



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:14 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

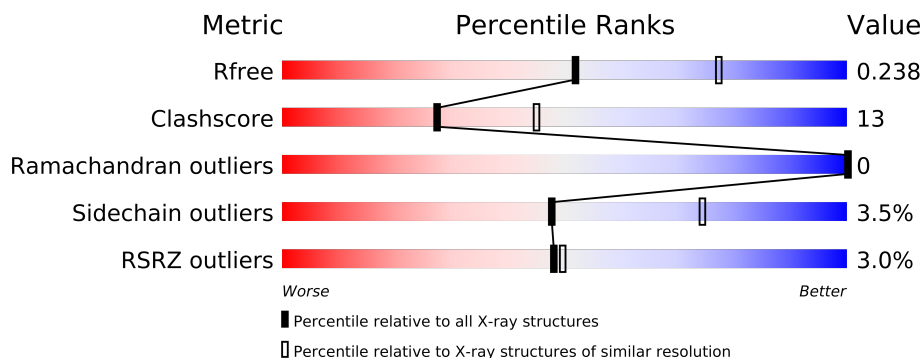
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	740	
1	B	740	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	815	-	X
3	NAG	B	802	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11785 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

There are 42 discrepancies between the modelled and reference sequences:

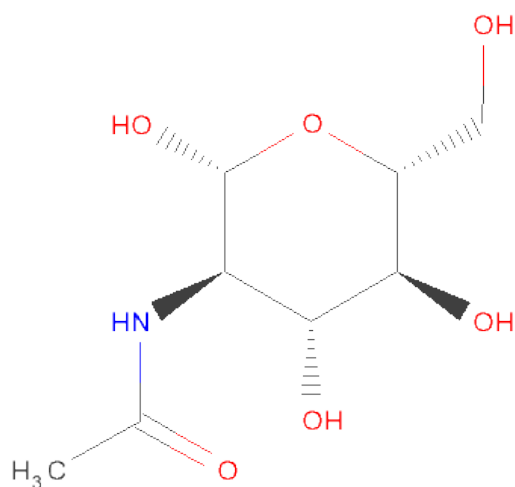
Chain	Residue	Modelled	Actual	Comment	Reference
A	759	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	760	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	761	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	762	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	763	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	764	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
A	759	HIS	-	EXPRESSION TAG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

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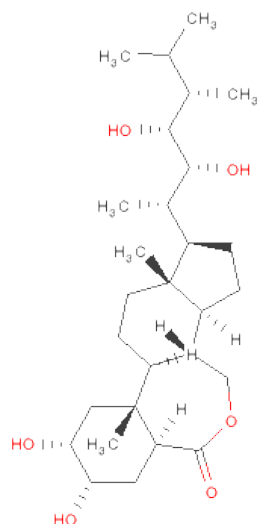
Chain	Residue	Modelled	Actual	Comment	Reference
B	761	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	762	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	763	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	764	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	759	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	760	HIS	-	EXPRESSION TAG	UNP Q9ZWC8
B	761	HIS	-	EXPRESSION TAG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

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



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

- Molecule 4 is BRASSINOLIDE (three-letter code: BLD) (formula: $C_{28}H_{48}O_6$).



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

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			72	40	2	30		
5	B	6	Total	C	N	O	0	0
			72	40	2	30		

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	764	HIS	-	EXPRESSION TAG	UNP Q9ZWC8

- Molecule 6 is water.

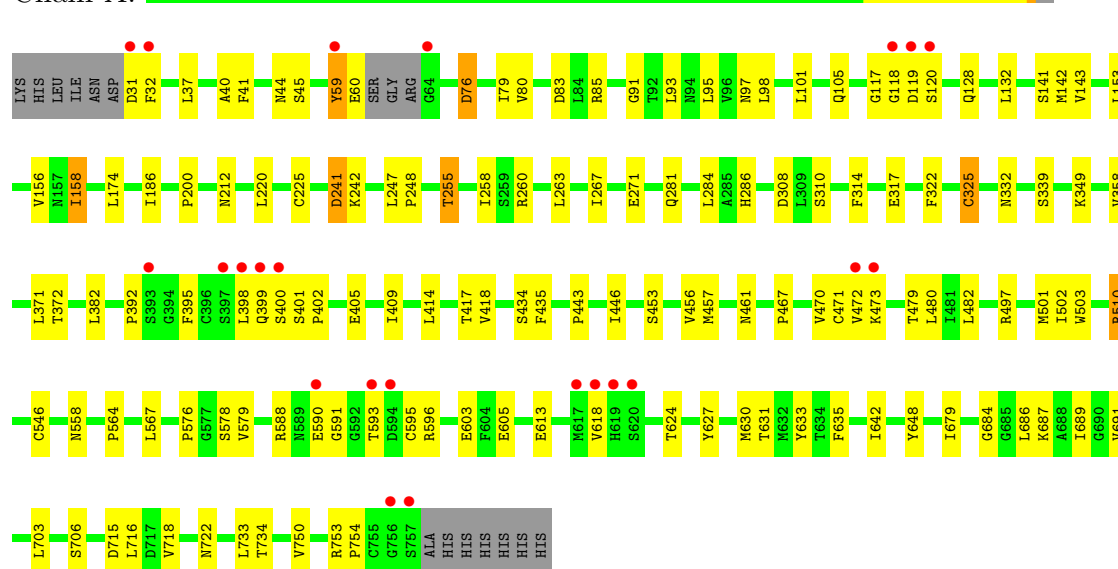
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total 210	O 210	0	0
6	B	201	Total 201	O 201	0	0

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.

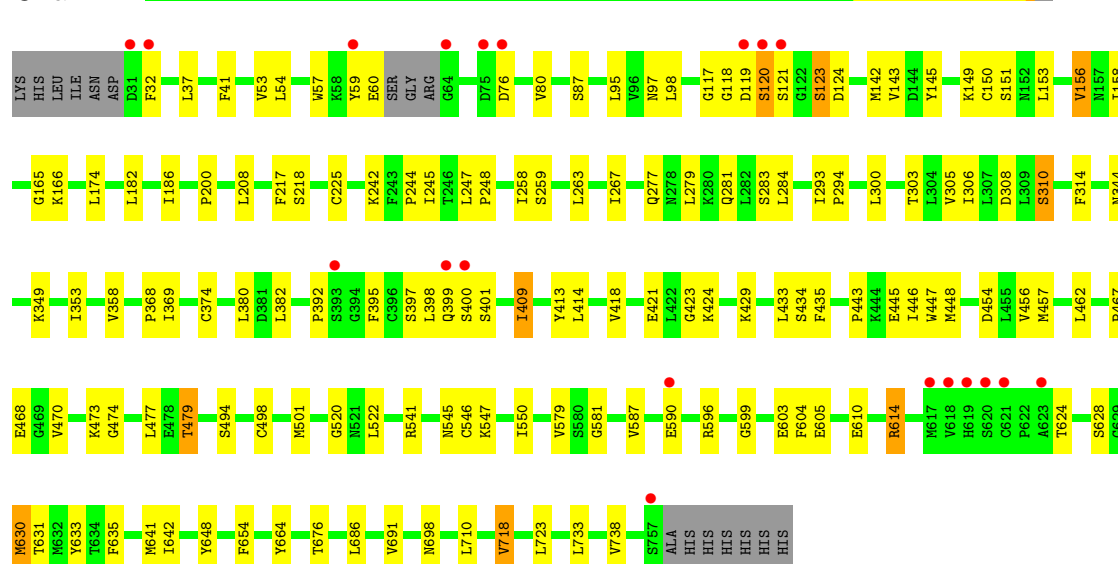
- Molecule 1: Serine/threonine-proteinkinase BRI1-like 1

Chain A:



- Molecule 1: Serine/threonine-proteinkinase BRI1-like 1

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.187 , 0.239 0.188 , 0.238	Depositor DCC
R_{free} test set	3780 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 19.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 75143 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11785	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	84	0	74	3	0
2	B	112	0	100	1	0
3	A	28	0	26	2	0
3	B	28	0	26	0	0
4	A	34	0	48	5	0
4	B	34	0	48	5	0
5	A	72	0	55	7	0
5	B	72	0	54	1	0
6	A	210	0	0	8	0
6	B	201	0	0	11	0
All	All	11785	0	11212	291	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (291) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:399:GLN:HG2	1:B:400:SER:H	1.20	1.02
1:A:153:LEU:HD21	1:A:156:VAL:HG22	1.41	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	Distance(Å)	Clash(Å)
1:A:510:ARG:NH1	1:A:510:ARG:HG2	1.85	0.90
1:B:590:GLU:CG	1:B:624:THR:HG21	2.01	0.89
1:A:400:SER:N	1:A:401:SER:HA	1.88	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
3:A:815:NAG:O3	3:A:815:NAG:H82	1.75	0.87
1:A:281:GLN:HB3	5:A:805:NAG:H81	1.55	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	5: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
1:B:400:SER:N	1:B:401:SER:CA	2.53	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
4:A:804:BLD:H221	4: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	5: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
1:B:418:VAL:CG2	1:B:457:MET:HE3	2.29	0.62
4:A:804:BLD:C12	4:A:804:BLD:H221	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:B:399:GLN:C	1:B:401:SER:HA	2.20	0.61
1:A:631:THR:HG22	4:A:804:BLD:H228	1.81	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
5:A:806:NAG:H83	5:A:806:NAG:H3	1.82	0.60
1:A:642:ILE:HD13	1:A:642:ILE:N	2.16	0.60
1:B:95:LEU:HB2	1:B:142:MET:HE2	1.82	0.60
1:A:399:GLN:CG	1:A:400:SER:N	2.60	0.60
1:A:119:ASP:CG	1:A:120:SER:N	2.54	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:448:MET:HE2	1:B:473:LYS:HD2	1.79	0.60
1:B:392:PRO:HG2	1:B:395:PHE:HE2	1.66	0.60
4:B:801:BLD:H112	4: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
3:A:815:NAG:HO3	3: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	4: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:59:TYR:CE1	1:B:60:GLU:HG3	2.39	0.57
1:B:279:LEU:HD23	1:B:300:LEU:HD22	1.87	0.57
1:A:510:ARG:NH1	1:A:510:ARG:CG	2.61	0.56
1:B:477:LEU:HB2	1:B:501:MET:CE	2.31	0.56
1:B:418:VAL:HG12	1:B:446:ILE:HD11	1.87	0.56
1:B:41:PHE:CE1	1:B:98:LEU:HD11	2.40	0.56
1:B:676:THR:HG22	1:B:698:ASN:HB2	1.86	0.56
1:A:716:LEU:HD22	1:A:733:LEU:CD1	2.36	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:B:166:LYS:N	6:B:1018:HOH:O	2.38	0.55
1:A:317:GLU:HG2	1:A:339:SER:O	2.07	0.55
1:B:358:VAL:CG2	1:B:382:LEU:HD23	2.36	0.55
1:B:433:LEU:HB2	1:B:457:MET:HG2	1.87	0.55
1:A:37:LEU:HD21	1:A:97:ASN:O	2.06	0.55
1:B:418:VAL:HG12	1:B:446:ILE:CD1	2.37	0.55
1:B:308:ASP:OD1	1:B:310:SER:HB2	2.07	0.55
1:B:358:VAL:HG23	1:B:382:LEU:HD23	1.89	0.54
1:B:281:GLN:HB3	5:B:808:NAG:H81	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
5:A:806:NAG:C3	5: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
4:B:801:BLD:H221	4: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:409:ILE:HG21	1:A:414:LEU:HD11	1.93	0.50
1:A:247:LEU:N	1:A:248:PRO:CD	2.74	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
5:A:806:NAG:C8	5:A:806:NAG:H3	2.43	0.48
1:B:398:LEU:HD22	1:B:399:GLN:O	2.13	0.48
1:A:79:ILE:HD12	1:A:101:LEU:HD22	1.95	0.48
1:B:95:LEU:HB2	1:B:142:MET:CE	2.43	0.48
1:A:308:ASP:OD1	1:A:310:SER:HB2	2.13	0.48
1:A:241:ASP:C	1:A:242:LYS:HG3	2.34	0.48
1:B:247:LEU:N	1:B:248:PRO:CD	2.76	0.48
1:A:467:PRO:O	1:A:470:VAL:HG23	2.14	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:ASP:N	1:A:76:ASP:OD2	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:738:VAL:HG12	6:B:1044:HOH:O	2.14	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: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
5:A:806:NAG:C3	5: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:B:153:LEU:CD2	1:B:156:VAL:HG22	2.38	0.45
1:A:418:VAL:HG12	1:A:446:ILE:CD1	2.44	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:B:392:PRO:HB2	1:B:395:PHE:CE2	2.52	0.45
1:A:398:LEU:HG	1:A:398:LEU:O	2.16	0.45
1:B:398:LEU:CD2	1:B:399:GLN:N	2.64	0.45
1:B:691:VAL:HG23	4:B:801:BLD:H02	1.98	0.44
4:A:804:BLD:H20	4:A:804:BLD:H24	1.79	0.44
2:A:811:NAG:H62	2:A:812:NAG:C1	2.47	0.44
1:A:564:PRO:HG2	1:A:567:LEU:HG	2.00	0.44
1:A:470:VAL:HG12	1:A:471:CYS:SG	2.58	0.44
1:A:405:GLU:OE2	6:A:999:HOH:O	2.21	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:B:37:LEU:C	1:B:37:LEU:HD23	2.38	0.44
1:A:576:PRO:HA	1:A:633:TYR:CE1	2.53	0.44
1:B:153:LEU:HD21	1:B:156:VAL:CG2	2.41	0.44
1:B:258:ILE:HD12	1:B:263:LEU:HD11	1.98	0.44
1:B:218:SER:HB3	1:B:242:LYS:O	2.17	0.44
1:B:635:PHE:HB3	1:B:664:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:ASP:OD1	1:A:85:ARG:NH2	2.47	0.43
1:B:457:MET:CE	1:B:462:LEU:HD11	2.39	0.43
1:B:174:LEU:O	1:B:200:PRO:HG3	2.18	0.43
1:A:32:PHE:HE2	1:A:59:TYR:OH	2.01	0.43
1:B:434:SER:OG	1:B:456:VAL:HG12	2.18	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:B:654:PHE:C	1:B:654:PHE:CD2	2.92	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: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:B:143:VAL:HG22	1:B:158:ILE:HD12	2.00	0.42
1:A:679:ILE:HD12	1:A:703:LEU:HD23	2.01	0.42
1:A:417:THR:HB	6:A:971:HOH:O	2.19	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
4:B:801:BLD:O06	4: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:B:380:LEU:HD22	1:B:395:PHE:CZ	2.55	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:53:VAL:HG21	1:B:87:SER:HB3	2.02	0.41
1:B:590:GLU:HG2	1:B:624:THR:CB	2.50	0.41
1:A:80:VAL:HG22	1:A:80:VAL:O	2.21	0.41
1:A:372:THR:HG22	1:A:395:PHE:CE1	2.55	0.41
1:A:31:ASP:C	1:A:32:PHE:CD2	2.93	0.41
1:B:546:CYS:HB3	6:B:901:HOH:O	2.19	0.41
1:A:281:GLN:N	1:A:281:GLN:OE1	2.54	0.41
4:A:804:BLD:H119	4:A:804:BLD:H08	1.85	0.41
1:A:596:ARG:CD	1:A:648:TYR:CD2	3.04	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:686:LEU:HD23	1:A:686:LEU:HA	1.86	0.41
1:B:80:VAL:HG22	1:B:80:VAL:O	2.21	0.41
1:B:423:GLY:HA3	1:B:445:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:ARG:HG2	1:A:286:HIS:HB2	2.02	0.41
1:B:117:GLY:CA	1:B:142:MET:CE	2.95	0.41
1:A:457:MET:HB2	1:A:482:LEU:CD2	2.51	0.41
1:A:93:LEU:O	1:A:117:GLY:CA	2.69	0.41
1:A:470:VAL:C	1:A:472:VAL:H	2.23	0.41
1:B:550:ILE:HB	1:B:642:ILE:HG12	2.03	0.41
1:B:550:ILE:HA	1:B:641:MET:HA	2.02	0.41
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.19	0.41
1:B:305:VAL:HG21	6:B:983:HOH:O	2.21	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: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:B:520:GLY:O	1:B:545:ASN:ND2	2.49	0.40
1:A:588:ARG:NH1	1:A:627:TYR:OH	2.54	0.40
1:B:477:LEU:O	1:B:501:MET:CE	2.60	0.40
1:A:546:CYS:HB3	6:A:901:HOH:O	2.22	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	Distance(Å)	Clash(Å)
1:B:124:ASP:OD1	1:B:541:ARG:NH1[1_545]	1.99	0.21

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	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%)	45	72
1	B	627/641 (98%)	606 (97%)	21 (3%)	50	76
All	All	1254/1282 (98%)	1210 (96%)	44 (4%)	48	74

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
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

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Mol	Chain	Res	Type
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 chains 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 ⓘ

26 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	801	1,2	12,14,15	0.50	0	15,19,21	1.25	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	802	2	12,14,15	0.52	0	15,19,21	0.91	1 (6%)
5	NAG	A	805	1,5	12,14,15	0.68	0	15,19,21	1.78	5 (33%)
5	NAG	A	806	5	12,14,15	1.97	4 (33%)	15,19,21	1.99	4 (26%)
5	BMA	A	807	5	10,11,12	1.17	1 (10%)	11,15,17	1.56	2 (18%)
5	MAN	A	808	5	10,11,12	1.49	3 (30%)	11,15,17	2.11	3 (27%)
5	MAN	A	809	5	10,11,12	4.02	1 (10%)	11,15,17	1.12	1 (9%)
5	MAN	A	810	5	10,11,12	2.14	4 (40%)	11,15,17	1.49	2 (18%)
2	NAG	A	811	1,2	12,14,15	2.16	3 (25%)	15,19,21	1.99	4 (26%)
2	NAG	A	812	2	12,14,15	1.86	2 (16%)	15,19,21	2.92	6 (40%)
2	NAG	A	813	1,2	12,14,15	0.76	1 (8%)	15,19,21	0.96	1 (6%)
2	NAG	A	814	2	12,14,15	0.65	0	15,19,21	0.85	1 (6%)
2	NAG	B	803	1,2	12,14,15	0.50	0	15,19,21	1.92	4 (26%)
2	NAG	B	804	2	12,14,15	0.66	0	15,19,21	0.74	0
2	NAG	B	806	1,2	12,14,15	0.57	0	15,19,21	0.93	1 (6%)
2	NAG	B	807	2	12,14,15	0.54	0	15,19,21	1.10	2 (13%)
5	NAG	B	808	1,5	12,14,15	2.08	5 (41%)	15,19,21	1.35	2 (13%)
5	NAG	B	809	5	12,14,15	2.33	4 (33%)	15,19,21	2.00	3 (20%)
5	BMA	B	810	5	10,11,12	1.19	1 (10%)	11,15,17	1.33	2 (18%)
5	MAN	B	811	5	10,11,12	1.50	3 (30%)	11,15,17	2.09	4 (36%)
5	MAN	B	812	5	10,11,12	2.09	3 (30%)	11,15,17	4.04	2 (18%)
5	MAN	B	813	5	10,11,12	2.29	4 (40%)	11,15,17	1.62	2 (18%)
2	NAG	B	814	1,2	12,14,15	0.84	0	15,19,21	1.01	1 (6%)
2	NAG	B	815	2	12,14,15	0.68	0	15,19,21	1.08	1 (6%)
2	NAG	B	816	1,2	12,14,15	0.75	1 (8%)	15,19,21	1.08	1 (6%)
2	NAG	B	817	2	12,14,15	0.64	0	15,19,21	0.79	1 (6%)

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
5	NAG	A	805	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	806	5	-	0/6/23/26	0/1/1/1
5	BMA	A	807	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	808	5	-	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	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	806	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	807	2	-	0/6/23/26	0/1/1/1
5	NAG	B	808	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	809	5	-	0/6/23/26	0/1/1/1
5	BMA	B	810	5	-	0/2/19/22	0/1/1/1
5	MAN	B	811	5	-	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 (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	809	MAN	O6-C6	-12.42	0.88	1.42
5	B	813	MAN	O5-C5	-4.95	1.36	1.45
5	B	809	NAG	O5-C5	-4.95	1.36	1.45
2	A	811	NAG	C2-N2	-4.87	1.40	1.46
5	A	810	MAN	O5-C5	-4.83	1.36	1.45
5	A	806	NAG	O5-C5	-4.55	1.37	1.45
5	B	808	NAG	C2-N2	-4.42	1.41	1.46
5	B	812	MAN	O5-C5	-4.25	1.37	1.45
5	B	809	NAG	C2-N2	-4.07	1.41	1.46
2	A	812	NAG	C2-N2	-3.68	1.42	1.46
5	B	808	NAG	O5-C5	-3.48	1.38	1.45
5	B	810	BMA	O5-C5	-3.34	1.39	1.45
2	A	812	NAG	O5-C5	-3.32	1.39	1.45
5	B	813	MAN	O2-C2	-3.13	1.36	1.43
5	A	810	MAN	O4-C4	-3.01	1.35	1.43
2	A	811	NAG	O5-C5	-2.96	1.39	1.45
5	B	812	MAN	O3-C3	-2.95	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	807	BMA	O5-C5	-2.95	1.39	1.45
5	B	812	MAN	O4-C4	-2.84	1.36	1.43
5	B	813	MAN	O4-C4	-2.84	1.36	1.43
5	A	806	NAG	O3-C3	-2.84	1.36	1.43
2	A	811	NAG	O3-C3	-2.83	1.36	1.43
5	B	811	MAN	O5-C5	-2.79	1.40	1.45
5	A	808	MAN	O5-C5	-2.64	1.40	1.45
5	B	811	MAN	O4-C4	-2.64	1.36	1.43
5	A	808	MAN	O2-C2	-2.62	1.37	1.43
5	B	808	NAG	O3-C3	-2.61	1.36	1.43
5	B	809	NAG	O7-C7	-2.60	1.17	1.23
5	B	809	NAG	O3-C3	-2.59	1.36	1.43
5	B	813	MAN	O3-C3	-2.46	1.37	1.43
5	B	811	MAN	O2-C2	-2.41	1.38	1.43
5	A	808	MAN	O4-C4	-2.40	1.37	1.43
5	B	808	NAG	O4-C4	-2.36	1.37	1.43
2	A	813	NAG	O5-C5	-2.35	1.41	1.45
2	B	816	NAG	O5-C5	-2.31	1.41	1.45
5	A	810	MAN	O3-C3	-2.27	1.37	1.43
5	A	810	MAN	O2-C2	-2.08	1.39	1.43
5	A	806	NAG	C7-N2	-2.07	1.25	1.34
5	B	808	NAG	O7-C7	-2.06	1.18	1.23
5	A	806	NAG	C2-N2	-2.01	1.44	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	812	MAN	O5-C5-C6	-13.01	93.33	106.98
2	A	812	NAG	C3-C4-C5	-6.47	98.65	110.20
5	A	806	NAG	C3-C2-N2	5.95	120.82	111.76
5	B	809	NAG	C3-C4-C5	-5.52	100.34	110.20
5	A	808	MAN	C4-C3-C2	-5.42	103.23	110.50
2	A	811	NAG	C6-C5-C4	-5.37	100.02	113.00
5	B	811	MAN	C4-C3-C2	-5.24	103.48	110.50
2	B	803	NAG	O5-C5-C4	4.96	116.94	110.65
2	A	812	NAG	C3-C2-N2	-4.86	104.36	111.76
2	A	812	NAG	O5-C5-C4	-4.26	105.25	110.65
2	A	812	NAG	O5-C5-C6	4.22	111.41	106.98
2	A	801	NAG	C3-C2-N2	-3.96	105.72	111.76
5	A	805	NAG	C2-N2-C7	-3.77	116.77	123.09
2	A	811	NAG	O3-C3-C4	-3.74	101.97	110.35
2	B	803	NAG	C3-C2-N2	-3.68	106.16	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	812	NAG	C2-N2-C7	-3.52	117.18	123.09
5	B	809	NAG	C3-C2-N2	-3.47	106.47	111.76
2	B	815	NAG	C2-N2-C7	-3.47	117.27	123.09
5	B	808	NAG	C3-C2-N2	-3.29	106.76	111.76
5	A	807	BMA	O3-C3-C2	3.10	115.60	109.94
5	B	813	MAN	C6-C5-C4	-2.93	105.93	113.00
5	A	805	NAG	O5-C5-C4	2.81	114.22	110.65
5	B	810	BMA	O5-C5-C6	2.71	109.82	106.98
5	B	809	NAG	O5-C5-C4	-2.70	107.22	110.65
5	B	811	MAN	O5-C5-C6	2.59	109.70	106.98
5	A	805	NAG	C3-C4-C5	2.55	114.76	110.20
5	A	808	MAN	O6-C6-C5	2.53	120.06	111.36
5	A	810	MAN	C6-C5-C4	-2.51	106.94	113.00
5	B	813	MAN	O4-C4-C3	-2.51	104.74	110.35
5	A	808	MAN	O5-C5-C6	2.48	109.58	106.98
5	A	806	NAG	C2-N2-C7	2.46	127.23	123.09
5	A	805	NAG	O5-C5-C6	2.45	109.55	106.98
5	A	810	MAN	O5-C5-C6	-2.44	104.42	106.98
5	B	808	NAG	C6-C5-C4	-2.42	107.15	113.00
5	A	806	NAG	O3-C3-C2	2.39	114.10	109.09
5	B	812	MAN	O2-C2-C3	-2.37	105.06	110.18
5	B	811	MAN	O6-C6-C5	2.36	119.48	111.36
2	A	811	NAG	C3-C2-N2	-2.35	108.18	111.76
2	B	814	NAG	C3-C2-N2	-2.34	108.19	111.76
2	B	816	NAG	C3-C2-N2	-2.34	108.20	111.76
2	A	812	NAG	C4-C3-C2	-2.32	105.64	111.32
2	B	807	NAG	C3-C2-N2	-2.29	108.27	111.76
5	B	810	BMA	O3-C3-C2	2.28	114.10	109.94
5	B	811	MAN	O3-C3-C2	2.26	114.07	109.94
2	B	806	NAG	C3-C2-N2	-2.26	108.33	111.76
2	B	803	NAG	C6-C5-C4	-2.17	107.76	113.00
2	A	802	NAG	O5-C5-C4	2.17	113.40	110.65
5	A	805	NAG	C6-C5-C4	-2.09	107.94	113.00
2	B	803	NAG	C3-C4-C5	2.09	113.94	110.20
5	A	809	MAN	O3-C3-C2	-2.08	106.13	109.94
2	B	817	NAG	O5-C5-C6	2.07	109.15	106.98
2	B	807	NAG	O5-C5-C6	2.06	109.15	106.98
2	A	814	NAG	O5-C5-C6	2.05	109.14	106.98
5	A	806	NAG	C3-C4-C5	-2.04	106.56	110.20
5	A	807	BMA	O5-C5-C6	2.03	109.11	106.98
2	A	811	NAG	C3-C4-C5	-2.02	106.59	110.20
2	A	813	NAG	O5-C5-C6	2.02	109.11	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	803	1	12,14,15	0.69	0	15,19,21	1.12	0
4	BLD	A	804	-	37,37,37	2.25	8 (21%)	59,59,59	2.63	20 (33%)
3	NAG	A	815	1	12,14,15	0.68	0	15,19,21	1.03	1 (6%)
4	BLD	B	801	-	37,37,37	2.29	9 (24%)	59,59,59	2.63	20 (33%)
3	NAG	B	802	1	12,14,15	0.57	0	15,19,21	0.82	0
3	NAG	B	805	1	12,14,15	0.64	0	15,19,21	1.51	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
4	BLD	A	804	-	-	0/20/85/85	0/0/4/4
3	NAG	A	815	1	-	0/6/23/26	0/1/1/1
4	BLD	B	801	-	-	0/20/85/85	0/0/4/4
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	805	1	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	BLD	C05-C06	7.26	1.58	1.51
4	B	801	BLD	C05-C06	7.12	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	BLD	O06-C06	6.69	1.38	1.21
4	A	804	BLD	O06-C06	6.58	1.37	1.21
4	B	801	BLD	O07-C07	-5.66	1.37	1.45
4	A	804	BLD	O07-C07	-5.59	1.37	1.45
4	B	801	BLD	C20-C17	-2.86	1.49	1.54
4	A	804	BLD	C19-C10	-2.71	1.49	1.54
4	B	801	BLD	C19-C10	-2.70	1.49	1.54
4	A	804	BLD	C20-C17	-2.49	1.50	1.54
4	B	801	BLD	C08-C14	2.33	1.58	1.53
4	B	801	BLD	O07-C06	2.26	1.37	1.34
4	A	804	BLD	C10-C05	-2.24	1.52	1.56
4	A	804	BLD	O22-C22	-2.18	1.37	1.43
4	B	801	BLD	O22-C22	-2.04	1.38	1.43
4	A	804	BLD	C13-C14	-2.03	1.50	1.55
4	B	801	BLD	C10-C05	-2.01	1.52	1.56

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	BLD	O06-C06-C05	-8.56	108.20	124.33
4	A	804	BLD	O06-C06-C05	-6.50	112.08	124.33
4	B	801	BLD	C13-C17-C20	-6.42	111.24	119.01
4	A	804	BLD	O07-C06-O06	-6.00	106.74	116.61
4	A	804	BLD	C19-C10-C05	-5.96	99.36	109.94
4	B	801	BLD	C19-C10-C05	-5.74	99.76	109.94
4	B	801	BLD	C18-C13-C12	-5.55	101.37	110.55
4	A	804	BLD	C01-C10-C05	5.51	115.76	107.23
4	A	804	BLD	C18-C13-C12	-5.43	101.57	110.55
4	B	801	BLD	C12-C13-C17	4.94	125.79	116.53
4	B	801	BLD	C10-C01-C02	4.88	122.43	114.20
4	A	804	BLD	C01-C10-C09	4.86	115.28	106.21
4	A	804	BLD	C13-C17-C20	-4.85	113.15	119.01
4	A	804	BLD	C01-C02-C03	4.65	116.80	111.33
4	A	804	BLD	C19-C10-C09	-4.57	105.03	111.65
4	B	801	BLD	C01-C02-C03	4.41	116.53	111.33
4	A	804	BLD	C10-C01-C02	4.33	121.50	114.20
4	B	801	BLD	C01-C10-C05	4.33	113.92	107.23
3	B	805	NAG	O5-C5-C6	4.30	111.49	106.98
4	B	801	BLD	O07-C06-O06	-4.10	109.87	116.61
4	A	804	BLD	C16-C17-C20	3.94	117.95	112.56
4	A	804	BLD	C12-C13-C17	3.88	123.80	116.53
4	B	801	BLD	C01-C10-C09	3.63	112.98	106.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	804	BLD	C04-C03-C02	3.53	114.87	110.37
4	B	801	BLD	C16-C17-C13	3.24	108.37	103.82
4	B	801	BLD	C16-C17-C20	3.19	116.92	112.56
4	A	804	BLD	C07-O07-C06	-2.86	116.72	120.75
4	B	801	BLD	C07-O07-C06	-2.85	116.73	120.75
4	B	801	BLD	C10-C05-C06	2.83	119.03	112.39
4	B	801	BLD	C21-C20-C17	-2.74	107.42	112.63
4	A	804	BLD	C16-C17-C13	2.71	107.64	103.82
4	B	801	BLD	C14-C08-C09	2.68	112.60	109.04
4	B	801	BLD	C19-C10-C09	-2.65	107.80	111.65
4	B	801	BLD	C04-C03-C02	2.62	113.72	110.37
4	A	804	BLD	C10-C09-C08	-2.50	113.06	116.71
3	A	815	NAG	C2-N2-C7	-2.38	119.09	123.09
4	B	801	BLD	C26-C25-C27	2.22	116.96	110.65
4	A	804	BLD	C12-C13-C14	2.21	110.98	107.28
3	B	805	NAG	C3-C2-N2	-2.18	108.44	111.76
4	A	804	BLD	C14-C08-C09	2.14	111.89	109.04
4	A	804	BLD	C11-C12-C13	2.14	116.70	112.83
4	A	804	BLD	O07-C06-C05	-2.12	116.36	119.61
4	B	801	BLD	C13-C14-C08	2.05	117.73	114.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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 ²)	Q<0.9
1	A	724/740 (97%)	-0.23	23 (3%)	45 47	11, 22, 48, 88	0
1	B	724/740 (97%)	-0.22	20 (2%)	50 53	12, 23, 50, 97	0
All	All	1448/1480 (97%)	-0.23	43 (2%)	48 50	11, 22, 49, 97	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	SER	9.4
1	A	400	SER	6.3
1	B	119	ASP	4.6
1	B	31	ASP	4.5
1	A	32	PHE	4.4
1	B	619	HIS	4.3
1	A	59	TYR	4.2
1	A	64	GLY	4.1
1	A	619	HIS	3.9
1	A	399	GLN	3.9
1	B	617	MET	3.9
1	B	59	TYR	3.8
1	B	32	PHE	3.7
1	B	120	SER	3.5
1	B	618	VAL	3.4
1	A	120	SER	3.2
1	A	620	SER	3.2
1	B	76	ASP	3.0
1	B	64	GLY	2.9
1	B	590	GLU	2.9
1	A	617	MET	2.9
1	A	757	SER	2.9
1	B	757	SER	2.8
1	A	31	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	756	GLY	2.8
1	A	590	GLU	2.7
1	A	393	SER	2.6
1	B	393	SER	2.6
1	A	593	THR	2.5
1	A	118	GLY	2.4
1	A	398	LEU	2.4
1	A	119	ASP	2.4
1	A	397	SER	2.4
1	B	121	SER	2.4
1	B	75	ASP	2.3
1	B	621	CYS	2.2
1	B	399	GLN	2.2
1	A	618	VAL	2.2
1	B	623	ALA	2.2
1	B	620	SER	2.2
1	A	594	ASP	2.1
1	A	473	LYS	2.1
1	A	472	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	812	14/15	0.26	34.60	28,34,44,45	0
2	NAG	B	816	14/15	0.24	10.41	29,42,54,54	0
2	NAG	A	801	14/15	0.30	9.84	25,41,51,52	0
2	NAG	B	815	14/15	0.25	5.69	22,35,43,46	0
2	NAG	B	803	14/15	0.23	5.67	28,41,47,52	0
2	NAG	B	807	14/15	0.39	3.03	49,68,74,77	0
2	NAG	A	802	14/15	0.35	3.03	38,54,62,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	813	14/15	0.20	2.75	28,38,46,46	0
5	NAG	A	806	14/15	0.16	2.63	16,26,32,32	0
2	NAG	B	804	14/15	0.32	1.49	35,44,48,49	0
2	NAG	B	806	14/15	0.22	1.30	40,50,57,58	0
5	NAG	B	809	14/15	0.13	0.92	19,25,30,31	0
2	NAG	B	814	14/15	0.11	0.09	16,23,29,31	0
2	NAG	A	811	14/15	0.10	-0.39	16,24,33,33	0
5	MAN	A	809	11/12	0.13	-0.80	16,20,24,42	0
5	NAG	B	808	14/15	0.10	-0.94	18,23,32,32	0
5	MAN	A	810	11/12	0.12	-1.38	16,19,23,29	0
5	NAG	A	805	14/15	0.11	-1.46	17,22,25,33	0
5	MAN	B	812	11/12	0.09	-1.74	16,22,26,33	0
5	MAN	B	813	11/12	0.09	-9.42	15,20,24,32	0
5	MAN	B	811	11/12	0.13	-	16,22,24,25	0
5	MAN	A	808	11/12	0.14	-	18,23,25,27	0
2	NAG	B	817	14/15	0.33	-	44,60,63,64	0
2	NAG	A	814	14/15	0.39	-	31,52,62,66	0
5	BMA	A	807	11/12	0.23	-	28,34,41,43	0
5	BMA	B	810	11/12	0.20	-	25,29,36,38	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	802	14/15	0.25	8.27	37,48,54,59	0
3	NAG	A	815	14/15	0.31	2.59	33,49,60,64	0
3	NAG	B	805	14/15	0.20	0.17	30,39,48,52	0
4	BLD	B	801	34/34	0.14	0.10	17,23,28,29	23
4	BLD	A	804	34/34	0.14	-0.12	15,22,30,35	23
3	NAG	A	803	14/15	0.15	-0.60	30,40,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.