



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:52 PM JST

PDB ID : 7VOI  
Title : Structure of the human CNOT1(MIF4G)-CNOT6L-CNOT7 complex  
Authors : Bartlam, M.; Zhang, Q.  
Deposited on : 2021-10-13  
Resolution : 4.38 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

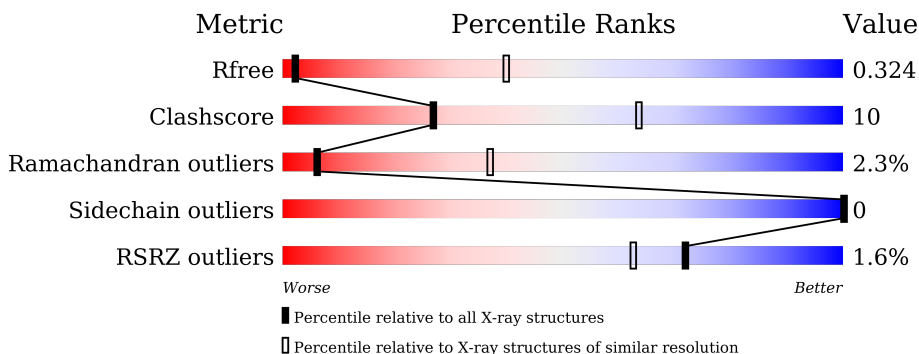
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.38 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	1022 (4.92-3.80)
Clashscore	141614	1085 (4.92-3.80)
Ramachandran outliers	138981	1036 (4.92-3.80)
Sidechain outliers	138945	1019 (4.92-3.80)
RSRZ outliers	127900	1094 (5.06-3.70)

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  $\geq 3$ , 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	B	285	 2% 78% 15% 7%
2	A	229	 % 82% 18%
3	C	555	 19% 11% 68%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5449 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 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	264	2137	1372	341	409	15	0	0	0

- Molecule 2 is a protein called CCR4-NOT transcription complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	229	1859	1198	310	342	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	HIS	-	expression tag	UNP A5YKK6
A	1090	MET	-	expression tag	UNP A5YKK6
A	1091	LEU	-	expression tag	UNP A5YKK6
A	1092	GLU	-	expression tag	UNP A5YKK6

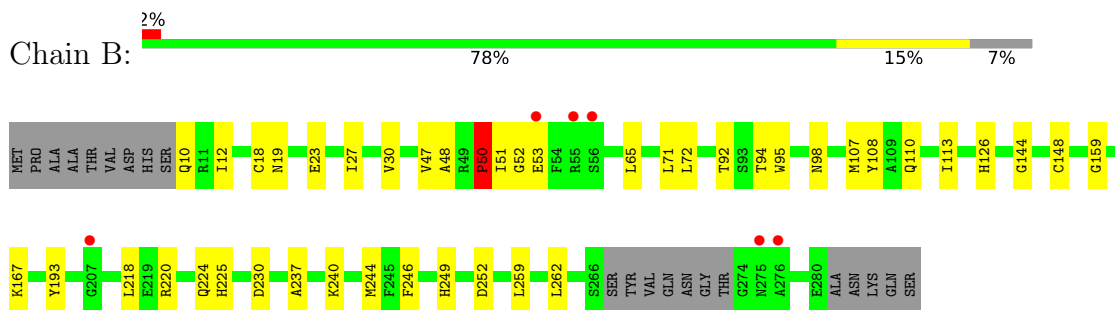
- Molecule 3 is a protein called CCR4-NOT transcription complex subunit 6-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	180	1453	932	253	263	5	0	0	0

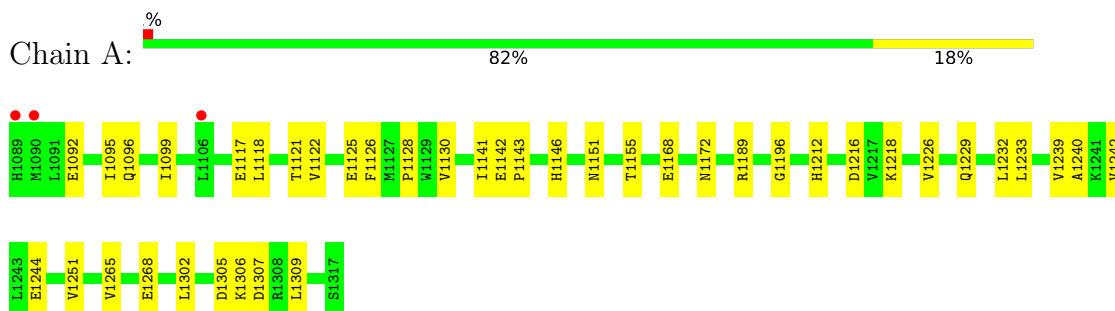
### 3 Residue-property plots [i](#)

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.

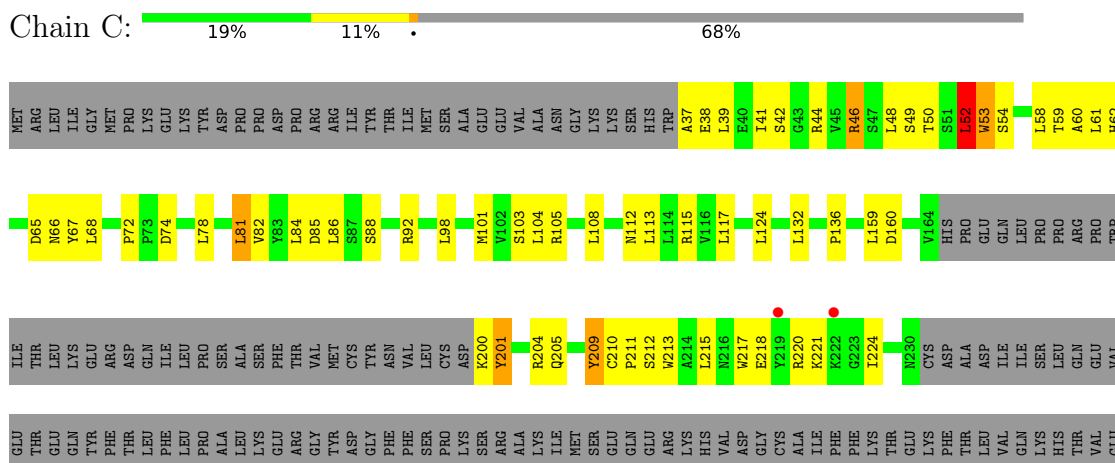
- Molecule 1: CCR4-NOT transcription complex subunit 7



- Molecule 2: CCR4-NOT transcription complex subunit 1



- Molecule 3: CCR4-NOT transcription complex subunit 6-like



PHE ASN GLN VAL ALA MET ALA ASN SER GLY ASP LEU ILE GLN ALA	HIS TRP ASP ASN GLY TYR SER VAL LYS ILE THR MET PHE VAL SER GLU VAL LYS ASN ILE LEU GLU LYS ALA SER VAL SER GLY ARG PRO GLY SER PRO THR ALA ASP GLY ASN SER ILE PRO LEU VAL LEU CYS ALA ASP LEU ASN SER ILE PHE LEU VAL LEU SER PRO MET ASP TYR THR ASN TYR THR VAL THR	TYR LEU SER ASN GLY VAL ALA ASP ASN HIS LYS ASP PHE LYS GLU LEU ARG TYR ASN GLU CYS LEU MET ASN PHE SER CYS GLY LYS ASN GLY SER GLU GLY ARG ILE THR HIS PHE GLN LEU LYS SER ALA THR TYR GLU ASN ASN LEU MET PRO TYR THR ASN TYR THR	PHE ASP PHE LYS GLY VAL ILE ASP TYR ILE PHE TYR SER LYS THR HIS MET ASN VAL LEU GLY VAL LEU GLY P506	L512 V513 E514 N515 I516 I517	C520 P521 H522 P523 H524 I525 P526	SER ASP HIS PHE SER LEU LEU THR GLN LEU GLU LEU HIS PRO PRO LEU LEU PRO LEU LEU VAL	ASN GLY VAL HIS LEU PRO ASN ARG ARG
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.99Å 110.99Å 242.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.74 – 4.38 38.74 – 4.38	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.74-4.38) 94.2 (38.74-4.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.68 (at 4.44Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.263 , 0.324 0.263 , 0.324	Depositor DCC
$R_{free}$ test set	1009 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	157.7	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 129.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5449	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	B	0.30	0/2185	0.47	0/2947
2	A	0.31	0/1894	0.54	2/2562 (0.1%)
3	C	0.48	1/1485 (0.1%)	0.75	4/2020 (0.2%)
All	All	0.36	1/5564 (0.0%)	0.58	6/7529 (0.1%)

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	B	0	1
3	C	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	514	GLU	CD-OE2	9.28	1.35	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1121	THR	CA-CB-CG2	8.15	123.81	112.40
2	A	1118	LEU	CB-CG-CD2	6.89	122.71	111.00
3	C	514	GLU	OE1-CD-OE2	5.58	129.99	123.30
3	C	209	TYR	CB-CG-CD2	5.57	124.34	121.00
3	C	209	TYR	CB-CG-CD1	-5.20	117.88	121.00
3	C	52	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	50	PRO	Peptide
3	C	52	LEU	Peptide
3	C	520	CYS	Peptide
3	C	522	HIS	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	B	2137	0	2040	43	0
2	A	1859	0	1899	19	1
3	C	1453	0	1475	64	1
All	All	5449	0	5414	111	1

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 (111) 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)
3:C:215:LEU:O	3:C:220:ARG:NH1	2.09	0.85
1:B:51:ILE:O	1:B:53:GLU:N	2.13	0.82
1:B:51:ILE:HG23	3:C:38:GLU:H	1.49	0.78
1:B:72:LEU:O	1:B:167:LYS:NZ	2.19	0.75
3:C:52:LEU:O	3:C:54:SER:N	2.17	0.73
3:C:53:TRP:HE3	3:C:53:TRP:H	1.39	0.71
3:C:61:LEU:HB3	3:C:81:LEU:HD11	1.73	0.70
3:C:82:VAL:HA	3:C:104:LEU:HA	1.75	0.68
1:B:18:CYS:SG	1:B:19:ASN:N	2.66	0.68
2:A:1141:ILE:HG13	2:A:1142:GLU:HG3	1.76	0.67
3:C:37:ALA:HB1	3:C:59:THR:OG1	1.95	0.67
1:B:51:ILE:CG2	3:C:38:GLU:H	2.08	0.67
1:B:48:ALA:HB2	3:C:41:ILE:HG12	1.77	0.67
3:C:115:ARG:HD3	3:C:136:PRO:HG2	1.75	0.66
1:B:220:ARG:NH2	1:B:230:ASP:OD1	2.21	0.66
3:C:217:TRP:C	3:C:221:LYS:HZ3	1.97	0.66
2:A:1218:LYS:HG3	2:A:1265:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:TYR:CD1	1:B:113:ILE:HG13	2.33	0.63
3:C:53:TRP:NE1	3:C:74:ASP:HB2	2.13	0.63
2:A:1226:VAL:HG11	2:A:1309:LEU:HB3	1.81	0.62
3:C:103:SER:O	3:C:105:ARG:HG3	2.00	0.62
1:B:27:ILE:HA	1:B:30:VAL:HG22	1.80	0.62
3:C:78:LEU:HB3	3:C:81:LEU:HD23	1.82	0.61
3:C:52:LEU:C	3:C:54:SER:H	2.03	0.60
1:B:108:TYR:CE1	3:C:46:ARG:NH2	2.70	0.60
1:B:110:GLN:OE1	3:C:46:ARG:NH1	2.34	0.60
3:C:53:TRP:CD1	3:C:74:ASP:HB2	2.37	0.59
3:C:53:TRP:HE1	3:C:72:PRO:HB2	1.67	0.59
1:B:51:ILE:HD11	3:C:39:LEU:HB2	1.84	0.58
1:B:51:ILE:C	1:B:53:GLU:H	2.04	0.58
1:B:108:TYR:HE1	3:C:46:ARG:NH2	2.03	0.57
1:B:110:GLN:HE22	3:C:46:ARG:HH12	1.51	0.57
3:C:217:TRP:O	3:C:221:LYS:HG3	2.05	0.56
1:B:51:ILE:HD13	3:C:58:LEU:HD21	1.87	0.56
1:B:220:ARG:HE	1:B:224:GLN:HA	1.71	0.56
2:A:1305:ASP:O	2:A:1307:ASP:N	2.38	0.55
3:C:37:ALA:O	3:C:60:ALA:N	2.39	0.55
3:C:218:GLU:HA	3:C:221:LYS:NZ	2.21	0.55
2:A:1092:GLU:O	2:A:1096:GLN:N	2.39	0.55
3:C:46:ARG:HD2	3:C:67:TYR:HB2	1.89	0.54
3:C:512:LEU:HD12	3:C:512:LEU:O	2.08	0.54
3:C:44:ARG:HH21	3:C:67:TYR:HE2	1.54	0.54
1:B:98:ASN:HB3	1:B:126:HIS:CE1	2.41	0.54
3:C:44:ARG:HA	3:C:66:ASN:HA	1.89	0.53
3:C:61:LEU:O	3:C:84:LEU:HA	2.09	0.53
1:B:51:ILE:HG12	3:C:38:GLU:O	2.08	0.53
3:C:117:LEU:HD11	3:C:132:LEU:HD21	1.91	0.53
2:A:1143:PRO:HA	2:A:1146:HIS:CE1	2.45	0.52
1:B:220:ARG:HH21	1:B:224:GLN:HA	1.76	0.51
2:A:1122:VAL:HG11	2:A:1130:VAL:HG21	1.91	0.51
2:A:1239:VAL:HA	2:A:1242:VAL:HG22	1.92	0.51
1:B:71:LEU:HG	1:B:107:MET:CE	2.41	0.50
1:B:144:GLY:HA2	1:B:148:CYS:SG	2.50	0.50
1:B:220:ARG:NE	1:B:224:GLN:HA	2.27	0.50
3:C:46:ARG:H	3:C:46:ARG:CD	2.24	0.50
1:B:193:TYR:OH	1:B:252:ASP:OD1	2.28	0.49
1:B:23:GLU:HB3	1:B:95:TRP:HE1	1.77	0.49
1:B:51:ILE:C	1:B:53:GLU:N	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:VAL:HG22	3:C:103:SER:O	2.13	0.49
1:B:220:ARG:NH2	1:B:224:GLN:HA	2.28	0.49
3:C:53:TRP:HE1	3:C:74:ASP:HB2	1.78	0.49
3:C:160:ASP:OD2	3:C:212:SER:HB2	2.13	0.48
3:C:224:ILE:HG13	3:C:526:PRO:HB3	1.95	0.48
3:C:217:TRP:CE2	3:C:221:LYS:HD3	2.49	0.48
3:C:217:TRP:CD1	3:C:221:LYS:NZ	2.69	0.48
3:C:204:ARG:NH1	3:C:210:CYS:O	2.47	0.48
3:C:520:CYS:O	3:C:522:HIS:N	2.47	0.48
1:B:48:ALA:HB1	3:C:39:LEU:HD11	1.96	0.47
2:A:1099:ILE:HG21	2:A:1130:VAL:HG22	1.96	0.47
2:A:1196:GLY:O	2:A:1242:VAL:HG12	2.14	0.47
2:A:1212:HIS:NE2	2:A:1216:ASP:OD2	2.47	0.47
1:B:23:GLU:HB3	1:B:95:TRP:NE1	2.30	0.46
3:C:84:LEU:HG	3:C:86:LEU:HG	1.98	0.46
1:B:110:GLN:NE2	3:C:46:ARG:HH12	2.13	0.46
1:B:10:GLN:O	1:B:92:THR:HG22	2.16	0.46
3:C:52:LEU:C	3:C:54:SER:N	2.68	0.46
2:A:1189:ARG:NH1	2:A:1233:LEU:HD21	2.30	0.45
3:C:112:ASN:HB3	3:C:113:LEU:H	1.58	0.45
2:A:1229:GLN:HA	2:A:1232:LEU:HD12	1.98	0.45
3:C:65:ASP:H	3:C:88:SER:HB2	1.82	0.45
3:C:521:PRO:HA	3:C:525:ILE:HB	1.98	0.45
3:C:39:LEU:O	3:C:62:HIS:N	2.39	0.44
1:B:12:ILE:HG12	1:B:94:THR:HB	1.98	0.44
2:A:1240:ALA:O	2:A:1244:GLU:HG3	2.17	0.44
2:A:1095:ILE:HD13	2:A:1126:PHE:CZ	2.53	0.44
3:C:522:HIS:CE1	3:C:523:PRO:HD2	2.53	0.44
2:A:1151:ASN:O	2:A:1155:THR:N	2.48	0.44
1:B:108:TYR:HE1	3:C:46:ARG:HH22	1.66	0.44
3:C:160:ASP:OD1	3:C:212:SER:N	2.51	0.44
3:C:200:LYS:HB2	3:C:201:TYR:H	1.56	0.43
1:B:47:VAL:O	3:C:42:SER:N	2.50	0.43
1:B:218:LEU:HD11	1:B:237:ALA:HA	2.01	0.43
3:C:217:TRP:HA	3:C:220:ARG:NH1	2.33	0.43
3:C:211:PRO:HB2	3:C:213:TRP:CD1	2.53	0.42
3:C:159:LEU:HD23	3:C:204:ARG:HH22	1.84	0.42
3:C:98:LEU:HD12	3:C:101:MET:CE	2.50	0.42
1:B:51:ILE:HD13	3:C:58:LEU:CD2	2.49	0.42
1:B:71:LEU:HG	1:B:107:MET:HE3	2.02	0.42
3:C:49:SER:OG	3:C:50:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ASP:HA	3:C:108:LEU:HB2	2.01	0.41
1:B:65:LEU:HD11	1:B:159:GLY:C	2.41	0.41
3:C:92:ARG:HD3	3:C:113:LEU:HD13	2.03	0.41
2:A:1125:GLU:O	2:A:1128:PRO:HD2	2.21	0.41
1:B:259:LEU:HD12	1:B:262:LEU:HD12	2.03	0.41
2:A:1168:GLU:O	2:A:1172:ASN:ND2	2.50	0.41
2:A:1268:GLU:OE2	2:A:1302:LEU:N	2.53	0.41
1:B:246:PHE:HB3	1:B:249:HIS:O	2.20	0.40
1:B:220:ARG:NH2	1:B:225:HIS:H	2.19	0.40
1:B:240:LYS:HE2	1:B:244:MET:CE	2.51	0.40
1:B:50:PRO:C	1:B:51:ILE:HG13	2.41	0.40
3:C:48:LEU:HG	3:C:68:LEU:HD21	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1117:GLU:O	3:C:205:GLN:NE2[8_767]	1.89	0.31

## 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	B	260/285 (91%)	243 (94%)	15 (6%)	2 (1%)	19	60
2	A	227/229 (99%)	217 (96%)	8 (4%)	2 (1%)	17	56
3	C	174/555 (31%)	148 (85%)	15 (9%)	11 (6%)	1	19
All	All	661/1069 (62%)	608 (92%)	38 (6%)	15 (2%)	6	37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	53	TRP
3	C	201	TYR
3	C	520	CYS
3	C	521	PRO
1	B	52	GLY
3	C	46	ARG
3	C	52	LEU
3	C	124	LEU
3	C	209	TYR
3	C	516	ASN
1	B	50	PRO
2	A	1306	LYS
3	C	81	LEU
2	A	1251	VAL
3	C	517	ILE

### 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	B	229/249 (92%)	229 (100%)	0	100	100
2	A	212/215 (99%)	212 (100%)	0	100	100
3	C	164/497 (33%)	164 (100%)	0	100	100
All	All	605/961 (63%)	605 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	ASN
3	C	522	HIS

### 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 [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	264/285 (92%)	-0.07	6 (2%) 60 51	132, 185, 265, 537	0
2	A	229/229 (100%)	-0.10	3 (1%) 77 68	138, 195, 272, 329	0
3	C	180/555 (32%)	-0.02	2 (1%) 80 72	145, 187, 271, 340	0
All	All	673/1069 (62%)	-0.07	11 (1%) 72 62	132, 189, 275, 537	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1089	HIS	4.3
1	B	55	ARG	3.9
1	B	56	SER	3.6
2	A	1106	LEU	3.1
1	B	207	GLY	2.7
1	B	53	GLU	2.7
3	C	222	LYS	2.7
2	A	1090	MET	2.2
3	C	219	TYR	2.1
1	B	276	ALA	2.1
1	B	275	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.