



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2016 – 09:49 AM EDT

PDB ID : 5IXT
Title : The crystal structure of the Arabidopsis receptor kinase HAESA LRR ectdo-
main in complex with a N-terminal extended IDA peptide hormone ligand.
Authors : Santiago, J.; Hothorn, M.
Deposited on : 2016-03-23
Resolution : 1.94 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

<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027939

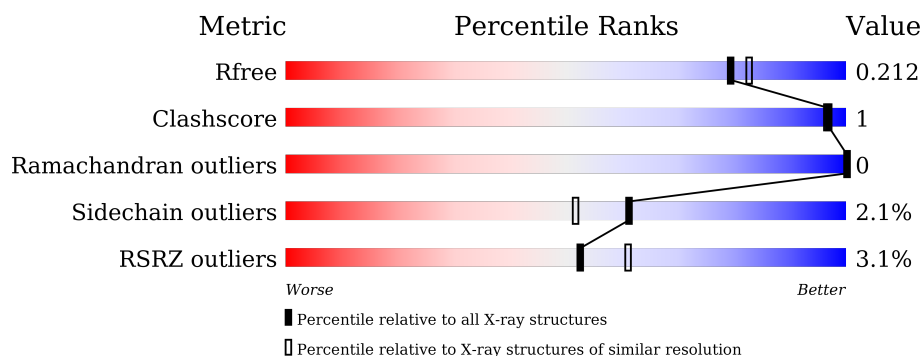
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	616	<div> <div>3%</div> <div>92%</div> <div>• •</div> </div>
2	B	17	<div> <div>6%</div> <div>71%</div> <div>29%</div> </div>

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
3	NAG	A	711	-	-	-	X
3	NAG	A	712	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4860 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-like protein kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	7	0
			4545	2887	759	885	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP P47735
A	16	SER	-	expression tag	UNP P47735
A	17	SER	-	expression tag	UNP P47735
A	18	MET	-	expression tag	UNP P47735
A	19	GLY	-	expression tag	UNP P47735
A	621	LEU	-	expression tag	UNP P47735
A	622	GLU	-	expression tag	UNP P47735
A	623	GLY	-	expression tag	UNP P47735
A	624	SER	-	expression tag	UNP P47735
A	625	GLU	-	expression tag	UNP P47735
A	626	ASN	-	expression tag	UNP P47735
A	627	LEU	-	expression tag	UNP P47735
A	628	TYR	-	expression tag	UNP P47735
A	629	PHE	-	expression tag	UNP P47735
A	630	GLN	-	expression tag	UNP P47735

- Molecule 2 is a protein called Protein IDA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			93	57	19	17			

There is a discrepancy between the modelled and reference sequences:

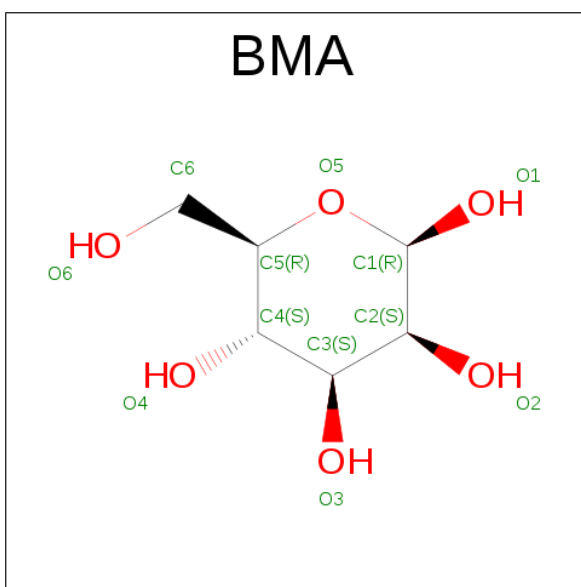
Chain	Residue	Modelled	Actual	Comment	Reference
B	53	TYR	LEU	conflict	UNP Q8LAD7

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



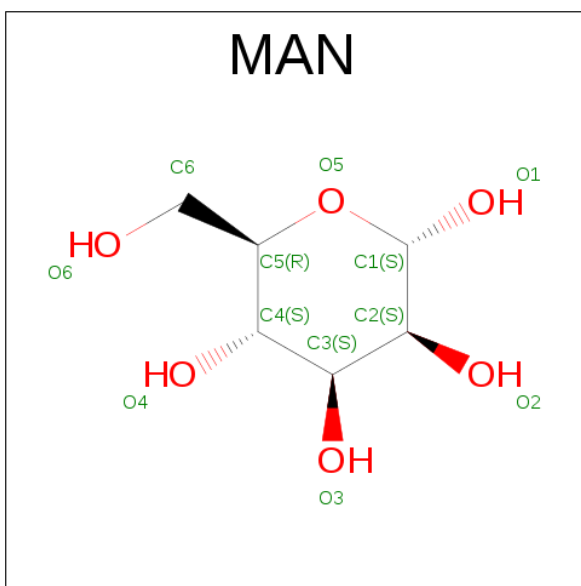
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

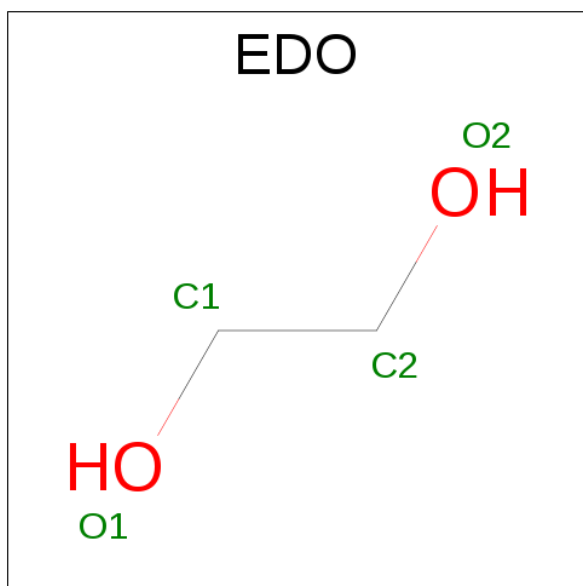


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

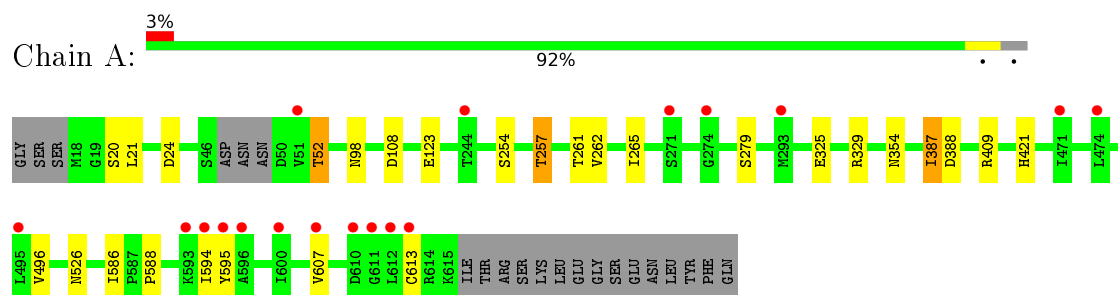
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	39	Total	O	0	0
			39	39		
8	B	1	Total	O	0	0
			1	1		

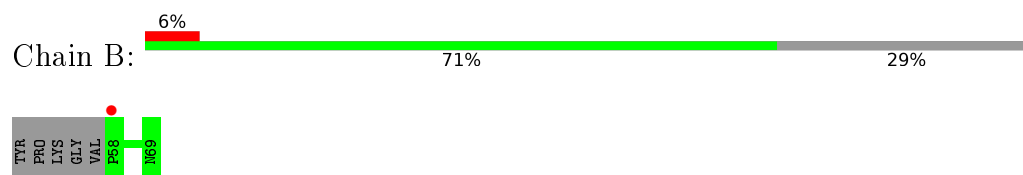
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Molecule 1: Receptor-like protein kinase 5



- Molecule 2: Protein IDA



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.92Å 148.92Å 58.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	128.97 – 1.94 48.75 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.4 (128.97-1.94) 99.4 (48.75-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.208 0.187 , 0.212	Depositor DCC
R_{free} test set	2644 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4860	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: MG, BMA, NAG, EDO, HYP, MAN

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	0.72	0/4652	0.83	3/6325 (0.0%)
2	B	0.69	0/87	0.62	0/114
All	All	0.72	0/4739	0.82	3/6439 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	387	ILE	CB-CA-C	-6.01	99.57	111.60
1	A	329	ARG	NE-CZ-NH1	5.94	123.27	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	4545	0	4558	12	1
2	B	93	0	92	0	0
3	A	154	0	138	0	0
4	A	11	0	9	0	0
5	A	11	0	10	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	6	0	0
8	A	39	0	0	1	0
8	B	1	0	0	0	0
All	All	4860	0	4813	12	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 1.

The worst 5 of 12 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:387:ILE:HD11	1:A:409:ARG:HB3	1.39	0.99
1:A:257:THR:HG21	1:A:279:SER:OG	1.91	0.71
1:A:254:SER:O	1:A:257:THR:HB	1.99	0.63
1:A:387:ILE:CD1	1:A:409:ARG:HB3	2.25	0.59
1:A:387:ILE:HD11	1:A:409:ARG:CB	2.25	0.58

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:526:ASN:OD1	1:A:526:ASN:ND2[6_555]	2.16	0.04

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	598/616 (97%)	561 (94%)	37 (6%)	0	100	100
2	B	9/17 (53%)	8 (89%)	1 (11%)	0	100	100
All	All	607/633 (96%)	569 (94%)	38 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	528/552 (96%)	517 (98%)	11 (2%)	61	52
2	B	10/14 (71%)	10 (100%)	0	100	100
All	All	538/566 (95%)	527 (98%)	11 (2%)	61	53

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	GLU
1	A	354	ASN
1	A	496	VAL
1	A	257	THR
1	A	421	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	ASN
1	A	397	ASN
1	A	558	GLN
2	B	69	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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	HYP	B	64	2	6,8,9	0.41	0	5,10,12	2.01	2 (40%)

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	HYP	B	64	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	64	HYP	O-C-CA	-2.91	117.75	125.69
2	B	64	HYP	CB-CG-CD	2.51	106.15	103.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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
3	NAG	A	701	1,3	14,14,15	0.31	0	15,19,21	0.79	0
3	NAG	A	702	3	14,14,15	0.40	0	15,19,21	0.59	0
3	NAG	A	703	1	14,14,15	0.58	0	15,19,21	1.72	3 (20%)
3	NAG	A	704	1,3	14,14,15	0.52	0	15,19,21	1.26	1 (6%)
3	NAG	A	705	3	14,14,15	0.71	0	15,19,21	2.01	5 (33%)
3	NAG	A	706	1	14,14,15	0.74	0	15,19,21	1.80	3 (20%)
3	NAG	A	707	1,3	14,14,15	0.30	0	15,19,21	1.09	1 (6%)
3	NAG	A	708	3,4	14,14,15	0.75	0	15,19,21	1.01	1 (6%)
4	BMA	A	709	3,5	11,11,12	0.75	0	15,15,17	1.38	2 (13%)
5	MAN	A	710	4	11,11,12	0.70	0	15,15,17	1.40	2 (13%)
3	NAG	A	711	1	14,14,15	0.64	0	15,19,21	1.59	3 (20%)
3	NAG	A	712	1,3	14,14,15	0.35	0	15,19,21	0.97	1 (6%)
3	NAG	A	713	3	14,14,15	0.35	0	15,19,21	1.25	1 (6%)
7	EDO	B	2000	-	3,3,3	0.68	0	2,2,2	0.35	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
3	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	704	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	705	3	-	0/6/23/26	0/1/1/1
3	NAG	A	706	1	-	0/6/23/26	0/1/1/1
3	NAG	A	707	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	708	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	709	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	710	4	-	0/2/19/22	1/1/1/1
3	NAG	A	711	1	-	0/6/23/26	0/1/1/1
3	NAG	A	712	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	713	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	2000	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	705	NAG	O7-C7-C8	-2.34	117.77	122.07
3	A	703	NAG	C3-C4-C5	-2.10	106.49	110.23
3	A	705	NAG	C4-C3-C2	2.00	114.44	111.34
3	A	711	NAG	O5-C5-C6	2.05	111.73	107.34
3	A	706	NAG	C1-O5-C5	2.05	115.16	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	710	MAN	C1-C2-C3-C4-C5-O5

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	595/616 (96%)	0.34	18 (3%) 54 62	65, 78, 104, 159	0
2	B	11/17 (64%)	0.21	1 (9%) 11 17	75, 84, 106, 128	0
All	All	606/633 (95%)	0.34	19 (3%) 52 61	65, 78, 104, 159	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	ASP	7.4
1	A	612	LEU	6.2
1	A	611	GLY	5.5
1	A	613	CYS	3.8
1	A	495	LEU	3.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	HYP	B	64	8/9	0.95	0.09	-	78,82,87,88	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

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
3	NAG	A	711	14/15	0.85	0.33	4.08	91,97,104,113	0
3	NAG	A	712	14/15	0.94	0.17	2.11	86,96,101,101	0
6	MG	A	715	1/1	0.97	0.10	-0.18	71,71,71,71	0
3	NAG	A	701	14/15	0.94	0.10	-0.47	82,94,103,104	0
3	NAG	A	707	14/15	0.96	0.14	-2.23	85,96,109,116	0
5	MAN	A	710	11/12	0.39	0.36	-	118,147,152,153	0
3	NAG	A	702	14/15	0.88	0.25	-	95,107,119,120	0
3	NAG	A	703	14/15	0.89	0.09	-	87,93,102,114	0
3	NAG	A	705	14/15	0.78	0.22	-	112,126,134,135	0
3	NAG	A	704	14/15	0.95	0.09	-	83,86,93,102	0
4	BMA	A	709	11/12	0.70	0.18	-	129,143,148,149	0
3	NAG	A	713	14/15	0.90	0.34	-	101,104,112,115	0
7	EDO	B	2000	4/4	0.59	0.28	-	89,92,94,94	0
6	MG	A	714	1/1	0.88	0.09	-	83,83,83,83	0
3	NAG	A	706	14/15	0.87	0.43	-	92,108,119,123	0
3	NAG	A	708	14/15	0.84	0.19	-	113,129,136,146	0

6.5 Other polymers

There are no such residues in this entry.