



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:59 PM GMT

PDB ID : 3VQ1  
Title : Crystal structure of mouse TLR4/MD-2/lipid IVa complex  
Authors : Ohto, U.; Shimizu, T.  
Deposited on : 2012-03-17  
Resolution : 2.70 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.

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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

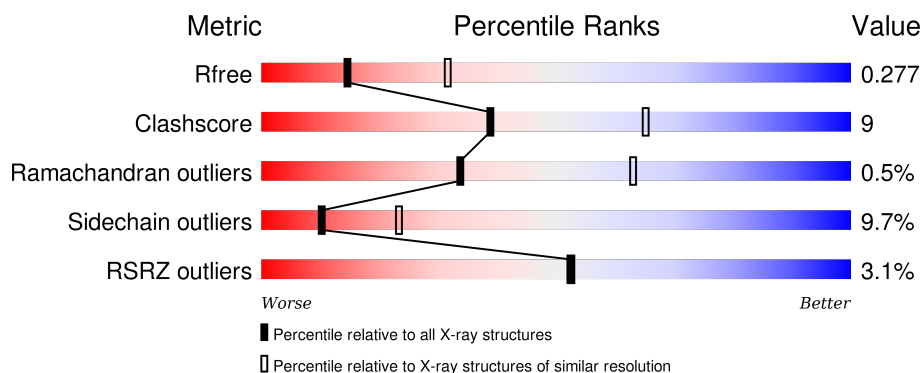
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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  $\geq 3$ , 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>2%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	606	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>
2	C	144	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>• 6%</div> </div> </div>
2	D	144	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	703	-	-	-	X
4	NAG	B	802	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12017 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	596	Total	C	N	O	S	3	0	0
			4749	3040	782	900	27			
1	B	596	Total	C	N	O	S	3	0	0
			4749	3040	782	900	27			

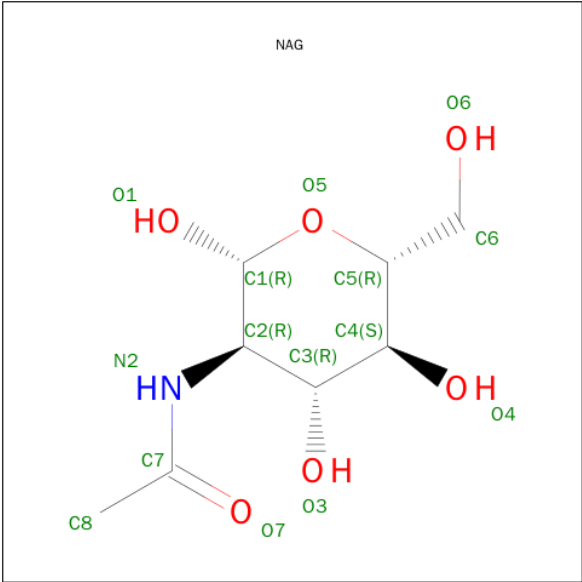
- Molecule 2 is a protein called Lymphocyte antigen 96.

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

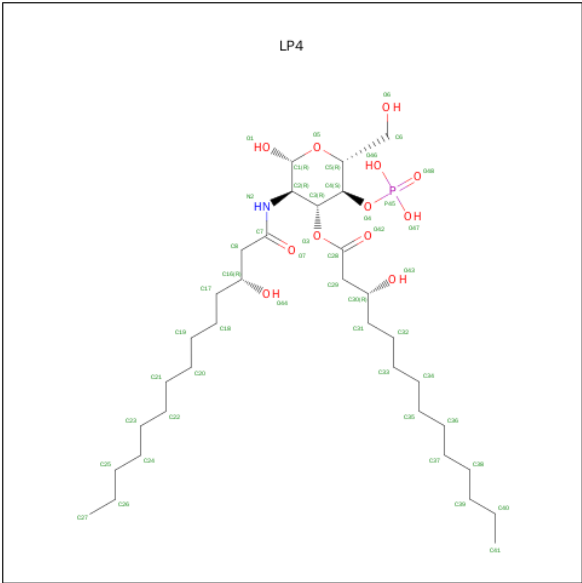
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is 2-DEOXY-3-O-[(3R)-3-HYDROXYTETRADECANOYL]-2-{[(3R)-3-HYDR OXYTETRADECANOYL]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).



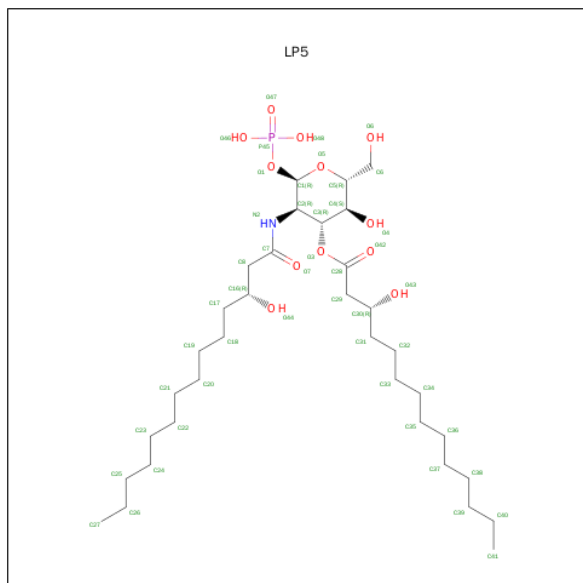
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			45	32	1	11	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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>N<sub>2</sub>O<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		

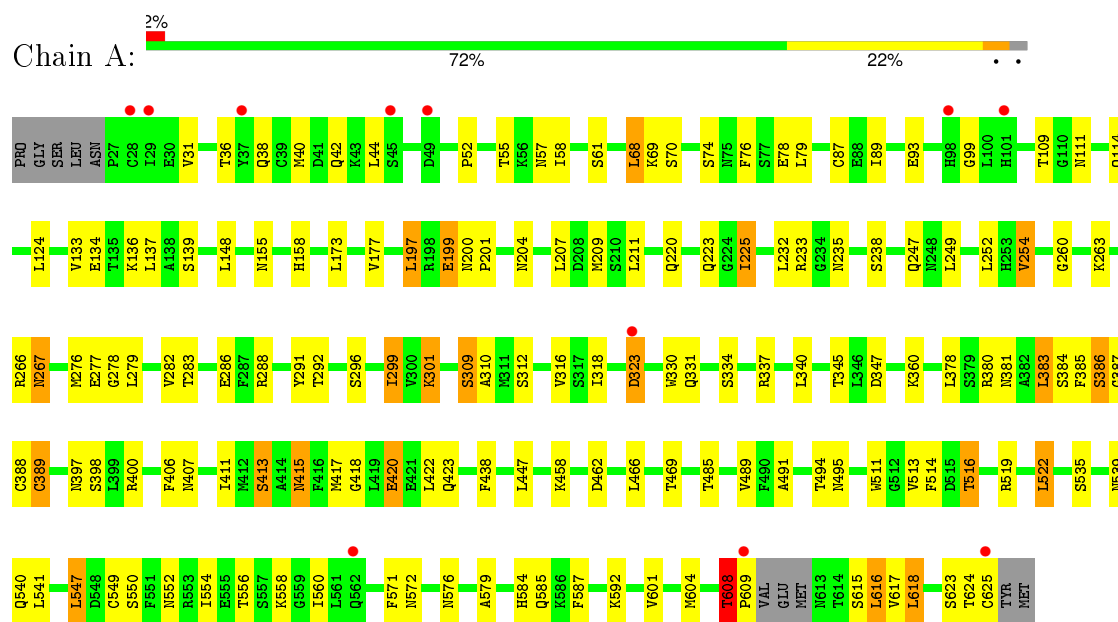
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	15	Total	O	0	0
			15	15		
7	C	4	Total	O	0	0
			4	4		
7	B	17	Total	O	0	0
			17	17		
7	D	1	Total	O	0	0
			1	1		

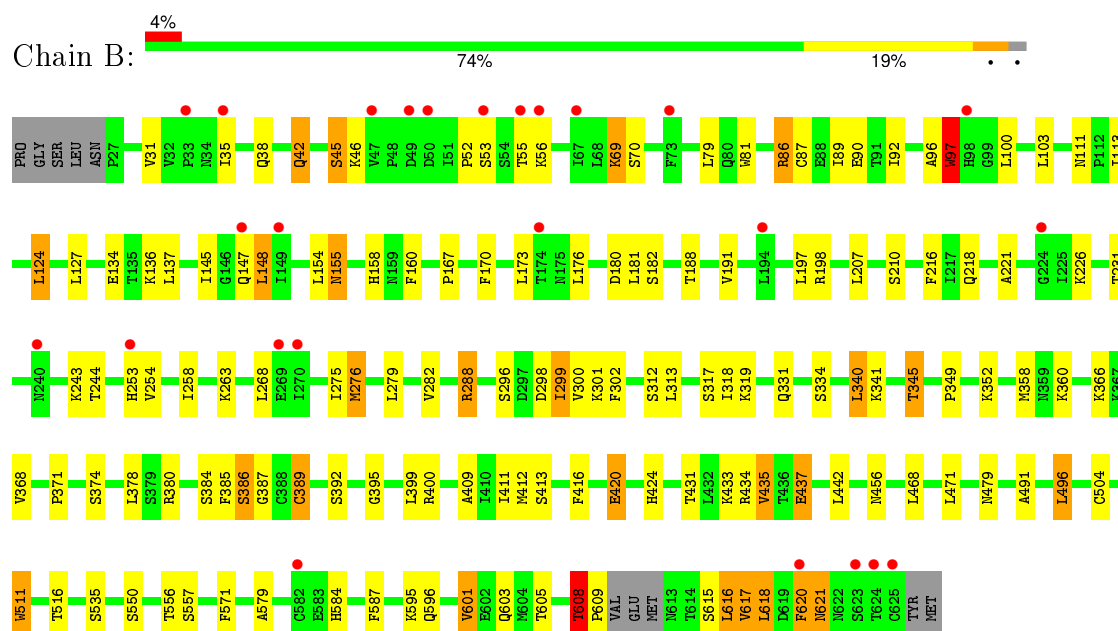
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

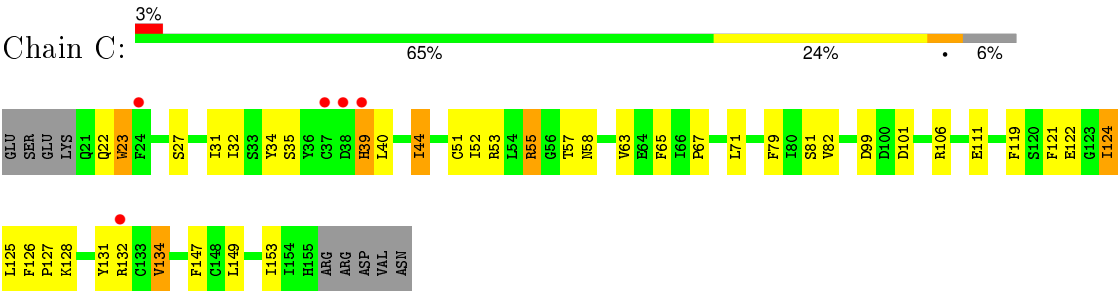
#### • Molecule 1: Toll-like receptor 4



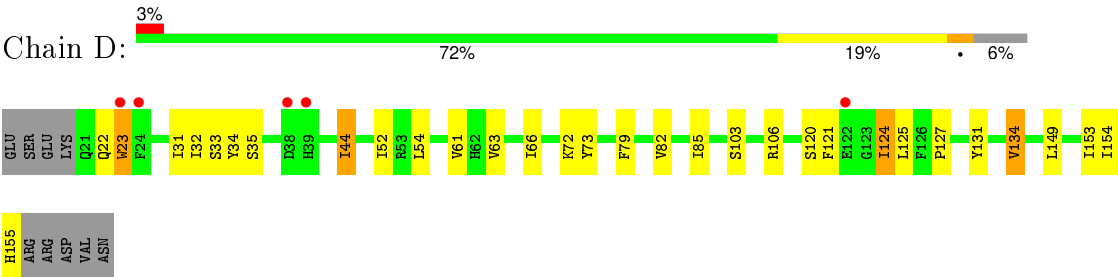
#### • Molecule 1: Toll-like receptor 4



● Molecule 2: Lymphocyte antigen 96



● Molecule 2: Lymphocyte antigen 96





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.16Å 150.52Å 181.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 39.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.70) 96.6 (39.17-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.234 , 0.277 0.223 , 0.277	Depositor DCC
$R_{free}$ test set	2981 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 57152 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: LP5, LP4, NAG

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	2/4848 (0.0%)	0.67	2/6569 (0.0%)
1	B	0.48	3/4848 (0.1%)	0.61	0/6569
2	C	0.50	1/1123 (0.1%)	0.61	0/1519
2	D	0.49	1/1123 (0.1%)	0.57	0/1519
All	All	0.49	7/11942 (0.1%)	0.63	2/16176 (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
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	23	TRP	CD2-CE2	5.54	1.48	1.41
1	A	511	TRP	CD2-CE2	5.43	1.47	1.41
1	B	511	TRP	CD2-CE2	5.39	1.47	1.41
2	C	23	TRP	CD2-CE2	5.31	1.47	1.41
1	B	97	TRP	CD2-CE2	5.25	1.47	1.41
1	A	330	TRP	CD2-CE2	5.19	1.47	1.41
1	B	81	TRP	CD2-CE2	5.15	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	522	LEU	CA-CB-CG	5.62	128.23	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ASP	Peptide
1	A	608	THR	Peptide
1	B	608	THR	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	4749	0	4714	85	0
1	B	4749	0	4714	75	0
2	C	1092	0	1051	32	0
2	D	1092	0	1051	25	0
3	A	56	0	49	0	0
3	B	28	0	25	1	0
4	A	14	0	13	2	0
4	B	14	0	13	1	0
5	C	45	0	55	5	0
5	D	45	0	55	4	0
6	C	48	0	63	5	0
6	D	48	0	63	4	0
7	A	15	0	0	0	0
7	B	17	0	0	2	0
7	C	4	0	0	1	0
7	D	1	0	0	0	0
All	All	12017	0	11866	214	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 9.

All (214) 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:296:SER:O	1:B:299:ILE:HG22	1.49	1.12
1:B:620:PHE:O	1:B:621:ASN:HB2	1.53	1.05
1:A:263:LYS:NZ	5:C:300:LP4:O46	2.04	0.90
1:A:572:ASN:HD22	4:A:705:NAG:C1	1.85	0.89
2:C:53:ARG:HE	2:C:55:ARG:HB3	1.44	0.80
2:C:127:PRO:HA	2:C:128:LYS:HB2	1.63	0.79
1:A:58:ILE:HG22	1:A:79:LEU:HD11	1.67	0.77
1:A:550:SER:OG	4:A:705:NAG:H82	1.85	0.76
2:C:127:PRO:HA	2:C:128:LYS:CB	2.15	0.76
1:A:556:THR:HG21	1:A:584:HIS:HB3	1.68	0.76
2:D:44:ILE:HD13	2:D:149:LEU:HD21	1.70	0.74
1:A:252:LEU:HG	1:A:254:VAL:HG22	1.70	0.73
1:A:207:LEU:HG	1:A:209:MET:HE1	1.71	0.73
1:A:608:THR:HB	1:A:609:PRO:CD	2.17	0.73
1:A:296:SER:O	1:A:299:ILE:HG22	1.88	0.72
1:A:554:ILE:H	1:A:576:ASN:HD22	1.37	0.72
1:A:388:CYS:HA	1:A:389:CYS:HB3	1.73	0.71
1:B:620:PHE:O	1:B:621:ASN:CB	2.35	0.70
2:C:79:PHE:HB2	2:C:134:VAL:HG23	1.72	0.69
1:B:556:THR:HG21	1:B:584:HIS:CG	2.29	0.68
1:B:479:ASN:O	1:B:504:CYS:HA	1.95	0.66
1:B:296:SER:O	1:B:299:ILE:CG2	2.38	0.65
2:D:54:LEU:HD12	2:D:155:HIS:CD2	2.31	0.65
2:D:63:VAL:HG21	5:D:300:LP4:H40A	1.78	0.65
1:B:556:THR:HG21	1:B:584:HIS:HB3	1.79	0.64
2:C:63:VAL:HG21	5:C:300:LP4:H40	1.80	0.64
1:A:286:GLU:HG2	1:A:310:ALA:HB3	1.80	0.64
1:B:124:LEU:O	1:B:148:LEU:HD12	1.98	0.63
1:A:381:ASN:H	1:A:407:ASN:ND2	1.96	0.63
1:A:539:ASN:O	1:A:540:GLN:HB2	1.99	0.63
1:A:388:CYS:HA	1:A:389:CYS:CB	2.28	0.63
1:B:617:VAL:HG22	7:B:912:HOH:O	2.00	0.62
1:A:554:ILE:H	1:A:576:ASN:ND2	1.97	0.62
2:D:72:LYS:HD2	2:D:73:TYR:CE1	2.34	0.62
1:B:608:THR:HB	1:B:609:PRO:CD	2.29	0.61
2:C:44:ILE:HD13	2:C:149:LEU:HD21	1.82	0.61
2:C:79:PHE:HB2	2:C:134:VAL:CG2	2.31	0.61
1:B:300:VAL:HG11	1:B:313:LEU:HD11	1.83	0.61
1:A:491:ALA:O	1:A:516:THR:HG21	2.01	0.60
2:D:44:ILE:CD1	2:D:149:LEU:HD21	2.32	0.60
1:B:97:TRP:HB3	1:B:100:LEU:HD12	1.81	0.60
1:A:296:SER:O	1:A:299:ILE:CG2	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LYS:HD2	1:B:341:LYS:HE2	1.82	0.60
1:B:288:ARG:HG2	1:B:312:SER:HB2	1.84	0.59
1:A:423:GLN:HA	1:A:447:LEU:HA	1.83	0.59
1:B:155:ASN:ND2	1:B:180:ASP:HB3	2.18	0.58
2:D:23:TRP:HB3	2:D:34:TYR:CE1	2.38	0.58
2:C:67:PRO:HD2	2:C:111:GLU:O	2.02	0.58
2:D:131:TYR:HB2	2:D:153:ILE:HB	1.85	0.58
1:B:491:ALA:O	1:B:516:THR:HG21	2.04	0.58
1:A:109:THR:HA	1:A:133:VAL:O	2.04	0.58
1:B:263:LYS:NZ	5:D:300:LP4:O46	2.36	0.57
1:B:345:THR:HG23	1:B:366:LYS:HE3	1.86	0.57
1:B:424:HIS:HE1	7:B:908:HOH:O	1.86	0.57
1:B:434:ARG:O	1:B:437:GLU:HB2	2.04	0.57
1:B:35:ILE:HG23	1:B:56:LYS:HB2	1.86	0.57
1:A:552:ASN:HB2	1:A:576:ASN:HD21	1.69	0.57
1:A:266:ARG:O	1:A:267:ASN:HB2	2.03	0.57
3:B:800:NAG:H62	3:B:801:NAG:C7	2.35	0.57
1:B:87:CYS:H	1:B:111:ASN:HD21	1.52	0.56
1:A:579:ALA:HA	1:A:608:THR:OG1	2.05	0.56
1:B:89:ILE:H	1:B:111:ASN:ND2	2.04	0.56
5:C:300:LP4:H22	6:C:301:LP5:H372	1.87	0.56
2:C:121:PHE:HB2	6:C:301:LP5:H292	1.87	0.56
1:B:550:SER:OG	4:B:802:NAG:H82	2.06	0.56
1:A:623:SER:O	1:A:625:CYS:N	2.32	0.55
1:B:52:PRO:HB2	1:B:55:THR:HG23	1.89	0.55
2:C:44:ILE:HG23	2:C:65:PHE:CG	2.42	0.55
1:A:87:CYS:H	1:A:111:ASN:HD21	1.55	0.55
1:B:556:THR:HG21	1:B:584:HIS:CB	2.36	0.54
1:B:615:SER:HB3	1:B:618:LEU:HD22	1.89	0.54
1:B:374:SER:HA	1:B:399:LEU:HA	1.90	0.54
1:A:207:LEU:CG	1:A:209:MET:HE1	2.38	0.54
1:B:45:SER:HB3	1:B:46:LYS:HD2	1.88	0.54
1:A:556:THR:HG21	1:A:584:HIS:CB	2.36	0.54
1:A:207:LEU:HG	1:A:209:MET:CE	2.37	0.54
1:A:316:VAL:HG12	1:A:318:ILE:H	1.72	0.54
1:A:197:LEU:HD23	1:A:225:ILE:HD13	1.89	0.54
2:C:27:SER:HB3	2:C:51:CYS:HB3	1.90	0.53
1:A:383:LEU:H	1:A:407:ASN:HD22	1.57	0.53
1:B:173:LEU:HD23	1:B:176:LEU:HD22	1.90	0.53
1:A:604:MET:O	1:A:616:LEU:HB3	2.08	0.53
1:B:182:SER:HA	1:B:210:SER:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:PHE:HB2	6:D:301:LP5:H292	1.91	0.52
2:C:131:TYR:HB2	2:C:153:ILE:HB	1.92	0.52
1:A:134:GLU:HA	1:A:158:HIS:O	2.09	0.52
1:A:462:ASP:HA	1:A:489:VAL:HG12	1.92	0.52
2:C:22:GLN:HG2	2:C:35:SER:HA	1.92	0.51
1:A:70:SER:HB2	1:A:93:GLU:OE2	2.09	0.51
1:A:585:GLN:CD	1:A:625:CYS:HB2	2.31	0.51
1:A:608:THR:CB	1:A:609:PRO:CD	2.88	0.51
1:A:199:GLU:HB3	1:A:200:ASN:ND2	2.26	0.51
2:C:44:ILE:HG23	2:C:65:PHE:HB3	1.92	0.51
1:A:89:ILE:H	1:A:111:ASN:HD22	1.57	0.51
1:B:191:VAL:HG12	1:B:221:ALA:HA	1.92	0.51
2:C:81:SER:HB3	2:C:132:ARG:HB3	1.92	0.51
2:D:31:ILE:HG13	2:D:154:ILE:HB	1.92	0.51
1:B:556:THR:HG22	1:B:587:PHE:CD2	2.46	0.50
1:B:579:ALA:HA	1:B:608:THR:OG1	2.11	0.50
2:D:22:GLN:HG2	2:D:35:SER:HA	1.93	0.50
2:C:127:PRO:CA	2:C:128:LYS:CB	2.87	0.50
1:A:52:PRO:O	1:A:55:THR:HG23	2.11	0.50
1:B:42:GLN:HA	1:B:42:GLN:HE21	1.75	0.50
1:A:539:ASN:O	1:A:540:GLN:CB	2.59	0.50
1:A:514:PHE:HB3	1:A:541:LEU:HD21	1.94	0.49
1:A:42:GLN:HB2	1:A:44:LEU:HG	1.95	0.49
2:C:82:VAL:HG22	2:C:131:TYR:CE2	2.47	0.49
1:B:191:VAL:HG22	1:B:218:GLN:OE1	2.13	0.49
2:C:32:ILE:CD1	2:C:52:ILE:HB	2.43	0.48
1:A:387:GLY:HA2	1:A:413:SER:HB3	1.94	0.48
2:D:124:ILE:CG2	2:D:125:LEU:N	2.76	0.48
1:A:288:ARG:NH1	2:C:99:ASP:OD1	2.43	0.48
2:D:52:ILE:HD13	6:D:301:LP5:H371	1.94	0.48
1:A:415:ASN:ND2	1:A:415:ASN:H	2.10	0.48
2:C:52:ILE:HG21	6:C:301:LP5:H371	1.96	0.48
1:B:616:LEU:C	1:B:618:LEU:H	2.15	0.48
1:A:263:LYS:HE3	7:C:404:HOH:O	2.13	0.48
5:D:300:LP4:H35A	5:D:300:LP4:H21	1.94	0.48
2:D:79:PHE:HB2	2:D:134:VAL:HG13	1.96	0.48
1:A:556:THR:HG22	1:A:587:PHE:CD2	2.49	0.47
1:B:608:THR:CB	1:B:609:PRO:CD	2.92	0.47
1:A:301:LYS:HB2	1:A:323:ASP:HB2	1.95	0.47
1:B:79:LEU:HD23	1:B:103:LEU:HD13	1.97	0.47
1:B:318:ILE:HG23	1:B:340:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:PHE:HE1	6:C:301:LP5:H241	1.80	0.47
1:B:136:LYS:HG2	1:B:160:PHE:HE2	1.80	0.47
1:A:615:SER:OG	1:A:616:LEU:N	2.46	0.46
1:A:40:MET:HG3	1:A:61:SER:OG	2.15	0.46
1:B:298:ASP:HB3	1:B:301:LYS:HE3	1.98	0.46
1:A:337:ARG:NH1	2:C:101:ASP:OD1	2.48	0.46
1:A:386:SER:HB2	1:A:411:ILE:HD12	1.98	0.46
1:B:188:THR:HA	1:B:216:PHE:O	2.14	0.46
1:B:331:GLN:HE21	1:B:352:LYS:HE2	1.81	0.46
1:B:389:CYS:O	1:B:416:PHE:HA	2.15	0.46
1:B:124:LEU:HB3	1:B:127:LEU:HB2	1.97	0.46
1:B:134:GLU:HA	1:B:158:HIS:O	2.15	0.46
1:A:233:ARG:HA	1:A:260:GLY:O	2.16	0.46
2:C:126:PHE:CE1	6:C:301:LP5:H241	2.50	0.46
1:B:46:LYS:HE2	1:B:69:LYS:HE3	1.96	0.46
1:A:462:ASP:HB2	2:D:85:ILE:HG23	1.97	0.46
1:B:387:GLY:HA2	1:B:413:SER:OG	2.15	0.46
2:C:44:ILE:HD11	2:C:147:PHE:HB2	1.98	0.46
1:B:409:ALA:HA	1:B:431:THR:HB	1.98	0.46
1:B:331:GLN:NE2	1:B:352:LYS:HE2	2.31	0.45
2:C:39:HIS:H	2:C:39:HIS:CD2	2.35	0.45
1:A:288:ARG:HG2	1:A:312:SER:HB3	1.98	0.45
1:A:309:SER:HB2	1:A:331:GLN:HE21	1.80	0.45
1:A:381:ASN:HB2	1:A:383:LEU:HB2	1.97	0.44
1:A:31:VAL:HG22	1:A:36:THR:HB	1.99	0.44
1:A:608:THR:CB	1:A:609:PRO:HD2	2.47	0.44
1:B:556:THR:HB	1:B:557:SER:H	1.64	0.44
1:B:386:SER:HB2	1:B:411:ILE:HD12	1.99	0.44
1:A:74:SER:HA	1:A:99:GLY:HA3	2.00	0.44
1:B:616:LEU:C	1:B:618:LEU:N	2.71	0.44
1:A:547:LEU:HD22	1:A:549:CYS:SG	2.58	0.44
2:C:119:PHE:CB	5:C:300:LP4:H31	2.47	0.44
1:A:608:THR:HB	1:A:609:PRO:HD2	1.99	0.44
1:A:418:GLY:N	1:A:420:GLU:OE2	2.50	0.44
2:D:61:VAL:HG21	5:D:300:LP4:H23	2.00	0.43
2:C:124:ILE:HG23	2:C:125:LEU:N	2.33	0.43
2:C:44:ILE:CD1	2:C:149:LEU:HD21	2.48	0.43
1:A:199:GLU:O	1:A:201:PRO:HD3	2.17	0.43
2:C:23:TRP:HB3	2:C:34:TYR:CE1	2.53	0.43
2:D:82:VAL:HG11	2:D:127:PRO:HG2	2.00	0.43
1:A:36:THR:HG23	1:A:57:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:MET:HB3	1:B:302:PHE:CE2	2.53	0.43
1:A:247:GLN:HA	1:A:278:GLY:HA3	2.01	0.43
5:C:300:LP4:H32	5:C:300:LP4:H29A	1.49	0.43
1:A:87:CYS:H	1:A:111:ASN:ND2	2.14	0.43
1:B:496:LEU:HA	1:B:496:LEU:HD12	1.87	0.43
1:B:412:MET:HG3	1:B:435:VAL:HG23	2.01	0.43
1:A:299:ILE:C	1:A:299:ILE:HD13	2.39	0.43
1:A:68:LEU:HA	1:A:68:LEU:HD12	1.93	0.43
1:B:92:ILE:HD11	1:B:113:ILE:HD13	2.00	0.43
2:D:121:PHE:CD2	6:D:301:LP5:H292	2.54	0.42
1:A:232:LEU:HA	1:A:235:ASN:HD21	1.85	0.42
2:C:127:PRO:HD3	1:B:442:LEU:HD21	2.01	0.42
1:B:243:LYS:HG3	1:B:275:ILE:HA	2.00	0.42
2:C:44:ILE:HG23	2:C:65:PHE:CB	2.50	0.42
1:A:232:LEU:HA	1:A:235:ASN:ND2	2.34	0.42
1:B:603:GLN:OE1	1:B:603:GLN:N	2.53	0.42
1:B:70:SER:HA	1:B:96:ALA:HA	2.01	0.42
2:D:31:ILE:HD11	2:D:154:ILE:HD12	2.01	0.42
1:A:415:ASN:HD21	2:D:125:LEU:H	1.68	0.42
1:B:468:LEU:HD13	1:B:471:LEU:HD22	2.01	0.42
1:A:266:ARG:O	1:A:267:ASN:CB	2.67	0.41
1:A:415:ASN:ND2	2:D:124:ILE:HG23	2.35	0.41
1:A:263:LYS:HE2	1:A:291:TYR:CE1	2.55	0.41
1:A:556:THR:HG21	1:A:584:HIS:CG	2.55	0.41
1:B:145:ILE:C	1:B:147:GLN:H	2.23	0.41
1:A:469:THR:O	1:A:495:ASN:ND2	2.50	0.41
2:D:32:ILE:HG12	2:D:153:ILE:HD12	2.02	0.41
1:B:349:PRO:HA	1:B:371:PRO:HD2	2.02	0.41
1:B:198:ARG:NH2	1:B:221:ALA:O	2.54	0.41
2:D:82:VAL:HG22	2:D:131:TYR:CE2	2.55	0.41
2:C:44:ILE:HA	2:C:65:PHE:HB3	2.03	0.41
1:B:371:PRO:HA	1:B:395:GLY:O	2.21	0.41
1:B:167:PRO:HD2	1:B:170:PHE:CE1	2.56	0.41
1:B:86:ARG:HD2	2:D:66:ILE:HG21	2.03	0.41
1:B:231:THR:HG23	1:B:258:ILE:HB	2.03	0.41
1:A:114:GLN:HG3	1:A:136:LYS:HB3	2.03	0.41
2:D:34:TYR:CD2	2:D:149:LEU:HD22	2.55	0.40
1:A:438:PHE:HB3	6:D:301:LP5:H201	2.02	0.40
1:B:420:GLU:H	1:B:420:GLU:CD	2.24	0.40
1:B:87:CYS:H	1:B:111:ASN:ND2	2.17	0.40
1:A:220:GLN:HE21	1:A:223:GLN:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:LYS:HB2	1:B:601:VAL:HG11	2.03	0.40
1:B:358:MET:HA	1:B:380:ARG:O	2.21	0.40
1:A:615:SER:HB3	1:A:618:LEU:HD23	2.03	0.40
1:B:226:LYS:HE3	1:B:253:HIS:CD2	2.56	0.40
1:A:380:ARG:HG3	1:A:406:PHE:HB2	2.02	0.40
1:A:420:GLU:HG2	1:A:420:GLU:H	1.59	0.40
1:A:177:VAL:HA	1:A:204:ASN:O	2.21	0.40
2:D:103:SER:O	2:D:106:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	592/606 (98%)	528 (89%)	60 (10%)	4 (1%)	26	55
1	B	592/606 (98%)	529 (89%)	60 (10%)	3 (0%)	34	63
2	C	133/144 (92%)	128 (96%)	5 (4%)	0	100	100
2	D	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
All	All	1450/1500 (97%)	1314 (91%)	129 (9%)	7 (0%)	34	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	621	ASN
1	A	267	ASN
1	A	624	THR
1	B	616	LEU
1	A	560	ILE
1	A	608	THR
1	B	608	THR

### 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	555/564 (98%)	493 (89%)	62 (11%)	7	17
1	B	555/564 (98%)	502 (90%)	53 (10%)	11	24
2	C	122/131 (93%)	110 (90%)	12 (10%)	10	23
2	D	122/131 (93%)	117 (96%)	5 (4%)	37	69
All	All	1354/1390 (97%)	1222 (90%)	132 (10%)	10	23

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	68	LEU
1	A	69	LYS
1	A	76	PHE
1	A	78	GLU
1	A	124	LEU
1	A	137	LEU
1	A	139	SER
1	A	148	LEU
1	A	155	ASN
1	A	173	LEU
1	A	197	LEU
1	A	199	GLU
1	A	211	LEU
1	A	225	ILE
1	A	238	SER
1	A	249	LEU
1	A	254	VAL
1	A	276	MET
1	A	277	GLU
1	A	279	LEU
1	A	282	VAL
1	A	283	THR
1	A	292	THR

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Mol	Chain	Res	Type
1	A	299	ILE
1	A	301	LYS
1	A	309	SER
1	A	334	SER
1	A	340	LEU
1	A	345	THR
1	A	347	ASP
1	A	360	LYS
1	A	378	LEU
1	A	384	SER
1	A	385	PHE
1	A	386	SER
1	A	389	CYS
1	A	397	ASN
1	A	398	SER
1	A	400	ARG
1	A	413	SER
1	A	415	ASN
1	A	417	MET
1	A	420	GLU
1	A	422	LEU
1	A	458	LYS
1	A	466	LEU
1	A	485	THR
1	A	494	THR
1	A	513	VAL
1	A	516	THR
1	A	519	ARG
1	A	522	LEU
1	A	535	SER
1	A	547	LEU
1	A	558	LYS
1	A	571	PHE
1	A	592	LYS
1	A	601	VAL
1	A	616	LEU
1	A	617	VAL
1	A	618	LEU
2	C	31	ILE
2	C	39	HIS
2	C	40	LEU
2	C	44	ILE

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Mol	Chain	Res	Type
2	C	55	ARG
2	C	57	THR
2	C	58	ASN
2	C	71	LEU
2	C	106	ARG
2	C	122	GLU
2	C	124	ILE
2	C	134	VAL
1	B	31	VAL
1	B	38	GLN
1	B	42	GLN
1	B	45	SER
1	B	53	SER
1	B	69	LYS
1	B	86	ARG
1	B	90	GLU
1	B	97	TRP
1	B	124	LEU
1	B	137	LEU
1	B	148	LEU
1	B	154	LEU
1	B	155	ASN
1	B	181	LEU
1	B	197	LEU
1	B	207	LEU
1	B	244	THR
1	B	254	VAL
1	B	268	LEU
1	B	276	MET
1	B	279	LEU
1	B	282	VAL
1	B	288	ARG
1	B	299	ILE
1	B	317	SER
1	B	334	SER
1	B	340	LEU
1	B	345	THR
1	B	360	LYS
1	B	368	VAL
1	B	378	LEU
1	B	384	SER
1	B	385	PHE

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Mol	Chain	Res	Type
1	B	386	SER
1	B	389	CYS
1	B	392	SER
1	B	400	ARG
1	B	420	GLU
1	B	433	LYS
1	B	435	VAL
1	B	437	GLU
1	B	456	ASN
1	B	496	LEU
1	B	511	TRP
1	B	535	SER
1	B	571	PHE
1	B	596	GLN
1	B	601	VAL
1	B	605	THR
1	B	617	VAL
1	B	618	LEU
1	B	620	PHE
2	D	33	SER
2	D	44	ILE
2	D	120	SER
2	D	124	ILE
2	D	134	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) 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	200	ASN
1	A	220	GLN
1	A	223	GLN
1	A	235	ASN
1	A	247	GLN
1	A	255	HIS
1	A	293	ASN
1	A	397	ASN
1	A	407	ASN
1	A	415	ASN

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Mol	Chain	Res	Type
1	A	456	ASN
1	A	539	ASN
1	A	563	HIS
1	A	576	ASN
2	C	39	HIS
2	C	155	HIS
1	B	42	GLN
1	B	57	ASN
1	B	105	ASN
1	B	111	ASN
1	B	129	ASN
1	B	155	ASN
1	B	235	ASN
1	B	253	HIS
1	B	255	HIS
1	B	267	ASN
1	B	331	GLN
1	B	339	GLN
1	B	359	ASN
1	B	424	HIS
1	B	456	ASN
1	B	472	ASN
1	B	518	HIS
1	B	521	GLN
1	B	539	ASN
1	B	562	GLN
1	B	584	HIS
1	B	600	ASN
1	B	621	ASN
2	D	21	GLN
2	D	62	HIS

### 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 ⓘ

6 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	701	1,3	14,14,15	1.60	1 (7%)	15,19,21	1.29	1 (6%)
3	NAG	A	702	3	14,14,15	0.33	0	15,19,21	1.40	2 (13%)
3	NAG	A	703	1,3	14,14,15	0.38	0	15,19,21	2.69	2 (13%)
3	NAG	A	704	3	14,14,15	0.57	0	15,19,21	1.59	2 (13%)
3	NAG	B	800	1,3	14,14,15	0.42	0	15,19,21	1.67	3 (20%)
3	NAG	B	801	3	14,14,15	0.57	0	15,19,21	1.58	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
3	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	704	3	-	0/6/23/26	0/1/1/1
3	NAG	B	800	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	801	3	-	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)
3	A	701	NAG	O5-C1	-5.74	1.34	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	NAG	C3-C4-C5	-4.24	102.80	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	C6-C5-C4	-3.43	104.55	113.02
3	A	702	NAG	C4-C3-C2	-2.83	106.83	111.23
3	B	800	NAG	C6-C5-C4	-2.73	106.27	113.02
3	A	704	NAG	O3-C3-C4	-2.17	105.46	110.34
3	B	800	NAG	C4-C3-C2	2.07	114.45	111.23
3	A	701	NAG	C3-C4-C5	2.12	113.89	110.20
3	A	702	NAG	C1-O5-C5	2.83	115.84	112.25
3	B	801	NAG	O5-C5-C6	3.09	114.05	107.35
3	A	704	NAG	C1-O5-C5	4.18	117.55	112.25
3	B	800	NAG	C1-O5-C5	4.67	118.17	112.25
3	A	703	NAG	C1-O5-C5	8.91	123.56	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	800	NAG	1	0
3	B	801	NAG	1	0

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
4	NAG	A	705	-	14,14,15	0.49	0	15,19,21	1.23	2 (13%)
4	NAG	B	802	1	14,14,15	0.49	0	15,19,21	0.95	0
5	LP4	C	300	6	45,45,48	0.78	1 (2%)	46,56,60	1.06	4 (8%)
6	LP5	C	301	5	47,48,48	0.87	3 (6%)	54,60,60	1.25	3 (5%)
5	LP4	D	300	6	45,45,48	0.74	1 (2%)	46,56,60	1.01	2 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LP5	D	301	5	47,48,48	0.87	2 (4%)	54,60,60	1.20	3 (5%)

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	705	-	-	0/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
5	LP4	C	300	6	-	0/43/60/65	0/1/1/1
6	LP5	C	301	5	-	0/44/65/65	0/1/1/1
5	LP4	D	300	6	-	0/43/60/65	0/1/1/1
6	LP5	D	301	5	-	0/44/65/65	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	LP5	O3-C3	-2.67	1.40	1.44
5	C	300	LP4	P45-O47	2.04	1.62	1.54
5	D	300	LP4	P45-O47	2.07	1.62	1.54
6	D	301	LP5	P45-O46	2.13	1.62	1.54
6	C	301	LP5	P45-O46	2.34	1.63	1.54
6	C	301	LP5	P45-O47	3.53	1.62	1.51
6	D	301	LP5	P45-O47	3.91	1.64	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	LP5	O5-C1-O1	-5.03	104.73	111.36
6	D	301	LP5	C3-O3-C28	-4.69	109.43	117.75
5	D	300	LP4	C3-O3-C28	-3.67	111.24	117.75
4	A	705	NAG	O7-C7-C8	-2.71	117.09	122.06
5	C	300	LP4	P45-O4-C4	-2.67	115.16	121.56
6	D	301	LP5	C3-C2-N2	-2.45	106.80	111.07
6	C	301	LP5	C8-C7-N2	-2.25	113.54	116.33
5	C	300	LP4	O5-C5-C4	-2.07	106.25	110.01
6	C	301	LP5	C3-O3-C28	-2.05	114.11	117.75
4	A	705	NAG	C1-O5-C5	2.03	114.82	112.25
6	D	301	LP5	O46-P45-O48	2.13	115.47	107.38
5	C	300	LP4	O5-C5-C6	2.27	112.26	107.35
5	D	300	LP4	O46-P45-O48	2.62	119.02	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	300	LP4	O46-P45-O48	2.74	119.39	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	NAG	2	0
4	B	802	NAG	1	0
5	C	300	LP4	5	0
6	C	301	LP5	5	0
5	D	300	LP4	4	0
6	D	301	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 ⓘ

### 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	596/606 (98%)	-0.07	11 (1%) 71 72	23, 43, 90, 127	1 (0%)
1	B	596/606 (98%)	0.09	25 (4%) 40 39	27, 56, 103, 136	1 (0%)
2	C	135/144 (93%)	0.12	5 (3%) 45 45	35, 51, 72, 85	1 (0%)
2	D	135/144 (93%)	0.06	5 (3%) 45 45	42, 57, 76, 96	2 (1%)
All	All	1462/1500 (97%)	0.02	46 (3%) 52 52	23, 50, 94, 136	5 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	623	SER	8.0
1	B	624	THR	5.4
1	B	270	ILE	5.3
1	B	625	CYS	4.9
1	B	98	HIS	4.8
1	A	49	ASP	4.1
1	A	323	ASP	4.1
1	B	49	ASP	4.1
1	A	29	ILE	4.0
1	B	35	ILE	3.7
2	D	39	HIS	3.5
1	B	147	GLN	3.4
2	C	24	PHE	3.2
2	D	23	TRP	3.1
2	C	39	HIS	3.1
1	A	28	CYS	3.0
1	A	625	CYS	2.9
1	A	98	HIS	2.9
1	B	50	ASP	2.9
1	B	620	PHE	2.9
1	A	609	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	149	ILE	2.8
1	B	33	PRO	2.7
1	B	73	PHE	2.7
1	B	224	GLY	2.6
1	B	67	ILE	2.6
1	B	240	ASN	2.5
1	B	56	LYS	2.4
2	C	132	ARG	2.4
1	B	47	VAL	2.4
1	A	101	HIS	2.4
1	B	174	THR	2.3
2	D	24	PHE	2.3
1	B	53	SER	2.3
1	B	253	HIS	2.3
1	A	562	GLN	2.2
2	D	122	GLU	2.2
2	D	38	ASP	2.2
2	C	38	ASP	2.1
1	B	194	LEU	2.1
1	B	269	GLU	2.1
1	A	37	TYR	2.1
2	C	37	CYS	2.1
1	B	55	THR	2.1
1	A	45	SER	2.1
1	B	582	CYS	2.0

## 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<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
3	NAG	A	703	14/15	0.93	0.20	4.12	39,43,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	800	14/15	0.96	0.13	-0.48	35,38,43,48	0
3	NAG	A	702	14/15	0.88	0.16	-	41,56,58,61	0
3	NAG	A	701	14/15	0.95	0.17	-	46,48,52,53	0
3	NAG	A	704	14/15	0.87	0.17	-	54,58,72,83	0
3	NAG	B	801	14/15	0.89	0.17	-	46,58,63,67	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
4	NAG	B	802	14/15	0.93	0.27	3.44	46,50,55,59	0
4	NAG	A	705	14/15	0.79	0.25	1.15	50,66,86,87	0
5	LP4	C	300	45/48	0.94	0.18	1.04	37,52,58,63	0
6	LP5	C	301	48/48	0.93	0.22	0.57	43,56,77,82	0
6	LP5	D	301	48/48	0.91	0.21	0.53	63,70,78,89	0
5	LP4	D	300	45/48	0.94	0.17	0.13	54,67,73,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.