



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:40 pm GMT

PDB ID : 4BXD  
Title : CRYSTAL STRUCTURE OF AMPDH3 FROM PSEUDOMONAS AERUGINOSA IN COMPLEX WITH TETRASACCHARIDE PENTAPEPTIDE  
Authors : Artola-Recolons, C.; Hermoso, J.A.  
Deposited on : 2013-07-10  
Resolution : 3.10 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.

---

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

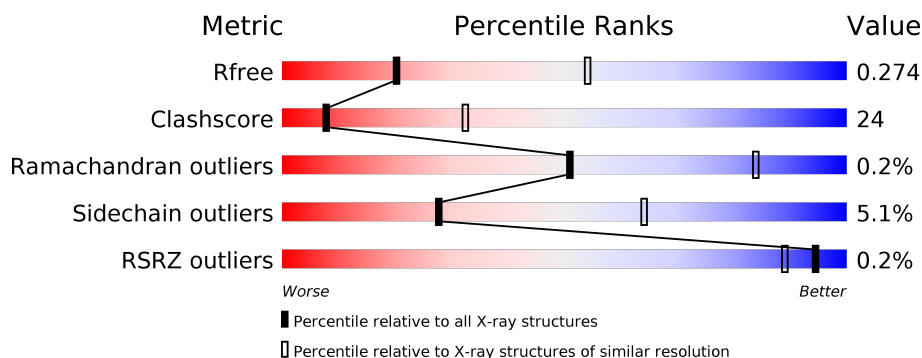
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	255	
1	B	255	
2	C	4	
2	D	4	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	6CL	D	3	-	-	X	-
2	DAL	D	4	-	-	X	-
3	MAG	A	1257	-	-	-	X
3	NAG	A	1258	-	-	-	X
3	NAG	A	1259	-	-	-	X
3	MAG	B	1257	-	-	-	X
3	NAG	B	1259	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8343 atoms, of which 4079 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 AMPDH3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	255	Total	C	H	N	O	S	0	0	0
			4005	1300	1969	354	379	3			
1	B	255	Total	C	H	N	O	S	0	0	0
			4004	1300	1968	354	379	3			

- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	0	0	0
			60	18	28	5	9			
2	D	4	Total	C	H	N	O	0	0	0
			60	18	28	5	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	3	Total	C	H	N	O	0	0
			87	25	43	3	16		
3	B	3	Total	C	H	N	O	0	0
			87	25	43	3	16		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

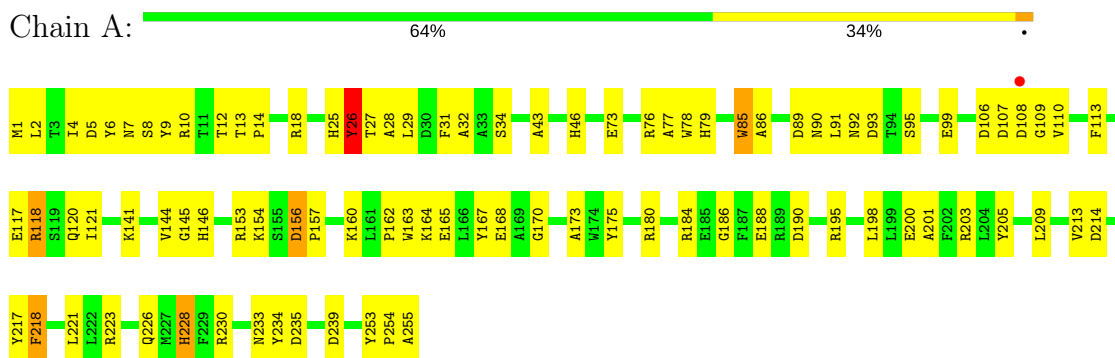
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	16	Total 16	O 16	0	0

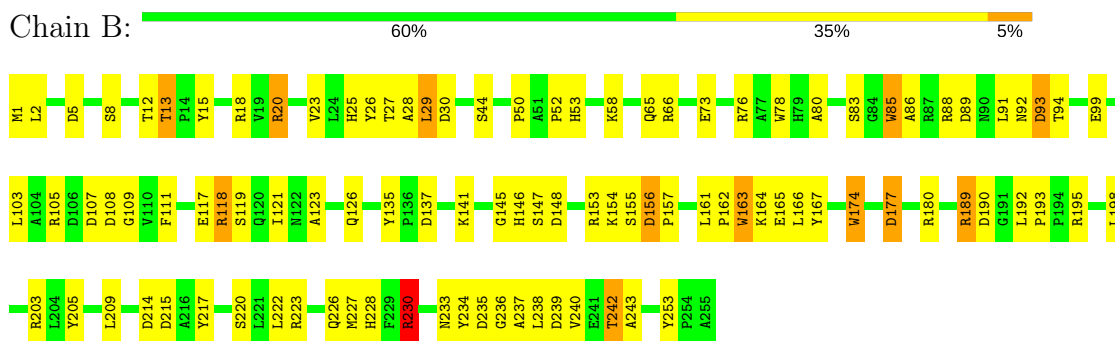
### 3 Residue-property plots

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

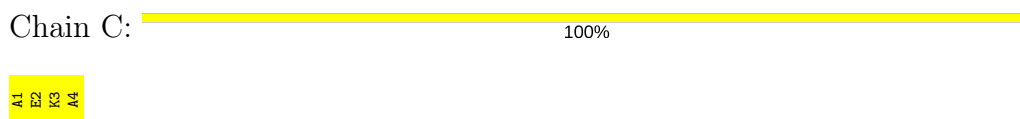
- Molecule 1: AMPDH3



- Molecule 1: AMPDH3



- Molecule 2: PEPTIDE



- Molecule 2: PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.19Å 101.19Å 162.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 3.10 48.30 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.30-3.10) 89.8 (48.30-3.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.85 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.224 , 0.277 0.227 , 0.274	Depositor DCC
$R_{free}$ test set	760 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: ZN, NAG, DAL, 6CL, MAG, FGA

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	1.34	4/2091 (0.2%)	0.89	1/2842 (0.0%)
1	B	1.25	3/2092 (0.1%)	0.88	1/2845 (0.0%)
2	C	1.94	0/4	2.54	0/4
2	D	1.56	0/4	1.01	0/4
All	All	1.30	7/4191 (0.2%)	0.89	2/5695 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	PHE	C-N	6.42	1.48	1.34
1	A	26	TYR	CE1-CZ	-6.19	1.30	1.38
1	A	85	TRP	NE1-CE2	-5.86	1.29	1.37
1	B	174	TRP	NE1-CE2	-5.31	1.30	1.37
1	B	163	TRP	NE1-CE2	-5.20	1.30	1.37
1	B	85	TRP	NE1-CE2	-5.10	1.30	1.37
1	A	99	GLU	CG-CD	-5.00	1.44	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ARG	C-N-CD	5.91	140.80	128.40
1	A	223	ARG	NE-CZ-NH2	-5.36	117.62	120.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	93	ASP	Peptide

## 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	2036	1969	1967	84	0
1	B	2036	1968	1968	111	0
2	C	32	28	28	5	0
2	D	32	28	29	10	0
3	A	44	43	41	4	0
3	B	44	43	41	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	22	0	0	1	0
5	B	16	0	0	0	0
All	All	4264	4079	4074	200	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 24.

All (200) 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:192:LEU:HD12	1:B:193:PRO:CD	1.83	1.07
1:B:192:LEU:HD12	1:B:193:PRO:HD3	1.41	1.03
1:B:154:LYS:NZ	3:B:1257:MAG:O3	1.94	1.01
1:A:107:ASP:CA	1:A:108:ASP:N	2.28	0.97
1:A:93:ASP:OD2	1:B:88:ARG:NH2	2.03	0.91
1:B:192:LEU:CD1	1:B:193:PRO:HD2	2.03	0.89
1:B:23:VAL:HG12	1:B:25:HIS:NE2	1.88	0.89
1:A:107:ASP:C	1:A:108:ASP:N	2.29	0.86
1:B:192:LEU:CD1	1:B:193:PRO:CD	2.55	0.84
1:A:5:ASP:OD2	1:A:8:SER:OG	1.96	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:CG	1:B:88:ARG:HH21	1.83	0.82
1:B:230:ARG:NH2	1:B:239:ASP:OD2	2.14	0.81
1:A:107:ASP:HA	1:A:108:ASP:N	1.96	0.79
1:B:28:ALA:O	1:B:29:LEU:HD13	1.81	0.79
3:B:1257:MAG:H83	3:B:1257:MAG:HM3	1.63	0.79
1:B:230:ARG:NH1	1:B:233:ASN:OD1	2.16	0.78
1:A:163:TRP:CD2	1:A:228:HIS:CE1	2.71	0.77
1:B:163:TRP:O	1:B:166:LEU:N	2.17	0.77
1:B:73:GLU:OE1	1:B:135:TYR:OH	2.02	0.76
1:B:118:ARG:O	1:B:121:ILE:N	2.18	0.76
1:B:111:PHE:HZ	3:B:1259:NAG:H81	1.51	0.75
1:B:76:ARG:NH1	1:B:93:ASP:OD1	2.20	0.74
2:D:3:6CL:N	2:D:4:DAL:HB3	2.03	0.73
1:B:235:ASP:O	1:B:237:ALA:N	2.20	0.73
1:A:12:THR:OG1	1:A:13:THR:N	2.20	0.72
1:B:156:ASP:HB2	1:B:157:PRO:HA	1.71	0.72
1:B:29:LEU:C	1:B:103:LEU:HD21	2.10	0.71
1:A:93:ASP:CG	1:B:88:ARG:NH2	2.43	0.71
1:A:27:THR:O	1:A:28:ALA:HB3	1.90	0.70
1:B:118:ARG:NH2	1:B:165:GLU:OE2	2.25	0.70
1:B:163:TRP:O	1:B:164:LYS:C	2.28	0.70
1:A:107:ASP:N	1:A:108:ASP:N	2.39	0.69
1:B:80:ALA:O	1:B:83:SER:OG	2.10	0.67
1:A:93:ASP:OD1	1:B:88:ARG:NH2	2.27	0.67
1:B:153:ARG:NH2	2:D:2:FGA:O	2.27	0.67
3:A:1257:MAG:H83	3:A:1257:MAG:O1	1.95	0.67
1:A:214:ASP:OD1	1:A:214:ASP:N	2.25	0.66
1:B:239:ASP:OD1	1:B:240:VAL:N	2.27	0.66
1:B:163:TRP:O	1:B:165:GLU:N	2.29	0.66
1:A:107:ASP:HB2	1:A:110:VAL:CG1	2.26	0.65
3:B:1257:MAG:H83	3:B:1257:MAG:CM	2.26	0.65
1:B:192:LEU:HD21	1:B:238:LEU:HD21	1.77	0.64
1:B:50:PRO:O	1:B:65:GLN:NE2	2.31	0.64
3:B:1258:NAG:O3	3:B:1259:NAG:O7	2.16	0.63
1:B:192:LEU:HD12	1:B:193:PRO:HD2	1.63	0.63
1:B:23:VAL:HG12	1:B:25:HIS:HE2	1.63	0.63
1:A:156:ASP:OD1	1:A:156:ASP:N	2.28	0.63
1:B:177:ASP:OD2	1:B:180:ARG:NH2	2.31	0.63
1:B:5:ASP:OD2	1:B:8:SER:OG	2.08	0.63
1:A:230:ARG:HH12	1:A:233:ASN:HB3	1.63	0.63
1:A:89:ASP:O	1:A:90:ASN:C	2.36	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASP:OD2	1:B:228:HIS:HD2	1.82	0.62
1:A:106:ASP:C	1:A:108:ASP:N	2.52	0.62
2:C:3:6CL:HB2	2:C:4:DAL:HB3	1.81	0.62
1:A:108:ASP:N	1:A:109:GLY:HA2	2.15	0.61
1:A:77:ALA:O	1:A:92:ASN:OD1	2.18	0.61
1:B:108:ASP:N	1:B:109:GLY:HA2	2.16	0.61
1:A:106:ASP:O	1:A:108:ASP:N	2.34	0.60
1:A:28:ALA:C	1:A:29:LEU:HD12	2.22	0.60
3:A:1259:NAG:H82	3:A:1259:NAG:O3	2.02	0.59
1:B:23:VAL:CG1	1:B:25:HIS:NE2	2.64	0.59
2:C:3:6CL:CB	2:C:4:DAL:HB3	2.33	0.59
1:A:91:LEU:O	1:A:95:SER:OG	2.21	0.59
1:B:223:ARG:NH1	1:B:227:MET:HE1	2.18	0.58
1:B:26:TYR:CE2	1:B:156:ASP:HA	2.38	0.58
1:A:146:HIS:CE1	1:A:154:LYS:HE3	2.38	0.58
1:A:27:THR:O	1:A:28:ALA:CB	2.51	0.57
1:A:186:GLY:O	1:A:190:ASP:N	2.37	0.57
2:D:3:6CL:CA	2:D:4:DAL:HB3	2.35	0.56
1:B:12:THR:OG1	1:B:13:THR:N	2.37	0.56
1:A:107:ASP:HB2	1:A:110:VAL:HG12	1.86	0.56
1:B:141:LYS:HD3	1:B:253:TYR:HB3	1.88	0.56
1:B:27:THR:HG22	1:B:99:GLU:CG	2.36	0.55
1:A:31:PHE:O	1:A:34:SER:N	2.39	0.54
1:A:46:HIS:CD2	1:A:73:GLU:HA	2.43	0.54
1:B:230:ARG:NH1	1:B:233:ASN:CG	2.60	0.54
1:B:226:GLN:C	1:B:228:HIS:H	2.11	0.53
1:B:26:TYR:OH	3:B:1258:NAG:H81	2.08	0.53
1:B:148:ASP:OD2	1:B:228:HIS:CD2	2.61	0.53
1:A:184:ARG:NH1	1:A:188:GLU:OE2	2.42	0.53
1:A:198:LEU:O	1:A:201:ALA:HB3	2.09	0.53
1:A:85:TRP:CE2	1:A:144:VAL:HG11	2.43	0.53
1:A:117:GLU:HB2	1:A:120:GLN:HG3	1.90	0.53
1:B:156:ASP:CB	1:B:157:PRO:HA	2.38	0.53
1:A:153:ARG:NH2	2:C:2:FGA:O	2.43	0.52
1:A:2:LEU:HB2	1:B:126:GLN:OE1	2.09	0.52
1:B:29:LEU:C	1:B:103:LEU:CD2	2.77	0.52
1:A:107:ASP:O	1:A:108:ASP:OD2	2.27	0.52
1:A:85:TRP:O	1:A:86:ALA:HB3	2.10	0.52
1:B:28:ALA:C	1:B:29:LEU:HD13	2.31	0.52
1:A:163:TRP:CE3	1:A:228:HIS:CE1	2.97	0.51
3:B:1257:MAG:H62	3:B:1258:NAG:C1	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:O	1:B:18:ARG:NH1	2.44	0.51
1:B:92:ASN:ND2	2:D:2:FGA:OE1	2.44	0.51
1:A:95:SER:O	1:B:18:ARG:NH2	2.34	0.50
1:A:43:ALA:HB1	1:A:78:TRP:O	2.12	0.50
1:A:118:ARG:HH22	1:A:165:GLU:CD	2.15	0.50
1:A:18:ARG:NH2	1:B:73:GLU:O	2.34	0.50
1:B:167:TYR:CD2	1:B:174:TRP:HB3	2.47	0.50
1:A:173:ALA:HB1	1:A:253:TYR:CE2	2.48	0.49
1:B:26:TYR:CD2	1:B:156:ASP:HB3	2.47	0.49
1:B:27:THR:HG22	1:B:99:GLU:HG3	1.93	0.49
1:B:76:ARG:NH2	2:D:3:6CL:O	2.46	0.49
1:B:195:ARG:HA	1:B:198:LEU:HD12	1.95	0.49
1:B:157:PRO:HB2	1:B:161:LEU:HD13	1.94	0.49
1:A:107:ASP:HB2	1:A:110:VAL:HG13	1.95	0.48
1:B:162:PRO:O	1:B:163:TRP:C	2.46	0.48
1:A:6:TYR:O	1:A:10:ARG:HD3	2.14	0.48
1:A:5:ASP:OD2	1:B:66:ARG:NH1	2.47	0.48
1:B:65:GLN:HG3	1:B:66:ARG:H	1.79	0.48
1:B:156:ASP:HB2	1:B:157:PRO:CA	2.43	0.48
1:A:7:ASN:ND2	5:A:2002:HOH:O	2.46	0.48
1:B:203:ARG:HG3	1:B:209:LEU:HD22	1.96	0.47
2:D:3:6CL:HB2	2:D:4:DAL:C	2.44	0.47
1:A:163:TRP:CE3	1:A:228:HIS:HE1	2.31	0.47
1:A:79:HIS:CE1	1:A:95:SER:HB2	2.49	0.47
1:B:123:ALA:O	1:B:126:GLN:HB3	2.14	0.47
1:B:189:ARG:CG	1:B:190:ASP:N	2.77	0.47
1:B:242:THR:CG2	1:B:243:ALA:N	2.78	0.47
3:A:1257:MAG:C7	2:C:1:ALA:H3	2.27	0.47
1:B:30:ASP:N	1:B:103:LEU:HD21	2.29	0.47
1:B:230:ARG:HH21	1:B:239:ASP:CG	2.18	0.47
1:B:161:LEU:O	1:B:163:TRP:N	2.45	0.46
1:B:230:ARG:NH2	1:B:239:ASP:CB	2.79	0.46
1:A:230:ARG:HH12	1:A:233:ASN:CB	2.29	0.46
1:B:226:GLN:OE1	1:B:234:TYR:HA	2.15	0.46
1:A:76:ARG:HB2	1:B:18:ARG:HA	1.97	0.46
1:B:27:THR:O	1:B:28:ALA:HB3	2.15	0.46
1:A:209:LEU:HD21	1:A:221:LEU:HD22	1.97	0.46
1:B:85:TRP:O	1:B:86:ALA:C	2.52	0.46
3:B:1257:MAG:N2	2:D:1:ALA:N	2.64	0.46
1:A:163:TRP:CE2	1:A:228:HIS:CE1	3.04	0.46
1:B:27:THR:HG22	1:B:99:GLU:HG2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:CE1	1:A:154:LYS:CE	2.98	0.45
1:A:198:LEU:O	1:A:201:ALA:N	2.48	0.45
1:B:222:LEU:O	1:B:223:ARG:C	2.55	0.45
1:B:145:GLY:O	1:B:146:HIS:C	2.52	0.45
1:B:65:GLN:CG	1:B:66:ARG:N	2.79	0.45
2:D:3:6CL:CB	2:D:4:DAL:HB3	2.46	0.45
1:A:254:PRO:O	1:A:255:ALA:HB2	2.17	0.45
1:B:78:TRP:N	1:B:78:TRP:CD1	2.81	0.45
1:A:8:SER:HB3	1:A:9:TYR:CD1	2.52	0.45
1:B:23:VAL:CG1	1:B:25:HIS:HE2	2.26	0.44
1:A:145:GLY:HA3	1:A:157:PRO:HD3	1.99	0.44
1:B:195:ARG:NH1	1:B:215:ASP:OD1	2.48	0.44
1:B:226:GLN:C	1:B:228:HIS:N	2.69	0.44
1:A:235:ASP:N	1:A:235:ASP:OD1	2.50	0.44
1:A:46:HIS:HD2	1:A:73:GLU:HA	1.82	0.44
1:A:4:ILE:HG22	1:A:5:ASP:N	2.32	0.44
1:B:29:LEU:CA	1:B:103:LEU:CD2	2.96	0.44
1:B:146:HIS:O	1:B:147:SER:C	2.56	0.44
1:A:78:TRP:HA	1:A:92:ASN:HD21	1.81	0.44
1:B:230:ARG:NH2	1:B:239:ASP:CG	2.71	0.44
1:B:118:ARG:O	1:B:119:SER:C	2.56	0.44
1:B:223:ARG:CZ	1:B:227:MET:HE1	2.47	0.44
2:D:3:6CL:N	2:D:4:DAL:CB	2.77	0.44
1:B:20:ARG:HD2	1:B:137:ASP:HB3	1.99	0.43
1:B:65:GLN:HG3	1:B:66:ARG:N	2.34	0.43
1:B:1:MET:HG2	1:B:2:LEU:N	2.33	0.43
1:A:76:ARG:NH1	2:C:3:6CL:O	2.41	0.43
1:A:113:PHE:O	1:A:160:LYS:HG3	2.18	0.43
1:B:161:LEU:HD22	1:B:163:TRP:CE2	2.53	0.43
1:A:195:ARG:NE	1:A:218:PHE:CD2	2.86	0.43
1:B:239:ASP:H	1:B:242:THR:CG2	2.32	0.43
1:A:29:LEU:HD11	3:A:1257:MAG:H1	2.01	0.43
1:A:141:LYS:HG2	1:A:205:TYR:CE1	2.54	0.43
1:A:175:TYR:CE2	1:A:180:ARG:HD3	2.53	0.43
1:B:105:ARG:NH2	1:B:107:ASP:OD1	2.51	0.43
1:B:1:MET:HG2	1:B:2:LEU:H	1.84	0.43
1:B:217:TYR:O	1:B:220:SER:HB2	2.19	0.43
1:B:239:ASP:HB3	1:B:242:THR:HB	2.00	0.42
1:A:118:ARG:O	1:A:121:ILE:N	2.50	0.42
1:B:111:PHE:CZ	3:B:1259:NAG:H81	2.40	0.42
1:B:92:ASN:ND2	2:D:3:6CL:O	2.52	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:N	1:A:14:PRO:CD	2.83	0.42
1:A:118:ARG:NH2	1:A:165:GLU:OE1	2.52	0.42
1:A:31:PHE:O	1:A:32:ALA:C	2.57	0.42
1:A:162:PRO:O	1:A:163:TRP:C	2.58	0.42
1:A:167:TYR:O	1:A:170:GLY:N	2.49	0.42
1:A:145:GLY:O	1:A:146:HIS:C	2.54	0.42
1:B:135:TYR:CD1	1:B:135:TYR:N	2.88	0.42
1:B:53:HIS:HA	1:B:58:LYS:HE3	2.02	0.42
1:B:141:LYS:HD2	1:B:205:TYR:CE1	2.54	0.41
1:B:189:ARG:HG2	1:B:190:ASP:N	2.35	0.41
1:A:10:ARG:HA	1:A:10:ARG:HD2	1.98	0.41
1:A:89:ASP:C	1:A:89:ASP:OD1	2.59	0.41
1:B:44:SER:O	1:B:78:TRP:O	2.37	0.41
1:A:213:VAL:HG13	1:A:217:TYR:CD1	2.56	0.41
1:B:89:ASP:N	1:B:89:ASP:OD1	2.54	0.41
1:A:18:ARG:HD2	1:B:93:ASP:O	2.21	0.41
1:A:226:GLN:OE1	1:A:234:TYR:HA	2.21	0.41
1:B:52:PRO:HD2	1:B:117:GLU:OE1	2.21	0.41
1:B:153:ARG:O	1:B:153:ARG:HG2	2.21	0.41
1:B:226:GLN:O	1:B:228:HIS:N	2.53	0.41
1:A:26:TYR:CE2	1:A:156:ASP:HA	2.56	0.41
1:A:200:GLU:OE2	1:A:203:ARG:NH1	2.50	0.41
1:B:230:ARG:O	1:B:230:ARG:CD	2.70	0.40
3:B:1258:NAG:O3	3:B:1259:NAG:C7	2.69	0.40
1:B:1:MET:CG	1:B:2:LEU:H	2.34	0.40
1:A:164:LYS:O	1:A:168:GLU:HG3	2.21	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	251/255 (98%)	220 (88%)	31 (12%)	0	100	100
1	B	253/255 (99%)	218 (86%)	34 (13%)	1 (0%)	38	75
All	All	504/510 (99%)	438 (87%)	65 (13%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	GLY

### 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	205/205 (100%)	198 (97%)	7 (3%)	42	77
1	B	205/205 (100%)	191 (93%)	14 (7%)	18	53
All	All	410/410 (100%)	389 (95%)	21 (5%)	28	64

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	25	HIS
1	A	26	TYR
1	A	118	ARG
1	A	156	ASP
1	A	228	HIS
1	A	239	ASP
1	B	13	THR
1	B	15	TYR
1	B	20	ARG
1	B	29	LEU
1	B	91	LEU
1	B	94	THR
1	B	118	ARG
1	B	155	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	156	ASP
1	B	177	ASP
1	B	189	ARG
1	B	214	ASP
1	B	230	ARG
1	B	242	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	92	ASN
1	B	228	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	FGA	C	2	2	3,8,9	0.67	0	2,9,11	1.18	0
2	6CL	C	3	2	6,11,12	1.31	1 (16%)	3,13,15	2.81	1 (33%)
2	DAL	C	4	2	2,5,5	1.88	1 (50%)	2,6,6	1.59	1 (50%)
2	FGA	D	2	2	3,8,9	0.58	0	2,9,11	1.04	0
2	6CL	D	3	2	6,11,12	1.81	2 (33%)	3,13,15	2.82	2 (66%)
2	DAL	D	4	2	2,5,5	1.99	1 (50%)	2,6,6	2.11	1 (50%)

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	FGA	C	2	2	-	0/3/8/9	0/0/0/0
2	6CL	C	3	2	-	0/6/12/14	0/0/0/0
2	DAL	C	4	2	-	0/0/4/4	0/0/0/0
2	FGA	D	2	2	-	0/3/8/9	0/0/0/0
2	6CL	D	3	2	-	0/6/12/14	0/0/0/0
2	DAL	D	4	2	-	0/0/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	6CL	CB-CA	-3.51	1.48	1.53
2	D	4	DAL	CA-N	-2.74	1.39	1.47
2	C	3	6CL	CB-CA	-2.70	1.49	1.53
2	C	4	DAL	CA-N	-2.60	1.39	1.47
2	D	3	6CL	CA-N	-2.50	1.39	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	6CL	O-C-CA	-4.84	111.66	125.02
2	D	3	6CL	O-C-CA	-4.41	112.84	125.02
2	D	3	6CL	CB-CA-C	-2.05	108.28	111.65
2	C	4	DAL	CB-CA-C	2.21	115.74	111.48
2	D	4	DAL	CB-CA-C	2.69	116.67	111.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	FGA	1	0
2	C	3	6CL	3	0
2	C	4	DAL	2	0
2	D	2	FGA	2	0
2	D	3	6CL	7	0
2	D	4	DAL	5	0

## 5.5 Carbohydrates [i](#)

6 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	MAG	A	1257	3	16,16,16	1.26	2 (12%)	21,22,22	2.25	7 (33%)
3	NAG	A	1258	3	14,14,15	1.42	3 (21%)	15,19,21	2.43	6 (40%)
3	NAG	A	1259	3	14,14,15	1.42	2 (14%)	15,19,21	2.77	9 (60%)
3	MAG	B	1257	3	16,16,16	1.26	1 (6%)	21,22,22	2.43	8 (38%)
3	NAG	B	1258	3	14,14,15	1.53	4 (28%)	15,19,21	2.86	9 (60%)
3	NAG	B	1259	3	14,14,15	1.46	2 (14%)	15,19,21	3.37	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
3	MAG	A	1257	3	-	0/8/28/28	0/1/1/1
3	NAG	A	1258	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1259	3	-	0/6/23/26	0/1/1/1
3	MAG	B	1257	3	-	0/8/28/28	0/1/1/1
3	NAG	B	1258	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1259	3	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1259	NAG	O5-C1	-3.29	1.38	1.43
3	B	1258	NAG	C1-C2	-2.82	1.48	1.52
3	A	1257	MAG	C1-C2	-2.76	1.48	1.53
3	B	1259	NAG	C3-C2	-2.73	1.46	1.52
3	A	1258	NAG	O5-C1	-2.64	1.39	1.43
3	B	1258	NAG	C2-N2	-2.59	1.41	1.46
3	A	1258	NAG	C2-N2	-2.36	1.42	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1257	MAG	O7-C7	-2.07	1.18	1.23
3	B	1258	NAG	O3-C3	-2.05	1.38	1.43
3	A	1258	NAG	C7-N2	2.09	1.42	1.34
3	A	1257	MAG	C7-N2	2.28	1.42	1.34
3	B	1259	NAG	C7-N2	2.32	1.42	1.34
3	B	1258	NAG	C7-N2	2.56	1.43	1.34
3	A	1259	NAG	C7-N2	2.77	1.44	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1258	NAG	O5-C1-C2	-5.58	103.72	111.47
3	B	1257	MAG	C3-C4-C5	-4.21	102.80	110.22
3	B	1258	NAG	C4-C3-C2	-4.13	104.97	111.02
3	A	1259	NAG	O5-C1-C2	-4.11	105.75	111.47
3	B	1259	NAG	O5-C1-C2	-4.11	105.76	111.47
3	B	1257	MAG	O5-C1-O1	-4.06	101.41	110.92
3	A	1259	NAG	O3-C3-C4	-4.02	101.61	110.36
3	A	1259	NAG	O7-C7-N2	-3.34	115.50	121.92
3	B	1257	MAG	O7-C7-C8	-3.29	116.06	122.06
3	A	1257	MAG	C1-C2-N2	-3.27	105.49	111.03
3	B	1258	NAG	O5-C1-C2	-3.00	107.30	111.47
3	B	1258	NAG	C3-C4-C5	-2.90	105.10	110.22
3	A	1258	NAG	O3-C3-C2	-2.88	103.22	109.39
3	B	1258	NAG	C2-N2-C7	-2.86	118.77	122.94
3	A	1257	MAG	O7-C7-C8	-2.57	117.39	122.06
3	B	1259	NAG	C6-C5-C4	-2.51	107.12	113.00
3	A	1259	NAG	O4-C4-C3	-2.51	104.90	110.36
3	B	1259	NAG	O7-C7-N2	-2.43	117.25	121.92
3	A	1259	NAG	C1-C2-N2	-2.39	106.41	110.49
3	A	1258	NAG	C2-N2-C7	-2.37	119.49	122.94
3	B	1257	MAG	C3-C2-N2	-2.28	106.25	110.61
3	A	1257	MAG	O7-C7-N2	-2.24	117.61	121.92
3	B	1257	MAG	O4-C4-C3	-2.20	105.57	110.36
3	B	1259	NAG	C4-C3-C2	-2.10	107.94	111.02
3	B	1257	MAG	O5-C5-C4	-2.05	105.88	109.66
3	A	1259	NAG	O7-C7-C8	-2.03	118.37	122.06
3	A	1259	NAG	C4-C3-C2	2.27	114.35	111.02
3	A	1257	MAG	O5-C1-C2	2.34	115.44	110.65
3	B	1258	NAG	C8-C7-N2	2.36	120.38	116.11
3	A	1258	NAG	C3-C4-C5	2.64	114.88	110.22
3	B	1258	NAG	C1-C2-N2	2.70	115.10	110.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1257	MAG	C3-C4-C5	2.72	115.02	110.22
3	A	1259	NAG	C2-N2-C7	2.93	127.21	122.94
3	A	1258	NAG	C1-O5-C5	3.25	116.64	112.17
3	B	1258	NAG	O4-C4-C3	3.57	118.13	110.36
3	B	1258	NAG	O3-C3-C4	3.74	118.49	110.36
3	B	1259	NAG	C8-C7-N2	3.91	123.17	116.11
3	A	1258	NAG	C4-C3-C2	4.30	117.32	111.02
3	B	1257	MAG	C1-O5-C5	4.58	122.35	113.72
3	B	1259	NAG	C1-C2-N2	4.91	118.87	110.49
3	A	1257	MAG	C8-C7-N2	4.92	125.00	116.11
3	B	1257	MAG	C8-C7-N2	5.18	125.47	116.11
3	B	1258	NAG	C1-O5-C5	5.52	119.77	112.17
3	A	1259	NAG	C8-C7-N2	5.55	126.13	116.11
3	A	1257	MAG	C1-O5-C5	5.70	124.45	113.72
3	B	1259	NAG	C1-O5-C5	9.11	124.73	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1257	MAG	3	0
3	A	1259	NAG	1	0
3	B	1257	MAG	5	0
3	B	1258	NAG	4	0
3	B	1259	NAG	4	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 [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	255/255 (100%)	-0.26	1 (0%) 92 84	17, 30, 48, 91	0
1	B	255/255 (100%)	-0.17	0 100 100	17, 34, 63, 89	0
2	C	1/4 (25%)	-0.03	0 100 100	49, 49, 49, 49	0
2	D	1/4 (25%)	1.18	0 100 100	47, 47, 47, 47	0
All	All	512/518 (98%)	-0.21	1 (0%) 94 89	17, 32, 59, 91	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ASP	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	FGA	C	2	9/10	0.84	0.23	-	24,33,58,80	0
2	FGA	D	2	9/10	0.92	0.23	-	32,53,65,65	0
2	DAL	C	4	6/6	0.95	0.20	-	13,18,32,33	0
2	6CL	C	3	12/13	0.87	0.23	-	29,46,55,60	0
2	DAL	D	4	6/6	0.77	0.27	-	29,42,58,70	0
2	6CL	D	3	12/13	0.91	0.26	-	23,49,59,59	0

### 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
3	MAG	A	1257	16/16	0.74	0.43	10.84	53,81,103,114	0
3	MAG	B	1257	16/16	0.88	0.36	3.13	52,75,93,94	0
3	NAG	A	1258	14/15	0.84	0.41	2.40	51,81,99,101	0
3	NAG	B	1259	14/15	0.86	0.38	2.11	57,75,95,101	0
3	NAG	B	1258	14/15	0.73	0.36	1.84	46,73,91,93	0
3	NAG	A	1259	14/15	0.82	0.43	1.65	58,88,103,112	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
4	ZN	B	1256	1/1	0.98	0.20	-0.06	36,36,36,36	0
4	ZN	A	1260	1/1	0.93	0.14	-2.48	35,35,35,35	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.