 90	20, 35, 55, 76	0
2	D	137/150 (91%)	-0.14	1 (0%) 89 90	23, 42, 65, 79	0
All	All	1456/1488 (97%)	-0.02	69 (4%) 35 34	9, 37, 95, 142	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	GLU	5.6
1	B	29	ILE	4.9
1	A	33	PRO	4.9
1	B	32	VAL	4.4
1	B	33	PRO	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
3	NAG	B	703	14/15	0.78	0.39	5.93	98,106,115,118	0
3	NAG	A	704	14/15	0.85	0.27	3.74	66,72,77,78	0
3	NAG	D	801	14/15	0.92	0.20	0.34	47,52,59,70	0
3	NAG	B	706	14/15	0.96	0.14	0.28	24,27,33,37	0
3	NAG	A	705	14/15	0.96	0.14	0.20	26,30,33,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	202	14/15	0.89	0.16	-0.49	45,48,53,62	0
3	NAG	C	201	14/15	0.87	0.34	-	66,74,83,92	0
3	NAG	B	704	14/15	0.65	0.34	-	95,108,117,122	0
3	NAG	B	702	14/15	0.83	0.31	-	70,82,103,104	0
3	NAG	C	203	14/15	0.91	0.35	-	65,74,85,87	0
3	NAG	A	701	14/15	0.87	0.20	-	59,65,74,75	0
3	NAG	B	701	14/15	0.87	0.31	-	84,88,91,94	0
3	NAG	D	803	14/15	0.84	0.21	-	68,74,77,77	0
3	NAG	D	802	14/15	0.87	0.44	-	78,86,88,90	0
3	NAG	A	703	14/15	0.74	0.27	-	52,76,83,84	0
3	NAG	B	705	14/15	0.76	0.20	-	67,75,83,85	0
3	NAG	A	706	14/15	0.86	0.25	-	39,52,57,60	0
3	NAG	B	707	14/15	0.88	0.26	-	42,48,52,56	0
3	NAG	A	702	14/15	0.88	0.22	-	64,76,82,86	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
7	MYR	C	207	15/16	0.85	0.36	7.32	52,62,77,89	0
6	DAO	C	206	13/14	0.85	0.29	7.05	39,44,59,65	0
3	NAG	B	703	14/15	0.78	0.39	5.93	98,106,115,118	0
7	MYR	D	807	15/16	0.84	0.34	5.03	46,50,65,66	0
3	NAG	A	704	14/15	0.85	0.27	3.74	66,72,77,78	0
6	DAO	D	806	13/14	0.92	0.18	1.36	45,51,63,69	0
4	LP4	C	204	45/48	0.94	0.16	0.86	28,37,52,56	0
4	LP4	D	804	45/48	0.93	0.17	0.34	35,50,59,68	0
3	NAG	D	801	14/15	0.92	0.20	0.34	47,52,59,70	0
5	LP5	D	805	48/48	0.94	0.16	0.28	31,45,63,67	0
3	NAG	B	706	14/15	0.96	0.14	0.28	24,27,33,37	0
3	NAG	A	705	14/15	0.96	0.14	0.20	26,30,33,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	LP5	C	205	48/48	0.94	0.15	0.16	38,46,56,61	0
3	NAG	C	202	14/15	0.89	0.16	-0.49	45,48,53,62	0
3	NAG	A	706	14/15	0.86	0.25	-	39,52,57,60	0
3	NAG	B	701	14/15	0.87	0.31	-	84,88,91,94	0
3	NAG	A	703	14/15	0.74	0.27	-	52,76,83,84	0
3	NAG	D	802	14/15	0.87	0.44	-	78,86,88,90	0
3	NAG	A	702	14/15	0.88	0.22	-	64,76,82,86	0
3	NAG	B	704	14/15	0.65	0.34	-	95,108,117,122	0
3	NAG	B	705	14/15	0.76	0.20	-	67,75,83,85	0
3	NAG	C	201	14/15	0.87	0.34	-	66,74,83,92	0
3	NAG	D	803	14/15	0.84	0.21	-	68,74,77,77	0
3	NAG	C	203	14/15	0.91	0.35	-	65,74,85,87	0
3	NAG	A	701	14/15	0.87	0.20	-	59,65,74,75	0
3	NAG	B	702	14/15	0.83	0.31	-	70,82,103,104	0
3	NAG	B	707	14/15	0.88	0.26	-	42,48,52,56	0

6.5 Other polymers

There are no such residues in this entry.