



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:17 PM GMT

PDB ID : 4QQF  
Title : Crystal structure of mitochondrial import inner membrane translocase subunit TIM50  
Authors : Li, J.Z.  
Deposited on : 2014-06-27  
Resolution : 2.67 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

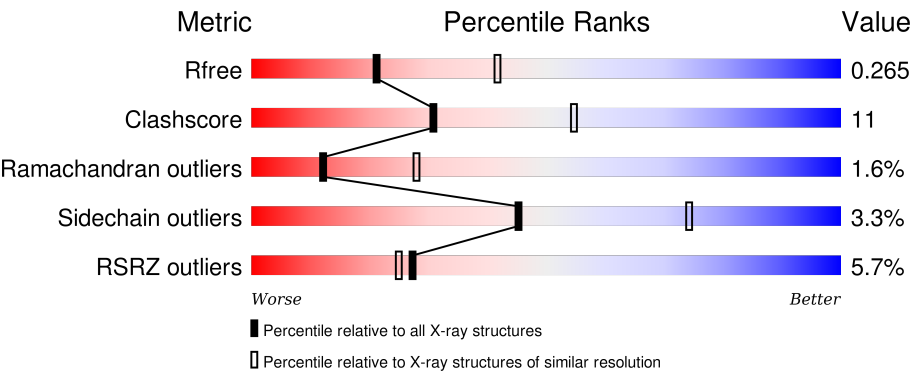
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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 <sub>free</sub>	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	202	<div><div>4%</div><div><div></div><div>80%</div><div>14%</div><div>•••</div></div></div>
1	B	202	<div><div>2%</div><div><div></div><div>76%</div><div>12%</div><div>•</div><div>10%</div></div></div>
1	C	202	<div><div>3%</div><div><div></div><div>85%</div><div>9%</div><div>••</div></div></div>
1	D	202	<div><div>6%</div><div><div></div><div>75%</div><div>14%</div><div>••</div><div>7%</div></div></div>
1	E	202	<div><div>3%</div><div><div></div><div>77%</div><div>12%</div><div></div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	202	

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	MG	A	401	-	-	-	X
2	MG	B	401	-	-	-	X
2	MG	C	401	-	-	-	X
2	MG	D	401	-	-	-	X
2	MG	E	401	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9432 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 import inner membrane translocase subunit TIM50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	187	Total	C	N	O	S	0	0	0
			1550	1011	249	286	4			
1	A	198	Total	C	N	O	S	0	0	0
			1641	1070	263	302	6			
1	B	181	Total	C	N	O	S	0	0	0
			1496	973	242	277	4			
1	C	193	Total	C	N	O	S	0	0	0
			1602	1045	256	296	5			
1	E	182	Total	C	N	O	S	0	0	0
			1504	981	241	278	4			
1	F	191	Total	C	N	O	S	0	0	0
			1584	1035	251	293	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	160	GLY	-	EXPRESSION TAG	UNP Q02776
D	161	SER	-	EXPRESSION TAG	UNP Q02776
D	162	HIS	-	EXPRESSION TAG	UNP Q02776
D	163	MET	-	EXPRESSION TAG	UNP Q02776
A	160	GLY	-	EXPRESSION TAG	UNP Q02776
A	161	SER	-	EXPRESSION TAG	UNP Q02776
A	162	HIS	-	EXPRESSION TAG	UNP Q02776
A	163	MET	-	EXPRESSION TAG	UNP Q02776
B	160	GLY	-	EXPRESSION TAG	UNP Q02776
B	161	SER	-	EXPRESSION TAG	UNP Q02776
B	162	HIS	-	EXPRESSION TAG	UNP Q02776
B	163	MET	-	EXPRESSION TAG	UNP Q02776
C	160	GLY	-	EXPRESSION TAG	UNP Q02776
C	161	SER	-	EXPRESSION TAG	UNP Q02776
C	162	HIS	-	EXPRESSION TAG	UNP Q02776
C	163	MET	-	EXPRESSION TAG	UNP Q02776

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Chain	Residue	Modelled	Actual	Comment	Reference
E	160	GLY	-	EXPRESSION TAG	UNP Q02776
E	161	SER	-	EXPRESSION TAG	UNP Q02776
E	162	HIS	-	EXPRESSION TAG	UNP Q02776
E	163	MET	-	EXPRESSION TAG	UNP Q02776
F	160	GLY	-	EXPRESSION TAG	UNP Q02776
F	161	SER	-	EXPRESSION TAG	UNP Q02776
F	162	HIS	-	EXPRESSION TAG	UNP Q02776
F	163	MET	-	EXPRESSION TAG	UNP Q02776

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

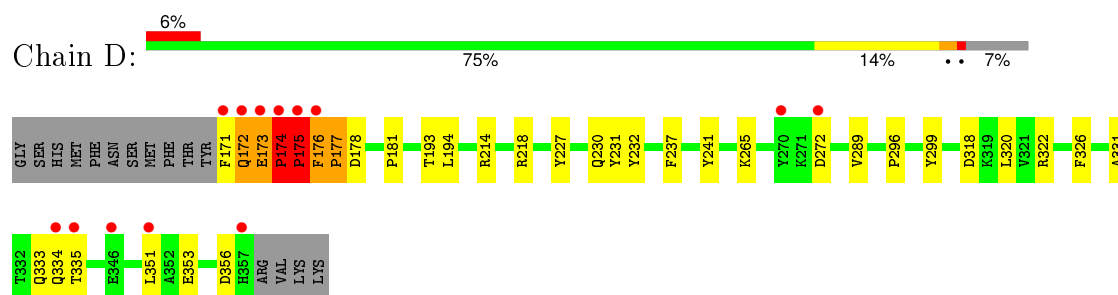
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	12	Total O 12 12	0	0
3	A	17	Total O 17 17	0	0
3	B	6	Total O 6 6	0	0
3	C	6	Total O 6 6	0	0
3	E	6	Total O 6 6	0	0
3	F	2	Total O 2 2	0	0

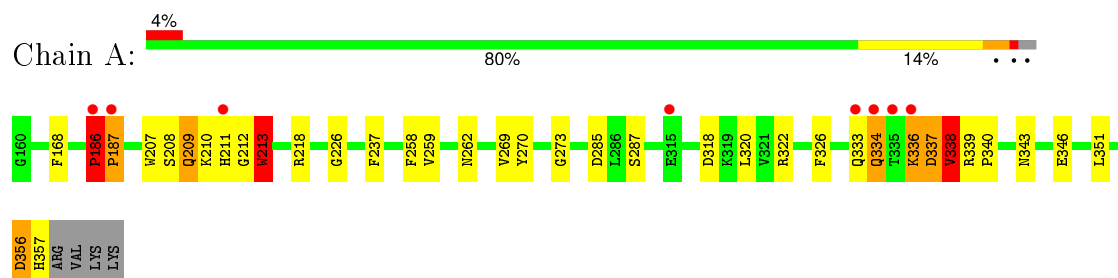
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

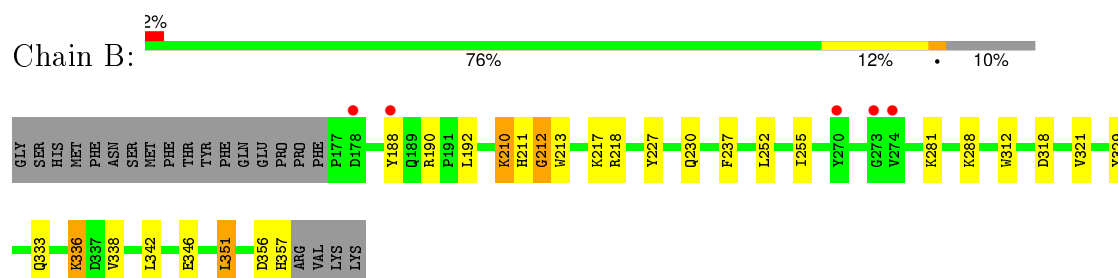
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



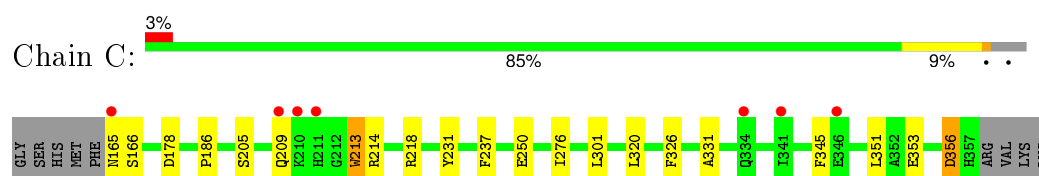
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



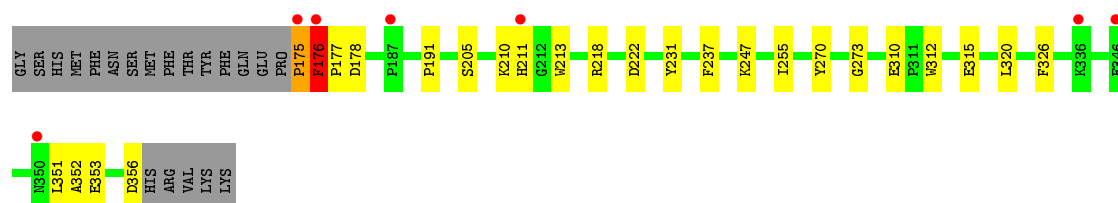
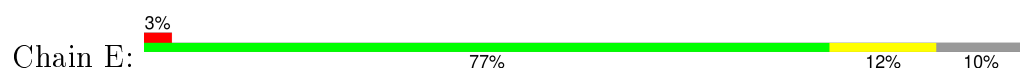
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



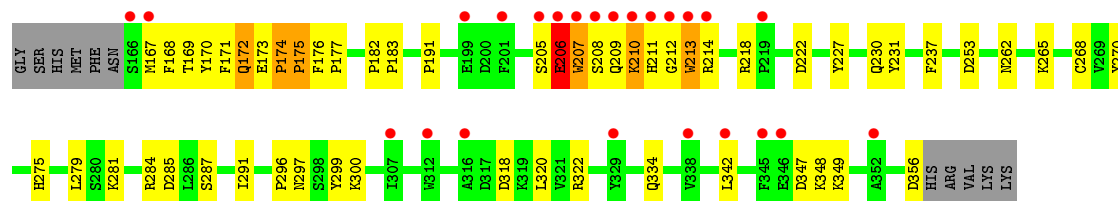
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.29Å 164.29Å 150.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.52 – 2.67 47.99 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.52-2.67) 95.7 (47.99-2.67)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.212 , 0.252 0.235 , 0.265	Depositor DCC
$R_{free}$ test set	2816 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.6	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 58660 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.60	2/1696 (0.1%)	0.78	1/2309 (0.0%)
1	B	0.51	0/1543	0.75	2/2101 (0.1%)
1	C	0.50	0/1655	0.71	1/2255 (0.0%)
1	D	0.56	2/1601 (0.1%)	0.79	3/2182 (0.1%)
1	E	0.53	1/1552 (0.1%)	0.68	1/2114 (0.0%)
1	F	0.50	2/1636 (0.1%)	0.72	2/2229 (0.1%)
All	All	0.54	7/9683 (0.1%)	0.74	10/13190 (0.1%)

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	B	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	PRO	N-CD	5.82	1.55	1.47
1	A	338	VAL	CB-CG2	-5.70	1.40	1.52
1	D	174	PRO	N-CD	5.54	1.55	1.47
1	F	174	PRO	N-CD	5.27	1.55	1.47
1	A	213	TRP	CB-CG	5.16	1.59	1.50
1	F	175	PRO	N-CD	5.05	1.54	1.47
1	E	175	PRO	N-CD	5.02	1.54	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	TRP	CA-CB-CG	6.43	125.91	113.70
1	D	176	PHE	N-CA-C	6.29	127.98	111.00
1	C	213	TRP	CA-CB-CG	6.27	125.61	113.70
1	B	351	LEU	CA-CB-CG	6.23	129.63	115.30
1	D	174	PRO	C-N-CD	6.12	141.25	128.40
1	E	176	PHE	C-N-CD	5.70	140.37	128.40
1	F	173	GLU	C-N-CD	5.60	140.16	128.40
1	F	174	PRO	C-N-CD	5.32	139.58	128.40
1	A	186	PRO	C-N-CD	-5.19	109.18	120.60
1	D	175	PRO	CA-N-CD	-5.08	104.39	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	212	GLY	Peptide
1	B	356	ASP	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1641	0	1590	40	0
1	B	1496	0	1467	15	0
1	C	1602	0	1557	11	0
1	D	1550	0	1512	47	0
1	E	1504	0	1476	28	0
1	F	1584	0	1544	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	17	0	0	0	1
3	B	6	0	0	3	0
3	C	6	0	0	0	0
3	D	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	6	0	0	0	0
3	F	2	0	0	0	0
All	All	9432	0	9146	202	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 11.

All (202) 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:F:207:TRP:CD1	1:F:213:TRP:HZ3	1.48	1.31
1:F:207:TRP:CE2	1:F:213:TRP:CH2	2.20	1.30
1:F:207:TRP:CD1	1:F:213:TRP:CZ3	2.20	1.30
1:A:337:ASP:OD1	1:A:339:ARG:NE	1.72	1.20
1:F:207:TRP:CE2	1:F:213:TRP:CZ3	2.36	1.13
1:F:207:TRP:NE1	1:F:213:TRP:CZ3	2.19	1.10
1:F:207:TRP:CG	1:F:213:TRP:CZ3	2.40	1.08
1:F:207:TRP:CZ3	1:F:212:GLY:HA2	1.95	1.01
1:F:207:TRP:CD2	1:F:213:TRP:CZ3	2.49	1.01
1:F:207:TRP:NE1	1:F:213:TRP:CH2	2.30	1.00
1:D:318:ASP:CG	1:D:322:ARG:NH1	2.15	1.00
1:D:318:ASP:OD2	1:D:322:ARG:NH1	2.00	0.94
1:F:171:PHE:O	1:F:172:GLN:HB2	1.67	0.93
1:F:207:TRP:CZ2	1:F:213:TRP:CH2	2.57	0.92
1:A:209:GLN:CD	1:F:183:PRO:HD2	1.91	0.91
1:A:337:ASP:CG	1:A:339:ARG:HE	1.74	0.90
1:F:207:TRP:HZ3	1:F:212:GLY:HA2	1.37	0.88
1:B:357:HIS:CD2	3:B:506:HOH:O	2.27	0.88
1:F:175:PRO:O	1:F:177:PRO:HD3	1.74	0.88
1:D:318:ASP:CG	1:D:322:ARG:HH11	1.77	0.87
1:F:265:LYS:CE	1:F:275:HIS:CD2	2.57	0.87
1:F:270:TYR:CD2	1:F:275:HIS:CE1	2.63	0.87
1:A:209:GLN:NE2	1:F:183:PRO:HD2	1.90	0.86
1:A:337:ASP:CG	1:A:339:ARG:HH21	1.81	0.84
1:D:175:PRO:HG2	1:D:176:PHE:CD2	2.12	0.84
1:B:288:LYS:HZ1	1:B:336:LYS:HG2	1.42	0.83
1:A:337:ASP:O	1:A:339:ARG:N	2.12	0.82
1:A:337:ASP:OD2	1:A:339:ARG:NH2	2.13	0.81
1:E:176:PHE:CE2	1:E:178:ASP:HB2	2.15	0.81
1:F:169:THR:O	1:F:171:PHE:N	2.13	0.80
1:F:208:SER:N	1:F:212:GLY:O	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:PHE:CE2	1:D:173:GLU:HB2	2.16	0.80
1:F:265:LYS:HE3	1:F:275:HIS:CD2	2.18	0.78
1:F:207:TRP:CG	1:F:213:TRP:CE3	2.72	0.77
1:B:357:HIS:HD2	3:B:506:HOH:O	1.66	0.77
1:F:265:LYS:NZ	1:F:275:HIS:CD2	2.54	0.76
1:D:172:GLN:HE22	1:C:178:ASP:H	1.36	0.74
1:A:209:GLN:NE2	1:F:183:PRO:CD	2.50	0.73
1:D:175:PRO:HG2	1:D:176:PHE:CE2	2.24	0.73
1:A:333:GLN:NE2	1:A:334:GLN:O	2.21	0.73
1:A:287:SER:HB2	1:A:337:ASP:HA	1.71	0.73
1:F:270:TYR:CE2	1:F:275:HIS:CE1	2.77	0.72
1:F:207:TRP:CE3	1:F:212:GLY:HA2	2.24	0.71
1:F:270:TYR:HD2	1:F:275:HIS:CE1	2.08	0.71
1:C:353:GLU:N	1:C:353:GLU:OE1	2.23	0.71
1:F:265:LYS:HE3	1:F:275:HIS:CG	2.26	0.71
1:D:174:PRO:HB2	1:D:178:ASP:O	1.91	0.70
1:E:176:PHE:HD2	1:E:177:PRO:N	1.92	0.68
1:B:288:LYS:NZ	1:B:336:LYS:HG2	2.08	0.67
1:F:207:TRP:CD2	1:F:213:TRP:CE3	2.83	0.66
1:A:336:LYS:O	1:A:338:VAL:N	2.28	0.66
1:B:192:LEU:HD23	1:B:288:LYS:HG3	1.77	0.66
1:F:297:ASN:HA	1:F:300:LYS:HG3	1.78	0.65
1:E:176:PHE:HE2	1:E:178:ASP:CB	2.09	0.65
1:D:175:PRO:HG2	1:D:176:PHE:HD2	1.58	0.65
1:E:176:PHE:HB2	1:E:177:PRO:HD2	1.81	0.63
1:D:173:GLU:HB3	1:D:174:PRO:HD2	1.80	0.63
1:F:207:TRP:CZ2	1:F:213:TRP:CZ2	2.87	0.63
1:D:333:GLN:O	1:D:335:THR:N	2.33	0.62
1:A:285:ASP:OD2	1:A:287:SER:OG	2.17	0.61
1:A:337:ASP:CG	1:A:339:ARG:NH2	2.50	0.61
1:D:318:ASP:OD1	1:D:322:ARG:NH1	2.31	0.61
1:D:171:PHE:CZ	1:D:173:GLU:HB2	2.36	0.60
1:F:227:TYR:O	1:F:230:GLN:HG2	2.02	0.60
1:A:207:TRP:HB2	1:A:213:TRP:CZ3	2.36	0.59
1:E:353:GLU:N	1:E:353:GLU:OE1	2.35	0.59
1:A:346:GLU:OE1	1:A:346:GLU:N	2.35	0.58
1:D:173:GLU:HG2	1:D:174:PRO:HD3	1.85	0.58
1:F:285:ASP:OD1	1:F:287:SER:OG	2.14	0.58
1:E:176:PHE:HE2	1:E:178:ASP:CG	2.07	0.57
1:D:173:GLU:CG	1:D:174:PRO:HD3	2.35	0.57
1:E:176:PHE:HD2	1:E:178:ASP:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:HG3	1:D:181:PRO:HD3	1.87	0.57
1:D:174:PRO:CB	1:D:178:ASP:O	2.52	0.57
1:F:206:GLU:HG2	1:F:207:TRP:N	2.19	0.56
1:D:227:TYR:O	1:D:230:GLN:HG2	2.05	0.56
1:E:176:PHE:CE2	1:E:178:ASP:CB	2.85	0.56
1:D:172:GLN:NE2	1:C:178:ASP:H	2.00	0.56
1:F:208:SER:O	1:F:212:GLY:N	2.39	0.56
1:A:209:GLN:OE1	1:F:182:PRO:HA	2.06	0.56
1:F:176:PHE:HD2	1:F:176:PHE:H	1.54	0.55
1:D:173:GLU:HB3	1:D:174:PRO:CD	2.37	0.55
1:D:171:PHE:CE2	1:D:173:GLU:CB	2.89	0.54
1:B:210:LYS:HD2	1:B:211:HIS:CE1	2.43	0.54
1:F:347:ASP:OD1	1:F:349:LYS:HE3	2.07	0.54
1:F:270:TYR:CD2	1:F:275:HIS:HE1	2.22	0.54
1:D:173:GLU:CG	1:D:174:PRO:CD	2.85	0.54
1:E:176:PHE:CD2	1:E:177:PRO:N	2.74	0.54
1:D:353:GLU:O	1:D:356:ASP:HB2	2.06	0.54
1:F:209:GLN:O	1:F:211:HIS:N	2.40	0.54
1:A:337:ASP:OD1	1:A:339:ARG:CZ	2.52	0.54
1:D:173:GLU:CB	1:D:174:PRO:CD	2.86	0.54
1:F:207:TRP:NE1	1:F:213:TRP:HH2	2.01	0.54
1:F:265:LYS:HZ1	1:F:275:HIS:CD2	2.25	0.54
1:E:176:PHE:CD2	1:E:177:PRO:CD	2.91	0.53
1:E:218:ARG:HD3	1:E:320:LEU:HD22	1.90	0.53
1:A:212:GLY:HA3	1:A:213:TRP:O	2.09	0.53
1:A:207:TRP:HB2	1:A:213:TRP:HZ3	1.74	0.53
1:C:276:ILE:HG21	1:C:301:LEU:HG	1.90	0.53
1:D:171:PHE:CZ	1:D:173:GLU:CB	2.92	0.52
1:E:191:PRO:HD2	1:E:231:TYR:O	2.10	0.52
1:F:206:GLU:OE2	1:F:214:ARG:HB3	2.09	0.52
1:B:227:TYR:O	1:B:230:GLN:HG2	2.10	0.52
1:D:218:ARG:HD3	1:D:320:LEU:HD22	1.92	0.51
1:E:326:PHE:CD2	1:E:351:LEU:HD21	2.45	0.51
1:F:206:GLU:CG	1:F:207:TRP:N	2.73	0.51
1:D:231:TYR:HB3	1:D:331:ALA:CB	2.40	0.51
1:F:205:SER:O	1:F:206:GLU:HB3	2.09	0.51
1:F:210:LYS:O	1:F:210:LYS:HG3	2.11	0.51
3:D:508:HOH:O	1:F:262:ASN:HB2	2.10	0.51
1:E:310:GLU:N	1:E:310:GLU:OE1	2.44	0.51
1:F:270:TYR:HD2	1:F:275:HIS:HE1	1.58	0.51
1:D:174:PRO:CG	1:D:178:ASP:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASP:CG	1:A:339:ARG:NE	2.46	0.50
1:D:173:GLU:HG2	1:D:174:PRO:CD	2.42	0.50
1:B:281:LYS:HD3	3:B:501:HOH:O	2.11	0.50
1:D:326:PHE:CD2	1:D:351:LEU:HD21	2.46	0.50
1:A:337:ASP:C	1:A:339:ARG:H	2.13	0.50
1:E:222:ASP:HA	1:E:255:ILE:HG12	1.94	0.49
1:B:217:LYS:HD3	1:B:252:LEU:HD23	1.93	0.49
1:D:175:PRO:CG	1:D:176:PHE:HD2	2.23	0.49
1:D:171:PHE:CE1	1:D:173:GLU:CD	2.86	0.49
1:A:337:ASP:OD2	1:A:339:ARG:CZ	2.60	0.48
1:F:222:ASP:OD1	1:F:222:ASP:N	2.47	0.48
1:F:342:LEU:HB3	1:F:348:LYS:HE2	1.95	0.48
1:E:176:PHE:HB2	1:E:177:PRO:CD	2.44	0.47
1:F:296:PRO:O	1:F:300:LYS:HG3	2.14	0.47
1:D:176:PHE:N	1:D:177:PRO:HA	2.28	0.47
1:E:176:PHE:CD2	1:E:177:PRO:HD2	2.49	0.47
1:E:176:PHE:CB	1:E:177:PRO:HD2	2.44	0.47
1:A:318:ASP:OD2	1:A:322:ARG:NH2	2.47	0.47
1:A:168:PHE:CD2	1:B:318:ASP:HB3	2.49	0.47
1:A:218:ARG:HD3	1:A:320:LEU:HD22	1.98	0.46
1:E:176:PHE:HE2	1:E:178:ASP:OD2	1.99	0.46
1:A:340:PRO:HA	1:A:343:ASN:HB3	1.98	0.46
1:D:175:PRO:CB	1:D:176:PHE:HD2	2.29	0.46
1:F:207:TRP:CZ3	1:F:212:GLY:CA	2.85	0.46
1:A:337:ASP:CG	1:A:339:ARG:CZ	2.85	0.46
1:C:218:ARG:HD3	1:C:320:LEU:HD22	1.97	0.46
1:E:210:LYS:HG3	1:E:211:HIS:CE1	2.51	0.46
1:A:208:SER:OG	1:A:211:HIS:O	2.24	0.46
1:C:209:GLN:CD	1:C:209:GLN:H	2.19	0.46
1:C:326:PHE:CD2	1:C:351:LEU:HD21	2.51	0.45
1:C:345:PHE:CE2	1:C:351:LEU:HG	2.51	0.45
1:D:296:PRO:HA	1:D:299:TYR:CZ	2.51	0.45
1:E:312:TRP:NE1	1:E:315:GLU:O	2.42	0.45
1:A:356:ASP:N	1:A:356:ASP:OD1	2.50	0.45
1:F:320:LEU:HA	1:F:320:LEU:HD12	1.82	0.45
1:E:175:PRO:O	1:E:176:PHE:CG	2.70	0.45
1:A:318:ASP:OD1	1:A:322:ARG:NH1	2.49	0.45
1:E:176:PHE:CE2	1:E:178:ASP:OD2	2.70	0.45
1:D:194:LEU:HB2	1:D:232:TYR:CD2	2.52	0.45
1:D:176:PHE:O	1:D:176:PHE:CD1	2.70	0.45
1:E:175:PRO:O	1:E:176:PHE:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLY:HA2	1:A:258:PHE:CD1	2.52	0.45
1:D:175:PRO:O	1:D:176:PHE:CD2	2.70	0.44
1:F:265:LYS:CE	1:F:275:HIS:CG	2.92	0.44
1:C:231:TYR:HB3	1:C:331:ALA:CB	2.47	0.44
1:E:176:PHE:CG	1:E:177:PRO:HD2	2.53	0.44
1:F:210:LYS:O	1:F:211:HIS:CD2	2.70	0.44
1:A:209:GLN:CG	1:F:183:PRO:HD2	2.48	0.44
1:F:279:LEU:HD11	1:F:291:ILE:HD12	2.00	0.44
1:A:207:TRP:HE3	1:A:213:TRP:CE3	2.35	0.43
1:D:171:PHE:CZ	1:D:173:GLU:CD	2.92	0.43
1:F:218:ARG:HD3	1:F:320:LEU:HD22	2.00	0.43
1:F:191:PRO:HD2	1:F:231:TYR:O	2.18	0.43
1:D:171:PHE:CE1	1:D:173:GLU:OE2	2.71	0.43
1:A:209:GLN:HG3	1:F:182:PRO:HB3	2.00	0.43
1:A:356:ASP:HA	1:A:357:HIS:HA	1.75	0.43
1:A:326:PHE:CD2	1:A:351:LEU:HD21	2.54	0.43
1:F:183:PRO:HD3	1:F:284:ARG:NH1	2.33	0.43
1:E:352:ALA:HB3	1:E:353:GLU:OE1	2.19	0.43
1:B:329:TYR:O	1:B:333:GLN:HB2	2.19	0.43
1:A:186:PRO:CB	1:A:187:PRO:HD2	2.48	0.43
1:D:241:TYR:CD1	1:D:265:LYS:HB3	2.53	0.43
1:A:337:ASP:C	1:A:339:ARG:N	2.72	0.43
1:D:175:PRO:C	1:D:176:PHE:CD2	2.92	0.43
1:B:188:TYR:HA	1:B:190:ARG:HH12	1.84	0.43
1:B:218:ARG:HA	1:B:312:TRP:CH2	2.54	0.43
1:F:176:PHE:N	1:F:176:PHE:CD2	2.79	0.43
1:F:265:LYS:CE	1:F:275:HIS:NE2	2.81	0.43
1:F:172:GLN:NE2	1:F:268:CYS:O	2.52	0.42
1:C:165:ASN:HA	1:C:166:SER:HA	1.70	0.42
1:A:259:VAL:HG11	1:A:262:ASN:OD1	2.19	0.42
1:F:206:GLU:CG	1:F:207:TRP:H	2.32	0.42
1:F:175:PRO:O	1:F:177:PRO:CD	2.57	0.42
1:B:252:LEU:O	1:B:255:ILE:HG22	2.20	0.42
1:F:318:ASP:O	1:F:322:ARG:HG2	2.19	0.42
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.92	0.42
1:D:193:THR:HB	1:D:289:VAL:HG22	2.02	0.41
1:E:213:TRP:CH2	1:E:247:LYS:HG2	2.55	0.41
1:F:172:GLN:O	1:F:176:PHE:CE1	2.73	0.41
1:D:272:ASP:O	1:D:272:ASP:OD1	2.38	0.41
1:A:270:TYR:OH	1:A:273:GLY:HA2	2.20	0.41
1:F:209:GLN:C	1:F:211:HIS:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:PRO:HA	1:F:175:PRO:HA	1.63	0.41
1:F:296:PRO:HA	1:F:299:TYR:CZ	2.56	0.41
1:C:356:ASP:N	1:C:356:ASP:OD1	2.53	0.41
1:D:333:GLN:O	1:D:335:THR:HG23	2.20	0.40
1:E:270:TYR:CZ	1:E:273:GLY:HA2	2.56	0.40
1:D:175:PRO:HB2	1:D:176:PHE:HD2	1.86	0.40
1:D:214:ARG:NH1	1:F:253:ASP:OD2	2.36	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)
3:A:511:HOH:O	3:A:511:HOH:O[8_554]	2.15	0.05

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	196/202 (97%)	183 (93%)	8 (4%)	5 (3%)	7	15
1	B	179/202 (89%)	176 (98%)	2 (1%)	1 (1%)	30	56
1	C	191/202 (95%)	181 (95%)	8 (4%)	2 (1%)	19	42
1	D	185/202 (92%)	177 (96%)	6 (3%)	2 (1%)	17	40
1	E	180/202 (89%)	176 (98%)	3 (2%)	1 (1%)	30	56
1	F	189/202 (94%)	171 (90%)	11 (6%)	7 (4%)	4	8
All	All	1120/1212 (92%)	1064 (95%)	38 (3%)	18 (2%)	12	28

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	334	GLN

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Mol	Chain	Res	Type
1	A	186	PRO
1	A	187	PRO
1	A	337	ASP
1	A	338	VAL
1	C	186	PRO
1	E	176	PHE
1	F	170	TYR
1	C	250	GLU
1	F	334	GLN
1	D	175	PRO
1	A	213	TRP
1	F	210	LYS
1	F	168	PHE
1	F	206	GLU
1	B	212	GLY
1	F	167	MET
1	F	172	GLN

### 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	184/188 (98%)	176 (96%)	8 (4%)	35	64
1	B	168/188 (89%)	161 (96%)	7 (4%)	36	65
1	C	180/188 (96%)	175 (97%)	5 (3%)	51	79
1	D	174/188 (93%)	169 (97%)	5 (3%)	50	78
1	E	169/188 (90%)	165 (98%)	4 (2%)	57	83
1	F	178/188 (95%)	172 (97%)	6 (3%)	44	73
All	All	1053/1128 (93%)	1018 (97%)	35 (3%)	45	74

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	172	GLN

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Mol	Chain	Res	Type
1	D	173	GLU
1	D	174	PRO
1	D	175	PRO
1	D	237	PHE
1	A	209	GLN
1	A	210	LYS
1	A	213	TRP
1	A	237	PHE
1	A	269	VAL
1	A	334	GLN
1	A	336	LYS
1	A	356	ASP
1	B	210	LYS
1	B	237	PHE
1	B	321	VAL
1	B	336	LYS
1	B	338	VAL
1	B	346	GLU
1	B	351	LEU
1	C	205	SER
1	C	213	TRP
1	C	214	ARG
1	C	237	PHE
1	C	356	ASP
1	E	176	PHE
1	E	205	SER
1	E	237	PHE
1	E	356	ASP
1	F	206	GLU
1	F	207	TRP
1	F	213	TRP
1	F	237	PHE
1	F	281	LYS
1	F	356	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	211	HIS
1	B	262	ASN
1	B	357	HIS
1	F	211	HIS

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Mol	Chain	Res	Type
1	F	275	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [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<sup>th</sup> 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(Å²)	Q<0.9
1	A	198/202 (98%)	0.34	8 (4%)	42	40	46, 60, 111, 192	0
1	B	181/202 (89%)	0.26	5 (2%)	56	55	48, 69, 104, 167	0
1	C	193/202 (95%)	0.29	7 (3%)	46	45	48, 69, 118, 141	0
1	D	187/202 (92%)	0.49	13 (6%)	19	17	24, 71, 117, 156	0
1	E	182/202 (90%)	0.32	7 (3%)	44	43	24, 68, 107, 131	0
1	F	191/202 (94%)	0.78	24 (12%)	5	4	57, 92, 148, 263	0
All	All	1132/1212 (93%)	0.41	64 (5%)	27	25	24, 70, 121, 263	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	PHE	6.5
1	D	175	PRO	5.9
1	D	174	PRO	5.8
1	E	176	PHE	5.8
1	A	335	THR	5.2
1	F	214	ARG	4.8
1	D	357	HIS	4.5
1	F	345	PHE	4.5
1	D	171	PHE	4.3
1	A	187	PRO	4.2
1	D	172	GLN	4.2
1	F	208	SER	4.1
1	D	272	ASP	3.8
1	D	334	GLN	3.8
1	D	173	GLU	3.8
1	F	212	GLY	3.8
1	A	334	GLN	3.8
1	C	210	LYS	3.8
1	A	336	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	205	SER	3.5
1	C	211	HIS	3.4
1	F	167	MET	3.3
1	C	209	GLN	3.3
1	C	165	ASN	3.2
1	F	201	PHE	3.2
1	F	338	VAL	3.1
1	C	334	GLN	3.0
1	F	213	TRP	3.0
1	E	346	GLU	3.0
1	B	270	TYR	3.0
1	F	210	LYS	3.0
1	D	351	LEU	2.8
1	E	175	PRO	2.7
1	F	207	TRP	2.7
1	F	211	HIS	2.7
1	A	333	GLN	2.7
1	F	316	ALA	2.6
1	A	315	GLU	2.6
1	E	336	LYS	2.6
1	D	270	TYR	2.6
1	B	274	VAL	2.6
1	F	312	TRP	2.5
1	B	178	ASP	2.5
1	E	211	HIS	2.5
1	F	199	GLU	2.4
1	F	307	ILE	2.4
1	F	206	GLU	2.4
1	E	187	PRO	2.4
1	F	352	ALA	2.4
1	F	346	GLU	2.4
1	F	342	LEU	2.3
1	D	335	THR	2.3
1	B	188	TYR	2.3
1	E	350	ASN	2.3
1	A	186	PRO	2.2
1	C	341	ILE	2.2
1	F	209	GLN	2.2
1	F	329	TYR	2.2
1	C	346	GLU	2.1
1	B	273	GLY	2.1
1	A	211	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	219	PRO	2.1
1	F	166	SER	2.0
1	D	346	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	D	401	1/1	0.88	0.73	25.46	68,68,68,68	0
2	MG	B	401	1/1	0.94	0.62	17.21	47,47,47,47	0
2	MG	E	401	1/1	0.97	0.53	13.76	39,39,39,39	0
2	MG	C	401	1/1	0.98	0.55	7.88	41,41,41,41	0
2	MG	A	401	1/1	0.97	0.49	6.98	41,41,41,41	0
2	MG	F	401	1/1	0.88	0.26	0.73	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.