



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:03 PM UTC

PDB ID : 6F4A / pdb_00006f4a
Title : Yeast mitochondrial RNA degradosome complex mtEXO
Authors : Razew, M.; Nowak, E.; Nowotny, M.
Deposited on : 2017-11-29
Resolution : 3.55 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

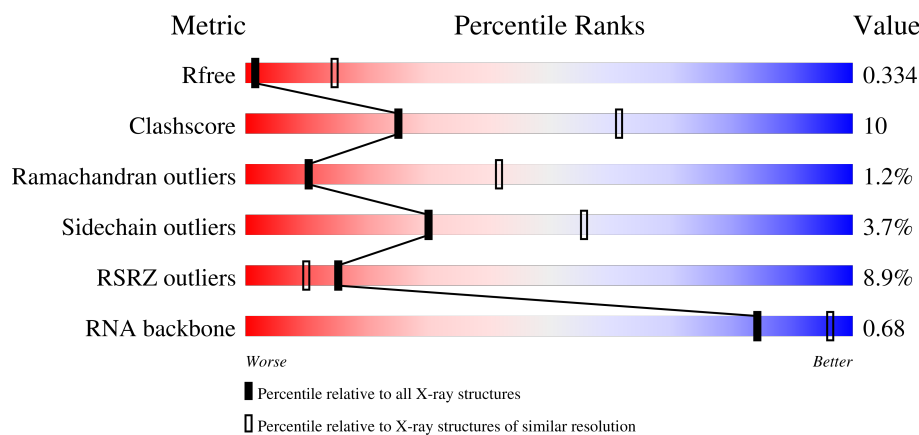
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)
RNA backbone	3983	1006 (4.02-3.06)

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	832	
2	B	644	
3	C	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7574 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 Exoribonuclease II, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	0	0
			4154	2598	730	813	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MET	-	initiating methionine	UNP A0A0W0CXR7
A	477	ASN	ASP	conflict	UNP A0A0W0CXR7
A	882	VAL	ILE	conflict	UNP A0A0W0CXR7

- Molecule 2 is a protein called Suv3 helicase.

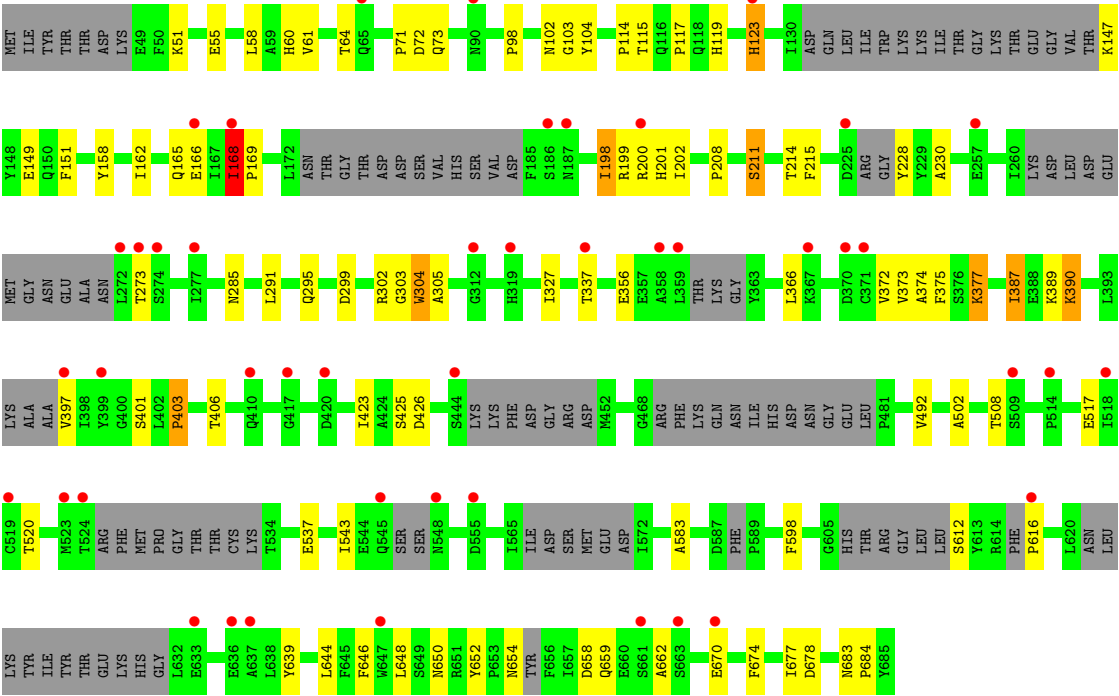
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	534	Total	C	N	O	S	0	0	0
			3301	2067	586	633	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	42	MET	-	initiating methionine	UNP Q6FKD7

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*GP*AP*UP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	P	0	0	0
			119	53	20	40	6			



● Molecule 3: RNA (5'-R(P*AP*GP*AP*UP*AP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.55Å 151.24Å 284.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 3.55 49.06 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.06-3.55) 95.4 (49.06-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.92 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.296 , 0.328 0.306 , 0.334	Depositor DCC
R_{free} test set	1318 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	139.5	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 247.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7574	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.45	0/4215	1.18	31/5792 (0.5%)
2	B	0.51	0/3351	1.25	30/4609 (0.7%)
3	C	0.14	0/132	0.34	0/203
All	All	0.48	0/7698	1.20	61/10604 (0.6%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	670	GLU	N-CA-C	11.23	123.09	111.07
1	A	590	PHE	CA-C-N	10.46	131.12	119.83
1	A	590	PHE	C-N-CA	10.46	131.12	119.83
1	A	886	HIS	CA-C-N	10.39	129.77	118.97
1	A	886	HIS	C-N-CA	10.39	129.77	118.97
1	A	279	ASP	CA-C-N	10.03	130.75	119.32
1	A	279	ASP	C-N-CA	10.03	130.75	119.32
1	A	267	ILE	N-CA-C	-9.11	103.02	111.67
1	A	199	SER	N-CA-C	-8.40	102.09	111.07
1	A	129	ASP	CA-C-N	8.17	130.05	119.84
1	A	129	ASP	C-N-CA	8.17	130.05	119.84
2	B	377	LYS	N-CA-C	-7.85	94.07	110.80
2	B	327	ILE	N-CA-C	7.80	121.71	112.35
2	B	543	ILE	N-CA-C	-7.71	102.93	110.72
2	B	537	GLU	N-CA-C	-7.57	102.97	111.07
2	B	215	PHE	N-CA-C	7.32	119.26	111.28
1	A	93	ASP	CA-C-N	7.08	127.68	119.47
1	A	93	ASP	C-N-CA	7.08	127.68	119.47
2	B	123	HIS	CB-CA-C	7.06	122.65	110.79
1	A	213	LEU	N-CA-C	6.82	122.03	112.75
2	B	677	ILE	N-CA-C	6.78	117.57	110.72
2	B	123	HIS	N-CA-CB	-6.71	100.20	110.13
2	B	214	THR	N-CA-C	6.65	118.53	111.28
2	B	327	ILE	CB-CA-C	-6.63	105.31	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	387	ILE	N-CA-C	6.59	116.74	110.42
2	B	303	GLY	N-CA-C	6.39	121.90	114.16
2	B	304	TRP	N-CA-C	6.38	118.24	111.28
2	B	502	ALA	CA-C-N	6.37	127.81	119.84
2	B	502	ALA	C-N-CA	6.37	127.81	119.84
1	A	127	THR	N-CA-C	-6.22	104.58	111.36
1	A	317	LEU	CA-C-N	6.06	126.38	119.83
1	A	317	LEU	C-N-CA	6.06	126.38	119.83
1	A	321	LYS	N-CA-C	5.99	117.81	111.28
1	A	738	SER	N-CA-C	5.96	118.56	111.71
1	A	232	GLY	N-CA-C	5.78	119.03	110.42
2	B	201	HIS	N-CA-C	5.73	118.29	109.07
2	B	508	THR	N-CA-C	-5.58	106.64	113.50
1	A	427	ASP	N-CA-C	-5.52	105.35	111.36
2	B	403	PRO	CA-C-N	5.51	124.97	119.24
2	B	403	PRO	C-N-CA	5.51	124.97	119.24
1	A	436	ILE	N-CA-C	-5.48	105.77	111.58
1	A	735	THR	N-CA-C	-5.47	105.39	111.36
1	A	771	GLY	O-C-N	5.41	123.02	121.07
2	B	583	ALA	CA-C-N	5.40	126.59	119.84
2	B	583	ALA	C-N-CA	5.40	126.59	119.84
2	B	168	ILE	CA-C-N	-5.34	113.03	120.25
2	B	168	ILE	C-N-CA	-5.34	113.03	120.25
1	A	364	ARG	N-CA-C	-5.33	105.47	111.28
2	B	366	LEU	N-CA-C	-5.32	103.11	110.35
1	A	97	LEU	N-CA-C	-5.28	105.61	111.36
2	B	492	VAL	N-CA-C	-5.25	104.40	111.44
1	A	292	GLU	N-CA-C	-5.25	105.64	111.36
1	A	461	GLY	N-CA-C	5.18	120.65	111.02
2	B	295	GLN	N-CA-C	5.17	118.68	112.38
1	A	122	ASN	N-CA-C	5.13	116.86	108.76
1	A	785	LYS	N-CA-C	-5.12	106.88	112.72
2	B	659	GLN	N-CA-C	5.11	121.69	110.80
2	B	678	ASP	N-CA-C	5.07	116.81	111.28
2	B	373	VAL	N-CA-C	5.03	115.58	107.73
1	A	671	LYS	N-CA-C	-5.02	105.81	111.28
1	A	792	LYS	N-CA-C	-5.01	103.79	110.55

There are no chirality outliers.

There are no planarity outliers.

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	4154	0	3132	89	0
2	B	3301	0	2356	37	0
3	C	119	0	61	3	0
All	All	7574	0	5549	127	0

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 10.

All (127) 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:209:ALA:HA	1:A:281:THR:HG23	1.69	0.75
1:A:770:ARG:NH1	1:A:773:ASP:OD1	2.22	0.73
1:A:553:ASP:N	1:A:588:SER:O	2.23	0.72
1:A:528:THR:HG23	1:A:537:PRO:HA	1.72	0.71
1:A:245:ILE:HD12	1:A:286:THR:HG23	1.73	0.70
2:B:652:TYR:O	2:B:654:ASN:N	2.22	0.69
1:A:527:PHE:HD2	1:A:770:ARG:HG2	1.62	0.64
1:A:326:TYR:OH	1:A:369:ASP:OD2	2.15	0.63
1:A:100:THR:OG1	1:A:152:ARG:NH2	2.32	0.62
1:A:670:THR:H	1:A:673:THR:HB	1.64	0.62
1:A:371:ALA:HA	1:A:402:ARG:HG3	1.82	0.61
1:A:229:ASP:OD1	1:A:231:ARG:HD3	2.01	0.61
1:A:509:TYR:HA	1:A:782:ARG:HH12	1.65	0.61
1:A:527:PHE:CE1	1:A:807:ALA:HB2	2.36	0.61
1:A:498:ASP:OD1	1:A:781:HIS:NE2	2.34	0.60
2:B:119:HIS:ND1	2:B:119:HIS:O	2.34	0.59
1:A:215:ILE:HG22	1:A:219:LYS:HE3	1.85	0.59
2:B:612:SER:N	2:B:658:ASP:OD2	2.36	0.59
2:B:403:PRO:HB3	2:B:639:TYR:CZ	2.38	0.58
1:A:226:TYR:HD2	1:A:263:VAL:HG11	1.69	0.58
2:B:158:TYR:O	2:B:162:ILE:HG12	2.03	0.58
2:B:200:ARG:HH11	2:B:337:THR:HG21	1.69	0.58
1:A:327:GLN:O	1:A:331:THR:HG23	2.04	0.57
1:A:105:GLY:HA2	1:A:119:MET:HE2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:O	1:A:436:ILE:N	2.38	0.57
1:A:529:THR:HB	1:A:536:VAL:HB	1.84	0.57
1:A:371:ALA:O	1:A:402:ARG:HD3	2.05	0.56
1:A:254:THR:O	1:A:257:ILE:N	2.39	0.56
1:A:455:THR:C	1:A:457:ARG:H	2.14	0.56
1:A:209:ALA:CA	1:A:281:THR:HG23	2.36	0.55
2:B:200:ARG:NH2	2:B:202:ILE:HD11	2.22	0.55
1:A:797:ASP:O	1:A:801:TRP:HD1	1.90	0.55
1:A:402:ARG:N	1:A:889:ASP:OD2	2.31	0.54
1:A:428:LEU:O	1:A:430:ILE:N	2.34	0.54
1:A:234:LYS:O	1:A:316:VAL:HG22	2.06	0.54
2:B:646:PHE:O	2:B:650:ASN:ND2	2.31	0.54
1:A:372:ALA:O	1:A:425:ASN:ND2	2.35	0.54
1:A:372:ALA:HB1	1:A:425:ASN:HA	1.89	0.53
1:A:434:SER:O	1:A:437:SER:N	2.42	0.52
1:A:432:LYS:O	1:A:434:SER:OG	2.27	0.52
1:A:338:TYR:HE2	1:A:387:LYS:HE3	1.73	0.52
2:B:299:ASP:OD2	2:B:302:ARG:N	2.41	0.52
1:A:219:LYS:HG2	1:A:250:ILE:HD11	1.93	0.51
2:B:658:ASP:HB3	2:B:662:ALA:HB2	1.93	0.51
2:B:147:LYS:N	2:B:149:GLU:OE1	2.43	0.51
1:A:338:TYR:N	1:A:338:TYR:CD1	2.78	0.51
1:A:444:TYR:CZ	1:A:540:PRO:HD3	2.47	0.50
1:A:407:LYS:O	1:A:410:VAL:HG22	2.11	0.50
1:A:334:GLU:HA	1:A:338:TYR:CD1	2.47	0.50
1:A:126:SER:C	1:A:712:ALA:HB2	2.36	0.50
1:A:449:PRO:HB3	1:A:543:PHE:CE2	2.47	0.50
1:A:782:ARG:HH21	1:A:789:LEU:C	2.20	0.49
2:B:117:PRO:HA	2:B:158:TYR:HE2	1.77	0.49
2:B:375:PHE:O	2:B:377:LYS:N	2.45	0.49
2:B:200:ARG:HH22	2:B:202:ILE:HD11	1.78	0.49
2:B:598:PHE:HE2	2:B:644:LEU:HD23	1.78	0.49
1:A:124:PRO:O	1:A:710:ASN:ND2	2.45	0.49
1:A:509:TYR:HA	1:A:782:ARG:NH1	2.28	0.49
2:B:374:ALA:O	2:B:425:SER:HA	2.14	0.48
1:A:460:PHE:O	1:A:463:MET:HG3	2.13	0.48
1:A:370:TYR:HE1	1:A:382:THR:HG22	1.77	0.48
1:A:197:ILE:O	1:A:201:THR:HG23	2.14	0.47
1:A:319:LEU:HD12	1:A:323:HIS:HB3	1.96	0.47
1:A:553:ASP:N	1:A:590:PHE:H	2.12	0.47
1:A:293:GLN:HB3	1:A:298:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:TYR:N	1:A:338:TYR:HD1	2.12	0.47
1:A:701:ARG:O	1:A:761:TYR:HB3	2.14	0.47
1:A:333:LEU:O	1:A:338:TYR:HA	2.15	0.47
1:A:744:SER:OG	3:C:2:A:OP1	2.25	0.47
2:B:648:LEU:O	2:B:652:TYR:N	2.48	0.47
2:B:51:LYS:O	2:B:55:GLU:HG2	2.15	0.46
1:A:402:ARG:HD2	1:A:888:LEU:O	2.14	0.46
1:A:435:GLY:O	1:A:439:VAL:HG23	2.15	0.46
2:B:304:TRP:CD1	2:B:305:ALA:N	2.84	0.46
1:A:754:LYS:HA	1:A:757:GLY:O	2.16	0.46
2:B:228:TYR:HA	2:B:273:THR:O	2.15	0.46
2:B:406:THR:HG22	2:B:674:PHE:HB2	1.97	0.46
1:A:278:ILE:O	1:A:280:PRO:HD3	2.16	0.45
1:A:747:SER:OG	1:A:749:PHE:O	2.31	0.45
1:A:345:ALA:HA	1:A:348:VAL:HG12	1.98	0.45
2:B:208:PRO:O	2:B:211:SER:OG	2.31	0.45
1:A:767:PRO:HA	1:A:773:ASP:HB2	1.98	0.45
2:B:372:VAL:O	2:B:423:ILE:HG23	2.16	0.45
2:B:166:GLU:O	2:B:169:PRO:HD2	2.17	0.45
1:A:344:PHE:HD1	1:A:360:TYR:CD2	2.34	0.44
1:A:428:LEU:C	1:A:430:ILE:H	2.24	0.44
1:A:149:VAL:HB	1:A:309:LEU:HD23	1.99	0.44
1:A:469:ASP:OD1	3:C:5:C:H5'	2.18	0.44
1:A:886:HIS:HA	1:A:887:PRO:HD2	1.73	0.43
1:A:291:ARG:O	1:A:294:GLN:HB2	2.18	0.43
1:A:240:SER:O	1:A:244:ILE:HG13	2.18	0.43
1:A:380:VAL:HA	1:A:383:THR:HG22	2.01	0.43
1:A:767:PRO:HG3	1:A:777:HIS:CE1	2.53	0.43
1:A:775:ILE:HG12	1:A:791:PHE:HE2	1.84	0.43
2:B:517:GLU:O	2:B:520:THR:OG1	2.37	0.43
2:B:102:ASN:O	2:B:104:TYR:N	2.50	0.43
2:B:230:ALA:HB3	2:B:291:LEU:HD23	2.01	0.43
2:B:683:ASN:HA	2:B:684:PRO:HD2	1.81	0.43
1:A:455:THR:C	1:A:457:ARG:N	2.77	0.43
1:A:782:ARG:NH2	1:A:790:CYS:HA	2.34	0.42
1:A:795:TYR:O	1:A:799:TYR:HD1	2.03	0.42
2:B:60:HIS:O	2:B:64:THR:HG23	2.19	0.42
1:A:129:ASP:HA	1:A:130:PRO:HD3	1.63	0.42
1:A:527:PHE:CD2	1:A:770:ARG:HG2	2.50	0.42
1:A:733:ASP:C	1:A:735:THR:H	2.27	0.42
2:B:168:ILE:H	2:B:169:PRO:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:O	1:A:334:GLU:HG2	2.20	0.42
2:B:387:ILE:HA	2:B:390:LYS:HE3	2.01	0.42
1:A:427:ASP:O	1:A:429:ASN:N	2.53	0.41
1:A:775:ILE:HD12	1:A:803:PHE:CE2	2.55	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.79	0.41
2:B:198:ILE:HG23	2:B:199:ARG:O	2.20	0.41
2:B:403:PRO:O	2:B:406:THR:OG1	2.37	0.41
1:A:398:GLN:HG3	1:A:399:ASP:N	2.35	0.41
2:B:165:GLN:O	2:B:169:PRO:HD3	2.20	0.41
2:B:61:VAL:O	2:B:64:THR:OG1	2.31	0.41
1:A:287:TYR:OH	1:A:291:ARG:NH1	2.52	0.41
1:A:289:GLY:O	1:A:293:GLN:HG3	2.21	0.41
1:A:305:ASN:HB2	1:A:312:THR:HG21	2.03	0.41
1:A:331:THR:HA	1:A:334:GLU:HG2	2.02	0.41
1:A:372:ALA:HB1	1:A:425:ASN:CA	2.51	0.41
1:A:431:PRO:HA	1:A:434:SER:HB2	2.03	0.40
1:A:770:ARG:NH2	1:A:773:ASP:OD2	2.55	0.40
2:B:426:ASP:OD1	2:B:426:ASP:N	2.53	0.40
3:C:0:A:O2'	3:C:1:G:H8	2.04	0.40
1:A:345:ALA:O	1:A:348:VAL:HG12	2.22	0.40
2:B:71:PRO:O	2:B:73:GLN:N	2.54	0.40

There are no symmetry-related clashes.

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	600/832 (72%)	571 (95%)	23 (4%)	6 (1%)	12	45
2	B	500/644 (78%)	446 (89%)	47 (9%)	7 (1%)	9	38
All	All	1100/1476 (74%)	1017 (92%)	70 (6%)	13 (1%)	10	42

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	ASN
1	A	435	GLY
1	A	456	ASP
2	B	168	ILE
2	B	356	GLU
2	B	72	ASP
2	B	114	PRO
2	B	115	THR
1	A	428	LEU
2	B	98	PRO
2	B	103	GLY
1	A	191	VAL
1	A	197	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/759 (39%)	287 (98%)	7 (2%)	43	63
2	B	194/568 (34%)	183 (94%)	11 (6%)	18	46
All	All	488/1327 (37%)	470 (96%)	18 (4%)	30	56

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	GLU
1	A	338	TYR
1	A	378	ASN
1	A	673	THR
1	A	711	GLN
1	A	759	THR
1	A	798	GLN
2	B	58	LEU
2	B	123	HIS
2	B	151	PHE

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Mol	Chain	Res	Type
2	B	198	ILE
2	B	211	SER
2	B	285	ASN
2	B	389	LYS
2	B	390	LYS
2	B	397	VAL
2	B	401	SER
2	B	616	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
2	B	123	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 oligosaccharides 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 [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, 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	644/832 (77%)	0.63	59 (9%) 14 9	75, 152, 237, 307	0
2	B	534/644 (82%)	0.59	45 (8%) 17 11	86, 152, 221, 287	0
3	C	6/6 (100%)	1.09	1 (16%) 4 4	149, 168, 179, 203	0
All	All	1184/1482 (79%)	0.61	105 (8%) 15 10	75, 152, 231, 307	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	780	LEU	7.1
2	B	519	CYS	5.0
1	A	781	HIS	4.4
1	A	560	SER	4.3
1	A	210	TRP	4.1
1	A	760	ALA	3.9
2	B	200	ARG	3.8
1	A	754	LYS	3.8
1	A	683	THR	3.8
1	A	819	THR	3.7
1	A	467	CYS	3.6
1	A	533	ASP	3.6
1	A	496	ILE	3.5
1	A	423	LEU	3.5
2	B	123	HIS	3.5
1	A	553	ASP	3.5
2	B	187	ASN	3.4
2	B	514	PRO	3.4
1	A	767	PRO	3.3
1	A	572	GLY	3.3
2	B	359	LEU	3.3
2	B	371	CYS	3.3
1	A	132	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	475	GLU	3.3
1	A	813	PHE	3.2
2	B	397	VAL	3.1
1	A	673	THR	3.1
1	A	736	LYS	3.1
2	B	417	GLY	3.1
1	A	777	HIS	3.1
1	A	815	ARG	3.0
2	B	257	GLU	3.0
1	A	442	LYS	3.0
2	B	670	GLU	2.9
2	B	661	SER	2.8
2	B	90	ASN	2.8
2	B	168	ILE	2.7
1	A	821	TRP	2.7
1	A	104	VAL	2.7
1	A	275	ASN	2.7
1	A	784	LEU	2.7
1	A	682	LEU	2.6
2	B	548	ASN	2.6
1	A	138	ASP	2.5
1	A	297	ASN	2.5
2	B	410	GLN	2.5
1	A	474	HIS	2.5
1	A	257	ILE	2.5
1	A	622	THR	2.5
2	B	523	MET	2.5
2	B	358	ALA	2.5
2	B	337	THR	2.5
2	B	663	SER	2.5
1	A	638	VAL	2.4
1	A	235	HIS	2.4
2	B	312	GLY	2.4
2	B	319	HIS	2.3
2	B	637	ALA	2.3
2	B	370	ASP	2.3
1	A	790	CYS	2.3
1	A	526	ALA	2.3
1	A	669	GLN	2.3
1	A	206	THR	2.3
1	A	236	VAL	2.3
2	B	277	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	660	CYS	2.2
2	B	524	THR	2.2
1	A	817	SER	2.2
2	B	444	SER	2.2
2	B	273	THR	2.2
2	B	186	SER	2.2
2	B	399	TYR	2.2
1	A	127	THR	2.2
2	B	545	GLN	2.1
2	B	647	TRP	2.1
1	A	105	GLY	2.1
1	A	328	GLU	2.1
1	A	213	LEU	2.1
1	A	147	ASN	2.1
1	A	315	ALA	2.1
1	A	478	ASP	2.1
1	A	309	LEU	2.1
1	A	549	LEU	2.1
1	A	759	THR	2.1
2	B	65	GLN	2.1
2	B	225	ASP	2.1
2	B	555	ASP	2.1
2	B	518	ILE	2.1
2	B	367	LYS	2.1
2	B	509	SER	2.1
1	A	882	VAL	2.1
2	B	166	GLU	2.1
2	B	636	GLU	2.1
2	B	274	SER	2.1
1	A	149	VAL	2.1
1	A	513	GLY	2.0
2	B	420	ASP	2.0
1	A	678	GLU	2.0
3	C	5	C	2.0
1	A	776	ASN	2.0
2	B	633	GLU	2.0
1	A	818	SER	2.0
2	B	272	LEU	2.0
2	B	616	PRO	2.0
1	A	576	ASP	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 oligosaccharides 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.