



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 AM UTC

PDB ID : 8BFI / pdb_00008bfi
Title : human CNOT1-CNOT10-CNOT11 module
Authors : Basquin, J.; Ozgur, S.; Conti, E.
Deposited on : 2022-10-26
Resolution : 3.00 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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

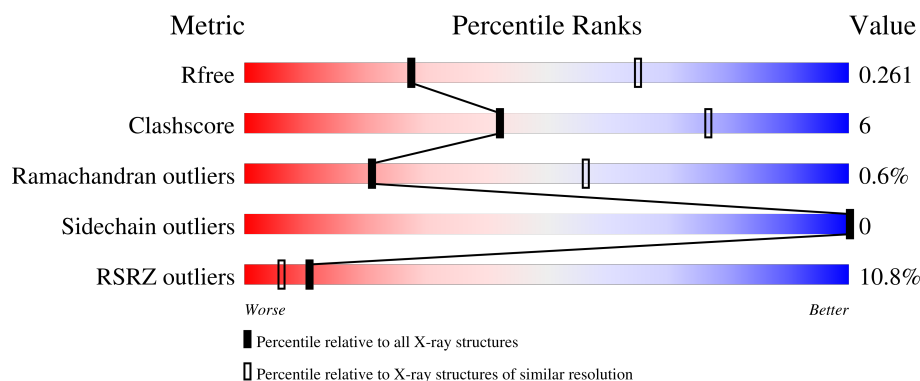
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	778	7% 63% 13% 23%
2	B	718	2% 68% 12% 20%
3	C	455	22% 80% 11% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11890 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 CCR4-NOT transcription complex subunit 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	Se	0	0	0
			4496	2878	780	817	10	11			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-90	MSE	-	initiating methionine	UNP A5YKK6
A	-89	HIS	-	expression tag	UNP A5YKK6
A	-88	HIS	-	expression tag	UNP A5YKK6
A	-87	HIS	-	expression tag	UNP A5YKK6
A	-86	HIS	-	expression tag	UNP A5YKK6
A	-85	HIS	-	expression tag	UNP A5YKK6
A	-84	HIS	-	expression tag	UNP A5YKK6
A	-83	GLY	-	expression tag	UNP A5YKK6
A	-82	MSE	-	expression tag	UNP A5YKK6
A	-81	GLU	-	expression tag	UNP A5YKK6
A	-80	GLY	-	expression tag	UNP A5YKK6
A	-79	GLU	-	expression tag	UNP A5YKK6
A	-78	TYR	-	expression tag	UNP A5YKK6
A	-77	ILE	-	expression tag	UNP A5YKK6
A	-76	LYS	-	expression tag	UNP A5YKK6
A	-75	LEU	-	expression tag	UNP A5YKK6
A	-74	LYS	-	expression tag	UNP A5YKK6
A	-73	VAL	-	expression tag	UNP A5YKK6
A	-72	ILE	-	expression tag	UNP A5YKK6
A	-71	GLY	-	expression tag	UNP A5YKK6
A	-70	GLN	-	expression tag	UNP A5YKK6
A	-69	ASP	-	expression tag	UNP A5YKK6
A	-68	SER	-	expression tag	UNP A5YKK6
A	-67	SER	-	expression tag	UNP A5YKK6
A	-66	GLU	-	expression tag	UNP A5YKK6
A	-65	ILE	-	expression tag	UNP A5YKK6
A	-64	HIS	-	expression tag	UNP A5YKK6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-63	PHE	-	expression tag	UNP A5YKK6
A	-62	LYS	-	expression tag	UNP A5YKK6
A	-61	VAL	-	expression tag	UNP A5YKK6
A	-60	LYS	-	expression tag	UNP A5YKK6
A	-59	MSE	-	expression tag	UNP A5YKK6
A	-58	THR	-	expression tag	UNP A5YKK6
A	-57	THR	-	expression tag	UNP A5YKK6
A	-56	HIS	-	expression tag	UNP A5YKK6
A	-55	LEU	-	expression tag	UNP A5YKK6
A	-54	LYS	-	expression tag	UNP A5YKK6
A	-53	LYS	-	expression tag	UNP A5YKK6
A	-52	LEU	-	expression tag	UNP A5YKK6
A	-51	LYS	-	expression tag	UNP A5YKK6
A	-50	GLU	-	expression tag	UNP A5YKK6
A	-49	SER	-	expression tag	UNP A5YKK6
A	-48	TYR	-	expression tag	UNP A5YKK6
A	-47	CYS	-	expression tag	UNP A5YKK6
A	-46	GLN	-	expression tag	UNP A5YKK6
A	-45	ARG	-	expression tag	UNP A5YKK6
A	-44	GLN	-	expression tag	UNP A5YKK6
A	-43	GLY	-	expression tag	UNP A5YKK6
A	-42	VAL	-	expression tag	UNP A5YKK6
A	-41	PRO	-	expression tag	UNP A5YKK6
A	-40	MSE	-	expression tag	UNP A5YKK6
A	-39	ASN	-	expression tag	UNP A5YKK6
A	-38	SER	-	expression tag	UNP A5YKK6
A	-37	LEU	-	expression tag	UNP A5YKK6
A	-36	ARG	-	expression tag	UNP A5YKK6
A	-35	PHE	-	expression tag	UNP A5YKK6
A	-34	LEU	-	expression tag	UNP A5YKK6
A	-33	PHE	-	expression tag	UNP A5YKK6
A	-32	GLU	-	expression tag	UNP A5YKK6
A	-31	GLY	-	expression tag	UNP A5YKK6
A	-30	GLN	-	expression tag	UNP A5YKK6
A	-29	ARG	-	expression tag	UNP A5YKK6
A	-28	ILE	-	expression tag	UNP A5YKK6
A	-27	ALA	-	expression tag	UNP A5YKK6
A	-26	ASP	-	expression tag	UNP A5YKK6
A	-25	ASN	-	expression tag	UNP A5YKK6
A	-24	HIS	-	expression tag	UNP A5YKK6
A	-23	THR	-	expression tag	UNP A5YKK6
A	-22	PRO	-	expression tag	UNP A5YKK6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	LYS	-	expression tag	UNP A5YKK6
A	-20	GLU	-	expression tag	UNP A5YKK6
A	-19	LEU	-	expression tag	UNP A5YKK6
A	-18	GLY	-	expression tag	UNP A5YKK6
A	-17	MSE	-	expression tag	UNP A5YKK6
A	-16	GLU	-	expression tag	UNP A5YKK6
A	-15	GLU	-	expression tag	UNP A5YKK6
A	-14	GLU	-	expression tag	UNP A5YKK6
A	-13	ASP	-	expression tag	UNP A5YKK6
A	-12	VAL	-	expression tag	UNP A5YKK6
A	-11	ILE	-	expression tag	UNP A5YKK6
A	-10	GLU	-	expression tag	UNP A5YKK6
A	-9	VAL	-	expression tag	UNP A5YKK6
A	-8	TYR	-	expression tag	UNP A5YKK6
A	-7	GLN	-	expression tag	UNP A5YKK6
A	-6	GLU	-	expression tag	UNP A5YKK6
A	-5	GLN	-	expression tag	UNP A5YKK6
A	-4	THR	-	expression tag	UNP A5YKK6
A	-3	GLY	-	expression tag	UNP A5YKK6
A	-2	GLY	-	expression tag	UNP A5YKK6
A	-1	ARG	-	expression tag	UNP A5YKK6
A	0	SER	-	expression tag	UNP A5YKK6
A	381	VAL	ILE	conflict	UNP A5YKK6
A	649	VAL	ALA	conflict	UNP A5YKK6
A	681	THR	MET	conflict	UNP A5YKK6

- Molecule 2 is a protein called CCR4-NOT transcription complex subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	574	Total	C	N	O	S	0	0	0
			4437	2818	767	824	28			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q9H9A5
B	-2	PRO	-	expression tag	UNP Q9H9A5
B	-1	ASP	-	expression tag	UNP Q9H9A5
B	0	SER	-	expression tag	UNP Q9H9A5

- Molecule 3 is a protein called CCR4-NOT transcription complex subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	410	Total	C	N	O	S	0	0	0
			2957	1900	499	543	15			

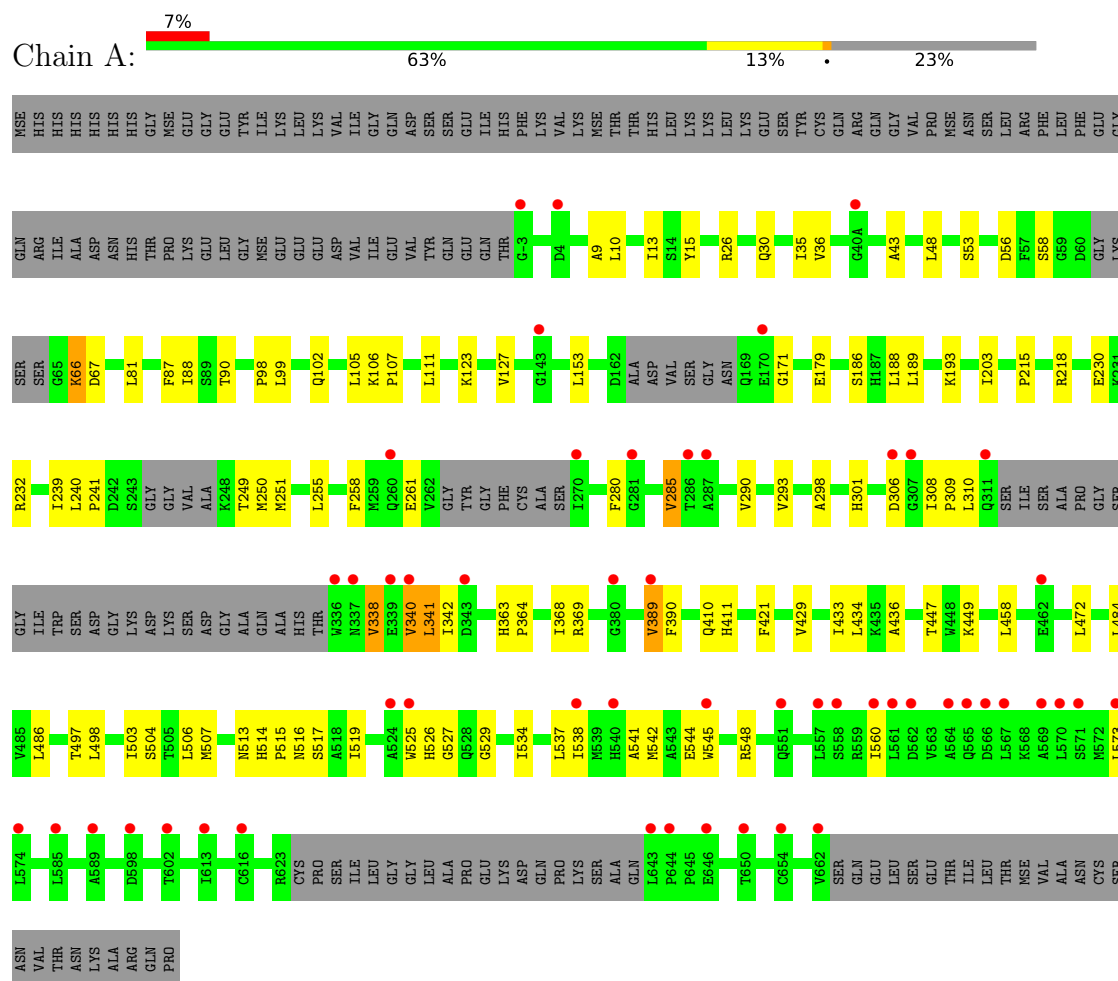
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	56	GLY	-	expression tag	UNP Q9UKZ1
C	57	PRO	-	expression tag	UNP Q9UKZ1
C	58	ASP	-	expression tag	UNP Q9UKZ1
C	59	ARG	-	expression tag	UNP Q9UKZ1
C	60	SER	-	expression tag	UNP Q9UKZ1
C	507	GLU	LYS	conflict	UNP Q9UKZ1

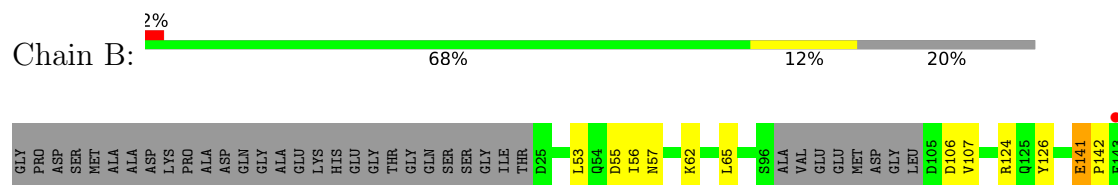
3 Residue-property plots

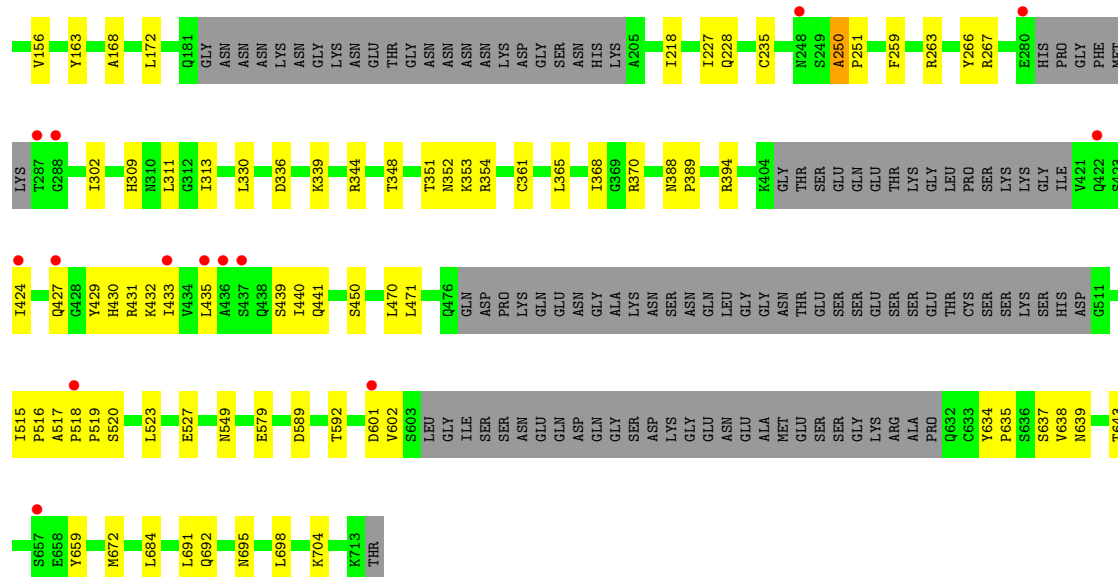
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CCR4-NOT transcription complex subunit 1

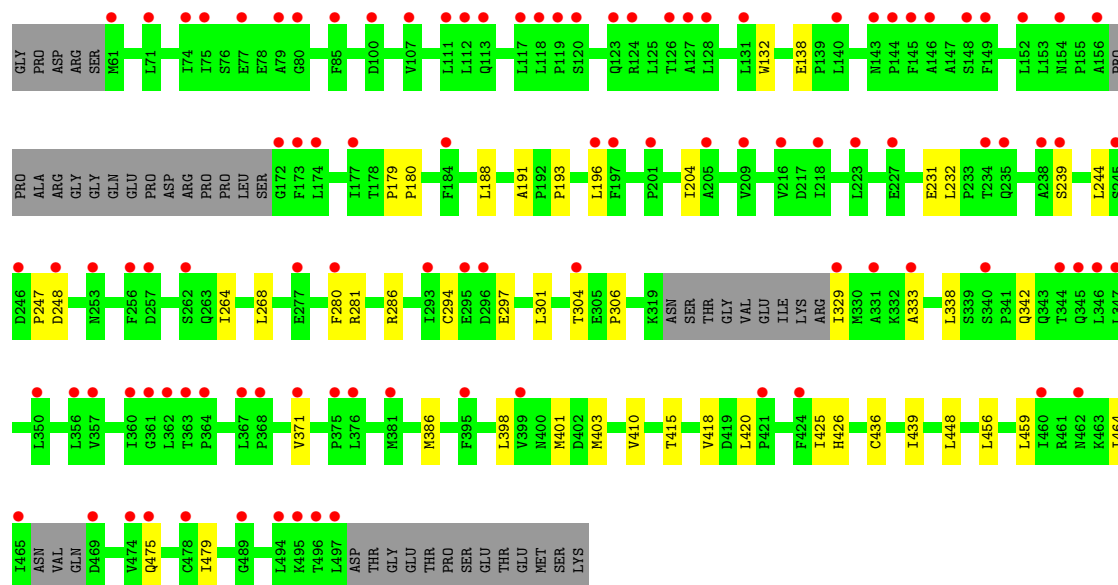
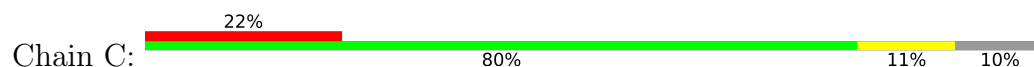


• Molecule 2: CCR4-NOT transcription complex subunit 10





• Molecule 3: CCR4-NOT transcription complex subunit 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.76Å 110.64Å 128.58Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	45.77 – 3.00 45.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.77-3.00) 99.9 (45.77-3.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.262 , 0.283 (Not available) , 0.261	Depositor DCC
R_{free} test set	2293 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11890	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	0.12	0/4577	0.45	4/6205 (0.1%)
2	B	0.10	0/4513	0.32	0/6107
3	C	0.12	0/3024	0.34	0/4136
All	All	0.11	0/12114	0.38	4/16448 (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	3
3	C	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	LYS	CA-C-N	9.25	138.35	121.70
1	A	66	LYS	C-N-CA	9.25	138.35	121.70
1	A	513	ASN	CA-C-N	9.07	138.02	121.70
1	A	513	ASN	C-N-CA	9.07	138.02	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	LEU	Peptide
1	A	285	VAL	Peptide
1	A	368	ILE	Peptide
3	C	248	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	4496	0	4271	71	0
2	B	4437	0	4406	65	0
3	C	2957	0	2801	37	0
All	All	11890	0	11478	148	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 6.

All (148) 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:389:VAL:HG12	1:A:390:PHE:H	1.34	0.93
3:C:459:LEU:HD23	3:C:464:ILE:HD12	1.68	0.75
1:A:251:MSE:HE1	2:B:361:CYS:HB3	1.68	0.74
3:C:415:THR:HG22	3:C:464:ILE:HG21	1.69	0.73
1:A:251:MSE:HE2	2:B:313:ILE:HD11	1.72	0.70
1:A:410:GLN:HG3	1:A:472:LEU:HD21	1.74	0.70
2:B:579:GLU:OE2	3:C:286:ARG:NH1	2.21	0.69
2:B:309:HIS:HB3	2:B:368:ILE:HG12	1.73	0.69
3:C:436:CYS:HA	3:C:439:ILE:HD12	1.76	0.67
2:B:163:TYR:HA	2:B:228:GLN:HE22	1.58	0.67
1:A:544:GLU:O	1:A:548:ARG:N	2.23	0.67
2:B:163:TYR:HA	2:B:228:GLN:NE2	2.11	0.66
1:A:306:ASP:OD2	2:B:267:ARG:NH2	2.29	0.66
1:A:99:LEU:HD22	3:C:231:GLU:HG2	1.79	0.65
1:A:433:ILE:HG22	1:A:519:ILE:HD11	1.79	0.65
2:B:643:THR:HG22	2:B:672:MET:HG3	1.79	0.65
1:A:188:LEU:HD21	1:A:203:ILE:HG12	1.77	0.65
3:C:456:LEU:HA	3:C:459:LEU:HD12	1.79	0.65
1:A:301:HIS:HB2	1:A:338:VAL:HG22	1.81	0.63
2:B:684:LEU:HG	3:C:280:PHE:HE1	1.63	0.63
2:B:250:ALA:HB3	2:B:251:PRO:HD3	1.80	0.63
1:A:504:SER:HA	1:A:537:LEU:HD21	1.79	0.63
1:A:66:LYS:HA	1:A:67:ASP:HB2	1.82	0.62
2:B:106:ASP:HB2	2:B:107:VAL:HG13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:MSE:HE3	2:B:365:LEU:HD11	1.83	0.60
1:A:525:TRP:HD1	1:A:526:HIS:CD2	2.21	0.59
3:C:403:MET:HE3	3:C:448:LEU:HD22	1.85	0.58
1:A:127:VAL:HG11	1:A:153:LEU:HD13	1.85	0.58
1:A:389:VAL:HG12	1:A:390:PHE:N	2.14	0.58
1:A:507:MSE:HE2	1:A:538:ILE:HG12	1.86	0.57
1:A:123:LYS:HD2	1:A:171:GLY:HA2	1.85	0.57
2:B:353:LYS:HD2	3:C:301:LEU:HD22	1.86	0.57
2:B:691:LEU:HD21	3:C:244:LEU:HD11	1.87	0.56
2:B:124:ARG:NH2	2:B:352:ASN:O	2.30	0.56
2:B:266:TYR:HB3	2:B:302:ILE:HG23	1.86	0.56
1:A:514:HIS:HB3	1:A:517:SER:OG	2.05	0.56
2:B:684:LEU:HG	3:C:280:PHE:CE1	2.40	0.56
2:B:602:VAL:HG23	2:B:638:VAL:HG22	1.88	0.55
1:A:338:VAL:HG12	1:A:340:VAL:HG22	1.89	0.55
3:C:191:ALA:O	3:C:193:PRO:HD3	2.05	0.55
2:B:394:ARG:NH2	3:C:297:GLU:OE1	2.38	0.54
1:A:186:SER:HA	2:B:470:LEU:HD21	1.91	0.53
1:A:542:MSE:SE	1:A:560:ILE:HG23	2.60	0.52
2:B:106:ASP:HB2	2:B:107:VAL:CG1	2.39	0.52
3:C:180:PRO:HB3	3:C:204:ILE:O	2.10	0.52
3:C:193:PRO:O	3:C:196:LEU:N	2.34	0.52
1:A:15:TYR:OH	3:C:138:GLU:OE2	2.14	0.52
2:B:348:THR:HA	2:B:351:THR:HG23	1.90	0.52
2:B:336:ASP:HB3	2:B:339:LYS:HB2	1.92	0.52
1:A:36:VAL:HA	1:A:43:ALA:HB3	1.91	0.51
2:B:602:VAL:HG11	2:B:635:PRO:HB2	1.91	0.51
1:A:434:LEU:HD13	1:A:486:LEU:HD11	1.91	0.51
1:A:88:ILE:HD12	1:A:88:ILE:H	1.75	0.51
1:A:106:LYS:HB2	1:A:107:PRO:C	2.35	0.51
3:C:329:ILE:HD12	3:C:342:GLN:HG2	1.93	0.51
2:B:433:ILE:HD13	3:C:268:LEU:HD11	1.93	0.51
3:C:371:VAL:HG21	3:C:410:VAL:HG11	1.93	0.50
1:A:249:THR:O	1:A:250:MSE:HB2	2.12	0.49
1:A:298:ALA:O	1:A:369:ARG:HG3	2.11	0.49
2:B:637:SER:O	2:B:639:ASN:N	2.40	0.49
1:A:534:ILE:O	1:A:538:ILE:HG13	2.12	0.49
1:A:10:LEU:HD23	1:A:13:ILE:HD12	1.94	0.49
3:C:132:TRP:CD2	3:C:188:LEU:HD13	2.47	0.49
1:A:255:LEU:HD22	1:A:285:VAL:HG22	1.94	0.49
2:B:424:ILE:N	2:B:435:LEU:O	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:VAL:O	1:A:342:ILE:N	2.46	0.49
2:B:388:ASN:HB2	2:B:518:PRO:HD2	1.94	0.49
2:B:589:ASP:O	2:B:592:THR:OG1	2.30	0.49
1:A:484:LEU:HD23	1:A:506:LEU:HD11	1.93	0.48
1:A:98:PRO:HB3	1:A:105:LEU:HD12	1.95	0.48
1:A:369:ARG:O	1:A:411:HIS:NE2	2.46	0.48
3:C:179:PRO:HB2	3:C:180:PRO:HD3	1.95	0.47
2:B:259:PHE:CE2	2:B:263:ARG:HD2	2.50	0.47
2:B:602:VAL:HG12	2:B:602:VAL:O	2.13	0.47
2:B:141:GLU:HB3	2:B:142:PRO:HD3	1.95	0.47
1:A:48:LEU:HD22	1:A:90:THR:HG22	1.97	0.47
2:B:433:ILE:HG21	3:C:268:LEU:HD21	1.96	0.46
3:C:333:ALA:HB2	3:C:338:LEU:HD11	1.98	0.46
3:C:475:GLN:O	3:C:479:ILE:HG13	2.16	0.46
1:A:105:LEU:HA	1:A:111:LEU:HD11	1.97	0.46
3:C:244:LEU:HD23	3:C:244:LEU:HA	1.80	0.46
1:A:436:ALA:HB3	1:A:516:ASN:HD21	1.80	0.45
1:A:541:ALA:O	1:A:545:TRP:N	2.40	0.45
1:A:458:LEU:HD23	1:A:498:LEU:HD23	1.97	0.45
3:C:294:CYS:SG	3:C:297:GLU:HB2	2.57	0.45
1:A:26:ARG:O	1:A:30:GLN:HG3	2.17	0.45
2:B:430:HIS:O	3:C:247:PRO:HB3	2.17	0.45
1:A:81:LEU:HG	1:A:87:PHE:HB2	1.99	0.44
2:B:439:SER:O	2:B:441:GLN:HG2	2.16	0.44
1:A:56:ASP:OD2	1:A:58:SER:HB2	2.17	0.44
1:A:241:PRO:HG2	2:B:354:ARG:HD2	1.98	0.44
1:A:261:GLU:HB3	2:B:311:LEU:HD12	1.98	0.44
1:A:230:GLU:HG2	1:A:232:ARG:HH12	1.82	0.44
2:B:344:ARG:HG3	2:B:348:THR:OG1	2.16	0.44
1:A:215:PRO:HG2	1:A:218:ARG:HB2	1.98	0.44
1:A:188:LEU:HD23	1:A:188:LEU:O	2.18	0.44
1:A:10:LEU:HD21	1:A:43:ALA:HA	1.99	0.44
1:A:250:MSE:HE3	2:B:370:ARG:HD3	2.00	0.44
1:A:258:PHE:HZ	1:A:310:LEU:HD11	1.83	0.43
2:B:517:ALA:O	2:B:520:SER:N	2.50	0.43
2:B:549:ASN:OD1	2:B:549:ASN:N	2.49	0.43
2:B:520:SER:OG	3:C:297:GLU:O	2.24	0.43
2:B:427:GLN:O	2:B:432:LYS:HG3	2.19	0.43
1:A:542:MSE:SE	1:A:573:LEU:HD11	2.68	0.43
2:B:695:ASN:HB3	2:B:698:LEU:HB2	2.00	0.43
2:B:124:ARG:HA	2:B:126:TYR:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:LEU:HD22	2:B:218:ILE:HG23	2.00	0.43
2:B:634:TYR:CD2	2:B:635:PRO:HD3	2.53	0.43
1:A:179:GLU:OE1	2:B:450:SER:OG	2.29	0.43
1:A:340:VAL:HB	1:A:341:LEU:H	1.67	0.43
3:C:304:THR:O	3:C:306:PRO:HD3	2.18	0.43
1:A:503:ILE:O	1:A:507:MSE:HG2	2.19	0.43
2:B:259:PHE:CZ	2:B:263:ARG:HD2	2.53	0.43
3:C:239:SER:HA	3:C:281:ARG:HB3	2.00	0.43
1:A:308:ILE:HA	1:A:309:PRO:HD3	1.91	0.42
1:A:527:GLY:C	1:A:529:GLY:H	2.27	0.42
1:A:340:VAL:HG23	1:A:341:LEU:HD12	2.01	0.42
1:A:363:HIS:HB2	1:A:364:PRO:HD2	2.00	0.42
2:B:431:ARG:O	3:C:264:ILE:HD13	2.19	0.42
1:A:239:ILE:HG23	1:A:240:LEU:HG	2.00	0.42
1:A:251:MSE:HE1	2:B:361:CYS:CB	2.45	0.42
3:C:398:LEU:O	3:C:401:MET:HG2	2.19	0.42
1:A:53:SER:HA	1:A:102:GLN:HE21	1.85	0.42
1:A:290:VAL:O	1:A:293:VAL:HG12	2.20	0.42
2:B:659:TYR:CD1	2:B:692:GLN:HG2	2.55	0.42
1:A:9:ALA:HB1	1:A:35:ILE:HG23	2.02	0.41
1:A:514:HIS:CG	1:A:515:PRO:HD2	2.55	0.41
2:B:429:TYR:HB3	2:B:430:HIS:H	1.67	0.41
1:A:497:THR:HG23	2:B:704:LYS:HZ3	1.85	0.41
1:A:429:VAL:HG23	1:A:449:LYS:O	2.20	0.41
3:C:386:MET:HE2	3:C:418:VAL:HG21	2.02	0.41
2:B:579:GLU:OE2	3:C:286:ARG:HD3	2.21	0.41
1:A:421:PHE:HB2	1:A:447:THR:HG23	2.03	0.41
2:B:388:ASN:HD22	2:B:519:PRO:HD2	1.86	0.41
1:A:66:LYS:HA	1:A:67:ASP:CB	2.50	0.41
1:A:255:LEU:HB2	1:A:280:PHE:CE2	2.55	0.41
3:C:420:LEU:HD23	3:C:425:ILE:HG23	2.03	0.41
3:C:232:LEU:HD23	3:C:232:LEU:HA	1.85	0.41
2:B:156:VAL:HG13	2:B:168:ALA:HB1	2.02	0.41
3:C:425:ILE:HD12	3:C:426:HIS:N	2.35	0.41
2:B:62:LYS:HA	2:B:65:LEU:HB3	2.03	0.41
2:B:227:ILE:HG13	2:B:235:CYS:SG	2.61	0.41
2:B:515:ILE:HA	2:B:516:PRO:HD3	1.95	0.40
2:B:330:LEU:HB3	2:B:344:ARG:HD2	2.03	0.40
2:B:389:PRO:HB3	2:B:471:LEU:HB2	2.04	0.40
2:B:55:ASP:OD2	2:B:56:ILE:HG12	2.22	0.40
2:B:523:LEU:HD22	2:B:527:GLU:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LEU:C	2:B:57:ASN:HB2	2.46	0.40

There are no symmetry-related clashes.

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	588/778 (76%)	576 (98%)	7 (1%)	5 (1%)	14	48
2	B	560/718 (78%)	550 (98%)	6 (1%)	4 (1%)	18	53
3	C	402/455 (88%)	395 (98%)	7 (2%)	0	100	100
All	All	1550/1951 (79%)	1521 (98%)	20 (1%)	9 (1%)	21	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	VAL
1	A	341	LEU
2	B	141	GLU
1	A	389	VAL
1	A	193	LYS
2	B	250	ALA
2	B	601	ASP
2	B	440	ILE
1	A	338	VAL

5.3.2 Protein sidechains [i](#)

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	446/660 (68%)	446 (100%)	0	100	100
2	B	472/607 (78%)	472 (100%)	0	100	100
3	C	295/406 (73%)	295 (100%)	0	100	100
All	All	1213/1673 (72%)	1213 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	30	GLN
1	A	151	GLN
1	A	279	GLN
1	A	337	ASN
1	A	349	ASN
1	A	401	HIS
2	B	77	GLN
2	B	92	ASN
2	B	109	ASN
2	B	228	GLN
2	B	258	ASN
2	B	442	ASN
2	B	446	ASN
3	C	302	ASN
3	C	311	GLN
3	C	373	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 [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	591/778 (75%)	0.63	53 (8%) 15 8	39, 83, 220, 262	0
2	B	574/718 (79%)	0.02	15 (2%) 57 34	30, 59, 110, 139	0
3	C	410/455 (90%)	1.49	102 (24%) 2 1	60, 142, 220, 246	0
All	All	1575/1951 (80%)	0.63	170 (10%) 11 6	30, 84, 214, 262	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	361	GLY	4.9
3	C	295	GLU	4.8
3	C	465	ILE	4.8
3	C	127	ALA	4.7
1	A	569	ALA	4.6
3	C	146	ALA	4.4
3	C	248	ASP	4.0
1	A	662	VAL	4.0
3	C	85	PHE	4.0
3	C	469	ASP	4.0
3	C	331	ALA	4.0
3	C	474	VAL	3.9
3	C	363	THR	3.7
2	B	518	PRO	3.7
1	A	585	LEU	3.7
3	C	257	ASP	3.6
3	C	346	LEU	3.6
1	A	560	ILE	3.6
3	C	128	LEU	3.6
3	C	496	THR	3.6
2	B	436	ALA	3.5
3	C	304	THR	3.5
3	C	475	GLN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	311	GLN	3.5
3	C	375	PRO	3.5
3	C	329	ILE	3.5
3	C	489	GLY	3.5
1	A	558	SER	3.4
1	A	598	ASP	3.4
1	A	561	LEU	3.4
3	C	209	VAL	3.3
1	A	564	ALA	3.3
3	C	360	ILE	3.3
3	C	100	ASP	3.3
3	C	173	PHE	3.3
1	A	562	ASP	3.2
3	C	61	MET	3.2
3	C	205	ALA	3.2
3	C	460	ILE	3.2
3	C	156	ALA	3.2
2	B	280	GLU	3.2
3	C	126	THR	3.2
3	C	131	LEU	3.2
3	C	80	GLY	3.2
3	C	149	PHE	3.2
2	B	287	THR	3.2
1	A	616	CYS	3.1
3	C	74	ILE	3.1
3	C	494	LEU	3.1
1	A	339	GLU	3.1
1	A	462	GLU	3.1
3	C	497	LEU	3.1
3	C	421	PRO	3.1
1	A	286	THR	3.0
3	C	293	ILE	3.0
3	C	119	PRO	3.0
1	A	573	LEU	3.0
2	B	143	PHE	3.0
3	C	112	LEU	3.0
3	C	140	LEU	2.9
2	B	657	SER	2.9
1	A	40(A)	GLY	2.9
3	C	172	GLY	2.9
3	C	201	PRO	2.9
3	C	277	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	235	GLN	2.9
1	A	524	ALA	2.9
3	C	362	LEU	2.9
3	C	345	GLN	2.8
3	C	296	ASP	2.8
3	C	381	MET	2.8
1	A	551	GLN	2.8
3	C	143	ASN	2.8
2	B	437	SER	2.8
1	A	574	LEU	2.8
3	C	184	PHE	2.7
3	C	117	LEU	2.7
3	C	399	VAL	2.7
1	A	570	LEU	2.7
3	C	71	LEU	2.7
3	C	152	LEU	2.7
3	C	223	LEU	2.7
2	B	433	ILE	2.7
3	C	145	PHE	2.7
1	A	336	TRP	2.7
3	C	357	VAL	2.7
3	C	113	GLN	2.6
3	C	280	PHE	2.6
3	C	367	LEU	2.6
3	C	148	SER	2.6
1	A	260	GLN	2.6
3	C	246	ASP	2.6
2	B	424	ILE	2.6
2	B	248	ASN	2.6
1	A	654	CYS	2.6
3	C	75	ILE	2.6
2	B	601	ASP	2.6
1	A	287	ALA	2.6
1	A	613	ILE	2.5
3	C	234	THR	2.5
1	A	-3	GLY	2.5
3	C	424	PHE	2.5
2	B	288	GLY	2.5
2	B	427	GLN	2.5
1	A	589	ALA	2.5
3	C	238	ALA	2.5
1	A	306	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	602	THR	2.5
3	C	123	GLN	2.5
3	C	120	SER	2.5
1	A	389	VAL	2.5
2	B	422	GLN	2.5
3	C	347	LEU	2.4
1	A	340	VAL	2.4
3	C	218	ILE	2.4
3	C	111	LEU	2.4
3	C	371	VAL	2.4
3	C	174	LEU	2.4
1	A	380	GLY	2.3
1	A	343	ASP	2.3
3	C	124	ARG	2.3
2	B	435	LEU	2.3
3	C	376	LEU	2.3
1	A	545	TRP	2.3
1	A	650	THR	2.3
3	C	495	LYS	2.3
1	A	565	GLN	2.3
1	A	646	GLU	2.3
1	A	307	GLY	2.3
3	C	216	VAL	2.3
1	A	281	GLY	2.3
1	A	571	SER	2.3
1	A	270	ILE	2.2
3	C	356	LEU	2.2
1	A	337	ASN	2.2
3	C	478	CYS	2.2
3	C	462	ASN	2.2
3	C	77	GLU	2.2
3	C	79	ALA	2.2
3	C	245	SER	2.2
3	C	262	SER	2.2
3	C	253	ASN	2.2
1	A	557	LEU	2.1
1	A	567	LEU	2.1
1	A	643	LEU	2.1
3	C	350	LEU	2.1
3	C	333	ALA	2.1
1	A	644	PRO	2.1
3	C	227	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	364	PRO	2.1
3	C	344	THR	2.1
3	C	177	ILE	2.1
1	A	540	HIS	2.1
1	A	4	ASP	2.1
1	A	566	ASP	2.1
3	C	239	SER	2.0
1	A	538	ILE	2.0
1	A	525	TRP	2.0
1	A	143	GLY	2.0
3	C	197	PHE	2.0
1	A	170	GLU	2.0
3	C	107	VAL	2.0
3	C	118	LEU	2.0
3	C	340	SER	2.0
3	C	154	ASN	2.0
3	C	256	PHE	2.0
3	C	395	PHE	2.0
3	C	144	PRO	2.0
3	C	368	PRO	2.0
3	C	196	LEU	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.