



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID : 3OJA  
Title : Crystal structure of LRIM1/APL1C complex  
Authors : Baxter, R.H.G.; Deisenhofer, J.  
Deposited on : 2010-08-20  
Resolution : 2.70 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

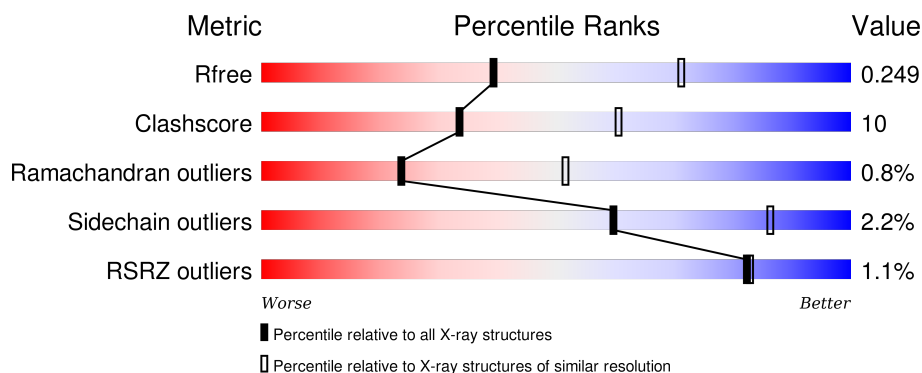
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	487	<div> <div>2%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	B	597	<div> <div>%</div> <div>70%</div> <div>18%</div> <div>• 11%</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
4	NAG	B	1017	X	-	-	-
5	MAN	B	1011	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9028 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 Leucine-rich Immune Molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3837	2386	691	749	11			

- Molecule 2 is a protein called Anopheles Plasmodium-responsive Leucine-rich repeat protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	534	Total	C	N	O	S	0	0	0
			4366	2748	774	832	12			

- 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	A	2	Total	C	N	O	0	0
			28	16	2	10		
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		

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



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

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	6	Total	C	N	O	0	0
			72	40	2	30		

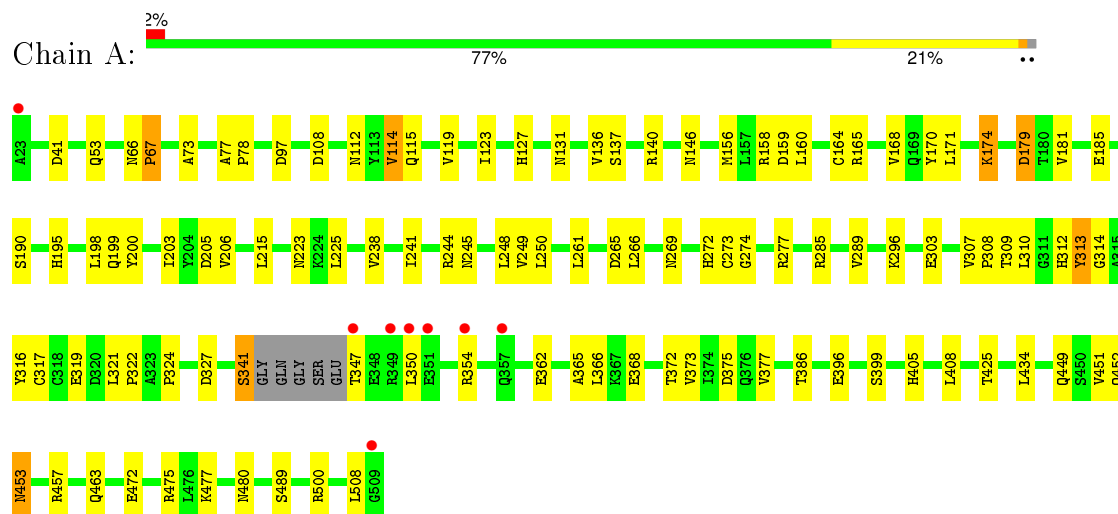
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	265	Total	O	0	0
			265	265		
6	B	348	Total	O	0	0
			348	348		

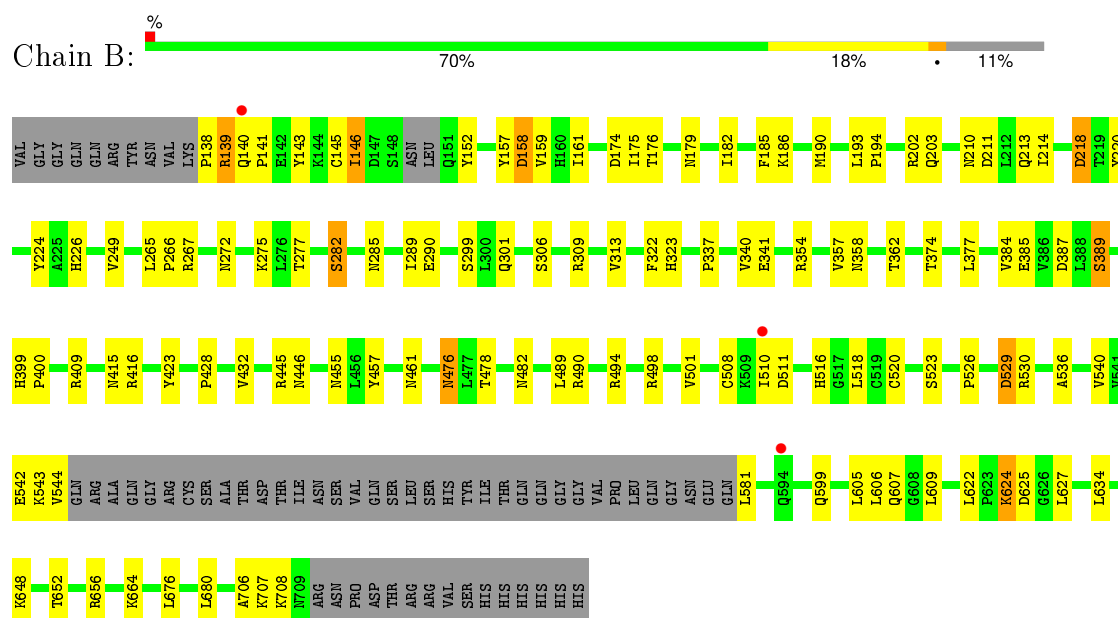
### 3 Residue-property plots

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: Leucine-rich Immune Molecule 1



#### • Molecule 2: Anopheles Plasmodium-responsive Leucine-rich repeat protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.89Å 110.89Å 168.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 2.70 45.56 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.56-2.70) 99.4 (45.56-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.205 , 0.265 0.180 , 0.249	Depositor DCC
$R_{free}$ test set	2881 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.4	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 56850 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.95	1/3884 (0.0%)	0.93	6/5238 (0.1%)
2	B	0.95	2/4441 (0.0%)	0.93	8/6019 (0.1%)
All	All	0.95	3/8325 (0.0%)	0.93	14/11257 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	VAL	CB-CG2	-5.15	1.42	1.52
2	B	341	GLU	CD-OE1	5.09	1.31	1.25
2	B	357	VAL	CB-CG2	-5.06	1.42	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	490	ARG	NE-CZ-NH2	-8.14	116.23	120.30
2	B	656	ARG	NE-CZ-NH2	-7.60	116.50	120.30
2	B	530	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	B	490	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	205	ASP	CB-CG-OD1	-6.29	112.64	118.30
2	B	529	ASP	CB-CG-OD1	-6.11	112.80	118.30
2	B	445	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	205	ASP	CB-CG-OD2	5.46	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASP	CB-CA-C	-5.41	99.58	110.40
2	B	656	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	41	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	314	GLY	N-CA-C	-5.16	100.19	113.10
1	A	327	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	341	GLU	OE1-CD-OE2	5.01	129.31	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1011	MAN	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	3837	0	3848	87	0
2	B	4366	0	4359	88	0
3	A	84	0	75	2	0
3	B	28	0	25	2	0
4	B	28	0	26	2	0
5	B	72	0	61	5	0
6	A	265	0	0	8	0
6	B	348	0	0	17	0
All	All	9028	0	8394	172	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 10.

All (172) 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:A:341:SER:HB3	6:B:942:HOH:O	1.66	0.93
2:B:140:GLN:HB2	2:B:141:PRO:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HB2	1:A:269:ASN:OD1	1.84	0.77
1:A:200:TYR:CE2	1:A:362:GLU:HG3	2.23	0.74
2:B:540:VAL:HG23	6:B:968:HOH:O	1.90	0.71
1:A:303:GLU:HG3	1:A:317:CYS:SG	2.31	0.70
2:B:581:LEU:HD12	2:B:581:LEU:O	1.92	0.69
1:A:136:VAL:HG12	1:A:164:CYS:SG	2.32	0.69
1:A:179:ASP:O	1:A:203:ILE:HA	1.93	0.69
5:B:1011:MAN:H2	5:B:1012:MAN:H2	1.76	0.68
1:A:277:ARG:HB2	1:A:313:TYR:CE1	2.31	0.66
1:A:449:GLN:NE2	6:A:754:HOH:O	2.29	0.65
3:A:1003:NAG:H61	3:A:1004:NAG:C1	2.26	0.65
1:A:170:TYR:CD1	1:A:195:HIS:HB2	2.32	0.65
2:B:625:ASP:OD1	2:B:627:LEU:HB2	1.97	0.65
1:A:66:ASN:HB3	1:A:67:PRO:CD	2.27	0.64
1:A:434:LEU:HD13	2:B:634:LEU:HD11	1.79	0.64
2:B:157:TYR:CE1	2:B:186:LYS:HD3	2.32	0.64
1:A:206:VAL:HG23	1:A:225:LEU:HD21	1.81	0.61
2:B:182:ILE:O	2:B:182:ILE:HG22	2.01	0.60
2:B:161:ILE:CD1	2:B:194:PRO:HG3	2.32	0.59
2:B:185:PHE:CE1	2:B:190:MET:CE	2.85	0.59
1:A:480:ASN:OD1	2:B:680:LEU:HD13	2.02	0.59
1:A:119:VAL:HB	1:A:123:ILE:HG13	1.83	0.59
2:B:185:PHE:CZ	2:B:190:MET:HE1	2.37	0.58
1:A:77:ALA:N	1:A:78:PRO:CD	2.66	0.58
2:B:145:CYS:O	2:B:146:ILE:HG12	2.03	0.58
1:A:508:LEU:HD11	2:B:707:LYS:O	2.03	0.57
2:B:476:ASN:OD1	4:B:1017:NAG:O5	2.23	0.56
1:A:248:LEU:CB	1:A:269:ASN:OD1	2.53	0.56
1:A:158:ARG:HH11	1:A:158:ARG:HG3	1.71	0.55
2:B:145:CYS:O	2:B:146:ILE:CG1	2.55	0.55
2:B:374:THR:HB	2:B:377:LEU:HD12	1.88	0.55
2:B:432:VAL:HG22	2:B:455:ASN:HB2	1.89	0.55
2:B:511:ASP:N	6:B:816:HOH:O	2.18	0.54
4:B:1007:NAG:O3	6:B:127:HOH:O	2.17	0.54
1:A:312:HIS:N	1:A:312:HIS:ND1	2.56	0.53
5:B:1011:MAN:C2	5:B:1012:MAN:H2	2.38	0.53
2:B:161:ILE:HD13	2:B:194:PRO:HG3	1.90	0.53
2:B:193:LEU:O	2:B:218:ASP:HB2	2.08	0.53
2:B:249:VAL:O	2:B:249:VAL:HG23	2.08	0.53
1:A:308:PRO:C	1:A:310:LEU:H	2.11	0.53
1:A:366:LEU:HD23	1:A:366:LEU:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:ASN:C	2:B:358:ASN:OD1	2.47	0.53
2:B:313:VAL:HG13	2:B:313:VAL:O	2.08	0.53
1:A:73:ALA:HB2	1:A:97:ASP:O	2.09	0.53
2:B:185:PHE:CE1	2:B:190:MET:HE2	2.44	0.52
1:A:452:GLN:HA	2:B:652:THR:HG23	1.91	0.52
2:B:322:PHE:CE2	2:B:323:HIS:CE1	2.97	0.52
2:B:185:PHE:CD1	2:B:190:MET:HE2	2.45	0.52
2:B:708:LYS:O	2:B:708:LYS:HG2	2.10	0.52
1:A:200:TYR:CZ	1:A:362:GLU:HG3	2.45	0.51
2:B:299:SER:O	2:B:301:GLN:HG3	2.11	0.51
1:A:249:VAL:O	1:A:250:LEU:HD23	2.10	0.51
2:B:152:TYR:HA	2:B:182:ILE:HG22	1.92	0.51
1:A:272:HIS:HA	1:A:319:GLU:O	2.10	0.51
2:B:202:ARG:HD3	2:B:224:TYR:HB3	1.93	0.51
2:B:536:ALA:O	6:B:968:HOH:O	2.19	0.50
1:A:146:ASN:N	1:A:146:ASN:HD22	2.09	0.50
1:A:408:LEU:HD13	2:B:609:LEU:CD2	2.41	0.50
2:B:282:SER:HA	2:B:306:SER:O	2.12	0.49
1:A:174:LYS:NZ	6:A:727:HOH:O	2.45	0.49
2:B:362:THR:HG23	2:B:384:VAL:CG2	2.42	0.49
1:A:53:GLN:HA	1:A:53:GLN:OE1	2.13	0.49
1:A:203:ILE:HG13	1:A:223:ASN:OD1	2.12	0.48
2:B:385:GLU:OE1	2:B:409:ARG:NH1	2.45	0.48
1:A:472:GLU:OE1	1:A:475:ARG:HD3	2.13	0.48
1:A:296:LYS:NZ	6:A:620:HOH:O	2.47	0.48
1:A:174:LYS:HB2	1:A:199:GLN:HG2	1.96	0.48
1:A:347:THR:N	6:A:731:HOH:O	2.46	0.48
1:A:307:VAL:O	1:A:310:LEU:HB2	2.14	0.48
1:A:261:LEU:O	1:A:285:ARG:NH2	2.46	0.48
1:A:265:ASP:O	1:A:266:LEU:HD23	2.14	0.48
1:A:273:CYS:O	1:A:274:GLY:C	2.51	0.48
1:A:140:ARG:HG3	6:A:674:HOH:O	2.14	0.47
1:A:365:ALA:O	1:A:368:GLU:HB2	2.14	0.47
1:A:308:PRO:O	1:A:310:LEU:N	2.47	0.47
1:A:66:ASN:HB3	1:A:67:PRO:HD2	1.97	0.47
2:B:510:ILE:CG2	6:B:816:HOH:O	2.63	0.47
1:A:249:VAL:HG11	1:A:324:PRO:HG2	1.96	0.47
2:B:185:PHE:CE1	2:B:190:MET:HE1	2.49	0.47
2:B:526:PRO:O	2:B:529:ASP:HB3	2.14	0.47
1:A:500:ARG:HG3	6:A:635:HOH:O	2.15	0.47
1:A:215:LEU:HD23	1:A:238:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASP:OD2	2:B:543:LYS:HE2	2.14	0.47
2:B:272:ASN:HB2	6:B:57:HOH:O	2.15	0.46
2:B:289:ILE:HB	2:B:313:VAL:HG23	1.98	0.46
1:A:308:PRO:C	1:A:310:LEU:N	2.69	0.46
2:B:143:TYR:HA	6:B:751:HOH:O	2.15	0.46
2:B:542:GLU:C	2:B:544:VAL:H	2.17	0.46
2:B:581:LEU:N	6:B:860:HOH:O	2.48	0.46
1:A:405:HIS:CE1	2:B:606:LEU:HD21	2.51	0.46
1:A:405:HIS:ND1	2:B:606:LEU:HD11	2.29	0.46
1:A:165:ARG:HD2	1:A:185:GLU:O	2.15	0.46
2:B:140:GLN:HB2	2:B:141:PRO:CD	2.36	0.46
2:B:461:ASN:HB2	2:B:482:ASN:OD1	2.16	0.46
1:A:372:THR:HG22	1:A:373:VAL:N	2.31	0.46
1:A:77:ALA:N	1:A:78:PRO:HD2	2.31	0.45
1:A:303:GLU:HG2	1:A:316:TYR:HA	1.99	0.45
1:A:181:VAL:HG23	1:A:203:ILE:HD13	1.98	0.45
1:A:277:ARG:NH1	6:A:666:HOH:O	2.48	0.45
1:A:248:LEU:HB2	1:A:269:ASN:CG	2.35	0.45
1:A:160:LEU:N	1:A:160:LEU:CD1	2.80	0.45
1:A:181:VAL:HG21	1:A:198:LEU:HD13	1.99	0.45
1:A:115:GLN:OE1	3:A:1003:NAG:O6	2.26	0.44
2:B:152:TYR:HA	2:B:182:ILE:CG2	2.46	0.44
2:B:428:PRO:HD2	6:B:95:HOH:O	2.17	0.44
5:B:1012:MAN:C1	6:B:738:HOH:O	2.65	0.44
1:A:108:ASP:HA	1:A:127:HIS:HB2	1.98	0.44
1:A:313:TYR:CD2	1:A:313:TYR:C	2.91	0.44
3:B:1016:NAG:H2	3:B:1016:NAG:H61	2.00	0.44
2:B:387:ASP:OD1	2:B:389:SER:HB2	2.18	0.44
5:B:1010:NAG:H62	5:B:1011:MAN:C1	2.47	0.43
1:A:457:ARG:HA	1:A:457:ARG:HD2	1.69	0.43
1:A:158:ARG:HH11	1:A:158:ARG:CG	2.29	0.43
1:A:273:CYS:SG	1:A:319:GLU:N	2.91	0.43
1:A:112:ASN:HB2	1:A:131:ASN:OD1	2.17	0.43
2:B:267:ARG:NH2	2:B:290:GLU:HG3	2.33	0.43
1:A:313:TYR:C	1:A:313:TYR:HD2	2.20	0.43
1:A:170:TYR:CD1	1:A:195:HIS:CB	3.00	0.43
1:A:285:ARG:NH2	1:A:289:VAL:HG21	2.33	0.43
2:B:494:ARG:HG2	6:B:934:HOH:O	2.19	0.43
2:B:508:CYS:HA	6:B:823:HOH:O	2.17	0.43
1:A:140:ARG:HD2	6:A:529:HOH:O	2.18	0.43
2:B:143:TYR:CD1	2:B:159:VAL:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:HIS:N	2:B:400:PRO:CD	2.81	0.43
1:A:168:VAL:HG11	1:A:171:LEU:HB2	2.01	0.43
2:B:202:ARG:NH1	2:B:224:TYR:CD1	2.87	0.43
1:A:244:ARG:HG2	1:A:245:ASN:N	2.33	0.43
2:B:179:ASN:HB2	2:B:203:GLN:NE2	2.33	0.43
2:B:138:PRO:O	2:B:139:ARG:HB2	2.19	0.43
3:B:1016:NAG:C6	3:B:1016:NAG:H2	2.49	0.42
2:B:457:TYR:HA	2:B:478:THR:OG1	2.19	0.42
2:B:190:MET:O	2:B:214:ILE:HA	2.19	0.42
2:B:210:ASN:O	2:B:211:ASP:HB3	2.20	0.42
1:A:350:LEU:O	1:A:354:ARG:HG2	2.19	0.42
2:B:605:LEU:HD12	2:B:605:LEU:O	2.19	0.42
1:A:241:ILE:O	1:A:241:ILE:HG23	2.19	0.42
1:A:123:ILE:HA	1:A:123:ILE:HD13	1.82	0.42
2:B:157:TYR:CZ	2:B:186:LYS:HD3	2.54	0.42
2:B:423:TYR:HB3	2:B:446:ASN:HA	2.02	0.42
2:B:385:GLU:HB2	2:B:409:ARG:NH1	2.34	0.42
2:B:664:LYS:HD2	2:B:664:LYS:HA	1.76	0.41
1:A:266:LEU:HB2	1:A:316:TYR:CE2	2.55	0.41
1:A:321:LEU:HA	1:A:322:PRO:HD3	1.91	0.41
2:B:706:ALA:C	2:B:708:LYS:H	2.24	0.41
2:B:624:LYS:HD3	2:B:624:LYS:N	2.35	0.41
2:B:337:PRO:HD2	2:B:340:VAL:HG11	2.03	0.41
2:B:498:ARG:NH1	2:B:516:HIS:O	2.52	0.41
2:B:489:LEU:HD12	2:B:520:CYS:HB3	2.02	0.41
1:A:453:ASN:ND2	5:B:1010:NAG:H81	2.35	0.41
2:B:622:LEU:HD22	6:B:956:HOH:O	2.19	0.41
1:A:114:VAL:HG12	1:A:115:GLN:N	2.35	0.41
2:B:218:ASP:O	2:B:220:TYR:N	2.54	0.41
2:B:498:ARG:HG2	2:B:501:VAL:O	2.21	0.41
1:A:477:LYS:HG3	2:B:676:LEU:CD1	2.51	0.41
1:A:508:LEU:O	1:A:508:LEU:HD23	2.21	0.40
2:B:523:SER:HB3	6:B:65:HOH:O	2.22	0.40
2:B:265:LEU:HA	2:B:266:PRO:HD3	1.90	0.40
2:B:174:ASP:O	2:B:176:THR:N	2.53	0.40
1:A:375:ASP:OD1	1:A:377:VAL:HG12	2.21	0.40
2:B:285:ASN:HB3	2:B:309:ARG:NH1	2.36	0.40
2:B:174:ASP:O	2:B:175:ILE:C	2.60	0.40
1:A:463:GLN:O	1:A:463:GLN:HG3	2.17	0.40
2:B:607:GLN:O	2:B:609:LEU:N	2.54	0.40
2:B:275:LYS:HD2	6:B:802:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:CG1	1:A:164:CYS:SG	3.07	0.40
1:A:449:GLN:OE1	2:B:648:LYS:HE2	2.21	0.40
1:A:156:MET:O	1:A:159:ASP:HB2	2.21	0.40
2:B:415:ASN:HB3	2:B:416:ARG:H	1.76	0.40
2:B:540:VAL:N	6:B:968:HOH:O	2.54	0.40
1:A:451:VAL:HG12	2:B:652:THR:HG21	2.03	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	478/487 (98%)	430 (90%)	46 (10%)	2 (0%)	39	69
2	B	528/597 (88%)	478 (90%)	44 (8%)	6 (1%)	17	42
All	All	1006/1084 (93%)	908 (90%)	90 (9%)	8 (1%)	24	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	226	HIS
2	B	146	ILE
2	B	158	ASP
2	B	139	ARG
1	A	309	THR
2	B	213	GLN
2	B	282	SER
1	A	67	PRO

### 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	420/423 (99%)	409 (97%)	11 (3%)	54	83
2	B	495/550 (90%)	486 (98%)	9 (2%)	66	89
All	All	915/973 (94%)	895 (98%)	20 (2%)	60	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	SER
1	A	174	LYS
1	A	190	SER
1	A	313	TYR
1	A	341	SER
1	A	386	THR
1	A	396	GLU
1	A	399	SER
1	A	425	THR
1	A	453	ASN
1	A	489	SER
2	B	158	ASP
2	B	218	ASP
2	B	277	THR
2	B	354	ARG
2	B	389	SER
2	B	476	ASN
2	B	518	LEU
2	B	599	GLN
2	B	624	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	146	ASN

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Mol	Chain	Res	Type
1	A	199	GLN
1	A	453	ASN
2	B	405	GLN
2	B	414	ASN
2	B	455	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 ⓘ

14 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$
3	NAG	A	1001	1,3	14,14,15	0.76	0	15,19,21	1.66	3 (20%)
3	NAG	A	1002	3	14,14,15	1.04	1 (7%)	15,19,21	2.02	6 (40%)
3	NAG	A	1003	1,3	14,14,15	0.80	0	15,19,21	1.91	3 (20%)
3	NAG	A	1004	3	14,14,15	0.89	0	15,19,21	3.70	5 (33%)
3	NAG	A	1005	1,3	14,14,15	0.77	0	15,19,21	2.36	3 (20%)
3	NAG	A	1006	3	14,14,15	0.94	1 (7%)	15,19,21	1.84	4 (26%)
5	NAG	B	1009	2,5	14,14,15	1.36	1 (7%)	15,19,21	2.15	5 (33%)
5	NAG	B	1010	5	14,14,15	1.13	2 (14%)	15,19,21	2.80	6 (40%)
5	MAN	B	1011	5	11,11,12	1.21	2 (18%)	14,15,17	1.72	1 (7%)
5	MAN	B	1012	5	11,11,12	1.20	1 (9%)	14,15,17	1.86	5 (35%)
5	MAN	B	1013	5	11,11,12	1.22	2 (18%)	14,15,17	1.58	4 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	B	1014	5	11,11,12	1.18	0	14,15,17	2.22	7 (50%)
3	NAG	B	1015	3,2	14,14,15	1.00	2 (14%)	15,19,21	2.08	4 (26%)
3	NAG	B	1016	3	14,14,15	0.57	0	15,19,21	1.74	2 (13%)

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
3	NAG	A	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1003	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1004	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1005	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1006	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1009	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1010	5	-	0/6/23/26	0/1/1/1
5	MAN	B	1011	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	1012	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1013	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1014	5	-	0/2/19/22	0/1/1/1
3	NAG	B	1015	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	1016	3	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1009	NAG	O5-C1	-4.01	1.37	1.43
3	A	1002	NAG	O5-C1	-3.50	1.37	1.43
5	B	1011	MAN	O5-C1	-2.98	1.38	1.43
5	B	1013	MAN	O5-C1	-2.91	1.38	1.43
5	B	1010	NAG	O5-C1	-2.35	1.39	1.43
5	B	1013	MAN	O2-C2	-2.25	1.38	1.43
3	B	1015	NAG	C2-N2	-2.25	1.42	1.46
3	B	1015	NAG	O5-C1	-2.22	1.40	1.43
5	B	1011	MAN	O5-C5	-2.19	1.38	1.43
5	B	1010	NAG	O7-C7	2.03	1.27	1.23
3	A	1006	NAG	C1-C2	2.35	1.55	1.52
5	B	1012	MAN	C2-C3	3.23	1.56	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	NAG	C2-N2-C7	-6.74	114.39	123.04
3	B	1015	NAG	C2-N2-C7	-5.86	115.51	123.04
3	A	1005	NAG	C2-N2-C7	-4.33	117.48	123.04
5	B	1009	NAG	O6-C6-C5	-4.25	97.29	111.33
5	B	1014	MAN	C1-O5-C5	-3.82	107.40	112.25
3	A	1002	NAG	C2-N2-C7	-3.76	118.20	123.04
5	B	1010	NAG	C6-C5-C4	-3.35	104.75	113.02
5	B	1009	NAG	C6-C5-C4	-3.20	105.13	113.02
3	A	1001	NAG	O7-C7-C8	-3.00	116.56	122.06
5	B	1013	MAN	O5-C1-C2	-2.71	106.47	110.86
3	B	1015	NAG	C3-C2-N2	-2.58	104.37	110.56
5	B	1010	NAG	O6-C6-C5	-2.54	102.93	111.33
3	A	1006	NAG	C3-C2-N2	-2.46	104.67	110.56
3	A	1003	NAG	C2-N2-C7	-2.45	119.89	123.04
3	A	1002	NAG	O4-C4-C3	-2.38	104.97	110.34
3	A	1005	NAG	O7-C7-C8	-2.31	117.83	122.06
3	A	1004	NAG	O3-C3-C4	-2.26	105.26	110.34
5	B	1010	NAG	O4-C4-C3	-2.25	105.27	110.34
5	B	1014	MAN	O3-C3-C2	-2.22	105.98	110.00
5	B	1014	MAN	O6-C6-C5	-2.18	104.11	111.33
3	A	1002	NAG	O6-C6-C5	-2.09	104.43	111.33
5	B	1010	NAG	C3-C2-N2	-2.04	105.66	110.56
5	B	1009	NAG	C3-C2-N2	-2.01	105.75	110.56
3	A	1002	NAG	O5-C5-C6	-2.00	103.01	107.35
5	B	1014	MAN	C2-C3-C4	2.07	114.55	111.04
5	B	1013	MAN	O5-C5-C6	2.16	112.02	107.35
5	B	1014	MAN	O2-C2-C1	2.26	113.73	109.21
5	B	1012	MAN	O2-C2-C1	2.27	113.76	109.21
5	B	1012	MAN	O4-C4-C3	2.29	115.50	110.34
5	B	1013	MAN	O3-C3-C4	2.47	115.89	110.34
3	B	1015	NAG	O3-C3-C2	2.51	114.08	109.11
3	A	1001	NAG	O7-C7-N2	2.58	127.13	121.86
5	B	1009	NAG	C2-N2-C7	2.65	126.44	123.04
3	A	1002	NAG	O4-C4-C5	2.65	116.27	109.24
5	B	1012	MAN	C2-C3-C4	2.71	115.65	111.04
3	B	1015	NAG	C1-O5-C5	2.80	115.80	112.25
5	B	1012	MAN	O2-C2-C3	2.87	115.89	110.12
3	A	1004	NAG	C3-C4-C5	2.91	115.27	110.20
5	B	1013	MAN	C2-C3-C4	3.03	116.19	111.04
3	A	1001	NAG	C1-O5-C5	3.07	116.15	112.25
5	B	1012	MAN	O5-C5-C6	3.09	114.04	107.35
3	A	1003	NAG	O3-C3-C2	3.12	115.29	109.11
3	A	1006	NAG	C2-N2-C7	3.13	127.06	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1014	MAN	O2-C2-C3	3.14	116.44	110.12
3	A	1006	NAG	C3-C4-C5	3.19	115.75	110.20
3	A	1006	NAG	C4-C3-C2	3.19	116.19	111.23
3	A	1004	NAG	C4-C3-C2	3.20	116.20	111.23
5	B	1010	NAG	C4-C3-C2	3.60	116.82	111.23
5	B	1009	NAG	C1-O5-C5	3.68	116.91	112.25
3	B	1016	NAG	O5-C5-C6	3.75	115.47	107.35
3	A	1002	NAG	C1-O5-C5	3.90	117.20	112.25
5	B	1014	MAN	C3-C4-C5	4.34	117.77	110.20
3	B	1016	NAG	C1-O5-C5	4.38	117.81	112.25
3	A	1003	NAG	C1-O5-C5	4.89	118.45	112.25
5	B	1011	MAN	O3-C3-C2	5.02	119.08	110.00
3	A	1005	NAG	C1-O5-C5	6.61	120.63	112.25
5	B	1010	NAG	C1-O5-C5	8.27	122.75	112.25
3	A	1004	NAG	C1-O5-C5	11.31	126.60	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1011	MAN	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	NAG	2	0
3	A	1004	NAG	1	0
5	B	1010	NAG	2	0
5	B	1011	MAN	3	0
5	B	1012	MAN	3	0
3	B	1016	NAG	2	0

## 5.6 Ligand geometry ⓘ

2 ligands 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	$\# Z  > 2$
4	NAG	B	1007	2	14,14,15	1.07	1 (7%)	15,19,21	3.04	8 (53%)
4	NAG	B	1017	2	14,14,15	0.83	0	15,19,21	2.48	7 (46%)

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
4	NAG	B	1007	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1017	2	1/1/5/7	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)
4	B	1007	NAG	O7-C7	2.58	1.29	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1007	NAG	C4-C3-C2	-6.95	100.43	111.23
4	B	1007	NAG	C2-N2-C7	-4.95	116.68	123.04
4	B	1017	NAG	O7-C7-C8	-2.19	118.04	122.06
4	B	1007	NAG	C3-C4-C5	-2.10	106.53	110.20
4	B	1017	NAG	O4-C4-C5	-2.03	103.85	109.24
4	B	1007	NAG	O5-C5-C6	2.31	112.34	107.35
4	B	1017	NAG	O3-C3-C2	2.36	113.78	109.11
4	B	1017	NAG	O5-C5-C6	2.56	112.88	107.35
4	B	1007	NAG	C3-C2-N2	2.56	116.70	110.56
4	B	1017	NAG	C3-C2-N2	2.87	117.44	110.56
4	B	1017	NAG	C6-C5-C4	3.02	120.47	113.02
4	B	1007	NAG	O3-C3-C4	3.25	117.66	110.34
4	B	1007	NAG	O4-C4-C3	3.75	118.78	110.34
4	B	1007	NAG	C1-O5-C5	3.90	117.20	112.25
4	B	1017	NAG	C1-O5-C5	6.67	120.72	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1017	NAG	C1

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	1007	NAG	1	0
4	B	1017	NAG	1	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	482/487 (98%)	-0.41	8 (1%) 73 74	18, 36, 62, 97	0
2	B	534/597 (89%)	-0.43	3 (0%) 90 91	13, 31, 65, 87	0
All	All	1016/1084 (93%)	-0.42	11 (1%) 82 83	13, 34, 64, 97	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	4.7
1	A	23	ALA	3.7
1	A	347	THR	3.4
1	A	354	ARG	3.1
2	B	140	GLN	3.0
1	A	349	ARG	2.9
1	A	351	GLU	2.9
1	A	509	GLY	2.8
1	A	357	GLN	2.0
2	B	594	GLN	2.0
2	B	510	ILE	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1001	14/15	0.98	0.13	0.24	12,28,35,40	0
5	NAG	B	1009	14/15	0.98	0.15	-0.59	15,25,35,37	0
3	NAG	A	1003	14/15	0.97	0.12	-	28,44,49,54	0
5	MAN	B	1014	11/12	0.93	0.16	-	40,49,70,84	0
5	MAN	B	1013	11/12	0.94	0.15	-	39,42,55,56	0
3	NAG	B	1016	14/15	0.94	0.17	-	30,61,79,81	0
5	MAN	B	1012	11/12	0.88	0.16	-	35,63,93,99	0
3	NAG	A	1002	14/15	0.97	0.14	-	37,52,63,65	0
3	NAG	B	1015	14/15	0.97	0.10	-	20,33,46,51	0
3	NAG	A	1006	14/15	0.80	0.42	-	59,84,99,100	0
5	MAN	B	1011	11/12	0.96	0.13	-	29,41,45,46	0
5	NAG	B	1010	14/15	0.97	0.13	-	14,31,43,46	0
3	NAG	A	1005	14/15	0.87	0.28	-	59,69,77,87	0
3	NAG	A	1004	14/15	0.92	0.15	-	39,55,71,72	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
4	NAG	B	1017	14/15	0.83	0.26	1.82	47,62,80,93	0
4	NAG	B	1007	14/15	0.90	0.15	-0.17	47,56,67,81	0

## 6.5 Other polymers

There are no such residues in this entry.