



# Full wwPDB X-ray Structure Validation 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 full wwPDB 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/ValidationPDFNotes.html>

---

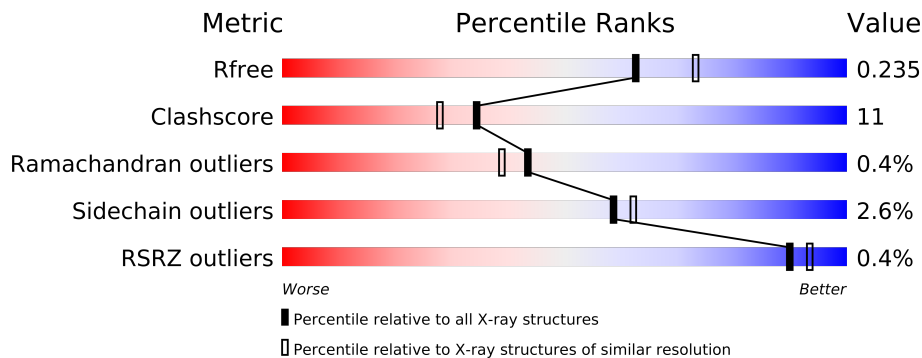
The following versions of software and data (see [references](#)) were used in the production of this report:

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

*Continued on next page...*

*Continued from previous page...*

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

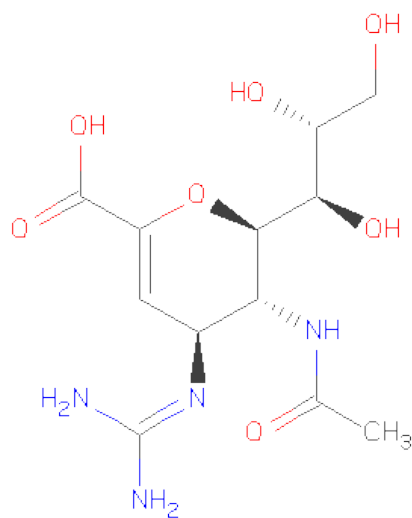
There are 7 unique types of molecules in this entry. The entry contains 13060 atoms, of which 0 are hydrogen and 0 are deuterium.

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:  $C_{12}H_{20}N_4O_7$ ).



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		

*Continued on next page...*

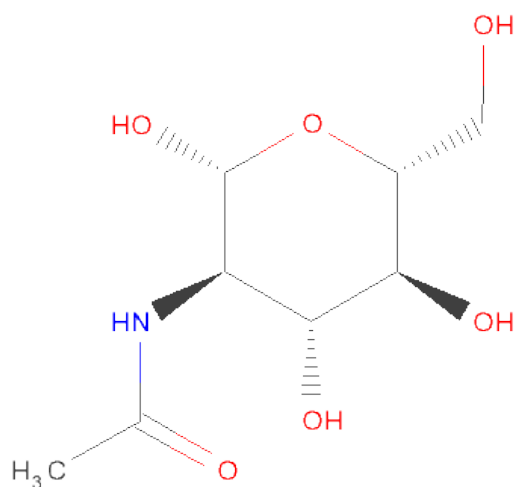
Continued from previous page...

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).

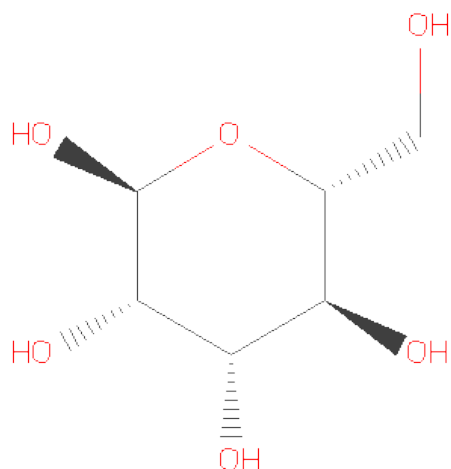
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- 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>).



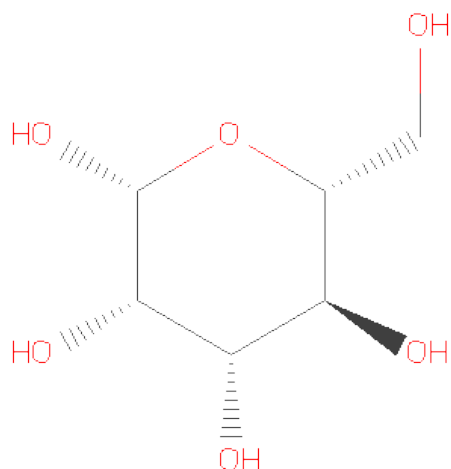
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

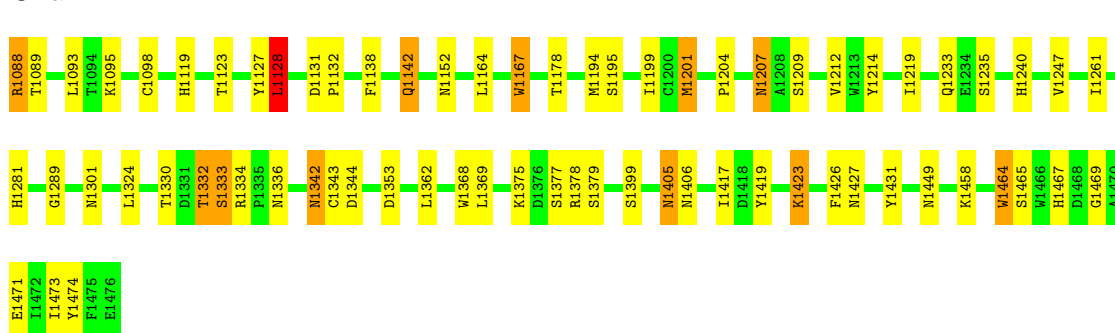
#### • Molecule 1: NEURAMINIDASE

Chain A:



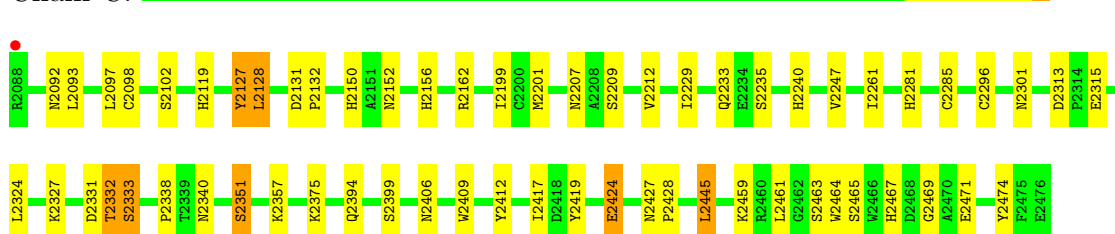
#### • Molecule 1: NEURAMINIDASE

Chain B:



#### • Molecule 1: NEURAMINIDASE

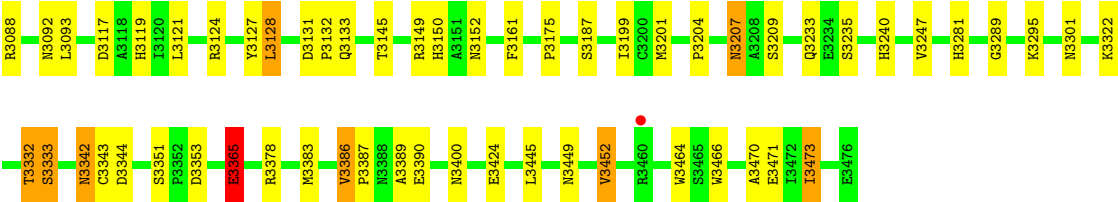
Chain C:



#### • Molecule 1: NEURAMINIDASE

Chain D:





## 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

All (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
1	C	2127	TYR	CD1-CE1	-5.06	1.31	1.39

All (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
1	D	3378	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	3128	LEU	CB-CG-CD2	5.98	121.17	111.00
1	B	1128	LEU	CB-CG-CD2	5.72	120.73	111.00
1	B	1333	SER	CB-CA-C	5.70	120.93	110.10
1	D	3149	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	331	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	2162	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	2331	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	2313	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	2445	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	196	ARG	NE-CZ-NH1	-5.10	117.75	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:B:1152:ASN:HD21	4:B:2480:NAG:C1	0.88	1.50
1:D:3207:ASN:HD21	4:D:4484:NAG:C1	1.25	1.45
1:D:3092:ASN:ND2	4:D:4482:NAG:H2	1.17	1.41
5:A:1485:MAN:HO6	5:A:1486:MAN:C1	1.53	1.22
1:C:2207:ASN:HD22	4:C:3489:NAG:C1	1.46	1.20
1:D:3207:ASN:ND2	4:D:4484:NAG:C1	2.09	1.14
1:D:3092:ASN:ND2	4:D:4482:NAG:C2	2.13	1.10
1:B:1207:ASN:HD21	4:B:2482:NAG:C2	1.73	1.02
5:A:1485:MAN:C1	6:A:1709:BMA:O6	2.07	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:3092:ASN:HD22	4:D:4482:NAG:C2	1.73	1.01
4:B:2482:NAG:O4	4:B:2483:NAG:C1	2.09	1.00
6:C:1709:BMA:O3	5:C:3490:MAN:C1	2.10	0.99
1:B:1093:LEU:H	1:B:1240:HIS:HD2	0.97	0.96
6:A:1709:BMA:C1	4:B:2483:NAG:O4	2.14	0.96
5:C:3483:MAN:O6	5:C:3484:MAN:C1	2.13	0.95
6:C:3493:BMA:C1	4:C:3494:NAG:O4	2.15	0.93
1:B:1207:ASN:HD21	4:B:2482:NAG:H2	1.33	0.92
1:D:3092:ASN:HD21	4:D:4482:NAG:H2	1.09	0.92
1:C:2150:HIS:HE1	1:D:3471:GLU:H	1.13	0.92
1:C:2092:ASN:HD21	4:C:3486:NAG:C1	1.83	0.92
1:C:2207:ASN:HD21	4:C:3489:NAG:C1	1.76	0.91
1:B:1471:GLU:H	1:D:3150:HIS:HE1	1.07	0.91
1:D:3333:SER:HB2	1:D:3353:ASP:O	1.70	0.91
1:B:1093:LEU:H	1:B:1240:HIS:CD2	1.88	0.89
1:D:3233:GLN:HE21	1:D:3247:VAL:H	1.22	0.88
1:C:2093:LEU:H	1:C:2240:HIS:HD2	1.20	0.88
1:D:3295:LYS:NZ	1:D:3390:GLU:OE2	2.08	0.85
1:D:3092:ASN:HD22	4:D:4482:NAG:H2	1.02	0.84
1:B:1333:SER:HB2	1:B:1353:ASP:O	1.78	0.83
1:A:152:ASN:HD21	4:A:1482:NAG:C2	1.89	0.82
1:A:150:HIS:HE1	1:C:2471:GLU:H	1.25	0.82
4:D:4485:NAG:O4	6:D:4486:BMA:C1	2.27	0.81
1:D:3093:LEU:H	1:D:3240:HIS:HD2	1.27	0.81
1:C:2152:ASN:HD21	4:C:3487:NAG:C2	1.92	0.81
4:A:1482:NAG:O4	4:A:1483:NAG:C1	2.28	0.81
1:B:1233:GLN:HE21	1:B:1247:VAL:H	1.29	0.80
5:B:2484:MAN:O6	5:B:2485:MAN:C1	2.30	0.79
5:B:2484:MAN:O3	5:B:2486:MAN:H2	1.83	0.79
1:C:2207:ASN:ND2	4:C:3489:NAG:N2	2.31	0.78
1:C:2233:GLN:HE21	1:C:2247:VAL:H	1.30	0.78
1:A:93:LEU:H	1:A:240:HIS:HD2	1.30	0.78
1:A:333:SER:HB2	1:A:353:ASP:O	1.85	0.77
1:A:92:ASN:CG	4:A:1480:NAG:C1	2.53	0.77
1:D:3386:VAL:HG22	1:D:3389:ALA:HB2	1.66	0.77
1:C:2207:ASN:ND2	4:C:3489:NAG:C2	2.47	0.77
1:B:1207:ASN:ND2	4:B:2482:NAG:H2	2.01	0.76
1:B:1471:GLU:H	1:D:3150:HIS:CE1	1.98	0.75
1:B:1207:ASN:HD21	4:B:2482:NAG:C1	1.98	0.75
5:C:3490:MAN:O2	5:C:3492:MAN:H3	1.86	0.75
1:C:2092:ASN:ND2	4:C:3486:NAG:C1	2.51	0.74
1:C:2102:SER:HB2	1:C:2459:LYS:O	1.90	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1333:SER:CB	1:B:1353:ASP:O	2.38	0.71
1:A:240:HIS:HE1	1:A:315:GLU:OE2	1.75	0.68
1:B:1405:ASN:C	1:B:1405:ASN:HD22	1.97	0.68
1:B:1471:GLU:N	1:D:3150:HIS:HE1	1.87	0.67
1:B:1281:HIS:HD2	1:B:1301:ASN:H	1.42	0.66
1:D:3093:LEU:H	1:D:3240:HIS:CD2	2.12	0.66
1:A:92:ASN:HD21	4:A:1480:NAG:C2	2.03	0.66
1:A:233:GLN:HE21	1:A:247:VAL:H	1.41	0.66
1:C:2465:SER:OG	1:C:2467:HIS:HD2	1.79	0.66
5:C:3483:MAN:C3	5:C:3485:MAN:C1	2.74	0.65
6:C:1709:BMA:C6	5:C:3483:MAN:C1	2.74	0.65
1:A:342:ASN:HD22	1:A:344:ASP:H	1.44	0.65
5:B:2484:MAN:O6	5:B:2485:MAN:H2	1.96	0.64
1:C:2399:SER:HB2	4:C:3481:NAG:O3	1.97	0.64
1:C:2092:ASN:HD21	4:C:3486:NAG:C2	2.10	0.64
6:C:3493:BMA:O6	5:D:4480:MAN:C1	2.47	0.63
1:D:3471:GLU:HG3	1:D:3473:ILE:HG22	1.79	0.63
1:C:2150:HIS:CE1	1:D:3471:GLU:H	2.05	0.63
4:B:2480:NAG:O4	4:B:2481:NAG:C1	2.47	0.62
1:B:1093:LEU:N	1:B:1240:HIS:HD2	1.83	0.62
1:C:2281:HIS:HD2	1:C:2301:ASN:H	1.46	0.62
1:A:92:ASN:ND2	4:A:1480:NAG:C2	2.61	0.62
5:B:2484:MAN:O6	5:B:2485:MAN:C2	2.46	0.62
1:A:467:HIS:H	1:A:467:HIS:CD2	2.16	0.61
1:C:2207:ASN:HD21	4:C:3489:NAG:C2	2.12	0.61
4:D:4484:NAG:C4	4:D:4485:NAG:C1	2.78	0.61
1:C:2461:LEU:O	4:C:3480:NAG:H61	2.01	0.61
6:C:1709:BMA:O3	5:C:3490:MAN:C2	2.50	0.60
1:D:3342:ASN:HD22	1:D:3344:ASP:H	1.50	0.60
1:A:93:LEU:H	1:A:240:HIS:CD2	2.16	0.60
1:A:412:TYR:HB2	1:A:433:GLU:OE2	2.02	0.59
1:A:235:SER:HB3	1:A:357:LYS:HE2	1.84	0.59
1:A:152:ASN:CG	4:A:1482:NAG:C1	2.63	0.59
1:C:2131:ASP:HB2	1:C:2132:PRO:HD2	1.83	0.59
1:B:1465:SER:OG	1:B:1467:HIS:HD2	1.85	0.58
5:B:2484:MAN:O5	6:D:4486:BMA:O6	2.22	0.57
1:A:284:GLU:OE2	1:A:412:TYR:OH	2.20	0.57
4:C:3480:NAG:O4	4:C:3481:NAG:O5	2.22	0.57
1:D:3365:GLU:HA	1:D:3387:PRO:HB3	1.86	0.57
1:C:2119:HIS:HD2	1:D:3117:ASP:OD1	1.88	0.57
5:B:2484:MAN:C6	5:B:2485:MAN:C1	2.83	0.57
1:D:3281:HIS:CD2	1:D:3301:ASN:H	2.23	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:3490:MAN:C1	5:C:3492:MAN:H5	2.35	0.56
1:C:2093:LEU:H	1:C:2240:HIS:CD2	2.12	0.56
1:D:3424:GLU:H	1:D:3424:GLU:CD	2.08	0.56
6:C:1709:BMA:C3	5:C:3490:MAN:C1	2.83	0.56
1:C:2333:SER:HB3	1:C:2351:SER:N	2.20	0.56
1:B:1142:GLN:NE2	7:B:2017:HOH:O	2.38	0.56
1:A:262:ILE:HG12	1:A:272:ILE:HG12	1.87	0.56
1:D:3152:ASN:ND2	4:D:4483:NAG:C2	2.68	0.55
1:C:2092:ASN:OD1	4:C:3486:NAG:C1	2.54	0.55
1:D:3131:ASP:HB2	1:D:3132:PRO:HD2	1.88	0.55
1:C:2097:LEU:HD22	1:C:2428:PRO:HG3	1.88	0.55
1:A:92:ASN:ND2	4:A:1480:NAG:O5	2.19	0.55
5:C:3483:MAN:O3	5:C:3485:MAN:C2	2.54	0.55
1:B:1342:ASN:ND2	1:B:1344:ASP:H	2.05	0.55
1:C:2152:ASN:CG	4:C:3487:NAG:C1	2.73	0.54
1:B:1207:ASN:ND2	4:B:2482:NAG:C2	2.56	0.54
1:B:1281:HIS:CD2	1:B:1301:ASN:H	2.24	0.54
1:A:119:HIS:CE1	1:B:1119:HIS:CE1	2.96	0.54
1:A:207:ASN:CG	4:C:3480:NAG:C1	2.72	0.54
5:A:1485:MAN:C3	5:A:1487:MAN:C1	2.84	0.54
1:A:91:LEU:HD11	1:A:419:TYR:HB3	1.89	0.54
1:A:281:HIS:HD2	1:A:301:ASN:H	1.55	0.54
1:C:2417:ILE:HB	1:C:2419:TYR:CZ	2.43	0.54
4:B:2480:NAG:O4	4:B:2481:NAG:O5	2.25	0.54
1:C:2152:ASN:ND2	4:C:3487:NAG:C2	2.59	0.54
1:C:2233:GLN:HB3	1:C:2285:CYS:O	2.08	0.53
1:D:3332:THR:HG22	1:D:3333:SER:H	1.72	0.53
1:C:2233:GLN:NE2	1:C:2247:VAL:H	2.03	0.53
1:D:3088:ARG:NH2	1:D:3133:GLN:OE1	2.36	0.53
1:B:1098:CYS:HB2	1:B:1427:ASN:HD22	1.73	0.53
1:D:3233:GLN:NE2	1:D:3247:VAL:H	1.98	0.53
1:C:2424:GLU:CD	1:C:2424:GLU:H	2.11	0.53
1:A:400:ASN:HB2	5:A:1487:MAN:O6	2.08	0.53
1:B:1379:SER:OG	1:B:1406:ASN:ND2	2.42	0.53
1:A:285:CYS:HB3	1:A:296:CYS:HB3	1.89	0.53
1:B:1131:ASP:HB2	1:B:1132:PRO:CD	2.38	0.53
1:B:1336:ASN:OD1	1:B:1375:LYS:HE3	2.09	0.52
1:D:3207:ASN:HD21	4:D:4484:NAG:C2	2.13	0.52
1:D:3281:HIS:HD2	1:D:3301:ASN:H	1.57	0.52
1:D:3201:MET:HA	1:D:3209:SER:O	2.10	0.52
1:D:3093:LEU:HD13	1:D:3289:GLY:HA3	1.92	0.51
1:D:3322:LYS:HB2	1:D:3343:CYS:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1342:ASN:HD22	1:B:1344:ASP:H	1.56	0.51
1:D:3092:ASN:HD21	4:D:4482:NAG:C2	1.99	0.51
1:B:1195:SER:HB2	1:B:1214:TYR:CZ	2.46	0.50
4:C:3487:NAG:O4	4:C:3488:NAG:C1	2.59	0.50
1:C:2156:HIS:CE1	7:C:4020:HOH:O	2.64	0.50
1:B:1123:THR:OG1	1:B:1449:ASN:ND2	2.43	0.50
1:A:119:HIS:HE1	1:B:1119:HIS:HE1	1.59	0.50
1:B:1199:ILE:HG12	1:B:1212:VAL:HG13	1.93	0.50
1:A:342:ASN:ND2	1:A:344:ASP:H	2.09	0.50
1:D:3332:THR:CG2	1:D:3333:SER:H	2.25	0.50
1:C:2131:ASP:HB2	1:C:2132:PRO:CD	2.40	0.50
1:A:119:HIS:CE1	1:B:1119:HIS:HE1	2.29	0.50
1:C:2152:ASN:ND2	4:C:3487:NAG:O5	2.36	0.50
5:A:1485:MAN:C1	6:A:1709:BMA:C6	2.88	0.50
1:A:460:ARG:O	1:A:460:ARG:HG3	2.12	0.49
1:C:2406:ASN:O	2:C:3478:ZMR:H4	2.13	0.49
5:B:2484:MAN:O3	5:B:2486:MAN:C2	2.58	0.49
1:A:332:THR:HG22	1:A:333:SER:H	1.75	0.49
1:B:1399:SER:HA	6:D:4486:BMA:H62	1.94	0.49
1:A:238:VAL:O	1:A:245:PRO:HD2	2.13	0.49
1:A:150:HIS:CE1	1:C:2471:GLU:H	2.17	0.49
1:A:92:ASN:OD1	4:A:1480:NAG:C1	2.61	0.48
4:C:3489:NAG:C4	4:C:3494:NAG:C1	2.85	0.48
1:A:417:ILE:HB	1:A:419:TYR:CZ	2.48	0.48
1:B:1332:THR:CG2	1:B:1333:SER:H	2.25	0.48
1:A:332:THR:CG2	1:A:333:SER:H	2.26	0.48
1:C:2409:TRP:CD2	2:C:3478:ZMR:H112	2.48	0.48
1:A:282:ILE:HD12	1:A:310:ILE:HD11	1.95	0.48
1:A:152:ASN:ND2	4:A:1482:NAG:C2	2.63	0.48
1:D:3187:SER:HA	1:D:3199:ILE:O	2.13	0.48
1:C:2127:TYR:CG	1:C:2235:SER:HA	2.49	0.48
2:B:2478:ZMR:H3	2:B:2478:ZMR:HN21	1.79	0.48
1:B:1471:GLU:HB2	1:B:1474:TYR:CD1	2.49	0.48
1:D:3127:TYR:CG	1:D:3235:SER:HA	2.49	0.48
1:A:281:HIS:CD2	1:A:301:ASN:H	2.32	0.48
1:B:1330:THR:HG21	1:B:1369:LEU:HB3	1.96	0.48
1:D:3092:ASN:HD22	4:D:4482:NAG:C7	2.26	0.47
1:C:2119:HIS:CE1	1:D:3119:HIS:CE1	3.01	0.47
1:B:1127:TYR:CG	1:B:1235:SER:HA	2.49	0.47
1:B:1088:ARG:HA	1:B:1088:ARG:HE	1.78	0.47
1:A:151:ALA:HB1	1:A:446:TRP:HB3	1.96	0.47
1:C:2240:HIS:HE1	1:C:2315:GLU:OE1	1.98	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1464:TRP:HB3	1:D:3204:PRO:HD3	1.96	0.47
1:B:1417:ILE:HG21	1:B:1426:PHE:HB3	1.97	0.47
1:B:1334:ARG:HG3	1:B:1375:LYS:HB2	1.97	0.47
1:C:2399:SER:CB	4:C:3481:NAG:O3	2.63	0.47
2:B:2478:ZMR:C3	2:B:2478:ZMR:HN21	2.27	0.47
1:B:1095:LYS:NZ	1:B:1423:LYS:O	2.44	0.47
1:D:3342:ASN:ND2	1:D:3344:ASP:H	2.13	0.46
1:C:2119:HIS:HE1	1:D:3119:HIS:CE1	2.33	0.46
1:C:2102:SER:CB	1:C:2459:LYS:O	2.61	0.46
1:C:2150:HIS:HD2	7:D:2009:HOH:O	1.99	0.46
1:A:324:LEU:HD21	1:A:362:LEU:HD21	1.98	0.46
1:A:127:TYR:CG	1:A:235:SER:HA	2.51	0.46
1:D:3332:THR:CG2	1:D:3333:SER:N	2.79	0.45
1:A:119:HIS:O	1:A:175:PRO:HD3	2.15	0.45
1:C:2199:ILE:HG12	1:C:2212:VAL:HG13	1.98	0.45
1:A:149:ARG:NH1	1:C:2474:TYR:O	2.49	0.45
1:A:330:THR:HG21	1:A:369:LEU:HB3	1.97	0.45
1:B:1138:PHE:HB3	1:B:1164:LEU:HD11	1.98	0.45
1:B:1204:PRO:HG2	1:B:1207:ASN:HB2	1.99	0.45
4:D:4484:NAG:O4	4:D:4485:NAG:O5	2.34	0.45
1:C:2412:TYR:OH	2:C:3477:ZMR:C2	2.65	0.44
1:A:452:VAL:HG21	1:A:466:TRP:HB3	2.00	0.44
1:C:2285:CYS:HB3	1:C:2296:CYS:HB3	1.99	0.44
1:B:1093:LEU:HD13	1:B:1289:GLY:HA3	1.98	0.44
1:B:1342:ASN:HD22	1:B:1343:CYS:N	2.15	0.44
1:B:1333:SER:HB3	1:B:1353:ASP:O	2.18	0.44
1:B:1088:ARG:NE	1:B:1088:ARG:HA	2.31	0.44
1:B:1247:VAL:HG22	1:B:1261:ILE:HD12	2.00	0.44
1:B:1167:TRP:HB3	1:B:1178:THR:HG22	1.99	0.43
1:C:2092:ASN:CG	4:C:3486:NAG:C1	2.87	0.43
1:A:124:ARG:HA	1:A:449:ASN:ND2	2.34	0.43
1:A:407:GLN:C	2:A:1478:ZMR:H113	2.39	0.43
1:D:3119:HIS:O	1:D:3175:PRO:HD3	2.18	0.43
1:C:2333:SER:HA	1:C:2375:LYS:O	2.18	0.43
1:B:1119:HIS:CE1	1:D:3119:HIS:CE1	3.07	0.43
1:B:1214:TYR:HB3	1:B:1219:ILE:HG13	1.99	0.43
1:C:2098:CYS:HB2	1:C:2427:ASN:HD22	1.83	0.43
1:C:2327:LYS:O	1:C:2338:PRO:HD2	2.18	0.43
1:C:2150:HIS:HE1	1:D:3471:GLU:N	1.96	0.43
1:A:161:PHE:CE2	1:C:2469:GLY:HA3	2.53	0.43
1:C:2340:ASN:ND2	1:C:2394:GLN:HG2	2.34	0.43
1:B:1417:ILE:HB	1:B:1419:TYR:CZ	2.54	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1128:LEU:HD23	1:B:1431:TYR:HB3	2.01	0.42
1:D:3121:LEU:HA	1:D:3145:THR:HA	2.01	0.42
1:B:1324:LEU:HD21	1:B:1362:LEU:HD21	2.01	0.42
1:B:1152:ASN:ND2	4:B:2480:NAG:O5	2.40	0.42
5:C:3490:MAN:O2	5:C:3492:MAN:C3	2.64	0.42
1:B:1332:THR:CG2	1:B:1333:SER:N	2.82	0.42
1:A:97:LEU:HD12	1:A:363:ASP:HB2	2.02	0.42
5:C:3483:MAN:H2	5:C:3485:MAN:O5	2.20	0.42
1:B:1201:MET:HA	1:B:1209:SER:O	2.19	0.42
1:C:2332:THR:HG22	1:C:2333:SER:N	2.34	0.42
1:C:2229:ILE:HG22	1:C:2229:ILE:O	2.19	0.41
1:D:3383:MET:O	1:D:3400:ASN:HA	2.21	0.41
1:C:2332:THR:HG22	1:C:2333:SER:H	1.85	0.41
1:D:3207:ASN:CG	4:D:4484:NAG:C1	2.83	0.41
1:C:2150:HIS:CE1	1:D:3470:ALA:HA	2.55	0.41
1:D:3124:ARG:HA	1:D:3449:ASN:ND2	2.36	0.41
1:C:2357:LYS:HB3	1:C:2412:TYR:CG	2.55	0.41
1:C:2201:MET:HA	1:C:2209:SER:O	2.21	0.41
1:C:2463:SER:HB2	7:C:4073:HOH:O	2.20	0.41
1:A:131:ASP:HB2	1:A:132:PRO:CD	2.51	0.41
1:B:1152:ASN:CG	4:B:2480:NAG:C1	2.72	0.41
1:A:189:SER:HA	1:A:197:MET:O	2.21	0.40
1:A:336:ASN:OD1	1:A:375:LYS:NZ	2.26	0.40
1:D:3452:VAL:HG21	1:D:3466:TRP:HB3	2.03	0.40
1:A:197:MET:HA	1:A:213:TRP:O	2.21	0.40
1:B:1469:GLY:HA3	1:D:3161:PHE:CE2	2.56	0.40
2:A:1478:ZMR:HN21	2:A:1478:ZMR:C3	2.35	0.40
1:A:402:VAL:HG23	5:A:1487:MAN:H61	2.03	0.40

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

Continued on next page...

*Continued from previous page...*

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

All (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
1	B	1207	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

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	155	ILE
1	A	342	ASN
1	A	406	ASN
1	A	445	LEU
1	A	460	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	464	TRP
1	B	1088	ARG
1	B	1089	THR
1	B	1128	LEU
1	B	1142	GLN
1	B	1194	MET
1	B	1201	MET
1	B	1342	ASN
1	B	1377	SER
1	B	1405	ASN
1	B	1423	LYS
1	B	1458	LYS
1	B	1464	TRP
1	B	1473	ILE
1	C	2128	LEU
1	C	2261	ILE
1	C	2324	LEU
1	C	2351	SER
1	C	2424	GLU
1	C	2445	LEU
1	C	2464	TRP
1	D	3128	LEU
1	D	3342	ASN
1	D	3351	SER
1	D	3365	GLU
1	D	3386	VAL
1	D	3445	LEU
1	D	3464	TRP
1	D	3473	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	119	HIS
1	A	150	HIS
1	A	152	ASN
1	A	207	ASN
1	A	233	GLN
1	A	240	HIS
1	A	281	HIS
1	A	340	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	342	ASN
1	A	406	ASN
1	A	408	ASN
1	A	422	ASN
1	A	427	ASN
1	A	449	ASN
1	A	467	HIS
1	B	1119	HIS
1	B	1142	GLN
1	B	1152	ASN
1	B	1207	ASN
1	B	1233	GLN
1	B	1240	HIS
1	B	1281	HIS
1	B	1340	ASN
1	B	1342	ASN
1	B	1405	ASN
1	B	1406	ASN
1	B	1408	ASN
1	B	1427	ASN
1	B	1449	ASN
1	B	1467	HIS
1	C	2092	ASN
1	C	2119	HIS
1	C	2150	HIS
1	C	2152	ASN
1	C	2207	ASN
1	C	2233	GLN
1	C	2240	HIS
1	C	2281	HIS
1	C	2340	ASN
1	C	2406	ASN
1	C	2408	ASN
1	C	2427	ASN
1	C	2449	ASN
1	C	2467	HIS
1	D	3119	HIS
1	D	3150	HIS
1	D	3152	ASN
1	D	3207	ASN
1	D	3233	GLN
1	D	3240	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	3281	HIS
1	D	3340	ASN
1	D	3342	ASN
1	D	3406	ASN
1	D	3422	ASN
1	D	3427	ASN
1	D	3449	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%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
2	A	1478	ZMR	C8-C7	-8.96	1.34	1.53
2	B	2478	ZMR	C8-C7	-8.81	1.35	1.53
4	B	2483	NAG	O4-C4	-8.80	1.21	1.43
4	B	2482	NAG	O4-C4	-8.74	1.21	1.43
2	A	1477	ZMR	C8-C7	-8.72	1.35	1.53
4	A	1482	NAG	O4-C4	-8.70	1.22	1.43
4	A	1480	NAG	O4-C4	-8.64	1.22	1.43
2	C	3478	ZMR	C8-C7	-8.60	1.35	1.53
2	B	2478	ZMR	O7-C7	-8.51	1.22	1.43
2	D	4478	ZMR	C8-C7	-8.42	1.36	1.53
2	A	1477	ZMR	O7-C7	-8.39	1.22	1.43
2	D	4478	ZMR	O7-C7	-8.34	1.22	1.43
4	C	3494	NAG	O4-C4	-8.33	1.22	1.43
4	C	3487	NAG	O4-C4	-8.32	1.22	1.43
2	C	3478	ZMR	O7-C7	-8.26	1.23	1.43
4	B	2480	NAG	O4-C4	-8.24	1.23	1.43
4	B	2481	NAG	O4-C4	-8.23	1.23	1.43
4	D	4484	NAG	O4-C4	-8.16	1.23	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1481	NAG	O4-C4	-7.99	1.23	1.43
4	C	3488	NAG	O4-C4	-7.93	1.23	1.43
2	B	2477	ZMR	O7-C7	-7.86	1.24	1.43
4	A	1483	NAG	O4-C4	-7.84	1.24	1.43
4	D	4482	NAG	O4-C4	-7.83	1.24	1.43
4	D	4485	NAG	O4-C4	-7.81	1.24	1.43
2	A	1478	ZMR	O7-C7	-7.70	1.24	1.43
2	D	4477	ZMR	O7-C7	-7.62	1.24	1.43
4	C	3486	NAG	O4-C4	-7.59	1.24	1.43
2	C	3477	ZMR	C8-C7	-7.47	1.38	1.53
2	B	2477	ZMR	C8-C7	-7.31	1.38	1.53
4	D	4483	NAG	O4-C4	-5.83	1.28	1.43
2	A	1478	ZMR	O8-C8	-4.34	1.33	1.43
2	C	3478	ZMR	O8-C8	-4.32	1.33	1.43
2	A	1477	ZMR	O8-C8	-4.22	1.33	1.43
2	B	2478	ZMR	O8-C8	-4.17	1.33	1.43
2	D	4477	ZMR	O8-C8	-4.07	1.34	1.43
2	D	4478	ZMR	O8-C8	-3.74	1.34	1.43
2	D	4477	ZMR	CZ-NE	3.69	1.36	1.29
4	D	4482	NAG	C2-N2	3.55	1.50	1.46
2	A	1477	ZMR	CZ-NE	3.52	1.36	1.29
2	B	2477	ZMR	O8-C8	-3.35	1.35	1.43
2	C	3477	ZMR	CZ-NE	3.18	1.35	1.29
2	C	3477	ZMR	O8-C8	-3.17	1.36	1.43
2	D	4478	ZMR	CZ-NE	3.15	1.35	1.29
2	B	2477	ZMR	O6-C6	-2.85	1.40	1.46
2	C	3477	ZMR	C7-C6	-2.80	1.49	1.52
2	B	2478	ZMR	CZ-NE	2.72	1.34	1.29
2	A	1478	ZMR	CZ-NE	2.70	1.34	1.29
2	C	3477	ZMR	O6-C6	-2.61	1.41	1.46
2	C	3478	ZMR	CZ-NE	2.24	1.33	1.29
2	B	2477	ZMR	CZ-NH2	-2.22	1.29	1.33
2	B	2477	ZMR	C5-N5	2.21	1.49	1.45
2	B	2477	ZMR	O1A-C1	-2.20	1.23	1.30
2	B	2477	ZMR	CZ-NE	2.16	1.33	1.29
2	C	3477	ZMR	C3-C2	2.14	1.37	1.33
4	D	4484	NAG	C2-N2	2.12	1.48	1.46
2	D	4477	ZMR	O6-C6	-2.08	1.42	1.46
4	C	3489	NAG	C2-N2	2.01	1.48	1.46

All (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
2	D	4478	ZMR	C4-C5-N5	-7.93	102.83	110.81
4	C	3488	NAG	C3-C2-N2	-7.87	99.77	111.76
4	C	3481	NAG	C3-C4-C5	7.61	123.79	110.20
2	A	1478	ZMR	C4-C3-C2	-7.45	117.14	122.77
4	D	4484	NAG	C3-C4-C5	7.38	123.39	110.20
2	B	2478	ZMR	C8-C7-C6	6.96	126.48	112.99
5	D	4480	MAN	O5-C5-C4	6.93	119.45	110.65
4	C	3480	NAG	C3-C4-C5	6.78	122.31	110.20
4	D	4485	NAG	C3-C4-C5	6.67	122.12	110.20
2	B	2477	ZMR	O6-C6-C7	-6.54	93.60	105.73
4	A	1482	NAG	C3-C2-N2	-6.40	102.01	111.76
2	A	1478	ZMR	O7-C7-C6	6.36	123.21	109.45
4	C	3489	NAG	C2-N2-C7	-6.15	112.76	123.09
4	B	2480	NAG	O5-C5-C6	6.07	113.35	106.98
4	D	4483	NAG	O4-C4-C5	6.06	125.25	109.28
5	B	2486	MAN	O5-C5-C6	5.95	113.22	106.98
2	D	4478	ZMR	C6-C5-N5	-5.91	100.68	110.99
4	A	1480	NAG	C3-C4-C5	5.87	120.69	110.20
2	A	1477	ZMR	C6-O6-C2	5.86	123.48	114.72
2	C	3477	ZMR	O7-C7-C8	5.77	123.33	108.74
4	B	2482	NAG	C3-C4-C5	5.66	120.31	110.20
2	D	4478	ZMR	O8-C8-C7	5.63	123.07	109.05
2	B	2478	ZMR	O8-C8-C7	5.53	122.82	109.05
4	C	3489	NAG	C3-C2-N2	-5.51	103.38	111.76
2	B	2477	ZMR	O8-C8-C7	5.50	122.74	109.05
2	B	2477	ZMR	O7-C7-C8	5.43	122.46	108.74
4	C	3480	NAG	O5-C5-C4	-5.43	103.77	110.65
2	D	4478	ZMR	C8-C7-C6	5.42	123.50	112.99
2	A	1478	ZMR	O6-C2-C3	-5.38	117.36	124.33
2	A	1478	ZMR	C6-C5-N5	-5.37	101.62	110.99
4	D	4482	NAG	C3-C4-C5	5.37	119.79	110.20
2	A	1477	ZMR	O8-C8-C7	5.34	122.34	109.05
2	B	2478	ZMR	C6-C5-N5	-5.29	101.77	110.99
6	C	3493	BMA	O5-C5-C6	5.28	112.52	106.98
2	C	3478	ZMR	C5-C4-NE	-5.25	103.63	109.17
5	D	4480	MAN	O5-C5-C6	5.24	112.48	106.98
5	C	3484	MAN	O5-C5-C4	-5.22	104.03	110.65
2	A	1477	ZMR	C4-C5-N5	-5.20	105.58	110.81

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3478	ZMR	C8-C7-C6	5.18	123.03	112.99
4	D	4484	NAG	C2-N2-C7	-5.13	114.48	123.09
4	C	3487	NAG	C3-C4-C5	5.10	119.32	110.20
4	C	3494	NAG	C3-C4-C5	5.09	119.29	110.20
4	A	1483	NAG	O4-C4-C5	5.07	122.65	109.28
4	D	4484	NAG	O5-C5-C6	5.05	112.28	106.98
2	A	1477	ZMR	O7-C7-C6	5.01	120.29	109.45
2	C	3477	ZMR	O6-C6-C7	-4.98	96.48	105.73
4	C	3481	NAG	C3-C2-N2	-4.97	104.19	111.76
4	A	1481	NAG	O4-C4-C3	4.96	121.47	110.35
4	C	3487	NAG	O5-C5-C6	4.96	112.18	106.98
4	D	4485	NAG	O4-C4-C3	4.94	121.42	110.35
2	A	1477	ZMR	O7-C7-C8	4.91	121.16	108.74
5	D	4481	MAN	O5-C5-C6	4.91	112.13	106.98
4	B	2480	NAG	C3-C4-C5	4.91	118.97	110.20
2	C	3477	ZMR	C4-C5-N5	-4.90	105.87	110.81
4	A	1483	NAG	O4-C4-C3	4.89	121.32	110.35
4	C	3488	NAG	C3-C4-C5	4.89	118.93	110.20
4	C	3486	NAG	C3-C4-C5	4.89	118.93	110.20
4	C	3488	NAG	O4-C4-C5	4.86	122.10	109.28
2	A	1478	ZMR	O6-C2-C1	4.86	121.46	111.88
4	C	3488	NAG	O5-C5-C6	4.85	112.07	106.98
2	C	3478	ZMR	O8-C8-C7	4.78	120.95	109.05
5	C	3485	MAN	O5-C5-C6	4.78	112.00	106.98
4	B	2480	NAG	O4-C4-C5	4.77	121.86	109.28
4	C	3486	NAG	O4-C4-C5	4.74	121.78	109.28
4	A	1482	NAG	O4-C4-C5	4.73	121.74	109.28
4	D	4483	NAG	O4-C4-C3	4.73	120.95	110.35
4	B	2481	NAG	O4-C4-C5	4.69	121.63	109.28
2	C	3477	ZMR	O8-C8-C7	4.67	120.69	109.05
2	D	4477	ZMR	O8-C8-C7	4.66	120.65	109.05
2	D	4478	ZMR	O6-C6-C5	4.64	116.10	110.29
2	D	4477	ZMR	O6-C6-C7	-4.63	97.14	105.73
2	C	3477	ZMR	C9-C8-C7	4.63	122.88	112.38
4	C	3494	NAG	O4-C4-C3	4.63	120.72	110.35
2	D	4477	ZMR	O8-C8-C9	4.56	119.83	109.20
2	B	2478	ZMR	O6-C2-C1	4.52	120.80	111.88
2	A	1478	ZMR	O7-C7-C8	4.52	120.16	108.74
5	A	1487	MAN	O5-C5-C6	4.52	111.72	106.98
2	C	3478	ZMR	O7-C7-C6	4.49	119.16	109.45
4	B	2481	NAG	O4-C4-C3	4.48	120.40	110.35
2	D	4477	ZMR	O7-C7-C8	4.44	119.97	108.74

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3494	NAG	O5-C5-C6	4.44	111.64	106.98
2	B	2478	ZMR	O6-C2-C3	-4.43	118.59	124.33
4	A	1481	NAG	O4-C4-C5	4.42	120.93	109.28
4	A	1482	NAG	C3-C4-C5	4.42	118.10	110.20
4	C	3487	NAG	O4-C4-C5	4.39	120.86	109.28
2	C	3477	ZMR	O9-C9-C8	-4.39	101.24	111.05
2	D	4478	ZMR	O7-C7-C6	4.38	118.92	109.45
4	C	3480	NAG	O5-C5-C6	4.37	111.56	106.98
6	A	1709	BMA	O3-C3-C4	4.36	120.14	110.35
4	B	2482	NAG	O5-C5-C4	-4.36	105.12	110.65
4	A	1482	NAG	O4-C4-C3	4.35	120.11	110.35
4	B	2481	NAG	C3-C4-C5	4.34	117.96	110.20
5	B	2484	MAN	O5-C5-C6	4.33	111.53	106.98
2	D	4477	ZMR	O7-C7-C6	4.33	118.81	109.45
4	D	4482	NAG	O4-C4-C5	4.32	120.68	109.28
4	C	3489	NAG	O4-C4-C5	4.23	120.44	109.28
2	A	1478	ZMR	O8-C8-C7	4.22	119.56	109.05
2	A	1478	ZMR	C9-C8-C7	4.20	121.90	112.38
4	A	1480	NAG	O4-C4-C5	4.20	120.34	109.28
4	C	3480	NAG	O4-C4-C3	4.19	119.74	110.35
2	C	3478	ZMR	O8-C8-C9	4.19	118.95	109.20
4	C	3487	NAG	O4-C4-C3	4.18	119.74	110.35
2	B	2477	ZMR	C8-C7-C6	4.17	121.08	112.99
4	B	2482	NAG	O4-C4-C5	4.15	120.21	109.28
4	A	1481	NAG	C3-C2-N2	-4.15	105.45	111.76
2	B	2477	ZMR	C4-C3-C2	-4.14	119.65	122.77
4	A	1481	NAG	C3-C4-C5	4.14	117.59	110.20
4	C	3481	NAG	O4-C4-C3	4.10	119.55	110.35
4	D	4482	NAG	O4-C4-C3	4.09	119.51	110.35
4	B	2482	NAG	O4-C4-C3	4.06	119.46	110.35
2	D	4477	ZMR	C8-C7-C6	4.06	120.86	112.99
4	C	3494	NAG	O4-C4-C5	4.06	119.97	109.28
4	B	2482	NAG	O5-C5-C6	4.05	111.23	106.98
4	D	4483	NAG	O5-C5-C6	4.04	111.22	106.98
2	B	2478	ZMR	C4-C5-N5	-4.03	106.75	110.81
2	A	1478	ZMR	O8-C8-C9	4.01	118.54	109.20
6	C	1709	BMA	C4-C3-C2	4.00	115.88	110.50
4	C	3486	NAG	O4-C4-C3	3.96	119.23	110.35
4	B	2480	NAG	O4-C4-C3	3.92	119.15	110.35
2	A	1477	ZMR	C9-C8-C7	3.91	121.25	112.38
5	C	3484	MAN	C4-C3-C2	3.89	115.72	110.50
2	D	4477	ZMR	C6-O6-C2	3.84	120.46	114.72

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3488	NAG	O4-C4-C3	3.84	118.96	110.35
4	C	3480	NAG	C3-C2-N2	-3.83	105.93	111.76
4	A	1480	NAG	O4-C4-C3	3.83	118.93	110.35
4	A	1482	NAG	O5-C5-C6	3.80	110.97	106.98
4	D	4484	NAG	O4-C4-C5	3.78	119.25	109.28
2	B	2478	ZMR	O6-C6-C5	3.78	115.02	110.29
4	D	4482	NAG	O5-C5-C6	3.73	110.89	106.98
4	C	3489	NAG	O5-C5-C6	3.68	110.84	106.98
2	D	4478	ZMR	O8-C8-C9	3.67	117.75	109.20
2	B	2477	ZMR	O8-C8-C9	3.63	117.66	109.20
2	B	2478	ZMR	O8-C8-C9	3.60	117.58	109.20
5	D	4480	MAN	C3-C4-C5	3.59	116.62	110.20
2	C	3478	ZMR	O7-C7-C8	3.59	117.81	108.74
2	C	3478	ZMR	C6-C5-C4	3.57	116.58	110.31
2	C	3477	ZMR	C8-C7-C6	3.51	119.79	112.99
2	D	4478	ZMR	O7-C7-C8	3.49	117.57	108.74
4	B	2481	NAG	C3-C2-N2	-3.49	106.45	111.76
2	A	1477	ZMR	O6-C6-C7	-3.44	99.35	105.73
2	C	3478	ZMR	C9-C8-C7	3.40	120.09	112.38
2	B	2477	ZMR	C4-C5-N5	-3.39	107.40	110.81
4	D	4483	NAG	O5-C5-C4	3.36	114.91	110.65
2	C	3478	ZMR	O6-C2-C3	-3.35	119.99	124.33
4	C	3486	NAG	C3-C2-N2	-3.31	106.72	111.76
2	B	2478	ZMR	O7-C7-C6	3.31	116.62	109.45
4	C	3480	NAG	O4-C4-C5	3.28	117.93	109.28
6	A	1709	BMA	C3-C4-C5	-3.27	104.37	110.20
4	A	1483	NAG	C3-C4-C5	3.26	116.03	110.20
5	B	2485	MAN	C4-C3-C2	3.25	114.86	110.50
2	D	4478	ZMR	C6-O6-C2	3.23	119.54	114.72
4	B	2483	NAG	O4-C4-C5	3.22	117.78	109.28
4	C	3494	NAG	O5-C5-C4	-3.23	106.56	110.65
2	B	2478	ZMR	O7-C7-C8	3.23	116.89	108.74
4	A	1480	NAG	O3-C3-C4	3.22	117.57	110.35
4	C	3494	NAG	C2-N2-C7	3.21	128.49	123.09
5	A	1485	MAN	C3-C4-C5	-3.20	104.49	110.20
2	C	3477	ZMR	O7-C7-C6	3.20	116.37	109.45
2	B	2478	ZMR	C9-C8-C7	3.18	119.60	112.38
5	B	2486	MAN	C3-C4-C5	-3.18	104.52	110.20
2	C	3477	ZMR	O6-C6-C5	3.15	114.24	110.29
5	C	3484	MAN	O2-C2-C3	3.14	116.95	110.18
4	A	1483	NAG	C4-C3-C2	-3.14	103.63	111.32
4	A	1480	NAG	O5-C5-C6	3.14	110.27	106.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2477	ZMR	O7-C7-C6	3.13	116.22	109.45
5	B	2485	MAN	O5-C5-C6	3.13	110.26	106.98
4	D	4482	NAG	C2-N2-C7	3.12	128.33	123.09
2	C	3478	ZMR	O6-C2-C1	3.12	118.03	111.88
4	C	3481	NAG	O5-C5-C6	3.12	110.25	106.98
2	A	1477	ZMR	C4-C3-C2	-3.12	120.42	122.77
4	B	2483	NAG	O5-C5-C6	3.11	110.25	106.98
4	B	2483	NAG	O4-C4-C3	3.10	117.30	110.35
4	D	4484	NAG	O4-C4-C3	3.09	117.29	110.35
2	B	2477	ZMR	C9-C8-C7	3.09	119.39	112.38
2	B	2477	ZMR	O9-C9-C8	-3.09	104.15	111.05
4	D	4484	NAG	C6-C5-C4	3.08	120.43	113.00
2	A	1477	ZMR	O8-C8-C9	3.04	116.29	109.20
2	D	4477	ZMR	C9-C8-C7	3.04	119.27	112.38
4	D	4485	NAG	C2-N2-C7	3.03	128.18	123.09
2	D	4477	ZMR	C4-C3-C2	-3.02	120.50	122.77
2	D	4478	ZMR	C9-C8-C7	3.00	119.18	112.38
2	A	1478	ZMR	C3-C4-NE	2.97	115.72	109.17
6	C	3493	BMA	C3-C4-C5	2.96	115.49	110.20
2	C	3477	ZMR	O8-C8-C9	2.95	116.08	109.20
2	D	4478	ZMR	O6-C2-C1	2.94	117.68	111.88
2	A	1477	ZMR	C6-C5-N5	-2.94	105.86	110.99
2	A	1478	ZMR	C4-C5-N5	-2.93	107.86	110.81
5	C	3483	MAN	O2-C2-C3	2.91	116.46	110.18
2	B	2478	ZMR	C5-N5-C10	2.89	130.73	123.02
2	A	1477	ZMR	O6-C2-C3	-2.84	120.64	124.33
2	D	4478	ZMR	C3-C4-NE	2.84	115.43	109.17
2	D	4477	ZMR	O1A-C1-C2	2.82	121.77	114.66
5	A	1485	MAN	O6-C6-C5	-2.81	101.68	111.36
2	D	4478	ZMR	O6-C2-C3	-2.80	120.70	124.33
4	B	2483	NAG	C3-C2-N2	-2.78	107.52	111.76
4	A	1480	NAG	C6-C5-C4	2.78	119.72	113.00
5	D	4481	MAN	O5-C5-C4	-2.77	107.14	110.65
2	A	1477	ZMR	O1A-C1-C2	2.76	121.60	114.66
4	C	3488	NAG	C8-C7-N2	2.75	121.49	116.11
5	A	1486	MAN	C3-C4-C5	2.74	115.09	110.20
4	C	3481	NAG	O4-C4-C5	2.73	116.47	109.28
6	D	4486	BMA	O5-C5-C6	2.73	109.84	106.98
6	A	1709	BMA	O2-C2-C3	2.72	116.04	110.18
4	B	2482	NAG	C3-C2-N2	2.72	115.90	111.76
4	D	4485	NAG	O4-C4-C5	2.71	116.42	109.28
5	C	3492	MAN	O5-C5-C6	2.70	109.82	106.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2478	ZMR	C3-C4-NE	2.69	115.11	109.17
5	B	2484	MAN	C3-C4-C5	-2.68	105.42	110.20
2	B	2477	ZMR	C6-O6-C2	2.68	118.72	114.72
4	A	1481	NAG	O5-C5-C6	2.67	109.79	106.98
4	D	4485	NAG	O5-C5-C6	2.67	109.79	106.98
6	C	3493	BMA	O2-C2-C3	2.67	115.93	110.18
2	C	3477	ZMR	O1A-C1-C2	2.64	121.30	114.66
4	D	4482	NAG	C3-C2-N2	2.62	115.76	111.76
2	B	2477	ZMR	O1A-C1-C2	2.62	121.26	114.66
2	A	1477	ZMR	C8-C7-C6	2.61	118.05	112.99
5	D	4481	MAN	C4-C3-C2	2.60	114.00	110.50
2	B	2477	ZMR	C5-C4-NE	-2.59	106.44	109.17
4	D	4482	NAG	O5-C5-C4	2.59	113.94	110.65
5	D	4480	MAN	O2-C2-C3	2.58	115.75	110.18
2	C	3477	ZMR	C3-C4-NE	2.55	114.80	109.17
2	D	4477	ZMR	O6-C6-C5	-2.54	107.11	110.29
2	D	4477	ZMR	NH2-CZ-NH1	-2.53	114.64	118.28
5	C	3485	MAN	O2-C2-C3	2.53	115.63	110.18
5	B	2484	MAN	O4-C4-C3	2.52	116.01	110.35
4	D	4485	NAG	C3-C2-N2	-2.50	107.95	111.76
5	D	4481	MAN	C3-C4-C5	2.48	114.62	110.20
2	C	3478	ZMR	O6-C6-C5	2.47	113.38	110.29
4	D	4484	NAG	C3-C2-N2	2.46	115.51	111.76
4	A	1483	NAG	O5-C5-C6	2.46	109.56	106.98
5	D	4480	MAN	O4-C4-C5	-2.40	102.95	109.28
4	C	3487	NAG	C2-N2-C7	-2.37	119.11	123.09
5	D	4480	MAN	O3-C3-C2	2.35	114.24	109.94
4	A	1483	NAG	O3-C3-C2	2.35	114.03	109.09
4	D	4484	NAG	O3-C3-C2	-2.35	104.16	109.09
2	C	3477	ZMR	C6-C5-N5	-2.34	106.90	110.99
5	A	1486	MAN	O2-C2-C3	2.34	115.22	110.18
2	A	1478	ZMR	O1A-C1-C2	2.34	120.54	114.66
5	C	3490	MAN	O5-C5-C4	-2.33	107.69	110.65
4	C	3489	NAG	O7-C7-N2	-2.32	117.05	121.90
5	A	1486	MAN	C4-C3-C2	2.31	113.60	110.50
4	C	3494	NAG	C3-C2-N2	-2.31	108.25	111.76
6	D	4486	BMA	O4-C4-C3	2.30	115.52	110.35
4	C	3481	NAG	O3-C3-C2	2.30	113.91	109.09
5	B	2484	MAN	C4-C3-C2	-2.29	107.43	110.50
5	C	3485	MAN	C4-C3-C2	2.29	113.58	110.50
5	C	3485	MAN	O4-C4-C3	2.28	115.47	110.35
6	C	3493	BMA	O5-C5-C4	2.27	113.54	110.65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1485	MAN	O4-C4-C3	2.25	115.39	110.35
2	C	3477	ZMR	C5-C4-NE	-2.23	106.82	109.17
2	D	4478	ZMR	C6-C5-C4	2.23	114.22	110.31
2	A	1477	ZMR	C3-C2-C1	2.22	128.50	124.12
6	D	4486	BMA	O3-C3-C4	2.21	115.32	110.35
2	A	1478	ZMR	C6-O6-C2	-2.20	111.43	114.72
2	A	1478	ZMR	O9-C9-C8	-2.16	106.21	111.05
5	D	4480	MAN	C6-C5-C4	-2.16	107.79	113.00
4	C	3481	NAG	O6-C6-C5	-2.16	103.94	111.36
4	A	1480	NAG	C3-C2-N2	-2.15	108.49	111.76
6	C	3493	BMA	C4-C3-C2	2.14	113.38	110.50
2	B	2477	ZMR	C7-C6-C5	2.14	117.40	114.24
4	A	1480	NAG	O3-C3-C2	-2.14	104.59	109.09
4	D	4484	NAG	O5-C5-C4	-2.13	107.95	110.65
2	D	4477	ZMR	O1B-C1-C2	-2.13	115.16	120.19
4	B	2483	NAG	C2-N2-C7	-2.10	119.56	123.09
5	B	2485	MAN	O2-C2-C3	2.10	114.70	110.18
6	A	1709	BMA	O4-C4-C3	2.10	115.05	110.35
2	D	4477	ZMR	C4-C5-N5	-2.09	108.70	110.81
4	C	3488	NAG	O7-C7-N2	-2.08	117.57	121.90
5	A	1485	MAN	O2-C2-C3	2.07	114.65	110.18
2	A	1477	ZMR	C5-C4-NE	-2.07	106.98	109.17
2	C	3478	ZMR	O10-C10-N5	2.06	126.21	121.90
2	C	3478	ZMR	C7-C6-C5	-2.06	111.21	114.24
4	D	4485	NAG	O6-C6-C5	-2.05	104.30	111.36
4	C	3487	NAG	O3-C3-C4	2.04	114.94	110.35
2	C	3477	ZMR	O1B-C1-C2	-2.04	115.36	120.19
2	C	3477	ZMR	C7-C6-C5	2.04	117.25	114.24
6	A	1709	BMA	O6-C6-C5	-2.04	104.34	111.36
4	A	1482	NAG	O5-C5-C4	-2.03	108.08	110.65
5	C	3485	MAN	O6-C6-C5	-2.00	104.47	111.36

All (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
4	B	2483	NAG	C4
4	C	3488	NAG	C4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
4	C	3481	NAG	C4
4	A	1481	NAG	C4
4	A	1481	NAG	C1
2	D	4478	ZMR	C8
2	D	4478	ZMR	C7
4	C	3487	NAG	C4
4	C	3480	NAG	C4
4	C	3494	NAG	C4
2	D	4477	ZMR	C8
2	D	4477	ZMR	C7
2	C	3477	ZMR	C8
2	C	3477	ZMR	C7
4	D	4482	NAG	C4
2	C	3478	ZMR	C8
2	C	3478	ZMR	C7
4	D	4484	NAG	C4
4	A	1480	NAG	C4
4	D	4485	NAG	C4
4	A	1483	NAG	C4
4	C	3489	NAG	C4
4	C	3489	NAG	C1
2	B	2478	ZMR	C8
2	B	2478	ZMR	C7
4	A	1482	NAG	C4
4	D	4483	NAG	C4
4	B	2482	NAG	C4
2	A	1477	ZMR	C8
2	A	1477	ZMR	C7
4	B	2480	NAG	C4
4	B	2481	NAG	C4

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

Continued on next page...

*Continued from previous page...*

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.