



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 05:23 PM EDT

PDB ID : 2PE4  
Title : Structure of Human Hyaluronidase 1, a Hyaluronan Hydrolyzing Enzyme Involved in Tumor Growth and Angiogenesis  
Authors : Chao, K.L.; Herzberg, O.  
Deposited on : unknown  
Resolution : 2.00 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](mailto: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.

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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 : rb-20030345  
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) : rb-20030345

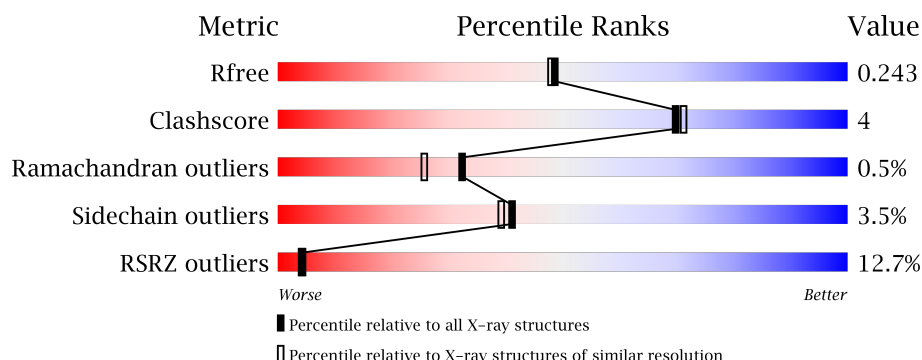
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 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	424	<div> <div>13%</div> <div>85%</div> <div>12%</div> <div>.</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
5	ACT	A	901	-	-	-	X
5	ACT	A	904	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	905	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3753 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 Hyaluronidase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3284	2102	575	590	17			

There are 10 discrepancies between the modelled and reference sequences:

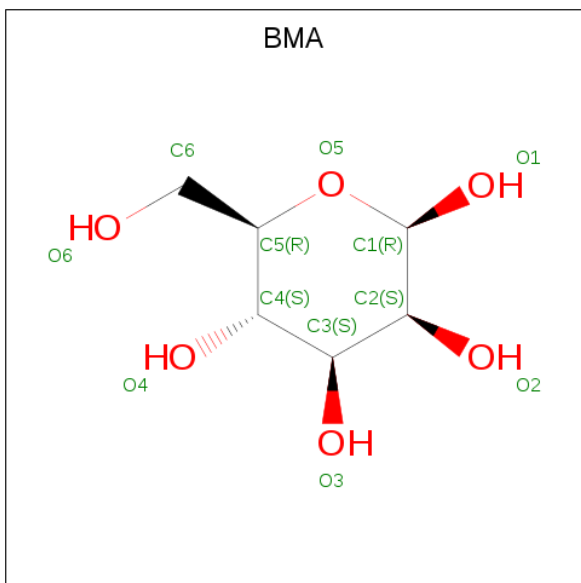
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ARG	-	CLONING ARTIFACT	UNP Q12794
A	21	SER	-	CLONING ARTIFACT	UNP Q12794
A	436	THR	-	CLONING ARTIFACT	UNP Q12794
A	437	GLY	-	CLONING ARTIFACT	UNP Q12794
A	438	HIS	-	EXPRESSION TAG	UNP Q12794
A	439	HIS	-	EXPRESSION TAG	UNP Q12794
A	440	HIS	-	EXPRESSION TAG	UNP Q12794
A	441	HIS	-	EXPRESSION TAG	UNP Q12794
A	442	HIS	-	EXPRESSION TAG	UNP Q12794
A	443	HIS	-	EXPRESSION TAG	UNP Q12794

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



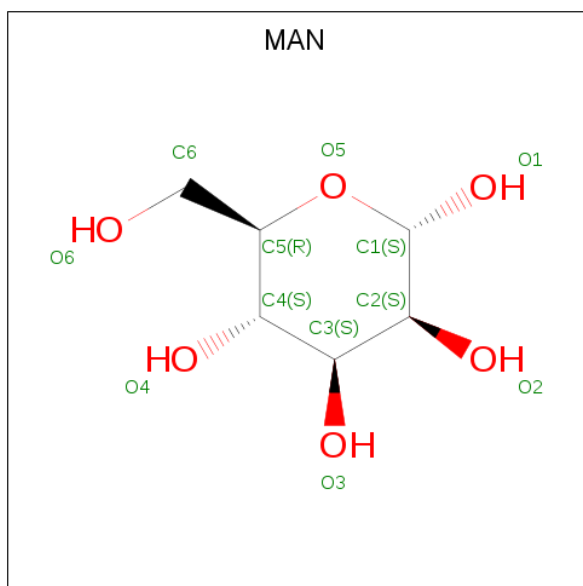
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



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

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



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 7 is water.

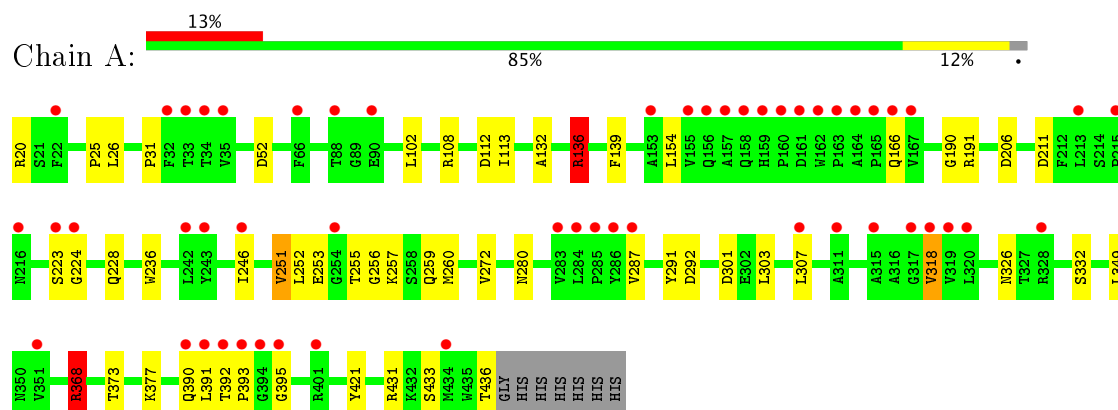
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	335	Total	O	0	0
			335	335		



### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: Hyaluronidase-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.05Å 92.05Å 143.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.65 – 2.00 30.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.65-2.00) 99.3 (30.65-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.190 , 0.230 0.217 , 0.243	Depositor DCC
$R_{free}$ test set	2420 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, GOL, BMA, NAG, ACT

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	0.89	1/3390 (0.0%)	0.99	16/4635 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	ARG	CD-NE	-5.76	1.36	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ARG	NE-CZ-NH2	-22.83	108.88	120.30
1	A	368	ARG	NE-CZ-NH1	20.14	130.37	120.30
1	A	368	ARG	CD-NE-CZ	8.47	135.46	123.60
1	A	191	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	318	VAL	CG1-CB-CG2	7.39	122.73	110.90
1	A	211	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	368	ARG	CG-CD-NE	-5.92	99.36	111.80
1	A	52	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	206	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	301	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	A	136	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	251	VAL	CB-CA-C	-5.28	101.37	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	191	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	292	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	136	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	368	ARG	Sidechain

## 5.2 Too-close contacts

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	3284	0	3145	28	1
2	A	56	0	48	1	0
3	A	11	0	8	0	0
4	A	33	0	29	0	0
5	A	28	0	21	0	0
6	A	6	0	8	3	0
7	A	335	0	0	6	0
All	All	3753	0	3259	28	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 4.

All (28) 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:252:LEU:O	1:A:255:THR:HG22	1.91	0.71
1:A:154:LEU:HD13	2:A:599:NAG:H82	1.79	0.65
1:A:20:ARG:N	6:A:601:GOL:HO1	2.00	0.59
1:A:260:MET:HG3	7:A:1137:HOH:O	2.05	0.57
1:A:259:GLN:HG2	7:A:1216:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:NZ	7:A:1102:HOH:O	2.38	0.56
1:A:31:PRO:O	1:A:368:ARG:HD3	2.07	0.54
1:A:246:ILE:HD11	1:A:287:VAL:HG12	1.89	0.54
1:A:280:ASN:HD22	6:A:601:GOL:H11	1.76	0.51
1:A:136:ARG:HD3	1:A:228:GLN:OE1	2.12	0.50
1:A:390:GLN:NE2	7:A:1112:HOH:O	2.45	0.49
1:A:224:GLY:O	1:A:228:GLN:HG2	2.14	0.48
1:A:253:GLU:HA	1:A:291:TYR:CZ	2.49	0.46
1:A:255:THR:HG23	1:A:257:LYS:H	1.82	0.44
1:A:20:ARG:N	6:A:601:GOL:C1	2.81	0.44
1:A:25:PRO:HD3	1:A:421:TYR:CE1	2.53	0.43
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.87	0.42
1:A:431:ARG:NH1	7:A:1142:HOH:O	2.39	0.42
1:A:326:ASN:O	1:A:332:SER:HB3	2.19	0.42
1:A:260:MET:HE2	7:A:950:HOH:O	2.19	0.41
1:A:393:PRO:C	1:A:395:GLY:H	2.23	0.41
1:A:113:ILE:HD13	1:A:190:GLY:HA2	2.01	0.41
1:A:255:THR:OG1	1:A:256:GLY:N	2.54	0.41
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.89	0.41
1:A:139:PHE:CZ	1:A:228:GLN:HB2	2.55	0.41
1:A:287:VAL:HG21	1:A:307:LEU:HD11	2.02	0.41
1:A:246:ILE:CG1	1:A:287:VAL:HG12	2.51	0.40
1:A:236:TRP:CD1	1:A:272:VAL:HB	2.56	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:390:GLN:OE1	1:A:393:PRO:CB[4_645]	1.47	0.73

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	415/424 (98%)	392 (94%)	21 (5%)	2 (0%)	32 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	132	ALA

### 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	341/347 (98%)	329 (96%)	12 (4%)	41 39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	108	ARG
1	A	136	ARG
1	A	166	GLN
1	A	251	VAL
1	A	303	LEU
1	A	318	VAL
1	A	349	LEU
1	A	373	THR
1	A	392	THR
1	A	433	SER
1	A	436	THR

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	280	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are 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	NAG	A	550	1,2	14,14,15	1.20	1 (7%)	15,19,21	2.95	4 (26%)
2	NAG	A	551	3,2	14,14,15	0.61	0	15,19,21	0.98	0
3	BMA	A	552	2,4	11,11,12	0.65	0	13,15,17	1.66	4 (30%)
4	MAN	A	553	3,4	11,11,12	0.72	0	13,15,17	1.75	2 (15%)
4	MAN	A	554	4	11,11,12	0.66	0	13,15,17	2.25	1 (7%)
4	MAN	A	555	3	11,11,12	0.79	0	13,15,17	2.29	3 (23%)
2	NAG	A	599	1,2	14,14,15	0.60	0	15,19,21	1.51	4 (26%)
2	NAG	A	600	2	14,14,15	0.70	0	15,19,21	1.29	2 (13%)
6	GOL	A	601	-	5,5,5	0.34	0	5,5,5	0.45	0
5	ACT	A	901	-	1,3,3	1.27	0	0,3,3	0.00	-
5	ACT	A	902	-	1,3,3	1.95	0	0,3,3	0.00	-
5	ACT	A	903	-	1,3,3	0.76	0	0,3,3	0.00	-
5	ACT	A	904	-	1,3,3	1.37	0	0,3,3	0.00	-
5	ACT	A	905	-	1,3,3	0.44	0	0,3,3	0.00	-
5	ACT	A	906	-	1,3,3	1.16	0	0,3,3	0.00	-
5	ACT	A	907	-	1,3,3	2.62	1 (100%)	0,3,3	0.00	-

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	550	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	551	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	552	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	553	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	554	4	-	0/2/19/22	0/1/1/1
4	MAN	A	555	3	-	0/2/19/22	0/1/1/1
2	NAG	A	599	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	600	2	-	0/6/23/26	0/1/1/1
6	GOL	A	601	-	-	0/4/4/4	0/0/0/0
5	ACT	A	901	-	-	0/0/0/0	0/0/0/0
5	ACT	A	902	-	-	0/0/0/0	0/0/0/0
5	ACT	A	903	-	-	0/0/0/0	0/0/0/0
5	ACT	A	904	-	-	0/0/0/0	0/0/0/0
5	ACT	A	905	-	-	0/0/0/0	0/0/0/0
5	ACT	A	906	-	-	0/0/0/0	0/0/0/0
5	ACT	A	907	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	NAG	O5-C1	-2.41	1.39	1.43
5	A	907	ACT	CH3-C	2.62	1.52	1.48

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	555	MAN	C1-C2-C3	-5.48	102.70	109.65
2	A	550	NAG	C6-C5-C4	-4.94	101.44	113.00
2	A	550	NAG	O5-C1-C2	-3.96	105.97	111.47
3	A	552	BMA	C3-C4-C5	-3.66	103.76	110.22
2	A	599	NAG	O7-C7-C8	-2.87	116.83	122.06
2	A	599	NAG	O5-C1-C2	-2.65	107.79	111.47
3	A	552	BMA	O6-C6-C5	-2.16	104.07	111.34
2	A	600	NAG	O4-C4-C5	2.05	114.45	109.28
2	A	599	NAG	C1-O5-C5	2.06	115.01	112.17
2	A	599	NAG	C2-N2-C7	2.23	126.20	122.94
3	A	552	BMA	O3-C3-C2	2.33	114.27	110.02
3	A	552	BMA	C1-O5-C5	2.62	115.77	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	NAG	C1-O5-C5	2.87	116.13	112.17
4	A	553	MAN	O2-C2-C3	3.10	116.26	110.17
2	A	550	NAG	C2-N2-C7	3.60	128.19	122.94
4	A	555	MAN	O3-C3-C4	3.81	118.64	110.36
4	A	555	MAN	O2-C2-C3	3.93	117.89	110.17
4	A	553	MAN	C1-O5-C5	4.48	118.34	112.17
4	A	554	MAN	C1-O5-C5	7.57	122.61	112.17
2	A	550	NAG	C1-O5-C5	7.71	122.79	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	599	NAG	1	0
6	A	601	GOL	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	417/424 (98%)	0.47	53 (12%) 4 4	20, 31, 58, 70	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ALA	6.5
1	A	394	GLY	6.2
1	A	157	ALA	5.6
1	A	161	ASP	5.6
1	A	162	TRP	5.4
1	A	393	PRO	5.3
1	A	66	PHE	5.0
1	A	167	VAL	4.9
1	A	213	LEU	4.7
1	A	318	VAL	4.5
1	A	390	GLN	4.1
1	A	155	VAL	4.1
1	A	319	VAL	4.0
1	A	215	PRO	3.9
1	A	307	LEU	3.7
1	A	391	LEU	3.6
1	A	284	LEU	3.6
1	A	242	LEU	3.5
1	A	216	ASN	3.5
1	A	153	ALA	3.4
1	A	285	PRO	3.4
1	A	287	VAL	3.4
1	A	165	PRO	3.4
1	A	395	GLY	3.2
1	A	22	PHE	3.2
1	A	286	TYR	3.1
1	A	401	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	158	GLN	3.0
1	A	163	PRO	2.8
1	A	392	THR	2.8
1	A	159	HIS	2.8
1	A	315	ALA	2.7
1	A	33	THR	2.7
1	A	328	ARG	2.7
1	A	160	PRO	2.7
1	A	320	LEU	2.7
1	A	243	TYR	2.6
1	A	224	GLY	2.6
1	A	90	GLU	2.6
1	A	32	PHE	2.5
1	A	35	VAL	2.5
1	A	88	THR	2.4
1	A	351	VAL	2.4
1	A	317	GLY	2.4
1	A	223	SER	2.3
1	A	434	MET	2.3
1	A	34	THR	2.2
1	A	166	GLN	2.2
1	A	156	GLN	2.2
1	A	254	GLY	2.1
1	A	283	VAL	2.1
1	A	246	ILE	2.1
1	A	311	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	ACT	A	901	4/4	0.74	0.27	3.75	69,70,70,70	0
5	ACT	A	905	4/4	0.90	0.34	3.74	54,56,56,57	0
5	ACT	A	904	4/4	0.84	0.26	3.22	64,64,64,66	0
5	ACT	A	902	4/4	0.78	0.23	1.36	64,64,65,66	0
5	ACT	A	906	4/4	0.94	0.19	1.28	65,65,65,66	0
5	ACT	A	903	4/4	0.87	0.16	1.13	61,62,63,63	0
6	GOL	A	601	6/6	0.71	0.13	-0.10	69,72,73,73	0
2	NAG	A	550	14/15	0.95	0.11	-0.38	31,37,40,43	0
2	NAG	A	599	14/15	0.88	0.11	-0.94	53,59,64,69	0
2	NAG	A	600	14/15	0.84	0.28	-	74,78,81,81	0
4	MAN	A	554	11/12	0.87	0.17	-	72,74,75,77	0
2	NAG	A	551	14/15	0.92	0.09	-	39,45,52,53	0
3	BMA	A	552	11/12	0.93	0.09	-	51,55,60,69	0
4	MAN	A	555	11/12	0.84	0.21	-	79,84,87,87	0
4	MAN	A	553	11/12	0.80	0.15	-	64,68,71,73	0
5	ACT	A	907	4/4	0.83	0.15	-	70,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.