



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:09 am GMT

PDB ID : 1IVC  
Title : STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS  
NEURAMINIDASE  
Authors : Jedrzejewski, M.J.; Luo, M.  
Deposited on : 1994-12-12  
Resolution : 2.40 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	:	trunk28620
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)	:	recalc28949

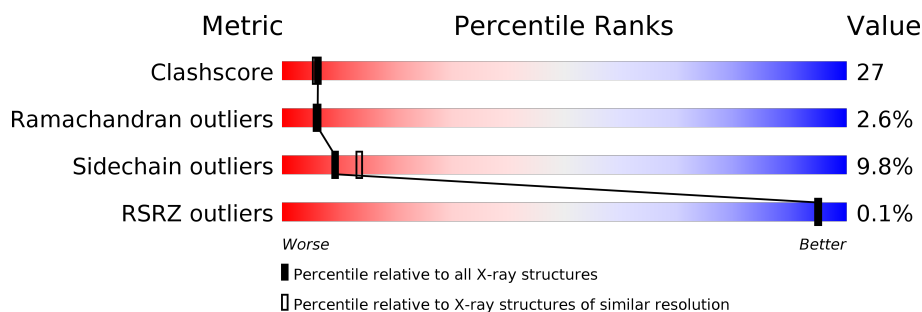
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	388	
1	B	388	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	472	-	-	-	X
2	NAG	A	484	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	472	-	-	-	X
2	NAG	B	484	-	-	-	X
3	FUL	A	477	-	-	X	-
4	NAG	A	478	-	-	X	X
4	MAN	A	481	-	-	X	-
4	MAN	A	483	-	-	X	X
4	NAG	B	478	-	-	-	X
4	MAN	B	483	-	-	X	X
5	FUC	B	477	X	-	-	-
7	ST2	A	471	-	-	-	X
7	ST2	B	471	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8220 atoms, of which 1790 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 INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			
1	B	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820
B	339	ASP	ASN	CONFLICT	UNP P06820

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
2	A	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
2	B	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
2	B	2	Total	C	H	N	O		0	0
			55	16	27	2	10			

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	4	Total	C	H	N	O		0	0
			96	28	47	2	19			

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	6	Total	C	H	N	O	0	0
			139	40	67	2	30		
4	B	6	Total	C	H	N	O	0	0
			139	40	67	2	30		

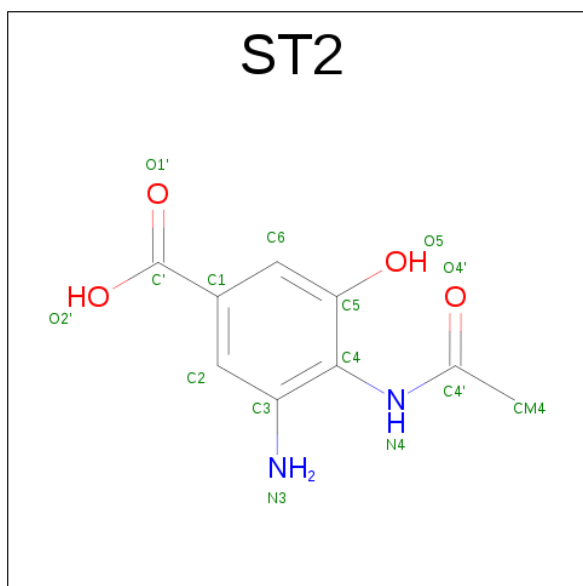
- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	4	Total	C	H	N	O	0	0
			96	28	47	2	19		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 4-(ACETYLAMINO)-5-AMINO-3-HYDROXYBENZOIC ACID (three-letter code: ST2) (formula: C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			19	9	4	2	4		
7	B	1	Total	C	H	N	O	0	0
			19	9	4	2	4		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.35Å 139.72Å 140.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.40 25.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.40) 61.4 (25.94-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.39Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.204 , (Not available) 0.217 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	1.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: BMA, NAG, CA, FUC, ST2, FUL, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.65	0/3092	0.91	3/4194 (0.1%)
1	B	0.65	0/3092	0.91	3/4194 (0.1%)
All	All	0.65	0/6184	0.91	6/8388 (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
5	B	1	0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	430	ARG	N-CA-C	5.66	126.28	111.00
1	B	430	ARG	N-CA-C	5.66	126.28	111.00
1	A	321	LEU	CA-CB-CG	-5.48	102.69	115.30
1	B	321	LEU	CA-CB-CG	-5.48	102.69	115.30
1	A	345	GLY	N-CA-C	5.15	125.97	113.10
1	B	345	GLY	N-CA-C	5.15	125.97	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	477	FUC	C1

There are no planarity outliers.



## 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	3022	723	2852	143	3
1	B	3022	723	2852	159	1
2	A	56	54	50	6	0
2	B	56	54	50	6	0
3	A	49	47	43	1	6
4	A	72	67	61	28	6
4	B	72	67	61	15	2
5	B	49	47	43	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	15	4	9	3	0
7	B	15	4	9	3	0
All	All	6430	1790	6030	334	9

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 27.

All (334) 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)
4:B:483:MAN:C4	4:B:483:MAN:C5	1.76	1.61
4:A:483:MAN:C4	4:A:483:MAN:C5	1.76	1.56
4:A:478:NAG:H61	1:B:455:THR:CG2	1.60	1.32
4:A:478:NAG:C6	1:B:455:THR:HG21	1.59	1.31
4:A:483:MAN:H2	1:B:455:THR:CG2	1.82	1.10
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.20	1.06
1:B:334:ASN:HA	1:B:387:ASN:HD21	1.20	1.01
1:B:177:ALA:HB2	1:B:193:CYS:HB3	1.48	0.96
4:A:478:NAG:H61	1:B:455:THR:HG21	0.98	0.95
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.48	0.95
4:A:483:MAN:H2	1:B:455:THR:HG22	1.47	0.93
1:B:184:HIS:HD2	1:B:186:GLY:H	1.23	0.86
1:B:437:TRP:H	1:B:469:ILE:HG21	1.43	0.82
1:A:184:HIS:HD2	1:A:186:GLY:H	1.23	0.82
1:A:437:TRP:H	1:A:469:ILE:HG21	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:HIS:CD2	1:B:186:GLY:H	1.99	0.81
1:A:184:HIS:CD2	1:A:186:GLY:H	1.99	0.80
1:B:406:TYR:OH	7:B:471:ST2:H2	1.83	0.78
1:A:311:SER:O	1:A:312:ILE:HD13	1.83	0.78
1:A:406:TYR:OH	7:A:471:ST2:H2	1.83	0.78
1:B:311:SER:O	1:B:312:ILE:HD13	1.83	0.78
1:B:338:ARG:HG2	1:B:338:ARG:HH11	1.51	0.75
1:A:338:ARG:HH11	1:A:338:ARG:HG2	1.51	0.74
1:B:411:SER:HB3	1:B:418:ILE:CD1	2.19	0.73
1:A:411:SER:HB3	1:A:418:ILE:CD1	2.19	0.72
1:A:334:ASN:HA	1:A:387:ASN:ND2	2.01	0.72
4:A:483:MAN:C2	1:B:455:THR:CG2	2.64	0.72
1:A:176:ILE:HG22	1:A:195:THR:HG21	1.73	0.71
4:A:483:MAN:H2	1:B:455:THR:HG21	1.71	0.70
4:B:483:MAN:C6	4:B:483:MAN:C4	2.70	0.70
4:A:483:MAN:C6	4:A:483:MAN:C4	2.70	0.69
1:B:334:ASN:HA	1:B:387:ASN:ND2	2.01	0.69
1:B:176:ILE:HG22	1:B:195:THR:HG21	1.73	0.69
1:A:273:GLN:HG3	1:A:340:PRO:HG3	1.75	0.68
1:A:270:GLY:HA3	1:A:314:SER:H	1.58	0.68
1:A:352:TRP:HD1	1:A:407:SER:HG	1.42	0.68
1:A:144:HIS:HE1	1:B:462:ALA:HA	1.59	0.67
4:A:478:NAG:O6	4:A:479:NAG:N2	2.28	0.67
1:B:273:GLN:HG3	1:B:340:PRO:HG3	1.75	0.67
1:B:270:GLY:HA3	1:B:314:SER:H	1.58	0.67
4:A:478:NAG:H61	1:B:455:THR:CB	2.23	0.67
1:B:184:HIS:HD2	1:B:186:GLY:N	1.92	0.66
4:B:478:NAG:O6	4:B:479:NAG:N2	2.28	0.66
1:A:184:HIS:HD2	1:A:186:GLY:N	1.92	0.66
1:B:245:SER:O	1:B:274:HIS:HE1	1.79	0.66
1:B:366:ILE:HG12	1:B:375:GLU:HG2	1.77	0.66
1:A:245:SER:O	1:A:274:HIS:HE1	1.79	0.65
1:A:366:ILE:HG12	1:A:375:GLU:HG2	1.77	0.65
4:A:478:NAG:O6	1:B:455:THR:HG21	1.96	0.65
1:A:411:SER:HB3	1:A:418:ILE:HD13	1.79	0.65
1:B:366:ILE:CG1	1:B:375:GLU:HG2	2.27	0.64
1:B:352:TRP:HD1	1:B:407:SER:HG	1.46	0.64
1:B:258:GLU:HG3	1:B:263:VAL:HG21	1.80	0.64
1:A:366:ILE:CG1	1:A:375:GLU:HG2	2.27	0.64
1:A:427:ILE:HD11	1:A:439:THR:HG23	1.80	0.64
2:A:473:NAG:H61	2:A:473:NAG:H2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:HD13	1:B:265:ILE:HG12	1.79	0.64
7:B:471:ST2:HN32	7:B:471:ST2:HM43	1.63	0.64
1:A:255:LEU:HD13	1:A:265:ILE:HG12	1.79	0.63
1:A:258:GLU:HG3	1:A:263:VAL:HG21	1.80	0.63
1:A:144:HIS:CD2	1:B:466:PHE:HD2	2.16	0.63
4:A:483:MAN:H4	4:A:483:MAN:C5	2.15	0.63
1:B:427:ILE:HD11	1:B:439:THR:HG23	1.80	0.63
1:B:411:SER:HB3	1:B:418:ILE:HD13	1.79	0.63
1:B:347:GLN:N	1:B:347:GLN:OE1	2.32	0.62
4:A:478:NAG:O5	1:B:455:THR:HB	1.98	0.62
7:A:471:ST2:HM43	7:A:471:ST2:HN32	1.63	0.62
1:A:347:GLN:OE1	1:A:347:GLN:N	2.32	0.62
1:B:338:ARG:HD3	1:B:339:ASP:OD2	2.00	0.62
1:B:359:ASP:OD1	1:B:380:ILE:HA	1.99	0.62
1:B:274:HIS:HD2	1:B:294:ASN:H	1.48	0.62
1:A:359:ASP:OD1	1:A:380:ILE:HA	1.99	0.62
1:A:274:HIS:HD2	1:A:294:ASN:H	1.48	0.61
2:B:473:NAG:H2	2:B:473:NAG:H61	1.80	0.61
1:B:136:GLN:CD	1:B:156:ARG:HH11	2.04	0.61
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.83	0.61
1:A:136:GLN:CD	1:A:156:ARG:HH11	2.04	0.61
1:B:281:TYR:HB2	1:B:420:ARG:HH21	1.66	0.61
1:A:338:ARG:HD3	1:A:339:ASP:OD2	2.00	0.61
1:B:328:ASN:O	1:B:329:ASP:HB3	2.01	0.61
1:B:224:ARG:NH2	1:B:244:GLY:N	2.49	0.60
1:A:328:ASN:O	1:A:329:ASP:HB3	2.01	0.60
1:A:281:TYR:HB2	1:A:420:ARG:HH21	1.66	0.60
1:A:227:GLU:HA	1:A:227:GLU:OE1	2.02	0.60
1:A:224:ARG:NH2	1:A:244:GLY:N	2.49	0.59
1:B:131:GLN:HE21	1:B:163:LEU:HD12	1.67	0.59
1:A:131:GLN:HE21	1:A:163:LEU:HD12	1.67	0.59
1:A:202:THR:HB	1:B:454:GLY:H	1.67	0.59
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.83	0.59
1:B:226:GLN:O	1:B:227:GLU:HB2	2.03	0.58
1:A:109:SER:HB3	1:A:140:LEU:HD13	1.85	0.58
1:B:109:SER:HB3	1:B:140:LEU:HD13	1.85	0.58
1:B:257:ILE:O	1:B:257:ILE:HD13	2.04	0.58
1:A:125:ASP:OD1	1:A:127:VAL:HG22	2.03	0.57
1:A:226:GLN:O	1:A:227:GLU:HB2	2.03	0.57
1:B:125:ASP:OD1	1:B:127:VAL:HG22	2.03	0.57
1:B:227:GLU:OE1	1:B:227:GLU:HA	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ILE:HG12	1:B:393:ASN:H	1.69	0.57
1:A:378:LYS:HG2	1:A:379:VAL:N	2.20	0.57
1:A:257:ILE:HD13	1:A:257:ILE:O	2.04	0.57
4:A:480:BMA:O6	4:A:483:MAN:C6	2.53	0.57
1:B:378:LYS:HG2	1:B:379:VAL:N	2.20	0.57
4:B:480:BMA:O6	4:B:483:MAN:C6	2.53	0.56
1:A:392:ILE:HG12	1:A:393:ASN:H	1.69	0.56
1:A:144:HIS:ND1	1:B:107:ARG:HG2	2.21	0.56
1:A:295:TRP:O	1:A:346:THR:HA	2.06	0.56
1:B:295:TRP:O	1:B:346:THR:HA	2.06	0.56
1:A:84:TYR:CE1	1:A:187:LYS:HD2	2.42	0.55
1:B:84:TYR:CE1	1:B:187:LYS:HD2	2.42	0.55
4:A:478:NAG:C1	1:B:455:THR:OG1	2.54	0.55
2:A:473:NAG:C6	2:A:473:NAG:H2	2.36	0.55
1:B:338:ARG:HG2	1:B:338:ARG:NH1	2.21	0.55
2:B:473:NAG:H2	2:B:473:NAG:C6	2.36	0.55
1:B:281:TYR:OH	1:B:288:ARG:HD2	2.07	0.55
1:A:203:ALA:HB3	1:A:215:ILE:HG22	1.89	0.55
1:A:281:TYR:OH	1:A:288:ARG:HD2	2.07	0.55
1:B:179:SER:HB3	1:B:194:ILE:HD12	1.88	0.55
1:B:203:ALA:HB3	1:B:215:ILE:HG22	1.89	0.55
1:B:118:ARG:HD2	1:B:427:ILE:HG13	1.89	0.55
1:A:258:GLU:HG3	1:A:263:VAL:CG2	2.38	0.54
1:B:292:ARG:NH1	1:B:294:ASN:OD1	2.40	0.54
1:A:179:SER:HB3	1:A:194:ILE:HD12	1.88	0.54
1:B:258:GLU:HG3	1:B:263:VAL:CG2	2.38	0.54
1:B:365:THR:HG21	1:B:371:ARG:HA	1.90	0.54
1:A:118:ARG:HD2	1:A:427:ILE:HG13	1.89	0.53
4:B:483:MAN:H4	4:B:483:MAN:C5	2.15	0.53
1:A:109:SER:CB	1:A:140:LEU:HD13	2.39	0.53
1:A:338:ARG:NH1	1:A:338:ARG:HG2	2.21	0.53
4:A:480:BMA:O6	4:A:483:MAN:H62	2.08	0.53
1:A:263:VAL:O	1:A:264:HIS:HB2	2.09	0.53
1:A:365:THR:HG21	1:A:371:ARG:HA	1.90	0.53
1:B:430:ARG:HG3	1:B:431:LYS:H	1.73	0.53
1:B:109:SER:CB	1:B:140:LEU:HD13	2.39	0.53
4:B:480:BMA:O6	4:B:483:MAN:H62	2.08	0.53
1:A:144:HIS:CE1	1:B:462:ALA:HA	2.40	0.53
1:A:430:ARG:HG3	1:A:431:LYS:H	1.73	0.52
4:A:483:MAN:C2	1:B:455:THR:HG21	2.38	0.52
1:B:263:VAL:O	1:B:264:HIS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ALA:O	1:A:274:HIS:NE2	2.43	0.52
4:A:478:NAG:C6	1:B:455:THR:CG2	2.45	0.52
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.92	0.52
1:A:437:TRP:N	1:A:469:ILE:HG21	2.21	0.51
1:B:246:ALA:O	1:B:274:HIS:NE2	2.43	0.51
4:A:478:NAG:O6	4:A:479:NAG:C1	2.58	0.51
1:B:256:PHE:CD2	1:B:310:TYR:HD1	2.29	0.51
4:B:478:NAG:O6	4:B:479:NAG:C1	2.58	0.51
1:A:377:PHE:HB3	1:A:394:ARG:HA	1.93	0.51
1:B:377:PHE:HB3	1:B:394:ARG:HA	1.93	0.51
1:A:292:ARG:NH1	1:A:294:ASN:OD1	2.40	0.51
1:A:273:GLN:OE1	1:A:296:LYS:HE3	2.11	0.51
1:B:253:ARG:C	1:B:254:ILE:HD12	2.31	0.51
1:A:253:ARG:C	1:A:254:ILE:HD12	2.31	0.50
1:A:86:ASN:HB3	1:A:234:ASN:OD1	2.11	0.50
1:A:176:ILE:HG22	1:A:195:THR:CG2	2.42	0.50
1:B:176:ILE:HG22	1:B:195:THR:CG2	2.42	0.50
1:B:273:GLN:OE1	1:B:296:LYS:HE3	2.11	0.50
1:A:331:ARG:HA	1:A:331:ARG:NH1	2.27	0.50
1:B:86:ASN:HB3	1:B:234:ASN:OD1	2.11	0.50
1:B:331:ARG:HA	1:B:331:ARG:NH1	2.27	0.50
1:A:89:LYS:NZ	1:A:414:GLY:O	2.44	0.50
1:A:256:PHE:CD2	1:A:310:TYR:HD1	2.29	0.49
4:A:478:NAG:O5	1:B:455:THR:CB	2.59	0.49
1:B:136:GLN:NE2	1:B:156:ARG:NH1	2.61	0.49
1:B:240:VAL:HG12	1:B:254:ILE:HG13	1.95	0.49
1:B:89:LYS:NZ	1:B:414:GLY:O	2.44	0.49
1:A:378:LYS:HG2	1:A:379:VAL:H	1.77	0.49
1:B:378:LYS:HG2	1:B:379:VAL:H	1.77	0.49
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.92	0.49
1:A:198:ASP:HB3	1:A:222:ILE:CG1	2.43	0.49
1:B:117:THR:HG22	1:B:135:GLY:HA2	1.95	0.48
1:B:198:ASP:HB3	1:B:222:ILE:CG1	2.43	0.48
1:B:258:GLU:OE2	1:B:263:VAL:HG21	2.13	0.48
1:A:136:GLN:NE2	1:A:156:ARG:NH1	2.61	0.48
1:B:198:ASP:HB3	1:B:222:ILE:HG12	1.95	0.48
1:A:296:LYS:HE2	1:A:340:PRO:HG3	1.95	0.48
1:A:437:TRP:H	1:A:469:ILE:CG2	2.22	0.48
1:A:298:SER:O	1:A:324:ASP:HB2	2.14	0.48
4:A:479:NAG:HN2	4:A:483:MAN:C1	2.27	0.48
1:A:240:VAL:HG12	1:A:254:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLN:N	1:A:347:GLN:CD	2.67	0.48
4:A:480:BMA:H2	4:A:481:MAN:O6	2.14	0.48
1:B:257:ILE:HD13	1:B:257:ILE:C	2.34	0.48
1:B:347:GLN:CD	1:B:347:GLN:N	2.67	0.48
1:A:198:ASP:HB3	1:A:222:ILE:HG12	1.95	0.48
1:A:100:PHE:HB3	1:A:445:VAL:HG22	1.96	0.48
1:A:258:GLU:OE2	1:A:263:VAL:HG21	2.13	0.48
1:A:399:ASP:CG	1:A:402:ASN:HD22	2.17	0.48
1:B:296:LYS:HE2	1:B:340:PRO:HG3	1.95	0.48
1:B:100:PHE:HB3	1:B:445:VAL:HG22	1.96	0.48
1:B:149:VAL:HG22	1:B:430:ARG:HB3	1.95	0.48
1:B:399:ASP:CG	1:B:402:ASN:HD22	2.17	0.48
1:A:257:ILE:HD13	1:A:257:ILE:C	2.34	0.47
4:A:480:BMA:C2	4:A:481:MAN:O6	2.62	0.47
1:B:437:TRP:N	1:B:469:ILE:HG21	2.21	0.47
4:B:480:BMA:C2	4:B:481:MAN:O6	2.62	0.47
1:A:427:ILE:HG12	1:A:440:SER:O	2.14	0.47
2:B:484:NAG:O6	2:B:485:NAG:C1	2.62	0.47
1:A:210:ARG:HE	1:A:210:ARG:N	2.12	0.47
1:A:149:VAL:HG22	1:A:430:ARG:HB3	1.95	0.47
2:A:484:NAG:O6	2:A:485:NAG:C1	2.62	0.47
1:B:298:SER:O	1:B:324:ASP:HB2	2.14	0.47
1:B:437:TRP:HD1	1:B:469:ILE:CG2	2.28	0.47
1:B:427:ILE:HG12	1:B:440:SER:O	2.14	0.47
4:B:479:NAG:HN2	4:B:483:MAN:C1	2.27	0.47
1:A:117:THR:HG22	1:A:135:GLY:HA2	1.95	0.47
1:A:256:PHE:CD2	1:A:310:TYR:CD1	3.03	0.47
1:B:154:PRO:HG2	1:B:155:HIS:CE1	2.50	0.47
1:B:97:PHE:HB3	1:B:446:PHE:HB3	1.96	0.47
1:A:154:PRO:HG2	1:A:155:HIS:CE1	2.50	0.47
1:A:245:SER:O	1:A:274:HIS:CE1	2.64	0.47
4:A:483:MAN:C6	4:A:483:MAN:H4	2.43	0.47
1:B:210:ARG:HE	1:B:210:ARG:N	2.12	0.47
1:A:385:THR:HA	1:A:386:PRO:HD2	1.74	0.47
1:A:144:HIS:CE1	1:B:463:ASN:H	2.33	0.47
1:B:256:PHE:CD2	1:B:310:TYR:CD1	3.03	0.47
1:A:97:PHE:HB3	1:A:446:PHE:HB3	1.96	0.47
4:B:479:NAG:H3	4:B:483:MAN:C6	2.45	0.47
1:A:269:ALA:HB3	1:A:312:ILE:O	2.15	0.46
4:B:480:BMA:H2	4:B:481:MAN:O6	2.14	0.46
1:B:245:SER:O	1:B:274:HIS:CE1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:483:MAN:H4	4:B:483:MAN:C6	2.43	0.46
1:A:197:ASP:O	1:A:201:ALA:HB2	2.15	0.46
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.44	0.46
1:A:139:THR:O	1:A:142:ASN:HB3	2.15	0.46
1:A:328:ASN:O	1:A:329:ASP:CB	2.64	0.46
1:B:139:THR:O	1:B:142:ASN:HB3	2.15	0.46
1:B:468:PRO:O	1:B:469:ILE:HB	2.15	0.46
1:A:299:ASN:HB3	1:A:322:VAL:HG22	1.98	0.46
1:A:308:GLU:HG3	2:A:484:NAG:H82	1.97	0.46
4:A:479:NAG:H3	4:A:483:MAN:C6	2.45	0.46
1:B:269:ALA:HB3	1:B:312:ILE:O	2.15	0.46
1:B:328:ASN:O	1:B:329:ASP:CB	2.64	0.46
2:B:473:NAG:C6	2:B:473:NAG:C2	2.94	0.46
1:A:437:TRP:HD1	1:A:469:ILE:CG2	2.28	0.46
1:A:136:GLN:CD	1:A:156:ARG:NH1	2.69	0.46
1:B:331:ARG:HA	1:B:331:ARG:HH11	1.81	0.46
1:A:468:PRO:O	1:A:469:ILE:HB	2.15	0.46
1:B:184:HIS:CD2	1:B:186:GLY:N	2.75	0.45
1:B:197:ASP:O	1:B:201:ALA:HB2	2.15	0.45
1:B:344:ARG:HH22	1:B:369:ASP:CG	2.19	0.45
1:A:176:ILE:CG2	1:A:195:THR:HG21	2.45	0.45
1:A:331:ARG:HH11	1:A:331:ARG:HA	1.81	0.45
4:A:480:BMA:O2	4:A:481:MAN:H5	2.16	0.45
1:B:294:ASN:OD1	1:B:347:GLN:HA	2.17	0.45
4:B:480:BMA:O2	4:B:481:MAN:H5	2.16	0.45
1:A:358:ASN:HB3	1:A:384:SER:OG	2.17	0.45
1:B:136:GLN:CD	1:B:156:ARG:NH1	2.69	0.45
1:B:165:VAL:HA	1:B:166:PRO:HD3	1.77	0.45
1:A:294:ASN:OD1	1:A:347:GLN:HA	2.17	0.45
1:A:344:ARG:HH22	1:A:369:ASP:CG	2.19	0.45
1:B:256:PHE:CE2	1:B:310:TYR:HD1	2.35	0.45
2:A:473:NAG:C2	2:A:473:NAG:C6	2.94	0.45
1:B:326:PRO:HA	1:B:368:LYS:O	2.17	0.45
1:A:184:HIS:CD2	1:A:186:GLY:N	2.75	0.45
1:A:256:PHE:CE2	1:A:310:TYR:HD1	2.35	0.45
1:B:288:ARG:NH1	1:B:383:TRP:CZ2	2.85	0.45
1:B:308:GLU:HG3	2:B:484:NAG:H82	1.97	0.45
1:A:288:ARG:NH1	1:A:383:TRP:CZ2	2.85	0.44
1:B:238:THR:HG21	1:B:305:ILE:HD13	1.99	0.44
1:A:165:VAL:HA	1:A:166:PRO:HD3	1.77	0.44
1:A:326:PRO:HA	1:A:368:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:ND2	1:B:387:ASN:OD1	2.50	0.44
1:A:224:ARG:HH21	1:A:244:GLY:N	2.16	0.44
1:B:320:GLY:HA3	1:B:387:ASN:ND2	2.33	0.44
1:A:334:ASN:ND2	1:A:387:ASN:OD1	2.50	0.44
1:B:358:ASN:HB3	1:B:384:SER:OG	2.17	0.44
1:B:229:GLU:OE2	1:B:410:PHE:HA	2.18	0.44
1:B:299:ASN:HB3	1:B:322:VAL:HG22	1.98	0.44
1:A:320:GLY:HA3	1:A:387:ASN:ND2	2.33	0.43
1:A:329:ASP:C	1:A:329:ASP:OD1	2.57	0.43
1:A:229:GLU:OE2	1:A:410:PHE:HA	2.18	0.43
1:A:241:MET:HE2	1:A:255:LEU:HG	2.00	0.43
1:B:385:THR:HA	1:B:386:PRO:HD2	1.74	0.43
4:A:479:NAG:H3	4:A:483:MAN:O5	2.19	0.43
1:A:366:ILE:HG13	1:A:375:GLU:HG2	2.01	0.43
1:B:329:ASP:C	1:B:329:ASP:OD1	2.57	0.43
1:A:173:GLN:OE1	1:B:103:ASP:O	2.36	0.43
1:B:142:ASN:HD22	1:B:143:LYS:N	2.16	0.42
1:B:419:ASN:HD21	1:B:448:GLY:HA3	1.84	0.42
1:B:151:ASP:HB3	7:B:471:ST2:O4'	2.19	0.42
1:B:254:ILE:HD12	1:B:254:ILE:N	2.35	0.42
1:A:238:THR:HG21	1:A:305:ILE:HD13	1.99	0.42
1:A:392:ILE:HG12	1:A:393:ASN:N	2.33	0.42
1:A:169:LEU:HD11	1:B:112:GLY:HA3	2.01	0.42
1:A:142:ASN:HD22	1:A:143:LYS:N	2.16	0.42
1:B:224:ARG:NH2	1:B:244:GLY:H	2.17	0.42
1:B:241:MET:HE2	1:B:255:LEU:HG	2.01	0.42
4:B:479:NAG:H3	4:B:483:MAN:O5	2.19	0.42
3:A:475:NAG:H5	3:A:476:BMA:O6	2.20	0.42
1:B:157:THR:HG22	1:B:176:ILE:HA	2.02	0.42
1:B:437:TRP:H	1:B:469:ILE:CG2	2.22	0.42
1:A:419:ASN:HD21	1:A:448:GLY:HA3	1.84	0.42
1:A:151:ASP:HB3	7:A:471:ST2:O4'	2.19	0.42
1:A:162:GLU:O	1:A:165:VAL:HG13	2.20	0.42
1:B:84:TYR:HE1	1:B:185:ASP:OD2	2.03	0.42
1:B:224:ARG:HH21	1:B:244:GLY:N	2.16	0.42
1:B:320:GLY:CA	1:B:387:ASN:HD22	2.33	0.42
5:B:475:NAG:H5	5:B:476:BMA:O6	2.20	0.42
1:B:176:ILE:CG2	1:B:195:THR:HG21	2.45	0.42
1:A:157:THR:HG22	1:A:176:ILE:HA	2.02	0.41
1:A:426:LEU:HD11	1:A:444:VAL:CG2	2.50	0.41
1:B:431:LYS:HD2	1:B:431:LYS:HA	1.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:O	1:B:107:ARG:NH2	2.49	0.41
1:B:426:LEU:HD11	1:B:444:VAL:CG2	2.50	0.41
1:A:320:GLY:CA	1:A:387:ASN:HD22	2.33	0.41
1:A:430:ARG:HG3	1:A:431:LYS:N	2.36	0.41
1:B:288:ARG:CZ	1:B:383:TRP:CZ2	3.04	0.41
1:B:118:ARG:HG2	1:B:425:GLU:OE2	2.20	0.41
1:A:399:ASP:OD2	1:A:402:ASN:ND2	2.53	0.41
1:A:84:TYR:HE1	1:A:185:ASP:OD2	2.03	0.41
1:B:399:ASP:OD2	1:B:402:ASN:ND2	2.53	0.41
1:B:162:GLU:O	1:B:165:VAL:HG13	2.20	0.41
1:B:430:ARG:CG	1:B:431:LYS:H	2.33	0.41
4:B:478:NAG:C6	4:B:479:NAG:C1	2.99	0.41
1:A:224:ARG:NH2	1:A:244:GLY:H	2.17	0.41
1:A:284:TYR:CE1	2:A:484:NAG:O7	2.74	0.41
1:A:254:ILE:N	1:A:254:ILE:HD12	2.35	0.41
1:A:90:PRO:O	1:A:417:CYS:HB2	2.21	0.41
1:B:246:ALA:O	1:B:274:HIS:CE1	2.74	0.40
1:B:320:GLY:CA	1:B:387:ASN:ND2	2.84	0.40
1:B:392:ILE:HG12	1:B:393:ASN:N	2.33	0.40
1:B:284:TYR:CE1	2:B:484:NAG:O7	2.74	0.40
1:A:118:ARG:HG2	1:A:425:GLU:OE2	2.20	0.40
1:B:125:ASP:OD2	1:B:130:TYR:HE1	2.04	0.40
1:B:430:ARG:HG3	1:B:431:LYS:N	2.36	0.40
1:A:272:ALA:HA	1:A:316:TYR:HE1	1.86	0.40
1:A:246:ALA:O	1:A:274:HIS:CE1	2.74	0.40
1:A:319:SER:OG	1:A:321:LEU:HB2	2.22	0.40
1:A:288:ARG:CZ	1:A:383:TRP:CZ2	3.04	0.40
1:A:430:ARG:CG	1:A:431:LYS:H	2.33	0.40
1:B:85:ARG:HD2	1:B:184:HIS:O	2.22	0.40
1:A:320:GLY:CA	1:A:387:ASN:ND2	2.84	0.40
1:B:182:SER:HA	1:B:190:LEU:O	2.21	0.40
1:B:319:SER:OG	1:B:321:LEU:HB2	2.22	0.40

All (9) 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)
3:A:477:FUL:H4	4:A:481:MAN:H1[3_654]	0.90	0.70
3:A:477:FUL:H1	4:A:481:MAN:O3[3_654]	0.96	0.64
3:A:477:FUL:H5	4:A:481:MAN:O5[3_654]	1.26	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:THR:HG1	4:B:478:NAG:H1[4_555]	1.31	0.29
1:A:338:ARG:HH21	1:B:315:SER:HG[7_554]	1.34	0.26
1:A:455:THR:CG2	4:B:478:NAG:H61[4_555]	1.42	0.18
3:A:477:FUL:O5	4:A:481:MAN:O5[3_654]	2.05	0.15
3:A:477:FUL:C4	4:A:481:MAN:H1[3_654]	1.59	0.01
3:A:477:FUL:O5	4:A:481:MAN:H4[3_654]	1.60	0.00

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/388 (100%)	338 (88%)	38 (10%)	10 (3%)	6	6
1	B	386/388 (100%)	338 (88%)	38 (10%)	10 (3%)	6	6
All	All	772/776 (100%)	676 (88%)	76 (10%)	20 (3%)	6	6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	330	ASP
1	A	346	THR
1	A	347	GLN
1	B	329	ASP
1	B	330	ASP
1	B	346	THR
1	B	347	GLN
1	A	322	VAL
1	A	382	GLY
1	B	322	VAL
1	B	382	GLY
1	A	264	HIS
1	A	430	ARG

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Mol	Chain	Res	Type
1	B	264	HIS
1	B	430	ARG
1	A	431	LYS
1	B	431	LYS
1	A	222	ILE
1	B	222	ILE

### 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	338/338 (100%)	305 (90%)	33 (10%)	9	14
1	B	338/338 (100%)	305 (90%)	33 (10%)	9	14
All	All	676/676 (100%)	610 (90%)	66 (10%)	9	14

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	165	VAL
1	A	174	VAL
1	A	179	SER
1	A	190	LEU
1	A	192	VAL
1	A	195	THR
1	A	199	LYS
1	A	202	THR
1	A	210	ARG
1	A	213	ASP
1	A	227	GLU
1	A	230	CYS
1	A	239	VAL
1	A	249	ARG
1	A	257	ILE
1	A	292	ARG

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Mol	Chain	Res	Type
1	A	315	SER
1	A	329	ASP
1	A	337	CYS
1	A	338	ARG
1	A	347	GLN
1	A	375	GLU
1	A	385	THR
1	A	387	ASN
1	A	390	SER
1	A	412	VAL
1	A	418	ILE
1	A	420	ARG
1	A	427	ILE
1	A	430	ARG
1	A	431	LYS
1	A	445	VAL
1	B	142	ASN
1	B	165	VAL
1	B	174	VAL
1	B	179	SER
1	B	190	LEU
1	B	192	VAL
1	B	195	THR
1	B	199	LYS
1	B	202	THR
1	B	210	ARG
1	B	213	ASP
1	B	227	GLU
1	B	230	CYS
1	B	239	VAL
1	B	249	ARG
1	B	257	ILE
1	B	292	ARG
1	B	315	SER
1	B	329	ASP
1	B	337	CYS
1	B	338	ARG
1	B	347	GLN
1	B	375	GLU
1	B	385	THR
1	B	387	ASN
1	B	390	SER

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Mol	Chain	Res	Type
1	B	412	VAL
1	B	418	ILE
1	B	420	ARG
1	B	427	ILE
1	B	430	ARG
1	B	431	LYS
1	B	445	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	131	GLN
1	A	142	ASN
1	A	144	HIS
1	A	173	GLN
1	A	184	HIS
1	A	274	HIS
1	A	334	ASN
1	A	387	ASN
1	A	393	ASN
1	A	402	ASN
1	A	419	ASN
1	B	104	ASN
1	B	131	GLN
1	B	142	ASN
1	B	155	HIS
1	B	184	HIS
1	B	274	HIS
1	B	334	ASN
1	B	387	ASN
1	B	393	ASN
1	B	402	ASN
1	B	419	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 ⓘ

28 carbohydrates 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	472	1,2	14,14,15	2.10	6 (42%)	15,19,21	3.10	5 (33%)
2	NAG	A	473	2	14,14,15	3.56	6 (42%)	15,19,21	3.26	8 (53%)
3	NAG	A	474	1,3	14,14,15	1.75	3 (21%)	15,19,21	3.04	7 (46%)
3	NAG	A	475	3	14,14,15	2.50	7 (50%)	15,19,21	3.98	8 (53%)
3	BMA	A	476	3	11,11,12	3.65	7 (63%)	13,15,17	3.01	5 (38%)
3	FUL	A	477	3,4	9,10,11	3.36	5 (55%)	13,14,16	2.85	7 (53%)
4	NAG	A	478	1,4	14,14,15	3.57	7 (50%)	15,19,21	3.46	10 (66%)
4	NAG	A	479	4	14,14,15	3.37	4 (28%)	15,19,21	2.56	5 (33%)
4	BMA	A	480	4	11,11,12	5.02	8 (72%)	13,15,17	3.40	8 (61%)
4	MAN	A	481	3,4	11,11,12	2.70	6 (54%)	13,15,17	2.88	8 (61%)
4	MAN	A	482	4	11,11,12	3.90	8 (72%)	13,15,17	1.78	3 (23%)
4	MAN	A	483	4	11,11,12	4.95	9 (81%)	13,15,17	2.92	8 (61%)
2	NAG	A	484	1,2	14,14,15	3.37	6 (42%)	15,19,21	3.62	10 (66%)
2	NAG	A	485	2	14,14,15	1.78	4 (28%)	15,19,21	4.12	11 (73%)
2	NAG	B	472	1,2	14,14,15	2.10	6 (42%)	15,19,21	3.10	5 (33%)
2	NAG	B	473	2	14,14,15	3.56	6 (42%)	15,19,21	3.26	8 (53%)
5	NAG	B	474	1,5	14,14,15	1.75	3 (21%)	15,19,21	3.04	7 (46%)
5	NAG	B	475	5	14,14,15	2.50	7 (50%)	15,19,21	3.98	8 (53%)
5	BMA	B	476	5	11,11,12	3.65	7 (63%)	13,15,17	3.01	5 (38%)
5	FUC	B	477	5	9,10,11	3.36	5 (55%)	13,14,16	2.85	7 (53%)
4	NAG	B	478	1,4	14,14,15	3.57	7 (50%)	15,19,21	3.46	10 (66%)
4	NAG	B	479	4	14,14,15	3.37	4 (28%)	15,19,21	2.56	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	B	480	4	11,11,12	5.02	8 (72%)	13,15,17	3.40	8 (61%)
4	MAN	B	481	4	11,11,12	2.70	6 (54%)	13,15,17	2.88	8 (61%)
4	MAN	B	482	4	11,11,12	3.90	8 (72%)	13,15,17	1.78	3 (23%)
4	MAN	B	483	4	11,11,12	4.95	9 (81%)	13,15,17	2.92	8 (61%)
2	NAG	B	484	1,2	14,14,15	3.37	6 (42%)	15,19,21	3.62	10 (66%)
2	NAG	B	485	2	14,14,15	1.78	4 (28%)	15,19,21	4.12	11 (73%)

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	472	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	473	2	-	0/6/23/26	0/1/1/1
3	NAG	A	474	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	475	3	-	0/6/23/26	0/1/1/1
3	BMA	A	476	3	-	0/2/19/22	0/1/1/1
3	FUL	A	477	3,4	-	0/0/17/20	0/1/1/1
4	NAG	A	478	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	479	4	-	0/6/23/26	0/1/1/1
4	BMA	A	480	4	-	0/2/19/22	1/1/1/1
4	MAN	A	481	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	482	4	-	0/2/19/22	1/1/1/1
4	MAN	A	483	4	-	0/2/19/22	0/1/1/1
2	NAG	A	484	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	485	2	-	0/6/23/26	0/1/1/1
2	NAG	B	472	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	473	2	-	0/6/23/26	0/1/1/1
5	NAG	B	474	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	475	5	-	0/6/23/26	0/1/1/1
5	BMA	B	476	5	-	0/2/19/22	0/1/1/1
5	FUC	B	477	5	1/1/5/5	0/0/17/20	0/1/1/1
4	NAG	B	478	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	479	4	-	0/6/23/26	0/1/1/1
4	BMA	B	480	4	-	0/2/19/22	1/1/1/1
4	MAN	B	481	4	-	0/2/19/22	0/1/1/1
4	MAN	B	482	4	-	0/2/19/22	1/1/1/1
4	MAN	B	483	4	-	0/2/19/22	0/1/1/1
2	NAG	B	484	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	485	2	-	0/6/23/26	0/1/1/1

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	484	NAG	C3-C2	-2.73	1.46	1.52
2	A	484	NAG	C3-C2	-2.73	1.46	1.52
5	B	476	BMA	O5-C5	-2.41	1.38	1.43
3	A	476	BMA	O5-C5	-2.41	1.38	1.43
2	A	485	NAG	C1-C2	-2.33	1.49	1.52
2	B	485	NAG	C1-C2	-2.33	1.49	1.52
5	B	476	BMA	O3-C3	2.03	1.47	1.43
3	A	476	BMA	O3-C3	2.03	1.47	1.43
5	B	476	BMA	C6-C5	2.06	1.59	1.51
3	A	476	BMA	C6-C5	2.06	1.59	1.51
2	A	472	NAG	C8-C7	2.07	1.55	1.50
2	B	472	NAG	C8-C7	2.07	1.55	1.50
2	A	473	NAG	C8-C7	2.22	1.55	1.50
2	B	473	NAG	C8-C7	2.22	1.55	1.50
2	B	484	NAG	C6-C5	2.32	1.59	1.51
2	A	484	NAG	C6-C5	2.32	1.59	1.51
4	A	483	MAN	O2-C2	2.34	1.48	1.43
4	B	483	MAN	O2-C2	2.34	1.48	1.43
4	B	478	NAG	O4-C4	2.35	1.48	1.43
4	A	478	NAG	O4-C4	2.35	1.48	1.43
2	B	484	NAG	O4-C4	2.38	1.48	1.43
2	A	484	NAG	O4-C4	2.38	1.48	1.43
3	A	475	NAG	O4-C4	2.39	1.48	1.43
5	B	475	NAG	O4-C4	2.39	1.48	1.43
3	A	474	NAG	C8-C7	2.44	1.55	1.50
5	B	474	NAG	C8-C7	2.44	1.55	1.50
2	A	485	NAG	C4-C5	2.50	1.58	1.53
2	B	485	NAG	C4-C5	2.50	1.58	1.53
4	A	483	MAN	O4-C4	2.50	1.48	1.43
4	B	483	MAN	O4-C4	2.50	1.48	1.43
4	A	480	BMA	O5-C1	2.51	1.47	1.43
4	B	480	BMA	O5-C1	2.51	1.47	1.43
3	A	477	FUL	O3-C3	2.57	1.48	1.43
5	B	477	FUC	O3-C3	2.57	1.48	1.43
4	B	478	NAG	C2-N2	2.59	1.50	1.46
4	A	478	NAG	C2-N2	2.59	1.50	1.46
4	B	481	MAN	O4-C4	2.63	1.49	1.43
4	A	481	MAN	O4-C4	2.63	1.49	1.43
2	A	472	NAG	O4-C4	2.65	1.49	1.43
2	B	472	NAG	O4-C4	2.65	1.49	1.43
4	A	480	BMA	O4-C4	2.71	1.49	1.43
4	B	480	BMA	O4-C4	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	476	BMA	O2-C2	2.78	1.49	1.43
3	A	476	BMA	O2-C2	2.78	1.49	1.43
2	A	485	NAG	C3-C2	2.80	1.58	1.52
2	B	485	NAG	C3-C2	2.80	1.58	1.52
4	B	481	MAN	C6-C5	2.82	1.61	1.51
4	A	481	MAN	C6-C5	2.82	1.61	1.51
3	A	474	NAG	C4-C3	2.88	1.59	1.52
5	B	474	NAG	C4-C3	2.88	1.59	1.52
2	A	485	NAG	C8-C7	2.90	1.56	1.50
2	B	485	NAG	C8-C7	2.90	1.56	1.50
2	A	472	NAG	O3-C3	2.94	1.49	1.43
2	B	472	NAG	O3-C3	2.94	1.49	1.43
2	A	472	NAG	C3-C2	2.95	1.58	1.52
2	B	472	NAG	C3-C2	2.95	1.58	1.52
5	B	476	BMA	C4-C3	3.09	1.60	1.52
3	A	476	BMA	C4-C3	3.09	1.60	1.52
2	A	472	NAG	O5-C1	3.14	1.48	1.43
2	B	472	NAG	O5-C1	3.14	1.48	1.43
4	A	483	MAN	O3-C3	3.18	1.50	1.43
4	B	483	MAN	O3-C3	3.18	1.50	1.43
4	B	482	MAN	O2-C2	3.20	1.50	1.43
4	A	482	MAN	O2-C2	3.20	1.50	1.43
4	B	482	MAN	O5-C1	3.22	1.49	1.43
4	A	482	MAN	O5-C1	3.22	1.49	1.43
3	A	475	NAG	C8-C7	3.23	1.57	1.50
5	B	475	NAG	C8-C7	3.23	1.57	1.50
4	B	478	NAG	C8-C7	3.28	1.57	1.50
4	A	478	NAG	C8-C7	3.28	1.57	1.50
3	A	475	NAG	C3-C2	3.31	1.59	1.52
5	B	475	NAG	C3-C2	3.31	1.59	1.52
4	B	481	MAN	C1-C2	3.34	1.60	1.52
4	A	481	MAN	C1-C2	3.34	1.60	1.52
4	B	482	MAN	C2-C3	3.35	1.57	1.52
4	A	482	MAN	C2-C3	3.35	1.57	1.52
4	A	483	MAN	C4-C3	3.36	1.60	1.52
4	B	483	MAN	C4-C3	3.36	1.60	1.52
3	A	475	NAG	C1-C2	3.36	1.57	1.52
5	B	475	NAG	C1-C2	3.36	1.57	1.52
4	A	480	BMA	C6-C5	3.37	1.63	1.51
4	B	480	BMA	C6-C5	3.37	1.63	1.51
4	B	479	NAG	C4-C5	3.42	1.60	1.53
4	A	479	NAG	C4-C5	3.42	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	481	MAN	C4-C5	3.47	1.60	1.53
4	A	481	MAN	C4-C5	3.47	1.60	1.53
2	B	484	NAG	C2-N2	3.64	1.52	1.46
2	A	484	NAG	C2-N2	3.64	1.52	1.46
5	B	476	BMA	C1-C2	3.66	1.60	1.52
3	A	476	BMA	C1-C2	3.66	1.60	1.52
4	B	479	NAG	C3-C2	3.74	1.60	1.52
4	A	479	NAG	C3-C2	3.74	1.60	1.52
4	B	481	MAN	C4-C3	3.76	1.61	1.52
4	A	481	MAN	C4-C3	3.76	1.61	1.52
3	A	475	NAG	C2-N2	3.76	1.53	1.46
5	B	475	NAG	C2-N2	3.76	1.53	1.46
2	A	473	NAG	C6-C5	3.79	1.64	1.51
2	B	473	NAG	C6-C5	3.79	1.64	1.51
3	A	477	FUL	C1-C2	3.88	1.61	1.52
5	B	477	FUC	C1-C2	3.88	1.61	1.52
3	A	475	NAG	C4-C3	3.89	1.62	1.52
5	B	475	NAG	C4-C3	3.89	1.62	1.52
2	A	473	NAG	O5-C1	3.96	1.50	1.43
2	B	473	NAG	O5-C1	3.96	1.50	1.43
2	B	484	NAG	O5-C1	4.05	1.50	1.43
2	A	484	NAG	O5-C1	4.05	1.50	1.43
4	A	483	MAN	C6-C5	4.08	1.65	1.51
4	B	483	MAN	C6-C5	4.08	1.65	1.51
4	B	478	NAG	C3-C2	4.08	1.61	1.52
4	A	478	NAG	C3-C2	4.08	1.61	1.52
4	B	482	MAN	C6-C5	4.10	1.65	1.51
4	A	482	MAN	C6-C5	4.10	1.65	1.51
3	A	475	NAG	O5-C1	4.16	1.50	1.43
5	B	475	NAG	O5-C1	4.16	1.50	1.43
3	A	474	NAG	C1-C2	4.30	1.58	1.52
5	B	474	NAG	C1-C2	4.30	1.58	1.52
4	B	482	MAN	O3-C3	4.34	1.52	1.43
4	A	482	MAN	O3-C3	4.34	1.52	1.43
2	A	472	NAG	C4-C3	4.40	1.63	1.52
2	B	472	NAG	C4-C3	4.40	1.63	1.52
4	B	479	NAG	C6-C5	4.50	1.67	1.51
4	A	479	NAG	C6-C5	4.50	1.67	1.51
4	A	480	BMA	O5-C5	4.72	1.53	1.43
4	B	480	BMA	O5-C5	4.72	1.53	1.43
4	B	478	NAG	O5-C5	4.76	1.53	1.43
4	A	478	NAG	O5-C5	4.76	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	473	NAG	C4-C3	4.76	1.64	1.52
2	B	473	NAG	C4-C3	4.76	1.64	1.52
4	B	482	MAN	C4-C5	4.80	1.63	1.53
4	A	482	MAN	C4-C5	4.80	1.63	1.53
4	B	481	MAN	O2-C2	4.87	1.54	1.43
4	A	481	MAN	O2-C2	4.87	1.54	1.43
3	A	477	FUL	C4-C5	4.89	1.62	1.53
5	B	477	FUC	C4-C5	4.89	1.62	1.53
4	A	483	MAN	O5-C5	4.94	1.53	1.43
4	B	483	MAN	O5-C5	4.94	1.53	1.43
3	A	477	FUL	C2-C3	5.02	1.59	1.52
5	B	477	FUC	C2-C3	5.02	1.59	1.52
4	A	483	MAN	C2-C3	5.03	1.59	1.52
4	B	483	MAN	C2-C3	5.03	1.59	1.52
3	A	477	FUL	O5-C1	5.07	1.52	1.43
5	B	477	FUC	O5-C1	5.07	1.52	1.43
4	A	480	BMA	C1-C2	5.31	1.64	1.52
4	B	480	BMA	C1-C2	5.31	1.64	1.52
2	A	473	NAG	C4-C5	5.63	1.65	1.53
2	B	473	NAG	C4-C5	5.63	1.65	1.53
4	A	480	BMA	C4-C5	5.71	1.65	1.53
4	B	480	BMA	C4-C5	5.71	1.65	1.53
4	B	482	MAN	O5-C5	5.83	1.55	1.43
4	A	482	MAN	O5-C5	5.83	1.55	1.43
4	B	482	MAN	C4-C3	6.22	1.68	1.52
4	A	482	MAN	C4-C3	6.22	1.68	1.52
4	A	483	MAN	C1-C2	6.48	1.67	1.52
4	B	483	MAN	C1-C2	6.48	1.67	1.52
4	A	480	BMA	O3-C3	6.82	1.58	1.43
4	B	480	BMA	O3-C3	6.82	1.58	1.43
4	B	478	NAG	O5-C1	7.06	1.55	1.43
4	A	478	NAG	O5-C1	7.06	1.55	1.43
4	B	478	NAG	C1-C2	7.77	1.63	1.52
4	A	478	NAG	C1-C2	7.77	1.63	1.52
2	A	473	NAG	C1-C2	8.65	1.64	1.52
2	B	473	NAG	C1-C2	8.65	1.64	1.52
5	B	476	BMA	C2-C3	9.83	1.65	1.52
3	A	476	BMA	C2-C3	9.83	1.65	1.52
2	B	484	NAG	C1-C2	10.06	1.66	1.52
2	A	484	NAG	C1-C2	10.06	1.66	1.52
4	B	479	NAG	C1-C2	10.12	1.66	1.52
4	A	479	NAG	C1-C2	10.12	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	480	BMA	C2-C3	10.80	1.67	1.52
4	B	480	BMA	C2-C3	10.80	1.67	1.52
4	A	483	MAN	C4-C5	11.03	1.76	1.53
4	B	483	MAN	C4-C5	11.03	1.76	1.53

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	475	NAG	O7-C7-C8	-8.76	106.12	122.06
5	B	475	NAG	O7-C7-C8	-8.76	106.12	122.06
2	A	485	NAG	C4-C3-C2	-7.97	99.34	111.02
2	B	485	NAG	C4-C3-C2	-7.97	99.34	111.02
2	A	473	NAG	C4-C3-C2	-7.71	99.71	111.02
2	B	473	NAG	C4-C3-C2	-7.71	99.71	111.02
2	A	485	NAG	O5-C1-C2	-6.75	102.08	111.47
2	B	485	NAG	O5-C1-C2	-6.75	102.08	111.47
2	A	472	NAG	C1-C2-N2	-6.29	99.74	110.49
2	B	472	NAG	C1-C2-N2	-6.29	99.74	110.49
2	B	484	NAG	O7-C7-C8	-6.03	111.08	122.06
2	A	484	NAG	O7-C7-C8	-6.03	111.08	122.06
4	B	478	NAG	O3-C3-C4	-5.93	97.46	110.36
4	A	478	NAG	O3-C3-C4	-5.93	97.46	110.36
4	B	479	NAG	C1-C2-N2	-5.60	100.92	110.49
4	A	479	NAG	C1-C2-N2	-5.60	100.92	110.49
3	A	475	NAG	C2-N2-C7	-5.44	115.01	122.94
5	B	475	NAG	C2-N2-C7	-5.44	115.01	122.94
2	A	473	NAG	C2-N2-C7	-4.90	115.79	122.94
2	B	473	NAG	C2-N2-C7	-4.90	115.79	122.94
3	A	475	NAG	C4-C3-C2	-4.33	104.67	111.02
5	B	475	NAG	C4-C3-C2	-4.33	104.67	111.02
3	A	474	NAG	C4-C3-C2	-4.24	104.80	111.02
5	B	474	NAG	C4-C3-C2	-4.24	104.80	111.02
2	B	484	NAG	C4-C3-C2	-3.82	105.43	111.02
2	A	484	NAG	C4-C3-C2	-3.82	105.43	111.02
2	A	485	NAG	O4-C4-C3	-3.79	102.10	110.36
2	B	485	NAG	O4-C4-C3	-3.79	102.10	110.36
4	B	478	NAG	C3-C4-C5	-3.79	103.54	110.22
4	A	478	NAG	C3-C4-C5	-3.79	103.54	110.22
3	A	477	FUL	C1-C2-C3	-3.72	104.94	109.65
5	B	477	FUC	C1-C2-C3	-3.72	104.94	109.65
4	B	479	NAG	O5-C1-C2	-3.71	106.31	111.47
4	A	479	NAG	O5-C1-C2	-3.71	106.31	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	480	BMA	O4-C4-C3	-3.65	102.42	110.36
4	B	480	BMA	O4-C4-C3	-3.65	102.42	110.36
4	A	483	MAN	C6-C5-C4	-3.64	104.48	113.00
4	B	483	MAN	C6-C5-C4	-3.64	104.48	113.00
4	B	482	MAN	O3-C3-C2	-3.58	103.52	110.02
4	A	482	MAN	O3-C3-C2	-3.58	103.52	110.02
4	B	478	NAG	O7-C7-C8	-3.57	115.55	122.06
4	A	478	NAG	O7-C7-C8	-3.57	115.55	122.06
5	B	476	BMA	O3-C3-C4	-3.43	102.89	110.36
3	A	476	BMA	O3-C3-C4	-3.43	102.89	110.36
4	A	483	MAN	O3-C3-C4	-3.39	102.98	110.36
4	B	483	MAN	O3-C3-C4	-3.39	102.98	110.36
2	A	485	NAG	C2-N2-C7	-3.11	118.41	122.94
2	B	485	NAG	C2-N2-C7	-3.11	118.41	122.94
2	A	472	NAG	C6-C5-C4	-3.11	105.73	113.00
2	B	472	NAG	C6-C5-C4	-3.11	105.73	113.00
3	A	477	FUL	O4-C4-C3	-3.01	103.80	110.36
5	B	477	FUC	O4-C4-C3	-3.01	103.80	110.36
4	A	483	MAN	O4-C4-C3	-3.01	103.82	110.36
4	B	483	MAN	O4-C4-C3	-3.01	103.82	110.36
4	B	478	NAG	O4-C4-C3	-2.97	103.89	110.36
4	A	478	NAG	O4-C4-C3	-2.97	103.89	110.36
4	B	478	NAG	C1-O5-C5	-2.93	108.13	112.17
4	A	478	NAG	C1-O5-C5	-2.93	108.13	112.17
2	A	472	NAG	C8-C7-N2	-2.89	110.89	116.11
2	B	472	NAG	C8-C7-N2	-2.89	110.89	116.11
2	A	485	NAG	C3-C4-C5	-2.84	105.21	110.22
2	B	485	NAG	C3-C4-C5	-2.84	105.21	110.22
3	A	475	NAG	O5-C1-C2	-2.76	107.64	111.47
5	B	475	NAG	O5-C1-C2	-2.76	107.64	111.47
4	B	481	MAN	O2-C2-C3	-2.75	104.77	110.17
4	A	481	MAN	O2-C2-C3	-2.75	104.77	110.17
3	A	474	NAG	O7-C7-C8	-2.66	117.22	122.06
5	B	474	NAG	O7-C7-C8	-2.66	117.22	122.06
2	B	484	NAG	O4-C4-C3	-2.48	104.97	110.36
2	A	484	NAG	O4-C4-C3	-2.48	104.97	110.36
2	A	473	NAG	O7-C7-C8	-2.27	117.92	122.06
2	B	473	NAG	O7-C7-C8	-2.27	117.92	122.06
4	A	480	BMA	O2-C2-C3	-2.19	105.88	110.17
4	B	480	BMA	O2-C2-C3	-2.19	105.88	110.17
4	B	481	MAN	O3-C3-C4	-2.15	105.68	110.36
4	A	481	MAN	O3-C3-C4	-2.15	105.68	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	480	BMA	C2-C3-C4	-2.14	107.15	110.88
4	B	480	BMA	C2-C3-C4	-2.14	107.15	110.88
3	A	475	NAG	O6-C6-C5	-2.13	104.17	111.34
5	B	475	NAG	O6-C6-C5	-2.13	104.17	111.34
3	A	477	FUL	O5-C5-C4	-2.08	106.19	109.62
5	B	477	FUC	O5-C5-C4	-2.08	106.19	109.62
4	B	482	MAN	O2-C2-C3	-2.08	106.08	110.17
4	A	482	MAN	O2-C2-C3	-2.08	106.08	110.17
2	A	473	NAG	O4-C4-C3	-2.07	105.85	110.36
2	B	473	NAG	O4-C4-C3	-2.07	105.85	110.36
2	B	484	NAG	O4-C4-C5	-2.03	104.16	109.28
2	A	484	NAG	O4-C4-C5	-2.03	104.16	109.28
3	A	474	NAG	C8-C7-N2	2.10	119.89	116.11
5	B	474	NAG	C8-C7-N2	2.10	119.89	116.11
2	A	485	NAG	O3-C3-C4	2.12	114.97	110.36
2	B	485	NAG	O3-C3-C4	2.12	114.97	110.36
2	B	484	NAG	O6-C6-C5	2.14	118.56	111.34
2	A	484	NAG	O6-C6-C5	2.14	118.56	111.34
4	B	479	NAG	O3-C3-C2	2.24	114.19	109.39
4	A	479	NAG	O3-C3-C2	2.24	114.19	109.39
2	A	485	NAG	C1-C2-N2	2.36	114.52	110.49
2	B	485	NAG	C1-C2-N2	2.36	114.52	110.49
2	B	484	NAG	O3-C3-C4	2.37	115.51	110.36
2	A	484	NAG	O3-C3-C4	2.37	115.51	110.36
4	A	483	MAN	C1-O5-C5	2.42	115.50	112.17
4	B	483	MAN	C1-O5-C5	2.42	115.50	112.17
2	B	484	NAG	C3-C4-C5	2.43	114.49	110.22
2	A	484	NAG	C3-C4-C5	2.43	114.49	110.22
4	A	480	BMA	C6-C5-C4	2.49	118.84	113.00
4	B	480	BMA	C6-C5-C4	2.49	118.84	113.00
5	B	476	BMA	C1-C2-C3	2.56	112.90	109.65
3	A	476	BMA	C1-C2-C3	2.56	112.90	109.65
2	A	485	NAG	O4-C4-C5	2.58	115.79	109.28
2	B	485	NAG	O4-C4-C5	2.58	115.79	109.28
3	A	475	NAG	O3-C3-C2	2.63	115.03	109.39
5	B	475	NAG	O3-C3-C2	2.63	115.03	109.39
2	A	473	NAG	O3-C3-C4	2.69	116.22	110.36
2	B	473	NAG	O3-C3-C4	2.69	116.22	110.36
4	B	481	MAN	C6-C5-C4	2.71	119.34	113.00
4	A	481	MAN	C6-C5-C4	2.71	119.34	113.00
3	A	474	NAG	O3-C3-C2	2.77	115.31	109.39
5	B	474	NAG	O3-C3-C2	2.77	115.31	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	483	MAN	C2-C3-C4	2.81	115.78	110.88
4	B	483	MAN	C2-C3-C4	2.81	115.78	110.88
5	B	476	BMA	O5-C1-C2	2.84	115.24	110.79
3	A	476	BMA	O5-C1-C2	2.84	115.24	110.79
4	B	481	MAN	C3-C4-C5	2.89	115.31	110.22
4	A	481	MAN	C3-C4-C5	2.89	115.31	110.22
3	A	474	NAG	C2-N2-C7	2.90	127.17	122.94
5	B	474	NAG	C2-N2-C7	2.90	127.17	122.94
4	B	482	MAN	O5-C1-C2	2.97	115.44	110.79
4	A	482	MAN	O5-C1-C2	2.97	115.44	110.79
2	A	473	NAG	C3-C4-C5	2.97	115.45	110.22
2	B	473	NAG	C3-C4-C5	2.97	115.45	110.22
4	B	478	NAG	C6-C5-C4	3.01	120.05	113.00
4	A	478	NAG	C6-C5-C4	3.01	120.05	113.00
4	B	481	MAN	C1-C2-C3	3.01	113.47	109.65
4	A	481	MAN	C1-C2-C3	3.01	113.47	109.65
4	B	478	NAG	C8-C7-N2	3.01	121.55	116.11
4	A	478	NAG	C8-C7-N2	3.01	121.55	116.11
3	A	474	NAG	O3-C3-C4	3.02	116.93	110.36
5	B	474	NAG	O3-C3-C4	3.02	116.93	110.36
3	A	477	FUL	O3-C3-C2	3.13	115.72	110.02
5	B	477	FUC	O3-C3-C2	3.13	115.72	110.02
4	B	481	MAN	C2-C3-C4	3.15	116.37	110.88
4	A	481	MAN	C2-C3-C4	3.15	116.37	110.88
4	B	478	NAG	O4-C4-C5	3.22	117.41	109.28
4	A	478	NAG	O4-C4-C5	3.22	117.41	109.28
5	B	476	BMA	C2-C3-C4	3.25	116.55	110.88
3	A	476	BMA	C2-C3-C4	3.25	116.55	110.88
3	A	477	FUL	C1-O5-C5	3.27	119.63	112.39
5	B	477	FUC	C1-O5-C5	3.27	119.63	112.39
2	A	485	NAG	C1-O5-C5	3.28	116.68	112.17
2	B	485	NAG	C1-O5-C5	3.28	116.68	112.17
4	A	480	BMA	O6-C6-C5	3.37	122.68	111.34
4	B	480	BMA	O6-C6-C5	3.37	122.68	111.34
4	A	483	MAN	C1-C2-C3	3.70	114.35	109.65
4	B	483	MAN	C1-C2-C3	3.70	114.35	109.65
4	B	478	NAG	O5-C1-C2	3.71	116.64	111.47
4	A	478	NAG	O5-C1-C2	3.71	116.64	111.47
3	A	475	NAG	O4-C4-C3	3.77	118.56	110.36
5	B	475	NAG	O4-C4-C3	3.77	118.56	110.36
4	A	483	MAN	C3-C4-C5	4.02	117.30	110.22
4	B	483	MAN	C3-C4-C5	4.02	117.30	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	479	NAG	C2-N2-C7	4.31	129.22	122.94
4	A	479	NAG	C2-N2-C7	4.31	129.22	122.94
2	A	473	NAG	O3-C3-C2	4.31	118.62	109.39
2	B	473	NAG	O3-C3-C2	4.31	118.62	109.39
4	A	480	BMA	C1-C2-C3	4.45	115.30	109.65
4	B	480	BMA	C1-C2-C3	4.45	115.30	109.65
4	B	481	MAN	O5-C1-C2	4.54	117.90	110.79
4	A	481	MAN	O5-C1-C2	4.54	117.90	110.79
3	A	477	FUL	C3-C4-C5	4.74	117.13	109.68
5	B	477	FUC	C3-C4-C5	4.74	117.13	109.68
2	B	484	NAG	C1-O5-C5	4.77	118.74	112.17
2	A	484	NAG	C1-O5-C5	4.77	118.74	112.17
2	A	473	NAG	C6-C5-C4	4.85	124.36	113.00
2	B	473	NAG	C6-C5-C4	4.85	124.36	113.00
2	A	472	NAG	O4-C4-C3	5.05	121.35	110.36
2	B	472	NAG	O4-C4-C3	5.05	121.35	110.36
3	A	477	FUL	C6-C5-C4	5.10	122.16	113.07
5	B	477	FUC	C6-C5-C4	5.10	122.16	113.07
4	B	479	NAG	C1-O5-C5	5.12	119.22	112.17
4	A	479	NAG	C1-O5-C5	5.12	119.22	112.17
4	A	483	MAN	O5-C1-C2	5.41	119.26	110.79
4	B	483	MAN	O5-C1-C2	5.41	119.26	110.79
4	B	481	MAN	C1-O5-C5	5.75	120.09	112.17
4	A	481	MAN	C1-O5-C5	5.75	120.09	112.17
2	B	484	NAG	C8-C7-N2	5.84	126.65	116.11
2	A	484	NAG	C8-C7-N2	5.84	126.65	116.11
2	A	485	NAG	C6-C5-C4	6.10	127.27	113.00
2	B	485	NAG	C6-C5-C4	6.10	127.27	113.00
4	A	480	BMA	C1-O5-C5	6.28	120.82	112.17
4	B	480	BMA	C1-O5-C5	6.28	120.82	112.17
2	A	485	NAG	O3-C3-C2	6.46	123.22	109.39
2	B	485	NAG	O3-C3-C2	6.46	123.22	109.39
4	A	480	BMA	O3-C3-C2	6.68	122.18	110.02
4	B	480	BMA	O3-C3-C2	6.68	122.18	110.02
2	A	472	NAG	C1-O5-C5	7.14	122.00	112.17
2	B	472	NAG	C1-O5-C5	7.14	122.00	112.17
4	B	478	NAG	C4-C3-C2	7.23	121.61	111.02
4	A	478	NAG	C4-C3-C2	7.23	121.61	111.02
2	B	484	NAG	C1-C2-N2	7.82	123.85	110.49
2	A	484	NAG	C1-C2-N2	7.82	123.85	110.49
3	A	475	NAG	C8-C7-N2	8.38	131.23	116.11
5	B	475	NAG	C8-C7-N2	8.38	131.23	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	476	BMA	C1-O5-C5	8.57	123.98	112.17
3	A	476	BMA	C1-O5-C5	8.57	123.98	112.17
3	A	474	NAG	C1-O5-C5	8.85	124.37	112.17
5	B	474	NAG	C1-O5-C5	8.85	124.37	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	477	FUC	C1

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	482	MAN	C1-C2-C3-C4-C5-O5
4	A	482	MAN	C1-C2-C3-C4-C5-O5
4	A	480	BMA	C1-C2-C3-C4-C5-O5
4	B	480	BMA	C1-C2-C3-C4-C5-O5

21 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	473	NAG	3	0
3	A	475	NAG	1	0
3	A	476	BMA	1	0
3	A	477	FUL	0	6
4	A	478	NAG	11	0
4	A	479	NAG	5	0
4	A	480	BMA	5	0
4	A	481	MAN	3	6
4	A	483	MAN	14	0
2	A	484	NAG	3	0
2	A	485	NAG	1	0
2	B	473	NAG	3	0
5	B	475	NAG	1	0
5	B	476	BMA	1	0
4	B	478	NAG	3	2
4	B	479	NAG	6	0
4	B	480	BMA	5	0
4	B	481	MAN	3	0
4	B	483	MAN	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	484	NAG	3	0
2	B	485	NAG	1	0

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
7	ST2	A	471	-	12,15,15	1.27	2 (16%)	13,21,21	2.28	3 (23%)
7	ST2	B	471	-	12,15,15	1.27	2 (16%)	13,21,21	2.28	3 (23%)

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
7	ST2	A	471	-	-	0/4/8/8	0/1/1/1
7	ST2	B	471	-	-	0/4/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	471	ST2	C6-C5	2.15	1.41	1.38
7	B	471	ST2	C6-C5	2.15	1.41	1.38
7	A	471	ST2	C3-C4	2.67	1.43	1.40
7	B	471	ST2	C3-C4	2.67	1.43	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	471	ST2	C4-N4-C4'	-6.63	112.28	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	471	ST2	C4-N4-C4'	-6.63	112.28	122.79
7	A	471	ST2	O4'-C4'-CM4	-2.09	118.26	122.06
7	B	471	ST2	O4'-C4'-CM4	-2.09	118.26	122.06
7	A	471	ST2	CM4-C4'-N4	3.53	120.20	115.02
7	B	471	ST2	CM4-C4'-N4	3.53	120.20	115.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	471	ST2	3	0
7	B	471	ST2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	388/388 (100%)	-0.50	0 <b>100</b> <b>100</b>	4, 13, 23, 31	0
1	B	388/388 (100%)	-0.49	1 (0%) <b>93</b> <b>93</b>	4, 13, 23, 31	0
All	All	776/776 (100%)	-0.49	1 (0%) <b>95</b> <b>95</b>	4, 13, 23, 31	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	346	THR	2.5

### 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](#)

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
4	MAN	A	483	11/12	0.53	0.62	<b>16.04</b>	15,15,36,41	0
4	MAN	B	483	11/12	0.46	0.66	<b>14.52</b>	15,15,36,41	0
2	NAG	B	472	14/15	0.88	0.25	<b>4.93</b>	15,15,31,31	0
4	NAG	B	478	14/15	0.63	0.29	<b>4.29</b>	15,18,31,33	0
4	NAG	A	478	14/15	0.63	0.28	<b>4.02</b>	15,18,31,33	0
2	NAG	A	472	14/15	0.86	0.32	<b>3.75</b>	15,15,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	484	14/15	0.81	0.22	3.52	15,15,35,36	0
2	NAG	A	484	14/15	0.89	0.26	2.92	15,15,35,36	0
4	BMA	A	480	11/12	0.73	0.48	-	15,15,35,36	0
4	NAG	B	479	14/15	0.69	0.64	-	15,15,38,38	0
2	NAG	A	473	14/15	0.69	0.41	-	15,15,35,37	0
5	NAG	B	475	14/15	0.78	0.37	-	15,15,34,36	0
2	NAG	A	485	14/15	0.84	0.35	-	15,15,37,37	0
4	MAN	A	481	11/12	0.57	0.49	-	15,15,34,35	0
5	BMA	B	476	11/12	0.66	0.45	-	15,15,38,39	0
4	NAG	A	479	14/15	0.68	0.63	-	15,15,38,38	0
2	NAG	B	485	14/15	0.87	0.42	-	15,15,37,37	0
2	NAG	B	473	14/15	0.82	0.42	-	15,15,35,37	0
5	FUC	B	477	10/11	0.78	0.47	-	15,15,33,36	0
4	MAN	B	481	11/12	0.61	0.46	-	15,15,34,35	0
3	NAG	A	474	14/15	0.94	0.11	-	15,20,27,31	0
5	NAG	B	474	14/15	0.86	0.18	-	15,20,27,31	0
3	BMA	A	476	11/12	0.56	0.55	-	15,15,38,39	0
4	MAN	B	482	11/12	0.62	0.54	-	15,15,38,40	0
3	NAG	A	475	14/15	0.77	0.29	-	15,15,34,36	0
3	FUL	A	477	10/11	0.55	0.51	-	15,15,33,36	0
4	BMA	B	480	11/12	0.64	0.64	-	15,15,35,36	0
4	MAN	A	482	11/12	0.67	0.60	-	15,15,38,40	0

## 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ST2	B	471	15/15	0.77	0.30	7.80	15,33,38,40	0
7	ST2	A	471	15/15	0.82	0.26	6.19	15,33,38,40	0
6	CA	B	470	1/1	0.90	0.07	-1.42	21,21,21,21	0
6	CA	A	470	1/1	0.94	0.06	-1.64	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.