Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:51 pm GMT

PDB ID	:	5M6O
Title	:	Frutapin complexed with alpha-D-mannose
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Deposited on	:	2016-10-25
Resolution	:	1.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

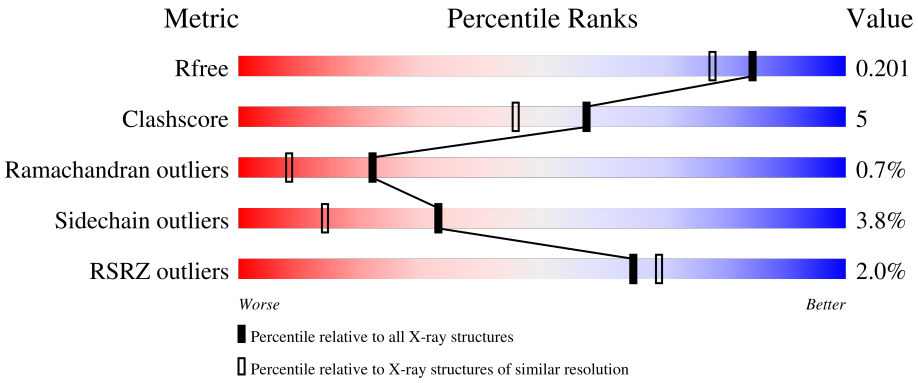
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	150	73% 27%
1	B	150	2% 77% 19%
1	C	150	4% 85% 13%
1	D	150	2% 86% 13%

2 Entry composition

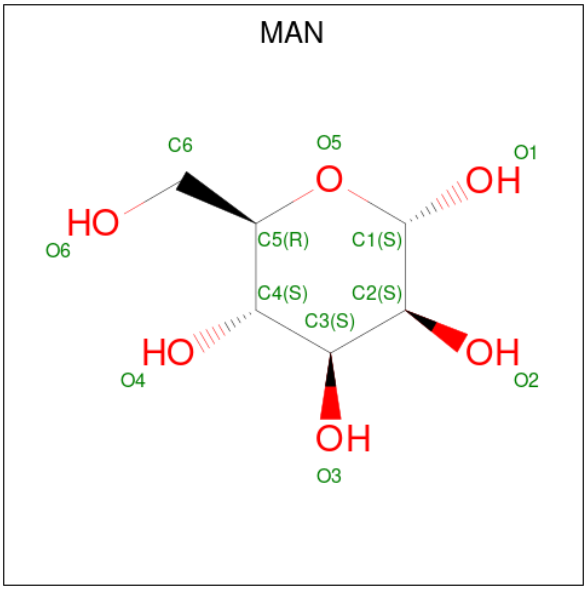
There are 3 unique types of molecules in this entry. The entry contains 5212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Frutapin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	4	0
			1169	756	187	224	2			
1	B	150	Total	C	N	O	S	0	10	0
			1213	781	194	235	3			
1	C	150	Total	C	N	O	S	0	5	0
			1187	761	193	231	2			
1	D	150	Total	C	N	O	S	0	3	0
			1168	750	189	227	2			

- Molecule 2 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0

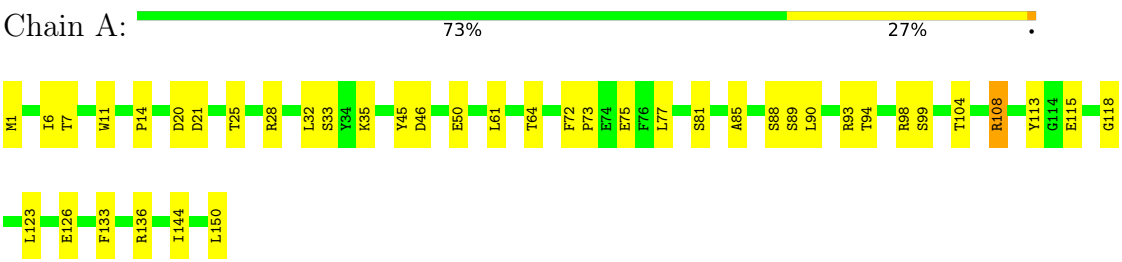
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	113	Total O 113 113	0	0
3	B	107	Total O 107 107	0	0
3	C	101	Total O 101 101	0	0
3	D	106	Total O 106 106	0	0

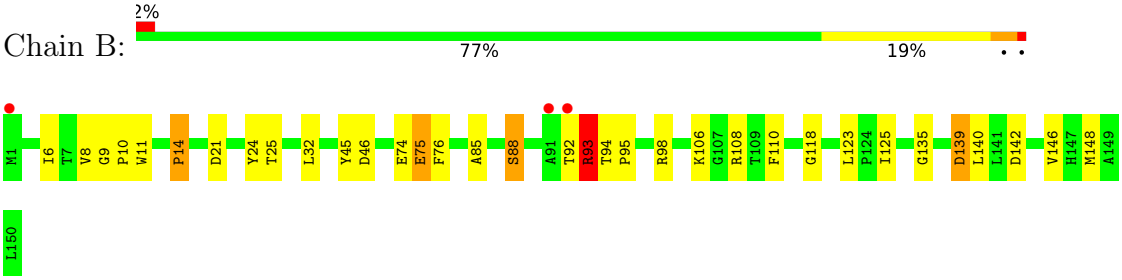
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

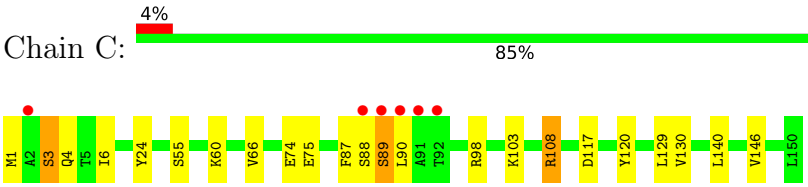
• Molecule 1: Frutapin



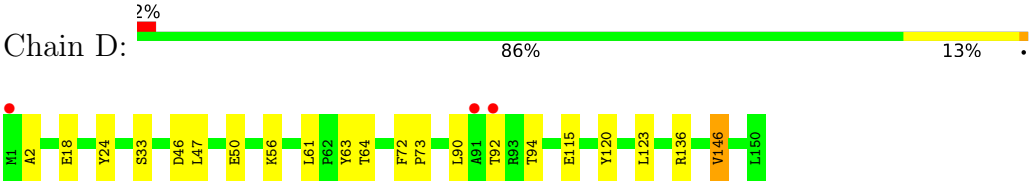
• Molecule 1: Frutapin



• Molecule 1: Frutapin



• Molecule 1: Frutapin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	73.96Å 73.96Å 185.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.05 – 1.70 64.05 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.05-1.70) 99.8 (64.05-1.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.141 , 0.191 0.153 , 0.201	Depositor DCC
R_{free} test set	3343 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
Reported twinning fraction	0.609 for H, K, L 0.391 for -h,-k,l	Depositor
Outliers	0 of 65549 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5212	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9493e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.41	6/1211 (0.5%)	1.38	14/1642 (0.9%)
1	B	1.44	5/1255 (0.4%)	1.43	12/1702 (0.7%)
1	C	1.24	1/1217 (0.1%)	1.24	4/1649 (0.2%)
1	D	1.22	1/1201 (0.1%)	1.22	3/1628 (0.2%)
All	All	1.33	13/4884 (0.3%)	1.32	33/6621 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	TYR	CE2-CZ	-8.40	1.27	1.38
1	B	45	TYR	CG-CD1	-6.62	1.30	1.39
1	A	7	THR	CB-CG2	-6.03	1.32	1.52
1	A	81	SER	CA-CB	-5.97	1.44	1.52
1	B	75	GLU	CD-OE1	5.78	1.32	1.25
1	A	11	TRP	CB-CG	5.68	1.60	1.50
1	D	50	GLU	CD-OE2	5.65	1.31	1.25
1	C	24	TYR	CE1-CZ	5.56	1.45	1.38
1	B	135	GLY	C-O	-5.34	1.15	1.23
1	B	24	TYR	CG-CD1	-5.30	1.32	1.39
1	B	74	GLU	CD-OE1	-5.29	1.19	1.25
1	A	45	TYR	CB-CG	5.23	1.59	1.51
1	A	104	THR	CB-CG2	-5.02	1.35	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	142	ASP	CB-CG-OD2	-10.89	108.50	118.30
1	B	21	ASP	CB-CG-OD1	10.22	127.50	118.30
1	C	108	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	C	108	ARG	NE-CZ-NH2	-8.46	116.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	76	PHE	CB-CG-CD1	8.42	126.69	120.80
1	A	136	ARG	NE-CZ-NH1	-8.40	116.10	120.30
1	A	50	GLU	OE1-CD-OE2	-8.02	113.68	123.30
1	A	46	ASP	CB-CG-OD1	-7.78	111.30	118.30
1	A	20	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	110	PHE	CB-CG-CD1	-7.23	115.74	120.80
1	A	108	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	25	THR	OG1-CB-CG2	-6.95	94.01	110.00
1	A	133	PHE	CB-CG-CD2	6.64	125.45	120.80
1	A	108	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	133	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	B	93	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	24	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	C	129	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	46	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	93	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	76	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	98	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	98	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	139[A]	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	139[B]	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	28	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	46	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	C	87	PHE	CB-CA-C	5.38	121.15	110.40
1	B	140	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	A	21	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	77	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	B	140	LEU	CB-CG-CD1	5.16	119.78	111.00
1	D	47	LEU	CB-CG-CD2	-5.02	102.47	111.00

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	1169	0	1162	14	1
1	B	1213	0	1199	19	0
1	C	1187	0	1160	9	1
1	D	1168	0	1143	12	0
2	A	12	0	12	0	0
2	B	12	0	12	1	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	113	0	0	0	0
3	B	107	0	0	2	0
3	C	101	0	0	5	0
3	D	106	0	0	5	0
All	All	5212	0	4712	47	1

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 5.

All (47) 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:14:PRO:HD2	1:B:94:THR:OG1	1.77	0.84
1:B:85:ALA:HB2	1:B:118:GLY:HA3	1.69	0.75
1:B:94:THR:HG23	3:B:307:HOH:O	1.87	0.75
1:C:89:SER:OG	3:C:301:HOH:O	2.03	0.73
1:D:115:GLU:OE2	3:D:301:HOH:O	2.12	0.67
1:C:120:TYR:HB3	3:C:380:HOH:O	1.96	0.64
1:D:94:THR:HG23	3:D:320:HOH:O	1.98	0.63
1:C:98:ARG:NH1	1:C:117:ASP:OD2	2.35	0.60
1:C:75:GLU:OE2	1:C:108:ARG:HD3	2.02	0.60
1:A:85:ALA:HB2	1:A:118:GLY:HA3	1.88	0.56
1:D:94:THR:HG22	3:D:370:HOH:O	2.05	0.56
1:A:6:ILE:HD12	1:B:6:ILE:HD12	1.88	0.55
1:B:106[A]:LYS:NZ	3:B:304:HOH:O	2.41	0.53
1:A:32:LEU:HD12	1:A:32:LEU:C	2.30	0.52
1:B:32:LEU:C	1:B:32:LEU:HD12	2.33	0.49
1:A:99:SER:HA	1:A:113:TYR:O	2.14	0.48
1:B:139[B]:ASP:OD1	2:B:201:MAN:H62	2.14	0.48
1:D:18:GLU:CG	1:D:136:ARG:NH2	2.77	0.47
1:A:75:GLU:OE2	1:A:108:ARG:HD3	2.14	0.47
1:A:123:LEU:HD12	1:B:8[B]:VAL:HG11	1.97	0.47
1:B:125:ILE:HG12	1:B:148[A]:MET:HE1	1.97	0.47
1:B:75:GLU:OE1	1:B:108:ARG:NH2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PRO:HD2	1:A:94:THR:HB	1.97	0.46
1:B:93:ARG:O	1:B:93:ARG:NH1	2.48	0.46
1:C:130:VAL:HG13	1:C:146[B]:VAL:HG13	1.96	0.46
1:D:61:LEU:HB3	1:D:63:TYR:CE1	2.51	0.46
1:B:8[B]:VAL:HG12	1:B:11:TRP:CH2	2.51	0.45
3:C:380:HOH:O	1:D:120:TYR:HB3	2.16	0.44
1:B:123:LEU:CD2	1:B:146[A]:VAL:HG21	2.47	0.44
1:D:18:GLU:HG3	3:D:377:HOH:O	2.16	0.44
1:A:61:LEU:HD11	1:A:90:LEU:CD2	2.48	0.43
1:A:123:LEU:HD12	1:B:8[B]:VAL:CG1	2.49	0.43
1:D:56:LYS:HG2	3:D:388:HOH:O	2.18	0.42
1:B:94:THR:OG1	1:B:95:PRO:CD	2.67	0.42
1:A:126:GLU:HG3	1:B:9:GLY:O	2.19	0.42
1:A:150:LEU:HD21	1:C:3:SER:HA	2.02	0.42
1:A:126:GLU:OE2	1:B:10:PRO:HD3	2.20	0.41
1:D:123:LEU:CD2	1:D:146[A]:VAL:HG21	2.50	0.41
1:B:25[A]:THR:HG22	1:D:2:ALA:HB1	2.02	0.41
1:C:90:LEU:HD12	3:C:336:HOH:O	2.20	0.41
1:A:33:SER:HA	1:A:64:THR:O	2.21	0.41
1:D:72:PHE:CD1	1:D:73:PRO:HA	2.56	0.41
1:D:33:SER:HA	1:D:64:THR:O	2.20	0.41
1:A:72:PHE:CD2	1:A:73:PRO:HA	2.57	0.40
1:B:106[B]:LYS:HD2	1:B:106[B]:LYS:HA	1.66	0.40
1:C:103[B]:LYS:CE	3:C:313:HOH:O	2.69	0.40
1:C:6:ILE:HG23	1:C:6:ILE:HD12	1.88	0.40

All (1) 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)
1:A:115:GLU:OE1	1:C:117:ASP:OD1[1_655]	2.08	0.12

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	152/150 (101%)	145 (95%)	5 (3%)	2 (1%)	12 2
1	B	158/150 (105%)	148 (94%)	9 (6%)	1 (1%)	25 11
1	C	153/150 (102%)	145 (95%)	7 (5%)	1 (1%)	22 8
1	D	151/150 (101%)	143 (95%)	8 (5%)	0	100 100
All	All	614/600 (102%)	581 (95%)	29 (5%)	4 (1%)	22 8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	SER
1	C	89	SER
1	A	35	LYS
1	B	88	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	128/124 (103%)	124 (97%)	4 (3%)	40 21
1	B	134/124 (108%)	130 (97%)	4 (3%)	41 22
1	C	129/124 (104%)	120 (93%)	9 (7%)	15 3
1	D	127/124 (102%)	123 (97%)	4 (3%)	40 21
All	All	518/496 (104%)	497 (96%)	21 (4%)	33 12

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	89	SER
1	A	144[A]	ILE
1	A	144[B]	ILE

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Mol	Chain	Res	Type
1	B	14	PRO
1	B	88	SER
1	B	92	THR
1	B	93	ARG
1	C	1	MET
1	C	3	SER
1	C	4	GLN
1	C	55	SER
1	C	60	LYS
1	C	66	VAL
1	C	74	GLU
1	C	88	SER
1	C	140	LEU
1	D	90	LEU
1	D	92	THR
1	D	146[A]	VAL
1	D	146[B]	VAL

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

Mol	Chain	Res	Type
1	A	4	GLN
1	C	4	GLN
1	D	127	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	MAN	C	201	-	12,12,12	0.97	1 (8%)	17,17,17	1.33	2 (11%)
2	MAN	B	201	-	12,12,12	0.88	0	17,17,17	1.65	5 (29%)
2	MAN	A	201	-	12,12,12	1.16	1 (8%)	17,17,17	1.89	3 (17%)
2	MAN	D	201	-	12,12,12	1.00	1 (8%)	17,17,17	1.04	1 (5%)

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	C	201	-	-	2/2/22/22	0/1/1/1
2	MAN	B	201	-	-	0/2/22/22	0/1/1/1
2	MAN	A	201	-	-	0/2/22/22	0/1/1/1
2	MAN	D	201	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	MAN	C4-C5	2.38	1.58	1.53
2	C	201	MAN	O1-C1	2.23	1.46	1.39
2	D	201	MAN	O1-C1	2.05	1.46	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	MAN	O2-C2-C3	4.89	121.66	110.35
2	A	201	MAN	O5-C1-C2	3.21	116.02	110.28
2	B	201	MAN	O5-C5-C4	3.20	115.51	109.69
2	A	201	MAN	O2-C2-C1	-3.10	101.97	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201	MAN	O3-C3-C4	-3.02	103.37	110.35
2	B	201	MAN	C1-O5-C5	2.82	118.98	113.66
2	B	201	MAN	O5-C1-C2	2.63	114.97	110.28
2	D	201	MAN	O2-C2-C1	2.56	115.10	109.16
2	B	201	MAN	O1-C1-O5	-2.32	103.42	110.38
2	C	201	MAN	O4-C4-C5	2.12	114.57	109.30
2	B	201	MAN	O4-C4-C3	-2.10	105.49	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	MAN	O5-C5-C6-O6
2	C	201	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	MAN	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^{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	150/150 (100%)	-0.42	0 100 100	8, 17, 33, 53	2 (1%)
1	B	150/150 (100%)	-0.33	3 (2%) 65 69	7, 15, 40, 67	7 (4%)
1	C	150/150 (100%)	-0.17	6 (4%) 38 42	9, 18, 48, 93	4 (2%)
1	D	150/150 (100%)	-0.26	3 (2%) 65 69	9, 19, 43, 71	3 (2%)
All	All	600/600 (100%)	-0.30	12 (2%) 65 69	7, 17, 43, 93	16 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	ALA	14.6
1	B	91	ALA	6.9
1	D	91	ALA	6.0
1	C	92	THR	5.4
1	D	1	MET	4.7
1	C	90	LEU	4.1
1	B	92	THR	3.7
1	D	92	THR	3.5
1	C	2	ALA	3.2
1	C	88	SER	2.9
1	B	1	MET	2.9
1	C	89	SER	2.1

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

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	MAN	D	201	12/12	0.88	0.13	25,33,42,44	0
2	MAN	B	201	12/12	0.89	0.11	20,25,35,36	0
2	MAN	C	201	12/12	0.90	0.11	28,32,37,41	0
2	MAN	A	201	12/12	0.92	0.10	19,22,25,31	0

6.5 Other polymers

There are no such residues in this entry.