



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:12 pm GMT

PDB ID : 5E62  
Title : HEF-mut with Tr323 complex  
Authors : Song, H.; Qi, J.; Shi, Y.; Gao, G.F.  
Deposited on : 2015-10-09  
Resolution : 2.20 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

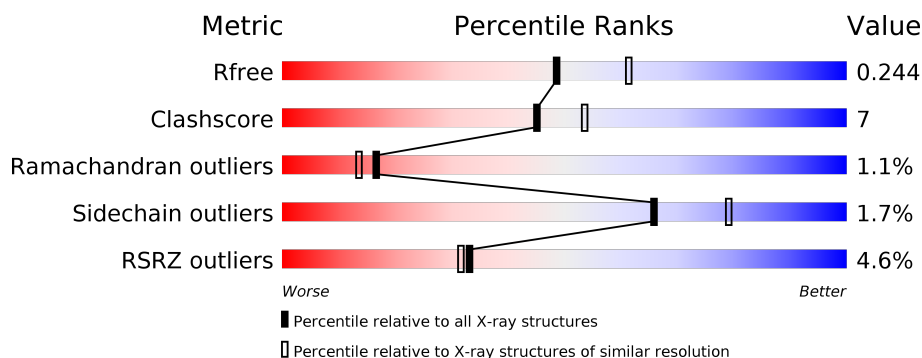
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	427	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	C	427	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	B	149	<div> <div>12%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	D	149	<div> <div>9%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9821 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 Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3240	2039	540	639	22			
1	C	424	Total	C	N	O	S	0	0	0
			3240	2039	540	639	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	SER	engineered mutation	UNP K9LG83
A	356	ALA	ASP	engineered mutation	UNP K9LG83
A	359	ALA	HIS	engineered mutation	UNP K9LG83
C	57	ALA	SER	engineered mutation	UNP K9LG83
C	356	ALA	ASP	engineered mutation	UNP K9LG83
C	359	ALA	HIS	engineered mutation	UNP K9LG83

- Molecule 2 is a protein called Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1110	695	194	217	4			
2	D	149	Total	C	N	O	S	0	0	0
			1110	695	194	217	4			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



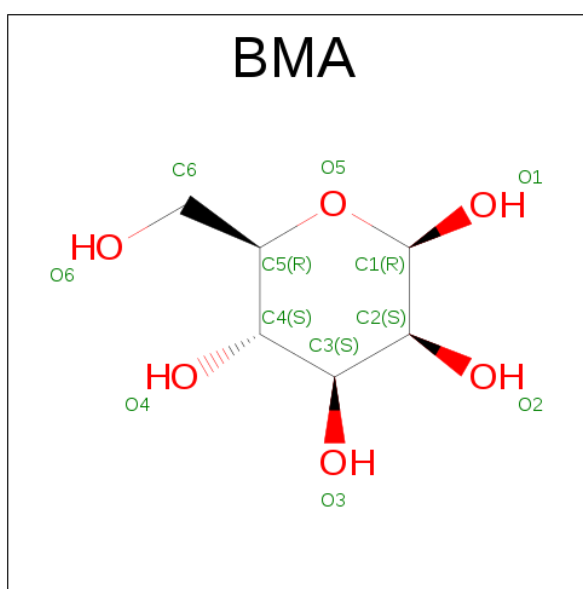
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

*Continued on next page...*

Continued from previous page...

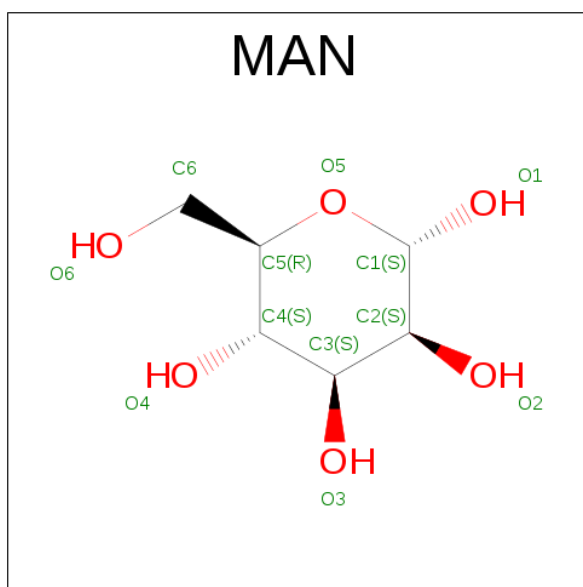
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



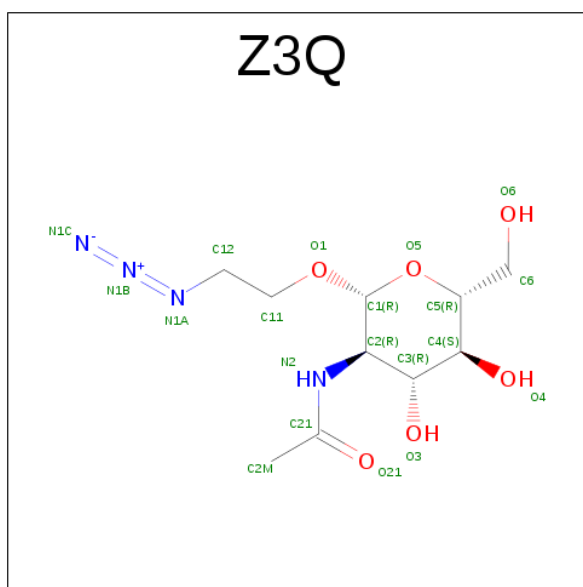
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



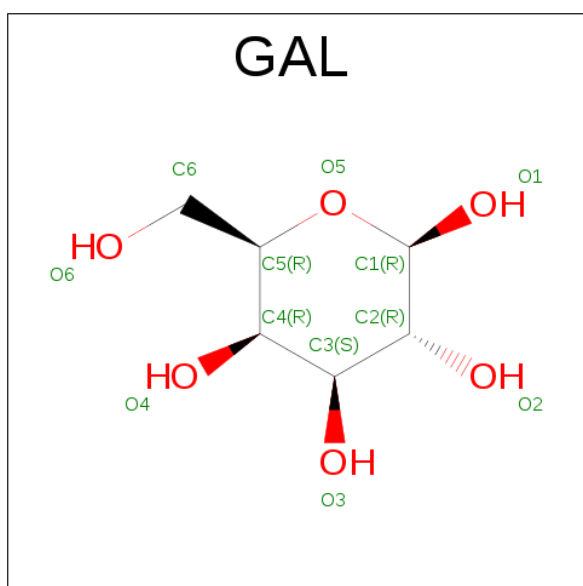
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 2-azidoethyl 2-(acetylamino)-2-deoxy-beta-D-glucopyranoside (three-letter code: Z3Q) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).



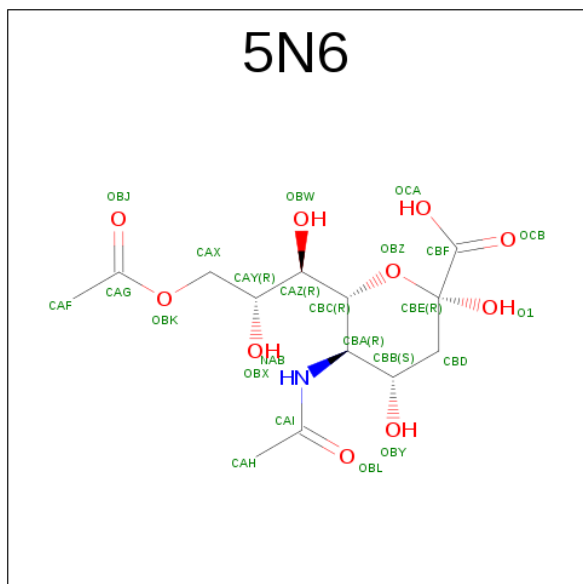
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	10	4	6		
6	C	1	Total	C	N	O	0	0
			20	10	4	6		

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is (2 {R},4 {S},5 {R},6 {R})-5-acetamido-6-[(1 {R},2 {R})-3-acetyloxy-1,2-bis(oxidanyl)propyl]-2,4-bis(oxidanyl)oxane-2-carboxylic acid (three-letter code: 5N6) (formula:  $C_{13}H_{21}NO_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			23	13	1	9		
8	C	1	Total	C	N	O	0	0
			23	13	1	9		

- Molecule 9 is water.

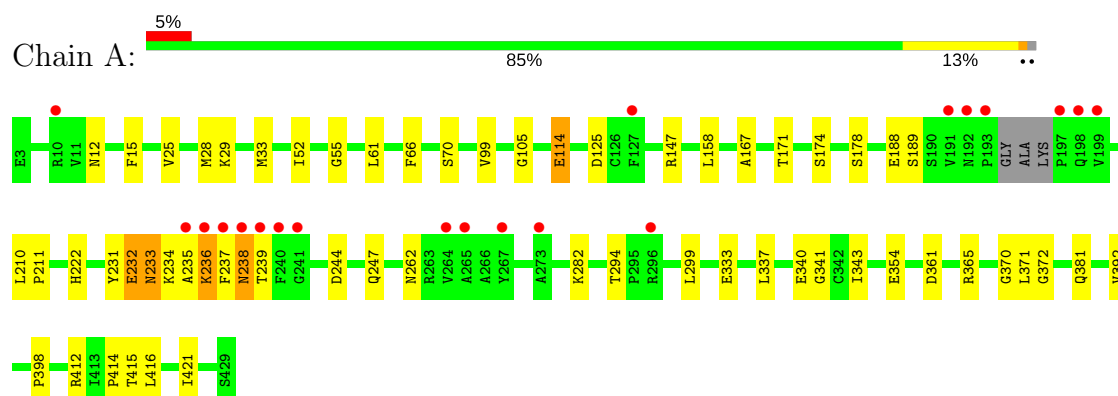
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	239	Total	O	0	0
			239	239		
9	B	66	Total	O	0	0
			66	66		
9	C	280	Total	O	0	0
			280	280		
9	D	44	Total	O	0	0
			44	44		



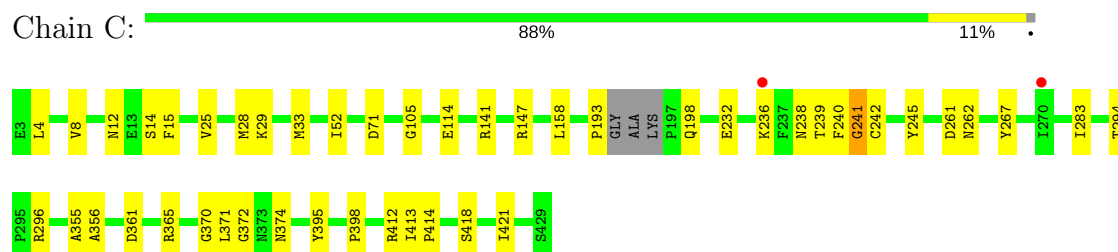
### 3 Residue-property plots [i](#)

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.

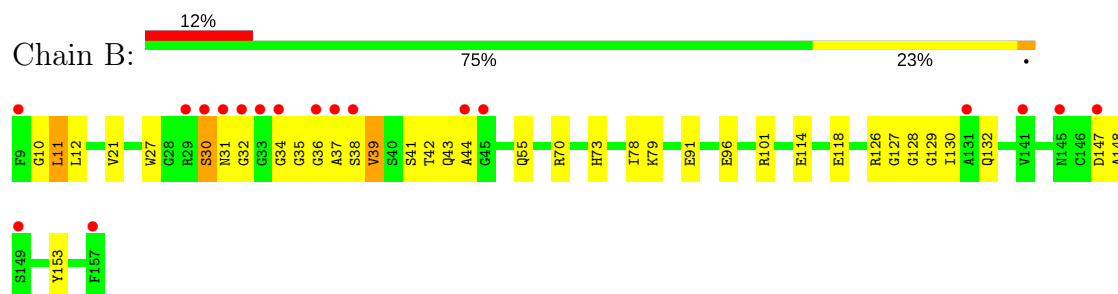
#### • Molecule 1: Hemagglutinin-esterase



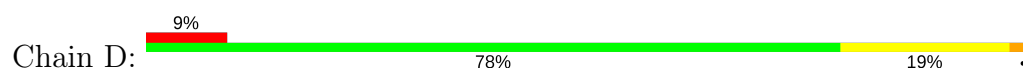
#### • Molecule 1: Hemagglutinin-esterase



#### • Molecule 2: Hemagglutinin-esterase



#### • Molecule 2: Hemagglutinin-esterase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.82Å 164.82Å 164.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.20 49.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.70-2.20) 96.0 (49.70-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.204 , 0.244 0.204 , 0.244	Depositor DCC
$R_{free}$ test set	3665 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, Z3Q, 5N6, GAL, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/3315	0.63	1/4494 (0.0%)
1	C	0.46	0/3315	0.61	0/4494
2	B	0.44	0/1127	0.62	0/1515
2	D	0.38	0/1127	0.55	0/1515
All	All	0.46	0/8884	0.61	1/12018 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASN	C-N-CA	-5.47	108.01	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3240	0	3114	47	0
1	C	3240	0	3114	38	0
2	B	1110	0	1067	25	0
2	D	1110	0	1067	28	0
3	A	84	0	73	3	0
3	B	42	0	38	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	84	0	74	1	0
3	D	42	0	38	1	0
4	A	22	0	17	2	0
4	C	11	0	9	0	0
5	A	66	0	57	0	0
5	C	33	0	28	0	0
6	A	20	0	0	1	0
6	C	20	0	0	0	0
7	A	11	0	9	3	0
7	C	11	0	9	2	0
8	A	23	0	0	5	0
8	C	23	0	0	2	0
9	A	239	0	0	5	1
9	B	66	0	0	5	1
9	C	280	0	0	7	1
9	D	44	0	0	7	0
All	All	9821	0	8714	132	2

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 7.

All (132) 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:234:LYS:O	1:A:238:ASN:ND2	1.89	1.06
1:A:244:ASP:OD1	1:A:262:ASN:HB2	1.70	0.92
1:A:29:LYS:NZ	9:A:804:HOH:O	2.05	0.90
8:A:717:5N6:OBW	8:A:717:5N6:OBL	1.90	0.90
2:D:80:ASN:OD1	9:D:801:HOH:O	1.91	0.87
1:C:193:PRO:O	9:C:801:HOH:O	1.96	0.82
1:A:340:GLU:OE1	9:A:802:HOH:O	1.98	0.81
1:A:114:GLU:OE2	9:A:803:HOH:O	1.99	0.79
2:D:80:ASN:ND2	9:D:802:HOH:O	2.14	0.77
1:C:198:GLN:OE1	9:C:802:HOH:O	2.03	0.77
2:D:30:SER:OG	2:D:31:ASN:ND2	2.19	0.76
1:A:415:THR:O	2:B:101:ARG:NH1	2.19	0.74
3:B:702:NAG:O4	9:B:801:HOH:O	2.06	0.72
1:A:233:ASN:O	1:A:234:LYS:C	2.19	0.72
1:C:240:PHE:O	1:C:296:ARG:NH1	2.23	0.72
7:C:712:GAL:H4	8:C:713:5N6:CBF	2.19	0.72
1:C:232:GLU:OE1	1:C:236:LYS:NZ	2.19	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:708:NAG:O3	4:A:709:BMA:H2	1.91	0.70
1:C:261:ASP:OD2	9:C:803:HOH:O	2.08	0.70
1:A:114:GLU:HG2	9:A:803:HOH:O	1.92	0.70
1:C:245:TYR:O	1:C:262:ASN:HB2	1.92	0.70
1:A:232:GLU:HG3	1:A:236:LYS:HG3	1.72	0.69
1:A:236:LYS:O	1:A:239:THR:OG1	2.06	0.69
1:C:238:ASN:HA	1:C:241:GLY:O	1.92	0.69
2:D:30:SER:OG	2:D:31:ASN:N	2.24	0.66
1:A:237:PHE:HZ	1:A:294:THR:HG21	1.61	0.66
3:A:702:NAG:O3	4:A:703:BMA:C1	2.43	0.66
1:C:236:LYS:O	1:C:239:THR:OG1	2.13	0.65
1:C:25:VAL:HG13	1:C:421:ILE:HG23	1.77	0.65
1:A:33:MET:HE1	2:B:101:ARG:HB2	1.79	0.65
1:A:234:LYS:HG3	1:A:238:ASN:HD21	1.61	0.65
2:B:38:SER:OG	2:B:39:VAL:N	2.30	0.63
1:C:412:ARG:NE	9:C:809:HOH:O	2.31	0.63
2:B:101:ARG:NH1	9:B:804:HOH:O	2.31	0.63
1:A:33:MET:HG3	1:A:416:LEU:HG	1.80	0.63
1:C:52:ILE:HD13	1:C:105:GLY:HA3	1.81	0.63
1:A:114:GLU:OE1	1:A:114:GLU:N	2.32	0.62
1:A:361:ASP:O	1:A:365:ARG:HG3	2.00	0.62
2:D:101:ARG:NE	9:D:804:HOH:O	2.25	0.60
1:C:242:CYS:HB2	9:C:901:HOH:O	2.02	0.60
2:D:79:LYS:NZ	9:D:805:HOH:O	2.35	0.60
1:A:233:ASN:O	1:A:235:ALA:N	2.35	0.59
1:C:33:MET:HE2	1:C:414:PRO:HB2	1.84	0.58
1:A:232:GLU:HG3	1:A:236:LYS:CG	2.34	0.58
1:C:418:SER:HB2	2:D:57:ARG:HH11	1.68	0.58
2:B:96:GLU:OE2	9:B:803:HOH:O	2.17	0.58
1:C:8:VAL:HG13	2:D:26:PHE:HB2	1.86	0.56
1:A:238:ASN:H	1:A:238:ASN:HD22	1.52	0.56
2:B:27:TRP:CD1	2:B:44:ALA:HB2	2.43	0.54
1:A:28:MET:SD	3:A:713:NAG:H5	2.48	0.53
2:D:26:PHE:HD1	2:D:43:GLN:H	1.57	0.53
1:A:25:VAL:HG13	1:A:421:ILE:HG23	1.90	0.53
2:B:126:ARG:NE	2:B:153:TYR:O	2.28	0.53
2:B:42:THR:O	2:B:43:GLN:HB2	2.09	0.53
1:C:361:ASP:O	1:C:365:ARG:HG3	2.09	0.52
1:C:147:ARG:NH1	2:D:75:GLU:OE1	2.42	0.52
1:A:333:GLU:OE1	9:A:805:HOH:O	2.19	0.52
1:A:412:ARG:NH2	2:B:91:GLU:HA	2.25	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ASN:HB3	1:C:14:SER:H	1.76	0.51
1:C:294:THR:OG1	9:C:805:HOH:O	2.19	0.51
1:C:4:LEU:H	2:D:30:SER:CB	2.24	0.51
1:A:354:GLU:O	1:C:29:LYS:HE2	2.10	0.51
1:A:61:LEU:HA	1:A:66:PHE:CD1	2.47	0.50
1:A:371:LEU:N	1:A:372:GLY:HA3	2.27	0.50
2:D:27:TRP:CD1	2:D:44:ALA:HB2	2.47	0.50
1:C:4:LEU:HB3	2:D:30:SER:HB2	1.93	0.50
1:A:167:ALA:HA	1:A:188:GLU:HG3	1.93	0.49
1:C:232:GLU:HB3	1:C:236:LYS:HE2	1.94	0.49
1:A:55:GLY:HA2	1:A:114:GLU:HB3	1.94	0.49
1:C:371:LEU:N	1:C:372:GLY:HA3	2.28	0.49
7:A:716:GAL:H4	8:A:717:5N6:CBF	2.43	0.48
1:A:52:ILE:HD13	1:A:105:GLY:HA3	1.95	0.48
1:C:240:PHE:H	1:C:241:GLY:HA3	1.78	0.48
1:A:12:ASN:H	1:A:15:PHE:HD1	1.60	0.47
7:A:716:GAL:C4	8:A:717:5N6:CBF	2.93	0.47
1:A:147:ARG:HD3	1:A:341:GLY:HA3	1.96	0.47
2:B:10:GLY:O	2:B:12:LEU:N	2.40	0.47
2:B:37:ALA:O	2:B:38:SER:HB3	2.15	0.47
2:D:101:ARG:NH2	9:D:804:HOH:O	2.47	0.46
2:D:34:GLY:HA2	2:D:35:GLY:HA2	1.68	0.46
7:C:712:GAL:C4	8:C:713:5N6:CBF	2.86	0.46
3:D:702:NAG:O4	9:D:803:HOH:O	2.20	0.46
2:B:34:GLY:HA2	2:B:35:GLY:HA2	1.67	0.46
2:D:149:SER:O	2:D:153:TYR:N	2.49	0.46
2:D:147:ASP:OD2	2:D:148:ALA:N	2.40	0.45
2:D:51:LYS:O	2:D:51:LYS:HD2	2.16	0.45
1:C:33:MET:CE	2:D:101:ARG:HB2	2.46	0.45
1:C:52:ILE:CD1	1:C:105:GLY:HA3	2.47	0.45
1:A:231:TYR:OH	8:A:717:5N6:OBJ	2.28	0.45
1:C:370:GLY:C	1:C:372:GLY:HA3	2.36	0.45
1:A:343:ILE:HG23	1:A:381:GLN:HA	1.99	0.45
1:A:412:ARG:HH22	2:B:91:GLU:HG3	1.82	0.45
1:C:71:ASP:HA	1:C:365:ARG:HG2	1.98	0.45
2:B:73:HIS:HE1	9:B:806:HOH:O	2.00	0.45
1:A:282:LYS:HB2	1:A:282:LYS:HE2	1.86	0.44
2:B:114:GLU:O	2:B:118:GLU:HG3	2.17	0.44
2:B:31:ASN:HA	2:B:36:GLY:HA3	1.99	0.44
1:C:395:TYR:HD2	2:D:86:GLU:HG2	1.82	0.44
1:A:412:ARG:HH22	2:B:91:GLU:HA	1.83	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ILE:HA	1:C:414:PRO:HD3	1.87	0.44
1:A:171:THR:HG22	1:A:178:SER:HA	1.99	0.44
1:C:12:ASN:H	1:C:15:PHE:HD1	1.65	0.43
2:D:128:GLY:HA2	2:D:129:GLY:HA2	1.52	0.43
2:B:30:SER:HB3	2:B:31:ASN:H	1.50	0.43
2:B:55:GLN:NE2	3:B:702:NAG:H83	2.33	0.43
1:A:232:GLU:HG2	1:A:232:GLU:H	1.50	0.42
1:A:337:LEU:O	2:B:79:LYS:HD3	2.19	0.42
1:A:125:ASP:HB3	1:A:174:SER:O	2.19	0.42
1:A:211:PRO:HD2	1:A:222:HIS:CE1	2.54	0.42
2:B:128:GLY:HA2	2:B:129:GLY:HA2	1.71	0.42
2:B:127:GLY:O	2:B:130:ILE:N	2.52	0.42
2:B:70:ARG:NH1	9:B:807:HOH:O	2.52	0.42
1:C:262:ASN:ND2	1:C:267:TYR:CD1	2.88	0.42
1:C:374:ASN:ND2	9:C:826:HOH:O	2.53	0.42
6:A:715:Z3Q:C2M	7:A:716:GAL:H2	2.50	0.41
1:C:395:TYR:CD2	2:D:86:GLU:HG2	2.55	0.41
2:B:147:ASP:OD2	2:B:148:ALA:N	2.44	0.41
2:D:38:SER:OG	2:D:39:VAL:N	2.53	0.41
1:A:210:LEU:HB3	1:A:222:HIS:CD2	2.56	0.41
2:D:142:ASP:C	2:D:144:GLU:H	2.24	0.41
1:A:370:GLY:C	1:A:372:GLY:HA3	2.40	0.41
1:A:247:GLN:NE2	1:A:299:LEU:O	2.51	0.41
1:C:398:PRO:HB2	2:D:78:ILE:O	2.21	0.41
1:A:70:SER:O	1:A:365:ARG:HD3	2.21	0.41
1:C:141:ARG:HD2	1:C:283:ILE:HG13	2.01	0.41
1:C:28:MET:SD	3:C:709:NAG:H5	2.61	0.41
2:D:126:ARG:HD3	2:D:154:ILE:HA	2.03	0.41
2:D:42:THR:O	2:D:42:THR:HG23	2.21	0.40
2:D:51:LYS:HG3	9:D:827:HOH:O	2.21	0.40
1:A:33:MET:CE	1:A:414:PRO:HB2	2.50	0.40
1:A:398:PRO:HB2	2:B:78:ILE:O	2.21	0.40
8:A:717:5N6:OBL	8:A:717:5N6:CAZ	2.70	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:977:HOH:O	9:C:1012:HOH:O[3_554]	1.99	0.21
9:B:807:HOH:O	9:B:829:HOH:O[10_554]	2.19	0.01



## 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	420/427 (98%)	399 (95%)	21 (5%)	0	100	100
1	C	420/427 (98%)	402 (96%)	15 (4%)	3 (1%)	25	24
2	B	147/149 (99%)	124 (84%)	17 (12%)	6 (4%)	3	1
2	D	147/149 (99%)	127 (86%)	16 (11%)	4 (3%)	6	3
All	All	1134/1152 (98%)	1052 (93%)	69 (6%)	13 (1%)	17	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	11	LEU
1	C	355	ALA
2	D	128	GLY
2	B	21	VAL
2	B	41	SER
2	B	132	GLN
2	D	41	SER
2	D	132	GLN
2	D	43	GLN
1	C	356	ALA
2	B	32	GLY
1	C	241	GLY
2	B	39	VAL

### 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	357/358 (100%)	349 (98%)	8 (2%)	57	70
1	C	357/358 (100%)	355 (99%)	2 (1%)	89	94
2	B	109/109 (100%)	107 (98%)	2 (2%)	64	77
2	D	109/109 (100%)	105 (96%)	4 (4%)	39	49
All	All	932/934 (100%)	916 (98%)	16 (2%)	66	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	A	114	GLU
1	A	158	LEU
1	A	189	SER
1	A	232	GLU
1	A	236	LYS
1	A	238	ASN
1	A	392	VAL
2	B	11	LEU
2	B	30	SER
1	C	114	GLU
1	C	158	LEU
2	D	9	PHE
2	D	11	LEU
2	D	126	ARG
2	D	144	GLU

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	238	ASN
2	B	156	ASN
2	D	31	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

36 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	$\# Z  > 2$
3	NAG	A	701	1,3	14,14,15	0.42	0	15,19,21	0.90	0
3	NAG	A	702	3,4	14,14,15	0.29	0	15,19,21	0.63	0
4	BMA	A	703	3,5	11,11,12	0.90	1 (9%)	13,15,17	2.99	5 (38%)
5	MAN	A	704	5,4	11,11,12	0.40	0	13,15,17	1.31	1 (7%)
5	MAN	A	705	5	11,11,12	0.39	0	13,15,17	1.03	0
5	MAN	A	706	5	11,11,12	0.33	0	13,15,17	1.12	1 (7%)
3	NAG	A	707	1,3	14,14,15	0.42	0	15,19,21	0.80	0
3	NAG	A	708	3,4	14,14,15	0.55	0	15,19,21	1.78	4 (26%)
4	BMA	A	709	3,5	11,11,12	0.62	0	13,15,17	3.46	6 (46%)
5	MAN	A	710	5,4	11,11,12	0.48	0	13,15,17	2.18	3 (23%)
5	MAN	A	711	5	11,11,12	0.34	0	13,15,17	0.80	0
5	MAN	A	712	4	11,11,12	0.48	0	13,15,17	0.82	0
3	NAG	A	713	1,3	14,14,15	0.77	1 (7%)	15,19,21	1.27	1 (6%)
3	NAG	A	714	3	14,14,15	0.31	0	15,19,21	1.45	3 (20%)
6	Z3Q	A	715	7	19,20,20	1.73	3 (15%)	23,26,26	3.93	7 (30%)
7	GAL	A	716	8,6	11,11,12	1.00	0	13,15,17	2.13	3 (23%)
8	5N6	A	717	7	20,23,24	1.84	5 (25%)	22,32,35	1.55	5 (22%)
3	NAG	B	701	3,2	14,14,15	0.43	0	15,19,21	0.84	0
3	NAG	B	702	3	14,14,15	0.39	0	15,19,21	1.44	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	703	2	14,14,15	0.38	0	15,19,21	1.42	3 (20%)
3	NAG	C	701	1,3	14,14,15	0.45	0	15,19,21	0.88	0
3	NAG	C	702	3,4	14,14,15	0.49	0	15,19,21	1.30	1 (6%)
4	BMA	C	703	3,5	11,11,12	0.49	0	13,15,17	1.09	1 (7%)
5	MAN	C	704	5,4	11,11,12	0.50	0	13,15,17	1.72	4 (30%)
5	MAN	C	705	5	11,11,12	0.39	0	13,15,17	0.69	0
5	MAN	C	706	5	11,11,12	0.51	0	13,15,17	1.01	0
3	NAG	C	707	1,3	14,14,15	0.49	0	15,19,21	1.12	2 (13%)
3	NAG	C	708	3	14,14,15	0.49	0	15,19,21	0.91	0
3	NAG	C	709	1,3	14,14,15	0.37	0	15,19,21	1.17	2 (13%)
3	NAG	C	710	3	14,14,15	0.35	0	15,19,21	1.32	1 (6%)
6	Z3Q	C	711	7	19,20,20	1.20	2 (10%)	23,26,26	1.07	2 (8%)
7	GAL	C	712	8,6	11,11,12	1.20	0	13,15,17	1.20	2 (15%)
8	5N6	C	713	7	20,23,24	2.43	9 (45%)	22,32,35	0.95	0
3	NAG	D	701	3,2	14,14,15	0.44	0	15,19,21	0.91	2 (13%)
3	NAG	D	702	3	14,14,15	0.48	0	15,19,21	1.51	3 (20%)
3	NAG	D	703	2	14,14,15	0.32	0	15,19,21	1.42	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	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	703	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	704	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	705	5	-	0/2/19/22	0/1/1/1
5	MAN	A	706	5	-	0/2/19/22	0/1/1/1
3	NAG	A	707	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	708	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	709	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	710	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	711	5	-	0/2/19/22	0/1/1/1
5	MAN	A	712	4	-	0/2/19/22	0/1/1/1
3	NAG	A	713	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	714	3	-	0/6/23/26	0/1/1/1
6	Z3Q	A	715	7	-	1/12/32/32	0/1/1/1
7	GAL	A	716	8,6	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	5N6	A	717	7	-	0/17/37/41	0/1/1/1
3	NAG	B	701	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	2	-	0/6/23/26	0/1/1/1
3	NAG	C	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	702	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	703	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	704	5,4	-	0/2/19/22	0/1/1/1
5	MAN	C	705	5	-	0/2/19/22	0/1/1/1
5	MAN	C	706	5	-	0/2/19/22	0/1/1/1
3	NAG	C	707	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	708	3	-	0/6/23/26	0/1/1/1
3	NAG	C	709	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	710	3	-	0/6/23/26	0/1/1/1
6	Z3Q	C	711	7	-	0/12/32/32	0/1/1/1
7	GAL	C	712	8,6	-	0/2/19/22	0/1/1/1
8	5N6	C	713	7	-	0/17/37/41	0/1/1/1
3	NAG	D	701	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	702	3	-	0/6/23/26	0/1/1/1
3	NAG	D	703	2	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	715	Z3Q	N1B-N1A	-6.10	1.07	1.23
8	C	713	5N6	CBB-CBA	-4.84	1.48	1.53
8	C	713	5N6	OBY-CBB	-4.61	1.33	1.43
6	C	711	Z3Q	N1B-N1A	-4.20	1.12	1.23
8	A	717	5N6	CBB-CBA	-4.17	1.49	1.53
8	C	713	5N6	CAZ-CBC	-4.15	1.47	1.52
8	C	713	5N6	OBK-CAX	-3.38	1.37	1.45
8	A	717	5N6	OBY-CBB	-3.16	1.36	1.43
8	C	713	5N6	CAY-CAZ	-2.87	1.47	1.53
8	C	713	5N6	CBD-CBB	-2.80	1.48	1.52
8	A	717	5N6	OBK-CAX	-2.76	1.39	1.45
4	A	703	BMA	O5-C1	-2.59	1.39	1.43
8	A	717	5N6	CBD-CBB	-2.57	1.48	1.52
8	C	713	5N6	OBZ-CBC	-2.57	1.39	1.43
8	A	717	5N6	CAX-CAY	-2.39	1.48	1.51
8	C	713	5N6	OBX-CAY	-2.37	1.38	1.43
8	C	713	5N6	OBZ-CBE	-2.11	1.38	1.43
6	A	715	Z3Q	O4-C4	-2.02	1.38	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	713	NAG	C1-C2	2.13	1.55	1.52
6	C	711	Z3Q	O1-C1	2.17	1.44	1.40
6	A	715	Z3Q	O1-C1	3.22	1.45	1.40

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	715	Z3Q	C1-C2-N2	-12.43	90.00	111.03
6	A	715	Z3Q	O5-C1-O1	-11.53	82.64	110.02
4	A	709	BMA	C2-C3-C4	-8.24	96.51	110.88
4	A	703	BMA	C1-O5-C5	-7.09	102.39	112.17
4	A	703	BMA	O2-C2-C3	-6.28	97.83	110.17
7	A	716	GAL	C1-O5-C5	-4.11	106.50	112.17
7	A	716	GAL	O3-C3-C4	-3.93	101.80	110.36
6	A	715	Z3Q	C3-C2-N2	-3.76	103.42	110.61
8	A	717	5N6	CAX-OBK-CAG	-3.72	107.69	117.17
6	A	715	Z3Q	O5-C5-C6	-3.34	98.41	106.41
4	A	709	BMA	O6-C6-C5	-3.06	101.05	111.34
3	D	702	NAG	C2-N2-C7	-2.95	118.64	122.94
4	A	709	BMA	O3-C3-C2	-2.91	104.73	110.02
5	A	706	MAN	C6-C5-C4	-2.89	106.24	113.00
6	C	711	Z3Q	C1-O5-C5	-2.74	108.55	113.72
3	B	702	NAG	C2-N2-C7	-2.71	118.99	122.94
3	A	708	NAG	O4-C4-C5	-2.68	102.52	109.28
3	C	702	NAG	O4-C4-C5	-2.56	102.83	109.28
6	C	711	Z3Q	C11-O1-C1	-2.56	109.48	113.87
3	A	708	NAG	O3-C3-C2	-2.54	103.95	109.39
4	A	703	BMA	O6-C6-C5	-2.54	102.81	111.34
3	B	703	NAG	C4-C3-C2	-2.51	107.34	111.02
8	A	717	5N6	CBB-CBA-NAB	-2.49	105.27	110.40
5	A	710	MAN	O3-C3-C4	-2.44	105.04	110.36
6	A	715	Z3Q	O4-C4-C5	-2.40	103.24	109.28
5	C	704	MAN	O3-C3-C4	-2.37	105.21	110.36
3	C	707	NAG	C2-N2-C7	-2.36	119.50	122.94
5	C	704	MAN	C6-C5-C4	-2.33	107.56	113.00
3	D	703	NAG	C2-N2-C7	-2.27	119.63	122.94
7	C	712	GAL	O3-C3-C4	-2.26	105.44	110.36
8	A	717	5N6	OBX-CAY-CAX	-2.23	105.03	110.00
3	A	714	NAG	C1-C2-N2	-2.22	106.70	110.49
3	D	702	NAG	O5-C1-C2	-2.16	108.47	111.47
4	A	703	BMA	O5-C1-C2	-2.13	107.45	110.79
4	A	703	BMA	O3-C3-C4	-2.08	105.83	110.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	709	NAG	O4-C4-C3	-2.04	105.92	110.36
3	D	701	NAG	O4-C4-C5	-2.02	104.20	109.28
3	B	703	NAG	C2-N2-C7	-2.01	120.00	122.94
8	A	717	5N6	CBB-CBA-CBC	-2.00	103.63	108.89
3	A	714	NAG	C2-N2-C7	2.02	125.89	122.94
5	C	704	MAN	C1-C2-C3	2.18	112.42	109.65
4	C	703	BMA	O3-C3-C2	2.19	114.01	110.02
3	C	707	NAG	C1-O5-C5	2.23	115.24	112.17
5	A	704	MAN	C1-C2-C3	2.25	112.50	109.65
3	D	701	NAG	C1-O5-C5	2.35	115.40	112.17
8	A	717	5N6	OBL-CAI-NAB	2.36	126.46	121.92
3	A	708	NAG	C1-O5-C5	2.40	115.48	112.17
7	C	712	GAL	C2-C3-C4	2.44	115.13	110.88
3	C	709	NAG	C1-O5-C5	2.89	116.15	112.17
7	A	716	GAL	C2-C3-C4	3.03	116.16	110.88
4	A	709	BMA	O3-C3-C4	3.08	117.06	110.36
3	C	710	NAG	C1-O5-C5	3.24	116.63	112.17
6	A	715	Z3Q	C2-N2-C21	3.43	131.88	123.19
3	D	702	NAG	C1-O5-C5	3.47	116.95	112.17
3	B	703	NAG	C1-O5-C5	3.53	117.03	112.17
3	A	713	NAG	C1-O5-C5	3.57	117.08	112.17
6	A	715	Z3Q	C11-O1-C1	3.59	120.03	113.87
4	A	709	BMA	O4-C4-C3	3.61	118.22	110.36
3	B	702	NAG	C1-O5-C5	3.63	117.17	112.17
5	C	704	MAN	C1-O5-C5	3.75	117.34	112.17
3	A	714	NAG	C1-O5-C5	3.80	117.41	112.17
3	D	703	NAG	C1-O5-C5	3.95	117.62	112.17
5	A	710	MAN	C1-C2-C3	4.13	114.88	109.65
3	A	708	NAG	O4-C4-C3	4.92	121.07	110.36
5	A	710	MAN	C1-O5-C5	5.39	119.60	112.17
4	A	709	BMA	C1-C2-C3	5.87	117.09	109.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	715	Z3Q	C11-O1-C1-C2

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NAG	1	0
4	A	703	BMA	1	0
3	A	708	NAG	1	0
4	A	709	BMA	1	0
3	A	713	NAG	1	0
6	A	715	Z3Q	1	0
7	A	716	GAL	3	0
8	A	717	5N6	5	0
3	B	702	NAG	2	0
3	C	709	NAG	1	0
7	C	712	GAL	2	0
8	C	713	5N6	2	0
3	D	702	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	424/427 (99%)	-0.18	20 (4%) 32 31	28, 40, 98, 144	0
1	C	424/427 (99%)	-0.48	2 (0%) 90 90	24, 36, 60, 78	0
2	B	149/149 (100%)	0.52	18 (12%) 5 4	26, 55, 120, 198	0
2	D	149/149 (100%)	0.53	13 (8%) 11 10	30, 51, 127, 190	0
All	All	1146/1152 (99%)	-0.11	53 (4%) 33 32	24, 40, 98, 198	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	32	GLY	17.9
2	B	37	ALA	14.5
2	D	33	GLY	14.3
2	B	34	GLY	14.1
2	D	37	ALA	11.0
2	B	32	GLY	10.4
2	D	35	GLY	10.2
1	A	191	VAL	8.1
1	A	193	PRO	7.8
2	D	36	GLY	7.0
2	B	33	GLY	6.8
2	D	34	GLY	6.3
1	A	237	PHE	6.1
2	B	36	GLY	5.7
2	B	44	ALA	5.3
1	A	264	VAL	5.3
2	D	149	SER	4.6
2	D	143	SER	4.4
1	A	265	ALA	4.2
1	A	199	VAL	4.1
2	D	31	ASN	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	141	VAL	4.0
2	D	38	SER	3.8
2	B	45	GLY	3.7
2	D	30	SER	3.5
1	A	241	GLY	3.4
2	B	157	PHE	3.4
1	A	273	ALA	3.3
2	B	30	SER	3.3
1	A	236	LYS	3.2
1	A	197	PRO	3.1
2	B	131	ALA	3.1
1	A	267	TYR	3.1
1	A	240	PHE	2.9
1	A	235	ALA	2.8
1	A	238	ASN	2.7
2	B	38	SER	2.7
1	C	270	ILE	2.7
1	A	192	ASN	2.6
2	B	147	ASP	2.5
2	B	9	PHE	2.5
2	B	149	SER	2.5
2	B	31	ASN	2.5
1	A	296	ARG	2.3
1	A	198	GLN	2.3
2	D	142	ASP	2.3
1	A	127	PHE	2.3
1	C	236	LYS	2.2
2	D	45	GLY	2.2
2	B	145	ASN	2.2
2	B	29	ARG	2.2
1	A	10	ARG	2.0
1	A	239	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
3	NAG	B	702	14/15	0.94	0.12	0.29	43,48,56,58	0
3	NAG	D	702	14/15	0.94	0.12	0.19	36,44,50,54	0
8	5N6	C	713	23/24	0.96	0.14	0.04	43,52,60,62	0
3	NAG	B	701	14/15	0.94	0.10	-0.05	30,35,39,41	0
3	NAG	C	709	14/15	0.96	0.10	-0.18	51,52,64,68	0
5	MAN	A	706	11/12	0.92	0.09	-0.51	32,38,42,46	0
8	5N6	A	717	23/24	0.94	0.18	-0.62	71,81,85,87	0
5	MAN	C	706	11/12	0.94	0.09	-0.62	38,40,45,48	0
3	NAG	D	701	14/15	0.96	0.09	-0.99	29,34,36,36	0
3	NAG	A	713	14/15	0.94	0.09	-1.14	60,63,69,72	0
3	NAG	A	714	14/15	0.81	0.13	-	58,65,73,79	0
6	Z3Q	A	715	20/20	0.61	0.61	-	129,139,148,148	0
5	MAN	C	704	11/12	0.96	0.07	-	30,34,39,41	0
4	BMA	C	703	11/12	0.93	0.09	-	33,35,39,41	0
5	MAN	A	711	11/12	0.89	0.16	-	52,58,65,65	0
5	MAN	A	705	11/12	0.93	0.09	-	37,40,43,44	0
7	GAL	C	712	11/12	0.85	0.23	-	68,84,101,102	0
5	MAN	C	705	11/12	0.94	0.09	-	41,46,52,59	0
3	NAG	A	708	14/15	0.95	0.10	-	31,36,38,39	0
3	NAG	C	707	14/15	0.98	0.08	-	25,30,36,39	0
3	NAG	C	710	14/15	0.90	0.10	-	53,57,63,68	0
3	NAG	C	708	14/15	0.91	0.14	-	39,46,51,52	0
3	NAG	A	702	14/15	0.93	0.12	-	36,42,46,50	0
3	NAG	C	702	14/15	0.96	0.09	-	28,33,38,40	0
4	BMA	A	703	11/12	0.95	0.10	-	35,38,42,43	0
3	NAG	C	701	14/15	0.96	0.08	-	34,37,41,42	0
5	MAN	A	710	11/12	0.94	0.10	-	42,47,48,51	0
3	NAG	A	707	14/15	0.96	0.08	-	29,37,40,42	0
3	NAG	B	703	14/15	0.87	0.21	-	70,77,81,82	0
3	NAG	D	703	14/15	0.78	0.25	-	88,99,103,103	0
4	BMA	A	709	11/12	0.88	0.17	-	43,47,54,60	0
6	Z3Q	C	711	20/20	0.45	0.66	-	109,126,133,138	0
7	GAL	A	716	11/12	0.77	0.31	-	96,109,120,121	0
3	NAG	A	701	14/15	0.95	0.09	-	38,40,49,50	0
5	MAN	A	704	11/12	0.97	0.09	-	28,32,37,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	A	712	11/12	0.93	0.09	-	39,42,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.