Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 06:37 PM EDT

PDB ID	:	4OVA
Title	:	Structure of the two tandem Tudor domains and a new identified KH0 domain from human Fragile X Mental Retardation Protein
Authors	:	Chen, Z.H.; Chen, Z.Z.
Deposited on	:	2014-02-21
Resolution	:	3.00 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:

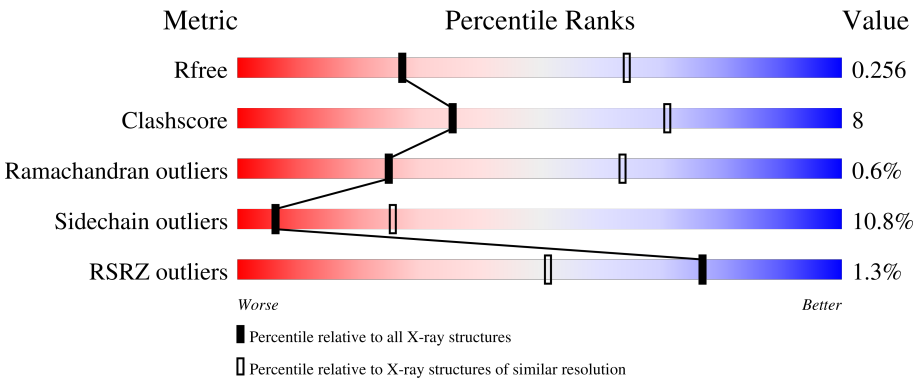
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	209	76% 18% • •
1	B	209	% 72% 21% • •
1	C	209	% 75% 18% • 5%
1	D	209	% 71% 22% • •

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	TRS	C	301	-	-	-	X

2 Entry composition (i)

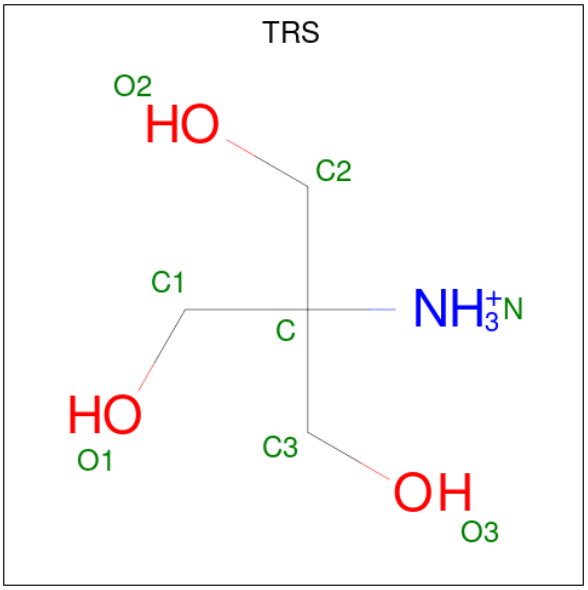
There are 3 unique types of molecules in this entry. The entry contains 6416 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fragile X mental retardation protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1568	998	268	293	9	0	0	0
1	B	200	1594	1014	274	298	8	0	0	0
1	C	199	1507	958	258	285	6	0	0	0
1	D	200	1560	993	271	287	9	0	0	0

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	8	4	1	3	0	0
2	D	1	8	4	1	3	0	0

- Molecule 3 is water.

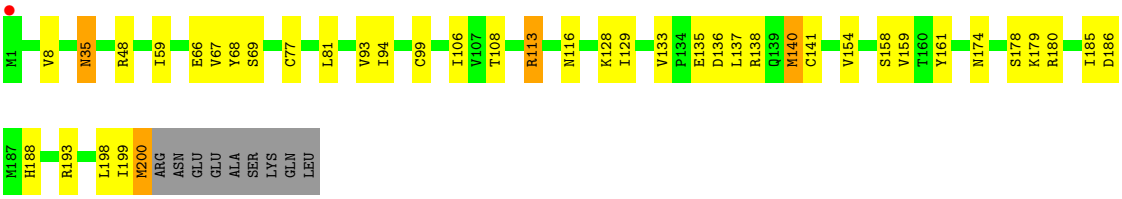
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	36	36	36	0	0
			Total	O		
3	B	64	64	64	0	0
			Total	O		
3	C	25	25	25	0	0
			Total	O		
3	D	46	46	46	0	0

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.

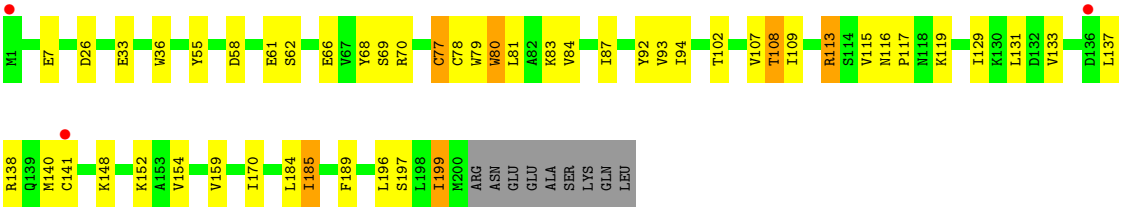
• Molecule 1: Fragile X mental retardation protein 1

Chain A: 76% 18%



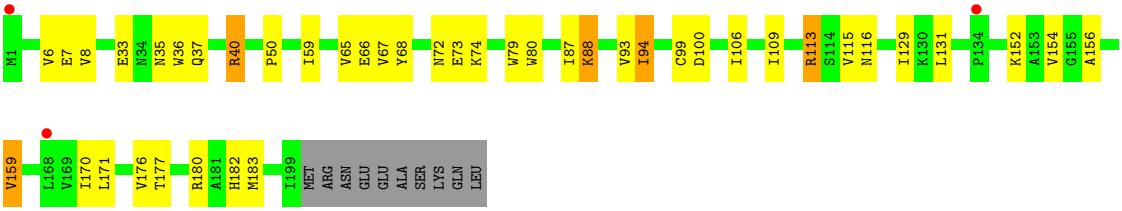
• Molecule 1: Fragile X mental retardation protein 1

Chain B: % 72% 21%



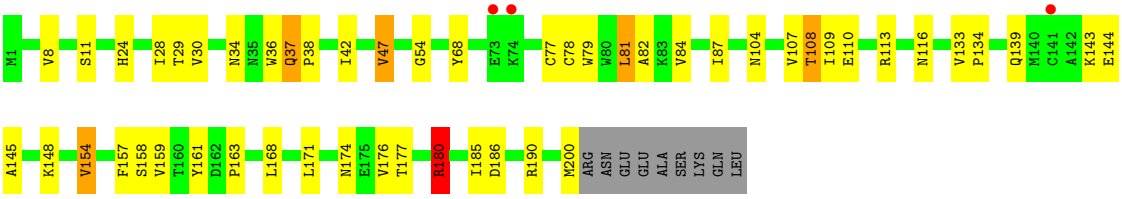
• Molecule 1: Fragile X mental retardation protein 1

Chain C: % 75% 18% 5%



• Molecule 1: Fragile X mental retardation protein 1

Chain D: % 71% 22%


M1
V8
S11
H24
I28
T29
V30
N34
N35
W36
Q37
P38
I42
V47
G54
Y68
E73
K74
C77
C78
W79
W80
L81
A82
K83
V84
I87
N104
V107
T108
I109
E110
R113
N116
V133
P134
Q139
M140
C141
A142
K143
E144
A145
K148
V154
F157
S158
V159
T160
Y161
D162
P163
L168
L171
N174
E175
V176
T177
R180
I185
D186
R190
M200
ARG
ASN
GLU
GLU
ALA
SER
LYS
GLN
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	232.64Å 60.84Å 168.86Å 90.00° 122.99° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 48.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-3.00) 95.9 (48.78-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.219 , 0.259 0.218 , 0.256	Depositor DCC
R_{free} test set	1928 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	106.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 84.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6416	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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, 0.333 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: TRS

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	0.47	0/1605	0.69	0/2182
1	B	0.42	0/1632	0.66	0/2215
1	C	0.46	0/1544	0.69	1/2111 (0.0%)
1	D	0.50	0/1596	0.73	1/2165 (0.0%)
All	All	0.46	0/6377	0.69	2/8673 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	180	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	40	ARG	NE-CZ-NH1	5.98	123.29	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	34	ASN	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	1568	0	1489	15	0
1	B	1594	0	1529	29	0
1	C	1507	0	1368	31	0
1	D	1560	0	1478	26	0
2	C	8	0	12	0	0
2	D	8	0	12	0	0
3	A	36	0	0	1	0
3	B	64	0	0	1	0
3	C	25	0	0	5	0
3	D	46	0	0	2	0
All	All	6416	0	5888	98	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 8.

All (98) 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:8:VAL:HG21	1:D:42:ILE:HD13	1.48	0.95
1:D:108:THR:HG23	1:D:110:GLU:OE1	1.79	0.82
1:C:116:ASN:ND2	3:C:418:HOH:O	2.13	0.80
1:D:24:HIS:HE2	1:D:29:THR:HG1	1.32	0.75
1:B:66:GLU:OE1	1:B:113:ARG:NH2	2.23	0.72
1:C:50:PRO:HA	3:C:418:HOH:O	1.92	0.68
1:B:87:ILE:O	1:C:88:LYS:NZ	2.28	0.67
1:B:78:CYS:SG	1:B:80:TRP:CZ3	2.89	0.64
1:C:79:TRP:CZ3	1:C:113:ARG:HG2	2.34	0.63
1:A:174:ASN:HB3	3:A:404:HOH:O	1.97	0.63
1:C:115:VAL:N	3:C:419:HOH:O	2.33	0.62
1:D:68:TYR:CZ	1:D:77:CYS:HB2	2.35	0.61
1:B:84:VAL:HA	1:B:94:ILE:HG22	1.82	0.61
1:C:93:VAL:HG22	1:C:106:ILE:HG12	1.85	0.59
1:B:129:ILE:N	1:B:129:ILE:HD12	2.18	0.59
1:A:106:ILE:HD12	1:D:104:ASN:HB3	1.86	0.58
1:A:93:VAL:HG22	1:A:106:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:O	1:A:188:HIS:HB3	2.04	0.58
1:A:66:GLU:OE1	1:A:113:ARG:NH1	2.37	0.57
1:B:92:TYR:CZ	1:B:109:ILE:HD13	2.39	0.57
1:D:37:GLN:HG2	1:D:38:PRO:HD2	1.87	0.57
1:D:158:SER:HB3	1:D:171:LEU:HB2	1.87	0.56
1:B:79:TRP:CZ3	1:B:113:ARG:HG2	2.42	0.55
1:B:159:VAL:HG12	1:B:170:ILE:HG12	1.88	0.55
1:C:65:VAL:HA	3:C:419:HOH:O	2.04	0.55
1:C:73:GLU:O	1:C:74:LYS:CB	2.54	0.55
1:D:157:PHE:CZ	1:D:171:LEU:HB3	2.42	0.55
1:C:67:VAL:HG12	1:C:68:TYR:N	2.22	0.54
1:A:93:VAL:HG22	1:A:106:ILE:CG1	2.40	0.52
1:A:66:GLU:HB2	1:A:113:ARG:HD2	1.90	0.52
1:B:78:CYS:SG	1:B:80:TRP:CH2	3.03	0.52
1:D:28:ILE:HD11	1:D:47:VAL:HG21	1.92	0.52
1:B:68:TYR:CZ	1:B:77:CYS:HB3	2.45	0.51
1:B:131:LEU:HD13	1:B:185:ILE:HG13	1.92	0.51
1:A:129:ILE:HD13	1:A:178:SER:HA	1.93	0.51
1:C:87:ILE:O	1:C:87:ILE:HG22	2.12	0.50
1:B:199:ILE:HG22	1:B:199:ILE:O	2.11	0.50
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.76	0.49
1:C:66:GLU:HB2	1:C:113:ARG:HD2	1.94	0.49
1:B:199:ILE:O	1:B:199:ILE:CG2	2.61	0.49
1:B:131:LEU:HD13	1:B:185:ILE:CG1	2.42	0.48
1:B:94:ILE:HD12	1:B:94:ILE:O	2.13	0.48
1:C:66:GLU:HA	1:C:80:TRP:O	2.14	0.48
1:C:68:TYR:HB2	1:C:79:TRP:CZ3	2.49	0.48
1:C:59:ILE:HD12	1:C:109:ILE:HD11	1.96	0.47
1:D:113:ARG:HH12	1:D:116:ASN:HB2	1.79	0.47
1:D:180:ARG:CG	1:D:180:ARG:HH11	2.27	0.47
1:D:180:ARG:HH11	1:D:180:ARG:HG3	1.79	0.47
1:B:68:TYR:CE1	1:B:77:CYS:HB3	2.50	0.47
1:C:66:GLU:N	3:C:419:HOH:O	2.47	0.47
1:C:66:GLU:OE1	1:C:113:ARG:NH1	2.38	0.47
1:D:154:VAL:HG13	1:D:177:THR:HG23	1.97	0.47
1:B:137:LEU:O	1:B:138:ARG:C	2.52	0.46
1:A:141:CYS:O	1:A:161:TYR:HB2	2.15	0.46
1:A:137:LEU:O	1:A:140:MET:N	2.49	0.46
1:C:67:VAL:CG1	1:C:68:TYR:N	2.79	0.46
1:C:154:VAL:CG1	1:C:177:THR:HG23	2.46	0.46
1:C:159:VAL:HG13	1:C:170:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:OE2	1:B:113:ARG:NH1	2.48	0.45
1:D:109:ILE:HD11	3:D:415:HOH:O	2.16	0.45
1:C:33:GLU:O	1:C:36:TRP:HD1	2.00	0.45
1:D:8:VAL:CG2	1:D:42:ILE:HD13	2.33	0.45
1:D:79:TRP:CZ3	1:D:113:ARG:HG2	2.52	0.45
1:C:154:VAL:HG13	1:C:177:THR:HG23	1.99	0.45
1:C:154:VAL:CG1	1:C:154:VAL:O	2.65	0.45
1:A:67:VAL:HG21	1:A:94:ILE:HD13	1.99	0.45
1:B:55:TYR:N	3:B:305:HOH:O	2.49	0.44
1:D:174:ASN:HB3	1:D:176:VAL:HG12	1.99	0.44
1:B:116:ASN:HA	1:B:117:PRO:HD3	1.90	0.44
1:D:159:VAL:HG12	1:D:168:LEU:HD22	2.00	0.44
1:B:115:VAL:O	1:B:116:ASN:C	2.56	0.43
1:B:133:VAL:HG21	1:B:141:CYS:SG	2.58	0.43
1:B:185:ILE:HD12	1:B:189:PHE:CZ	2.53	0.43
1:D:148:LYS:NZ	3:D:416:HOH:O	2.50	0.43
1:C:176:VAL:HG22	1:C:180:ARG:HG2	2.00	0.43
1:D:145:ALA:HA	1:D:148:LYS:HE2	2.01	0.42
1:A:128:LYS:C	1:A:129:ILE:HG13	2.40	0.42
1:B:93:VAL:HG11	1:C:106:ILE:HD11	2.00	0.42
1:D:81:LEU:HD13	1:D:82:ALA:N	2.34	0.42
1:D:133:VAL:HG23	1:D:134:PRO:HD2	2.02	0.42
1:B:61:GLU:O	1:B:62:SER:CB	2.67	0.42
1:C:131:LEU:HD21	1:C:182:HIS:CE1	2.55	0.42
1:A:185:ILE:HG23	1:A:186:ASP:N	2.35	0.41
1:B:107:VAL:HG22	1:B:108:THR:N	2.35	0.41
1:D:36:TRP:CZ3	1:D:37:GLN:HG3	2.55	0.41
1:A:68:TYR:CZ	1:A:77:CYS:HB2	2.55	0.41
1:C:129:ILE:HB	1:C:170:ILE:HB	2.02	0.41
1:C:7:GLU:OE2	1:C:113:ARG:NH2	2.47	0.41
1:A:199:ILE:C	1:A:200:MET:HG2	2.41	0.41
1:B:185:ILE:HD13	1:B:185:ILE:HA	1.94	0.41
1:B:61:GLU:HG2	1:B:87:ILE:HG13	2.03	0.41
1:B:33:GLU:O	1:B:36:TRP:HD1	2.04	0.41
1:D:30:VAL:HG22	1:D:42:ILE:HD12	2.03	0.41
1:C:67:VAL:HG21	1:C:94:ILE:HG13	2.03	0.40
1:C:156:ALA:HB1	1:C:171:LEU:O	2.21	0.40
1:C:6:VAL:HA	1:C:50:PRO:HD3	2.04	0.40
1:D:161:TYR:CE2	1:D:163:PRO:HA	2.56	0.40
1:D:185:ILE:HG23	1:D:186:ASP:N	2.36	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	198/209 (95%)	177 (89%)	19 (10%)	2 (1%)	15	53
1	B	198/209 (95%)	173 (87%)	25 (13%)	0	100	100
1	C	197/209 (94%)	180 (91%)	15 (8%)	2 (1%)	15	53
1	D	198/209 (95%)	183 (92%)	14 (7%)	1 (0%)	29	68
All	All	791/836 (95%)	713 (90%)	73 (9%)	5 (1%)	25	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	35	ASN
1	C	99	CYS
1	D	54	GLY
1	A	35	ASN
1	A	138	ARG

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	164/188 (87%)	142 (87%)	22 (13%)	4	17
1	B	169/188 (90%)	148 (88%)	21 (12%)	4	20
1	C	148/188 (79%)	138 (93%)	10 (7%)	16	48
1	D	157/188 (84%)	141 (90%)	16 (10%)	7	28
All	All	638/752 (85%)	569 (89%)	69 (11%)	6	26

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	35	ASN
1	A	48	ARG
1	A	59	ILE
1	A	69	SER
1	A	81	LEU
1	A	99	CYS
1	A	108	THR
1	A	113	ARG
1	A	116	ASN
1	A	133	VAL
1	A	135	GLU
1	A	136	ASP
1	A	140	MET
1	A	154	VAL
1	A	158	SER
1	A	159	VAL
1	A	179	LYS
1	A	180	ARG
1	A	193	ARG
1	A	198	LEU
1	A	200	MET
1	B	26	ASP
1	B	58	ASP
1	B	69	SER
1	B	70	ARG
1	B	77	CYS
1	B	80	TRP
1	B	81	LEU
1	B	83	LYS
1	B	102	THR
1	B	108	THR
1	B	113	ARG
1	B	119	LYS
1	B	140	MET
1	B	148	LYS
1	B	152	LYS
1	B	154	VAL
1	B	184	LEU
1	B	185	ILE
1	B	196	LEU
1	B	197	SER

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Mol	Chain	Res	Type
1	B	199	ILE
1	C	8	VAL
1	C	37	GLN
1	C	72	ASN
1	C	88	LYS
1	C	94	ILE
1	C	100	ASP
1	C	113	ARG
1	C	152	LYS
1	C	159	VAL
1	C	183	MET
1	D	11	SER
1	D	37	GLN
1	D	47	VAL
1	D	78	CYS
1	D	81	LEU
1	D	84	VAL
1	D	87	ILE
1	D	107	VAL
1	D	108	THR
1	D	139	GLN
1	D	143	LYS
1	D	144	GLU
1	D	154	VAL
1	D	180	ARG
1	D	190	ARG
1	D	200	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	37	GLN
1	A	41	GLN
1	A	116	ASN
1	A	118	ASN
1	B	41	GLN
1	B	139	GLN
1	B	147	HIS
1	B	182	HIS
1	C	37	GLN
1	C	118	ASN

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Mol	Chain	Res	Type
1	C	147	HIS
1	C	182	HIS
1	D	45	HIS
1	D	147	HIS
1	D	182	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	TRS	D	301	-	7,7,7	0.34	0	9,9,9	0.55	0
2	TRS	C	301	-	7,7,7	0.33	0	9,9,9	0.48	0

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	TRS	D	301	-	-	0/9/9/9	-
2	TRS	C	301	-	-	6/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	TRS	C1-C-C2-O2
2	C	301	TRS	C3-C-C2-O2
2	C	301	TRS	N-C-C2-O2
2	C	301	TRS	C2-C-C3-O3
2	C	301	TRS	C1-C-C3-O3
2	C	301	TRS	N-C-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	200/209 (95%)	-0.16	1 (0%)	91	75	65, 96, 137, 175	0
1	B	200/209 (95%)	0.00	3 (1%)	73	46	67, 103, 153, 200	3 (1%)
1	C	199/209 (95%)	-0.03	3 (1%)	73	46	58, 98, 148, 173	2 (1%)
1	D	200/209 (95%)	-0.10	3 (1%)	73	46	59, 98, 151, 175	5 (2%)
All	All	799/836 (95%)	-0.07	10 (1%)	77	51	58, 99, 150, 200	10 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	CYS	4.2
1	C	1	MET	3.7
1	C	134	PRO	3.6
1	D	74	LYS	3.5
1	B	1	MET	2.8
1	A	1	MET	2.6
1	D	141	CYS	2.5
1	B	136	ASP	2.4
1	C	168	LEU	2.3
1	D	73	GLU	2.2

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	TRS	C	301	8/8	0.80	0.40	86,94,101,103	0
2	TRS	D	301	8/8	0.87	0.32	116,130,135,137	0

6.5 Other polymers (i)

There are no such residues in this entry.