



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:49 PM GMT

PDB ID : 4G8A  
Title : Crystal structure of human TLR4 polymorphic variant D299G and T399I in complex with MD-2 and LPS  
Authors : Ohto, U.; Shimizu, T.  
Deposited on : 2012-07-23  
Resolution : 2.40 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](mailto: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.

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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

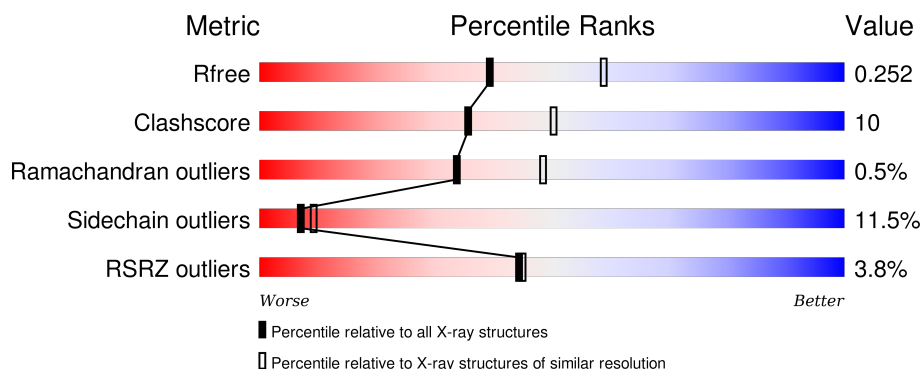
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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  $\geq 3$ , 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	635	<div> <div>4%</div> <div>69% 21% 5% 5%</div> </div>
1	B	635	<div> <div>3%</div> <div>68% 23% 5%</div> </div>
2	C	144	<div> <div>6%</div> <div>68% 27% . .</div> </div>
2	D	144	<div> <div>4%</div> <div>63% 30% . . .</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
7	DAO	C	204	-	-	-	X
7	DAO	D	204	-	-	-	X
8	MYR	C	205	-	-	-	X
8	MYR	D	205	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12381 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
			4800	3075	790	908	27			
1	B	605	Total	C	N	O	S	0	0	0
			4836	3099	795	915	27			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ARG	-	EXPRESSION TAG	UNP O00206
A	4	SER	-	EXPRESSION TAG	UNP O00206
A	5	PRO	-	EXPRESSION TAG	UNP O00206
A	6	TRP	-	EXPRESSION TAG	UNP O00206
A	7	ASP	-	EXPRESSION TAG	UNP O00206
A	8	TYR	-	EXPRESSION TAG	UNP O00206
A	9	LYS	-	EXPRESSION TAG	UNP O00206
A	10	ASP	-	EXPRESSION TAG	UNP O00206
A	11	ASP	-	EXPRESSION TAG	UNP O00206
A	12	ASP	-	EXPRESSION TAG	UNP O00206
A	13	ASP	-	EXPRESSION TAG	UNP O00206
A	14	LYS	-	EXPRESSION TAG	UNP O00206
A	15	LEU	-	EXPRESSION TAG	UNP O00206
A	16	ALA	-	EXPRESSION TAG	UNP O00206
A	17	ALA	-	EXPRESSION TAG	UNP O00206
A	18	ALA	-	EXPRESSION TAG	UNP O00206
A	19	ASN	-	EXPRESSION TAG	UNP O00206
A	20	SER	-	EXPRESSION TAG	UNP O00206
A	21	SER	-	EXPRESSION TAG	UNP O00206
A	22	ILE	-	EXPRESSION TAG	UNP O00206
A	299	GLY	ASP	ENGINEERED MUTATION	UNP O00206
A	399	ILE	THR	ENGINEERED MUTATION	UNP O00206
A	630	THR	-	EXPRESSION TAG	UNP O00206
A	631	GLY	-	EXPRESSION TAG	UNP O00206
A	632	HIS	-	EXPRESSION TAG	UNP O00206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	633	HIS	-	EXPRESSION TAG	UNP O00206
A	634	HIS	-	EXPRESSION TAG	UNP O00206
A	635	HIS	-	EXPRESSION TAG	UNP O00206
A	636	HIS	-	EXPRESSION TAG	UNP O00206
A	637	HIS	-	EXPRESSION TAG	UNP O00206
B	3	ARG	-	EXPRESSION TAG	UNP O00206
B	4	SER	-	EXPRESSION TAG	UNP O00206
B	5	PRO	-	EXPRESSION TAG	UNP O00206
B	6	TRP	-	EXPRESSION TAG	UNP O00206
B	7	ASP	-	EXPRESSION TAG	UNP O00206
B	8	TYR	-	EXPRESSION TAG	UNP O00206
B	9	LYS	-	EXPRESSION TAG	UNP O00206
B	10	ASP	-	EXPRESSION TAG	UNP O00206
B	11	ASP	-	EXPRESSION TAG	UNP O00206
B	12	ASP	-	EXPRESSION TAG	UNP O00206
B	13	ASP	-	EXPRESSION TAG	UNP O00206
B	14	LYS	-	EXPRESSION TAG	UNP O00206
B	15	LEU	-	EXPRESSION TAG	UNP O00206
B	16	ALA	-	EXPRESSION TAG	UNP O00206
B	17	ALA	-	EXPRESSION TAG	UNP O00206
B	18	ALA	-	EXPRESSION TAG	UNP O00206
B	19	ASN	-	EXPRESSION TAG	UNP O00206
B	20	SER	-	EXPRESSION TAG	UNP O00206
B	21	SER	-	EXPRESSION TAG	UNP O00206
B	22	ILE	-	EXPRESSION TAG	UNP O00206
B	299	GLY	ASP	ENGINEERED MUTATION	UNP O00206
B	399	ILE	THR	ENGINEERED MUTATION	UNP O00206
B	630	THR	-	EXPRESSION TAG	UNP O00206
B	631	GLY	-	EXPRESSION TAG	UNP O00206
B	632	HIS	-	EXPRESSION TAG	UNP O00206
B	633	HIS	-	EXPRESSION TAG	UNP O00206
B	634	HIS	-	EXPRESSION TAG	UNP O00206
B	635	HIS	-	EXPRESSION TAG	UNP O00206
B	636	HIS	-	EXPRESSION TAG	UNP O00206
B	637	HIS	-	EXPRESSION TAG	UNP O00206

- 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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	56	GLY	ARG	ENGINEERED MUTATION	UNP Q9Y6Y9
D	56	GLY	ARG	ENGINEERED MUTATION	UNP Q9Y6Y9

- Molecule 3 is SUGAR (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	B	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		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

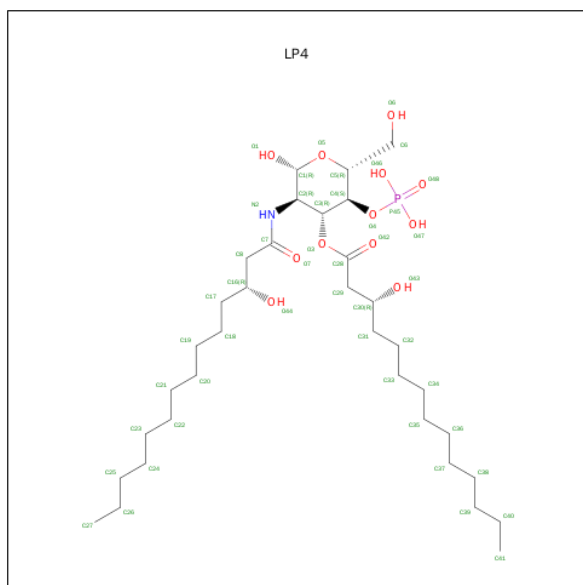
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

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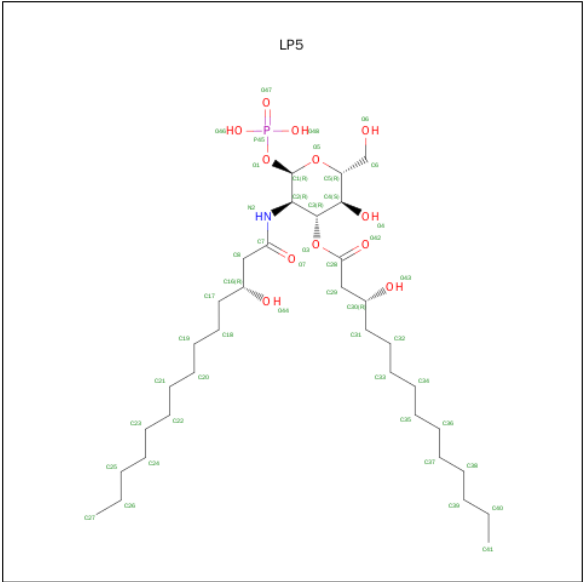
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-DEOXY-3-O-[(3R)-3-HYDROXYTETRADECANOYL]-2-[[[(3R)-3-HYDROXYTETRADECANOYL]AMINO}-4-O-PHOSPHONO-BETA-D-GLUCOPYRANOSE (three-letter code: LP4) (formula: C<sub>34</sub>H<sub>66</sub>NO<sub>12</sub>P).



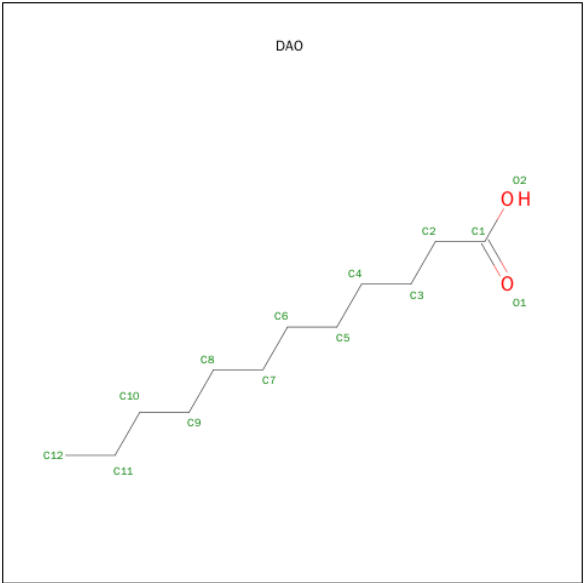
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			45	32	1	11	1		
5	D	1	Total	C	N	O	P	0	0
			45	32	1	11	1		

- Molecule 6 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: C<sub>34</sub>H<sub>66</sub>NO<sub>12</sub>P).



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

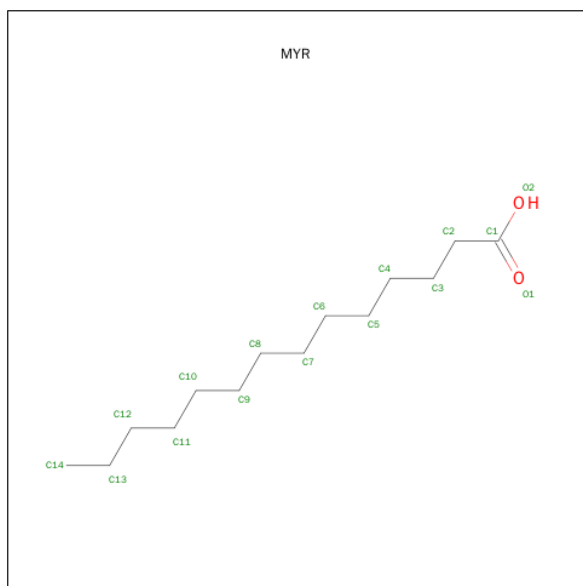
- Molecule 7 is LAURIC ACID (three-letter code: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



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

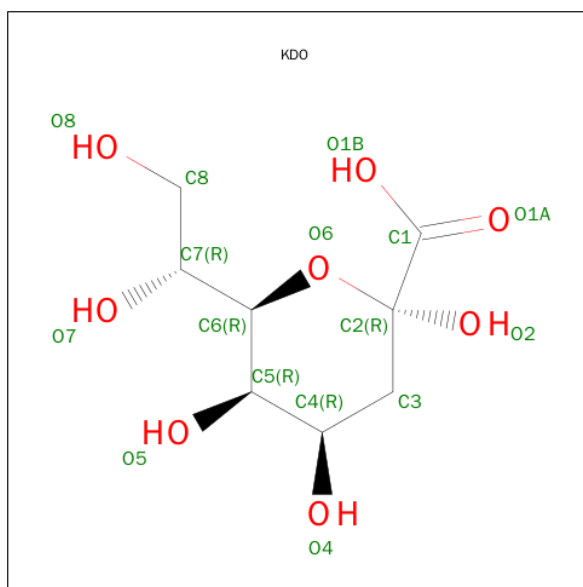


- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



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

- Molecule 9 is SUGAR (3-DEOXY-D-MANNO-OCT-2-ULOSONIC ACID) (three-letter code: KDO) (formula:  $C_8H_{14}O_8$ ).

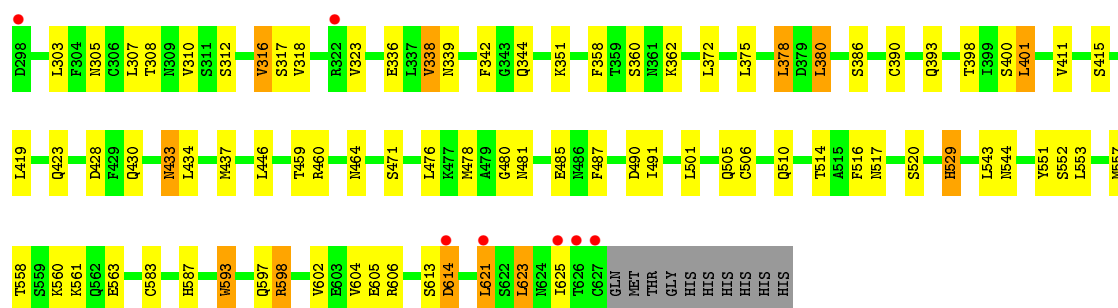


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			15	8	7		
9	D	1	Total	C	O	0	0
			15	8	7		

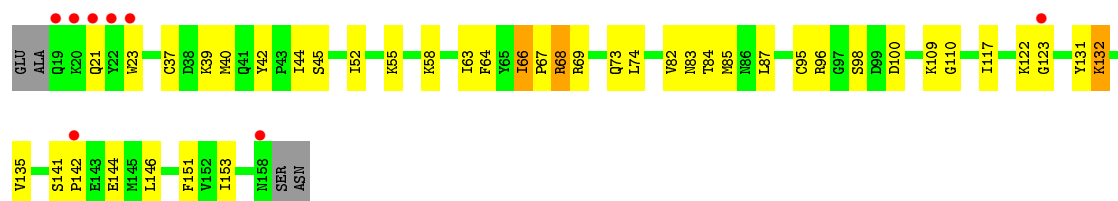
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	15	Total	O	0	0
			15	15		
10	B	21	Total	O	0	0
			21	21		
10	D	3	Total	O	0	0
			3	3		

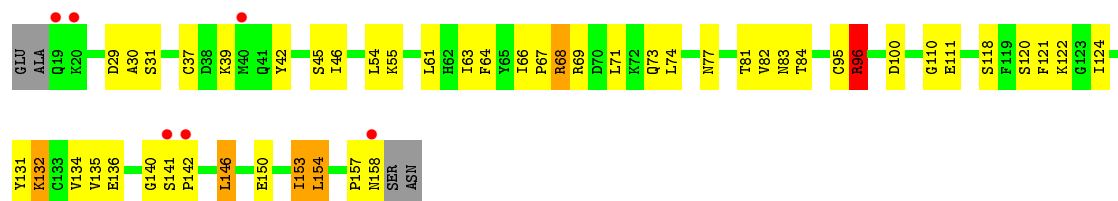




• Molecule 2: Lymphocyte antigen 96



• Molecule 2: Lymphocyte antigen 96



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.04Å 124.68Å 109.14Å 90.00° 115.72° 90.00°	Depositor
Resolution (Å)	39.18 – 2.40 39.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.18-2.40) 99.6 (39.18-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.199 , 0.249 0.201 , 0.252	Depositor DCC
$R_{free}$ test set	3753 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74484 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, KDO, NAG, LP5, MYR, 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	0.51	1/4900 (0.0%)	0.68	1/6634 (0.0%)
1	B	0.51	1/4939 (0.0%)	0.68	2/6688 (0.0%)
2	C	0.53	1/1159 (0.1%)	0.75	0/1562
2	D	0.52	0/1159	0.75	1/1562 (0.1%)
All	All	0.51	3/12157 (0.0%)	0.69	4/16446 (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	1
2	C	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	593	TRP	CD2-CE2	5.31	1.47	1.41
2	C	23	TRP	CD2-CE2	5.25	1.47	1.41
1	A	332	TRP	CD2-CE2	5.18	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	283	LEU	CA-CB-CG	5.25	127.38	115.30
2	D	96	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	283	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	610	ALA	Peptide
2	C	122	LYS	Peptide
2	C	141	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4800	0	4750	92	0
1	B	4836	0	4779	97	0
2	C	1133	0	1129	23	0
2	D	1133	0	1129	29	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	56	0	50	1	0
4	B	56	0	50	2	0
5	C	45	0	52	5	0
5	D	45	0	52	3	0
6	C	48	0	63	4	0
6	D	48	0	63	4	0
7	C	13	0	23	1	0
7	D	13	0	23	0	0
8	C	15	0	27	0	0
8	D	15	0	27	0	0
9	C	15	0	12	0	0
9	D	15	0	12	0	0
10	A	15	0	0	1	0
10	B	21	0	0	0	0
10	D	3	0	0	0	0
All	All	12381	0	12293	238	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 10.

The worst 5 of 238 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:604:VAL:HG11	1:B:621:LEU:HG	1.50	0.94
2:D:81:THR:HB	2:D:132:LYS:HG3	1.49	0.93
2:C:42:TYR:CE1	2:C:68:ARG:HG3	2.04	0.93
2:D:96:ARG:HH21	2:D:96:ARG:HG2	1.38	0.84
1:B:287:GLU:HG2	1:B:312:SER:HB3	1.62	0.82

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	599/635 (94%)	559 (93%)	37 (6%)	3 (0%)	34	48
1	B	603/635 (95%)	562 (93%)	37 (6%)	4 (1%)	26	38
2	C	138/144 (96%)	131 (95%)	6 (4%)	1 (1%)	26	38
2	D	138/144 (96%)	133 (96%)	5 (4%)	0	100	100
All	All	1478/1558 (95%)	1385 (94%)	85 (6%)	8 (0%)	34	48

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	142	PRO
1	A	564	LEU
1	B	202	PRO
1	B	292	TYR
1	A	292	TYR



### 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	558/588 (95%)	493 (88%)	65 (12%)	7	9
1	B	562/588 (96%)	500 (89%)	62 (11%)	8	10
2	C	130/133 (98%)	115 (88%)	15 (12%)	7	9
2	D	130/133 (98%)	113 (87%)	17 (13%)	5	6
All	All	1380/1442 (96%)	1221 (88%)	159 (12%)	7	9

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	LEU
1	B	266	GLU
2	D	55	LYS
1	B	141	LEU
1	B	204	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	129	GLN
1	B	236	ASN
2	C	26	ASN
1	B	185	ASN
1	B	268	ASN

### 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 ⓘ

8 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$
4	NAG	A	702	1,4	14,14,15	0.67	0	15,19,21	1.01	1 (6%)
4	NAG	A	703	4	14,14,15	0.46	0	15,19,21	1.93	3 (20%)
4	NAG	A	704	1,4	14,14,15	0.47	0	15,19,21	1.56	3 (20%)
4	NAG	A	705	4	14,14,15	0.42	0	15,19,21	2.01	3 (20%)
4	NAG	B	702	1,4	14,14,15	0.65	0	15,19,21	1.24	2 (13%)
4	NAG	B	703	4	14,14,15	0.44	0	15,19,21	2.24	5 (33%)
4	NAG	B	704	1,4	14,14,15	0.72	1 (7%)	15,19,21	2.25	2 (13%)
4	NAG	B	705	4	14,14,15	0.52	0	15,19,21	1.14	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	NAG	A	702	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	703	4	-	0/6/23/26	0/1/1/1
4	NAG	A	704	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	4	-	0/6/23/26	0/1/1/1
4	NAG	B	702	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	703	4	-	0/6/23/26	0/1/1/1
4	NAG	B	704	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	705	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	704	NAG	O5-C1	-2.15	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	NAG	C2-N2-C7	-3.74	118.23	123.04
4	B	702	NAG	C2-N2-C7	-3.02	119.16	123.04
4	A	705	NAG	C6-C5-C4	-3.00	105.63	113.02
4	B	703	NAG	C4-C3-C2	-2.97	106.61	111.23
4	B	704	NAG	C6-C5-C4	-2.88	105.92	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	NAG	1	0
4	A	704	NAG	1	0
4	B	704	NAG	2	0

## 5.6 Ligand geometry [i](#)

14 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	14,14,15	0.48	0	15,19,21	1.04	0
3	NAG	B	701	1	14,14,15	0.63	0	15,19,21	1.75	2 (13%)
3	NAG	C	201	2	14,14,15	0.47	0	15,19,21	1.25	1 (6%)
5	LP4	C	202	9,8,7,6	45,45,48	0.63	0	46,56,60	1.18	3 (6%)
6	LP5	C	203	5	47,48,48	0.90	2 (4%)	54,60,60	1.26	7 (12%)
7	DAO	C	204	5	12,12,13	0.91	1 (8%)	11,11,13	0.68	0
8	MYR	C	205	5	14,14,15	0.84	1 (7%)	13,13,15	0.87	0
9	KDO	C	206	5	12,15,16	0.45	0	12,21,24	0.78	0
3	NAG	D	201	2	14,14,15	0.49	0	15,19,21	1.35	1 (6%)
5	LP4	D	202	9,8,7,6	45,45,48	0.78	2 (4%)	46,56,60	1.44	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LP5	D	203	5	47,48,48	0.79	2 (4%)	54,60,60	1.33	6 (11%)
7	DAO	D	204	5	12,12,13	0.94	1 (8%)	11,11,13	0.76	0
8	MYR	D	205	5	14,14,15	0.82	1 (7%)	13,13,15	0.80	0
9	KDO	D	206	5	12,15,16	0.68	0	12,21,24	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1	-	0/6/23/26	0/1/1/1
3	NAG	C	201	2	-	0/6/23/26	0/1/1/1
5	LP4	C	202	9,8,7,6	-	0/43/60/65	0/1/1/1
6	LP5	C	203	5	-	0/44/65/65	0/1/1/1
7	DAO	C	204	5	-	0/10/10/11	0/0/0/0
8	MYR	C	205	5	-	0/12/12/13	0/0/0/0
9	KDO	C	206	5	-	0/6/26/30	0/1/1/1
3	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	LP4	D	202	9,8,7,6	-	0/43/60/65	0/1/1/1
6	LP5	D	203	5	-	0/44/65/65	0/1/1/1
7	DAO	D	204	5	-	0/10/10/11	0/0/0/0
8	MYR	D	205	5	-	0/12/12/13	0/0/0/0
9	KDO	D	206	5	-	0/6/26/30	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	204	DAO	O2-C1	-3.18	1.24	1.42
7	C	204	DAO	O2-C1	-3.09	1.25	1.42
8	C	205	MYR	O2-C1	-3.05	1.25	1.42
8	D	205	MYR	O2-C1	-3.00	1.25	1.42
5	D	202	LP4	O3-C3	-2.32	1.41	1.44

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	202	LP4	C1-O5-C5	-5.41	105.38	112.25
5	C	202	LP4	C1-O5-C5	-3.98	107.20	112.25
6	D	203	LP5	O5-C1-O1	-3.81	106.33	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	202	LP4	C8-C7-N2	-3.80	111.62	116.33
6	D	203	LP5	C8-C7-N2	-3.33	112.21	116.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	202	LP4	5	0
6	C	203	LP5	4	0
7	C	204	DAO	1	0
5	D	202	LP4	3	0
6	D	203	LP5	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	601/635 (94%)	0.12	27 (4%) 37 38	26, 44, 79, 120	0
1	B	605/635 (95%)	0.06	16 (2%) 59 58	27, 44, 69, 106	0
2	C	140/144 (97%)	0.28	8 (5%) 27 27	32, 49, 83, 103	0
2	D	140/144 (97%)	0.12	6 (4%) 39 40	33, 44, 76, 102	0
All	All	1486/1558 (95%)	0.11	57 (3%) 44 45	26, 45, 74, 120	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	11.3
2	D	19	GLN	6.5
1	A	625	ILE	6.3
1	A	75	PHE	6.1
1	A	301	ILE	5.9

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	702	14/15	0.96	0.17	1.38	37,43,47,51	0
4	NAG	A	704	14/15	0.95	0.21	0.30	46,49,50,55	0
4	NAG	B	704	14/15	0.96	0.13	-0.21	35,36,44,51	0
4	NAG	B	702	14/15	0.95	0.12	-0.32	34,37,45,47	0
4	NAG	A	705	14/15	0.91	0.25	-	57,58,61,63	0
4	NAG	B	705	14/15	0.90	0.19	-	41,49,59,60	0
4	NAG	A	703	14/15	0.83	0.33	-	53,59,64,66	0
4	NAG	B	703	14/15	0.91	0.20	-	51,55,59,64	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	DAO	D	204	13/14	0.93	0.20	3.63	48,51,53,56	0
7	DAO	C	204	13/14	0.92	0.20	3.06	50,52,54,58	0
8	MYR	C	205	15/16	0.91	0.24	2.57	51,54,60,66	0
8	MYR	D	205	15/16	0.96	0.19	2.16	41,50,55,55	0
3	NAG	A	701	14/15	0.66	0.27	1.33	90,101,105,108	0
6	LP5	D	203	48/48	0.92	0.17	1.01	40,52,58,65	0
5	LP4	C	202	45/48	0.94	0.17	0.97	36,45,53,56	0
5	LP4	D	202	45/48	0.94	0.15	0.91	37,45,52,57	0
6	LP5	C	203	48/48	0.89	0.19	0.31	49,54,64,70	0
3	NAG	C	201	14/15	0.87	0.26	-	66,73,81,81	0
3	NAG	B	701	14/15	0.65	0.40	-	95,105,111,112	0
9	KDO	C	206	15/16	0.94	0.14	-	62,67,71,73	0
3	NAG	D	201	14/15	0.88	0.25	-	61,69,72,73	0
9	KDO	D	206	15/16	0.71	0.18	-	62,66,78,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.