



Full wwPDB X-ray Structure Validation Report i

Dec 20, 2022 – 12:26 pm GMT

PDB ID : 8BFI
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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

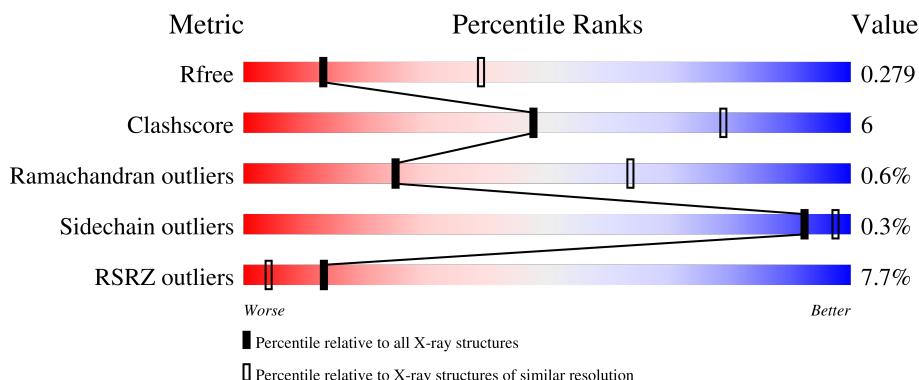
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

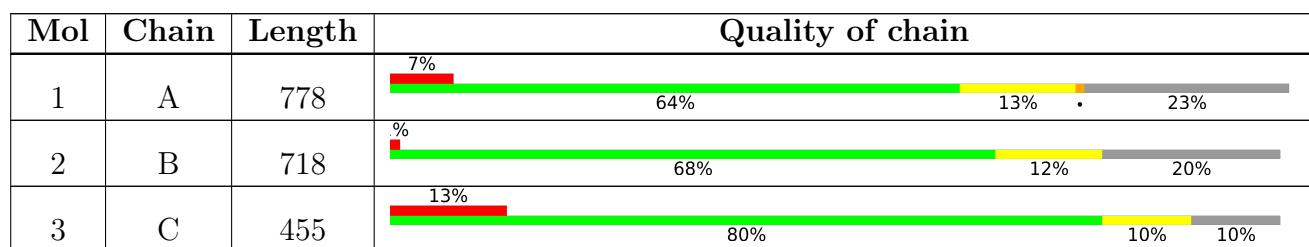
The reported resolution of this entry is 3.00 Å.

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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.



2 Entry composition (i)

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
			Total	C	N	O	S	Se			
1	A	602	4496	2878	780	817	10	11	0	0	0

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

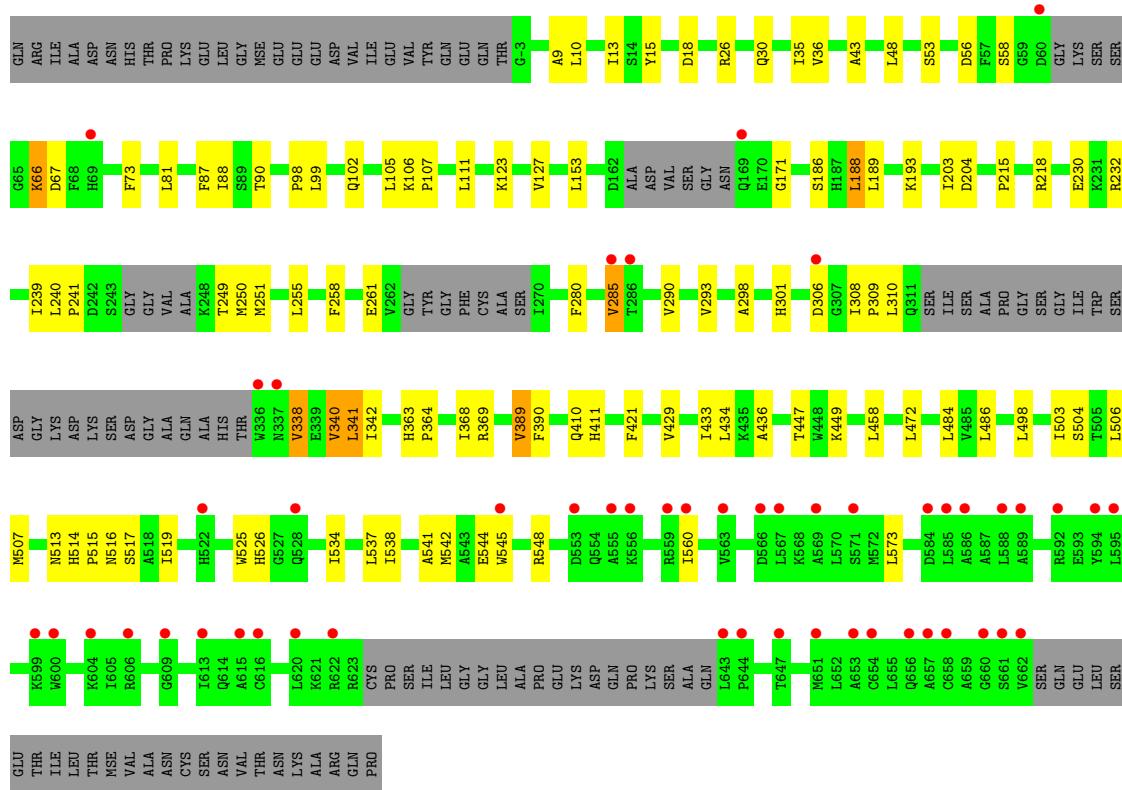
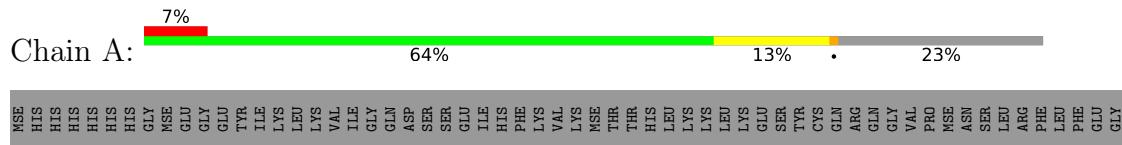
There are 6 discrepancies between the modelled and reference sequences:

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



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.76 Å 110.64 Å 128.58 Å 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) 100.0 (45.77-3.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.18 (at 3.01 Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R , R_{free}	0.262 , 0.283 0.260 , 0.279	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 , 74.0	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality 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	0.24	0/4577	0.48	3/6205 (0.0%)
2	B	0.24	0/4513	0.43	0/6107
3	C	0.24	0/3024	0.45	1/4136 (0.0%)
All	All	0.24	0/12114	0.45	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($^{\circ}$)	Ideal($^{\circ}$)
1	A	66	LYS	C-N-CA	6.66	138.35	121.70
1	A	513	ASN	C-N-CA	6.53	138.02	121.70
3	C	414	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	188	LEU	CA-CB-CG	5.03	126.86	115.30

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 [\(i\)](#)

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	68	0
2	B	4437	0	4406	62	0
3	C	2957	0	2801	35	0
All	All	11890	0	11478	142	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 (142) 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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:106:LYS:HB2	1:A:107:PRO:C	2.35	0.46
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
2:B:172:LEU:HD22	2:B:218:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:634:TYR:CD2	2:B:635:PRO:HD3	2.53	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: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:429:VAL:HG23	1:A:449:LYS:O	2.20	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

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%)	17 55
2	B	560/718 (78%)	550 (98%)	6 (1%)	4 (1%)	22 60
3	C	402/455 (88%)	395 (98%)	7 (2%)	0	100 100
All	All	1550/1951 (79%)	1521 (98%)	20 (1%)	9 (1%)	25 64

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%)	443 (99%)	3 (1%)	84 94
2	B	472/607 (78%)	471 (100%)	1 (0%)	93 98
3	C	295/406 (73%)	295 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1213/1673 (72%)	1209 (100%)	4 (0%)	92 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	73	PHE
1	A	204	ASP
2	B	258	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	228	GLN

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 monosaccharides 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	591/778 (75%)	0.30	51 (8%) 10 3	39, 83, 220, 262	0
2	B	574/718 (79%)	-0.16	10 (1%) 70 41	30, 59, 110, 139	0
3	C	410/455 (90%)	0.84	61 (14%) 2 1	60, 142, 220, 246	0
All	All	1575/1951 (80%)	0.27	122 (7%) 13 4	30, 84, 214, 262	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	PRO	11.4
1	A	661	SER	10.6
3	C	361	GLY	9.6
3	C	331	ALA	9.3
3	C	345	GLN	9.0
3	C	346	LEU	7.8
1	A	660	GLY	7.7
3	C	209	VAL	7.4
1	A	653	ALA	6.3
3	C	363	THR	6.2
3	C	253	ASN	6.2
1	A	657	ALA	6.1
3	C	362	LEU	5.8
1	A	616	CYS	5.8
1	A	60	ASP	5.8
3	C	156	ALA	5.7
3	C	334	PHE	5.6
1	A	643	LEU	5.6
3	C	359	HIS	5.6
3	C	342	GLN	5.4
1	A	656	GLN	5.1
2	B	96	SER	4.6
1	A	662	VAL	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	364	PRO	4.5
1	A	589	ALA	4.4
1	A	569	ALA	4.4
3	C	356	LEU	4.4
1	A	585	LEU	4.4
3	C	85	PHE	4.4
1	A	563	VAL	4.3
1	A	613	ILE	4.3
3	C	256	PHE	4.2
1	A	553	ASP	4.2
2	B	244	ASN	4.1
3	C	339	SER	4.1
3	C	394	TYR	4.1
3	C	259	SER	4.0
1	A	567	LEU	4.0
3	C	248	ASP	4.0
3	C	257	ASP	3.9
3	C	205	ALA	3.8
1	A	566	ASP	3.8
3	C	79	ALA	3.8
1	A	560	ILE	3.7
1	A	545	TRP	3.7
3	C	367	LEU	3.6
1	A	595	LEU	3.6
1	A	586	ALA	3.6
2	B	713	LYS	3.6
1	A	600	TRP	3.5
3	C	341	PRO	3.5
3	C	332	LYS	3.5
1	A	647	THR	3.4
1	A	654	CYS	3.4
3	C	352	LYS	3.4
1	A	286	THR	3.4
3	C	381	MET	3.4
1	A	594	TYR	3.4
1	A	584	ASP	3.3
1	A	658	CYS	3.3
3	C	375	PRO	3.3
1	A	169	GLN	3.2
3	C	373	ASN	3.1
3	C	210	GLY	3.1
3	C	333	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	258	SER	3.1
3	C	219	SER	3.0
3	C	349	GLU	3.0
3	C	360	ILE	3.0
3	C	357	VAL	3.0
3	C	358	TYR	2.9
1	A	588	LEU	2.9
3	C	254	SER	2.9
3	C	377	VAL	2.9
1	A	556	LYS	2.9
2	B	657	SER	2.9
1	A	592	ARG	2.8
1	A	604	LYS	2.8
1	A	622	ARG	2.8
3	C	371	VAL	2.8
3	C	127	ALA	2.8
1	A	606	ARG	2.8
3	C	387	GLN	2.7
1	A	559	ARG	2.7
1	A	620	LEU	2.7
2	B	712	VAL	2.7
1	A	336	TRP	2.7
1	A	615	ALA	2.7
3	C	201	PRO	2.6
1	A	528	GLN	2.6
2	B	247	GLY	2.6
1	A	571	SER	2.5
3	C	370	LEU	2.5
1	A	651	MET	2.5
1	A	285	VAL	2.5
3	C	335	LYS	2.5
1	A	599	LYS	2.5
3	C	187	GLN	2.4
3	C	260	VAL	2.4
2	B	245	THR	2.4
2	B	246	ALA	2.4
3	C	376	LEU	2.4
3	C	146	ALA	2.4
3	C	227	GLU	2.4
3	C	329	ILE	2.3
3	C	120	SER	2.3
3	C	218	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	372	GLU	2.2
1	A	306	ASP	2.2
2	B	287	THR	2.2
3	C	393	GLU	2.2
2	B	248	ASN	2.2
1	A	609	GLY	2.2
3	C	353	ASP	2.1
1	A	337	ASN	2.1
1	A	522	HIS	2.1
1	A	555	ALA	2.1
3	C	479	ILE	2.1
3	C	497	LEU	2.1
3	C	337	PRO	2.0
3	C	172	GLY	2.0
1	A	69	HIS	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 [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.