WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 01:09 PM JST

PDB ID	:	6JFM
Title	:	Mitofusin2 (MFN2)_T111D
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Deposited on	:	2019-02-10
Resolution	:	2.09 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36
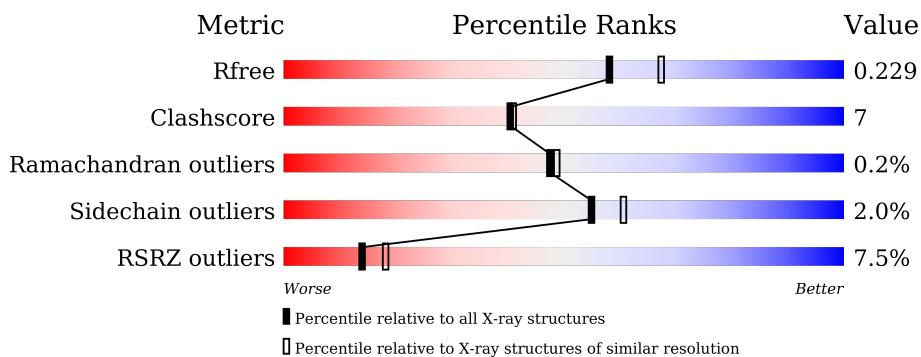
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
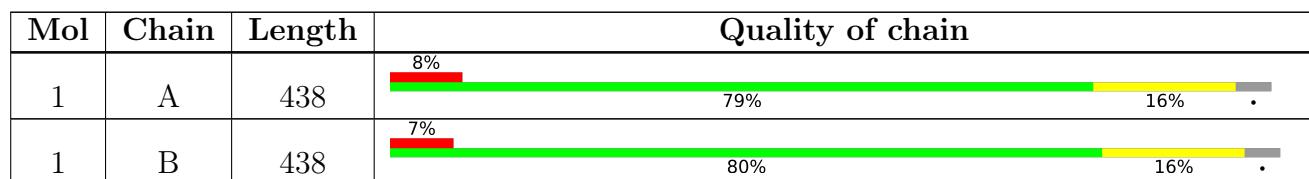
The reported resolution of this entry is 2.09 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	438	8% / 79% / 16% / ·
1	B	438	7% / 80% / 16% / ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7099 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.
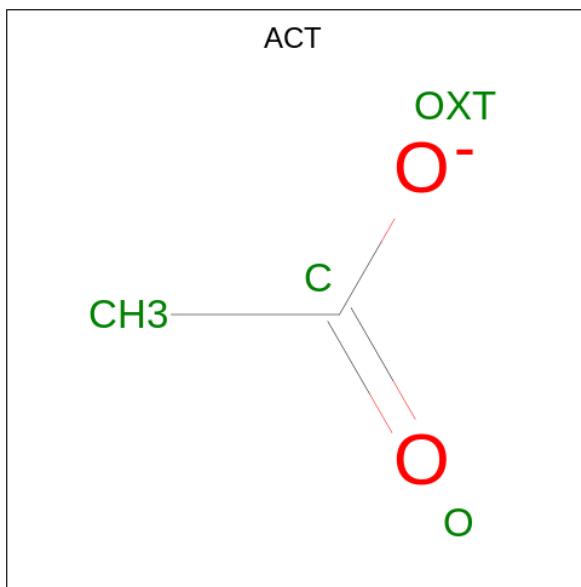
- Molecule 1 is a protein called Mitofusin-2,Mitofusin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total 3393	C 2127	N 599	O 646	S 21	0	4	0
1	B	422	Total 3427	C 2148	N 608	O 651	S 20	0	6	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP O95140
A	16	PRO	-	expression tag	UNP O95140
A	17	HIS	-	expression tag	UNP O95140
A	18	MET	-	expression tag	UNP O95140
A	19	GLY	-	expression tag	UNP O95140
A	20	GLY	-	expression tag	UNP O95140
A	21	SER	-	expression tag	UNP O95140
A	111	ASP	THR	engineered mutation	UNP O95140
B	15	GLY	-	expression tag	UNP O95140
B	16	PRO	-	expression tag	UNP O95140
B	17	HIS	-	expression tag	UNP O95140
B	18	MET	-	expression tag	UNP O95140
B	19	GLY	-	expression tag	UNP O95140
B	20	GLY	-	expression tag	UNP O95140
B	21	SER	-	expression tag	UNP O95140
B	111	ASP	THR	engineered mutation	UNP O95140

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O⁻

C

CH3

O

O

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total C O 4 2 2			0	0
2	A	1	Total C O 4 2 2			0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total Ca 2 2		0	0
3	B	1	Total Ca 1 1		0	0
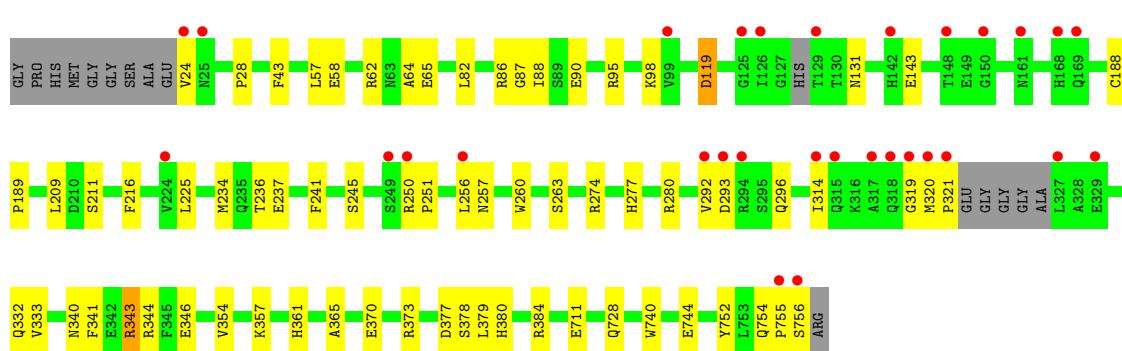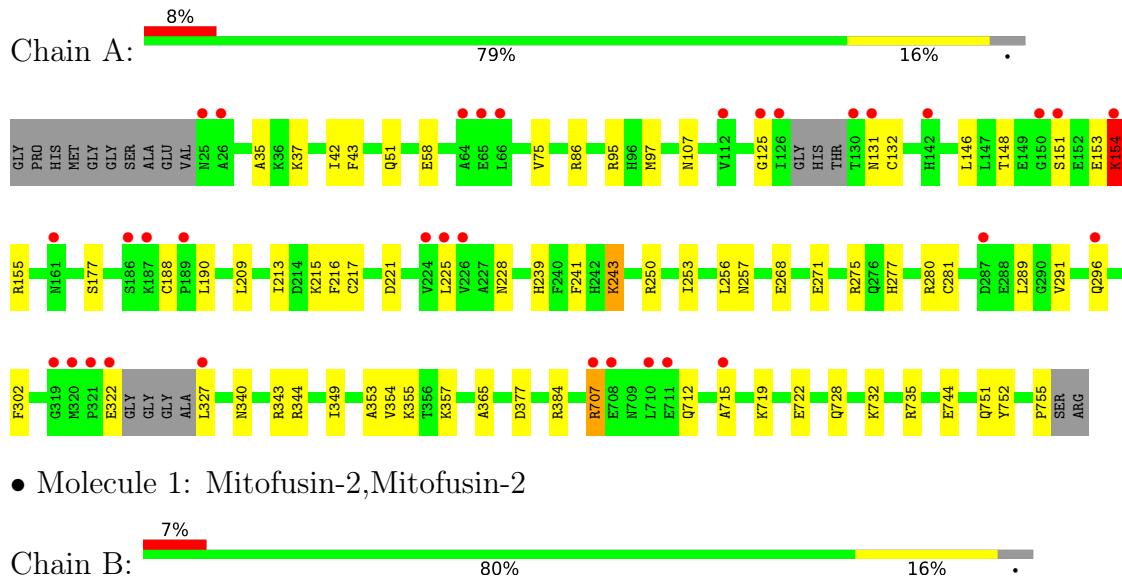
• Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total O 137 137		0	0
4	B	131	Total O 131 131		0	0

3 Residue-property plots ⓘ

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: Mitofusin-2,Mitofusin-2

• Molecule 1: Mitofusin-2,Mitofusin-2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.44Å 126.56Å 79.97Å 90.00° 102.46° 90.00°	Depositor
Resolution (Å)	31.64 – 2.09 31.64 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (31.64-2.09) 98.7 (31.64-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???), REFMAC	Depositor
R, R_{free}	0.176 , 0.229 0.176 , 0.229	Depositor DCC
R_{free} test set	2467 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7099	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACT

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	0.43	1/3462 (0.0%)	0.57	2/4659 (0.0%)
1	B	0.41	0/3500	0.56	0/4709
All	All	0.42	1/6962 (0.0%)	0.57	2/9368 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	LYS	CD-CE	-5.62	1.37	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	LYS	CD-CE-NZ	6.25	126.06	111.70
1	A	154	LYS	CG-CD-CE	-5.75	94.65	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ASN	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	3393	0	3355	51	3
1	B	3427	0	3398	51	3
2	A	8	0	6	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	137	0	0	7	0
4	B	131	0	0	2	0
All	All	7099	0	6759	98	3

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 7.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:HIS:HD2	1:B:280:ARG:HE	1.25	0.85
1:B:320:MET:HB3	1:B:321:PRO:HD2	1.60	0.84
1:A:37:LYS:NZ	4:A:1002:HOH:O	2.18	0.77
1:A:154:LYS:O	1:A:154:LYS:HD2	1.85	0.76
1:A:154:LYS:HD2	1:A:154:LYS:C	2.06	0.76
1:A:322:GLU:HG3	1:A:327:LEU:HD23	1.72	0.72
1:A:281:CYS:SG	4:A:1124:HOH:O	2.45	0.72
2:A:901:ACT:OXT	4:A:1001:HOH:O	2.09	0.71
1:A:384:ARG:HD3	1:A:728:GLN:HE22	1.57	0.68
1:A:146:LEU:O	1:A:154:LYS:HA	1.93	0.68
1:A:751:GLN:NE2	4:A:1004:HOH:O	2.28	0.65
1:A:95:ARG:HD3	1:A:357:LYS:HB3	1.78	0.65
1:B:119:ASP:HA	1:B:314:ILE:HD11	1.79	0.63
1:A:271:GLU:O	1:A:275:ARG:HG3	1.99	0.62
1:A:719:LYS:HA	1:A:722:GLU:HG2	1.82	0.60
1:A:340:ASN:O	1:A:344:ARG:HG2	2.01	0.60
1:A:37:LYS:HZ1	1:B:24:VAL:N	2.00	0.60
1:B:277:HIS:HD2	1:B:280:ARG:NE	1.99	0.59
1:B:87:GLY:O	1:B:90:GLU:HG2	2.03	0.59
1:A:343:ARG:HG2	1:A:344:ARG:NH1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:SER:HA	1:B:251:PRO:HG3	1.85	0.57
1:A:343:ARG:HD3	1:B:744:GLU:OE1	2.05	0.57
1:A:277:HIS:CD2	1:A:280:ARG:HH21	2.22	0.56
1:B:98:LYS:NZ	1:B:216:PHE:O	2.38	0.56
1:B:260:TRP:CH2	1:B:274:ARG:HB2	2.40	0.56
1:A:253:ILE:HD12	1:A:291:VAL:HG21	1.88	0.56
1:B:754:GLN:O	1:B:756:SER:N	2.39	0.55
1:B:263:SER:OG	4:B:901:HOH:O	2.18	0.55
1:B:58:GLU:OE2	1:B:62:ARG:NH1	2.40	0.54
1:A:735:ARG:NH2	4:A:1006:HOH:O	2.39	0.54
1:A:51:GLN:HE21	1:A:86[A]:ARG:HH12	1.56	0.54
1:A:277:HIS:HD2	1:A:280:ARG:HH21	1.56	0.53
1:B:225:LEU:HB2	1:B:241:PHE:CZ	2.43	0.53
1:A:43:PHE:CZ	1:A:365:ALA:HB2	2.44	0.53
1:A:215:LYS:HG2	1:A:216:PHE:CZ	2.43	0.53
1:B:293[A]:ASP:H	1:B:296:GLN:HE21	1.57	0.53
1:A:188[A]:CYS:SG	1:A:190:LEU:HB2	2.49	0.53
1:B:343:ARG:HG2	1:B:344:ARG:NH1	2.24	0.53
1:B:319:GLY:O	1:B:320:MET:HG2	2.09	0.52
1:B:293[B]:ASP:H	1:B:296:GLN:NE2	2.08	0.52
1:B:293[A]:ASP:H	1:B:296:GLN:NE2	2.08	0.51
1:B:293[B]:ASP:H	1:B:296:GLN:HE21	1.59	0.51
1:B:380:HIS:HD2	1:B:728:GLN:O	1.94	0.51
1:B:370:GLU:HG3	1:B:373:ARG:HH12	1.75	0.50
1:A:256:LEU:HD22	1:A:302:PHE:HB2	1.94	0.50
1:B:234:MET:HG2	1:B:237:GLU:OE1	2.12	0.49
1:B:332[B]:GLN:H	1:B:332[B]:GLN:CD	2.13	0.49
1:A:132:CYS:HB2	1:A:177:SER:O	2.13	0.48
1:A:42:ILE:HG13	1:B:24:VAL:HG21	1.96	0.48
1:A:221:ASP:HB2	1:A:349:ILE:HG13	1.95	0.48
1:B:332[B]:GLN:HE21	1:B:333:VAL:H	1.62	0.48
1:B:57:LEU:HD23	1:B:379:LEU:HD12	1.95	0.47
1:B:740:TRP:CZ3	1:B:744:GLU:HG3	2.48	0.47
1:A:154:LYS:C	1:A:154:LYS:CD	2.81	0.47
1:A:355:LYS:HE3	1:A:755:PRO:HA	1.95	0.47
1:A:107:ASN:OD1	1:A:228:ASN:HB2	2.15	0.46
1:A:384:ARG:HD3	1:A:728:GLN:NE2	2.30	0.46
1:B:143:GLU:HA	1:B:143:GLU:OE1	2.16	0.46
1:B:380:HIS:HE1	1:B:384[B]:ARG:HH11	1.64	0.46
1:B:257:ASN:OD1	1:B:277:HIS:CE1	2.69	0.46
1:B:95:ARG:HD2	1:B:357:LYS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:OD1	1:B:277:HIS:HE1	2.00	0.45
1:A:153:GLU:OE1	1:A:155:ARG:NH2	2.47	0.45
1:B:250:ARG:HG3	1:B:250:ARG:HH11	1.80	0.45
1:B:354:VAL:HG11	1:B:752:TYR:HB3	1.98	0.45
1:A:289:LEU:HB3	1:A:291:VAL:HG13	1.98	0.44
1:A:715:ALA:O	1:A:719:LYS:HE3	2.16	0.44
1:A:225:LEU:HB2	1:A:241:PHE:CZ	2.53	0.44
1:B:380:HIS:CE1	1:B:384[B]:ARG:HH11	2.35	0.44
1:B:90:GLU:OE2	4:B:902:HOH:O	2.21	0.44
1:A:213:ILE:HA	1:A:217:CYS:HB2	1.99	0.44
1:B:340:ASN:O	1:B:344:ARG:HG2	2.16	0.44
1:A:354:VAL:HG11	1:A:752:TYR:HB3	1.99	0.44
1:B:209:LEU:HD21	1:B:236:THR:HG22	2.00	0.43
1:A:42:ILE:CG1	1:B:24:VAL:HG21	2.48	0.43
1:B:277:HIS:CD2	1:B:280:ARG:HH21	2.36	0.43
1:A:257:ASN:OD1	1:A:277:HIS:CE1	2.72	0.43
1:B:88:ILE:HG23	1:B:361:HIS:CD2	2.53	0.43
1:A:239:HIS:CE1	1:A:243:LYS:HD2	2.54	0.43
1:A:707:ARG:NH1	4:A:1014:HOH:O	2.51	0.43
1:A:148:THR:HG23	1:A:151:SER:O	2.18	0.43
1:B:43:PHE:CZ	1:B:365:ALA:HB2	2.53	0.42
1:A:97:MET:HG2	1:A:353:ALA:CB	2.49	0.42
1:A:296:GLN:OE1	1:A:296:GLN:N	2.49	0.42
1:B:256:LEU:HD21	1:B:341:PHE:CD1	2.54	0.42
1:B:332[B]:GLN:NE2	1:B:333:VAL:H	2.16	0.42
1:A:35:ALA:HB2	1:A:752:TYR:CD1	2.55	0.42
1:A:744:GLU:HG2	4:A:1049:HOH:O	2.19	0.41
1:B:188:CYS:HA	1:B:189:PRO:HD3	1.98	0.41
1:A:154:LYS:H	1:A:154:LYS:HG3	1.56	0.41
1:B:293[A]:ASP:OD1	1:B:296:GLN:HG3	2.21	0.41
1:A:322:GLU:CG	1:A:327:LEU:HD23	2.47	0.41
1:B:28:PRO:HD2	1:B:346:GLU:OE1	2.22	0.40
1:A:257:ASN:OD1	1:A:277:HIS:HE1	2.03	0.40
1:A:268:GLU:OE2	1:B:384[A]:ARG:NH2	2.54	0.40
1:A:58[A]:GLU:HG2	1:A:75:VAL:CG1	2.51	0.40
1:B:82:LEU:O	1:B:86:ARG:HG2	2.22	0.40
1:B:292:VAL:CG2	1:B:296:GLN:HB2	2.51	0.40

All (3) 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:154:LYS:CE	1:B:65:GLU:N[2_656]	2.01	0.19
1:A:154:LYS:NZ	1:B:64:ALA:N[2_656]	2.12	0.08
1:A:154:LYS:NZ	1:B:64:ALA:C[2_656]	2.13	0.07

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	417/438 (95%)	410 (98%)	6 (1%)	1 (0%)	47	49
1	B	422/438 (96%)	415 (98%)	6 (1%)	1 (0%)	47	49
All	All	839/876 (96%)	825 (98%)	12 (1%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	755	PRO
1	A	125	GLY

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	373/380 (98%)	365 (98%)	8 (2%)	53	59
1	B	378/380 (100%)	370 (98%)	8 (2%)	53	59
All	All	751/760 (99%)	735 (98%)	16 (2%)	55	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	209	LEU
1	A	243	LYS
1	A	250	ARG
1	A	377	ASP
1	A	707	ARG
1	A	712	GLN
1	A	732	LYS
1	B	119	ASP
1	B	131	ASN
1	B	211[A]	SER
1	B	211[B]	SER
1	B	343	ARG
1	B	377	ASP
1	B	378	SER
1	B	711	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	51	GLN
1	A	162	GLN
1	A	169	GLN
1	A	185	ASN
1	A	276	GLN
1	A	277	HIS
1	A	318	GLN
1	A	367	GLN
1	A	386	GLN
1	A	387	GLN
1	A	728	GLN
1	A	750	HIS
1	A	751	GLN
1	B	107	ASN
1	B	277	HIS
1	B	296	GLN
1	B	315	GLN
1	B	318	GLN
1	B	360	GLN
1	B	380	HIS

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Mol	Chain	Res	Type
1	B	728	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	ACT	A	901	-	3,3,3	1.20	0	3,3,3	1.40	0
2	ACT	A	902	3	3,3,3	1.31	0	3,3,3	1.59	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	902	ACT	O-C-CH3	-2.01	114.53	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ACT	1	0

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(Å²)	Q<0.9
1	A	419/438 (95%)	0.49	33 (7%)	12	16	26, 42, 78, 130	0
1	B	422/438 (96%)	0.49	30 (7%)	16	20	26, 40, 77, 140	0
All	All	841/876 (96%)	0.49	63 (7%)	14	18	26, 41, 77, 140	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	MET	7.6
1	B	319	GLY	7.3
1	A	151	SER	7.3
1	B	321	PRO	7.0
1	B	327	LEU	6.6
1	A	64	ALA	6.4
1	A	189	PRO	5.6
1	B	756	SER	5.2
1	B	126	ILE	5.0
1	B	318	GLN	4.8
1	A	150	GLY	4.6
1	A	25	ASN	4.2
1	B	142[A]	HIS	4.2
1	B	755	PRO	4.1
1	B	150	GLY	4.1
1	A	327	LEU	4.0
1	A	126	ILE	3.9
1	A	186	SER	3.8
1	B	293[A]	ASP	3.7
1	A	319	GLY	3.7
1	A	125	GLY	3.7
1	B	129	THR	3.5
1	B	169[A]	GLN	3.4
1	B	24	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	329	GLU	3.2
1	A	154	LYS	3.2
1	A	322	GLU	3.2
1	B	317	ALA	3.2
1	A	142	HIS	3.2
1	A	187	LYS	3.2
1	A	65	GLU	3.2
1	A	710	LEU	3.2
1	A	130	THR	3.2
1	B	292	VAL	3.1
1	A	711[A]	GLU	3.1
1	A	320	MET	3.1
1	A	26	ALA	3.0
1	B	25	ASN	3.0
1	B	125	GLY	2.9
1	A	225	LEU	2.9
1	B	250	ARG	2.7
1	B	148	THR	2.6
1	A	707	ARG	2.5
1	B	161	ASN	2.5
1	A	321	PRO	2.5
1	A	66	LEU	2.5
1	A	224	VAL	2.4
1	A	131	ASN	2.4
1	A	226	VAL	2.3
1	B	294	ARG	2.3
1	B	314	ILE	2.3
1	B	168	HIS	2.3
1	B	99	VAL	2.2
1	A	287	ASP	2.2
1	A	708	GLU	2.2
1	A	112	VAL	2.2
1	B	224	VAL	2.2
1	A	715	ALA	2.2
1	B	315	GLN	2.1
1	B	256	LEU	2.1
1	A	296	GLN	2.1
1	B	249	SER	2.0
1	A	161	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	A	903	1/1	0.68	0.12	93,93,93,93	0
2	ACT	A	902	4/4	0.79	0.17	41,53,53,56	0
3	CA	B	801	1/1	0.86	0.08	88,88,88,88	0
2	ACT	A	901	4/4	0.94	0.29	52,57,59,59	0
3	CA	A	904	1/1	0.96	0.07	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.