Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:33 am BST

PDB ID	:	3UUX
Title	:	Crystal structure of yeast Fis1 in complex with Mdv1 fragment containing N-terminal extension and coiled coil domains
Authors	:	Zhang, Y.; Chan, N.C.; Gristick, H.; Chan, D.C.
Deposited on	:	2011-11-28
Resolution	:	3.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

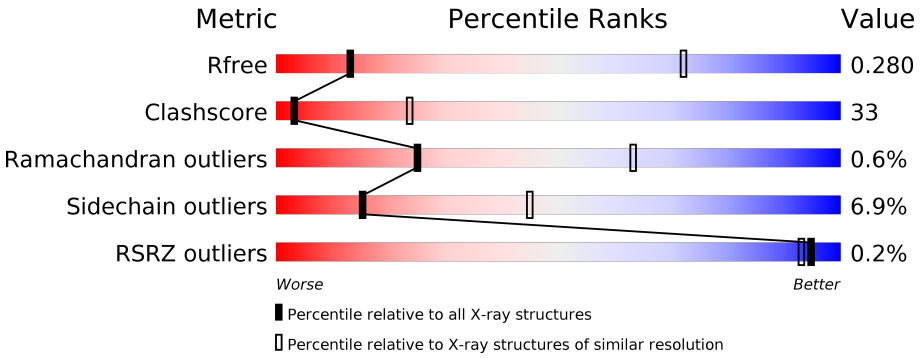
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 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	129	49% 45% 5%
1	C	129	% 51% 43%
2	B	242	27% 25% 45%
2	D	242	26% 25% 5% 44%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4076 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 Mitochondria fission 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1028	654	172	198	4			
1	C	125	Total	C	N	O	S	0	0	0
			1004	638	168	194	4			

- Molecule 2 is a protein called Mitochondrial division protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1013	641	164	206	2			
2	D	135	Total	C	N	O	S	0	0	0
			1031	651	169	209	2			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	MET	-	EXPRESSION TAG	UNP P47025
B	74	GLY	-	EXPRESSION TAG	UNP P47025
B	75	SER	-	EXPRESSION TAG	UNP P47025
B	76	SER	-	EXPRESSION TAG	UNP P47025
B	77	HIS	-	EXPRESSION TAG	UNP P47025
B	78	HIS	-	EXPRESSION TAG	UNP P47025
B	79	HIS	-	EXPRESSION TAG	UNP P47025
B	80	HIS	-	EXPRESSION TAG	UNP P47025
B	81	HIS	-	EXPRESSION TAG	UNP P47025
B	82	HIS	-	EXPRESSION TAG	UNP P47025
B	83	SER	-	EXPRESSION TAG	UNP P47025
B	84	SER	-	EXPRESSION TAG	UNP P47025
B	85	GLY	-	EXPRESSION TAG	UNP P47025
B	86	LEU	-	EXPRESSION TAG	UNP P47025
B	87	VAL	-	EXPRESSION TAG	UNP P47025
B	88	PRO	-	EXPRESSION TAG	UNP P47025

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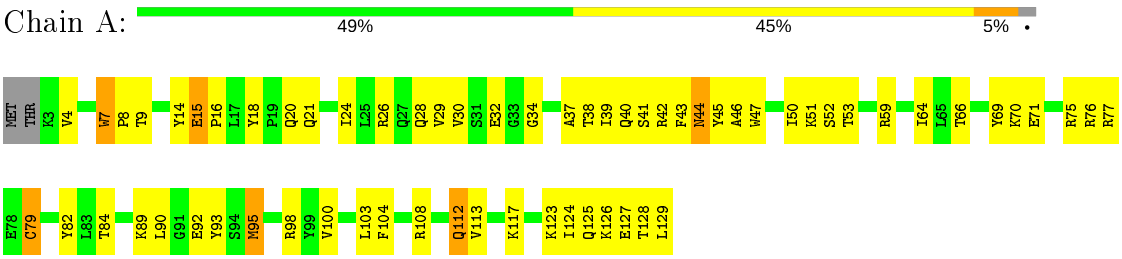
Chain	Residue	Modelled	Actual	Comment	Reference
B	89	ARG	-	EXPRESSION TAG	UNP P47025
B	90	GLY	-	EXPRESSION TAG	UNP P47025
B	91	SER	-	EXPRESSION TAG	UNP P47025
B	92	HIS	-	EXPRESSION TAG	UNP P47025
B	93	MET	-	EXPRESSION TAG	UNP P47025
B	215	ALA	LYS	ENGINEERED MUTATION	UNP P47025
B	216	ALA	LYS	ENGINEERED MUTATION	UNP P47025
D	73	MET	-	EXPRESSION TAG	UNP P47025
D	74	GLY	-	EXPRESSION TAG	UNP P47025
D	75	SER	-	EXPRESSION TAG	UNP P47025
D	76	SER	-	EXPRESSION TAG	UNP P47025
D	77	HIS	-	EXPRESSION TAG	UNP P47025
D	78	HIS	-	EXPRESSION TAG	UNP P47025
D	79	HIS	-	EXPRESSION TAG	UNP P47025
D	80	HIS	-	EXPRESSION TAG	UNP P47025
D	81	HIS	-	EXPRESSION TAG	UNP P47025
D	82	HIS	-	EXPRESSION TAG	UNP P47025
D	83	SER	-	EXPRESSION TAG	UNP P47025
D	84	SER	-	EXPRESSION TAG	UNP P47025
D	85	GLY	-	EXPRESSION TAG	UNP P47025
D	86	LEU	-	EXPRESSION TAG	UNP P47025
D	87	VAL	-	EXPRESSION TAG	UNP P47025
D	88	PRO	-	EXPRESSION TAG	UNP P47025
D	89	ARG	-	EXPRESSION TAG	UNP P47025
D	90	GLY	-	EXPRESSION TAG	UNP P47025
D	91	SER	-	EXPRESSION TAG	UNP P47025
D	92	HIS	-	EXPRESSION TAG	UNP P47025
D	93	MET	-	EXPRESSION TAG	UNP P47025
D	215	ALA	LYS	ENGINEERED MUTATION	UNP P47025
D	216	ALA	LYS	ENGINEERED MUTATION	UNP P47025

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 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.

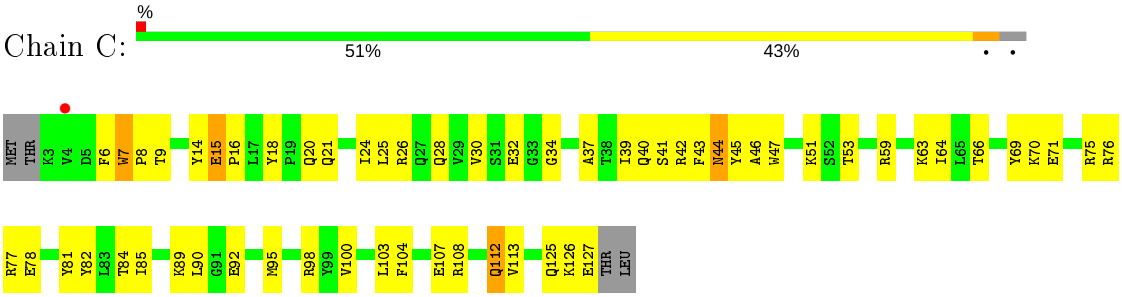
- Molecule 1: Mitochondria fission 1 protein

Chain A:



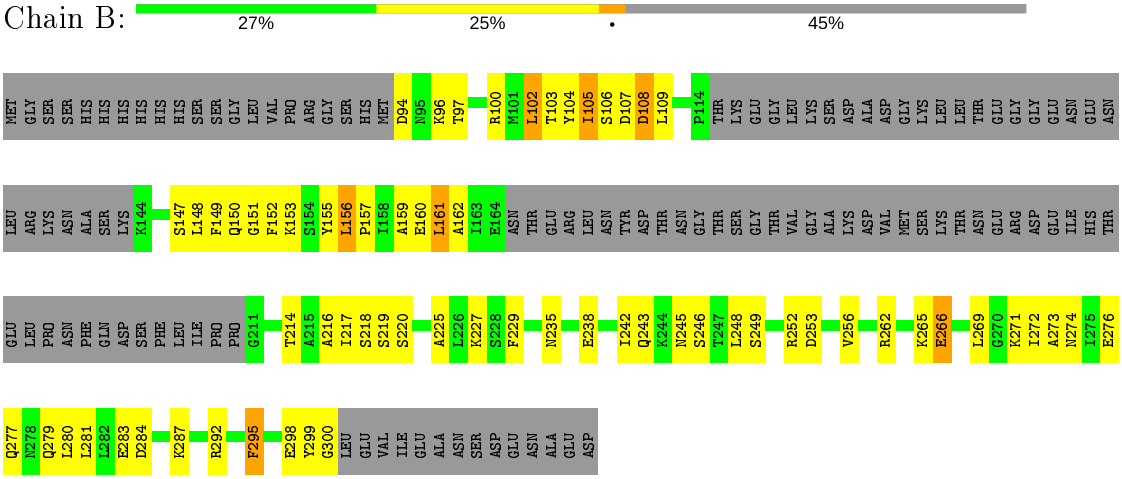
- Molecule 1: Mitochondria fission 1 protein

Chain C:



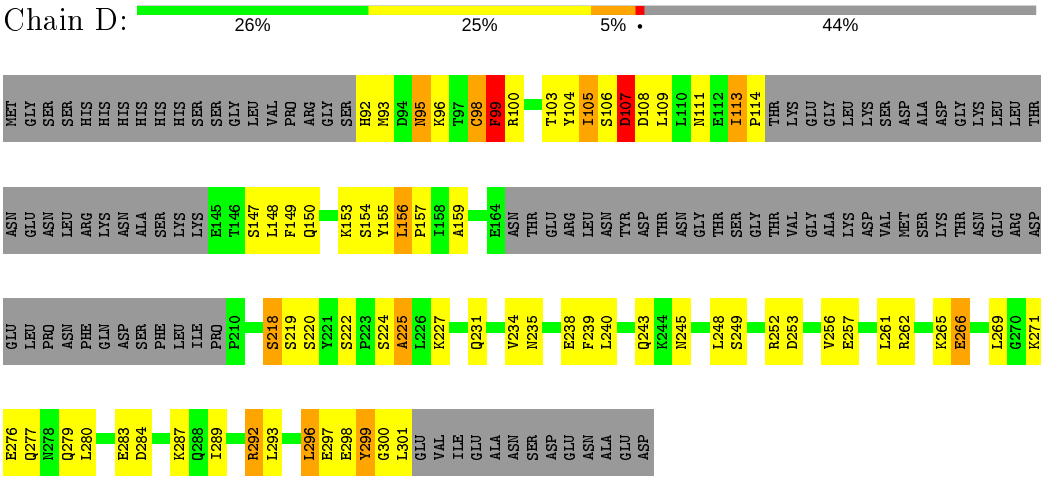
- Molecule 2: Mitochondrial division protein 1

Chain B:



- Molecule 2: Mitochondrial division protein 1

Chain D:


26%
25%
5%
44%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER H92 M93 D94 N95 K96 T97 C98 F99 R100 T103 Y104 I105 S106 D107 D108 L109 L110 N111 E112 I113 P114 THR LYS GLU GLY LEU LYS SER ASP ALA ASP GLY LYS LEU LEU THR GLU GLY GLY GLU
ASN GLU ASN LEU ARG LYS ASN ALA SER LYS LYS E145 T146 S147 L148 F149 Q150 K153 S154 Y155 L156 P157 I158 A159 E164 ASN THR GLU ARG LEU ASN TYR ASP THR ASN GLY THR SER GLY THR VAL GLY ALA LYS ASP VAL MET SER LYS THR ASN GLU ARG ASP GLU ILE HIS THR
GLU LEU PRO ASN PHE GLN ASP SER PHE LEU ILE PRO P210 S218 S219 S220 Y221 S222 P223 S224 A225 L226 K227 Q231 V234 N235 E238 F239 L240 Q243 K244 N245 L248 S249 R252 D253 V256 E257 L261 R262 K265 E266 L269 G270 K271 I272 A273 N274 I275
E276 Q277 N278 Q279 L280 E283 D284 K287 Q288 I289 R292 L293 L296 E297 E298 Y299 G300 L301 GLU VAL ILE GLU ALA ASN SER ASP GLU ASN ALA GLU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	174.68Å 174.68Å 167.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.51 – 3.90 19.81 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (123.51-3.90) 99.6 (19.81-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 3.94Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.270 , 0.284 0.266 , 0.280	Depositor DCC
R_{free} test set	1178 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å^2)	122.5	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 107.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.028 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4076	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

5.1 Standard geometry

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	0.87	3/1048 (0.3%)	0.87	1/1417 (0.1%)
1	C	0.86	2/1024 (0.2%)	0.85	1/1388 (0.1%)
2	B	0.96	2/1023 (0.2%)	1.00	4/1382 (0.3%)
2	D	1.33	5/1042 (0.5%)	1.06	4/1407 (0.3%)
All	All	1.02	12/4137 (0.3%)	0.95	10/5594 (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
2	B	0	1
2	D	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	218	SER	CB-OG	18.31	1.66	1.42
2	D	225	ALA	C-O	13.78	1.49	1.23
1	C	127	GLU	C-O	9.32	1.41	1.23
2	B	225	ALA	C-O	-9.14	1.05	1.23
1	C	44	ASN	CB-CG	-7.00	1.34	1.51
2	B	225	ALA	CA-CB	6.72	1.66	1.52
2	D	99	PHE	C-O	5.79	1.34	1.23
1	A	44	ASN	CB-CG	-5.57	1.38	1.51
1	A	79	CYS	CB-SG	-5.48	1.72	1.81
1	A	127	GLU	C-O	5.17	1.33	1.23
2	D	222	SER	CB-OG	5.09	1.48	1.42
2	D	224	SER	CB-OG	5.01	1.48	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	44	ASN	CB-CA-C	-7.88	94.63	110.40
2	B	161	LEU	CA-CB-CG	6.80	130.95	115.30
2	D	98	CYS	CA-CB-SG	-6.67	101.99	114.00
2	D	292	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	D	107	ASP	N-CA-C	-6.41	93.71	111.00
2	B	105	ILE	CG1-CB-CG2	-6.08	98.02	111.40
2	D	106	SER	N-CA-C	5.44	125.70	111.00
2	B	106	SER	N-CA-C	5.43	125.66	111.00
2	B	102	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	44	ASN	CB-CA-C	5.22	120.85	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	220	SER	Peptide
2	D	225	ALA	Mainchain

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	1028	0	1001	70	0
1	C	1004	0	961	72	0
2	B	1013	0	975	70	0
2	D	1031	0	986	105	2
All	All	4076	0	3923	266	2

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 33.

All (266) 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)
2:D:113:ILE:CG1	2:D:113:ILE:CD1	1.82	1.54
2:D:218:SER:OG	2:D:218:SER:CB	1.66	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:NH2	2:D:114:PRO:HD3	1.46	1.26
1:C:59:ARG:HD2	2:D:99:PHE:HD1	1.02	1.15
1:A:126:LYS:HB3	2:D:104:TYR:CE2	1.86	1.10
2:D:99:PHE:CE2	2:D:103:THR:HG21	1.93	1.04
1:C:59:ARG:HD2	2:D:99:PHE:CD1	1.94	1.03
1:C:59:ARG:CD	2:D:99:PHE:HD1	1.72	1.02
2:D:113:ILE:HD13	2:D:114:PRO:N	1.76	1.00
1:C:77:ARG:HH22	2:D:114:PRO:HD3	1.02	0.99
1:C:77:ARG:HH22	2:D:114:PRO:CD	1.76	0.98
1:A:126:LYS:HB3	2:D:104:TYR:CD2	2.05	0.92
2:D:99:PHE:C	2:D:99:PHE:HD2	1.73	0.91
1:C:59:ARG:HG2	1:C:90:LEU:HD11	1.53	0.90
1:A:44:ASN:HB2	2:B:152:PHE:HD1	1.38	0.88
1:C:28:GLN:HG2	2:D:155:TYR:OH	1.73	0.88
1:A:59:ARG:HG2	1:A:90:LEU:HD11	1.55	0.87
2:B:214:THR:O	2:B:229:PHE:HZ	1.55	0.86
1:A:4:VAL:HG11	2:B:153:LYS:HG3	1.56	0.86
1:A:43:PHE:CD2	2:B:148:LEU:HG	2.11	0.85
2:D:269:LEU:O	2:D:272:ILE:HG12	1.76	0.84
2:B:298:GLU:HA	2:B:298:GLU:OE1	1.78	0.83
2:D:99:PHE:HE2	2:D:103:THR:HG21	1.41	0.83
2:D:99:PHE:CE2	2:D:103:THR:CG2	2.62	0.83
2:B:272:ILE:HG13	2:B:273:ALA:N	1.91	0.83
2:B:269:LEU:O	2:B:272:ILE:HG12	1.79	0.82
1:C:77:ARG:NH2	2:D:114:PRO:CD	2.36	0.82
2:D:99:PHE:HE2	2:D:103:THR:CG2	1.93	0.81
2:D:113:ILE:C	2:D:113:ILE:HD13	2.00	0.81
2:D:92:HIS:CG	2:D:93:MET:H	1.99	0.81
2:D:99:PHE:C	2:D:99:PHE:CD2	2.52	0.80
2:D:99:PHE:O	2:D:99:PHE:HD2	1.65	0.80
2:D:272:ILE:HG13	2:D:273:ALA:N	1.96	0.80
2:B:214:THR:OG1	2:B:229:PHE:HE2	1.65	0.80
2:B:214:THR:HG1	2:B:229:PHE:HE2	1.34	0.76
2:D:293:LEU:O	2:D:297:GLU:HG2	1.85	0.75
1:A:7:TRP:HD1	1:A:8:PRO:HD2	1.52	0.75
2:D:108:ASP:O	2:D:111:ASN:OD1	2.05	0.74
2:D:113:ILE:HD13	2:D:114:PRO:CD	2.17	0.73
1:C:46:ALA:HB2	1:C:64:ILE:CG2	2.19	0.73
1:C:59:ARG:CD	2:D:99:PHE:CD1	2.61	0.73
1:A:41:SER:HA	1:A:44:ASN:OD1	1.89	0.72
1:A:46:ALA:HB2	1:A:64:ILE:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLU:OE2	2:D:148:LEU:HB2	1.89	0.72
2:B:147:SER:HB3	2:B:150:GLN:HG3	1.71	0.72
2:D:147:SER:HB3	2:D:150:GLN:HG3	1.71	0.72
2:D:272:ILE:O	2:D:276:GLU:HB2	1.89	0.72
1:C:46:ALA:HB2	1:C:64:ILE:HG21	1.73	0.71
2:D:249:SER:HA	2:D:252:ARG:NH1	2.06	0.71
1:A:8:PRO:HB3	2:B:149:PHE:CE1	2.25	0.70
1:A:92:GLU:OE1	2:B:100:ARG:CD	2.40	0.70
1:C:92:GLU:OE1	2:D:100:ARG:NE	2.24	0.70
2:B:253:ASP:O	2:B:256:VAL:HG12	1.92	0.70
1:A:126:LYS:CB	2:D:104:TYR:CE2	2.73	0.70
1:A:112:GLN:HE21	1:A:112:GLN:H	1.40	0.69
2:B:105:ILE:HG13	2:B:109:LEU:HD11	1.74	0.69
2:D:99:PHE:HE2	2:D:103:THR:HG1	1.40	0.69
1:A:46:ALA:HB2	1:A:64:ILE:HG21	1.75	0.68
1:C:43:PHE:CD2	2:D:148:LEU:HG	2.28	0.68
2:D:253:ASP:O	2:D:256:VAL:HG12	1.94	0.67
2:D:92:HIS:CG	2:D:93:MET:N	2.62	0.67
2:B:96:LYS:O	2:B:100:ARG:HG3	1.94	0.67
2:B:272:ILE:O	2:B:276:GLU:HB2	1.95	0.66
2:D:292:ARG:O	2:D:296:LEU:HG	1.96	0.66
1:A:69:TYR:CZ	1:A:76:ARG:HD3	2.30	0.66
1:A:125:GLN:HG3	1:A:126:LYS:N	2.09	0.66
1:C:69:TYR:CZ	1:C:76:ARG:HD3	2.31	0.65
2:D:289:ILE:HG22	2:D:292:ARG:HH22	1.61	0.65
1:A:7:TRP:CD1	1:A:8:PRO:HD2	2.32	0.65
1:C:41:SER:HA	1:C:44:ASN:OD1	1.97	0.65
2:D:107:ASP:C	2:D:107:ASP:OD2	2.34	0.64
1:C:7:TRP:HD1	1:C:8:PRO:HD2	1.62	0.64
2:D:245:ASN:HA	2:D:248:LEU:HB3	1.80	0.64
1:A:93:TYR:CE1	1:A:123:LYS:HD2	2.33	0.64
1:A:124:ILE:O	1:A:128:THR:HG23	1.99	0.63
2:D:113:ILE:CD1	2:D:113:ILE:CB	2.75	0.63
1:A:39:ILE:HG13	1:A:40:GLN:H	1.64	0.62
1:A:84:THR:HG21	1:A:100:VAL:HB	1.81	0.62
1:A:39:ILE:HG13	1:A:40:GLN:N	2.16	0.61
1:C:84:THR:HG21	1:C:100:VAL:HB	1.81	0.61
1:C:18:TYR:O	1:C:21:GLN:N	2.33	0.61
2:D:155:TYR:CD2	2:D:155:TYR:C	2.74	0.61
2:B:298:GLU:C	2:B:299:TYR:HD2	2.04	0.60
2:D:113:ILE:C	2:D:113:ILE:CD1	2.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLU:O	1:C:15:GLU:HG2	2.00	0.60
1:C:39:ILE:HG13	1:C:40:GLN:H	1.67	0.60
2:D:113:ILE:CD1	2:D:114:PRO:HD2	2.32	0.60
1:A:18:TYR:O	1:A:21:GLN:N	2.34	0.59
1:A:126:LYS:C	2:D:104:TYR:HE2	2.06	0.59
2:D:92:HIS:CD2	2:D:93:MET:N	2.71	0.59
1:C:39:ILE:HG13	1:C:40:GLN:N	2.18	0.58
2:B:249:SER:HA	2:B:252:ARG:NH1	2.19	0.58
1:A:8:PRO:HB3	2:B:149:PHE:CD1	2.38	0.58
2:B:245:ASN:HA	2:B:248:LEU:HB3	1.86	0.58
1:C:6:PHE:CD1	2:D:147:SER:HB2	2.39	0.58
2:D:299:TYR:CD2	2:D:299:TYR:N	2.70	0.58
1:C:77:ARG:HH21	2:D:114:PRO:HD3	1.58	0.58
2:B:105:ILE:O	2:B:109:LEU:HD13	2.04	0.57
2:D:280:LEU:HA	2:D:283:GLU:OE2	2.05	0.57
2:D:92:HIS:CD2	2:D:93:MET:H	2.21	0.57
1:A:44:ASN:HB2	2:B:152:PHE:CD1	2.29	0.57
2:B:155:TYR:C	2:B:155:TYR:CD2	2.78	0.57
1:A:50:ILE:O	1:A:89:LYS:NZ	2.31	0.56
1:A:93:TYR:CZ	1:A:123:LYS:HD2	2.40	0.56
1:C:112:GLN:HE21	1:C:112:GLN:H	1.52	0.56
1:A:92:GLU:OE1	2:B:100:ARG:HD2	2.05	0.56
1:A:15:GLU:O	1:A:15:GLU:HG2	2.04	0.56
2:B:272:ILE:HG13	2:B:273:ALA:H	1.69	0.56
1:C:43:PHE:O	1:C:46:ALA:N	2.39	0.56
1:A:28:GLN:NE2	1:A:32:GLU:HG3	2.21	0.56
1:C:16:PRO:HG3	1:C:53:THR:HG23	1.87	0.56
1:A:42:ARG:NH2	1:A:71:GLU:OE1	2.35	0.55
2:D:218:SER:HG	2:D:218:SER:CB	2.09	0.55
1:A:103:LEU:HD21	1:A:113:VAL:HG22	1.88	0.55
2:B:298:GLU:CA	2:B:298:GLU:OE1	2.48	0.55
2:B:262:ARG:O	2:B:265:LYS:HB3	2.06	0.55
1:C:77:ARG:HD3	1:C:107:GLU:OE2	2.06	0.55
2:B:280:LEU:HA	2:B:283:GLU:OE2	2.06	0.55
2:D:272:ILE:HG13	2:D:273:ALA:H	1.71	0.55
2:D:113:ILE:CD1	2:D:114:PRO:CD	2.85	0.55
1:A:15:GLU:O	1:A:51:LYS:HG2	2.07	0.55
1:A:16:PRO:HG3	1:A:53:THR:HG23	1.89	0.55
1:A:40:GLN:HG2	2:B:243:GLN:HE22	1.72	0.54
1:A:28:GLN:HE21	1:A:32:GLU:HG3	1.72	0.54
1:A:92:GLU:OE1	2:B:100:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:TRP:CD1	1:C:8:PRO:HD2	2.43	0.54
1:A:39:ILE:HD12	1:A:75:ARG:HD2	1.90	0.53
1:A:43:PHE:CE2	2:B:148:LEU:HG	2.43	0.53
2:D:113:ILE:CG1	2:D:114:PRO:HD2	2.38	0.53
2:D:107:ASP:OD2	2:D:108:ASP:N	2.42	0.52
1:A:28:GLN:HG2	2:B:155:TYR:OH	2.10	0.52
1:C:7:TRP:CD1	1:C:81:TYR:CD2	2.97	0.52
2:D:99:PHE:HE2	2:D:103:THR:CB	2.22	0.52
1:C:28:GLN:NE2	1:C:32:GLU:HG3	2.25	0.52
1:C:15:GLU:O	1:C:51:LYS:HG2	2.10	0.51
1:A:20:GLN:O	1:A:24:ILE:HG12	2.11	0.51
2:D:113:ILE:HG12	2:D:114:PRO:HD2	1.90	0.51
2:D:300:GLY:O	2:D:301:LEU:CB	2.57	0.51
2:D:99:PHE:HE2	2:D:103:THR:OG1	1.92	0.51
1:C:78:GLU:OE2	2:D:148:LEU:CB	2.56	0.51
2:D:95:ASN:HB3	2:D:96:LYS:CB	2.41	0.51
1:C:32:GLU:HB3	1:C:37:ALA:HA	1.91	0.51
1:C:28:GLN:HG2	2:D:155:TYR:HH	1.75	0.51
1:C:77:ARG:HH22	2:D:114:PRO:CG	2.24	0.51
1:C:66:THR:O	1:C:70:LYS:HG3	2.11	0.51
1:A:32:GLU:HB3	1:A:37:ALA:HA	1.92	0.51
1:C:14:TYR:CZ	1:C:89:LYS:HD2	2.46	0.51
2:D:272:ILE:O	2:D:276:GLU:N	2.44	0.51
2:B:271:LYS:O	2:B:274:ASN:HB3	2.11	0.51
1:C:40:GLN:HG2	2:D:243:GLN:HE22	1.76	0.51
1:A:39:ILE:HD12	1:A:75:ARG:CD	2.41	0.50
1:C:63:LYS:HA	2:D:103:THR:HG22	1.93	0.50
2:B:298:GLU:O	2:B:299:TYR:HD2	1.95	0.50
2:D:105:ILE:HG22	2:D:108:ASP:HB3	1.93	0.50
2:B:276:GLU:O	2:B:279:GLN:HG2	2.11	0.49
1:C:20:GLN:O	1:C:24:ILE:HG12	2.11	0.49
1:A:126:LYS:O	2:D:104:TYR:HE2	1.95	0.49
1:C:76:ARG:HH11	2:D:111:ASN:HB2	1.76	0.49
2:D:155:TYR:O	2:D:155:TYR:CD2	2.65	0.49
2:B:269:LEU:HD23	2:B:269:LEU:O	2.12	0.49
1:C:43:PHE:O	1:C:44:ASN:C	2.51	0.49
2:D:235:ASN:O	2:D:238:GLU:HG2	2.11	0.49
2:B:104:TYR:C	2:B:105:ILE:HG23	2.33	0.49
2:B:102:LEU:HB2	2:B:103:THR:HG23	1.94	0.49
2:B:153:LYS:O	2:B:157:PRO:HD2	2.13	0.48
1:C:8:PRO:HB3	2:D:149:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:LEU:O	2:D:269:LEU:HD23	2.13	0.48
2:B:214:THR:O	2:B:229:PHE:CZ	2.48	0.48
2:B:298:GLU:O	2:B:299:TYR:CD2	2.66	0.48
1:C:39:ILE:HD12	1:C:75:ARG:HD2	1.95	0.48
2:D:249:SER:HA	2:D:252:ARG:HH12	1.78	0.48
2:B:292:ARG:HB3	2:B:292:ARG:CZ	2.43	0.48
2:B:295:PHE:C	2:B:295:PHE:CD2	2.87	0.48
1:C:108:ARG:NH1	1:C:108:ARG:HB2	2.29	0.48
1:C:28:GLN:HE21	1:C:32:GLU:HG3	1.79	0.47
1:A:108:ARG:HB2	1:A:108:ARG:NH1	2.29	0.47
1:A:32:GLU:OE1	1:A:38:THR:N	2.44	0.47
2:B:272:ILE:O	2:B:276:GLU:N	2.47	0.47
1:A:43:PHE:CG	2:B:148:LEU:HG	2.49	0.47
1:C:103:LEU:HD21	1:C:113:VAL:HG22	1.95	0.47
2:D:266:GLU:HA	2:D:269:LEU:HB3	1.95	0.47
2:B:271:LYS:HA	2:B:274:ASN:HB3	1.97	0.47
2:D:271:LYS:O	2:D:274:ASN:HB3	2.15	0.47
1:A:66:THR:O	1:A:70:LYS:HG3	2.15	0.46
1:C:47:TRP:NE1	1:C:51:LYS:HD2	2.30	0.46
1:C:76:ARG:O	1:C:77:ARG:C	2.53	0.46
2:D:147:SER:HB3	2:D:150:GLN:CG	2.44	0.46
1:C:43:PHE:CG	2:D:148:LEU:HG	2.50	0.46
2:B:155:TYR:O	2:B:155:TYR:CD2	2.69	0.46
1:C:125:GLN:HG3	1:C:126:LYS:N	2.31	0.46
2:D:269:LEU:O	2:D:272:ILE:CG1	2.56	0.46
1:C:82:TYR:CE2	2:D:148:LEU:HD23	2.49	0.46
1:A:79:CYS:HA	1:A:82:TYR:HD2	1.80	0.46
2:D:276:GLU:O	2:D:279:GLN:HG2	2.16	0.46
2:D:292:ARG:HB3	2:D:292:ARG:CZ	2.44	0.46
2:D:99:PHE:CZ	2:D:103:THR:HG21	2.48	0.46
2:D:153:LYS:O	2:D:157:PRO:HD2	2.15	0.46
1:C:104:PHE:O	1:C:108:ARG:HA	2.16	0.45
1:A:125:GLN:O	1:A:128:THR:N	2.39	0.45
2:B:277:GLN:O	2:B:280:LEU:HB3	2.16	0.45
1:A:92:GLU:OE1	2:B:100:ARG:HG2	2.17	0.45
2:D:262:ARG:O	2:D:265:LYS:HB3	2.17	0.45
2:D:298:GLU:HB2	2:D:299:TYR:CD2	2.52	0.45
2:D:156:LEU:HD22	2:D:159:ALA:HB3	1.98	0.45
1:A:26:ARG:HB2	1:A:45:TYR:CE1	2.52	0.45
1:C:26:ARG:O	1:C:30:VAL:HG23	2.17	0.45
1:C:43:PHE:CE2	2:D:148:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:THR:OG1	2:B:229:PHE:CE2	2.52	0.45
1:A:52:SER:OG	1:A:53:THR:N	2.50	0.45
1:A:123:LYS:CE	1:C:98:ARG:HH12	2.29	0.44
2:D:154:SER:O	2:D:157:PRO:HG2	2.17	0.44
2:D:239:PHE:HD2	2:D:240:LEU:HD12	1.80	0.44
2:D:277:GLN:O	2:D:280:LEU:HB3	2.17	0.44
2:B:108:ASP:O	2:B:109:LEU:C	2.52	0.44
2:B:105:ILE:HG21	2:B:105:ILE:HD13	1.52	0.44
1:A:47:TRP:NE1	1:A:51:LYS:HD2	2.32	0.44
1:C:14:TYR:CE1	1:C:89:LYS:HD2	2.52	0.44
2:B:235:ASN:O	2:B:238:GLU:HG2	2.18	0.44
1:A:90:LEU:O	1:A:90:LEU:HD23	2.17	0.44
1:C:6:PHE:CE1	2:D:147:SER:HB2	2.53	0.44
1:C:59:ARG:HB3	2:D:99:PHE:CD1	2.52	0.43
1:C:42:ARG:NH2	1:C:71:GLU:OE1	2.45	0.43
2:D:271:LYS:HA	2:D:274:ASN:HB3	2.00	0.43
1:A:104:PHE:O	1:A:108:ARG:HA	2.18	0.43
1:A:123:LYS:HZ1	1:C:98:ARG:HH12	1.67	0.43
2:D:284:ASP:O	2:D:287:LYS:HB3	2.19	0.43
2:B:266:GLU:HA	2:B:269:LEU:HB3	1.99	0.43
2:B:94:ASP:O	2:B:97:THR:N	2.44	0.43
1:C:25:LEU:HD21	2:D:156:LEU:HD21	2.01	0.43
2:D:98:CYS:O	2:D:99:PHE:C	2.56	0.43
1:A:40:GLN:HB2	2:B:246:SER:OG	2.19	0.43
1:A:43:PHE:O	1:A:46:ALA:N	2.52	0.42
1:C:90:LEU:HD23	1:C:90:LEU:O	2.20	0.42
1:A:123:LYS:HE3	1:C:98:ARG:HH12	1.83	0.42
1:A:76:ARG:O	1:A:77:ARG:C	2.56	0.42
2:B:281:LEU:HD23	2:B:281:LEU:C	2.40	0.42
1:A:104:PHE:CD1	1:A:117:LYS:HD2	2.54	0.41
2:B:97:THR:HA	2:B:100:ARG:HG3	2.02	0.41
1:C:69:TYR:CE1	1:C:76:ARG:HB3	2.55	0.41
1:C:43:PHE:C	1:C:45:TYR:N	2.73	0.41
1:A:39:ILE:HD12	1:A:75:ARG:NE	2.34	0.41
2:B:161:LEU:HD23	2:B:161:LEU:O	2.19	0.41
2:B:271:LYS:HA	2:B:274:ASN:CB	2.50	0.41
2:B:284:ASP:O	2:B:287:LYS:HB3	2.21	0.41
2:B:299:TYR:O	2:B:300:GLY:C	2.59	0.41
1:A:26:ARG:O	1:A:30:VAL:HG23	2.21	0.41
1:A:95:MET:O	1:A:98:ARG:HB3	2.20	0.41
2:B:156:LEU:N	2:B:157:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ILE:HD12	1:C:85:ILE:HG23	1.75	0.41
2:B:160:GLU:C	2:B:162:ALA:N	2.74	0.41
2:B:216:ALA:C	2:B:218:SER:H	2.24	0.41
2:B:298:GLU:C	2:B:299:TYR:CD2	2.90	0.41
1:A:126:LYS:HA	1:A:129:LEU:HG	2.03	0.41
1:C:39:ILE:HD12	1:C:75:ARG:CD	2.50	0.41
1:C:76:ARG:NH1	2:D:111:ASN:HB2	2.36	0.41
2:D:231:GLN:HA	2:D:234:VAL:HG12	2.02	0.41
2:D:238:GLU:HG3	2:D:239:PHE:N	2.35	0.41
1:C:7:TRP:NE1	1:C:81:TYR:CG	2.89	0.40
1:A:14:TYR:CE1	1:A:89:LYS:HD2	2.56	0.40
2:B:108:ASP:N	2:B:108:ASP:OD2	2.54	0.40
1:A:26:ARG:O	1:A:29:VAL:N	2.55	0.40
2:B:105:ILE:HG13	2:B:109:LEU:CD1	2.47	0.40
2:B:156:LEU:HD22	2:B:159:ALA:HB3	2.03	0.40
2:D:257:GLU:O	2:D:261:LEU:HB2	2.20	0.40
2:B:151:GLY:HA2	2:B:242:ILE:HG21	2.04	0.40
2:D:245:ASN:HA	2:D:248:LEU:CB	2.47	0.40

All (2) 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)
2:D:98:CYS:SG	2:D:98:CYS:SG[5_555]	1.04	1.16
2:D:218:SER:OG	2:D:292:ARG:NH2[5_555]	1.82	0.38

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	125/129 (97%)	118 (94%)	6 (5%)	1 (1%)	19 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	123/129 (95%)	115 (94%)	7 (6%)	1 (1%)	19 57
2	B	126/242 (52%)	118 (94%)	7 (6%)	1 (1%)	19 57
2	D	129/242 (53%)	119 (92%)	10 (8%)	0	100 100
All	All	503/742 (68%)	470 (93%)	30 (6%)	3 (1%)	25 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLY
1	C	34	GLY
2	B	217	ILE

5.3.2 Protein sidechains

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	109/116 (94%)	104 (95%)	5 (5%)	27 55
1	C	105/116 (90%)	100 (95%)	5 (5%)	25 54
2	B	110/217 (51%)	103 (94%)	7 (6%)	17 47
2	D	111/217 (51%)	98 (88%)	13 (12%)	5 26
All	All	435/666 (65%)	405 (93%)	30 (7%)	15 45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TRP
1	A	9	THR
1	A	15	GLU
1	A	95	MET
1	A	112	GLN
2	B	107	ASP
2	B	108	ASP
2	B	156	LEU

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Mol	Chain	Res	Type
2	B	219	SER
2	B	227	LYS
2	B	266	GLU
2	B	295	PHE
1	C	7	TRP
1	C	9	THR
1	C	15	GLU
1	C	95	MET
1	C	112	GLN
2	D	95	ASN
2	D	99	PHE
2	D	105	ILE
2	D	107	ASP
2	D	109	LEU
2	D	113	ILE
2	D	156	LEU
2	D	219	SER
2	D	220	SER
2	D	227	LYS
2	D	266	GLU
2	D	296	LEU
2	D	299	TYR

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

Mol	Chain	Res	Type
1	A	28	GLN
1	A	109	ASN
1	A	112	GLN
2	B	231	GLN
2	B	243	GLN
2	B	285	ASN
1	C	28	GLN
1	C	109	ASN
1	C	112	GLN
2	D	231	GLN
2	D	243	GLN
2	D	285	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	127/129 (98%)	-0.42	0 100 100	101, 123, 134, 138	0
1	C	125/129 (96%)	-0.28	1 (0%) 86 79	108, 124, 135, 145	0
2	B	132/242 (54%)	-0.56	0 100 100	104, 128, 138, 145	0
2	D	135/242 (55%)	-0.39	0 100 100	108, 133, 146, 152	0
All	All	519/742 (69%)	-0.42	1 (0%) 95 93	101, 127, 142, 152	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	VAL	2.0

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.