Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 05:38 pm GMT

PDB ID	:	2J5W
Title	:	Ceruloplasmin revisited: structural and functional roles of various metal cation binding sites
Authors	:	Bento, I.; Peixoto, C.; Zaitsev, V.N.; Lindley, P.F.
Deposited on	:	2006-09-19
Resolution	:	2.80 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:

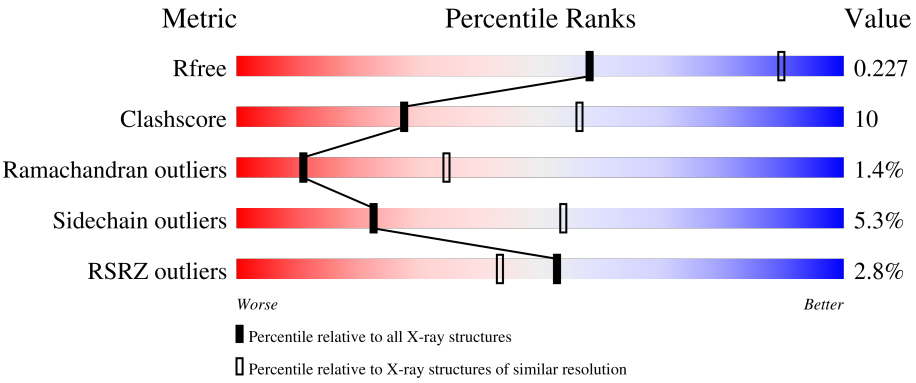
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	1065	3% 76% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	A	3056	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8728 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	1029	Total	C	N	O	S	0	0	0
			8333	5304	1394	1597	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	GLN	GLU	conflict	UNP P00450
A	252	SER	PRO	conflict	UNP P00450

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		

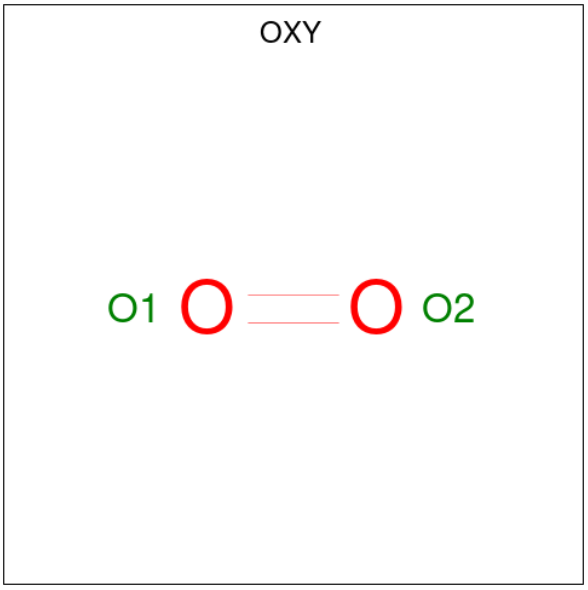
- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	Cu	0	0
			7	7		

- Molecule 5 is OXYGEN ATOM (three-letter code: O) (formula: O).

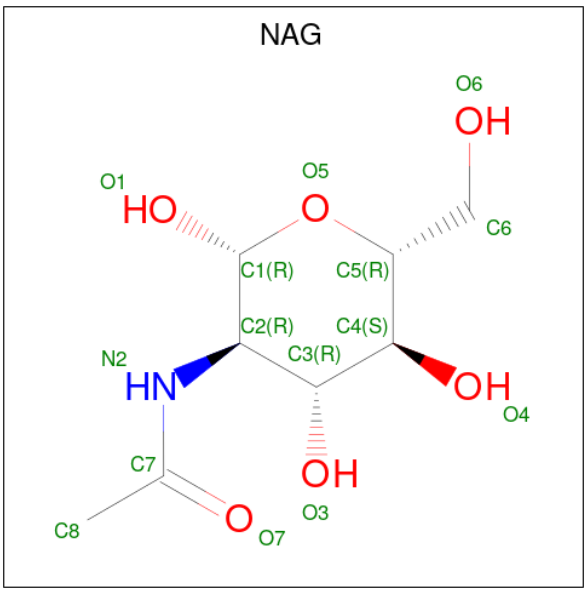
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



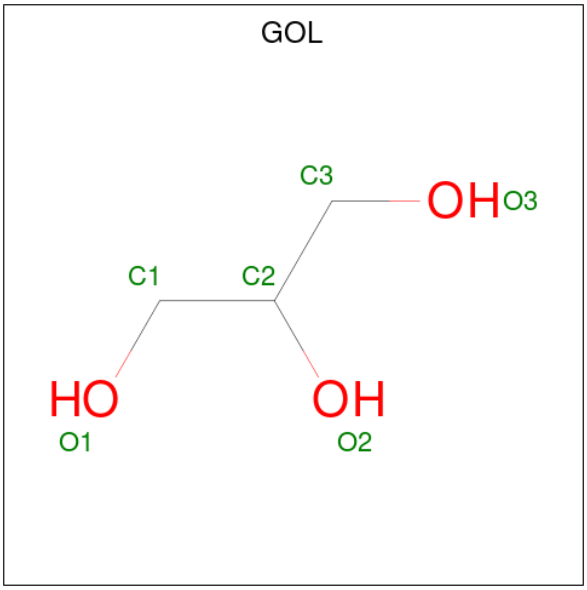
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

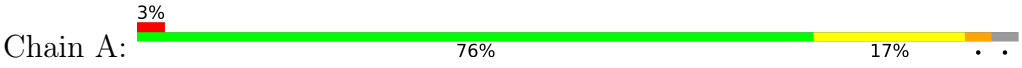
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	341	Total O 341 341	0	0

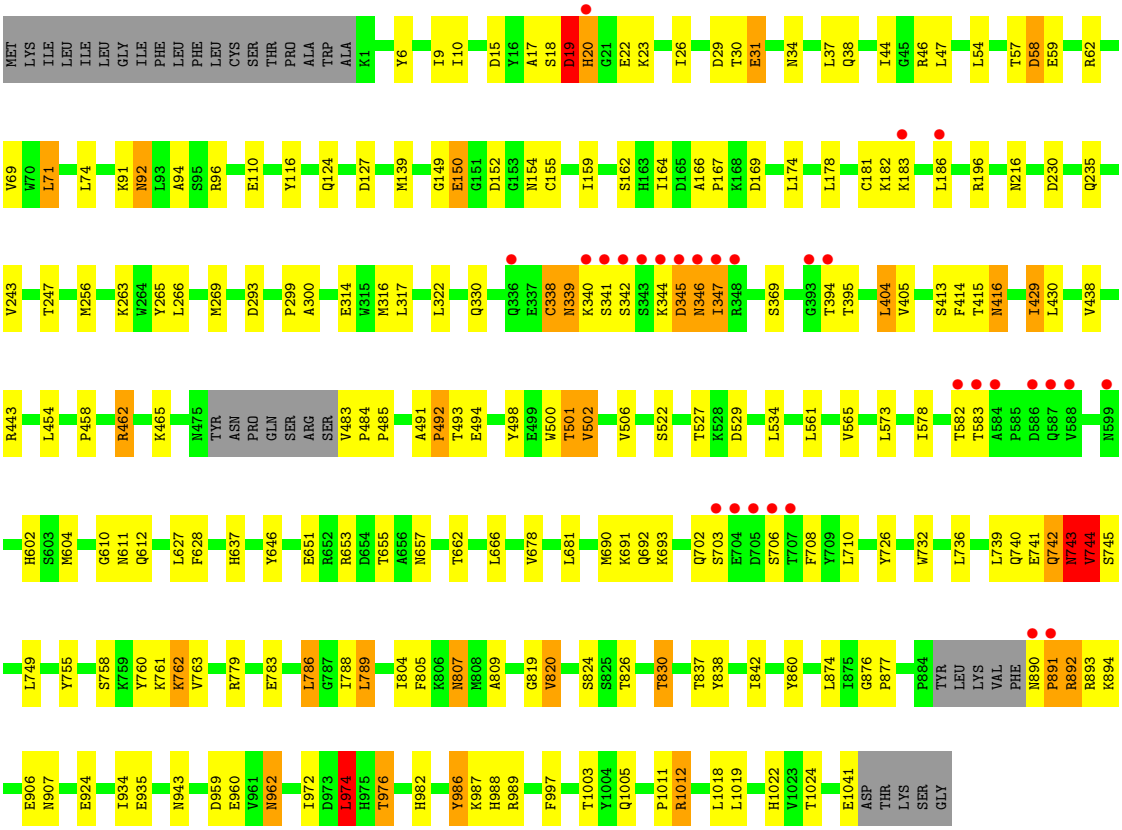
3 Residue-property plots (i)

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 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.14Å 209.14Å 82.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.52 – 2.80 68.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.52-2.80) 100.0 (68.46-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.226 0.180 , 0.227	Depositor DCC
R_{free} test set	2608 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8728	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: OXY, CA, O, NA, GOL, CU, NAG

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	0.56	3/8565 (0.0%)	0.67	5/11620 (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	A	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1012	ARG	N-CA	6.39	1.59	1.46
1	A	1012	ARG	CA-C	-6.11	1.37	1.52
1	A	986	TYR	CD2-CE2	-5.32	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	974	LEU	CA-CB-CG	6.10	129.33	115.30
1	A	462	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	58	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	19	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	152	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ASP	Peptide
1	A	22	GLU	Peptide
1	A	340	LYS	Peptide
1	A	483	VAL	Peptide
1	A	57	THR	Peptide
1	A	742	GLN	Peptide
1	A	743	ASN	Peptide
1	A	744	VAL	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	8333	0	7899	162	0
2	A	1	0	0	0	0
3	A	3	0	0	0	0
4	A	7	0	0	0	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	28	0	26	0	0
8	A	12	0	16	2	0
9	A	341	0	0	23	0
All	All	8728	0	7941	164	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 10.

All (164) 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:19:ASP:CB	1:A:20:HIS:HA	1.69	1.22
1:A:743:ASN:HA	1:A:744:VAL:CG1	1.68	1.21
1:A:743:ASN:HA	1:A:744:VAL:HG12	1.28	1.13
1:A:19:ASP:CB	1:A:20:HIS:CA	2.30	1.09
1:A:743:ASN:HA	1:A:744:VAL:CB	1.79	1.08
1:A:19:ASP:HB3	1:A:20:HIS:C	1.72	1.08
1:A:19:ASP:HB2	1:A:20:HIS:HA	1.09	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:HE3	9:A:2072:HOH:O	1.56	1.03
1:A:484:PRO:HB2	1:A:485:PRO:HD2	1.41	1.02
1:A:743:ASN:CA	1:A:744:VAL:HG12	1.90	1.00
1:A:743:ASN:OD1	1:A:744:VAL:HG12	1.65	0.97
1:A:986:TYR:O	1:A:987:LYS:HB2	1.65	0.97
1:A:743:ASN:HA	1:A:744:VAL:HB	1.50	0.94
1:A:19:ASP:HB3	1:A:20:HIS:CA	1.98	0.91
1:A:19:ASP:HB3	1:A:20:HIS:O	1.70	0.89
1:A:744:VAL:HG22	1:A:744:VAL:O	1.72	0.89
1:A:345:ASP:HA	1:A:346:ASN:HB2	1.53	0.87
1:A:37:LEU:HD21	1:A:247:THR:HG21	1.59	0.85
1:A:760:TYR:CD2	1:A:906:GLU:HG2	2.14	0.82
1:A:988:HIS:O	1:A:989:ARG:HB2	1.79	0.81
1:A:1041:GLU:C	9:A:2336:HOH:O	2.20	0.80
1:A:71:LEU:HD22	1:A:74:LEU:HB2	1.62	0.79
1:A:743:ASN:CA	1:A:744:VAL:CB	2.60	0.79
1:A:454:LEU:HD22	1:A:534:LEU:HD13	1.66	0.78
1:A:34:ASN:HB2	1:A:38:GLN:HB2	1.66	0.78
1:A:744:VAL:O	1:A:744:VAL:CG2	2.31	0.77
1:A:743:ASN:OD1	1:A:744:VAL:CG1	2.33	0.76
1:A:484:PRO:HB2	1:A:485:PRO:CD	2.15	0.76
1:A:783:GLU:HB2	1:A:786:LEU:HD22	1.68	0.75
1:A:653:ARG:HH21	1:A:1005:GLN:HE22	1.34	0.74
8:A:3058:GOL:H32	9:A:2050:HOH:O	1.87	0.74
1:A:760:TYR:CE2	1:A:906:GLU:HG2	2.23	0.73
1:A:394:THR:HG22	1:A:395:THR:HG23	1.70	0.73
1:A:743:ASN:CA	1:A:744:VAL:HB	2.20	0.71
1:A:150:GLU:OE1	1:A:989:ARG:NH2	2.23	0.71
1:A:561:LEU:HB2	1:A:627:LEU:HD22	1.73	0.69
1:A:491:ALA:HB1	1:A:492:PRO:HD2	1.75	0.69
1:A:830:THR:HG22	1:A:838:TYR:OH	1.93	0.69
1:A:604:MET:HE2	1:A:690:MET:HG2	1.74	0.68
1:A:755:TYR:CZ	9:A:2215:HOH:O	2.46	0.68
1:A:761:LYS:NZ	9:A:2220:HOH:O	2.25	0.68
1:A:604:MET:CE	1:A:690:MET:HG2	2.24	0.67
1:A:1012:ARG:CG	9:A:2323:HOH:O	2.43	0.67
1:A:743:ASN:CA	1:A:744:VAL:CG1	2.56	0.67
1:A:602:HIS:NE2	9:A:2147:HOH:O	2.28	0.66
1:A:159:ILE:HD12	1:A:269:MET:HE1	1.78	0.65
1:A:1012:ARG:HG2	9:A:2323:HOH:O	1.96	0.65
1:A:892:ARG:HD2	1:A:960:GLU:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:H	1:A:330:GLN:HE22	1.43	0.64
1:A:493:THR:HG22	1:A:493:THR:O	1.99	0.62
1:A:484:PRO:CB	1:A:485:PRO:HD2	2.24	0.62
1:A:893:ARG:HB3	1:A:959:ASP:OD1	2.00	0.61
1:A:743:ASN:CG	1:A:744:VAL:HG12	2.21	0.61
1:A:164:ILE:HB	9:A:2019:HOH:O	2.00	0.60
1:A:653:ARG:HH21	1:A:1005:GLN:NE2	1.99	0.60
1:A:462:ARG:HG3	1:A:462:ARG:HH11	1.67	0.60
8:A:3058:GOL:C3	9:A:2050:HOH:O	2.45	0.60
1:A:755:TYR:CE1	9:A:2215:HOH:O	2.54	0.59
1:A:166:ALA:HB3	1:A:167:PRO:HD3	1.84	0.59
1:A:988:HIS:HD2	9:A:2274:HOH:O	1.85	0.59
1:A:150:GLU:CD	1:A:989:ARG:HH22	2.04	0.59
1:A:502:VAL:O	1:A:502:VAL:HG22	2.03	0.58
1:A:338:CYS:N	1:A:339:ASN:HA	2.19	0.57
1:A:17:ALA:HB2	1:A:247:THR:CG2	2.33	0.57
1:A:314:GLU:O	1:A:465:LYS:HE2	2.05	0.57
1:A:894:LYS:HD3	9:A:2308:HOH:O	2.06	0.56
1:A:763:VAL:HG22	1:A:874:LEU:HD21	1.88	0.55
1:A:404:LEU:HD13	1:A:573:LEU:HD11	1.88	0.55
1:A:18:SER:O	1:A:19:ASP:C	2.45	0.55
1:A:10:ILE:HD11	1:A:54:LEU:HD11	1.89	0.54
1:A:347:ILE:HD11	1:A:501:THR:HG22	1.87	0.54
1:A:92:ASN:HD21	1:A:94:ALA:HB3	1.71	0.54
1:A:17:ALA:O	1:A:46:ARG:NH1	2.41	0.54
1:A:414:PHE:HB3	9:A:2105:HOH:O	2.08	0.54
1:A:988:HIS:CD2	9:A:2274:HOH:O	2.61	0.54
1:A:484:PRO:CB	1:A:485:PRO:CD	2.82	0.53
1:A:651:GLU:OE2	1:A:987:LYS:HE2	2.08	0.53
1:A:369:SER:OG	1:A:611:ASN:ND2	2.34	0.53
1:A:743:ASN:CB	1:A:744:VAL:HG12	2.38	0.53
1:A:230:ASP:HA	1:A:235:GLN:HE21	1.74	0.53
1:A:485:PRO:HB3	1:A:494:GLU:OE1	2.09	0.53
1:A:976:THR:HG23	1:A:1022:HIS:H	1.73	0.53
1:A:69:VAL:HG12	9:A:2015:HOH:O	2.09	0.52
1:A:345:ASP:HA	1:A:346:ASN:CB	2.34	0.52
1:A:6:TYR:CE1	1:A:59:GLU:HG3	2.45	0.52
1:A:830:THR:CG2	1:A:838:TYR:OH	2.56	0.52
1:A:162:SER:HB3	1:A:169:ASP:HB3	1.92	0.51
1:A:779:ARG:HG3	1:A:783:GLU:HG3	1.92	0.51
1:A:17:ALA:HB2	1:A:247:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:ILE:C	1:A:972:ILE:HD12	2.31	0.50
1:A:322:LEU:HD13	1:A:527:THR:HA	1.93	0.50
1:A:655:THR:HG21	1:A:681:LEU:HD12	1.91	0.50
1:A:502:VAL:O	1:A:502:VAL:CG2	2.60	0.50
1:A:314:GLU:O	1:A:465:LYS:CE	2.60	0.50
1:A:491:ALA:HB1	1:A:492:PRO:CD	2.41	0.49
1:A:29:ASP:O	1:A:31:GLU:N	2.46	0.49
1:A:299:PRO:O	1:A:300:ALA:HB3	2.13	0.49
1:A:997:PHE:CZ	1:A:1005:GLN:HG2	2.47	0.49
1:A:96:ARG:NH1	9:A:2019:HOH:O	2.43	0.49
1:A:637:HIS:O	1:A:657:ASN:HA	2.13	0.49
1:A:196:ARG:HD2	1:A:256:MET:HB3	1.95	0.48
1:A:988:HIS:HB3	9:A:2314:HOH:O	2.14	0.48
1:A:159:ILE:CD1	1:A:269:MET:HE1	2.44	0.48
1:A:565:VAL:HG22	1:A:602:HIS:CD2	2.48	0.48
1:A:44:ILE:HD13	1:A:216:ASN:HB3	1.94	0.48
1:A:610:GLY:HA2	1:A:692:GLN:HA	1.95	0.47
1:A:646:TYR:CE1	1:A:666:LEU:HD22	2.49	0.47
1:A:890:ASN:N	1:A:891:PRO:CD	2.77	0.47
1:A:438:VAL:HA	1:A:502:VAL:HG22	1.95	0.47
1:A:196:ARG:HE	1:A:256:MET:HA	1.80	0.47
1:A:17:ALA:O	1:A:19:ASP:N	2.48	0.46
1:A:92:ASN:ND2	1:A:94:ALA:H	2.13	0.46
1:A:149:GLY:O	1:A:150:GLU:C	2.53	0.46
1:A:693:LYS:NZ	9:A:2186:HOH:O	2.44	0.46
1:A:345:ASP:CA	1:A:346:ASN:HB2	2.37	0.46
1:A:760:TYR:CD2	1:A:906:GLU:CG	2.93	0.46
1:A:299:PRO:O	1:A:976:THR:HG21	2.16	0.46
1:A:316:MET:CE	1:A:330:GLN:HE21	2.29	0.46
1:A:807:ASN:ND2	1:A:809:ALA:H	2.14	0.46
1:A:740:GLN:O	1:A:741:GLU:HB2	2.16	0.45
1:A:443:ARG:HA	1:A:498:TYR:O	2.17	0.45
1:A:10:ILE:CD1	1:A:54:LEU:HD11	2.47	0.45
1:A:960:GLU:OE2	1:A:962:ASN:ND2	2.50	0.44
1:A:804:ILE:HD13	1:A:837:THR:HG23	1.99	0.44
1:A:820:VAL:HG22	1:A:842:ILE:HD13	1.99	0.44
1:A:139:MET:HE2	9:A:2032:HOH:O	2.17	0.44
1:A:110:GLU:HG3	1:A:124:GLN:HG2	1.98	0.44
1:A:726:TYR:OH	1:A:762:LYS:HE2	2.17	0.44
1:A:974:LEU:H	1:A:974:LEU:HD13	1.83	0.44
1:A:394:THR:HA	1:A:583:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:C	1:A:416:ASN:HD22	2.20	0.44
1:A:578:ILE:O	1:A:582:THR:OG1	2.34	0.44
1:A:982:HIS:CD2	1:A:1011:PRO:HA	2.52	0.43
1:A:612:GLN:HE21	1:A:692:GLN:HG3	1.84	0.43
1:A:110:GLU:O	1:A:127:ASP:HB3	2.18	0.43
1:A:522:SER:HB3	1:A:529:ASP:HB3	2.00	0.43
1:A:860:TYR:CZ	1:A:876:GLY:HA3	2.53	0.43
1:A:458:PRO:HG3	1:A:500:TRP:CE2	2.53	0.43
1:A:974:LEU:HD22	1:A:974:LEU:O	2.18	0.43
1:A:805:PHE:HD2	1:A:830:THR:HG21	1.84	0.42
1:A:786:LEU:O	1:A:789:LEU:HB2	2.20	0.42
1:A:820:VAL:HG22	1:A:842:ILE:CD1	2.49	0.42
1:A:155:CYS:HB2	1:A:265:TYR:OH	2.19	0.42
1:A:749:LEU:HD22	1:A:758:SER:HB3	2.02	0.42
1:A:628:PHE:HA	1:A:662:THR:O	2.20	0.42
1:A:986:TYR:O	1:A:987:LYS:CB	2.45	0.42
1:A:405:VAL:HG23	1:A:429:ILE:HD13	2.01	0.42
1:A:935:GLU:HG2	9:A:2299:HOH:O	2.19	0.42
1:A:789:LEU:HD22	1:A:943:ASN:CG	2.41	0.41
1:A:732:TRP:CZ3	1:A:736:LEU:HD22	2.55	0.41
1:A:762:LYS:HD3	1:A:788:ILE:HD11	2.02	0.41
1:A:23:LYS:NZ	9:A:2004:HOH:O	2.52	0.41
1:A:691:LYS:NZ	9:A:2185:HOH:O	2.38	0.41
1:A:154:ASN:O	1:A:181:CYS:HA	2.21	0.41
1:A:154:ASN:HA	1:A:182:LYS:HG3	2.02	0.41
1:A:907:ASN:ND2	1:A:934:ILE:HG23	2.36	0.41
1:A:413:SER:HB2	1:A:415:THR:HG23	2.02	0.41
1:A:462:ARG:HH11	1:A:462:ARG:CG	2.34	0.41
1:A:15:ASP:HA	1:A:47:LEU:HD23	2.03	0.41
1:A:657:ASN:ND2	1:A:1003:THR:OG1	2.54	0.41
1:A:9:ILE:HG23	1:A:174:LEU:HD21	2.03	0.40
1:A:493:THR:O	1:A:493:THR:CG2	2.67	0.40
1:A:116:TYR:CZ	1:A:1018:LEU:HB2	2.56	0.40
1:A:167:PRO:HB3	1:A:1024:THR:HG23	2.02	0.40

There are no symmetry-related clashes.

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	1023/1065 (96%)	953 (93%)	56 (6%)	14 (1%)	11 34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	150	GLU
1	A	346	ASN
1	A	347	ILE
1	A	744	VAL
1	A	344	LYS
1	A	743	ASN
1	A	342	SER
1	A	492	PRO
1	A	703	SER
1	A	30	THR
1	A	877	PRO
1	A	891	PRO
1	A	819	GLY

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	904/937 (96%)	856 (95%)	48 (5%)	22 54

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	31	GLU
1	A	58	ASP
1	A	62	ARG
1	A	71	LEU
1	A	91	LYS
1	A	92	ASN
1	A	178	LEU
1	A	183	LYS
1	A	186	LEU
1	A	243	VAL
1	A	266	LEU
1	A	293	ASP
1	A	317	LEU
1	A	338	CYS
1	A	339	ASN
1	A	341	SER
1	A	345	ASP
1	A	404	LEU
1	A	416	ASN
1	A	429	ILE
1	A	430	LEU
1	A	501	THR
1	A	502	VAL
1	A	506	VAL
1	A	678	VAL
1	A	702	GLN
1	A	706	SER
1	A	708	PHE
1	A	710	LEU
1	A	739	LEU
1	A	742	GLN
1	A	744	VAL
1	A	745	SER
1	A	762	LYS
1	A	786	LEU
1	A	789	LEU
1	A	807	ASN
1	A	820	VAL
1	A	824	SER
1	A	826	THR
1	A	830	THR
1	A	892	ARG

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Mol	Chain	Res	Type
1	A	924	GLU
1	A	962	ASN
1	A	974	LEU
1	A	976	THR
1	A	1019	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	235	GLN
1	A	238	ASN
1	A	296	ASN
1	A	320	GLN
1	A	330	GLN
1	A	416	ASN
1	A	602	HIS
1	A	611	ASN
1	A	612	GLN
1	A	657	ASN
1	A	677	ASN
1	A	698	GLN
1	A	702	GLN
1	A	740	GLN
1	A	807	ASN
1	A	962	ASN
1	A	1005	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
7	NAG	A	3056	1	14,14,15	0.93	1 (7%)	17,19,21	1.28	2 (11%)
6	OXY	A	3054	4	1,1,1	0.83	0	-		
7	NAG	A	3055	1	14,14,15	0.74	1 (7%)	17,19,21	0.96	0
8	GOL	A	3058	-	5,5,5	0.40	0	5,5,5	0.44	0
8	GOL	A	3057	-	5,5,5	0.43	0	5,5,5	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	3058	-	-	2/4/4/4	-
7	NAG	A	3055	1	-	0/6/23/26	0/1/1/1
8	GOL	A	3057	-	-	2/4/4/4	-
7	NAG	A	3056	1	1/1/5/7	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3056	NAG	C1-C2	2.66	1.56	1.52
7	A	3055	NAG	C1-C2	2.13	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	3056	NAG	O5-C5-C4	-3.20	103.05	110.83
7	A	3056	NAG	C6-C5-C4	2.01	117.72	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	3056	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3056	NAG	C8-C7-N2-C2
7	A	3056	NAG	O7-C7-N2-C2
8	A	3057	GOL	C1-C2-C3-O3
8	A	3058	GOL	O1-C1-C2-C3
7	A	3056	NAG	O5-C5-C6-O6
8	A	3057	GOL	O2-C2-C3-O3
8	A	3058	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	3058	GOL	2	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, 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	1029/1065 (96%)	0.02	29 (2%) 53 43	20, 47, 72, 100	7 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	890	ASN	5.2
1	A	891	PRO	5.0
1	A	704	GLU	4.8
1	A	342	SER	4.8
1	A	705	ASP	4.8
1	A	343	SER	4.7
1	A	707	THR	4.7
1	A	706	SER	4.4
1	A	703	SER	3.8
1	A	341	SER	3.5
1	A	183	LYS	3.5
1	A	348	ARG	3.5
1	A	583	THR	3.5
1	A	345	ASP	3.4
1	A	20	HIS	3.0
1	A	340	LYS	3.0
1	A	344	LYS	2.7
1	A	394	THR	2.7
1	A	582	THR	2.6
1	A	347	ILE	2.4
1	A	186	LEU	2.4
1	A	588	VAL	2.4
1	A	336	GLN	2.4
1	A	586	ASP	2.2
1	A	599	ASN	2.2
1	A	587	GLN	2.1
1	A	584	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	346	ASN	2.1
1	A	393	GLY	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
7	NAG	A	3056	14/15	0.85	0.46	79,81,84,85	0
3	NA	A	3044	1/1	0.86	0.32	55,55,55,55	0
7	NAG	A	3055	14/15	0.91	0.14	57,60,62,62	0
3	NA	A	3043	1/1	0.94	0.14	55,55,55,55	0
4	CU	A	3053	1/1	0.96	0.10	53,53,53,53	1
8	GOL	A	3058	6/6	0.96	0.26	63,64,65,65	0
8	GOL	A	3057	6/6	0.98	0.17	46,46,47,47	0
3	NA	A	3045	1/1	0.99	0.09	43,43,43,43	0
4	CU	A	3048	1/1	0.99	0.15	40,40,40,40	0
2	CA	A	3042	1/1	0.99	0.15	43,43,43,43	0
5	O	A	3050	1/1	0.99	0.19	51,51,51,51	1
4	CU	A	3046	1/1	1.00	0.16	44,44,44,44	0
6	OXY	A	3054	2/2	1.00	0.14	34,34,34,35	0
4	CU	A	3049	1/1	1.00	0.12	43,43,43,43	0
4	CU	A	3051	1/1	1.00	0.15	43,43,43,43	0
4	CU	A	3052	1/1	1.00	0.17	41,41,41,41	0
4	CU	A	3047	1/1	1.00	0.16	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.