



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:23 AM UTC

PDB ID : 3U4T / pdb_00003u4t
Title : Crystal Structure of the C-terminal part of the TPR repeat-containing protein Q11TI6_CYTH3 from *Cytophaga hutchinsonii*. Northeast Structural Genomics Consortium Target ChR11B.
Authors : Vorobiev, S.; Neely, H.; Chen, Y.; Seetharaman, J.; Patel, P.; Xiao, R.; Ciccosanti, C.; Maglaqui, M.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-10-10
Resolution : 2.28 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

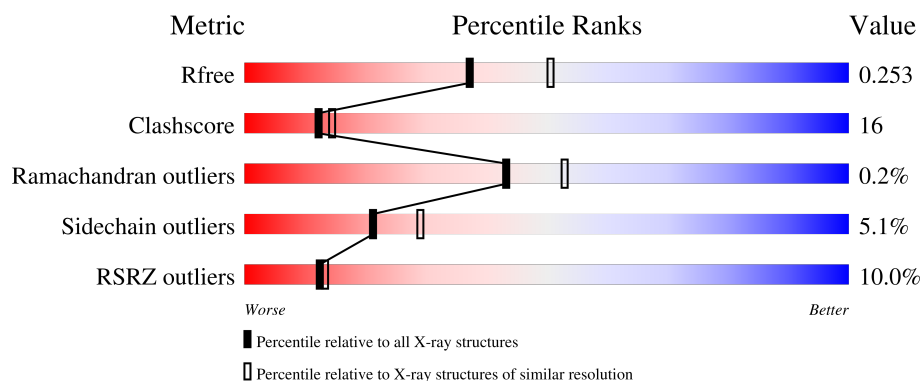
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	272	10% 60% 32% • 5%
1	B	272	9% 68% 23% • 5%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4366 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 TPR repeat-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	Se	0	0	0
			2128	1381	344	398	2	3			
1	B	258	Total	C	N	O	S	Se	0	0	0
			2129	1381	344	398	2	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	MSE	-	expression tag	UNP Q11TI6
A	357	GLU	SER	engineered mutation	UNP Q11TI6
A	490	LEU	-	expression tag	UNP Q11TI6
A	491	GLU	-	expression tag	UNP Q11TI6
A	492	HIS	-	expression tag	UNP Q11TI6
A	493	HIS	-	expression tag	UNP Q11TI6
A	494	HIS	-	expression tag	UNP Q11TI6
A	495	HIS	-	expression tag	UNP Q11TI6
A	496	HIS	-	expression tag	UNP Q11TI6
A	497	HIS	-	expression tag	UNP Q11TI6
B	226	MSE	-	expression tag	UNP Q11TI6
B	357	GLU	SER	engineered mutation	UNP Q11TI6
B	490	LEU	-	expression tag	UNP Q11TI6
B	491	GLU	-	expression tag	UNP Q11TI6
B	492	HIS	-	expression tag	UNP Q11TI6
B	493	HIS	-	expression tag	UNP Q11TI6
B	494	HIS	-	expression tag	UNP Q11TI6
B	495	HIS	-	expression tag	UNP Q11TI6
B	496	HIS	-	expression tag	UNP Q11TI6
B	497	HIS	-	expression tag	UNP Q11TI6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total 56	O 56	0	0
2	B	53	Total 53	O 53	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.67Å 42.82Å 104.95Å 90.00° 92.83° 90.00°	Depositor
Resolution (Å)	42.28 – 2.28 42.28 – 2.28	Depositor EDS
% Data completeness (in resolution range)	92.5 (42.28-2.28) 95.8 (42.28-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.238 , 0.256 0.234 , 0.253	Depositor DCC
R_{free} test set	1688 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4366	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.57% 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	0.48	0/2177	1.01	15/2936 (0.5%)
1	B	0.49	0/2177	1.04	12/2933 (0.4%)
All	All	0.48	0/4354	1.02	27/5869 (0.5%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	PHE	N-CA-C	-12.61	97.61	111.36
1	A	287	THR	N-CA-C	-7.43	103.26	111.36
1	B	258	LYS	N-CA-C	6.41	120.49	111.52
1	A	407	ARG	N-CA-C	-6.06	104.67	111.28
1	A	476	ASP	CA-C-N	6.00	125.67	119.56
1	A	476	ASP	C-N-CA	6.00	125.67	119.56
1	B	305	TYR	N-CA-C	-5.99	104.76	111.28
1	B	315	ASP	N-CA-C	5.93	118.23	111.11
1	B	407	ARG	N-CA-C	-5.82	104.94	111.28
1	B	458	ILE	N-CA-C	-5.80	104.85	110.42
1	B	415	ASP	CA-C-N	5.73	125.85	119.32
1	B	415	ASP	C-N-CA	5.73	125.85	119.32
1	A	258	LYS	N-CA-C	5.67	119.21	111.39
1	A	305	TYR	N-CA-C	-5.57	105.12	111.14
1	A	242	ASN	N-CA-C	5.54	124.62	113.31
1	A	415	ASP	CA-C-N	5.54	125.64	119.32
1	A	415	ASP	C-N-CA	5.54	125.64	119.32
1	A	240	LYS	N-CA-C	-5.49	106.28	112.87
1	B	391	VAL	N-CA-C	-5.46	105.18	110.42
1	B	264	ILE	N-CA-C	-5.33	105.22	113.16
1	A	480	LYS	N-CA-C	5.20	117.03	111.36
1	B	232	PHE	N-CA-CB	5.17	117.81	110.16
1	B	263	TYR	N-CA-C	5.17	121.80	110.80
1	A	457	THR	N-CA-C	-5.10	105.80	111.36
1	A	264	ILE	N-CA-C	-5.09	105.17	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	LYS	CA-C-N	5.03	125.31	119.93
1	A	397	LYS	C-N-CA	5.03	125.31	119.93

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	2128	0	2095	69	0
1	B	2129	0	2095	62	0
2	A	56	0	0	2	0
2	B	53	0	0	0	0
All	All	4366	0	4190	131	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 16.

All (131) 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:322:TYR:HA	1:B:335:MSE:HE3	1.34	1.09
1:A:322:TYR:HA	1:A:335:MSE:HE3	1.38	1.02
1:A:435:ALA:HB3	1:A:436:PRO:HD3	1.52	0.92
1:B:231:GLU:HG3	1:B:254:LEU:HD11	1.52	0.90
1:B:481:LYS:N	1:B:481:LYS:HE3	1.90	0.86
1:B:325:ALA:CB	1:B:335:MSE:HE2	2.07	0.85
1:A:325:ALA:HB3	1:A:335:MSE:HE2	1.63	0.81
1:B:481:LYS:HE3	1:B:481:LYS:H	1.47	0.80
1:B:322:TYR:CA	1:B:335:MSE:HE3	2.12	0.78
1:B:322:TYR:HA	1:B:335:MSE:CE	2.10	0.78
1:A:481:LYS:H	1:A:481:LYS:HZ2	1.31	0.75
1:B:232:PHE:HA	1:B:254:LEU:HD21	1.69	0.75
1:A:325:ALA:CB	1:A:335:MSE:HE2	2.17	0.75
1:B:325:ALA:HB3	1:B:335:MSE:HE2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:TYR:O	1:B:248:ILE:HG13	1.86	0.74
1:A:238:LEU:N	1:A:238:LEU:HD23	2.02	0.73
1:B:258:LYS:N	1:B:258:LYS:HD2	2.04	0.72
1:A:234:TYR:O	1:A:237:PHE:HB3	1.91	0.71
1:A:244:TYR:O	1:A:248:ILE:HG13	1.91	0.70
1:B:398:PRO:O	1:B:399:ASN:HB2	1.90	0.70
1:A:322:TYR:CA	1:A:335:MSE:HE3	2.18	0.70
1:A:258:LYS:HD2	1:A:258:LYS:N	2.07	0.69
1:A:356:MSE:HA	2:A:609:HOH:O	1.93	0.69
1:B:361:ARG:C	1:B:363:THR:H	2.01	0.68
1:A:322:TYR:HA	1:A:335:MSE:CE	2.20	0.68
1:B:231:GLU:HG3	1:B:254:LEU:CD1	2.26	0.66
1:B:232:PHE:C	1:B:232:PHE:CD2	2.73	0.66
1:A:234:TYR:CE2	1:A:238:LEU:HD21	2.34	0.63
1:B:245:ALA:O	1:B:249:GLU:HG2	1.99	0.62
1:A:245:ALA:O	1:A:249:GLU:HG2	1.98	0.62
1:A:435:ALA:HB3	1:A:436:PRO:CD	2.27	0.62
1:B:361:ARG:HH11	1:B:361:ARG:HG2	1.64	0.62
1:B:435:ALA:HB3	1:B:436:PRO:HD3	1.82	0.61
1:A:309:LEU:HD13	1:A:317:LEU:HB3	1.82	0.61
1:B:361:ARG:O	1:B:363:THR:N	2.31	0.61
1:A:481:LYS:HE3	1:A:481:LYS:N	2.16	0.60
1:B:481:LYS:H	1:B:481:LYS:CE	2.13	0.60
1:A:481:LYS:H	1:A:481:LYS:NZ	1.99	0.60
1:B:469:TRP:CE3	1:B:482:ALA:HA	2.36	0.59
1:B:232:PHE:CD2	1:B:232:PHE:O	2.55	0.59
1:B:232:PHE:C	1:B:232:PHE:HD2	2.12	0.58
1:A:238:LEU:HD23	1:A:238:LEU:H	1.67	0.57
1:B:361:ARG:HB3	1:B:363:THR:HG22	1.85	0.57
1:A:236:ASP:O	1:A:240:LYS:HB2	2.05	0.56
1:A:371:TYR:HE2	1:A:406:TRP:CD1	2.23	0.55
1:B:235:ALA:HB2	1:B:250:VAL:CG2	2.36	0.55
1:B:361:ARG:HG2	1:B:361:ARG:NH1	2.21	0.55
1:B:361:ARG:C	1:B:363:THR:N	2.64	0.55
1:B:403:GLY:O	1:B:407:ARG:HG3	2.07	0.55
1:A:418:THR:HG22	1:A:418:THR:O	2.07	0.55
1:A:312:LYS:HA	1:A:312:LYS:HE2	1.89	0.55
1:A:391:VAL:O	1:A:395:GLU:HG3	2.07	0.55
1:A:315:ASP:O	1:A:319:ILE:HG12	2.07	0.54
1:A:469:TRP:CE3	1:A:482:ALA:HA	2.43	0.54
1:A:435:ALA:CB	1:A:436:PRO:HD3	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:PHE:O	1:B:232:PHE:HD2	1.90	0.52
1:A:462:LYS:HE2	2:A:593:HOH:O	2.10	0.52
1:A:239:PHE:C	1:A:241:ASN:H	2.18	0.52
1:A:303:GLU:CD	1:A:332:ARG:HH22	2.18	0.52
1:A:303:GLU:HA	1:A:335:MSE:HE1	1.91	0.52
1:B:282:GLN:O	1:B:286:GLU:HG3	2.10	0.52
1:B:424:LYS:O	1:B:428:GLU:HG3	2.10	0.52
1:A:481:LYS:N	1:A:481:LYS:CE	2.73	0.52
1:A:481:LYS:H	1:A:481:LYS:CE	2.23	0.51
1:B:430:LEU:O	1:B:434:CYS:HB2	2.11	0.51
1:B:322:TYR:HD1	1:B:335:MSE:HE1	1.74	0.51
1:B:361:ARG:HB3	1:B:363:THR:CG2	2.41	0.50
1:A:230:VAL:HG23	1:A:231:GLU:N	2.27	0.50
1:A:349:PHE:O	1:A:353:ILE:HG13	2.12	0.50
1:A:434:CYS:O	1:A:435:ALA:C	2.56	0.49
1:A:239:PHE:C	1:A:241:ASN:N	2.69	0.49
1:A:325:ALA:HB3	1:A:335:MSE:CE	2.39	0.49
1:A:392:LYS:O	1:A:396:LEU:HG	2.12	0.49
1:A:234:TYR:CD2	1:A:238:LEU:HD21	2.47	0.49
1:A:266:ASN:HB3	1:A:288:TYR:CD1	2.48	0.48
1:B:392:LYS:O	1:B:396:LEU:HG	2.13	0.48
1:A:299:SER:HB2	1:A:329:ASP:HB2	1.96	0.48
1:B:312:LYS:HA	1:B:312:LYS:HE2	1.95	0.48
1:A:343:PHE:CD1	1:A:351:LEU:HD23	2.48	0.48
1:A:430:LEU:HD23	1:A:448:ALA:HB2	1.96	0.47
1:A:430:LEU:O	1:A:434:CYS:HB2	2.14	0.47
1:B:484:ASP:HA	1:B:487:LYS:HG2	1.95	0.47
1:A:323:GLN:O	1:A:326:VAL:HG12	2.15	0.47
1:A:473:LEU:HA	1:A:476:ASP:O	2.15	0.47
1:B:238:LEU:HD12	1:B:247:ALA:HA	1.97	0.47
1:B:235:ALA:HB2	1:B:250:VAL:HG22	1.97	0.47
1:B:235:ALA:HB2	1:B:250:VAL:HG21	1.96	0.46
1:B:356:MSE:O	1:B:359:GLN:HB2	2.15	0.46
1:B:325:ALA:HB3	1:B:335:MSE:CE	2.42	0.46
1:A:243:ASN:HB3	1:A:246:GLU:HB2	1.96	0.46
1:B:233:ARG:HE	1:B:233:ARG:HB2	1.49	0.46
1:B:398:PRO:O	1:B:399:ASN:CB	2.62	0.46
1:B:243:ASN:HB3	1:B:246:GLU:OE1	2.16	0.45
1:A:361:ARG:C	1:A:363:THR:H	2.23	0.45
1:A:312:LYS:HE2	1:A:312:LYS:CA	2.45	0.45
1:B:400:ILE:O	1:B:400:ILE:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:VAL:O	1:B:251:PHE:C	2.60	0.44
1:B:315:ASP:O	1:B:319:ILE:HG12	2.17	0.44
1:A:435:ALA:CB	1:A:436:PRO:CD	2.92	0.44
1:B:253:LYS:O	1:B:257:LYS:HG2	2.18	0.44
1:B:427:TYR:CD1	1:B:448:ALA:HA	2.53	0.44
1:B:322:TYR:CD1	1:B:335:MSE:HE1	2.52	0.44
1:B:322:TYR:HD1	1:B:335:MSE:CE	2.31	0.44
1:B:357:GLU:C	1:B:359:GLN:N	2.75	0.43
1:A:292:VAL:HG22	1:A:293:ASN:N	2.34	0.43
1:A:243:ASN:HB3	1:A:246:GLU:OE1	2.18	0.43
1:A:430:LEU:HD21	1:A:444:GLU:HB3	2.00	0.43
1:A:282:GLN:O	1:A:286:GLU:HG3	2.19	0.43
1:A:398:PRO:O	1:A:399:ASN:HB2	2.18	0.43
1:A:399:ASN:HA	1:A:404:TYR:CE2	2.53	0.43
1:A:448:ALA:O	1:A:452:ILE:HG12	2.19	0.43
1:A:386:ALA:O	1:A:390:PHE:CD2	2.72	0.43
1:B:299:SER:HB2	1:B:329:ASP:HB2	1.99	0.43
1:A:244:TYR:CD1	1:A:271:CYS:HA	2.54	0.42
1:B:429:LYS:O	1:B:432:GLU:HB2	2.20	0.42
1:B:231:GLU:CG	1:B:254:LEU:HD11	2.37	0.42
1:B:453:ALA:HB2	1:B:468:ALA:HB3	2.02	0.42
1:A:415:ASP:HB2	1:A:422:LEU:HD12	2.02	0.42
1:A:424:LYS:HB3	1:A:425:PRO:CD	2.50	0.42
1:A:263:TYR:HB3	1:A:267:ARG:NH1	2.35	0.41
1:A:405:LEU:O	1:A:408:ALA:HB3	2.21	0.41
1:A:479:ASN:O	1:A:483:ILE:HG13	2.20	0.41
1:B:312:LYS:HE2	1:B:312:LYS:CA	2.50	0.41
1:B:479:ASN:O	1:B:483:ILE:HG13	2.21	0.41
1:A:399:ASN:HA	1:A:404:TYR:HE2	1.84	0.41
1:A:240:LYS:HA	1:A:240:LYS:HE2	2.02	0.40
1:B:233:ARG:HH11	1:B:233:ARG:HD2	1.72	0.40
1:A:266:ASN:HB3	1:A:288:TYR:CG	2.57	0.40
1:B:373:LEU:HG	1:B:377:TYR:CE2	2.56	0.40
1:A:235:ALA:HA	1:A:238:LEU:HG	2.03	0.40
1:B:263:TYR:HB3	1:B:267:ARG:NH1	2.36	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	256/272 (94%)	243 (95%)	12 (5%)	1 (0%)	30	36
1	B	256/272 (94%)	239 (93%)	17 (7%)	0	100	100
All	All	512/544 (94%)	482 (94%)	29 (6%)	1 (0%)	43	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	THR

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	217/226 (96%)	206 (95%)	11 (5%)	21	29
1	B	217/226 (96%)	206 (95%)	11 (5%)	21	29
All	All	434/452 (96%)	412 (95%)	22 (5%)	21	29

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LEU
1	A	240	LYS
1	A	250	VAL
1	A	254	LEU
1	A	280	LEU

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Mol	Chain	Res	Type
1	A	312	LYS
1	A	317	LEU
1	A	328	ARG
1	A	402	ILE
1	A	464	LYS
1	A	481	LYS
1	B	232	PHE
1	B	233	ARG
1	B	250	VAL
1	B	254	LEU
1	B	280	LEU
1	B	314	GLN
1	B	317	LEU
1	B	328	ARG
1	B	363	THR
1	B	480	LYS
1	B	481	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	A	449	ASN
1	A	471	ASN
1	B	243	ASN
1	B	252	ASN
1	B	338	GLN
1	B	354	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	255/272 (93%)	0.52	26 (10%) 12 13	22, 40, 71, 93	0
1	B	254/272 (93%)	0.51	25 (9%) 13 14	22, 40, 75, 99	0
All	All	509/544 (93%)	0.51	51 (10%) 12 13	22, 40, 72, 99	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	4.5
1	A	363	THR	4.3
1	B	459	ASN	4.1
1	B	363	THR	3.8
1	B	231	GLU	3.8
1	A	256	ALA	3.7
1	A	253	LYS	3.7
1	B	232	PHE	3.7
1	A	243	ASN	3.5
1	B	238	LEU	3.5
1	B	463	VAL	3.4
1	B	454	TYR	3.3
1	B	460	ARG	3.2
1	A	487	LYS	3.2
1	A	254	LEU	3.2
1	A	230	VAL	3.1
1	A	237	PHE	3.0
1	A	257	LYS	3.0
1	B	257	LYS	2.9
1	B	256	ALA	2.9
1	A	232	PHE	2.9
1	B	458	ILE	2.9
1	A	454	TYR	2.8
1	B	234	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	362	PRO	2.8
1	A	420	GLN	2.8
1	B	240	LYS	2.7
1	B	259	TYR	2.7
1	B	249	GLU	2.7
1	B	480	LYS	2.7
1	A	277	LYS	2.6
1	B	250	VAL	2.5
1	A	460	ARG	2.5
1	A	241	ASN	2.4
1	B	253	LYS	2.4
1	A	419	LYS	2.4
1	B	487	LYS	2.4
1	A	234	TYR	2.3
1	A	470	LYS	2.3
1	B	473	LEU	2.2
1	A	365	THR	2.2
1	A	233	ARG	2.2
1	A	259	TYR	2.2
1	A	246	GLU	2.2
1	A	398	PRO	2.1
1	A	275	LEU	2.1
1	B	243	ASN	2.1
1	B	399	ASN	2.1
1	A	362	PRO	2.1
1	B	367	PRO	2.1
1	B	479	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 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.