



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:38 am BST

PDB ID : 1YY3  
Title : Structure of S-Adenosylmethionine:tRNA Ribosyltransferase-Isomerase (QueA)  
Authors : Grimm, C.; Ficner, R.; Reuter, K.  
Deposited on : 2005-02-23  
Resolution : 2.88 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.

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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	:	2.11
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)	:	2.11

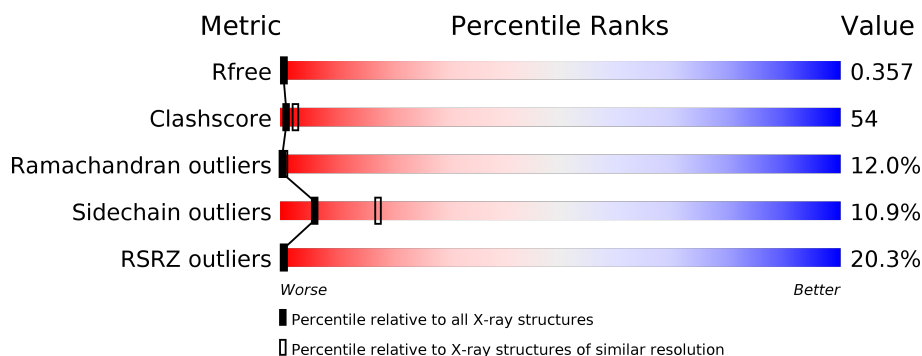
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 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	346	<div> <div>21%</div> <div>29%</div> <div>49%</div> <div>11%</div> <div>•</div> <div>9%</div> </div>
1	B	346	<div> <div>16%</div> <div>28%</div> <div>49%</div> <div>12%</div> <div>•</div> <div>9%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4990 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 S-adenosylmethionine:tRNA ribosyltransferase-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2495	1593	418	474	10			
1	B	315	Total	C	N	O	S	0	0	0
			2495	1593	418	474	10			

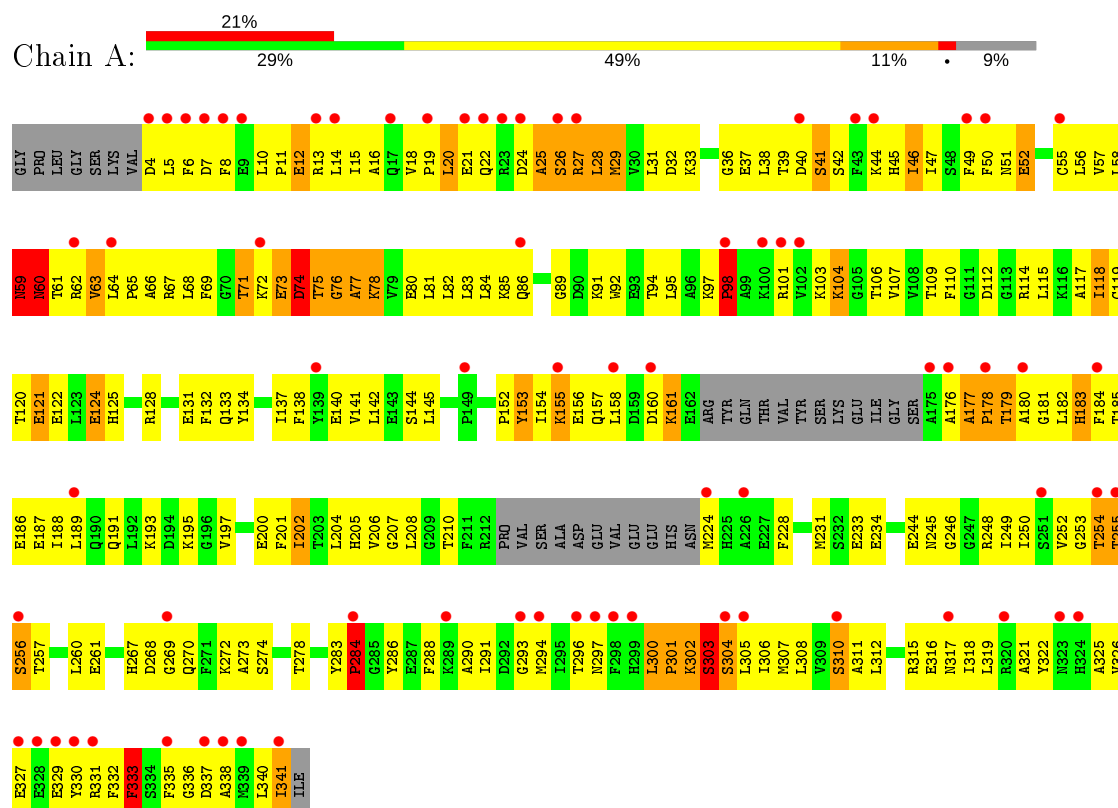
There are 10 discrepancies between the modelled and reference sequences:

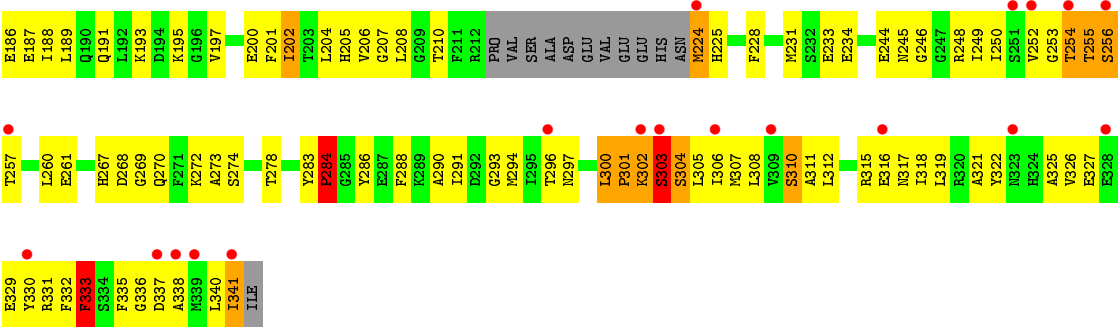
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	CLONING ARTIFACT	UNP O32054
A	-2	PRO	-	CLONING ARTIFACT	UNP O32054
A	-1	LEU	-	CLONING ARTIFACT	UNP O32054
A	0	GLY	-	CLONING ARTIFACT	UNP O32054
A	1	SER	-	CLONING ARTIFACT	UNP O32054
B	-3	GLY	-	CLONING ARTIFACT	UNP O32054
B	-2	PRO	-	CLONING ARTIFACT	UNP O32054
B	-1	LEU	-	CLONING ARTIFACT	UNP O32054
B	0	GLY	-	CLONING ARTIFACT	UNP O32054
B	1	SER	-	CLONING ARTIFACT	UNP O32054

### 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 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: S-adenosylmethionine:tRNA ribosyltransferase-isomerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.67Å 101.67Å 152.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.00 – 2.88 29.37 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.8 (61.00-2.88) 98.5 (29.37-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.364 , 0.386 0.362 , 0.357	Depositor DCC
$R_{free}$ test set	733 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.5	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 76.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% 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

### 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	0.55	0/2543	0.75	0/3425
1	B	0.53	0/2543	0.74	0/3425
All	All	0.54	0/5086	0.75	0/6850

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

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	2495	0	2474	265	0
1	B	2495	0	2474	269	0
All	All	4990	0	4948	534	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 54.

All (534) 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:B:18:VAL:HG22	1:B:19:PRO:HD2	1.25	1.14
1:B:254:THR:HG23	1:B:296:THR:OG1	1.51	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:HG22	1:A:19:PRO:HD2	1.25	1.10
1:A:254:THR:HG23	1:A:296:THR:OG1	1.47	1.09
1:B:97:LYS:HB3	1:B:98:PRO:HD2	1.32	1.08
1:A:97:LYS:HB3	1:A:98:PRO:HD2	1.33	1.08
1:A:185:THR:HB	1:A:188:ILE:HG13	1.54	0.90
1:B:141:VAL:O	1:B:144:SER:HB3	1.71	0.90
1:B:185:THR:HB	1:B:188:ILE:HG13	1.54	0.89
1:A:141:VAL:O	1:A:144:SER:HB3	1.72	0.89
1:B:19:PRO:HB3	1:B:335:PHE:HB3	1.58	0.85
1:B:62:ARG:HD2	1:B:64:LEU:HD13	1.57	0.85
1:B:186:GLU:HA	1:B:189:LEU:HD12	1.57	0.85
1:A:63:VAL:C	1:A:65:PRO:HD2	1.98	0.84
1:A:19:PRO:HB3	1:A:335:PHE:HB3	1.59	0.84
1:A:186:GLU:HA	1:A:189:LEU:HD12	1.58	0.84
1:A:112:ASP:OD2	1:A:114:ARG:HG2	1.77	0.84
1:A:36:GLY:HA3	1:A:317:ASN:HD22	1.42	0.83
1:A:62:ARG:HD2	1:A:64:LEU:HD13	1.57	0.83
1:B:63:VAL:C	1:B:65:PRO:HD2	1.99	0.83
1:A:6:PHE:HB3	1:A:306:ILE:HD13	1.60	0.83
1:B:46:ILE:HG23	1:B:47:ILE:H	1.44	0.83
1:A:46:ILE:HG23	1:A:47:ILE:H	1.44	0.83
1:B:36:GLY:HA3	1:B:317:ASN:HD22	1.42	0.82
1:A:261:GLU:HG3	1:A:286:TYR:OH	1.80	0.81
1:B:254:THR:HG23	1:B:296:THR:HG1	1.45	0.81
1:B:6:PHE:HB3	1:B:306:ILE:HD13	1.61	0.81
1:B:261:GLU:HG3	1:B:286:TYR:OH	1.82	0.80
1:A:31:LEU:HD12	1:A:32:ASP:N	1.97	0.80
1:A:254:THR:HG23	1:A:296:THR:HG1	1.43	0.79
1:B:112:ASP:OD2	1:B:114:ARG:HG2	1.82	0.79
1:B:10:LEU:HD23	1:B:301:PRO:HD3	1.65	0.79
1:A:62:ARG:HD2	1:A:64:LEU:HB2	1.65	0.78
1:B:62:ARG:HD2	1:B:64:LEU:HB2	1.65	0.77
1:B:318:ILE:HD12	1:B:319:LEU:N	2.00	0.76
1:A:10:LEU:HD23	1:A:301:PRO:HD3	1.67	0.76
1:B:18:VAL:CG2	1:B:19:PRO:HD2	2.14	0.75
1:A:318:ILE:HD12	1:A:319:LEU:N	2.00	0.75
1:A:82:LEU:HD21	1:A:208:LEU:HD22	1.68	0.74
1:A:322:TYR:O	1:A:326:VAL:HG23	1.88	0.74
1:B:31:LEU:HD12	1:B:32:ASP:N	2.03	0.74
1:B:82:LEU:HD21	1:B:208:LEU:HD22	1.70	0.74
1:A:18:VAL:CG2	1:A:19:PRO:HD2	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:CA	1:A:317:ASN:HD22	2.00	0.73
1:B:62:ARG:C	1:B:64:LEU:H	1.91	0.73
1:B:36:GLY:CA	1:B:317:ASN:HD22	2.01	0.73
1:A:62:ARG:C	1:A:64:LEU:H	1.91	0.72
1:A:183:HIS:CE1	1:A:338:ALA:HB2	2.25	0.72
1:B:118:ILE:HD12	1:B:118:ILE:H	1.53	0.72
1:A:304:SER:HA	1:A:307:MET:CE	2.19	0.72
1:B:161:LYS:N	1:B:161:LYS:HD2	2.04	0.72
1:B:59:ASN:O	1:B:59:ASN:ND2	2.22	0.72
1:B:306:ILE:HD12	1:B:307:MET:H	1.55	0.72
1:A:161:LYS:N	1:A:161:LYS:HD2	2.04	0.71
1:B:124:GLU:H	1:B:124:GLU:CD	1.91	0.71
1:B:322:TYR:O	1:B:326:VAL:HG23	1.90	0.71
1:A:118:ILE:H	1:A:118:ILE:HD12	1.55	0.71
1:B:183:HIS:CE1	1:B:338:ALA:HB2	2.25	0.71
1:A:257:THR:HG23	1:A:291:ILE:HD13	1.73	0.70
1:A:59:ASN:ND2	1:A:59:ASN:O	2.24	0.70
1:A:124:GLU:H	1:A:124:GLU:CD	1.94	0.69
1:A:137:ILE:HD13	1:A:140:GLU:OE1	1.91	0.69
1:A:97:LYS:CB	1:A:98:PRO:HD2	2.18	0.69
1:B:257:THR:HG23	1:B:291:ILE:HD13	1.74	0.69
1:A:306:ILE:HD12	1:A:307:MET:H	1.55	0.69
1:B:304:SER:HA	1:B:307:MET:CE	2.23	0.69
1:A:254:THR:CG2	1:A:296:THR:OG1	2.35	0.69
1:A:82:LEU:CD2	1:A:208:LEU:HD22	2.23	0.69
1:B:137:ILE:HD13	1:B:140:GLU:OE1	1.92	0.69
1:B:14:LEU:HD12	1:B:326:VAL:HG13	1.75	0.69
1:B:46:ILE:HG23	1:B:47:ILE:N	2.07	0.69
1:A:31:LEU:HD13	1:A:38:LEU:HD23	1.75	0.68
1:B:97:LYS:HB3	1:B:98:PRO:CD	2.17	0.68
1:A:255:THR:CG2	1:A:256:SER:N	2.57	0.68
1:B:50:PHE:HE2	1:B:56:LEU:HD21	1.59	0.68
1:B:40:ASP:O	1:B:41:SER:HB2	1.94	0.67
1:A:46:ILE:HG23	1:A:47:ILE:N	2.08	0.67
1:A:318:ILE:O	1:A:322:TYR:HD1	1.77	0.67
1:B:82:LEU:CD2	1:B:208:LEU:HD22	2.25	0.67
1:A:14:LEU:HD22	1:A:330:TYR:O	1.94	0.67
1:A:115:LEU:HD11	1:A:132:PHE:CD2	2.31	0.66
1:B:306:ILE:HD12	1:B:307:MET:N	2.11	0.66
1:A:40:ASP:O	1:A:41:SER:HB2	1.96	0.66
1:B:64:LEU:O	1:B:66:ALA:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ILE:O	1:B:322:TYR:HD1	1.78	0.66
1:B:97:LYS:O	1:B:98:PRO:C	2.33	0.66
1:B:31:LEU:HD13	1:B:38:LEU:HD23	1.76	0.66
1:A:14:LEU:HD12	1:A:326:VAL:HG13	1.78	0.66
1:B:255:THR:CG2	1:B:256:SER:N	2.59	0.66
1:A:306:ILE:HD12	1:A:307:MET:N	2.11	0.65
1:A:50:PHE:HE2	1:A:56:LEU:HD21	1.60	0.65
1:B:38:LEU:HD22	1:B:321:ALA:HB2	1.77	0.65
1:A:31:LEU:HD13	1:A:38:LEU:CD2	2.27	0.65
1:A:185:THR:HG22	1:A:187:GLU:H	1.62	0.65
1:A:80:GLU:HB3	1:A:97:LYS:HB2	1.78	0.64
1:B:185:THR:HG22	1:B:187:GLU:H	1.62	0.64
1:B:18:VAL:HG22	1:B:19:PRO:CD	2.17	0.64
1:B:31:LEU:HD13	1:B:38:LEU:CD2	2.27	0.64
1:A:64:LEU:O	1:A:66:ALA:N	2.31	0.64
1:B:14:LEU:HD22	1:B:330:TYR:O	1.97	0.64
1:A:25:ALA:O	1:A:26:SER:C	2.35	0.64
1:A:304:SER:HA	1:A:307:MET:HE3	1.80	0.63
1:B:115:LEU:HD11	1:B:132:PHE:CD2	2.33	0.63
1:B:25:ALA:O	1:B:26:SER:C	2.37	0.63
1:B:5:LEU:HB3	1:B:315:ARG:HH11	1.64	0.63
1:B:8:PHE:H	1:B:301:PRO:HB3	1.65	0.62
1:A:6:PHE:CB	1:A:306:ILE:HD13	2.28	0.62
1:B:6:PHE:CE1	1:B:315:ARG:HG3	2.35	0.62
1:A:6:PHE:CE1	1:A:315:ARG:HG3	2.34	0.62
1:A:5:LEU:HB3	1:A:315:ARG:HH11	1.64	0.62
1:A:206:VAL:HG23	1:A:207:GLY:H	1.64	0.62
1:A:234:GLU:OE1	1:A:234:GLU:N	2.28	0.62
1:B:80:GLU:HB3	1:B:97:LYS:HB2	1.80	0.62
1:A:104:LYS:O	1:A:119:CYS:O	2.18	0.62
1:A:38:LEU:HD22	1:A:321:ALA:HB2	1.82	0.62
1:B:104:LYS:O	1:B:119:CYS:O	2.18	0.62
1:B:6:PHE:CB	1:B:306:ILE:HD13	2.28	0.62
1:B:254:THR:CG2	1:B:296:THR:OG1	2.38	0.62
1:A:97:LYS:HB3	1:A:98:PRO:CD	2.18	0.61
1:B:76:GLY:O	1:B:77:ALA:HB2	1.99	0.61
1:A:18:VAL:HG22	1:A:19:PRO:CD	2.17	0.61
1:A:76:GLY:O	1:A:77:ALA:HB2	2.01	0.61
1:A:14:LEU:HD21	1:A:329:GLU:HA	1.82	0.61
1:B:94:THR:HB	1:B:128:ARG:O	2.01	0.61
1:B:294:MET:HG2	1:B:312:LEU:CD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:O	1:A:41:SER:CB	2.49	0.61
1:A:19:PRO:CB	1:A:335:PHE:HB3	2.31	0.60
1:A:50:PHE:CE2	1:A:56:LEU:HD21	2.37	0.60
1:B:50:PHE:CE2	1:B:56:LEU:HD21	2.35	0.60
1:A:97:LYS:O	1:A:98:PRO:C	2.37	0.60
1:B:267:HIS:CD2	1:B:272:LYS:HG3	2.37	0.60
1:B:179:THR:C	1:B:181:GLY:H	2.03	0.60
1:A:55:CYS:SG	1:A:200:GLU:HG2	2.41	0.60
1:B:14:LEU:HD21	1:B:329:GLU:HA	1.84	0.60
1:A:179:THR:C	1:A:181:GLY:H	2.04	0.60
1:A:182:LEU:C	1:A:184:PHE:H	2.04	0.60
1:B:55:CYS:SG	1:B:200:GLU:HG2	2.41	0.60
1:B:306:ILE:HD12	1:B:307:MET:HG3	1.84	0.59
1:B:72:LYS:HE3	1:B:74:ASP:HB2	1.84	0.59
1:A:12:GLU:HA	1:A:15:ILE:HD12	1.85	0.59
1:B:114:ARG:HG3	1:B:114:ARG:O	2.02	0.59
1:B:36:GLY:HA3	1:B:317:ASN:ND2	2.16	0.59
1:A:114:ARG:HG3	1:A:114:ARG:O	2.03	0.59
1:B:302:LYS:C	1:B:303:SER:O	2.39	0.59
1:A:14:LEU:HD21	1:A:329:GLU:CA	2.33	0.59
1:A:59:ASN:HB2	1:A:256:SER:HB3	1.82	0.59
1:A:115:LEU:HA	1:A:133:GLN:O	2.02	0.59
1:A:58:LEU:HD12	1:A:252:VAL:HB	1.85	0.59
1:A:302:LYS:C	1:A:303:SER:O	2.39	0.59
1:B:303:SER:O	1:B:306:ILE:HD11	2.02	0.59
1:B:16:ALA:HB2	1:B:331:ARG:HB3	1.85	0.58
1:A:91:LYS:HE2	1:A:120:THR:HG21	1.85	0.58
1:A:302:LYS:O	1:A:303:SER:O	2.22	0.58
1:A:47:ILE:CD1	1:A:191:GLN:HB3	2.32	0.58
1:A:283:TYR:CG	1:A:284:PRO:HD2	2.38	0.58
1:A:294:MET:HG2	1:A:312:LEU:CD2	2.33	0.58
1:B:91:LYS:HE2	1:B:120:THR:HG21	1.85	0.58
1:B:182:LEU:C	1:B:184:PHE:H	2.05	0.58
1:B:284:PRO:HD3	1:B:307:MET:O	2.04	0.58
1:A:301:PRO:O	1:A:302:LYS:CB	2.52	0.58
1:B:304:SER:HA	1:B:307:MET:HE2	1.84	0.58
1:A:8:PHE:H	1:A:301:PRO:HB3	1.68	0.57
1:B:103:LYS:O	1:B:104:LYS:C	2.43	0.57
1:B:14:LEU:HD21	1:B:329:GLU:CA	2.34	0.57
1:A:114:ARG:O	1:A:115:LEU:HB3	2.05	0.57
1:A:94:THR:HB	1:A:128:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:HB2	1:A:331:ARG:HB3	1.86	0.57
1:B:115:LEU:HA	1:B:133:GLN:O	2.03	0.57
1:A:286:TYR:HE1	1:A:288:PHE:HA	1.68	0.57
1:B:117:ALA:HB2	1:B:132:PHE:CD2	2.40	0.57
1:B:40:ASP:O	1:B:41:SER:CB	2.51	0.57
1:A:267:HIS:CD2	1:A:272:LYS:HG3	2.39	0.57
1:B:114:ARG:O	1:B:115:LEU:HB3	2.03	0.57
1:B:5:LEU:HD22	1:B:315:ARG:HH12	1.68	0.57
1:A:117:ALA:HB2	1:A:132:PHE:CD2	2.40	0.57
1:A:185:THR:HB	1:A:188:ILE:CG1	2.32	0.57
1:B:14:LEU:CD1	1:B:326:VAL:HG13	2.35	0.57
1:B:283:TYR:CG	1:B:284:PRO:HD2	2.40	0.57
1:A:255:THR:HG23	1:A:256:SER:N	2.19	0.57
1:B:206:VAL:HG23	1:B:207:GLY:H	1.70	0.57
1:B:59:ASN:HB2	1:B:256:SER:HB3	1.86	0.57
1:B:4:ASP:OD2	1:B:302:LYS:HG2	2.04	0.57
1:A:29:MET:CE	1:A:321:ALA:HB1	2.35	0.57
1:B:301:PRO:O	1:B:302:LYS:CB	2.52	0.57
1:A:284:PRO:HD3	1:A:307:MET:O	2.05	0.56
1:B:58:LEU:HD12	1:B:252:VAL:HB	1.87	0.56
1:B:255:THR:HG23	1:B:256:SER:N	2.20	0.56
1:B:19:PRO:CB	1:B:335:PHE:HB3	2.32	0.56
1:B:137:ILE:N	1:B:137:ILE:HD12	2.20	0.56
1:B:302:LYS:O	1:B:303:SER:O	2.23	0.56
1:B:51:ASN:O	1:B:197:VAL:HG22	2.05	0.56
1:A:82:LEU:HD21	1:A:208:LEU:CD2	2.33	0.56
1:B:234:GLU:OE1	1:B:234:GLU:N	2.28	0.56
1:B:306:ILE:CD1	1:B:307:MET:HG3	2.36	0.56
1:A:233:GLU:HB3	1:A:234:GLU:OE1	2.05	0.56
1:B:286:TYR:HE1	1:B:288:PHE:HA	1.71	0.56
1:B:204:LEU:HD12	1:B:228:PHE:O	2.06	0.56
1:B:233:GLU:HB3	1:B:234:GLU:OE1	2.06	0.56
1:A:304:SER:HA	1:A:307:MET:HE2	1.88	0.56
1:A:36:GLY:HA3	1:A:317:ASN:ND2	2.16	0.56
1:A:28:LEU:HD12	1:A:28:LEU:C	2.25	0.55
1:A:301:PRO:O	1:A:302:LYS:HB2	2.07	0.55
1:A:4:ASP:OD2	1:A:302:LYS:HG2	2.05	0.55
1:A:137:ILE:N	1:A:137:ILE:HD12	2.21	0.55
1:B:301:PRO:O	1:B:302:LYS:HB2	2.06	0.55
1:A:154:ILE:O	1:A:157:GLN:N	2.40	0.55
1:B:179:THR:C	1:B:181:GLY:N	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:CD1	1:B:191:GLN:HB3	2.36	0.55
1:B:62:ARG:C	1:B:64:LEU:N	2.60	0.55
1:A:5:LEU:HD22	1:A:315:ARG:HH12	1.71	0.55
1:B:82:LEU:HD21	1:B:208:LEU:CD2	2.35	0.55
1:A:14:LEU:CD1	1:A:326:VAL:HG13	2.36	0.55
1:B:176:ALA:O	1:B:178:PRO:HD3	2.06	0.55
1:A:306:ILE:HD12	1:A:307:MET:HG3	1.89	0.55
1:A:176:ALA:O	1:A:178:PRO:HD3	2.07	0.55
1:B:28:LEU:HD12	1:B:28:LEU:C	2.27	0.55
1:B:97:LYS:CB	1:B:98:PRO:HD2	2.17	0.55
1:A:62:ARG:CD	1:A:64:LEU:HD13	2.33	0.55
1:B:12:GLU:HA	1:B:15:ILE:HD12	1.87	0.55
1:A:51:ASN:O	1:A:197:VAL:HG22	2.07	0.54
1:A:62:ARG:HD2	1:A:64:LEU:CD1	2.32	0.54
1:A:152:PRO:HA	1:A:155:LYS:HB3	1.89	0.54
1:A:62:ARG:C	1:A:64:LEU:N	2.60	0.54
1:A:41:SER:OG	1:A:42:SER:N	2.32	0.54
1:A:57:VAL:HG21	1:A:260:LEU:HD11	1.88	0.54
1:A:72:LYS:HE3	1:A:74:ASP:HB2	1.89	0.54
1:B:154:ILE:O	1:B:157:GLN:N	2.41	0.54
1:B:152:PRO:O	1:B:156:GLU:HG3	2.07	0.54
1:A:24:ASP:O	1:A:25:ALA:C	2.46	0.54
1:A:305:LEU:HD22	1:A:305:LEU:N	2.21	0.54
1:B:36:GLY:O	1:B:38:LEU:HG	2.08	0.54
1:B:118:ILE:N	1:B:118:ILE:HD12	2.23	0.54
1:B:24:ASP:HB2	1:B:44:LYS:HG2	1.90	0.54
1:A:152:PRO:O	1:A:156:GLU:HG3	2.08	0.53
1:B:118:ILE:HD12	1:B:131:GLU:O	2.08	0.53
1:B:152:PRO:HA	1:B:155:LYS:HB3	1.90	0.53
1:B:46:ILE:CG2	1:B:47:ILE:H	2.17	0.53
1:A:103:LYS:O	1:A:104:LYS:C	2.46	0.53
1:A:301:PRO:O	1:A:302:LYS:HG3	2.09	0.53
1:A:250:ILE:N	1:A:250:ILE:HD12	2.22	0.53
1:B:4:ASP:CB	1:B:302:LYS:HD3	2.38	0.53
1:A:78:LYS:HB3	1:A:101:ARG:NH1	2.24	0.53
1:A:204:LEU:HD12	1:A:228:PHE:O	2.07	0.53
1:A:63:VAL:O	1:A:65:PRO:HD2	2.08	0.53
1:B:296:THR:HG23	1:B:297:ASN:N	2.24	0.53
1:A:52:GLU:OE1	1:A:195:LYS:HG2	2.08	0.53
1:B:304:SER:HA	1:B:307:MET:HE3	1.91	0.53
1:A:179:THR:C	1:A:181:GLY:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLY:C	1:A:255:THR:N	2.59	0.53
1:B:24:ASP:O	1:B:25:ALA:C	2.48	0.53
1:A:19:PRO:HD3	1:A:335:PHE:CD2	2.43	0.52
1:A:46:ILE:CG2	1:A:47:ILE:H	2.18	0.52
1:A:36:GLY:O	1:A:38:LEU:HG	2.10	0.52
1:B:62:ARG:HD2	1:B:64:LEU:CD1	2.33	0.52
1:A:255:THR:HG22	1:A:256:SER:H	1.75	0.52
1:B:284:PRO:HA	1:B:311:ALA:HA	1.91	0.52
1:A:24:ASP:HB2	1:A:44:LYS:HG2	1.89	0.52
1:B:249:ILE:C	1:B:250:ILE:HD12	2.30	0.52
1:B:4:ASP:HB3	1:B:302:LYS:HD3	1.90	0.52
1:B:137:ILE:O	1:B:140:GLU:HB2	2.10	0.52
1:B:160:ASP:C	1:B:161:LYS:HD2	2.30	0.52
1:B:134:TYR:CZ	1:B:138:PHE:HB2	2.45	0.52
1:B:62:ARG:CD	1:B:64:LEU:HD13	2.33	0.52
1:B:305:LEU:N	1:B:305:LEU:HD22	2.24	0.52
1:A:78:LYS:HB3	1:A:101:ARG:HH12	1.74	0.52
1:B:57:VAL:HG21	1:B:260:LEU:HD11	1.92	0.52
1:A:250:ILE:HA	1:A:293:GLY:O	2.09	0.52
1:A:160:ASP:C	1:A:161:LYS:HD2	2.31	0.51
1:B:52:GLU:OE1	1:B:195:LYS:HG2	2.09	0.51
1:A:72:LYS:HD2	1:A:73:GLU:N	2.25	0.51
1:B:63:VAL:O	1:B:65:PRO:HD2	2.09	0.51
1:A:29:MET:HE3	1:A:321:ALA:HB1	1.92	0.51
1:A:69:PHE:CE2	1:A:158:LEU:HD11	2.45	0.51
1:B:41:SER:OG	1:B:42:SER:N	2.39	0.51
1:A:296:THR:HG23	1:A:297:ASN:N	2.25	0.51
1:A:4:ASP:CB	1:A:302:LYS:HD3	2.40	0.51
1:B:301:PRO:O	1:B:302:LYS:HG3	2.09	0.51
1:B:327:GLU:C	1:B:329:GLU:H	2.14	0.51
1:A:249:ILE:C	1:A:250:ILE:HD12	2.30	0.51
1:A:315:ARG:O	1:A:318:ILE:HG13	2.10	0.51
1:A:4:ASP:HB3	1:A:302:LYS:HD3	1.92	0.51
1:A:284:PRO:HA	1:A:311:ALA:HA	1.92	0.51
1:A:59:ASN:OD1	1:A:255:THR:HG22	2.10	0.51
1:A:118:ILE:HD12	1:A:131:GLU:O	2.10	0.51
1:A:19:PRO:HB3	1:A:335:PHE:CB	2.36	0.51
1:B:59:ASN:HD22	1:B:59:ASN:C	2.14	0.51
1:A:327:GLU:C	1:A:329:GLU:H	2.14	0.51
1:A:120:THR:O	1:A:121:GLU:CB	2.59	0.50
1:A:306:ILE:CD1	1:A:307:MET:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HA	1:B:338:ALA:O	2.11	0.50
1:B:59:ASN:OD1	1:B:255:THR:HG22	2.10	0.50
1:B:61:THR:OG1	1:B:177:ALA:HB2	2.11	0.50
1:A:28:LEU:HA	1:A:338:ALA:O	2.12	0.50
1:B:315:ARG:O	1:B:318:ILE:HG13	2.11	0.50
1:B:120:THR:O	1:B:121:GLU:CB	2.59	0.50
1:B:185:THR:HB	1:B:188:ILE:CG1	2.33	0.50
1:B:253:GLY:C	1:B:255:THR:N	2.61	0.50
1:A:303:SER:O	1:A:306:ILE:HD11	2.12	0.50
1:A:118:ILE:N	1:A:118:ILE:HD12	2.26	0.50
1:A:137:ILE:O	1:A:140:GLU:HB2	2.12	0.50
1:B:250:ILE:HD12	1:B:250:ILE:N	2.27	0.50
1:A:59:ASN:C	1:A:59:ASN:HD22	2.15	0.49
1:B:62:ARG:NH1	1:B:64:LEU:HD22	2.27	0.49
1:A:189:LEU:O	1:A:193:LYS:HG3	2.11	0.49
1:A:134:TYR:CZ	1:A:138:PHE:HB2	2.47	0.49
1:A:316:GLU:OE1	1:A:316:GLU:HA	2.13	0.49
1:B:78:LYS:HB3	1:B:101:ARG:HH12	1.77	0.49
1:B:189:LEU:O	1:B:193:LYS:HG3	2.12	0.49
1:B:72:LYS:HD2	1:B:73:GLU:N	2.28	0.49
1:B:78:LYS:HB3	1:B:101:ARG:NH1	2.27	0.49
1:B:29:MET:CE	1:B:321:ALA:HB1	2.42	0.49
1:B:179:THR:O	1:B:181:GLY:N	2.46	0.49
1:A:286:TYR:CE1	1:A:288:PHE:HA	2.47	0.49
1:B:255:THR:HG22	1:B:256:SER:H	1.77	0.49
1:B:268:ASP:O	1:B:270:GLN:N	2.46	0.49
1:B:250:ILE:HA	1:B:293:GLY:O	2.13	0.49
1:B:273:ALA:O	1:B:274:SER:HB3	2.12	0.49
1:A:72:LYS:C	1:A:72:LYS:HD2	2.34	0.48
1:A:244:GLU:C	1:A:246:GLY:H	2.17	0.48
1:B:56:LEU:CD2	1:B:250:ILE:HB	2.43	0.48
1:B:5:LEU:HD22	1:B:315:ARG:NH1	2.28	0.48
1:A:179:THR:O	1:A:181:GLY:N	2.46	0.48
1:A:56:LEU:CD2	1:A:250:ILE:HB	2.43	0.48
1:A:67:ARG:HD2	1:A:80:GLU:OE1	2.13	0.48
1:A:5:LEU:HB3	1:A:315:ARG:NH1	2.29	0.48
1:B:38:LEU:CD2	1:B:321:ALA:HB2	2.43	0.48
1:A:268:ASP:O	1:A:270:GLN:N	2.46	0.48
1:A:46:ILE:O	1:A:49:PHE:HD1	1.97	0.48
1:A:94:THR:CG2	1:A:95:LEU:N	2.76	0.48
1:B:142:LEU:O	1:B:145:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:O	1:B:27:ARG:O	2.32	0.48
1:A:61:THR:OG1	1:A:177:ALA:HB2	2.13	0.48
1:A:261:GLU:OE1	1:A:290:ALA:HB3	2.13	0.48
1:A:261:GLU:HG3	1:A:286:TYR:CZ	2.49	0.48
1:B:67:ARG:HD2	1:B:80:GLU:OE1	2.14	0.48
1:A:273:ALA:O	1:A:274:SER:HB3	2.14	0.47
1:A:62:ARG:NH1	1:A:64:LEU:HD22	2.29	0.47
1:A:86:GLN:HB2	1:A:92:TRP:CZ2	2.50	0.47
1:B:62:ARG:O	1:B:64:LEU:N	2.47	0.47
1:A:62:ARG:O	1:A:64:LEU:N	2.47	0.47
1:A:284:PRO:N	1:A:311:ALA:HB2	2.29	0.47
1:A:142:LEU:O	1:A:145:LEU:N	2.47	0.47
1:A:182:LEU:C	1:A:184:PHE:N	2.67	0.47
1:B:14:LEU:HD13	1:B:326:VAL:HA	1.96	0.47
1:B:316:GLU:OE1	1:B:316:GLU:HA	2.15	0.47
1:A:67:ARG:HE	1:A:69:PHE:HZ	1.63	0.47
1:B:137:ILE:HB	1:B:140:GLU:OE1	2.14	0.47
1:B:19:PRO:HB3	1:B:335:PHE:CB	2.37	0.47
1:B:244:GLU:C	1:B:246:GLY:H	2.17	0.47
1:B:86:GLN:HB2	1:B:92:TRP:CZ2	2.49	0.47
1:A:47:ILE:HD12	1:A:191:GLN:HB3	1.96	0.47
1:A:59:ASN:O	1:A:60:ASN:C	2.52	0.47
1:B:106:THR:HG22	1:B:107:VAL:N	2.29	0.47
1:B:62:ARG:CD	1:B:64:LEU:HB2	2.42	0.47
1:A:47:ILE:HD13	1:A:191:GLN:HB3	1.96	0.47
1:A:84:LEU:HD11	1:A:95:LEU:HG	1.97	0.47
1:B:72:LYS:HD2	1:B:72:LYS:C	2.35	0.47
1:A:206:VAL:HG23	1:A:207:GLY:N	2.29	0.47
1:B:59:ASN:O	1:B:60:ASN:C	2.53	0.47
1:A:71:THR:HB	1:A:77:ALA:HB1	1.97	0.47
1:A:283:TYR:O	1:A:284:PRO:C	2.53	0.46
1:B:69:PHE:CE2	1:B:158:LEU:HD11	2.50	0.46
1:A:120:THR:O	1:A:121:GLU:HB2	2.16	0.46
1:A:62:ARG:CD	1:A:64:LEU:HB2	2.42	0.46
1:B:86:GLN:HB2	1:B:92:TRP:CE2	2.51	0.46
1:A:137:ILE:HB	1:A:140:GLU:HG3	1.97	0.46
1:A:13:ARG:HG3	1:A:14:LEU:N	2.31	0.46
1:A:330:TYR:HD2	1:A:337:ASP:OD2	1.98	0.46
1:A:83:LEU:N	1:A:83:LEU:CD1	2.78	0.46
1:B:182:LEU:C	1:B:184:PHE:N	2.68	0.46
1:A:5:LEU:HD22	1:A:315:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:HA2	1:B:148:MET:HE2	1.98	0.46
1:B:19:PRO:HD3	1:B:335:PHE:CD2	2.50	0.46
1:B:45:HIS:CD2	1:B:45:HIS:N	2.84	0.46
1:B:120:THR:O	1:B:121:GLU:HB2	2.16	0.46
1:B:60:ASN:HB3	1:B:201:PHE:HD2	1.81	0.46
1:B:137:ILE:HB	1:B:140:GLU:HG3	1.97	0.45
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.76	0.45
1:B:255:THR:CG2	1:B:256:SER:H	2.28	0.45
1:A:32:ASP:OD2	1:A:37:GLU:HB3	2.16	0.45
1:B:284:PRO:N	1:B:311:ALA:HB2	2.31	0.45
1:A:157:GLN:HG3	1:A:157:GLN:O	2.17	0.45
1:B:306:ILE:H	1:B:306:ILE:HG13	1.62	0.45
1:B:94:THR:CG2	1:B:95:LEU:N	2.79	0.45
1:A:106:THR:HG22	1:A:107:VAL:N	2.31	0.45
1:B:84:LEU:HD11	1:B:95:LEU:HG	1.98	0.45
1:B:47:ILE:HD12	1:B:191:GLN:HB3	1.98	0.45
1:B:32:ASP:O	1:B:33:LYS:C	2.55	0.45
1:A:152:PRO:HG2	1:A:153:TYR:H	1.82	0.45
1:B:7:ASP:HB2	1:B:302:LYS:HG3	1.98	0.45
1:B:46:ILE:O	1:B:49:PHE:HD1	2.00	0.45
1:A:31:LEU:HD12	1:A:31:LEU:C	2.36	0.45
1:B:224:MET:HB3	1:B:225:HIS:H	1.55	0.45
1:B:62:ARG:HD2	1:B:64:LEU:CB	2.42	0.45
1:A:186:GLU:O	1:A:186:GLU:OE1	2.35	0.45
1:A:38:LEU:CD2	1:A:321:ALA:HB2	2.46	0.45
1:B:5:LEU:HB3	1:B:315:ARG:NH1	2.29	0.45
1:B:157:GLN:O	1:B:157:GLN:HG3	2.16	0.45
1:B:261:GLU:HG3	1:B:286:TYR:CZ	2.52	0.44
1:B:81:LEU:HD22	1:B:94:THR:HG21	1.99	0.44
1:A:86:GLN:HB2	1:A:92:TRP:CE2	2.52	0.44
1:A:81:LEU:HD22	1:A:94:THR:HG21	1.98	0.44
1:B:13:ARG:C	1:B:15:ILE:H	2.20	0.44
1:B:186:GLU:OE1	1:B:186:GLU:O	2.35	0.44
1:A:137:ILE:HB	1:A:140:GLU:OE1	2.16	0.44
1:A:65:PRO:HD3	1:A:205:HIS:CE1	2.53	0.44
1:A:45:HIS:CD2	1:A:45:HIS:N	2.85	0.44
1:B:13:ARG:HG3	1:B:14:LEU:N	2.32	0.44
1:B:11:PRO:O	1:B:13:ARG:N	2.51	0.44
1:B:283:TYR:O	1:B:284:PRO:C	2.56	0.44
1:B:80:GLU:OE2	1:B:97:LYS:HG3	2.18	0.44
1:A:80:GLU:OE2	1:A:97:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PRO:HD3	1:B:205:HIS:CE1	2.52	0.44
1:B:286:TYR:CE1	1:B:288:PHE:HA	2.50	0.44
1:A:8:PHE:CE1	1:A:301:PRO:HG3	2.53	0.44
1:B:68:LEU:HB3	1:B:110:PHE:CE2	2.51	0.43
1:B:8:PHE:CE1	1:B:301:PRO:HG3	2.52	0.43
1:B:71:THR:HB	1:B:77:ALA:HB1	2.00	0.43
1:A:117:ALA:HA	1:A:131:GLU:O	2.18	0.43
1:A:6:PHE:CZ	1:A:284:PRO:HG2	2.52	0.43
1:A:29:MET:HE1	1:A:321:ALA:HB1	2.01	0.43
1:B:137:ILE:HB	1:B:140:GLU:CG	2.48	0.43
1:B:14:LEU:HD21	1:B:329:GLU:CB	2.49	0.43
1:A:177:ALA:O	1:A:178:PRO:O	2.36	0.43
1:A:284:PRO:HG3	1:A:310:SER:HB3	1.99	0.43
1:A:300:LEU:HD13	1:A:333:PHE:CE1	2.53	0.43
1:B:50:PHE:O	1:B:195:LYS:HE2	2.18	0.43
1:B:294:MET:HG2	1:B:312:LEU:HD21	1.99	0.43
1:B:14:LEU:HD21	1:B:329:GLU:HB3	1.99	0.43
1:A:109:THR:HG22	1:A:110:PHE:N	2.33	0.43
1:A:67:ARG:HB3	1:A:82:LEU:HD12	2.00	0.43
1:B:183:HIS:CD2	1:B:183:HIS:H	2.37	0.43
1:B:67:ARG:HE	1:B:69:PHE:HZ	1.63	0.43
1:A:14:LEU:HD13	1:A:326:VAL:HA	2.00	0.43
1:A:325:ALA:HB3	1:A:332:PHE:HZ	1.84	0.43
1:A:340:LEU:HD23	1:A:341:ILE:N	2.34	0.43
1:B:13:ARG:C	1:B:15:ILE:N	2.71	0.43
1:B:176:ALA:O	1:B:178:PRO:CD	2.67	0.43
1:B:248:ARG:HB2	1:B:248:ARG:HE	1.59	0.43
1:B:284:PRO:HG3	1:B:310:SER:HB3	2.00	0.43
1:A:32:ASP:O	1:A:33:LYS:C	2.56	0.43
1:A:202:ILE:HD12	1:A:202:ILE:HA	1.77	0.43
1:A:310:SER:OG	1:A:318:ILE:HG12	2.18	0.43
1:A:82:LEU:HA	1:A:82:LEU:HD12	1.83	0.43
1:B:202:ILE:HD12	1:B:202:ILE:HA	1.73	0.43
1:B:310:SER:OG	1:B:318:ILE:HG12	2.19	0.43
1:A:14:LEU:HD21	1:A:329:GLU:CB	2.49	0.43
1:A:50:PHE:O	1:A:195:LYS:HE2	2.19	0.43
1:A:176:ALA:O	1:A:178:PRO:CD	2.67	0.42
1:A:71:THR:CB	1:A:77:ALA:HB1	2.49	0.42
1:B:330:TYR:HD2	1:B:337:ASP:OD2	2.03	0.42
1:A:183:HIS:CD2	1:A:183:HIS:N	2.86	0.42
1:A:183:HIS:CD2	1:A:183:HIS:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:O	1:A:257:THR:N	2.52	0.42
1:A:6:PHE:CE2	1:A:307:MET:HG2	2.54	0.42
1:A:14:LEU:HD21	1:A:329:GLU:HB3	2.01	0.42
1:A:325:ALA:O	1:A:330:TYR:HB2	2.19	0.42
1:B:109:THR:HG22	1:B:110:PHE:N	2.34	0.42
1:B:67:ARG:HB3	1:B:82:LEU:HD12	2.00	0.42
1:A:7:ASP:HB2	1:A:302:LYS:HG3	2.01	0.42
1:A:137:ILE:HB	1:A:140:GLU:CG	2.49	0.42
1:A:300:LEU:O	1:A:302:LYS:N	2.50	0.42
1:A:301:PRO:O	1:A:302:LYS:CG	2.67	0.42
1:B:142:LEU:O	1:B:143:GLU:C	2.58	0.42
1:B:152:PRO:HG2	1:B:153:TYR:H	1.84	0.42
1:B:47:ILE:HD13	1:B:191:GLN:HB3	2.00	0.42
1:B:6:PHE:CZ	1:B:284:PRO:HG2	2.55	0.42
1:A:68:LEU:HB3	1:A:110:PHE:CE2	2.54	0.42
1:A:13:ARG:C	1:A:15:ILE:N	2.73	0.42
1:A:85:LYS:HB3	1:A:85:LYS:HE2	1.91	0.42
1:B:105:GLY:HA2	1:B:119:CYS:O	2.19	0.42
1:B:31:LEU:HD12	1:B:31:LEU:C	2.38	0.42
1:B:31:LEU:HD13	1:B:38:LEU:HD21	2.01	0.42
1:A:202:ILE:HD11	1:A:231:MET:CE	2.50	0.42
1:A:27:ARG:CB	1:A:330:TYR:CE2	3.03	0.42
1:A:308:LEU:HD23	1:A:308:LEU:C	2.40	0.42
1:B:183:HIS:CD2	1:B:183:HIS:N	2.86	0.42
1:A:182:LEU:O	1:A:184:PHE:N	2.52	0.42
1:A:253:GLY:C	1:A:255:THR:H	2.23	0.42
1:B:117:ALA:HA	1:B:131:GLU:O	2.19	0.42
1:B:254:THR:HA	1:B:296:THR:OG1	2.20	0.42
1:B:300:LEU:N	1:B:300:LEU:HD13	2.34	0.42
1:A:20:LEU:C	1:A:22:GLN:H	2.23	0.41
1:A:60:ASN:HB3	1:A:201:PHE:HD2	1.84	0.41
1:B:177:ALA:O	1:B:178:PRO:O	2.38	0.41
1:B:206:VAL:HG23	1:B:207:GLY:N	2.33	0.41
1:A:233:GLU:HA	1:A:273:ALA:HB2	2.02	0.41
1:B:253:GLY:C	1:B:255:THR:H	2.23	0.41
1:A:325:ALA:HB3	1:A:332:PHE:CZ	2.55	0.41
1:A:62:ARG:HD2	1:A:64:LEU:CB	2.42	0.41
1:B:43:PHE:CE2	1:B:183:HIS:O	2.73	0.41
1:B:340:LEU:HD23	1:B:341:ILE:N	2.34	0.41
1:B:85:LYS:HB3	1:B:85:LYS:HE2	1.89	0.41
1:A:255:THR:CG2	1:A:256:SER:H	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HB2	1:A:330:TYR:CE2	2.55	0.41
1:B:182:LEU:O	1:B:184:PHE:N	2.54	0.41
1:B:325:ALA:HB3	1:B:332:PHE:HZ	1.84	0.41
1:B:83:LEU:CD1	1:B:83:LEU:N	2.83	0.41
1:A:11:PRO:O	1:A:13:ARG:N	2.53	0.41
1:A:248:ARG:HE	1:A:248:ARG:HB2	1.62	0.41
1:B:11:PRO:C	1:B:13:ARG:N	2.74	0.41
1:B:202:ILE:HD11	1:B:231:MET:HE3	2.03	0.41
1:B:20:LEU:C	1:B:22:GLN:H	2.24	0.41
1:B:308:LEU:HD23	1:B:308:LEU:C	2.40	0.41
1:B:318:ILE:CD1	1:B:319:LEU:N	2.78	0.41
1:B:29:MET:HE3	1:B:321:ALA:HB1	2.03	0.41
1:A:318:ILE:CD1	1:A:319:LEU:N	2.78	0.41
1:B:325:ALA:HB3	1:B:332:PHE:CZ	2.56	0.41
1:B:58:LEU:C	1:B:60:ASN:H	2.24	0.41
1:A:300:LEU:HD13	1:A:300:LEU:N	2.36	0.41
1:A:300:LEU:HD13	1:A:333:PHE:CD1	2.56	0.41
1:B:6:PHE:CE2	1:B:307:MET:HG2	2.55	0.41
1:A:13:ARG:C	1:A:15:ILE:H	2.23	0.41
1:A:33:LYS:HB2	1:A:341:ILE:HG22	2.02	0.41
1:B:257:THR:O	1:B:261:GLU:HB2	2.20	0.41
1:B:261:GLU:OE1	1:B:290:ALA:HB3	2.20	0.41
1:B:29:MET:HE1	1:B:321:ALA:HB1	2.02	0.41
1:A:306:ILE:H	1:A:306:ILE:HG13	1.66	0.41
1:B:152:PRO:O	1:B:153:TYR:C	2.59	0.41
1:A:45:HIS:O	1:A:46:ILE:C	2.60	0.41
1:B:261:GLU:HG3	1:B:286:TYR:HH	1.83	0.41
1:B:301:PRO:O	1:B:302:LYS:CG	2.68	0.41
1:B:300:LEU:HD13	1:B:333:PHE:CE1	2.56	0.41
1:A:26:SER:O	1:A:27:ARG:O	2.39	0.40
1:B:268:ASP:C	1:B:270:GLN:H	2.24	0.40
1:B:33:LYS:HB2	1:B:341:ILE:HG22	2.03	0.40
1:A:268:ASP:C	1:A:270:GLN:H	2.24	0.40
1:B:121:GLU:OE1	1:B:129:LYS:HE2	2.22	0.40
1:A:185:THR:C	1:A:187:GLU:N	2.72	0.40
1:A:183:HIS:ND1	1:A:338:ALA:HB2	2.37	0.40
1:B:62:ARG:CZ	1:B:64:LEU:HD22	2.51	0.40
1:A:234:GLU:H	1:A:234:GLU:CD	2.14	0.40
1:B:13:ARG:HH11	1:B:13:ARG:HG2	1.86	0.40
1:B:300:LEU:CD1	1:B:300:LEU:N	2.84	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	309/346 (89%)	213 (69%)	59 (19%)	37 (12%)	0	1
1	B	309/346 (89%)	215 (70%)	57 (18%)	37 (12%)	0	1
All	All	618/692 (89%)	428 (69%)	116 (19%)	74 (12%)	0	1

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	41	SER
1	A	73	GLU
1	A	98	PRO
1	A	104	LYS
1	A	178	PRO
1	A	302	LYS
1	A	303	SER
1	B	27	ARG
1	B	41	SER
1	B	73	GLU
1	B	98	PRO
1	B	104	LYS
1	B	178	PRO
1	B	302	LYS
1	B	303	SER
1	A	21	GLU
1	A	26	SER
1	A	46	ILE
1	A	75	THR
1	A	76	GLY
1	A	121	GLU
1	A	179	THR
1	A	245	ASN
1	A	256	SER

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Mol	Chain	Res	Type
1	A	269	GLY
1	A	333	PHE
1	A	336	GLY
1	B	21	GLU
1	B	25	ALA
1	B	26	SER
1	B	46	ILE
1	B	75	THR
1	B	76	GLY
1	B	121	GLU
1	B	179	THR
1	B	245	ASN
1	B	256	SER
1	B	269	GLY
1	B	333	PHE
1	B	336	GLY
1	A	25	ALA
1	A	59	ASN
1	A	183	HIS
1	B	59	ASN
1	B	155	LYS
1	B	183	HIS
1	A	39	THR
1	A	74	ASP
1	A	77	ALA
1	A	155	LYS
1	A	180	ALA
1	B	12	GLU
1	B	63	VAL
1	B	74	ASP
1	B	77	ALA
1	B	180	ALA
1	A	12	GLU
1	A	60	ASN
1	A	63	VAL
1	A	284	PRO
1	B	60	ASN
1	B	78	LYS
1	B	153	TYR
1	A	78	LYS
1	A	153	TYR
1	B	24	ASP

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Mol	Chain	Res	Type
1	B	39	THR
1	B	284	PRO
1	A	177	ALA
1	B	177	ALA
1	A	301	PRO
1	B	301	PRO
1	A	89	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/293 (91%)	238 (90%)	28 (10%)	7	19
1	B	266/293 (91%)	236 (89%)	30 (11%)	6	16
All	All	532/586 (91%)	474 (89%)	58 (11%)	6	17

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	28	LEU
1	A	29	MET
1	A	52	GLU
1	A	59	ASN
1	A	60	ASN
1	A	71	THR
1	A	74	ASP
1	A	75	THR
1	A	98	PRO
1	A	118	ILE
1	A	122	GLU
1	A	124	GLU
1	A	125	HIS
1	A	161	LYS
1	A	202	ILE

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Mol	Chain	Res	Type
1	A	210	THR
1	A	224	MET
1	A	254	THR
1	A	255	THR
1	A	278	THR
1	A	284	PRO
1	A	300	LEU
1	A	303	SER
1	A	304	SER
1	A	310	SER
1	A	333	PHE
1	A	341	ILE
1	B	18	VAL
1	B	20	LEU
1	B	28	LEU
1	B	29	MET
1	B	31	LEU
1	B	52	GLU
1	B	59	ASN
1	B	60	ASN
1	B	71	THR
1	B	74	ASP
1	B	75	THR
1	B	98	PRO
1	B	118	ILE
1	B	122	GLU
1	B	124	GLU
1	B	125	HIS
1	B	161	LYS
1	B	202	ILE
1	B	210	THR
1	B	224	MET
1	B	254	THR
1	B	255	THR
1	B	278	THR
1	B	284	PRO
1	B	300	LEU
1	B	303	SER
1	B	304	SER
1	B	310	SER
1	B	333	PHE
1	B	341	ILE



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	45	HIS
1	A	51	ASN
1	A	133	GLN
1	A	183	HIS
1	A	205	HIS
1	A	270	GLN
1	B	22	GLN
1	B	45	HIS
1	B	51	ASN
1	B	133	GLN
1	B	183	HIS
1	B	205	HIS
1	B	270	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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	315/346 (91%)	1.22	73 (23%) <span>0</span> <span>0</span>	49, 87, 111, 126	0
1	B	315/346 (91%)	1.08	55 (17%) <span>1</span> <span>1</span>	48, 85, 111, 126	0
All	All	630/692 (91%)	1.15	128 (20%) <span>1</span> <span>0</span>	48, 86, 111, 126	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	LEU	11.1
1	A	324	HIS	8.5
1	B	177	ALA	8.0
1	A	62	ARG	7.5
1	A	9	GLU	6.9
1	A	6	PHE	6.7
1	B	9	GLU	6.0
1	B	18	VAL	5.8
1	A	19	PRO	5.4
1	B	21	GLU	5.3
1	A	341	ILE	5.2
1	B	24	ASP	5.2
1	B	175	ALA	4.7
1	A	175	ALA	4.6
1	A	8	PHE	4.6
1	A	224	MET	4.4
1	A	23	ARG	4.3
1	A	330	TYR	4.3
1	B	254	THR	4.2
1	A	102	VAL	4.1
1	B	38	LEU	4.1
1	A	335	PHE	4.0
1	B	224	MET	4.0
1	A	5	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	156	GLU	3.9
1	B	316	GLU	3.9
1	A	64	LEU	3.9
1	B	251	SER	3.9
1	B	19	PRO	3.8
1	A	158	LEU	3.8
1	B	75	THR	3.8
1	A	22	GLN	3.6
1	A	7	ASP	3.6
1	B	7	ASP	3.6
1	B	328	GLU	3.6
1	A	328	GLU	3.6
1	B	8	PHE	3.5
1	A	139	TYR	3.5
1	A	254	THR	3.5
1	B	341	ILE	3.4
1	B	64	LEU	3.3
1	A	40	ASP	3.3
1	B	35	THR	3.3
1	A	100	LYS	3.2
1	B	59	ASN	3.2
1	A	13	ARG	3.2
1	A	4	ASP	3.2
1	A	155	LYS	3.1
1	B	40	ASP	3.1
1	A	317	ASN	3.1
1	A	337	ASP	3.1
1	A	27	ARG	3.0
1	B	303	SER	3.0
1	B	6	PHE	3.0
1	B	257	THR	3.0
1	B	153	TYR	3.0
1	B	98	PRO	2.9
1	B	23	ARG	2.9
1	B	256	SER	2.9
1	B	339	MET	2.9
1	A	269	GLY	2.8
1	B	22	GLN	2.8
1	A	293	GLY	2.8
1	A	323	ASN	2.8
1	A	339	MET	2.8
1	A	320	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	139	TYR	2.7
1	A	17	GLN	2.7
1	A	21	GLU	2.7
1	A	160	ASP	2.7
1	A	298	PHE	2.6
1	A	289	LYS	2.6
1	B	4	ASP	2.6
1	A	26	SER	2.6
1	A	98	PRO	2.6
1	B	74	ASP	2.6
1	B	296	THR	2.5
1	A	299	HIS	2.5
1	A	14	LEU	2.5
1	B	162	GLU	2.5
1	A	149	PRO	2.5
1	A	310	SER	2.5
1	A	297	ASN	2.5
1	A	49	PHE	2.5
1	A	50	PHE	2.4
1	A	327	GLU	2.4
1	A	43	PHE	2.4
1	B	338	ALA	2.4
1	A	284	PRO	2.4
1	A	86	GLN	2.4
1	A	305	LEU	2.4
1	A	44	LYS	2.3
1	B	161	LYS	2.3
1	A	176	ALA	2.3
1	A	338	ALA	2.3
1	A	24	ASP	2.3
1	B	13	ARG	2.3
1	B	330	TYR	2.3
1	A	226	ALA	2.3
1	B	302	LYS	2.3
1	A	251	SER	2.3
1	A	72	LYS	2.3
1	B	5	LEU	2.2
1	B	154	ILE	2.2
1	B	252	VAL	2.2
1	A	331	ARG	2.2
1	B	17	GLN	2.2
1	A	189	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	143	GLU	2.2
1	A	304	SER	2.2
1	B	58	LEU	2.2
1	A	255	THR	2.2
1	B	337	ASP	2.2
1	A	329	GLU	2.2
1	A	55	CYS	2.1
1	A	184	PHE	2.1
1	B	306	ILE	2.1
1	A	294	MET	2.1
1	B	309	VAL	2.1
1	A	256	SER	2.1
1	B	10	LEU	2.1
1	A	101	ARG	2.1
1	A	178	PRO	2.1
1	B	99	ALA	2.1
1	B	323	ASN	2.0
1	A	180	ALA	2.0
1	A	296	THR	2.0
1	B	57	VAL	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.