



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:10 AM GMT

PDB ID : 2CML  
Title : STRUCTURE OF NEURAMINIDASE FROM ENGLISH DUCK SUBTYPE  
N6 COMPLEXED WITH 30 MM ZANAMIVIR, CRYSTAL SOAKED FOR  
3 HOURS AT 291 K.  
Authors : Rudino-Pinera, E.; Tunnah, P.; Lukacik, P.; Crennell, S.J.; Webster, R.G.;  
Laver, W.G.; Garman, E.F.  
Deposited on : 2006-05-10  
Resolution : 2.15 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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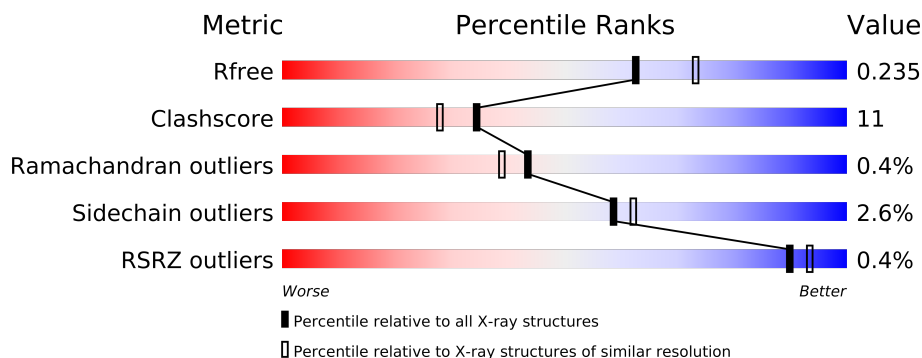
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.15 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))
$R_{free}$	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	389	
1	B	389	
1	C	389	
1	D	389	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZMR	A	1478	-	X
2	ZMR	B	2478	-	X
2	ZMR	C	3478	-	X
2	ZMR	D	4478	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	1482	-	X
4	NAG	B	2480	-	X
4	NAG	C	3480	-	X
4	NAG	C	3486	-	X
4	NAG	C	3487	-	X
4	NAG	C	3489	-	X
4	NAG	D	4482	-	X
4	NAG	D	4483	-	X
4	NAG	D	4484	-	X
4	NAG	D	4485	-	X
5	MAN	A	1485	-	X
5	MAN	A	1486	-	X
5	MAN	A	1487	-	X
5	MAN	B	2484	-	X
5	MAN	B	2485	-	X
5	MAN	B	2486	-	X
5	MAN	C	3483	-	X
5	MAN	C	3484	-	X
5	MAN	C	3485	-	X
5	MAN	C	3490	-	X
5	MAN	D	4480	-	X
5	MAN	D	4481	-	X
6	BMA	A	1709	-	X
6	BMA	C	1709	-	X
6	BMA	C	3493	-	X
6	BMA	D	4486	-	X

## 2 Entry composition i

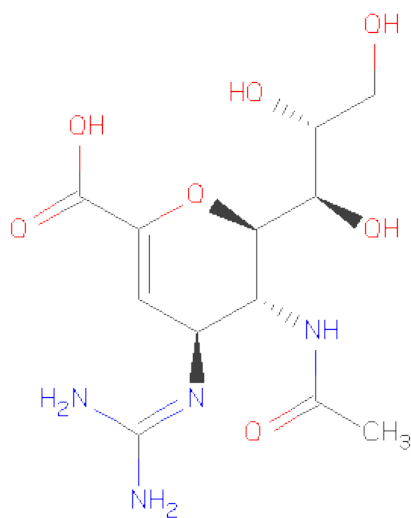
There are 7 unique types of molecules in this entry. The entry contains 13060 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	B	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	C	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

- Molecule 2 is ZANAMIVIR (three-letter code: ZMR) (formula: C<sub>12</sub>H<sub>20</sub>N<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	12	4	7		
2	A	1	Total	C	N	O	0	0
			23	12	4	7		

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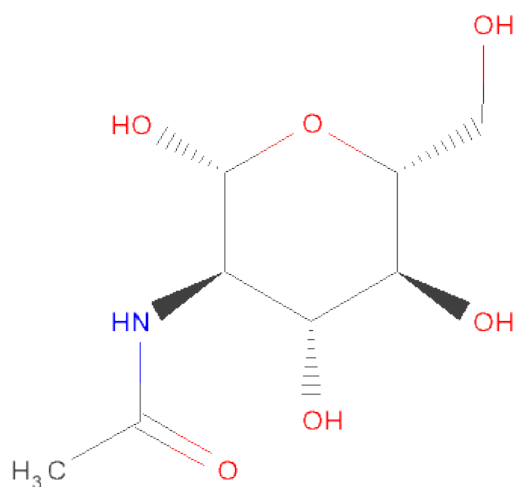
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			23	12	4	7		
2	B	1	Total	C	N	O	0	0
			23	12	4	7		
2	C	1	Total	C	N	O	0	0
			23	12	4	7		
2	C	1	Total	C	N	O	0	0
			23	12	4	7		
2	D	1	Total	C	N	O	0	0
			23	12	4	7		
2	D	1	Total	C	N	O	0	0
			23	12	4	7		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

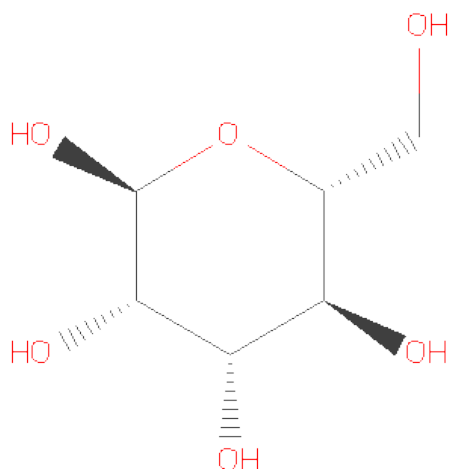
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



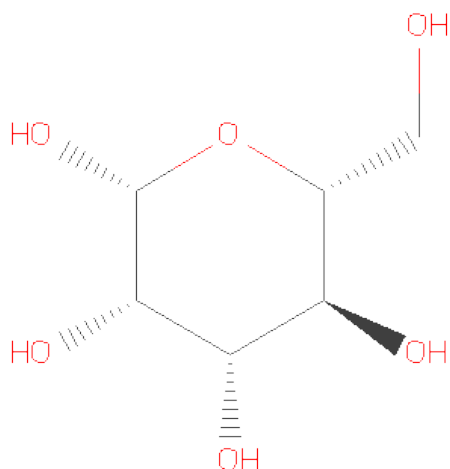
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 6 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	103	Total	O	0	0
			103	103		
7	B	109	Total	O	0	0
			109	109		
7	C	96	Total	O	0	0
			96	96		
7	D	78	Total	O	0	0
			78	78		



### 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 ( $RSRZ > 2$ ). 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.

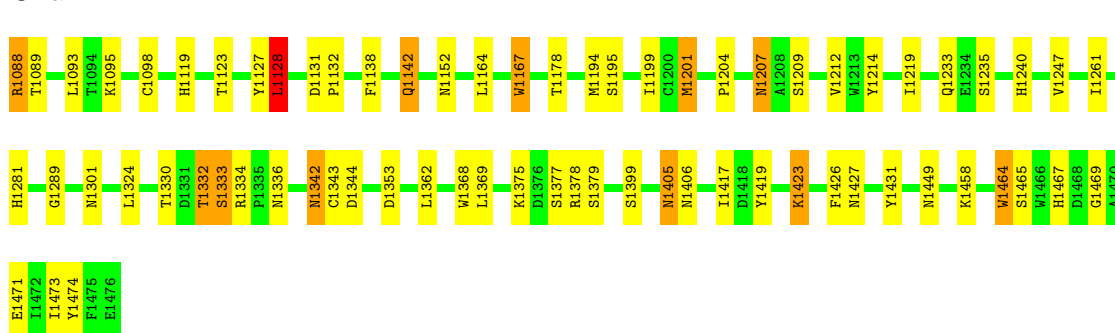
#### • Molecule 1: NEURAMINIDASE

Chain A:



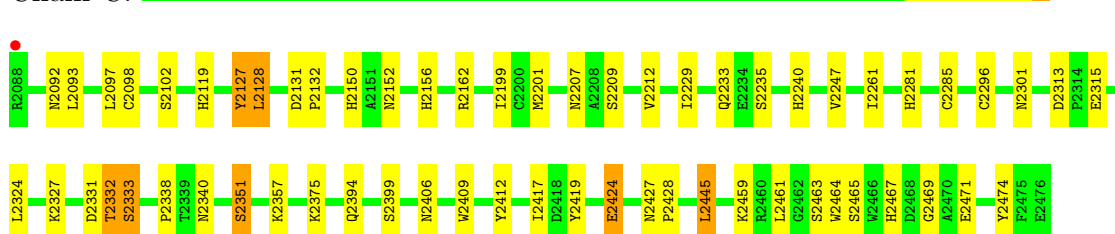
#### • Molecule 1: NEURAMINIDASE

Chain B:



#### • Molecule 1: NEURAMINIDASE

Chain C:



#### • Molecule 1: NEURAMINIDASE

Chain D:

R3088	T3332
N3092	S3333
L3093	N3342
D3117	C3343
A3118	D3344
H3119	S3351
I3120	P3352
L3121	D3353
R3124	E3365
Y3127	R3378
L3128	N3383
D3131	V3386
P3132	P3387
Q3133	N3388
T3145	A3389
R3149	E3390
H3150	N3400
A3151	E3424
N3152	L3445
F3161	N3449
P3175	V3452
P3175	R3460
S3187	W3464
I3199	S3465
C3200	W3466
M3201	A3470
P3204	E3471
N3207	I3472
A3208	I3473
S3209	E3476
Q3233	
E3234	
S3235	
H3240	
V3247	
H3281	
G3289	
K3295	
N3301	
K3322	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.24Å 73.69Å 106.68Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	30.70 – 2.15 30.62 – 2.15	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.70-2.15) 90.3 (30.62-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.180 , 0.232 0.186 , 0.235	Depositor DCC
$R_{free}$ test set	4038 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 16.2	EDS
Estimated twinning fraction	0.017 for l,k,-h 0.025 for h,-k,-l 0.021 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 80655 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMR, CA, BMA, NAG, 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	1.02	1/3083 (0.0%)	0.92	2/4185 (0.0%)
1	B	1.00	2/3083 (0.1%)	0.92	5/4185 (0.1%)
1	C	1.02	1/3083 (0.0%)	0.91	5/4185 (0.1%)
1	D	1.04	2/3084 (0.1%)	0.96	4/4185 (0.1%)
All	All	1.02	6/12333 (0.0%)	0.93	16/16740 (0.1%)

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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	GLU	CG-CD	7.61	1.63	1.51
1	B	1368	TRP	CB-CG	5.55	1.60	1.50
1	B	1167	TRP	CB-CG	5.51	1.60	1.50
1	D	3452	VAL	CB-CG1	5.44	1.64	1.52
1	D	3365	GLU	CG-CD	5.20	1.59	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3128	LEU	CA-CB-CG	8.13	133.99	115.30
1	C	2128	LEU	CA-CB-CG	7.87	133.41	115.30
1	B	1378	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	B	1128	LEU	CA-CB-CG	7.21	131.87	115.30
1	B	1378	ARG	NE-CZ-NH2	-6.76	116.92	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	THR	Peptide
1	B	1332	THR	Peptide
1	C	2332	THR	Peptide
1	D	3332	THR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3008	0	2888	56	0
1	B	3008	0	2888	60	0
1	C	3008	0	2888	63	0
1	D	3009	0	2888	55	0
2	A	46	0	30	2	0
2	B	46	0	30	2	0
2	C	46	0	30	3	0
2	D	46	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	56	0	44	11	0
4	B	56	0	44	12	0
4	C	98	0	77	24	0
4	D	56	0	44	16	0
5	A	33	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	33	0	30	7	0
5	C	55	0	50	11	0
5	D	22	0	20	1	0
6	A	11	0	10	3	0
6	C	22	0	19	6	0
6	D	11	0	10	3	0
7	A	103	0	0	0	0
7	B	109	0	0	1	0
7	C	96	0	0	2	0
7	D	78	0	0	1	0
All	All	13060	0	12050	252	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 252 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:3152:ASN:HD21	4:D:4483:NAG:C1	1.01	1.60
1:C:2152:ASN:HD21	4:C:3487:NAG:C1	1.15	1.59
1:A:152:ASN:HD21	4:A:1482:NAG:C1	0.98	1.59
1:A:207:ASN:HD21	4:C:3480:NAG:C1	0.97	1.57
1:A:92:ASN:HD21	4:A:1480:NAG:C1	1.10	1.56

There are no symmetry-related clashes.

## 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	387/389 (100%)	365 (94%)	20 (5%)	2 (0%)	38	31
1	B	387/389 (100%)	368 (95%)	18 (5%)	1 (0%)	50	47
1	C	387/389 (100%)	370 (96%)	16 (4%)	1 (0%)	50	47
1	D	387/389 (100%)	373 (96%)	12 (3%)	2 (0%)	38	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1548/1556 (100%)	1476 (95%)	66 (4%)	6 (0%)	43	39

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	C	2333	SER
1	D	3333	SER
1	A	207	ASN
1	D	3207	ASN

### 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	331/331 (100%)	324 (98%)	7 (2%)	66	72
1	B	331/331 (100%)	318 (96%)	13 (4%)	43	43
1	C	331/331 (100%)	324 (98%)	7 (2%)	66	72
1	D	331/331 (100%)	323 (98%)	8 (2%)	61	67
All	All	1324/1324 (100%)	1289 (97%)	35 (3%)	59	62

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1405	ASN
1	B	1473	ILE
1	D	3445	LEU
1	B	1423	LYS
1	B	1458	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1406	ASN
1	C	2119	HIS

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Mol	Chain	Res	Type
1	D	3342	ASN
1	B	1408	ASN
1	B	1449	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 48 ligands modelled in this entry, 4 are monoatomic - leaving 44 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	ZMR	A	1477	-	23,23,23	2.89	4 (17%)	32,32,32	2.75	15 (46%)
2	ZMR	A	1478	-	23,23,23	2.80	4 (17%)	32,32,32	3.08	14 (43%)
4	NAG	A	1480	1,4	12,14,15	2.60	1 (8%)	15,19,21	2.70	8 (53%)
4	NAG	A	1481	4	12,14,15	2.34	1 (8%)	15,19,21	2.48	5 (33%)
4	NAG	A	1482	1	12,14,15	2.59	1 (8%)	15,19,21	2.94	6 (40%)
4	NAG	A	1483	-	12,14,15	2.28	1 (8%)	15,19,21	2.43	6 (40%)
5	MAN	A	1485	5	10,11,12	0.64	0	11,15,17	1.80	4 (36%)
5	MAN	A	1486	5	10,11,12	0.68	0	11,15,17	1.49	3 (27%)
5	MAN	A	1487	5	10,11,12	0.67	0	11,15,17	1.63	1 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	A	1709	-	10,11,12	0.87	0	11,15,17	2.14	5 (45%)
2	ZMR	B	2477	-	23,23,23	2.71	8 (34%)	32,32,32	2.70	14 (43%)
2	ZMR	B	2478	-	23,23,23	2.85	4 (17%)	32,32,32	3.28	14 (43%)
4	NAG	B	2480	1	12,14,15	2.42	1 (8%)	15,19,21	2.69	4 (26%)
4	NAG	B	2481	-	12,14,15	2.48	1 (8%)	15,19,21	2.30	4 (26%)
4	NAG	B	2482	-	12,14,15	2.62	1 (8%)	15,19,21	2.81	6 (40%)
4	NAG	B	2483	-	12,14,15	2.60	1 (8%)	15,19,21	2.82	6 (40%)
5	MAN	B	2484	-	10,11,12	0.57	0	11,15,17	2.12	4 (36%)
5	MAN	B	2485	-	10,11,12	0.80	0	11,15,17	1.62	3 (27%)
5	MAN	B	2486	-	10,11,12	0.67	0	11,15,17	2.22	2 (18%)
6	BMA	C	1709	5,4	10,11,12	0.68	0	11,15,17	1.65	1 (9%)
2	ZMR	C	3477	-	23,23,23	2.90	7 (30%)	32,32,32	2.68	16 (50%)
2	ZMR	C	3478	-	23,23,23	2.79	4 (17%)	32,32,32	2.99	14 (43%)
4	NAG	C	3480	1,4	12,14,15	2.68	1 (8%)	15,19,21	3.15	6 (40%)
4	NAG	C	3481	4,6	12,14,15	2.84	1 (8%)	15,19,21	3.04	7 (46%)
5	MAN	C	3483	5,6	10,11,12	0.55	0	11,15,17	1.24	1 (9%)
5	MAN	C	3484	-	10,11,12	0.68	0	11,15,17	2.34	3 (27%)
5	MAN	C	3485	5	10,11,12	0.82	0	11,15,17	2.09	5 (45%)
4	NAG	C	3486	-	12,14,15	2.25	1 (8%)	15,19,21	2.41	4 (26%)
4	NAG	C	3487	1	12,14,15	2.45	1 (8%)	15,19,21	2.59	6 (40%)
4	NAG	C	3488	-	12,14,15	2.34	1 (8%)	15,19,21	3.35	7 (46%)
4	NAG	C	3489	1,4	12,14,15	2.82	2 (16%)	15,19,21	3.48	6 (40%)
5	MAN	C	3490	-	10,11,12	0.73	0	11,15,17	1.34	1 (9%)
5	MAN	C	3492	-	10,11,12	0.51	0	11,15,17	1.12	1 (9%)
6	BMA	C	3493	-	10,11,12	0.92	0	11,15,17	2.34	5 (45%)
4	NAG	C	3494	4	12,14,15	2.48	1 (8%)	15,19,21	2.73	7 (46%)
2	ZMR	D	4477	-	23,23,23	2.97	5 (21%)	32,32,32	2.46	14 (43%)
2	ZMR	D	4478	-	23,23,23	2.77	4 (17%)	32,32,32	3.65	15 (46%)
5	MAN	D	4480	-	10,11,12	0.79	0	11,15,17	3.24	7 (63%)
5	MAN	D	4481	-	10,11,12	0.87	0	11,15,17	2.22	4 (36%)
4	NAG	D	4482	-	12,14,15	2.55	2 (16%)	15,19,21	2.74	7 (46%)
4	NAG	D	4483	1	12,14,15	1.80	1 (8%)	15,19,21	2.60	4 (26%)
4	NAG	D	4484	4	12,14,15	2.54	2 (16%)	15,19,21	3.26	9 (60%)
4	NAG	D	4485	4,6	12,14,15	2.29	1 (8%)	15,19,21	2.70	7 (46%)
6	BMA	D	4486	4	10,11,12	0.55	0	11,15,17	1.66	3 (27%)

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	ZMR	A	1477	-	2/2/9/11	0/21/38/38	0/1/1/1
2	ZMR	A	1478	-	2/2/9/11	1/21/38/38	0/1/1/1
4	NAG	A	1480	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1481	4	2/2/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1482	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1483	-	1/1/5/7	0/6/23/26	0/1/1/1
5	MAN	A	1485	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1486	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1487	5	-	0/2/19/22	0/1/1/1
6	BMA	A	1709	-	-	0/2/19/22	0/1/1/1
2	ZMR	B	2477	-	2/2/9/11	0/21/38/38	0/1/1/1
2	ZMR	B	2478	-	2/2/9/11	0/21/38/38	0/1/1/1
4	NAG	B	2480	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	2481	-	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	2482	-	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	2483	-	1/1/5/7	0/6/23/26	0/1/1/1
5	MAN	B	2484	-	-	0/2/19/22	0/1/1/1
5	MAN	B	2485	-	-	0/2/19/22	0/1/1/1
5	MAN	B	2486	-	-	0/2/19/22	0/1/1/1
6	BMA	C	1709	5,4	-	0/2/19/22	0/1/1/1
2	ZMR	C	3477	-	2/2/9/11	0/21/38/38	0/1/1/1
2	ZMR	C	3478	-	2/2/9/11	0/21/38/38	0/1/1/1
4	NAG	C	3480	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	3481	4,6	1/1/5/7	0/6/23/26	0/1/1/1
5	MAN	C	3483	5,6	-	0/2/19/22	0/1/1/1
5	MAN	C	3484	-	-	0/2/19/22	0/1/1/1
5	MAN	C	3485	5	-	0/2/19/22	0/1/1/1
4	NAG	C	3486	-	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	3487	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	3488	-	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	3489	1,4	2/2/5/7	0/6/23/26	0/1/1/1
5	MAN	C	3490	-	-	0/2/19/22	0/1/1/1
5	MAN	C	3492	-	-	0/2/19/22	0/1/1/1
6	BMA	C	3493	-	-	0/2/19/22	0/1/1/1
4	NAG	C	3494	4	1/1/5/7	0/6/23/26	0/1/1/1
2	ZMR	D	4477	-	2/2/9/11	0/21/38/38	0/1/1/1
2	ZMR	D	4478	-	2/2/9/11	1/21/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	D	4480	-	-	0/2/19/22	0/1/1/1
5	MAN	D	4481	-	-	0/2/19/22	0/1/1/1
4	NAG	D	4482	-	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	4483	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	4484	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	4485	4,6	1/1/5/7	0/6/23/26	0/1/1/1
6	BMA	D	4486	4	-	0/2/19/22	0/1/1/1

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4477	ZMR	C8-C7	-9.58	1.33	1.53
4	C	3481	NAG	O4-C4	-9.56	1.19	1.43
4	C	3489	NAG	O4-C4	-9.40	1.20	1.43
2	C	3477	ZMR	O7-C7	-9.16	1.20	1.43
4	C	3480	NAG	O4-C4	-8.97	1.21	1.43

The worst 5 of 284 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4478	ZMR	C4-C3-C2	-11.72	113.92	122.77
2	B	2478	ZMR	C4-C3-C2	-8.98	115.99	122.77
2	C	3478	ZMR	C4-C5-N5	-8.86	101.89	110.81
4	B	2483	NAG	C3-C4-C5	8.24	124.92	110.20
4	C	3489	NAG	C3-C4-C5	8.14	124.74	110.20

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2477	ZMR	C8
2	B	2477	ZMR	C7
4	C	3486	NAG	C4
2	A	1478	ZMR	C8
2	A	1478	ZMR	C7

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4478	ZMR	C5-C4-NE-CZ
2	A	1478	ZMR	C5-C4-NE-CZ

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	389/389 (100%)	-0.47	1 (0%) 91 95	5, 11, 18, 30	0
1	B	389/389 (100%)	-0.43	0 100 100	5, 12, 20, 36	0
1	C	389/389 (100%)	-0.43	1 (0%) 91 95	5, 12, 20, 37	0
1	D	389/389 (100%)	-0.42	1 (0%) 91 95	5, 12, 19, 32	0
All	All	1556/1556 (100%)	-0.44	3 (0%) 90 96	5, 12, 20, 37	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	ARG	2.8
1	D	3460	ARG	2.4
1	C	2088	ARG	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	A	1486	11/12	0.17	14.09	32,36,41,46	0
2	ZMR	C	3478	23/23	0.36	11.10	28,35,37,39	23
2	ZMR	B	2478	23/23	0.43	10.80	35,42,44,45	23
6	BMA	D	4486	11/12	0.22	9.84	41,43,45,46	0
5	MAN	D	4480	11/12	0.30	9.77	44,49,52,52	0
2	ZMR	D	4478	23/23	0.45	9.33	38,44,48,49	23
6	BMA	C	1709	11/12	0.18	8.70	26,31,32,33	0
5	MAN	B	2485	11/12	0.24	8.54	42,47,49,49	0
5	MAN	B	2486	11/12	0.26	7.66	48,49,50,50	0
5	MAN	C	3483	11/12	0.15	7.49	24,27,30,30	0
4	NAG	D	4482	14/15	0.31	7.26	73,78,79,80	0
2	ZMR	A	1478	23/23	0.45	7.12	36,41,45,47	23
5	MAN	A	1485	11/12	0.18	7.11	31,35,40,40	0
6	BMA	A	1709	11/12	0.21	6.61	31,36,37,37	0
5	MAN	D	4481	11/12	0.36	6.34	65,69,70,70	0
4	NAG	A	1482	14/15	0.19	5.89	23,28,32,34	0
5	MAN	C	3485	11/12	0.14	5.12	19,25,28,30	0
5	MAN	C	3490	11/12	0.16	4.62	29,33,35,36	0
4	NAG	C	3489	14/15	0.22	4.33	34,41,44,44	0
5	MAN	B	2484	11/12	0.20	4.20	41,44,45,46	0
4	NAG	C	3487	14/15	0.17	4.19	19,22,30,31	0
6	BMA	C	3493	11/12	0.20	4.16	33,34,36,37	0
5	MAN	C	3484	11/12	0.15	3.96	29,30,34,37	0
4	NAG	D	4483	14/15	0.16	3.78	16,25,26,27	0
4	NAG	D	4484	14/15	0.21	3.69	24,30,31,32	0
5	MAN	A	1487	11/12	0.13	3.28	21,31,32,33	0
4	NAG	C	3486	14/15	0.20	2.15	42,47,49,49	0
4	NAG	C	3480	14/15	0.20	2.11	33,41,46,47	0
4	NAG	D	4485	14/15	0.20	2.10	21,30,36,36	0
4	NAG	B	2480	14/15	0.14	2.06	14,26,30,30	0
4	NAG	B	2483	14/15	0.21	1.20	30,36,37,38	0
4	NAG	C	3488	14/15	0.33	1.15	63,68,70,70	0
4	NAG	A	1480	14/15	0.12	0.98	16,25,27,27	0
4	NAG	C	3494	14/15	0.19	0.90	21,28,31,31	0
4	NAG	B	2482	14/15	0.23	0.69	44,52,53,53	0
4	NAG	C	3481	14/15	0.13	0.68	21,25,27,29	0
2	ZMR	A	1477	23/23	0.07	-0.78	6,10,13,15	0
2	ZMR	B	2477	23/23	0.07	-0.78	2,10,13,16	0
2	ZMR	C	3477	23/23	0.07	-0.87	5,11,16,16	0
2	ZMR	D	4477	23/23	0.07	-0.95	5,10,13,16	0
3	CA	D	4479	1/1	0.04	-1.57	19,19,19,19	0
3	CA	C	3479	1/1	0.03	-1.95	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	2479	1/1	0.04	-2.53	25,25,25,25	0
3	CA	A	1479	1/1	0.04	-3.31	20,20,20,20	0
4	NAG	A	1481	14/15	0.38	-	71,74,75,75	0
4	NAG	A	1483	14/15	0.36	-	71,77,79,80	0
5	MAN	C	3492	11/12	0.30	-	60,65,67,67	0
4	NAG	B	2481	14/15	0.40	-	66,72,74,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.