



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:02 PM UTC

PDB ID : 5N0K / pdb_00005n0k
Title : Rat ceruloplasmin orthorhombic form
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Deposited on : 2017-02-03
Resolution : 2.30 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

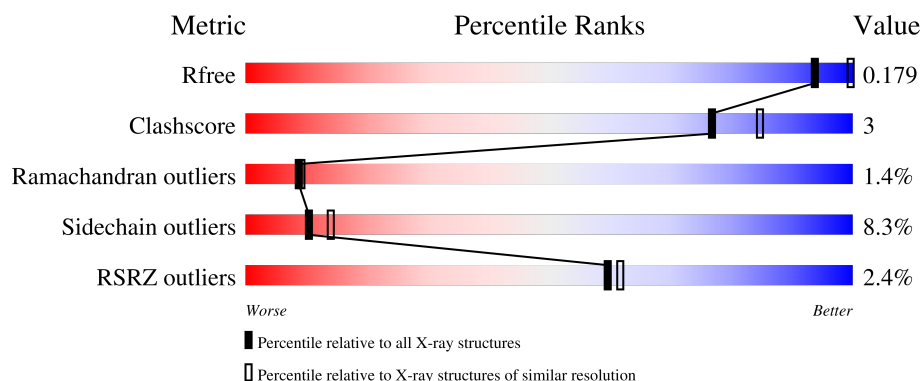
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

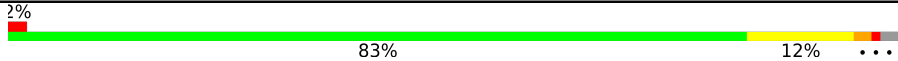
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	1059	

2 Entry composition [i](#)

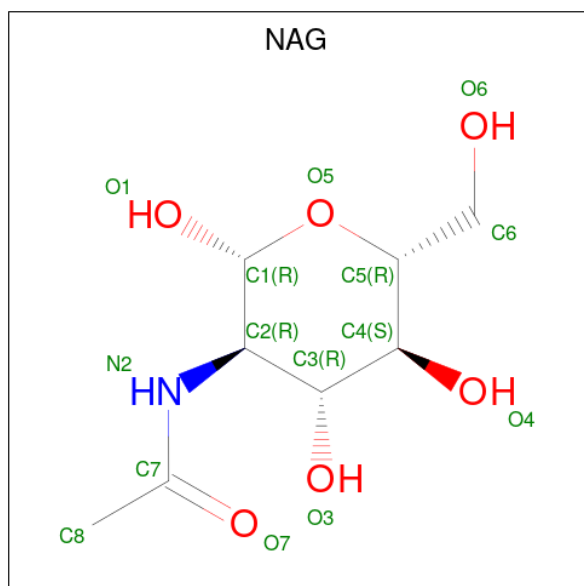
There are 6 unique types of molecules in this entry. The entry contains 8566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ceruloplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1034	Total	C	N	O	S	0	4	0
			8334	5299	1390	1603	42			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	Cu	0	0
			9	9		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Na 2	0	0

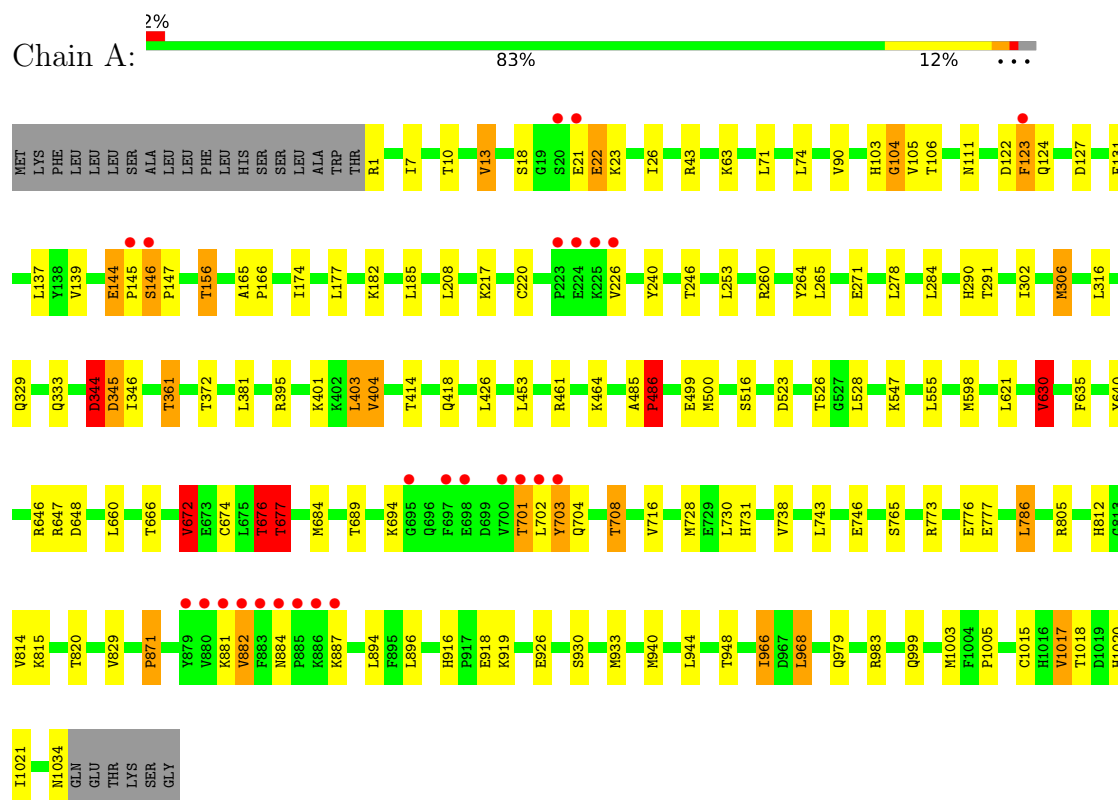
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	206	Total 206	O 206	0	0

3 Residue-property plots [i](#)

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: Ceruloplasmin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.36Å 103.81Å 172.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.30 14.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.98-2.30) 99.5 (14.98-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.175 , 0.226 0.183 , 0.179	Depositor DCC
R_{free} test set	3082 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8566	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: CU, NAG, NA, CA

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	0.95	5/8570 (0.1%)	1.05	30/11615 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	884	ASN	N-CA	6.66	1.50	1.46
1	A	290	HIS	C-O	-5.27	1.17	1.23
1	A	131	PHE	C-O	5.25	1.30	1.23
1	A	703	TYR	CA-C	5.24	1.58	1.52
1	A	884	ASN	CA-C	5.12	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	VAL	CB-CA-C	-9.03	97.95	110.77
1	A	1021	ILE	N-CA-CB	6.67	118.35	110.55
1	A	702	LEU	N-CA-C	6.64	118.96	108.67
1	A	547	LYS	CA-C-N	-6.39	112.34	122.95
1	A	547	LYS	C-N-CA	-6.39	112.34	122.95
1	A	103	HIS	N-CA-C	6.19	118.95	111.40
1	A	676	THR	N-CA-CB	6.15	119.19	109.71
1	A	485	ALA	CA-C-N	6.06	127.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ALA	C-N-CA	6.06	127.42	119.84
1	A	486	PRO	N-CA-C	5.94	124.70	112.47
1	A	404	VAL	N-CA-CB	-5.91	101.76	111.45
1	A	672	VAL	N-CA-CB	5.70	119.05	111.64
1	A	43	ARG	N-CA-C	5.70	118.24	109.07
1	A	968	LEU	CA-CB-CG	5.61	135.93	116.30
1	A	676	THR	CB-CA-C	5.57	118.61	110.26
1	A	344	ASP	CA-C-N	5.47	131.55	121.70
1	A	344	ASP	C-N-CA	5.47	131.55	121.70
1	A	346	ILE	N-CA-C	5.45	116.08	108.89
1	A	708	THR	CB-CA-C	5.44	119.66	109.71
1	A	404	VAL	CB-CA-C	5.37	120.01	110.71
1	A	104	GLY	N-CA-C	5.34	121.93	115.31
1	A	63	LYS	N-CA-C	5.28	117.42	109.23
1	A	630	VAL	CB-CA-C	5.25	117.81	110.99
1	A	127	ASP	N-CA-C	5.18	117.67	111.71
1	A	882	VAL	N-CA-C	5.16	120.06	109.34
1	A	677	THR	CB-CA-C	5.13	119.02	110.81
1	A	361	THR	CB-CA-C	-5.09	100.22	110.30
1	A	983	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	A	676	THR	CA-C-N	5.01	127.30	120.54
1	A	676	THR	C-N-CA	5.01	127.30	120.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLY	Peptide
1	A	182	LYS	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	8334	0	7949	48	0
2	A	14	0	13	0	0
3	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	2	0	0	1	0
6	A	206	0	0	6	0
All	All	8566	0	7962	48	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 3.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HB3	1:A:147:PRO:HD3	1.47	0.95
1:A:630:VAL:O	1:A:676:THR:HG21	1.72	0.89
1:A:220:CYS:SG	5:A:1113:NA:NA	1.88	0.86
1:A:674:CYS:SG	1:A:676:THR:HG23	2.17	0.85
1:A:344:ASP:HA	1:A:345:ASP:HB2	1.58	0.83
1:A:146:SER:HB3	1:A:147:PRO:CD	2.16	0.75
1:A:1003:MET:HE3	1:A:1005:PRO:HG3	1.77	0.66
1:A:344:ASP:CA	1:A:345:ASP:HB2	2.26	0.66
1:A:916:HIS:ND1	6:A:1203:HOH:O	2.30	0.64
1:A:701:THR:HG21	1:A:815:LYS:HE3	1.80	0.63
1:A:555:LEU:HB2	1:A:621:LEU:HD22	1.84	0.59
1:A:648:ASP:OD1	1:A:812:HIS:HD2	1.86	0.58
1:A:26:ILE:H	1:A:329:GLN:HE22	1.49	0.58
1:A:146:SER:CB	1:A:147:PRO:CD	2.82	0.58
1:A:598:MET:HE2	1:A:684:MET:HG2	1.84	0.58
1:A:21:GLU:HA	1:A:23:LYS:H	1.69	0.57
1:A:701:THR:HG21	1:A:815:LYS:CE	2.38	0.54
1:A:1015:CYS:SG	1:A:1017:VAL:HG13	2.49	0.53
1:A:156:THR:HG22	1:A:264:TYR:HD1	1.74	0.52
1:A:144:GLU:HB2	1:A:145:PRO:HD2	1.91	0.52
1:A:71:LEU:HD22	1:A:74:LEU:HB2	1.92	0.51
1:A:516:SER:HB3	1:A:523:ASP:HB3	1.93	0.50
1:A:933:MET:HB3	1:A:940:MET:CE	2.42	0.49
1:A:111:ASN:ND2	1:A:139:VAL:H	2.11	0.49
1:A:728[A]:MET:HE1	6:A:1240:HOH:O	2.12	0.49
1:A:731:HIS:HE1	6:A:1389:HOH:O	1.96	0.49
1:A:786:LEU:HD13	1:A:871:PRO:HG2	1.95	0.49
1:A:635:PHE:CD1	1:A:672:VAL:HG13	2.49	0.48
1:A:1017:VAL:HG22	1:A:1020:HIS:CG	2.49	0.47
1:A:647:ARG:HH21	1:A:999:GLN:HE22	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG12	6:A:1373:HOH:O	2.14	0.46
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.97	0.46
1:A:240:TYR:O	1:A:246[B]:THR:HG23	2.16	0.46
1:A:344:ASP:OD1	1:A:344:ASP:C	2.59	0.46
1:A:453:LEU:HD22	1:A:528:LEU:HD13	1.97	0.45
1:A:677:THR:CG2	6:A:1392:HOH:O	2.64	0.44
1:A:933:MET:HB3	1:A:940:MET:HE1	1.99	0.44
1:A:640:TYR:CE2	1:A:660:LEU:HD22	2.54	0.43
1:A:933:MET:HE3	1:A:940:MET:HE1	2.01	0.43
1:A:284:LEU:HD13	1:A:306:MET:HB2	2.00	0.42
1:A:7:ILE:O	1:A:90:VAL:HA	2.18	0.42
1:A:208:LEU:HD11	1:A:1018:THR:HG21	2.02	0.42
1:A:344:ASP:CA	1:A:345:ASP:CB	2.97	0.42
1:A:930:SER:O	6:A:1201:HOH:O	2.22	0.42
1:A:144:GLU:HB2	1:A:145:PRO:CD	2.50	0.42
1:A:403:LEU:HB2	1:A:526:THR:HG22	2.01	0.42
1:A:156:THR:HG21	1:A:302:ILE:O	2.20	0.41
1:A:271:GLU:CD	1:A:966:ILE:HG13	2.46	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	1036/1059 (98%)	975 (94%)	47 (4%)	14 (1%)	9 9

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	A	226	VAL
1	A	738	VAL

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Mol	Chain	Res	Type
1	A	887	LYS
1	A	122	ASP
1	A	123	PHE
1	A	345	ASP
1	A	694	LYS
1	A	881	LYS
1	A	882	VAL
1	A	22	GLU
1	A	124	GLN
1	A	486	PRO
1	A	871	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	913/931 (98%)	838 (92%)	75 (8%)	10	14

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	10	THR
1	A	13	VAL
1	A	18	SER
1	A	22	GLU
1	A	105	VAL
1	A	106	THR
1	A	123	PHE
1	A	137	LEU
1	A	144	GLU
1	A	156	THR
1	A	174	ILE
1	A	177	LEU
1	A	185	LEU
1	A	217	LYS

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	260	ARG
1	A	265	LEU
1	A	278	LEU
1	A	291	THR
1	A	306	MET
1	A	316	LEU
1	A	333	GLN
1	A	344	ASP
1	A	361	THR
1	A	372	THR
1	A	381	LEU
1	A	395	ARG
1	A	401	LYS
1	A	403	LEU
1	A	404	VAL
1	A	414	THR
1	A	418	GLN
1	A	426	LEU
1	A	461	ARG
1	A	464	LYS
1	A	486	PRO
1	A	499	GLU
1	A	500	MET
1	A	630	VAL
1	A	646	ARG
1	A	666	THR
1	A	672	VAL
1	A	676	THR
1	A	677	THR
1	A	689	THR
1	A	701	THR
1	A	703	TYR
1	A	704	GLN
1	A	708	THR
1	A	716	VAL
1	A	730	LEU
1	A	743	LEU
1	A	746	GLU
1	A	765	SER
1	A	773	ARG
1	A	776	GLU

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Mol	Chain	Res	Type
1	A	777	GLU
1	A	786	LEU
1	A	805	ARG
1	A	814	VAL
1	A	820	THR
1	A	829	VAL
1	A	894	LEU
1	A	896	LEU
1	A	918	GLU
1	A	919	LYS
1	A	926	GLU
1	A	944	LEU
1	A	948	THR
1	A	966	ILE
1	A	968	LEU
1	A	979	GLN
1	A	1017	VAL
1	A	1034	ASN

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

Mol	Chain	Res	Type
1	A	39	ASN
1	A	89	HIS
1	A	92	ASN
1	A	111	ASN
1	A	195	GLN
1	A	234	GLN
1	A	237	ASN
1	A	329	GLN
1	A	338	ASN
1	A	456	GLN
1	A	483	HIS
1	A	581	ASN
1	A	605	ASN
1	A	651	ASN
1	A	655	HIS
1	A	679	HIS
1	A	731	HIS
1	A	736	GLN
1	A	801	ASN
1	A	812	HIS

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Mol	Chain	Res	Type
1	A	911	ASN
1	A	945	GLN
1	A	956	ASN
1	A	999	GLN
1	A	1034	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1101	1	14,14,15	1.03	0	17,19,21	2.17	3 (17%)

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	1101	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	NAG	C1-O5-C5	6.94	121.49	112.19
2	A	1101	NAG	C2-N2-C7	3.61	127.73	122.90
2	A	1101	NAG	C1-C2-N2	2.98	115.13	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	NAG	C4-C5-C6-O6
2	A	1101	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	1034/1059 (97%)	-0.36	25 (2%) 59 62	23, 40, 78, 174	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	702	LEU	8.8
1	A	882	VAL	7.4
1	A	885	PRO	5.7
1	A	883	PHE	5.6
1	A	703	TYR	5.4
1	A	701	THR	5.3
1	A	146	SER	5.3
1	A	226	VAL	5.0
1	A	697	PHE	4.7
1	A	700	VAL	4.4
1	A	123	PHE	4.4
1	A	881	LYS	3.7
1	A	880	VAL	3.7
1	A	879	TYR	3.6
1	A	223	PRO	3.5
1	A	887	LYS	3.0
1	A	20	SER	3.0
1	A	695	GLY	2.9
1	A	884	ASN	2.7
1	A	145	PRO	2.5
1	A	698	GLU	2.5
1	A	224	GLU	2.1
1	A	225	LYS	2.1
1	A	21	GLU	2.0
1	A	886	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	NAG	A	1101	14/15	0.75	0.12	78,86,92,93	0
5	NA	A	1113	1/1	0.89	0.14	25,25,25,25	0
5	NA	A	1112	1/1	0.96	0.06	54,54,54,54	0
4	CA	A	1111	1/1	0.98	0.04	44,44,44,44	0
3	CU	A	1107	1/1	0.99	0.02	30,30,30,30	0
3	CU	A	1108	1/1	0.99	0.03	38,38,38,38	0
3	CU	A	1109	1/1	0.99	0.01	34,34,34,34	0
3	CU	A	1110	1/1	0.99	0.03	40,40,40,40	0
3	CU	A	1102	1/1	0.99	0.02	40,40,40,40	0
3	CU	A	1104	1/1	0.99	0.04	41,41,41,41	0
3	CU	A	1106	1/1	0.99	0.02	37,37,37,37	0
3	CU	A	1103	1/1	1.00	0.02	30,30,30,30	0
3	CU	A	1105	1/1	1.00	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.