



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2016 – 08:12 PM EST

PDB ID : 5GNU
Title : the structure of mini-MFN1 apo
Authors : Yan, L.; Yu, C.; Ming, Z.; Lou, Z.; Rao, Z.; Lou, J.
Deposited on : 2016-07-25
Resolution : 4.11 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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-20028320

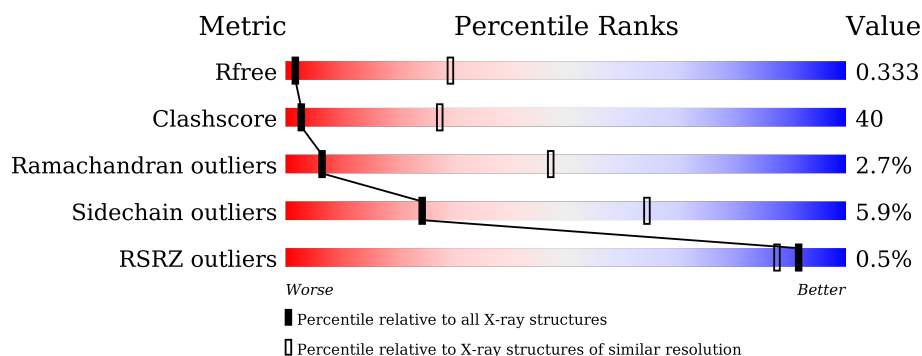
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.11 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}	91344	1020 (4.62-3.60)
Clashscore	102246	1119 (4.62-3.60)
Ramachandran outliers	100387	1065 (4.62-3.60)
Sidechain outliers	100360	1051 (4.62-3.60)
RSRZ outliers	91569	1024 (4.62-3.60)

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. 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	421	<div> <div style="width: 37%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 10%; background-color: grey;"></div> </div> <div>37% 46% 5% • 10%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3021 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 Mitofusin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	3021	1916	516	575	14	0	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	GLY	-	expression tag	UNP Q8IWA4
A	366	SER	-	expression tag	UNP Q8IWA4
A	367	GLY	-	expression tag	UNP Q8IWA4
A	368	SER	-	expression tag	UNP Q8IWA4
A	369	GLY	-	expression tag	UNP Q8IWA4
A	370	SER	-	expression tag	UNP Q8IWA4
A	371	GLY	-	expression tag	UNP Q8IWA4
A	372	GLY	-	expression tag	UNP Q8IWA4
A	373	SER	-	expression tag	UNP Q8IWA4
A	374	GLU	-	expression tag	UNP Q8IWA4
A	375	ILE	-	expression tag	UNP Q8IWA4
A	376	ALA	-	expression tag	UNP Q8IWA4
A	377	ARG	-	expression tag	UNP Q8IWA4
A	378	LEU	-	expression tag	UNP Q8IWA4
A	379	PRO	-	expression tag	UNP Q8IWA4
A	380	LYS	-	expression tag	UNP Q8IWA4
A	381	GLU	-	expression tag	UNP Q8IWA4
A	382	ILE	-	expression tag	UNP Q8IWA4
A	383	ASP	-	expression tag	UNP Q8IWA4
A	384	GLN	-	expression tag	UNP Q8IWA4
A	385	LEU	-	expression tag	UNP Q8IWA4
A	386	GLU	-	expression tag	UNP Q8IWA4
A	387	LYS	-	expression tag	UNP Q8IWA4
A	388	ILE	-	expression tag	UNP Q8IWA4
A	389	GLN	-	expression tag	UNP Q8IWA4
A	390	ASN	-	expression tag	UNP Q8IWA4
A	391	ASN	-	expression tag	UNP Q8IWA4

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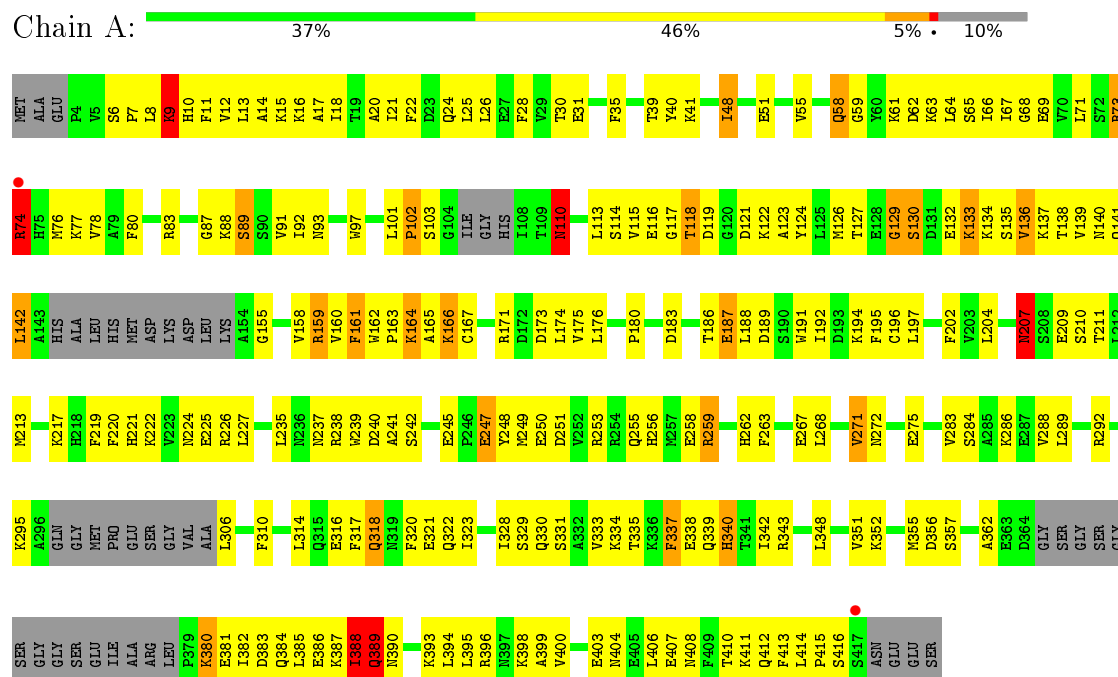
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Chain	Residue	Modelled	Actual	Comment	Reference
A	392	SER	-	expression tag	UNP Q8IWA4
A	393	LYS	-	expression tag	UNP Q8IWA4
A	394	LEU	-	expression tag	UNP Q8IWA4
A	395	LEU	-	expression tag	UNP Q8IWA4
A	396	ARG	-	expression tag	UNP Q8IWA4
A	397	ASN	-	expression tag	UNP Q8IWA4
A	398	LYS	-	expression tag	UNP Q8IWA4
A	399	ALA	-	expression tag	UNP Q8IWA4
A	400	VAL	-	expression tag	UNP Q8IWA4
A	401	GLN	-	expression tag	UNP Q8IWA4
A	402	LEU	-	expression tag	UNP Q8IWA4
A	403	GLU	-	expression tag	UNP Q8IWA4
A	404	ASN	-	expression tag	UNP Q8IWA4
A	405	GLU	-	expression tag	UNP Q8IWA4
A	406	LEU	-	expression tag	UNP Q8IWA4
A	407	GLU	-	expression tag	UNP Q8IWA4
A	408	ASN	-	expression tag	UNP Q8IWA4
A	409	PHE	-	expression tag	UNP Q8IWA4
A	410	THR	-	expression tag	UNP Q8IWA4
A	411	LYS	-	expression tag	UNP Q8IWA4
A	412	GLN	-	expression tag	UNP Q8IWA4
A	413	PHE	-	expression tag	UNP Q8IWA4
A	414	LEU	-	expression tag	UNP Q8IWA4
A	415	PRO	-	expression tag	UNP Q8IWA4
A	416	SER	-	expression tag	UNP Q8IWA4
A	417	SER	-	expression tag	UNP Q8IWA4
A	418	ASN	-	expression tag	UNP Q8IWA4
A	419	GLU	-	expression tag	UNP Q8IWA4
A	420	GLU	-	expression tag	UNP Q8IWA4
A	421	SER	-	expression tag	UNP Q8IWA4

3 Residue-property plots

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: Mitofusin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.00 Å 76.49 Å 95.36 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 4.11 46.20 – 4.11	Depositor EDS
% Data completeness (in resolution range)	75.8 (46.20-4.11) 67.0 (46.20-4.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 4.14 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.284 , 0.350 0.274 , 0.333	Depositor DCC
R_{free} test set	296 reflections (9.94%)	DCC
Wilson B-factor (Å ²)	129.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 108.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.084 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3021	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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

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	0.38	0/3070	0.83	8/4132 (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
1	A	0	7

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	389	GLN	N-CA-CB	-9.69	93.15	110.60
1	A	388	ILE	CB-CA-C	-8.66	94.28	111.60
1	A	9	LYS	CB-CA-C	-6.64	97.12	110.40
1	A	389	GLN	N-CA-C	6.00	127.21	111.00
1	A	337	PHE	CB-CA-C	-5.67	99.06	110.40
1	A	110	ASN	N-CA-C	5.63	126.19	111.00
1	A	191	TRP	CA-CB-CG	5.14	123.47	113.70
1	A	88	LYS	CB-CA-C	-5.06	100.29	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	GLY	Peptide
1	A	207	ASN	Peptide
1	A	247	GLU	Peptide
1	A	318	GLN	Peptide
1	A	388	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	389	GLN	Peptide
1	A	73	ARG	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	3021	0	3027	242	1
All	All	3021	0	3027	242	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 40.

All (242) 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:A:383:ASP:HA	1:A:386:GLU:HB3	1.38	1.05
1:A:209:GLU:HG2	1:A:238:ARG:HH22	1.31	0.96
1:A:314:LEU:HG	1:A:318:GLN:HE21	1.37	0.88
1:A:138:THR:HG22	1:A:139:VAL:HG13	1.54	0.88
1:A:283:VAL:HG11	1:A:317:PHE:HB2	1.57	0.87
1:A:207:ASN:OD1	1:A:238:ARG:NH2	2.09	0.85
1:A:388:ILE:O	1:A:388:ILE:HG22	1.75	0.83
1:A:389:GLN:HG3	1:A:390:ASN:H	1.41	0.83
1:A:130:SER:OG	1:A:132:GLU:OE1	1.97	0.82
1:A:334:LYS:NZ	1:A:413:PHE:O	2.12	0.81
1:A:41:LYS:HD2	1:A:41:LYS:O	1.79	0.81
1:A:162:TRP:HE3	1:A:166:LYS:HD3	1.45	0.81
1:A:240:ASP:OD2	1:A:286:LYS:NZ	2.16	0.78
1:A:186:THR:HG22	1:A:188:LEU:H	1.47	0.78
1:A:28:PHE:HD1	1:A:398:LYS:HG2	1.48	0.76
1:A:389:GLN:HG3	1:A:390:ASN:N	2.01	0.76
1:A:321:GLU:HG3	1:A:322:GLN:N	2.00	0.75
1:A:338:GLU:HG2	1:A:339:GLN:HG3	1.68	0.74
1:A:9:LYS:O	1:A:13:LEU:HG	1.88	0.74
1:A:159:ARG:NH2	1:A:161:PHE:HD2	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:HD12	1:A:21:ILE:HD12	1.70	0.73
1:A:62:ASP:HB3	1:A:63:LYS:HD2	1.70	0.72
1:A:159:ARG:NH1	1:A:159:ARG:O	2.21	0.71
1:A:71:LEU:HD22	1:A:337:PHE:HE1	1.56	0.71
1:A:110:ASN:O	1:A:110:ASN:ND2	2.23	0.71
1:A:18:ILE:HG21	1:A:337:PHE:CZ	2.25	0.70
1:A:89:SER:HB3	1:A:103:SER:HA	1.74	0.70
1:A:135:SER:OG	1:A:138:THR:OG1	2.10	0.69
1:A:314:LEU:HG	1:A:318:GLN:NE2	2.06	0.69
1:A:356:ASP:OD1	1:A:396:ARG:NH2	2.26	0.69
1:A:390:ASN:HA	1:A:393:LYS:HB3	1.74	0.69
1:A:26:LEU:HD11	1:A:65:SER:HA	1.76	0.68
1:A:389:GLN:OE1	1:A:390:ASN:ND2	2.28	0.67
1:A:10:HIS:CD2	1:A:329:SER:HB2	2.29	0.67
1:A:186:THR:O	1:A:188:LEU:O	2.12	0.67
1:A:28:PHE:CD1	1:A:398:LYS:HG2	2.29	0.66
1:A:135:SER:O	1:A:138:THR:HB	1.95	0.66
1:A:6:SER:O	1:A:8:LEU:N	2.27	0.66
1:A:124:TYR:HB2	1:A:161:PHE:HB3	1.78	0.66
1:A:338:GLU:O	1:A:342:ILE:HG12	1.96	0.66
1:A:101:LEU:HD21	1:A:113:LEU:HD13	1.77	0.66
1:A:15:LYS:HZ2	1:A:74:ARG:CZ	2.09	0.65
1:A:258:GLU:O	1:A:262:HIS:HB2	1.97	0.65
1:A:395:LEU:HA	1:A:398:LYS:HB2	1.77	0.65
1:A:139:VAL:HB	1:A:142:LEU:HD22	1.77	0.65
1:A:271:VAL:HG13	1:A:275:GLU:HG3	1.79	0.64
1:A:97:TRP:CD1	1:A:292:ARG:HD3	2.32	0.64
1:A:12:VAL:HA	1:A:15:LYS:HD2	1.80	0.64
1:A:390:ASN:O	1:A:394:LEU:N	2.25	0.64
1:A:97:TRP:HD1	1:A:292:ARG:HD3	1.62	0.64
1:A:101:LEU:HD12	1:A:102:PRO:HD2	1.79	0.63
1:A:334:LYS:HZ1	1:A:415:PRO:HD2	1.62	0.63
1:A:386:GLU:HA	1:A:389:GLN:HB3	1.81	0.63
1:A:129:GLY:O	1:A:130:SER:HB3	1.97	0.63
1:A:83:ARG:HH21	1:A:213:MET:HG3	1.63	0.62
1:A:410:THR:HG22	1:A:414:LEU:HD12	1.82	0.62
1:A:314:LEU:O	1:A:318:GLN:HG3	1.99	0.61
1:A:217:LYS:HG2	1:A:263:PHE:CE1	2.35	0.61
1:A:6:SER:O	1:A:9:LYS:HG3	2.00	0.60
1:A:118:THR:HG23	1:A:161:PHE:CZ	2.36	0.60
1:A:356:ASP:N	1:A:396:ARG:HH22	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TRP:C	1:A:166:LYS:HZ1	2.05	0.60
1:A:283:VAL:HG22	1:A:316:GLU:HB3	1.82	0.60
1:A:384:GLN:HE21	1:A:385:LEU:HD23	1.67	0.60
1:A:15:LYS:HZ2	1:A:74:ARG:NH2	2.00	0.60
1:A:18:ILE:HA	1:A:21:ILE:HD12	1.84	0.59
1:A:39:THR:HG22	1:A:48:ILE:HD11	1.84	0.59
1:A:39:THR:CG2	1:A:48:ILE:HD11	2.34	0.58
1:A:114:SER:OG	1:A:159:ARG:HB2	2.04	0.58
1:A:63:LYS:HA	1:A:66:ILE:HG13	1.85	0.58
1:A:338:GLU:OE1	1:A:338:GLU:N	2.38	0.57
1:A:11:PHE:CZ	1:A:76:MET:HG3	2.39	0.57
1:A:118:THR:O	1:A:164:LYS:HB2	2.04	0.57
1:A:224:ASN:HB2	1:A:268:LEU:HD22	1.87	0.57
1:A:387:LYS:HA	1:A:389:GLN:NE2	2.20	0.57
1:A:69:GLU:OE2	1:A:73:ARG:NH1	2.38	0.57
1:A:20:ALA:O	1:A:24:GLN:HG3	2.04	0.57
1:A:239:TRP:H	1:A:284:SER:HB3	1.68	0.57
1:A:330:GLN:OE1	1:A:334:LYS:NZ	2.35	0.57
1:A:245:GLU:HB2	1:A:248:TYR:HD2	1.70	0.56
1:A:292:ARG:O	1:A:295:LYS:HE2	2.04	0.56
1:A:209:GLU:HG2	1:A:238:ARG:NH2	2.10	0.56
1:A:15:LYS:HE3	1:A:74:ARG:HG3	1.87	0.56
1:A:22:PHE:HA	1:A:25:LEU:HB3	1.87	0.56
1:A:192:ILE:HG23	1:A:219:PHE:HE1	1.69	0.56
1:A:162:TRP:CE3	1:A:166:LYS:HD3	2.35	0.56
1:A:40:TYR:CZ	1:A:51:GLU:HB2	2.41	0.55
1:A:71:LEU:HD21	1:A:340:HIS:ND1	2.22	0.55
1:A:92:ILE:HG23	1:A:176:LEU:HD22	1.88	0.55
1:A:166:LYS:HG2	1:A:167:CYS:N	2.22	0.55
1:A:334:LYS:NZ	1:A:415:PRO:HD2	2.21	0.55
1:A:333:VAL:O	1:A:337:PHE:HB2	2.08	0.54
1:A:77:LYS:HD3	1:A:175:VAL:HB	1.88	0.54
1:A:116:GLU:HA	1:A:175:VAL:HG22	1.89	0.54
1:A:318:GLN:C	1:A:321:GLU:HG2	2.28	0.54
1:A:126:MET:HG2	1:A:133:LYS:HD2	1.90	0.54
1:A:385:LEU:O	1:A:389:GLN:N	2.41	0.54
1:A:164:LYS:NZ	1:A:171:ARG:HG3	2.24	0.53
1:A:134:LYS:HG2	1:A:138:THR:HG21	1.90	0.53
1:A:393:LYS:O	1:A:396:ARG:HB3	2.08	0.53
1:A:256:HIS:HA	1:A:259:ARG:NE	2.24	0.53
1:A:93:ASN:HD21	1:A:289:LEU:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:HB2	1:A:263:PHE:HZ	1.74	0.53
1:A:162:TRP:HB3	1:A:166:LYS:CE	2.38	0.53
1:A:395:LEU:HD22	1:A:398:LYS:HZ3	1.71	0.53
1:A:115:VAL:HA	1:A:160:VAL:O	2.10	0.52
1:A:387:LYS:CA	1:A:389:GLN:HG2	2.40	0.52
1:A:117:GLY:C	1:A:161:PHE:HE1	2.13	0.52
1:A:408:ASN:HA	1:A:411:LYS:HE2	1.91	0.51
1:A:207:ASN:CG	1:A:238:ARG:HE	2.14	0.51
1:A:328:ILE:HG12	1:A:328:ILE:O	2.10	0.51
1:A:15:LYS:HG2	1:A:74:ARG:NE	2.25	0.51
1:A:284:SER:HB2	1:A:286:LYS:HZ2	1.75	0.51
1:A:101:LEU:HD12	1:A:102:PRO:CD	2.40	0.51
1:A:31:GLU:HB3	1:A:398:LYS:HZ1	1.75	0.51
1:A:116:GLU:HG2	1:A:161:PHE:CZ	2.46	0.50
1:A:166:LYS:HG3	1:A:167:CYS:SG	2.51	0.50
1:A:348:LEU:O	1:A:352:LYS:HG3	2.11	0.50
1:A:390:ASN:HB3	1:A:393:LYS:HE2	1.92	0.50
1:A:137:LYS:HD2	1:A:141:GLN:HE22	1.76	0.50
1:A:124:TYR:HB2	1:A:161:PHE:O	2.12	0.50
1:A:187:GLU:O	1:A:188:LEU:HB2	2.12	0.50
1:A:64:LEU:HD23	1:A:67:ILE:HD12	1.93	0.50
1:A:362:ALA:O	1:A:385:LEU:HD22	2.12	0.50
1:A:272:ASN:ND2	1:A:275:GLU:OE1	2.45	0.50
1:A:31:GLU:HB3	1:A:398:LYS:NZ	2.27	0.50
1:A:71:LEU:O	1:A:74:ARG:HD3	2.12	0.50
1:A:380:LYS:C	1:A:382:ILE:H	2.13	0.50
1:A:93:ASN:OD1	1:A:289:LEU:HD13	2.11	0.50
1:A:136:VAL:HG13	1:A:137:LYS:H	1.77	0.49
1:A:263:PHE:HA	1:A:267:GLU:OE2	2.13	0.49
1:A:118:THR:N	1:A:161:PHE:CE1	2.80	0.49
1:A:356:ASP:CA	1:A:396:ARG:HH22	2.25	0.49
1:A:93:ASN:HD21	1:A:289:LEU:HD13	1.78	0.49
1:A:196:CYS:HB3	1:A:202:PHE:HE2	1.78	0.49
1:A:310:PHE:CZ	1:A:314:LEU:HD22	2.48	0.49
1:A:318:GLN:HA	1:A:321:GLU:HG2	1.95	0.49
1:A:124:TYR:CB	1:A:161:PHE:HB3	2.43	0.49
1:A:306:LEU:CD1	1:A:310:PHE:HB3	2.42	0.49
1:A:388:ILE:N	1:A:389:GLN:HG2	2.28	0.49
1:A:399:ALA:O	1:A:403:GLU:HG3	2.13	0.48
1:A:163:PRO:N	1:A:166:LYS:HE2	2.28	0.48
1:A:271:VAL:CG1	1:A:275:GLU:HG3	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:C	1:A:226:ARG:HG2	2.33	0.48
1:A:30:THR:HA	1:A:61:LYS:HD3	1.96	0.48
1:A:48:ILE:CD1	1:A:388:ILE:HD13	2.44	0.48
1:A:408:ASN:O	1:A:412:GLN:HB2	2.14	0.47
1:A:194:LYS:HD3	1:A:194:LYS:N	2.28	0.47
1:A:247:GLU:HA	1:A:250:GLU:H	1.78	0.47
1:A:71:LEU:HD22	1:A:337:PHE:CE1	2.43	0.47
1:A:404:ASN:HA	1:A:407:GLU:HG3	1.96	0.47
1:A:110:ASN:HA	1:A:180:PRO:HB3	1.95	0.47
1:A:117:GLY:CA	1:A:161:PHE:HE1	2.27	0.47
1:A:11:PHE:CE2	1:A:76:MET:HG3	2.50	0.47
1:A:189:ASP:C	1:A:192:ILE:HB	2.34	0.47
1:A:68:GLY:HA2	1:A:71:LEU:HB2	1.95	0.47
1:A:17:ALA:O	1:A:21:ILE:HG13	2.15	0.47
1:A:242:SER:O	1:A:249:MET:HG3	2.15	0.47
1:A:396:ARG:O	1:A:400:VAL:HG23	2.15	0.47
1:A:159:ARG:NH2	1:A:161:PHE:CD2	2.74	0.46
1:A:55:VAL:HA	1:A:58:GLN:OE1	2.15	0.46
1:A:211:THR:HG23	1:A:259:ARG:HH11	1.80	0.46
1:A:210:SER:OG	1:A:211:THR:N	2.47	0.46
1:A:211:THR:HG23	1:A:259:ARG:NH1	2.30	0.46
1:A:348:LEU:O	1:A:351:VAL:HG12	2.16	0.46
1:A:395:LEU:HD22	1:A:398:LYS:CE	2.46	0.46
1:A:83:ARG:HG3	1:A:183:ASP:HB2	1.98	0.46
1:A:283:VAL:HG12	1:A:284:SER:N	2.30	0.46
1:A:118:THR:N	1:A:161:PHE:HE1	2.13	0.46
1:A:134:LYS:HE3	1:A:134:LYS:HB2	1.58	0.46
1:A:255:GLN:O	1:A:258:GLU:HB3	2.15	0.46
1:A:159:ARG:C	1:A:159:ARG:HD2	2.36	0.45
1:A:93:ASN:ND2	1:A:289:LEU:HD13	2.30	0.45
1:A:123:ALA:HB1	1:A:136:VAL:HB	1.98	0.45
1:A:237:ASN:HA	1:A:283:VAL:O	2.17	0.45
1:A:115:VAL:C	1:A:175:VAL:HG13	2.37	0.45
1:A:6:SER:C	1:A:8:LEU:H	2.18	0.45
1:A:381:GLU:HB3	1:A:384:GLN:OE1	2.17	0.45
1:A:114:SER:O	1:A:160:VAL:N	2.47	0.45
1:A:238:ARG:HA	1:A:284:SER:HB2	1.98	0.45
1:A:74:ARG:NH2	1:A:337:PHE:CZ	2.84	0.45
1:A:121:ASP:C	1:A:122:LYS:HD3	2.37	0.45
1:A:263:PHE:CE1	1:A:268:LEU:HG	2.52	0.44
1:A:339:GLN:HA	1:A:342:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE2	1:A:395:LEU:HD12	1.99	0.44
1:A:395:LEU:HD22	1:A:398:LYS:NZ	2.32	0.44
1:A:58:GLN:HG2	1:A:59:GLY:N	2.32	0.44
1:A:192:ILE:HG23	1:A:219:PHE:CE1	2.51	0.44
1:A:117:GLY:N	1:A:161:PHE:CE1	2.85	0.44
1:A:163:PRO:O	1:A:165:ALA:N	2.50	0.44
1:A:348:LEU:HD12	1:A:406:LEU:HD12	1.99	0.44
1:A:412:GLN:HG3	1:A:413:PHE:CZ	2.52	0.44
1:A:14:ALA:HA	1:A:413:PHE:CE2	2.53	0.43
1:A:388:ILE:O	1:A:388:ILE:CG2	2.48	0.43
1:A:235:LEU:HD11	1:A:320:PHE:CZ	2.53	0.43
1:A:226:ARG:CZ	1:A:226:ARG:HA	2.48	0.43
1:A:18:ILE:HG23	1:A:71:LEU:HD13	2.01	0.43
1:A:400:VAL:HA	1:A:403:GLU:CD	2.39	0.43
1:A:114:SER:HA	1:A:176:LEU:O	2.19	0.43
1:A:118:THR:HG23	1:A:161:PHE:CE2	2.54	0.42
1:A:272:ASN:OD1	1:A:275:GLU:HG2	2.19	0.42
1:A:331:SER:O	1:A:335:THR:HG23	2.19	0.42
1:A:67:ILE:O	1:A:71:LEU:HG	2.19	0.42
1:A:41:LYS:HD2	1:A:41:LYS:C	2.38	0.42
1:A:101:LEU:HD21	1:A:113:LEU:CD1	2.47	0.42
1:A:59:GLY:O	1:A:63:LYS:HD3	2.19	0.42
1:A:209:GLU:H	1:A:238:ARG:NH2	2.17	0.42
1:A:256:HIS:HA	1:A:259:ARG:HE	1.84	0.42
1:A:380:LYS:C	1:A:382:ILE:N	2.73	0.42
1:A:137:LYS:HD2	1:A:140:ASN:HB2	2.00	0.42
1:A:221:HIS:O	1:A:225:GLU:HG3	2.19	0.42
1:A:22:PHE:CD2	1:A:25:LEU:HD23	2.54	0.42
1:A:288:VAL:HG22	1:A:314:LEU:HD12	2.02	0.42
1:A:164:LYS:HZ3	1:A:171:ARG:HG3	1.85	0.42
1:A:226:ARG:C	1:A:227:LEU:HD23	2.40	0.42
1:A:255:GLN:HA	1:A:258:GLU:HB3	2.02	0.42
1:A:415:PRO:HA	1:A:416:SER:HA	1.44	0.42
1:A:15:LYS:HG2	1:A:74:ARG:HG2	2.03	0.41
1:A:209:GLU:HB3	1:A:238:ARG:HH12	1.85	0.41
1:A:118:THR:HG23	1:A:161:PHE:CE1	2.55	0.41
1:A:18:ILE:O	1:A:21:ILE:HB	2.19	0.41
1:A:155:GLY:HA3	1:A:195:PHE:HE2	1.84	0.41
1:A:255:GLN:O	1:A:259:ARG:HG2	2.20	0.41
1:A:310:PHE:O	1:A:314:LEU:N	2.45	0.41
1:A:251:ASP:O	1:A:255:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:HG23	1:A:61:LYS:NZ	2.35	0.41
1:A:387:LYS:HA	1:A:389:GLN:HE21	1.86	0.41
1:A:78:VAL:HG12	1:A:174:LEU:HD11	2.01	0.41
1:A:187:GLU:HG2	1:A:187:GLU:O	2.21	0.41
1:A:403:GLU:O	1:A:407:GLU:HG3	2.21	0.41
1:A:80:PHE:CE1	1:A:92:ILE:HG12	2.56	0.41
1:A:162:TRP:HA	1:A:163:PRO:HD3	1.76	0.41
1:A:139:VAL:CG1	1:A:142:LEU:HD13	2.51	0.41
1:A:16:LYS:HB2	1:A:16:LYS:HE3	1.77	0.41
1:A:318:GLN:CA	1:A:321:GLU:HG2	2.51	0.40
1:A:329:SER:OG	1:A:330:GLN:N	2.52	0.40
1:A:384:GLN:CG	1:A:385:LEU:N	2.84	0.40
1:A:87:GLY:O	1:A:91:VAL:HG23	2.22	0.40
1:A:204:LEU:HB2	1:A:220:PHE:CZ	2.57	0.40
1:A:35:PHE:O	1:A:39:THR:OG1	2.22	0.40
1:A:127:THR:HA	1:A:158:VAL:HG22	2.04	0.40
1:A:330:GLN:O	1:A:334:LYS:HE2	2.20	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)
1:A:241:ALA:O	1:A:343:ARG:NH1[2_454]	2.17	0.03

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	368/421 (87%)	302 (82%)	56 (15%)	10 (3%)	6 47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	74	ARG
1	A	130	SER
1	A	164	LYS
1	A	173	ASP
1	A	271	VAL
1	A	110	ASN
1	A	357	SER
1	A	102	PRO
1	A	136	VAL

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	337/368 (92%)	317 (94%)	20 (6%)	24 64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	48	ILE
1	A	58	GLN
1	A	74	ARG
1	A	89	SER
1	A	118	THR
1	A	119	ASP
1	A	133	LYS
1	A	142	LEU
1	A	159	ARG
1	A	161	PHE
1	A	166	LYS
1	A	187	GLU
1	A	197	LEU
1	A	207	ASN
1	A	253	ARG
1	A	259	ARG

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Mol	Chain	Res	Type
1	A	323	ILE
1	A	340	HIS
1	A	380	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	93	ASN
1	A	141	GLN
1	A	221	HIS
1	A	315	GLN
1	A	318	GLN
1	A	384	GLN
1	A	390	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [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	378/421 (89%)	-0.19	2 (0%) 91 88	126, 157, 193, 213	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	SER	2.2
1	A	74	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.