



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:42 AM UTC

PDB ID : 4QQF / pdb_00004qqf
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

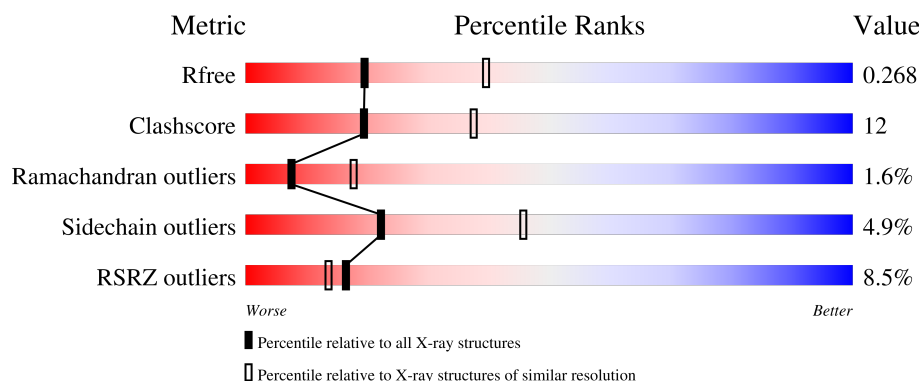
1 Overall quality at a glance

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_{free}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 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 $\leq 5\%$. 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	7% 78% 14% . . .
1	B	202	5% 73% 14% . 10%
1	C	202	5% 81% 12% . .
1	D	202	7% 73% 16% . . 7%
1	E	202	4% 75% 13% . 10%

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Mol	Chain	Length	Quality of chain
1	F	202	18% 63% 26% 5% 5%

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 (CCD ID: MG) (formula: Mg).

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

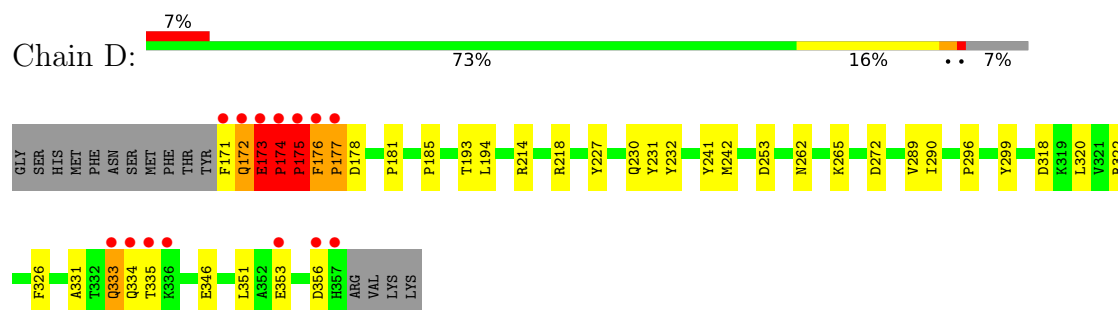
- Molecule 3 is water.

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

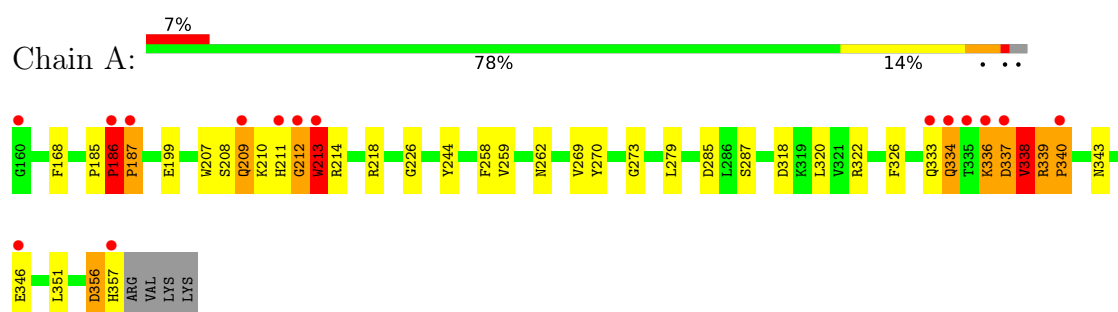
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

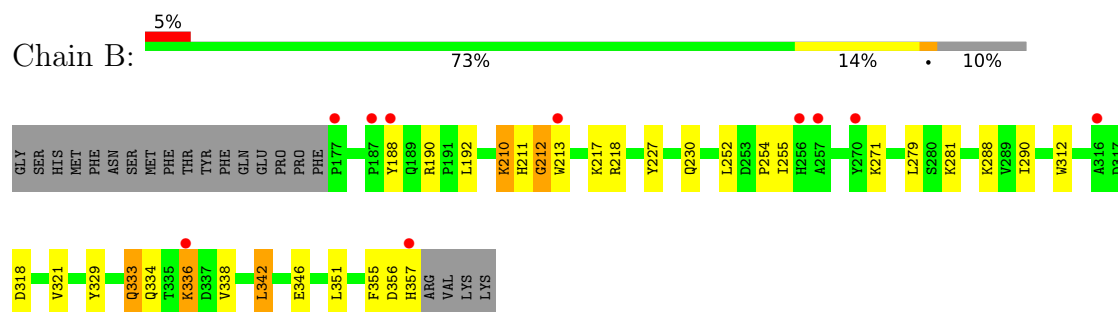
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



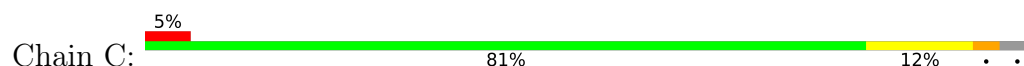
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50

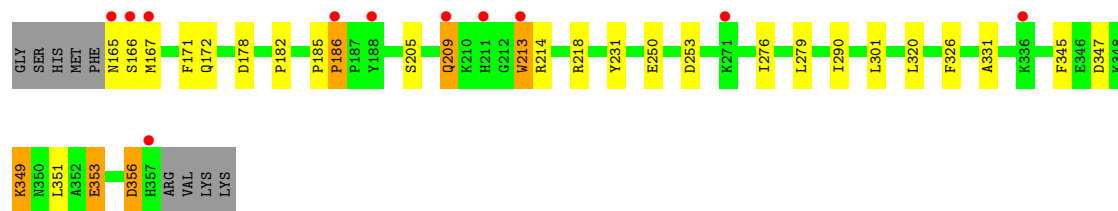


- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50

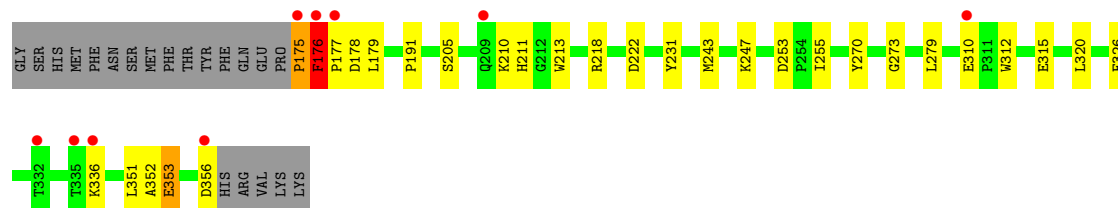
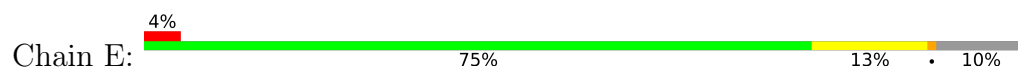


- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50

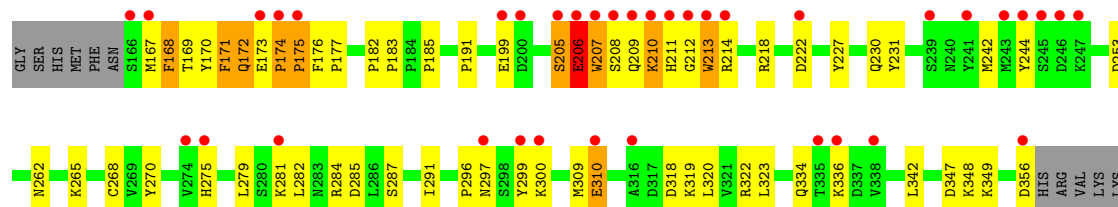




- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



- 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, α , β , γ	164.29Å 164.29Å 150.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.52 – 2.67 38.52 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.52-2.67) 95.6 (38.52-2.67)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.212 , 0.252 0.238 , 0.268	Depositor DCC
R_{free} test set	2937 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.73	1/1696 (0.1%)	1.19	11/2309 (0.5%)
1	B	0.64	0/1543	1.02	4/2101 (0.2%)
1	C	0.63	1/1655 (0.1%)	1.10	10/2255 (0.4%)
1	D	0.68	3/1601 (0.2%)	1.13	9/2182 (0.4%)
1	E	0.65	2/1552 (0.1%)	0.98	5/2114 (0.2%)
1	F	0.64	3/1636 (0.2%)	1.08	9/2229 (0.4%)
All	All	0.66	10/9683 (0.1%)	1.09	48/13190 (0.4%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	173	GLU	C-N	6.61	1.41	1.33
1	F	173	GLU	C-N	6.55	1.41	1.33
1	D	177	PRO	N-CD	5.82	1.55	1.47
1	D	174	PRO	N-CD	5.61	1.55	1.47
1	F	174	PRO	N-CD	5.34	1.55	1.47
1	A	339	ARG	CA-C	5.33	1.58	1.52
1	C	182	PRO	CA-C	5.26	1.54	1.51
1	E	176	PHE	C-N	5.24	1.41	1.34
1	E	175	PRO	N-CD	5.09	1.54	1.47
1	F	175	PRO	N-CD	5.05	1.54	1.47

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	185	PRO	CA-C-N	12.67	133.43	120.38
1	C	185	PRO	C-N-CA	12.67	133.43	120.38
1	A	339	ARG	CA-C-N	-11.36	108.09	119.56
1	A	339	ARG	C-N-CA	-11.36	108.09	119.56
1	C	186	PRO	CA-C-N	-10.34	108.87	120.04
1	C	186	PRO	C-N-CA	-10.34	108.87	120.04
1	A	185	PRO	CA-C-N	10.16	130.85	120.38
1	A	185	PRO	C-N-CA	10.16	130.85	120.38
1	A	186	PRO	CA-C-N	9.51	131.73	119.84
1	A	186	PRO	C-N-CA	9.51	131.73	119.84
1	F	174	PRO	C-N-CD	8.63	139.58	120.60
1	D	176	PHE	N-CA-C	8.22	127.98	109.81
1	D	185	PRO	CA-C-N	-7.81	113.96	119.66
1	D	185	PRO	C-N-CA	-7.81	113.96	119.66
1	D	176	PHE	C-N-CD	7.77	137.69	120.60
1	D	174	PRO	N-CA-C	7.58	119.95	110.70
1	E	179	LEU	N-CA-C	7.53	119.57	111.36
1	C	186	PRO	N-CA-C	7.52	119.88	110.70
1	B	333	GLN	N-CA-C	-7.34	103.92	113.17
1	C	185	PRO	O-C-N	7.26	124.56	121.15
1	F	173	GLU	CA-C-N	-7.18	112.98	120.38
1	F	173	GLU	C-N-CA	-7.18	112.98	120.38
1	D	253	ASP	CA-C-N	-7.11	112.38	119.56
1	D	253	ASP	C-N-CA	-7.11	112.38	119.56
1	F	171	PHE	N-CA-C	-6.99	99.21	110.32
1	A	339	ARG	N-CA-C	6.66	121.27	112.35
1	B	213	TRP	CA-CB-CG	6.48	125.91	113.60
1	C	253	ASP	CA-C-N	-6.37	113.13	119.56
1	C	253	ASP	C-N-CA	-6.37	113.13	119.56
1	C	213	TRP	CA-CB-CG	6.32	125.61	113.60
1	E	253	ASP	CA-C-N	-6.30	113.20	119.56
1	E	253	ASP	C-N-CA	-6.30	113.20	119.56
1	C	171	PHE	N-CA-C	5.85	117.96	109.71
1	A	214	ARG	N-CA-C	-5.81	99.71	109.07
1	F	310	GLU	CA-C-N	5.66	125.67	119.90
1	F	310	GLU	C-N-CA	5.66	125.67	119.90
1	D	175	PRO	CA-N-CD	-5.44	104.39	112.00
1	D	242	MET	N-CA-C	5.41	116.86	111.07
1	F	205	SER	N-CA-C	5.41	117.90	109.52
1	F	185	PRO	CA-C-N	5.24	123.48	119.66
1	F	185	PRO	C-N-CA	5.24	123.48	119.66
1	A	212	GLY	CA-C-N	5.22	131.10	121.70
1	A	212	GLY	C-N-CA	5.22	131.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	176	PHE	CA-C-N	-5.18	113.30	119.05
1	E	176	PHE	C-N-CA	-5.18	113.30	119.05
1	B	355	PHE	CA-C-N	-5.14	115.15	123.23
1	B	355	PHE	C-N-CA	-5.14	115.15	123.23
1	A	340	PRO	N-CA-C	5.04	120.17	113.86

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	41	0
1	B	1496	0	1467	16	0
1	C	1602	0	1557	14	0
1	D	1550	0	1512	48	0
1	E	1504	0	1476	30	0
1	F	1584	0	1544	77	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
3	E	6	0	0	0	0
3	F	2	0	0	0	0
All	All	9432	0	9146	214	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 12.

All (214) 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:D:318:ASP:CG	1:D:322:ARG:NH1	2.15	1.04
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:A:209:GLN:CD	1:F:183:PRO:HD2	1.91	0.95
1:A:337:ASP:CG	1:A:339:ARG:HE	1.74	0.95
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:D:318:ASP:CG	1:D:322:ARG:HH11	1.77	0.92
1:B:288:LYS:HZ1	1:B:336:LYS:HG2	1.35	0.90
1:A:337:ASP:CG	1:A:339:ARG:HH21	1.81	0.89
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: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	0.85
1:D:175:PRO:HG2	1:D:176:PHE:CD2	2.12	0.84
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:D:171:PHE:CE2	1:D:173:GLU:HB2	2.16	0.80
1:F:208:SER:N	1:F:212:GLY:O	2.11	0.80
1:F:265:LYS:HE3	1:F:275:HIS:CD2	2.18	0.78
1:B:357:HIS:HD2	3:B:506:HOH:O	1.66	0.77
1:F:207:TRP:CG	1:F:213:TRP:CE3	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:C:353:GLU:N	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:A:337:ASP:CG	1:A:339:ARG:NH2	2.50	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:D:173:GLU:HB3	1:D:174:PRO:HD2	1.80	0.63
1:E:176:PHE:HB2	1:E:177:PRO:HD2	1.81	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:E:176:PHE:HE2	1:E:178:ASP:CG	2.07	0.62
1:A:285:ASP:OD2	1:A:287:SER:OG	2.17	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:N	1:A:346:GLU:OE1	2.35	0.58
1:D:173:GLU:HG2	1:D:174:PRO:HD3	1.85	0.58
1:D:173:GLU:CG	1:D:174:PRO:HD3	2.35	0.57
1:D:173:GLU:HG3	1:D:181:PRO:HD3	1.87	0.57
1:E:176:PHE:HD2	1:E:178:ASP:H	1.53	0.57
1:D:174:PRO:CB	1:D:178:ASP:O	2.52	0.57
1:D:227:TYR:O	1:D:230:GLN:HG2	2.05	0.56
1:F:206:GLU:HG2	1:F:207:TRP:N	2.19	0.56
1:D:172:GLN:NE2	1:C:178:ASP:H	2.00	0.56
1:E:176:PHE:CE2	1:E:178:ASP:CB	2.85	0.56
1:F:208:SER:O	1:F:212:GLY:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLN:OE1	1:F:182:PRO:HA	2.06	0.56
1:F:176:PHE:H	1:F:176:PHE:HD2	1.54	0.55
1:A:337:ASP:CG	1:A:339:ARG:NE	2.46	0.55
1:C:353:GLU:H	1:C:353:GLU:CD	2.15	0.55
1:D:173:GLU:HB3	1:D:174:PRO:CD	2.37	0.55
1:A:337:ASP:C	1:A:339:ARG:H	2.13	0.54
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:D:173:GLU:CG	1:D:174:PRO:CD	2.85	0.54
1:F:270:TYR:CD2	1:F:275:HIS:HE1	2.22	0.54
1:E:176:PHE:CD2	1:E:177:PRO:N	2.74	0.54
1:D:171:PHE:CE1	1:D:173:GLU:CD	2.86	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:D:173:GLU:CB	1:D:174:PRO:CD	2.86	0.54
1:A:337:ASP:OD1	1:A:339:ARG:CZ	2.52	0.54
1:F:285:ASP:OD1	1:F:287:SER:OG	2.14	0.54
1:A:208:SER:OG	1:A:211:HIS:O	2.24	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
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:205:SER:O	1:F:206:GLU:HB3	2.09	0.51
1:F:210:LYS:HG3	1:F:210:LYS:O	2.11	0.51
1:D:174:PRO:CG	1:D:178:ASP:O	2.59	0.51
1:F:270:TYR:HD2	1:F:275:HIS:HE1	1.58	0.51
1:D:173:GLU:HG2	1:D:174:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASP:CG	1:A:339:ARG:CZ	2.85	0.50
1:C:209:GLN:H	1:C:209:GLN:CD	2.19	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:B:217:LYS:HD3	1:B:252:LEU:HD23	1.93	0.49
1:E:222:ASP:HA	1:E:255:ILE:HG12	1.94	0.49
1:D:175:PRO:CG	1:D:176:PHE:HD2	2.23	0.49
1:D:171:PHE:CZ	1:D:173:GLU:CD	2.92	0.48
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:A:337:ASP:C	1:A:339:ARG:N	2.72	0.48
1:D:175:PRO:C	1:D:176:PHE:CD2	2.92	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:A:318:ASP:OD2	1:A:322:ARG:NH2	2.47	0.47
1:E:176:PHE:CB	1:E:177:PRO:HD2	2.44	0.47
1:F:309:MET:HE1	1:F:319:LYS:HB3	1.96	0.47
1:B:254:PRO:HB3	1:E:243:MET:HE2	1.97	0.47
1:F:168:PHE:CD2	1:F:242:MET:HE1	2.50	0.47
1:D:262:ASN:HB2	1:C:167:MET:HE1	1.96	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:A:340:PRO:HA	1:A:343:ASN:HB3	1.98	0.46
1:E:176:PHE:HE2	1:E:178:ASP:OD2	1.99	0.46
1:D:175:PRO:CB	1:D:176:PHE:HD2	2.29	0.46
1:F:209:GLN:C	1:F:211:HIS:N	2.73	0.46
1:C:218:ARG:HD3	1:C:320:LEU:HD22	1.97	0.46
1:F:207:TRP:CZ3	1:F:212:GLY:CA	2.85	0.46
1:E:210:LYS:HG3	1:E:211:HIS:CE1	2.51	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:HD12	1:F:320:LEU:HA	1.82	0.45
1:A:318:ASP:OD1	1:A:322:ARG:NH1	2.49	0.45
1:C:347:ASP:OD1	1:C:349:LYS:NZ	2.44	0.45
1:E:175:PRO:O	1:E:176:PHE:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LEU:HB2	1:D:232:TYR:CD2	2.52	0.45
1:E:176:PHE:CE2	1:E:178:ASP:OD2	2.70	0.45
1:D:176:PHE:O	1:D:176:PHE:CD1	2.70	0.45
1:A:226:GLY:HA2	1:A:258:PHE:CD1	2.52	0.45
1:E:175:PRO:O	1:E:176:PHE:CD1	2.70	0.45
1:D:175:PRO:O	1:D:176:PHE:CD2	2.70	0.44
1:C:231:TYR:HB3	1:C:331:ALA:CB	2.47	0.44
1:F:265:LYS:CE	1:F:275:HIS:CG	2.92	0.44
1:E:176:PHE:CG	1:E:177:PRO:HD2	2.53	0.44
1:F:199:GLU:OE2	1:F:244:TYR:OH	2.29	0.44
1:F:210:LYS:O	1:F:211:HIS:CD2	2.70	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:F:191:PRO:HD2	1:F:231:TYR:O	2.18	0.43
1:F:218:ARG:HD3	1:F:320:LEU:HD22	2.00	0.43
1:D:171:PHE:CE1	1:D:173:GLU:OE2	2.71	0.43
1:A:199:GLU:OE2	1:A:244:TYR:OH	2.33	0.43
1:A:209:GLN:HG3	1:F:182:PRO:HB3	2.00	0.43
1:A:326:PHE:CD2	1:A:351:LEU:HD21	2.54	0.43
1:A:356:ASP:HA	1:A:357:HIS:HA	1.75	0.43
1:D:241:TYR:CD1	1:D:265:LYS:HB3	2.53	0.43
1:A:186:PRO:CB	1:A:187:PRO:HD2	2.48	0.43
1:B:329:TYR:O	1:B:333:GLN:HB2	2.19	0.43
1:E:352:ALA:HB3	1:E:353:GLU:OE1	2.19	0.43
1:F:183:PRO:HD3	1:F:284:ARG:NH1	2.33	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:CD2	1:F:176:PHE:N	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:F:297:ASN:CG	1:F:300:LYS:HE3	2.44	0.42
1:E:176:PHE:CD2	1:E:176:PHE:C	2.97	0.42
1:A:259:VAL:HG11	1:A:262:ASN:OD1	2.19	0.42
1:F:175:PRO:O	1:F:177:PRO:CD	2.57	0.42
1:F:206:GLU:CG	1:F:207:TRP:H	2.32	0.42
1:B:252:LEU:O	1:B:255:ILE:HG22	2.20	0.42
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.92	0.42
1:F:318:ASP:O	1:F:322:ARG:HG2	2.19	0.42
1:F:209:GLN:C	1:F:211:HIS:H	2.28	0.42
1:D:193:THR:HB	1:D:289:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:TRP:CH2	1:E:247:LYS:HG2	2.55	0.41
1:D:272:ASP:OD1	1:D:272:ASP:O	2.38	0.41
1:F:172:GLN:O	1:F:176:PHE:CE1	2.73	0.41
1:A:270:TYR:OH	1:A:273:GLY:HA2	2.20	0.41
1:A:209:GLN:CG	1:F:183:PRO:HD2	2.48	0.41
1:C:356:ASP:OD1	1:C:356:ASP:N	2.53	0.41
1:F:174:PRO:HA	1:F:175:PRO:HA	1.63	0.41
1:F:242:MET:HE3	1:F:242:MET:HB2	1.89	0.41
1:F:296:PRO:HA	1:F:299:TYR:CZ	2.56	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 [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	196/202 (97%)	183 (93%)	8 (4%)	5 (3%)	4 9
1	B	179/202 (89%)	176 (98%)	2 (1%)	1 (1%)	21 41
1	C	191/202 (95%)	181 (95%)	8 (4%)	2 (1%)	12 28
1	D	185/202 (92%)	177 (96%)	6 (3%)	2 (1%)	11 26
1	E	180/202 (89%)	176 (98%)	3 (2%)	1 (1%)	21 41
1	F	189/202 (94%)	171 (90%)	11 (6%)	7 (4%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1120/1212 (92%)	1064 (95%)	38 (3%)	18 (2%)	7	18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	334	GLN
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%)	175 (95%)	9 (5%)	22	46
1	B	168/188 (89%)	157 (94%)	11 (6%)	15	34
1	C	180/188 (96%)	170 (94%)	10 (6%)	19	40
1	D	174/188 (93%)	167 (96%)	7 (4%)	28	53
1	E	169/188 (90%)	163 (96%)	6 (4%)	31	57
1	F	178/188 (95%)	169 (95%)	9 (5%)	21	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1053/1128 (93%)	1001 (95%)	52 (5%)	22	46

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	172	GLN
1	D	173	GLU
1	D	174	PRO
1	D	175	PRO
1	D	290	ILE
1	D	333	GLN
1	D	346	GLU
1	A	209	GLN
1	A	210	LYS
1	A	213	TRP
1	A	269	VAL
1	A	279	LEU
1	A	334	GLN
1	A	336	LYS
1	A	338	VAL
1	A	356	ASP
1	B	210	LYS
1	B	271	LYS
1	B	279	LEU
1	B	290	ILE
1	B	321	VAL
1	B	334	GLN
1	B	336	LYS
1	B	338	VAL
1	B	342	LEU
1	B	346	GLU
1	B	351	LEU
1	C	172	GLN
1	C	205	SER
1	C	209	GLN
1	C	213	TRP
1	C	214	ARG
1	C	279	LEU
1	C	290	ILE
1	C	349	LYS
1	C	353	GLU
1	C	356	ASP

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Mol	Chain	Res	Type
1	E	176	PHE
1	E	205	SER
1	E	279	LEU
1	E	336	LYS
1	E	353	GLU
1	E	356	ASP
1	F	206	GLU
1	F	207	TRP
1	F	213	TRP
1	F	281	LYS
1	F	282	LEU
1	F	310	GLU
1	F	323	LEU
1	F	336	LYS
1	F	356	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	ASN
1	B	211	HIS
1	B	357	HIS
1	E	189	GLN
1	E	204	HIS
1	F	172	GLN
1	F	211	HIS
1	F	275	HIS
1	F	343	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 oligosaccharides in this entry.

5.6 Ligand geometry

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

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, 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	198/202 (98%)	0.25	15 (7%)	20 17	46, 60, 111, 192	0
1	B	181/202 (89%)	0.23	10 (5%)	30 26	48, 69, 104, 167	0
1	C	193/202 (95%)	0.22	11 (5%)	29 25	48, 69, 118, 141	0
1	D	187/202 (92%)	0.62	14 (7%)	20 17	24, 71, 117, 156	0
1	E	182/202 (90%)	0.31	9 (4%)	35 30	24, 68, 107, 131	0
1	F	191/202 (94%)	1.04	37 (19%)	3 2	57, 92, 148, 263	0
All	All	1132/1212 (93%)	0.44	96 (8%)	16 14	24, 70, 121, 263	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	176	PHE	8.9
1	D	176	PHE	8.7
1	A	336	LYS	7.9
1	D	174	PRO	7.8
1	A	187	PRO	7.8
1	D	175	PRO	7.4
1	D	172	GLN	7.2
1	A	335	THR	6.6
1	D	357	HIS	6.6
1	D	173	GLU	6.2
1	F	207	TRP	6.0
1	A	334	GLN	5.9
1	D	171	PHE	5.9
1	F	205	SER	5.0
1	E	177	PRO	4.7
1	B	188	TYR	4.7
1	A	333	GLN	4.6
1	F	247	LYS	4.3
1	D	336	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	175	PRO	4.2
1	B	177	PRO	4.1
1	F	199	GLU	4.0
1	A	160	GLY	3.9
1	F	211	HIS	3.9
1	A	337	ASP	3.9
1	C	213	TRP	3.9
1	F	174	PRO	3.8
1	D	177	PRO	3.8
1	F	208	SER	3.7
1	F	281	LYS	3.7
1	B	336	LYS	3.7
1	F	316	ALA	3.6
1	E	356	ASP	3.5
1	A	357	HIS	3.5
1	B	213	TRP	3.4
1	B	187	PRO	3.3
1	F	245	SER	3.2
1	F	274	VAL	3.2
1	F	213	TRP	3.2
1	C	357	HIS	3.1
1	A	186	PRO	3.1
1	F	167	MET	3.1
1	A	209	GLN	3.1
1	F	206	GLU	3.0
1	F	246	ASP	3.0
1	F	356	ASP	3.0
1	F	275	HIS	3.0
1	F	244	TYR	3.0
1	F	210	LYS	2.9
1	F	241	TYR	2.9
1	F	209	GLN	2.9
1	F	173	GLU	2.9
1	F	175	PRO	2.8
1	A	213	TRP	2.8
1	C	166	SER	2.8
1	E	336	LYS	2.8
1	D	335	THR	2.8
1	F	214	ARG	2.8
1	F	212	GLY	2.7
1	C	209	GLN	2.7
1	F	335	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	243	MET	2.7
1	C	336	LYS	2.6
1	A	340	PRO	2.6
1	E	209	GLN	2.6
1	F	310	GLU	2.6
1	C	165	ASN	2.6
1	B	316	ALA	2.6
1	E	332	THR	2.5
1	C	188	TYR	2.5
1	B	257	ALA	2.5
1	A	346	GLU	2.5
1	E	310	GLU	2.5
1	A	212	GLY	2.4
1	A	211	HIS	2.4
1	F	297	ASN	2.4
1	D	356	ASP	2.4
1	C	186	PRO	2.3
1	C	211	HIS	2.2
1	F	299	TYR	2.2
1	F	239	SER	2.2
1	D	353	GLU	2.2
1	F	166	SER	2.2
1	B	357	HIS	2.2
1	D	334	GLN	2.2
1	F	222	ASP	2.2
1	B	270	TYR	2.1
1	D	333	GLN	2.1
1	F	200	ASP	2.1
1	E	335	THR	2.1
1	C	271	LYS	2.1
1	F	336	LYS	2.1
1	B	256	HIS	2.1
1	F	338	VAL	2.1
1	F	300	LYS	2.0
1	C	167	MET	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MG	D	401	1/1	0.81	0.42	68,68,68,68	0
2	MG	F	401	1/1	0.90	0.28	55,55,55,55	0
2	MG	B	401	1/1	0.95	0.33	47,47,47,47	0
2	MG	C	401	1/1	0.97	0.39	41,41,41,41	0
2	MG	E	401	1/1	0.98	0.40	39,39,39,39	0
2	MG	A	401	1/1	0.98	0.43	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.