Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 09:29 AM EDT

PDB ID	:	4ENZ
Title	:	Structure of human ceruloplasmin at 2.6 A resolution
Authors	:	Samygina, V.R.; Sokolov, A.V.; Bourenkov, G.; Vasilyev, V.B.; Bartunik, H.
Deposited on	:	2012-04-13
Resolution	:	2.60 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 (i)) were used in the production of this report:

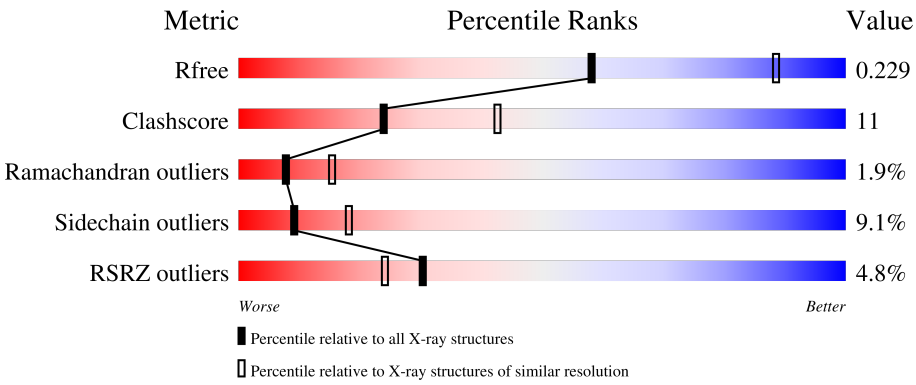
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

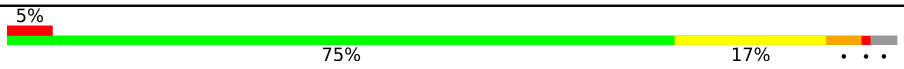
The reported resolution of this entry is 2.60 Å.

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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	

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
2	NAG	A	1111	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	O	A	1108	-	-	-	X

2 Entry composition (i)

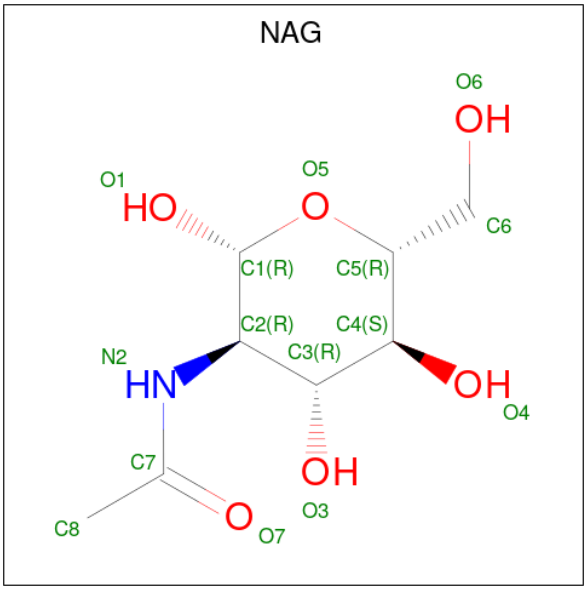
There are 9 unique types of molecules in this entry. The entry contains 8468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1029	8337	5311	1393	1595	38	0	1	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
2	A	1	14	8	1	5	0	0

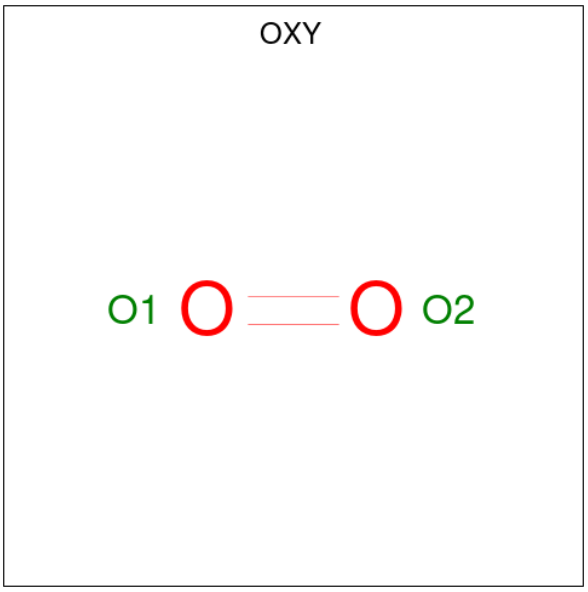
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
3	A	6	6	6	0	0

- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



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

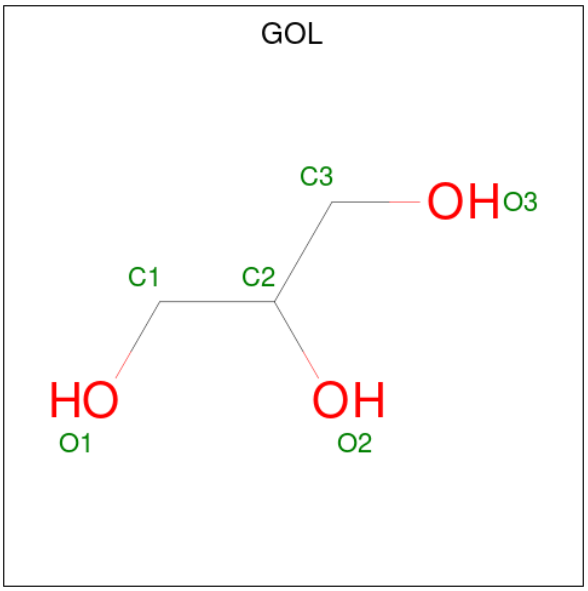
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

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



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

- Molecule 9 is water.

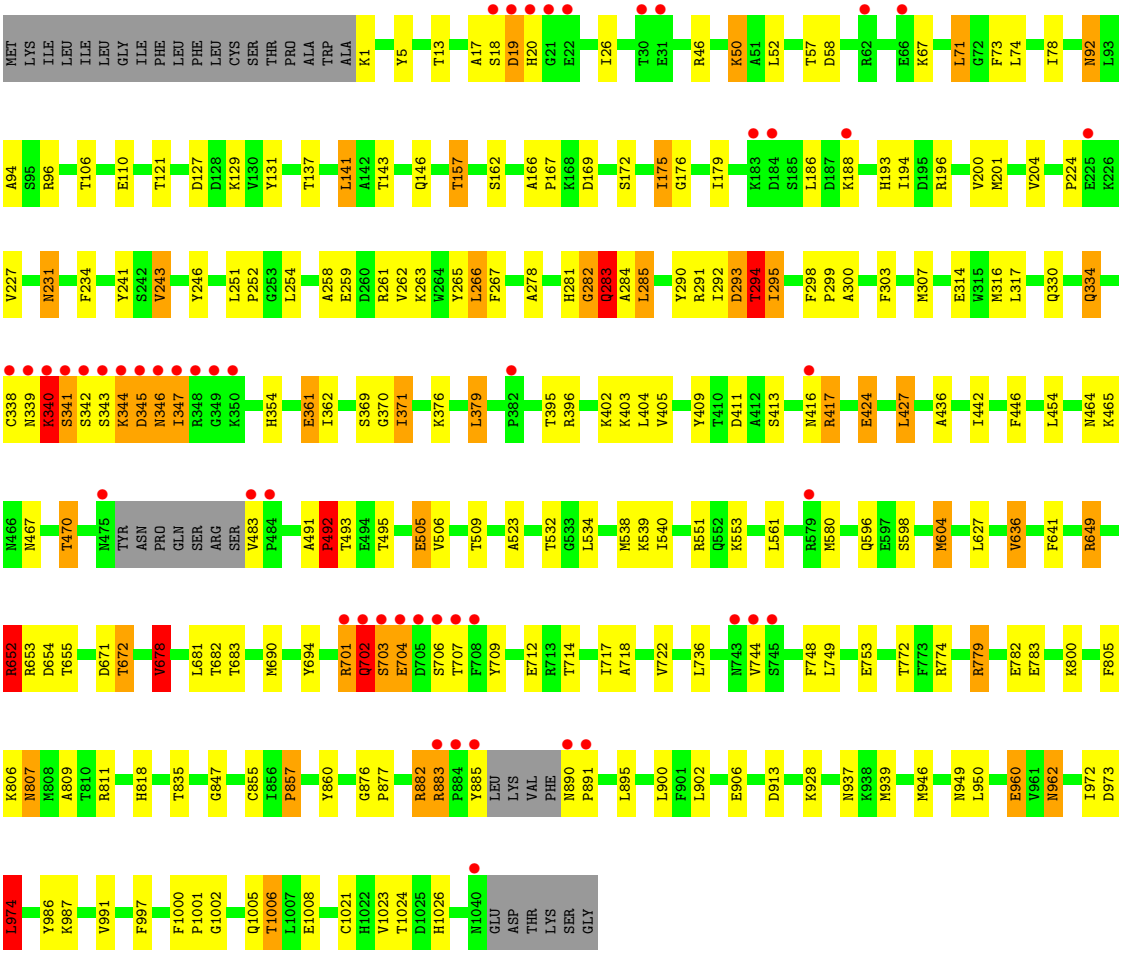
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	86	86	86	0	0

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	210.78Å 210.78Å 84.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.90 – 2.60 14.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (14.90-2.60) 95.2 (14.90-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.234 0.200 , 0.229	Depositor DCC
R_{free} test set	3091 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	69.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8468	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, CU, NAG, CA, GOL, O, NA

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	0.79	2/8575 (0.0%)	0.83	7/11637 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1008	GLU	CG-CD	6.54	1.61	1.51
1	A	361	GLU	CG-CD	5.33	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	974	LEU	CA-CB-CG	6.99	131.37	115.30
1	A	678	VAL	CB-CA-C	-6.81	98.46	111.40
1	A	266	LEU	CA-CB-CG	6.73	130.78	115.30
1	A	551	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	345	ASP	C-N-CA	5.20	134.69	121.70
1	A	652	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	779	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	THR	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	8337	0	7895	181	1
2	A	28	0	26	0	0
3	A	6	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	6	0	8	0	0
9	A	86	0	0	6	0
All	All	8468	0	7929	181	1

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 11.

All (181) 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:340:LYS:HB3	1:A:341:SER:CA	1.56	1.35
1:A:340:LYS:CB	1:A:341:SER:HA	1.43	1.34
1:A:282:GLY:HA3	1:A:283:GLN:CB	1.52	1.30
1:A:282:GLY:CA	1:A:283:GLN:HB2	1.68	1.22
1:A:701:ARG:HA	1:A:702:GLN:CB	1.74	1.16
1:A:701:ARG:CG	1:A:702:GLN:HB3	1.78	1.13
1:A:701:ARG:CA	1:A:702:GLN:HB2	1.79	1.12
1:A:19:ASP:HB3	1:A:20:HIS:HA	1.32	1.08
1:A:282:GLY:HA3	1:A:283:GLN:CG	1.84	1.05
1:A:701:ARG:CA	1:A:702:GLN:CB	2.35	1.04
1:A:282:GLY:HA3	1:A:283:GLN:HB2	1.02	1.01
1:A:340:LYS:HB2	1:A:341:SER:HA	1.44	1.00
1:A:281:HIS:O	1:A:282:GLY:O	1.80	0.99
1:A:157:THR:HG22	1:A:265:TYR:HD1	1.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ARG:HA	1:A:702:GLN:HB2	1.00	0.98
1:A:340:LYS:HB3	1:A:341:SER:HA	0.98	0.95
1:A:282:GLY:CA	1:A:283:GLN:CB	2.37	0.93
1:A:294:THR:O	1:A:295:ILE:O	1.89	0.90
1:A:939:MET:HB3	1:A:946:MET:CE	2.01	0.90
1:A:340:LYS:CB	1:A:341:SER:CA	2.27	0.88
1:A:701:ARG:CB	1:A:702:GLN:HB3	2.04	0.88
1:A:19:ASP:CB	1:A:20:HIS:HA	2.06	0.85
1:A:293:ASP:O	1:A:294:THR:HB	1.77	0.84
1:A:604:MET:HE1	1:A:690:MET:HG2	1.59	0.83
1:A:416:ASN:O	1:A:417:ARG:HB3	1.76	0.83
1:A:986:TYR:O	1:A:987:LYS:HB2	1.75	0.83
1:A:258:ALA:O	1:A:259:GLU:HB2	1.79	0.83
1:A:857:PRO:HD3	1:A:1006:THR:HG22	1.61	0.83
1:A:71:LEU:HD22	1:A:74:LEU:HB2	1.62	0.82
1:A:342:SER:OG	1:A:343:SER:N	2.09	0.81
1:A:343:SER:O	1:A:344:LYS:HB2	1.79	0.81
1:A:701:ARG:HG2	1:A:702:GLN:HB3	1.60	0.79
1:A:340:LYS:HB3	1:A:341:SER:C	2.05	0.78
1:A:347:ILE:HD12	1:A:347:ILE:O	1.83	0.78
1:A:343:SER:O	1:A:344:LYS:CB	2.33	0.77
1:A:157:THR:HG22	1:A:265:TYR:CD1	2.16	0.76
1:A:604:MET:CE	1:A:690:MET:HG2	2.16	0.74
1:A:470:THR:HG23	1:A:523:ALA:HB1	1.68	0.74
1:A:299:PRO:O	1:A:300:ALA:HB3	1.86	0.74
1:A:285:LEU:HD13	1:A:307:MET:HB2	1.70	0.73
1:A:106:THR:HG23	1:A:146:GLN:HG3	1.70	0.72
1:A:282:GLY:HA2	1:A:283:GLN:HE21	1.54	0.72
1:A:1021:CYS:SG	1:A:1023:VAL:HG13	2.30	0.72
1:A:702:GLN:HE21	1:A:702:GLN:HA	1.56	0.71
1:A:50:LYS:HB2	1:A:172:SER:O	1.90	0.71
1:A:200:VAL:HG13	1:A:243:VAL:HG23	1.72	0.71
1:A:636:VAL:O	1:A:682:THR:HG21	1.91	0.70
1:A:141:LEU:HD13	1:A:143:THR:HG23	1.73	0.70
1:A:141:LEU:HD13	1:A:143:THR:CG2	2.22	0.70
1:A:702:GLN:HE21	1:A:702:GLN:CA	2.04	0.70
1:A:491:ALA:HB1	1:A:492:PRO:HD2	1.74	0.70
1:A:701:ARG:CB	1:A:702:GLN:CB	2.67	0.69
1:A:293:ASP:O	1:A:294:THR:CB	2.41	0.69
1:A:702:GLN:HA	1:A:702:GLN:NE2	2.08	0.69
1:A:157:THR:HG21	1:A:303:PHE:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ARG:HG3	1:A:702:GLN:HB3	1.71	0.68
1:A:278:ALA:O	1:A:294:THR:O	2.12	0.68
1:A:748:PHE:O	9:A:1207:HOH:O	2.11	0.68
1:A:129:LYS:HD3	1:A:131:TYR:CZ	2.29	0.67
1:A:939:MET:HB3	1:A:946:MET:HE1	1.75	0.67
1:A:282:GLY:HA3	1:A:283:GLN:HG2	1.76	0.65
1:A:464:ASN:OD1	1:A:467:ASN:ND2	2.30	0.64
1:A:671:ASP:OD1	1:A:672:THR:HG22	1.98	0.64
1:A:454:LEU:HD22	1:A:534:LEU:HD13	1.79	0.63
1:A:281:HIS:O	1:A:282:GLY:C	2.36	0.63
1:A:653:ARG:HH21	1:A:1005:GLN:HE22	1.44	0.63
1:A:701:ARG:CG	1:A:702:GLN:CB	2.68	0.63
1:A:299:PRO:O	1:A:300:ALA:CB	2.46	0.62
1:A:652:ARG:HD2	1:A:847:GLY:O	2.00	0.62
1:A:655:THR:HG21	1:A:681:LEU:HD12	1.81	0.61
1:A:243:VAL:HG22	1:A:251:LEU:HD22	1.84	0.60
1:A:347:ILE:O	1:A:347:ILE:CD1	2.50	0.60
1:A:855:CYS:O	1:A:1006:THR:HG21	2.02	0.59
1:A:343:SER:O	1:A:344:LYS:HG2	2.02	0.58
1:A:561:LEU:HB2	1:A:627:LEU:HD22	1.85	0.58
1:A:807:ASN:HD22	1:A:809:ALA:H	1.51	0.58
1:A:654:ASP:OD1	1:A:818:HIS:HD2	1.87	0.58
1:A:973:ASP:OD2	9:A:1275:HOH:O	2.17	0.58
1:A:166:ALA:HB3	1:A:167:PRO:HD3	1.85	0.58
1:A:224:PRO:O	1:A:227:VAL:HG22	2.04	0.58
1:A:818:HIS:HE1	9:A:1203:HOH:O	1.87	0.57
1:A:890:ASN:HB3	1:A:891:PRO:HD3	1.86	0.57
1:A:470:THR:HG23	1:A:523:ALA:CB	2.34	0.57
1:A:26:ILE:H	1:A:330:GLN:HE22	1.54	0.56
1:A:345:ASP:HB2	1:A:505:GLU:OE2	2.05	0.56
1:A:1006:THR:HG23	9:A:1205:HOH:O	2.06	0.56
1:A:200:VAL:HG13	1:A:243:VAL:CG2	2.36	0.56
1:A:19:ASP:CB	1:A:20:HIS:CA	2.81	0.55
1:A:251:LEU:HD12	1:A:252:PRO:HD2	1.87	0.55
1:A:807:ASN:HD21	1:A:809:ALA:HB3	1.72	0.55
1:A:110:GLU:O	1:A:127:ASP:HB3	2.07	0.55
1:A:807:ASN:ND2	1:A:809:ALA:H	2.03	0.54
1:A:424:GLU:CB	1:A:427:LEU:HD22	2.38	0.54
1:A:483:VAL:HG13	1:A:483:VAL:O	2.08	0.54
1:A:196:ARG:HB2	1:A:262:VAL:HG22	1.90	0.54
1:A:338:CYS:N	1:A:339:ASN:HA	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:MET:CB	1:A:946:MET:HE1	2.37	0.54
1:A:294:THR:HG23	1:A:295:ILE:N	2.22	0.53
1:A:343:SER:O	1:A:344:LYS:CG	2.56	0.53
1:A:409:TYR:HA	1:A:417:ARG:HA	1.90	0.53
1:A:906:GLU:HB2	1:A:937:ASN:HB3	1.90	0.53
1:A:282:GLY:CA	1:A:283:GLN:HE21	2.21	0.52
1:A:682:THR:HG22	1:A:1001:PRO:HG2	1.91	0.52
1:A:193:HIS:O	1:A:194:ILE:HD13	2.11	0.51
1:A:316:MET:SD	1:A:330:GLN:HB3	2.50	0.51
1:A:17:ALA:O	1:A:19:ASP:N	2.34	0.51
1:A:491:ALA:HB1	1:A:492:PRO:CD	2.40	0.51
1:A:294:THR:CG2	1:A:295:ILE:N	2.73	0.51
1:A:986:TYR:O	1:A:987:LYS:CB	2.53	0.51
1:A:702:GLN:CA	1:A:702:GLN:NE2	2.70	0.51
1:A:282:GLY:CA	1:A:283:GLN:NE2	2.74	0.50
1:A:539:LYS:C	1:A:540:ILE:HD12	2.31	0.50
1:A:960:GLU:OE1	1:A:962:ASN:ND2	2.44	0.50
1:A:204:VAL:HG22	1:A:241:TYR:CD2	2.47	0.50
1:A:106:THR:HG22	1:A:146:GLN:HE21	1.77	0.50
1:A:282:GLY:CA	1:A:283:GLN:CG	2.75	0.49
1:A:340:LYS:HB3	1:A:342:SER:N	2.28	0.49
1:A:92:ASN:ND2	1:A:94:ALA:H	2.11	0.49
1:A:436:ALA:CB	1:A:442:ILE:HD11	2.43	0.48
1:A:604:MET:CE	1:A:690:MET:CG	2.89	0.48
1:A:913:ASP:OD1	1:A:928:LYS:NZ	2.35	0.47
1:A:314:GLU:O	1:A:465:LYS:NZ	2.47	0.47
1:A:446:PHE:O	1:A:495:THR:HA	2.15	0.47
1:A:282:GLY:HA2	1:A:283:GLN:NE2	2.24	0.47
1:A:298:PHE:HB3	1:A:299:PRO:CD	2.45	0.47
1:A:292:ILE:C	1:A:292:ILE:HD12	2.35	0.46
1:A:404:LEU:HB2	1:A:532:THR:HG22	1.96	0.46
1:A:282:GLY:N	1:A:283:GLN:HB2	2.23	0.46
1:A:369:SER:HB2	1:A:371:ILE:HD13	1.98	0.46
1:A:1023:VAL:HG22	1:A:1026:HIS:CG	2.51	0.46
1:A:416:ASN:O	1:A:417:ARG:CB	2.51	0.46
1:A:5:TYR:CE1	1:A:78:ILE:HG23	2.51	0.46
1:A:997:PHE:CZ	1:A:1005:GLN:HG2	2.51	0.45
1:A:598:SER:HB2	9:A:1274:HOH:O	2.16	0.45
1:A:701:ARG:HG3	1:A:702:GLN:CB	2.42	0.45
1:A:939:MET:CE	1:A:946:MET:HE1	2.47	0.45
1:A:974:LEU:H	1:A:974:LEU:HD13	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASP:O	1:A:413:SER:O	2.35	0.44
1:A:718:ALA:HA	1:A:806:LYS:O	2.17	0.44
1:A:939:MET:CB	1:A:946:MET:CE	2.86	0.44
1:A:263:LYS:HG2	1:A:265:TYR:OH	2.17	0.44
1:A:334:GLN:HE21	1:A:334:GLN:HB2	1.62	0.44
1:A:772:THR:HB	1:A:774:ARG:HD2	1.99	0.44
1:A:655:THR:HG21	1:A:1002:GLY:HA3	1.99	0.44
1:A:201:MET:HB2	1:A:267:PHE:CZ	2.53	0.44
1:A:370:GLY:C	1:A:379:LEU:HD22	2.38	0.43
1:A:294:THR:O	1:A:295:ILE:C	2.54	0.43
1:A:231:ASN:HD22	1:A:234:PHE:H	1.64	0.43
1:A:162:SER:HB3	1:A:169:ASP:HB3	1.99	0.43
1:A:361:GLU:HA	1:A:403:LYS:O	2.19	0.43
1:A:641:PHE:CD1	1:A:678:VAL:HG13	2.53	0.43
1:A:52:LEU:HD22	1:A:73:PHE:HB2	2.01	0.43
1:A:706:SER:O	1:A:707:THR:C	2.57	0.42
1:A:141:LEU:HD13	1:A:143:THR:HG22	1.99	0.42
1:A:709:TYR:CE2	1:A:800:LYS:HB2	2.54	0.42
1:A:246:TYR:CD2	1:A:251:LEU:HD13	2.54	0.42
1:A:538:MET:HG2	1:A:540:ILE:CD1	2.49	0.42
1:A:883:ARG:O	1:A:883:ARG:HD2	2.19	0.42
1:A:807:ASN:HD22	1:A:807:ASN:C	2.23	0.42
1:A:345:ASP:HA	1:A:346:ASN:CB	2.49	0.42
1:A:703:SER:O	1:A:704:GLU:HG2	2.20	0.42
1:A:939:MET:CE	1:A:946:MET:CE	2.98	0.42
1:A:860:TYR:CZ	1:A:876:GLY:HA3	2.55	0.41
1:A:946:MET:O	1:A:949:ASN:HB2	2.20	0.41
1:A:175:ILE:HG13	1:A:176:GLY:N	2.34	0.41
1:A:424:GLU:HB3	1:A:427:LEU:HD22	2.00	0.41
1:A:604:MET:HE2	1:A:690:MET:HG2	1.99	0.41
1:A:939:MET:HA	1:A:946:MET:HE1	2.02	0.41
1:A:717:ILE:O	1:A:805:PHE:HA	2.21	0.41
1:A:882:ARG:HB3	1:A:883:ARG:H	1.70	0.41
1:A:939:MET:CA	1:A:946:MET:HE1	2.51	0.41
1:A:436:ALA:HB2	1:A:442:ILE:HD11	2.03	0.41
1:A:284:ALA:C	1:A:285:LEU:HD22	2.41	0.41
1:A:92:ASN:C	1:A:92:ASN:HD22	2.24	0.41
1:A:290:TYR:CZ	1:A:649:ARG:HG2	2.56	0.41
1:A:678:VAL:HG22	1:A:694:TYR:HD1	1.86	0.41
1:A:1000:PHE:HB3	1:A:1001:PRO:CD	2.50	0.40
1:A:179:ILE:N	1:A:179:ILE:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:MET:HE2	1:A:690:MET:CG	2.50	0.40
1:A:483:VAL:O	1:A:483:VAL:CG1	2.68	0.40
1:A:882:ARG:HG2	9:A:1277:HOH:O	2.20	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LYS:O	1:A:712:GLU:OE2[3_565]	2.10	0.10

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	1024/1065 (96%)	962 (94%)	43 (4%)	19 (2%)	8 15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	GLY
1	A	283	GLN
1	A	295	ILE
1	A	344	LYS
1	A	346	ASN
1	A	702	GLN
1	A	704	GLU
1	A	744	VAL
1	A	882	ARG
1	A	294	THR
1	A	340	LYS
1	A	18	SER
1	A	492	PRO

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Mol	Chain	Res	Type
1	A	19	ASP
1	A	1024	THR
1	A	417	ARG
1	A	877	PRO
1	A	857	PRO
1	A	347	ILE

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	903/937 (96%)	821 (91%)	82 (9%)	9 18

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	13	THR
1	A	46	ARG
1	A	50	LYS
1	A	58	ASP
1	A	67	LYS
1	A	71	LEU
1	A	92	ASN
1	A	96	ARG
1	A	121	THR
1	A	137	THR
1	A	141	LEU
1	A	157	THR
1	A	175	ILE
1	A	186	LEU
1	A	188	LYS
1	A	231	ASN
1	A	243	VAL
1	A	254	LEU
1	A	261	ARG

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Mol	Chain	Res	Type
1	A	266	LEU
1	A	283	GLN
1	A	285	LEU
1	A	291	ARG
1	A	293	ASP
1	A	294	THR
1	A	317	LEU
1	A	334	GLN
1	A	340	LYS
1	A	341	SER
1	A	354	HIS
1	A	362	ILE
1	A	371	ILE
1	A	376	LYS
1	A	379	LEU
1	A	395	THR
1	A	396	ARG
1	A	402	LYS
1	A	405	VAL
1	A	424	GLU
1	A	427	LEU
1	A	470	THR
1	A	492	PRO
1	A	493	THR
1	A	505	GLU
1	A	506	VAL
1	A	509	THR
1	A	580	MET
1	A	596	GLN
1	A	604	MET
1	A	636	VAL
1	A	649	ARG
1	A	652	ARG
1	A	672	THR
1	A	678	VAL
1	A	683	THR
1	A	701	ARG
1	A	702	GLN
1	A	703	SER
1	A	714	THR
1	A	722	VAL
1	A	736	LEU

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Mol	Chain	Res	Type
1	A	749	LEU
1	A	753	GLU
1	A	779	ARG
1	A	782	GLU
1	A	783	GLU
1	A	807	ASN
1	A	811	ARG
1	A	835	THR
1	A	883	ARG
1	A	885	TYR
1	A	895	LEU
1	A	900	LEU
1	A	902	LEU
1	A	950	LEU
1	A	960	GLU
1	A	962	ASN
1	A	972	ILE
1	A	974	LEU
1	A	991	VAL
1	A	1006	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	231	ASN
1	A	238	ASN
1	A	281	HIS
1	A	283	GLN
1	A	287	ASN
1	A	296	ASN
1	A	330	GLN
1	A	334	GLN
1	A	611	ASN
1	A	612	GLN
1	A	657	ASN
1	A	661	GLN
1	A	677	ASN
1	A	702	GLN
1	A	807	ASN
1	A	818	HIS
1	A	962	ASN

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Mol	Chain	Res	Type
1	A	1005	GLN
1	A	1028	HIS

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 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	OXY	A	1109	3	1,1,1	0.09	0	-		
8	GOL	A	1113	-	5,5,5	0.32	0	5,5,5	0.66	0
2	NAG	A	1101	1	14,14,15	0.71	0	17,19,21	1.77	6 (35%)
2	NAG	A	1111	1	14,14,15	0.65	0	17,19,21	1.72	2 (11%)

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	1113	-	-	2/4/4/4	-
2	NAG	A	1101	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1111	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1111	NAG	C1-O5-C5	3.99	117.60	112.19
2	A	1101	NAG	C3-C4-C5	-3.97	103.16	110.24
2	A	1101	NAG	C1-O5-C5	3.50	116.94	112.19
2	A	1111	NAG	O5-C5-C6	3.34	112.44	107.20
2	A	1101	NAG	O4-C4-C5	2.43	115.33	109.30
2	A	1101	NAG	O5-C5-C6	2.32	110.84	107.20
2	A	1101	NAG	O4-C4-C3	2.06	115.12	110.35
2	A	1101	NAG	O7-C7-C8	-2.03	118.28	122.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1111	NAG	O5-C5-C6-O6
8	A	1113	GOL	C1-C2-C3-O3
8	A	1113	GOL	O2-C2-C3-O3

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	1029/1065 (96%)	-0.22	49 (4%)	30	24	44, 68, 107, 139	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	706	SER	8.2
1	A	707	THR	8.0
1	A	890	ASN	7.1
1	A	21	GLY	6.8
1	A	705	ASP	6.7
1	A	704	GLU	6.4
1	A	343	SER	6.0
1	A	344	LYS	6.0
1	A	346	ASN	5.9
1	A	885	TYR	5.9
1	A	340	LYS	5.7
1	A	345	ASP	5.4
1	A	347	ILE	5.4
1	A	703	SER	5.3
1	A	20	HIS	5.1
1	A	349	GLY	4.8
1	A	708	PHE	4.6
1	A	342	SER	4.5
1	A	884	PRO	4.5
1	A	743	ASN	4.3
1	A	891	PRO	4.3
1	A	22	GLU	4.2
1	A	483	VAL	4.1
1	A	702	GLN	3.9
1	A	744	VAL	3.8
1	A	18	SER	3.8
1	A	341	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	416	ASN	3.7
1	A	348	ARG	3.3
1	A	484	PRO	3.1
1	A	19	ASP	2.9
1	A	339	ASN	2.8
1	A	62	ARG	2.7
1	A	188	LYS	2.7
1	A	66	GLU	2.7
1	A	701	ARG	2.5
1	A	745	SER	2.5
1	A	183	LYS	2.5
1	A	475	ASN	2.5
1	A	350	LYS	2.4
1	A	883	ARG	2.4
1	A	579	ARG	2.3
1	A	338	CYS	2.3
1	A	382	PRO	2.2
1	A	184	ASP	2.2
1	A	225	GLU	2.1
1	A	31	GLU	2.1
1	A	1040	ASN	2.1
1	A	30	THR	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, 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(Å^2)	Q<0.9
2	NAG	A	1111	14/15	0.71	0.49	106,110,116,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	O	A	1108	1/1	0.76	0.79	22,22,22,22	1
7	NA	A	1112	1/1	0.88	0.29	85,85,85,85	0
2	NAG	A	1101	14/15	0.92	0.24	71,81,86,88	0
8	GOL	A	1113	6/6	0.92	0.16	60,61,62,64	0
5	OXY	A	1109	2/2	0.94	0.14	66,66,66,66	0
6	CA	A	1110	1/1	0.97	0.11	58,58,58,58	0
3	CU	A	1106	1/1	0.98	0.07	61,61,61,61	0
3	CU	A	1104	1/1	0.98	0.12	60,60,60,60	0
3	CU	A	1107	1/1	0.99	0.09	62,62,62,62	0
3	CU	A	1105	1/1	0.99	0.04	62,62,62,62	0
3	CU	A	1103	1/1	0.99	0.10	59,59,59,59	0
3	CU	A	1102	1/1	1.00	0.10	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.