Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 01:03 am GMT

PDB ID	:	5N0K
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 (i) 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 (1)) were used in the production of this report:

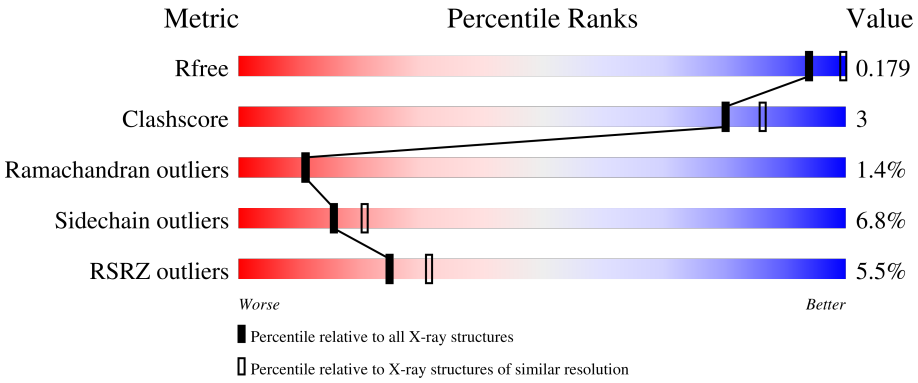
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	5% 85% 10%

2 Entry composition

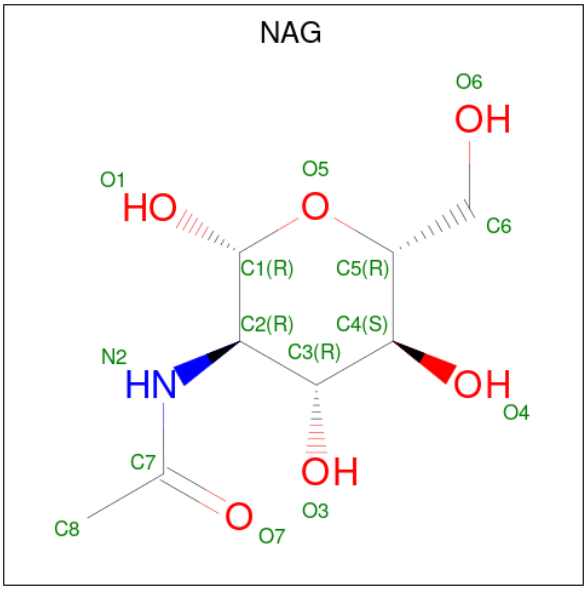
There are 6 unique types of molecules in this entry. The entry contains 8566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	1034	8334	5299	1390	1603	42	0	4	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

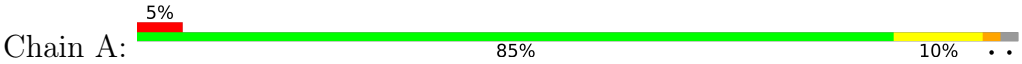
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	206	Total O 206 206	0	0

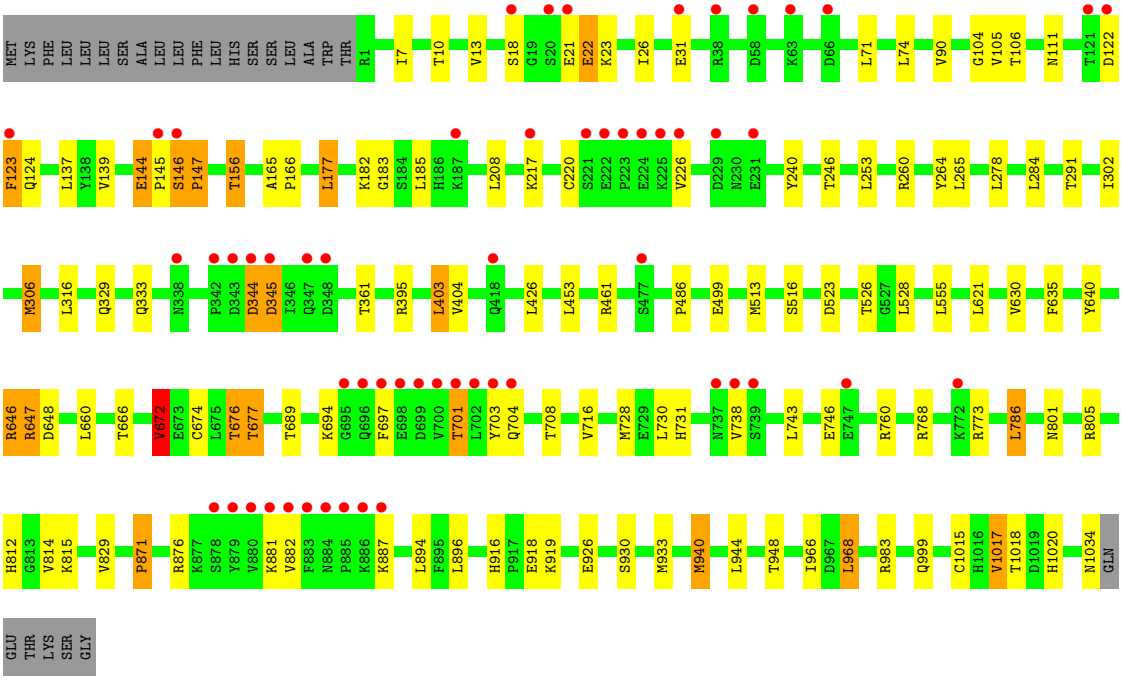
3 Residue-property plots (i)

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

Chain A:





4 Data and refinement statistics (i)

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) 100.0 (14.98-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NA, NAG, 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	0.73	0/8570	0.93	16/11615 (0.1%)

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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	983	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	A	646	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	968	LEU	CA-CB-CG	8.97	135.93	115.30
1	A	647	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	983	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	672	VAL	CB-CA-C	-7.08	97.95	111.40
1	A	177	LEU	CA-CB-CG	6.80	130.95	115.30
1	A	876	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	768[A]	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	768[B]	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	646	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	940	MET	CG-SD-CE	-5.83	90.88	100.20
1	A	513	MET	CG-SD-CE	-5.67	91.13	100.20
1	A	647	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	760	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	183	GLY	N-CA-C	-5.20	100.11	113.10

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 (i)

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	44	0
2	A	14	0	13	0	0
3	A	9	0	0	0	0
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	44	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 (44) 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: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:728[A]:MET:HE1	6:A:1240:HOH:O	1.99	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:CB	1:A:147:PRO:CD	2.82	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: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
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: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:HA	1:A:940:MET:HE1	2.00	0.44
1:A:640:TYR:CE2	1:A:660:LEU:HD22	2.54	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:344:ASP:OD1	1:A:344:ASP:C	2.59	0.41
1:A:156:THR:HG21	1:A:302:ILE:O	2.20	0.41

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%)	11 11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	A	226	VAL
1	A	738	VAL
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	913/931 (98%)	851 (93%)	62 (7%)	16 21

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	18	SER
1	A	22	GLU
1	A	31	GLU
1	A	105	VAL

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Mol	Chain	Res	Type
1	A	106	THR
1	A	123	PHE
1	A	137	LEU
1	A	144	GLU
1	A	147	PRO
1	A	156	THR
1	A	177	LEU
1	A	185	LEU
1	A	217	LYS
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	395	ARG
1	A	403	LEU
1	A	404	VAL
1	A	426	LEU
1	A	461	ARG
1	A	499	GLU
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	697	PHE
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	773	ARG
1	A	786	LEU

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Mol	Chain	Res	Type
1	A	801	ASN
1	A	805	ARG
1	A	814	VAL
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	1017	VAL
1	A	1034	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	92	ASN
1	A	111	ASN
1	A	195	GLN
1	A	230	ASN
1	A	234	GLN
1	A	319	GLN
1	A	329	GLN
1	A	456	GLN
1	A	581	ASN
1	A	605	ASN
1	A	651	ASN
1	A	655	HIS
1	A	679	HIS
1	A	801	ASN
1	A	812	HIS
1	A	945	GLN
1	A	956	ASN
1	A	979	GLN
1	A	999	GLN
1	A	1034	ASN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	1.00	0	17,19,21	2.13	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(^{o})	Ideal(^{o})
2	A	1101	NAG	C1-O5-C5	6.86	121.49	112.19
2	A	1101	NAG	C2-N2-C7	3.39	127.73	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	NAG	C1-C2-N2	2.72	115.13	110.49

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, 95^{th} 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%)	-0.00	57 (5%)	25	31	23, 41, 78, 174	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	882	VAL	21.6
1	A	700	VAL	19.4
1	A	701	THR	15.7
1	A	884	ASN	15.4
1	A	703	TYR	14.5
1	A	702	LEU	13.7
1	A	883	PHE	12.4
1	A	697	PHE	10.5
1	A	885	PRO	9.4
1	A	881	LYS	9.1
1	A	696	GLN	8.0
1	A	225	LYS	7.7
1	A	695	GLY	7.3
1	A	224	GLU	7.3
1	A	699	ASP	7.1
1	A	698	GLU	6.8
1	A	123	PHE	6.5
1	A	879	TYR	5.9
1	A	704	GLN	5.3
1	A	226	VAL	5.2
1	A	343	ASP	5.1
1	A	146	SER	4.7
1	A	21	GLU	4.7
1	A	887	LYS	4.4
1	A	344	ASP	4.3
1	A	20	SER	4.3
1	A	345	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	878	SER	3.8
1	A	477	SER	3.5
1	A	886	LYS	3.5
1	A	217	LYS	3.5
1	A	229	ASP	3.5
1	A	347	GLN	3.2
1	A	145	PRO	3.0
1	A	418	GLN	3.0
1	A	187	LYS	2.9
1	A	221	SER	2.8
1	A	747	GLU	2.8
1	A	737	ASN	2.8
1	A	121	THR	2.7
1	A	66	ASP	2.7
1	A	348	ASP	2.7
1	A	223	PRO	2.7
1	A	122	ASP	2.7
1	A	738	VAL	2.6
1	A	880	VAL	2.6
1	A	338	ASN	2.4
1	A	18	SER	2.4
1	A	231	GLU	2.4
1	A	222	GLU	2.4
1	A	38	ARG	2.4
1	A	58[A]	ASP	2.3
1	A	739	SER	2.3
1	A	342	PRO	2.3
1	A	31	GLU	2.2
1	A	63	LYS	2.2
1	A	772	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	1101	14/15	0.81	0.36	78,86,92,93	0
5	NA	A	1113	1/1	0.89	0.27	25,25,25,25	0
5	NA	A	1112	1/1	0.95	0.13	54,54,54,54	0
3	CU	A	1110	1/1	0.98	0.02	40,40,40,40	0
4	CA	A	1111	1/1	0.98	0.04	44,44,44,44	0
3	CU	A	1107	1/1	0.99	0.05	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	0.03	34,34,34,34	0
3	CU	A	1102	1/1	0.99	0.05	40,40,40,40	0
3	CU	A	1104	1/1	0.99	0.02	41,41,41,41	0
3	CU	A	1105	1/1	0.99	0.05	29,29,29,29	0
3	CU	A	1106	1/1	0.99	0.04	37,37,37,37	0
3	CU	A	1103	1/1	1.00	0.04	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.