



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:09 PM GMT

PDB ID : 4KQA  
Title : Crystal structure of the golgi casein kinase  
Authors : Xiao, J.  
Deposited on : 2013-05-14  
Resolution : 2.60 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 (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

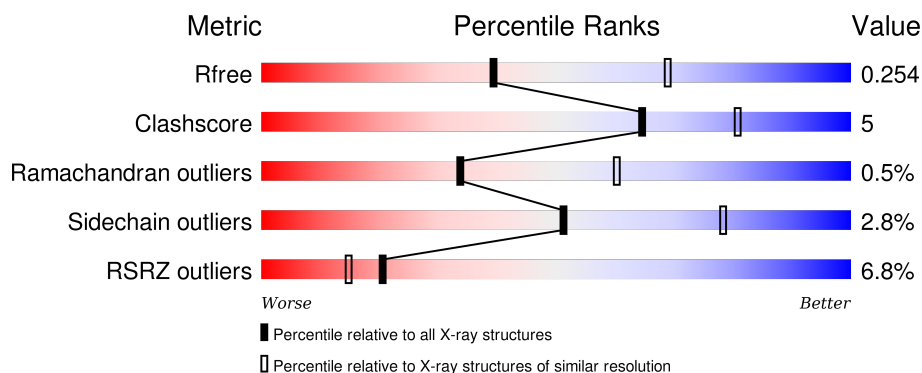
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	453	<div> <div>2%</div> <div>79%</div> <div>13%</div> <div>8%</div> </div>
1	B	453	<div> <div>9%</div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
1	C	453	<div> <div>2%</div> <div>80%</div> <div>11%</div> <div>8%</div> </div>
1	D	453	<div> <div>13%</div> <div>74%</div> <div>17%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	B	603	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14391 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 Protein H03A11.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	Se	0	0	0
			3453	2198	604	632	10	9			
1	B	426	Total	C	N	O	S	Se	0	0	0
			3516	2234	618	645	10	9			
1	C	419	Total	C	N	O	S	Se	0	0	0
			3454	2198	605	632	10	9			
1	D	416	Total	C	N	O	S	Se	0	0	0
			3427	2181	601	626	10	9			

- 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	B	3	Total	C	N	O	0	0
			39	22	2	15		
2	C	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 a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		
4	A	1	Total	Ni	0	0
			1	1		

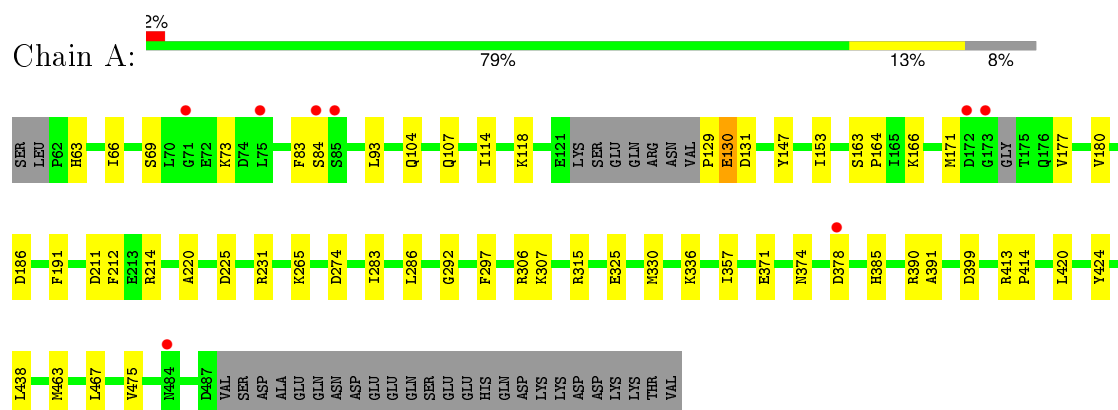
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	B	54	Total	O	0	0
			54	54		
5	C	99	Total	O	0	0
			99	99		
5	D	42	Total	O	0	0
			42	42		

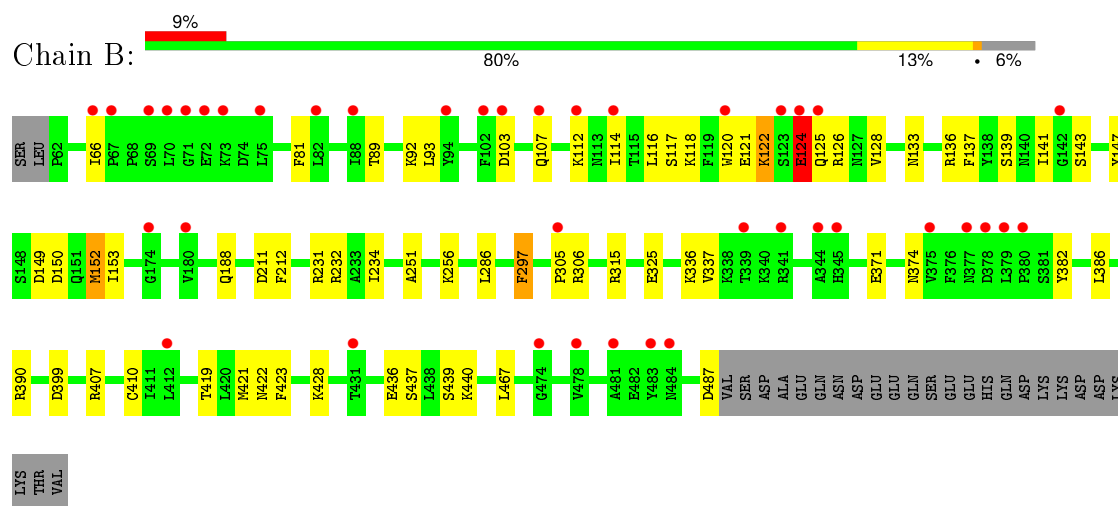
### 3 Residue-property plots

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.

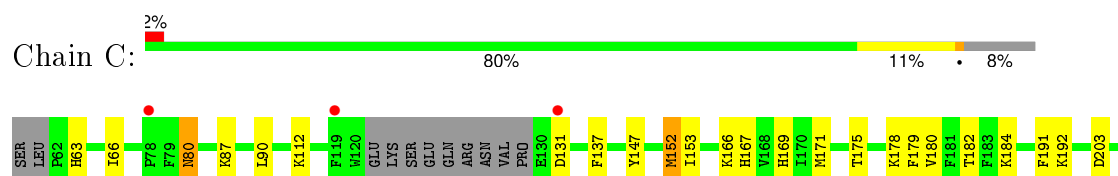
#### • Molecule 1: Protein H03A11.1

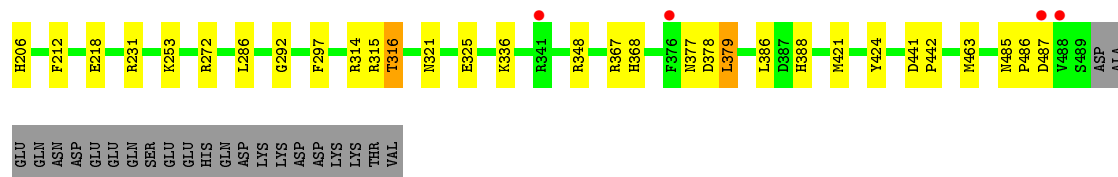


#### • Molecule 1: Protein H03A11.1

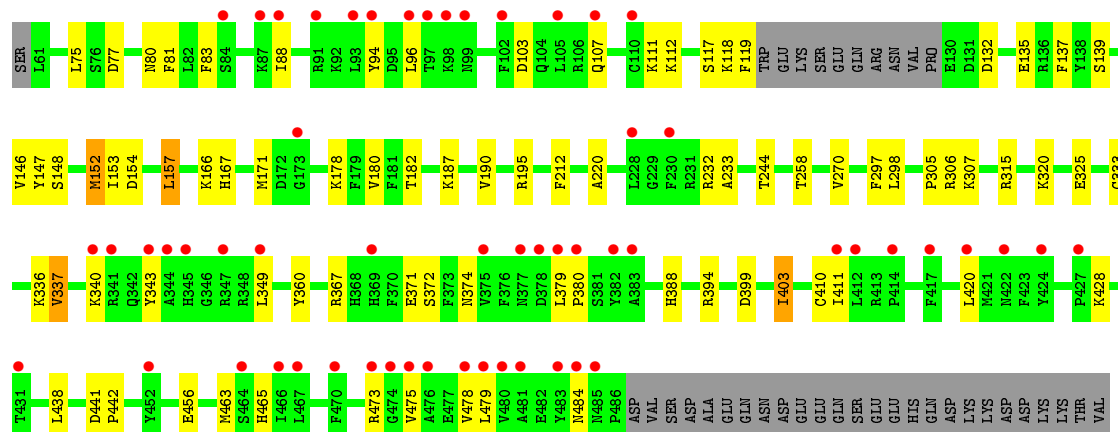
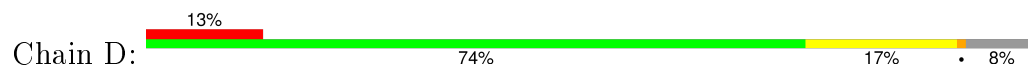


#### • Molecule 1: Protein H03A11.1





- Molecule 1: Protein H03A11.1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.79Å 157.31Å 168.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.46 – 2.60 46.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.46-2.60) 94.1 (46.46-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.217 , 0.254 0.215 , 0.254	Depositor DCC
$R_{free}$ test set	6137 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 64068 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14391	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.22	0/3538	0.40	0/4762
1	B	0.22	0/3603	0.41	0/4852
1	C	0.22	0/3539	0.40	0/4765
1	D	0.22	0/3510	0.40	0/4725
All	All	0.22	0/14190	0.40	0/19104

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
2	B	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	603	BMA	C1

There are no planarity outliers.

### 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	3453	0	3331	31	0
1	B	3516	0	3395	32	0
1	C	3454	0	3335	31	0
1	D	3427	0	3315	47	0
2	A	39	0	34	0	0
2	B	39	0	34	0	0
2	C	39	0	34	0	0
2	D	39	0	34	1	0
3	A	28	0	25	0	0
3	B	28	0	25	1	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	76	0	0	1	0
5	B	54	0	0	3	0
5	C	99	0	0	3	0
5	D	42	0	0	2	0
All	All	14391	0	13612	140	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 5.

All (140) 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:B:150:ASP:OD1	1:B:231:ARG:NH1	2.12	0.82
1:B:419:THR:O	5:B:722:HOH:O	1.97	0.81
1:B:306:ARG:NH1	1:B:371:GLU:OE2	2.15	0.80
1:D:306:ARG:NH1	1:D:371:GLU:OE2	2.16	0.78
1:A:306:ARG:NH1	1:A:371:GLU:OE1	2.18	0.77
1:B:120:TRP:O	1:B:122:LYS:N	2.24	0.70
1:A:274:ASP:OD1	1:C:272:ARG:NH1	2.27	0.68
1:D:77:ASP:HB3	1:D:80:ASN:HB2	1.77	0.67
1:B:124:GLU:HG2	1:B:125:GLN:HG2	1.77	0.65
1:B:234:ILE:HD12	1:B:386:LEU:HD13	1.78	0.65
1:B:133:ASN:HA	1:B:136:ARG:HG2	1.79	0.65
1:A:129:PRO:O	1:A:131:ASP:N	2.30	0.64
1:C:137:PHE:HA	1:C:152:MSE:HE1	1.78	0.64
1:B:137:PHE:HA	1:B:152:MSE:HE1	1.80	0.63
1:C:112:LYS:HB2	1:C:379:LEU:HD21	1.80	0.63
1:A:211:ASP:OD2	1:A:214:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HG23	1:B:286:LEU:HD23	1.80	0.63
1:C:66:ILE:HG23	1:C:286:LEU:HD23	1.81	0.62
1:A:325:GLU:OE2	1:A:336:LYS:NZ	2.33	0.62
1:C:316:THR:HG21	1:C:321:ASN:O	2.00	0.61
1:D:137:PHE:HA	1:D:152:MSE:HE1	1.81	0.60
1:D:307:LYS:HG3	1:D:374:ASN:HB2	1.83	0.59
1:B:81:PHE:O	1:B:428:LYS:NZ	2.31	0.58
1:B:407:ARG:NH1	1:B:407:ARG:O	2.37	0.58
1:C:325:GLU:OE2	1:C:336:LYS:NZ	2.36	0.58
1:D:410:CYS:SG	5:D:730:HOH:O	2.57	0.57
1:B:325:GLU:OE2	1:B:336:LYS:NZ	2.36	0.57
1:B:315:ARG:NH2	1:B:399:ASP:OD2	2.37	0.57
1:D:171:MSE:HE1	1:D:190:VAL:HG13	1.87	0.56
1:A:93:LEU:HD22	1:A:467:LEU:HD13	1.87	0.56
1:A:214:ARG:NH1	1:A:391:ALA:O	2.39	0.55
1:A:274:ASP:CG	1:C:272:ARG:HH12	2.09	0.55
1:D:305:PRO:HG2	1:D:374:ASN:O	2.07	0.54
1:A:315:ARG:NH2	1:A:399:ASP:OD2	2.41	0.54
1:B:423:PHE:N	5:B:722:HOH:O	2.12	0.54
1:C:147:TYR:CZ	1:C:231:ARG:HG2	2.43	0.54
1:D:146:VAL:HG23	1:D:147:TYR:HD1	1.73	0.54
1:C:80:ASN:ND2	1:C:80:ASN:O	2.31	0.54
1:A:66:ILE:HG23	1:A:286:LEU:HD23	1.89	0.53
1:C:314:ARG:NH1	1:C:368:HIS:HB2	2.24	0.53
1:D:325:GLU:OE2	1:D:336:LYS:NZ	2.41	0.52
1:D:83:PHE:CE2	1:D:456:GLU:HB3	2.44	0.52
1:D:333:CYS:HA	1:D:337:VAL:HG13	1.89	0.52
1:C:314:ARG:NH2	5:C:716:HOH:O	2.42	0.52
1:B:437:SER:O	1:B:440:LYS:HG2	2.10	0.52
1:C:192:LYS:NZ	1:C:218:GLU:OE2	2.32	0.52
1:A:147:TYR:CD2	1:A:153:ILE:HG13	2.44	0.52
1:D:135:GLU:HG3	1:D:187:LYS:NZ	2.26	0.51
1:B:407:ARG:NH1	1:B:410:CYS:SG	2.83	0.51
1:D:336:LYS:O	1:D:340:LYS:NZ	2.30	0.51
1:D:132:ASP:OD1	1:D:187:LYS:NZ	2.43	0.51
1:A:424:TYR:CG	1:A:463:MSE:HG3	2.46	0.51
1:A:147:TYR:CZ	1:A:231:ARG:HG2	2.45	0.51
1:D:111:LYS:HE2	1:D:380:PRO:HD3	1.93	0.50
1:B:147:TYR:CD1	1:B:153:ILE:HG13	2.47	0.50
1:A:166:LYS:NZ	1:A:186:ASP:OD1	2.42	0.50
1:D:154:ASP:HA	1:D:157:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:TYR:HB3	1:D:349:LEU:HG	1.93	0.50
1:D:315:ARG:NH2	1:D:399:ASP:OD2	2.45	0.50
1:D:146:VAL:HG22	1:D:232:ARG:HA	1.94	0.50
1:B:92:LYS:HG2	1:B:467:LEU:HD11	1.94	0.49
1:D:81:PHE:O	1:D:428:LYS:NZ	2.30	0.49
1:B:89:THR:HG23	1:B:467:LEU:HD22	1.95	0.49
1:B:251:ALA:O	1:B:256:LYS:NZ	2.46	0.49
1:A:225:ASP:OD2	1:A:385:HIS:ND1	2.34	0.49
1:C:379:LEU:H	1:C:379:LEU:HD12	1.78	0.48
1:D:367:ARG:HH22	1:D:388:HIS:CE1	2.32	0.48
1:D:148:SER:O	2:D:602:NAG:H2	2.13	0.48
1:D:410:CYS:O	1:D:478:VAL:HG12	2.14	0.47
1:A:177:VAL:HG11	1:A:283:ILE:HD11	1.97	0.47
1:D:117:SER:HB3	1:D:139:SER:HB3	1.97	0.47
1:D:349:LEU:HB3	1:D:411:ILE:HD11	1.97	0.46
1:D:171:MSE:HB2	1:D:180:VAL:HG23	1.97	0.46
1:C:421:MSE:HE3	1:C:421:MSE:HA	1.97	0.46
1:C:147:TYR:CD2	1:C:153:ILE:HG13	2.51	0.46
1:C:315:ARG:NH1	5:C:734:HOH:O	2.48	0.46
1:A:93:LEU:HD21	1:A:467:LEU:HB2	1.96	0.46
1:A:104:GLN:O	1:A:107:GLN:HG2	2.16	0.46
1:C:169:HIS:HB2	1:C:180:VAL:HG13	1.98	0.45
1:C:87:LYS:HD2	1:C:90:LEU:HD23	1.97	0.45
1:D:112:LYS:HB3	1:D:379:LEU:HD11	1.99	0.45
1:A:357:ILE:HD13	1:A:420:LEU:HD11	1.98	0.45
1:D:258:THR:HB	1:D:270:VAL:HB	1.98	0.45
1:A:211:ASP:HB3	1:A:390:ARG:HG2	1.99	0.45
1:D:420:LEU:HB3	1:D:463:MSE:HE1	1.98	0.44
1:B:211:ASP:HB3	1:B:390:ARG:HG2	1.98	0.44
1:B:436:GLU:O	1:B:439:SER:OG	2.32	0.44
1:B:116:LEU:HD12	1:B:141:ILE:HB	1.99	0.44
1:D:320:LYS:N	1:D:320:LYS:HD2	2.33	0.44
1:B:112:LYS:O	1:B:143:SER:OG	2.32	0.44
1:D:441:ASP:HA	1:D:442:PRO:HD3	1.88	0.44
1:D:146:VAL:HG23	1:D:147:TYR:CD1	2.52	0.43
1:D:403:ILE:HD12	1:D:465:HIS:CD2	2.53	0.43
1:D:478:VAL:HG23	1:D:479:LEU:N	2.33	0.43
1:D:147:TYR:CD2	1:D:153:ILE:HG13	2.54	0.43
1:D:167:HIS:HB2	1:D:182:THR:HB	2.00	0.43
1:D:195:ARG:NH2	5:D:711:HOH:O	2.44	0.43
1:C:191:PHE:CE1	1:C:292:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD13	1:B:421:MSE:HE1	2.01	0.43
1:A:191:PHE:CE1	1:A:292:GLY:HA3	2.53	0.43
1:D:220:ALA:HA	1:D:438:LEU:HD21	2.00	0.43
1:A:69:SER:HA	1:A:73:LYS:NZ	2.34	0.43
1:C:179:PHE:HB2	1:C:191:PHE:HB3	2.01	0.43
1:D:103:ASP:O	1:D:107:GLN:HG2	2.19	0.43
1:A:220:ALA:HA	1:A:438:LEU:HD21	2.00	0.42
1:B:232:ARG:HD2	1:B:382:TYR:CD1	2.53	0.42
1:A:163:SER:HA	1:A:164:PRO:HD3	1.92	0.42
1:A:63:HIS:N	5:A:713:HOH:O	2.49	0.42
1:A:114:ILE:HG13	1:A:118:LYS:HE3	2.01	0.42
1:C:203:ASP:HB3	1:C:206:HIS:CG	2.55	0.42
1:C:424:TYR:CG	1:C:463:MSE:HG3	2.55	0.42
1:D:171:MSE:HE3	1:D:178:LYS:HB3	2.02	0.42
1:D:360:TYR:CD1	1:D:403:ILE:HG12	2.55	0.42
1:C:178:LYS:HG2	1:C:192:LYS:HG2	2.01	0.42
1:B:117:SER:HB2	1:B:139:SER:HB2	2.01	0.42
1:D:135:GLU:HG3	1:D:187:LYS:HZ1	1.85	0.41
1:C:166:LYS:HE3	1:C:184:LYS:HA	2.01	0.41
1:D:146:VAL:HG21	1:D:233:ALA:O	2.20	0.41
1:A:171:MSE:HB2	1:A:180:VAL:HG23	2.02	0.41
1:D:475:VAL:HA	1:D:478:VAL:HG22	2.02	0.41
1:C:167:HIS:HB2	1:C:182:THR:HB	2.03	0.41
1:C:153:ILE:HA	1:C:153:ILE:HD13	1.95	0.41
1:A:147:TYR:CE2	1:A:231:ARG:HG2	2.55	0.41
1:D:166:LYS:HE3	1:D:167:HIS:CD2	2.55	0.41
1:A:413:ARG:HA	1:A:414:PRO:HD3	1.89	0.41
1:C:253:LYS:HB3	1:C:253:LYS:HE2	1.93	0.41
1:A:83:PHE:O	1:A:84:SER:HB3	2.21	0.41
1:B:305:PRO:HG2	1:B:374:ASN:O	2.20	0.41
1:D:307:LYS:N	1:D:372:SER:O	2.43	0.41
1:A:307:LYS:HG3	1:A:374:ASN:HB2	2.03	0.41
1:C:367:ARG:HH22	1:C:388:HIS:CD2	2.39	0.41
1:C:63:HIS:N	5:C:733:HOH:O	2.53	0.41
1:C:485:ASN:HA	1:C:486:PRO:HD2	1.88	0.40
1:B:422:ASN:N	5:B:722:HOH:O	2.55	0.40
1:B:407:ARG:HA	1:B:407:ARG:HD2	1.77	0.40
1:B:188:GLN:O	1:B:297:PHE:HB2	2.21	0.40
1:C:441:ASP:HA	1:C:442:PRO:HD3	1.90	0.40
1:D:337:VAL:HG23	1:D:349:LEU:HD21	2.04	0.40
1:B:103:ASP:O	1:B:107:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:604:NAG:H61	3:B:605:NAG:HN2	1.87	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	412/453 (91%)	393 (95%)	17 (4%)	2 (0%)	34	60
1	B	424/453 (94%)	405 (96%)	15 (4%)	4 (1%)	21	42
1	C	415/453 (92%)	398 (96%)	14 (3%)	3 (1%)	26	51
1	D	412/453 (91%)	394 (96%)	18 (4%)	0	100	100
All	All	1663/1812 (92%)	1590 (96%)	64 (4%)	9 (0%)	34	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	B	121	GLU
1	B	122	LYS
1	C	377	ASN
1	C	378	ASP
1	B	124	GLU
1	C	379	LEU
1	B	149	ASP
1	A	378	ASP

### 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	386/410 (94%)	380 (98%)	6 (2%)	70	89
1	B	393/410 (96%)	383 (98%)	10 (2%)	55	81
1	C	386/410 (94%)	375 (97%)	11 (3%)	51	78
1	D	383/410 (93%)	366 (96%)	17 (4%)	35	63
All	All	1548/1640 (94%)	1504 (97%)	44 (3%)	51	78

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	A	212	PHE
1	A	265	LYS
1	A	297	PHE
1	A	330	MSE
1	A	475	VAL
1	B	114	ILE
1	B	118	LYS
1	B	124	GLU
1	B	126	ARG
1	B	128	VAL
1	B	152	MSE
1	B	212	PHE
1	B	297	PHE
1	B	337	VAL
1	B	487	ASP
1	C	80	ASN
1	C	131	ASP
1	C	152	MSE
1	C	171	MSE
1	C	175	THR
1	C	212	PHE
1	C	297	PHE
1	C	316	THR
1	C	348	ARG
1	C	386	LEU
1	C	487	ASP
1	D	75	LEU

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Mol	Chain	Res	Type
1	D	88	ILE
1	D	94	TYR
1	D	96	LEU
1	D	118	LYS
1	D	119	PHE
1	D	152	MSE
1	D	157	LEU
1	D	212	PHE
1	D	244	THR
1	D	297	PHE
1	D	298	LEU
1	D	337	VAL
1	D	394	ARG
1	D	403	ILE
1	D	473	ARG
1	D	484	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

20 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	0.56	0	15,19,21	1.19	1 (6%)
2	NAG	A	602	2	14,14,15	0.21	0	15,19,21	0.26	0
2	BMA	A	603	2	11,11,12	0.59	0	14,15,17	0.74	0
3	NAG	A	604	1,3	14,14,15	0.30	0	15,19,21	0.85	1 (6%)
3	NAG	A	605	3	14,14,15	0.19	0	15,19,21	0.30	0
2	NAG	B	601	1,2	14,14,15	0.31	0	15,19,21	1.38	2 (13%)
2	NAG	B	602	2	14,14,15	0.33	0	15,19,21	0.28	0
2	BMA	B	603	2	11,11,12	0.55	0	14,15,17	0.75	0
3	NAG	B	604	1,3	14,14,15	0.20	0	15,19,21	2.08	1 (6%)
3	NAG	B	605	3	14,14,15	0.26	0	15,19,21	0.30	0
2	NAG	C	601	1,2	14,14,15	0.65	1 (7%)	15,19,21	1.76	2 (13%)
2	NAG	C	602	2	14,14,15	0.30	0	15,19,21	0.22	0
2	BMA	C	603	2	11,11,12	0.59	0	14,15,17	0.78	0
3	NAG	C	604	1,3	14,14,15	0.33	0	15,19,21	0.46	0
3	NAG	C	605	3	14,14,15	0.26	0	15,19,21	0.21	0
2	NAG	D	601	1,2	14,14,15	0.21	0	15,19,21	1.96	2 (13%)
2	NAG	D	602	2	14,14,15	0.19	0	15,19,21	0.37	0
2	BMA	D	603	2	11,11,12	0.59	0	14,15,17	0.75	0
3	NAG	D	604	1,3	14,14,15	0.30	0	15,19,21	1.66	1 (6%)
3	NAG	D	605	3	14,14,15	0.21	0	15,19,21	0.30	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
3	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	605	3	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	2	-	0/6/23/26	0/1/1/1
2	BMA	B	603	2	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	B	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	605	3	-	0/6/23/26	0/1/1/1
2	NAG	C	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	602	2	-	0/6/23/26	0/1/1/1
2	BMA	C	603	2	-	0/2/19/22	0/1/1/1
3	NAG	C	604	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	605	3	-	0/6/23/26	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
3	NAG	D	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	605	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAG	O5-C1	-2.04	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	NAG	O4-C4-C3	-6.33	96.09	110.34
2	C	601	NAG	O4-C4-C5	-2.35	103.02	109.24
3	A	604	NAG	O4-C4-C3	-2.29	105.19	110.34
2	B	601	NAG	O4-C4-C5	3.45	118.39	109.24
2	B	601	NAG	O4-C4-C3	3.79	118.88	110.34
2	A	601	NAG	O4-C4-C5	4.10	120.11	109.24
2	D	601	NAG	O4-C4-C5	4.64	121.53	109.24
2	D	601	NAG	O4-C4-C3	5.84	123.49	110.34
3	D	604	NAG	O4-C4-C3	6.07	124.00	110.34
3	B	604	NAG	O4-C4-C5	7.77	129.84	109.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	603	BMA	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	604	NAG	1	0
3	B	605	NAG	1	0
2	D	602	NAG	1	0

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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<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	409/453 (90%)	0.14	8 (1%) 68 63	31, 47, 82, 118	0
1	B	417/453 (92%)	0.49	40 (9%) 10 6	33, 53, 88, 164	0
1	C	410/453 (90%)	0.14	7 (1%) 73 68	31, 47, 81, 119	0
1	D	407/453 (89%)	0.55	57 (14%) 4 2	36, 54, 83, 118	0
All	All	1643/1812 (90%)	0.33	112 (6%) 20 15	31, 51, 83, 164	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	344	ALA	7.6
1	B	123	SER	5.2
1	D	424	TYR	5.2
1	A	85	SER	4.9
1	B	71	GLY	4.8
1	D	414	PRO	4.8
1	D	474	GLY	4.6
1	D	479	LEU	4.5
1	B	378	ASP	4.5
1	D	484	ASN	4.5
1	D	483	TYR	4.5
1	B	75	LEU	4.4
1	B	66	ILE	4.3
1	B	67	PRO	4.2
1	D	412	LEU	4.2
1	D	94	TYR	4.2
1	D	93	LEU	4.0
1	B	94	TYR	4.0
1	B	124	GLU	4.0
1	B	344	ALA	3.8
1	D	102	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	91	ARG	3.7
1	D	345	HIS	3.6
1	B	70	LEU	3.5
1	D	417	PHE	3.5
1	D	470	PHE	3.5
1	D	476	ALA	3.4
1	B	72	GLU	3.4
1	D	341	ARG	3.3
1	D	379	LEU	3.3
1	B	174	GLY	3.3
1	D	377	ASN	3.3
1	D	475	VAL	3.2
1	B	103	ASP	3.2
1	B	379	LEU	3.2
1	D	485	ASN	3.1
1	D	105	LEU	3.0
1	D	228	LEU	3.0
1	D	478	VAL	3.0
1	A	378	ASP	2.9
1	B	412	LEU	2.9
1	B	483	TYR	2.9
1	B	102	PHE	2.9
1	A	71	GLY	2.8
1	B	112	LYS	2.8
1	D	382	TYR	2.8
1	D	420	LEU	2.8
1	D	375	VAL	2.8
1	B	82	LEU	2.8
1	B	107	GLN	2.8
1	D	84	SER	2.8
1	B	484	ASN	2.7
1	B	380	PRO	2.7
1	B	341	ARG	2.7
1	D	466	ILE	2.7
1	A	172	ASP	2.7
1	D	411	ILE	2.7
1	C	119	PHE	2.7
1	B	69	SER	2.7
1	D	480	VAL	2.6
1	D	452	TYR	2.6
1	D	378	ASP	2.6
1	D	88	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	131	ASP	2.5
1	B	481	ALA	2.5
1	D	347	ARG	2.5
1	D	343	TYR	2.5
1	A	84	SER	2.5
1	B	114	ILE	2.5
1	D	340	LYS	2.5
1	A	75	LEU	2.5
1	D	380	PRO	2.4
1	B	125	GLN	2.4
1	B	375	VAL	2.4
1	D	464	SER	2.4
1	D	349	LEU	2.4
1	D	97	THR	2.4
1	A	484	ASN	2.4
1	D	173	GLY	2.3
1	B	431	THR	2.3
1	C	487	ASP	2.3
1	C	376	PHE	2.3
1	D	230	PHE	2.3
1	B	305	PRO	2.3
1	D	107	GLN	2.3
1	D	481	ALA	2.3
1	D	87	LYS	2.3
1	D	427	PRO	2.2
1	D	369	HIS	2.2
1	D	110	CYS	2.2
1	B	73	LYS	2.2
1	B	474	GLY	2.2
1	A	173	GLY	2.2
1	B	142	GLY	2.2
1	B	88	ILE	2.2
1	C	488	VAL	2.2
1	B	120	TRP	2.1
1	D	98	LYS	2.1
1	B	377	ASN	2.1
1	B	345	HIS	2.1
1	D	422	ASN	2.1
1	D	96	LEU	2.1
1	B	180	VAL	2.1
1	C	78	PRO	2.1
1	D	431	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	478	VAL	2.0
1	D	473	ARG	2.0
1	D	383	ALA	2.0
1	D	99	ASN	2.0
1	D	467	LEU	2.0
1	C	341	ARG	2.0
1	B	339	THR	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<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
2	NAG	D	602	14/15	0.91	0.15	-	46,69,77,81	0
2	BMA	D	603	11/12	0.67	0.27	-	97,125,139,147	0
2	NAG	B	602	14/15	0.90	0.17	-	55,75,95,101	0
3	NAG	B	605	14/15	0.73	0.30	-	86,102,125,127	0
3	NAG	A	605	14/15	0.86	0.19	-	78,106,131,143	0
3	NAG	A	604	14/15	0.92	0.17	-	40,51,74,82	0
2	BMA	B	603	11/12	0.72	0.27	-	106,122,135,136	0
3	NAG	D	604	14/15	0.96	0.15	-	32,54,84,85	0
2	NAG	A	602	14/15	0.97	0.11	-	38,54,65,69	0
3	NAG	B	604	14/15	0.92	0.22	-	45,54,71,94	0
3	NAG	C	605	14/15	0.88	0.25	-	51,68,83,88	0
3	NAG	C	604	14/15	0.93	0.14	-	31,47,56,72	0
2	NAG	C	602	14/15	0.95	0.14	-	48,70,90,98	0
2	BMA	A	603	11/12	0.80	0.16	-	60,72,100,103	0
2	NAG	B	601	14/15	0.91	0.20	-	53,72,93,97	0
2	BMA	C	603	11/12	0.84	0.12	-	60,80,92,97	0
2	NAG	D	601	14/15	0.92	0.14	-	54,68,103,103	0
2	NAG	A	601	14/15	0.94	0.13	-	29,55,102,107	0
2	NAG	C	601	14/15	0.94	0.15	-	46,66,93,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	605	14/15	0.85	0.20	-	64,97,115,115	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<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
4	NI	B	606	1/1	0.98	0.19	-	42,42,42,42	0
4	NI	A	606	1/1	0.98	0.16	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.