



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 07:22 pm GMT

PDB ID : 4J0M  
Title : Crystal structure of BRL1 (LRR) in complex with brassinolide  
Authors : Chai, J.; She, J.; Han, Z.; Zhou, B.  
Deposited on : 2013-01-31  
Resolution : 2.50 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

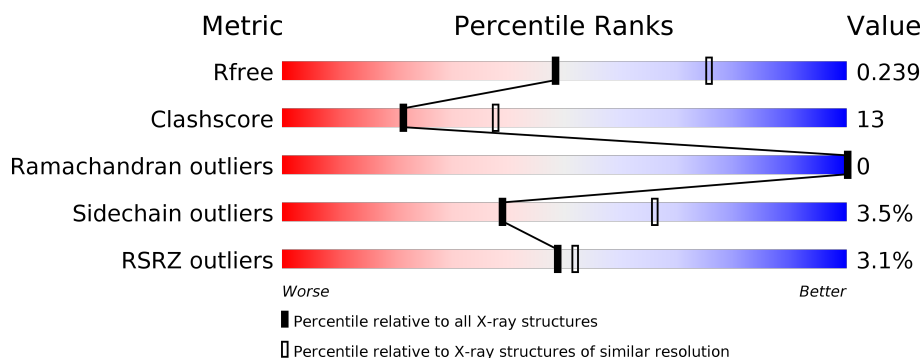
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	740	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>••</div> </div> </div>
1	B	740	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11785 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 Serine/threonine-protein kinase BRI1-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5455	3446	913	1067	29			
1	B	724	Total	C	N	O	S	0	0	0
			5455	3446	913	1067	29			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	760	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	761	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	762	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	763	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	764	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	759	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	760	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	761	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	762	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	763	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	764	HIS	-	EXPRESSION TAG	UNP Q9ZWC8

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



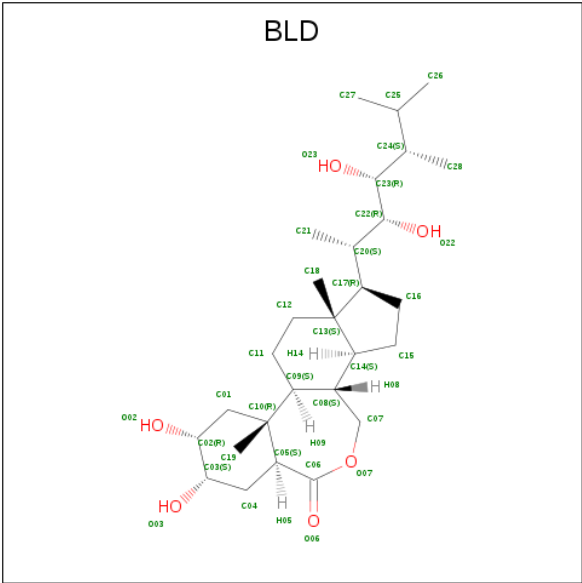
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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

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

- Molecule 3 is Brassinolide (three-letter code: BLD) (formula: C<sub>28</sub>H<sub>48</sub>O<sub>6</sub>).



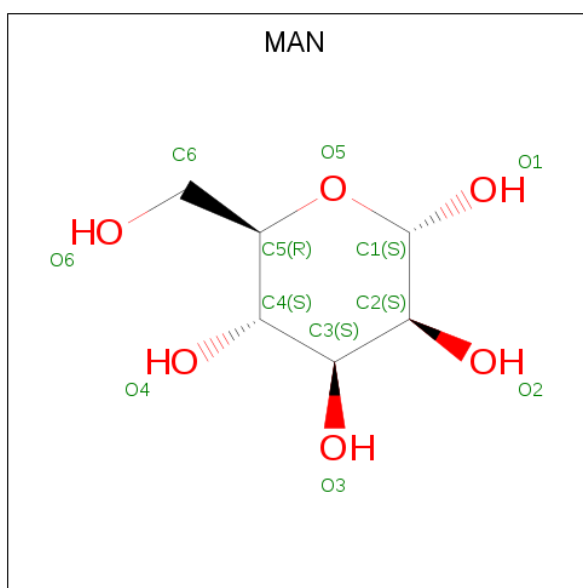
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			34	28	6		
3	B	1	Total	C	O	0	0
			34	28	6		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

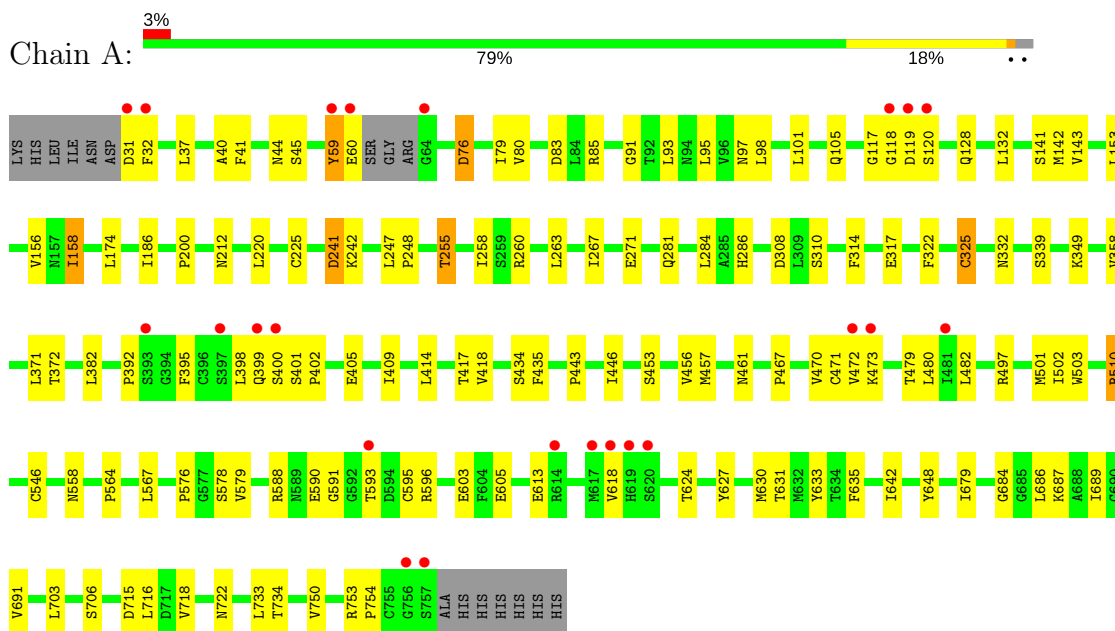
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	201	Total	O	0	0
			201	201		

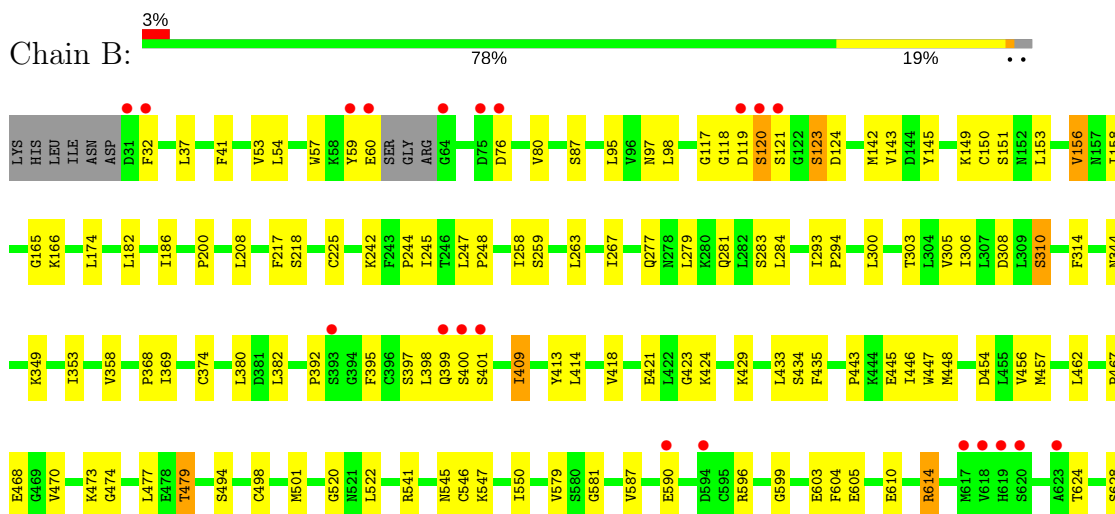
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Serine/threonine-protein kinase BRI1-like 1



- Molecule 1: Serine/threonine-protein kinase BRI1-like 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.86Å 83.40Å 264.06Å 90.00° 97.24° 90.00°	Depositor
Resolution (Å)	29.83 – 2.50 29.83 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.83-2.50) 93.9 (29.83-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.187 , 0.239 0.188 , 0.239	Depositor DCC
$R_{free}$ test set	3786 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLD, BMA, NAG, MAN

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	0.43	0/5561	0.67	0/7559
1	B	0.42	0/5561	0.66	1/7559 (0.0%)
All	All	0.42	0/11122	0.66	1/15118 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	156	VAL	CB-CA-C	-5.11	101.69	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	SER	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	5455	0	5391	144	0
1	B	5455	0	5390	133	1
2	A	140	0	122	12	0
2	B	168	0	148	2	0
3	A	34	0	48	5	0
3	B	34	0	48	5	0
4	A	11	0	9	0	0
4	B	11	0	9	0	0
5	A	33	0	24	0	0
5	B	33	0	23	0	0
6	A	210	0	0	8	0
6	B	201	0	0	11	0
All	All	11785	0	11212	291	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 13.

All (291) 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:120:SER:HB3	1:B:145:TYR:HB2	1.26	1.17
1:B:118:GLY:H	1:B:142:MET:HE3	1.06	1.15
1:A:95:LEU:HD22	1:A:142:MET:HE2	1.30	1.12
1:B:590:GLU:HG2	1:B:624:THR:HG21	1.25	1.12
1:A:510:ARG:HH11	1:A:510:ARG:HG2	1.06	1.11
1:A:95:LEU:H	1:A:118:GLY:HA2	1.07	1.11
1:A:399:GLN:HG3	1:A:402:PRO:HD3	1.28	1.11
1:B:398:LEU:HD23	1:B:399:GLN:H	1.01	1.09
1:A:590:GLU:HG2	1:A:624:THR:HG21	1.12	1.08
1:A:95:LEU:HB2	1:A:142:MET:HE3	1.34	1.07
1:A:153:LEU:HD21	1:A:156:VAL:HG22	1.41	1.02
1:B:399:GLN:HG2	1:B:400:SER:H	1.20	1.02
1:A:399:GLN:HG2	1:A:401:SER:HA	1.41	1.01
1:A:95:LEU:H	1:A:118:GLY:CA	1.75	0.98
1:B:448:MET:CE	1:B:473:LYS:HD2	1.98	0.94
1:A:590:GLU:HG2	1:A:624:THR:CG2	1.97	0.93
1:B:398:LEU:HD23	1:B:399:GLN:N	1.83	0.93
1:A:95:LEU:N	1:A:118:GLY:HA2	1.82	0.93
1:A:480:LEU:N	1:A:501:MET:HE1	1.83	0.93
1:B:477:LEU:HB2	1:B:501:MET:HE1	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ARG:NH1	1:A:510:ARG:HG2	1.85	0.90
1:A:400:SER:N	1:A:401:SER:HA	1.88	0.89
1:B:590:GLU:CG	1:B:624:THR:HG21	2.01	0.89
1:A:590:GLU:CG	1:A:624:THR:HG21	2.02	0.89
1:B:498:CYS:O	1:B:522:LEU:HD22	1.73	0.88
1:B:400:SER:N	1:B:401:SER:HA	1.89	0.88
1:A:281:GLN:HB3	2:A:805:NAG:H81	1.55	0.87
2:A:815:NAG:O3	2:A:815:NAG:H82	1.75	0.87
1:B:118:GLY:N	1:B:142:MET:HE3	1.90	0.86
1:B:305:VAL:HG23	1:B:306:ILE:HG13	1.56	0.86
1:A:399:GLN:CG	1:A:402:PRO:HD3	2.04	0.85
1:B:398:LEU:CD2	1:B:399:GLN:H	1.90	0.85
1:B:117:GLY:HA2	1:B:142:MET:HE1	1.55	0.84
1:A:399:GLN:OE1	6:A:1080:HOH:O	1.94	0.84
1:A:153:LEU:HD21	1:A:156:VAL:CG2	2.06	0.84
1:B:120:SER:HB3	1:B:145:TYR:CB	2.08	0.83
1:B:590:GLU:HG2	1:B:624:THR:CG2	2.08	0.83
1:B:477:LEU:O	1:B:501:MET:HE2	1.78	0.83
1:B:457:MET:HE2	1:B:462:LEU:HD11	1.60	0.82
1:A:399:GLN:HG2	1:A:400:SER:H	1.44	0.82
1:A:119:ASP:CG	1:A:120:SER:H	1.83	0.81
1:B:153:LEU:HD21	1:B:156:VAL:HG22	1.62	0.81
1:A:399:GLN:HG2	1:A:400:SER:N	1.95	0.80
1:A:281:GLN:HB3	2:A:805:NAG:C8	2.12	0.79
1:A:258:ILE:HD12	1:A:263:LEU:CD1	2.12	0.78
1:A:497:ARG:HD2	6:A:1104:HOH:O	1.83	0.77
1:B:477:LEU:CB	1:B:501:MET:HE1	2.13	0.77
1:B:418:VAL:HG21	1:B:457:MET:CE	2.16	0.76
1:A:399:GLN:CG	1:A:400:SER:H	1.96	0.76
1:A:119:ASP:HA	1:A:141:SER:OG	1.85	0.75
1:B:118:GLY:H	1:B:142:MET:CE	1.94	0.75
1:B:418:VAL:HG21	1:B:457:MET:HE3	1.68	0.75
1:B:468:GLU:OE1	6:B:1007:HOH:O	2.03	0.75
1:B:603:GLU:OE2	1:B:605:GLU:HB2	1.87	0.74
1:B:399:GLN:HG2	1:B:400:SER:N	2.00	0.74
1:B:258:ILE:HD11	1:B:284:LEU:HD22	1.69	0.74
1:B:501:MET:SD	6:B:1000:HOH:O	2.46	0.72
1:B:117:GLY:CA	1:B:142:MET:HE1	2.19	0.72
1:A:558:ASN:OD1	2:A:801:NAG:H2	1.88	0.72
1:B:467:PRO:O	1:B:470:VAL:HG23	1.89	0.72
1:B:448:MET:HE1	1:B:473:LYS:HD2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:SER:N	1:B:401:SER:CA	2.53	0.71
1:A:603:GLU:OE2	1:A:605:GLU:HB2	1.91	0.71
1:A:480:LEU:H	1:A:501:MET:HE1	1.57	0.70
1:B:258:ILE:HD12	1:B:263:LEU:CD1	2.22	0.70
1:B:443:PRO:HD2	1:B:446:ILE:HD12	1.73	0.69
1:A:95:LEU:HB2	1:A:142:MET:CE	2.17	0.69
1:B:165:GLY:HA3	6:B:1018:HOH:O	1.92	0.69
1:A:258:ILE:HD12	1:A:263:LEU:HD11	1.72	0.69
1:A:443:PRO:HD2	1:A:446:ILE:HD12	1.73	0.69
1:B:151:SER:HA	1:B:174:LEU:HD22	1.75	0.69
1:A:310:SER:OG	1:A:332:ASN:OD1	2.11	0.69
1:A:418:VAL:HG21	1:A:457:MET:CE	2.23	0.68
3:A:804:BLD:H221	3:A:804:BLD:H112	1.73	0.68
1:A:479:THR:C	1:A:501:MET:HE1	2.14	0.68
1:A:105:GLN:HB3	1:A:128:GLN:HG3	1.75	0.66
1:A:41:PHE:CD1	1:A:98:LEU:HD21	2.30	0.66
1:A:95:LEU:HD22	1:A:142:MET:CE	2.18	0.66
1:A:558:ASN:OD1	2:A:801:NAG:C2	2.40	0.66
1:B:374:CYS:HB3	6:B:1054:HOH:O	1.94	0.65
1:A:479:THR:HA	1:A:501:MET:CE	2.26	0.65
1:B:501:MET:CE	6:B:1000:HOH:O	2.44	0.65
1:A:281:GLN:CB	2:A:805:NAG:H81	2.28	0.64
1:A:399:GLN:HG2	1:A:401:SER:CA	2.24	0.64
1:A:418:VAL:HG12	1:A:446:ILE:HD11	1.79	0.64
1:B:277:GLN:O	1:B:303:THR:HG21	1.98	0.64
1:A:174:LEU:O	1:A:200:PRO:HG3	1.99	0.63
1:A:95:LEU:HB3	1:A:118:GLY:HA3	1.81	0.63
1:A:418:VAL:HG21	1:A:457:MET:HE3	1.81	0.62
3:A:804:BLD:C12	3:A:804:BLD:H221	2.29	0.62
1:B:418:VAL:CG2	1:B:457:MET:HE3	2.29	0.62
1:A:372:THR:HG22	1:A:395:PHE:CD1	2.35	0.62
1:B:392:PRO:HB2	1:B:395:PHE:CD2	2.34	0.62
1:A:132:LEU:HD13	1:A:142:MET:HE1	1.82	0.61
1:A:631:THR:HG22	3:A:804:BLD:H228	1.81	0.61
1:B:399:GLN:C	1:B:401:SER:HA	2.20	0.61
1:A:153:LEU:CD2	1:A:156:VAL:CG2	2.78	0.61
1:A:258:ILE:HD11	1:A:284:LEU:HD22	1.80	0.61
1:B:123:SER:OG	1:B:124:ASP:N	2.33	0.60
1:A:642:ILE:HD13	1:A:642:ILE:N	2.16	0.60
2:A:806:NAG:H83	2:A:806:NAG:H3	1.82	0.60
1:A:119:ASP:CG	1:A:120:SER:N	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLN:CG	1:A:400:SER:N	2.60	0.60
1:B:95:LEU:HB2	1:B:142:MET:HE2	1.82	0.60
1:B:392:PRO:HG2	1:B:395:PHE:HE2	1.66	0.60
1:B:448:MET:HE2	1:B:473:LYS:HD2	1.79	0.60
3:B:801:BLD:H112	3:B:801:BLD:H221	1.82	0.60
1:B:41:PHE:CD1	1:B:98:LEU:HD21	2.36	0.60
1:A:119:ASP:OD2	1:A:120:SER:N	2.33	0.59
1:A:684:GLY:HA3	1:A:706:SER:OG	2.02	0.59
1:A:510:ARG:HH11	1:A:510:ARG:CG	1.95	0.59
2:A:815:NAG:HO3	2:A:815:NAG:H82	1.68	0.59
1:A:358:VAL:CG2	1:A:382:LEU:HD23	2.33	0.58
1:A:255:THR:HB	1:A:281:GLN:HB2	1.85	0.58
1:A:59:TYR:CE1	1:A:60:GLU:HG3	2.39	0.58
1:A:479:THR:CA	1:A:501:MET:HE1	2.33	0.58
1:A:596:ARG:HD3	1:A:648:TYR:CE2	2.38	0.58
1:B:501:MET:HE3	6:B:1000:HOH:O	2.02	0.58
1:A:753:ARG:NH1	1:A:754:PRO:HD2	2.18	0.57
1:B:631:THR:HG22	3:B:801:BLD:H228	1.85	0.57
1:B:118:GLY:HA3	1:B:120:SER:OG	2.04	0.57
1:A:399:GLN:C	1:A:401:SER:HA	2.24	0.57
1:B:279:LEU:HD23	1:B:300:LEU:HD22	1.87	0.57
1:B:59:TYR:CE1	1:B:60:GLU:HG3	2.39	0.57
1:A:510:ARG:NH1	1:A:510:ARG:CG	2.61	0.56
1:B:41:PHE:CE1	1:B:98:LEU:HD11	2.40	0.56
1:B:418:VAL:HG12	1:B:446:ILE:HD11	1.87	0.56
1:B:477:LEU:HB2	1:B:501:MET:CE	2.31	0.56
1:A:716:LEU:HD22	1:A:733:LEU:CD1	2.36	0.56
1:B:676:THR:HG22	1:B:698:ASN:HB2	1.86	0.56
1:A:400:SER:N	1:A:401:SER:CA	2.67	0.56
1:A:501:MET:CE	1:A:503:TRP:O	2.53	0.56
1:A:479:THR:HA	1:A:501:MET:HE1	1.88	0.56
1:A:479:THR:HA	1:A:501:MET:HE3	1.87	0.56
1:B:718:VAL:HG13	1:B:723:LEU:HD12	1.88	0.55
1:A:32:PHE:HE2	1:A:59:TYR:HH	1.52	0.55
1:A:480:LEU:H	1:A:501:MET:CE	2.19	0.55
1:A:317:GLU:HG2	1:A:339:SER:O	2.07	0.55
1:B:166:LYS:N	6:B:1018:HOH:O	2.38	0.55
1:B:358:VAL:CG2	1:B:382:LEU:HD23	2.36	0.55
1:A:37:LEU:HD21	1:A:97:ASN:O	2.06	0.55
1:B:433:LEU:HB2	1:B:457:MET:HG2	1.87	0.55
1:B:308:ASP:OD1	1:B:310:SER:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:VAL:HG12	1:B:446:ILE:CD1	2.37	0.55
1:B:358:VAL:HG23	1:B:382:LEU:HD23	1.89	0.54
1:B:281:GLN:HB3	2:B:808:NAG:H81	1.90	0.54
1:B:59:TYR:CZ	1:B:60:GLU:HG3	2.43	0.54
1:B:590:GLU:CB	1:B:624:THR:HG21	2.38	0.54
2:A:806:NAG:C3	2:A:806:NAG:H83	2.37	0.54
1:B:32:PHE:HZ	1:B:59:TYR:HH	1.50	0.54
1:B:614:ARG:HB2	1:B:614:ARG:NH1	2.23	0.53
1:A:418:VAL:HG21	1:A:457:MET:HE1	1.90	0.53
1:B:54:LEU:HD22	1:B:57:TRP:CE2	2.44	0.53
1:B:468:GLU:OE2	1:B:494:SER:HB2	2.07	0.53
1:A:80:VAL:HG23	1:A:105:GLN:HG3	1.90	0.53
1:B:421:GLU:O	1:B:424:LYS:HB2	2.09	0.53
1:B:418:VAL:HG11	1:B:446:ILE:HD13	1.91	0.52
1:A:716:LEU:CD2	1:A:733:LEU:CD1	2.88	0.52
1:A:706:SER:HB2	6:A:916:HOH:O	2.10	0.52
1:B:150:CYS:O	1:B:174:LEU:HD22	2.10	0.52
1:A:501:MET:HE3	1:A:503:TRP:O	2.10	0.51
3:B:801:BLD:H221	3:B:801:BLD:C12	2.40	0.51
1:A:322:PHE:O	1:A:325:CYS:HB2	2.10	0.51
1:B:409:ILE:HG21	1:B:414:LEU:HD11	1.91	0.51
1:A:716:LEU:HD22	1:A:733:LEU:HD11	1.93	0.51
1:A:418:VAL:CG2	1:A:457:MET:HE3	2.40	0.51
1:B:418:VAL:HG21	1:B:457:MET:HE1	1.91	0.51
1:B:738:VAL:CG1	6:B:1044:HOH:O	2.59	0.51
1:A:395:PHE:HB2	6:A:1015:HOH:O	2.10	0.50
1:A:247:LEU:N	1:A:248:PRO:CD	2.74	0.50
1:A:409:ILE:HG21	1:A:414:LEU:HD11	1.93	0.50
1:B:217:PHE:O	1:B:244:PRO:HG3	2.12	0.50
1:A:132:LEU:CD1	1:A:142:MET:HE1	2.42	0.50
1:A:502:ILE:HD11	1:A:578:SER:HB3	1.94	0.49
1:B:267:ILE:HD11	1:B:314:PHE:CZ	2.48	0.49
1:A:392:PRO:HG2	1:A:395:PHE:HE2	1.77	0.49
1:B:344:ASN:HB2	1:B:368:PRO:HB3	1.95	0.49
1:B:454:ASP:HA	1:B:479:THR:HG22	1.94	0.49
2:A:806:NAG:C8	2:A:806:NAG:H3	2.43	0.48
1:A:79:ILE:HD12	1:A:101:LEU:HD22	1.95	0.48
1:B:398:LEU:HD22	1:B:399:GLN:O	2.13	0.48
1:A:308:ASP:OD1	1:A:310:SER:HB2	2.13	0.48
1:B:95:LEU:HB2	1:B:142:MET:CE	2.43	0.48
1:A:241:ASP:C	1:A:242:LYS:HG3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:PRO:O	1:A:470:VAL:HG23	2.14	0.48
1:B:247:LEU:N	1:B:248:PRO:CD	2.76	0.48
1:A:691:VAL:HG22	1:A:715:ASP:HB3	1.96	0.48
1:A:418:VAL:CG1	1:A:446:ILE:CD1	2.92	0.47
1:A:76:ASP:OD2	1:A:76:ASP:N	2.47	0.47
1:A:267:ILE:HD11	1:A:314:PHE:CZ	2.50	0.47
1:A:461:ASN:HB2	6:A:1053:HOH:O	2.15	0.47
1:B:418:VAL:CG1	1:B:446:ILE:CD1	2.93	0.47
1:B:429:LYS:HB3	1:B:429:LYS:HE3	1.66	0.47
1:B:447:TRP:O	1:B:474:GLY:HA3	2.14	0.47
1:B:738:VAL:HG12	6:B:1044:HOH:O	2.14	0.47
1:A:153:LEU:CD2	1:A:156:VAL:HG22	2.27	0.47
1:A:635:PHE:HE2	1:A:642:ILE:HD11	1.78	0.47
1:A:93:LEU:HD21	1:A:142:MET:HE1	1.96	0.47
2:A:806:NAG:C3	2:A:806:NAG:C8	2.92	0.46
1:B:579:VAL:HG12	1:B:633:TYR:OH	2.15	0.46
1:B:581:GLY:HA2	1:B:630:MET:HG3	1.97	0.46
1:A:41:PHE:CE1	1:A:98:LEU:HD11	2.50	0.46
1:B:380:LEU:CD2	1:B:395:PHE:CZ	2.98	0.46
1:B:37:LEU:HD21	1:B:97:ASN:O	2.15	0.46
1:B:686:LEU:O	1:B:710:LEU:HD22	2.16	0.46
1:B:610:GLU:OE1	2:B:807:NAG:H82	2.16	0.46
1:A:358:VAL:HG23	1:A:382:LEU:HD23	1.98	0.46
1:A:434:SER:OG	1:A:456:VAL:HG12	2.16	0.46
1:A:418:VAL:HG12	1:A:446:ILE:CD1	2.44	0.45
1:B:153:LEU:CD2	1:B:156:VAL:HG22	2.38	0.45
1:B:545:ASN:O	1:B:547:LYS:HD2	2.16	0.45
1:A:45:SER:O	1:A:91:GLY:HA3	2.16	0.45
1:A:734:THR:HB	1:A:750:VAL:HG12	1.97	0.45
1:A:398:LEU:HG	1:A:398:LEU:O	2.16	0.45
1:B:392:PRO:HB2	1:B:395:PHE:CE2	2.52	0.45
1:B:398:LEU:CD2	1:B:399:GLN:N	2.64	0.45
1:B:691:VAL:HG23	3:B:801:BLD:H02	1.98	0.44
1:A:564:PRO:HG2	1:A:567:LEU:HG	2.00	0.44
3:A:804:BLD:H20	3:A:804:BLD:H24	1.79	0.44
2:A:811:NAG:H62	2:A:812:NAG:C1	2.47	0.44
1:A:405:GLU:OE2	6:A:999:HOH:O	2.21	0.44
1:A:470:VAL:HG12	1:A:471:CYS:SG	2.58	0.44
1:B:418:VAL:CG1	1:B:446:ILE:HD13	2.47	0.44
1:A:241:ASP:HB3	1:A:242:LYS:HG3	2.00	0.44
1:A:576:PRO:HA	1:A:633:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:C	1:B:37:LEU:HD23	2.38	0.44
1:B:153:LEU:HD21	1:B:156:VAL:CG2	2.41	0.44
1:B:218:SER:HB3	1:B:242:LYS:O	2.17	0.44
1:B:258:ILE:HD12	1:B:263:LEU:HD11	1.98	0.44
1:A:83:ASP:OD1	1:A:85:ARG:NH2	2.47	0.43
1:B:635:PHE:HB3	1:B:664:TYR:CE1	2.53	0.43
1:A:32:PHE:HE2	1:A:59:TYR:OH	2.01	0.43
1:B:174:LEU:O	1:B:200:PRO:HG3	2.18	0.43
1:B:434:SER:OG	1:B:456:VAL:HG12	2.18	0.43
1:B:457:MET:CE	1:B:462:LEU:HD11	2.39	0.43
1:A:392:PRO:HB2	1:A:395:PHE:CE2	2.52	0.43
1:A:392:PRO:HB2	1:A:395:PHE:CD2	2.54	0.43
1:B:718:VAL:HG13	1:B:718:VAL:O	2.18	0.43
1:A:473:LYS:HA	1:A:473:LYS:HD2	1.81	0.43
1:B:413:TYR:CD2	1:B:413:TYR:N	2.87	0.43
1:A:143:VAL:HG22	1:A:158:ILE:HD12	1.99	0.43
1:A:40:ALA:O	1:A:44:ASN:HB2	2.19	0.43
1:B:654:PHE:C	1:B:654:PHE:CD2	2.92	0.43
1:B:158:ILE:O	1:B:158:ILE:HG22	2.18	0.42
1:B:259:SER:HB3	1:B:283:SER:OG	2.19	0.42
1:B:32:PHE:CE2	1:B:59:TYR:CE1	3.07	0.42
1:A:689:ILE:O	1:A:689:ILE:HG23	2.18	0.42
1:A:417:THR:HB	6:A:971:HOH:O	2.19	0.42
1:A:679:ILE:HD12	1:A:703:LEU:HD23	2.01	0.42
1:B:143:VAL:HG22	1:B:158:ILE:HD12	2.00	0.42
1:B:596:ARG:HD3	1:B:648:TYR:CD2	2.54	0.42
1:A:95:LEU:CB	1:A:118:GLY:HA3	2.49	0.42
3:B:801:BLD:O06	3:B:801:BLD:C19	2.67	0.42
1:B:587:VAL:HB	1:B:599:GLY:CA	2.49	0.42
1:A:418:VAL:HG11	1:A:446:ILE:HD13	2.01	0.42
1:A:59:TYR:HD1	1:A:60:GLU:N	2.18	0.42
1:B:245:ILE:O	1:B:248:PRO:HD2	2.20	0.42
1:B:380:LEU:HD22	1:B:395:PHE:CZ	2.55	0.42
1:B:53:VAL:HG21	1:B:87:SER:HB3	2.02	0.41
1:A:31:ASP:C	1:A:32:PHE:CD2	2.93	0.41
1:A:372:THR:HG22	1:A:395:PHE:CE1	2.55	0.41
1:A:80:VAL:HG22	1:A:80:VAL:O	2.21	0.41
1:B:546:CYS:HB3	6:B:901:HOH:O	2.19	0.41
1:B:590:GLU:HG2	1:B:624:THR:CB	2.50	0.41
1:A:281:GLN:N	1:A:281:GLN:OE1	2.54	0.41
1:A:596:ARG:CD	1:A:648:TYR:CD2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:804:BLD:H119	3:A:804:BLD:H08	1.85	0.41
1:B:477:LEU:C	1:B:501:MET:HE2	2.39	0.41
1:A:247:LEU:HB3	1:A:248:PRO:HD3	2.03	0.41
1:A:260:ARG:HG2	1:A:286:HIS:HB2	2.02	0.41
1:A:686:LEU:HD23	1:A:686:LEU:HA	1.86	0.41
1:B:423:GLY:HA3	1:B:445:GLU:HB3	2.02	0.41
1:B:80:VAL:HG22	1:B:80:VAL:O	2.21	0.41
1:A:457:MET:HB2	1:A:482:LEU:CD2	2.51	0.41
1:B:117:GLY:CA	1:B:142:MET:CE	2.95	0.41
1:A:470:VAL:C	1:A:472:VAL:H	2.23	0.41
1:A:93:LEU:O	1:A:117:GLY:CA	2.69	0.41
1:B:550:ILE:HB	1:B:642:ILE:HG12	2.03	0.41
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.19	0.41
1:B:550:ILE:HA	1:B:641:MET:HA	2.02	0.41
1:A:32:PHE:N	1:A:32:PHE:CD2	2.89	0.41
1:B:293:ILE:HA	1:B:294:PRO:HD3	1.94	0.41
1:B:305:VAL:HG21	6:B:983:HOH:O	2.21	0.41
1:A:591:GLY:HA3	1:A:595:CYS:SG	2.60	0.40
1:A:733:LEU:HD13	1:A:733:LEU:HA	1.89	0.40
1:B:182:LEU:HB2	1:B:208:LEU:HD23	2.02	0.40
1:A:132:LEU:CD1	1:A:142:MET:CE	2.99	0.40
1:A:588:ARG:NH1	1:A:627:TYR:OH	2.54	0.40
1:B:520:GLY:O	1:B:545:ASN:ND2	2.49	0.40
1:A:546:CYS:HB3	6:A:901:HOH:O	2.22	0.40
1:B:477:LEU:O	1:B:501:MET:CE	2.60	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:B:124:ASP:OD1	1:B:541:ARG:NH1[1_545]	1.99	0.21

## 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	720/740 (97%)	685 (95%)	35 (5%)	0	100	100
1	B	720/740 (97%)	693 (96%)	27 (4%)	0	100	100
All	All	1440/1480 (97%)	1378 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	627/641 (98%)	604 (96%)	23 (4%)	37	64
1	B	627/641 (98%)	606 (97%)	21 (3%)	41	68
All	All	1254/1282 (98%)	1210 (96%)	44 (4%)	39	66

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	76	ASP
1	A	158	ILE
1	A	186	ILE
1	A	212	ASN
1	A	220	LEU
1	A	225	CYS
1	A	241	ASP
1	A	255	THR
1	A	325	CYS
1	A	349	LYS
1	A	371	LEU
1	A	435	PHE
1	A	453	SER
1	A	510	ARG

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Mol	Chain	Res	Type
1	A	579	VAL
1	A	593	THR
1	A	613	GLU
1	A	618	VAL
1	A	630	MET
1	A	687	LYS
1	A	718	VAL
1	A	722	ASN
1	B	76	ASP
1	B	119	ASP
1	B	121	SER
1	B	123	SER
1	B	149	LYS
1	B	186	ILE
1	B	225	CYS
1	B	310	SER
1	B	349	LYS
1	B	353	ILE
1	B	369	ILE
1	B	397	SER
1	B	409	ILE
1	B	435	PHE
1	B	479	THR
1	B	604	PHE
1	B	614	ARG
1	B	628	SER
1	B	630	MET
1	B	718	VAL
1	B	733	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

32 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
2	NAG	A	801	1,2	14,14,15	0.49	0	17,19,21	1.65	1 (5%)
2	NAG	A	802	2	14,14,15	0.44	0	17,19,21	1.30	1 (5%)
2	NAG	A	803	1	14,14,15	0.54	0	17,19,21	1.31	2 (11%)
3	BLD	A	804	-	36,37,37	1.98	7 (19%)	46,59,59	2.65	16 (34%)
2	NAG	A	805	1,2	14,14,15	0.58	0	17,19,21	1.83	5 (29%)
2	NAG	A	806	2,4	14,14,15	1.86	4 (28%)	17,19,21	2.30	5 (29%)
4	BMA	A	807	2,5	11,11,12	1.09	1 (9%)	15,15,17	1.57	3 (20%)
5	MAN	A	808	5,4	11,11,12	1.42	3 (27%)	15,15,17	1.84	3 (20%)
5	MAN	A	809	5	11,11,12	3.93	1 (9%)	15,15,17	1.36	3 (20%)
5	MAN	A	810	5	11,11,12	2.01	4 (36%)	15,15,17	1.61	3 (20%)
2	NAG	A	811	1,2	14,14,15	1.92	3 (21%)	17,19,21	2.78	5 (29%)
2	NAG	A	812	2	14,14,15	1.64	3 (21%)	17,19,21	2.43	6 (35%)
2	NAG	A	813	1,2	14,14,15	0.59	0	17,19,21	0.80	0
2	NAG	A	814	2	14,14,15	0.47	0	17,19,21	0.89	1 (5%)
2	NAG	A	815	1	14,14,15	0.52	0	17,19,21	1.30	2 (11%)
3	BLD	B	801	-	36,37,37	2.04	9 (25%)	46,59,59	2.65	17 (36%)
2	NAG	B	802	1	14,14,15	0.45	0	17,19,21	0.95	0
2	NAG	B	803	1,2	14,14,15	0.45	0	17,19,21	2.27	5 (29%)
2	NAG	B	804	2	14,14,15	0.47	0	17,19,21	1.03	2 (11%)
2	NAG	B	805	1	14,14,15	0.61	0	17,19,21	1.23	2 (11%)
2	NAG	B	806	1,2	14,14,15	0.50	0	17,19,21	1.73	1 (5%)
2	NAG	B	807	2	14,14,15	0.46	0	17,19,21	1.49	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	808	1,2	14,14,15	2.06	6 (42%)	17,19,21	2.23	3 (17%)
2	NAG	B	809	2,4	14,14,15	2.29	5 (35%)	17,19,21	2.75	2 (11%)
4	BMA	B	810	2,5	11,11,12	1.05	2 (18%)	15,15,17	1.54	3 (20%)
5	MAN	B	811	5,4	11,11,12	1.68	3 (27%)	15,15,17	1.78	4 (26%)
5	MAN	B	812	5	11,11,12	2.17	4 (36%)	15,15,17	3.24	5 (33%)
5	MAN	B	813	5	11,11,12	2.34	5 (45%)	15,15,17	1.44	3 (20%)
2	NAG	B	814	1,2	14,14,15	0.66	0	17,19,21	1.16	2 (11%)
2	NAG	B	815	2	14,14,15	0.56	0	17,19,21	1.18	1 (5%)
2	NAG	B	816	1,2	14,14,15	0.62	0	17,19,21	1.04	1 (5%)
2	NAG	B	817	2	14,14,15	0.50	0	17,19,21	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	BLD	A	804	-	-	0/20/85/85	0/4/4/4
2	NAG	A	805	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	806	2,4	-	0/6/23/26	0/1/1/1
4	BMA	A	807	2,5	-	0/2/19/22	0/1/1/1
5	MAN	A	808	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	809	5	-	0/2/19/22	0/1/1/1
5	MAN	A	810	5	-	0/2/19/22	0/1/1/1
2	NAG	A	811	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	812	2	-	0/6/23/26	0/1/1/1
2	NAG	A	813	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	814	2	-	0/6/23/26	0/1/1/1
2	NAG	A	815	1	-	0/6/23/26	0/1/1/1
3	BLD	B	801	-	-	0/20/85/85	0/4/4/4
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	804	2	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	-	0/6/23/26	0/1/1/1
2	NAG	B	806	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	807	2	-	0/6/23/26	0/1/1/1
2	NAG	B	808	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	809	2,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	B	810	2,5	-	0/2/19/22	0/1/1/1
5	MAN	B	811	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	812	5	-	0/2/19/22	0/1/1/1
5	MAN	B	813	5	-	0/2/19/22	0/1/1/1
2	NAG	B	814	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	815	2	-	0/6/23/26	0/1/1/1
2	NAG	B	816	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	817	2	-	0/6/23/26	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	809	MAN	O6-C6	-12.84	0.88	1.42
3	B	801	BLD	O07-C07	-5.63	1.37	1.45
3	A	804	BLD	O07-C07	-5.56	1.37	1.45
2	B	809	NAG	O5-C1	-5.08	1.35	1.43
5	B	813	MAN	O5-C1	-4.60	1.36	1.43
2	B	808	NAG	O5-C1	-4.55	1.36	1.43
5	B	812	MAN	O5-C1	-4.21	1.36	1.43
5	B	811	MAN	O5-C1	-3.88	1.37	1.43
2	A	806	NAG	O5-C1	-3.74	1.37	1.43
2	A	811	NAG	O5-C1	-3.48	1.38	1.43
2	B	809	NAG	O5-C5	-3.48	1.36	1.43
5	B	813	MAN	O5-C5	-3.48	1.36	1.43
5	A	810	MAN	O5-C1	-3.45	1.38	1.43
5	A	810	MAN	O5-C5	-3.37	1.36	1.43
2	A	811	NAG	C2-N2	-3.34	1.40	1.46
2	A	812	NAG	O5-C1	-3.15	1.38	1.43
2	A	806	NAG	O5-C5	-3.12	1.37	1.43
3	B	801	BLD	C20-C17	-3.11	1.49	1.54
2	B	808	NAG	C2-N2	-3.03	1.41	1.46
5	B	813	MAN	O2-C2	-2.99	1.36	1.43
5	A	810	MAN	O4-C4	-2.97	1.35	1.43
5	B	812	MAN	O3-C3	-2.91	1.35	1.43
3	A	804	BLD	C19-C10	-2.90	1.49	1.54
3	B	801	BLD	C19-C10	-2.90	1.49	1.54
5	B	812	MAN	O5-C5	-2.85	1.37	1.43
5	B	812	MAN	O4-C4	-2.80	1.36	1.43
5	B	813	MAN	O4-C4	-2.79	1.36	1.43
2	A	806	NAG	O3-C3	-2.79	1.36	1.43
2	B	809	NAG	C2-N2	-2.79	1.41	1.46
2	A	811	NAG	O3-C3	-2.79	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	BLD	C20-C17	-2.71	1.50	1.54
5	B	811	MAN	O4-C4	-2.60	1.36	1.43
2	B	808	NAG	O3-C3	-2.57	1.36	1.43
2	B	809	NAG	O3-C3	-2.56	1.36	1.43
2	A	812	NAG	C2-N2	-2.52	1.42	1.46
2	B	809	NAG	O7-C7	-2.50	1.17	1.23
5	A	808	MAN	O2-C2	-2.49	1.37	1.43
4	A	807	BMA	O5-C1	-2.48	1.39	1.43
5	B	813	MAN	O3-C3	-2.42	1.37	1.43
3	A	804	BLD	C10-C05	-2.42	1.52	1.56
5	A	808	MAN	O5-C1	-2.38	1.39	1.43
2	A	806	NAG	C7-N2	-2.37	1.25	1.34
5	A	808	MAN	O4-C4	-2.37	1.37	1.43
2	B	808	NAG	O4-C4	-2.32	1.37	1.43
2	B	808	NAG	C1-C2	-2.29	1.49	1.52
3	A	804	BLD	C13-C14	-2.28	1.50	1.55
5	B	811	MAN	O2-C2	-2.28	1.38	1.43
4	B	810	BMA	O5-C1	-2.26	1.40	1.43
5	A	810	MAN	O3-C3	-2.24	1.37	1.43
3	B	801	BLD	C10-C05	-2.17	1.52	1.56
2	B	808	NAG	O5-C5	-2.17	1.38	1.43
3	A	804	BLD	O22-C22	-2.15	1.37	1.43
3	B	801	BLD	C13-C14	-2.08	1.50	1.55
4	B	810	BMA	O5-C5	-2.04	1.39	1.43
2	A	812	NAG	O5-C5	-2.02	1.39	1.43
3	B	801	BLD	O22-C22	-2.01	1.38	1.43
3	B	801	BLD	O07-C06	2.36	1.37	1.34
3	B	801	BLD	C08-C14	2.45	1.58	1.53
3	A	804	BLD	O06-C06	6.65	1.37	1.21
3	B	801	BLD	O06-C06	6.76	1.38	1.21

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	809	NAG	O5-C1-C2	-8.91	99.22	111.52
5	B	812	MAN	O5-C5-C6	-8.73	93.33	107.15
2	A	806	NAG	O5-C1-C2	-7.55	101.10	111.52
2	A	811	NAG	O5-C1-C2	-7.41	101.30	111.52
3	B	801	BLD	C13-C17-C20	-6.58	111.24	118.91
2	A	812	NAG	C3-C4-C5	-6.48	98.65	110.24
2	B	808	NAG	O5-C1-C2	-6.37	102.72	111.52
3	A	804	BLD	O07-C06-O06	-6.22	106.74	116.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	BLD	C19-C10-C05	-6.11	99.36	109.91
3	B	801	BLD	C19-C10-C05	-5.88	99.76	109.91
3	B	801	BLD	C18-C13-C12	-5.68	101.37	110.59
3	A	804	BLD	C18-C13-C12	-5.56	101.57	110.59
2	B	809	NAG	C3-C4-C5	-5.54	100.34	110.24
2	A	811	NAG	C6-C5-C4	-5.49	100.02	112.99
3	A	804	BLD	C13-C17-C20	-4.94	113.15	118.91
5	A	808	MAN	C2-C3-C4	-4.40	103.23	110.87
3	B	801	BLD	O07-C06-O06	-4.26	109.87	116.68
5	B	811	MAN	C2-C3-C4	-4.25	103.48	110.87
2	A	805	NAG	C2-N2-C7	-4.23	116.77	122.94
2	A	812	NAG	C2-N2-C7	-3.95	117.18	122.94
2	B	815	NAG	C2-N2-C7	-3.89	117.27	122.94
2	A	812	NAG	C4-C3-C2	-3.67	105.64	111.02
2	A	811	NAG	O3-C3-C4	-3.59	101.97	110.34
4	B	810	BMA	O5-C1-C2	-3.52	105.30	110.78
5	B	812	MAN	C1-C2-C3	-3.38	105.38	109.66
5	B	813	MAN	C6-C5-C4	-2.99	105.93	112.99
2	A	806	NAG	C4-C3-C2	-2.98	106.65	111.02
3	A	804	BLD	C07-O07-C06	-2.95	116.72	120.99
3	B	801	BLD	C07-O07-C06	-2.94	116.73	120.99
3	B	801	BLD	C21-C20-C17	-2.94	107.42	112.69
2	B	814	NAG	O5-C1-C2	-2.82	107.62	111.52
4	A	807	BMA	O5-C1-C2	-2.77	106.45	110.78
2	A	815	NAG	C2-N2-C7	-2.64	119.09	122.94
5	B	812	MAN	O2-C2-C3	-2.63	105.06	110.19
5	A	810	MAN	C6-C5-C4	-2.56	106.94	112.99
2	B	808	NAG	C6-C5-C4	-2.47	107.15	112.99
5	B	813	MAN	O4-C4-C3	-2.40	104.74	110.34
2	A	812	NAG	O5-C5-C4	-2.29	105.25	110.83
2	B	805	NAG	O5-C1-C2	-2.28	108.37	111.52
2	A	805	NAG	O5-C1-C2	-2.23	108.44	111.52
2	B	803	NAG	C6-C5-C4	-2.21	107.76	112.99
5	B	812	MAN	O5-C1-C2	-2.15	107.42	110.78
2	A	805	NAG	C6-C5-C4	-2.14	107.94	112.99
2	B	804	NAG	C2-N2-C7	-2.10	119.88	122.94
5	A	809	MAN	O3-C3-C2	-2.10	106.13	110.04
5	A	809	MAN	O2-C2-C3	-2.07	106.15	110.19
2	A	806	NAG	C3-C4-C5	-2.06	106.56	110.24
5	A	810	MAN	O4-C4-C5	-2.06	104.15	109.31
2	A	811	NAG	C3-C4-C5	-2.04	106.59	110.24
3	B	801	BLD	C26-C25-C24	2.01	116.55	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	807	BMA	C1-O5-C5	2.03	114.98	112.19
2	B	803	NAG	C3-C4-C5	2.07	113.94	110.24
3	A	804	BLD	C14-C08-C09	2.07	111.89	109.09
5	B	813	MAN	C1-C2-C3	2.10	112.32	109.66
5	B	811	MAN	O3-C3-C2	2.17	114.07	110.04
3	A	804	BLD	C15-C14-C13	2.17	106.53	103.84
4	B	810	BMA	O3-C3-C2	2.19	114.10	110.04
2	A	806	NAG	O3-C3-C2	2.20	114.10	109.39
3	B	801	BLD	C13-C14-C08	2.21	117.73	114.38
3	B	801	BLD	C26-C25-C27	2.22	116.96	110.63
3	A	804	BLD	C11-C12-C13	2.26	116.70	112.79
4	B	810	BMA	C1-O5-C5	2.28	115.32	112.19
2	A	812	NAG	C1-C2-N2	2.35	114.49	110.49
5	B	811	MAN	O6-C6-C5	2.35	119.48	111.29
3	A	804	BLD	C12-C13-C14	2.39	110.98	107.26
2	A	803	NAG	C4-C3-C2	2.43	114.58	111.02
2	B	816	NAG	C4-C3-C2	2.47	114.63	111.02
2	A	814	NAG	C1-O5-C5	2.51	115.64	112.19
5	A	808	MAN	O6-C6-C5	2.51	120.06	111.29
2	B	803	NAG	O5-C5-C4	2.51	116.94	110.83
2	A	805	NAG	C3-C4-C5	2.53	114.76	110.24
2	B	804	NAG	C1-O5-C5	2.55	115.69	112.19
3	B	801	BLD	C14-C08-C09	2.60	112.60	109.09
2	B	814	NAG	C1-O5-C5	2.63	115.80	112.19
2	A	812	NAG	O5-C5-C6	2.69	111.41	107.15
2	B	805	NAG	O5-C5-C6	2.74	111.49	107.15
3	B	801	BLD	C04-C03-C02	2.77	113.72	110.27
5	B	811	MAN	C1-O5-C5	2.80	116.04	112.19
2	A	806	NAG	C2-N2-C7	2.94	127.23	122.94
3	B	801	BLD	C16-C17-C20	2.95	116.92	112.63
4	A	807	BMA	O3-C3-C2	2.99	115.60	110.04
3	A	804	BLD	C16-C17-C13	3.07	107.64	103.84
2	A	805	NAG	C1-O5-C5	3.25	116.66	112.19
5	A	809	MAN	C1-O5-C5	3.35	116.79	112.19
5	A	810	MAN	C1-O5-C5	3.36	116.81	112.19
2	A	803	NAG	C1-O5-C5	3.40	116.86	112.19
2	A	815	NAG	C1-O5-C5	3.54	117.06	112.19
3	B	801	BLD	C16-C17-C13	3.66	108.37	103.84
3	A	804	BLD	C16-C17-C20	3.66	117.95	112.63
3	A	804	BLD	C04-C03-C02	3.70	114.87	110.27
2	B	803	NAG	O5-C1-C2	3.84	116.82	111.52
5	A	808	MAN	C1-O5-C5	3.91	117.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	BLD	C01-C10-C05	4.22	113.92	107.09
2	A	811	NAG	C1-O5-C5	4.26	118.05	112.19
2	A	802	NAG	C1-O5-C5	4.35	118.17	112.19
3	B	801	BLD	C01-C02-C03	4.42	116.53	111.36
3	A	804	BLD	C10-C01-C02	4.53	121.50	113.97
3	A	804	BLD	C01-C02-C03	4.66	116.80	111.36
3	A	804	BLD	C12-C13-C17	4.75	123.80	116.56
2	B	808	NAG	C1-O5-C5	5.00	119.07	112.19
3	B	801	BLD	C10-C01-C02	5.09	122.43	113.97
2	B	807	NAG	C1-O5-C5	5.09	119.19	112.19
3	A	804	BLD	C01-C10-C05	5.36	115.76	107.09
3	B	801	BLD	C12-C13-C17	6.06	125.79	116.56
2	A	801	NAG	C1-O5-C5	6.16	120.66	112.19
2	B	806	NAG	C1-O5-C5	6.42	121.02	112.19
2	B	803	NAG	C1-O5-C5	6.75	121.48	112.19
5	B	812	MAN	C1-O5-C5	7.32	122.26	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	2	0
3	A	804	BLD	5	0
2	A	805	NAG	3	0
2	A	806	NAG	4	0
2	A	811	NAG	1	0
2	A	812	NAG	1	0
2	A	815	NAG	2	0
3	B	801	BLD	5	0
2	B	807	NAG	1	0
2	B	808	NAG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	724/740 (97%)	-0.25	23 (3%)	47 51	11, 22, 48, 88	0
1	B	724/740 (97%)	-0.26	22 (3%)	50 53	12, 23, 50, 97	0
All	All	1448/1480 (97%)	-0.26	45 (3%)	49 52	11, 22, 49, 97	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	SER	10.3
1	A	400	SER	6.5
1	B	31	ASP	4.7
1	B	617	MET	4.6
1	A	619	HIS	4.5
1	A	59	TYR	4.3
1	B	619	HIS	4.3
1	B	59	TYR	4.2
1	B	618	VAL	4.2
1	A	32	PHE	4.2
1	A	64	GLY	4.1
1	B	119	ASP	4.1
1	A	399	GLN	4.1
1	A	617	MET	3.7
1	A	620	SER	3.5
1	B	32	PHE	3.5
1	B	76	ASP	3.4
1	B	757	SER	3.4
1	A	120	SER	3.2
1	B	120	SER	3.2
1	A	393	SER	3.1
1	A	757	SER	3.0
1	A	756	GLY	3.0
1	A	618	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	31	ASP	2.9
1	B	121	SER	2.9
1	B	64	GLY	2.8
1	B	75	ASP	2.6
1	B	399	GLN	2.6
1	B	590	GLU	2.4
1	A	593	THR	2.4
1	B	393	SER	2.4
1	B	401	SER	2.4
1	A	473	LYS	2.3
1	A	397	SER	2.3
1	A	118	GLY	2.3
1	B	620	SER	2.2
1	A	614	ARG	2.2
1	A	481	ILE	2.2
1	B	594	ASP	2.2
1	B	60	GLU	2.2
1	A	472	VAL	2.1
1	A	60	GLU	2.1
1	A	119	ASP	2.1
1	B	623	ALA	2.1

## 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. 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	815	14/15	0.80	0.31	33,49,60,64	0
2	NAG	B	807	14/15	0.83	0.39	49,68,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	806	14/15	0.85	0.25	40,50,57,58	0
2	NAG	B	803	14/15	0.86	0.23	28,41,47,52	0
2	NAG	B	802	14/15	0.86	0.26	37,48,54,59	0
5	MAN	A	808	11/12	0.86	0.17	18,23,25,27	0
2	NAG	A	801	14/15	0.86	0.30	25,41,51,52	0
2	NAG	B	817	14/15	0.87	0.36	44,60,63,64	0
2	NAG	A	803	14/15	0.89	0.16	30,40,48,48	0
2	NAG	B	804	14/15	0.90	0.35	35,44,48,49	0
2	NAG	A	814	14/15	0.90	0.42	31,52,62,66	0
2	NAG	A	802	14/15	0.90	0.38	38,54,62,63	0
2	NAG	B	805	14/15	0.91	0.22	30,39,48,52	0
5	MAN	B	811	11/12	0.92	0.14	16,22,24,25	0
3	BLD	A	804	34/34	0.93	0.15	15,22,30,35	23
4	BMA	B	810	11/12	0.93	0.21	25,29,36,38	0
2	NAG	A	813	14/15	0.94	0.24	28,38,46,46	0
2	NAG	B	815	14/15	0.94	0.27	22,35,43,46	0
3	BLD	B	801	34/34	0.94	0.15	17,23,28,29	23
4	BMA	A	807	11/12	0.94	0.24	28,34,41,43	0
2	NAG	A	812	14/15	0.94	0.27	28,34,44,45	0
5	MAN	A	809	11/12	0.94	0.13	16,20,24,42	0
2	NAG	A	806	14/15	0.95	0.16	16,26,32,32	0
2	NAG	B	816	14/15	0.95	0.27	29,42,54,54	0
5	MAN	A	810	11/12	0.96	0.12	16,19,23,29	0
2	NAG	B	814	14/15	0.96	0.14	16,23,29,31	0
2	NAG	A	811	14/15	0.96	0.10	16,24,33,33	0
5	MAN	B	812	11/12	0.96	0.09	16,22,26,33	0
2	NAG	A	805	14/15	0.97	0.11	17,22,25,33	0
5	MAN	B	813	11/12	0.97	0.10	15,20,24,32	0
2	NAG	B	809	14/15	0.97	0.13	19,25,30,31	0
2	NAG	B	808	14/15	0.97	0.09	18,23,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.