



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:49 pm GMT

PDB ID : 1GAL  
Title : CRYSTAL STRUCTURE OF GLUCOSE OXIDASE FROM ASPERGILLUS  
NIGER: REFINED AT 2.3 ANGSTROMS RESOLUTION  
Authors : Hecht, H.J.; Kalisz, K.; Hendle, J.; Schmid, R.D.; Schomburg, D.  
Deposited on : 1992-08-27  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

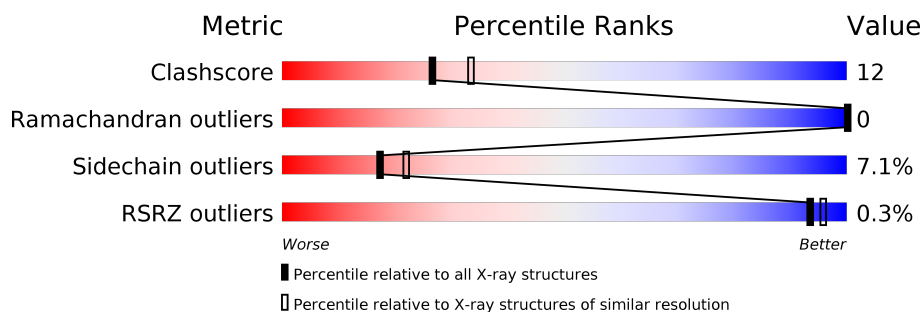
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	583	

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
3	NAG	A	608	-	-	-	X
3	NAG	A	609	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4774 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.

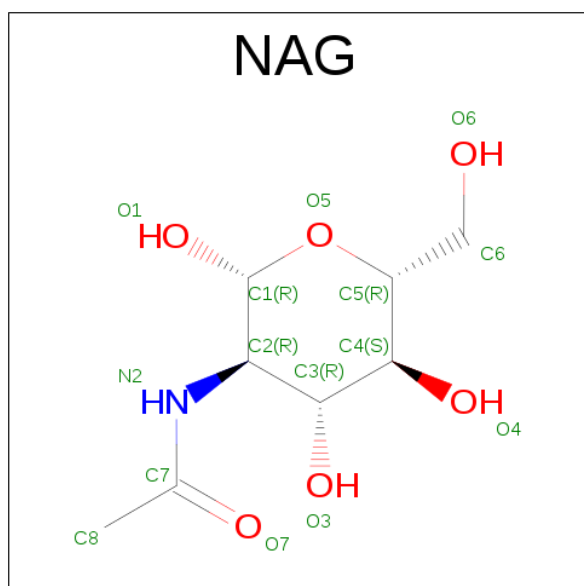
- Molecule 1 is a protein called GLUCOSE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4452	2801	764	873	14			

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



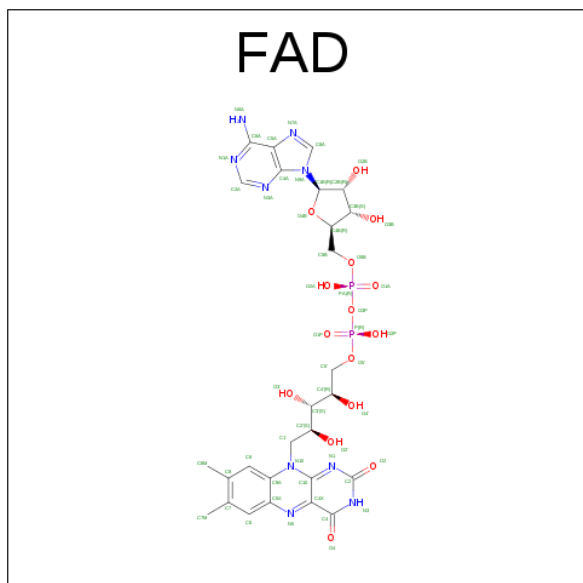
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

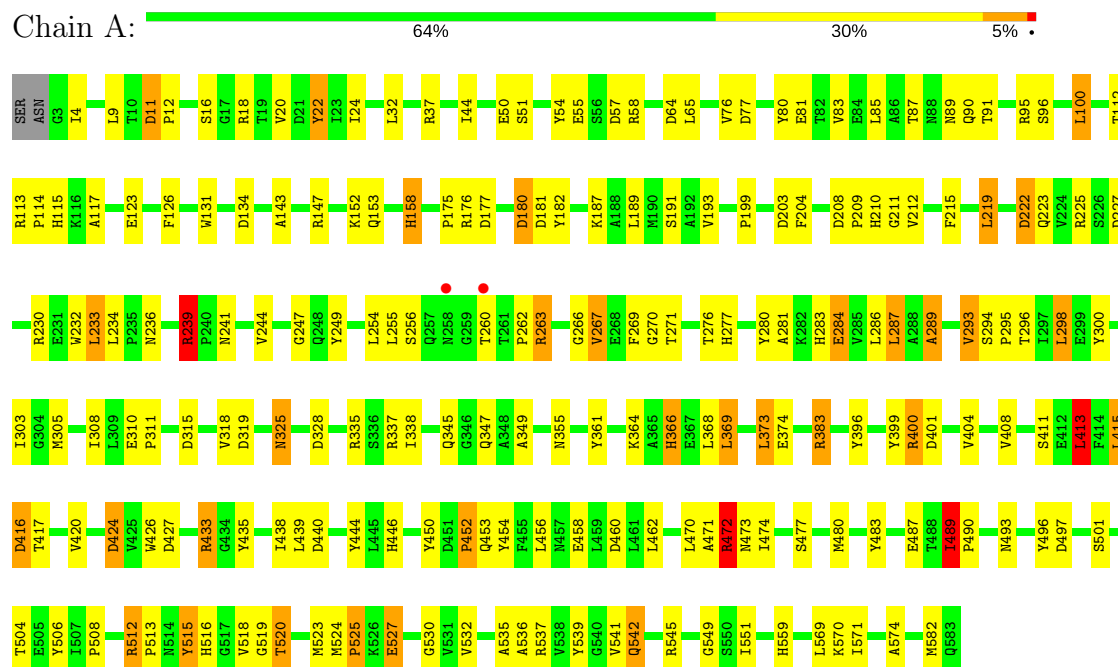
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		

### 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 the various outlier classes 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: GLUCOSE OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.50Å 66.50Å 214.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 19.41 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 85.1 (19.41-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.30Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.181 , (Not available) 0.163 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, FAD, 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	0.83	0/4560	1.95	103/6219 (1.7%)

There are no bond length outliers.

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	545	ARG	NE-CZ-NH2	-25.90	107.35	120.30
1	A	545	ARG	NE-CZ-NH1	24.57	132.59	120.30
1	A	512	ARG	NE-CZ-NH1	21.22	130.91	120.30
1	A	95	ARG	NE-CZ-NH1	20.86	130.73	120.30
1	A	472	ARG	NE-CZ-NH1	17.48	129.04	120.30
1	A	383	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	A	95	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	A	230	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	A	433	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	A	433	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	A	400	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	A	328	ASP	CB-CG-OD1	12.34	129.40	118.30
1	A	239	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	A	337	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	A	18	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	A	400	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	147	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	208	ASP	CB-CG-OD1	10.61	127.85	118.30
1	A	176	ARG	NE-CZ-NH2	-10.13	115.24	120.30
1	A	239	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	A	512	ARG	NE-CZ-NH2	-9.47	115.57	120.30
1	A	433	ARG	CD-NE-CZ	9.40	136.76	123.60
1	A	203	ASP	CB-CG-OD1	8.95	126.35	118.30
1	A	58	ARG	NE-CZ-NH2	-8.78	115.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	A	383	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	18	ARG	CD-NE-CZ	8.14	134.99	123.60
1	A	435	TYR	CB-CG-CD2	-8.08	116.15	121.00
1	A	515	TYR	CB-CG-CD1	-7.87	116.28	121.00
1	A	230	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	22	TYR	CB-CG-CD1	7.56	125.53	121.00
1	A	225	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	191	SER	N-CA-CB	7.39	121.58	110.50
1	A	512	ARG	CD-NE-CZ	7.36	133.90	123.60
1	A	374	GLU	CG-CD-OE1	-7.31	103.69	118.30
1	A	539	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	A	181	ASP	CB-CG-OD2	-7.18	111.83	118.30
1	A	263	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	80	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	A	542	GLN	CA-CB-CG	6.90	128.57	113.40
1	A	374	GLU	OE1-CD-OE2	6.87	131.54	123.30
1	A	472	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	208	ASP	N-CA-CB	6.72	122.69	110.60
1	A	65	LEU	CA-CB-CG	6.61	130.50	115.30
1	A	337	ARG	NH1-CZ-NH2	6.59	126.65	119.40
1	A	493	ASN	CA-CB-CG	6.57	127.86	113.40
1	A	219	LEU	CA-CB-CG	6.40	130.02	115.30
1	A	180	ASP	CB-CA-C	6.40	123.19	110.40
1	A	319	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	366	HIS	CA-CB-CG	-6.20	103.05	113.60
1	A	399	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	A	54	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	A	537	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	551	ILE	N-CA-C	6.08	127.42	111.00
1	A	460	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	444	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	A	369	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	191	SER	CB-CA-C	-5.80	99.07	110.10
1	A	77	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	497	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	222	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	284	GLU	CA-CB-CG	5.75	126.05	113.40
1	A	58	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	452	PRO	N-CD-CG	-5.59	94.81	103.20
1	A	519	GLY	N-CA-C	5.58	127.06	113.10
1	A	177	ASP	CB-CG-OD1	5.57	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	239	ARG	CD-NE-CZ	5.47	131.25	123.60
1	A	134	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	267	VAL	N-CA-CB	-5.44	99.53	111.50
1	A	180	ASP	N-CA-CB	-5.38	100.91	110.60
1	A	512	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
1	A	525	PRO	N-CD-CG	-5.33	95.21	103.20
1	A	446	HIS	O-C-N	5.32	131.21	122.70
1	A	234	LEU	CB-CA-C	5.30	120.27	110.20
1	A	411	SER	CB-CA-C	-5.29	100.05	110.10
1	A	446	HIS	CA-CB-CG	-5.29	104.61	113.60
1	A	227	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	11	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	57	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	559	HIS	CA-CB-CG	-5.26	104.66	113.60
1	A	267	VAL	CG1-CB-CG2	5.25	119.30	110.90
1	A	415	LEU	O-C-N	5.22	131.05	122.70
1	A	383	ARG	CA-C-N	5.18	126.57	116.20
1	A	520	THR	CA-CB-CG2	-5.18	105.14	112.40
1	A	289	ALA	N-CA-CB	-5.17	102.87	110.10
1	A	123	GLU	CG-CD-OE1	-5.16	107.99	118.30
1	A	123	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	A	64	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	427	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	458	GLU	CG-CD-OE2	5.13	128.57	118.30
1	A	427	ASP	N-CA-C	-5.10	97.24	111.00
1	A	90	GLN	O-C-N	5.09	130.85	122.70
1	A	57	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	315	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	401	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	271	THR	CA-CB-OG1	-5.06	98.37	109.00
1	A	489	ILE	CG1-CB-CG2	-5.06	100.28	111.40
1	A	413	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	208	ASP	O-C-N	5.03	130.65	121.10
1	A	18	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	A	337	ARG	CD-NE-CZ	-5.01	116.59	123.60
1	A	400	ARG	CG-CD-NE	-5.00	101.29	111.80

There are no chirality outliers.

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	4452	0	4239	104	0
2	A	61	0	52	0	0
3	A	56	0	52	0	0
4	A	53	0	31	2	0
5	A	152	0	0	7	0
All	All	4774	0	4374	104	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 12.

All (104) 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:383:ARG:NH1	5:A:838:HOH:O	1.84	1.09
1:A:325:ASN:ND2	1:A:433:ARG:HD2	1.91	0.85
1:A:115:HIS:HD2	1:A:117:ALA:H	1.24	0.84
1:A:4:ILE:HD11	1:A:233:LEU:HD13	1.65	0.79
1:A:22:TYR:CE2	1:A:284:GLU:HG2	2.18	0.78
1:A:22:TYR:HE2	1:A:284:GLU:HG2	1.49	0.77
1:A:283:HIS:HD2	1:A:582:MET:SD	2.09	0.76
1:A:400:ARG:O	1:A:404:VAL:HB	1.94	0.67
1:A:50:GLU:HG2	1:A:100:LEU:CD1	2.28	0.64
1:A:417:THR:HA	1:A:420:VAL:O	1.99	0.63
1:A:187:LYS:HD3	5:A:761:HOH:O	1.99	0.63
1:A:490:PRO:HB3	1:A:506:TYR:OH	1.98	0.63
1:A:296:THR:HB	1:A:438:ILE:HG22	1.81	0.61
1:A:81:GLU:HB2	1:A:91:THR:HG23	1.82	0.61
1:A:472:ARG:HD3	1:A:487:GLU:OE1	2.01	0.60
1:A:126:PHE:O	1:A:525:PRO:HD3	2.01	0.60
1:A:4:ILE:CD1	1:A:233:LEU:HD13	2.31	0.60
1:A:325:ASN:HD22	1:A:433:ARG:HD2	1.66	0.60
1:A:338:ILE:HA	1:A:483:TYR:O	2.03	0.59
1:A:152:LYS:HE2	1:A:182:TYR:CE1	2.39	0.58
1:A:472:ARG:NH1	1:A:487:GLU:OE2	2.37	0.57
1:A:477:SER:O	1:A:480:MET:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:MET:HA	1:A:532:VAL:HG23	1.87	0.56
1:A:383:ARG:NH2	5:A:839:HOH:O	2.37	0.56
1:A:355:ASN:OD1	1:A:366:HIS:HE1	1.89	0.56
1:A:189:LEU:HD11	1:A:474:ILE:HD12	1.88	0.56
1:A:143:ALA:HB2	1:A:569:LEU:HD11	1.89	0.55
1:A:383:ARG:HD3	1:A:456:LEU:HD13	1.89	0.55
1:A:44:ILE:O	1:A:241:ASN:HB2	2.07	0.55
1:A:16:SER:HB3	1:A:277:HIS:HB3	1.87	0.55
1:A:50:GLU:HG2	1:A:100:LEU:HD12	1.89	0.54
1:A:51:SER:O	1:A:247:GLY:HA2	2.07	0.54
1:A:153:GLN:O	1:A:158:HIS:HB2	2.08	0.54
1:A:152:LYS:HE2	1:A:182:TYR:CD1	2.44	0.54
1:A:289:ALA:HB1	1:A:293:VAL:HG22	1.89	0.54
1:A:364:LYS:HE3	1:A:462:LEU:HD13	1.90	0.53
1:A:269:PHE:O	1:A:276:THR:HA	2.08	0.53
1:A:193:VAL:HG21	1:A:212:VAL:HG23	1.91	0.53
1:A:115:HIS:CD2	1:A:117:ALA:H	2.16	0.53
1:A:284:GLU:HG3	1:A:286:LEU:HD21	1.90	0.53
1:A:158:HIS:CE1	1:A:175:PRO:HB3	2.45	0.52
1:A:236:ASN:O	1:A:239:ARG:HB2	2.10	0.52
1:A:325:ASN:ND2	1:A:433:ARG:CD	2.68	0.52
1:A:50:GLU:OE1	4:A:600:FAD:H1B	2.10	0.52
1:A:295:PRO:HG3	1:A:520:THR:HB	1.92	0.52
1:A:263:ARG:HG3	1:A:542:GLN:OE1	2.10	0.51
1:A:222:ASP:O	1:A:223:GLN:HB2	2.10	0.51
1:A:408:VAL:O	5:A:834:HOH:O	2.19	0.51
1:A:4:ILE:HD11	1:A:233:LEU:CD1	2.38	0.50
1:A:76:VAL:O	1:A:76:VAL:HG12	2.12	0.50
1:A:373:LEU:HG	1:A:396:TYR:HB3	1.94	0.50
1:A:212:VAL:HA	1:A:349:ALA:O	2.12	0.49
1:A:294:SER:N	1:A:295:PRO:HD2	2.28	0.49
1:A:501:SER:O	1:A:504:THR:HB	2.13	0.49
1:A:287:LEU:CD2	1:A:298:LEU:HD13	2.43	0.49
1:A:325:ASN:HD21	1:A:433:ARG:HD2	1.74	0.48
1:A:255:LEU:HD11	1:A:303:ILE:HD11	1.94	0.48
1:A:413:LEU:HD13	1:A:471:ALA:HB2	1.95	0.48
1:A:232:TRP:O	1:A:236:ASN:ND2	2.44	0.48
1:A:300:TYR:HE1	1:A:440:ASP:O	1.95	0.48
1:A:383:ARG:HD2	1:A:453:GLN:OE1	2.14	0.48
1:A:87:THR:OG1	1:A:508:PRO:HB3	2.14	0.47
1:A:490:PRO:HB3	1:A:506:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:HH11	1:A:487:GLU:CD	2.18	0.47
1:A:571:ILE:O	1:A:574:ALA:HB3	2.14	0.47
1:A:453:GLN:HB3	1:A:456:LEU:HD12	1.96	0.46
1:A:474:ILE:O	1:A:480:MET:HG3	2.15	0.46
1:A:347:GLN:HA	1:A:415:LEU:O	2.15	0.46
1:A:310:GLU:HB3	1:A:311:PRO:HD3	1.98	0.46
1:A:249:TYR:HB2	1:A:270:GLY:O	2.15	0.46
1:A:204:PHE:CD1	1:A:209:PRO:HA	2.51	0.46
1:A:85:LEU:O	1:A:89:ASN:N	2.48	0.46
1:A:55:GLU:OE2	5:A:854:HOH:O	2.21	0.45
1:A:112:THR:HB	1:A:204:PHE:HB3	1.98	0.45
1:A:489:ILE:HD11	5:A:766:HOH:O	2.15	0.45
1:A:489:ILE:HA	1:A:490:PRO:C	2.36	0.45
1:A:373:LEU:HB2	5:A:846:HOH:O	2.17	0.45
1:A:472:ARG:HD2	1:A:496:TYR:CE1	2.52	0.45
1:A:450:TYR:CE2	1:A:452:PRO:HG3	2.52	0.45
1:A:335:ARG:HB3	1:A:489:ILE:HG23	1.99	0.44
1:A:266:GLY:HA3	1:A:280:TYR:HA	1.98	0.44
1:A:269:PHE:CZ	1:A:277:HIS:HB2	2.53	0.44
1:A:11:ASP:HA	1:A:12:PRO:HD2	1.81	0.44
1:A:424:ASP:HB3	1:A:426:TRP:HZ3	1.82	0.44
1:A:518:VAL:HA	1:A:549:GLY:O	2.18	0.43
1:A:24:ILE:HG12	1:A:286:LEU:HD12	1.99	0.43
1:A:20:VAL:O	1:A:281:ALA:HA	2.18	0.43
1:A:369:LEU:O	1:A:373:LEU:HD13	2.19	0.43
1:A:81:GLU:HB2	1:A:91:THR:CG2	2.49	0.43
1:A:318:VAL:HG21	1:A:541:VAL:HG22	2.01	0.43
1:A:305:MET:CE	1:A:308:ILE:HD13	2.49	0.42
1:A:527:GLU:CD	1:A:527:GLU:H	2.23	0.42
1:A:182:TYR:HA	1:A:345:GLN:O	2.19	0.42
1:A:113:ARG:HB3	1:A:114:PRO:HD2	2.02	0.42
1:A:325:ASN:HD22	1:A:433:ARG:CD	2.29	0.41
1:A:256:SER:O	1:A:262:PRO:HA	2.21	0.41
1:A:535:ALA:O	1:A:536:ALA:HB3	2.21	0.41
1:A:210:HIS:CD2	1:A:211:GLY:N	2.89	0.41
1:A:524:MET:O	1:A:530:GLY:HA3	2.21	0.41
1:A:131:TRP:CZ2	1:A:570:LYS:HD3	2.56	0.41
1:A:454:TYR:OH	1:A:513:PRO:HB3	2.21	0.41
1:A:515:TYR:CD2	4:A:600:FAD:HM73	2.56	0.41
1:A:199:PRO:O	1:A:211:GLY:HA3	2.20	0.40
1:A:24:ILE:HA	1:A:286:LEU:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/583 (99%)	554 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	466/468 (100%)	433 (93%)	33 (7%)	17	22

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	32	LEU
1	A	37	ARG
1	A	83	VAL
1	A	96	SER
1	A	100	LEU
1	A	158	HIS
1	A	180	ASP
1	A	215	PHE
1	A	219	LEU

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Mol	Chain	Res	Type
1	A	233	LEU
1	A	239	ARG
1	A	244	VAL
1	A	254	LEU
1	A	260	THR
1	A	267	VAL
1	A	287	LEU
1	A	293	VAL
1	A	298	LEU
1	A	325	ASN
1	A	368	LEU
1	A	373	LEU
1	A	413	LEU
1	A	416	ASP
1	A	424	ASP
1	A	439	LEU
1	A	470	LEU
1	A	472	ARG
1	A	473	ASN
1	A	489	ILE
1	A	512	ARG
1	A	516	HIS
1	A	527	GLU

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	115	HIS
1	A	158	HIS
1	A	275	ASN
1	A	278	ASN
1	A	283	HIS
1	A	325	ASN
1	A	476	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 ⓘ

5 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	1.14	1 (7%)	15,19,21	0.83	0
2	NAG	A	602	2	14,14,15	1.01	1 (7%)	15,19,21	1.94	5 (33%)
2	BMA	A	613	2	11,11,12	0.76	0	13,15,17	2.53	4 (30%)
2	MAN	A	615	2	11,11,12	0.91	0	13,15,17	1.94	3 (23%)
2	MAN	A	616	2	11,11,12	0.96	0	13,15,17	2.29	7 (53%)

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	613	2	-	0/2/19/22	0/1/1/1
2	MAN	A	615	2	-	0/2/19/22	0/1/1/1
2	MAN	A	616	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAG	O7-C7	-2.99	1.16	1.23
2	A	602	NAG	O7-C7	-2.83	1.16	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	613	BMA	C1-C2-C3	-5.15	103.13	109.65
2	A	615	MAN	C1-C2-C3	-4.25	104.27	109.65
2	A	613	BMA	O3-C3-C2	-4.06	102.64	110.02
2	A	613	BMA	O5-C1-C2	-3.69	105.01	110.79
2	A	602	NAG	O5-C1-C2	-3.46	106.66	111.47
2	A	616	MAN	C1-C2-C3	-3.09	105.73	109.65
2	A	602	NAG	O7-C7-C8	-3.06	116.49	122.06
2	A	616	MAN	O5-C1-C2	-2.22	107.30	110.79
2	A	616	MAN	O3-C3-C2	-2.20	106.03	110.02
2	A	615	MAN	C6-C5-C4	2.27	118.31	113.00
2	A	602	NAG	C1-O5-C5	2.38	115.44	112.17
2	A	616	MAN	C2-C3-C4	2.45	115.14	110.88
2	A	602	NAG	O7-C7-N2	2.59	126.90	121.92
2	A	616	MAN	O3-C3-C4	2.63	116.08	110.36
2	A	616	MAN	O2-C2-C3	3.09	116.25	110.17
2	A	602	NAG	C1-C2-N2	3.64	116.71	110.49
2	A	613	BMA	C2-C3-C4	3.85	117.59	110.88
2	A	615	MAN	O2-C2-C3	4.29	118.61	110.17
2	A	616	MAN	C1-O5-C5	4.59	118.49	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

5 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	FAD	A	600	-	51,58,58	1.83	16 (31%)	54,89,89	2.90	23 (42%)
3	NAG	A	604	1	14,14,15	1.21	2 (14%)	15,19,21	2.72	11 (73%)
3	NAG	A	605	1	14,14,15	1.31	3 (21%)	15,19,21	2.07	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	608	1	14,14,15	1.06	1 (7%)	15,19,21	3.22	5 (33%)
3	NAG	A	609	1	14,14,15	1.13	1 (7%)	15,19,21	1.51	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
4	FAD	A	600	-	-	0/28/50/50	0/6/6/6
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	0/6/23/26	0/1/1/1
3	NAG	A	608	1	-	0/6/23/26	0/1/1/1
3	NAG	A	609	1	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	NAG	O7-C7	-3.50	1.15	1.23
4	A	600	FAD	PA-O2A	-3.49	1.37	1.55
3	A	604	NAG	O7-C7	-3.10	1.16	1.23
3	A	609	NAG	O7-C7	-2.64	1.17	1.23
3	A	608	NAG	O7-C7	-2.61	1.17	1.23
4	A	600	FAD	P-O2P	-2.55	1.42	1.55
4	A	600	FAD	O3B-C3B	-2.51	1.37	1.43
4	A	600	FAD	PA-O5B	-2.47	1.48	1.59
4	A	600	FAD	C1'-N10	-2.27	1.46	1.48
4	A	600	FAD	C9-C9A	-2.24	1.36	1.40
3	A	605	NAG	O5-C5	-2.04	1.39	1.43
3	A	605	NAG	C2-N2	2.05	1.49	1.46
4	A	600	FAD	C9A-N10	2.09	1.41	1.38
4	A	600	FAD	C10-N1	2.15	1.36	1.33
3	A	604	NAG	O5-C1	2.23	1.47	1.43
4	A	600	FAD	O4B-C1B	2.42	1.44	1.41
4	A	600	FAD	C2-N3	2.62	1.43	1.38
4	A	600	FAD	C5X-N5	2.84	1.39	1.35
4	A	600	FAD	C4-C4X	2.93	1.46	1.41
4	A	600	FAD	C4X-C10	3.29	1.46	1.41
4	A	600	FAD	O5'-C5'	3.62	1.59	1.44
4	A	600	FAD	C4-N3	3.83	1.40	1.33
4	A	600	FAD	C8-C7	4.17	1.51	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C4X-C4-N3	-7.94	112.18	123.48
3	A	608	NAG	C4-C3-C2	-6.25	101.86	111.02
3	A	608	NAG	O5-C1-C2	-5.44	103.91	111.47
3	A	605	NAG	O5-C1-C2	-5.28	104.12	111.47
4	A	600	FAD	C5A-C6A-N1A	-4.90	104.89	119.70
3	A	604	NAG	O5-C1-C2	-4.61	105.06	111.47
4	A	600	FAD	C1B-N9A-C4A	-4.48	118.90	126.64
4	A	600	FAD	N3A-C2A-N1A	-4.20	125.20	128.86
4	A	600	FAD	C9-C9A-C5X	-3.32	113.84	119.58
4	A	600	FAD	C4X-C10-N10	-3.18	118.31	120.52
4	A	600	FAD	C6-C5X-N5	-3.15	115.27	118.97
3	A	604	NAG	C6-C5-C4	-3.06	105.83	113.00
4	A	600	FAD	O2B-C2B-C1B	-3.04	102.11	111.61
4	A	600	FAD	O5B-C5B-C4B	-3.04	98.23	109.00
3	A	604	NAG	O3-C3-C4	-2.90	104.04	110.36
3	A	604	NAG	C4-C3-C2	-2.90	106.78	111.02
3	A	605	NAG	C1-C2-N2	-2.68	105.91	110.49
3	A	604	NAG	C8-C7-N2	-2.61	111.39	116.11
4	A	600	FAD	C1'-C2'-C3'	-2.55	102.51	109.82
4	A	600	FAD	C2B-C3B-C4B	-2.53	97.70	102.62
3	A	604	NAG	O4-C4-C5	-2.38	103.30	109.28
3	A	604	NAG	C1-O5-C5	-2.36	108.91	112.17
4	A	600	FAD	C8-C9-C9A	2.12	125.85	119.11
4	A	600	FAD	O3'-C3'-C4'	2.14	114.12	108.82
3	A	604	NAG	O4-C4-C3	2.16	115.05	110.36
3	A	604	NAG	O7-C7-C8	2.30	126.23	122.06
4	A	600	FAD	O2P-P-O1P	2.39	124.63	112.28
3	A	609	NAG	C1-C2-N2	2.47	114.71	110.49
4	A	600	FAD	C4-C4X-C10	2.54	122.02	119.96
3	A	608	NAG	O3-C3-C2	2.61	114.97	109.39
4	A	600	FAD	O2B-C2B-C3B	2.68	120.40	111.83
3	A	604	NAG	O3-C3-C2	2.68	115.14	109.39
4	A	600	FAD	C4X-N5-C5X	3.23	120.17	116.76
4	A	600	FAD	O3B-C3B-C4B	3.60	121.59	111.09
3	A	605	NAG	C1-O5-C5	3.69	117.25	112.17
4	A	600	FAD	C5A-C6A-N6A	3.77	128.15	120.47
4	A	600	FAD	C6-C5X-C9A	3.96	124.14	119.00
4	A	600	FAD	N6A-C6A-N1A	4.13	126.96	118.77
3	A	609	NAG	O6-C6-C5	4.42	126.22	111.34
3	A	604	NAG	C2-N2-C7	4.71	129.82	122.94
3	A	608	NAG	C1-O5-C5	5.60	119.89	112.17
3	A	608	NAG	C1-C2-N2	6.50	121.59	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C2A-N1A-C6A	8.14	133.02	118.77
4	A	600	FAD	C4-N3-C2	8.36	122.47	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	FAD	2	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	581/583 (99%)	-0.65	2 (0%) 93 96	2, 11, 29, 67	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	THR	3.7
1	A	258	ASN	2.7

### 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	BMA	A	613	11/12	0.83	0.19	1.38	54,54,54,54	0
2	NAG	A	602	14/15	0.89	0.16	0.93	30,30,30,30	0
2	MAN	A	615	11/12	0.85	0.14	0.70	57,57,57,57	0
2	NAG	A	601	14/15	0.93	0.12	0.50	22,22,22,22	0
2	MAN	A	616	11/12	0.86	0.23	-	68,68,68,68	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(Å <sup>2</sup> )	Q<0.9
3	NAG	A	609	14/15	0.59	0.38	6.56	76,76,76,76	0
3	NAG	A	608	14/15	0.82	0.25	3.72	65,65,65,65	0
3	NAG	A	604	14/15	0.90	0.14	0.74	23,23,23,23	0
3	NAG	A	605	14/15	0.96	0.12	0.70	17,17,17,17	0
4	FAD	A	600	53/53	0.97	0.08	-0.05	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.