Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:01 AM GMT

PDB ID	:	2P34
Title	:	Crystal structure of a lectin from Canavalia maritima seeds (CML) in complex with man1-4man-OMe
Authors	:	Moreno, F.B.M.B.; Bezerra, G.A.; Oliveira, T.M.; Souza, E.P.; Rocha, B.A.M.; Benevides, R.G.; Delatorre, P.; Cavada, B.S.; de Azevedo Jr., W.
Deposited on	:	2007-03-08
Resolution	:	2.10 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
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:

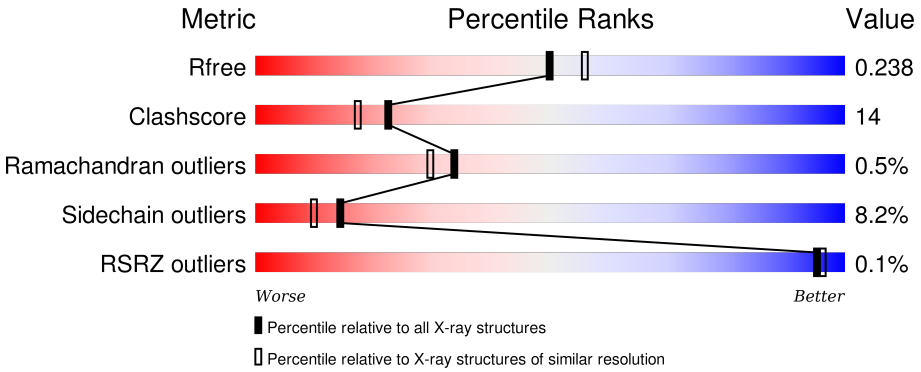
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	237	78% 17%
1	B	237	70% 22% 5%
1	C	237	65% 30%
1	D	237	68% 27%

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
2	MMA	O	2	X	-	-	X
2	MMA	P	2	X	-	-	-
2	MMA	Q	2	X	-	-	-
2	MMA	R	2	X	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7655 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 Lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1775	1120	297	357	1			
1	B	234	Total	C	N	O	S	0	0	0
			1778	1122	297	358	1			
1	C	234	Total	C	N	O	S	0	0	0
			1775	1120	297	357	1			
1	D	234	Total	C	N	O	S	0	0	0
			1778	1122	297	358	1			

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	2	Total	C	O	0	0
			24	13	11		
2	P	2	Total	C	O	0	0
			24	13	11		
2	Q	2	Total	C	O	0	0
			24	13	11		
2	R	2	Total	C	O	0	0
			24	13	11		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is water.

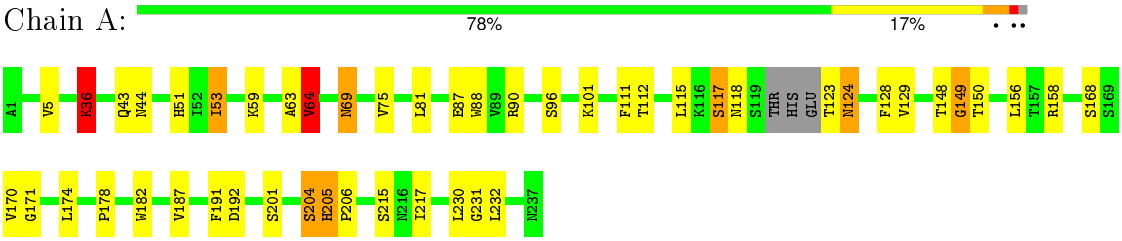
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	132	Total O 132 132	0	0
5	B	131	Total O 131 131	0	0
5	C	91	Total O 91 91	0	0
5	D	87	Total O 87 87	0	0
5	P	2	Total O 2 2	0	0
5	Q	2	Total O 2 2	0	0

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.

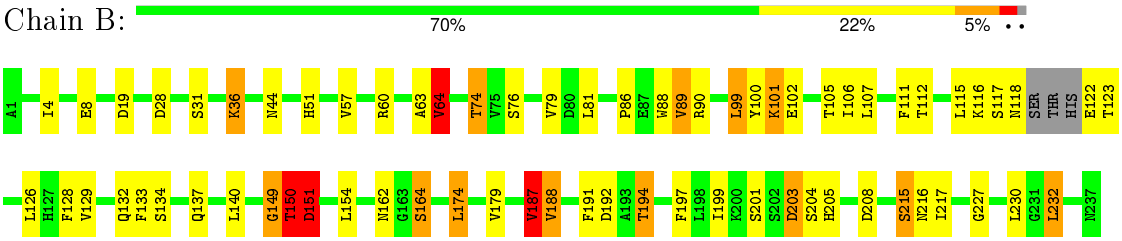
- Molecule 1: Lectin

Chain A:



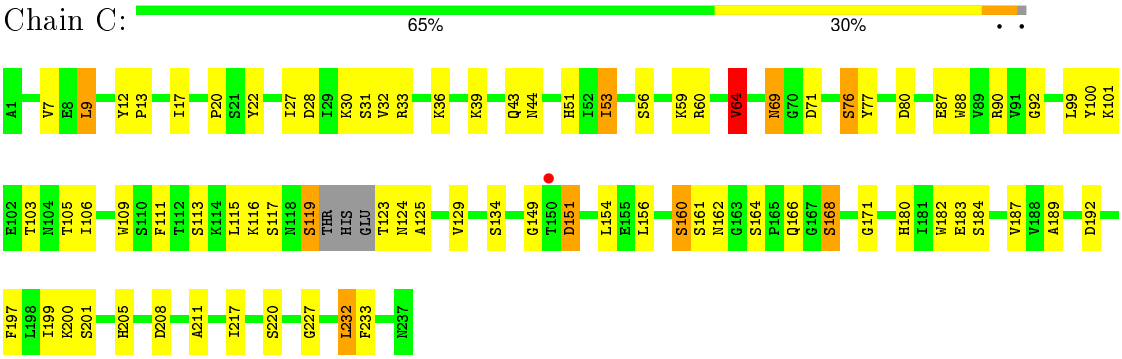
- Molecule 1: Lectin

Chain B:



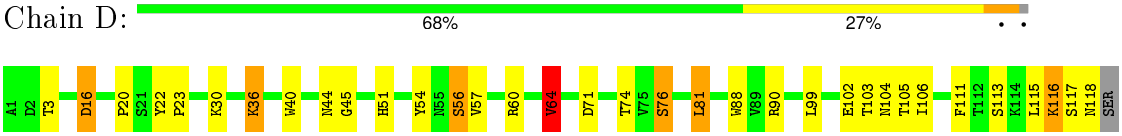
- Molecule 1: Lectin

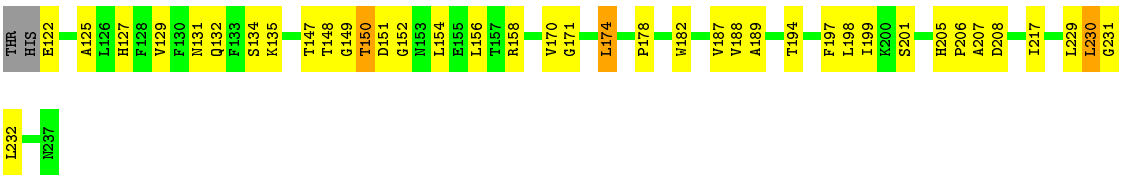
Chain C:



- Molecule 1: Lectin

Chain D:




THR
HIS
E122
A125
L126
H127
F128
V129
F130
N131
Q132
F133
S134
K135
T147
T148
G149
T150
D151
G152
N153
L154
E155
L156
T157
R158
V170
G171
L174
P178
W182
V187
V188
A189
T194
F197
L198
I199
K200
S201
H205
P206
A207
D208
I217
L229
L230
G231
L232
N237

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	69.45Å 69.45Å 161.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.52 – 2.10 33.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (33.52-2.10) 96.5 (33.52-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.239 0.174 , 0.238	Depositor DCC
R_{free} test set	2489 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 21.1	EDS
Estimated twinning fraction	0.024 for -h,-k,l 0.488 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 49047 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7655	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: CA, MN, MMA, 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	1.00	2/1814 (0.1%)	1.01	2/2469 (0.1%)
1	B	1.04	6/1817 (0.3%)	1.06	8/2473 (0.3%)
1	C	0.97	1/1815 (0.1%)	1.09	5/2472 (0.2%)
1	D	0.90	2/1817 (0.1%)	1.02	9/2473 (0.4%)
All	All	0.98	11/7263 (0.2%)	1.05	24/9887 (0.2%)

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	1
1	B	0	3
1	D	0	2
2	O	1	0
2	P	1	0
2	Q	1	0
2	R	1	0
All	All	4	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	SER	C-N	18.32	1.76	1.34
1	D	36	LYS	CE-NZ	8.87	1.71	1.49
1	B	203	ASP	CB-CG	6.89	1.66	1.51
1	D	36	LYS	CD-CE	6.61	1.67	1.51
1	B	129	VAL	CB-CG2	-5.74	1.40	1.52
1	A	36	LYS	CE-NZ	5.47	1.62	1.49
1	A	36	LYS	CD-CE	5.15	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	LYS	CE-NZ	5.14	1.61	1.49
1	B	89	VAL	CB-CG1	5.11	1.63	1.52
1	B	79	VAL	CB-CG1	5.09	1.63	1.52
1	B	187	VAL	CB-CG1	-5.02	1.42	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	119	SER	O-C-N	-22.28	87.06	122.70
1	C	119	SER	CA-C-N	15.40	151.08	117.20
1	C	119	SER	C-N-CA	10.43	147.79	121.70
1	D	229	LEU	C-N-CA	10.11	146.98	121.70
1	D	230	LEU	N-CA-C	-9.34	85.79	111.00
1	D	36	LYS	CD-CE-NZ	8.79	131.91	111.70
1	B	151	ASP	N-CA-CB	-8.57	95.17	110.60
1	A	64	VAL	CB-CA-C	-8.13	95.95	111.40
1	B	203	ASP	CB-CG-OD2	7.94	125.45	118.30
1	D	229	LEU	O-C-N	-7.72	110.35	122.70
1	B	64	VAL	CB-CA-C	-7.50	97.15	111.40
1	D	64	VAL	CG1-CB-CG2	6.99	122.09	110.90
1	D	64	VAL	CB-CA-C	-6.90	98.30	111.40
1	B	174	LEU	CA-CB-CG	6.88	131.12	115.30
1	D	229	LEU	CA-C-N	6.78	132.11	117.20
1	C	64	VAL	CB-CA-C	-6.42	99.21	111.40
1	B	19	ASP	CB-CG-OD1	5.90	123.61	118.30
1	D	174	LEU	CA-CB-CG	5.83	128.71	115.30
1	D	229	LEU	N-CA-C	5.70	126.40	111.00
1	B	232	LEU	CA-CB-CG	5.59	128.15	115.30
1	C	64	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	A	205	HIS	N-CA-CB	-5.24	101.17	110.60
1	B	151	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	116	LYS	C-N-CA	5.02	134.25	121.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	O	2	MMA	C1
2	P	2	MMA	C1
2	Q	2	MMA	C1
2	R	2	MMA	C1

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	SER	Peptide
1	B	149	GLY	Peptide
1	B	150	THR	Peptide
1	B	187	VAL	Peptide
1	D	116	LYS	Peptide
1	D	148	THR	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	1775	0	1727	36	0
1	B	1778	0	1728	54	0
1	C	1775	0	1727	54	0
1	D	1778	0	1727	60	0
2	O	24	0	23	1	0
2	P	24	0	23	0	0
2	Q	24	0	23	0	0
2	R	24	0	23	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	132	0	0	6	0
5	B	131	0	0	7	0
5	C	91	0	0	3	0
5	D	87	0	0	5	0
5	P	2	0	0	0	0
5	Q	2	0	0	0	0
All	All	7655	0	7001	195	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 14.

All (195) 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:D:36:LYS:NZ	1:D:36:LYS:CE	1.71	1.51
1:C:119:SER:C	1:C:123:THR:N	1.76	1.37
1:D:150:THR:HA	1:D:152:GLY:H	1.00	1.09
1:D:117:SER:HB3	1:D:118:ASN:CA	1.82	1.08
1:D:117:SER:CB	1:D:118:ASN:HA	1.78	1.06
1:B:117:SER:HB3	1:B:118:ASN:HA	1.08	1.05
1:B:117:SER:CB	1:B:118:ASN:HA	1.92	0.99
1:C:36:LYS:NZ	5:C:252:HOH:O	1.97	0.98
1:A:158:ARG:HG3	5:A:327:HOH:O	1.68	0.94
1:A:44:ASN:HD21	1:A:201:SER:H	1.11	0.94
1:D:150:THR:HA	1:D:152:GLY:N	1.85	0.92
1:C:44:ASN:HD21	1:C:201:SER:H	0.98	0.91
1:D:64:VAL:HG13	1:D:74:THR:HG22	1.51	0.91
1:A:53:ILE:CD1	5:A:266:HOH:O	2.19	0.90
1:B:74:THR:CG2	5:B:315:HOH:O	2.20	0.90
1:D:44:ASN:HD21	1:D:201:SER:H	1.20	0.90
1:C:44:ASN:ND2	1:C:201:SER:H	1.73	0.87
1:B:44:ASN:HD21	1:B:201:SER:H	1.22	0.85
1:D:117:SER:HB3	1:D:118:ASN:HA	0.90	0.84
1:C:119:SER:O	1:C:123:THR:N	2.11	0.84
1:A:205:HIS:HD2	1:A:206:PRO:O	1.60	0.84
1:D:36:LYS:HE3	5:D:324:HOH:O	1.78	0.83
1:B:74:THR:HG22	5:B:315:HOH:O	1.74	0.83
1:B:203:ASP:C	1:B:205:HIS:H	1.79	0.83
1:A:53:ILE:HD12	5:A:266:HOH:O	1.76	0.81
1:D:150:THR:HB	1:D:151:ASP:HA	1.63	0.81
1:D:150:THR:CA	1:D:152:GLY:H	1.89	0.80
1:D:99:LEU:HD12	2:O:2:MMA:H4	1.64	0.79
1:B:117:SER:HB3	1:B:118:ASN:CA	2.03	0.78
1:A:59:LYS:CE	5:A:356:HOH:O	2.31	0.78
1:A:59:LYS:HE3	5:A:356:HOH:O	1.86	0.74
1:B:194:THR:CG2	5:B:289:HOH:O	2.34	0.74
1:B:118:ASN:ND2	5:B:360:HOH:O	2.17	0.74
1:C:44:ASN:HD21	1:C:201:SER:N	1.80	0.74
1:B:137:GLN:HG2	1:B:140:LEU:HD12	1.69	0.72
1:B:122:GLU:OE2	1:B:123:THR:OG1	2.08	0.71
1:A:148:THR:O	1:A:149:GLY:O	2.08	0.70
1:D:36:LYS:HD3	1:D:76:SER:O	1.91	0.70
1:B:57:VAL:HG23	1:B:188:VAL:HG13	1.74	0.69
1:C:156:LEU:O	1:C:171:GLY:HA3	1.92	0.68
1:C:53:ILE:C	1:C:53:ILE:HD13	2.14	0.67
1:D:36:LYS:CE	5:D:324:HOH:O	2.37	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:HB3	1:A:217:ILE:HD11	1.75	0.67
1:B:149:GLY:HA3	1:B:150:THR:C	2.15	0.66
1:A:44:ASN:HD21	1:A:201:SER:N	1.89	0.66
1:C:88:TRP:HB3	1:C:217:ILE:HD11	1.77	0.66
1:D:135:LYS:HD2	1:D:149:GLY:O	1.96	0.66
1:D:150:THR:CB	1:D:151:ASP:HA	2.26	0.66
1:D:116:LYS:HG3	1:D:188:VAL:HB	1.79	0.65
1:C:160:SER:O	1:C:162:ASN:N	2.29	0.65
1:B:88:TRP:HB3	1:B:217:ILE:HD11	1.78	0.64
1:B:44:ASN:HD21	1:B:201:SER:N	1.96	0.64
1:D:44:ASN:ND2	1:D:201:SER:H	1.92	0.64
1:B:203:ASP:C	1:B:205:HIS:N	2.50	0.64
1:B:194:THR:HG22	5:B:289:HOH:O	1.98	0.63
1:A:117:SER:HA	1:A:187:VAL:HG22	1.81	0.63
1:B:51:HIS:HE1	5:D:259:HOH:O	1.81	0.62
1:C:149:GLY:O	1:C:151:ASP:OD2	2.16	0.62
1:A:43:GLN:HE22	1:A:69:ASN:HD21	1.45	0.62
1:D:60:ARG:HD3	1:D:76:SER:OG	2.02	0.60
1:D:88:TRP:HB3	1:D:217:ILE:HD11	1.83	0.59
1:D:51:HIS:HB2	1:D:64:VAL:HG23	1.83	0.59
1:A:115:LEU:O	1:A:123:THR:HA	2.03	0.59
1:B:36:LYS:HE3	5:B:334:HOH:O	2.03	0.58
1:A:178:PRO:HB3	1:A:217:ILE:CD1	2.32	0.58
1:B:60:ARG:HH11	1:D:60:ARG:NH1	2.01	0.58
1:C:60:ARG:HD3	1:C:76:SER:OG	2.04	0.58
1:A:124:ASN:HD21	1:B:132:GLN:H	1.52	0.56
1:C:111:PHE:CE2	1:C:113:SER:HB2	2.40	0.56
1:D:64:VAL:HG13	1:D:74:THR:CG2	2.32	0.56
1:C:7:VAL:HG22	1:C:27:ILE:CD1	2.34	0.56
1:A:51:HIS:HB2	1:A:64:VAL:HG23	1.88	0.56
1:A:90:ARG:NH1	1:A:217:ILE:CG2	2.68	0.56
1:C:90:ARG:NH1	1:C:217:ILE:HG23	2.21	0.56
1:B:162:ASN:OD1	1:B:164:SER:HB2	2.07	0.55
1:C:43:GLN:HE22	1:C:69:ASN:HD21	1.54	0.55
1:C:92:GLY:HA2	1:C:109:TRP:CH2	2.42	0.54
1:B:149:GLY:CA	1:B:150:THR:C	2.75	0.54
1:D:88:TRP:HB3	1:D:217:ILE:CD1	2.37	0.54
1:A:36:LYS:HD2	1:A:75:VAL:HG23	1.88	0.54
1:B:99:LEU:HD13	1:B:100:TYR:CZ	2.42	0.54
1:C:115:LEU:HD21	1:C:182:TRP:HA	1.91	0.53
1:A:112:THR:O	1:A:191:PHE:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TYR:CE1	1:D:81:LEU:HD22	2.45	0.52
1:C:124:ASN:ND2	1:D:131:ASN:H	2.08	0.52
1:A:148:THR:C	1:A:149:GLY:O	2.47	0.52
1:C:106:ILE:HB	1:C:154:LEU:HB3	1.90	0.52
1:D:205:HIS:HD2	1:D:206:PRO:O	1.92	0.52
1:C:111:PHE:CZ	1:C:113:SER:HB2	2.45	0.52
1:C:51:HIS:HB2	1:C:64:VAL:HG23	1.91	0.52
1:B:57:VAL:HG21	1:D:64:VAL:HG22	1.90	0.52
1:B:4:ILE:HD13	1:B:215:SER:OG	2.10	0.51
1:B:150:THR:OG1	1:B:151:ASP:HA	2.10	0.51
1:B:28:ASP:HB3	1:B:31:SER:O	2.10	0.51
1:C:22:TYR:CD2	1:C:39:LYS:HE2	2.44	0.51
1:C:43:GLN:HE22	1:C:69:ASN:ND2	2.08	0.51
1:C:232:LEU:HB3	1:C:233:PHE:CD2	2.46	0.51
1:D:170:VAL:HG21	1:D:231:GLY:HA2	1.93	0.51
1:B:115:LEU:O	1:B:123:THR:HA	2.11	0.51
1:C:99:LEU:HD22	2:R:2:MMA:H4	1.93	0.51
1:B:60:ARG:HH21	1:B:76:SER:CB	2.24	0.50
1:A:5:VAL:HG21	1:A:81:LEU:HD22	1.93	0.50
1:B:133:PHE:HA	1:B:137:GLN:HE22	1.75	0.50
1:A:96:SER:OG	1:A:230:LEU:HA	2.10	0.50
1:B:194:THR:HG23	5:B:289:HOH:O	2.06	0.50
1:D:54:TYR:CD1	1:D:81:LEU:HD22	2.46	0.50
1:D:90:ARG:NH1	1:D:217:ILE:HG23	2.26	0.50
1:A:156:LEU:O	1:A:171:GLY:HA3	2.12	0.50
1:C:119:SER:HB3	1:D:131:ASN:HB3	1.93	0.50
1:D:116:LYS:O	1:D:187:VAL:N	2.45	0.49
1:C:99:LEU:CD2	2:R:2:MMA:H4	2.42	0.49
1:C:100:TYR:HB3	1:C:205:HIS:O	2.12	0.49
1:A:205:HIS:CD2	1:A:206:PRO:HD2	2.47	0.49
1:B:90:ARG:NH1	1:B:217:ILE:CG2	2.75	0.49
1:A:90:ARG:NH1	1:A:217:ILE:HG22	2.28	0.48
1:D:149:GLY:HA2	1:D:150:THR:O	2.12	0.48
1:C:20:PRO:HB2	1:C:22:TYR:CZ	2.48	0.48
1:A:205:HIS:CD2	1:A:206:PRO:O	2.51	0.48
1:B:126:LEU:CD2	1:B:179:VAL:HG22	2.44	0.48
1:D:105:THR:O	1:D:197:PHE:HA	2.13	0.48
1:B:203:ASP:O	1:B:205:HIS:N	2.47	0.47
1:C:87:GLU:HG3	1:C:180:HIS:CD2	2.50	0.47
1:B:111:PHE:HB3	1:B:128:PHE:CZ	2.50	0.47
1:C:36:LYS:HE3	1:C:76:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:THR:O	1:B:197:PHE:HA	2.15	0.47
1:B:117:SER:H	1:B:187:VAL:HG12	1.79	0.46
1:C:125:ALA:HB3	1:D:129:VAL:HG12	1.97	0.46
1:B:90:ARG:NH1	1:B:217:ILE:HG23	2.31	0.46
1:D:56:SER:CB	1:D:189:ALA:H	2.29	0.46
1:D:115:LEU:HD21	1:D:182:TRP:HA	1.97	0.45
1:D:156:LEU:O	1:D:171:GLY:HA3	2.15	0.45
1:B:122:GLU:CD	1:B:123:THR:HG1	2.19	0.45
1:A:51:HIS:O	1:A:63:ALA:HA	2.17	0.45
1:C:105:THR:O	1:C:197:PHE:HA	2.16	0.45
1:D:102:GLU:OE2	1:D:104:ASN:OD1	2.35	0.45
1:A:90:ARG:NH1	1:A:217:ILE:HG23	2.32	0.45
1:C:36:LYS:HG3	1:C:77:TYR:HD1	1.82	0.45
1:B:64:VAL:HG22	1:D:57:VAL:CG1	2.47	0.44
1:D:106:ILE:HB	1:D:154:LEU:HB3	1.99	0.44
1:C:69:ASN:HD21	1:C:71:ASP:HB2	1.81	0.44
1:B:111:PHE:HB3	1:B:128:PHE:CE2	2.53	0.44
1:C:56:SER:HB2	1:C:189:ALA:O	2.17	0.44
1:D:20:PRO:HB2	1:D:22:TYR:CZ	2.52	0.44
1:A:201:SER:HB2	1:A:206:PRO:HB3	2.00	0.44
1:A:87:GLU:HG3	1:A:182:TRP:O	2.18	0.44
1:C:17:ILE:O	1:C:33:ARG:HG2	2.17	0.44
1:A:124:ASN:N	1:A:124:ASN:HD22	2.15	0.44
1:C:44:ASN:ND2	1:C:200:LYS:HA	2.33	0.44
1:D:103:THR:O	1:D:199:ILE:HA	2.18	0.43
1:C:7:VAL:O	1:C:211:ALA:HA	2.18	0.43
1:D:205:HIS:CD2	1:D:206:PRO:HD2	2.54	0.43
1:C:129:VAL:HG12	1:D:125:ALA:HB3	2.01	0.43
1:D:147:THR:HG21	1:D:158:ARG:HH12	1.84	0.43
1:A:59:LYS:HE2	5:A:356:HOH:O	2.09	0.43
1:C:69:ASN:ND2	1:C:71:ASP:H	2.16	0.43
1:B:112:THR:O	1:B:191:PHE:HA	2.19	0.43
1:C:59:LYS:HD3	1:C:80:ASP:HB2	2.00	0.43
1:D:45:GLY:HA2	1:D:198:LEU:HD21	2.01	0.43
1:C:208:ASP:OD2	1:C:227:GLY:HA2	2.19	0.43
1:C:56:SER:CB	1:C:189:ALA:H	2.32	0.43
1:D:16:ASP:HB2	5:D:326:HOH:O	2.17	0.43
1:A:111:PHE:HB3	1:A:128:PHE:CZ	2.53	0.43
1:A:111:PHE:HB3	1:A:128:PHE:CE2	2.54	0.42
1:D:150:THR:HG22	1:D:152:GLY:N	2.34	0.42
1:B:57:VAL:CG2	1:D:64:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:THR:O	1:C:199:ILE:HA	2.18	0.42
1:C:28:ASP:HB3	1:C:31:SER:O	2.19	0.42
1:D:207:ALA:HA	1:D:208:ASP:HA	1.82	0.42
1:B:133:PHE:HA	1:B:137:GLN:NE2	2.35	0.42
1:D:3:THR:HG23	1:D:30:LYS:HD3	2.02	0.42
1:D:23:PRO:HB2	1:D:40:TRP:O	2.19	0.42
1:C:12:TYR:HA	1:C:13:PRO:HD3	1.90	0.42
1:D:117:SER:CB	1:D:118:ASN:CA	2.67	0.42
1:C:9:LEU:CD1	1:C:9:LEU:N	2.83	0.41
1:D:111:PHE:CE2	1:D:113:SER:HB2	2.55	0.41
1:B:102:GLU:HB2	1:B:199:ILE:HG23	2.02	0.41
1:A:170:VAL:HG21	1:A:231:GLY:HA2	2.02	0.41
1:B:8:GLU:OE1	1:B:28:ASP:OD2	2.39	0.41
1:B:86:PRO:HG2	1:B:89:VAL:HG12	2.03	0.41
1:C:205:HIS:HB3	5:C:314:HOH:O	2.19	0.41
1:C:117:SER:HA	1:C:187:VAL:HG12	2.01	0.41
1:B:36:LYS:HE2	1:B:36:LYS:HB2	1.79	0.41
1:B:106:ILE:HB	1:B:154:LEU:HB3	2.02	0.41
1:D:111:PHE:CZ	1:D:113:SER:HB2	2.56	0.41
1:B:208:ASP:OD2	1:B:227:GLY:HA2	2.21	0.41
1:B:60:ARG:HH21	1:B:76:SER:HB3	1.86	0.41
1:B:51:HIS:HB2	1:B:64:VAL:HG23	2.02	0.41
1:C:99:LEU:HA	1:C:99:LEU:HD12	1.86	0.41
1:D:111:PHE:O	1:D:127:HIS:HA	2.21	0.41
1:C:30:LYS:HA	5:C:304:HOH:O	2.20	0.41
1:D:178:PRO:HB3	1:D:217:ILE:HD11	2.03	0.40
1:A:174:LEU:N	1:A:174:LEU:HD12	2.36	0.40
1:B:51:HIS:O	1:B:63:ALA:HA	2.21	0.40
1:D:30:LYS:HA	5:D:245:HOH:O	2.22	0.40
1:C:116:LYS:O	1:C:187:VAL:HG12	2.22	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	230/237 (97%)	220 (96%)	9 (4%)	1 (0%)	39 37
1	B	230/237 (97%)	223 (97%)	6 (3%)	1 (0%)	39 37
1	C	232/237 (98%)	218 (94%)	11 (5%)	3 (1%)	15 9
1	D	230/237 (97%)	218 (95%)	12 (5%)	0	100 100
All	All	922/948 (97%)	879 (95%)	38 (4%)	5 (0%)	34 30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	SER
1	B	204	SER
1	C	151	ASP
1	A	149	GLY
1	C	168	SER

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	199/202 (98%)	184 (92%)	15 (8%)	17 13
1	B	199/202 (98%)	180 (90%)	19 (10%)	11 7
1	C	199/202 (98%)	182 (92%)	17 (8%)	13 9
1	D	199/202 (98%)	185 (93%)	14 (7%)	19 15
All	All	796/808 (98%)	731 (92%)	65 (8%)	14 10

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	53	ILE
1	A	64	VAL

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Mol	Chain	Res	Type
1	A	69	ASN
1	A	101	LYS
1	A	117	SER
1	A	118	ASN
1	A	124	ASN
1	A	129	VAL
1	A	150	THR
1	A	168	SER
1	A	192	ASP
1	A	204	SER
1	A	215	SER
1	A	232	LEU
1	B	36	LYS
1	B	64	VAL
1	B	74	THR
1	B	81	LEU
1	B	99	LEU
1	B	101	LYS
1	B	107	LEU
1	B	134	SER
1	B	150	THR
1	B	151	ASP
1	B	164	SER
1	B	174	LEU
1	B	188	VAL
1	B	192	ASP
1	B	194	THR
1	B	215	SER
1	B	216	ASN
1	B	230	LEU
1	B	232	LEU
1	C	9	LEU
1	C	32	VAL
1	C	53	ILE
1	C	64	VAL
1	C	69	ASN
1	C	76	SER
1	C	101	LYS
1	C	134	SER
1	C	160	SER
1	C	164	SER
1	C	166	GLN

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Mol	Chain	Res	Type
1	C	168	SER
1	C	183	GLU
1	C	184	SER
1	C	192	ASP
1	C	220	SER
1	C	232	LEU
1	D	16	ASP
1	D	56	SER
1	D	64	VAL
1	D	71	ASP
1	D	76	SER
1	D	81	LEU
1	D	122	GLU
1	D	132	GLN
1	D	134	SER
1	D	150	THR
1	D	174	LEU
1	D	194	THR
1	D	230	LEU
1	D	232	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	83	ASN
1	A	104	ASN
1	A	124	ASN
1	A	166	GLN
1	A	205	HIS
1	B	41	ASN
1	B	44	ASN
1	B	51	HIS
1	B	104	ASN
1	B	137	GLN
1	B	166	GLN
1	C	41	ASN
1	C	44	ASN
1	C	69	ASN
1	C	104	ASN
1	C	124	ASN

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Mol	Chain	Res	Type
1	D	44	ASN
1	D	51	HIS
1	D	104	ASN
1	D	132	GLN
1	D	205	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
2	MAN	O	1	2	11,11,12	0.91	1 (9%)	14,15,17	1.19	1 (7%)
2	MMA	O	2	2	13,13,13	0.85	1 (7%)	18,18,18	2.03	4 (22%)
2	MAN	P	1	2	11,11,12	1.37	2 (18%)	14,15,17	1.55	1 (7%)
2	MMA	P	2	2	13,13,13	0.71	0	18,18,18	3.81	8 (44%)
2	MAN	Q	1	2	11,11,12	1.53	2 (18%)	14,15,17	1.67	2 (14%)
2	MMA	Q	2	2	13,13,13	0.97	1 (7%)	18,18,18	4.34	7 (38%)
2	MAN	R	1	2	11,11,12	0.99	1 (9%)	14,15,17	1.43	2 (14%)
2	MMA	R	2	2	13,13,13	0.66	0	18,18,18	2.12	8 (44%)

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	MAN	O	1	2	-	0/2/19/22	0/1/1/1
2	MMA	O	2	2	1/1/5/5	0/4/24/24	0/1/1/1
2	MAN	P	1	2	-	0/2/19/22	0/1/1/1
2	MMA	P	2	2	1/1/5/5	0/4/24/24	0/1/1/1
2	MAN	Q	1	2	-	0/2/19/22	0/1/1/1
2	MMA	Q	2	2	1/1/5/5	0/4/24/24	0/1/1/1
2	MAN	R	1	2	-	0/2/19/22	0/1/1/1
2	MMA	R	2	2	1/1/5/5	0/4/24/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	1	MAN	O5-C1	-3.49	1.37	1.43
2	P	1	MAN	O5-C1	-2.80	1.39	1.43
2	P	1	MAN	O2-C2	-2.31	1.38	1.43
2	Q	2	MMA	O3-C3	-2.28	1.37	1.43
2	O	2	MMA	O1-C1	2.07	1.43	1.40
2	O	1	MAN	C2-C3	2.48	1.55	1.52
2	Q	1	MAN	C2-C3	2.57	1.56	1.52
2	R	1	MAN	C2-C3	2.84	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	2	MMA	C1-C2-C3	-8.77	92.68	109.97
2	Q	2	MMA	C1-C2-C3	-7.98	94.25	109.97
2	P	2	MMA	C1-O5-C5	-7.24	99.70	113.75
2	Q	2	MMA	C1-O5-C5	-6.28	101.55	113.75
2	R	2	MMA	C1-C2-C3	-3.45	103.18	109.97
2	Q	2	MMA	O6-C6-C5	-2.32	103.68	111.33
2	R	2	MMA	O5-C1-C2	-2.20	105.76	110.28
2	O	2	MMA	C4-C3-C2	2.03	114.58	110.79
2	P	2	MMA	O2-C2-C1	2.05	114.51	110.02
2	Q	2	MMA	O2-C2-C1	2.07	114.55	110.02
2	Q	1	MAN	O4-C4-C3	2.11	115.09	110.34
2	P	2	MMA	O5-C1-C2	2.20	114.79	110.28
2	R	2	MMA	O5-C1-O1	2.21	116.20	110.88
2	Q	2	MMA	O5-C5-C6	2.25	112.03	106.36
2	R	2	MMA	O5-C5-C6	2.27	112.10	106.36
2	O	2	MMA	O5-C5-C4	2.34	114.07	109.68
2	O	2	MMA	O5-C5-C6	2.59	112.90	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	2	MMA	C7-O1-C1	2.62	117.58	113.29
2	R	1	MAN	O2-C2-C3	2.73	115.61	110.12
2	R	1	MAN	C1-O5-C5	2.76	115.75	112.25
2	R	2	MMA	O5-C5-C4	2.84	115.01	109.68
2	O	1	MAN	O3-C3-C4	2.86	116.77	110.34
2	R	2	MMA	O1-C1-C2	3.03	111.78	108.21
2	Q	2	MMA	O5-C1-O1	3.15	118.44	110.88
2	P	2	MMA	O5-C1-O1	3.22	118.61	110.88
2	R	2	MMA	C3-C4-C5	3.32	115.98	110.20
2	P	2	MMA	O5-C5-C6	3.60	115.45	106.36
2	R	2	MMA	C7-O1-C1	4.51	120.68	113.29
2	Q	1	MAN	C1-O5-C5	4.80	118.34	112.25
2	P	1	MAN	C1-O5-C5	4.92	118.49	112.25
2	O	2	MMA	C7-O1-C1	6.84	124.50	113.29
2	P	2	MMA	O1-C1-C2	9.07	118.91	108.21
2	Q	2	MMA	O1-C1-C2	14.16	124.91	108.21

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Q	2	MMA	C1
2	O	2	MMA	C1
2	P	2	MMA	C1
2	R	2	MMA	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	2	MMA	1	0
2	R	2	MMA	2	0

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	234/237 (98%)	-0.63	0 100 100	8, 15, 28, 46	6 (2%)
1	B	234/237 (98%)	-0.63	0 100 100	9, 16, 28, 43	4 (1%)
1	C	234/237 (98%)	-0.41	1 (0%) 93 94	13, 22, 37, 51	6 (2%)
1	D	234/237 (98%)	-0.44	0 100 100	12, 21, 37, 49	6 (2%)
All	All	936/948 (98%)	-0.53	1 (0%) 95 96	8, 18, 34, 51	22 (2%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	THR	2.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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	MMA	O	2	13/13	0.80	0.29	6.48	47,56,64,64	0
2	MMA	R	2	13/13	0.83	0.27	3.13	46,56,62,63	0
2	MMA	Q	2	13/13	0.97	0.11	1.02	19,26,29,31	0
2	MAN	P	1	11/12	0.98	0.09	1.01	9,16,18,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAN	O	1	11/12	0.94	0.13	0.90	21,34,40,41	0
2	MAN	R	1	11/12	0.94	0.14	0.70	27,34,40,41	0
2	MAN	Q	1	11/12	0.98	0.08	-0.04	11,13,16,17	0
2	MMA	P	2	13/13	0.96	0.08	-0.73	20,24,28,30	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^{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	MN	A	238	1/1	1.00	0.08	0.06	14,14,14,14	0
3	MN	B	238	1/1	1.00	0.08	-0.05	14,14,14,14	0
4	CA	C	239	1/1	0.99	0.07	-0.94	16,16,16,16	0
4	CA	B	239	1/1	1.00	0.07	-1.23	13,13,13,13	0
3	MN	D	238	1/1	1.00	0.07	-1.25	21,21,21,21	0
3	MN	C	238	1/1	1.00	0.07	-1.66	18,18,18,18	0
4	CA	D	239	1/1	0.99	0.07	-1.78	17,17,17,17	0
4	CA	A	239	1/1	1.00	0.04	-3.47	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.