Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:16 AM GMT

PDB ID	:	2CH8
Title	:	STRUCTURE OF THE EPSTEIN-BARR VIRUS ONCOGENE BARF1
Authors	:	Tarbouriech, N.; Ruggiero, F.; Deturenne-Tessier, M.; Ooka, T.; Burmeister, W.P.
Deposited on	:	2006-03-13
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

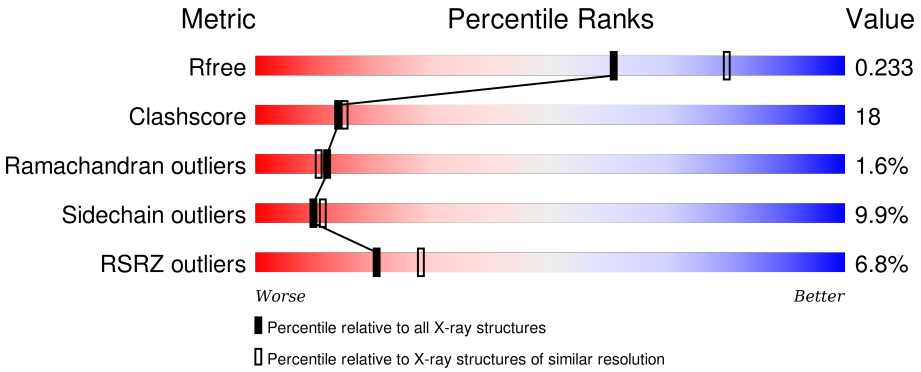
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 >=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 <=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	201	7% 63% 23% 6% • 6%
1	B	201	6% 62% 26% • • 7%
1	C	201	4% 68% 19% • • 7%
1	D	201	8% 69% 17% • • 7%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	1225	X	-	-	-
4	MAN	B	1225	X	-	-	-
4	MAN	C	1226	X	-	-	-
4	MAN	D	1225	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6701 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 33 KDA EARLY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	2	0
			1505	972	257	269	7			
1	B	186	Total	C	N	O	S	0	2	0
			1496	967	256	266	7			
1	C	186	Total	C	N	O	S	0	3	0
			1502	969	258	268	7			
1	D	186	Total	C	N	O	S	0	2	0
			1497	968	255	267	7			

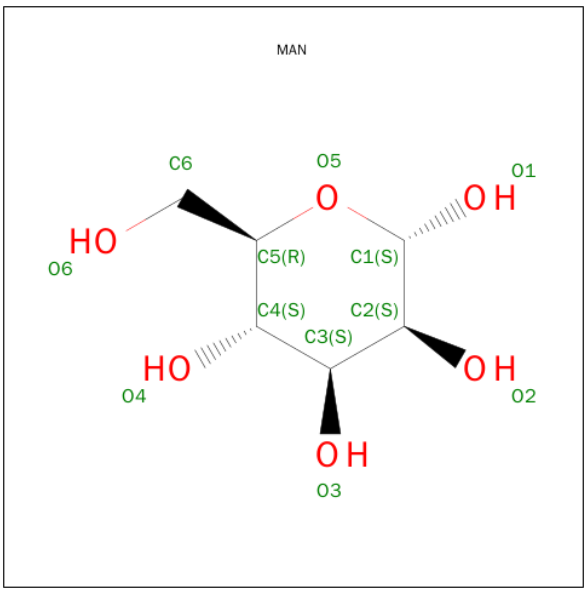
- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Pt	0	0
			3	3		
2	A	3	Total	Pt	0	0
			3	3		
2	D	3	Total	Pt	0	0
			3	3		
2	C	3	Total	Pt	0	0
			3	3		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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



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

- Molecule 5 is water.

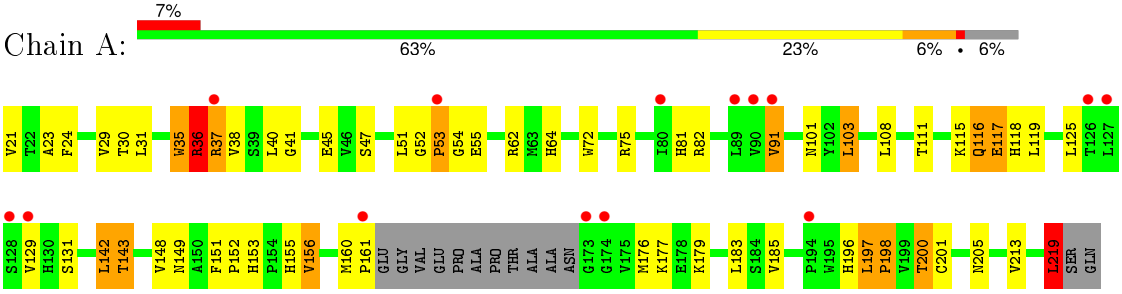
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	128	Total O 128 128	0	0
5	B	131	Total O 131 131	0	0
5	C	145	Total O 145 145	0	0
5	D	129	Total O 129 129	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

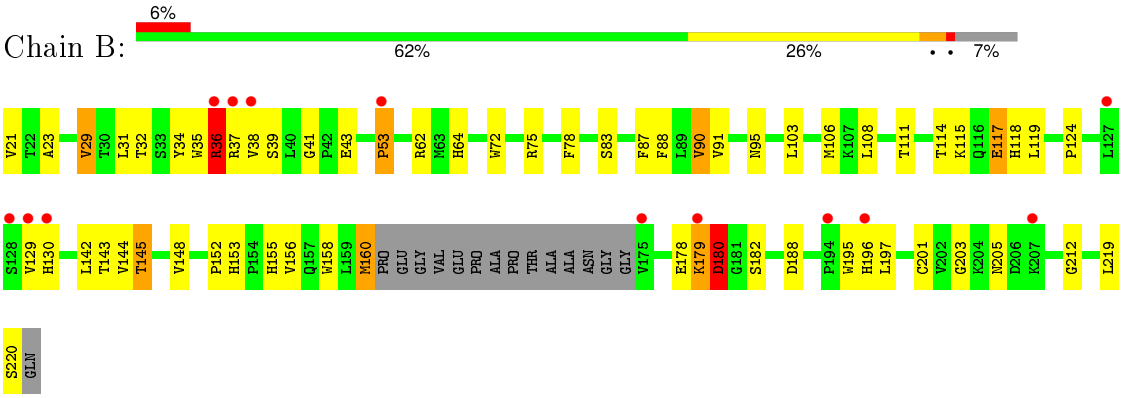
- Molecule 1: 33 KDA EARLY PROTEIN

Chain A:



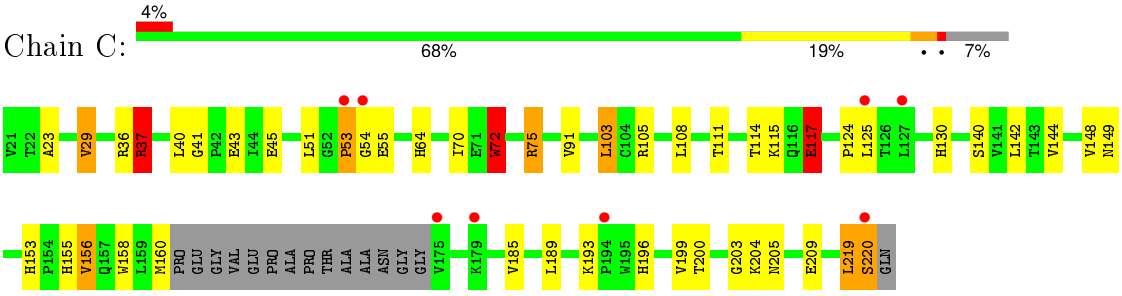
- Molecule 1: 33 KDA EARLY PROTEIN

Chain B:



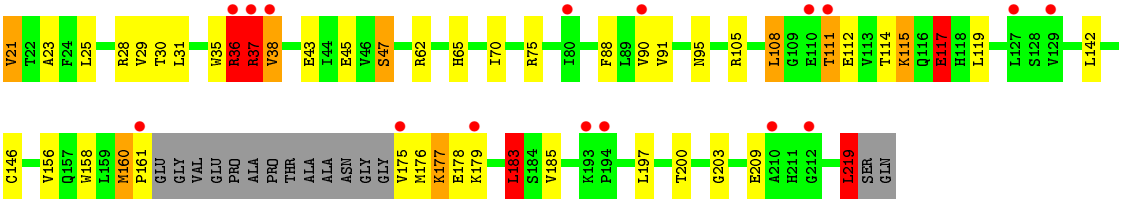
- Molecule 1: 33 KDA EARLY PROTEIN

Chain C:



- Molecule 1: 33 KDA EARLY PROTEIN

Chain D:


V21 T22 A23 F24 L25 R28 V29 T30 L31 W35 R36 R37 V38 E43 I44 E45 V46 S47 R62 H65 I70 R75 I80 F88 L89 V90 V91 N95 R105 L108 G109 E110 T111 E112 V113 T114 K115 Q116 E117 H118 L119 L127 S128 V129 L142
C146 V156 Q157 W158 L159 M160 P161 GLU GLY VAL GLU PRO ALA PRO THR ALA ALA ASN GLY GLY V175 M176 K177 E178 K179 L183 S184 V185 K193 P194 L197 T200 G203 E209 A210 H211 G212 L219 SER GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	179.25Å 179.25Å 95.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.30) 100.0 (29.87-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.233 0.175 , 0.233	Depositor DCC
R_{free} test set	2583 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.5	EDS
Estimated twinning fraction	0.116 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 50910 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6701	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PT, 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	1.13	3/1560 (0.2%)	1.06	7/2122 (0.3%)
1	B	1.03	1/1550 (0.1%)	1.03	6/2107 (0.3%)
1	C	1.09	4/1561 (0.3%)	1.01	7/2122 (0.3%)
1	D	1.02	2/1552 (0.1%)	0.94	4/2112 (0.2%)
All	All	1.07	10/6223 (0.2%)	1.01	24/8463 (0.3%)

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	A	0	3
1	B	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	CYS	CB-SG	-8.08	1.68	1.82
1	B	201	CYS	CB-SG	-7.07	1.70	1.82
1	D	117[A]	GLU	CB-CG	5.89	1.63	1.52
1	D	117[B]	GLU	CB-CG	5.89	1.63	1.52
1	A	117	GLU	CD-OE2	5.58	1.31	1.25
1	C	72	TRP	CE3-CZ3	5.48	1.47	1.38
1	C	72	TRP	CB-CG	5.30	1.59	1.50
1	C	117	GLU	CG-CD	5.22	1.59	1.51
1	C	43	GLU	CG-CD	5.20	1.59	1.51
1	A	177	LYS	CB-CG	5.03	1.66	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	B	180	ASP	CB-CG-OD1	-9.87	109.42	118.30
1	C	37	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	105	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	75	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	62	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	201	CYS	CA-CB-SG	-6.32	102.63	114.00
1	B	180	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	201	CYS	CA-CB-SG	-5.92	103.34	114.00
1	D	219	LEU	CB-CG-CD1	5.79	120.84	111.00
1	A	103	LEU	CA-CB-CG	5.76	128.54	115.30
1	D	183	LEU	CA-CB-CG	5.69	128.38	115.30
1	C	105	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	53	PRO	O-C-N	5.60	132.73	123.20
1	C	75	ARG	CG-CD-NE	-5.56	100.12	111.80
1	A	37	ARG	N-CA-C	5.48	125.79	111.00
1	A	82	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	36	ARG	C-N-CA	5.46	135.36	121.70
1	A	219	LEU	CA-CB-CG	5.42	127.76	115.30
1	C	75	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	36	ARG	C-N-CA	5.28	134.89	121.70
1	C	144	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	D	37	ARG	N-CA-C	5.17	124.95	111.00
1	A	82	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	LEU	Peptide
1	A	35	TRP	Peptide
1	A	36	ARG	Peptide
1	B	53	PRO	Peptide

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	1505	0	1474	63	0
1	B	1496	0	1474	54	0
1	C	1502	0	1475	41	0
1	D	1497	0	1468	55	0
2	A	3	0	0	0	0
2	B	3	0	0	1	0
2	C	3	0	0	1	0
2	D	3	0	0	0	0
3	A	28	0	25	2	0
3	B	28	0	25	6	0
3	C	28	0	25	1	0
3	D	28	0	25	2	0
4	A	11	0	10	2	0
4	B	11	0	10	3	0
4	C	11	0	10	1	0
4	D	11	0	10	2	0
5	A	128	0	0	8	0
5	B	131	0	0	7	0
5	C	145	0	0	13	0
5	D	129	0	0	14	0
All	All	6701	0	6031	217	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 18.

All (217) 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:95:ASN:HD21	3:B:1223:NAG:C1	1.11	1.59
1:B:160:MET:SD	2:B:1222:PT:PT	1.03	1.39
1:C:160:MET:SD	2:C:1222:PT:PT	1.06	1.31
1:C:36[B]:ARG:CZ	5:C:2017:HOH:O	1.80	1.30
1:D:23:ALA:CB	1:D:29:VAL:HG21	1.65	1.25
1:B:36:ARG:N	1:B:37:ARG:HA	1.61	1.14
1:B:36:ARG:H	1:B:37:ARG:CA	1.52	1.14
1:D:23:ALA:HB2	1:D:29:VAL:HG21	1.08	1.03
1:C:160:MET:SD	5:C:2132:HOH:O	2.20	1.00
1:A:23:ALA:HB2	1:A:29:VAL:HG21	1.41	0.98
1:C:36[B]:ARG:NH1	5:C:2017:HOH:O	1.90	0.98
1:B:36:ARG:H	1:B:37:ARG:HA	0.82	0.98
1:A:23:ALA:HB2	1:A:29:VAL:CG2	1.94	0.97
1:B:87:PHE:HE2	1:B:106:MET:HE2	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ALA:HB2	1:D:29:VAL:CG2	1.97	0.94
1:B:87:PHE:HE2	1:B:106:MET:CE	1.80	0.94
1:D:115:LYS:HG3	5:D:2013:HOH:O	1.68	0.93
1:D:117[B]:GLU:HB2	5:D:2078:HOH:O	1.69	0.93
1:C:36[B]:ARG:NH2	5:C:2020:HOH:O	1.95	0.91
1:A:156:VAL:HG22	1:A:185:VAL:CG1	2.00	0.91
1:D:177:LYS:HE3	5:D:2113:HOH:O	1.70	0.91
1:A:156:VAL:HG22	1:A:185:VAL:HG12	1.49	0.91
1:B:87:PHE:CE2	1:B:106:MET:HE2	2.05	0.91
3:A:1224:NAG:C4	4:A:1225:MAN:C1	2.50	0.89
3:C:1225:NAG:HO4	4:C:1226:MAN:C1	1.85	0.87
1:B:35:TRP:HA	1:B:36:ARG:HB2	1.55	0.87
1:B:87:PHE:CE2	1:B:106:MET:CE	2.58	0.86
1:A:143:THR:HG23	5:A:2098:HOH:O	1.74	0.85
1:B:29:VAL:HG11	1:B:119:LEU:HD11	1.58	0.84
1:D:156:VAL:HG23	1:D:185:VAL:HG13	1.61	0.83
1:A:36:ARG:HG3	1:A:37:ARG:HB2	1.62	0.81
1:D:117[A]:GLU:HB2	5:D:2078:HOH:O	1.79	0.81
1:A:155:HIS:HD2	5:A:2115:HOH:O	1.63	0.81
1:C:117:GLU:HB2	5:C:2091:HOH:O	1.81	0.80
1:A:160:MET:SD	1:A:196:HIS:ND1	2.56	0.79
1:D:23:ALA:HB1	1:D:29:VAL:HG21	1.63	0.79
1:A:160:MET:HB3	1:A:196:HIS:CE1	2.18	0.78
1:A:72:TRP:HE3	5:A:2049:HOH:O	1.66	0.78
1:B:34:TYR:HE1	1:B:37:ARG:HG3	1.47	0.78
1:C:156:VAL:CG2	1:C:185:VAL:HG13	2.15	0.76
1:D:29:VAL:HG11	1:D:119:LEU:HD11	1.67	0.75
1:C:36[B]:ARG:NH2	5:C:2017:HOH:O	1.98	0.75
1:A:160:MET:HB3	1:A:196:HIS:HE1	1.51	0.75
1:A:161:PRO:HD3	1:A:198:PRO:O	1.88	0.74
1:B:29:VAL:CG2	5:B:2003:HOH:O	2.35	0.73
1:A:29:VAL:HG12	1:A:91:VAL:HG13	1.71	0.73
1:B:29:VAL:HG12	1:B:91:VAL:CG1	2.17	0.72
1:C:219:LEU:O	1:C:220:SER:HB2	1.88	0.72
1:D:29:VAL:HG11	1:D:119:LEU:CD1	2.19	0.72
1:C:204:LYS:HE3	1:C:209:GLU:HB2	1.71	0.71
1:A:51:LEU:HD21	1:A:103:LEU:HD22	1.71	0.71
1:D:177:LYS:HG2	1:D:183:LEU:CD1	2.21	0.71
1:D:177:LYS:HG2	1:D:183:LEU:HD12	1.71	0.71
1:B:23:ALA:HB2	1:B:29:VAL:HG21	1.72	0.71
1:A:40:LEU:HD12	1:A:108:LEU:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:HG23	5:B:2009:HOH:O	1.91	0.70
1:C:54:GLY:O	1:C:55:GLU:HB2	1.92	0.69
1:B:36:ARG:N	1:B:37:ARG:CA	2.37	0.69
1:A:23:ALA:CB	1:A:29:VAL:HG21	2.19	0.69
3:B:1224:NAG:C4	4:B:1225:MAN:C1	2.70	0.69
1:A:156:VAL:CG2	1:A:185:VAL:CG1	2.70	0.69
1:B:155:HIS:HD2	5:B:2117:HOH:O	1.75	0.69
1:C:51:LEU:HD21	1:C:103:LEU:HD22	1.74	0.69
1:A:23:ALA:CB	1:A:29:VAL:CG2	2.71	0.68
1:B:95:ASN:CG	3:B:1223:NAG:C1	2.61	0.68
1:B:180:ASP:HB3	1:B:182:SER:H	1.60	0.68
1:C:156:VAL:HG23	1:C:185:VAL:HG13	1.76	0.67
1:B:35:TRP:HA	1:B:36:ARG:CB	2.25	0.66
1:B:87:PHE:CE2	1:B:106:MET:HE3	2.30	0.65
1:A:148:VAL:HG23	1:A:156:VAL:HG13	1.78	0.65
1:D:200:THR:HG22	5:D:2106:HOH:O	1.96	0.65
1:A:29:VAL:HG13	1:A:30:THR:N	2.11	0.64
1:B:145:THR:HB	1:B:188:ASP:OD2	1.97	0.64
1:D:105:ARG:CG	1:D:114:THR:HG22	2.26	0.64
1:D:38:VAL:HG23	5:D:2022:HOH:O	1.97	0.64
3:B:1224:NAG:O4	4:B:1225:MAN:C2	2.44	0.64
1:D:35:TRP:HH2	1:D:111:THR:HG23	1.63	0.64
1:B:29:VAL:HG11	1:B:119:LEU:CD1	2.26	0.64
1:A:29:VAL:CG1	1:A:91:VAL:HG13	2.27	0.64
1:D:29:VAL:HG22	5:D:2010:HOH:O	1.96	0.63
1:D:105:ARG:HG2	1:D:114:THR:HG22	1.80	0.63
1:A:36:ARG:HB3	1:A:37:ARG:CA	2.29	0.63
1:B:29:VAL:HG12	1:B:91:VAL:HG11	1.79	0.62
1:A:161:PRO:HD2	1:A:196:HIS:CE1	2.34	0.62
1:B:29:VAL:HG12	1:B:91:VAL:HG12	1.81	0.62
1:C:23:ALA:HB2	1:C:29:VAL:HG11	1.81	0.62
3:D:1224:NAG:C4	4:D:1225:MAN:C1	2.78	0.62
1:D:23:ALA:CB	1:D:29:VAL:CG2	2.60	0.61
1:D:21:VAL:HG13	1:D:31:LEU:CD2	2.30	0.61
1:C:155:HIS:HD2	5:C:2134:HOH:O	1.83	0.61
1:B:29:VAL:HG22	5:B:2012:HOH:O	2.00	0.60
1:D:36:ARG:HG2	5:D:2018:HOH:O	2.01	0.59
1:A:47:SER:HB3	1:A:62:ARG:HG2	1.84	0.59
1:A:131:SER:HB2	1:A:142:LEU:HD22	1.85	0.59
1:D:115:LYS:CG	5:D:2013:HOH:O	2.37	0.58
3:A:1224:NAG:H4	4:A:1225:MAN:C1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LYS:CD	1:D:117[B]:GLU:OE1	2.52	0.57
1:C:51:LEU:HD11	1:C:103:LEU:HD13	1.86	0.56
1:D:47:SER:HB3	1:D:62:ARG:HG2	1.87	0.56
1:A:148:VAL:CG2	1:A:156:VAL:HG13	2.36	0.56
1:A:156:VAL:CG2	1:A:185:VAL:HG12	2.30	0.56
1:C:36[B]:ARG:HG3	1:C:37:ARG:N	2.21	0.56
1:B:32:THR:HG22	1:B:88:PHE:CD1	2.41	0.56
1:C:36[A]:ARG:HG3	1:C:37:ARG:N	2.22	0.55
1:D:37:ARG:O	1:D:38:VAL:C	2.43	0.55
1:A:200:THR:HB	1:A:213:VAL:HG22	1.87	0.55
1:D:29:VAL:HB	1:D:91:VAL:CG1	2.37	0.55
1:C:36[B]:ARG:CG	1:C:37:ARG:N	2.70	0.55
1:C:37:ARG:HD3	5:C:2024:HOH:O	2.06	0.54
1:A:55:GLU:HA	1:A:55:GLU:OE2	2.07	0.54
1:B:95:ASN:ND2	3:B:1223:NAG:C2	2.66	0.54
1:D:36:ARG:HB3	1:D:37:ARG:HB2	1.90	0.53
1:D:25:LEU:HD12	1:D:95:ASN:HA	1.90	0.53
1:A:36:ARG:HB3	1:A:38:VAL:N	2.23	0.53
1:B:148:VAL:HG23	1:B:156:VAL:HG22	1.91	0.53
1:A:24:PHE:HZ	1:D:219:LEU:HD22	1.73	0.53
1:C:196:HIS:HB3	5:C:2132:HOH:O	2.07	0.53
1:B:144:VAL:HG23	1:B:158:TRP:CZ2	2.44	0.53
1:B:43:GLU:O	1:B:64:HIS:HE1	1.92	0.53
1:D:156:VAL:CG2	1:D:185:VAL:HG13	2.35	0.53
1:A:219:LEU:HD12	1:A:219:LEU:C	2.30	0.52
1:A:143:THR:CG2	5:A:2098:HOH:O	2.42	0.52
1:D:108:LEU:O	1:D:111:THR:HG22	2.10	0.52
1:A:153:HIS:H	1:A:205:ASN:ND2	2.07	0.52
1:D:28:ARG:O	1:D:29:VAL:HG23	2.09	0.52
1:B:31:LEU:HD13	1:B:117:GLU:HB3	1.92	0.52
1:A:35:TRP:HD1	1:A:36:ARG:HB2	1.75	0.51
1:A:36:ARG:CG	1:A:37:ARG:HB2	2.38	0.51
1:D:105:ARG:HG3	1:D:114:THR:HG22	1.92	0.51
1:D:30:THR:HG21	1:D:88:PHE:HD1	1.74	0.51
1:D:115:LYS:HD3	1:D:117[B]:GLU:OE1	2.10	0.50
1:A:81:HIS:HE1	5:A:2056:HOH:O	1.92	0.50
1:D:21:VAL:CG1	1:D:31:LEU:HD23	2.41	0.50
1:B:23:ALA:HB2	1:B:29:VAL:CG2	2.41	0.50
1:D:35:TRP:CH2	1:D:111:THR:HG23	2.45	0.50
1:C:45:GLU:HG2	1:C:64:HIS:CE1	2.47	0.50
1:C:72:TRP:NE1	5:C:2059:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HB3	1:A:37:ARG:C	2.32	0.49
1:A:152:PRO:HD2	1:A:205:ASN:HD21	1.77	0.49
1:B:29:VAL:HG23	5:B:2003:HOH:O	2.10	0.49
1:B:130[B]:HIS:CE1	1:C:124:PRO:HB2	2.47	0.49
3:B:1224:NAG:H4	4:B:1225:MAN:C1	2.42	0.49
1:A:29:VAL:HG21	1:A:119:LEU:HD11	1.96	0.48
1:A:101:ASN:ND2	1:A:118:HIS:ND1	2.62	0.48
1:A:155:HIS:CD2	5:A:2115:HOH:O	2.50	0.48
1:B:35:TRP:HD1	1:B:38:VAL:O	1.97	0.48
1:B:87:PHE:CD2	1:B:106:MET:HE3	2.49	0.47
1:A:219:LEU:CD1	1:A:219:LEU:C	2.82	0.47
1:A:156:VAL:CG2	1:A:185:VAL:HG13	2.43	0.47
1:C:158:TRP:CZ3	1:C:199:VAL:HG13	2.50	0.47
1:A:21:VAL:HG13	1:A:31:LEU:CD2	2.45	0.46
1:D:36:ARG:HA	5:D:2018:HOH:O	2.15	0.46
1:C:54:GLY:O	1:C:55:GLU:CB	2.63	0.46
1:C:53:PRO:HB2	1:C:54:GLY:HA3	1.97	0.46
1:C:36[A]:ARG:HG2	5:C:2018:HOH:O	2.15	0.46
1:C:70:ILE:HB	1:C:75:ARG:HD2	1.96	0.46
1:D:43:GLU:OE2	1:D:65:HIS:NE2	2.47	0.46
1:A:23:ALA:CB	1:A:29:VAL:HG23	2.46	0.46
1:A:53:PRO:HB2	1:A:54:GLY:CA	2.46	0.46
1:B:143:THR:HG22	5:B:2098:HOH:O	2.15	0.46
1:D:29:VAL:HG11	1:D:119:LEU:HD13	1.98	0.45
1:A:29:VAL:HG12	1:A:29:VAL:O	2.13	0.45
1:A:103:LEU:CD1	1:A:116:GLN:HG2	2.46	0.45
1:A:54:GLY:O	1:A:55:GLU:HB2	2.17	0.45
1:C:125:LEU:HA	1:C:149:ASN:O	2.17	0.45
1:A:35:TRP:CD1	1:A:36:ARG:HB2	2.51	0.44
1:B:153:HIS:H	1:B:205:ASN:ND2	2.14	0.44
1:A:45:GLU:HG2	1:A:64:HIS:CD2	2.52	0.44
1:C:156:VAL:HG22	1:C:185:VAL:HG13	1.99	0.44
1:C:29:VAL:HG12	5:C:2009:HOH:O	2.18	0.44
1:C:36[B]:ARG:NH1	5:C:2014:HOH:O	2.49	0.44
1:D:175:VAL:HG12	1:D:176:MET:N	2.33	0.44
1:D:36:ARG:CB	5:D:2022:HOH:O	2.65	0.44
1:D:160:MET:N	1:D:161:PRO:HD3	2.33	0.44
1:D:115:LYS:CB	5:D:2013:HOH:O	2.66	0.44
1:C:148:VAL:HG21	1:C:203:GLY:HA3	1.99	0.44
1:A:24:PHE:CZ	1:D:219:LEU:HD22	2.51	0.44
1:D:115:LYS:HB2	5:D:2013:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:VAL:CG2	5:D:2010:HOH:O	2.60	0.43
1:B:91:VAL:O	1:B:91:VAL:HG13	2.18	0.43
1:B:145:THR:CG2	5:B:2099:HOH:O	2.66	0.43
1:D:70:ILE:HB	1:D:75:ARG:HD2	1.99	0.43
1:B:160:MET:SD	1:B:196:HIS:ND1	2.91	0.43
1:B:103:LEU:HD11	1:B:114:THR:HG22	1.99	0.43
1:A:115:LYS:HE2	1:A:117:GLU:HG2	1.99	0.43
1:A:125:LEU:HA	1:A:149:ASN:O	2.18	0.43
1:D:28:ARG:C	1:D:29:VAL:HG23	2.39	0.43
3:D:1224:NAG:O4	4:D:1225:MAN:C2	2.64	0.43
1:C:153:HIS:H	1:C:205:ASN:ND2	2.16	0.43
1:B:129:VAL:HG11	1:B:212:GLY:HA3	2.01	0.43
1:B:34:TYR:C	1:B:106:MET:HE3	2.39	0.43
1:A:196:HIS:HB2	5:A:2113:HOH:O	2.19	0.43
1:B:148:VAL:HG21	1:B:203:GLY:HA3	2.00	0.42
1:A:151:PHE:CD1	1:A:152:PRO:HA	2.54	0.42
1:B:124:PRO:HB2	1:C:130[B]:HIS:CE1	2.55	0.42
1:A:196:HIS:CG	5:A:2113:HOH:O	2.72	0.42
1:C:37:ARG:HD2	1:C:40:LEU:HG	2.01	0.41
1:B:35:TRP:CG	1:B:36:ARG:HB3	2.56	0.41
1:A:35:TRP:HE1	1:A:36:ARG:NH2	2.18	0.41
1:A:125:LEU:HD12	1:A:125:LEU:C	2.41	0.41
1:D:29:VAL:HB	1:D:91:VAL:HG12	2.02	0.41
1:A:161:PRO:HD2	1:A:196:HIS:ND1	2.34	0.41
1:D:21:VAL:CG1	1:D:31:LEU:CD2	2.95	0.41
1:A:52:GLY:O	1:A:53:PRO:C	2.58	0.41
1:D:203:GLY:O	1:D:209:GLU:HA	2.21	0.41
1:B:21:VAL:N	1:B:118:HIS:O	2.53	0.41
1:D:146:CYS:HB2	1:D:158:TRP:CZ2	2.55	0.41
1:B:179:LYS:HD2	1:B:179:LYS:O	2.21	0.41
1:C:189:LEU:CD2	1:C:199:VAL:HG21	2.51	0.41
1:C:204:LYS:HB3	1:C:204:LYS:HE2	1.77	0.41
1:D:25:LEU:CD1	1:D:95:ASN:HA	2.50	0.41
1:B:152:PRO:HD2	1:B:205:ASN:HD21	1.84	0.41
1:C:140:SER:HB2	1:C:193:LYS:HD2	2.03	0.41
1:C:103:LEU:HG	1:C:114:THR:CG2	2.51	0.40
1:B:78:PHE:HA	1:B:90:VAL:O	2.21	0.40
1:B:35:TRP:CD2	1:B:36:ARG:CB	3.05	0.40
1:A:40:LEU:HD12	1:A:108:LEU:CD1	2.47	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	186/201 (92%)	174 (94%)	8 (4%)	4 (2%)	8 6
1	B	184/201 (92%)	173 (94%)	7 (4%)	4 (2%)	8 6
1	C	185/201 (92%)	177 (96%)	6 (3%)	2 (1%)	17 18
1	D	184/201 (92%)	175 (95%)	7 (4%)	2 (1%)	17 18
All	All	739/804 (92%)	699 (95%)	28 (4%)	12 (2%)	12 11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	PRO
1	A	198	PRO
1	B	39	SER
1	B	195	TRP
1	C	53	PRO
1	D	36	ARG
1	A	36	ARG
1	B	36	ARG
1	B	41	GLY
1	D	38	VAL
1	A	41	GLY
1	C	41	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/176 (96%)	154 (91%)	15 (9%)	12 14
1	B	169/176 (96%)	151 (89%)	18 (11%)	8 9
1	C	170/176 (97%)	156 (92%)	14 (8%)	14 17
1	D	169/176 (96%)	149 (88%)	20 (12%)	6 7
All	All	677/704 (96%)	610 (90%)	67 (10%)	10 11

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	75	ARG
1	A	91	VAL
1	A	111	THR
1	A	116	GLN
1	A	129	VAL
1	A	142	LEU
1	A	143	THR
1	A	156	VAL
1	A	176	MET
1	A	179	LYS
1	A	183	LEU
1	A	197	LEU
1	A	200	THR
1	A	219	LEU
1	B	29	VAL
1	B	36	ARG
1	B	72	TRP
1	B	83	SER
1	B	90	VAL
1	B	108	LEU
1	B	111	THR
1	B	115	LYS
1	B	117	GLU
1	B	142	LEU
1	B	145	THR
1	B	160	MET
1	B	178	GLU
1	B	179	LYS
1	B	180	ASP
1	B	197	LEU
1	B	219	LEU
1	B	220	SER

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Mol	Chain	Res	Type
1	C	29	VAL
1	C	37	ARG
1	C	72	TRP
1	C	91	VAL
1	C	103	LEU
1	C	108	LEU
1	C	111	THR
1	C	115	LYS
1	C	117	GLU
1	C	142	LEU
1	C	156	VAL
1	C	200	THR
1	C	219	LEU
1	C	220	SER
1	D	21	VAL
1	D	36	ARG
1	D	37	ARG
1	D	45	GLU
1	D	47	SER
1	D	90	VAL
1	D	108	LEU
1	D	111	THR
1	D	112	GLU
1	D	115	LYS
1	D	117[A]	GLU
1	D	117[B]	GLU
1	D	142	LEU
1	D	160	MET
1	D	177	LYS
1	D	178	GLU
1	D	179	LYS
1	D	183	LEU
1	D	197	LEU
1	D	219	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	81	HIS
1	A	101	ASN
1	A	135	GLN

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Mol	Chain	Res	Type
1	A	155	HIS
1	A	157	GLN
1	A	205	ASN
1	B	64	HIS
1	B	155	HIS
1	B	205	ASN
1	C	155	HIS
1	C	205	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

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	1223	1,3	14,14,15	0.67	0	15,19,21	1.60	3 (20%)
3	NAG	A	1224	3,4	14,14,15	1.03	2 (14%)	15,19,21	1.71	5 (33%)
3	NAG	B	1223	1,3	14,14,15	0.74	0	15,19,21	1.14	1 (6%)
3	NAG	B	1224	3,4	14,14,15	0.77	0	15,19,21	1.90	4 (26%)
3	NAG	C	1224	1,3	14,14,15	0.71	0	15,19,21	1.39	2 (13%)
3	NAG	C	1225	3,4	14,14,15	0.96	1 (7%)	15,19,21	1.43	2 (13%)
3	NAG	D	1223	1,3	14,14,15	0.75	0	15,19,21	2.24	3 (20%)
3	NAG	D	1224	3,4	14,14,15	0.91	0	15,19,21	1.26	1 (6%)

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	1223	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1224	3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	1223	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1224	3,4	-	0/6/23/26	0/1/1/1
3	NAG	C	1224	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	1225	3,4	-	0/6/23/26	0/1/1/1
3	NAG	D	1223	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1224	3,4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1225	NAG	O5-C1	-2.25	1.40	1.43
3	A	1224	NAG	O5-C1	-2.14	1.40	1.43
3	A	1224	NAG	O4-C4	-2.06	1.38	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1223	NAG	C4-C3-C2	-6.95	100.42	111.23
3	B	1224	NAG	C2-N2-C7	-4.28	117.54	123.04
3	B	1224	NAG	C1-O5-C5	-4.10	107.04	112.25
3	C	1225	NAG	C4-C3-C2	-3.72	105.44	111.23
3	A	1224	NAG	O4-C4-C5	-3.55	99.84	109.24
3	A	1223	NAG	C6-C5-C4	-3.44	104.53	113.02
3	C	1224	NAG	C6-C5-C4	-2.66	106.46	113.02
3	C	1225	NAG	C2-N2-C7	-2.63	119.66	123.04
3	B	1223	NAG	C4-C3-C2	-2.55	107.27	111.23
3	D	1224	NAG	O6-C6-C5	-2.48	103.12	111.33
3	A	1224	NAG	C4-C3-C2	-2.23	107.77	111.23
3	A	1224	NAG	O4-C4-C3	-2.02	105.78	110.34
3	C	1224	NAG	C1-O5-C5	2.08	114.89	112.25
3	A	1223	NAG	O5-C5-C6	2.11	111.92	107.35
3	B	1224	NAG	C8-C7-N2	2.15	120.22	116.11
3	A	1223	NAG	C3-C4-C5	2.41	114.40	110.20
3	B	1224	NAG	C3-C4-C5	2.43	114.44	110.20
3	D	1223	NAG	C3-C4-C5	2.73	114.96	110.20
3	A	1224	NAG	C3-C4-C5	2.80	115.07	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1224	NAG	O5-C5-C6	2.94	113.70	107.35
3	D	1223	NAG	C3-C2-N2	3.69	119.39	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1224	NAG	2	0
3	B	1223	NAG	3	0
3	B	1224	NAG	3	0
3	C	1225	NAG	1	0
3	D	1224	NAG	2	0

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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	MAN	A	1225	3	11,11,12	0.86	0	14,15,17	1.90	3 (21%)
4	MAN	B	1225	3	11,11,12	0.91	1 (9%)	14,15,17	1.89	4 (28%)
4	MAN	C	1226	3	11,11,12	0.93	0	14,15,17	2.03	5 (35%)
4	MAN	D	1225	3	11,11,12	1.12	1 (9%)	14,15,17	1.85	4 (28%)

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	MAN	A	1225	3	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	1225	3	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	C	1226	3	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	D	1225	3	1/1/4/5	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)
4	B	1225	MAN	O5-C1	-2.21	1.40	1.43
4	D	1225	MAN	O5-C1	-2.08	1.40	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1225	MAN	O4-C4-C3	-4.16	100.96	110.34
4	C	1226	MAN	C1-O5-C5	-3.86	107.36	112.25
4	C	1226	MAN	C1-C2-C3	-3.30	105.63	109.54
4	D	1225	MAN	C1-C2-C3	-3.20	105.76	109.54
4	B	1225	MAN	O5-C1-C2	-2.74	106.42	110.86
4	C	1226	MAN	O4-C4-C3	-2.45	104.82	110.34
4	D	1225	MAN	O5-C1-C2	-2.34	107.06	110.86
4	B	1225	MAN	O4-C4-C3	-2.19	105.42	110.34
4	B	1225	MAN	C2-C3-C4	2.03	114.49	111.04
4	C	1226	MAN	O3-C3-C4	2.37	115.67	110.34
4	A	1225	MAN	C6-C5-C4	2.44	119.02	113.02
4	C	1226	MAN	C3-C4-C5	2.67	114.84	110.20
4	D	1225	MAN	O3-C3-C4	2.95	116.98	110.34
4	D	1225	MAN	C3-C4-C5	3.90	116.99	110.20
4	A	1225	MAN	O5-C1-C2	4.24	117.73	110.86
4	B	1225	MAN	C3-C4-C5	4.81	118.57	110.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1225	MAN	C1
4	D	1225	MAN	C1
4	C	1226	MAN	C1
4	A	1225	MAN	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1225	MAN	2	0
4	B	1225	MAN	3	0
4	C	1226	MAN	1	0
4	D	1225	MAN	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

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^{th} 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^2)	Q<0.9
1	A	188/201 (93%)	0.32	14 (7%)	17	25	20, 28, 40, 52	0
1	B	186/201 (92%)	0.24	13 (6%)	19	27	20, 29, 39, 51	0
1	C	186/201 (92%)	0.05	8 (4%)	39	48	21, 29, 38, 47	0
1	D	186/201 (92%)	0.27	16 (8%)	13	18	19, 29, 39, 52	0
All	All	746/804 (92%)	0.22	51 (6%)	20	28	19, 29, 40, 52	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	PRO	4.9
1	C	220	SER	4.8
1	B	127	LEU	4.5
1	A	174	GLY	4.5
1	A	127	LEU	4.3
1	D	37	ARG	4.1
1	A	90	VAL	3.8
1	A	129	VAL	3.8
1	A	173	GLY	3.7
1	A	161	PRO	3.7
1	B	37	ARG	3.7
1	D	129	VAL	3.6
1	D	36	ARG	3.5
1	D	127	LEU	3.3
1	A	80	ILE	3.3
1	D	193	LYS	3.2
1	D	161	PRO	3.1
1	D	175	VAL	3.1
1	D	38	VAL	3.0
1	B	129	VAL	2.9
1	D	194	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	196	HIS	2.8
1	B	179	LYS	2.8
1	A	89	LEU	2.7
1	C	127	LEU	2.7
1	B	128	SER	2.7
1	C	54	GLY	2.7
1	B	175	VAL	2.6
1	C	179	LYS	2.6
1	B	130[A]	HIS	2.5
1	D	111	THR	2.5
1	D	90	VAL	2.5
1	B	38	VAL	2.4
1	A	91	VAL	2.4
1	A	53	PRO	2.4
1	C	53	PRO	2.4
1	B	53	PRO	2.3
1	C	194	PRO	2.3
1	A	194	PRO	2.3
1	B	36	ARG	2.3
1	D	80	ILE	2.3
1	D	212	GLY	2.2
1	A	37	ARG	2.2
1	C	125	LEU	2.2
1	A	128	SER	2.2
1	B	207	LYS	2.1
1	C	175	VAL	2.1
1	D	179	LYS	2.1
1	D	110	GLU	2.1
1	A	126	THR	2.0
1	D	210	ALA	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
3	NAG	D	1223	14/15	0.95	0.14	0.44	24,30,39,40	0
3	NAG	B	1223	14/15	0.98	0.14	-0.17	24,27,34,35	0
3	NAG	A	1223	14/15	0.97	0.12	-0.43	21,27,35,36	0
3	NAG	C	1224	14/15	0.97	0.10	-0.49	22,30,38,40	0
3	NAG	D	1224	14/15	0.93	0.18	-	26,34,40,41	0
3	NAG	C	1225	14/15	0.97	0.16	-	25,35,39,40	0
3	NAG	A	1224	14/15	0.95	0.23	-	29,32,38,43	0
3	NAG	B	1224	14/15	0.95	0.22	-	28,35,41,42	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
2	PT	A	1221	1/1	0.99	0.03	-	40,40,40,40	1
2	PT	C	1221	1/1	0.97	0.03	-	38,38,38,38	1
2	PT	B	1226	1/1	0.96	0.16	-	31,31,31,31	1
2	PT	C	1222	1/1	0.99	0.03	-	32,32,32,32	1
2	PT	D	1222	1/1	0.96	0.11	-	41,41,41,41	1
2	PT	A	1222	1/1	0.73	0.23	-	45,45,45,45	1
2	PT	B	1222	1/1	0.99	0.02	-	44,44,44,44	1
4	MAN	B	1225	11/12	0.88	0.34	-	47,52,57,59	0
4	MAN	D	1225	11/12	0.83	0.36	-	53,57,58,59	0
2	PT	B	1221	1/1	0.99	0.02	-	44,44,44,44	1
2	PT	C	1223	1/1	0.96	0.41	-	32,32,32,32	1
4	MAN	C	1226	11/12	0.83	0.36	-	59,63,66,66	0
2	PT	D	1220	1/1	0.99	0.03	-	44,44,44,44	1
2	PT	A	1220	1/1	0.96	0.06	-	41,41,41,41	1
2	PT	D	1221	1/1	0.99	0.03	-	36,36,36,36	1
4	MAN	A	1225	11/12	0.88	0.41	-	52,54,56,57	0

6.5 Other polymers

There are no such residues in this entry.