



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 10:31 AM EDT

PDB ID : 2AHX
Title : Crystal structure of ErbB4/HER4 extracellular domain
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Deposited on : 2005-07-28
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

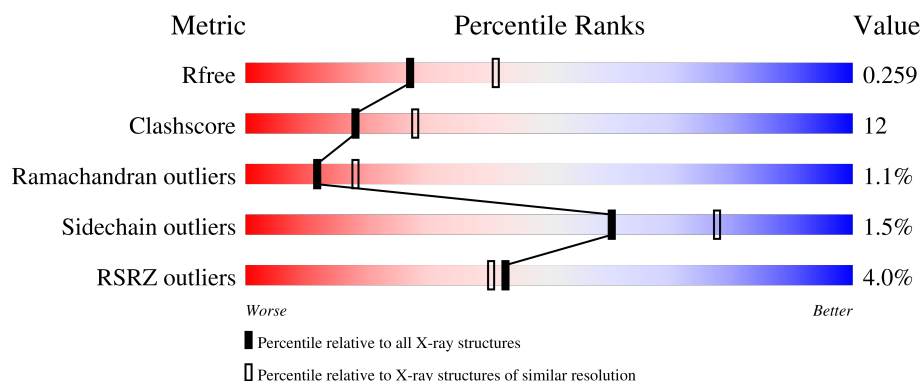
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 $\leq 5\%$. 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	617	
1	B	617	

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	1004	X	-	-	-
2	NAG	A	1006	X	-	-	-
2	NAG	A	1007	X	-	-	-
2	NAG	B	1010	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9940 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.

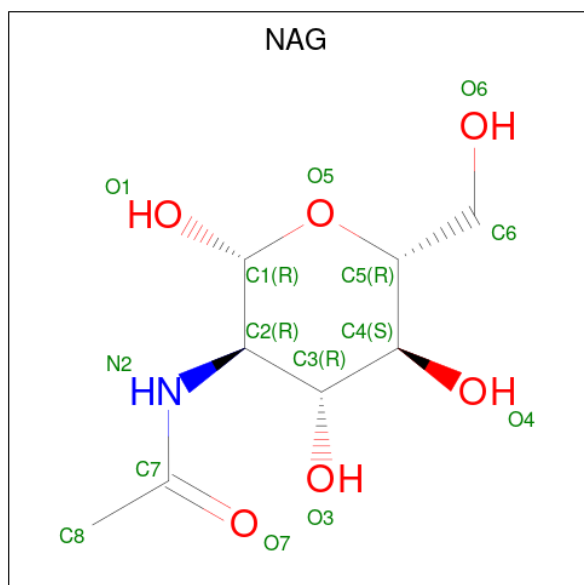
- Molecule 1 is a protein called Receptor tyrosine-protein kinase erbB-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4767	2961	831	917	58			
1	B	615	Total	C	N	O	S	0	0	0
			4795	2975	837	925	58			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ARG	-	cloning artifact	UNP Q15303
A	524	ASP	GLY	engineered mutation	UNP Q15303
B	0	ARG	-	cloning artifact	UNP Q15303
B	524	ASP	GLY	engineered mutation	UNP Q15303

- 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
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Y	0	0
			1	1		

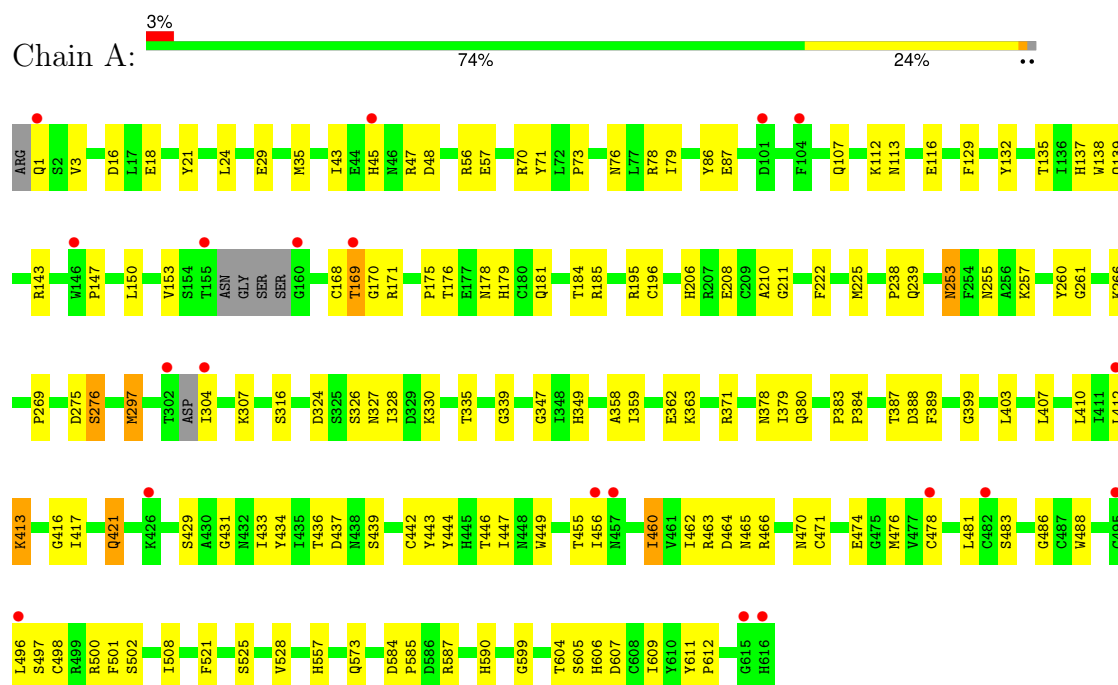
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	82	Total	O	0	0
			82	82		

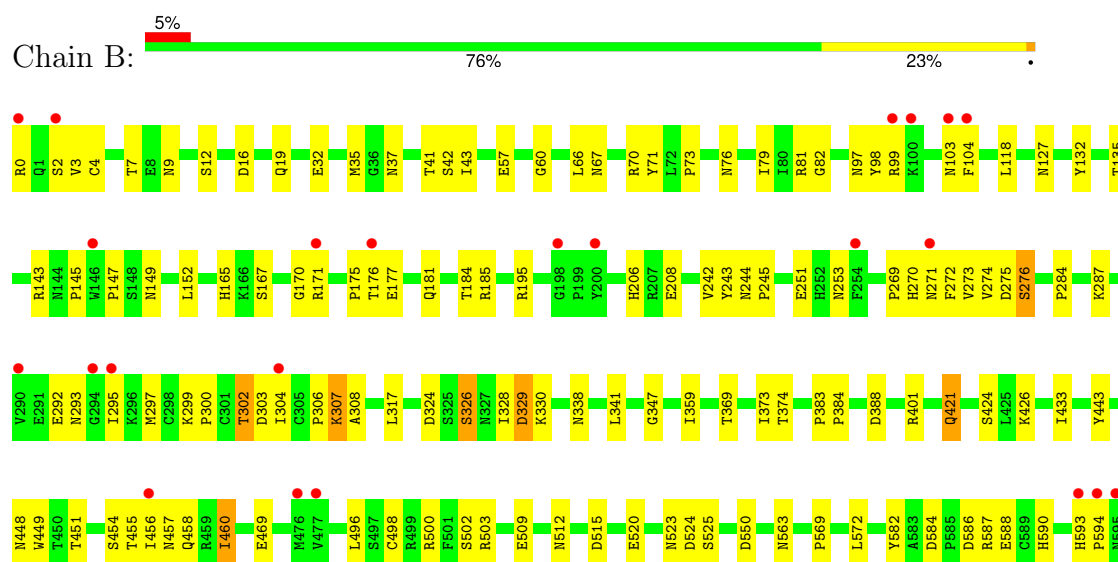
3 Residue-property plots [i](#)

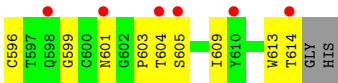
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Receptor tyrosine-protein kinase erbB-4



- Molecule 1: Receptor tyrosine-protein kinase erbB-4





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.96Å 203.09Å 261.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.40 29.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.88-2.40) 96.1 (29.88-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.235 , 0.265 0.227 , 0.259	Depositor DCC
R_{free} test set	4047 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: YT3, SO4, 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	0.40	0/4872	0.67	0/6601
1	B	0.42	0/4901	0.69	1/6644 (0.0%)
All	All	0.41	0/9773	0.68	1/13245 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	THR	C-N-CA	-6.73	104.88	121.70

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	4767	0	4496	127	0
1	B	4795	0	4526	102	0
2	A	112	0	104	8	0
2	B	112	0	104	4	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	B	1	0	0	1	0
5	A	56	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	82	0	0	2	0
All	All	9940	0	9230	229	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 12.

The worst 5 of 229 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:407:LEU:HD13	1:A:410:LEU:HD21	1.29	1.11
1:A:78:ARG:HD3	1:A:222:PHE:HB3	1.46	0.94
1:A:470:ASN:OD1	2:A:1007:NAG:H3	1.66	0.94
1:A:446:THR:HG21	1:A:478:CYS:SG	2.07	0.94
1:B:152:LEU:HD11	2:B:1011:NAG:H83	1.54	0.90

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	605/617 (98%)	545 (90%)	53 (9%)	7 (1%)	11	16
1	B	613/617 (99%)	564 (92%)	42 (7%)	7 (1%)	12	18
All	All	1218/1234 (99%)	1109 (91%)	95 (8%)	14 (1%)	12	18

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	169	THR
1	B	307	LYS

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Mol	Chain	Res	Type
1	A	316	SER
1	A	413	LYS

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	541/546 (99%)	535 (99%)	6 (1%)	70	84
1	B	545/546 (100%)	535 (98%)	10 (2%)	54	73
All	All	1086/1092 (100%)	1070 (98%)	16 (2%)	60	77

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	496	LEU
1	B	460	ILE
1	B	145	PRO
1	B	421	GLN
1	B	104	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	ASN
1	B	321	GLN
1	B	601	ASN
1	B	206	HIS
1	B	338	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	B	1010	1	14,14,15	0.75	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	B	1014	1	14,14,15	0.57	0	17,19,21	0.72	0
3	SO4	B	2002	-	4,4,4	0.37	0	6,6,6	0.11	0
2	NAG	A	1004	1	14,14,15	0.49	0	17,19,21	0.81	1 (5%)
2	NAG	B	1013	1	14,14,15	0.68	0	17,19,21	1.04	1 (5%)
2	NAG	A	1005	1	14,14,15	0.72	0	17,19,21	0.65	0
2	NAG	A	1001	1	14,14,15	0.73	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	B	1015	1	14,14,15	0.55	0	17,19,21	0.97	1 (5%)
2	NAG	B	1011	1	14,14,15	0.47	0	17,19,21	0.86	1 (5%)
2	NAG	A	1006	1	14,14,15	0.87	1 (7%)	17,19,21	0.75	0
2	NAG	A	1008	1	14,14,15	0.73	1 (7%)	17,19,21	0.72	0
3	SO4	B	2003	-	4,4,4	0.37	0	6,6,6	0.13	0
2	NAG	B	1012	1	14,14,15	0.70	0	17,19,21	0.80	1 (5%)
2	NAG	A	1003	1	14,14,15	0.52	0	17,19,21	1.01	1 (5%)
2	NAG	B	1016	1	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
2	NAG	A	1002	1	14,14,15	0.45	0	17,19,21	0.95	1 (5%)
2	NAG	B	1009	1	14,14,15	0.54	0	17,19,21	1.00	1 (5%)
2	NAG	A	1007	1	14,14,15	0.86	1 (7%)	17,19,21	0.66	0
3	SO4	A	2001	-	4,4,4	0.37	0	6,6,6	0.08	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
2	NAG	B	1013	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1010	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	1014	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1015	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1011	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1016	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1006	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1012	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1007	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	1004	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1007	NAG	C1-C2	2.46	1.55	1.52
2	B	1010	NAG	C1-C2	2.40	1.55	1.52
2	A	1008	NAG	C1-C2	2.33	1.55	1.52
2	A	1001	NAG	C1-C2	2.25	1.55	1.52
2	A	1006	NAG	C1-C2	2.04	1.55	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1009	NAG	C1-C2-N2	-3.36	105.13	110.43
2	B	1013	NAG	C2-N2-C7	-2.99	118.89	122.90
2	A	1002	NAG	C2-N2-C7	-2.95	118.95	122.90
2	A	1003	NAG	C2-N2-C7	-2.75	119.22	122.90
2	A	1001	NAG	C2-N2-C7	-2.63	119.37	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1004	NAG	C1
2	A	1006	NAG	C1
2	A	1007	NAG	C1
2	B	1010	NAG	C1

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1004	NAG	C8-C7-N2-C2
2	A	1004	NAG	O7-C7-N2-C2
2	A	1005	NAG	C8-C7-N2-C2
2	A	1005	NAG	O7-C7-N2-C2
2	A	1007	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1014	NAG	2	0
2	A	1001	NAG	3	0
2	B	1011	NAG	1	0
2	B	1009	NAG	1	0
2	A	1007	NAG	5	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 [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	611/617 (99%)	0.13	20 (3%)	49 46	8, 26, 40, 53	0
1	B	615/617 (99%)	0.18	29 (4%)	37 34	11, 26, 43, 72	0
All	All	1226/1234 (99%)	0.15	49 (3%)	43 40	8, 26, 41, 72	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	614	THR	6.1
1	B	0	ARG	5.0
1	B	295	ILE	4.1
1	B	304	ILE	4.0
1	B	601	ASN	3.9

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(\AA^2)	Q<0.9
2	NAG	A	1007	14/15	0.39	0.25	61,66,67,68	0
2	NAG	A	1004	14/15	0.72	0.17	48,56,59,61	0
2	NAG	A	1006	14/15	0.74	0.15	44,48,52,52	0
2	NAG	A	1005	14/15	0.75	0.14	53,59,68,68	0
2	NAG	B	1011	14/15	0.76	0.13	35,48,55,58	0
2	NAG	B	1014	14/15	0.76	0.16	46,54,61,64	0
2	NAG	B	1013	14/15	0.79	0.13	33,35,42,44	0
2	NAG	B	1015	14/15	0.83	0.13	24,37,50,52	0
2	NAG	A	1001	14/15	0.84	0.15	22,28,46,54	0
2	NAG	B	1010	14/15	0.85	0.18	26,36,43,54	0
2	NAG	A	1002	14/15	0.87	0.14	18,23,25,31	0
2	NAG	B	1012	14/15	0.88	0.10	24,41,49,53	0
2	NAG	A	1008	14/15	0.88	0.12	34,44,55,56	0
2	NAG	A	1003	14/15	0.89	0.09	29,34,46,49	0
3	SO4	B	2002	5/5	0.89	0.14	73,74,76,76	0
2	NAG	B	1009	14/15	0.90	0.12	16,25,39,45	0
3	SO4	B	2003	5/5	0.90	0.18	57,58,70,71	0
2	NAG	B	1016	14/15	0.91	0.09	37,42,45,47	0
3	SO4	A	2001	5/5	0.93	0.10	57,58,66,71	0
4	YT3	B	3001	1/1	0.94	0.06	38,38,38,38	1

6.5 Other polymers [i](#)

There are no such residues in this entry.