



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:55 am GMT

PDB ID : 4R3Z  
Title : Crystal structure of human ArgRS-GlnRS-AIMP1 complex  
Authors : Fu, Y.; Kim, Y.; Cho, Y.  
Deposited on : 2014-08-18  
Resolution : 4.03 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.

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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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

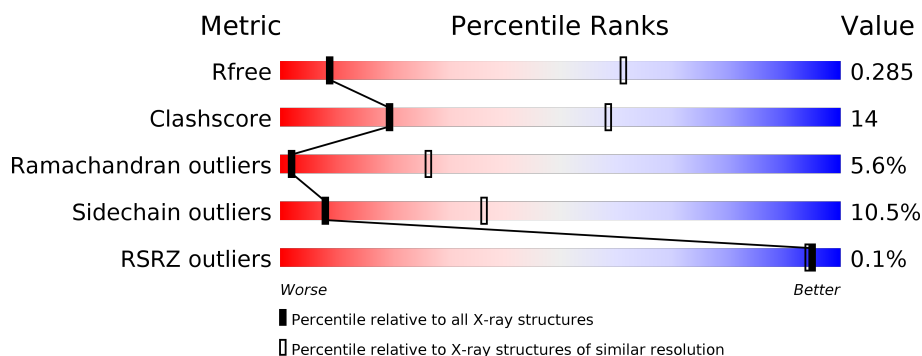
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



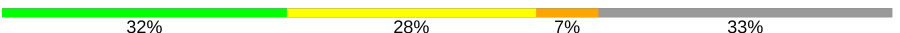
The reported resolution of this entry is 4.03 Å.

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))
$R_{free}$	100719	1094 (4.48-3.60)
Clashscore	112137	1194 (4.48-3.60)
Ramachandran outliers	110173	1145 (4.48-3.60)
Sidechain outliers	110143	1132 (4.48-3.60)
RSRZ outliers	101464	1105 (4.48-3.60)

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	312	 16% 8% 76%
2	B	675	 67% 28%
3	C	799	 32% 28% 7% 33%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10242 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 Aminoacyl tRNA synthase complex-interacting multifunctional protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	0	0	0
			617	393	108	116			

- Molecule 2 is a protein called Arginine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	659	Total	C	N	O	S	0	0	0
			5286	3364	905	987	30			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	MET	-	EXPRESSION TAG	UNP P54136
B	-13	GLY	-	EXPRESSION TAG	UNP P54136
B	-12	SER	-	EXPRESSION TAG	UNP P54136
B	-11	SER	-	EXPRESSION TAG	UNP P54136
B	-10	HIS	-	EXPRESSION TAG	UNP P54136
B	-9	HIS	-	EXPRESSION TAG	UNP P54136
B	-8	HIS	-	EXPRESSION TAG	UNP P54136
B	-7	HIS	-	EXPRESSION TAG	UNP P54136
B	-6	HIS	-	EXPRESSION TAG	UNP P54136
B	-5	HIS	-	EXPRESSION TAG	UNP P54136
B	-4	SER	-	EXPRESSION TAG	UNP P54136
B	-3	GLN	-	EXPRESSION TAG	UNP P54136
B	-2	ASP	-	EXPRESSION TAG	UNP P54136
B	-1	PRO	-	EXPRESSION TAG	UNP P54136
B	0	MET	-	EXPRESSION TAG	UNP P54136

- Molecule 3 is a protein called Glutamine-tRNA ligase.

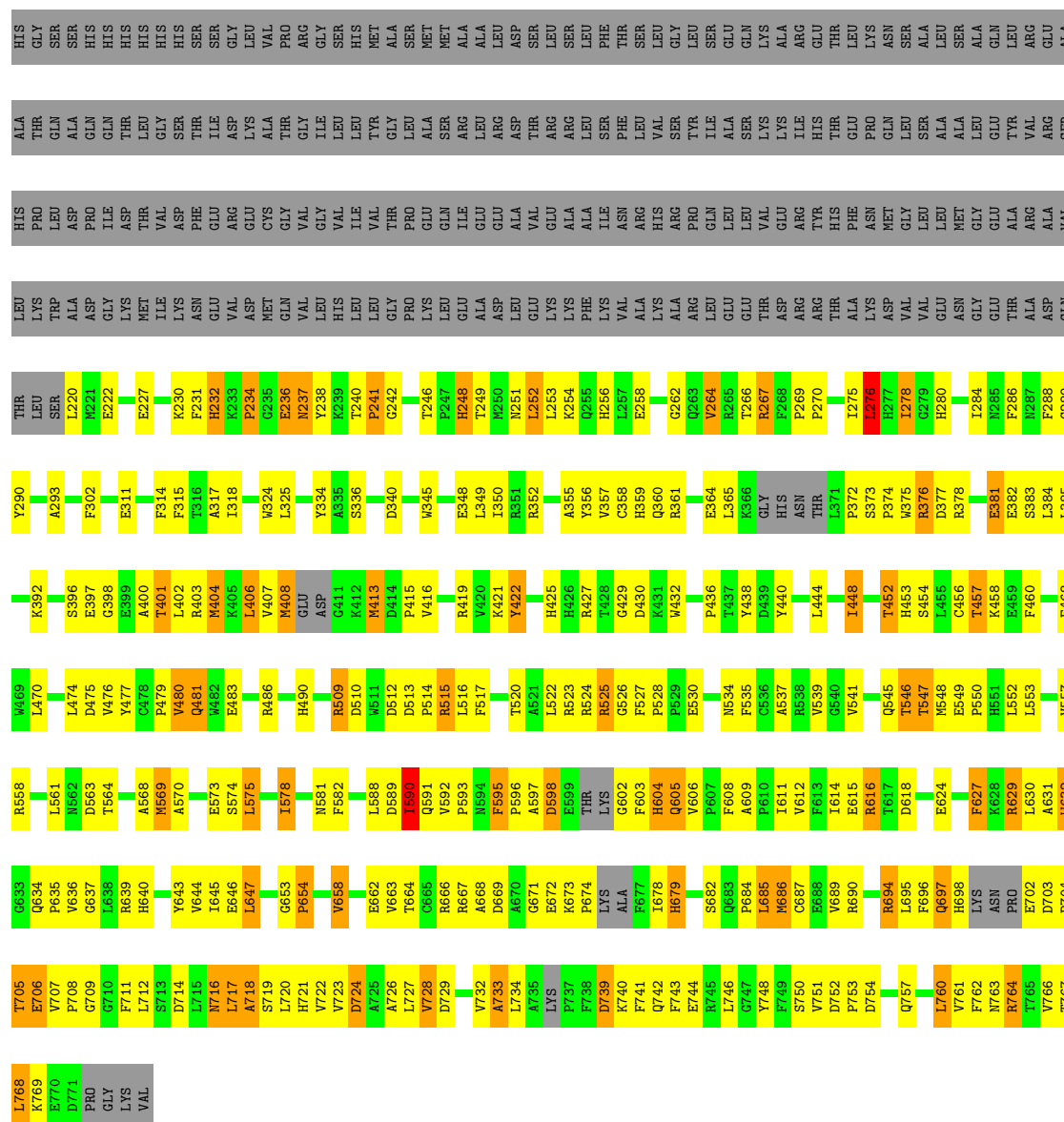
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	538	Total	C	N	O	S	0	0	0
			4339	2786	753	774	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	HIS	-	EXPRESSION TAG	UNP P47897
C	-22	GLY	-	EXPRESSION TAG	UNP P47897
C	-21	SER	-	EXPRESSION TAG	UNP P47897
C	-20	SER	-	EXPRESSION TAG	UNP P47897
C	-19	HIS	-	EXPRESSION TAG	UNP P47897
C	-18	HIS	-	EXPRESSION TAG	UNP P47897
C	-17	HIS	-	EXPRESSION TAG	UNP P47897
C	-16	HIS	-	EXPRESSION TAG	UNP P47897
C	-15	HIS	-	EXPRESSION TAG	UNP P47897
C	-14	HIS	-	EXPRESSION TAG	UNP P47897
C	-13	SER	-	EXPRESSION TAG	UNP P47897
C	-12	SER	-	EXPRESSION TAG	UNP P47897
C	-11	GLY	-	EXPRESSION TAG	UNP P47897
C	-10	LEU	-	EXPRESSION TAG	UNP P47897
C	-9	VAL	-	EXPRESSION TAG	UNP P47897
C	-8	PRO	-	EXPRESSION TAG	UNP P47897
C	-7	ARG	-	EXPRESSION TAG	UNP P47897
C	-6	GLY	-	EXPRESSION TAG	UNP P47897
C	-5	SER	-	EXPRESSION TAG	UNP P47897
C	-4	HIS	-	EXPRESSION TAG	UNP P47897
C	-3	MET	-	EXPRESSION TAG	UNP P47897
C	-2	ALA	-	EXPRESSION TAG	UNP P47897
C	-1	SER	-	EXPRESSION TAG	UNP P47897
C	0	MET	-	EXPRESSION TAG	UNP P47897



Chain C:  32% 28% 7% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.64Å 313.25Å 161.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.92 – 4.03 37.92 – 4.03	Depositor EDS
% Data completeness (in resolution range)	70.1 (37.92-4.03) 70.2 (37.92-4.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.20 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1745)	Depositor
R, $R_{free}$	0.229 , 0.285 0.229 , 0.285	Depositor DCC
$R_{free}$ test set	765 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 113.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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	A	0.28	0/619	0.48	0/824
2	B	0.28	0/5379	0.47	0/7246
3	C	0.32	0/4457	0.53	0/6044
All	All	0.30	0/10455	0.50	0/14114

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	617	0	668	19	0
2	B	5286	0	5347	119	0
3	C	4339	0	4255	162	0
All	All	10242	0	10270	295	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 14.

All (295) 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:733:ALA:H	3:C:734:LEU:HG	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:LYS:HG2	2:B:629:LYS:HB2	1.55	0.87
3:C:637:GLY:HA2	3:C:644:VAL:HG22	1.59	0.82
3:C:558:ARG:HD3	3:C:769:LYS:HA	1.63	0.80
3:C:276:LEU:HD11	3:C:318:ILE:HG12	1.63	0.79
3:C:458:LYS:HZ3	3:C:483:GLU:HG3	1.49	0.76
2:B:105:SER:HA	2:B:106:GLN:HB2	1.68	0.76
3:C:635:PRO:HB3	3:C:646:GLU:HA	1.66	0.76
2:B:627:ILE:HG23	2:B:628:LEU:HB2	1.71	0.72
3:C:591:GLN:HB3	3:C:603:PHE:HB3	1.70	0.72
2:B:101:LEU:HD23	2:B:116:ASN:HB2	1.72	0.71
3:C:718:ALA:HB1	3:C:720:LEU:HD12	1.72	0.71
3:C:716:ASN:O	3:C:718:ALA:N	2.24	0.70
3:C:358:CYS:SG	3:C:359:HIS:N	2.65	0.69
1:A:67:ILE:HA	1:A:70:GLU:HG2	1.73	0.69
3:C:697:GLN:HE21	3:C:716:ASN:HB2	1.57	0.68
1:A:64:GLN:HA	1:A:67:ILE:HG22	1.75	0.67
3:C:734:LEU:HB2	3:C:757:GLN:HG3	1.77	0.66
3:C:375:TRP:HB3	3:C:378:ARG:HD3	1.77	0.66
2:B:186:PRO:O	2:B:188:LEU:N	2.28	0.66
3:C:754:ASP:HB2	3:C:761:VAL:HG11	1.78	0.66
3:C:509:ARG:HD3	3:C:510:ASP:HB2	1.78	0.66
3:C:396:SER:O	3:C:398:GLY:N	2.29	0.65
2:B:600:TYR:HA	2:B:603:GLU:HB2	1.78	0.64
3:C:548:MET:HB3	3:C:552:LEU:HD21	1.79	0.64
3:C:248:HIS:HB2	3:C:252:LEU:HD12	1.79	0.64
1:A:24:TYR:HD2	1:A:25:LEU:HD12	1.63	0.64
3:C:515:ARG:HG3	3:C:695:LEU:HB2	1.79	0.63
3:C:598:ASP:N	3:C:598:ASP:OD1	2.31	0.63
2:B:628:LEU:HD21	2:B:630:VAL:HG22	1.80	0.63
2:B:626:LYS:HG3	2:B:627:ILE:HB	1.79	0.63
3:C:733:ALA:N	3:C:734:LEU:HG	2.10	0.63
1:A:48:LEU:O	1:A:52:ASN:ND2	2.30	0.63
2:B:545:ALA:HA	2:B:635:MET:HE1	1.80	0.63
2:B:485:VAL:HG22	2:B:490:GLU:HB3	1.79	0.63
3:C:570:ALA:HB2	3:C:728:VAL:HG23	1.81	0.62
3:C:514:PRO:HB3	3:C:525:ARG:HG3	1.82	0.62
3:C:667:ARG:O	3:C:669:ASP:N	2.32	0.62
2:B:66:ARG:NH2	2:B:82:GLU:OE1	2.32	0.62
3:C:430:ASP:O	3:C:432:TRP:N	2.29	0.62
3:C:530:GLU:O	3:C:534:ASN:ND2	2.33	0.62
3:C:719:SER:HA	3:C:720:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD13	2:B:62:LEU:HA	1.82	0.61
3:C:760:LEU:HD12	3:C:762:PHE:HE1	1.66	0.61
3:C:358:CYS:HB3	3:C:403:ARG:HD2	1.83	0.61
2:B:542:ARG:NH1	2:B:639:GLU:OE2	2.34	0.60
3:C:241:PRO:HG3	3:C:480:VAL:HG12	1.81	0.60
3:C:631:ALA:HB3	3:C:634:GLN:HB3	1.81	0.60
3:C:549:GLU:H	3:C:552:LEU:HD21	1.67	0.60
3:C:690:ARG:HG2	3:C:722:VAL:HG23	1.83	0.60
3:C:732:VAL:HG11	3:C:762:PHE:HZ	1.67	0.60
3:C:636:VAL:HG23	3:C:674:PRO:HB3	1.83	0.59
3:C:732:VAL:HA	3:C:733:ALA:HB2	1.84	0.59
3:C:267:ARG:NH1	3:C:267:ARG:O	2.36	0.59
3:C:525:ARG:HH22	3:C:694:ARG:HH21	1.49	0.59
3:C:302:PHE:HE1	3:C:318:ILE:HD12	1.69	0.58
3:C:760:LEU:HD23	3:C:760:LEU:H	1.67	0.58
2:B:366:VAL:HG21	2:B:418:THR:HG23	1.85	0.58
2:B:237:HIS:NE2	2:B:388:ASP:OD1	2.26	0.58
3:C:647:LEU:H	3:C:663:VAL:HG21	1.69	0.58
2:B:238:VAL:HG12	2:B:334:GLY:HA3	1.87	0.57
2:B:243:THR:HB	2:B:291:TYR:HE1	1.70	0.57
3:C:643:TYR:HA	3:C:667:ARG:HA	1.85	0.57
3:C:561:LEU:HA	3:C:564:THR:HG22	1.86	0.57
2:B:223:ARG:HH21	2:B:653:GLY:HA2	1.70	0.56
2:B:313:ASP:HA	2:B:316:ARG:HG2	1.86	0.56
3:C:719:SER:N	3:C:720:LEU:HB2	2.20	0.56
2:B:180:VAL:HG13	2:B:181:ASN:H	1.70	0.56
3:C:679:HIS:CD2	3:C:679:HIS:H	2.24	0.56
3:C:696:PHE:HB3	3:C:714:ASP:HB3	1.88	0.56
2:B:123:GLN:O	2:B:125:LEU:N	2.39	0.56
2:B:627:ILE:HG12	2:B:628:LEU:HD23	1.88	0.56
3:C:732:VAL:HG22	3:C:741:PHE:CZ	2.41	0.56
3:C:729:ASP:N	3:C:729:ASP:OD1	2.37	0.56
2:B:185:LEU:HD11	2:B:582:PRO:HB3	1.87	0.55
2:B:251:HIS:HD2	2:B:279:ARG:HG3	1.71	0.55
3:C:234:PRO:HB3	3:C:262:GLY:CA	2.36	0.55
3:C:266:THR:HG22	3:C:453:HIS:HB2	1.88	0.55
3:C:647:LEU:H	3:C:663:VAL:CG2	2.20	0.55
3:C:515:ARG:NH1	3:C:719:SER:O	2.40	0.55
2:B:241:TRP:CH2	2:B:298:GLN:HG2	2.41	0.55
2:B:48:ASN:O	2:B:52:LYS:HB2	2.06	0.55
2:B:61:SER:HB3	3:C:392:LYS:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:LYS:NZ	2:B:281:ASP:OD2	2.40	0.55
1:A:24:TYR:OH	1:A:28:GLN:NE2	2.41	0.54
2:B:268:ASP:HB3	2:B:271:VAL:HG12	1.88	0.54
2:B:497:SER:OG	2:B:655:LYS:O	2.22	0.54
3:C:740:LYS:HG3	3:C:750:SER:HB2	1.88	0.54
2:B:163:ASN:N	2:B:163:ASN:OD1	2.38	0.54
2:B:76:ILE:HD11	2:B:579:LEU:HB3	1.90	0.54
3:C:743:PHE:HB3	3:C:746:LEU:HD13	1.89	0.54
2:B:247:MET:HG2	2:B:276:SER:HB2	1.89	0.54
3:C:276:LEU:HA	3:C:280:HIS:ND1	2.23	0.54
3:C:421:LYS:O	3:C:422:TYR:HB2	2.08	0.54
3:C:349:LEU:HG	3:C:474:LEU:HD21	1.89	0.54
3:C:525:ARG:HH11	3:C:527:PHE:HE1	1.54	0.54
3:C:705:THR:O	3:C:707:VAL:N	2.41	0.54
2:B:483:ASP:OD1	2:B:484:LYS:N	2.40	0.53
3:C:720:LEU:HB3	3:C:721:HIS:HB3	1.91	0.53
2:B:243:THR:HB	2:B:291:TYR:CE1	2.44	0.53
1:A:68:GLN:O	2:B:79:ARG:NH2	2.41	0.53
3:C:513:ASP:O	3:C:516:LEU:HB2	2.09	0.53
3:C:314:PHE:O	3:C:318:ILE:HG13	2.08	0.53
3:C:528:PRO:HD2	3:C:557:VAL:HG23	1.91	0.53
3:C:724:ASP:N	3:C:724:ASP:OD1	2.39	0.53
3:C:739:ASP:O	3:C:751:VAL:HG23	2.09	0.53
3:C:752:ASP:OD2	3:C:763:ASN:ND2	2.37	0.52
3:C:227:GLU:HB2	3:C:290:TYR:HE2	1.74	0.52
3:C:350:ILE:HA	3:C:355:ALA:HB3	1.92	0.52
3:C:416:VAL:HG11	3:C:419:ARG:NH1	2.24	0.52
3:C:404:MET:H	3:C:415:PRO:HB2	1.75	0.52
2:B:206:GLU:HG2	2:B:461:ARG:HG3	1.91	0.52
2:B:225:PHE:HB3	2:B:230:TYR:HB2	1.92	0.52
3:C:517:PHE:HZ	3:C:550:PRO:HB3	1.75	0.52
3:C:605:GLN:HE21	3:C:605:GLN:N	2.08	0.52
3:C:361:ARG:HD2	3:C:365:LEU:HD13	1.93	0.51
2:B:254:ASP:OD1	2:B:289:ARG:NH1	2.44	0.51
3:C:234:PRO:HB3	3:C:262:GLY:HA3	1.93	0.51
3:C:561:LEU:HD21	3:C:740:LYS:HG2	1.92	0.51
3:C:373:SER:HB3	3:C:376:ARG:HH21	1.75	0.51
3:C:525:ARG:NH2	3:C:694:ARG:HH21	2.08	0.51
3:C:635:PRO:HG3	3:C:666:ARG:HH12	1.76	0.51
2:B:194:VAL:HG11	2:B:225:PHE:CD2	2.46	0.51
3:C:602:GLY:O	3:C:603:PHE:HD1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:632:TRP:HA	3:C:647:LEU:HD23	1.93	0.50
2:B:535:LEU:HD22	2:B:657:VAL:HG22	1.93	0.50
3:C:413:MET:O	3:C:415:PRO:HD3	2.12	0.50
3:C:406:LEU:HB2	3:C:415:PRO:HB3	1.93	0.50
2:B:366:VAL:HG12	2:B:368:GLY:H	1.76	0.50
2:B:647:LYS:O	2:B:651:ILE:HG12	2.11	0.50
3:C:764:ARG:HG3	3:C:764:ARG:O	2.12	0.50
3:C:348:GLU:HG3	3:C:352:ARG:HD2	1.93	0.50
3:C:345:TRP:HE3	3:C:444:LEU:HD13	1.77	0.50
2:B:105:SER:HB3	2:B:114:GLN:HE21	1.76	0.50
3:C:573:GLU:HB2	3:C:615:GLU:HB2	1.94	0.49
1:A:79:PRO:HD2	1:A:80:PHE:CG	2.47	0.49
2:B:269:LEU:HD12	2:B:270:GLN:N	2.27	0.49
2:B:9:SER:O	2:B:13:LEU:N	2.45	0.49
3:C:490:HIS:HB3	3:C:702:GLU:HG3	1.94	0.49
3:C:574:SER:HB3	3:C:727:LEU:HD13	1.94	0.49
3:C:452:THR:O	3:C:453:HIS:ND1	2.46	0.49
3:C:314:PHE:HA	3:C:317:ALA:HB3	1.93	0.49
3:C:717:LEU:O	3:C:719:SER:N	2.45	0.49
2:B:326:LEU:HB2	2:B:328:VAL:HG23	1.93	0.49
1:A:47:LYS:O	1:A:50:VAL:HG12	2.13	0.49
2:B:198:PHE:HB2	2:B:214:SER:O	2.13	0.48
3:C:618:ASP:HA	3:C:629:ARG:HD3	1.95	0.48
2:B:81:GLN:HB3	2:B:100:LEU:HD13	1.95	0.48
2:B:316:ARG:HA	2:B:319:LEU:HB2	1.96	0.48
2:B:3:VAL:HA	2:B:6:SER:HB3	1.96	0.48
2:B:67:ASN:O	2:B:69:PRO:HD3	2.13	0.48
3:C:458:LYS:HA	3:C:458:LYS:HD2	1.53	0.48
2:B:119:MET:SD	2:B:119:MET:N	2.87	0.48
2:B:209:VAL:HB	2:B:444:VAL:HG11	1.95	0.48
2:B:456:SER:OG	2:B:457:GLY:HA2	2.13	0.48
2:B:236:ASN:HB2	2:B:330:LEU:HD22	1.96	0.47
3:C:517:PHE:HA	3:C:522:LEU:HD21	1.95	0.47
3:C:236:GLU:O	3:C:238:TYR:N	2.43	0.47
3:C:612:VAL:HG12	3:C:682:SER:HB2	1.96	0.47
2:B:454:THR:HB	2:B:457:GLY:HA3	1.96	0.47
3:C:356:TYR:O	3:C:402:LEU:HD12	2.14	0.47
2:B:632:MET:O	2:B:636:LEU:HG	2.14	0.47
3:C:396:SER:C	3:C:398:GLY:H	2.17	0.47
2:B:350:GLU:OE2	2:B:362:LYS:NZ	2.41	0.47
2:B:512:ARG:HG3	2:B:513:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:ILE:HA	2:B:633:TRP:HB2	1.96	0.47
3:C:249:THR:O	3:C:253:LEU:HB2	2.15	0.47
2:B:119:MET:HE1	2:B:159:PRO:HB2	1.97	0.47
3:C:378:ARG:NH1	3:C:382:GLU:OE1	2.47	0.47
3:C:545:GLN:O	3:C:547:THR:N	2.48	0.47
2:B:581:PHE:HB3	2:B:582:PRO:HD3	1.97	0.46
2:B:192:LYS:HD3	2:B:230:TYR:HE1	1.80	0.46
2:B:534:LEU:HB3	2:B:649:PHE:HZ	1.81	0.46
3:C:604:HIS:CD2	3:C:604:HIS:H	2.32	0.46
2:B:408:VAL:HG12	2:B:409:ASP:H	1.80	0.46
2:B:174:GLN:HB3	2:B:579:LEU:HD21	1.98	0.46
3:C:457:THR:HG23	3:C:460:PHE:HE2	1.80	0.46
2:B:74:ILE:HD11	2:B:174:GLN:HG2	1.96	0.46
3:C:324:TRP:CE2	3:C:523:ARG:HG3	2.50	0.46
2:B:502:CYS:HB3	2:B:523:MET:HG2	1.97	0.46
2:B:223:ARG:NH2	2:B:653:GLY:HA2	2.31	0.45
3:C:454:SER:O	3:C:481:GLN:HA	2.16	0.45
2:B:508:LEU:O	2:B:595:HIS:HA	2.15	0.45
2:B:139:GLU:O	2:B:142:THR:HG22	2.17	0.45
2:B:236:ASN:HB3	2:B:332:GLU:HA	1.99	0.45
3:C:535:PHE:CG	3:C:553:LEU:HD13	2.52	0.45
2:B:80:LEU:HA	2:B:83:VAL:HG22	1.98	0.45
2:B:39:PRO:O	2:B:43:GLN:HB3	2.17	0.45
3:C:401:THR:HG22	3:C:419:ARG:HA	1.99	0.45
1:A:24:TYR:CD2	1:A:25:LEU:HD12	2.48	0.44
3:C:440:TYR:CD1	3:C:470:LEU:HD21	2.52	0.44
3:C:733:ALA:HB3	3:C:734:LEU:HA	1.99	0.44
3:C:456:CYS:HB2	3:C:481:GLN:HE21	1.82	0.44
3:C:742:GLN:NE2	3:C:748:TYR:HE1	2.15	0.44
3:C:645:ILE:HB	3:C:663:VAL:HG21	1.99	0.44
2:B:485:VAL:HG13	2:B:490:GLU:HB2	2.00	0.44
3:C:526:GLY:HA2	3:C:740:LYS:HE3	1.99	0.44
3:C:616:ARG:HD2	3:C:658:VAL:HB	1.98	0.44
2:B:217:ILE:HG12	2:B:508:LEU:HD21	1.99	0.44
3:C:582:PHE:CD2	3:C:609:ALA:HB3	2.53	0.44
1:A:56:LYS:HA	1:A:59:ILE:HB	2.00	0.44
2:B:616:TYR:HB3	2:B:619:GLU:HB3	1.99	0.44
2:B:54:ARG:HA	2:B:57:ILE:HG22	2.00	0.44
3:C:697:GLN:NE2	3:C:716:ASN:HB2	2.28	0.44
2:B:604:LEU:HD13	2:B:641:VAL:HG13	1.99	0.44
3:C:232:HIS:ND1	3:C:232:HIS:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:LYS:O	2:B:310:LEU:HG	2.17	0.43
3:C:457:THR:OG1	3:C:458:LYS:N	2.50	0.43
3:C:595:PHE:C	3:C:597:ALA:H	2.22	0.43
3:C:614:ILE:HD13	3:C:679:HIS:O	2.18	0.43
2:B:454:THR:HG22	2:B:455:ARG:H	1.84	0.43
3:C:231:PHE:HB3	3:C:232:HIS:H	1.46	0.43
1:A:79:PRO:HB2	1:A:80:PHE:HA	1.99	0.43
3:C:425:HIS:H	3:C:429:GLY:HA2	1.83	0.43
3:C:444:LEU:HG	3:C:470:LEU:HD23	2.00	0.43
2:B:194:VAL:HG11	2:B:225:PHE:HD2	1.84	0.43
3:C:630:LEU:HD11	3:C:647:LEU:HB2	2.00	0.43
3:C:256:HIS:NE2	3:C:452:THR:HG23	2.34	0.43
3:C:592:VAL:HB	3:C:604:HIS:CD2	2.52	0.43
2:B:394:GLN:NE2	2:B:398:GLU:OE1	2.51	0.43
3:C:284:ILE:HG23	3:C:288:PHE:HD2	1.84	0.43
3:C:608:PHE:CG	3:C:609:ALA:N	2.87	0.43
3:C:403:ARG:HB3	3:C:415:PRO:HB2	2.00	0.43
3:C:673:LYS:HB3	3:C:674:PRO:HD2	2.01	0.43
1:A:17:GLU:O	1:A:21:ILE:HG12	2.19	0.43
2:B:301:ASN:HB3	2:B:304:ILE:HB	2.00	0.43
2:B:568:HIS:CE1	2:B:570:LYS:HB2	2.53	0.43
2:B:280:PHE:CE1	2:B:287:LYS:HG3	2.54	0.42
3:C:289:GLY:O	3:C:293:ALA:N	2.48	0.42
3:C:361:ARG:CZ	3:C:419:ARG:HH11	2.32	0.42
3:C:706:GLU:C	3:C:708:PRO:HD3	2.39	0.42
1:A:71:ILE:HG22	1:A:76:LYS:HB2	2.01	0.42
2:B:501:GLY:HA2	2:B:654:ILE:HG12	2.02	0.42
2:B:622:ARG:HA	2:B:622:ARG:HD2	1.89	0.42
3:C:575:LEU:HA	3:C:575:LEU:HD22	1.73	0.42
3:C:614:ILE:HD12	3:C:615:GLU:H	1.84	0.42
2:B:628:LEU:HD22	2:B:629:LYS:N	2.34	0.42
2:B:191:ASN:HD22	2:B:191:ASN:HA	1.71	0.42
2:B:481:GLU:O	2:B:485:VAL:HB	2.18	0.42
3:C:510:ASP:HB3	3:C:512:ASP:OD1	2.19	0.42
2:B:243:THR:HA	2:B:294:VAL:HG21	2.00	0.42
2:B:259:TYR:CE2	2:B:307:ALA:HB2	2.54	0.42
3:C:246:THR:O	3:C:248:HIS:N	2.48	0.42
3:C:653:GLY:HA3	3:C:654:PRO:HD2	1.85	0.42
3:C:696:PHE:HA	3:C:714:ASP:O	2.20	0.42
3:C:254:LYS:O	3:C:258:GLU:HB2	2.19	0.42
3:C:237:ASN:ND2	3:C:480:VAL:HG13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:537:ALA:O	2:B:541:ILE:HG13	2.20	0.42
3:C:581:ASN:HB2	3:C:664:THR:OG1	2.20	0.42
2:B:408:VAL:O	2:B:440:GLY:HA2	2.20	0.41
2:B:523:MET:HA	2:B:530:THR:HG21	2.01	0.41
3:C:220:LEU:HD12	3:C:537:ALA:HB2	2.02	0.41
3:C:470:LEU:HD12	3:C:470:LEU:HA	1.76	0.41
1:A:73:ASN:N	1:A:73:ASN:OD1	2.53	0.41
3:C:357:VAL:HG23	3:C:383:SER:OG	2.19	0.41
3:C:578:ILE:HG23	3:C:662:GLU:HB3	2.02	0.41
2:B:456:SER:CB	2:B:457:GLY:HA2	2.51	0.41
3:C:590:ILE:HG13	3:C:590:ILE:O	2.18	0.41
3:C:689:VAL:HB	3:C:723:VAL:HG23	2.01	0.41
1:A:21:ILE:H	1:A:21:ILE:HG12	1.59	0.41
2:B:258:ASP:N	2:B:258:ASP:OD1	2.48	0.41
3:C:444:LEU:O	3:C:448:ILE:HG13	2.20	0.41
2:B:453:LYS:O	2:B:457:GLY:HA3	2.20	0.41
3:C:430:ASP:C	3:C:432:TRP:H	2.18	0.41
3:C:720:LEU:HA	3:C:721:HIS:HA	1.83	0.41
2:B:452:PHE:CD1	2:B:453:LYS:HB2	2.56	0.41
3:C:381:GLU:HA	3:C:384:LEU:HB2	2.02	0.41
3:C:624:GLU:O	3:C:627:PHE:HB2	2.20	0.41
2:B:134:PRO:HA	2:B:137:ILE:HB	2.02	0.41
2:B:133:ASN:HA	2:B:134:PRO:HD3	1.86	0.41
2:B:264:PRO:HA	2:B:265:PRO:HD2	1.94	0.41
3:C:539:VAL:HG11	3:C:548:MET:SD	2.61	0.41
1:A:49:ARG:HA	1:A:49:ARG:HD3	1.90	0.41
2:B:126:LYS:HB3	2:B:127:THR:H	1.63	0.41
2:B:588:ILE:HG21	2:B:594:LEU:HD23	2.01	0.41
3:C:407:VAL:HG13	3:C:408:MET:H	1.86	0.41
3:C:733:ALA:N	3:C:734:LEU:HA	2.35	0.41
2:B:465:LEU:HD13	2:B:465:LEU:HA	1.86	0.41
1:A:66:LEU:HA	2:B:62:LEU:HD13	2.02	0.41
2:B:72:ASN:ND2	2:B:184:GLN:HG3	2.36	0.41
2:B:58:LEU:HA	2:B:58:LEU:HD23	1.84	0.41
2:B:503:ILE:HA	2:B:523:MET:SD	2.60	0.40
3:C:374:PRO:HB2	3:C:375:TRP:CD1	2.56	0.40
2:B:50:LYS:HE2	3:C:421:LYS:O	2.21	0.40
2:B:70:THR:HG23	2:B:71:LYS:H	1.86	0.40
3:C:302:PHE:HB2	3:C:334:TYR:HD1	1.86	0.40
2:B:335:GLU:HG2	2:B:387:SER:HB2	2.03	0.40
1:A:77:GLN:HG2	1:A:78:ILE:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:GLN:HA	2:B:273:TYR:HB3	2.03	0.40
2:B:505:TYR:HB2	2:B:654:ILE:HD11	2.03	0.40
2:B:68:LYS:HA	2:B:69:PRO:HD3	1.77	0.40
2:B:452:PHE:CG	2:B:453:LYS:HB2	2.56	0.40
2:B:570:LYS:HA	2:B:570:LYS:HD3	1.90	0.40
3:C:241:PRO:HB2	3:C:242:GLY:H	1.58	0.40
3:C:336:SER:HB3	3:C:425:HIS:NE2	2.37	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	74/312 (24%)	69 (93%)	4 (5%)	1 (1%)	13	55
2	B	657/675 (97%)	586 (89%)	58 (9%)	13 (2%)	9	49
3	C	524/799 (66%)	372 (71%)	96 (18%)	56 (11%)	0	10
All	All	1255/1786 (70%)	1027 (82%)	158 (13%)	70 (6%)	2	26

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	187	ALA
3	C	264	VAL
3	C	269	PRO
3	C	372	PRO
3	C	397	GLU
3	C	668	ALA
3	C	717	LEU
2	B	32	CYS
2	B	104	PRO
2	B	124	MET

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Mol	Chain	Res	Type
2	B	199	SER
2	B	453	LYS
3	C	241	PRO
3	C	276	LEU
3	C	311	GLU
3	C	400	ALA
3	C	422	TYR
3	C	590	ILE
3	C	611	ILE
3	C	629	ARG
3	C	706	GLU
3	C	716	ASN
3	C	718	ALA
3	C	726	ALA
3	C	733	ALA
3	C	768	LEU
2	B	75	ASN
2	B	106	GLN
3	C	230	LYS
3	C	236	GLU
3	C	360	GLN
3	C	376	ARG
3	C	438	TYR
3	C	479	PRO
3	C	486	ARG
3	C	546	THR
3	C	593	PRO
3	C	685	LEU
3	C	704	PRO
3	C	705	THR
2	B	614	SER
3	C	278	ILE
3	C	364	GLU
3	C	448	ILE
3	C	481	GLN
3	C	509	ARG
3	C	588	LEU
3	C	654	PRO
3	C	671	GLY
3	C	686	MET
2	B	454	THR
2	B	487	THR

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Mol	Chain	Res	Type
3	C	240	THR
3	C	475	ASP
3	C	547	THR
3	C	568	ALA
3	C	569	MET
3	C	647	LEU
3	C	658	VAL
3	C	684	PRO
3	C	753	PRO
3	C	596	PRO
3	C	709	GLY
2	B	160	GLY
3	C	234	PRO
3	C	436	PRO
2	B	69	PRO
3	C	270	PRO
3	C	541	VAL
1	A	79	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/269 (24%)	61 (92%)	5 (8%)	15	51
2	B	579/594 (98%)	539 (93%)	40 (7%)	18	54
3	C	466/685 (68%)	394 (84%)	72 (16%)	3	22
All	All	1111/1548 (72%)	994 (90%)	117 (10%)	8	36

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	21	ILE
1	A	32	LEU
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	80	PHE
2	B	13	LEU
2	B	51	LEU
2	B	70	THR
2	B	74	ILE
2	B	80	LEU
2	B	107	GLN
2	B	119	MET
2	B	124	MET
2	B	125	LEU
2	B	126	LYS
2	B	128	LYS
2	B	163	ASN
2	B	185	LEU
2	B	188	LEU
2	B	195	ILE
2	B	208	HIS
2	B	219	GLU
2	B	238	VAL
2	B	244	GLN
2	B	245	PHE
2	B	324	ASP
2	B	330	LEU
2	B	340	ASP
2	B	344	ASP
2	B	418	THR
2	B	453	LYS
2	B	454	THR
2	B	456	SER
2	B	461	ARG
2	B	464	ASP
2	B	465	LEU
2	B	509	SER
2	B	517	ILE
2	B	520	PHE
2	B	525	ASP
2	B	551	ASP
2	B	596	THR
2	B	627	ILE
2	B	629	LYS
2	B	659	ARG
3	C	222	GLU

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Mol	Chain	Res	Type
3	C	232	HIS
3	C	237	ASN
3	C	248	HIS
3	C	251	ASN
3	C	252	LEU
3	C	264	VAL
3	C	267	ARG
3	C	275	ILE
3	C	276	LEU
3	C	278	ILE
3	C	286	PHE
3	C	315	PHE
3	C	325	LEU
3	C	340	ASP
3	C	377	ASP
3	C	381	GLU
3	C	385	LEU
3	C	401	THR
3	C	404	MET
3	C	406	LEU
3	C	408	MET
3	C	413	MET
3	C	427	ARG
3	C	452	THR
3	C	457	THR
3	C	468	PHE
3	C	476	VAL
3	C	477	TYR
3	C	480	VAL
3	C	515	ARG
3	C	520	THR
3	C	524	ARG
3	C	525	ARG
3	C	546	THR
3	C	563	ASP
3	C	569	MET
3	C	575	LEU
3	C	578	ILE
3	C	589	ASP
3	C	590	ILE
3	C	595	PHE
3	C	598	ASP

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Mol	Chain	Res	Type
3	C	604	HIS
3	C	605	GLN
3	C	606	VAL
3	C	616	ARG
3	C	627	PHE
3	C	632	TRP
3	C	639	ARG
3	C	640	HIS
3	C	672	GLU
3	C	678	ILE
3	C	679	HIS
3	C	685	LEU
3	C	686	MET
3	C	687	CYS
3	C	694	ARG
3	C	697	GLN
3	C	698	HIS
3	C	703	ASP
3	C	711	PHE
3	C	712	LEU
3	C	724	ASP
3	C	728	VAL
3	C	739	ASP
3	C	744	GLU
3	C	760	LEU
3	C	764	ARG
3	C	766	VAL
3	C	767	THR
3	C	768	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
2	B	114	GLN
2	B	181	ASN
2	B	191	ASN
2	B	320	ASN
2	B	438	HIS
2	B	568	HIS
2	B	631	ASN
3	C	263	GLN

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Mol	Chain	Res	Type
3	C	360	GLN
3	C	426	HIS
3	C	604	HIS
3	C	605	GLN
3	C	648	GLN
3	C	649	HIS
3	C	679	HIS
3	C	697	GLN
3	C	742	GLN
3	C	756	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 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 [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	A	76/312 (24%)	-0.24	0 <a href="#">100</a>   <a href="#">100</a>	89, 159, 206, 234	0
2	B	659/675 (97%)	-0.29	1 (0%) <a href="#">94</a>   <a href="#">93</a>	77, 161, 235, 299	0
3	C	538/799 (67%)	-0.37	0 <a href="#">100</a>   <a href="#">100</a>	67, 129, 231, 318	4 (0%)
All	All	1273/1786 (71%)	-0.32	1 (0%) <a href="#">95</a>   <a href="#">94</a>	67, 150, 232, 318	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	16	GLU	2.1

### 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.