



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2022 – 06:02 pm BST

PDB ID : 7ZU9  
Title : CRYSTAL STRUCTURE OF THE C89A\_C113A GMP SYNTHETASE IN-ACTIVE DOUBLE MUTANT FROM PLASMODIUM FALCIPARUM  
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Deposited on : 2022-05-11  
Resolution : 2.80 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	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

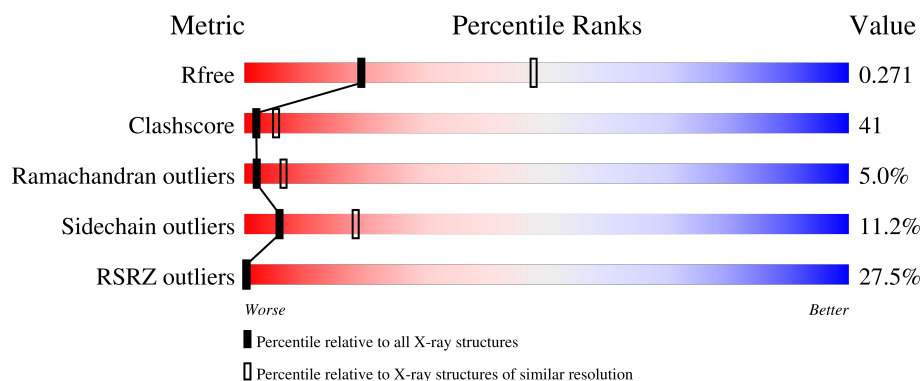
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	A	568	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4084 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 Glutamine amidotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4074	2615	666	774	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q8IJR9
A	-11	ARG	-	expression tag	UNP Q8IJR9
A	-10	GLY	-	expression tag	UNP Q8IJR9
A	-9	SER	-	expression tag	UNP Q8IJR9
A	-8	HIS	-	expression tag	UNP Q8IJR9
A	-7	HIS	-	expression tag	UNP Q8IJR9
A	-6	HIS	-	expression tag	UNP Q8IJR9
A	-5	HIS	-	expression tag	UNP Q8IJR9
A	-4	HIS	-	expression tag	UNP Q8IJR9
A	-3	HIS	-	expression tag	UNP Q8IJR9
A	-2	GLY	-	expression tag	UNP Q8IJR9
A	-1	SER	-	expression tag	UNP Q8IJR9
A	0	MET	-	expression tag	UNP Q8IJR9
A	1	ALA	-	expression tag	UNP Q8IJR9
A	89	ALA	CYS	engineered mutation	UNP Q8IJR9
A	113	ALA	CYS	engineered mutation	UNP Q8IJR9

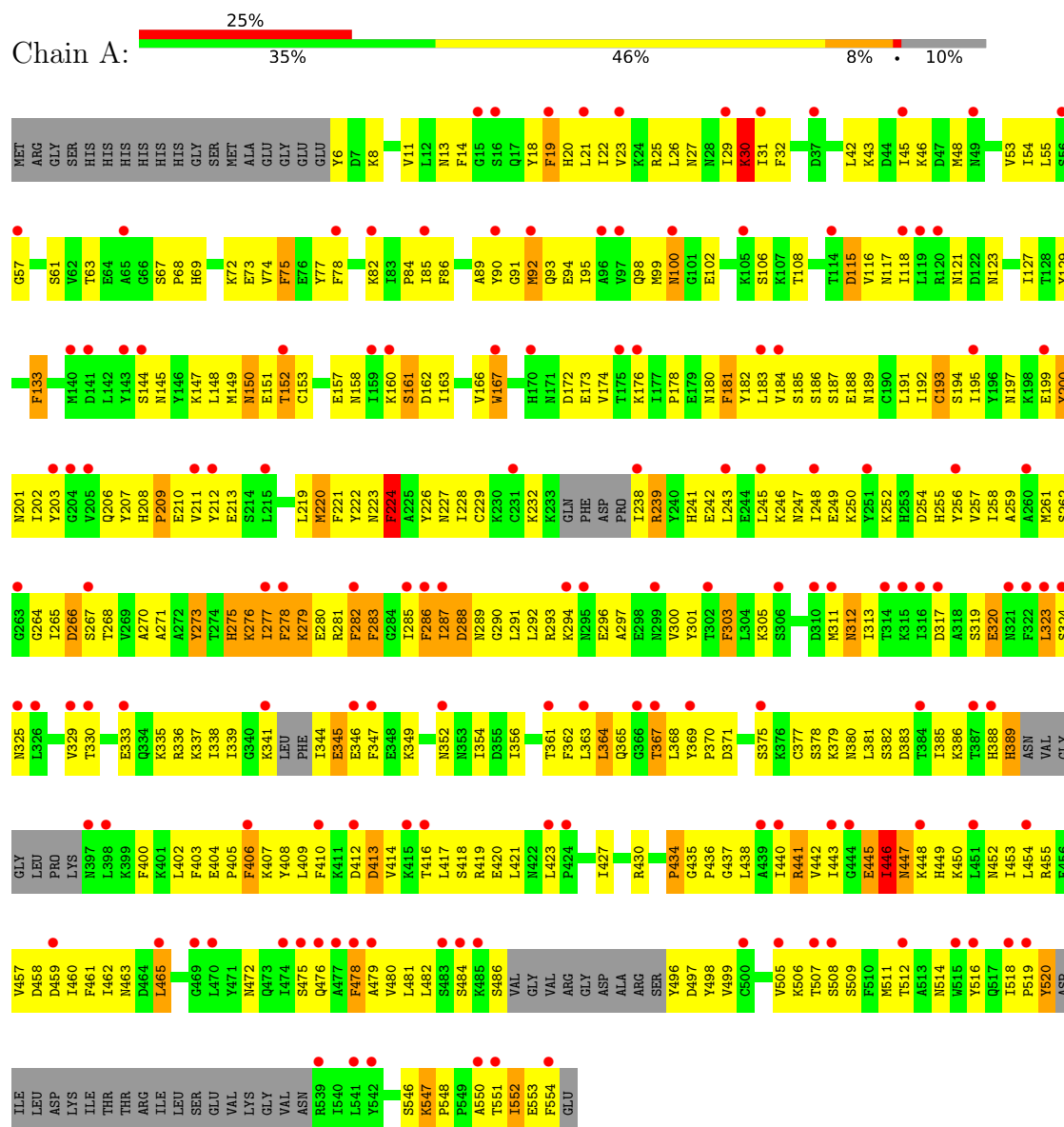
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		

### 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: Glutamine amidotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.65Å 64.54Å 56.33Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	28.16 – 2.80 28.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (28.16-2.80) 92.1 (28.16-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.270 , 0.314 0.243 , 0.271	Depositor DCC
$R_{free}$ test set	462 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.360 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.326 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.397 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.398 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.305 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4084	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.60% 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	0.38	0/4157	0.64	0/5615

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	4074	0	3971	332	0
2	A	10	0	0	0	0
All	All	4084	0	3971	332	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 41.

All (332) 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:29:ILE:CD1	1:A:222:TYR:HA	1.55	1.36
1:A:29:ILE:HD11	1:A:222:TYR:CA	1.72	1.19
1:A:291:LEU:CD2	1:A:454:LEU:HD23	1.88	1.03
1:A:291:LEU:HD22	1:A:454:LEU:CD2	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:CD2	1:A:454:LEU:CD2	2.40	0.99
1:A:144:SER:HA	1:A:548:PRO:HD2	1.46	0.94
1:A:29:ILE:HD11	1:A:222:TYR:HA	0.94	0.92
1:A:276:LYS:HB2	1:A:281:ARG:HH12	1.39	0.87
1:A:192:ILE:HD11	1:A:195:ILE:HD11	1.55	0.87
1:A:220:MET:O	1:A:224:PHE:HB2	1.75	0.86
1:A:54:ILE:HD12	1:A:86:PHE:HB2	1.57	0.86
1:A:291:LEU:HD23	1:A:454:LEU:HD23	1.55	0.85
1:A:323:LEU:HD22	1:A:447:ASN:HA	1.63	0.81
1:A:294:LYS:HD2	1:A:455:ARG:HG2	1.63	0.80
1:A:121:ASN:ND2	1:A:511:MET:SD	2.56	0.78
1:A:267:SER:HA	1:A:270:ALA:HB3	1.67	0.78
1:A:414:VAL:HA	1:A:417:LEU:HB2	1.66	0.76
1:A:181:PHE:O	1:A:512:THR:HG21	1.84	0.76
1:A:86:PHE:HD1	1:A:203:TYR:HB2	1.49	0.76
1:A:385:ILE:HA	1:A:434:PRO:HB3	1.68	0.75
1:A:507:THR:CG2	1:A:512:THR:O	2.33	0.75
1:A:291:LEU:HD22	1:A:454:LEU:HD21	1.69	0.74
1:A:291:LEU:HD23	1:A:454:LEU:CD2	2.10	0.73
1:A:8:LYS:HE3	1:A:48:MET:HB2	1.70	0.73
1:A:29:ILE:HD11	1:A:222:TYR:CB	2.17	0.73
1:A:276:LYS:HB3	1:A:281:ARG:HH22	1.52	0.73
1:A:442:VAL:HG22	1:A:481:LEU:HB3	1.70	0.73
1:A:264:GLY:O	1:A:268:THR:N	2.21	0.72
1:A:445:GLU:O	1:A:446:ILE:HG12	1.89	0.72
1:A:507:THR:HG21	1:A:512:THR:H	1.55	0.72
1:A:552:ILE:HG22	1:A:553:GLU:HG2	1.71	0.72
1:A:305:LYS:HE3	1:A:312:ASN:HA	1.71	0.72
1:A:336:ARG:HE	1:A:440:ILE:HD13	1.55	0.71
1:A:377:CYS:SG	1:A:378:SER:N	2.64	0.71
1:A:149:MET:SD	1:A:149:MET:N	2.62	0.70
1:A:84:PRO:HB2	1:A:86:PHE:CZ	2.26	0.70
1:A:507:THR:HG23	1:A:512:THR:O	1.91	0.70
1:A:29:ILE:CD1	1:A:222:TYR:HD1	2.04	0.70
1:A:276:LYS:CB	1:A:281:ARG:HH22	2.04	0.70
1:A:167:TRP:HH2	1:A:213:GLU:HB2	1.55	0.70
1:A:368:LEU:H	1:A:371:ASP:HB2	1.57	0.70
1:A:85:ILE:O	1:A:203:TYR:N	2.25	0.69
1:A:209:PRO:HG3	1:A:221:PHE:CE2	2.28	0.69
1:A:150:ASN:HB2	1:A:511:MET:HB3	1.75	0.69
1:A:259:ALA:HA	1:A:364:LEU:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLY:HA3	1:A:453:ILE:HG23	1.74	0.69
1:A:385:ILE:HG22	1:A:386:LYS:HG3	1.74	0.67
1:A:443:ILE:HG12	1:A:482:LEU:HA	1.76	0.67
1:A:323:LEU:O	1:A:325:ASN:N	2.26	0.67
1:A:199:GLU:H	1:A:508:SER:HB2	1.60	0.66
1:A:123:ASN:HB3	1:A:127:ILE:HD11	1.77	0.66
1:A:305:LYS:HD2	1:A:313:ILE:HG22	1.78	0.66
1:A:197:ASN:ND2	1:A:200:TYR:HB2	2.11	0.66
1:A:518:ILE:O	1:A:520:TYR:N	2.28	0.66
1:A:106:SER:HB2	1:A:173:GLU:HB2	1.77	0.66
1:A:29:ILE:HD12	1:A:222:TYR:HA	1.70	0.65
1:A:29:ILE:CD1	1:A:222:TYR:CD1	2.80	0.65
1:A:29:ILE:HD11	1:A:222:TYR:CD1	2.32	0.65
1:A:57:GLY:HA3	1:A:90:TYR:HB3	1.79	0.65
1:A:264:GLY:O	1:A:268:THR:HG23	1.97	0.65
1:A:507:THR:CG2	1:A:512:THR:H	2.09	0.64
1:A:482:LEU:O	1:A:498:TYR:HA	1.98	0.64
1:A:271:ALA:HB1	1:A:311:MET:HE1	1.78	0.64
1:A:255:HIS:HB2	1:A:361:THR:HA	1.79	0.64
1:A:330:THR:OG1	1:A:443:ILE:HB	1.98	0.64
1:A:29:ILE:O	1:A:31:ILE:N	2.31	0.63
1:A:265:ILE:HA	1:A:268:THR:OG1	1.99	0.62
1:A:287:ILE:HG21	1:A:292:LEU:HD13	1.81	0.62
1:A:67:SER:O	1:A:69:HIS:ND1	2.28	0.61
1:A:336:ARG:HE	1:A:440:ILE:CD1	2.13	0.61
1:A:344:ILE:O	1:A:388:HIS:CD2	2.54	0.61
1:A:437:GLY:O	1:A:440:ILE:HG22	2.01	0.61
1:A:29:ILE:HG12	1:A:222:TYR:HD1	1.65	0.60
1:A:183:LEU:CD1	1:A:192:ILE:HG13	2.31	0.60
1:A:43:LYS:HA	1:A:46:LYS:HE2	1.83	0.60
1:A:23:VAL:O	1:A:27:ASN:HB2	2.01	0.60
1:A:25:ARG:HH12	1:A:209:PRO:HB2	1.67	0.59
1:A:289:ASN:HA	1:A:319:SER:HA	1.83	0.59
1:A:287:ILE:HG22	1:A:287:ILE:O	2.03	0.59
1:A:89:ALA:HA	1:A:206:GLN:HA	1.84	0.59
1:A:548:PRO:HA	1:A:550:ALA:N	2.18	0.59
1:A:84:PRO:HB3	1:A:201:ASN:HB3	1.84	0.59
1:A:283:PHE:CE2	1:A:352:ASN:HA	2.38	0.58
1:A:547:LYS:HB3	1:A:548:PRO:HD3	1.83	0.58
1:A:283:PHE:HE1	1:A:285:ILE:HD11	1.66	0.58
1:A:323:LEU:HD13	1:A:446:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:HA	1:A:273:TYR:HD2	1.66	0.58
1:A:288:ASP:HB3	1:A:317:ASP:CG	2.22	0.58
1:A:127:ILE:HD12	1:A:127:ILE:H	1.69	0.58
1:A:197:ASN:HD22	1:A:200:TYR:HB2	1.68	0.58
1:A:241:HIS:ND1	1:A:242:GLU:HG2	2.18	0.58
1:A:277:ILE:HG22	1:A:278:PHE:H	1.68	0.57
1:A:296:GLU:O	1:A:300:VAL:HB	2.04	0.57
1:A:29:ILE:CG1	1:A:222:TYR:HD1	2.17	0.57
1:A:346:GLU:HG3	1:A:347:PHE:CE1	2.38	0.57
1:A:11:VAL:HG23	1:A:54:ILE:HG23	1.85	0.57
1:A:93:GLN:HG2	1:A:174:VAL:HG22	1.86	0.57
1:A:115:ASP:HB3	1:A:163:ILE:HG23	1.85	0.57
1:A:416:THR:O	1:A:419:ARG:N	2.36	0.57
1:A:278:PHE:HB2	1:A:281:ARG:HH21	1.70	0.57
1:A:290:GLY:HA2	1:A:297:ALA:HB2	1.86	0.57
1:A:447:ASN:CG	1:A:448:LYS:H	2.08	0.57
1:A:301:TYR:O	1:A:313:ILE:HG21	2.05	0.57
1:A:333:GLU:O	1:A:337:LYS:HB2	2.05	0.56
1:A:446:ILE:HA	1:A:450:LYS:HD2	1.86	0.56
1:A:145:ASN:O	1:A:514:ASN:ND2	2.38	0.56
1:A:266:ASP:OD1	1:A:266:ASP:N	2.37	0.56
1:A:346:GLU:HA	1:A:388:HIS:CE1	2.41	0.56
1:A:262:SER:O	1:A:292:LEU:HD11	2.06	0.56
1:A:90:TYR:HA	1:A:93:GLN:HB2	1.88	0.55
1:A:276:LYS:HB2	1:A:281:ARG:NH1	2.16	0.55
1:A:291:LEU:HA	1:A:454:LEU:HD23	1.88	0.55
1:A:21:LEU:HD22	1:A:210:GLU:HA	1.88	0.55
1:A:99:MET:HE1	1:A:202:ILE:HG21	1.89	0.55
1:A:29:ILE:CD1	1:A:222:TYR:CA	2.49	0.55
1:A:365:GLN:HB2	1:A:406:PHE:CE1	2.42	0.55
1:A:72:LYS:O	1:A:75:PHE:N	2.40	0.55
1:A:273:TYR:CD1	1:A:273:TYR:C	2.81	0.54
1:A:250:LYS:NZ	1:A:256:TYR:HA	2.22	0.54
1:A:30:LYS:HB3	1:A:232:LYS:HZ1	1.72	0.54
1:A:277:ILE:HG22	1:A:278:PHE:N	2.23	0.54
1:A:446:ILE:HB	1:A:450:LYS:HD2	1.89	0.54
1:A:445:GLU:CD	1:A:445:GLU:H	2.11	0.54
1:A:441:ARG:HG3	1:A:480:VAL:HG13	1.90	0.54
1:A:148:LEU:HD12	1:A:183:LEU:O	2.07	0.54
1:A:300:VAL:HG13	1:A:301:TYR:HD1	1.73	0.54
1:A:336:ARG:NE	1:A:440:ILE:HD13	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:VAL:HG12	1:A:212:TYR:H	1.73	0.53
1:A:442:VAL:HA	1:A:481:LEU:O	2.08	0.53
1:A:209:PRO:HG3	1:A:221:PHE:CZ	2.44	0.53
1:A:224:PHE:O	1:A:228:ILE:HG12	2.09	0.53
1:A:291:LEU:HD13	1:A:437:GLY:HA3	1.90	0.53
1:A:250:LYS:HZ1	1:A:256:TYR:HA	1.73	0.53
1:A:99:MET:O	1:A:100:ASN:CB	2.56	0.53
1:A:287:ILE:H	1:A:317:ASP:HB2	1.73	0.53
1:A:445:GLU:OE2	1:A:484:SER:HA	2.09	0.53
1:A:46:LYS:HG2	1:A:77:TYR:CE1	2.43	0.53
1:A:267:SER:HA	1:A:270:ALA:CB	2.36	0.53
1:A:286:PHE:O	1:A:287:ILE:HB	2.08	0.53
1:A:46:LYS:HG2	1:A:77:TYR:HE1	1.75	0.52
1:A:184:VAL:HB	1:A:194:SER:HB3	1.90	0.52
1:A:27:ASN:ND2	1:A:31:ILE:O	2.43	0.52
1:A:365:GLN:HB2	1:A:406:PHE:HE1	1.74	0.52
1:A:6:TYR:HE2	1:A:31:ILE:HA	1.74	0.52
1:A:30:LYS:HD2	1:A:32:PHE:HE1	1.75	0.52
1:A:117:ASN:HD21	1:A:163:ILE:HG12	1.74	0.52
1:A:271:ALA:HB1	1:A:311:MET:CE	2.40	0.52
1:A:448:LYS:C	1:A:450:LYS:H	2.13	0.52
1:A:255:HIS:CB	1:A:361:THR:HA	2.39	0.52
1:A:300:VAL:HG13	1:A:301:TYR:CD1	2.45	0.52
1:A:258:ILE:HD12	1:A:283:PHE:CD2	2.44	0.52
1:A:329:VAL:HG12	1:A:330:THR:H	1.73	0.52
1:A:293:ARG:NH2	1:A:430:ARG:HB2	2.25	0.52
1:A:507:THR:HG22	1:A:512:THR:N	2.25	0.52
1:A:149:MET:SD	1:A:182:TYR:HB3	2.49	0.52
1:A:406:PHE:O	1:A:407:LYS:CB	2.58	0.51
1:A:507:THR:CG2	1:A:512:THR:N	2.71	0.51
1:A:551:THR:HG22	1:A:552:ILE:H	1.74	0.51
1:A:133:PHE:CZ	1:A:191:LEU:HD12	2.45	0.51
1:A:551:THR:HG22	1:A:552:ILE:N	2.24	0.51
1:A:73:GLU:HG2	1:A:74:VAL:N	2.25	0.51
1:A:435:GLY:N	1:A:436:PRO:HD3	2.26	0.51
1:A:185:SER:HB2	1:A:193:CYS:HB3	1.93	0.51
1:A:300:VAL:HA	1:A:303:PHE:CD2	2.45	0.51
1:A:475:SER:OG	1:A:506:LYS:HA	2.11	0.51
1:A:199:GLU:HB3	1:A:412:ASP:HB2	1.93	0.51
1:A:221:PHE:O	1:A:224:PHE:HB3	2.11	0.50
1:A:19:PHE:O	1:A:23:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:HD13	1:A:186:SER:O	2.11	0.50
1:A:257:VAL:O	1:A:258:ILE:HD13	2.12	0.50
1:A:266:ASP:OD2	1:A:368:LEU:HD11	2.11	0.50
1:A:435:GLY:H	1:A:436:PRO:HD3	1.76	0.50
1:A:116:VAL:HG13	1:A:187:SER:HA	1.94	0.50
1:A:185:SER:CB	1:A:193:CYS:HB3	2.42	0.50
1:A:238:ILE:HG12	1:A:239:ARG:N	2.27	0.50
1:A:291:LEU:CD2	1:A:452:ASN:O	2.60	0.49
1:A:277:ILE:O	1:A:278:PHE:HB2	2.11	0.49
1:A:427:ILE:HG12	1:A:430:ARG:NH1	2.27	0.49
1:A:200:TYR:HB3	1:A:202:ILE:HG13	1.94	0.49
1:A:150:ASN:C	1:A:150:ASN:HD22	2.15	0.49
1:A:301:TYR:CD2	1:A:313:ILE:HG13	2.47	0.49
1:A:330:THR:CG2	1:A:335:LYS:HE2	2.43	0.49
1:A:380:ASN:OD1	1:A:381:LEU:N	2.46	0.49
1:A:182:TYR:CE1	1:A:512:THR:OG1	2.58	0.49
1:A:108:THR:HG21	1:A:189:ASN:HB3	1.94	0.49
1:A:293:ARG:HE	1:A:430:ARG:HD2	1.79	0.48
1:A:53:VAL:HB	1:A:78:PHE:CZ	2.48	0.48
1:A:261:MET:HG2	1:A:285:ILE:H	1.78	0.48
1:A:275:HIS:O	1:A:276:LYS:HB2	2.14	0.48
1:A:286:PHE:O	1:A:287:ILE:CB	2.62	0.48
1:A:441:ARG:HD3	1:A:554:PHE:N	2.29	0.48
1:A:446:ILE:CA	1:A:450:LYS:HD2	2.44	0.48
1:A:178:PRO:HD3	1:A:195:ILE:HD13	1.96	0.47
1:A:409:LEU:HD13	1:A:413:ASP:HB3	1.96	0.47
1:A:55:LEU:HB3	1:A:91:GLY:HA3	1.96	0.47
1:A:258:ILE:O	1:A:364:LEU:N	2.46	0.47
1:A:270:ALA:HA	1:A:273:TYR:CD2	2.48	0.47
1:A:29:ILE:HG22	1:A:31:ILE:HG12	1.97	0.47
1:A:250:LYS:HA	1:A:255:HIS:NE2	2.29	0.47
1:A:409:LEU:HB3	1:A:413:ASP:HB2	1.95	0.47
1:A:406:PHE:O	1:A:407:LYS:HB3	2.14	0.47
1:A:246:LYS:HA	1:A:246:LYS:HD2	1.51	0.47
1:A:291:LEU:HA	1:A:454:LEU:HB2	1.96	0.47
1:A:486:SER:O	1:A:486:SER:OG	2.26	0.47
1:A:223:ASN:O	1:A:227:ASN:HB2	2.14	0.47
1:A:445:GLU:HG2	1:A:446:ILE:H	1.78	0.47
1:A:283:PHE:CD1	1:A:283:PHE:C	2.88	0.47
1:A:367:THR:HG21	1:A:389:HIS:HB3	1.96	0.47
1:A:369:TYR:HB3	1:A:370:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ARG:HB3	1:A:420:GLU:H	1.32	0.47
1:A:547:LYS:HB3	1:A:548:PRO:CD	2.44	0.47
1:A:345:GLU:C	1:A:347:PHE:H	2.18	0.47
1:A:147:LYS:HE2	1:A:547:LYS:HE2	1.97	0.47
1:A:291:LEU:CB	1:A:454:LEU:HD23	2.46	0.46
1:A:129:TYR:CD1	1:A:188:GLU:HA	2.50	0.46
1:A:20:HIS:HA	1:A:23:VAL:HG22	1.97	0.46
1:A:186:SER:HB3	1:A:191:LEU:O	2.15	0.46
1:A:239:ARG:HG3	1:A:243:LEU:HD22	1.96	0.46
1:A:149:MET:HG3	1:A:182:TYR:CD1	2.51	0.46
1:A:183:LEU:HD11	1:A:192:ILE:HG13	1.97	0.46
1:A:197:ASN:O	1:A:201:ASN:HA	2.15	0.46
1:A:167:TRP:CH2	1:A:213:GLU:HB2	2.44	0.46
1:A:404:GLU:N	1:A:405:PRO:HD3	2.31	0.46
1:A:427:ILE:O	1:A:430:ARG:HG2	2.16	0.46
1:A:454:LEU:HD12	1:A:458:ASP:OD1	2.15	0.46
1:A:92:MET:HA	1:A:95:ILE:HG22	1.98	0.46
1:A:511:MET:O	1:A:512:THR:OG1	2.34	0.46
1:A:278:PHE:O	1:A:279:LYS:HB2	2.16	0.45
1:A:61:SER:HB3	1:A:63:THR:HG22	1.97	0.45
1:A:461:PHE:O	1:A:465:LEU:HD23	2.15	0.45
1:A:300:VAL:HA	1:A:303:PHE:HD2	1.81	0.45
1:A:312:ASN:N	1:A:312:ASN:ND2	2.64	0.45
1:A:94:GLU:O	1:A:98:GLN:HG3	2.16	0.45
1:A:178:PRO:HG2	1:A:195:ILE:HG21	1.98	0.45
1:A:209:PRO:HG2	1:A:210:GLU:H	1.81	0.45
1:A:172:ASP:OD1	1:A:172:ASP:N	2.49	0.45
1:A:460:ILE:HA	1:A:463:ASN:ND2	2.31	0.45
1:A:144:SER:O	1:A:147:LYS:NZ	2.50	0.45
1:A:339:ILE:HB	1:A:346:GLU:OE1	2.17	0.45
1:A:413:ASP:OD1	1:A:413:ASP:N	2.49	0.45
1:A:117:ASN:ND2	1:A:163:ILE:HG12	2.32	0.45
1:A:280:GLU:CB	1:A:312:ASN:OD1	2.65	0.45
1:A:443:ILE:HG21	1:A:482:LEU:HD23	1.98	0.45
1:A:199:GLU:HG3	1:A:508:SER:HB2	1.99	0.44
1:A:277:ILE:CG2	1:A:278:PHE:H	2.26	0.44
1:A:345:GLU:HB2	1:A:346:GLU:H	1.57	0.44
1:A:181:PHE:HB2	1:A:512:THR:HG21	2.00	0.44
1:A:228:ILE:HG13	1:A:229:CYS:N	2.33	0.44
1:A:291:LEU:HD23	1:A:452:ASN:O	2.18	0.44
1:A:160:LYS:O	1:A:161:SER:C	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ILE:O	1:A:435:GLY:N	2.50	0.44
1:A:516:TYR:CD1	1:A:518:ILE:HG13	2.52	0.44
1:A:354:ILE:C	1:A:356:ILE:H	2.21	0.44
1:A:446:ILE:O	1:A:447:ASN:HB2	2.17	0.44
1:A:160:LYS:O	1:A:162:ASP:N	2.51	0.44
1:A:245:LEU:C	1:A:247:ASN:H	2.20	0.44
1:A:182:TYR:OH	1:A:509:SER:N	2.50	0.43
1:A:286:PHE:CB	1:A:341:LYS:HB3	2.48	0.43
1:A:507:THR:HG22	1:A:512:THR:HB	2.00	0.43
1:A:86:PHE:CD1	1:A:203:TYR:HB2	2.39	0.43
1:A:186:SER:CB	1:A:191:LEU:O	2.66	0.43
1:A:254:ASP:O	1:A:356:ILE:HG13	2.18	0.43
1:A:85:ILE:HB	1:A:202:ILE:HG12	2.01	0.43
1:A:238:ILE:HG12	1:A:239:ARG:H	1.82	0.43
1:A:354:ILE:HG23	1:A:356:ILE:HB	1.99	0.43
1:A:375:SER:HA	1:A:379:LYS:HE3	2.01	0.43
1:A:551:THR:H	1:A:554:PHE:HA	1.83	0.43
1:A:157:GLU:OE1	1:A:227:ASN:ND2	2.52	0.43
1:A:239:ARG:HD3	1:A:239:ARG:HA	1.48	0.43
1:A:19:PHE:CD1	1:A:19:PHE:N	2.86	0.43
1:A:250:LYS:HG2	1:A:255:HIS:CE1	2.54	0.43
1:A:287:ILE:HA	1:A:289:ASN:OD1	2.18	0.43
1:A:459:ASP:HA	1:A:462:ILE:HB	2.00	0.43
1:A:82:LYS:HB3	1:A:82:LYS:HE2	1.79	0.43
1:A:261:MET:O	1:A:261:MET:HG3	2.19	0.43
1:A:102:GLU:HB3	1:A:176:LYS:HG3	2.01	0.43
1:A:194:SER:O	1:A:195:ILE:HG13	2.18	0.43
1:A:219:LEU:HD12	1:A:222:TYR:HB3	2.01	0.43
1:A:438:LEU:HD21	1:A:479:ALA:HB3	2.01	0.43
1:A:86:PHE:CG	1:A:224:PHE:HZ	2.36	0.42
1:A:166:VAL:HB	1:A:207:TYR:HB2	2.01	0.42
1:A:252:LYS:HD3	1:A:252:LYS:HA	1.80	0.42
1:A:278:PHE:O	1:A:280:GLU:N	2.51	0.42
1:A:445:GLU:C	1:A:446:ILE:HG23	2.39	0.42
1:A:368:LEU:HB3	1:A:370:PRO:HD2	2.00	0.42
1:A:29:ILE:HD11	1:A:222:TYR:HD1	1.73	0.42
1:A:209:PRO:HG3	1:A:221:PHE:HE2	1.82	0.42
1:A:89:ALA:O	1:A:93:GLN:HG3	2.18	0.42
1:A:42:LEU:HD23	1:A:45:ILE:HD11	2.01	0.42
1:A:336:ARG:NH2	1:A:382:SER:O	2.51	0.42
1:A:182:TYR:HE2	1:A:508:SER:OG	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.91	0.42
1:A:481:LEU:HD12	1:A:499:VAL:O	2.20	0.42
1:A:84:PRO:HB3	1:A:201:ASN:CB	2.50	0.42
1:A:282:PHE:CD1	1:A:282:PHE:N	2.87	0.42
1:A:409:LEU:HD22	1:A:413:ASP:OD2	2.20	0.42
1:A:476:GLN:HB2	1:A:505:VAL:HG22	2.01	0.42
1:A:14:PHE:CG	1:A:68:PRO:HB2	2.54	0.41
1:A:29:ILE:HD11	1:A:222:TYR:CG	2.55	0.41
1:A:427:ILE:HG12	1:A:430:ARG:HH11	1.84	0.41
1:A:476:GLN:HB2	1:A:505:VAL:CG2	2.49	0.41
1:A:283:PHE:HE2	1:A:352:ASN:HA	1.82	0.41
1:A:291:LEU:HG	1:A:320:GLU:HA	2.01	0.41
1:A:478:PHE:CE2	1:A:552:ILE:HG23	2.56	0.41
1:A:271:ALA:O	1:A:275:HIS:HB2	2.20	0.41
1:A:29:ILE:HG12	1:A:222:TYR:CD1	2.52	0.41
1:A:278:PHE:HD2	1:A:281:ARG:HE	1.68	0.41
1:A:410:PHE:O	1:A:414:VAL:HG22	2.20	0.41
1:A:262:SER:HB2	1:A:386:LYS:HE3	2.03	0.41
1:A:75:PHE:HE1	1:A:85:ILE:HD13	1.86	0.41
1:A:95:ILE:HG13	1:A:99:MET:HE2	2.02	0.41
1:A:380:ASN:ND2	1:A:383:ASP:H	2.19	0.41
1:A:89:ALA:O	1:A:93:GLN:N	2.39	0.41
1:A:447:ASN:OD1	1:A:448:LYS:N	2.54	0.41
1:A:180:ASN:ND2	1:A:197:ASN:OD1	2.54	0.41
1:A:435:GLY:N	1:A:436:PRO:CD	2.84	0.41
1:A:446:ILE:CB	1:A:450:LYS:HD2	2.51	0.41
1:A:14:PHE:O	1:A:68:PRO:HG2	2.21	0.40
1:A:187:SER:O	1:A:191:LEU:HD23	2.21	0.40
1:A:386:LYS:HB3	1:A:386:LYS:HE2	1.97	0.40
1:A:22:ILE:O	1:A:26:LEU:HG	2.21	0.40
1:A:150:ASN:O	1:A:152:THR:N	2.55	0.40
1:A:152:THR:OG1	1:A:153:CYS:N	2.44	0.40
1:A:283:PHE:C	1:A:283:PHE:HD1	2.24	0.40
1:A:320:GLU:OE2	1:A:452:ASN:HB3	2.22	0.40
1:A:363:LEU:C	1:A:363:LEU:HD12	2.41	0.40
1:A:497:ASP:OD1	1:A:499:VAL:HG13	2.21	0.40
1:A:85:ILE:HG22	1:A:202:ILE:HG23	2.03	0.40
1:A:418:SER:O	1:A:421:LEU:HB2	2.21	0.40
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.86	0.40
1:A:30:LYS:C	1:A:30:LYS:HD3	2.41	0.40
1:A:454:LEU:HD13	1:A:454:LEU:HA	1.80	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	497/568 (88%)	381 (77%)	91 (18%)	25 (5%)	<b>2</b> <b>6</b>

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	100	ASN
1	A	152	THR
1	A	287	ILE
1	A	324	SER
1	A	445	GLU
1	A	446	ILE
1	A	457	VAL
1	A	519	PRO
1	A	151	GLU
1	A	447	ASN
1	A	286	PHE
1	A	320	GLU
1	A	349	LYS
1	A	224	PHE
1	A	275	HIS
1	A	277	ILE
1	A	434	PRO
1	A	449	HIS
1	A	345	GLU
1	A	400	PHE
1	A	161	SER
1	A	248	ILE
1	A	249	GLU
1	A	209	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	447/514 (87%)	397 (89%)	50 (11%)	6 18

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	18	TYR
1	A	19	PHE
1	A	30	LYS
1	A	75	PHE
1	A	92	MET
1	A	115	ASP
1	A	133	PHE
1	A	150	ASN
1	A	158	ASN
1	A	167	TRP
1	A	181	PHE
1	A	193	CYS
1	A	200	TYR
1	A	208	HIS
1	A	220	MET
1	A	224	PHE
1	A	226	TYR
1	A	239	ARG
1	A	266	ASP
1	A	273	TYR
1	A	276	LYS
1	A	278	PHE
1	A	279	LYS
1	A	282	PHE
1	A	283	PHE
1	A	288	ASP
1	A	303	PHE
1	A	312	ASN
1	A	323	LEU

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Mol	Chain	Res	Type
1	A	338	ILE
1	A	362	PHE
1	A	364	LEU
1	A	367	THR
1	A	389	HIS
1	A	402	LEU
1	A	403	PHE
1	A	406	PHE
1	A	408	TYR
1	A	413	ASP
1	A	441	ARG
1	A	446	ILE
1	A	465	LEU
1	A	472	ASN
1	A	478	PHE
1	A	496	TYR
1	A	520	TYR
1	A	546	SER
1	A	547	LYS
1	A	552	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

### 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	509/568 (89%)	1.53	140 (27%) 0 0	20, 44, 85, 165	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	8.7
1	A	310	ASP	8.0
1	A	256	TYR	7.8
1	A	477	ALA	7.6
1	A	57	GLY	7.4
1	A	469	GLY	7.4
1	A	251	TYR	7.3
1	A	118	ILE	7.1
1	A	306	SER	7.1
1	A	508	SER	6.7
1	A	346	GLU	6.6
1	A	195	ILE	6.6
1	A	287	ILE	6.2
1	A	483	SER	6.1
1	A	361	THR	6.1
1	A	140	MET	6.0
1	A	286	PHE	5.9
1	A	412	ASP	5.8
1	A	316	ILE	5.6
1	A	484	SER	5.6
1	A	326	LEU	5.5
1	A	479	ALA	5.4
1	A	505	VAL	5.4
1	A	295	ASN	5.4
1	A	119	LEU	5.3
1	A	518	ILE	5.3
1	A	551	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASN	5.2
1	A	519	PRO	5.2
1	A	367	THR	5.1
1	A	443	ILE	5.1
1	A	444	GLY	4.8
1	A	144	SER	4.7
1	A	397	ASN	4.7
1	A	325	ASN	4.7
1	A	92	MET	4.6
1	A	176	LYS	4.6
1	A	415	LYS	4.5
1	A	159	ILE	4.5
1	A	515	TRP	4.5
1	A	347	PHE	4.4
1	A	282	PHE	4.3
1	A	459	ASP	4.3
1	A	416	THR	4.2
1	A	65	ALA	4.2
1	A	500	CYS	4.1
1	A	439	ALA	4.0
1	A	485	LYS	3.8
1	A	105	LYS	3.7
1	A	323	LEU	3.7
1	A	322	PHE	3.6
1	A	82	LYS	3.6
1	A	478	PHE	3.6
1	A	470	LEU	3.5
1	A	474	ILE	3.4
1	A	114	THR	3.4
1	A	120	ARG	3.4
1	A	175	THR	3.3
1	A	31	ILE	3.3
1	A	204	GLY	3.2
1	A	410	PHE	3.2
1	A	516	TYR	3.2
1	A	245	LEU	3.2
1	A	56	SER	3.2
1	A	314	THR	3.1
1	A	406	PHE	3.1
1	A	315	LYS	3.1
1	A	507	THR	3.1
1	A	294	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	260	ALA	3.1
1	A	203	TYR	3.1
1	A	448	LYS	3.0
1	A	152	THR	3.0
1	A	363	LEU	3.0
1	A	16	SER	3.0
1	A	183	LEU	2.9
1	A	352	ASN	2.9
1	A	277	ILE	2.9
1	A	143	TYR	2.9
1	A	141	ASP	2.9
1	A	554	PHE	2.9
1	A	85	ILE	2.8
1	A	263	GLY	2.8
1	A	78	PHE	2.8
1	A	317	ASP	2.8
1	A	231	CYS	2.8
1	A	424	PRO	2.7
1	A	285	ILE	2.7
1	A	387	THR	2.7
1	A	21	LEU	2.7
1	A	311	MET	2.6
1	A	15	GLY	2.6
1	A	90	TYR	2.6
1	A	243	LEU	2.6
1	A	205	VAL	2.6
1	A	398	LEU	2.6
1	A	321	ASN	2.6
1	A	388	HIS	2.6
1	A	278	PHE	2.6
1	A	329	VAL	2.5
1	A	475	SER	2.5
1	A	199	GLU	2.5
1	A	454	LEU	2.5
1	A	539	ARG	2.5
1	A	476	GLN	2.5
1	A	299	ASN	2.5
1	A	170	HIS	2.5
1	A	215	LEU	2.5
1	A	542	TYR	2.4
1	A	550	ALA	2.4
1	A	302	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	366	GLY	2.4
1	A	238	ILE	2.4
1	A	384	THR	2.4
1	A	440	ILE	2.4
1	A	97	VAL	2.4
1	A	341	LYS	2.4
1	A	333	GLU	2.3
1	A	160	LYS	2.3
1	A	512	THR	2.3
1	A	211	VAL	2.2
1	A	45	ILE	2.2
1	A	96	ALA	2.2
1	A	267	SER	2.2
1	A	167	TRP	2.2
1	A	184	VAL	2.2
1	A	369	TYR	2.2
1	A	29	ILE	2.2
1	A	451	LEU	2.2
1	A	23	VAL	2.1
1	A	324	SER	2.1
1	A	465	LEU	2.1
1	A	375	SER	2.1
1	A	37	ASP	2.1
1	A	423	LEU	2.1
1	A	212	TYR	2.0
1	A	49	ASN	2.0
1	A	330	THR	2.0
1	A	19	PHE	2.0
1	A	541	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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.