Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 04:58 AM EDT

PDB ID	:	6FCO
Title	:	Structural and functional characterisation of Frataxin (FXN) like protein from Chaetomium thermophilum
Authors	:	Jamshidiha, M.; Rasheed, M.; Pastore, A.; Cota, E.
Deposited on	:	2017-12-20
Resolution	:	2.03 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 (i) 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 (i)) were used in the production of this report:

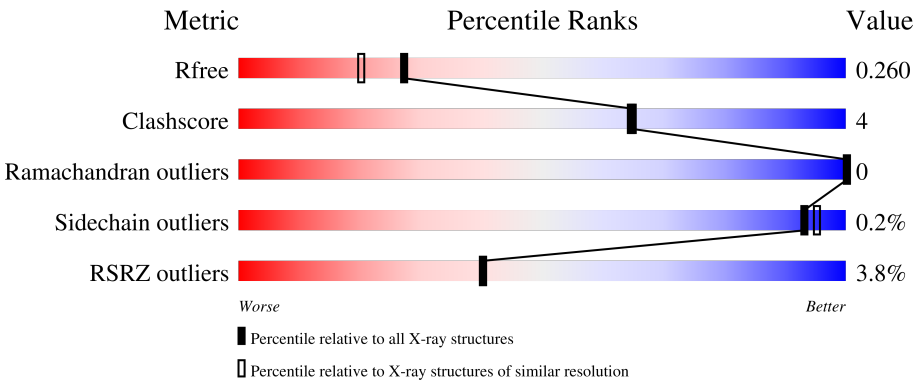
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	126	7%, 87%, 7%, • 6%
1	B	126	4%, 83%, 11%, 6%
1	C	126	2%, 86%, 10%, •
1	D	126	2%, 82%, 7%, 11%
1	E	126	6%, 75%, 10%, 15%

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Mol	Chain	Length	Quality of chain
1	F	126	76% 8% • 15%

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	MLA	C	301	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5382 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.

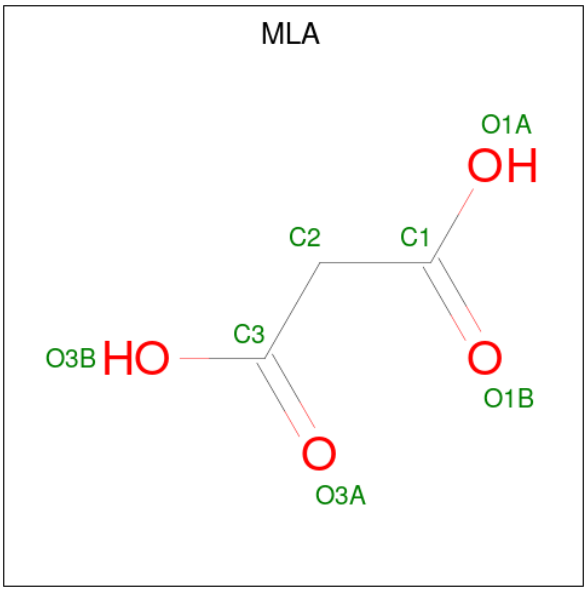
- Molecule 1 is a protein called Mitochondrial frataxin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	119	892	566	148	176	2	0	0	0
1	B	118	904	571	151	180	2	0	0	0
1	C	121	911	576	146	187	2	0	0	0
1	D	112	850	540	138	170	2	0	0	0
1	E	107	828	529	133	165	1	0	0	0
1	F	107	824	525	133	164	2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	SER	-	expression tag	UNP G0S1Z8
A	86	MET	-	expression tag	UNP G0S1Z8
B	85	SER	-	expression tag	UNP G0S1Z8
B	86	MET	-	expression tag	UNP G0S1Z8
C	85	SER	-	expression tag	UNP G0S1Z8
C	86	MET	-	expression tag	UNP G0S1Z8
D	85	SER	-	expression tag	UNP G0S1Z8
D	86	MET	-	expression tag	UNP G0S1Z8
E	85	SER	-	expression tag	UNP G0S1Z8
E	86	MET	-	expression tag	UNP G0S1Z8
F	85	SER	-	expression tag	UNP G0S1Z8
F	86	MET	-	expression tag	UNP G0S1Z8

- Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	7	3	4	0	0
			Total	C	O		
2	A	1	7	3	4	0	0
			Total	C	O		
2	C	1	7	3	4	0	0
			Total	C	O		
2	C	1	7	3	4	0	0

- Molecule 3 is water.

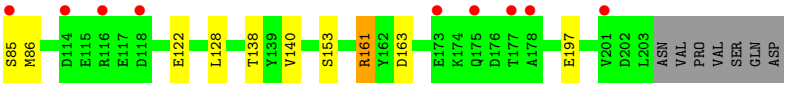
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	22	22	22	0	0
			Total	O		
3	B	33	33	33	0	0
			Total	O		
3	C	28	28	28	0	0
			Total	O		
3	D	28	28	28	0	0
			Total	O		
3	E	18	18	18	0	0
			Total	O		
3	F	16	16	16	0	0

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.

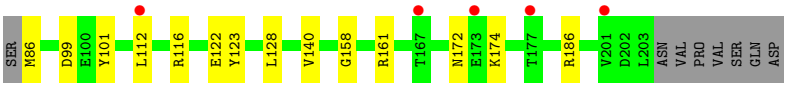
• Molecule 1: Mitochondrial frataxin-like protein

Chain A:



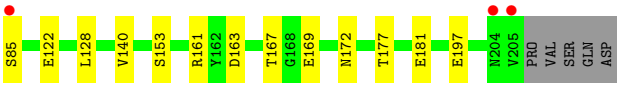
• Molecule 1: Mitochondrial frataxin-like protein

Chain B:



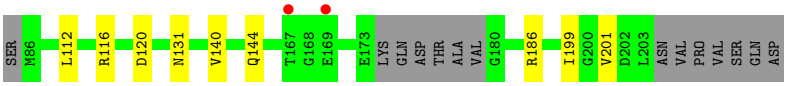
• Molecule 1: Mitochondrial frataxin-like protein

Chain C:



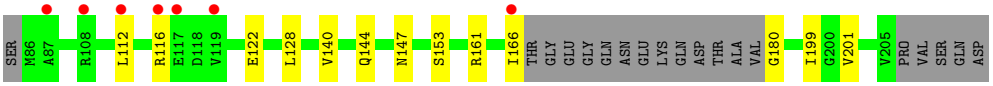
• Molecule 1: Mitochondrial frataxin-like protein

Chain D:



• Molecule 1: Mitochondrial frataxin-like protein

Chain E:



• Molecule 1: Mitochondrial frataxin-like protein

Chain F:

76%
8%
•
15%

SER
M96
L112
R116
Q124
T138
Y139
V140
Q144
N147
S153
R161
I166
THR
GLY
GLU
GLY
GLN
ASN
GLU
LYS
GLN
ASP
THR
ALA
VAL
G180
L185
R186
V205
PRO
VAL
SER
GLN
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.06Å 89.06Å 185.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.29 – 2.03 80.29 – 2.03	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.29-2.03) 100.0 (80.29-2.03)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.219 , 0.260 0.227 , 0.260	Depositor DCC
R_{free} test set	2444 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5382	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 41.57 % 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 2.3143e-04. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLA

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	0.71	1/908 (0.1%)	0.83	1/1240 (0.1%)
1	B	0.75	0/920	0.85	1/1254 (0.1%)
1	C	0.77	1/927 (0.1%)	0.81	0/1267
1	D	0.73	0/865	0.82	0/1179
1	E	0.76	1/843 (0.1%)	0.87	1/1150 (0.1%)
1	F	0.72	1/839 (0.1%)	0.85	2/1144 (0.2%)
All	All	0.74	4/5302 (0.1%)	0.84	5/7234 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	153	SER	CB-OG	-6.18	1.34	1.42
1	C	153	SER	CB-OG	-5.84	1.34	1.42
1	A	153	SER	CB-OG	-5.47	1.35	1.42
1	E	153	SER	CB-OG	-5.46	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	F	161	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	161	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	F	186	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	B	101	TYR	CB-CG-CD2	-5.12	117.93	121.00

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	892	0	837	8	0
1	B	904	0	862	10	0
1	C	911	0	846	10	0
1	D	850	0	798	7	0
1	E	828	0	790	9	0
1	F	824	0	779	9	0
2	A	14	0	4	2	0
2	C	14	0	4	2	0
3	A	22	0	0	1	0
3	B	33	0	0	3	0
3	C	28	0	0	2	0
3	D	28	0	0	0	0
3	E	18	0	0	0	0
3	F	16	0	0	0	0
All	All	5382	0	4920	42	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 4.

All (42) 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:120:ASP:OD1	1:D:131:ASN:HB3	1.78	0.83
1:C:85:SER:CB	1:C:163:ASP:HB3	2.10	0.82
1:E:144:GLN:HE22	1:F:138:THR:H	1.26	0.81
1:A:138:THR:H	1:D:144:GLN:HE22	1.34	0.76
1:A:161:ARG:HD3	2:A:301:MLA:O1A	1.95	0.64
1:E:140:VAL:HG11	1:F:140:VAL:HG11	1.78	0.64
3:A:419:HOH:O	1:F:186:ARG:HD3	1.99	0.62
1:B:172:ASN:ND2	1:B:174:LYS:H	2.01	0.59
1:E:112:LEU:HD11	1:E:116:ARG:CZ	2.34	0.58
1:A:140:VAL:HG11	1:D:140:VAL:HG11	1.89	0.55
1:B:140:VAL:HG11	1:C:140:VAL:HG11	1.91	0.53
1:C:177:THR:OG1	3:C:401:HOH:O	2.19	0.53
1:C:167:THR:OG1	1:C:181:GLU:OE1	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:HD11	1:D:116:ARG:CZ	2.40	0.52
1:A:85:SER:O	1:A:86:MET:C	2.47	0.51
1:E:144:GLN:HE22	1:F:138:THR:N	2.03	0.51
1:C:172:ASN:ND2	1:C:177:THR:HG21	2.26	0.50
1:F:112:LEU:HD11	1:F:116:ARG:CZ	2.42	0.49
1:C:197:GLU:OE2	1:D:186:ARG:NE	2.45	0.49
1:B:99:ASP:OD1	3:B:301:HOH:O	2.20	0.48
1:A:197:GLU:OE2	1:B:186:ARG:HD3	2.14	0.48
1:E:199:ILE:HG22	1:E:201:VAL:HG23	1.96	0.47
1:C:169:GLU:O	3:C:401:HOH:O	2.20	0.47
1:E:166:ILE:HA	1:E:180:GLY:HA2	1.97	0.47
1:B:172:ASN:HD22	1:B:174:LYS:H	1.62	0.47
1:A:85:SER:CB	1:A:163:ASP:HB3	2.45	0.46
1:B:161:ARG:NH1	3:B:305:HOH:O	2.47	0.46
1:F:144:GLN:HG3	1:F:147:ASN:HD22	1.81	0.46
2:C:301:MLA:HC22	1:F:186:ARG:HA	1.97	0.45
1:B:158:GLY:HA3	1:F:185:LEU:O	2.16	0.45
1:E:122:GLU:OE1	1:F:124:GLN:CB	2.64	0.45
1:B:112:LEU:HD11	1:B:116:ARG:CZ	2.48	0.44
1:D:199:ILE:HG22	1:D:201:VAL:HG23	1.98	0.44
1:B:123:TYR:OH	3:B:301:HOH:O	2.17	0.44
1:E:144:GLN:HG3	1:E:147:ASN:HD22	1.83	0.44
1:C:122:GLU:O	1:C:128:LEU:HD12	2.18	0.43
1:B:122:GLU:O	1:B:128:LEU:HD12	2.20	0.41
1:A:122:GLU:O	1:A:128:LEU:HD12	2.21	0.41
1:A:161:ARG:HD3	2:A:301:MLA:C1	2.50	0.41
1:C:197:GLU:OE2	1:D:186:ARG:CZ	2.69	0.41
1:E:122:GLU:O	1:E:128:LEU:HD12	2.21	0.41
1:C:161:ARG:HD2	2:C:301:MLA:HC21	2.03	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	117/126 (93%)	116 (99%)	1 (1%)	0	100	100
1	B	116/126 (92%)	116 (100%)	0	0	100	100
1	C	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
1	D	108/126 (86%)	108 (100%)	0	0	100	100
1	E	103/126 (82%)	101 (98%)	2 (2%)	0	100	100
1	F	103/126 (82%)	102 (99%)	1 (1%)	0	100	100
All	All	666/756 (88%)	661 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	89/112 (80%)	89 (100%)	0	100	100
1	B	94/112 (84%)	93 (99%)	1 (1%)	73	77
1	C	93/112 (83%)	93 (100%)	0	100	100
1	D	87/112 (78%)	87 (100%)	0	100	100
1	E	87/112 (78%)	87 (100%)	0	100	100
1	F	86/112 (77%)	86 (100%)	0	100	100
All	All	536/672 (80%)	535 (100%)	1 (0%)	93	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	GLN

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Mol	Chain	Res	Type
1	B	172	ASN
1	C	147	ASN
1	C	172	ASN
1	D	144	GLN
1	D	147	ASN
1	E	113	GLN
1	E	144	GLN
1	F	113	GLN
1	F	147	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	MLA	A	302	-	6,6,6	2.28	2 (33%)	7,7,7	3.32	4 (57%)
2	MLA	C	301	-	6,6,6	2.29	2 (33%)	7,7,7	2.38	3 (42%)
2	MLA	A	301	-	6,6,6	1.68	1 (16%)	7,7,7	1.81	2 (28%)
2	MLA	C	302	-	6,6,6	2.27	2 (33%)	7,7,7	3.34	4 (57%)

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	MLA	A	302	-	-	0/4/4/4	-
2	MLA	C	301	-	-	2/4/4/4	-
2	MLA	A	301	-	-	2/4/4/4	-
2	MLA	C	302	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	MLA	C2-C1	4.38	1.57	1.51
2	C	301	MLA	C2-C1	4.22	1.57	1.51
2	C	302	MLA	C2-C3	3.71	1.56	1.51
2	A	301	MLA	C2-C1	3.07	1.55	1.51
2	C	302	MLA	C2-C1	2.92	1.55	1.51
2	C	301	MLA	O3A-C3	2.57	1.30	1.22
2	A	302	MLA	O3B-C3	-2.28	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	302	MLA	C3-C2-C1	6.03	134.23	112.95
2	A	302	MLA	O1A-C1-C2	6.00	133.09	114.51
2	A	302	MLA	O1A-C1-O1B	-4.83	110.90	123.33
2	C	301	MLA	O1A-C1-C2	3.96	126.79	114.51
2	C	301	MLA	O1A-C1-O1B	-3.83	113.49	123.33
2	C	302	MLA	O3B-C3-O3A	-3.56	114.17	123.33
2	C	302	MLA	O1B-C1-C2	3.41	131.81	122.11
2	A	302	MLA	C3-C2-C1	3.39	124.90	112.95
2	C	302	MLA	O3A-C3-C2	3.37	131.72	122.11
2	A	301	MLA	C3-C2-C1	3.18	124.19	112.95
2	A	301	MLA	O1A-C1-O1B	-2.51	116.87	123.33
2	C	301	MLA	C3-C2-C1	2.33	121.16	112.95
2	A	302	MLA	O1B-C1-C2	-2.16	115.97	122.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MLA	O1A-C1-C2-C3
2	A	301	MLA	O1B-C1-C2-C3
2	C	301	MLA	O1B-C1-C2-C3
2	C	301	MLA	O1A-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	MLA	2	0
2	A	301	MLA	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	119/126 (94%)	0.49	9 (7%)	13	13	26, 44, 73, 86	0
1	B	118/126 (93%)	0.28	5 (4%)	36	35	24, 36, 67, 80	0
1	C	121/126 (96%)	0.31	3 (2%)	57	57	26, 37, 61, 72	0
1	D	112/126 (88%)	0.29	2 (1%)	68	67	26, 38, 70, 83	0
1	E	107/126 (84%)	0.37	7 (6%)	18	18	23, 39, 66, 79	0
1	F	107/126 (84%)	0.23	0	100	100	23, 39, 68, 84	0
All	All	684/756 (90%)	0.33	26 (3%)	40	40	23, 39, 69, 86	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	SER	4.5
1	E	166	ILE	4.4
1	B	173	GLU	3.6
1	C	204	ASN	3.4
1	D	167	THR	3.2
1	E	119	VAL	3.1
1	B	177	THR	3.1
1	A	175	GLN	3.0
1	A	201	VAL	2.8
1	E	117	GLU	2.7
1	A	116	ARG	2.6
1	A	85	SER	2.6
1	B	167	THR	2.6
1	A	114	ASP	2.5
1	B	201	VAL	2.5
1	C	205	VAL	2.5
1	A	173	GLU	2.5
1	A	118	ASP	2.4
1	E	112	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	178	ALA	2.3
1	D	169	GLU	2.3
1	E	87	ALA	2.2
1	B	112	LEU	2.2
1	E	108	ARG	2.1
1	E	116	ARG	2.0
1	A	177	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 monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th 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	MLA	C	302	7/7	0.84	0.17	37,39,47,54	0
2	MLA	A	301	7/7	0.86	0.16	33,40,44,50	0
2	MLA	A	302	7/7	0.87	0.20	37,38,42,48	0
2	MLA	C	301	7/7	0.90	0.18	37,39,43,52	0

6.5 Other polymers (i)

There are no such residues in this entry.