wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:59 PM GMT

PDB ID	:	3VQ2
Title	:	Crystal structure of mouse TLR4/MD-2/LPS complex
Authors	:	Ohto, U.; Shimizu, T.
Deposited on	:	2012-03-17
Resolution	:	2.48 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 (i) symbol.

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

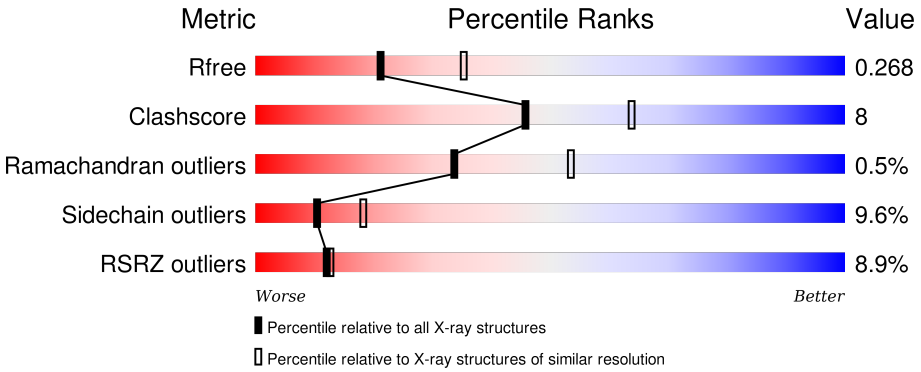
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	606	8% 74% 18%
1	B	606	12% 73% 20%
2	C	144	3% 66% 24% 6%
2	D	144	3% 64% 26% 6%

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
7	DAO	C	302	-	-	-	X
7	DAO	D	302	-	-	-	X
8	MYR	C	303	-	-	-	X
8	MYR	D	303	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11815 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.

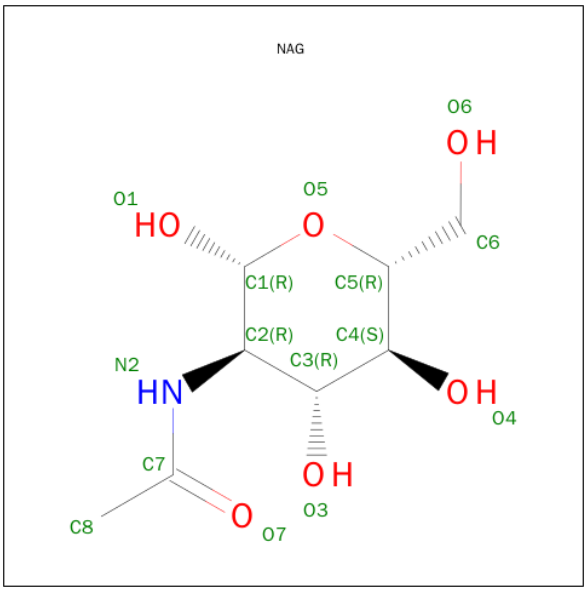
- Molecule 1 is a protein called Toll-like receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4637	2972	764	875	26			
1	B	581	Total	C	N	O	S	0	0	0
			4637	2972	764	875	26			

- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	135	Total	C	N	O	S	0	0	0
			1092	706	182	197	7			
2	D	135	Total	C	N	O	S	0	0	0
			1092	706	182	197	7			

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

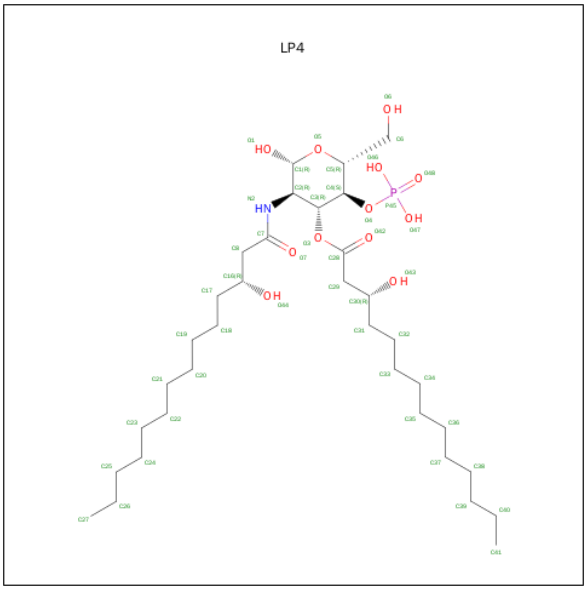


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	B	2	Total	C	N	O	0	0
			28	16	2	10		

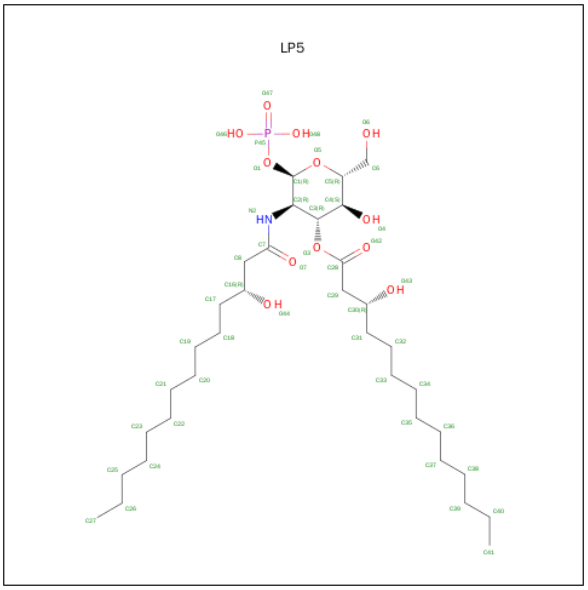
- Molecule 5 is 2-DEOXY-3-O-[(3R)-3-HYDROXYTETRADECANOYL]-2-{[(3R)-3-HYDROXYTETRADECANOYL]AMINO}-4-O-PHOSPHONO-BETA-D-GLUCOPYRANOSE (three-letter code: LP4) (formula: $C_{34}H_{66}NO_{12}P$).



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		

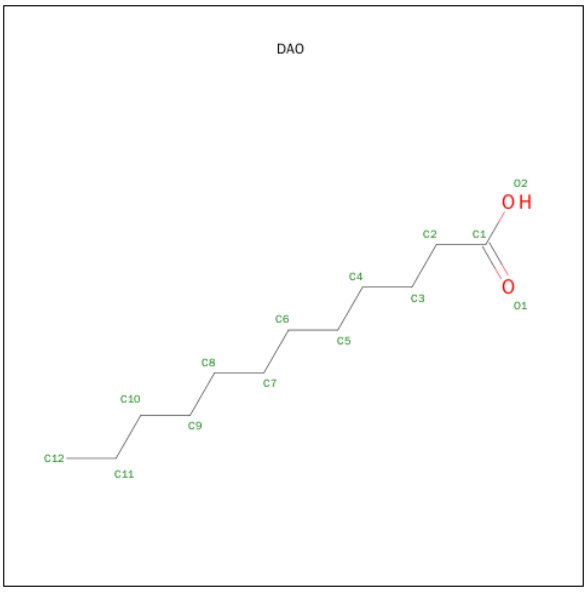
- Molecule 6 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOOXY)TETRAHYDRO-2H-PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (three-letter code: LP5) (formula:

$C_{34}H_{66}NO_{12}P$).



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: $C_{12}H_{24}O_2$).



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

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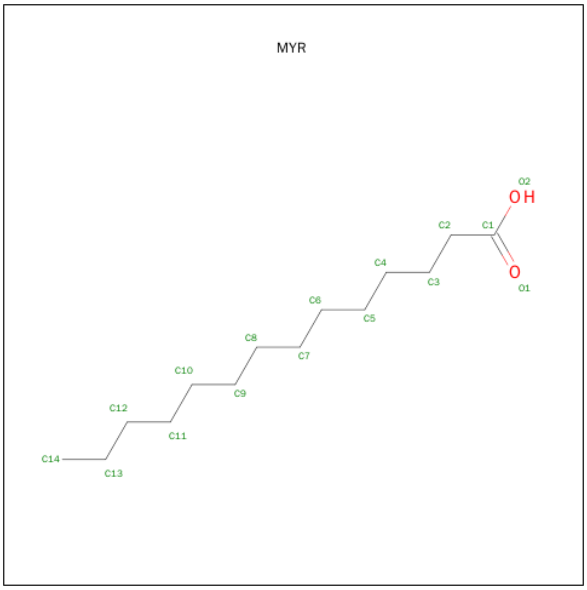
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 13 12 1	0	0

- 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 15 14 1	0	0
8	D	1	Total C O 15 14 1	0	0

- Molecule 9 is water.

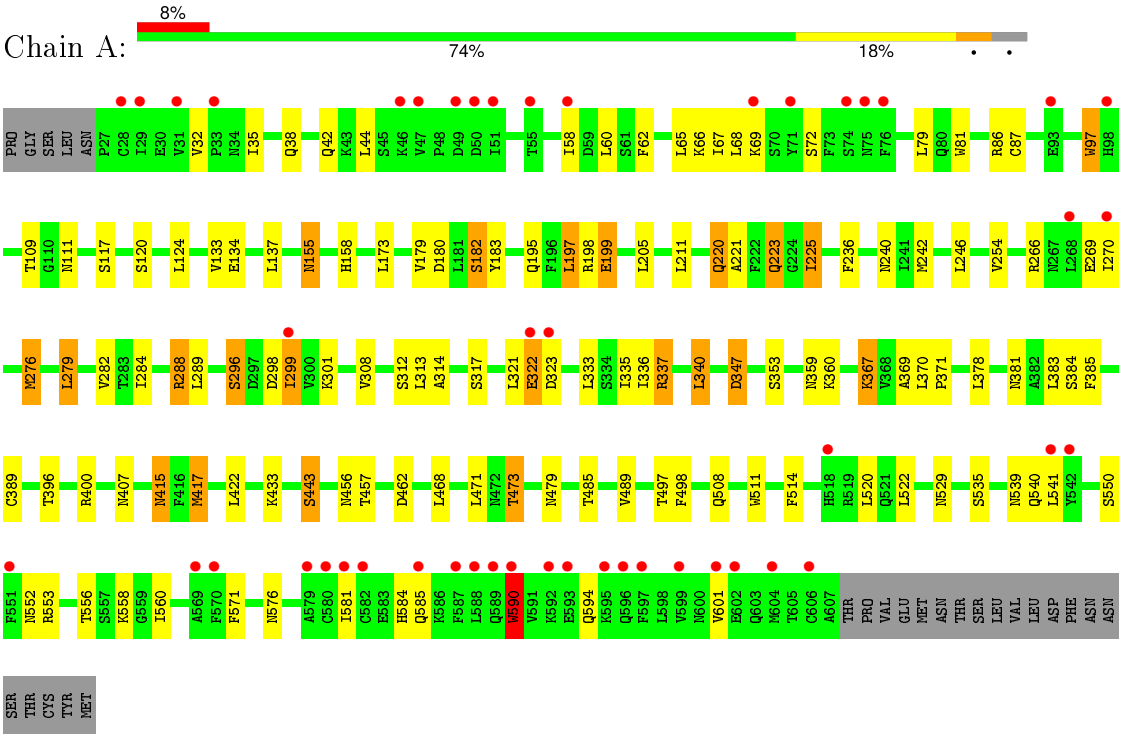
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total O 8 8	0	0
9	B	9	Total O 9 9	0	0

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.

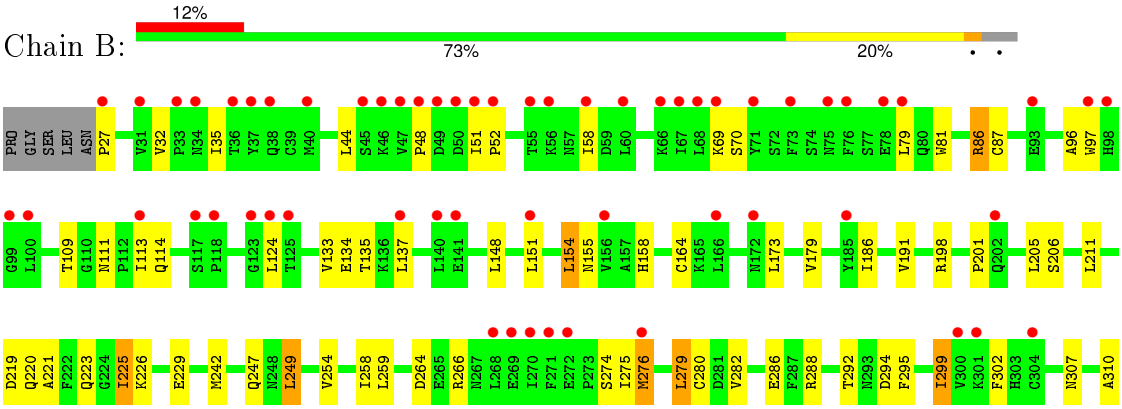
- Molecule 1: Toll-like receptor 4

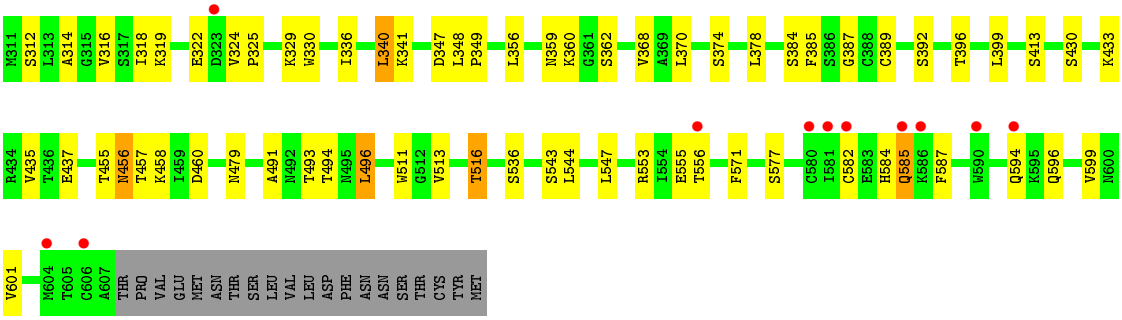
Chain A:



- Molecule 1: Toll-like receptor 4

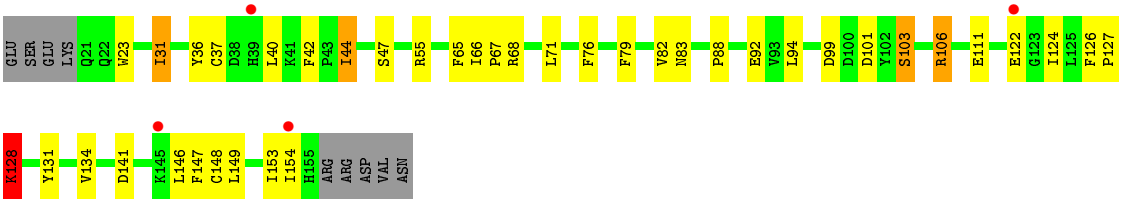
Chain B:





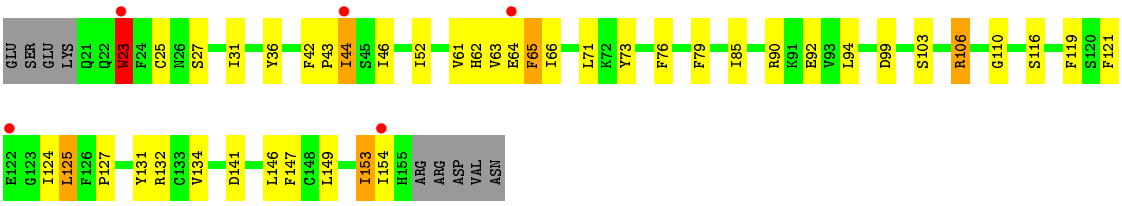
- Molecule 2: Lymphocyte antigen 96

Chain C:



- Molecule 2: Lymphocyte antigen 96

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.81Å 144.32Å 86.94Å 90.00° 95.16° 90.00°	Depositor
Resolution (Å)	86.59 – 2.48 72.16 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.4 (86.59-2.48) 98.4 (72.16-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.221 , 0.267 0.226 , 0.268	Depositor DCC
R_{free} test set	3758 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.6	EDS
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 73743 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11815	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.375 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: 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	0.50	4/4735 (0.1%)	0.66	2/6414 (0.0%)
1	B	0.50	4/4735 (0.1%)	0.62	0/6414
2	C	0.52	1/1123 (0.1%)	0.68	1/1519 (0.1%)
2	D	0.50	1/1123 (0.1%)	0.60	0/1519
All	All	0.50	10/11716 (0.1%)	0.64	3/15866 (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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	23	TRP	CD2-CE2	5.82	1.48	1.41
1	B	511	TRP	CD2-CE2	5.56	1.48	1.41
1	A	97	TRP	CD2-CE2	5.46	1.47	1.41
1	A	81	TRP	CD2-CE2	5.40	1.47	1.41
1	B	97	TRP	CD2-CE2	5.24	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	383	LEU	CA-CB-CG	5.98	129.06	115.30
2	C	128	LYS	N-CA-C	-5.56	95.99	111.00
1	A	337	ARG	NE-CZ-NH1	-5.47	117.56	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ASP	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	4637	0	4611	74	0
1	B	4637	0	4613	62	0
2	C	1092	0	1051	26	0
2	D	1092	0	1051	34	0
3	A	42	0	39	2	0
4	A	28	0	25	1	0
4	B	28	0	25	0	0
5	C	45	0	53	0	0
5	D	45	0	53	0	0
6	C	48	0	63	1	0
6	D	48	0	63	2	0
7	C	13	0	23	0	0
7	D	13	0	23	2	0
8	C	15	0	27	0	0
8	D	15	0	27	0	0
9	A	8	0	0	0	0
9	B	9	0	0	0	0
All	All	11815	0	11747	181	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 8.

The worst 5 of 181 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:556:THR:HG21	1:B:584:HIS:CG	2.12	0.84
1:A:87:CYS:H	1:A:111:ASN:HD21	1.25	0.84
2:C:44:ILE:HD13	2:C:149:LEU:HD21	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PHE:CE1	1:B:299:ILE:HG21	2.22	0.74
1:B:387:GLY:HA2	1:B:413:SER:HB3	1.70	0.73

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	579/606 (96%)	533 (92%)	43 (7%)	3 (0%)	34	53
1	B	579/606 (96%)	529 (91%)	47 (8%)	3 (0%)	34	53
2	C	133/144 (92%)	127 (96%)	5 (4%)	1 (1%)	24	39
2	D	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
All	All	1424/1500 (95%)	1318 (93%)	99 (7%)	7 (0%)	34	53

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	581	ILE
2	C	128	LYS
1	B	52	PRO
1	A	317	SER
1	A	560	ILE

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	540/564 (96%)	487 (90%)	53 (10%)	10 17
1	B	540/564 (96%)	485 (90%)	55 (10%)	9 16
2	C	122/131 (93%)	112 (92%)	10 (8%)	14 25
2	D	122/131 (93%)	113 (93%)	9 (7%)	17 30
All	All	1324/1390 (95%)	1197 (90%)	127 (10%)	10 18

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	65	PHE
1	B	173	LEU
1	B	601	VAL
2	C	103	SER
1	B	86	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	540	GLN
1	B	98	HIS
2	D	21	GLN
2	C	155	HIS
1	B	102	HIS

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)

4 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	802	1,4	14,14,15	1.50	1 (7%)	15,19,21	1.25	2 (13%)
4	NAG	A	803	4	14,14,15	0.65	0	15,19,21	1.47	2 (13%)
4	NAG	B	701	1,4	14,14,15	0.54	0	15,19,21	1.38	3 (20%)
4	NAG	B	702	4	14,14,15	0.57	0	15,19,21	1.35	2 (13%)

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	802	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	803	4	-	0/6/23/26	0/1/1/1
4	NAG	B	701	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	702	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	A	802	NAG	O5-C1	-5.27	1.34	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	802	NAG	C2-N2-C7	-3.13	119.02	123.04
4	A	803	NAG	C3-C2-N2	-2.51	104.54	110.56
4	B	701	NAG	C6-C5-C4	-2.36	107.19	113.02
4	A	802	NAG	C6-C5-C4	-2.05	107.97	113.02
4	B	701	NAG	O4-C4-C5	-2.01	103.92	109.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	NAG	1	0

5.6 Ligand geometry

11 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	800	1	14,14,15	1.78	1 (7%)	15,19,21	2.53	4 (26%)
3	NAG	A	801	1	14,14,15	0.70	1 (7%)	15,19,21	2.01	3 (20%)
3	NAG	A	804	-	14,14,15	0.50	0	15,19,21	0.87	0
5	LP4	C	300	8,7,6	45,45,48	0.77	0	46,56,60	0.91	1 (2%)
6	LP5	C	301	5	47,48,48	0.83	3 (6%)	54,60,60	1.31	6 (11%)
7	DAO	C	302	5	12,12,13	0.91	1 (8%)	11,11,13	0.61	0
8	MYR	C	303	5	14,14,15	0.84	1 (7%)	13,13,15	0.69	0
5	LP4	D	300	8,7,6	45,45,48	0.70	0	46,56,60	1.04	4 (8%)
6	LP5	D	301	5	47,48,48	0.81	1 (2%)	54,60,60	1.12	6 (11%)
7	DAO	D	302	5	12,12,13	0.93	1 (8%)	11,11,13	0.61	0
8	MYR	D	303	5	14,14,15	0.84	1 (7%)	13,13,15	0.73	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	800	1	-	0/6/23/26	0/1/1/1
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	804	-	-	0/6/23/26	0/1/1/1
5	LP4	C	300	8,7,6	-	0/43/60/65	0/1/1/1
6	LP5	C	301	5	-	0/44/65/65	0/1/1/1
7	DAO	C	302	5	-	0/10/10/11	0/0/0/0
8	MYR	C	303	5	-	0/12/12/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LP4	D	300	8,7,6	-	0/43/60/65	0/1/1/1
6	LP5	D	301	5	-	0/44/65/65	0/1/1/1
7	DAO	D	302	5	-	0/10/10/11	0/0/0/0
8	MYR	D	303	5	-	0/12/12/13	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	NAG	O5-C1	-6.40	1.33	1.43
7	D	302	DAO	O2-C1	-3.12	1.25	1.42
7	C	302	DAO	O2-C1	-3.05	1.25	1.42
8	D	303	MYR	O2-C1	-3.04	1.25	1.42
8	C	303	MYR	O2-C1	-3.03	1.25	1.42

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	800	NAG	C1-O5-C5	-8.47	101.49	112.25
6	C	301	LP5	C8-C7-N2	-3.92	111.47	116.33
3	A	801	NAG	C2-N2-C7	-3.79	118.17	123.04
5	D	300	LP4	C3-O3-C28	-2.75	112.87	117.75
3	A	800	NAG	C4-C3-C2	-2.60	107.19	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	NAG	2	0
6	C	301	LP5	1	0
6	D	301	LP5	2	0
7	D	302	DAO	2	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	581/606 (95%)	0.66	48 (8%) 14 15	42, 65, 119, 169	0
1	B	581/606 (95%)	0.80	70 (12%) 6 6	38, 68, 128, 184	0
2	C	135/144 (93%)	0.41	4 (2%) 54 58	46, 64, 92, 112	2 (1%)
2	D	135/144 (93%)	0.45	5 (3%) 45 50	57, 72, 97, 142	2 (1%)
All	All	1432/1500 (95%)	0.68	127 (8%) 12 13	38, 68, 121, 184	4 (0%)

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	CYS	10.7
1	B	50	ASP	7.3
1	B	31	VAL	6.5
1	B	55	THR	5.3
1	A	579	ALA	5.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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
4	NAG	A	802	14/15	0.91	0.19	0.38	65,75,85,96	0
4	NAG	B	701	14/15	0.98	0.18	0.10	47,54,70,80	0
4	NAG	B	702	14/15	0.93	0.19	-	63,78,94,120	0
4	NAG	A	803	14/15	0.91	0.14	-	79,94,120,130	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^{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
8	MYR	C	303	15/16	0.90	0.38	7.81	68,79,99,122	0
8	MYR	D	303	15/16	0.89	0.33	6.07	66,91,101,116	0
7	DAO	C	302	13/14	0.92	0.28	3.63	68,75,88,90	0
7	DAO	D	302	13/14	0.94	0.26	2.27	72,82,97,103	0
5	LP4	C	300	45/48	0.91	0.21	1.32	45,64,81,99	0
6	LP5	C	301	48/48	0.94	0.22	0.68	48,68,102,109	0
5	LP4	D	300	45/48	0.93	0.20	0.51	60,72,90,96	0
6	LP5	D	301	48/48	0.94	0.19	0.09	52,78,102,119	0
3	NAG	A	804	14/15	0.83	0.20	-0.07	81,105,125,136	0
3	NAG	A	800	14/15	0.91	0.17	-0.81	59,73,84,85	0
3	NAG	A	801	14/15	0.85	0.20	-	71,82,105,111	0

6.5 Other polymers (i)

There are no such residues in this entry.