Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2023 – 01:01 PM EDT

PDB ID	:	1QX1
Title	:	Golgi alpha-mannosidase II D341N mutant complex with 2-F-mannosyl-F
Authors	:	Numao, S.; Kuntz, D.A.; Withers, S.G.; Rose, D.R.
Deposited on	:	2003-09-04
Resolution	:	1.30 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 (i)) were used in the production of this report:

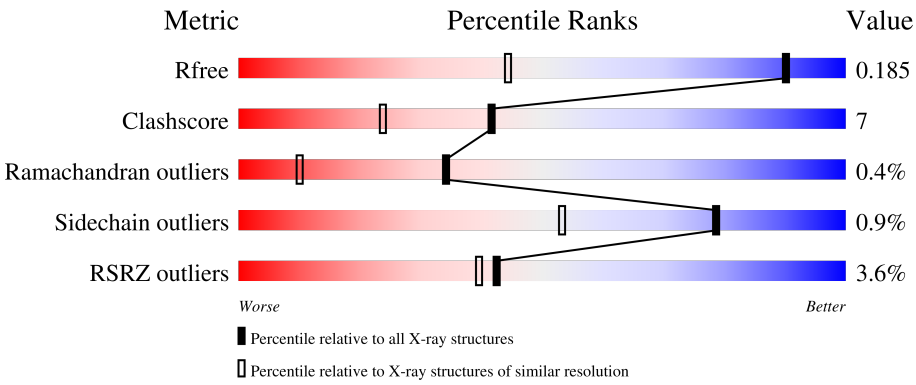
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	1045	3% 84% 12% • •

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	2001	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	2002	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9520 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.

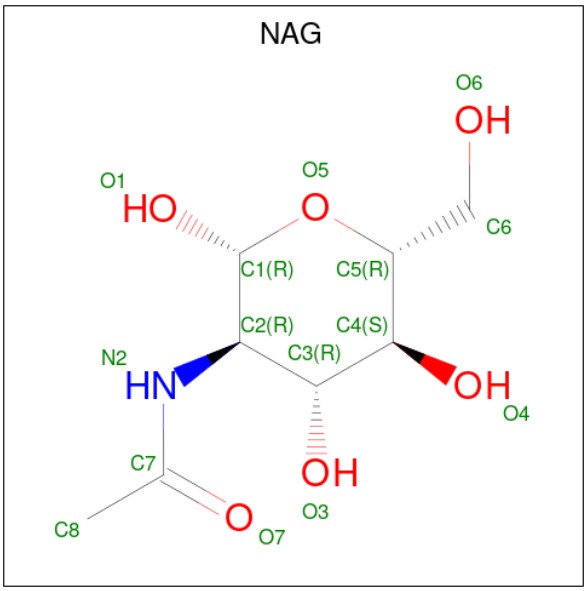
- Molecule 1 is a protein called Alpha-mannosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1014	8433	5356	1482	1552	43	0	29	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	cloning artifact	UNP Q24451
A	2	SER	-	cloning artifact	UNP Q24451
A	3	SER	-	cloning artifact	UNP Q24451
A	4	HIS	-	expression tag	UNP Q24451
A	5	HIS	-	expression tag	UNP Q24451
A	6	HIS	-	expression tag	UNP Q24451
A	7	HIS	-	expression tag	UNP Q24451
A	8	HIS	-	expression tag	UNP Q24451
A	9	HIS	-	expression tag	UNP Q24451
A	10	GLY	-	cloning artifact	UNP Q24451
A	11	GLU	-	cloning artifact	UNP Q24451
A	12	PHE	-	cloning artifact	UNP Q24451
A	341	ASN	ASP	engineered mutation	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

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

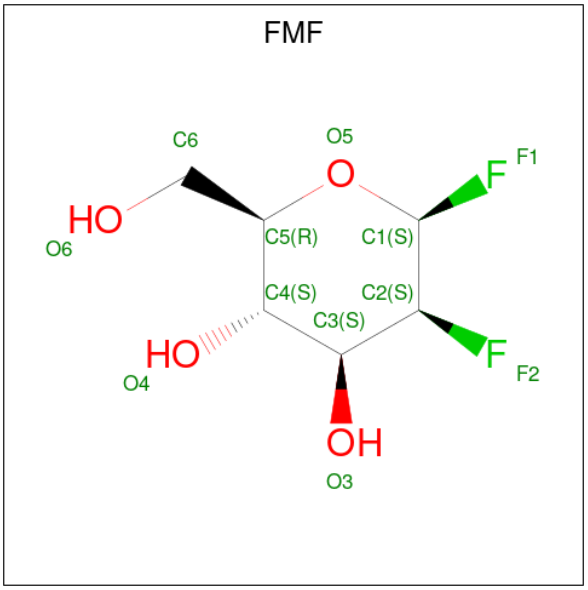


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

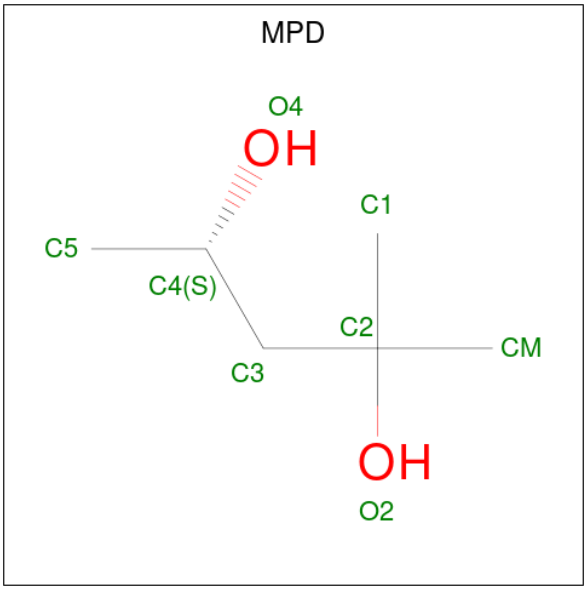
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is 2-deoxy-2-fluoro-beta-D-mannopyranosyl fluoride (three-letter code: FMF) (formula: $C_6H_{10}F_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
4	A	1	22	12	2	8	0	1

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	8	6	2	0	0

- Molecule 6 is water.

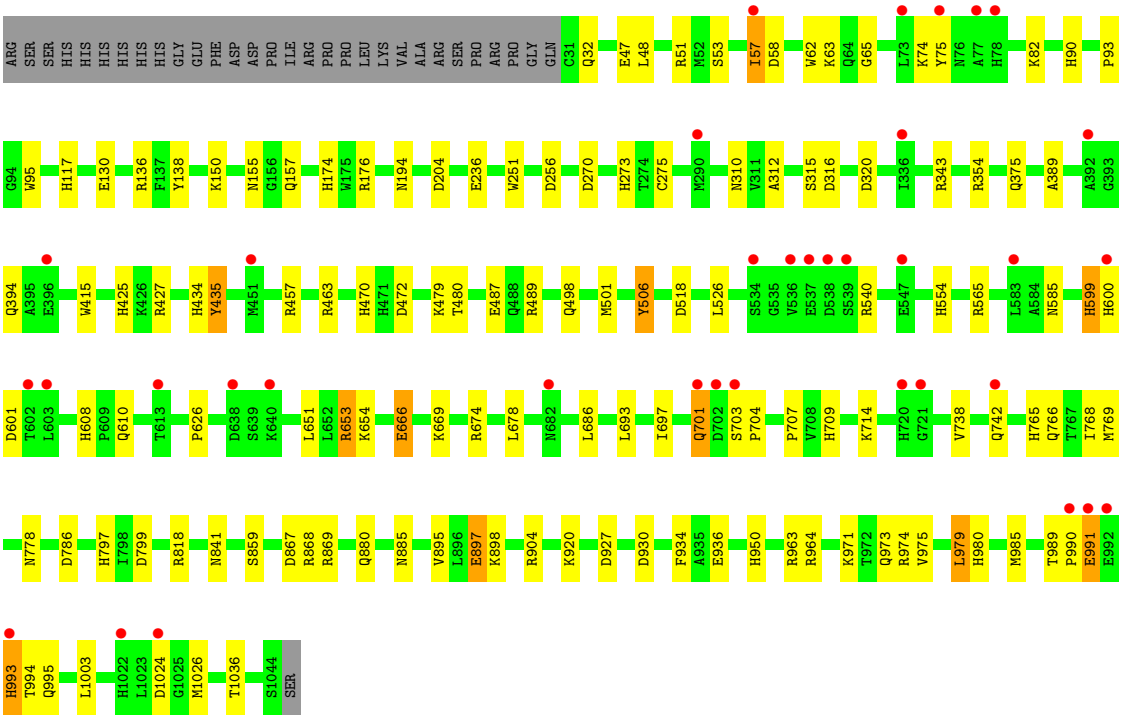
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	1042	1042	1042	0	0

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: Alpha-mannosidase II

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	69.05Å 109.83Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.23 – 1.30 29.86 – 1.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.23-1.30) 92.9 (29.86-1.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 1.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.170 , 0.189 0.165 , 0.185	Depositor DCC
R_{free} test set	2321 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9520	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: FMF, ZN, NAG, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.01	7/8666 (0.1%)	1.03	28/11760 (0.2%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	MET	SD-CE	-6.79	1.39	1.77
1	A	506[A]	TYR	CD2-CE2	6.00	1.48	1.39
1	A	506[B]	TYR	CD2-CE2	6.00	1.48	1.39
1	A	312	ALA	CA-CB	5.72	1.64	1.52
1	A	859	SER	CB-OG	-5.25	1.35	1.42
1	A	415	TRP	CG-CD1	5.09	1.43	1.36
1	A	897	GLU	CG-CD	5.07	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	427	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	979[A]	LEU	CA-CB-CG	6.93	131.25	115.30
1	A	979[B]	LEU	CA-CB-CG	6.93	131.25	115.30
1	A	501	MET	CG-SD-CE	-6.93	89.12	100.20
1	A	963	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	427	ARG	NE-CZ-NH2	-6.29	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	565	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	457	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	343	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	974	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	674	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	818	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	540	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	320	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	463	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	518	ASP	N-CA-C	-5.46	96.25	111.00
1	A	63	LYS	CD-CE-NZ	5.45	124.24	111.70
1	A	506[A]	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	506[B]	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	489	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	867	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	786	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	993	HIS	N-CA-C	5.20	125.04	111.00
1	A	818	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	868	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	868	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	457	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	799	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	435[B]	TYR	Mainchain
1	A	599[B]	HIS	Mainchain

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	8433	0	8183	111	1
2	A	14	0	13	7	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	13	1	0
5	A	8	0	14	3	0
6	A	1042	0	0	42	1
All	All	9520	0	8223	116	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 7.

All (116) 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:194:ASN:HD21	2:A:2001:NAG:C1	1.25	1.46
1:A:435[B]:TYR:CE1	6:A:2594:HOH:O	1.80	1.30
1:A:75[B]:TYR:CE1	6:A:2992:HOH:O	2.02	1.12
1:A:707:PRO:HG2	1:A:797[B]:HIS:CE1	1.87	1.09
1:A:82[A]:LYS:HD2	1:A:375:GLN:HE22	1.24	1.03
1:A:506[B]:TYR:OH	6:A:2896:HOH:O	1.55	1.02
1:A:75[B]:TYR:HD1	6:A:2781:HOH:O	1.44	0.99
1:A:435[B]:TYR:HE1	6:A:2594:HOH:O	1.30	0.95
1:A:709[A]:HIS:CD2	6:A:3045:HOH:O	2.16	0.95
1:A:707:PRO:HG2	1:A:797[B]:HIS:HE1	1.27	0.94
1:A:117[B]:HIS:HE1	1:A:354:ARG:HE	1.08	0.93
1:A:117[B]:HIS:CE1	1:A:354:ARG:HE	1.86	0.91
1:A:47:GLU:OE1	1:A:51:ARG:NH1	2.03	0.91
1:A:707:PRO:CG	1:A:797[B]:HIS:CE1	2.54	0.91
1:A:707:PRO:CG	1:A:797[B]:HIS:HE1	1.82	0.90
1:A:75[B]:TYR:HE1	6:A:2992:HOH:O	1.43	0.88
1:A:707:PRO:CB	1:A:797[B]:HIS:CE1	2.58	0.87
1:A:82[A]:LYS:HD2	1:A:375:GLN:NE2	1.95	0.81
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.27	0.80
1:A:989:THR:HG22	1:A:991:GLU:HG3	1.66	0.78
1:A:136:ARG:HD3	6:A:2887:HOH:O	1.83	0.78
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.66	0.78
1:A:971[B]:LYS:HB2	1:A:971[B]:LYS:NZ	1.99	0.77
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.32	0.77
1:A:75[B]:TYR:CD1	6:A:2781:HOH:O	2.26	0.76
1:A:693:LEU:HD13	6:A:3029:HOH:O	1.85	0.76
1:A:707:PRO:HB2	1:A:797[B]:HIS:CE1	2.21	0.76
1:A:989:THR:CG2	1:A:991:GLU:HG3	2.16	0.76
1:A:117[B]:HIS:HE1	1:A:354:ARG:NE	1.82	0.74
1:A:669[B]:LYS:CD	1:A:669[B]:LYS:NZ	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASN:HD21	2:A:2001:NAG:C2	2.01	0.73
1:A:498:GLN:HE21	1:A:526:LEU:H	1.37	0.72
1:A:971[B]:LYS:HB2	1:A:971[B]:LYS:HZ3	1.54	0.71
1:A:256:ASP:HB2	6:A:3023:HOH:O	1.90	0.70
1:A:130:GLU:OE2	6:A:2891:HOH:O	2.10	0.69
1:A:82[B]:LYS:HE3	6:A:2745:HOH:O	1.93	0.69
1:A:82[B]:LYS:CE	6:A:2745:HOH:O	2.40	0.68
2:A:2001:NAG:N2	6:A:2914:HOH:O	2.27	0.68
5:A:2002:MPD:H13	6:A:2693:HOH:O	1.95	0.67
5:A:2002:MPD:H11	6:A:2844:HOH:O	1.96	0.65
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.79	0.65
1:A:194:ASN:ND2	2:A:2001:NAG:N2	2.45	0.65
1:A:75[B]:TYR:OH	6:A:3042:HOH:O	2.14	0.64
1:A:742:GLN:HG3	6:A:2682:HOH:O	1.97	0.64
1:A:990:PRO:O	1:A:991:GLU:O	2.17	0.63
1:A:765:HIS:HE1	6:A:2611:HOH:O	1.81	0.62
1:A:980:HIS:HE1	6:A:2083:HOH:O	1.83	0.61
1:A:707:PRO:CB	1:A:797[B]:HIS:HE1	2.05	0.61
1:A:703:SER:HB2	1:A:704:PRO:HD2	1.82	0.61
1:A:194:ASN:ND2	2:A:2001:NAG:C2	2.62	0.60
1:A:709[A]:HIS:HD2	6:A:3045:HOH:O	1.62	0.60
1:A:701:GLN:HE21	1:A:701:GLN:HA	1.66	0.60
1:A:904:ARG:HG2	1:A:985:MET:SD	2.43	0.59
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.31	0.59
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.86	0.58
1:A:950:HIS:HE1	6:A:2616:HOH:O	1.88	0.57
1:A:480:THR:H	1:A:880:GLN:HE22	1.53	0.57
1:A:74:LYS:HE3	6:A:3042:HOH:O	2.05	0.56
1:A:990:PRO:O	1:A:991:GLU:C	2.43	0.56
1:A:626:PRO:O	1:A:950:HIS:HD2	1.88	0.56
1:A:273:HIS:HE1	5:A:2002:MPD:O4	1.88	0.55
1:A:57:ILE:HD12	1:A:58:ASP:N	2.22	0.54
1:A:270:ASP:OD1	1:A:273:HIS:HD2	1.90	0.54
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.91	0.54
1:A:554:HIS:HD2	6:A:2799:HOH:O	1.91	0.54
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.91	0.53
1:A:994:THR:HA	6:A:2575:HOH:O	2.08	0.53
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.39	0.53
1:A:599[A]:HIS:CD2	1:A:610:GLN:HG3	2.44	0.53
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.92	0.52
1:A:601:ASP:OD2	1:A:608:HIS:HE1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:GLN:HE21	1:A:701:GLN:CA	2.22	0.52
1:A:654:LYS:HG3	1:A:742:GLN:NE2	2.25	0.52
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.44	0.51
1:A:766[B]:GLN:HG2	1:A:768:ILE:HG13	1.91	0.51
1:A:554:HIS:HE1	6:A:2803:HOH:O	1.93	0.51
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.46	0.50
1:A:599[A]:HIS:HD2	1:A:610:GLN:CG	2.24	0.50
1:A:678:LEU:HD12	1:A:769[A]:MET:HE1	1.93	0.50
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.57	0.50
1:A:600:HIS:N	1:A:600:HIS:ND1	2.59	0.50
1:A:57:ILE:HD12	1:A:58:ASP:O	2.11	0.49
1:A:251:TRP:C	1:A:251:TRP:CD1	2.85	0.49
1:A:599[A]:HIS:HD2	1:A:610:GLN:HG3	1.78	0.49
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.95	0.48
1:A:82[A]:LYS:NZ	6:A:2822:HOH:O	2.47	0.48
1:A:155:ASN:HB3	6:A:2363:HOH:O	2.12	0.48
2:A:2001:NAG:H2	6:A:2914:HOH:O	2.13	0.48
1:A:435[B]:TYR:CZ	6:A:2594:HOH:O	2.26	0.48
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.62	0.47
1:A:989:THR:HG21	1:A:991:GLU:HG3	1.96	0.47
1:A:498:GLN:NE2	1:A:526:LEU:H	2.10	0.46
1:A:389:ALA:HB1	1:A:394:GLN:CG	2.45	0.46
1:A:714:LYS:HE3	1:A:738:VAL:HG22	1.97	0.46
1:A:666[A]:GLU:CG	6:A:2198:HOH:O	2.64	0.46
1:A:608:HIS:HD2	6:A:2841:HOH:O	1.99	0.45
1:A:47:GLU:CD	1:A:51:ARG:HH11	2.21	0.44
1:A:138:TYR:OH	1:A:150:LYS:HE2	2.17	0.44
1:A:707:PRO:HG2	1:A:797[B]:HIS:ND1	2.28	0.43
1:A:934:PHE:CE2	1:A:936:GLU:HB2	2.54	0.43
2:A:2001:NAG:C2	6:A:2914:HOH:O	2.66	0.43
1:A:686:LEU:HD22	1:A:697:ILE:HG12	2.00	0.43
1:A:32:GLN:NE2	6:A:3023:HOH:O	2.51	0.42
1:A:701:GLN:HA	1:A:701:GLN:NE2	2.33	0.42
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.54	0.42
1:A:600:HIS:CE1	6:A:2660:HOH:O	2.73	0.42
1:A:920:LYS:HG3	6:A:2990:HOH:O	2.20	0.41
1:A:472:ASP:OD2	4:A:2003[B]:FMF:O3	2.38	0.41
1:A:599[B]:HIS:CE1	1:A:601:ASP:HA	2.54	0.41
1:A:310:ASN:HA	6:A:2824:HOH:O	2.21	0.41
1:A:315:SER:O	1:A:316[B]:ASP:C	2.57	0.41
1:A:90:HIS:HA	6:A:2891:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026[A]:MET:HE3	6:A:2720:HOH:O	2.20	0.40
1:A:479:LYS:HD3	6:A:2836:HOH:O	2.20	0.40
1:A:995:GLN:HG3	6:A:2575:HOH:O	2.22	0.40
1:A:841:ASN:O	1:A:898[A]:LYS:HE2	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:53[B]:SER:OG	6:A:2448:HOH:O[1_455]	2.19	0.01

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	1041/1045 (100%)	1010 (97%)	27 (3%)	4 (0%)	34 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	991	GLU
1	A	95	TRP
1	A	993	HIS
1	A	204	ASP

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	930/929 (100%)	920 (99%)	10 (1%)	73 45

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	275	CYS
1	A	585	ASN
1	A	653	ARG
1	A	666[A]	GLU
1	A	666[B]	GLU
1	A	701	GLN
1	A	979[A]	LEU
1	A	979[B]	LEU
1	A	1024	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	91	ASN
1	A	121	ASN
1	A	148	GLN
1	A	157	GLN
1	A	194	ASN
1	A	240	GLN
1	A	249	GLN
1	A	273	HIS
1	A	347	ASN
1	A	388	GLN
1	A	394	GLN
1	A	425	HIS
1	A	434	HIS
1	A	460	GLN
1	A	469	GLN
1	A	470	HIS
1	A	488	GLN
1	A	498	GLN
1	A	554	HIS
1	A	608	HIS

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Mol	Chain	Res	Type
1	A	655	ASN
1	A	701	GLN
1	A	742	GLN
1	A	765	HIS
1	A	809	ASN
1	A	812	GLN
1	A	880	GLN
1	A	885	ASN
1	A	901	ASN
1	A	919	HIS
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	986	GLN
1	A	1018	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 5 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
2	NAG	A	2001	1	14,14,15	0.85	1 (7%)	17,19,21	1.02	1 (5%)
5	MPD	A	2002	-	7,7,7	0.86	0	9,10,10	0.70	0
4	FMF	A	2003[A]	1,3	11,11,12	2.93	5 (45%)	10,15,17	3.24	4 (40%)
4	FMF	A	2003[B]	1,3	11,11,12	2.61	5 (45%)	10,15,17	2.28	2 (20%)

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	2001	1	-	4/6/23/26	0/1/1/1
5	MPD	A	2002	-	1/1/2/2	2/5/5/5	-
4	FMF	A	2003[A]	1,3	-	0/2/19/22	0/1/1/1
4	FMF	A	2003[B]	1,3	-	0/2/19/22	1/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2003[A]	FMF	C2-C3	6.91	1.61	1.51
4	A	2003[B]	FMF	C2-C3	6.05	1.60	1.51
4	A	2003[A]	FMF	O5-C1	-3.82	1.37	1.43
4	A	2003[B]	FMF	C4-C3	3.65	1.61	1.52
4	A	2003[A]	FMF	O4-C4	-3.35	1.35	1.43
4	A	2003[B]	FMF	O3-C3	3.08	1.50	1.43
4	A	2003[A]	FMF	F2-C2	-2.64	1.34	1.40
4	A	2003[B]	FMF	C1-C2	2.61	1.55	1.52
4	A	2003[A]	FMF	O3-C3	2.17	1.48	1.43
4	A	2003[B]	FMF	O4-C4	-2.14	1.37	1.43
2	A	2001	NAG	C1-C2	2.09	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2003[A]	FMF	C1-O5-C5	7.26	122.03	112.19
4	A	2003[A]	FMF	C3-C4-C5	-5.70	100.07	110.24
4	A	2003[B]	FMF	C1-O5-C5	4.96	118.91	112.19
4	A	2003[B]	FMF	C3-C4-C5	-4.55	102.13	110.24
2	A	2001	NAG	C4-C3-C2	-3.07	106.52	111.02
4	A	2003[A]	FMF	C6-C5-C4	-2.94	106.11	113.00
4	A	2003[A]	FMF	O4-C4-C5	2.52	115.54	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	2002	MPD	C4

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	NAG	C3-C2-N2-C7
2	A	2001	NAG	C8-C7-N2-C2
2	A	2001	NAG	O7-C7-N2-C2
5	A	2002	MPD	C2-C3-C4-O4
2	A	2001	NAG	O5-C5-C6-O6
5	A	2002	MPD	C2-C3-C4-C5

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2003[B]	FMF	C1-C2-C3-C4-C5-O5

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	NAG	7	0
5	A	2002	MPD	3	0
4	A	2003[B]	FMF	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	316[B]:ASP	C	317:LEU	N	1.65

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	1014/1045 (97%)	-0.07	36 (3%) 42 39	7, 13, 27, 49	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	702	ASP	6.0
1	A	701	GLN	5.4
1	A	993	HIS	5.1
1	A	78	HIS	4.9
1	A	638	ASP	4.5
1	A	720	HIS	4.5
1	A	992	GLU	4.0
1	A	991	GLU	4.0
1	A	602	THR	3.9
1	A	536	VAL	3.8
1	A	547	GLU	3.4
1	A	1024	ASP	3.3
1	A	603	LEU	3.3
1	A	721	GLY	3.2
1	A	537	GLU	3.2
1	A	600	HIS	3.2
1	A	290	MET	2.9
1	A	682	ASN	2.8
1	A	613	THR	2.7
1	A	538[A]	ASP	2.5
1	A	534	SER	2.4
1	A	703	SER	2.4
1	A	539	SER	2.3
1	A	73	LEU	2.3
1	A	392	ALA	2.3
1	A	57	ILE	2.2
1	A	990	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	396	GLU	2.2
1	A	1022	HIS	2.2
1	A	75[A]	TYR	2.2
1	A	77	ALA	2.1
1	A	640	LYS	2.1
1	A	451[A]	MET	2.0
1	A	336	ILE	2.0
1	A	742	GLN	2.0
1	A	583	LEU	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	2001	14/15	0.66	0.37	35,47,50,55	0
4	FMF	A	2003[A]	11/12	0.94	0.11	6,12,16,16	11
4	FMF	A	2003[B]	11/12	0.94	0.11	11,14,18,21	11
5	MPD	A	2002	8/8	0.94	0.12	14,17,22,25	0
3	ZN	A	2004	1/1	0.98	0.04	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.