



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2016 – 03:34 PM EDT

PDB ID : 5IJC  
Title : The crystal structure of mouse TLR4/MD-2/neoseptin-3 complex  
Authors : Wang, Y.; Su, L.; Morin, M.D.; Jones, B.T.; Whitby, L.R.; Surakattula, M.; Huang, H.; Shi, H.; Choi, J.H.; Wang, K.; Moresco, E.M.; Berger, M.; Zhan, X.; Zhang, H.; Boger, D.L.; Beutler, B.  
Deposited on : 2016-03-01  
Resolution : 2.57 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027257  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027257

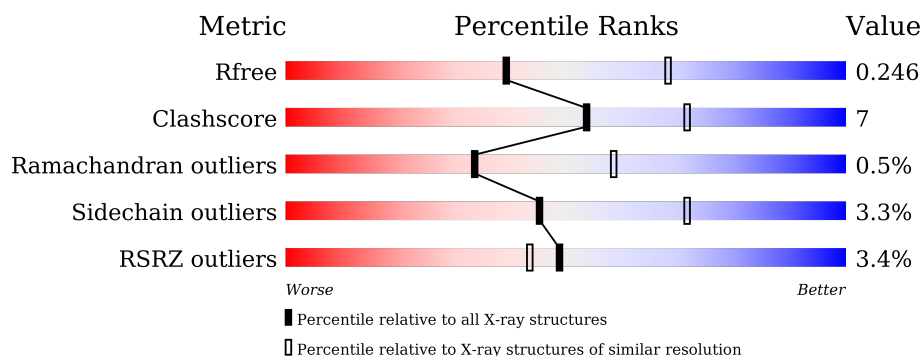
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	594	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	594	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
2	C	150	<div> <div></div> <div> <div>64%</div> <div>26%</div> <div>.</div> <div>9%</div> </div> </div>
2	D	150	<div> <div></div> <div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	703	X	-	-	-
3	NAG	A	704	-	-	-	X
3	NAG	A	706	X	-	-	-
3	NAG	A	707	-	-	-	X
3	NAG	B	701	X	-	-	-
3	NAG	B	704	X	-	-	-
3	NAG	B	706	X	-	-	X
3	NAG	B	708	X	-	-	-
3	NAG	C	203	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12459 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Toll-like receptor 4, Variable lymphocyte receptor B chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	592	Total	C	N	O	S	0	1	0
			4721	3019	786	891	25			
1	B	593	Total	C	N	O	S	0	0	0
			4720	3018	784	893	25			

- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	136	Total	C	N	O	S	0	0	0
			1103	712	186	198	7			
2	D	136	Total	C	N	O	S	0	1	0
			1111	717	189	198	7			

There are 16 discrepancies between the modelled and reference sequences:

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

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



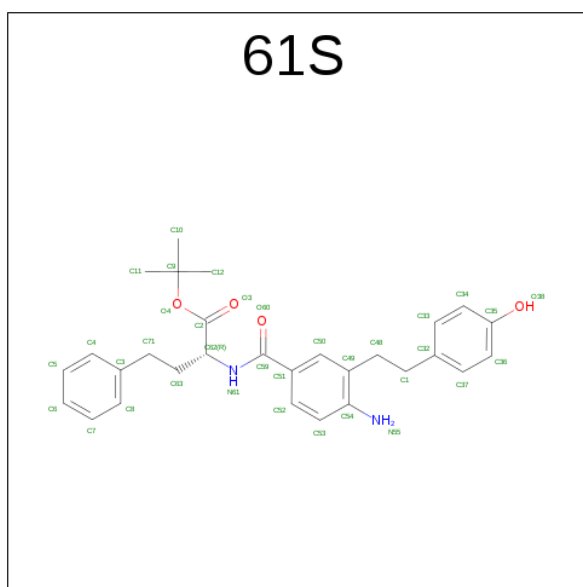
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

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

- Molecule 4 is tert-butyl (2R)-2-({4-amino-3-[2-(4-hydroxyphenyl)ethyl]benzoyl}amino)-4-phenylbutanoate (three-letter code: 61S) (formula: C<sub>29</sub>H<sub>34</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	29	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			35	29	2	4		
4	B	1	Total	C	N	O	0	0
			35	29	2	4		
4	D	1	Total	C	N	O	0	0
			35	29	2	4		

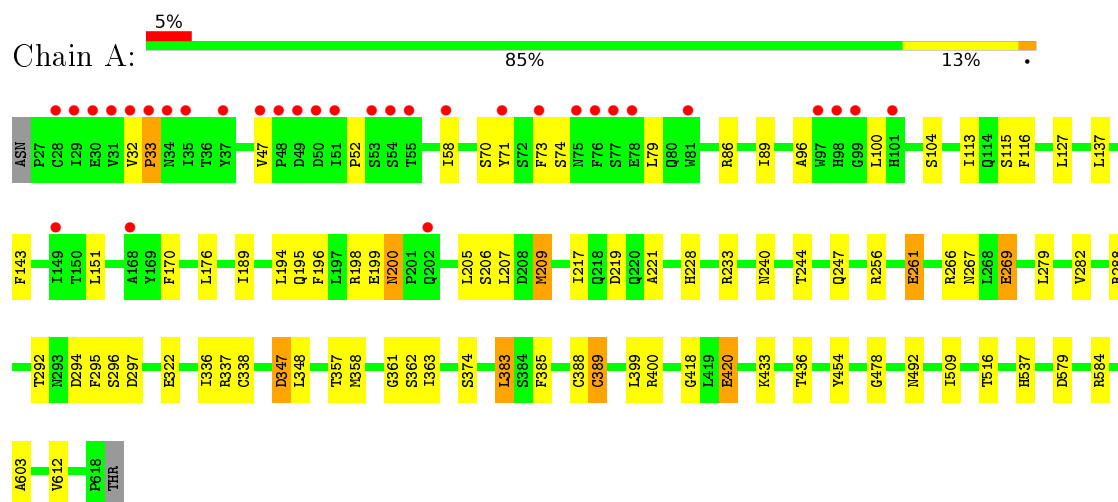
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	149	Total	O	0	0
			149	149		
5	C	33	Total	O	0	0
			33	33		
5	B	122	Total	O	0	0
			122	122		
5	D	38	Total	O	0	0
			38	38		

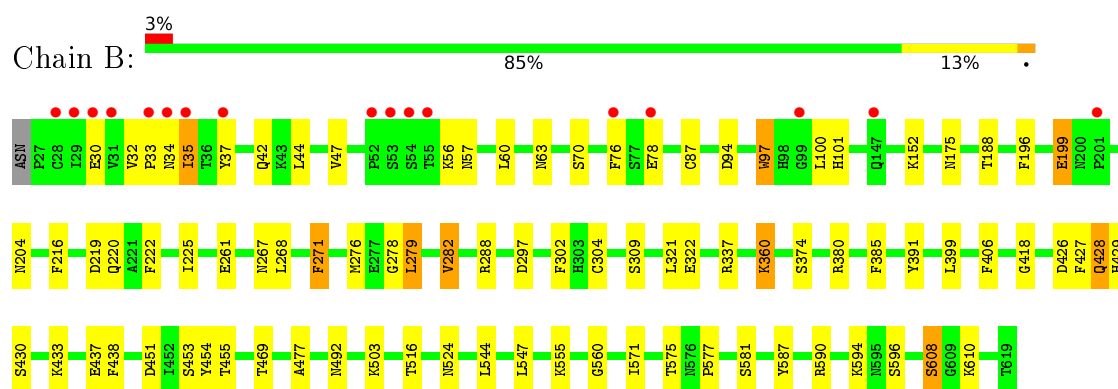
### 3 Residue-property plots

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

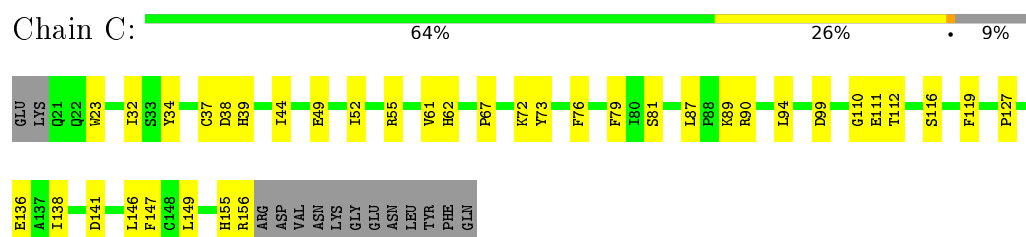
- Molecule 1: Toll-like receptor 4, Variable lymphocyte receptor B chimera



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

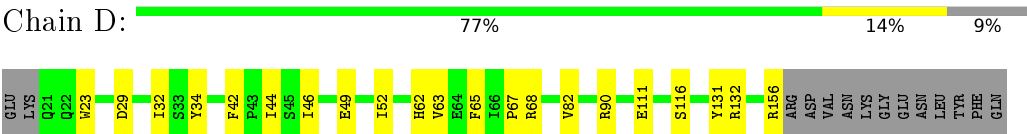


- Molecule 2: Lymphocyte antigen 96





● Molecule 2: Lymphocyte antigen 96



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.75Å 148.56Å 131.72Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	130.34 – 2.57 42.35 – 2.57	Depositor EDS
% Data completeness (in resolution range)	85.3 (130.34-2.57) 85.3 (42.35-2.57)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.197 , 0.247 0.200 , 0.246	Depositor DCC
$R_{free}$ test set	2000 reflections (2.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: 61S, 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	0.78	0/4825	0.90	10/6538 (0.2%)
1	B	0.78	0/4821	0.88	4/6534 (0.1%)
2	C	0.81	0/1134	0.83	0/1533
2	D	0.84	0/1145	0.87	0/1547
All	All	0.79	0/11925	0.88	14/16152 (0.1%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	LEU	CA-CB-CG	9.16	136.37	115.30
1	B	380	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	256	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	337	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	A	297	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	233	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	297	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	337	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	338	CYS	CA-CB-SG	-5.45	104.18	114.00
1	B	337	ARG	NE-CZ-NH1	-5.33	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	256	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	209	MET	CG-SD-CE	-5.21	91.86	100.20
1	A	198	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	GLY	Peptide
1	B	278	GLY	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	4721	0	4707	53	0
1	B	4720	0	4697	59	0
2	C	1103	0	1062	24	0
2	D	1111	0	1075	13	0
3	A	112	0	102	7	0
3	B	126	0	115	4	0
3	C	42	0	38	0	0
3	D	42	0	38	2	0
4	A	35	0	34	1	0
4	B	70	0	67	4	0
4	D	35	0	33	1	0
5	A	149	0	0	9	0
5	B	122	0	0	8	0
5	C	33	0	0	2	0
5	D	38	0	0	3	0
All	All	12459	0	11968	157	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 7.

All (157) 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)
3:A:707:NAG:H83	5:A:860:HOH:O	1.66	0.94
1:B:32:VAL:HB	1:B:35:ILE:HG23	1.52	0.91
1:B:196:PHE:O	1:B:199:GLU:HG3	1.73	0.89
1:B:196:PHE:O	1:B:199:GLU:CG	2.24	0.86
1:A:388:CYS:SG	1:A:389:CYS:HB2	2.17	0.84
1:B:222:PHE:CD2	1:B:225:ILE:HD11	2.18	0.78
1:B:32:VAL:HB	1:B:35:ILE:CG2	2.16	0.74
1:A:436:THR:HG22	5:A:925:HOH:O	1.89	0.71
1:B:516:THR:HB	5:B:877:HOH:O	1.91	0.70
1:A:433:LYS:NZ	5:A:801:HOH:O	2.24	0.70
1:A:189:ILE:CG2	1:A:217:ILE:HG12	2.22	0.69
1:A:288:ARG:HD3	2:C:99:ASP:OD2	1.95	0.66
1:B:406:PHE:CE2	5:B:890:HOH:O	2.48	0.66
1:A:70:SER:HA	1:A:96:ALA:HA	1.77	0.66
1:B:503:LYS:NZ	3:B:707:NAG:H81	2.12	0.65
1:A:86:ARG:NH1	2:C:110:GLY:O	2.30	0.65
1:B:428:GLN:HB3	5:B:890:HOH:O	1.96	0.65
2:C:72:LYS:HD3	2:C:73:TYR:CE2	2.32	0.65
2:D:62:HIS:ND1	2:D:116:SER:OG	2.30	0.64
1:B:391:TYR:HB2	1:B:418:GLY:HA3	1.79	0.64
1:B:35:ILE:HD12	1:B:56:LYS:HD2	1.79	0.63
2:D:90[A]:ARG:NH1	5:D:301:HOH:O	2.30	0.63
1:B:524:ASN:OD1	1:B:524:ASN:C	2.36	0.61
1:B:42:GLN:HB2	1:B:44:LEU:HG	1.81	0.61
3:D:201:NAG:H3	5:D:331:HOH:O	2.02	0.60
1:B:374:SER:HA	1:B:399:LEU:HA	1.83	0.59
2:D:46:ILE:HG12	2:D:63:VAL:HG22	1.83	0.59
1:A:261:GLU:OE2	1:A:267:ASN:HA	2.03	0.58
1:B:594:LYS:O	1:B:594:LYS:HG3	2.02	0.58
1:B:188:THR:HG22	1:B:216:PHE:HB3	1.86	0.57
1:A:104:SER:HA	1:A:127:LEU:HA	1.86	0.57
2:D:32:ILE:HD13	2:D:52:ILE:HB	1.87	0.56
1:A:266:ARG:NH1	3:A:703:NAG:H82	2.20	0.56
2:D:32:ILE:CD1	2:D:52:ILE:HB	2.36	0.56
1:B:276:MET:HB2	1:B:279:LEU:HD22	1.88	0.55
1:B:34:ASN:N	1:B:37:TYR:OH	2.36	0.55
2:D:42:PHE:CD2	2:D:68:ARG:HG3	2.42	0.55
1:A:195:GLN:HG3	5:A:926:HOH:O	2.06	0.55
1:A:418:GLY:N	1:A:420:GLU:OE2	2.40	0.54
1:A:418:GLY:CA	1:A:420:GLU:OE2	2.55	0.54
1:B:204:ASN:HD22	3:B:702:NAG:H83	1.72	0.54
2:D:23:TRP:HB3	2:D:34:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:87:LEU:HD21	4:B:710:61S:H33	1.90	0.53
1:B:555:LYS:HG2	1:B:577:PRO:O	2.08	0.53
1:A:32:VAL:HG13	1:A:33:PRO:HD2	1.91	0.53
3:D:202:NAG:O3	3:D:203:NAG:O5	2.20	0.53
1:A:206:SER:OG	1:A:228:HIS:HB3	2.10	0.52
4:B:710:61S:H15	4:B:711:61S:H15	1.92	0.52
1:B:321:LEU:HD23	1:B:321:LEU:C	2.30	0.52
1:B:271:PHE:CD1	1:B:271:PHE:C	2.83	0.52
1:B:426:ASP:OD1	1:B:451:ASP:HB3	2.10	0.52
2:C:76:PHE:HE1	2:C:94:LEU:HD12	1.75	0.52
1:A:266:ARG:HH11	3:A:703:NAG:H82	1.76	0.51
1:A:73:PHE:HB3	1:A:100:LEU:HD21	1.92	0.51
2:C:23:TRP:HB3	2:C:34:TYR:CE1	2.45	0.51
1:A:492:ASN:HB3	5:A:927:HOH:O	2.10	0.51
3:A:704:NAG:C8	5:A:922:HOH:O	2.58	0.51
1:B:360:LYS:HB3	5:B:902:HOH:O	2.12	0.50
1:A:294:ASP:C	1:A:294:ASP:OD1	2.50	0.50
1:A:137:LEU:HD11	1:A:143:PHE:CD1	2.47	0.50
1:A:189:ILE:HG23	1:A:217:ILE:HG23	1.94	0.49
1:A:199:GLU:HB2	1:A:200:ASN:OD1	2.13	0.49
1:A:189:ILE:HG22	1:A:217:ILE:HG12	1.93	0.49
1:A:516:THR:HB	5:A:902:HOH:O	2.13	0.49
2:D:46:ILE:HA	2:D:62:HIS:O	2.13	0.49
1:B:271:PHE:C	1:B:271:PHE:HD1	2.15	0.48
1:B:204:ASN:HA	5:B:909:HOH:O	2.12	0.48
2:D:44:ILE:HG13	2:D:65:PHE:HB3	1.94	0.48
3:A:707:NAG:H62	3:A:708:NAG:H82	1.95	0.48
1:B:469:THR:HG21	3:B:705:NAG:H82	1.95	0.48
1:A:244:THR:O	1:A:247:GLN:HB2	2.14	0.48
1:A:113:ILE:HD11	1:A:116:PHE:CZ	2.49	0.48
4:A:709:61S:H5	4:A:709:61S:O3	2.14	0.48
2:C:127:PRO:HD3	4:B:710:61S:H31	1.95	0.48
1:A:207:LEU:HD13	1:A:209:MET:CE	2.44	0.48
1:B:279:LEU:HA	1:B:282:VAL:HG13	1.96	0.48
3:A:705:NAG:H61	5:A:941:HOH:O	2.13	0.48
2:D:67:PRO:HD2	2:D:111:GLU:O	2.14	0.47
1:B:152:LYS:HA	1:B:175:ASN:O	2.14	0.47
1:B:575:THR:O	1:B:575:THR:HG22	2.14	0.47
1:B:63:ASN:O	1:B:87:CYS:HA	2.14	0.47
1:B:608:SER:HB2	1:B:610:LYS:HB2	1.96	0.47
1:B:78:GLU:O	1:B:78:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:LYS:HZ1	3:B:707:NAG:H81	1.79	0.47
1:B:97:TRP:CB	1:B:100:LEU:HD12	2.45	0.47
1:B:406:PHE:CD2	5:B:890:HOH:O	2.68	0.47
2:C:87:LEU:N	2:C:87:LEU:HD12	2.29	0.47
1:A:516:THR:HG22	1:A:516:THR:O	2.15	0.46
1:B:261:GLU:OE2	1:B:267:ASN:HA	2.16	0.46
2:C:32:ILE:HD13	2:C:52:ILE:HB	1.98	0.46
1:A:336:ILE:HG12	1:A:357:THR:HG22	1.97	0.46
2:C:112:THR:CG2	5:C:319:HOH:O	2.64	0.46
1:B:30:GLU:OE2	1:B:33:PRO:HA	2.16	0.46
1:B:70:SER:OG	1:B:94:ASP:O	2.25	0.46
1:B:97:TRP:HB3	1:B:100:LEU:HD12	1.98	0.46
1:A:151:LEU:HD23	1:A:176:LEU:HD13	1.98	0.45
1:B:437:GLU:O	1:B:438:PHE:HB3	2.16	0.45
2:C:76:PHE:CE1	2:C:94:LEU:HD12	2.52	0.45
1:A:363:ILE:O	1:A:383:LEU:HA	2.16	0.45
1:B:544:LEU:HD21	1:B:547:LEU:HB2	1.98	0.45
1:A:347:ASP:O	1:A:348:LEU:C	2.55	0.45
2:C:62:HIS:CE1	2:C:116:SER:HG	2.34	0.45
1:B:453:SER:HB3	1:B:454:TYR:CD2	2.52	0.45
1:A:269:GLU:H	1:A:269:GLU:HG3	1.68	0.44
1:A:89:ILE:O	1:A:113:ILE:HG22	2.17	0.44
2:D:62:HIS:CE1	2:D:116:SER:OG	2.70	0.44
1:A:170:PHE:HB3	1:A:196:PHE:CZ	2.52	0.44
1:B:596:SER:HA	5:B:838:HOH:O	2.17	0.44
1:A:537:HIS:ND1	5:A:804:HOH:O	2.32	0.44
3:A:705:NAG:H82	3:A:705:NAG:O3	2.18	0.44
1:A:47:VAL:HG23	1:A:47:VAL:O	2.16	0.44
1:A:374:SER:HA	1:A:399:LEU:HA	2.00	0.44
1:A:362:SER:O	1:A:363:ILE:HG23	2.18	0.44
1:A:400:ARG:HH11	1:A:400:ARG:HG2	1.82	0.44
2:C:55:ARG:HG3	5:C:302:HOH:O	2.18	0.44
1:B:430:SER:O	1:B:455:THR:HA	2.18	0.44
2:C:155:HIS:O	2:C:156:ARG:HB3	2.17	0.43
2:C:67:PRO:HD2	2:C:111:GLU:O	2.18	0.43
1:A:58:ILE:HG22	1:A:79:LEU:HD11	2.00	0.43
2:C:79:PHE:CE1	2:C:89:LYS:HG3	2.53	0.43
2:D:156:ARG:HD3	5:D:336:HOH:O	2.18	0.43
1:A:194:LEU:HD12	1:A:221:ALA:O	2.18	0.43
1:B:196:PHE:O	1:B:199:GLU:HG2	2.12	0.43
1:B:219:ASP:OD1	1:B:220:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HA	1:A:282:VAL:HG13	2.00	0.43
2:C:146:LEU:O	2:C:147:PHE:HB3	2.18	0.43
1:A:388:CYS:HA	1:A:389:CYS:HA	1.83	0.43
1:B:279:LEU:HA	1:B:282:VAL:CG1	2.48	0.43
2:C:131:TYR:N	2:C:131:TYR:CD1	2.87	0.43
2:C:61:VAL:HG23	2:C:119:PHE:CD2	2.53	0.43
2:C:136:GLU:HG2	2:C:138:ILE:HD11	2.01	0.43
1:A:603:ALA:O	1:A:612:VAL:HG23	2.19	0.42
1:B:47:VAL:HG11	1:B:76:PHE:HE2	1.85	0.42
1:B:34:ASN:H	1:B:37:TYR:HH	1.64	0.42
1:A:295:PHE:CD1	1:A:296:SER:N	2.87	0.42
4:B:710:61S:O3	4:B:710:61S:H14	2.19	0.42
1:B:560:GLY:HA2	1:B:587:TYR:CE2	2.54	0.42
1:A:579:ASP:OD1	1:A:579:ASP:C	2.57	0.42
1:A:516:THR:CG2	1:A:516:THR:O	2.67	0.41
2:C:34:TYR:CD2	2:C:149:LEU:HD22	2.55	0.41
1:B:35:ILE:HG13	1:B:35:ILE:O	2.20	0.41
2:C:155:HIS:O	2:C:156:ARG:CB	2.68	0.41
1:A:509:ILE:HB	1:A:537:HIS:CE1	2.55	0.41
1:A:454:TYR:CD1	1:A:478:GLY:HA3	2.55	0.41
1:B:453:SER:HA	1:B:477:ALA:O	2.20	0.41
1:A:86:ARG:O	1:A:86:ARG:CG	2.67	0.41
2:D:90[B]:ARG:HH12	4:D:204:61S:C59	2.34	0.41
1:B:32:VAL:CB	1:B:35:ILE:CG2	2.95	0.41
1:B:427:PHE:O	1:B:428:GLN:C	2.59	0.41
1:A:295:PHE:CD1	1:A:295:PHE:C	2.95	0.40
1:B:590:ARG:NH2	5:B:815:HOH:O	2.53	0.40
1:B:225:ILE:HG21	1:B:225:ILE:HD13	1.84	0.40
2:C:37:CYS:C	2:C:39:HIS:H	2.25	0.40
1:B:302:PHE:HE2	1:B:304:CYS:SG	2.45	0.40
1:B:547:LEU:O	1:B:571:ILE:HA	2.22	0.40
2:C:141:ASP:N	2:C:141:ASP:OD1	2.55	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	591/594 (100%)	524 (89%)	65 (11%)	2 (0%)	46	70
1	B	591/594 (100%)	538 (91%)	51 (9%)	2 (0%)	46	70
2	C	134/150 (89%)	123 (92%)	9 (7%)	2 (2%)	13	25
2	D	135/150 (90%)	130 (96%)	4 (3%)	1 (1%)	26	49
All	All	1451/1488 (98%)	1315 (91%)	129 (9%)	7 (0%)	34	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	GLN
1	B	429	HIS
2	D	29	ASP
2	C	38	ASP
2	C	44	ILE
1	A	33	PRO
1	A	52	PRO

### 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	550/551 (100%)	534 (97%)	16 (3%)	50	76
1	B	550/551 (100%)	531 (96%)	19 (4%)	43	70
2	C	123/136 (90%)	117 (95%)	6 (5%)	31	56
2	D	124/136 (91%)	120 (97%)	4 (3%)	46	73
All	All	1347/1374 (98%)	1302 (97%)	45 (3%)	45	71

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	74	SER
1	A	115	SER
1	A	200	ASN
1	A	205	LEU
1	A	219	ASP
1	A	240	ASN
1	A	261	GLU
1	A	269	GLU
1	A	292	THR
1	A	322	GLU
1	A	347	ASP
1	A	385	PHE
1	A	389	CYS
1	A	420	GLU
1	A	584	ARG
2	C	49	GLU
2	C	81	SER
2	C	90	ARG
2	C	130	HIS
2	C	131	TYR
2	C	134	VAL
1	B	35	ILE
1	B	57	ASN
1	B	60	LEU
1	B	97	TRP
1	B	101	HIS
1	B	199	GLU
1	B	268	LEU
1	B	271	PHE
1	B	279	LEU
1	B	282	VAL
1	B	288	ARG
1	B	309	SER
1	B	322	GLU
1	B	360	LYS
1	B	385	PHE
1	B	433	LYS
1	B	492	ASN
1	B	581	SER
1	B	608	SER
2	D	49	GLU
2	D	82	VAL

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Mol	Chain	Res	Type
2	D	131	TYR
2	D	132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	701	1,3	14,14,15	0.71	0	15,19,21	1.95	5 (33%)
3	NAG	A	702	3	14,14,15	0.71	0	15,19,21	1.07	0
3	NAG	A	703	1	14,14,15	0.80	1 (7%)	15,19,21	1.34	2 (13%)
3	NAG	A	704	1	14,14,15	0.66	0	15,19,21	1.95	6 (40%)
3	NAG	A	705	1	14,14,15	0.88	1 (7%)	15,19,21	2.51	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	706	1	14,14,15	1.07	1 (7%)	15,19,21	2.37	6 (40%)
3	NAG	A	707	1,3	14,14,15	0.61	0	15,19,21	3.26	9 (60%)
3	NAG	A	708	3	14,14,15	0.63	0	15,19,21	1.96	5 (33%)
4	61S	A	709	-	37,37,37	1.51	2 (5%)	50,51,51	2.13	11 (22%)
3	NAG	B	701	1	14,14,15	1.30	2 (14%)	15,19,21	2.33	4 (26%)
3	NAG	B	702	1	14,14,15	0.84	1 (7%)	15,19,21	2.12	5 (33%)
3	NAG	B	703	1	14,14,15	0.89	1 (7%)	15,19,21	1.95	5 (33%)
3	NAG	B	704	1	14,14,15	0.85	1 (7%)	15,19,21	1.89	3 (20%)
3	NAG	B	705	1	14,14,15	1.11	1 (7%)	15,19,21	2.62	9 (60%)
3	NAG	B	706	1,3	14,14,15	0.72	0	15,19,21	2.07	4 (26%)
3	NAG	B	707	3	14,14,15	0.79	0	15,19,21	1.24	3 (20%)
3	NAG	B	708	1,3	14,14,15	1.08	1 (7%)	15,19,21	2.24	8 (53%)
3	NAG	B	709	3	14,14,15	0.85	1 (7%)	15,19,21	2.24	5 (33%)
4	61S	B	710	-	37,37,37	1.34	1 (2%)	50,51,51	2.52	12 (24%)
4	61S	B	711	-	37,37,37	1.32	1 (2%)	50,51,51	1.70	9 (18%)
3	NAG	C	201	3,2	14,14,15	0.60	0	15,19,21	2.71	8 (53%)
3	NAG	C	202	3	14,14,15	0.83	1 (7%)	15,19,21	1.76	5 (33%)
3	NAG	C	203	2	14,14,15	0.81	1 (7%)	15,19,21	2.26	5 (33%)
3	NAG	D	201	2	14,14,15	0.63	0	15,19,21	1.68	4 (26%)
3	NAG	D	202	3,2	14,14,15	0.75	0	15,19,21	1.79	4 (26%)
3	NAG	D	203	3	14,14,15	0.88	0	15,19,21	1.31	2 (13%)
4	61S	D	204	-	37,37,37	1.49	3 (8%)	50,51,51	1.64	7 (14%)

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	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	704	1	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1	-	0/6/23/26	0/1/1/1
3	NAG	A	706	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	707	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	708	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	61S	A	709	-	-	0/27/27/27	0/3/3/3
3	NAG	B	701	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	704	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
3	NAG	B	706	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	707	3	-	0/6/23/26	0/1/1/1
3	NAG	B	708	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	709	3	-	0/6/23/26	0/1/1/1
4	61S	B	710	-	-	0/27/27/27	0/3/3/3
4	61S	B	711	-	-	0/27/27/27	0/3/3/3
3	NAG	C	201	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	202	3	-	0/6/23/26	0/1/1/1
3	NAG	C	203	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	201	2	-	0/6/23/26	0/1/1/1
3	NAG	D	202	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	203	3	-	0/6/23/26	0/1/1/1
4	61S	D	204	-	-	0/27/27/27	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	204	61S	O4-C9	-2.78	1.43	1.48
4	A	709	61S	C54-C49	-2.33	1.37	1.40
3	C	203	NAG	O5-C1	-2.13	1.40	1.43
3	C	202	NAG	O5-C1	-2.02	1.40	1.43
4	D	204	61S	C52-C51	2.01	1.42	1.39
3	B	709	NAG	C1-C2	2.04	1.55	1.52
3	B	701	NAG	C2-N2	2.11	1.50	1.46
3	A	705	NAG	C1-C2	2.19	1.55	1.52
3	B	702	NAG	C1-C2	2.22	1.55	1.52
3	A	703	NAG	C1-C2	2.35	1.55	1.52
3	B	703	NAG	C1-C2	2.38	1.55	1.52
3	B	704	NAG	C1-C2	2.44	1.55	1.52
3	B	705	NAG	C1-C2	2.62	1.56	1.52
3	A	706	NAG	C1-C2	2.95	1.56	1.52
3	B	708	NAG	C1-C2	3.17	1.57	1.52
3	B	701	NAG	C1-C2	3.80	1.57	1.52
4	B	711	61S	O4-C2	6.21	1.44	1.33
4	D	204	61S	O4-C2	7.26	1.46	1.33
4	B	710	61S	O4-C2	7.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	709	61S	O4-C2	7.62	1.46	1.33

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	706	NAG	O5-C5-C4	-5.02	101.82	110.13
4	B	710	61S	O4-C2-O3	-4.42	116.44	125.61
3	C	201	NAG	C4-C3-C2	-4.34	104.61	111.34
3	A	707	NAG	O7-C7-N2	-4.03	113.64	121.84
3	A	707	NAG	O3-C3-C2	-3.98	100.85	109.37
3	B	706	NAG	C2-N2-C7	-3.94	117.98	123.11
3	B	701	NAG	O7-C7-C8	-3.89	114.91	122.07
3	B	701	NAG	O5-C5-C4	-3.83	103.79	110.13
3	B	704	NAG	O5-C5-C4	-3.80	103.83	110.13
3	B	706	NAG	O3-C3-C2	-3.76	101.32	109.37
3	A	708	NAG	C2-N2-C7	-3.65	118.35	123.11
4	B	710	61S	C10-C9-C12	-3.64	101.01	111.17
3	A	707	NAG	C6-C5-C4	-3.60	103.96	112.99
4	A	709	61S	O4-C2-O3	-3.56	118.21	125.61
3	B	708	NAG	C4-C3-C2	-3.46	105.97	111.34
3	B	708	NAG	O7-C7-C8	-3.38	115.86	122.07
4	B	710	61S	O3-C2-C62	-3.17	115.27	124.08
3	A	706	NAG	O7-C7-C8	-3.15	116.28	122.07
3	A	708	NAG	C4-C3-C2	-3.10	106.52	111.34
3	C	203	NAG	C4-C3-C2	-3.09	106.54	111.34
3	B	703	NAG	C4-C3-C2	-3.02	106.65	111.34
3	C	201	NAG	O4-C4-C3	-3.00	103.58	110.36
3	A	703	NAG	O5-C5-C4	-2.99	105.18	110.13
4	B	711	61S	C48-C49-C54	-2.97	117.90	122.84
3	B	704	NAG	O7-C7-C8	-2.91	116.71	122.07
3	A	707	NAG	C4-C3-C2	-2.78	107.02	111.34
3	B	702	NAG	C3-C4-C5	-2.76	105.31	110.23
3	B	709	NAG	O7-C7-C8	-2.69	117.12	122.07
3	A	705	NAG	O7-C7-C8	-2.68	117.13	122.07
4	B	710	61S	C9-O4-C2	-2.62	117.72	121.68
4	D	204	61S	C51-C59-N61	-2.61	112.42	116.98
3	A	701	NAG	O4-C4-C5	-2.60	102.37	109.23
4	A	709	61S	O3-C2-C62	-2.59	116.87	124.08
3	B	705	NAG	O7-C7-C8	-2.58	117.32	122.07
3	D	202	NAG	O6-C6-C5	-2.43	103.19	111.30
3	B	702	NAG	O7-C7-C8	-2.40	117.64	122.07
4	B	710	61S	C53-C52-C51	-2.32	118.02	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	202	NAG	O7-C7-C8	-2.30	117.83	122.07
4	A	709	61S	C48-C49-C54	-2.29	119.03	122.84
4	B	710	61S	C51-C59-N61	-2.29	112.99	116.98
3	B	707	NAG	O3-C3-C4	-2.28	105.21	110.36
4	B	711	61S	C53-C54-N55	-2.28	115.60	120.16
3	A	705	NAG	O5-C5-C4	-2.27	106.37	110.13
3	B	703	NAG	O7-C7-C8	-2.24	117.94	122.07
3	A	701	NAG	O6-C6-C5	-2.22	103.88	111.30
4	A	709	61S	C12-C9-C11	-2.21	104.99	111.17
4	A	709	61S	C50-C49-C54	-2.19	117.18	118.97
3	D	202	NAG	O4-C4-C5	-2.18	103.49	109.23
3	A	704	NAG	C4-C3-C2	-2.17	107.98	111.34
3	B	707	NAG	C8-C7-N2	-2.13	112.00	116.10
3	B	702	NAG	O7-C7-N2	-2.08	117.61	121.84
3	A	704	NAG	O7-C7-C8	-2.05	118.29	122.07
4	D	204	61S	C52-C53-C54	-2.05	118.80	121.35
3	A	704	NAG	O5-C5-C4	2.01	113.46	110.13
3	C	202	NAG	O5-C5-C4	2.01	113.46	110.13
4	B	711	61S	C48-C49-C50	2.08	123.60	119.35
3	B	708	NAG	O5-C5-C4	2.12	113.64	110.13
3	B	705	NAG	O4-C4-C5	2.12	114.81	109.23
4	A	709	61S	C1-C48-C49	2.15	116.10	112.77
3	B	707	NAG	O4-C4-C5	2.15	114.89	109.23
4	A	709	61S	C48-C49-C50	2.17	123.79	119.35
3	B	708	NAG	O3-C3-C4	2.18	115.28	110.36
4	B	710	61S	C1-C48-C49	2.20	116.19	112.77
3	D	202	NAG	C1-O5-C5	2.23	115.42	112.14
3	B	705	NAG	O7-C7-N2	2.24	126.40	121.84
3	C	201	NAG	O3-C3-C2	2.29	114.27	109.37
3	C	201	NAG	C3-C4-C5	2.31	114.35	110.23
3	A	704	NAG	C3-C4-C5	2.31	114.35	110.23
3	D	201	NAG	C3-C4-C5	2.34	114.40	110.23
3	C	202	NAG	C2-N2-C7	2.35	126.16	123.11
3	B	703	NAG	O3-C3-C2	2.37	114.44	109.37
3	A	706	NAG	C8-C7-N2	2.37	120.65	116.10
3	B	709	NAG	O7-C7-N2	2.39	126.72	121.84
3	A	703	NAG	C1-O5-C5	2.40	115.66	112.14
3	A	708	NAG	O5-C5-C4	2.40	114.12	110.13
4	B	710	61S	C49-C54-N55	2.43	122.67	120.70
4	B	711	61S	C2-C62-N61	2.44	116.25	110.64
3	D	201	NAG	O5-C5-C4	2.46	114.20	110.13
4	B	711	61S	C49-C54-N55	2.48	122.71	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	711	61S	C63-C62-C2	2.53	115.99	109.95
3	A	705	NAG	O5-C5-C6	2.53	112.76	107.34
4	A	709	61S	C53-C54-C49	2.56	121.44	119.20
4	B	710	61S	O60-C59-N61	2.56	127.09	122.45
3	B	708	NAG	C1-O5-C5	2.57	115.92	112.14
3	D	203	NAG	C3-C4-C5	2.58	114.83	110.23
3	C	203	NAG	C2-N2-C7	2.59	126.47	123.11
3	B	705	NAG	O3-C3-C2	2.62	114.98	109.37
3	A	707	NAG	C3-C4-C5	2.63	114.92	110.23
3	B	708	NAG	O3-C3-C2	2.63	115.00	109.37
3	A	701	NAG	C1-O5-C5	2.64	116.02	112.14
3	C	201	NAG	C8-C7-N2	2.66	121.20	116.10
3	A	708	NAG	O4-C4-C5	2.67	116.27	109.23
4	A	709	61S	C62-N61-C59	2.78	129.09	121.49
3	D	203	NAG	O5-C5-C4	2.79	114.75	110.13
4	B	711	61S	C53-C54-C49	2.84	121.69	119.20
3	A	704	NAG	C8-C7-N2	2.84	121.54	116.10
3	B	709	NAG	O3-C3-C2	2.84	115.46	109.37
4	B	710	61S	C62-N61-C59	2.87	129.32	121.49
3	B	701	NAG	O7-C7-N2	2.90	127.76	121.84
3	B	703	NAG	C8-C7-N2	2.91	121.68	116.10
3	D	201	NAG	C4-C3-C2	2.99	115.99	111.34
3	B	706	NAG	C4-C3-C2	3.00	115.99	111.34
3	C	203	NAG	C3-C4-C5	3.06	115.69	110.23
4	B	710	61S	C63-C62-N61	3.08	116.61	110.81
3	A	701	NAG	C8-C7-N2	3.15	122.13	116.10
3	A	706	NAG	C2-N2-C7	3.15	127.20	123.11
3	C	201	NAG	C1-O5-C5	3.16	116.79	112.14
3	B	708	NAG	C2-N2-C7	3.22	127.29	123.11
3	B	705	NAG	C3-C4-C5	3.31	116.13	110.23
4	D	204	61S	C1-C48-C49	3.31	117.92	112.77
4	D	204	61S	C63-C62-C2	3.34	117.94	109.95
3	A	705	NAG	O3-C3-C2	3.42	116.69	109.37
4	B	711	61S	C62-N61-C59	3.45	130.90	121.49
3	C	202	NAG	C4-C3-C2	3.46	116.72	111.34
3	A	707	NAG	C2-N2-C7	3.48	127.63	123.11
3	C	203	NAG	C1-O5-C5	3.68	117.55	112.14
4	D	204	61S	C53-C54-C49	3.68	122.42	119.20
3	B	705	NAG	C4-C3-C2	3.71	117.09	111.34
3	C	202	NAG	C3-C4-C5	3.72	116.86	110.23
3	B	706	NAG	C1-O5-C5	3.73	117.62	112.14
3	A	705	NAG	C8-C7-N2	3.73	123.25	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	706	NAG	O5-C5-C6	3.74	115.35	107.34
3	D	201	NAG	C1-O5-C5	3.83	117.77	112.14
3	B	708	NAG	C8-C7-N2	3.84	123.46	116.10
3	A	708	NAG	C1-O5-C5	3.85	117.80	112.14
3	B	705	NAG	C1-O5-C5	3.90	117.88	112.14
3	B	705	NAG	C2-N2-C7	3.93	128.21	123.11
3	A	701	NAG	O5-C5-C4	3.94	116.67	110.13
3	A	706	NAG	C4-C3-C2	4.15	117.79	111.34
3	D	202	NAG	O5-C5-C4	4.16	117.02	110.13
3	B	702	NAG	C2-N2-C7	4.20	128.57	123.11
4	A	709	61S	C63-C62-N61	4.27	118.86	110.81
3	B	703	NAG	C2-N2-C7	4.31	128.72	123.11
3	A	707	NAG	C8-C7-N2	4.33	124.40	116.10
3	B	704	NAG	C2-N2-C7	4.38	128.80	123.11
3	A	707	NAG	O5-C5-C4	4.41	117.43	110.13
3	C	201	NAG	O5-C5-C4	4.48	117.55	110.13
3	B	702	NAG	C8-C7-N2	4.51	124.74	116.10
3	B	705	NAG	O5-C5-C4	4.63	117.80	110.13
3	B	709	NAG	C2-N2-C7	4.87	129.44	123.11
3	B	709	NAG	C1-O5-C5	4.92	119.38	112.14
3	A	704	NAG	C2-N2-C7	5.00	129.60	123.11
3	C	201	NAG	C2-N2-C7	5.00	129.61	123.11
4	D	204	61S	O4-C2-C62	5.14	117.33	110.61
3	C	203	NAG	O5-C5-C4	5.21	118.77	110.13
4	D	204	61S	C62-N61-C59	5.34	136.07	121.49
3	B	701	NAG	C2-N2-C7	5.99	130.89	123.11
3	A	705	NAG	C2-N2-C7	6.49	131.55	123.11
4	B	711	61S	O4-C2-C62	6.84	119.55	110.61
3	A	707	NAG	C1-O5-C5	6.86	122.23	112.14
4	A	709	61S	O4-C2-C62	10.93	124.90	110.61
4	B	710	61S	O4-C2-C62	13.51	128.27	110.61

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	706	NAG	C1
3	C	203	NAG	C1
3	A	706	NAG	C1
3	B	704	NAG	C1
3	A	703	NAG	C1
3	B	701	NAG	C1
3	B	708	NAG	C1

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	2	0
3	A	704	NAG	1	0
3	A	705	NAG	2	0
3	A	707	NAG	2	0
3	A	708	NAG	1	0
4	A	709	61S	1	0
3	B	702	NAG	1	0
3	B	705	NAG	1	0
3	B	707	NAG	2	0
4	B	710	61S	4	0
4	B	711	61S	1	0
3	D	201	NAG	1	0
3	D	202	NAG	1	0
3	D	203	NAG	1	0
4	D	204	61S	1	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	592/594 (99%)	-0.01	32 (5%) 29 24	13, 39, 83, 128	0
1	B	593/594 (99%)	-0.06	17 (2%) 55 51	12, 38, 77, 112	0
2	C	136/150 (90%)	-0.16	0 100 100	25, 40, 63, 76	0
2	D	136/150 (90%)	-0.23	0 100 100	24, 38, 65, 78	0
All	All	1457/1488 (97%)	-0.06	49 (3%) 49 43	12, 39, 78, 128	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	PRO	7.5
1	A	34	ASN	5.8
1	A	51	ILE	5.6
1	A	49	ASP	4.8
1	A	35	ILE	4.4
1	B	29	ILE	4.4
1	B	31	VAL	4.3
1	A	50	ASP	4.2
1	A	28	CYS	4.2
1	A	32	VAL	4.1
1	B	55	THR	4.1
1	A	101	HIS	4.0
1	A	31	VAL	3.9
1	B	35	ILE	3.9
1	B	99	GLY	3.8
1	B	201	PRO	3.8
1	A	48	PRO	3.6
1	B	37	TYR	3.6
1	A	75	ASN	3.6
1	A	54	SER	3.6
1	A	53	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	37	TYR	3.3
1	A	77	SER	3.1
1	A	81	TRP	3.1
1	A	98	HIS	3.1
1	B	147	GLN	3.1
1	A	73	PHE	3.1
1	A	58	ILE	3.1
1	A	29	ILE	3.0
1	A	55	THR	2.9
1	A	99	GLY	2.8
1	B	54	SER	2.8
1	A	76	PHE	2.7
1	B	28	CYS	2.7
1	A	168	ALA	2.5
1	B	33	PRO	2.5
1	A	78	GLU	2.5
1	A	97	TRP	2.4
1	B	76	PHE	2.4
1	A	47	VAL	2.4
1	B	30	GLU	2.4
1	B	52	PRO	2.3
1	B	34	ASN	2.3
1	B	78	GLU	2.2
1	A	30	GLU	2.2
1	A	149	ILE	2.2
1	A	71	TYR	2.1
1	B	53	SER	2.1
1	A	202	GLN	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	B	706	14/15	0.97	0.18	3.17	34,40,44,48	0
3	NAG	A	707	14/15	0.94	0.17	2.35	32,41,48,49	0
3	NAG	A	704	14/15	0.78	0.22	2.21	66,84,92,95	0
4	61S	A	709	35/35	0.95	0.14	0.43	30,33,37,40	0
4	61S	B	710	35/35	0.95	0.14	0.38	28,32,37,41	0
4	61S	B	711	35/35	0.97	0.14	0.36	28,37,53,55	0
4	61S	D	204	35/35	0.95	0.14	0.18	27,41,56,57	0
3	NAG	D	202	14/15	0.95	0.16	0.10	41,49,54,69	0
3	NAG	C	201	14/15	0.96	0.14	-0.97	41,46,58,68	0
3	NAG	B	707	14/15	0.82	0.33	-	60,72,85,86	0
3	NAG	A	702	14/15	0.89	0.14	-	50,70,81,88	0
3	NAG	A	701	14/15	0.93	0.14	-	54,59,77,79	0
3	NAG	D	203	14/15	0.91	0.23	-	64,81,90,91	0
3	NAG	C	203	14/15	0.86	0.27	-	72,81,90,92	0
3	NAG	C	202	14/15	0.88	0.24	-	63,77,85,88	0
3	NAG	B	709	14/15	0.81	0.20	-	80,94,105,106	0
3	NAG	D	201	14/15	0.86	0.20	-	70,85,96,97	0
3	NAG	A	705	14/15	0.85	0.13	-	66,76,84,87	0
3	NAG	B	703	14/15	0.79	0.23	-	73,100,116,122	0
3	NAG	A	706	14/15	0.78	0.29	-	77,94,99,99	0
3	NAG	B	704	14/15	0.77	0.22	-	62,92,101,108	0
3	NAG	A	703	14/15	0.83	0.17	-	82,95,101,102	0
3	NAG	B	701	14/15	0.76	0.29	-	67,91,99,99	0
3	NAG	A	708	14/15	0.91	0.19	-	58,61,67,68	0
3	NAG	B	708	14/15	0.79	0.21	-	79,94,96,96	0
3	NAG	B	705	14/15	0.83	0.15	-	64,74,80,86	0
3	NAG	B	702	14/15	0.90	0.14	-	65,74,82,87	0

## 6.5 Other polymers

There are no such residues in this entry.