



# Full wwPDB X-ray Structure Validation Report ⓘ

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 Full wwPDB X-ray Structure Validation 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.

---

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

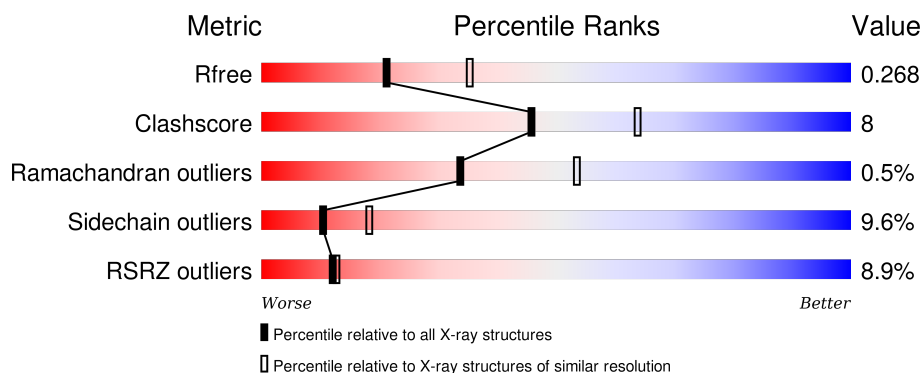
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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  $\geq 3$ , 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	606	<div> <div>8%</div> <div>74%</div> <div>18%</div> <div>• •</div> </div>
1	B	606	<div> <div>12%</div> <div>73%</div> <div>20%</div> <div>• •</div> </div>
2	C	144	<div> <div>3%</div> <div>66%</div> <div>24%</div> <div>• • 6%</div> </div>
2	D	144	<div> <div>3%</div> <div>64%</div> <div>26%</div> <div>• • 6%</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
7	DAO	C	302	-	-	-	X
7	DAO	D	302	-	-	-	X
8	MYR	C	303	-	-	-	X
8	MYR	D	303	-	-	-	X

## 2 Entry composition [i](#)

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.

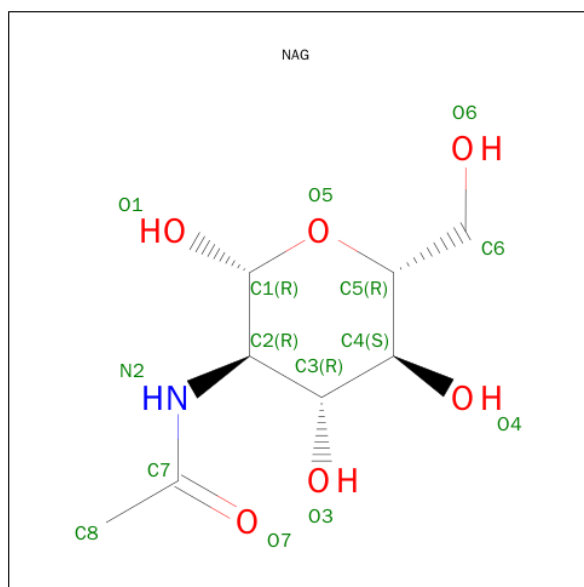
- Molecule 1 is a protein called Toll-like receptor 4.

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:  $C_8H_{15}NO_6$ ).

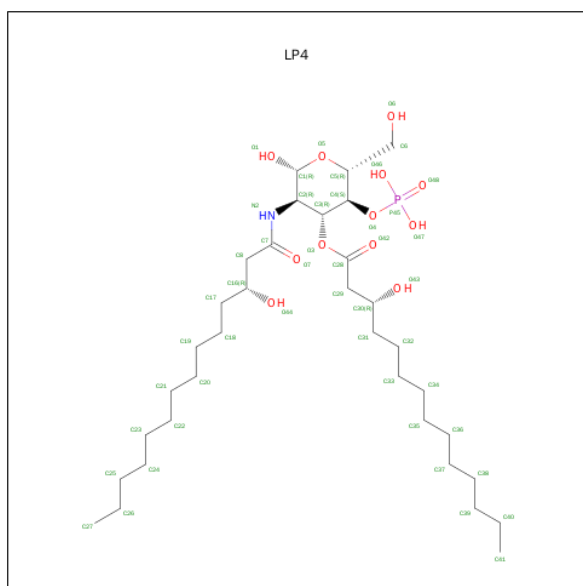


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		

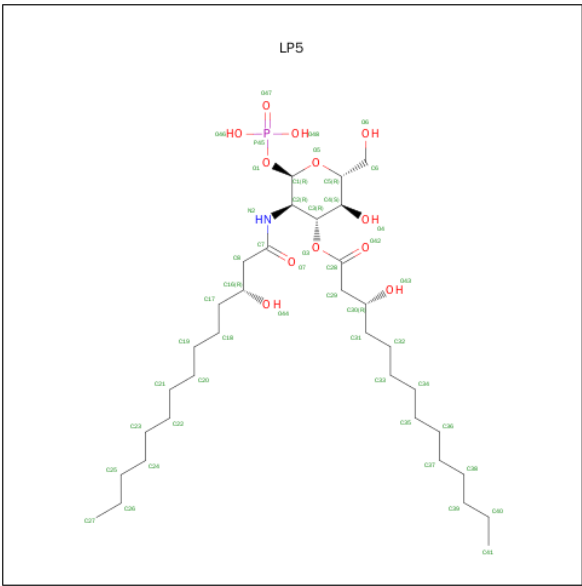
- Molecule 5 is 2-DEOXY-3-O-[(3R)-3-HYDROXYTETRADECANOYL]-2-([(3R)-3-HYDROXYTETRADECANOYL|AMINO}-4-O-PHOSPHONO-BETA-D-GLUCOPYRANOSE (three-letter code: LP4) (formula:  $C_{34}H_{66}NO_{12}P$ ).



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		

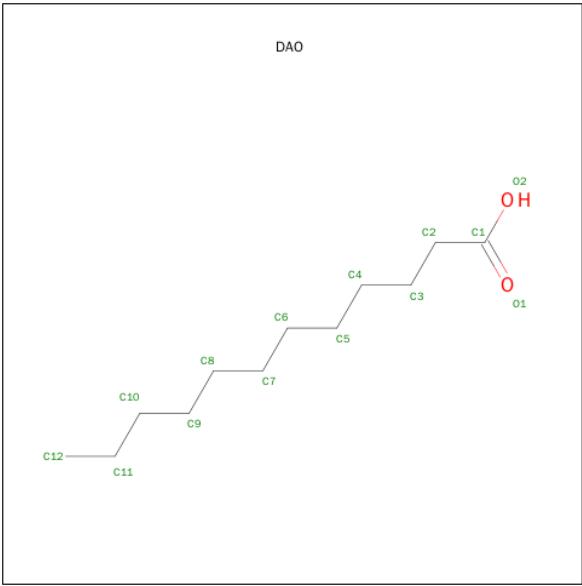
- Molecule 6 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOXY)TETRAHYDRO-2H-PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (three-letter code: LP5) (formula:

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>).



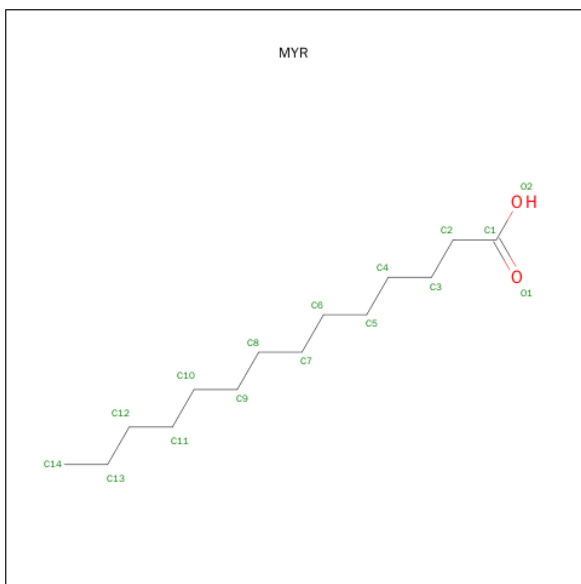
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			13	12	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

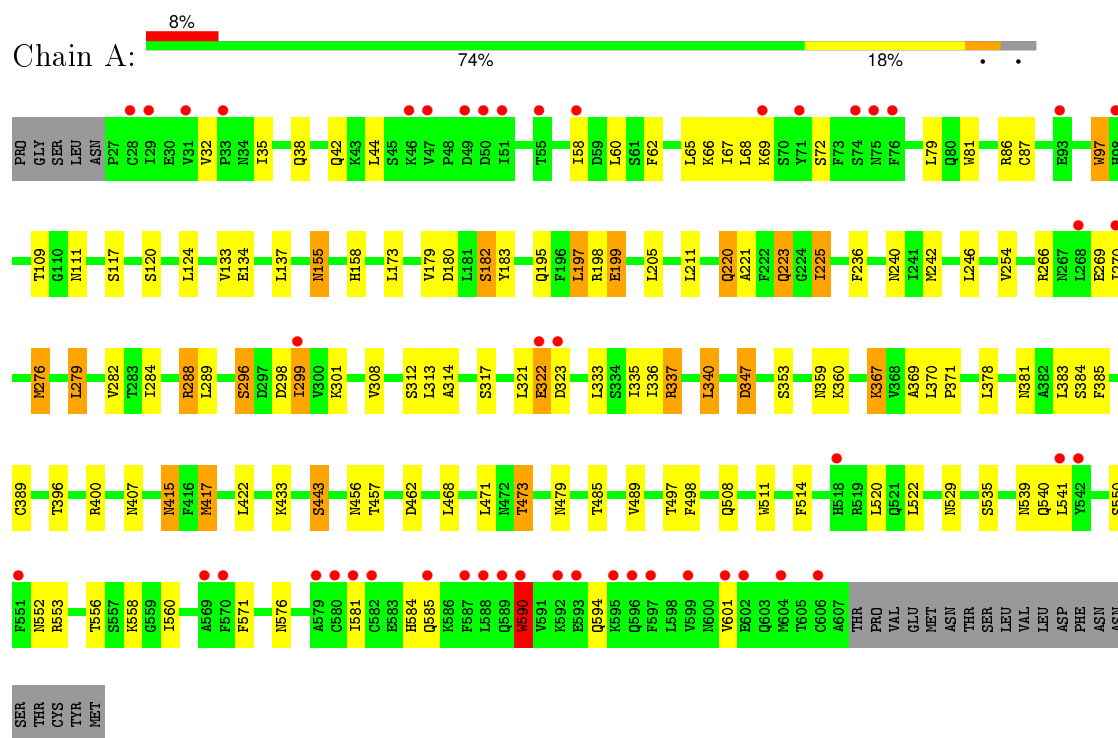
- Molecule 9 is water.

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

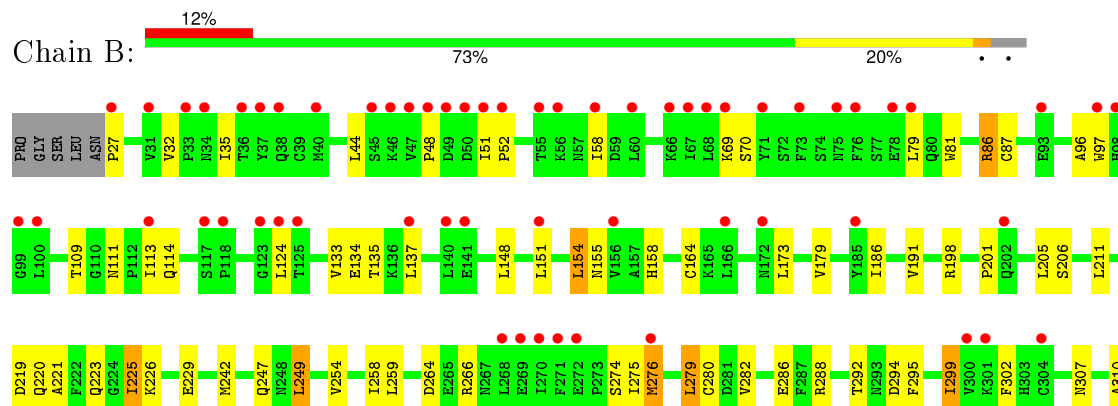
### 3 Residue-property plots

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.

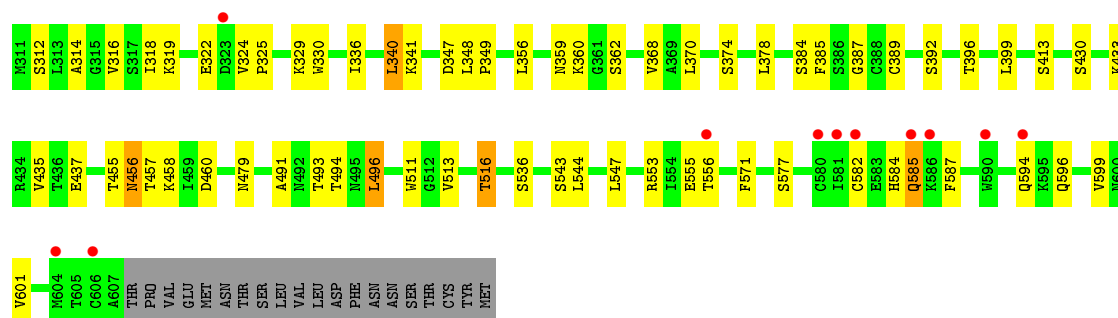
#### • Molecule 1: Toll-like receptor 4



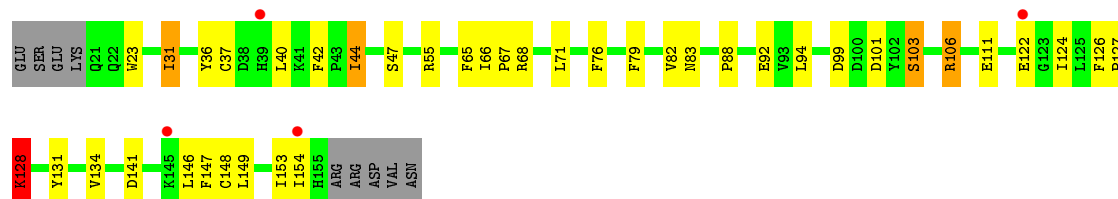
#### • Molecule 1: Toll-like receptor 4



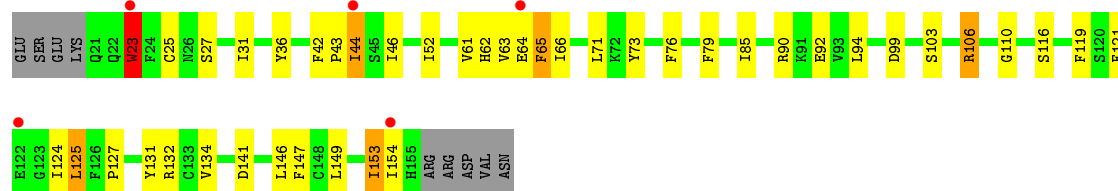




- Molecule 2: Lymphocyte antigen 96



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.6	EDS
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<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 ⓘ

### 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

All (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
1	A	511	TRP	CD2-CE2	5.13	1.47	1.41
2	C	23	TRP	CD2-CE2	5.13	1.47	1.41
1	B	330	TRP	CD2-CE2	5.13	1.47	1.41
1	A	590	TRP	CD2-CE2	5.07	1.47	1.41
1	B	81	TRP	CD2-CE2	5.01	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 ⓘ

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.

All (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
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
1:A:367:LYS:HD2	1:A:367:LYS:H	1.55	0.71
2:C:127:PRO:HB2	2:C:128:LYS:HB2	1.73	0.70
1:A:529:ASN:HB3	1:A:553:ARG:NH2	2.09	0.68
2:C:127:PRO:CB	2:C:128:LYS:HB2	2.25	0.67
2:D:36:TYR:HE2	2:D:44:ILE:HD12	1.60	0.66
1:B:86:ARG:NH1	2:D:110:GLY:O	2.29	0.66
2:D:127:PRO:HD2	2:D:131:TYR:OH	1.96	0.65
1:B:556:THR:HG22	1:B:587:PHE:CD2	2.31	0.65
1:A:367:LYS:HD2	1:A:367:LYS:N	2.11	0.65
2:C:44:ILE:CD1	2:C:149:LEU:HD21	2.26	0.64
2:D:62:HIS:HD2	2:D:116:SER:OG	1.79	0.64
1:B:286:GLU:HG3	1:B:310:ALA:HB3	1.80	0.63
1:B:86:ARG:HB2	1:B:86:ARG:HH11	1.64	0.63
4:A:802:NAG:H83	3:A:804:NAG:H5	1.79	0.63
6:D:301:LP5:H232	7:D:302:DAO:H81	1.81	0.62
2:D:79:PHE:HB2	2:D:134:VAL:HG22	1.81	0.62
1:B:276:MET:HG3	1:B:279:LEU:HD22	1.82	0.62
2:C:82:VAL:HG22	2:C:131:TYR:CE2	2.35	0.61
1:A:322:GLU:HG2	1:A:322:GLU:O	2.00	0.60
1:B:556:THR:HG21	1:B:584:HIS:HB3	1.83	0.59
1:B:340:LEU:H	1:B:359:ASN:HD21	1.50	0.59
1:A:550:SER:OG	3:A:804:NAG:H82	2.02	0.58
1:B:288:ARG:HG2	1:B:312:SER:HB2	1.84	0.58
1:A:220:GLN:HG3	1:A:223:GLN:HE21	1.68	0.58
1:A:134:GLU:HA	1:A:158:HIS:O	2.03	0.58
1:B:58:ILE:HG22	1:B:79:LEU:HD11	1.84	0.57
1:A:69:LYS:O	1:A:72:SER:OG	2.20	0.57
1:A:195:GLN:HG2	1:A:199:GLU:OE2	2.05	0.57
1:A:552:ASN:HB2	1:A:576:ASN:HD21	1.70	0.57
1:A:553:ARG:HH22	1:B:553:ARG:HH22	1.52	0.57
2:D:76:PHE:HE1	2:D:94:LEU:HD12	1.68	0.57
2:D:44:ILE:HD11	2:D:147:PHE:HB2	1.87	0.57
2:C:131:TYR:HB2	2:C:153:ILE:HB	1.86	0.57
2:C:103:SER:O	2:C:106:ARG:HG3	2.04	0.56
1:A:299:ILE:HG12	1:A:299:ILE:O	2.06	0.56
1:A:417:MET:HE1	2:D:125:LEU:N	2.20	0.56
1:B:295:PHE:CZ	1:B:299:ILE:CG2	2.88	0.56

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:THR:HG21	1:B:584:HIS:CB	2.35	0.55
1:A:462:ASP:HB2	2:D:85:ILE:HG23	1.87	0.55
1:B:87:CYS:H	1:B:111:ASN:HD21	1.52	0.55
2:C:88:PRO:HG3	1:B:460:ASP:HB3	1.87	0.55
1:A:313:LEU:HD12	1:A:335:ILE:HD12	1.87	0.55
1:A:556:THR:HG21	1:A:584:HIS:CB	2.37	0.55
1:A:42:GLN:HB2	1:A:44:LEU:HG	1.89	0.55
1:A:340:LEU:H	1:A:359:ASN:HD21	1.56	0.54
1:B:225:ILE:O	1:B:225:ILE:HG13	2.06	0.54
1:B:276:MET:HB3	1:B:302:PHE:CE2	2.43	0.54
1:B:374:SER:HA	1:B:399:LEU:HA	1.90	0.53
1:A:276:MET:HG3	1:A:279:LEU:CD2	2.38	0.53
1:B:206:SER:HB3	1:B:229:GLU:HG2	1.89	0.53
1:A:87:CYS:H	1:A:111:ASN:ND2	2.02	0.53
1:A:333:LEU:HD11	1:A:335:ILE:HD11	1.91	0.53
1:A:236:PHE:CD1	1:A:242:MET:HG3	2.44	0.52
1:B:279:LEU:O	1:B:282:VAL:HG22	2.10	0.52
1:B:387:GLY:HA2	1:B:413:SER:CB	2.39	0.52
1:B:201:PRO:HB3	1:B:226:LYS:HE3	1.92	0.52
1:B:258:ILE:HG13	1:B:288:ARG:HB2	1.92	0.52
1:B:27:PRO:HA	1:B:51:ILE:HD11	1.91	0.51
1:A:66:LYS:C	1:A:67:ILE:HG13	2.31	0.51
1:A:514:PHE:HB3	1:A:541:LEU:HD21	1.91	0.51
1:B:319:LYS:HD2	1:B:341:LYS:HE2	1.93	0.51
1:A:456:ASN:ND2	1:B:456:ASN:HD21	2.07	0.51
2:C:31:ILE:O	2:C:31:ILE:HG13	2.10	0.51
2:C:44:ILE:HD11	2:C:147:PHE:HB2	1.92	0.51
1:B:295:PHE:CZ	1:B:299:ILE:HG21	2.44	0.51
1:A:269:GLU:HG2	1:A:270:ILE:H	1.76	0.51
2:D:31:ILE:HG13	2:D:154:ILE:HB	1.93	0.51
2:D:36:TYR:CE2	2:D:44:ILE:HD12	2.45	0.50
1:A:32:VAL:HG12	1:A:35:ILE:HB	1.94	0.49
2:D:42:PHE:HD1	2:D:146:LEU:O	1.94	0.49
1:A:415:ASN:O	1:A:443:SER:OG	2.29	0.49
1:A:381:ASN:H	1:A:407:ASN:ND2	2.10	0.49
1:A:296:SER:O	1:A:299:ILE:HG22	2.12	0.49
1:B:288:ARG:NH1	2:D:99:ASP:OD2	2.46	0.49
2:D:103:SER:O	2:D:106:ARG:HG3	2.12	0.49
2:C:76:PHE:HE1	2:C:94:LEU:HD12	1.78	0.49
1:A:180:ASP:OD1	1:A:182:SER:HB2	2.13	0.49
1:A:539:ASN:O	1:A:540:GLN:HB2	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:NH1	2:C:99:ASP:OD2	2.46	0.49
2:D:124:ILE:CG2	2:D:125:LEU:N	2.75	0.48
1:A:415:ASN:ND2	1:A:415:ASN:H	2.11	0.48
1:B:87:CYS:H	1:B:111:ASN:ND2	2.11	0.48
1:A:556:THR:HG21	1:A:584:HIS:CG	2.49	0.48
2:D:62:HIS:CD2	2:D:116:SER:OG	2.65	0.48
1:B:314:ALA:HA	1:B:336:ILE:O	2.13	0.48
2:C:126:PHE:HZ	6:C:301:LP5:H321	1.78	0.48
1:A:415:ASN:HD21	2:D:125:LEU:H	1.62	0.47
1:A:370:LEU:O	1:A:396:THR:HB	2.14	0.47
1:B:249:LEU:HB3	1:B:282:VAL:HG11	1.95	0.47
1:A:58:ILE:HG22	1:A:79:LEU:HD11	1.97	0.47
1:A:197:LEU:HD23	1:A:225:ILE:HD12	1.95	0.47
2:D:134:VAL:HA	2:D:149:LEU:O	2.14	0.47
1:A:337:ARG:HH12	2:C:101:ASP:CG	2.16	0.47
1:B:307:ASN:HA	1:B:329:LYS:HG3	1.97	0.47
1:A:381:ASN:H	1:A:407:ASN:HD21	1.61	0.47
1:A:301:LYS:HG2	1:A:301:LYS:O	2.13	0.47
2:D:23:TRP:CZ2	2:D:25:CYS:HB3	2.50	0.47
1:A:296:SER:O	1:A:299:ILE:CG2	2.63	0.47
1:B:111:ASN:O	1:B:135:THR:HA	2.15	0.47
2:C:55:ARG:O	2:C:122:GLU:O	2.32	0.47
1:A:179:VAL:HG23	1:A:205:LEU:HD11	1.97	0.47
1:A:87:CYS:N	1:A:111:ASN:HD21	2.02	0.46
1:A:347:ASP:HB3	1:A:369:ALA:HB3	1.96	0.46
1:B:44:LEU:HD13	1:B:48:PRO:HG3	1.98	0.46
1:A:417:MET:HE3	2:D:125:LEU:HB2	1.98	0.46
1:B:134:GLU:HA	1:B:158:HIS:O	2.14	0.46
1:B:430:SER:O	1:B:455:THR:HA	2.15	0.46
1:A:282:VAL:HG23	1:A:284:ILE:HG13	1.96	0.46
2:C:79:PHE:HB2	2:C:134:VAL:HG22	1.97	0.46
1:B:544:LEU:HD21	1:B:547:LEU:HB2	1.97	0.46
1:A:62:PHE:CZ	2:C:68:ARG:HD3	2.51	0.46
1:B:109:THR:HA	1:B:133:VAL:O	2.16	0.46
1:B:370:LEU:O	1:B:396:THR:HB	2.16	0.46
1:B:491:ALA:O	1:B:516:THR:HG21	2.16	0.45
1:A:590:TRP:O	1:A:594:GLN:HB2	2.16	0.45
1:A:473:THR:HG23	1:A:498:PHE:HB3	1.98	0.45
2:C:92:GLU:HA	2:C:92:GLU:OE2	2.16	0.45
1:A:457:THR:O	1:A:479:ASN:HB3	2.17	0.45
1:A:65:LEU:O	1:A:67:ILE:N	2.41	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:ASN:HD21	2:C:128:LYS:HB3	1.81	0.45
2:C:37:CYS:HB2	2:C:148:CYS:HB3	1.86	0.44
1:A:468:LEU:HD13	1:A:471:LEU:HD22	1.99	0.44
6:D:301:LP5:H16	6:D:301:LP5:H191	1.81	0.44
1:B:457:THR:O	1:B:479:ASN:HB3	2.17	0.44
2:C:42:PHE:CD2	2:C:68:ARG:HG3	2.51	0.44
2:D:46:ILE:HG13	2:D:63:VAL:HG22	2.00	0.44
1:A:539:ASN:O	1:A:540:GLN:CB	2.65	0.44
2:D:61:VAL:HG23	2:D:119:PHE:CD2	2.52	0.44
1:B:316:VAL:HG12	1:B:318:ILE:H	1.82	0.44
2:D:73:TYR:CD1	2:D:141:ASP:HB3	2.52	0.44
1:B:242:MET:HG2	1:B:275:ILE:CG2	2.48	0.44
2:C:31:ILE:HD11	2:C:154:ILE:HD12	2.00	0.43
1:B:493:THR:HB	1:B:496:LEU:HD22	1.99	0.43
1:B:86:ARG:HD2	2:D:66:ILE:HG21	2.01	0.43
1:A:86:ARG:HD3	2:C:66:ILE:HG21	2.01	0.43
2:D:124:ILE:HG22	2:D:125:LEU:N	2.33	0.43
2:D:90:ARG:NH1	2:D:92:GLU:OE2	2.52	0.43
1:B:264:ASP:OD1	2:D:103:SER:HB3	2.19	0.43
2:D:90:ARG:NH1	7:D:302:DAO:H31	2.34	0.43
1:A:155:ASN:C	1:A:155:ASN:HD22	2.22	0.42
1:B:179:VAL:HG23	1:B:205:LEU:HD11	2.00	0.42
2:D:42:PHE:HA	2:D:43:PRO:HD3	1.94	0.42
2:D:131:TYR:HB2	2:D:153:ILE:HB	2.01	0.42
1:A:497:THR:HA	1:A:520:LEU:HA	2.02	0.42
1:A:485:THR:HG22	1:A:508:GLN:HB2	2.01	0.42
1:B:348:LEU:HA	1:B:349:PRO:HD3	1.87	0.42
1:A:220:GLN:HG3	1:A:223:GLN:NE2	2.34	0.42
1:A:417:MET:HE1	2:D:124:ILE:HA	2.01	0.42
1:A:276:MET:HG3	1:A:279:LEU:HD23	2.01	0.42
1:B:555:GLU:O	1:B:556:THR:HG23	2.20	0.42
1:A:242:MET:O	1:A:246:LEU:HG	2.19	0.42
1:B:585:GLN:H	1:B:585:GLN:HG3	1.66	0.42
2:C:67:PRO:HD2	2:C:111:GLU:O	2.19	0.42
1:B:70:SER:HA	1:B:96:ALA:HA	2.01	0.42
1:B:164:CYS:O	1:B:164:CYS:SG	2.77	0.42
1:A:462:ASP:HA	1:A:489:VAL:HG12	2.01	0.41
2:C:36:TYR:HE2	2:C:44:ILE:HD12	1.85	0.41
1:A:553:ARG:NH2	1:B:553:ARG:HH22	2.18	0.41
2:C:141:ASP:OD1	2:C:141:ASP:N	2.53	0.41
1:B:32:VAL:CG1	1:B:35:ILE:HB	2.51	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HA	1:A:133:VAL:O	2.21	0.41
1:B:324:VAL:HA	1:B:325:PRO:HD3	1.92	0.41
1:B:295:PHE:CZ	1:B:299:ILE:HG22	2.56	0.41
2:D:52:ILE:HG23	2:D:121:PHE:HZ	1.85	0.41
1:B:198:ARG:NH2	1:B:221:ALA:O	2.54	0.41
1:A:417:MET:HE1	2:D:125:LEU:H	1.83	0.41
1:A:276:MET:HG3	1:A:279:LEU:HD22	2.02	0.41
1:A:370:LEU:HA	1:A:371:PRO:HD2	1.97	0.41
1:B:164:CYS:HB2	1:B:186:ILE:HG21	2.03	0.41
1:B:292:THR:HG22	1:B:294:ASP:O	2.21	0.41
1:A:97:TRP:NE1	1:A:120:SER:O	2.54	0.40
2:D:64:GLU:O	2:D:65:PHE:HB3	2.21	0.40
1:B:151:LEU:HD21	1:B:154:LEU:HD23	2.03	0.40
1:A:556:THR:HG21	1:A:584:HIS:CD2	2.57	0.40
1:A:314:ALA:HA	1:A:336:ILE:O	2.20	0.40
1:A:198:ARG:NH2	1:A:221:ALA:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (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
1	B	114	GLN
1	B	362	SER

### 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	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

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	60	LEU
1	A	68	LEU
1	A	117	SER
1	A	124	LEU
1	A	137	LEU
1	A	155	ASN
1	A	173	LEU
1	A	182	SER
1	A	183	TYR
1	A	197	LEU
1	A	199	GLU
1	A	211	LEU
1	A	220	GLN
1	A	223	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	225	ILE
1	A	240	ASN
1	A	254	VAL
1	A	266	ARG
1	A	276	MET
1	A	279	LEU
1	A	288	ARG
1	A	289	LEU
1	A	296	SER
1	A	298	ASP
1	A	299	ILE
1	A	308	VAL
1	A	312	SER
1	A	321	LEU
1	A	322	GLU
1	A	340	LEU
1	A	347	ASP
1	A	353	SER
1	A	360	LYS
1	A	367	LYS
1	A	378	LEU
1	A	384	SER
1	A	385	PHE
1	A	389	CYS
1	A	400	ARG
1	A	415	ASN
1	A	417	MET
1	A	422	LEU
1	A	433	LYS
1	A	443	SER
1	A	473	THR
1	A	522	LEU
1	A	535	SER
1	A	558	LYS
1	A	571	PHE
1	A	585	GLN
1	A	590	TRP
1	A	601	VAL
2	C	31	ILE
2	C	40	LEU
2	C	44	ILE
2	C	47	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	65	PHE
2	C	71	LEU
2	C	103	SER
2	C	106	ARG
2	C	124	ILE
2	C	146	LEU
1	B	69	LYS
1	B	86	ARG
1	B	113	ILE
1	B	124	LEU
1	B	137	LEU
1	B	148	LEU
1	B	154	LEU
1	B	155	ASN
1	B	173	LEU
1	B	191	VAL
1	B	211	LEU
1	B	219	ASP
1	B	220	GLN
1	B	223	GLN
1	B	225	ILE
1	B	247	GLN
1	B	249	LEU
1	B	254	VAL
1	B	259	LEU
1	B	266	ARG
1	B	274	SER
1	B	276	MET
1	B	279	LEU
1	B	280	CYS
1	B	299	ILE
1	B	322	GLU
1	B	340	LEU
1	B	347	ASP
1	B	356	LEU
1	B	360	LYS
1	B	368	VAL
1	B	378	LEU
1	B	384	SER
1	B	385	PHE
1	B	389	CYS
1	B	392	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	433	LYS
1	B	435	VAL
1	B	437	GLU
1	B	456	ASN
1	B	458	LYS
1	B	494	THR
1	B	496	LEU
1	B	513	VAL
1	B	516	THR
1	B	536	SER
1	B	543	SER
1	B	571	PHE
1	B	577	SER
1	B	582	CYS
1	B	585	GLN
1	B	594	GLN
1	B	596	GLN
1	B	599	VAL
1	B	601	VAL
2	D	23	TRP
2	D	27	SER
2	D	44	ILE
2	D	65	PHE
2	D	71	LEU
2	D	106	ARG
2	D	125	LEU
2	D	132	ARG
2	D	153	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	111	ASN
1	A	129	ASN
1	A	155	ASN
1	A	175	ASN
1	A	223	GLN
1	A	235	ASN
1	A	267	ASN
1	A	359	ASN
1	A	407	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	415	ASN
1	A	428	GLN
1	A	456	ASN
1	A	472	ASN
1	A	521	GLN
1	A	539	ASN
1	A	540	GLN
1	A	576	ASN
2	C	155	HIS
1	B	42	GLN
1	B	98	HIS
1	B	102	HIS
1	B	111	ASN
1	B	155	ASN
1	B	223	GLN
1	B	235	ASN
1	B	267	ASN
1	B	339	GLN
1	B	359	ASN
1	B	484	ASN
1	B	589	GLN
1	B	596	GLN
1	B	600	ASN
2	D	21	GLN
2	D	62	HIS
2	D	83	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
4	B	702	NAG	C2-N2-C7	2.08	125.71	123.04
4	A	803	NAG	C4-C3-C2	3.72	117.01	111.23
4	B	701	NAG	C1-O5-C5	3.82	117.10	112.25
4	B	702	NAG	C1-O5-C5	4.00	117.32	112.25

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

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
6	C	301	LP5	P45-O48	-2.03	1.47	1.54
6	C	301	LP5	P45-O46	2.13	1.62	1.54
3	A	801	NAG	C1-C2	2.22	1.55	1.52
6	C	301	LP5	P45-O47	2.73	1.60	1.51
6	D	301	LP5	P45-O47	3.02	1.61	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
6	D	301	LP5	C8-C7-N2	-2.56	113.16	116.33
6	C	301	LP5	O1-P45-O47	-2.53	100.79	107.11
6	C	301	LP5	C1-C2-N2	-2.47	106.36	111.01
6	D	301	LP5	O46-P45-O47	-2.45	102.70	110.58
6	D	301	LP5	C3-O3-C28	-2.36	113.57	117.75
3	A	801	NAG	C3-C4-C5	-2.35	106.10	110.20
6	D	301	LP5	C3-C2-N2	-2.29	107.09	111.07
6	D	301	LP5	O5-C1-O1	-2.20	108.46	111.36
6	C	301	LP5	C17-C16-C8	-2.16	104.85	112.10
3	A	800	NAG	C2-N2-C7	-2.14	120.29	123.04
6	C	301	LP5	O46-P45-O47	-2.14	103.71	110.58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	300	LP4	C8-C7-N2	-2.01	113.83	116.33
5	D	300	LP4	O5-C5-C6	2.14	111.99	107.35
6	D	301	LP5	O46-P45-O48	2.17	115.64	107.38
5	C	300	LP4	O46-P45-O48	2.23	117.75	110.58
3	A	800	NAG	O5-C5-C6	2.47	112.69	107.35
5	D	300	LP4	O46-P45-O48	2.73	119.37	110.58
6	C	301	LP5	C3-O3-C28	3.04	123.13	117.75
3	A	801	NAG	C1-O5-C5	5.76	119.56	112.25

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 [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 ⓘ

### 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<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	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%)

All (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
1	A	587	PHE	5.0
1	B	97	TRP	5.0
1	A	581	ILE	4.9
1	A	593	GLU	4.7
1	A	33	PRO	4.7
1	B	594	GLN	4.7
1	B	52	PRO	4.6
1	A	589	GLN	4.6
1	A	596	GLN	4.5
1	B	123	GLY	4.5
1	B	27	PRO	4.4
1	B	46	LYS	4.3
1	A	49	ASP	4.3
1	A	590	TRP	4.2
1	B	124	LEU	4.2
2	D	122	GLU	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	99	GLY	4.1
1	A	580	CYS	4.0
1	B	73	PHE	4.0
1	B	300	VAL	4.0
1	A	51	ILE	4.0
1	A	585	GLN	4.0
1	A	55	THR	3.9
1	B	67	ILE	3.9
1	B	590	TRP	3.8
1	B	75	ASN	3.8
1	B	34	ASN	3.8
1	A	323	ASP	3.7
1	B	47	VAL	3.7
1	B	69	LYS	3.7
1	A	69	LYS	3.6
1	A	50	ASP	3.5
1	B	100	LEU	3.4
1	A	322	GLU	3.4
1	B	581	ILE	3.4
1	B	76	PHE	3.4
1	B	580	CYS	3.4
1	A	58	ILE	3.3
1	B	301	LYS	3.3
1	A	597	PHE	3.3
1	B	269	GLU	3.3
1	B	582	CYS	3.2
1	B	33	PRO	3.2
1	B	37	TYR	3.2
1	A	47	VAL	3.1
1	B	98	HIS	3.1
1	B	113	ILE	3.1
2	D	154	ILE	3.1
1	B	270	ILE	3.1
1	A	268	LEU	3.0
1	A	75	ASN	3.0
1	A	592	LYS	2.9
1	B	271	PHE	2.8
1	A	570	PHE	2.8
1	A	542	TYR	2.8
1	A	28	CYS	2.7
1	B	58	ILE	2.7
1	B	151	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	276	MET	2.7
1	B	68	LEU	2.6
1	B	36	THR	2.6
1	B	56	LYS	2.6
1	A	299	ILE	2.6
1	A	71	TYR	2.5
2	C	39	HIS	2.5
1	B	38	GLN	2.5
1	B	304	CYS	2.5
2	C	154	ILE	2.5
1	A	518	HIS	2.5
1	A	599	VAL	2.5
1	B	48	PRO	2.5
1	B	140	LEU	2.5
1	A	76	PHE	2.5
2	C	145	LYS	2.5
1	A	541	LEU	2.5
1	B	71	TYR	2.5
1	B	166	LEU	2.4
1	A	602	GLU	2.4
1	A	46	LYS	2.4
1	B	556	THR	2.4
1	A	551	PHE	2.4
1	A	601	VAL	2.4
2	D	23	TRP	2.3
1	B	79	LEU	2.3
1	B	40	MET	2.3
1	A	606	CYS	2.3
2	C	122	GLU	2.3
1	A	588	LEU	2.3
1	B	51	ILE	2.2
1	B	585	GLN	2.2
1	B	586	LYS	2.2
1	B	125	THR	2.2
1	B	78	GLU	2.2
1	B	156	VAL	2.2
1	B	202	GLN	2.2
1	B	323	ASP	2.2
1	A	98	HIS	2.2
1	A	270	ILE	2.2
1	B	137	LEU	2.2
1	A	31	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	49	ASP	2.2
1	A	74	SER	2.2
1	A	93	GLU	2.2
1	B	45	SER	2.1
1	B	185	TYR	2.1
1	B	60	LEU	2.1
1	B	172	ASN	2.1
1	A	569	ALA	2.1
1	A	595	LYS	2.1
1	B	604	MET	2.1
1	B	141	GLU	2.1
1	B	272	GLU	2.1
1	B	117	SER	2.1
1	A	29	ILE	2.1
1	B	268	LEU	2.1
1	B	118	PRO	2.1
1	A	604	MET	2.1
2	D	64	GLU	2.1
2	D	44	ILE	2.0
1	B	66	LYS	2.0
1	B	606	CYS	2.0
1	B	93	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	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 ⓘ

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(Å <sup>2</sup> )	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 ⓘ

There are no such residues in this entry.