



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:47 pm GMT

PDB ID : 3EJP
Title : Golgi alpha-Mannosidase II in complex with 5-substituted swainsonine analog:
(5R)-5-[2'-oxo-2'-(phenyl)ethyl]-swainsonine
Authors : Kuntz, D.A.; Rose, D.R.
Deposited on : 2008-09-18
Resolution : 1.32 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

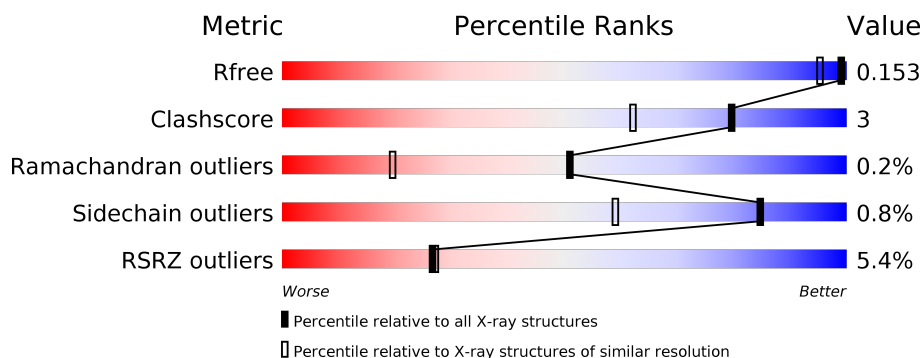
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 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}	100719	1164 (1.34-1.30)
Clashscore	112137	1223 (1.34-1.30)
Ramachandran outliers	110173	1179 (1.34-1.30)
Sidechain outliers	110143	1179 (1.34-1.30)
RSRZ outliers	101464	1167 (1.34-1.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1045	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9759 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1016	8415	5345	1480	1548	42	0	42	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	EXPRESSION TAG	UNP Q24451
A	2	SER	-	EXPRESSION TAG	UNP Q24451
A	3	SER	-	EXPRESSION TAG	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	-	EXPRESSION TAG	UNP Q24451
A	11	GLU	-	EXPRESSION TAG	UNP Q24451
A	12	PHE	-	EXPRESSION TAG	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

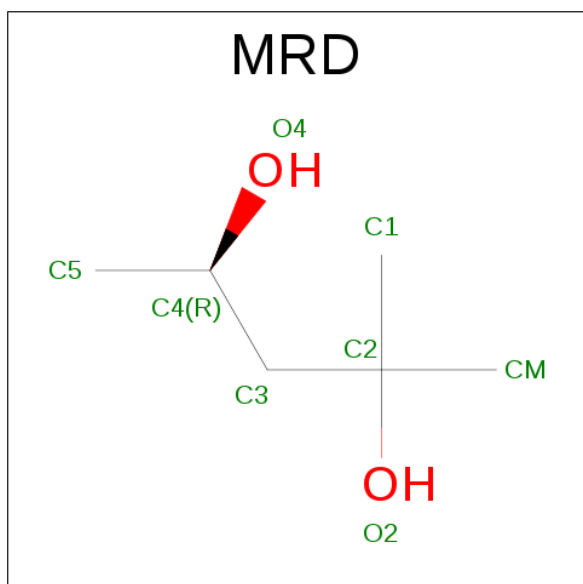


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

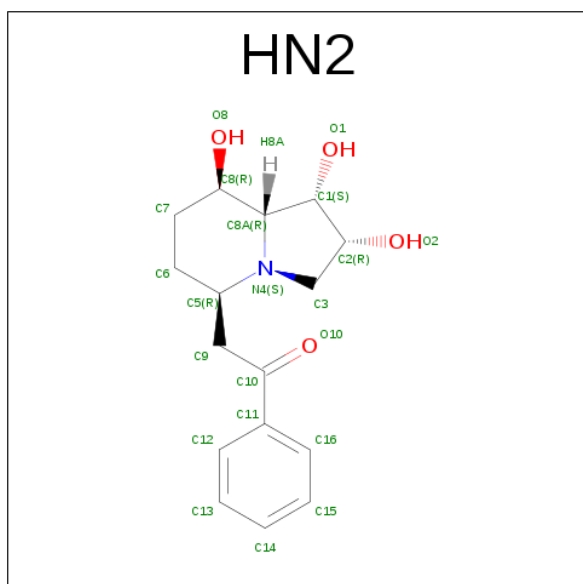
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



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

- Molecule 5 is 1-PHENYL-2-[(1S,2R,5R,8R,8AR)-1,2,8-TRIHIDROXYOCTAHYDROINDOLIZIN-5-YL]ETHANONE (three-letter code: HN2) (formula: C₁₆H₂₁NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	16	1	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1295	Total	O	0	5
			1300	1300		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

Amino Acid	Percentage
ARG	11%
SER	11%
SER	11%
HIS	11%
HIS	11%
HIS	11%
HIS	11%
HIS	11%
GLY	11%
GLU	11%
PHE	11%
ASP	11%
ASP	11%
PRO	11%
ILE	11%
ARG	11%
ARG	11%
PRO	11%
PRO	11%
LEU	11%
LYS	11%
VAL	11%
ALA	11%
ARG	11%
SER	11%
PRO	11%
ARG	11%
PRO	11%
GLY	11%
Q30	5%
N40	5%
E47	5%
L48	5%
R51	5%
M52	5%
W62	5%
Q65	5%
Y75	5%
N76	5%
A77	5%
H78	5%
K82	5%
W95	5%
I96	5%
H117	5%
W128	5%
R136	5%
V144	5%

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.03Å 109.88Å 138.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.22 – 1.32 28.60 – 1.32	Depositor EDS
% Data completeness (in resolution range)	92.1 (29.22-1.32) 92.1 (28.60-1.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.157 , 0.182 0.155 , 0.153	Depositor DCC
R_{free} test set	5091 reflections (2.29%)	DCC
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9759	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, ZN, HN2, 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	0.54	0/8781	0.67	1/11914 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	963	ARG	NE-CZ-NH2	-5.51	117.54	120.30

There are no chirality outliers.

There are no planarity outliers.

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	8415	0	8211	51	0
2	A	14	0	13	1	0
3	A	1	0	0	0	0
4	A	8	0	14	2	0
5	A	21	0	19	0	0
6	A	1300	0	0	15	0
All	All	9759	0	8257	54	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 (54) 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:610:GLN:HG3	6:A:1827:HOH:O	1.41	1.21
1:A:498[B]:GLN:HG2	1:A:526:LEU:HD12	1.16	1.12
1:A:136[A]:ARG:HD3	6:A:1338:HOH:O	1.72	0.89
1:A:599[A]:HIS:CD2	6:A:1827:HOH:O	2.34	0.80
1:A:75[A]:TYR:HD1	6:A:2154:HOH:O	1.65	0.79
1:A:96:ILE:CG2	6:A:2101:HOH:O	2.32	0.77
1:A:96:ILE:HG22	6:A:2101:HOH:O	1.84	0.76
1:A:380:GLN:HG2	6:A:1643:HOH:O	1.84	0.76
1:A:541:THR:HG23	6:A:1239:HOH:O	1.87	0.74
1:A:136[B]:ARG:HD2	6:A:1880:HOH:O	1.88	0.71
1:A:82[A]:LYS:HE3	1:A:375[A]:GLN:NE2	2.06	0.70
1:A:82[A]:LYS:HD2	1:A:375[A]:GLN:HE22	1.58	0.69
1:A:280:LYS:NZ	1:A:301:VAL:HG21	2.07	0.68
1:A:599[A]:HIS:HD2	1:A:610:GLN:CG	2.06	0.67
1:A:651[B]:LEU:HD22	1:A:659:LEU:HD11	1.77	0.67
1:A:1011[B]:ARG:NH1	6:A:1681:HOH:O	2.27	0.66
1:A:640:LYS:HD2	1:A:646:TYR:CE2	2.31	0.65
1:A:599[A]:HIS:CD2	1:A:610:GLN:HG3	2.32	0.64
4:A:1048:MRD:H1C3	6:A:1112:HOH:O	1.98	0.63
1:A:979[A]:LEU:HD21	1:A:999:VAL:HG11	1.81	0.62
1:A:904:ARG:HG2	1:A:985:MET:SD	2.40	0.61
1:A:742:GLN:HG3	6:A:1438:HOH:O	2.02	0.60
4:A:1048:MRD:H1C1	6:A:2192:HOH:O	2.00	0.59
1:A:47:GLU:OE2	1:A:51:ARG:HD3	2.03	0.58
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.34	0.58
1:A:280:LYS:HZ2	1:A:301:VAL:HG21	1.67	0.58
1:A:599[A]:HIS:HD2	1:A:610:GLN:HG3	1.68	0.56
1:A:498[B]:GLN:HG2	1:A:526:LEU:CD1	2.11	0.55
1:A:599[A]:HIS:CD2	1:A:610:GLN:CG	2.90	0.54
2:A:1046:NAG:H3	2:A:1046:NAG:H83	1.90	0.54
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.90	0.53
1:A:653:ARG:HD3	1:A:654:LYS:O	2.09	0.52
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.92	0.52
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.45	0.52
1:A:288:LYS:NZ	6:A:2093:HOH:O	2.43	0.52
1:A:47:GLU:OE2	1:A:51:ARG:CD	2.57	0.51
1:A:82[A]:LYS:CE	1:A:375[A]:GLN:NE2	2.73	0.51
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.46	0.49
1:A:653:ARG:HD2	1:A:656:PRO:HA	1.94	0.49
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:PRO:HG2	1:A:797[A]:HIS:CE1	2.48	0.48
1:A:313:ALA:O	1:A:316[B]:ASP:HB2	2.14	0.47
1:A:82[A]:LYS:CD	1:A:375[A]:GLN:HE22	2.26	0.47
1:A:651[B]:LEU:HD11	1:A:744:VAL:CG1	2.45	0.47
1:A:491[A]:GLN:NE2	6:A:1552:HOH:O	2.30	0.44
1:A:96:ILE:HG23	1:A:479:LYS:HE2	1.99	0.44
1:A:251:TRP:C	1:A:251:TRP:CD1	2.91	0.43
1:A:96:ILE:HG23	1:A:479:LYS:CE	2.49	0.43
1:A:48:LEU:HG	1:A:52[A]:MET:SD	2.59	0.42
1:A:204:ASP:H	1:A:205:PRO:HD3	1.85	0.42
1:A:599[A]:HIS:HD2	1:A:610:GLN:HG2	1.84	0.41
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	2.04	0.41
1:A:96:ILE:O	1:A:96:ILE:HG22	2.19	0.40
1:A:225:LEU:HD21	1:A:264[A]:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1056/1045 (101%)	1030 (98%)	24 (2%)	2 (0%)	51 19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
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	944/929 (102%)	936 (99%)	8 (1%)	85	59

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	PHE
1	A	275	CYS
1	A	585	ASN
1	A	651[A]	LEU
1	A	651[B]	LEU
1	A	653	ARG
1	A	828	TYR
1	A	898	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	1046	1	14,14,15	0.60	0	15,19,21	2.97	4 (26%)
4	MRD	A	1048	-	7,7,7	0.33	0	9,10,10	0.65	0
5	HN2	A	1049	-	23,23,23	0.85	0	25,33,33	0.89	1 (4%)

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	1046	1	-	0/6/23/26	0/1/1/1
4	MRD	A	1048	-	-	0/5/5/5	0/0/0/0
5	HN2	A	1049	-	-	0/8/37/37	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1049	HN2	C6-C5-N4	-2.33	105.31	110.86
2	A	1046	NAG	C8-C7-N2	2.95	121.44	116.11
2	A	1046	NAG	O5-C1-C2	3.86	116.85	111.47
2	A	1046	NAG	C2-N2-C7	5.85	131.47	122.94
2	A	1046	NAG	C1-O5-C5	7.89	123.05	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1046	NAG	1	0
4	A	1048	MRD	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, 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	1016/1045 (97%)	0.13	55 (5%) 26 27	6, 12, 24, 44	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	11.1
1	A	702	ASP	6.7
1	A	701	GLN	6.5
1	A	991	GLU	6.0
1	A	990	PRO	5.4
1	A	78	HIS	5.3
1	A	602	THR	5.2
1	A	1045	SER	4.9
1	A	603	LEU	4.6
1	A	682	ASN	4.4
1	A	77	ALA	4.3
1	A	703	SER	4.2
1	A	638	ASP	4.0
1	A	537	GLU	3.9
1	A	1024	ASP	3.7
1	A	721	GLY	3.6
1	A	613	THR	3.6
1	A	521	PHE	3.5
1	A	392	ALA	3.5
1	A	538	ASP	3.3
1	A	534	SER	3.3
1	A	614	THR	3.2
1	A	994	THR	3.2
1	A	720	HIS	3.2
1	A	290	MET	3.1
1	A	992	GLU	3.0
1	A	655	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	676	ILE	2.9
1	A	989	THR	2.9
1	A	144	ASN	2.8
1	A	30	GLN	2.8
1	A	600[A]	HIS	2.8
1	A	347	ASN	2.7
1	A	547	GLU	2.6
1	A	583	LEU	2.5
1	A	535	GLY	2.5
1	A	683	GLY	2.5
1	A	654	LYS	2.5
1	A	396	GLU	2.4
1	A	254	LYS	2.4
1	A	451	MET	2.4
1	A	1028	ALA	2.4
1	A	700	THR	2.4
1	A	40	ASN	2.3
1	A	1030	GLU	2.2
1	A	1044	SER	2.2
1	A	601	ASP	2.1
1	A	737	PRO	2.1
1	A	348	THR	2.1
1	A	1027	VAL	2.1
1	A	661	LEU	2.1
1	A	640	LYS	2.1
1	A	128	TRP	2.0
1	A	908	LEU	2.0
1	A	304	ARG	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	MRD	A	1048	8/8	0.92	0.12	1.01	14,18,20,22	0
5	HN2	A	1049	21/21	0.97	0.05	-0.30	7,9,15,16	0
3	ZN	A	1047	1/1	1.00	0.02	-2.45	8,8,8,8	0
2	NAG	A	1046	14/15	0.63	0.36	-	34,40,45,46	0

6.5 Other polymers

There are no such residues in this entry.