Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 PM GMT

PDB ID	:	4K3Y
Title	:	Crystal structure of a subtype N11 neuraminidase-like protein of A/flat-faced bat/Peru/033/2010 (H18N11)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2013-04-11
Resolution	:	2.68 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

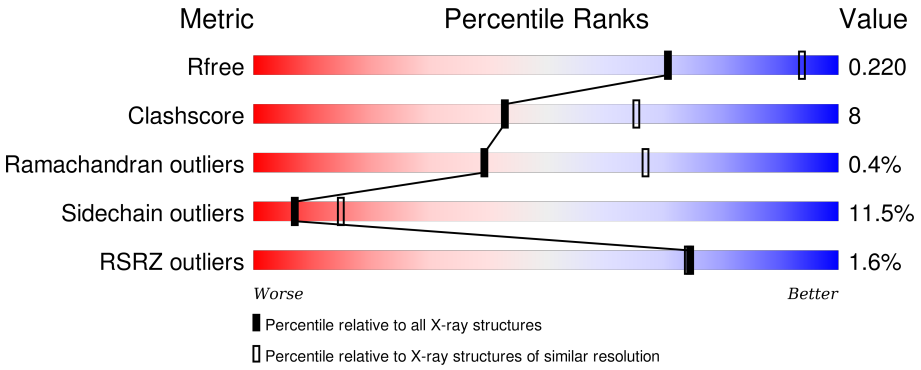
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	369	% 75% 19%
1	B	369	69% 25%
1	C	369	% 72% 21%
1	D	369	4% 69% 24%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	C	608	-	-	-	X
5	NAG	C	603	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11239 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2723	1719	451	534	19			
1	B	354	Total	C	N	O	S	0	0	0
			2723	1719	451	534	19			
1	C	355	Total	C	N	O	S	0	0	0
			2727	1721	452	535	19			
1	D	354	Total	C	N	O	S	0	0	0
			2723	1719	451	534	19			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 6 is water.

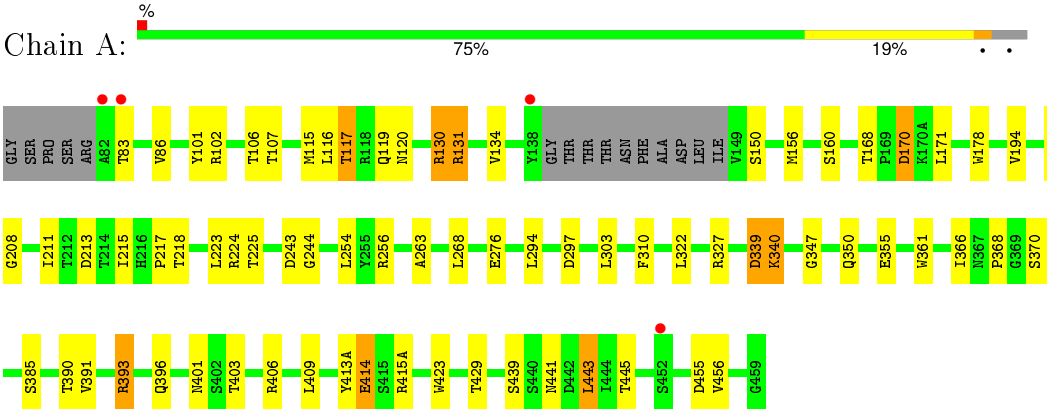
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	57	Total	O	0	0
			57	57		
6	B	27	Total	O	0	0
			27	27		
6	C	25	Total	O	0	0
			25	25		
6	D	8	Total	O	0	0
			8	8		

3 Residue-property plots (i)

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

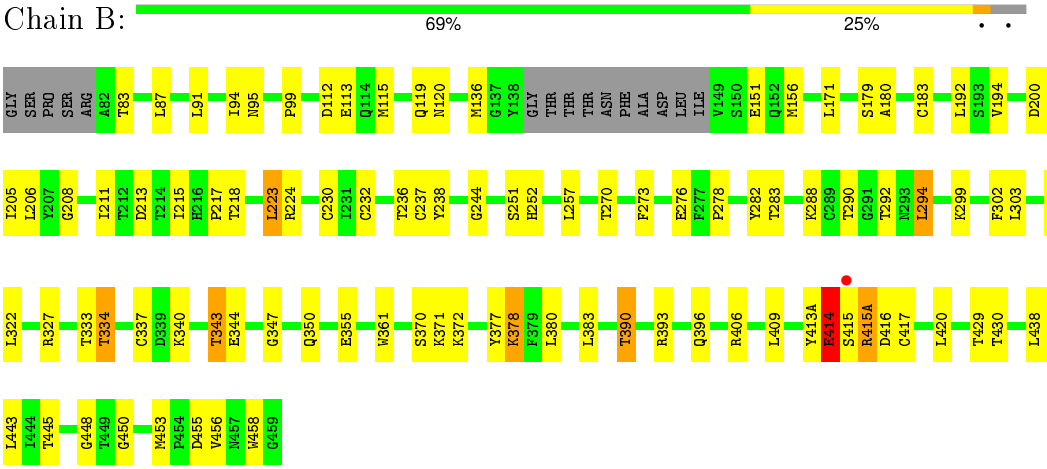
- Molecule 1: neuraminidase

Chain A:



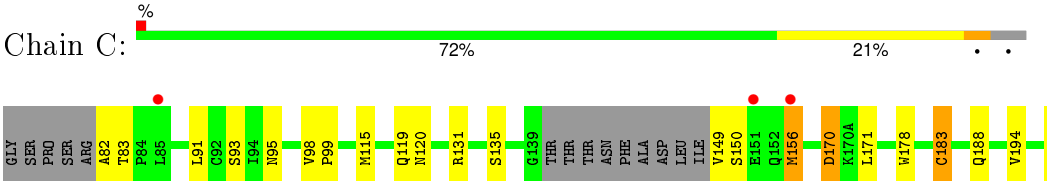
- Molecule 1: neuraminidase

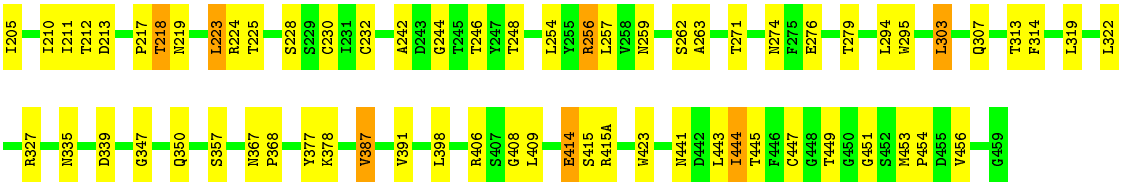
Chain B:



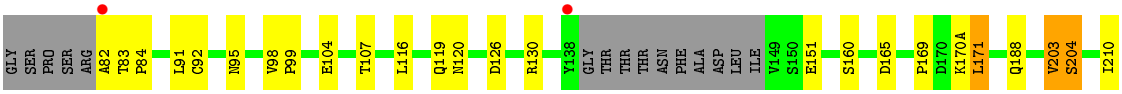
- Molecule 1: neuraminidase

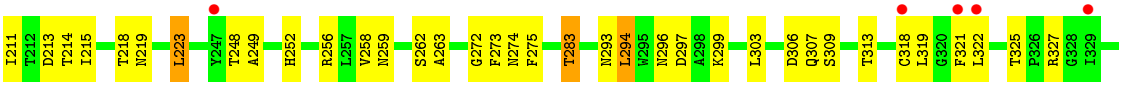
Chain C:

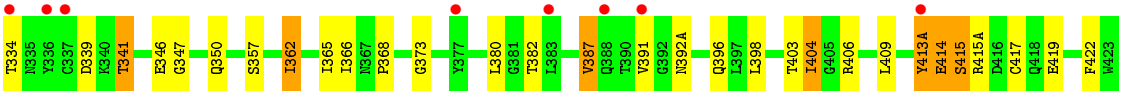


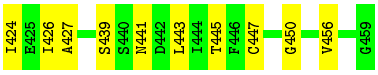


- Molecule 1: neuraminidase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	181.29Å 181.29Å 136.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 2.68 48.87 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.87-2.68) 98.5 (48.87-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.178 , 0.220 0.179 , 0.220	Depositor DCC
R_{free} test set	3547 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.0	EDS
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 70284 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11239	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.49	0/2790	0.66	1/3786 (0.0%)
1	B	0.47	0/2790	0.65	1/3786 (0.0%)
1	C	0.46	0/2794	0.62	0/3791
1	D	0.40	0/2790	0.57	0/3786
All	All	0.46	0/11164	0.63	2/15149 (0.0%)

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	4
1	C	0	1
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	GLY	N-CA-C	-5.32	99.79	113.10
1	B	208	GLY	N-CA-C	-5.19	100.12	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	441	ASN	Peptide
1	B	390	THR	Peptide
1	B	413(A)	TYR	Peptide
1	B	414	GLU	Peptide
1	B	441	ASN	Peptide
1	C	441	ASN	Peptide
1	D	415	SER	Peptide
1	D	441	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2723	0	2582	40	0
1	B	2723	0	2581	45	0
1	C	2727	0	2584	52	0
1	D	2723	0	2582	53	0
2	A	39	0	34	0	0
2	D	39	0	34	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	B	56	0	50	1	0
4	C	28	0	25	1	0
5	C	60	0	52	0	0
6	A	57	0	0	1	0
6	B	27	0	0	0	0
6	C	25	0	0	0	0
6	D	8	0	0	1	0
All	All	11239	0	10524	177	0

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 8.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:GLN:OE1	1:D:406:ARG:NH1	2.13	0.81
1:A:211:ILE:HD12	1:C:447:CYS:HB2	1.62	0.81
1:C:449:THR:HG22	1:C:451:GLY:H	1.47	0.80
1:B:120:ASN:O	1:B:406:ARG:NH2	2.15	0.79
1:A:254:LEU:HD13	1:A:268:LEU:HD21	1.66	0.78
1:C:274:ASN:HD22	1:C:294:LEU:H	1.29	0.78
1:B:203:VAL:HG22	1:B:215:ILE:HB	1.67	0.77
1:C:210:ILE:HD11	1:D:413(A):TYR:CE2	2.20	0.77
1:A:393:ARG:NH2	1:A:455:ASP:OD1	2.17	0.77
1:C:120:ASN:O	1:C:406:ARG:NH2	2.19	0.75
1:A:414:GLU:HG2	1:A:415(A):ARG:H	1.52	0.75
1:D:120:ASN:O	1:D:406:ARG:NH2	2.20	0.75
1:B:414:GLU:HG3	1:B:415(A):ARG:H	1.50	0.74
1:B:203:VAL:HG13	1:B:223:LEU:HD23	1.69	0.74
1:C:256:ARG:HG2	1:C:263:ALA:HB3	1.69	0.72
1:B:430:THR:HG22	1:B:438:LEU:H	1.55	0.71
1:B:415(A):ARG:NH2	1:D:259:ASN:O	2.22	0.71
1:B:333:THR:OG1	1:B:334:THR:N	2.23	0.71
1:B:294:LEU:HA	1:B:347:GLY:O	1.90	0.71
1:C:82:ALA:O	4:C:602:NAG:H81	1.91	0.70
1:C:294:LEU:HA	1:C:347:GLY:O	1.92	0.69
1:C:398:LEU:HD21	1:C:444:ILE:HD12	1.74	0.69
1:A:120:ASN:O	1:A:406:ARG:NH2	2.27	0.68
1:D:322:LEU:HB2	1:D:327:ARG:HD2	1.77	0.67
1:A:194:VAL:HG22	1:A:203:VAL:HG12	1.77	0.66
1:B:370:SER:O	1:B:372:LYS:N	2.26	0.65
1:B:205:ILE:HD12	1:B:213:ASP:HB3	1.79	0.65
1:C:350:GLN:OE1	1:C:406:ARG:NH1	2.30	0.65
1:C:211:ILE:HD12	1:D:447:CYS:HB2	1.79	0.64
1:D:95:ASN:ND2	1:D:450:GLY:O	2.27	0.64
1:A:322:LEU:HB2	1:A:327:ARG:HD2	1.80	0.64
4:B:603:NAG:H83	1:D:151:GLU:HB2	1.78	0.64
1:A:256:ARG:HG3	1:A:263:ALA:HB3	1.79	0.64
1:B:224:ARG:NH2	1:B:244:GLY:O	2.31	0.63
1:D:365:ILE:HG12	1:D:404:ILE:HD11	1.80	0.63
1:C:453:MET:HE3	1:C:454:PRO:HD2	1.81	0.62
1:D:91:LEU:HG	1:D:283:THR:HG21	1.80	0.62
1:A:294:LEU:HA	1:A:347:GLY:O	1.98	0.62
1:D:274:ASN:HD22	1:D:294:LEU:H	1.44	0.62
1:C:95:ASN:OD1	1:C:378:LYS:NZ	2.32	0.61
1:D:130:ARG:NH1	1:D:160:SER:OG	2.33	0.61
1:A:370:SER:O	1:A:372:LYS:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ARG:NH2	1:B:453:MET:O	2.34	0.60
1:D:203:VAL:HG13	1:D:215:ILE:HB	1.83	0.60
1:A:130:ARG:NH1	1:A:160:SER:OG	2.34	0.60
1:A:102:ARG:HH12	1:B:151:GLU:HG3	1.66	0.59
1:D:413(A):TYR:N	1:D:413(A):TYR:CD1	2.71	0.59
1:D:380:LEU:HD11	1:D:392(A):ASN:HB2	1.83	0.59
1:C:279:THR:HG21	1:C:408:GLY:HA2	1.84	0.59
1:D:82:ALA:C	1:D:83:THR:HG23	2.24	0.58
1:A:203:VAL:HG22	1:A:215:ILE:HB	1.84	0.58
1:C:228:SER:OG	1:C:279:THR:HG22	2.03	0.58
1:B:91:LEU:HG	1:B:283:THR:HG21	1.84	0.58
1:A:170:ASP:N	1:A:170:ASP:OD1	2.36	0.57
1:B:206:LEU:HG	1:B:211:ILE:HD13	1.86	0.57
1:A:102:ARG:NH1	1:B:151:GLU:O	2.37	0.57
1:D:426:ILE:HG22	1:D:427:ALA:O	2.06	0.56
1:C:335:ASN:HB3	1:C:387:VAL:HG12	1.88	0.56
1:D:248:THR:OG1	1:D:249:ALA:N	2.39	0.55
1:B:217:PRO:HD3	1:B:223:LEU:HD22	1.89	0.55
1:B:322:LEU:HB2	1:B:327:ARG:HD2	1.89	0.54
1:C:259:ASN:O	1:D:415(A):ARG:NH2	2.40	0.54
1:D:414:GLU:HG2	1:D:415(A):ARG:H	1.72	0.54
1:B:355:GLU:HG2	1:B:383:LEU:HD12	1.89	0.54
1:A:256:ARG:HB3	1:A:310:PHE:CZ	2.42	0.54
1:A:372:LYS:HG2	1:A:403:THR:HG22	1.88	0.54
1:A:385:SER:HB3	1:A:390:THR:HG23	1.88	0.53
1:C:224:ARG:NH1	1:C:276:GLU:OE2	2.41	0.53
1:A:276:GLU:HG3	1:A:294:LEU:HD12	1.91	0.53
1:D:188:GLN:HG3	6:D:706:HOH:O	2.09	0.52
1:C:274:ASN:ND2	1:C:294:LEU:H	2.04	0.52
1:D:299:LYS:HG3	1:D:341:THR:HG23	1.91	0.52
1:C:194:VAL:HG23	1:C:225:THR:HG23	1.92	0.51
1:C:217:PRO:HB3	1:C:223:LEU:HD13	1.92	0.51
1:C:205:ILE:HD12	1:C:213:ASP:HB3	1.92	0.51
1:D:318:CYS:HB3	1:D:387:VAL:HG13	1.91	0.51
1:B:282:TYR:O	1:B:283:THR:HG23	2.09	0.51
1:C:224:ARG:NH2	1:C:244:GLY:O	2.44	0.51
1:C:408:GLY:HA3	1:C:423:TRP:CE2	2.46	0.50
1:D:256:ARG:HG2	1:D:263:ALA:HB3	1.93	0.50
1:C:210:ILE:HD11	1:D:413(A):TYR:CZ	2.46	0.50
1:B:87:LEU:HD13	1:B:282:TYR:HB3	1.94	0.49
1:B:343:THR:OG1	1:B:344:GLU:OE1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LEU:HD21	1:C:444:ILE:CD1	2.42	0.49
1:B:94:ILE:HG12	1:B:448:GLY:HA3	1.94	0.49
1:C:408:GLY:HA3	1:C:423:TRP:CZ2	2.48	0.49
1:B:217:PRO:HB3	1:B:223:LEU:HD13	1.94	0.49
1:C:211:ILE:HD13	1:D:98:VAL:HB	1.94	0.49
1:B:273:PHE:HB3	1:B:340:LYS:HE2	1.94	0.49
1:B:288:LYS:HB3	1:B:302:PHE:CZ	2.48	0.49
1:C:322:LEU:HB2	1:C:327:ARG:HD2	1.95	0.48
1:B:183:CYS:HB3	1:B:230:CYS:O	2.14	0.48
1:C:414:GLU:HB2	1:C:415(A):ARG:H	1.79	0.48
1:C:256:ARG:NH1	1:C:307:GLN:O	2.32	0.48
1:D:169:PRO:HA	1:D:171:LEU:HD22	1.94	0.48
1:B:99:PRO:HA	1:B:445:THR:O	2.14	0.48
1:D:294:LEU:HA	1:D:347:GLY:O	2.13	0.47
1:D:414:GLU:HG2	1:D:415:SER:N	2.29	0.47
1:D:321:PHE:HD2	1:D:362:ILE:HD13	1.79	0.47
1:C:170:ASP:N	1:C:170:ASP:OD1	2.46	0.47
1:A:361:TRP:CH2	1:A:378:LYS:HB2	2.49	0.47
1:D:126:ASP:N	1:D:126:ASP:OD1	2.39	0.47
1:C:303:LEU:HG	1:C:314:PHE:CE1	2.49	0.47
1:C:183:CYS:HB2	1:C:232:CYS:SG	2.56	0.46
1:A:366:ILE:O	1:A:368:PRO:HD3	2.15	0.46
1:D:272:GLY:O	1:D:296:ASN:ND2	2.40	0.46
1:B:276:GLU:HG3	1:B:294:LEU:HD22	1.97	0.46
1:A:115:MET:SD	1:A:171:LEU:HD21	2.56	0.46
1:B:292:THR:HG22	1:B:294:LEU:HD13	1.98	0.46
1:B:252:HIS:CD2	1:B:270:THR:HG21	2.51	0.45
1:D:325:THR:HG23	1:D:368:PRO:HB3	1.98	0.45
1:D:165:ASP:HB3	1:D:170(A):LYS:HD2	1.97	0.45
1:B:294:LEU:HD12	1:B:347:GLY:O	2.17	0.45
1:A:361:TRP:CZ3	1:A:378:LYS:HB2	2.52	0.45
1:C:279:THR:HG21	1:C:408:GLY:CA	2.46	0.45
1:A:414:GLU:HG2	1:A:415(A):ARG:N	2.27	0.45
1:C:201:GLY:O	1:C:223:LEU:HB2	2.16	0.45
1:A:297:ASP:HB2	1:A:340:LYS:HG2	1.97	0.45
1:C:274:ASN:HD22	1:C:294:LEU:N	2.07	0.45
1:C:99:PRO:HA	1:C:445:THR:O	2.17	0.45
1:D:366:ILE:HD12	1:D:373:GLY:HA3	1.98	0.44
1:C:414:GLU:H	1:C:414:GLU:HG3	1.53	0.44
1:A:339:ASP:N	1:A:339:ASP:OD1	2.46	0.44
1:A:224:ARG:NH2	1:A:244:GLY:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:HB	6:A:714:HOH:O	2.17	0.44
1:B:350:GLN:OE1	1:B:406:ARG:NH1	2.49	0.44
1:C:115:MET:SD	1:C:135:SER:HB2	2.57	0.44
1:D:218:THR:OG1	1:D:219:ASN:N	2.49	0.44
1:D:82:ALA:O	1:D:83:THR:OG1	2.27	0.43
1:A:350:GLN:OE1	1:A:406:ARG:NH1	2.51	0.43
1:D:327:ARG:NH1	1:D:368:PRO:HG3	2.33	0.43
1:C:257:LEU:HD23	1:C:262:SER:HA	2.00	0.43
1:D:252:HIS:CE1	1:D:275:PHE:H	2.36	0.43
1:A:194:VAL:HG23	1:A:225:THR:HG23	2.00	0.43
1:A:117:THR:OG1	1:A:120:ASN:ND2	2.49	0.43
1:D:99:PRO:HA	1:D:445:THR:O	2.19	0.43
1:A:120:ASN:OD1	1:A:131:ARG:HD3	2.18	0.43
1:C:217:PRO:HD3	1:C:223:LEU:HD22	2.00	0.43
1:A:423:TRP:HB2	1:A:443:LEU:HD21	2.00	0.43
1:A:211:ILE:HD11	1:C:98:VAL:O	2.19	0.43
1:D:203:VAL:HG12	1:D:223:LEU:HD23	2.01	0.43
1:C:156:MET:SD	1:D:107:THR:HG21	2.59	0.43
1:B:232:CYS:HA	1:B:237:CYS:HA	2.01	0.43
1:A:217:PRO:HA	1:A:223:LEU:HD21	2.01	0.42
1:D:273:PHE:HB2	1:D:293:ASN:HD21	1.84	0.42
1:D:306:ASP:OD1	1:D:307:GLN:N	2.47	0.42
1:D:223:LEU:HD12	1:D:223:LEU:HA	1.77	0.42
1:B:361:TRP:CZ3	1:B:378:LYS:HB2	2.55	0.42
1:B:230:CYS:HB2	1:B:238:TYR:O	2.19	0.42
1:C:256:ARG:CG	1:C:263:ALA:HB3	2.46	0.42
1:D:419:GLU:OE2	1:D:447:CYS:HB3	2.20	0.42
1:C:194:VAL:HG22	1:C:203:VAL:HG22	2.02	0.42
1:C:212:THR:HG21	1:D:415(A):ARG:HH22	1.83	0.42
1:D:204:SER:HB3	1:D:211:ILE:CD1	2.49	0.42
1:A:202:PHE:CE2	1:C:453:MET:HE1	2.55	0.42
1:C:224:ARG:HB2	1:C:242:ALA:HB3	2.01	0.42
1:D:366:ILE:O	1:D:368:PRO:HD3	2.20	0.41
1:B:95:ASN:ND2	1:B:450:GLY:O	2.40	0.41
1:B:201:GLY:O	1:B:223:LEU:HB2	2.20	0.41
1:D:293:ASN:HB3	1:D:297:ASP:HB3	2.01	0.41
1:C:248:THR:HG22	1:C:295:TRP:CD1	2.55	0.41
1:D:422:PHE:HE2	1:D:424:ILE:HD11	1.84	0.41
1:A:243:ASP:OD1	1:A:244:GLY:N	2.47	0.41
1:C:218:THR:OG1	1:C:219:ASN:N	2.53	0.41
1:A:168:THR:O	1:A:171:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:HG2	1:B:414:GLU:O	2.20	0.41
1:D:83:THR:HA	1:D:84:PRO:HD3	1.86	0.41
1:A:101:TYR:HB3	1:A:445:THR:OG1	2.21	0.41
1:B:393:ARG:NH1	1:B:455:ASP:OD1	2.41	0.41
1:D:171:LEU:HA	1:D:171:LEU:HD12	1.88	0.41
1:B:299:LYS:NZ	1:B:317:PRO:O	2.45	0.41
1:C:327:ARG:CZ	1:C:368:PRO:HG3	2.51	0.41
1:B:278:PRO:HA	1:B:290:THR:O	2.20	0.40
1:A:134:VAL:HG11	1:A:178:TRP:HA	2.04	0.40
1:B:179:SER:HB3	1:B:194:VAL:HB	2.03	0.40
1:B:180:ALA:HA	1:B:192:LEU:O	2.21	0.40
1:B:99:PRO:HG3	1:B:458:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

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	350/369 (95%)	332 (95%)	17 (5%)	1 (0%)	46	73
1	B	350/369 (95%)	330 (94%)	19 (5%)	1 (0%)	46	73
1	C	351/369 (95%)	332 (95%)	18 (5%)	1 (0%)	46	73
1	D	350/369 (95%)	319 (91%)	29 (8%)	2 (1%)	30	56
All	All	1401/1476 (95%)	1313 (94%)	83 (6%)	5 (0%)	39	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	LYS
1	C	150	SER
1	D	391	VAL

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Mol	Chain	Res	Type
1	A	371	LYS
1	D	357	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	298/310 (96%)	269 (90%)	29 (10%)	10 22
1	B	298/310 (96%)	261 (88%)	37 (12%)	6 12
1	C	298/310 (96%)	264 (89%)	34 (11%)	7 15
1	D	298/310 (96%)	261 (88%)	37 (12%)	6 12
All	All	1192/1240 (96%)	1055 (88%)	137 (12%)	7 15

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	86	VAL
1	A	106	THR
1	A	107	THR
1	A	116	LEU
1	A	117	THR
1	A	119	GLN
1	A	130	ARG
1	A	131	ARG
1	A	150	SER
1	A	156	MET
1	A	170	ASP
1	A	204	SER
1	A	213	ASP
1	A	303	LEU
1	A	339	ASP
1	A	340	LYS
1	A	355	GLU
1	A	391	VAL

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Mol	Chain	Res	Type
1	A	393	ARG
1	A	396	GLN
1	A	401	ASN
1	A	409	LEU
1	A	413(A)	TYR
1	A	414	GLU
1	A	429	THR
1	A	439	SER
1	A	443	LEU
1	A	456	VAL
1	B	83	THR
1	B	112	ASP
1	B	113	GLU
1	B	115	MET
1	B	119	GLN
1	B	136	MET
1	B	156	MET
1	B	171	LEU
1	B	200	ASP
1	B	203	VAL
1	B	218	THR
1	B	223	LEU
1	B	236	THR
1	B	251	SER
1	B	257	LEU
1	B	294	LEU
1	B	303	LEU
1	B	319	LEU
1	B	334	THR
1	B	337	CYS
1	B	343	THR
1	B	377	TYR
1	B	378	LYS
1	B	380	LEU
1	B	390	THR
1	B	396	GLN
1	B	409	LEU
1	B	414	GLU
1	B	415	SER
1	B	415(A)	ARG
1	B	416	ASP
1	B	417	CYS

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Mol	Chain	Res	Type
1	B	420	LEU
1	B	429	THR
1	B	439	SER
1	B	443	LEU
1	B	456	VAL
1	C	83	THR
1	C	91	LEU
1	C	93	SER
1	C	119	GLN
1	C	131	ARG
1	C	149	VAL
1	C	156	MET
1	C	170	ASP
1	C	171	LEU
1	C	178	TRP
1	C	183	CYS
1	C	188	GLN
1	C	218	THR
1	C	223	LEU
1	C	230	CYS
1	C	246	THR
1	C	254	LEU
1	C	256	ARG
1	C	271	THR
1	C	303	LEU
1	C	313	THR
1	C	319	LEU
1	C	339	ASP
1	C	357	SER
1	C	367	ASN
1	C	377	TYR
1	C	387	VAL
1	C	391	VAL
1	C	409	LEU
1	C	414	GLU
1	C	415	SER
1	C	443	LEU
1	C	444	ILE
1	C	456	VAL
1	D	92	CYS
1	D	104	GLU
1	D	116	LEU

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Mol	Chain	Res	Type
1	D	119	GLN
1	D	171	LEU
1	D	203	VAL
1	D	204	SER
1	D	210	ILE
1	D	213	ASP
1	D	214	THR
1	D	223	LEU
1	D	258	VAL
1	D	262	SER
1	D	283	THR
1	D	294	LEU
1	D	303	LEU
1	D	309	SER
1	D	313	THR
1	D	319	LEU
1	D	334	THR
1	D	339	ASP
1	D	341	THR
1	D	346	GLU
1	D	362	ILE
1	D	382	THR
1	D	387	VAL
1	D	396	GLN
1	D	398	LEU
1	D	403	THR
1	D	404	ILE
1	D	409	LEU
1	D	413(A)	TYR
1	D	414	GLU
1	D	417	CYS
1	D	439	SER
1	D	443	LEU
1	D	456	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	HIS
1	C	219	ASN
1	C	274	ASN
1	D	274	ASN

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Mol	Chain	Res	Type
1	D	359	ASN
1	D	394	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

17 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	601	1,2	14,14,15	0.63	0	15,19,21	1.06	0
2	NAG	A	602	2	14,14,15	0.55	0	15,19,21	1.01	1 (6%)
2	BMA	A	603	2	11,11,12	0.58	0	14,15,17	0.70	0
4	NAG	B	601	1,4	14,14,15	0.52	0	15,19,21	1.61	2 (13%)
4	NAG	B	602	4	14,14,15	0.48	0	15,19,21	0.73	0
4	NAG	B	603	1,4	14,14,15	0.44	0	15,19,21	1.21	1 (6%)
4	NAG	B	604	4	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
4	NAG	C	601	1,4	14,14,15	0.49	0	15,19,21	0.87	1 (6%)
4	NAG	C	602	4	14,14,15	0.49	0	15,19,21	0.62	0
5	NAG	C	603	1,5	14,14,15	0.62	0	15,19,21	0.77	0
5	FUC	C	604	5	10,10,11	0.62	0	14,14,16	0.78	1 (7%)
5	NAG	C	605	5	14,14,15	0.56	0	15,19,21	1.00	0
5	BMA	C	606	5	11,11,12	0.55	0	14,15,17	0.71	0
5	MAN	C	607	5	11,11,12	0.54	0	14,15,17	0.66	0
2	NAG	D	601	1,2	14,14,15	0.58	0	15,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	602	2	14,14,15	0.54	0	15,19,21	1.15	1 (6%)
2	BMA	D	603	2	11,11,12	0.50	0	14,15,17	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	BMA	A	603	2	-	0/2/19/22	0/1/1/1
4	NAG	B	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	602	4	-	0/6/23/26	0/1/1/1
4	NAG	B	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	604	4	-	0/6/23/26	0/1/1/1
4	NAG	C	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	602	4	-	0/6/23/26	0/1/1/1
5	NAG	C	603	1,5	-	0/6/23/26	0/1/1/1
5	FUC	C	604	5	-	0/0/17/20	0/1/1/1
5	NAG	C	605	5	-	0/6/23/26	0/1/1/1
5	BMA	C	606	5	-	0/2/19/22	0/1/1/1
5	MAN	C	607	5	-	0/2/19/22	0/1/1/1
2	NAG	D	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	602	2	-	0/6/23/26	0/1/1/1
2	BMA	D	603	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	602	NAG	C2-N2-C7	-4.22	117.62	123.04
4	B	601	NAG	C2-N2-C7	-3.40	118.67	123.04
5	C	604	FUC	O5-C5-C6	2.03	109.49	106.13
4	C	601	NAG	C1-O5-C5	2.71	115.69	112.25
2	A	602	NAG	C3-C4-C5	2.74	114.98	110.20
4	B	604	NAG	C1-O5-C5	2.76	115.75	112.25
4	B	603	NAG	C1-O5-C5	3.89	117.19	112.25
4	B	601	NAG	C1-O5-C5	4.50	117.96	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	NAG	1	0
4	C	602	NAG	1	0

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	354/369 (95%)	-0.34	4 (1%)	82	82	41, 59, 90, 127	0
1	B	354/369 (95%)	-0.33	1 (0%)	94	95	44, 65, 99, 132	0
1	C	355/369 (96%)	-0.17	3 (0%)	87	88	47, 68, 98, 152	0
1	D	354/369 (95%)	0.11	15 (4%)	40	38	59, 93, 124, 153	0
All	All	1417/1476 (96%)	-0.18	23 (1%)	74	74	41, 69, 115, 153	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	318	CYS	3.8
1	D	138	TYR	3.8
1	D	321	PHE	3.8
1	D	247	TYR	3.5
1	D	82	ALA	3.3
1	D	377	TYR	3.1
1	D	322	LEU	3.1
1	A	82	ALA	3.0
1	A	83	THR	3.0
1	C	151	GLU	2.9
1	B	415	SER	2.7
1	A	138	TYR	2.7
1	C	156	MET	2.7
1	D	337	CYS	2.6
1	D	336	TYR	2.6
1	D	329	ILE	2.6
1	D	388	GLN	2.5
1	A	452	SER	2.3
1	D	383	LEU	2.3
1	D	391	VAL	2.1
1	D	334	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	413(A)	TYR	2.0
1	C	85	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	C	603	14/15	0.96	0.22	2.90	65,92,118,127	0
4	NAG	B	603	14/15	0.92	0.15	0.38	90,119,133,139	0
5	BMA	C	606	11/12	0.88	0.23	-	111,128,140,150	0
4	NAG	B	602	14/15	0.89	0.26	-	110,122,134,136	0
2	NAG	D	601	14/15	0.95	0.18	-	97,107,113,121	0
5	MAN	C	607	11/12	0.88	0.42	-	150,159,166,168	0
2	NAG	A	602	14/15	0.85	0.39	-	108,132,154,166	0
4	NAG	B	604	14/15	0.90	0.18	-	117,123,133,134	0
2	NAG	D	602	14/15	0.87	0.38	-	123,139,170,173	0
5	FUC	C	604	10/11	0.89	0.23	-	133,135,141,143	0
4	NAG	C	601	14/15	0.92	0.18	-	78,100,114,135	0
2	BMA	D	603	11/12	0.71	0.38	-	135,165,174,175	0
2	NAG	A	601	14/15	0.94	0.15	-	77,80,93,103	0
4	NAG	B	601	14/15	0.93	0.10	-	65,77,91,96	0
5	NAG	C	605	14/15	0.90	0.21	-	74,100,107,121	0
4	NAG	C	602	14/15	0.85	0.31	-	105,129,140,142	0
2	BMA	A	603	11/12	0.74	0.44	-	136,152,163,166	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	C	608	1/1	0.94	0.20	3.10	73,73,73,73	0
3	CA	B	605	1/1	0.96	0.19	1.50	68,68,68,68	0
3	CA	D	604	1/1	0.66	0.11	-0.86	110,110,110,110	0
3	CA	A	604	1/1	0.93	0.12	-0.97	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.