



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:38 PM BST

PDB ID : 3G5C  
Title : Structural and biochemical studies on the ectodomain of human ADAM22  
Authors : Liu, H.; Shim, A.; Chen, X.; He, X.  
Deposited on : 2009-02-04  
Resolution : 2.36 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

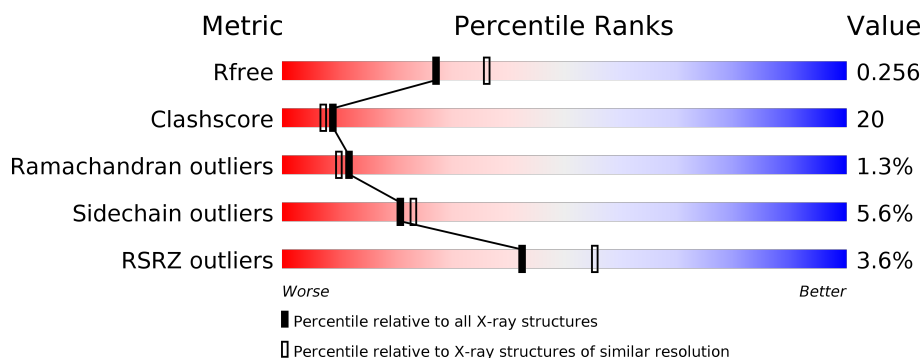
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 respectively. 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	510	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>• 5%</div> </div> </div>
1	B	510	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7915 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 ADAM 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			
1	B	486	Total	C	N	O	S	0	0	0
			3728	2303	643	731	51			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	737	HIS	-	expression tag	UNP Q9P0K1
A	738	HIS	-	expression tag	UNP Q9P0K1
A	739	HIS	-	expression tag	UNP Q9P0K1
A	740	HIS	-	expression tag	UNP Q9P0K1
A	741	HIS	-	expression tag	UNP Q9P0K1
A	742	HIS	-	expression tag	UNP Q9P0K1
B	737	HIS	-	expression tag	UNP Q9P0K1
B	738	HIS	-	expression tag	UNP Q9P0K1
B	739	HIS	-	expression tag	UNP Q9P0K1
B	740	HIS	-	expression tag	UNP Q9P0K1
B	741	HIS	-	expression tag	UNP Q9P0K1
B	742	HIS	-	expression tag	UNP Q9P0K1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is water.

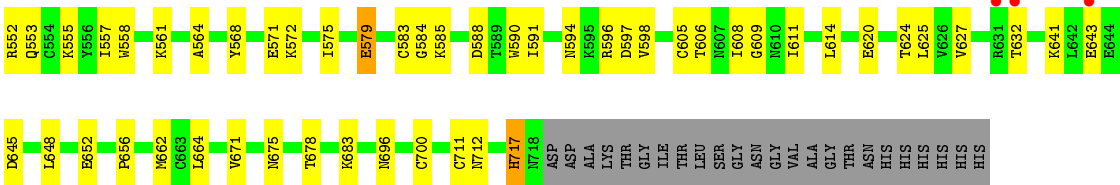
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	191	Total	O	0	0
			191	191		





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.09 Å   122.09 Å   208.69 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.36 47.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-2.36) 96.6 (47.16-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.29 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.245 , 0.273 0.247 , 0.256	Depositor DCC
$R_{free}$ test set	2522 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.39	0/3792	0.63	1/5105 (0.0%)
1	B	0.43	1/3792 (0.0%)	0.68	3/5105 (0.1%)
All	All	0.41	1/7584 (0.0%)	0.66	4/10210 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	456	GLU	C-N	-9.34	1.12	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	GLU	O-C-N	-13.15	101.66	122.70
1	B	444	PRO	CA-N-CD	-9.91	97.63	111.50
1	A	444	PRO	CA-N-CD	-8.01	100.29	111.50
1	B	456	GLU	CA-C-N	6.45	131.39	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	456	GLU	Mainchain

## 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	3728	0	3579	151	1
1	B	3728	0	3578	150	1
2	A	42	0	39	2	0
2	B	42	0	39	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	178	0	0	18	0
4	B	191	0	0	16	0
All	All	7915	0	7235	299	1

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 20.

All (299) 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:A:398:TRP:CZ3	1:A:413:LYS:NZ	2.23	1.06
1:A:398:TRP:CE3	1:A:413:LYS:NZ	2.28	1.01
1:A:504:ARG:HH11	1:A:514:GLU:HG3	1.31	0.94
1:B:605:CYS:HB2	1:B:608:ILE:HD13	1.54	0.87
1:B:504:ARG:HB3	1:B:514:GLU:HG3	1.57	0.85
1:A:398:TRP:HZ3	1:A:413:LYS:NZ	1.72	0.84
1:A:277:TYR:CD2	1:A:285:ILE:HD11	2.13	0.84
1:A:514:GLU:OE2	1:A:526:ASN:HA	1.80	0.82
1:A:551:ASP:OD1	1:A:555:LYS:HE2	1.81	0.81
1:A:249:HIS:H	1:A:297:ASN:HD21	1.26	0.81
1:B:504:ARG:HH11	1:B:514:GLU:HG3	1.45	0.80
1:A:585:LYS:HE3	1:A:588:ASP:HA	1.61	0.80
1:B:402:ILE:HD13	1:B:413:LYS:O	1.81	0.80
1:A:378:ILE:HG23	1:A:422:TYR:CD1	2.17	0.79
1:A:504:ARG:NH1	1:A:514:GLU:HG3	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:LYS:HE3	1:B:588:ASP:HA	1.64	0.78
1:B:317:ARG:HD3	1:B:352:LEU:HD21	1.66	0.78
1:B:378:ILE:HD11	1:B:434:LEU:HD21	1.66	0.78
1:B:504:ARG:NH1	1:B:514:GLU:HG3	1.99	0.77
1:B:594:ASN:HD22	1:B:596:ARG:H	1.30	0.77
1:B:249:HIS:H	1:B:297:ASN:HD21	1.33	0.76
1:A:280:GLN:HE22	1:A:413:LYS:HA	1.50	0.75
1:A:317:ARG:HD3	1:A:352:LEU:HD21	1.68	0.75
1:B:345:ILE:HD12	1:B:381:ILE:HG22	1.66	0.75
1:B:268:SER:O	1:B:272:MET:HG3	1.86	0.74
1:B:504:ARG:HB3	1:B:514:GLU:CG	2.17	0.74
1:A:594:ASN:HD22	1:A:596:ARG:H	1.35	0.73
1:A:398:TRP:HE3	1:A:413:LYS:NZ	1.83	0.73
4:A:178:HOH:O	1:B:317:ARG:HD2	1.88	0.72
1:B:662:MET:CE	1:B:671:VAL:HG12	2.19	0.71
1:A:440:LYS:HG2	4:A:757:HOH:O	1.90	0.71
1:B:348:ILE:HD11	1:B:425:PHE:CZ	2.26	0.70
1:B:280:GLN:HE22	1:B:413:LYS:HA	1.55	0.70
1:B:402:ILE:HD11	1:B:413:LYS:N	2.08	0.69
1:A:627:VAL:HG12	1:A:632:THR:HG22	1.76	0.68
1:B:551:ASP:OD1	1:B:555:LYS:HE2	1.92	0.68
1:B:594:ASN:ND2	1:B:596:ARG:H	1.92	0.68
1:A:268:SER:O	1:A:272:MET:HG3	1.94	0.68
1:B:571:GLU:HA	1:B:598:VAL:HG21	1.75	0.68
1:A:662:MET:CE	1:A:671:VAL:HG12	2.24	0.68
1:A:462:THR:H	1:A:465:GLU:HG3	1.59	0.67
1:B:316:ARG:HA	1:B:320:ILE:HG12	1.75	0.67
1:B:382:SER:HA	4:B:32:HOH:O	1.94	0.67
1:B:537:GLY:O	1:B:538:VAL:HG12	1.95	0.67
1:B:329:LEU:HD23	1:B:357:VAL:HG23	1.76	0.67
1:A:493:LYS:N	4:A:115:HOH:O	2.27	0.67
1:B:627:VAL:HG12	1:B:632:THR:HG22	1.76	0.67
1:B:541:ILE:HG13	1:B:656:PRO:HG3	1.77	0.67
1:A:553:GLN:HE22	1:A:652:GLU:H	1.43	0.66
1:A:329:LEU:HD23	1:A:357:VAL:HG23	1.76	0.66
1:A:504:ARG:HB3	1:A:514:GLU:CG	2.26	0.66
1:A:504:ARG:HB3	1:A:514:GLU:HG2	1.77	0.66
1:A:348:ILE:HD11	1:A:425:PHE:CZ	2.30	0.66
1:A:594:ASN:ND2	1:A:596:ARG:H	1.94	0.66
1:B:662:MET:HE1	1:B:671:VAL:HG12	1.79	0.65
1:A:249:HIS:H	1:A:297:ASN:ND2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ARG:HH11	1:B:514:GLU:CG	2.10	0.64
1:B:683:LYS:NZ	1:B:712:ASN:HD21	1.93	0.64
1:A:571:GLU:HA	1:A:598:VAL:HG21	1.77	0.64
1:A:348:ILE:HG13	1:A:377:ASN:O	1.97	0.64
1:A:594:ASN:HD22	1:A:596:ARG:HB2	1.63	0.64
1:B:402:ILE:H	1:B:402:ILE:HD13	1.63	0.64
1:A:662:MET:HE1	1:A:671:VAL:HG12	1.78	0.64
1:B:608:ILE:HG23	1:B:609:GLY:O	1.96	0.64
1:B:557:ILE:CD1	1:B:648:LEU:HD13	2.28	0.64
1:B:553:GLN:HE22	1:B:652:GLU:H	1.46	0.64
1:A:348:ILE:HD11	1:A:425:PHE:CE2	2.33	0.63
1:B:402:ILE:CD1	1:B:402:ILE:N	2.62	0.63
1:A:608:ILE:HG23	1:A:609:GLY:O	1.98	0.62
1:B:249:HIS:H	1:B:297:ASN:ND2	1.97	0.62
1:B:462:THR:H	1:B:465:GLU:HG3	1.64	0.62
1:A:440:LYS:HA	4:A:79:HOH:O	2.00	0.62
1:A:683:LYS:NZ	1:A:712:ASN:HD21	1.98	0.62
1:A:575:ILE:N	1:A:575:ILE:HD12	2.15	0.61
1:B:378:ILE:HG23	1:B:422:TYR:CD1	2.36	0.61
1:A:303:GLU:H	1:A:303:GLU:CD	2.04	0.60
1:B:348:ILE:HD11	1:B:425:PHE:CE2	2.36	0.60
1:B:493:LYS:N	4:B:42:HOH:O	2.34	0.60
1:A:568:TYR:OH	1:A:572:LYS:HE3	2.00	0.60
1:B:263:ASN:O	1:B:267:LYS:HG3	2.02	0.60
1:A:594:ASN:ND2	1:A:596:ARG:HB2	2.17	0.59
1:B:641:LYS:HG3	4:B:206:HOH:O	2.02	0.59
1:B:293:TRP:HE3	1:B:297:ASN:HD22	1.49	0.59
1:A:382:SER:HA	4:A:20:HOH:O	2.02	0.59
1:A:558:TRP:NE1	1:A:608:ILE:HD11	2.18	0.59
1:B:594:ASN:HD22	1:B:596:ARG:HB2	1.66	0.59
1:B:541:ILE:CD1	1:B:662:MET:HG2	2.33	0.58
1:A:549:THR:OG1	1:A:552:ARG:HG3	2.03	0.58
1:B:247:ASN:HB2	1:B:292:THR:HG23	1.84	0.58
1:B:594:ASN:ND2	1:B:596:ARG:HB2	2.18	0.58
1:B:514:GLU:OE1	1:B:526:ASN:HA	2.03	0.58
1:B:557:ILE:HD11	1:B:648:LEU:HD13	1.86	0.58
1:B:317:ARG:HG3	1:B:351:LEU:HD21	1.85	0.58
1:A:485:CYS:HB3	1:A:496:PHE:HE2	1.68	0.58
1:B:378:ILE:CD1	1:B:434:LEU:HD21	2.33	0.58
1:B:402:ILE:CD1	1:B:413:LYS:N	2.67	0.57
1:B:558:TRP:CD1	1:B:608:ILE:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HD13	1:A:302:SER:N	2.20	0.57
1:B:568:TYR:OH	1:B:572:LYS:HE3	2.03	0.57
1:B:683:LYS:HZ3	1:B:712:ASN:HD21	1.52	0.57
1:B:662:MET:HE2	1:B:671:VAL:HG12	1.84	0.57
1:A:579:GLU:H	1:A:579:GLU:CD	2.06	0.56
1:A:558:TRP:CD1	1:A:608:ILE:HD11	2.40	0.56
1:B:579:GLU:CD	1:B:579:GLU:H	2.09	0.56
1:B:348:ILE:HG13	1:B:377:ASN:O	2.06	0.56
1:B:257:LEU:HD22	1:B:257:LEU:N	2.21	0.56
1:A:263:ASN:O	1:A:267:LYS:HG3	2.06	0.56
1:B:378:ILE:HG23	1:B:422:TYR:CE1	2.41	0.56
1:B:579:GLU:HG3	1:B:590:TRP:HE1	1.70	0.56
1:A:575:ILE:HD12	1:A:575:ILE:H	1.69	0.56
1:A:541:ILE:CD1	1:A:656:PRO:HG3	2.36	0.55
1:B:432:ALA:HB3	4:B:127:HOH:O	2.06	0.55
1:A:298:LYS:HA	1:B:596:ARG:HH21	1.72	0.55
1:B:303:GLU:H	1:B:303:GLU:CD	2.09	0.55
1:A:248:ASP:OD1	1:A:331:SER:HA	2.06	0.55
1:B:402:ILE:HD11	1:B:412:LYS:C	2.28	0.54
1:B:402:ILE:HD13	1:B:402:ILE:N	2.22	0.54
1:A:257:LEU:HD22	1:A:257:LEU:N	2.22	0.54
1:B:541:ILE:CD1	1:B:656:PRO:HG3	2.36	0.54
1:A:398:TRP:HZ3	1:A:413:LYS:HZ1	1.52	0.54
1:B:584:GLY:C	1:B:591:ILE:HD13	2.27	0.54
1:A:527:ILE:HD11	4:A:28:HOH:O	2.07	0.54
1:A:301:ILE:C	1:A:301:ILE:HD13	2.27	0.54
1:A:453:GLU:HG2	4:A:79:HOH:O	2.07	0.54
1:B:497:GLN:HG3	1:B:498:PRO:HD2	1.89	0.54
1:B:242:GLU:HG2	1:B:288:VAL:HG11	1.88	0.54
1:B:316:ARG:HG3	1:B:317:ARG:N	2.22	0.54
1:B:624:THR:HG22	1:B:625:LEU:N	2.23	0.54
1:B:245:ILE:HD13	1:B:330:PHE:CE1	2.44	0.53
2:B:3:NAG:H62	2:B:3:NAG:O3	2.08	0.53
1:B:495:LYS:N	4:B:42:HOH:O	2.40	0.53
1:A:416:GLN:HB2	4:A:784:HOH:O	2.08	0.53
1:A:537:GLY:O	1:A:538:VAL:HG12	2.08	0.53
1:A:572:LYS:HE2	4:A:746:HOH:O	2.09	0.53
1:B:347:GLY:O	1:B:350:SER:HB3	2.09	0.53
1:A:241:ILE:HD12	1:A:285:ILE:CD1	2.39	0.53
1:A:298:LYS:HD3	1:B:596:ARG:NH2	2.23	0.53
1:B:402:ILE:HD12	1:B:411:PRO:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLY:H	1:A:366:MET:CE	2.22	0.52
1:A:316:ARG:HG3	1:A:317:ARG:N	2.24	0.52
1:A:378:ILE:HG23	1:A:422:TYR:CE1	2.44	0.52
1:A:512:ILE:HD11	1:A:529:LYS:HG3	1.91	0.52
1:A:541:ILE:HG13	1:A:656:PRO:HG3	1.91	0.52
1:B:675:ASN:HB3	4:B:208:HOH:O	2.10	0.52
1:A:551:ASP:HA	1:A:564:ALA:HB2	1.91	0.52
1:A:340:SER:O	1:A:359:GLU:HG2	2.10	0.52
1:B:541:ILE:CG1	1:B:656:PRO:HG3	2.40	0.51
1:A:683:LYS:HZ3	1:A:712:ASN:HD21	1.56	0.51
1:A:316:ARG:HA	1:A:320:ILE:HG12	1.91	0.51
1:A:624:THR:HG22	1:A:625:LEU:N	2.25	0.51
1:B:662:MET:CE	1:B:671:VAL:HA	2.39	0.51
1:A:347:GLY:O	1:A:350:SER:HB3	2.10	0.51
1:A:441:LEU:C	1:A:443:ASP:H	2.13	0.51
1:A:584:GLY:C	1:A:591:ILE:HD13	2.30	0.51
2:A:3:NAG:O3	2:A:3:NAG:H62	2.11	0.51
1:B:456:GLU:OE1	1:B:477:CYS:SG	2.69	0.51
1:A:311:GLU:HG3	4:A:196:HOH:O	2.11	0.51
1:A:441:LEU:O	1:A:443:ASP:N	2.44	0.51
1:A:662:MET:HE2	1:A:671:VAL:HG12	1.93	0.50
1:B:441:LEU:C	1:B:443:ASP:H	2.14	0.50
1:A:241:ILE:HD12	1:A:285:ILE:HD13	1.93	0.50
1:A:398:TRP:C	1:A:398:TRP:CD1	2.85	0.50
1:B:348:ILE:HD11	1:B:425:PHE:HZ	1.71	0.50
1:B:591:ILE:HD12	1:B:591:ILE:N	2.26	0.50
1:A:317:ARG:HG3	1:A:351:LEU:HD21	1.92	0.50
1:B:538:VAL:HG22	4:B:99:HOH:O	2.12	0.50
1:B:485:CYS:HB3	1:B:496:PHE:HE2	1.76	0.50
1:B:541:ILE:HD13	1:B:662:MET:SD	2.52	0.50
1:A:624:THR:HG22	1:A:625:LEU:H	1.77	0.50
1:A:717:HIS:HB2	4:A:139:HOH:O	2.11	0.50
1:A:323:LYS:HB3	4:A:105:HOH:O	2.12	0.50
1:A:272:MET:SD	1:A:363:THR:HG22	2.51	0.50
1:A:368:VAL:O	1:A:372:GLN:HG2	2.11	0.50
1:A:643:GLU:HG3	1:A:645:ASP:H	1.76	0.49
1:A:717:HIS:O	1:A:718:ASN:HB2	2.11	0.49
1:B:315:TYR:HE2	1:B:320:ILE:HD11	1.77	0.49
1:B:561:LYS:HD3	4:B:119:HOH:O	2.11	0.49
1:B:244:MET:SD	1:B:322:GLU:HG3	2.53	0.49
1:B:614:LEU:HD23	1:B:614:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:GLU:OE1	1:A:620:GLU:N	2.46	0.49
1:B:551:ASP:HA	1:B:564:ALA:HB2	1.95	0.49
1:B:614:LEU:HD23	1:B:614:LEU:H	1.78	0.49
1:B:624:THR:HG22	1:B:625:LEU:H	1.78	0.49
1:A:643:GLU:HB3	1:A:646:VAL:HG23	1.95	0.48
1:B:473:CYS:O	1:B:480:THR:HG23	2.13	0.48
1:B:504:ARG:NH1	1:B:514:GLU:OE1	2.45	0.48
1:A:323:LYS:HA	4:A:179:HOH:O	2.12	0.48
1:B:575:ILE:HG22	1:B:575:ILE:O	2.13	0.48
1:B:303:GLU:HB2	1:B:336:GLU:HG3	1.95	0.48
1:A:700:CYS:HB3	1:A:711:CYS:SG	2.53	0.48
1:A:293:TRP:HE3	1:A:297:ASN:HD22	1.62	0.48
1:A:444:PRO:HA	1:A:445:PRO:HD3	1.85	0.48
1:A:571:GLU:O	1:A:575:ILE:HD13	2.14	0.48
1:B:575:ILE:HG22	4:B:223:HOH:O	2.13	0.48
1:B:441:LEU:O	1:B:443:ASP:N	2.46	0.47
1:A:454:THR:HG23	4:A:117:HOH:O	2.15	0.47
1:A:360:PHE:CD1	1:A:366:MET:HE1	2.49	0.47
1:A:462:THR:HB	1:A:463:PRO:HD2	1.96	0.47
1:B:462:THR:HB	1:B:463:PRO:HD2	1.97	0.47
1:A:441:LEU:N	1:A:441:LEU:HD23	2.30	0.47
1:A:575:ILE:HG22	1:A:575:ILE:O	2.15	0.47
1:A:591:ILE:N	1:A:591:ILE:HD12	2.29	0.47
1:B:504:ARG:HH11	1:B:514:GLU:CD	2.18	0.47
1:A:473:CYS:O	1:A:480:THR:HG23	2.15	0.47
1:B:272:MET:SD	1:B:363:THR:HG22	2.55	0.46
1:B:248:ASP:HB2	1:B:297:ASN:HD21	1.80	0.46
1:A:580:LYS:HE2	1:A:624:THR:OG1	2.15	0.46
1:A:567:LYS:O	1:A:571:GLU:HG3	2.16	0.46
1:A:611:ILE:O	1:A:611:ILE:HG23	2.16	0.46
1:B:277:TYR:CG	1:B:285:ILE:HD11	2.51	0.45
1:B:474:CYS:HB2	1:B:486:SER:OG	2.16	0.45
1:A:596:ARG:HH21	1:B:298:LYS:HA	1.80	0.45
1:B:345:ILE:HD11	1:B:376:HIS:CE1	2.50	0.45
1:A:614:LEU:N	1:A:614:LEU:HD23	2.31	0.45
1:B:445:PRO:HA	1:B:453:GLU:OE2	2.16	0.45
1:A:361:GLY:H	1:A:366:MET:HE2	1.80	0.45
1:A:661:MET:HE3	1:A:670:PRO:N	2.31	0.45
1:A:293:TRP:CE3	1:A:297:ASN:HA	2.52	0.45
1:B:401:CYS:HB2	4:B:772:HOH:O	2.17	0.45
1:B:572:LYS:HE2	4:B:789:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASP:O	1:B:428:SER:HB3	2.17	0.45
1:A:345:ILE:N	1:A:345:ILE:HD12	2.32	0.45
1:A:456:GLU:HB2	1:A:477:CYS:HB3	1.99	0.45
1:A:595:LYS:HE3	1:B:296:ASP:OD1	2.17	0.45
1:B:557:ILE:HD12	1:B:648:LEU:HD13	1.98	0.45
1:B:272:MET:O	1:B:276:ILE:HG12	2.16	0.44
1:B:340:SER:O	1:B:359:GLU:HG2	2.18	0.44
1:A:417:CYS:O	1:A:421:GLU:HG3	2.17	0.44
1:B:536:ASP:OD2	1:B:552:ARG:NH1	2.50	0.44
1:B:643:GLU:HG3	1:B:645:ASP:H	1.81	0.44
1:A:246:VAL:O	1:A:329:LEU:HD12	2.18	0.44
1:A:242:GLU:HG2	1:A:288:VAL:HG11	2.00	0.44
1:B:502:VAL:HG11	4:B:763:HOH:O	2.17	0.44
1:B:504:ARG:NH1	1:B:514:GLU:CG	2.73	0.44
1:A:462:THR:OG1	1:A:465:GLU:HG2	2.18	0.44
2:A:3:NAG:H5	4:A:178:HOH:O	2.17	0.43
1:A:303:GLU:HB2	1:A:336:GLU:HG3	1.98	0.43
1:A:533:TYR:HB3	4:A:214:HOH:O	2.18	0.43
1:A:541:ILE:HD12	1:A:656:PRO:HG3	1.99	0.43
1:B:385:ARG:HG3	1:B:611:ILE:HG23	1.99	0.43
1:B:301:ILE:HG22	4:B:787:HOH:O	2.17	0.43
1:B:393:LYS:HE3	1:B:393:LYS:HA	2.00	0.43
1:B:453:GLU:HG2	4:B:80:HOH:O	2.18	0.43
1:A:240:TYR:CZ	1:A:437:LYS:HG2	2.53	0.43
1:A:289:ALA:HA	1:A:442:LEU:HD11	2.00	0.43
1:A:579:GLU:HG3	1:A:590:TRP:HE1	1.82	0.43
1:B:293:TRP:CE3	1:B:297:ASN:HA	2.52	0.43
1:B:301:ILE:HD13	1:B:302:SER:N	2.33	0.43
1:A:660:GLN:O	1:A:671:VAL:HG13	2.19	0.43
1:B:257:LEU:N	1:B:257:LEU:CD2	2.81	0.43
1:B:317:ARG:HG3	1:B:351:LEU:CD2	2.48	0.43
1:B:541:ILE:HD12	1:B:662:MET:HG2	1.98	0.43
1:A:398:TRP:CG	1:A:398:TRP:O	2.71	0.43
1:A:244:MET:SD	1:A:322:GLU:HG3	2.58	0.42
1:B:248:ASP:OD1	1:B:331:SER:HA	2.18	0.42
1:A:541:ILE:CG1	1:A:656:PRO:HG3	2.48	0.42
1:B:415:THR:O	1:B:418:ASN:HB2	2.20	0.42
1:B:485:CYS:HB3	1:B:496:PHE:CE2	2.53	0.42
1:B:611:ILE:HG23	1:B:611:ILE:O	2.19	0.42
1:A:309:LEU:HD12	1:A:309:LEU:O	2.20	0.42
1:A:393:LYS:HE3	1:A:393:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD23	1:A:374:LEU:HA	1.85	0.42
1:B:401:CYS:C	1:B:411:PRO:HB3	2.40	0.42
1:B:444:PRO:HA	1:B:445:PRO:HD3	1.84	0.42
1:A:485:CYS:HB3	1:A:496:PHE:CE2	2.51	0.42
1:A:548:LYS:HE2	1:A:652:GLU:OE2	2.20	0.42
1:B:402:ILE:CD1	1:B:402:ILE:H	2.26	0.42
1:B:528:HIS:CE1	1:B:696:ASN:HB3	2.54	0.42
1:A:257:LEU:N	1:A:257:LEU:CD2	2.82	0.42
1:A:437:LYS:HA	1:A:438:PRO:HD3	1.92	0.42
1:A:568:TYR:CZ	1:A:572:LYS:HG3	2.55	0.42
1:A:541:ILE:HD13	1:A:662:MET:SD	2.60	0.42
1:B:620:GLU:OE1	1:B:620:GLU:N	2.53	0.42
1:A:497:GLN:HG3	1:A:498:PRO:HD2	2.02	0.42
1:A:415:THR:O	1:A:418:ASN:HB2	2.19	0.42
1:A:512:ILE:HD11	1:A:693:VAL:HG11	2.01	0.42
1:A:628:GLN:HA	4:A:193:HOH:O	2.19	0.41
1:A:384:LYS:HE3	1:A:615:GLY:O	2.20	0.41
1:B:392:CYS:HB3	4:B:782:HOH:O	2.20	0.41
1:A:504:ARG:HB3	1:A:514:GLU:HG3	2.00	0.41
1:B:266:ALA:O	1:B:270:VAL:HG23	2.20	0.41
1:A:401:CYS:C	1:A:411:PRO:HB3	2.41	0.41
1:A:565:SER:HB3	1:A:569:CYS:SG	2.61	0.41
1:B:452:ILE:N	1:B:452:ILE:HD12	2.35	0.41
1:B:568:TYR:CZ	1:B:572:LYS:HG3	2.56	0.41
1:B:245:ILE:HD13	1:B:330:PHE:CZ	2.56	0.41
1:B:402:ILE:HD11	1:B:412:LYS:CA	2.51	0.41
1:A:313:MET:HA	1:A:316:ARG:HG2	2.02	0.41
1:A:316:ARG:NH1	4:A:35:HOH:O	2.52	0.41
1:B:700:CYS:HB3	1:B:711:CYS:SG	2.60	0.41
1:B:374:LEU:HA	1:B:374:LEU:HD23	1.92	0.40
1:A:628:GLN:NE2	1:A:631:ARG:HH21	2.19	0.40
1:A:260:VAL:HG13	1:A:261:HIS:N	2.37	0.40
1:B:462:THR:H	1:B:465:GLU:CG	2.32	0.40
1:B:717:HIS:HB3	4:B:138:HOH:O	2.21	0.40
1:A:317:ARG:HG3	1:A:351:LEU:CD2	2.51	0.40
1:A:463:PRO:O	1:A:467:VAL:HG23	2.22	0.40
1:B:258:SER:O	1:B:262:THR:HG23	2.22	0.40
1:A:596:ARG:NH2	1:B:298:LYS:HD3	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLU:O	1:B:391:GLU:O[8_544]	2.06	0.14

## 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	484/510 (95%)	447 (92%)	30 (6%)	7 (1%)	11	9
1	B	484/510 (95%)	446 (92%)	32 (7%)	6 (1%)	13	11
All	All	968/1020 (95%)	893 (92%)	62 (6%)	13 (1%)	12	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	LEU
1	A	538	VAL
1	B	442	LEU
1	B	538	VAL
1	A	461	GLY
1	B	461	GLY
1	A	492	LYS
1	A	606	THR
1	B	606	THR
1	A	629	GLN
1	B	492	LYS
1	A	463	PRO
1	B	463	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/438 (96%)	397 (94%)	23 (6%)	21	24
1	B	420/438 (96%)	396 (94%)	24 (6%)	20	22
All	All	840/876 (96%)	793 (94%)	47 (6%)	21	23

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	ILE
1	A	316	ARG
1	A	339	ARG
1	A	348	ILE
1	A	393	LYS
1	A	408	TYR
1	A	409	TYR
1	A	416	GLN
1	A	434	LEU
1	A	441	LEU
1	A	444	PRO
1	A	473	CYS
1	A	481	GLN
1	A	514	GLU
1	A	538	VAL
1	A	579	GLU
1	A	583	CYS
1	A	608	ILE
1	A	610	ASN
1	A	664	LEU
1	A	677	SER
1	A	678	THR
1	A	717	HIS
1	B	301	ILE
1	B	316	ARG
1	B	322	GLU
1	B	339	ARG
1	B	393	LYS
1	B	398	TRP
1	B	402	ILE
1	B	408	TYR
1	B	409	TYR
1	B	416	GLN

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Mol	Chain	Res	Type
1	B	428	SER
1	B	434	LEU
1	B	441	LEU
1	B	444	PRO
1	B	473	CYS
1	B	481	GLN
1	B	513	ARG
1	B	514	GLU
1	B	579	GLU
1	B	583	CYS
1	B	597	ASP
1	B	664	LEU
1	B	678	THR
1	B	717	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	297	ASN
1	A	372	GLN
1	A	377	ASN
1	A	416	GLN
1	A	418	ASN
1	A	539	GLN
1	A	553	GLN
1	A	592	GLN
1	A	594	ASN
1	A	628	GLN
1	A	712	ASN
1	B	247	ASN
1	B	263	ASN
1	B	297	ASN
1	B	372	GLN
1	B	376	HIS
1	B	416	GLN
1	B	418	ASN
1	B	539	GLN
1	B	553	GLN
1	B	592	GLN
1	B	594	ASN
1	B	628	GLN

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Mol	Chain	Res	Type
1	B	712	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z  > 2$
2	NAG	B	3	1	14,14,15	0.70	0	17,19,21	1.02	2 (11%)
2	NAG	A	3	1	14,14,15	0.64	0	17,19,21	1.03	2 (11%)
2	NAG	B	2	1	14,14,15	0.52	0	17,19,21	0.80	1 (5%)
2	NAG	A	1	1	14,14,15	0.57	0	17,19,21	0.64	0
2	NAG	B	1	1	14,14,15	0.58	0	17,19,21	0.64	0
2	NAG	A	2	1	14,14,15	0.43	0	17,19,21	0.72	1 (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
2	NAG	B	3	1	-	2/6/23/26	0/1/1/1
2	NAG	A	3	1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1	1	-	2/6/23/26	0/1/1/1
2	NAG	A	2	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	NAG	C1-O5-C5	2.74	115.90	112.19
2	A	3	NAG	C1-O5-C5	2.68	115.82	112.19
2	B	2	NAG	C2-N2-C7	-2.36	119.54	122.90
2	A	3	NAG	C2-N2-C7	-2.31	119.62	122.90
2	B	3	NAG	C2-N2-C7	-2.15	119.84	122.90
2	A	2	NAG	C2-N2-C7	-2.09	119.92	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	NAG	O5-C5-C6-O6
2	A	3	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
2	B	3	NAG	C4-C5-C6-O6
2	A	3	NAG	C4-C5-C6-O6
2	A	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	NAG	1	0
2	A	3	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	456:GLU	C	457:GLU	N	1.12

## 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	486/510 (95%)	0.05	19 (3%)	39 52	23, 55, 128, 184	1 (0%)
1	B	486/510 (95%)	0.07	16 (3%)	46 59	23, 55, 128, 184	1 (0%)
All	All	972/1020 (95%)	0.06	35 (3%)	42 55	23, 55, 128, 184	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	TRP	9.7
1	B	395	GLU	6.2
1	A	461	GLY	5.8
1	B	398	TRP	5.7
1	B	461	GLY	5.4
1	A	395	GLU	5.2
1	A	408	TYR	4.0
1	B	408	TYR	3.7
1	B	399	SER	3.3
1	A	360	PHE	3.3
1	B	482	ASP	3.2
1	B	409	TYR	2.9
1	B	643	GLU	2.8
1	A	301	ILE	2.8
1	A	397	THR	2.8
1	B	396	ASP	2.8
1	A	588	ASP	2.8
1	B	631	ARG	2.8
1	A	396	ASP	2.7
1	A	409	TYR	2.7
1	A	630	GLY	2.6
1	A	441	LEU	2.5
1	A	399	SER	2.4
1	A	717	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	631	ARG	2.3
1	B	465	GLU	2.3
1	A	259	VAL	2.3
1	A	470	GLY	2.2
1	A	338	SER	2.2
1	A	478	THR	2.2
1	B	441	LEU	2.2
1	B	360	PHE	2.2
1	B	397	THR	2.1
1	B	632	THR	2.1
1	B	410	LEU	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	1	14/15	0.67	0.18	113,116,125,127	0
2	NAG	A	3	14/15	0.78	0.21	104,107,108,109	0
2	NAG	B	3	14/15	0.81	0.18	104,107,108,109	0
2	NAG	A	1	14/15	0.82	0.22	113,116,125,127	0
3	CA	B	802	1/1	0.85	0.11	78,78,78,78	0
3	CA	A	802	1/1	0.86	0.11	78,78,78,78	0
2	NAG	A	2	14/15	0.87	0.15	73,82,85,86	0
2	NAG	B	2	14/15	0.92	0.17	73,82,85,86	0
3	CA	A	803	1/1	0.93	0.16	47,47,47,47	0
3	CA	B	803	1/1	0.96	0.18	47,47,47,47	0
3	CA	B	801	1/1	0.99	0.11	48,48,48,48	0
3	CA	A	801	1/1	1.00	0.09	48,48,48,48	0

## 6.5 Other polymers

There are no such residues in this entry.