



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:16 PM UTC

PDB ID : 6Q63 / pdb_00006q63
Title : BT0459
Authors : Basle, A.; Crouch, L.; Bolam, D.
Deposited on : 2018-12-10
Resolution : 2.44 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

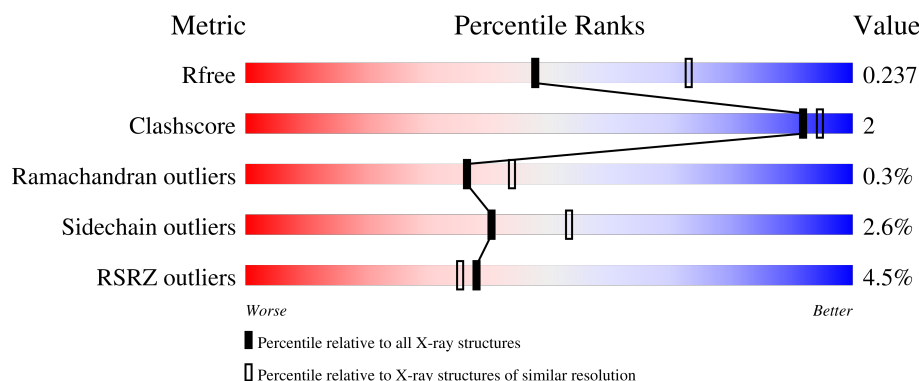
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	774	2% 94% • •
1	B	774	5% 89% 7% •
1	C	774	6% 90% 7% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18027 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 Beta-hexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			5945	3796	983	1147	19			
1	B	751	Total	C	N	O	S	0	0	0
			5945	3796	983	1147	19			
1	C	751	Total	C	N	O	S	0	0	0
			5945	3796	983	1147	19			

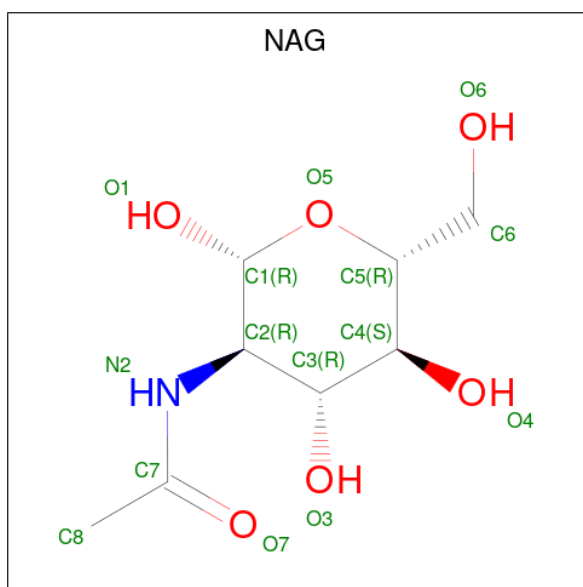
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	C	1	Total	C	N	O	0	0
			15	8	1	6		

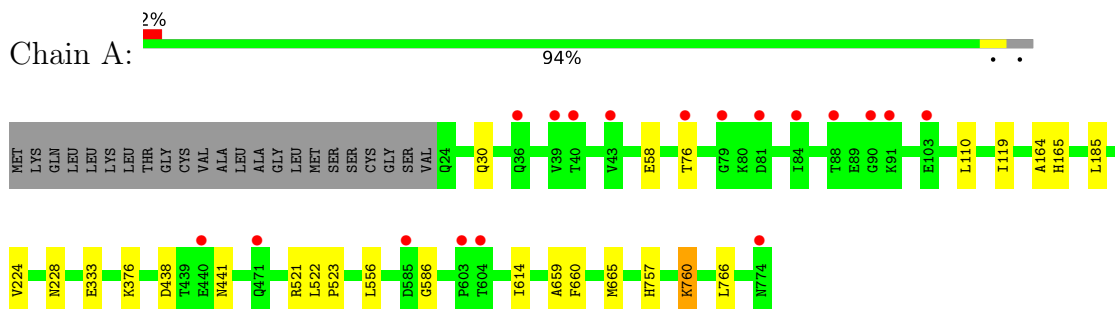
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	30	Total	O	0	0
			30	30		
5	C	44	Total	O	0	0
			44	44		

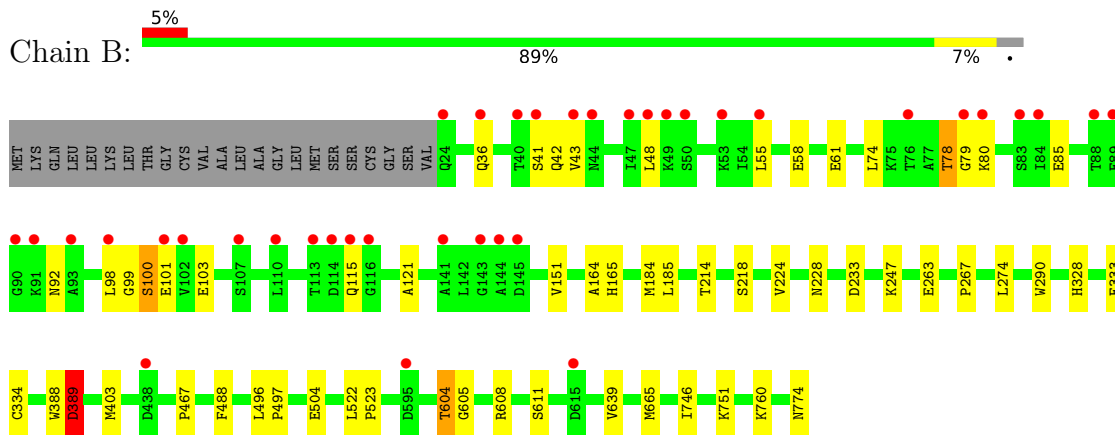
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

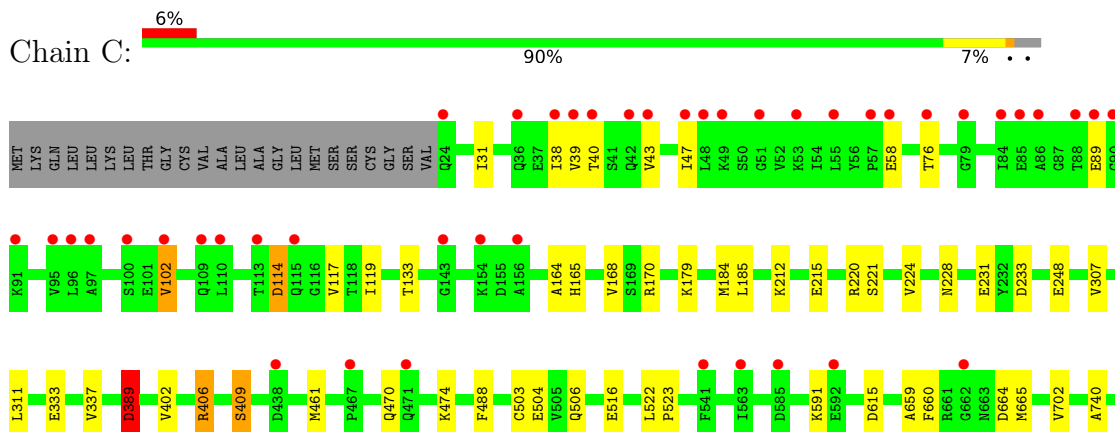
• Molecule 1: Beta-hexosaminidase



• Molecule 1: Beta-hexosaminidase



• Molecule 1: Beta-hexosaminidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	175.84Å 186.88Å 242.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 2.44 49.80 – 2.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-2.44) 99.9 (49.80-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.211 , 0.235 0.213 , 0.237	Depositor DCC
R_{free} test set	7654 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 18.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18027	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, CA, CU

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	1.00	0/6097	1.36	1/8289 (0.0%)
1	B	1.06	2/6097 (0.0%)	1.38	3/8289 (0.0%)
1	C	1.09	3/6097 (0.0%)	1.39	2/8289 (0.0%)
All	All	1.05	5/18291 (0.0%)	1.38	6/24867 (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
1	C	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	ASP	CG-OD2	27.75	1.78	1.25
1	B	389	ASP	CG-OD2	23.87	1.70	1.25
1	C	389	ASP	CG-OD1	14.13	1.52	1.25
1	B	389	ASP	CG-OD1	11.38	1.47	1.25
1	C	406	ARG	CZ-NH2	8.53	1.44	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	389	ASP	CB-CG-OD2	-9.74	95.99	118.40
1	B	389	ASP	CB-CG-OD2	-9.23	97.17	118.40
1	C	406	ARG	NE-CZ-NH2	5.81	124.43	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ASP	OD1-CG-OD2	5.60	136.34	122.90
1	B	389	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	586	GLY	CA-C-O	-5.11	118.19	122.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	389	ASP	Sidechain
1	C	389	ASP	Sidechain
1	C	664	ASP	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	5945	0	5775	11	0
1	B	5945	0	5775	21	0
1	C	5945	0	5775	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	15	1	0
4	B	15	0	15	1	0
4	C	15	0	15	1	0
5	A	67	0	0	0	0
5	B	30	0	0	0	0
5	C	44	0	0	2	0
All	All	18027	0	17370	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (56) 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:389:ASP:CG	1:B:389:ASP:OD2	1.70	1.34
1:C:389:ASP:OD2	1:C:389:ASP:CG	1.78	1.25
1:A:438:ASP:OD2	1:A:441:ASN:ND2	2.27	0.65
1:C:409:SER:OG	5:C:1001:HOH:O	2.15	0.63
1:B:389:ASP:OD2	1:B:389:ASP:CB	2.49	0.61
1:C:170:ARG:O	1:C:220:ARG:NH2	2.34	0.59
1:B:78:THR:C	1:B:80:LYS:H	2.12	0.56
1:A:30:GLN:HG3	1:A:521:ARG:HD3	1.88	0.56
1:C:389:ASP:OD2	1:C:389:ASP:CB	2.52	0.56
1:C:333:GLU:OE1	4:C:903:NAG:H2	2.06	0.55
1:A:333:GLU:OE1	4:A:903:NAG:H2	2.08	0.54
1:B:78:THR:O	1:B:80:LYS:N	2.39	0.53
1:A:556:LEU:HD23	1:A:614:ILE:HD12	1.89	0.52
1:C:461:MET:HE1	1:C:470:GLN:HG2	1.91	0.52
1:C:389:ASP:OD2	5:C:1002:HOH:O	2.18	0.52
1:C:224:VAL:HG21	1:C:228:ASN:HA	1.92	0.51
1:B:224:VAL:HG21	1:B:228:ASN:HA	1.93	0.51
1:A:164:ALA:HB3	1:A:185:LEU:HD21	1.93	0.50
1:A:224:VAL:HG21	1:A:228:ASN:HA	1.94	0.50
1:C:660:PHE:CZ	1:C:665:MET:HG3	2.47	0.49
1:B:214:THR:O	1:B:218:SER:OG	2.27	0.49
1:B:164:ALA:HB3	1:B:185:LEU:HD21	1.93	0.49
1:C:102:VAL:HG23	1:C:102:VAL:O	2.12	0.49
1:B:333:GLU:OE1	4:B:903:NAG:H2	2.13	0.48
1:B:48:LEU:HD21	1:B:74:LEU:HD22	1.97	0.47
1:A:110:LEU:HD13	1:A:119:ILE:HG12	1.97	0.46
1:B:55:LEU:HA	1:B:85:GLU:O	2.16	0.46
1:C:164:ALA:HB3	1:C:185:LEU:HD21	1.97	0.46
1:C:114:ASP:OD1	1:C:114:ASP:C	2.58	0.46
1:C:389:ASP:OD1	1:C:406:ARG:NE	2.45	0.46
1:B:98:LEU:HA	1:B:121:ALA:O	2.17	0.45
1:B:184:MET:HE1	1:B:488:PHE:CZ	2.52	0.44
1:A:660:PHE:CZ	1:A:665:MET:HG3	2.52	0.44
1:C:39:VAL:HG23	1:C:40:THR:N	2.33	0.43
1:C:212:LYS:HA	1:C:215:GLU:HB2	2.01	0.43
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.91	0.42
1:B:267:PRO:HG2	1:B:334:CYS:SG	2.60	0.42
1:B:665:MET:O	1:B:746:ILE:HA	2.20	0.42
1:C:179:LYS:NZ	1:C:248:GLU:OE2	2.52	0.42
1:C:522:LEU:N	1:C:523:PRO:CD	2.83	0.41
1:C:659:ALA:HA	1:C:766:LEU:O	2.19	0.41
1:C:31:ILE:HD11	1:C:133:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:N	1:A:523:PRO:CD	2.83	0.41
1:A:659:ALA:HA	1:A:766:LEU:O	2.21	0.41
1:B:99:GLY:O	1:B:100:SER:C	2.63	0.41
1:C:389:ASP:HA	1:C:402:VAL:HG13	2.02	0.41
1:C:503:CYS:HA	1:C:506:GLN:HB2	2.01	0.41
1:C:702:VAL:HB	1:C:740:ALA:CB	2.51	0.41
1:B:522:LEU:N	1:B:523:PRO:CD	2.84	0.41
1:B:604:THR:OG1	1:B:605:GLY:N	2.53	0.40
1:B:388:TRP:CZ3	1:B:403:MET:SD	3.15	0.40
1:B:496:LEU:HA	1:B:497:PRO:HA	1.91	0.40
1:A:757:HIS:O	1:A:760:LYS:HD3	2.21	0.40
1:C:184:MET:HE1	1:C:488:PHE:CE2	2.56	0.40
1:C:307:VAL:O	1:C:311:LEU:HG	2.21	0.40
1:B:263:GLU:HA	1:B:328:HIS:O	2.22	0.40

There are no symmetry-related clashes.

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	749/774 (97%)	725 (97%)	24 (3%)	0	100	100
1	B	749/774 (97%)	719 (96%)	26 (4%)	4 (0%)	24	29
1	C	749/774 (97%)	723 (96%)	24 (3%)	2 (0%)	36	44
All	All	2247/2322 (97%)	2167 (96%)	74 (3%)	6 (0%)	36	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	GLU
1	B	79	GLY
1	C	221	SER

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Mol	Chain	Res	Type
1	B	100	SER
1	C	102	VAL
1	B	43	VAL

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	638/656 (97%)	633 (99%)	5 (1%)	73	81
1	B	638/656 (97%)	614 (96%)	24 (4%)	29	41
1	C	638/656 (97%)	618 (97%)	20 (3%)	35	47
All	All	1914/1968 (97%)	1865 (97%)	49 (3%)	40	53

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	76	THR
1	A	165	HIS
1	A	376	LYS
1	A	760	LYS
1	B	36	GLN
1	B	41	SER
1	B	42	GLN
1	B	58	GLU
1	B	61	GLU
1	B	78	THR
1	B	92	ASN
1	B	103	GLU
1	B	115	GLN
1	B	151	VAL
1	B	165	HIS
1	B	233	ASP
1	B	247	LYS
1	B	274	LEU

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Mol	Chain	Res	Type
1	B	290	TRP
1	B	467	PRO
1	B	504	GLU
1	B	604	THR
1	B	608	ARG
1	B	611	SER
1	B	639	VAL
1	B	751	LYS
1	B	760	LYS
1	B	774	ASN
1	C	38	ILE
1	C	43	VAL
1	C	47	ILE
1	C	58	GLU
1	C	76	THR
1	C	89	GLU
1	C	114	ASP
1	C	117	VAL
1	C	119	ILE
1	C	165	HIS
1	C	168	VAL
1	C	231	GLU
1	C	233	ASP
1	C	337	VAL
1	C	409	SER
1	C	474	LYS
1	C	504	GLU
1	C	516	GLU
1	C	591	LYS
1	C	615	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	92	ASN
1	A	367	GLN
1	A	372	ASN
1	A	477	GLN
1	A	593	ASN
1	A	627	ASN
1	B	115	GLN

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Mol	Chain	Res	Type
1	B	379	ASN
1	B	399	ASN
1	B	490	HIS
1	C	219	GLN
1	C	306	GLN
1	C	367	GLN
1	C	379	ASN
1	C	399	ASN
1	C	477	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
4	NAG	B	903	-	15,15,15	0.84	0	21,21,21	1.45	2 (9%)
4	NAG	A	903	-	15,15,15	0.77	0	21,21,21	1.25	2 (9%)
4	NAG	C	903	-	15,15,15	0.82	0	21,21,21	1.35	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	903	-	-	4/6/26/26	0/1/1/1
4	NAG	A	903	-	-	4/6/26/26	0/1/1/1
4	NAG	C	903	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	NAG	O5-C1-C2	4.04	113.58	109.52
4	A	903	NAG	O5-C1-C2	3.53	113.06	109.52
4	B	903	NAG	C1-C2-N2	3.18	114.41	110.73
4	C	903	NAG	O5-C1-C2	3.09	112.62	109.52
4	C	903	NAG	C1-C2-N2	2.90	114.09	110.73
4	A	903	NAG	C1-C2-N2	2.76	113.93	110.73
4	C	903	NAG	C1-O5-C5	2.18	117.88	113.65

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	NAG	C1-C2-N2-C7
4	C	903	NAG	C1-C2-N2-C7
4	B	903	NAG	C4-C5-C6-O6
4	B	903	NAG	O5-C5-C6-O6
4	A	903	NAG	C4-C5-C6-O6
4	A	903	NAG	O5-C5-C6-O6
4	C	903	NAG	C4-C5-C6-O6
4	B	903	NAG	C1-C2-N2-C7
4	C	903	NAG	O5-C5-C6-O6
4	B	903	NAG	C3-C2-N2-C7
4	A	903	NAG	C3-C2-N2-C7
4	C	903	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	NAG	1	0
4	A	903	NAG	1	0
4	C	903	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	751/774 (97%)	0.06	18 (2%) 59 60	38, 52, 88, 110	0
1	B	751/774 (97%)	0.31	38 (5%) 33 30	43, 58, 107, 136	0
1	C	751/774 (97%)	0.42	45 (5%) 27 24	37, 62, 140, 178	0
All	All	2253/2322 (97%)	0.26	101 (4%) 38 35	37, 57, 115, 178	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	VAL	7.9
1	C	102	VAL	7.7
1	C	39	VAL	4.3
1	C	47	ILE	4.1
1	C	90	GLY	4.1
1	B	49	LYS	3.9
1	B	91	LYS	3.9
1	A	84	ILE	3.9
1	B	76	THR	3.9
1	C	43	VAL	3.8
1	C	91	LYS	3.7
1	B	144	ALA	3.6
1	A	39	VAL	3.5
1	B	90	GLY	3.3
1	B	143	GLY	3.3
1	C	88	THR	3.3
1	C	40	THR	3.3
1	B	113	THR	3.2
1	A	79	GLY	3.2
1	B	84	ILE	3.1
1	B	43	VAL	3.0
1	A	103	GLU	2.9
1	A	604	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	86	ALA	2.9
1	B	48	LEU	2.9
1	B	50	SER	2.8
1	A	43	VAL	2.8
1	B	47	ILE	2.8
1	C	471	GLN	2.8
1	C	143	GLY	2.8
1	B	438	ASP	2.8
1	B	116	GLY	2.7
1	C	51	GLY	2.7
1	B	83	SER	2.7
1	C	49	LYS	2.7
1	C	85	GLU	2.7
1	C	55	LEU	2.7
1	C	115	GLN	2.7
1	C	84	ILE	2.6
1	B	40	THR	2.6
1	C	53	LYS	2.6
1	C	113	THR	2.6
1	B	88	THR	2.6
1	C	89	GLU	2.6
1	A	88	THR	2.5
1	B	107	SER	2.5
1	C	154	LYS	2.5
1	B	36	GLN	2.5
1	C	95	VAL	2.5
1	C	100	SER	2.5
1	C	563	ILE	2.4
1	C	585	ASP	2.4
1	A	40	THR	2.4
1	C	79	GLY	2.4
1	C	76	THR	2.4
1	A	774	ASN	2.4
1	C	592	GLU	2.4
1	B	41	SER	2.4
1	C	24	GLN	2.4
1	C	42	GLN	2.4
1	B	89	GLU	2.4
1	C	36	GLN	2.3
1	B	80	LYS	2.3
1	C	58	GLU	2.3
1	B	79	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	114	ASP	2.3
1	C	57	PRO	2.3
1	B	55	LEU	2.3
1	B	145	ASP	2.3
1	C	541	PHE	2.3
1	B	115	GLN	2.2
1	C	467	PRO	2.2
1	B	93	ALA	2.2
1	A	90	GLY	2.2
1	A	585	ASP	2.2
1	B	615	ASP	2.2
1	B	44	ASN	2.2
1	B	141	ALA	2.2
1	A	76	THR	2.2
1	C	96	LEU	2.2
1	C	109	GLN	2.1
1	C	662	GLY	2.1
1	C	38	ILE	2.1
1	A	440	GLU	2.1
1	A	81	ASP	2.1
1	A	36	GLN	2.1
1	C	48	LEU	2.1
1	C	755	GLU	2.1
1	B	24	GLN	2.1
1	B	53	LYS	2.1
1	C	97	ALA	2.1
1	C	156	ALA	2.1
1	B	98	LEU	2.1
1	C	438	ASP	2.1
1	A	603	PRO	2.1
1	A	471	GLN	2.0
1	B	110	LEU	2.0
1	B	595	ASP	2.0
1	A	91	LYS	2.0
1	B	101	GLU	2.0
1	C	110	LEU	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 [i](#)

There are no oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	903	15/15	0.75	0.23	64,71,73,74	0
4	NAG	A	903	15/15	0.77	0.21	53,60,61,62	0
4	NAG	B	903	15/15	0.79	0.20	57,62,64,65	0
3	CA	B	902	1/1	0.99	0.03	50,50,50,50	0
2	CU	C	901	1/1	0.99	0.02	46,46,46,46	0
3	CA	C	902	1/1	1.00	0.02	40,40,40,40	0
2	CU	A	901	1/1	1.00	0.01	41,41,41,41	0
3	CA	A	902	1/1	1.00	0.01	46,46,46,46	0
2	CU	B	901	1/1	1.00	0.01	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.