



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:52 PM GMT

PDB ID : 4MYC  
Title : Structure of the mitochondrial ABC transporter, Atm1  
Authors : Srinivasan, V.  
Deposited on : 2013-09-27  
Resolution : 3.06 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

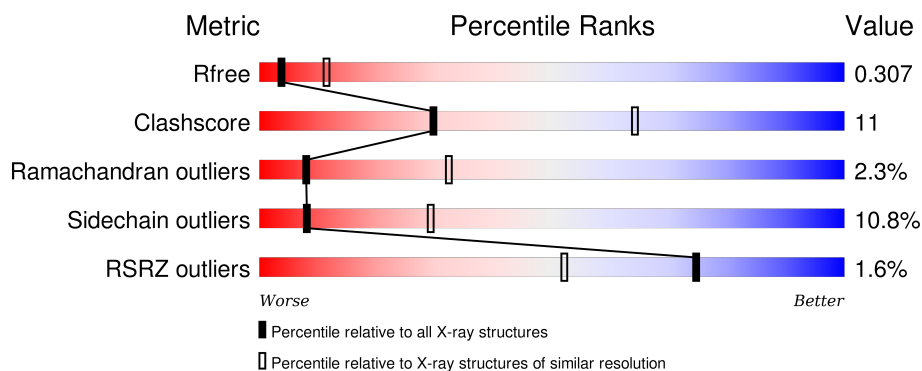
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 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))
$R_{free}$	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	598	 3% 68% 27% 5%
1	B	598	 2% 68% 27% 5%
1	C	598	 % 71% 24% 5%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14028 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 Iron-sulfur clusters transporter ATM1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4676	3002	802	855	17			
1	C	598	Total	C	N	O	S	0	0	0
			4676	3002	802	855	17			
1	B	598	Total	C	N	O	S	0	0	0
			4676	3002	802	855	17			

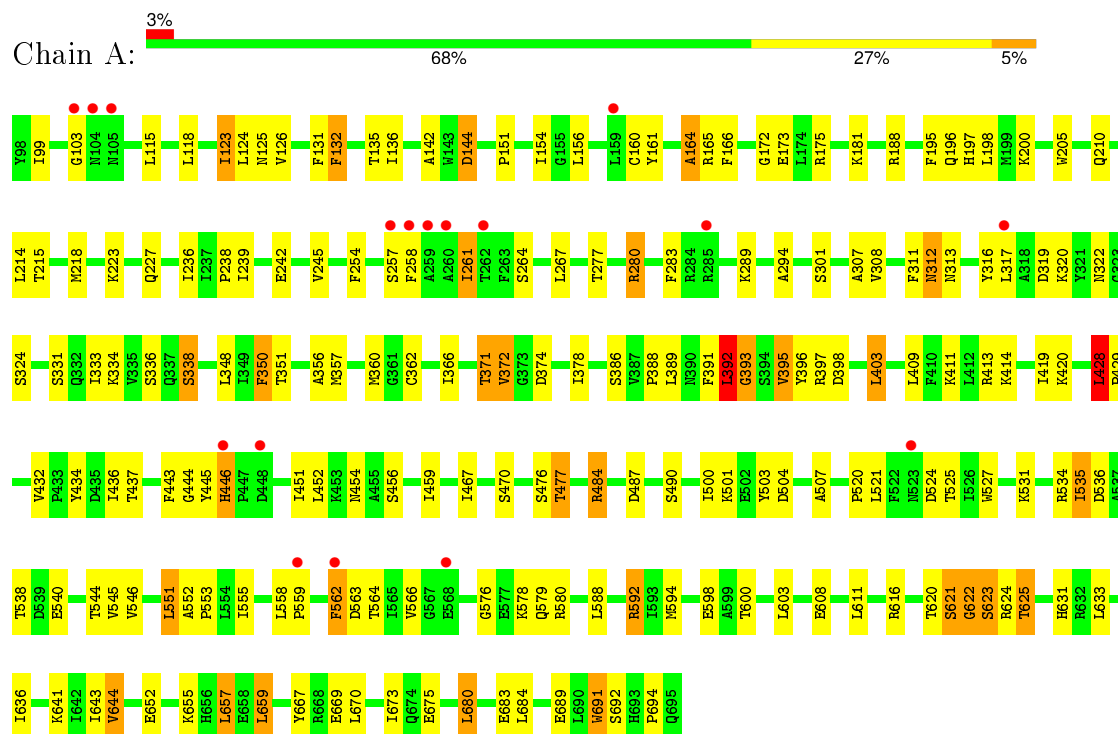
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	691	TRP	-	EXPRESSION TAG	UNP P40416
A	692	SER	-	EXPRESSION TAG	UNP P40416
A	693	HIS	-	EXPRESSION TAG	UNP P40416
A	694	PRO	-	EXPRESSION TAG	UNP P40416
A	695	GLN	-	EXPRESSION TAG	UNP P40416
C	691	TRP	-	EXPRESSION TAG	UNP P40416
C	692	SER	-	EXPRESSION TAG	UNP P40416
C	693	HIS	-	EXPRESSION TAG	UNP P40416
C	694	PRO	-	EXPRESSION TAG	UNP P40416
C	695	GLN	-	EXPRESSION TAG	UNP P40416
B	691	TRP	-	EXPRESSION TAG	UNP P40416
B	692	SER	-	EXPRESSION TAG	UNP P40416
B	693	HIS	-	EXPRESSION TAG	UNP P40416
B	694	PRO	-	EXPRESSION TAG	UNP P40416
B	695	GLN	-	EXPRESSION TAG	UNP P40416

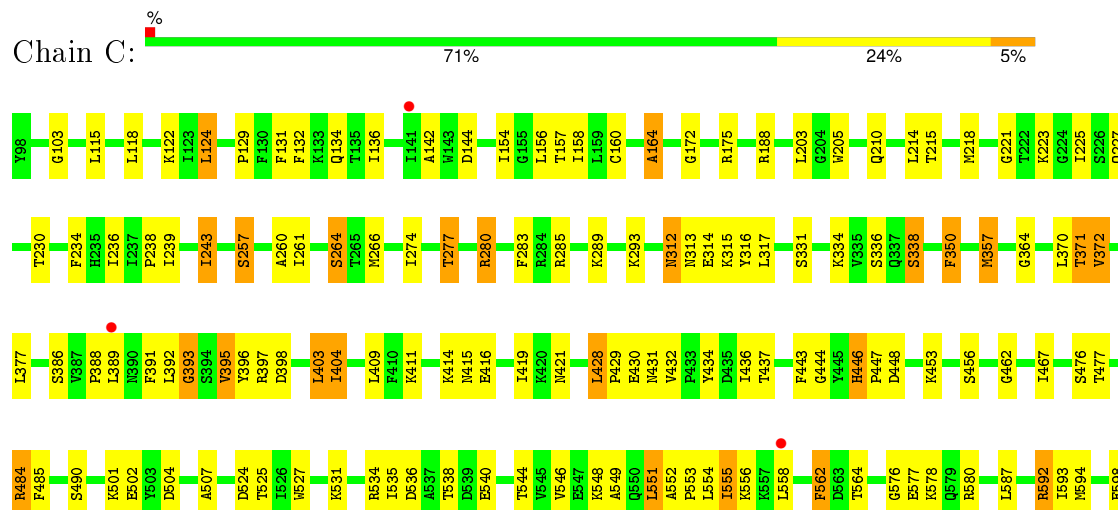
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Iron-sulfur clusters transporter ATM1, mitochondrial

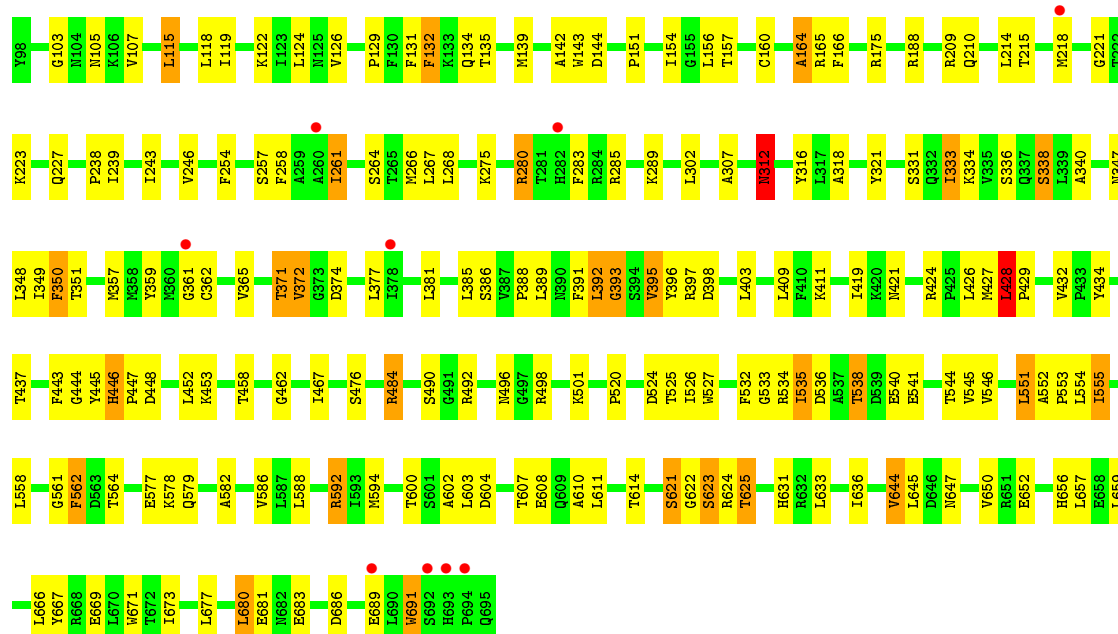


- Molecule 1: Iron-sulfur clusters transporter ATM1, mitochondrial





- Molecule 1: Iron-sulfur clusters transporter ATM1, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.62Å 156.62Å 520.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.60 – 3.06 48.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.60-3.06) 99.7 (48.60-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.251 , 0.298 0.259 , 0.307	Depositor DCC
$R_{free}$ test set	3611 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 19.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 76585 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	14028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/4763	0.65	0/6451
1	B	0.52	0/4763	0.67	1/6451 (0.0%)
1	C	0.53	0/4763	0.67	0/6451
All	All	0.52	0/14289	0.66	1/19353 (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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	LEU	C-N-CD	-6.17	107.02	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	428	LEU	Peptide
1	B	428	LEU	Peptide
1	C	428	LEU	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	4676	0	4738	130	0
1	B	4676	0	4738	125	0
1	C	4676	0	4738	95	0
All	All	14028	0	14214	317	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 11.

All (317) 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:C:453:LYS:NZ	1:C:647:ASN:OD1	2.04	0.90
1:A:546:VAL:HG13	1:A:551:LEU:HB3	1.57	0.86
1:B:526:ILE:HD11	1:B:558:LEU:HD12	1.57	0.86
1:A:631:HIS:HB2	1:B:691:TRP:HH2	1.47	0.80
1:C:261:ILE:HD11	1:C:357:MET:HG3	1.64	0.78
1:A:691:TRP:CH2	1:B:631:HIS:HB2	2.21	0.76
1:C:218:MET:HA	1:C:409:LEU:HD13	1.68	0.75
1:B:426:LEU:HB3	1:B:428:LEU:HD23	1.67	0.75
1:B:546:VAL:HG13	1:B:551:LEU:HB3	1.68	0.74
1:A:691:TRP:HH2	1:B:631:HIS:HB2	1.54	0.73
1:A:181:LYS:HA	1:B:333:ILE:HD11	1.70	0.72
1:C:436:ILE:HD11	1:C:593:ILE:HD13	1.71	0.72
1:A:261:ILE:HD11	1:A:357:MET:HG3	1.72	0.72
1:A:350:PHE:CE1	1:A:386:SER:HB3	2.27	0.69
1:C:124:LEU:HD13	1:C:164:ALA:HA	1.75	0.68
1:A:531:LYS:NZ	1:A:535:ILE:O	2.26	0.68
1:B:391:PHE:O	1:B:393:GLY:N	2.26	0.68
1:A:428:LEU:HB3	1:A:429:PRO:HD3	1.74	0.68
1:B:427:MET:H	1:B:428:LEU:HD22	1.59	0.67
1:A:484:ARG:NH1	1:A:501:LYS:HG2	2.11	0.66
1:A:280:ARG:NH1	1:A:338:SER:OG	2.29	0.66
1:B:124:LEU:HD22	1:B:164:ALA:HA	1.77	0.65
1:B:621:SER:O	1:B:623:SER:N	2.29	0.65
1:B:218:MET:HA	1:B:409:LEU:HD13	1.79	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ARG:NH1	1:C:338:SER:OG	2.28	0.64
1:C:350:PHE:CE1	1:C:386:SER:HB3	2.31	0.64
1:B:434:TYR:O	1:B:625:THR:HG21	1.97	0.64
1:B:600:THR:HB	1:B:608:GLU:HG3	1.80	0.63
1:A:218:MET:HA	1:A:409:LEU:HD13	1.81	0.63
1:A:633:LEU:HD23	1:A:667:TYR:CE1	2.33	0.63
1:A:118:LEU:HD11	1:A:238:PRO:HG3	1.81	0.63
1:C:668:ARG:NH2	1:C:669:GLU:OE2	2.32	0.62
1:A:125:ASN:ND2	1:A:242:GLU:OE2	2.30	0.62
1:A:631:HIS:HB2	1:B:691:TRP:CH2	2.34	0.62
1:C:632:ARG:HD3	1:C:634:ARG:HH21	1.64	0.62
1:A:616:ARG:O	1:A:620:THR:OG1	2.17	0.62
1:B:453:LYS:NZ	1:B:647:ASN:OD1	2.32	0.62
1:B:280:ARG:NH1	1:B:338:SER:OG	2.27	0.61
1:B:633:LEU:HD23	1:B:667:TYR:CE1	2.35	0.61
1:A:118:LEU:HD13	1:A:175:ARG:HD3	1.80	0.61
1:A:484:ARG:NH1	1:A:487:ASP:OD2	2.33	0.61
1:A:683:GLU:HG2	1:B:680:LEU:HD21	1.82	0.61
1:A:118:LEU:HD13	1:A:175:ARG:HH11	1.66	0.60
1:C:131:PHE:CE2	1:C:160:CYS:HB3	2.36	0.60
1:A:391:PHE:O	1:A:393:GLY:N	2.33	0.60
1:A:124:LEU:HD12	1:A:164:ALA:HA	1.83	0.60
1:C:633:LEU:HD23	1:C:667:TYR:CE1	2.37	0.59
1:C:391:PHE:O	1:C:393:GLY:N	2.34	0.59
1:A:411:LYS:HE2	1:A:414:LYS:HZ1	1.67	0.59
1:B:239:ILE:HD13	1:B:388:PRO:HG2	1.84	0.59
1:A:197:HIS:CD2	1:A:413:ARG:HA	2.39	0.58
1:A:680:LEU:HD21	1:B:683:GLU:HG2	1.84	0.58
1:A:644:VAL:HG13	1:A:652:GLU:HB2	1.85	0.58
1:B:261:ILE:HD11	1:B:357:MET:HG3	1.85	0.58
1:A:131:PHE:CE2	1:A:160:CYS:HB3	2.39	0.58
1:A:535:ILE:HG13	1:B:316:TYR:CD1	2.38	0.58
1:B:258:PHE:HD1	1:B:357:MET:HG2	1.68	0.58
1:B:645:LEU:HD23	1:B:650:VAL:HA	1.84	0.57
1:B:395:VAL:O	1:B:397:ARG:N	2.38	0.57
1:C:280:ARG:HH11	1:C:338:SER:HG	1.52	0.57
1:C:431:ASN:H	1:B:492:ARG:HH22	1.53	0.56
1:A:434:TYR:O	1:A:625:THR:HG21	2.05	0.56
1:A:395:VAL:O	1:A:397:ARG:N	2.38	0.56
1:A:205:TRP:HH2	1:A:214:LEU:HD21	1.71	0.56
1:C:462:GLY:H	1:C:625:THR:HB	1.69	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ASP:N	1:A:536:ASP:OD2	2.35	0.56
1:B:524:ASP:OD1	1:B:525:THR:N	2.34	0.55
1:A:527:TRP:HD1	1:A:562:PHE:CG	2.24	0.55
1:A:411:LYS:HG3	1:A:414:LYS:HZ3	1.69	0.55
1:A:205:TRP:CH2	1:A:214:LEU:HD21	2.41	0.55
1:C:395:VAL:O	1:C:397:ARG:N	2.40	0.55
1:C:536:ASP:N	1:C:536:ASP:OD2	2.37	0.55
1:B:421:ASN:OD1	1:B:421:ASN:N	2.40	0.54
1:A:166:PHE:CE1	1:B:348:LEU:HD13	2.42	0.54
1:A:411:LYS:HG3	1:A:414:LYS:HD3	1.88	0.54
1:B:350:PHE:CE1	1:B:386:SER:HB3	2.42	0.54
1:C:656:HIS:HE1	1:C:671:TRP:CZ3	2.26	0.54
1:A:316:TYR:CD1	1:B:535:ILE:HG13	2.43	0.53
1:B:446:HIS:ND1	1:B:447:PRO:HD2	2.23	0.53
1:A:283:PHE:CE1	1:A:334:LYS:HB3	2.44	0.53
1:B:594:MET:HE1	1:B:624:ARG:HH21	1.72	0.53
1:A:428:LEU:HB2	1:A:503:TYR:HE1	1.74	0.53
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.91	0.53
1:B:602:ALA:O	1:B:604:ASP:N	2.33	0.53
1:B:536:ASP:OD2	1:B:536:ASP:N	2.31	0.53
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.90	0.53
1:C:527:TRP:CZ3	1:C:531:LYS:HD2	2.43	0.53
1:C:411:LYS:O	1:C:414:LYS:HB3	2.09	0.53
1:A:527:TRP:CZ3	1:A:531:LYS:HD2	2.44	0.53
1:B:371:THR:OG1	1:B:372:VAL:N	2.41	0.52
1:A:411:LYS:HE2	1:A:414:LYS:NZ	2.24	0.52
1:C:609:GLN:O	1:C:613:ARG:HG3	2.09	0.52
1:A:131:PHE:HD2	1:A:161:TYR:HA	1.75	0.52
1:C:283:PHE:HE1	1:C:334:LYS:HB3	1.75	0.52
1:A:351:THR:HG23	1:B:165:ARG:HD3	1.91	0.52
1:C:446:HIS:ND1	1:C:447:PRO:HD2	2.24	0.51
1:A:428:LEU:HB3	1:A:429:PRO:CD	2.40	0.51
1:C:280:ARG:NH1	1:C:338:SER:HG	2.05	0.51
1:A:254:PHE:HE1	1:A:374:ASP:HB3	1.74	0.51
1:B:677:LEU:O	1:B:681:GLU:HG2	2.11	0.51
1:C:134:GLN:HB3	1:C:157:THR:HG21	1.92	0.51
1:B:258:PHE:HB3	1:B:357:MET:HE2	1.93	0.51
1:C:118:LEU:HD13	1:C:175:ARG:HD3	1.91	0.51
1:A:397:ARG:NH1	1:A:398:ASP:OD1	2.43	0.51
1:A:540:GLU:O	1:A:544:THR:HG23	2.10	0.51
1:B:540:GLU:O	1:B:544:THR:HG23	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:LEU:HD23	1:C:650:VAL:HA	1.93	0.50
1:B:462:GLY:H	1:B:625:THR:HG22	1.76	0.50
1:A:166:PHE:HE1	1:B:348:LEU:HB2	1.77	0.50
1:C:118:LEU:HD11	1:C:238:PRO:HB3	1.92	0.50
1:A:684:LEU:HA	1:B:680:LEU:HD23	1.92	0.50
1:A:366:ILE:HG12	1:B:143:TRP:CE3	2.47	0.50
1:B:496:ASN:O	1:B:498:ARG:HD2	2.12	0.50
1:C:632:ARG:HD3	1:C:634:ARG:NH2	2.26	0.50
1:A:198:LEU:HD13	1:B:302:LEU:HD21	1.94	0.50
1:B:644:VAL:HG13	1:B:652:GLU:HB2	1.93	0.50
1:C:600:THR:HB	1:C:608:GLU:HG3	1.94	0.50
1:A:451:ILE:HG21	1:A:477:THR:HG21	1.94	0.49
1:B:669:GLU:O	1:B:673:ILE:HG13	2.12	0.49
1:C:432:VAL:O	1:C:592:ARG:NH1	2.44	0.49
1:C:546:VAL:HG13	1:C:551:LEU:HB3	1.93	0.49
1:C:277:THR:HA	1:C:280:ARG:HG2	1.95	0.49
1:C:411:LYS:HG3	1:C:414:LYS:HD3	1.94	0.49
1:A:236:ILE:HD13	1:A:392:LEU:HD11	1.94	0.49
1:B:448:ASP:OD1	1:B:448:ASP:N	2.41	0.49
1:C:154:ILE:O	1:C:158:ILE:HG23	2.13	0.48
1:C:239:ILE:HD13	1:C:388:PRO:HG2	1.94	0.48
1:A:294:ALA:HB2	1:A:324:SER:HB3	1.95	0.48
1:A:195:PHE:CE2	1:B:318:ALA:HA	2.48	0.48
1:A:348:LEU:HD13	1:B:166:PHE:CD1	2.48	0.48
1:C:397:ARG:NH1	1:C:398:ASP:OD1	2.46	0.48
1:B:105:ASN:C	1:B:107:VAL:H	2.16	0.48
1:C:350:PHE:CD1	1:C:386:SER:HB3	2.48	0.48
1:C:313:ASN:HA	1:C:316:TYR:HB3	1.95	0.48
1:A:411:LYS:O	1:A:414:LYS:HB3	2.14	0.48
1:A:181:LYS:HG2	1:B:333:ILE:HD13	1.95	0.47
1:A:165:ARG:HD3	1:B:351:THR:HG23	1.97	0.47
1:C:540:GLU:O	1:C:544:THR:HG23	2.15	0.47
1:B:359:TYR:O	1:B:362:CYS:N	2.48	0.47
1:B:582:ALA:O	1:B:586:VAL:HG13	2.14	0.47
1:A:520:PRO:HG3	1:B:307:ALA:HB2	1.95	0.47
1:C:434:TYR:O	1:C:625:THR:HG21	2.14	0.47
1:C:129:PRO:HB2	1:C:377:LEU:HD12	1.97	0.47
1:B:209:ARG:HH12	1:B:411:LYS:HZ1	1.62	0.47
1:B:246:VAL:HG22	1:B:381:LEU:HG	1.96	0.47
1:A:307:ALA:HB2	1:B:520:PRO:HG3	1.97	0.47
1:C:656:HIS:CE1	1:C:671:TRP:CZ3	3.03	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLY:O	1:B:365:VAL:HG23	2.14	0.47
1:C:448:ASP:OD1	1:C:448:ASP:N	2.48	0.47
1:C:552:ALA:HB3	1:C:553:PRO:HD3	1.96	0.47
1:C:371:THR:OG1	1:C:372:VAL:N	2.48	0.47
1:A:576:GLY:O	1:A:580:ARG:HB2	2.15	0.47
1:B:122:LYS:HE3	1:B:238:PRO:O	2.15	0.47
1:C:274:ILE:O	1:C:277:THR:HG22	2.15	0.46
1:B:652:GLU:OE2	1:B:666:LEU:N	2.26	0.46
1:B:131:PHE:CD2	1:B:160:CYS:HB3	2.50	0.46
1:A:669:GLU:O	1:A:673:ILE:HG13	2.15	0.46
1:C:421:ASN:OD1	1:C:421:ASN:N	2.44	0.46
1:B:214:LEU:O	1:B:218:MET:HG2	2.15	0.46
1:A:633:LEU:O	1:A:636:ILE:HG13	2.15	0.46
1:A:173:GLU:HB3	1:B:340:ALA:HB1	1.96	0.46
1:A:521:LEU:HD13	1:A:566:VAL:HB	1.97	0.46
1:A:500:ILE:HA	1:A:503:TYR:HD2	1.80	0.46
1:C:555:ILE:HG21	1:C:562:PHE:CE1	2.51	0.46
1:A:301:SER:OG	1:A:317:LEU:HD13	2.15	0.46
1:C:524:ASP:OD1	1:C:525:THR:N	2.43	0.46
1:A:620:THR:O	1:A:622:GLY:N	2.49	0.46
1:B:656:HIS:HE1	1:B:671:TRP:CZ3	2.33	0.46
1:A:283:PHE:HE1	1:A:334:LYS:HD3	1.80	0.46
1:B:267:LEU:HA	1:B:267:LEU:HD12	1.76	0.46
1:C:462:GLY:H	1:C:625:THR:CB	2.28	0.45
1:C:644:VAL:HG13	1:C:652:GLU:HB2	1.97	0.45
1:C:443:PHE:CG	1:C:444:GLY:N	2.84	0.45
1:A:239:ILE:HD13	1:A:388:PRO:HG2	1.98	0.45
1:A:436:ILE:HB	1:A:459:ILE:HB	1.99	0.45
1:A:196:GLN:O	1:A:200:LYS:HG3	2.17	0.45
1:A:558:LEU:HA	1:A:559:PRO:HD2	1.71	0.45
1:C:429:PRO:HD2	1:C:434:TYR:HE1	1.81	0.45
1:B:462:GLY:H	1:B:625:THR:CG2	2.29	0.45
1:C:548:LYS:HB3	1:C:618:ASN:OD1	2.17	0.45
1:A:126:VAL:HG11	1:A:245:VAL:HG12	1.98	0.45
1:C:260:ALA:O	1:C:264:SER:HB2	2.17	0.45
1:B:389:LEU:HA	1:B:389:LEU:HD12	1.73	0.45
1:C:504:ASP:O	1:C:507:ALA:N	2.49	0.45
1:B:427:MET:H	1:B:428:LEU:CD2	2.29	0.45
1:C:403:LEU:HD22	1:C:403:LEU:HA	1.69	0.45
1:A:308:VAL:HG11	1:A:317:LEU:HD12	1.98	0.45
1:A:680:LEU:HD12	1:A:680:LEU:HA	1.67	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:THR:OG1	1:A:372:VAL:N	2.49	0.45
1:A:313:ASN:HA	1:A:316:TYR:HB3	1.97	0.45
1:B:118:LEU:HD13	1:B:175:ARG:HH11	1.82	0.45
1:B:266:MET:HE1	1:B:385:LEU:HB2	1.99	0.45
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.75	0.45
1:B:126:VAL:O	1:B:129:PRO:HD2	2.17	0.45
1:C:686:ASP:O	1:C:689:GLU:HB3	2.16	0.45
1:A:504:ASP:O	1:A:507:ALA:N	2.49	0.45
1:A:524:ASP:OD1	1:A:525:THR:N	2.40	0.44
1:B:428:LEU:HB3	1:B:498:ARG:NH1	2.32	0.44
1:A:283:PHE:HE1	1:A:334:LYS:HB3	1.82	0.44
1:C:317:LEU:HD23	1:C:317:LEU:HA	1.67	0.44
1:A:600:THR:HB	1:A:608:GLU:HG3	1.99	0.44
1:C:484:ARG:NH1	1:C:501:LYS:HG2	2.32	0.44
1:A:621:SER:O	1:A:623:SER:N	2.47	0.44
1:A:356:ALA:O	1:A:360:MET:HG3	2.17	0.44
1:A:594:MET:HE3	1:A:624:ARG:HH21	1.83	0.44
1:B:131:PHE:CE2	1:B:160:CYS:HB3	2.53	0.44
1:C:257:SER:O	1:C:261:ILE:HG23	2.18	0.44
1:A:655:LYS:O	1:A:659:LEU:HB2	2.18	0.44
1:A:657:LEU:HA	1:A:657:LEU:HD12	1.81	0.44
1:A:432:VAL:O	1:A:592:ARG:NH1	2.51	0.44
1:A:172:GLY:O	1:A:175:ARG:HB3	2.18	0.44
1:B:268:LEU:HD23	1:B:349:ILE:HG12	2.00	0.44
1:C:558:LEU:HD13	1:C:564:THR:HG21	2.00	0.44
1:C:122:LYS:HE3	1:C:238:PRO:O	2.17	0.43
1:C:604:ASP:OD1	1:C:607:THR:OG1	2.26	0.43
1:C:680:LEU:HD12	1:C:680:LEU:HA	1.78	0.43
1:B:432:VAL:O	1:B:592:ARG:NH1	2.50	0.43
1:C:205:TRP:CH2	1:C:214:LEU:HD21	2.53	0.43
1:A:181:LYS:HG2	1:B:333:ILE:CD1	2.48	0.43
1:A:622:GLY:O	1:A:624:ARG:HG3	2.17	0.43
1:A:694:PRO:HB2	1:B:647:ASN:HD22	1.84	0.43
1:B:283:PHE:CE1	1:B:334:LYS:HB3	2.53	0.43
1:C:689:GLU:O	1:C:692:SER:HB3	2.19	0.43
1:C:502:GLU:OE2	1:B:424:ARG:HD3	2.18	0.43
1:C:230:THR:O	1:C:234:PHE:HB2	2.19	0.43
1:A:258:PHE:HE1	1:A:378:ILE:HD12	1.84	0.43
1:B:555:ILE:HG21	1:B:562:PHE:CE1	2.53	0.43
1:A:132:PHE:HA	1:A:135:THR:HG22	2.01	0.43
1:B:554:LEU:HD22	1:B:577:GLU:HB3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:O	1:A:283:PHE:HB2	2.19	0.43
1:B:561:GLY:O	1:B:564:THR:OG1	2.27	0.43
1:A:452:LEU:HA	1:A:452:LEU:HD12	1.88	0.43
1:B:209:ARG:NH1	1:B:411:LYS:HZ1	2.17	0.43
1:B:118:LEU:HD11	1:B:238:PRO:HB3	1.99	0.43
1:C:243:ILE:HG12	1:C:266:MET:HG3	2.00	0.43
1:C:556:LYS:HD3	1:C:556:LYS:HA	1.77	0.43
1:B:686:ASP:O	1:B:689:GLU:HB3	2.18	0.43
1:B:644:VAL:CG1	1:B:652:GLU:HB2	2.49	0.43
1:C:554:LEU:HD22	1:C:577:GLU:HB3	2.00	0.43
1:B:283:PHE:HE1	1:B:334:LYS:HB3	1.84	0.42
1:B:538:THR:HG23	1:B:541:GLU:CD	2.40	0.42
1:A:311:PHE:CD1	1:B:533:GLY:HA2	2.54	0.42
1:A:579:GLN:HB2	1:A:611:LEU:HD11	2.01	0.42
1:C:214:LEU:O	1:C:218:MET:HG2	2.19	0.42
1:A:644:VAL:CG1	1:A:652:GLU:HB2	2.48	0.42
1:A:123:ILE:HD13	1:A:123:ILE:HA	1.75	0.42
1:A:319:ASP:HA	1:A:322:ASN:HB2	2.01	0.42
1:C:313:ASN:O	1:C:315:LYS:N	2.52	0.42
1:A:308:VAL:HG12	1:B:532:PHE:HZ	1.84	0.42
1:A:689:GLU:O	1:A:692:SER:HB3	2.19	0.42
1:C:280:ARG:O	1:C:283:PHE:HB2	2.19	0.42
1:A:403:LEU:HD22	1:A:403:LEU:HA	1.82	0.42
1:B:397:ARG:NH1	1:B:398:ASP:OD1	2.52	0.42
1:A:389:LEU:HA	1:A:389:LEU:HD12	1.80	0.42
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.67	0.42
1:C:549:ALA:O	1:C:580:ARG:HG3	2.20	0.42
1:C:221:GLY:O	1:C:225:ILE:HG13	2.20	0.42
1:B:428:LEU:HB3	1:B:498:ARG:HH12	1.85	0.42
1:B:254:PHE:HB3	1:B:258:PHE:CD2	2.54	0.42
1:A:362:CYS:O	1:B:139:MET:HE1	2.19	0.42
1:A:151:PRO:HB2	1:A:154:ILE:HG12	2.02	0.42
1:B:579:GLN:HB2	1:B:611:LEU:HD11	2.02	0.42
1:C:389:LEU:HD12	1:C:389:LEU:HA	1.79	0.42
1:B:452:LEU:HA	1:B:452:LEU:HD12	1.86	0.42
1:A:277:THR:HA	1:A:280:ARG:HG2	2.02	0.42
1:B:132:PHE:HA	1:B:135:THR:HG22	2.02	0.42
1:B:680:LEU:HD12	1:B:680:LEU:HA	1.66	0.41
1:C:462:GLY:H	1:C:625:THR:CG2	2.33	0.41
1:B:115:LEU:O	1:B:118:LEU:HB3	2.20	0.41
1:A:258:PHE:CE1	1:A:378:ILE:HD12	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:PHE:CE1	1:C:334:LYS:HB3	2.54	0.41
1:B:604:ASP:OD2	1:B:607:THR:OG1	2.25	0.41
1:A:641:LYS:HE2	1:A:643:ILE:HD11	2.02	0.41
1:B:545:VAL:HG11	1:B:588:LEU:HG	2.02	0.41
1:A:470:SER:HA	1:B:691:TRP:CH2	2.55	0.41
1:A:694:PRO:CB	1:B:647:ASN:HD22	2.34	0.41
1:A:525:THR:HA	1:A:564:THR:O	2.20	0.41
1:C:587:LEU:HD23	1:C:587:LEU:HA	1.91	0.41
1:B:151:PRO:O	1:B:154:ILE:HG12	2.20	0.41
1:B:446:HIS:ND1	1:B:448:ASP:OD1	2.53	0.41
1:A:525:THR:HG22	1:A:563:ASP:O	2.21	0.41
1:C:293:LYS:HA	1:C:293:LYS:HD3	1.73	0.41
1:B:134:GLN:HB3	1:B:157:THR:HG21	2.02	0.41
1:B:280:ARG:O	1:B:283:PHE:HB2	2.20	0.41
1:B:633:LEU:O	1:B:636:ILE:HG13	2.20	0.41
1:B:443:PHE:CG	1:B:444:GLY:N	2.88	0.41
1:C:364:GLY:O	1:C:370:LEU:N	2.45	0.41
1:A:527:TRP:HZ3	1:A:531:LYS:HD2	1.84	0.41
1:C:633:LEU:HD12	1:C:633:LEU:H	1.85	0.41
1:C:414:LYS:HE2	1:C:415:ASN:ND2	2.35	0.41
1:C:234:PHE:N	1:C:234:PHE:CD1	2.88	0.41
1:A:239:ILE:HG12	1:A:389:LEU:HD13	2.02	0.41
1:B:610:ALA:O	1:B:614:THR:HG23	2.20	0.41
1:B:221:GLY:HA3	1:B:409:LEU:HD22	2.02	0.41
1:C:576:GLY:O	1:C:580:ARG:HB2	2.20	0.41
1:C:608:GLU:OE2	1:C:632:ARG:HD2	2.21	0.41
1:B:254:PHE:HE1	1:B:374:ASP:HB3	1.85	0.41
1:C:429:PRO:HD2	1:C:434:TYR:CE1	2.56	0.41
1:B:318:ALA:O	1:B:321:TYR:HB3	2.21	0.41
1:B:312:ASN:OD1	1:B:312:ASN:N	2.42	0.41
1:A:545:VAL:HG11	1:A:588:LEU:HG	2.03	0.41
1:C:404:ILE:HG12	1:C:404:ILE:H	1.72	0.41
1:C:203:LEU:HD22	1:C:485:PHE:CD2	2.55	0.41
1:C:594:MET:HE1	1:C:624:ARG:HH21	1.86	0.41
1:A:443:PHE:CG	1:A:444:GLY:N	2.88	0.41
1:A:546:VAL:HG13	1:A:551:LEU:CB	2.38	0.40
1:B:254:PHE:CE1	1:B:374:ASP:HB3	2.56	0.40
1:A:166:PHE:HA	1:B:347:ASN:OD1	2.22	0.40
1:C:172:GLY:O	1:C:175:ARG:HB3	2.21	0.40
1:B:280:ARG:HH11	1:B:338:SER:HG	1.63	0.40
1:A:254:PHE:CE1	1:A:374:ASP:HB3	2.56	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLU:HB3	1:B:340:ALA:CB	2.52	0.40
1:A:239:ILE:HA	1:A:239:ILE:HD12	1.88	0.40
1:B:129:PRO:HB2	1:B:377:LEU:CD1	2.51	0.40
1:B:484:ARG:NH1	1:B:501:LYS:HG2	2.36	0.40
1:A:144:ASP:OD2	1:A:144:ASP:N	2.47	0.40
1:C:158:ILE:HD13	1:C:158:ILE:HG21	1.87	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	596/598 (100%)	540 (91%)	42 (7%)	14 (2%)	8	32
1	B	596/598 (100%)	540 (91%)	42 (7%)	14 (2%)	8	32
1	C	596/598 (100%)	544 (91%)	38 (6%)	14 (2%)	8	32
All	All	1788/1794 (100%)	1624 (91%)	122 (7%)	42 (2%)	8	32

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	ASN
1	A	392	LEU
1	A	395	VAL
1	A	396	TYR
1	A	603	LEU
1	A	621	SER
1	C	312	ASN
1	C	392	LEU
1	C	395	VAL
1	C	396	TYR
1	C	603	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	621	SER
1	B	312	ASN
1	B	392	LEU
1	B	395	VAL
1	B	396	TYR
1	B	603	LEU
1	A	164	ALA
1	C	164	ALA
1	B	164	ALA
1	B	393	GLY
1	B	429	PRO
1	B	621	SER
1	A	393	GLY
1	C	393	GLY
1	B	142	ALA
1	A	99	ILE
1	A	142	ALA
1	A	446	HIS
1	C	142	ALA
1	C	446	HIS
1	B	428	LEU
1	B	446	HIS
1	B	622	GLY
1	A	428	LEU
1	A	622	GLY
1	C	314	GLU
1	A	103	GLY
1	C	428	LEU
1	C	430	GLU
1	C	103	GLY
1	B	103	GLY

### 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.

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	501/514 (98%)	444 (89%)	57 (11%)	7 26
1	B	501/514 (98%)	449 (90%)	52 (10%)	9 31
1	C	501/514 (98%)	447 (89%)	54 (11%)	8 29
All	All	1503/1542 (98%)	1340 (89%)	163 (11%)	8 29

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	123	ILE
1	A	132	PHE
1	A	136	ILE
1	A	144	ASP
1	A	156	LEU
1	A	188	ARG
1	A	210	GLN
1	A	215	THR
1	A	223	LYS
1	A	227	GLN
1	A	257	SER
1	A	261	ILE
1	A	264	SER
1	A	280	ARG
1	A	289	LYS
1	A	312	ASN
1	A	320	LYS
1	A	331	SER
1	A	333	ILE
1	A	336	SER
1	A	338	SER
1	A	350	PHE
1	A	371	THR
1	A	372	VAL
1	A	392	LEU
1	A	403	LEU
1	A	419	ILE
1	A	420	LYS
1	A	428	LEU
1	A	437	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	445	TYR
1	A	446	HIS
1	A	454	ASN
1	A	456	SER
1	A	467	ILE
1	A	476	SER
1	A	477	THR
1	A	484	ARG
1	A	490	SER
1	A	534	ARG
1	A	535	ILE
1	A	538	THR
1	A	551	LEU
1	A	555	ILE
1	A	562	PHE
1	A	578	LYS
1	A	592	ARG
1	A	598	GLU
1	A	623	SER
1	A	625	THR
1	A	644	VAL
1	A	657	LEU
1	A	659	LEU
1	A	675	GLU
1	A	680	LEU
1	A	691	TRP
1	C	115	LEU
1	C	124	LEU
1	C	132	PHE
1	C	136	ILE
1	C	144	ASP
1	C	156	LEU
1	C	188	ARG
1	C	210	GLN
1	C	215	THR
1	C	223	LYS
1	C	227	GLN
1	C	236	ILE
1	C	243	ILE
1	C	257	SER
1	C	264	SER
1	C	277	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	280	ARG
1	C	285	ARG
1	C	289	LYS
1	C	312	ASN
1	C	331	SER
1	C	336	SER
1	C	338	SER
1	C	350	PHE
1	C	357	MET
1	C	371	THR
1	C	372	VAL
1	C	403	LEU
1	C	404	ILE
1	C	416	GLU
1	C	419	ILE
1	C	437	THR
1	C	456	SER
1	C	467	ILE
1	C	476	SER
1	C	477	THR
1	C	484	ARG
1	C	490	SER
1	C	534	ARG
1	C	535	ILE
1	C	538	THR
1	C	551	LEU
1	C	555	ILE
1	C	562	PHE
1	C	578	LYS
1	C	592	ARG
1	C	598	GLU
1	C	609	GLN
1	C	623	SER
1	C	625	THR
1	C	644	VAL
1	C	657	LEU
1	C	659	LEU
1	C	680	LEU
1	B	115	LEU
1	B	119	ILE
1	B	132	PHE
1	B	144	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	156	LEU
1	B	188	ARG
1	B	210	GLN
1	B	215	THR
1	B	223	LYS
1	B	227	GLN
1	B	243	ILE
1	B	257	SER
1	B	261	ILE
1	B	264	SER
1	B	275	LYS
1	B	280	ARG
1	B	285	ARG
1	B	289	LYS
1	B	312	ASN
1	B	331	SER
1	B	333	ILE
1	B	336	SER
1	B	338	SER
1	B	350	PHE
1	B	371	THR
1	B	372	VAL
1	B	392	LEU
1	B	403	LEU
1	B	419	ILE
1	B	437	THR
1	B	445	TYR
1	B	458	THR
1	B	467	ILE
1	B	476	SER
1	B	484	ARG
1	B	490	SER
1	B	527	TRP
1	B	534	ARG
1	B	535	ILE
1	B	538	THR
1	B	551	LEU
1	B	555	ILE
1	B	562	PHE
1	B	578	LYS
1	B	592	ARG
1	B	623	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	625	THR
1	B	644	VAL
1	B	657	LEU
1	B	659	LEU
1	B	680	LEU
1	B	691	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	B	140	ASN
1	B	379	ASN

### 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 carbohydrates 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, 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	A	598/598 (100%)	-0.06	17 (2%) 56 30	5, 41, 61, 87	0
1	B	598/598 (100%)	-0.15	9 (1%) 76 55	4, 37, 57, 77	0
1	C	598/598 (100%)	-0.20	3 (0%) 91 81	4, 28, 49, 69	0
All	All	1794/1794 (100%)	-0.14	29 (1%) 74 52	4, 33, 57, 87	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	ASN	7.8
1	A	103	GLY	5.7
1	B	692	SER	5.7
1	A	105	ASN	4.9
1	B	694	PRO	4.0
1	A	285	ARG	3.7
1	A	568	GLU	3.4
1	B	378	ILE	2.7
1	A	262	THR	2.7
1	C	389	LEU	2.7
1	A	258	PHE	2.6
1	B	260	ALA	2.6
1	A	260	ALA	2.5
1	A	523	ASN	2.5
1	B	282	HIS	2.4
1	C	558	LEU	2.4
1	A	448	ASP	2.4
1	B	218	MET	2.4
1	A	317	LEU	2.3
1	A	159	LEU	2.2
1	A	559	PRO	2.2
1	B	361	GLY	2.2
1	C	141	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	562	PHE	2.1
1	A	446	HIS	2.1
1	B	693	HIS	2.1
1	B	689	GLU	2.1
1	A	259	ALA	2.0
1	A	257	SER	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 carbohydrates 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.