



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:44 PM UTC

PDB ID : 6BA1 / pdb_00006ba1
Title : Purine-Preferring Ribonucleoside Hydrolase from Gardnerella vaginalis
Authors : Renner, N.; Jacques, D.A.
Deposited on : 2017-10-11
Resolution : 2.90 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

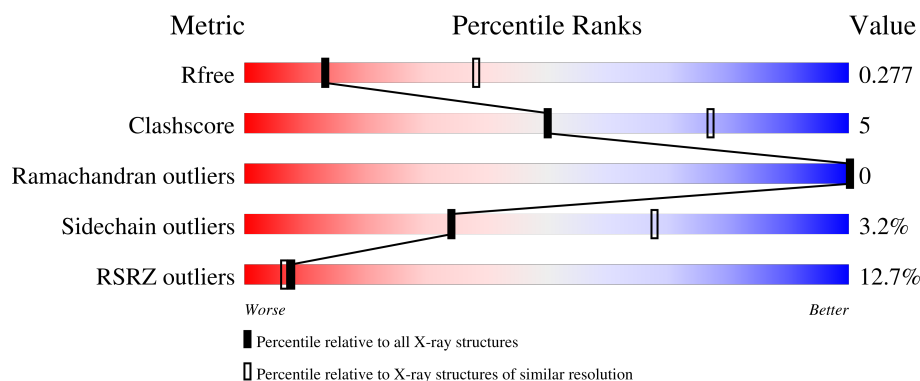
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



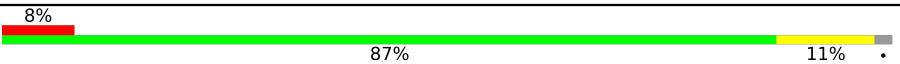
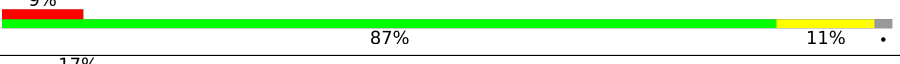
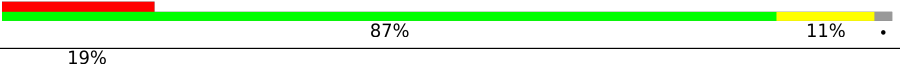
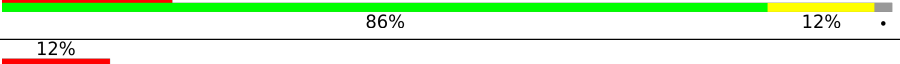
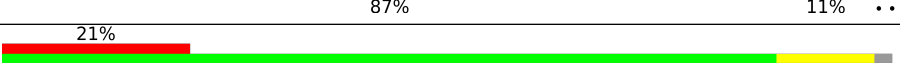
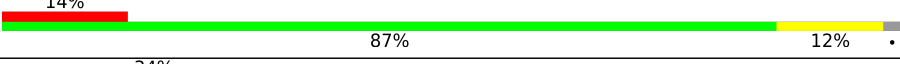
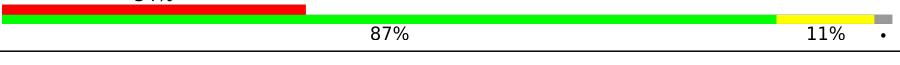
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 ≥ 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	321	7% 87% 11% .
1	B	321	12% 88% 11% .
1	C	321	5% 87% 12% .
1	D	321	11% 86% 12% .
1	E	321	8% 87% 11% .

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Mol	Chain	Length	Quality of chain
1	F	321	
1	G	321	
1	H	321	
1	I	321	
1	J	321	
1	K	321	
1	L	321	
1	M	321	
1	N	321	
1	O	321	
1	P	321	
1	Q	321	
1	R	321	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 42469 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 Inosine-uridine preferring nucleoside hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2362	1499	389	464	10			
1	B	316	Total	C	N	O	S	0	0	0
			2370	1505	391	464	10			
1	C	316	Total	C	N	O	S	0	0	0
			2370	1505	391	464	10			
1	D	316	Total	C	N	O	S	0	0	0
			2370	1505	391	464	10			
1	E	316	Total	C	N	O	S	0	0	0
			2358	1496	388	464	10			
1	F	316	Total	C	N	O	S	0	0	0
			2359	1498	389	462	10			
1	G	316	Total	C	N	O	S	0	0	0
			2358	1496	388	464	10			
1	H	316	Total	C	N	O	S	0	0	0
			2359	1498	389	462	10			
1	I	316	Total	C	N	O	S	0	0	0
			2355	1495	388	462	10			
1	J	316	Total	C	N	O	S	0	0	0
			2349	1491	384	464	10			
1	K	316	Total	C	N	O	S	0	0	0
			2355	1494	387	464	10			
1	L	316	Total	C	N	O	S	0	0	0
			2362	1499	389	464	10			
1	M	316	Total	C	N	O	S	0	0	0
			2349	1492	385	462	10			
1	N	316	Total	C	N	O	S	0	0	0
			2349	1492	385	462	10			
1	O	316	Total	C	N	O	S	0	0	0
			2363	1500	389	464	10			
1	P	316	Total	C	N	O	S	0	0	0
			2362	1499	389	464	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	316	Total	C	N	O	S	0	0	0
			2352	1493	385	464	10			
1	R	316	Total	C	N	O	S	0	0	0
			2349	1492	385	462	10			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP F5LUS2
A	-1	SER	-	expression tag	UNP F5LUS2
A	0	HIS	-	expression tag	UNP F5LUS2
B	-2	GLY	-	expression tag	UNP F5LUS2
B	-1	SER	-	expression tag	UNP F5LUS2
B	0	HIS	-	expression tag	UNP F5LUS2
C	-2	GLY	-	expression tag	UNP F5LUS2
C	-1	SER	-	expression tag	UNP F5LUS2
C	0	HIS	-	expression tag	UNP F5LUS2
D	-2	GLY	-	expression tag	UNP F5LUS2
D	-1	SER	-	expression tag	UNP F5LUS2
D	0	HIS	-	expression tag	UNP F5LUS2
E	-2	GLY	-	expression tag	UNP F5LUS2
E	-1	SER	-	expression tag	UNP F5LUS2
E	0	HIS	-	expression tag	UNP F5LUS2
F	-2	GLY	-	expression tag	UNP F5LUS2
F	-1	SER	-	expression tag	UNP F5LUS2
F	0	HIS	-	expression tag	UNP F5LUS2
G	-2	GLY	-	expression tag	UNP F5LUS2
G	-1	SER	-	expression tag	UNP F5LUS2
G	0	HIS	-	expression tag	UNP F5LUS2
H	-2	GLY	-	expression tag	UNP F5LUS2
H	-1	SER	-	expression tag	UNP F5LUS2
H	0	HIS	-	expression tag	UNP F5LUS2
I	-2	GLY	-	expression tag	UNP F5LUS2
I	-1	SER	-	expression tag	UNP F5LUS2
I	0	HIS	-	expression tag	UNP F5LUS2
J	-2	GLY	-	expression tag	UNP F5LUS2
J	-1	SER	-	expression tag	UNP F5LUS2
J	0	HIS	-	expression tag	UNP F5LUS2
K	-2	GLY	-	expression tag	UNP F5LUS2
K	-1	SER	-	expression tag	UNP F5LUS2
K	0	HIS	-	expression tag	UNP F5LUS2
L	-2	GLY	-	expression tag	UNP F5LUS2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	SER	-	expression tag	UNP F5LUS2
L	0	HIS	-	expression tag	UNP F5LUS2
M	-2	GLY	-	expression tag	UNP F5LUS2
M	-1	SER	-	expression tag	UNP F5LUS2
M	0	HIS	-	expression tag	UNP F5LUS2
N	-2	GLY	-	expression tag	UNP F5LUS2
N	-1	SER	-	expression tag	UNP F5LUS2
N	0	HIS	-	expression tag	UNP F5LUS2
O	-2	GLY	-	expression tag	UNP F5LUS2
O	-1	SER	-	expression tag	UNP F5LUS2
O	0	HIS	-	expression tag	UNP F5LUS2
P	-2	GLY	-	expression tag	UNP F5LUS2
P	-1	SER	-	expression tag	UNP F5LUS2
P	0	HIS	-	expression tag	UNP F5LUS2
Q	-2	GLY	-	expression tag	UNP F5LUS2
Q	-1	SER	-	expression tag	UNP F5LUS2
Q	0	HIS	-	expression tag	UNP F5LUS2
R	-2	GLY	-	expression tag	UNP F5LUS2
R	-1	SER	-	expression tag	UNP F5LUS2
R	0	HIS	-	expression tag	UNP F5LUS2

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0

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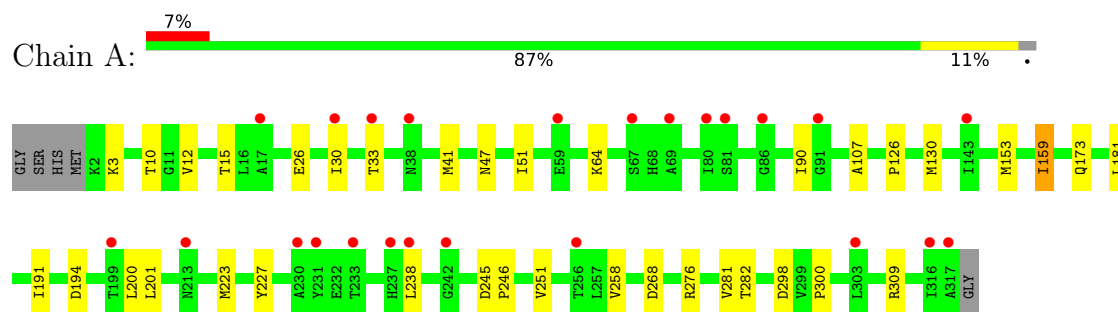
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	1	Total 1	Ca 1	0	0
2	K	1	Total 1	Ca 1	0	0
2	L	1	Total 1	Ca 1	0	0
2	M	1	Total 1	Ca 1	0	0
2	N	1	Total 1	Ca 1	0	0
2	O	1	Total 1	Ca 1	0	0
2	P	1	Total 1	Ca 1	0	0
2	Q	1	Total 1	Ca 1	0	0
2	R	1	Total 1	Ca 1	0	0

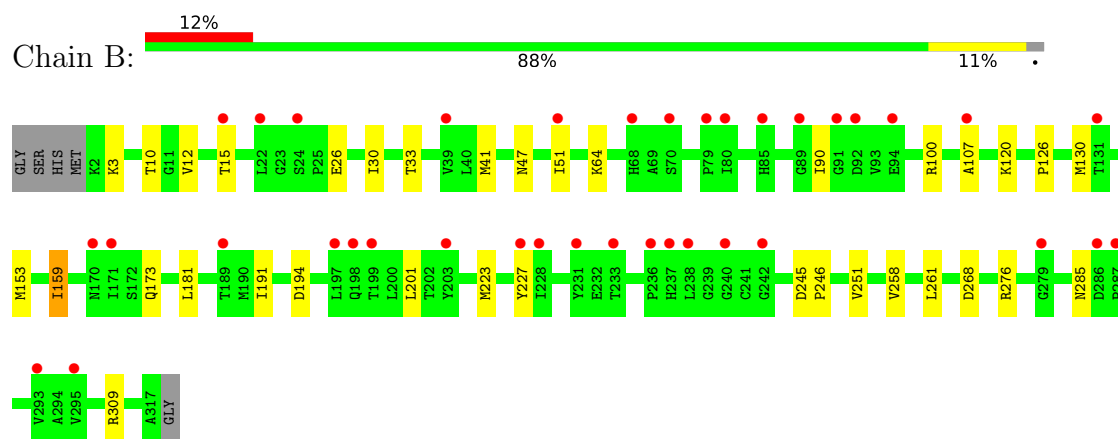
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

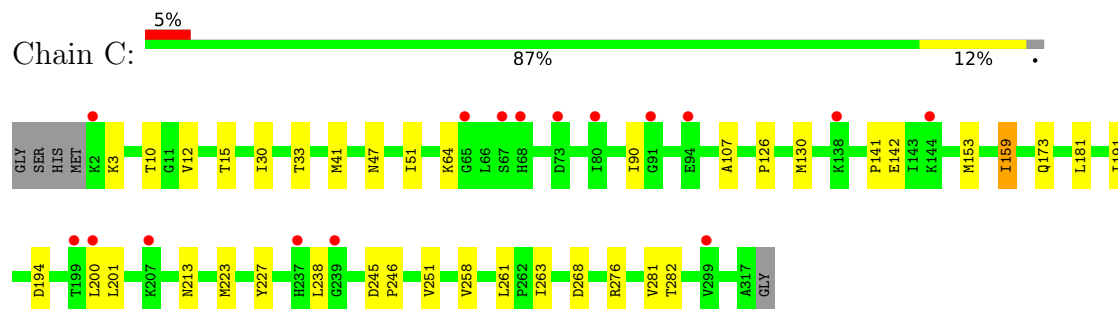
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



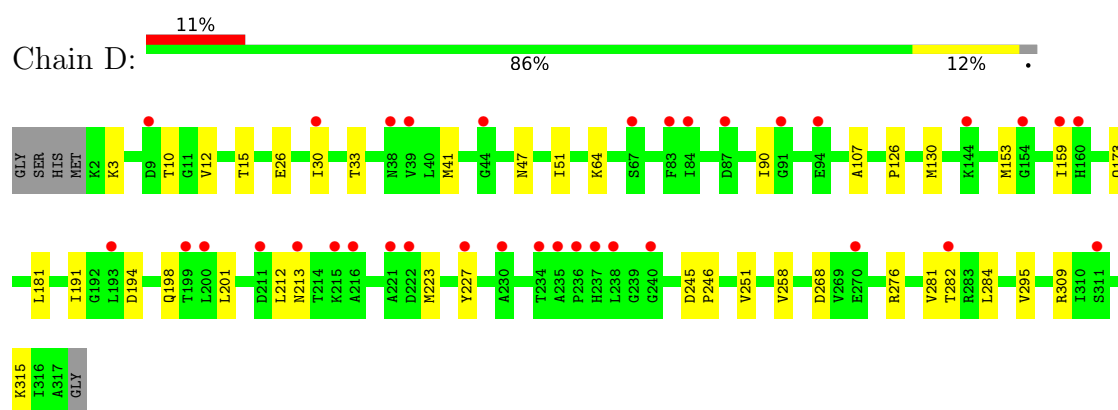
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



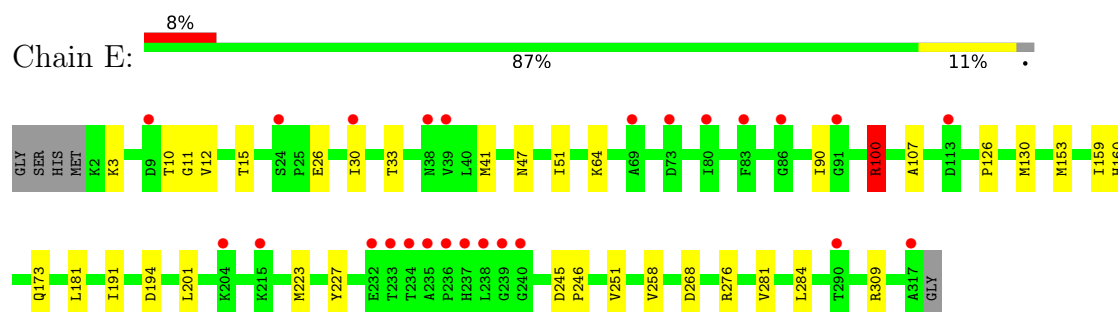
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



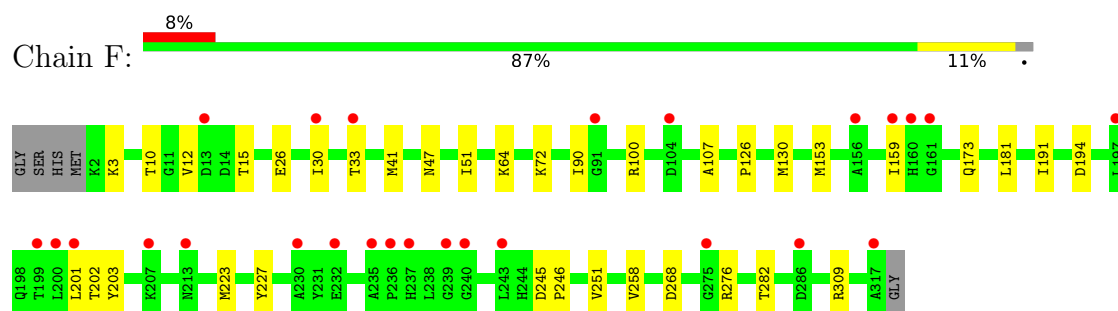
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



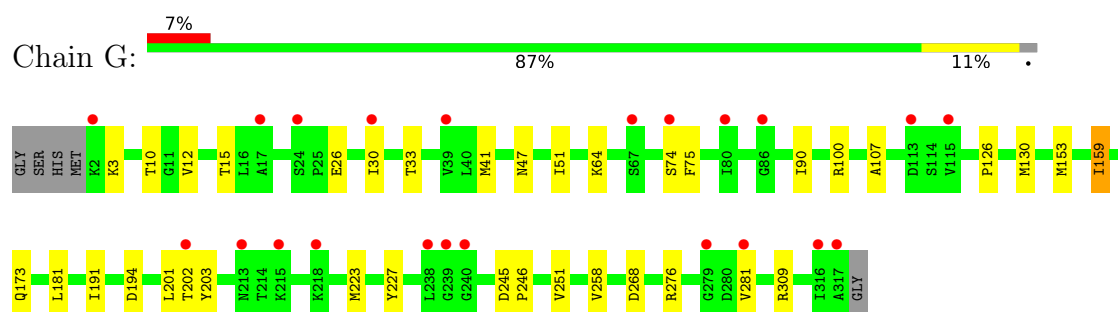
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



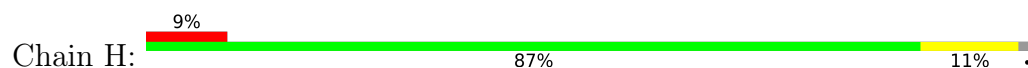
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase

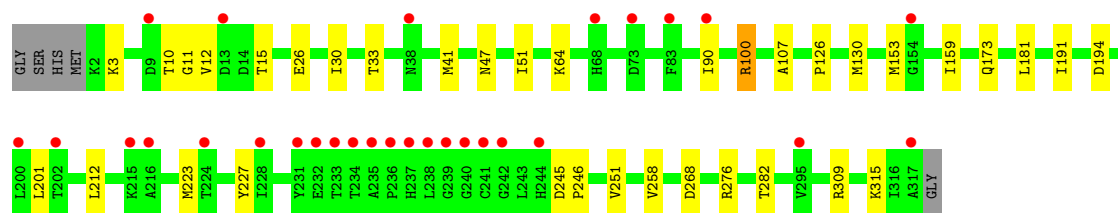


- Molecule 1: Inosine-uridine preferring nucleoside hydrolase

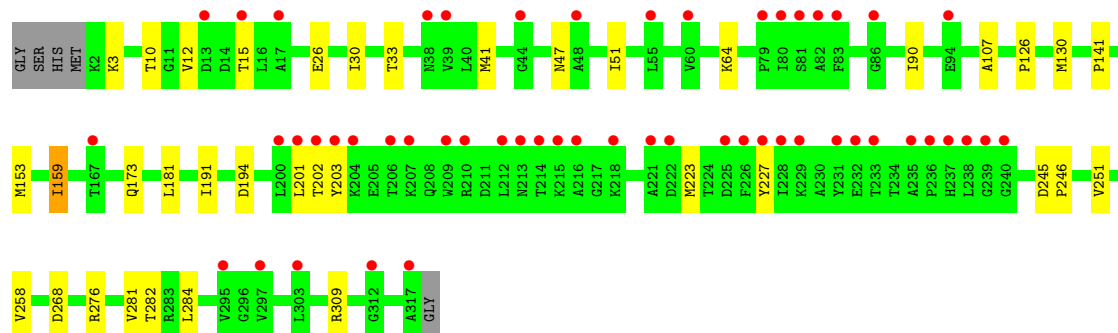
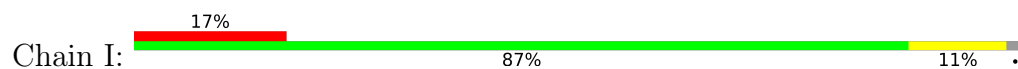


- Molecule 1: Inosine-uridine preferring nucleoside hydrolase

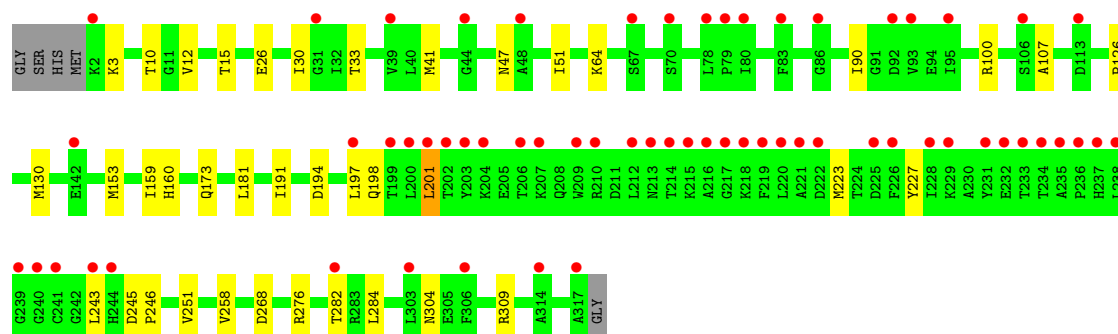
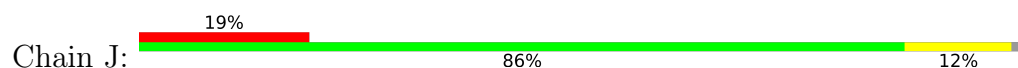




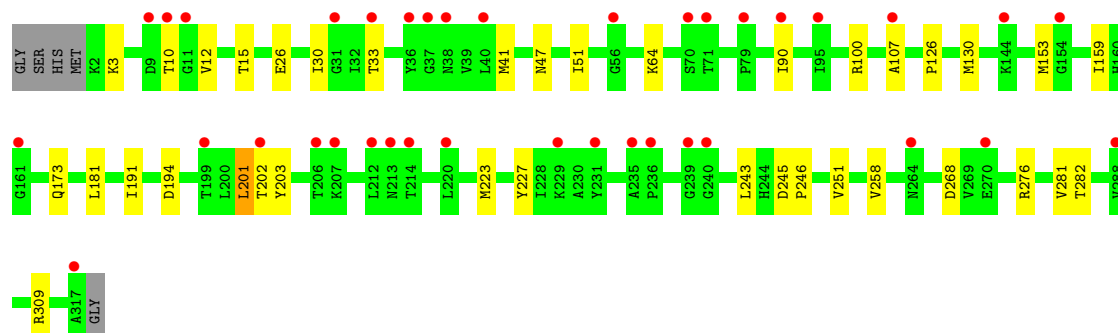
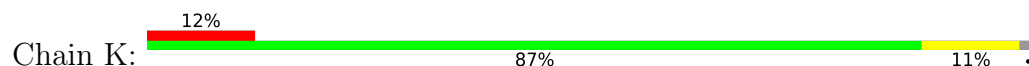
● Molecule 1: Inosine-uridine preferring nucleoside hydrolase



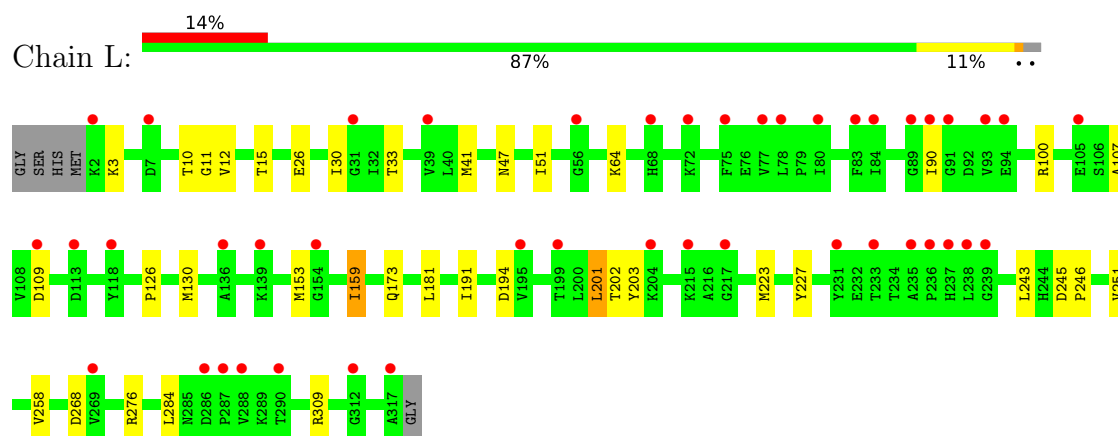
● Molecule 1: Inosine-uridine preferring nucleoside hydrolase



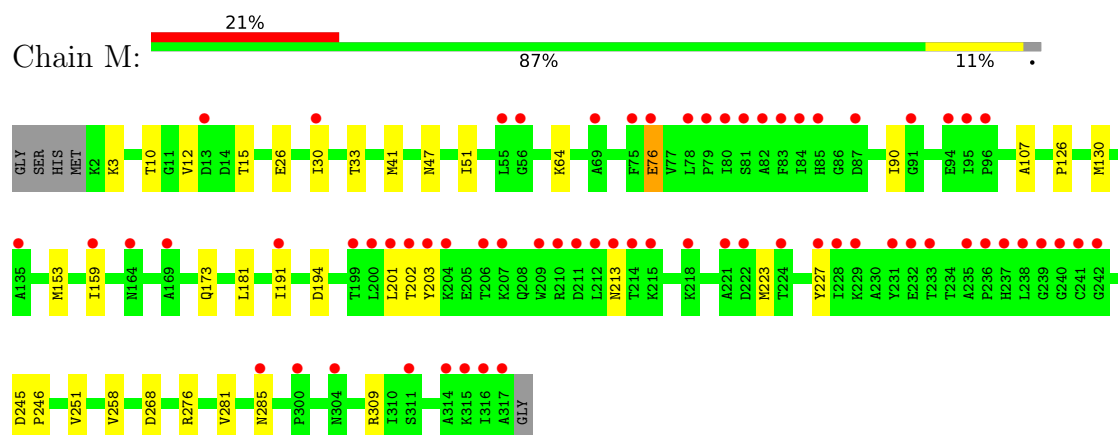
● Molecule 1: Inosine-uridine preferring nucleoside hydrolase



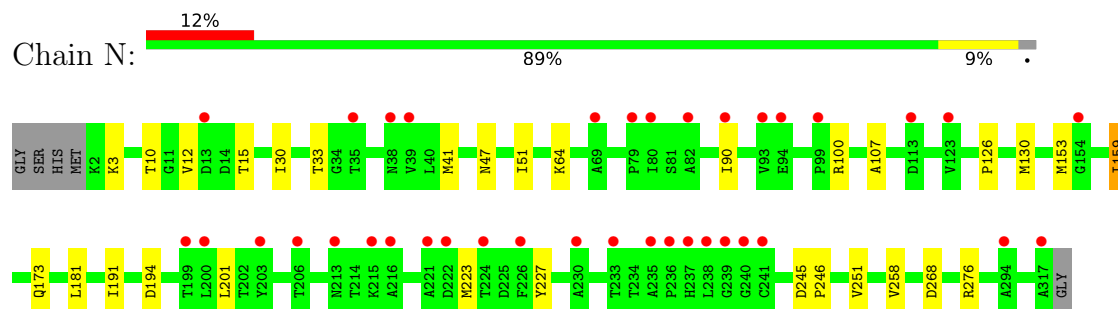
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



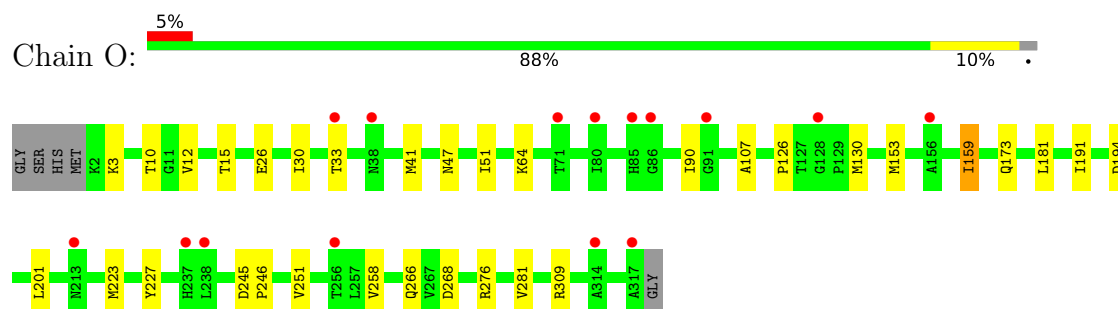
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



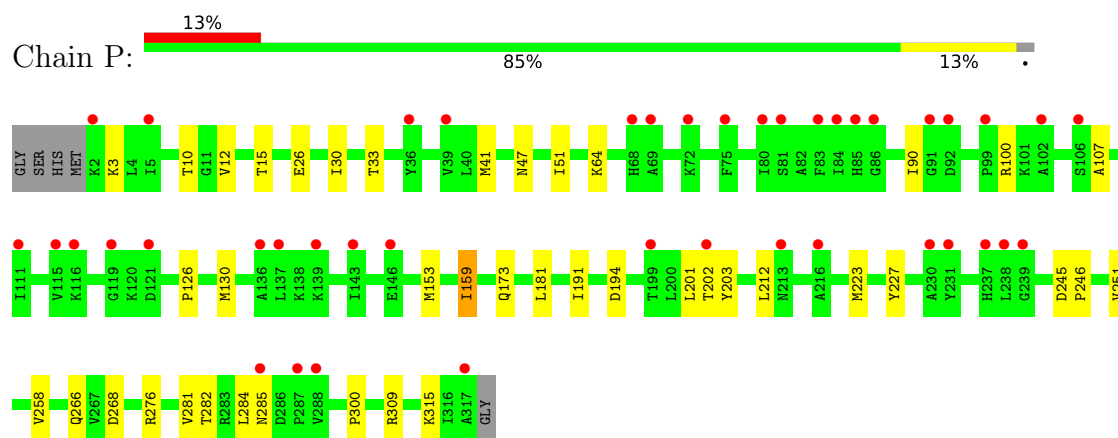
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



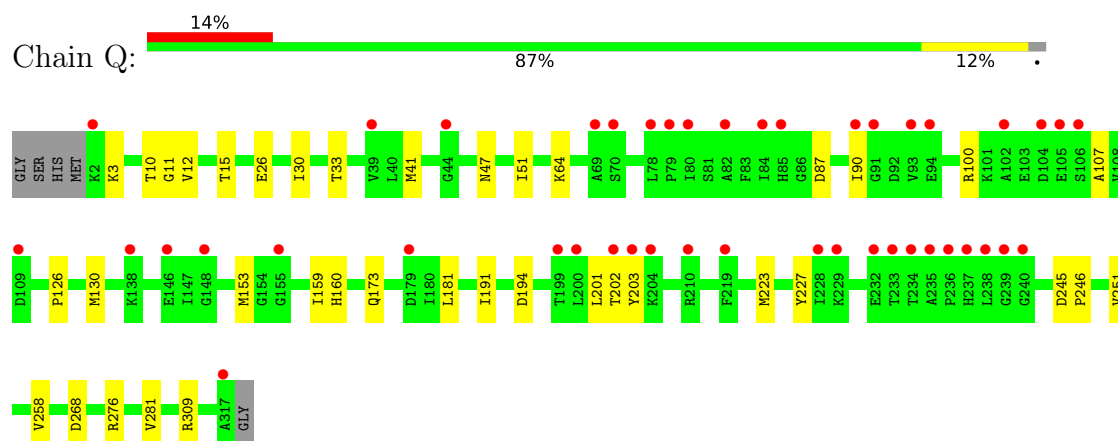
- Molecule 1: Inosine-uridine preferring nucleoside hydrolase



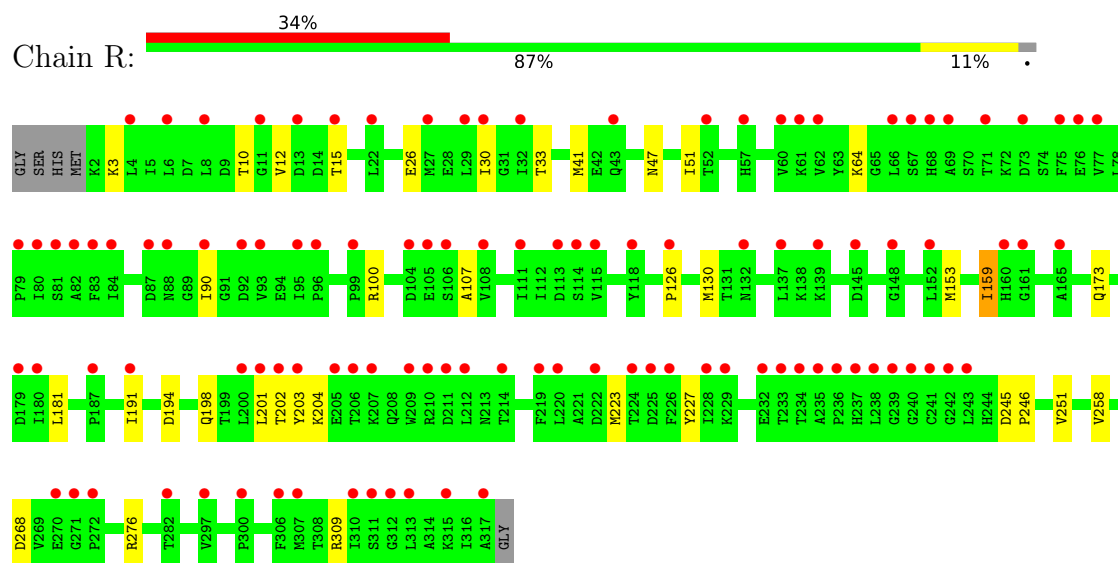
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase



• Molecule 1: Inosine-uridine preferring nucleoside hydrolase



• Molecule 1: Inosine-uridine preferring nucleoside hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	163.27Å 80.24Å 223.82Å 90.00° 106.50° 90.00°	Depositor
Resolution (Å)	80.24 – 2.90 80.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	77.0 (80.24-2.90) 77.0 (80.24-2.90)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.279 , 0.282 0.276 , 0.277	Depositor DCC
R_{free} test set	4795 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	42469	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.62	0/2404	0.89	0/3278
1	B	0.62	0/2412	0.88	0/3286
1	C	0.62	0/2412	0.89	0/3286
1	D	0.60	0/2412	0.87	0/3286
1	E	0.60	0/2400	0.91	2/3274 (0.1%)
1	F	0.63	0/2401	0.89	0/3274
1	G	0.59	0/2400	0.87	0/3274
1	H	0.60	0/2401	0.89	2/3274 (0.1%)
1	I	0.59	0/2397	0.87	0/3270
1	J	0.60	0/2391	0.87	0/3264
1	K	0.59	0/2397	0.87	0/3271
1	L	0.58	0/2404	0.87	0/3278
1	M	0.60	0/2391	0.88	0/3263
1	N	0.59	0/2391	0.87	0/3263
1	O	0.59	0/2405	0.87	0/3279
1	P	0.61	0/2404	0.88	0/3278
1	Q	0.59	0/2394	0.88	0/3267
1	R	0.61	0/2391	0.88	0/3263
All	All	0.60	0/43207	0.88	4/58928 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	100	ARG	NE-CZ-NH1	-10.91	110.59	121.50
1	H	100	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	H	100	ARG	NE-CZ-NH1	-7.02	114.48	121.50
1	E	100	ARG	NE-CZ-NH2	6.55	125.10	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	100	ARG	Sidechain
1	H	100	ARG	Sidechain

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	2362	0	2361	29	0
1	B	2370	0	2383	29	0
1	C	2370	0	2383	27	2
1	D	2370	0	2383	30	0
1	E	2358	0	2350	27	0
1	F	2359	0	2359	23	0
1	G	2358	0	2350	28	0
1	H	2359	0	2359	25	0
1	I	2355	0	2348	27	0
1	J	2349	0	2330	28	2
1	K	2355	0	2341	25	0
1	L	2362	0	2361	28	1
1	M	2349	0	2337	25	3
1	N	2349	0	2337	22	0
1	O	2363	0	2363	25	0
1	P	2362	0	2361	34	0
1	Q	2352	0	2339	32	0
1	R	2349	0	2337	25	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
All	All	42469	0	42382	453	5

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 5.

All (453) 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:P:300:PRO:HB3	1:Q:87:ASP:OD2	1.66	0.95
1:P:300:PRO:CB	1:Q:87:ASP:OD2	2.24	0.85
1:P:300:PRO:CB	1:Q:87:ASP:CG	2.57	0.77
1:P:300:PRO:HB2	1:Q:87:ASP:CG	2.10	0.76
1:A:300:PRO:HG2	1:G:75:PHE:O	1.86	0.76
1:H:90:ILE:HG23	1:H:223:MET:HE3	1.76	0.68
1:E:90:ILE:HG23	1:E:223:MET:HE3	1.76	0.68
1:L:90:ILE:HG23	1:L:223:MET:HE3	1.76	0.68
1:F:90:ILE:HG23	1:F:223:MET:HE3	1.76	0.68
1:G:90:ILE:HG23	1:G:223:MET:HE3	1.76	0.67
1:M:90:ILE:HG23	1:M:223:MET:HE3	1.76	0.67
1:B:90:ILE:HG23	1:B:223:MET:HE3	1.76	0.67
1:O:90:ILE:HG23	1:O:223:MET:HE3	1.76	0.67
1:J:90:ILE:HG23	1:J:223:MET:HE3	1.76	0.66
1:R:90:ILE:HG23	1:R:223:MET:HE3	1.77	0.66
1:I:90:ILE:HG23	1:I:223:MET:HE3	1.76	0.66
1:Q:90:ILE:HG23	1:Q:223:MET:HE3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HG23	1:A:223:MET:HE3	1.76	0.66
1:D:90:ILE:HG23	1:D:223:MET:HE3	1.76	0.66
1:K:90:ILE:HG23	1:K:223:MET:HE3	1.76	0.66
1:N:90:ILE:HG23	1:N:223:MET:HE3	1.77	0.66
1:P:90:ILE:HG23	1:P:223:MET:HE3	1.76	0.66
1:C:90:ILE:HG23	1:C:223:MET:HE3	1.76	0.65
1:M:285:ASN:OD1	1:R:198:GLN:HA	1.97	0.64
1:D:33:THR:HG23	1:D:107:ALA:HB1	1.82	0.62
1:F:33:THR:HG23	1:F:107:ALA:HB1	1.82	0.62
1:M:33:THR:HG23	1:M:107:ALA:HB1	1.83	0.61
1:Q:33:THR:HG23	1:Q:107:ALA:HB1	1.82	0.61
1:C:33:THR:HG23	1:C:107:ALA:HB1	1.82	0.61
1:P:33:THR:HG23	1:P:107:ALA:HB1	1.83	0.61
1:E:33:THR:HG23	1:E:107:ALA:HB1	1.83	0.61
1:G:33:THR:HG23	1:G:107:ALA:HB1	1.83	0.60
1:B:33:THR:HG23	1:B:107:ALA:HB1	1.83	0.60
1:J:33:THR:HG23	1:J:107:ALA:HB1	1.83	0.60
1:N:33:THR:HG23	1:N:107:ALA:HB1	1.83	0.60
1:H:33:THR:HG23	1:H:107:ALA:HB1	1.82	0.60
1:K:33:THR:HG23	1:K:107:ALA:HB1	1.83	0.60
1:O:33:THR:HG23	1:O:107:ALA:HB1	1.83	0.60
1:A:33:THR:HG23	1:A:107:ALA:HB1	1.83	0.60
1:L:33:THR:HG23	1:L:107:ALA:HB1	1.82	0.60
1:R:33:THR:HG23	1:R:107:ALA:HB1	1.83	0.60
1:I:33:THR:HG23	1:I:107:ALA:HB1	1.83	0.59
1:F:41:MET:HE1	1:F:64:LYS:HG2	1.86	0.57
1:J:90:ILE:CG2	1:J:223:MET:HE3	2.34	0.57
1:E:90:ILE:CG2	1:E:223:MET:HE3	2.35	0.57
1:N:90:ILE:CG2	1:N:223:MET:HE3	2.35	0.57
1:F:90:ILE:CG2	1:F:223:MET:HE3	2.34	0.57
1:P:126:PRO:HG2	1:P:130:MET:HE1	1.87	0.57
1:R:90:ILE:CG2	1:R:223:MET:HE3	2.35	0.57
1:M:90:ILE:CG2	1:M:223:MET:HE3	2.35	0.56
1:D:90:ILE:CG2	1:D:223:MET:HE3	2.35	0.56
1:D:126:PRO:HG2	1:D:130:MET:HE1	1.88	0.56
1:E:41:MET:HE1	1:E:64:LYS:HG2	1.87	0.56
1:E:126:PRO:HG2	1:E:130:MET:HE1	1.87	0.56
1:F:126:PRO:HG2	1:F:130:MET:HE1	1.87	0.56
1:K:90:ILE:CG2	1:K:223:MET:HE3	2.35	0.56
1:C:90:ILE:CG2	1:C:223:MET:HE3	2.35	0.56
1:I:90:ILE:CG2	1:I:223:MET:HE3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:90:ILE:CG2	1:O:223:MET:HE3	2.35	0.56
1:P:90:ILE:CG2	1:P:223:MET:HE3	2.35	0.56
1:Q:90:ILE:CG2	1:Q:223:MET:HE3	2.34	0.56
1:Q:126:PRO:HG2	1:Q:130:MET:HE1	1.88	0.56
1:R:126:PRO:HG2	1:R:130:MET:HE1	1.88	0.56
1:C:126:PRO:HG2	1:C:130:MET:HE1	1.87	0.56
1:L:90:ILE:CG2	1:L:223:MET:HE3	2.35	0.56
1:J:198:GLN:HA	1:P:285:ASN:OD1	2.05	0.56
1:I:126:PRO:HG2	1:I:130:MET:HE1	1.87	0.56
1:O:126:PRO:HG2	1:O:130:MET:HE1	1.87	0.56
1:R:41:MET:HE1	1:R:64:LYS:HG2	1.87	0.56
1:A:90:ILE:CG2	1:A:223:MET:HE3	2.35	0.56
1:A:126:PRO:HG2	1:A:130:MET:HE1	1.87	0.56
1:M:126:PRO:HG2	1:M:130:MET:HE1	1.88	0.56
1:B:90:ILE:CG2	1:B:223:MET:HE3	2.35	0.56
1:H:126:PRO:HG2	1:H:130:MET:HE1	1.88	0.56
1:B:126:PRO:HG2	1:B:130:MET:HE1	1.87	0.56
1:G:126:PRO:HG2	1:G:130:MET:HE1	1.88	0.56
1:G:90:ILE:CG2	1:G:223:MET:HE3	2.35	0.55
1:D:41:MET:HE1	1:D:64:LYS:HG2	1.88	0.55
1:K:126:PRO:HG2	1:K:130:MET:HE1	1.88	0.55
1:L:126:PRO:HG2	1:L:130:MET:HE1	1.87	0.55
1:Q:33:THR:HG23	1:Q:107:ALA:CB	2.37	0.55
1:C:33:THR:HG23	1:C:107:ALA:CB	2.37	0.55
1:H:90:ILE:CG2	1:H:223:MET:HE3	2.35	0.55
1:L:33:THR:HG23	1:L:107:ALA:CB	2.37	0.55
1:A:33:THR:HG23	1:A:107:ALA:CB	2.37	0.55
1:E:33:THR:HG23	1:E:107:ALA:CB	2.37	0.55
1:L:41:MET:HE1	1:L:64:LYS:HG2	1.89	0.55
1:Q:41:MET:HE1	1:Q:64:LYS:HG2	1.89	0.55
1:N:126:PRO:HG2	1:N:130:MET:HE1	1.88	0.55
1:J:126:PRO:HG2	1:J:130:MET:HE1	1.87	0.55
1:K:15:THR:CG2	1:K:223:MET:HE1	2.37	0.55
1:R:33:THR:HG23	1:R:107:ALA:CB	2.37	0.55
1:D:15:THR:CG2	1:D:223:MET:HE1	2.37	0.55
1:K:41:MET:HE1	1:K:64:LYS:HG2	1.89	0.55
1:O:33:THR:HG23	1:O:107:ALA:CB	2.37	0.55
1:B:15:THR:CG2	1:B:223:MET:HE1	2.37	0.55
1:H:15:THR:CG2	1:H:223:MET:HE1	2.37	0.55
1:R:15:THR:CG2	1:R:223:MET:HE1	2.37	0.55
1:F:15:THR:CG2	1:F:223:MET:HE1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:THR:HG23	1:F:107:ALA:CB	2.37	0.55
1:A:15:THR:CG2	1:A:223:MET:HE1	2.37	0.55
1:J:15:THR:CG2	1:J:223:MET:HE1	2.37	0.55
1:I:15:THR:CG2	1:I:223:MET:HE1	2.37	0.54
1:K:33:THR:HG23	1:K:107:ALA:CB	2.37	0.54
1:M:15:THR:CG2	1:M:223:MET:HE1	2.37	0.54
1:P:33:THR:HG23	1:P:107:ALA:CB	2.37	0.54
1:G:15:THR:CG2	1:G:223:MET:HE1	2.37	0.54
1:N:15:THR:CG2	1:N:223:MET:HE1	2.37	0.54
1:N:33:THR:HG23	1:N:107:ALA:CB	2.37	0.54
1:O:41:MET:HE1	1:O:64:LYS:HG2	1.89	0.54
1:B:33:THR:HG23	1:B:107:ALA:CB	2.37	0.54
1:E:15:THR:CG2	1:E:223:MET:HE1	2.37	0.54
1:G:33:THR:HG23	1:G:107:ALA:CB	2.37	0.54
1:I:33:THR:HG23	1:I:107:ALA:CB	2.37	0.54
1:A:159:ILE:HD11	1:E:281:VAL:HA	1.90	0.54
1:H:33:THR:HG23	1:H:107:ALA:CB	2.37	0.54
1:O:15:THR:CG2	1:O:223:MET:HE1	2.37	0.54
1:H:41:MET:HE1	1:H:64:LYS:HG2	1.89	0.54
1:L:15:THR:CG2	1:L:223:MET:HE1	2.37	0.54
1:D:33:THR:HG23	1:D:107:ALA:CB	2.37	0.54
1:J:33:THR:HG23	1:J:107:ALA:CB	2.37	0.54
1:A:41:MET:HE1	1:A:64:LYS:HG2	1.90	0.54
1:C:15:THR:CG2	1:C:223:MET:HE1	2.37	0.54
1:G:41:MET:HE1	1:G:64:LYS:HG2	1.90	0.54
1:J:41:MET:HE1	1:J:64:LYS:HG2	1.89	0.54
1:M:33:THR:HG23	1:M:107:ALA:CB	2.37	0.54
1:Q:15:THR:CG2	1:Q:223:MET:HE1	2.37	0.53
1:M:41:MET:HE1	1:M:64:LYS:HG2	1.89	0.53
1:P:15:THR:CG2	1:P:223:MET:HE1	2.37	0.53
1:P:41:MET:HE1	1:P:64:LYS:HG2	1.91	0.53
1:N:41:MET:HE1	1:N:64:LYS:HG2	1.89	0.53
1:B:41:MET:HE1	1:B:64:LYS:HG2	1.91	0.53
1:L:15:THR:OG1	1:L:223:MET:HE1	2.09	0.53
1:A:15:THR:OG1	1:A:223:MET:HE1	2.09	0.53
1:M:15:THR:OG1	1:M:223:MET:HE1	2.09	0.53
1:H:15:THR:OG1	1:H:223:MET:HE1	2.09	0.53
1:G:15:THR:OG1	1:G:223:MET:HE1	2.09	0.52
1:R:15:THR:OG1	1:R:223:MET:HE1	2.09	0.52
1:B:15:THR:OG1	1:B:223:MET:HE1	2.09	0.52
1:D:212:LEU:HD22	1:D:315:LYS:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:THR:OG1	1:E:223:MET:HE1	2.09	0.52
1:J:15:THR:OG1	1:J:223:MET:HE1	2.09	0.52
1:N:15:THR:OG1	1:N:223:MET:HE1	2.10	0.52
1:P:15:THR:OG1	1:P:223:MET:HE1	2.09	0.52
1:D:15:THR:HG21	1:D:51:ILE:HD13	1.92	0.52
1:L:15:THR:HG21	1:L:51:ILE:HD13	1.92	0.52
1:O:15:THR:OG1	1:O:223:MET:HE1	2.09	0.52
1:I:41:MET:HE1	1:I:64:LYS:HG2	1.91	0.52
1:F:15:THR:HG21	1:F:51:ILE:HD13	1.91	0.52
1:K:15:THR:OG1	1:K:223:MET:HE1	2.09	0.52
1:L:268:ASP:OD2	1:L:276:ARG:NH1	2.43	0.52
1:D:41:MET:HE1	1:D:64:LYS:CG	2.40	0.52
1:F:15:THR:CG2	1:F:51:ILE:HD13	2.40	0.52
1:G:159:ILE:CD1	1:L:284:LEU:HD22	2.40	0.52
1:O:268:ASP:OD2	1:O:276:ARG:NH1	2.43	0.52
1:A:281:VAL:CG2	1:E:160:HIS:HB2	2.40	0.51
1:C:15:THR:OG1	1:C:223:MET:HE1	2.09	0.51
1:C:268:ASP:OD2	1:C:276:ARG:NH1	2.43	0.51
1:P:268:ASP:OD2	1:P:276:ARG:NH1	2.43	0.51
1:A:41:MET:HE1	1:A:64:LYS:CG	2.40	0.51
1:C:15:THR:HG21	1:C:51:ILE:HD13	1.93	0.51
1:D:15:THR:OG1	1:D:223:MET:HE1	2.09	0.51
1:H:268:ASP:OD2	1:H:276:ARG:NH1	2.43	0.51
1:I:15:THR:HG21	1:I:51:ILE:HD13	1.92	0.51
1:J:268:ASP:OD2	1:J:276:ARG:NH1	2.43	0.51
1:M:268:ASP:OD2	1:M:276:ARG:NH1	2.43	0.51
1:P:41:MET:HE1	1:P:64:LYS:CG	2.41	0.51
1:Q:268:ASP:OD2	1:Q:276:ARG:NH1	2.43	0.51
1:J:41:MET:HE1	1:J:64:LYS:CG	2.41	0.51
1:K:41:MET:HE1	1:K:64:LYS:CG	2.40	0.51
1:P:15:THR:HG21	1:P:51:ILE:HD13	1.93	0.51
1:Q:15:THR:OG1	1:Q:223:MET:HE1	2.09	0.51
1:E:268:ASP:OD2	1:E:276:ARG:NH1	2.43	0.51
1:F:41:MET:HE1	1:F:64:LYS:CG	2.40	0.51
1:G:15:THR:HG21	1:G:51:ILE:HD13	1.92	0.51
1:K:268:ASP:OD2	1:K:276:ARG:NH1	2.43	0.51
1:L:41:MET:HE1	1:L:64:LYS:CG	2.41	0.51
1:O:41:MET:HE1	1:O:64:LYS:CG	2.41	0.51
1:D:268:ASP:OD2	1:D:276:ARG:NH1	2.43	0.51
1:G:268:ASP:OD2	1:G:276:ARG:NH1	2.43	0.51
1:I:15:THR:OG1	1:I:223:MET:HE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:268:ASP:OD2	1:N:276:ARG:NH1	2.43	0.51
1:Q:41:MET:HE1	1:Q:64:LYS:CG	2.41	0.51
1:R:15:THR:HG21	1:R:51:ILE:HD13	1.92	0.51
1:R:268:ASP:OD2	1:R:276:ARG:NH1	2.43	0.51
1:A:15:THR:HG21	1:A:51:ILE:HD13	1.93	0.51
1:F:268:ASP:OD2	1:F:276:ARG:NH1	2.43	0.51
1:I:41:MET:HE1	1:I:64:LYS:CG	2.41	0.51
1:M:41:MET:HE1	1:M:64:LYS:CG	2.41	0.51
1:C:41:MET:HE1	1:C:64:LYS:CG	2.41	0.51
1:E:15:THR:CG2	1:E:51:ILE:HD13	2.41	0.51
1:J:15:THR:HG21	1:J:51:ILE:HD13	1.92	0.51
1:M:15:THR:HG21	1:M:51:ILE:HD13	1.93	0.51
1:N:41:MET:HE1	1:N:64:LYS:CG	2.41	0.51
1:R:41:MET:HE1	1:R:64:LYS:CG	2.40	0.51
1:H:15:THR:HG21	1:H:51:ILE:HD13	1.92	0.51
1:K:15:THR:CG2	1:K:51:ILE:HD13	2.41	0.51
1:H:41:MET:HE1	1:H:64:LYS:CG	2.41	0.51
1:J:160:HIS:NE2	1:P:266:GLN:NE2	2.59	0.51
1:A:159:ILE:CD1	1:E:284:LEU:HD22	2.41	0.51
1:I:268:ASP:OD2	1:I:276:ARG:NH1	2.44	0.51
1:J:15:THR:CG2	1:J:51:ILE:HD13	2.41	0.51
1:K:15:THR:HG21	1:K:51:ILE:HD13	1.92	0.51
1:N:15:THR:HG21	1:N:51:ILE:HD13	1.93	0.51
1:Q:15:THR:CG2	1:Q:51:ILE:HD13	2.41	0.51
1:A:268:ASP:OD2	1:A:276:ARG:NH1	2.44	0.50
1:E:15:THR:HG21	1:E:51:ILE:HD13	1.92	0.50
1:F:15:THR:OG1	1:F:223:MET:HE1	2.09	0.50
1:O:15:THR:HG21	1:O:51:ILE:HD13	1.92	0.50
1:B:41:MET:HE1	1:B:64:LYS:CG	2.41	0.50
1:D:15:THR:CG2	1:D:51:ILE:HD13	2.41	0.50
1:E:41:MET:HE1	1:E:64:LYS:CG	2.41	0.50
1:G:15:THR:CG2	1:G:51:ILE:HD13	2.42	0.50
1:R:15:THR:CG2	1:R:51:ILE:HD13	2.41	0.50
1:C:41:MET:HE1	1:C:64:LYS:HG2	1.92	0.50
1:G:41:MET:HE1	1:G:64:LYS:CG	2.41	0.50
1:B:15:THR:CG2	1:B:51:ILE:HD13	2.42	0.50
1:B:268:ASP:OD2	1:B:276:ARG:NH1	2.44	0.50
1:L:12:VAL:HA	1:L:223:MET:HE2	1.94	0.50
1:L:15:THR:CG2	1:L:51:ILE:HD13	2.41	0.50
1:Q:15:THR:HG21	1:Q:51:ILE:HD13	1.92	0.50
1:L:202:THR:HG22	1:L:203:TYR:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:202:THR:HG22	1:Q:203:TYR:H	1.77	0.50
1:F:12:VAL:HA	1:F:223:MET:HE2	1.94	0.50
1:G:202:THR:HG22	1:G:203:TYR:H	1.76	0.50
1:H:15:THR:CG2	1:H:51:ILE:HD13	2.41	0.50
1:I:15:THR:CG2	1:I:51:ILE:HD13	2.42	0.50
1:M:202:THR:HG22	1:M:203:TYR:H	1.77	0.50
1:N:15:THR:CG2	1:N:51:ILE:HD13	2.42	0.50
1:F:202:THR:HG22	1:F:203:TYR:H	1.77	0.50
1:H:12:VAL:HA	1:H:223:MET:HE2	1.94	0.50
1:K:12:VAL:HA	1:K:223:MET:HE2	1.94	0.50
1:R:202:THR:HG22	1:R:203:TYR:H	1.77	0.50
1:B:15:THR:HG21	1:B:51:ILE:HD13	1.93	0.49
1:R:12:VAL:HA	1:R:223:MET:HE2	1.94	0.49
1:K:202:THR:HG22	1:K:203:TYR:H	1.77	0.49
1:C:15:THR:CG2	1:C:51:ILE:HD13	2.42	0.49
1:O:15:THR:CG2	1:O:51:ILE:HD13	2.42	0.49
1:Q:12:VAL:HA	1:Q:223:MET:HE2	1.94	0.49
1:M:15:THR:CG2	1:M:51:ILE:HD13	2.42	0.49
1:I:202:THR:HG22	1:I:203:TYR:H	1.77	0.49
1:J:12:VAL:HA	1:J:223:MET:HE2	1.94	0.49
1:P:202:THR:HG22	1:P:203:TYR:H	1.77	0.49
1:N:12:VAL:HA	1:N:223:MET:HE2	1.95	0.49
1:B:12:VAL:HA	1:B:223:MET:HE2	1.95	0.49
1:O:12:VAL:HA	1:O:223:MET:HE2	1.94	0.49
1:P:15:THR:CG2	1:P:51:ILE:HD13	2.42	0.49
1:M:12:VAL:HA	1:M:223:MET:HE2	1.94	0.49
1:O:159:ILE:HD11	1:Q:281:VAL:HA	1.95	0.49
1:R:3:LYS:HB3	1:R:30:ILE:HD11	1.95	0.49
1:G:12:VAL:HA	1:G:223:MET:HE2	1.94	0.49
1:E:12:VAL:HA	1:E:223:MET:HE2	1.94	0.49
1:J:3:LYS:HB3	1:J:30:ILE:HD11	1.95	0.49
1:F:3:LYS:HB3	1:F:30:ILE:HD11	1.95	0.48
1:A:12:VAL:HG11	1:A:227:TYR:HB2	1.95	0.48
1:A:15:THR:CG2	1:A:51:ILE:HD13	2.42	0.48
1:Q:3:LYS:HB3	1:Q:30:ILE:HD11	1.95	0.48
1:M:3:LYS:HB3	1:M:30:ILE:HD11	1.95	0.48
1:D:12:VAL:HA	1:D:223:MET:HE2	1.94	0.48
1:D:47:ASN:CG	1:D:90:ILE:HD11	2.39	0.48
1:I:12:VAL:HA	1:I:223:MET:HE2	1.94	0.48
1:M:12:VAL:HG11	1:M:227:TYR:HB2	1.96	0.48
1:N:3:LYS:HB3	1:N:30:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:12:VAL:HA	1:P:223:MET:HE2	1.95	0.48
1:A:12:VAL:HA	1:A:223:MET:HE2	1.95	0.48
1:C:12:VAL:HA	1:C:223:MET:HE2	1.94	0.48
1:G:12:VAL:HG11	1:G:227:TYR:HB2	1.96	0.48
1:N:47:ASN:CG	1:N:90:ILE:HD11	2.39	0.48
1:B:12:VAL:HG11	1:B:227:TYR:HB2	1.95	0.48
1:D:3:LYS:HB3	1:D:30:ILE:HD11	1.95	0.48
1:G:3:LYS:HB3	1:G:30:ILE:HD11	1.96	0.48
1:J:160:HIS:HB2	1:P:281:VAL:CG2	2.44	0.48
1:E:12:VAL:HG11	1:E:227:TYR:HB2	1.96	0.48
1:G:47:ASN:CG	1:G:90:ILE:HD11	2.39	0.48
1:I:3:LYS:HB3	1:I:30:ILE:HD11	1.96	0.48
1:L:47:ASN:CG	1:L:90:ILE:HD11	2.39	0.48
1:O:47:ASN:CG	1:O:90:ILE:HD11	2.39	0.48
1:P:12:VAL:HG11	1:P:227:TYR:HB2	1.96	0.48
1:F:47:ASN:CG	1:F:90:ILE:HD11	2.39	0.48
1:G:281:VAL:HA	1:L:159:ILE:HD11	1.96	0.48
1:C:47:ASN:CG	1:C:90:ILE:HD11	2.39	0.48
1:H:12:VAL:HG11	1:H:227:TYR:HB2	1.96	0.48
1:I:12:VAL:HG11	1:I:227:TYR:HB2	1.96	0.48
1:L:3:LYS:HB3	1:L:30:ILE:HD11	1.95	0.48
1:O:12:VAL:HG11	1:O:227:TYR:HB2	1.95	0.48
1:D:12:VAL:HG11	1:D:227:TYR:HB2	1.96	0.47
1:N:12:VAL:HG11	1:N:227:TYR:HB2	1.95	0.47
1:Q:12:VAL:HG11	1:Q:227:TYR:HB2	1.96	0.47
1:Q:47:ASN:CG	1:Q:90:ILE:HD11	2.39	0.47
1:C:159:ILE:CD1	1:I:284:LEU:HD22	2.44	0.47
1:K:3:LYS:HB3	1:K:30:ILE:HD11	1.95	0.47
1:M:47:ASN:CG	1:M:90:ILE:HD11	2.39	0.47
1:O:3:LYS:HB3	1:O:30:ILE:HD11	1.96	0.47
1:A:47:ASN:CG	1:A:90:ILE:HD11	2.39	0.47
1:C:200:LEU:HD13	1:C:238:LEU:HG	1.96	0.47
1:E:47:ASN:CG	1:E:90:ILE:HD11	2.39	0.47
1:J:197:LEU:HB2	1:P:284:LEU:HD23	1.96	0.47
1:L:12:VAL:HG11	1:L:227:TYR:HB2	1.96	0.47
1:P:3:LYS:HB3	1:P:30:ILE:HD11	1.97	0.47
1:B:3:LYS:HB3	1:B:30:ILE:HD11	1.96	0.47
1:B:47:ASN:CG	1:B:90:ILE:HD11	2.39	0.47
1:H:47:ASN:CG	1:H:90:ILE:HD11	2.39	0.47
1:R:47:ASN:CG	1:R:90:ILE:HD11	2.39	0.47
1:R:130:MET:HE2	1:R:181:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:HB3	1:C:30:ILE:HD11	1.96	0.47
1:C:12:VAL:HG11	1:C:227:TYR:HB2	1.95	0.47
1:C:159:ILE:HD11	1:I:281:VAL:HA	1.96	0.47
1:G:130:MET:HE2	1:G:181:LEU:CD2	2.45	0.47
1:I:130:MET:HE2	1:I:181:LEU:CD2	2.45	0.47
1:J:47:ASN:CG	1:J:90:ILE:HD11	2.39	0.47
1:B:285:ASN:OD1	1:D:198:GLN:HA	2.14	0.47
1:I:47:ASN:CG	1:I:90:ILE:HD11	2.39	0.47
1:A:159:ILE:HD12	1:E:284:LEU:HD22	1.95	0.47
1:A:298:ASP:OD1	1:G:74:SER:HB2	2.14	0.47
1:E:3:LYS:HB3	1:E:30:ILE:HD11	1.96	0.47
1:E:130:MET:HE2	1:E:181:LEU:CD2	2.45	0.47
1:H:3:LYS:HB3	1:H:30:ILE:HD11	1.95	0.47
1:H:130:MET:HE2	1:H:181:LEU:CD2	2.45	0.47
1:K:47:ASN:CG	1:K:90:ILE:HD11	2.39	0.47
1:K:281:VAL:HA	1:N:159:ILE:HD11	1.96	0.47
1:M:130:MET:HE2	1:M:181:LEU:CD2	2.45	0.47
1:N:130:MET:HE2	1:N:181:LEU:CD2	2.45	0.47
1:A:3:LYS:HB3	1:A:30:ILE:HD11	1.96	0.47
1:P:130:MET:HE2	1:P:181:LEU:CD2	2.45	0.47
1:B:120:LYS:HD3	1:C:213:ASN:CG	2.40	0.47
1:C:130:MET:HE2	1:C:181:LEU:CD2	2.45	0.47
1:F:130:MET:HE2	1:F:181:LEU:CD2	2.45	0.47
1:K:12:VAL:HG11	1:K:227:TYR:HB2	1.96	0.47
1:P:47:ASN:CG	1:P:90:ILE:HD11	2.39	0.47
1:Q:130:MET:HE2	1:Q:181:LEU:CD2	2.45	0.47
1:O:130:MET:HE2	1:O:181:LEU:CD2	2.45	0.46
1:A:130:MET:HE2	1:A:181:LEU:CD2	2.45	0.46
1:D:130:MET:HE2	1:D:181:LEU:CD2	2.45	0.46
1:B:159:ILE:HD11	1:D:281:VAL:HA	1.96	0.46
1:F:12:VAL:HG11	1:F:227:TYR:HB2	1.97	0.46
1:J:12:VAL:HG11	1:J:227:TYR:HB2	1.97	0.46
1:K:130:MET:HE2	1:K:181:LEU:CD2	2.45	0.46
1:B:130:MET:HE2	1:B:181:LEU:CD2	2.45	0.46
1:J:130:MET:HE2	1:J:181:LEU:CD2	2.45	0.46
1:P:212:LEU:HD22	1:P:315:LYS:HE3	1.97	0.46
1:G:159:ILE:HD12	1:L:284:LEU:HD22	1.97	0.46
1:L:130:MET:HE2	1:L:181:LEU:CD2	2.45	0.46
1:B:159:ILE:CD1	1:D:284:LEU:HD22	2.46	0.46
1:A:126:PRO:CG	1:A:130:MET:HE1	2.46	0.45
1:B:126:PRO:CG	1:B:130:MET:HE1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:PRO:CG	1:K:130:MET:HE1	2.47	0.45
1:O:126:PRO:CG	1:O:130:MET:HE1	2.47	0.45
1:B:159:ILE:HG12	1:D:281:VAL:HG22	1.99	0.45
1:R:12:VAL:HG11	1:R:227:TYR:HB2	1.97	0.45
1:M:126:PRO:CG	1:M:130:MET:HE1	2.47	0.45
1:A:200:LEU:HD13	1:A:238:LEU:HG	1.98	0.45
1:C:126:PRO:CG	1:C:130:MET:HE1	2.46	0.45
1:E:191:ILE:HD11	1:E:251:VAL:HG11	1.99	0.45
1:G:126:PRO:CG	1:G:130:MET:HE1	2.47	0.45
1:E:126:PRO:CG	1:E:130:MET:HE1	2.47	0.45
1:G:191:ILE:HD11	1:G:251:VAL:HG11	1.99	0.45
1:J:126:PRO:CG	1:J:130:MET:HE1	2.47	0.45
1:C:191:ILE:HD11	1:C:251:VAL:HG11	1.99	0.44
1:R:126:PRO:CG	1:R:130:MET:HE1	2.47	0.44
1:D:191:ILE:HD11	1:D:251:VAL:HG11	2.00	0.44
1:M:281:VAL:HA	1:R:159:ILE:HD11	1.97	0.44
1:F:191:ILE:HD11	1:F:251:VAL:HG11	1.99	0.44
1:N:191:ILE:HD11	1:N:251:VAL:HG11	2.00	0.44
1:P:191:ILE:HD11	1:P:251:VAL:HG11	1.99	0.44
1:B:261:LEU:HD11	1:D:295:VAL:HG11	1.98	0.44
1:L:126:PRO:CG	1:L:130:MET:HE1	2.47	0.44
1:F:126:PRO:CG	1:F:130:MET:HE1	2.46	0.44
1:Q:191:ILE:HD11	1:Q:251:VAL:HG11	2.00	0.44
1:F:15:THR:HG21	1:F:223:MET:HE1	2.00	0.44
1:J:191:ILE:HD11	1:J:251:VAL:HG11	1.99	0.44
1:L:191:ILE:HD11	1:L:251:VAL:HG11	1.99	0.44
1:O:191:ILE:HD11	1:O:251:VAL:HG11	2.00	0.44
1:Q:126:PRO:CG	1:Q:130:MET:HE1	2.47	0.44
1:C:245:ASP:N	1:C:246:PRO:CD	2.81	0.44
1:H:126:PRO:CG	1:H:130:MET:HE1	2.47	0.44
1:K:245:ASP:N	1:K:246:PRO:CD	2.81	0.44
1:M:191:ILE:HD11	1:M:251:VAL:HG11	2.00	0.44
1:O:245:ASP:N	1:O:246:PRO:CD	2.81	0.44
1:P:126:PRO:CG	1:P:130:MET:HE1	2.46	0.44
1:D:245:ASP:N	1:D:246:PRO:CD	2.81	0.43
1:H:191:ILE:HD11	1:H:251:VAL:HG11	1.99	0.43
1:I:245:ASP:N	1:I:246:PRO:CD	2.81	0.43
1:M:245:ASP:N	1:M:246:PRO:CD	2.81	0.43
1:N:126:PRO:CG	1:N:130:MET:HE1	2.47	0.43
1:Q:245:ASP:N	1:Q:246:PRO:CD	2.81	0.43
1:A:245:ASP:N	1:A:246:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:THR:HG21	1:I:223:MET:HE1	2.01	0.43
1:O:266:GLN:NE2	1:Q:160:HIS:NE2	2.67	0.43
1:R:245:ASP:N	1:R:246:PRO:CD	2.81	0.43
1:C:281:VAL:HA	1:I:159:ILE:HD11	2.01	0.43
1:I:126:PRO:CG	1:I:130:MET:HE1	2.47	0.43
1:K:15:THR:HG21	1:K:223:MET:HE1	2.00	0.43
1:L:245:ASP:N	1:L:246:PRO:CD	2.81	0.43
1:Q:15:THR:HG21	1:Q:223:MET:HE1	2.00	0.43
1:B:15:THR:HG21	1:B:223:MET:HE1	2.01	0.43
1:B:245:ASP:N	1:B:246:PRO:CD	2.81	0.43
1:C:15:THR:HG21	1:C:223:MET:HE1	2.01	0.43
1:J:245:ASP:N	1:J:246:PRO:CD	2.82	0.43
1:O:15:THR:HG21	1:O:223:MET:HE1	2.01	0.43
1:R:15:THR:HG21	1:R:223:MET:HE1	2.00	0.43
1:F:245:ASP:N	1:F:246:PRO:CD	2.81	0.43
1:H:245:ASP:N	1:H:246:PRO:CD	2.81	0.43
1:B:191:ILE:HD11	1:B:251:VAL:HG11	2.00	0.43
1:A:15:THR:HG21	1:A:223:MET:HE1	2.01	0.43
1:D:126:PRO:CG	1:D:130:MET:HE1	2.47	0.43
1:D:213:ASN:HD22	1:I:141:PRO:HG3	1.83	0.43
1:H:15:THR:HG21	1:H:223:MET:HE1	2.00	0.43
1:A:191:ILE:HD11	1:A:251:VAL:HG11	1.99	0.43
1:D:15:THR:HG21	1:D:223:MET:HE1	2.00	0.43
1:G:245:ASP:N	1:G:246:PRO:CD	2.81	0.43
1:N:15:THR:HG21	1:N:223:MET:HE1	2.00	0.43
1:N:245:ASP:N	1:N:246:PRO:CD	2.81	0.43
1:P:15:THR:HG21	1:P:223:MET:HE1	2.01	0.43
1:I:191:ILE:HD11	1:I:251:VAL:HG11	1.99	0.43
1:P:245:ASP:N	1:P:246:PRO:CD	2.81	0.43
1:J:284:LEU:HD22	1:P:159:ILE:CD1	2.49	0.42
1:E:245:ASP:N	1:E:246:PRO:CD	2.82	0.42
1:J:15:THR:HG21	1:J:223:MET:HE1	2.01	0.42
1:G:15:THR:HG21	1:G:223:MET:HE1	2.01	0.42
1:L:15:THR:HG21	1:L:223:MET:HE1	2.01	0.42
1:M:15:THR:HG21	1:M:223:MET:HE1	2.01	0.42
1:R:191:ILE:HD11	1:R:251:VAL:HG11	2.00	0.42
1:K:191:ILE:HD11	1:K:251:VAL:HG11	2.00	0.42
1:E:15:THR:HG21	1:E:223:MET:HE1	2.01	0.41
1:P:300:PRO:HG2	1:Q:87:ASP:OD1	2.20	0.41
1:A:26:GLU:OE1	1:A:309:ARG:NH2	2.54	0.41
1:O:281:VAL:CG2	1:Q:160:HIS:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:26:GLU:OE1	1:R:309:ARG:NH2	2.54	0.41
1:K:26:GLU:OE1	1:K:309:ARG:NH2	2.54	0.41
1:M:26:GLU:OE1	1:M:309:ARG:NH2	2.54	0.41
1:O:26:GLU:OE1	1:O:309:ARG:NH2	2.54	0.41
1:B:26:GLU:OE1	1:B:309:ARG:NH2	2.54	0.41
1:E:26:GLU:OE1	1:E:309:ARG:NH2	2.54	0.41
1:G:26:GLU:OE1	1:G:309:ARG:NH2	2.54	0.41
1:H:26:GLU:OE1	1:H:309:ARG:NH2	2.54	0.41
1:I:26:GLU:OE1	1:I:309:ARG:NH2	2.54	0.41
1:Q:26:GLU:OE1	1:Q:309:ARG:NH2	2.54	0.41
1:D:26:GLU:OE1	1:D:309:ARG:NH2	2.54	0.41
1:F:26:GLU:OE1	1:F:309:ARG:NH2	2.54	0.40
1:L:26:GLU:OE1	1:L:309:ARG:NH2	2.54	0.40
1:P:26:GLU:OE1	1:P:309:ARG:NH2	2.54	0.40
1:H:212:LEU:HD22	1:H:315:LYS:CG	2.52	0.40
1:J:26:GLU:OE1	1:J:309:ARG:NH2	2.54	0.40
1:B:261:LEU:CD1	1:D:295:VAL:HG11	2.51	0.40
1:E:11:GLY:O	1:E:15:THR:HG23	2.22	0.40
1:J:201:LEU:HG	1:J:243:LEU:HD21	2.04	0.40
1:H:11:GLY:O	1:H:15:THR:HG23	2.22	0.40
1:H:212:LEU:HD22	1:H:315:LYS:HG3	2.03	0.40
1:K:201:LEU:HG	1:K:243:LEU:HD21	2.04	0.40
1:L:201:LEU:HG	1:L:243:LEU:HD21	2.04	0.40
1:C:261:LEU:O	1:C:263:ILE:HG22	2.22	0.40
1:L:11:GLY:O	1:L:15:THR:HG23	2.22	0.40
1:Q:11:GLY:O	1:Q:15:THR:HG23	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:N	1:M:213:ASN:ND2[1_454]	1.96	0.24
1:J:304:ASN:OD1	1:R:204:LYS:CB[2_8514]	1.99	0.21
1:J:304:ASN:CG	1:R:204:LYS:CB[2_8514]	2.08	0.12
1:L:109:ASP:CG	1:M:76:GLU:OE2[2_9414]	2.15	0.05
1:C:141:PRO:C	1:M:213:ASN:ND2[1_454]	2.19	0.01

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	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	B	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	C	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	D	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	E	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	F	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	G	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	H	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	I	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	J	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	K	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	L	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	M	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	N	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	O	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	P	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	Q	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
1	R	314/321 (98%)	295 (94%)	19 (6%)	0	100	100
All	All	5652/5778 (98%)	5310 (94%)	342 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	255/263 (97%)	247 (97%)	8 (3%)	35	69
1	B	257/263 (98%)	249 (97%)	8 (3%)	35	69
1	C	257/263 (98%)	249 (97%)	8 (3%)	35	69
1	D	257/263 (98%)	249 (97%)	8 (3%)	35	69
1	E	254/263 (97%)	246 (97%)	8 (3%)	35	69
1	F	254/263 (97%)	244 (96%)	10 (4%)	28	63
1	G	254/263 (97%)	246 (97%)	8 (3%)	35	69
1	H	254/263 (97%)	246 (97%)	8 (3%)	35	69
1	I	253/263 (96%)	245 (97%)	8 (3%)	34	68
1	J	252/263 (96%)	243 (96%)	9 (4%)	31	65
1	K	253/263 (96%)	244 (96%)	9 (4%)	31	65
1	L	255/263 (97%)	247 (97%)	8 (3%)	35	69
1	M	252/263 (96%)	244 (97%)	8 (3%)	34	68
1	N	252/263 (96%)	244 (97%)	8 (3%)	34	68
1	O	255/263 (97%)	248 (97%)	7 (3%)	39	73
1	P	255/263 (97%)	246 (96%)	9 (4%)	32	66
1	Q	253/263 (96%)	245 (97%)	8 (3%)	34	68
1	R	252/263 (96%)	244 (97%)	8 (3%)	34	68
All	All	4574/4734 (97%)	4426 (97%)	148 (3%)	34	68

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	153	MET
1	A	159	ILE
1	A	173	GLN
1	A	194	ASP
1	A	201	LEU
1	A	258	VAL
1	A	282	THR
1	B	10	THR
1	B	100	ARG
1	B	153	MET

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Mol	Chain	Res	Type
1	B	159	ILE
1	B	173	GLN
1	B	194	ASP
1	B	201	LEU
1	B	258	VAL
1	C	10	THR
1	C	153	MET
1	C	159	ILE
1	C	173	GLN
1	C	194	ASP
1	C	201	LEU
1	C	258	VAL
1	C	282	THR
1	D	10	THR
1	D	153	MET
1	D	159	ILE
1	D	173	GLN
1	D	194	ASP
1	D	201	LEU
1	D	258	VAL
1	D	282	THR
1	E	10	THR
1	E	100	ARG
1	E	153	MET
1	E	159	ILE
1	E	173	GLN
1	E	194	ASP
1	E	201	LEU
1	E	258	VAL
1	F	10	THR
1	F	72	LYS
1	F	100	ARG
1	F	153	MET
1	F	159	ILE
1	F	173	GLN
1	F	194	ASP
1	F	201	LEU
1	F	258	VAL
1	F	282	THR
1	G	10	THR
1	G	100	ARG
1	G	153	MET

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Mol	Chain	Res	Type
1	G	159	ILE
1	G	173	GLN
1	G	194	ASP
1	G	201	LEU
1	G	258	VAL
1	H	10	THR
1	H	153	MET
1	H	159	ILE
1	H	173	GLN
1	H	194	ASP
1	H	201	LEU
1	H	258	VAL
1	H	282	THR
1	I	10	THR
1	I	153	MET
1	I	159	ILE
1	I	173	GLN
1	I	194	ASP
1	I	201	LEU
1	I	258	VAL
1	I	282	THR
1	J	10	THR
1	J	100	ARG
1	J	153	MET
1	J	159	ILE
1	J	173	GLN
1	J	194	ASP
1	J	201	LEU
1	J	258	VAL
1	J	282	THR
1	K	10	THR
1	K	100	ARG
1	K	153	MET
1	K	159	ILE
1	K	173	GLN
1	K	194	ASP
1	K	201	LEU
1	K	258	VAL
1	K	282	THR
1	L	10	THR
1	L	100	ARG
1	L	153	MET

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Mol	Chain	Res	Type
1	L	159	ILE
1	L	173	GLN
1	L	194	ASP
1	L	201	LEU
1	L	258	VAL
1	M	10	THR
1	M	76	GLU
1	M	153	MET
1	M	159	ILE
1	M	173	GLN
1	M	194	ASP
1	M	201	LEU
1	M	258	VAL
1	N	10	THR
1	N	100	ARG
1	N	153	MET
1	N	159	ILE
1	N	173	GLN
1	N	194	ASP
1	N	201	LEU
1	N	258	VAL
1	O	10	THR
1	O	153	MET
1	O	159	ILE
1	O	173	GLN
1	O	194	ASP
1	O	201	LEU
1	O	258	VAL
1	P	10	THR
1	P	100	ARG
1	P	153	MET
1	P	159	ILE
1	P	173	GLN
1	P	194	ASP
1	P	201	LEU
1	P	258	VAL
1	P	282	THR
1	Q	10	THR
1	Q	100	ARG
1	Q	153	MET
1	Q	159	ILE
1	Q	173	GLN

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Mol	Chain	Res	Type
1	Q	194	ASP
1	Q	201	LEU
1	Q	258	VAL
1	R	10	THR
1	R	100	ARG
1	R	153	MET
1	R	159	ILE
1	R	173	GLN
1	R	194	ASP
1	R	201	LEU
1	R	258	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	266	GLN
1	B	213	ASN
1	B	266	GLN
1	C	213	ASN
1	C	266	GLN
1	D	213	ASN
1	D	266	GLN
1	E	213	ASN
1	F	213	ASN
1	F	266	GLN
1	G	213	ASN
1	G	266	GLN
1	H	213	ASN
1	H	266	GLN
1	I	213	ASN
1	I	266	GLN
1	J	213	ASN
1	J	266	GLN
1	K	266	GLN
1	L	213	ASN
1	L	266	GLN
1	M	213	ASN
1	M	266	GLN
1	N	213	ASN
1	N	266	GLN
1	O	213	ASN

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Mol	Chain	Res	Type
1	O	266	GLN
1	P	213	ASN
1	P	266	GLN
1	Q	213	ASN
1	R	213	ASN
1	R	266	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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, 95th 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 ²)	Q<0.9
1	A	316/321 (98%)	0.78	24 (7%) 20 16	20, 30, 41, 47	0
1	B	316/321 (98%)	1.17	37 (11%) 9 8	26, 37, 51, 60	0
1	C	316/321 (98%)	0.74	16 (5%) 33 26	23, 33, 46, 51	0
1	D	316/321 (98%)	1.04	35 (11%) 10 9	25, 37, 59, 72	0
1	E	316/321 (98%)	0.88	25 (7%) 18 15	30, 39, 54, 101	0
1	F	316/321 (98%)	0.94	26 (8%) 17 14	29, 39, 51, 56	0
1	G	316/321 (98%)	0.94	22 (6%) 22 18	27, 39, 56, 72	0
1	H	316/321 (98%)	0.88	29 (9%) 14 12	31, 41, 64, 121	0
1	I	316/321 (98%)	1.20	53 (16%) 4 3	26, 42, 73, 96	0
1	J	316/321 (98%)	1.33	62 (19%) 3 2	26, 42, 80, 150	0
1	K	316/321 (98%)	1.18	37 (11%) 9 8	35, 50, 68, 78	0
1	L	316/321 (98%)	1.23	44 (13%) 6 5	34, 50, 69, 83	0
1	M	316/321 (98%)	1.35	66 (20%) 2 2	28, 45, 91, 121	0
1	N	316/321 (98%)	1.04	37 (11%) 9 8	36, 49, 68, 94	0
1	O	316/321 (98%)	0.94	15 (4%) 36 28	27, 41, 62, 74	0
1	P	316/321 (98%)	1.17	42 (13%) 7 6	27, 44, 68, 81	0
1	Q	316/321 (98%)	1.25	44 (13%) 6 5	33, 47, 68, 118	0
1	R	316/321 (98%)	1.75	109 (34%) 1 1	44, 62, 87, 104	0
All	All	5688/5778 (98%)	1.10	723 (12%) 8 6	20, 42, 69, 150	0

All (723) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	240	GLY	8.2
1	I	238	LEU	7.7
1	B	238	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
1	M	240	GLY	6.6
1	M	91	GLY	6.4
1	J	236	PRO	6.3
1	J	240	GLY	6.2
1	Q	238	LEU	6.0
1	J	235	ALA	5.9
1	I	317	ALA	5.8
1	R	235	ALA	5.8
1	J	239	GLY	5.8
1	E	91	GLY	5.7
1	M	238	LEU	5.6
1	I	225	ASP	5.5
1	J	238	LEU	5.5
1	H	236	PRO	5.4
1	F	200	LEU	5.3
1	E	240	GLY	5.3
1	R	317	ALA	5.2
1	I	240	GLY	5.1
1	Q	237	HIS	5.1
1	H	240	GLY	5.0
1	D	240	GLY	5.0
1	R	137	LEU	4.9
1	B	237	HIS	4.8
1	M	228	ILE	4.7
1	J	317	ALA	4.7
1	N	236	PRO	4.7
1	Q	240	GLY	4.6
1	P	91	GLY	4.6
1	J	237	HIS	4.5
1	R	209	TRP	4.5
1	H	235	ALA	4.5
1	Q	236	PRO	4.5
1	Q	239	GLY	4.5
1	I	237	HIS	4.5
1	E	236	PRO	4.4
1	O	91	GLY	4.4
1	M	239	GLY	4.4
1	P	86	GLY	4.4
1	J	203	TYR	4.4
1	J	202	THR	4.3
1	R	71	THR	4.3
1	F	199	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	238	LEU	4.3
1	J	228	ILE	4.3
1	A	237	HIS	4.3
1	B	240	GLY	4.3
1	R	80	ILE	4.2
1	M	237	HIS	4.2
1	E	235	ALA	4.2
1	R	95	ILE	4.2
1	J	200	LEU	4.2
1	G	317	ALA	4.1
1	E	237	HIS	4.1
1	J	303	LEU	4.1
1	I	236	PRO	4.1
1	Q	235	ALA	4.1
1	C	237	HIS	4.0
1	L	91	GLY	4.0
1	J	231	TYR	4.0
1	I	215	LYS	4.0
1	H	237	HIS	3.9
1	E	80	ILE	3.9
1	F	235	ALA	3.9
1	B	286	ASP	3.9
1	O	86	GLY	3.9
1	R	200	LEU	3.9
1	M	203	TYR	3.9
1	R	148	GLY	3.9
1	Q	233	THR	3.9
1	J	241	CYS	3.9
1	I	81	SER	3.9
1	O	238	LEU	3.8
1	I	44	GLY	3.8
1	M	79	PRO	3.8
1	J	206	THR	3.8
1	B	91	GLY	3.8
1	G	240	GLY	3.8
1	F	161	GLY	3.8
1	P	106	SER	3.7
1	A	80	ILE	3.7
1	J	225	ASP	3.7
1	M	80	ILE	3.7
1	E	238	LEU	3.7
1	M	317	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	213	ASN	3.7
1	M	233	THR	3.7
1	N	238	LEU	3.7
1	M	218	LYS	3.6
1	N	237	HIS	3.6
1	R	233	THR	3.6
1	N	239	GLY	3.6
1	R	211	ASP	3.6
1	O	213	ASN	3.6
1	M	241	CYS	3.6
1	L	237	HIS	3.6
1	I	218	LYS	3.6
1	F	91	GLY	3.6
1	R	240	GLY	3.6
1	R	236	PRO	3.6
1	M	242	GLY	3.5
1	R	13	ASP	3.5
1	I	213	ASN	3.5
1	J	233	THR	3.5
1	D	30	ILE	3.5
1	H	238	LEU	3.5
1	K	236	PRO	3.5
1	J	216	ALA	3.5
1	B	242	GLY	3.5
1	R	212	LEU	3.5
1	J	67	SER	3.5
1	I	209	TRP	3.5
1	J	209	TRP	3.5
1	J	226	PHE	3.4
1	I	232	GLU	3.4
1	M	210	ARG	3.4
1	M	209	TRP	3.4
1	H	234	THR	3.4
1	Q	80	ILE	3.4
1	R	75	PHE	3.4
1	A	91	GLY	3.4
1	N	235	ALA	3.4
1	E	233	THR	3.4
1	I	233	THR	3.4
1	M	229	LYS	3.4
1	P	239	GLY	3.4
1	R	242	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	236	PRO	3.4
1	P	237	HIS	3.4
1	R	81	SER	3.4
1	A	213	ASN	3.4
1	N	213	ASN	3.4
1	Q	91	GLY	3.4
1	I	203	TYR	3.4
1	K	154	GLY	3.3
1	R	83	PHE	3.3
1	J	222	ASP	3.3
1	E	86	GLY	3.3
1	K	240	GLY	3.3
1	R	232	GLU	3.3
1	J	207	LYS	3.3
1	I	206	THR	3.3
1	R	234	THR	3.3
1	C	239	GLY	3.3
1	I	312	GLY	3.3
1	J	113	ASP	3.3
1	M	84	ILE	3.3
1	D	311	SER	3.3
1	G	67	SER	3.3
1	E	73	ASP	3.2
1	J	234	THR	3.2
1	M	231	TYR	3.2
1	O	80	ILE	3.2
1	H	215	LYS	3.2
1	J	232	GLU	3.2
1	J	229	LYS	3.2
1	G	239	GLY	3.2
1	B	199	THR	3.2
1	M	94	GLU	3.2
1	Q	232	GLU	3.2
1	P	102	ALA	3.2
1	P	68	HIS	3.2
1	R	306	PHE	3.2
1	J	39	VAL	3.2
1	B	236	PRO	3.2
1	P	238	LEU	3.1
1	L	215	LYS	3.1
1	M	204	LYS	3.1
1	R	315	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	R	87	ASP	3.1
1	L	236	PRO	3.1
1	M	212	LEU	3.1
1	O	317	ALA	3.1
1	D	237	HIS	3.1
1	R	115	VAL	3.1
1	M	206	THR	3.1
1	Q	78	LEU	3.1
1	I	204	LYS	3.1
1	I	228	ILE	3.1
1	J	210	ARG	3.1
1	P	72	LYS	3.1
1	O	85	HIS	3.0
1	J	31	GLY	3.0
1	B	228	ILE	3.0
1	L	233	THR	3.0
1	J	92	ASP	3.0
1	D	91	GLY	3.0
1	E	239	GLY	3.0
1	J	218	LYS	3.0
1	R	84	ILE	3.0
1	R	229	LYS	3.0
1	I	55	LEU	3.0
1	N	224	THR	3.0
1	Q	234	THR	3.0
1	I	229	LYS	3.0
1	J	215	LYS	3.0
1	A	238	LEU	3.0
1	B	233	THR	3.0
1	J	219	PHE	3.0
1	L	204	LYS	3.0
1	F	239	GLY	3.0
1	R	69	ALA	3.0
1	R	77	VAL	3.0
1	F	237	HIS	3.0
1	P	80	ILE	2.9
1	R	310	ILE	2.9
1	K	212	LEU	2.9
1	B	231	TYR	2.9
1	D	213	ASN	2.9
1	H	83	PHE	2.9
1	I	226	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	214	THR	2.9
1	M	214	THR	2.9
1	I	214	THR	2.9
1	M	224	THR	2.9
1	A	30	ILE	2.9
1	J	95	ILE	2.9
1	F	243	LEU	2.9
1	R	22	LEU	2.9
1	N	154	GLY	2.9
1	Q	204	LYS	2.9
1	I	222	ASP	2.9
1	P	39	VAL	2.9
1	J	83	PHE	2.9
1	B	85	HIS	2.9
1	Q	210	ARG	2.9
1	G	202	THR	2.9
1	A	242	GLY	2.8
1	B	287	PRO	2.8
1	B	39	VAL	2.8
1	L	83	PHE	2.8
1	R	73	ASP	2.8
1	L	80	ILE	2.8
1	K	239	GLY	2.8
1	N	240	GLY	2.8
1	M	236	PRO	2.8
1	Q	79	PRO	2.8
1	R	76	GLU	2.8
1	R	118	TYR	2.8
1	F	230	ALA	2.8
1	G	115	VAL	2.8
1	P	285	ASN	2.8
1	H	13	ASP	2.8
1	L	90	ILE	2.8
1	M	13	ASP	2.8
1	N	233	THR	2.8
1	M	315	LYS	2.8
1	J	221	ALA	2.8
1	R	201	LEU	2.8
1	H	73	ASP	2.8
1	A	86	GLY	2.8
1	H	239	GLY	2.8
1	N	99	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	227	TYR	2.8
1	I	221	ALA	2.8
1	N	226	PHE	2.8
1	J	212	LEU	2.8
1	H	68	HIS	2.8
1	A	233	THR	2.8
1	M	211	ASP	2.8
1	G	2	LYS	2.8
1	P	287	PRO	2.8
1	I	60	VAL	2.7
1	E	83	PHE	2.7
1	J	80	ILE	2.7
1	P	5	ILE	2.7
1	Q	203	TYR	2.7
1	E	215	LYS	2.7
1	I	15	THR	2.7
1	R	113	ASP	2.7
1	C	91	GLY	2.7
1	M	311	SER	2.7
1	E	39	VAL	2.7
1	K	288	VAL	2.7
1	H	241	CYS	2.7
1	Q	84	ILE	2.7
1	B	227	TYR	2.7
1	R	203	TYR	2.7
1	C	94	GLU	2.7
1	K	270	GLU	2.7
1	M	235	ALA	2.7
1	P	83	PHE	2.7
1	R	82	ALA	2.7
1	A	38	ASN	2.7
1	M	300	PRO	2.7
1	Q	179	ASP	2.7
1	R	96	PRO	2.7
1	F	232	GLU	2.7
1	M	232	GLU	2.7
1	Q	90	ILE	2.7
1	R	4	LEU	2.7
1	I	216	ALA	2.7
1	M	221	ALA	2.7
1	N	203	TYR	2.7
1	D	199	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	213	ASN	2.7
1	R	272	PRO	2.7
1	F	286	ASP	2.7
1	D	39	VAL	2.7
1	Q	39	VAL	2.7
1	N	69	ALA	2.6
1	Q	102	ALA	2.6
1	K	31	GLY	2.6
1	R	239	GLY	2.6
1	N	38	ASN	2.6
1	B	295	VAL	2.6
1	G	238	LEU	2.6
1	G	316	ILE	2.6
1	B	70	SER	2.6
1	B	15	THR	2.6
1	I	212	LEU	2.6
1	A	143	ILE	2.6
1	P	146	GLU	2.6
1	D	9	ASP	2.6
1	M	314	ALA	2.6
1	Q	317	ALA	2.6
1	J	70	SER	2.6
1	J	106	SER	2.6
1	H	244	HIS	2.6
1	B	203	TYR	2.6
1	H	154	GLY	2.6
1	L	56	GLY	2.6
1	C	144	LYS	2.6
1	R	207	LYS	2.6
1	I	297	VAL	2.6
1	L	93	VAL	2.6
1	M	199	THR	2.6
1	R	60	VAL	2.6
1	H	232	GLU	2.6
1	P	213	ASN	2.6
1	R	132	ASN	2.6
1	I	48	ALA	2.6
1	J	48	ALA	2.6
1	R	67	SER	2.6
1	R	68	HIS	2.6
1	M	200	LEU	2.6
1	Q	200	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	80	ILE	2.6
1	A	317	ALA	2.6
1	L	75	PHE	2.6
1	Q	69	ALA	2.6
1	D	67	SER	2.5
1	Q	2	LYS	2.5
1	R	161	GLY	2.5
1	A	231	TYR	2.5
1	I	227	TYR	2.5
1	R	238	LEU	2.5
1	F	156	ALA	2.5
1	J	314	ALA	2.5
1	F	213	ASN	2.5
1	R	88	ASN	2.5
1	N	113	ASP	2.5
1	P	92	ASP	2.5
1	Q	85	HIS	2.5
1	K	144	LYS	2.5
1	I	86	GLY	2.5
1	K	220	LEU	2.5
1	R	187	PRO	2.5
1	N	80	ILE	2.5
1	A	33	THR	2.5
1	H	233	THR	2.5
1	P	199	THR	2.5
1	M	69	ALA	2.5
1	I	38	ASN	2.5
1	C	73	ASP	2.5
1	P	121	ASP	2.5
1	K	70	SER	2.5
1	D	238	LEU	2.5
1	R	313	LEU	2.5
1	B	279	GLY	2.5
1	M	56	GLY	2.5
1	Q	228	ILE	2.5
1	R	271	GLY	2.5
1	L	195	VAL	2.5
1	D	83	PHE	2.5
1	A	230	ALA	2.5
1	H	317	ALA	2.5
1	Q	82	ALA	2.5
1	G	113	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	200	LEU	2.5
1	J	243	LEU	2.5
1	P	137	LEU	2.5
1	C	80	ILE	2.5
1	P	84	ILE	2.5
1	Q	93	VAL	2.5
1	H	202	THR	2.5
1	M	82	ALA	2.5
1	G	215	LYS	2.5
1	K	229	LYS	2.5
1	P	2	LYS	2.5
1	O	237	HIS	2.5
1	F	201	LEU	2.4
1	J	79	PRO	2.4
1	P	143	ILE	2.4
1	G	39	VAL	2.4
1	R	106	SER	2.4
1	Q	146	GLU	2.4
1	I	235	ALA	2.4
1	J	2	LYS	2.4
1	P	136	ALA	2.4
1	N	35	THR	2.4
1	N	199	THR	2.4
1	N	206	THR	2.4
1	P	202	THR	2.4
1	F	197	LEU	2.4
1	R	145	ASP	2.4
1	R	225	ASP	2.4
1	Q	106	SER	2.4
1	K	317	ALA	2.4
1	K	10	THR	2.4
1	K	71	THR	2.4
1	O	71	THR	2.4
1	M	55	LEU	2.4
1	B	170	ASN	2.4
1	L	84	ILE	2.4
1	R	30	ILE	2.4
1	J	217	GLY	2.4
1	L	39	VAL	2.4
1	Q	44	GLY	2.4
1	R	108	VAL	2.4
1	R	222	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	229	LYS	2.4
1	I	83	PHE	2.4
1	Q	70	SER	2.4
1	N	221	ALA	2.4
1	P	317	ALA	2.4
1	R	202	THR	2.4
1	L	68	HIS	2.4
1	K	40	LEU	2.4
1	M	304	ASN	2.4
1	P	99	PRO	2.4
1	H	242	GLY	2.4
1	L	269	VAL	2.4
1	B	92	ASP	2.4
1	L	109	ASP	2.4
1	R	104	ASP	2.4
1	R	179	ASP	2.4
1	Q	219	PHE	2.4
1	R	219	PHE	2.4
1	O	156	ALA	2.4
1	A	67	SER	2.4
1	R	311	SER	2.4
1	H	231	TYR	2.4
1	J	282	THR	2.4
1	L	199	THR	2.4
1	Q	199	THR	2.4
1	R	206	THR	2.4
1	J	201	LEU	2.4
1	L	89	GLY	2.3
1	E	9	ASP	2.3
1	J	306	PHE	2.3
1	D	216	ALA	2.3
1	D	221	ALA	2.3
1	P	69	ALA	2.3
1	B	198	GLN	2.3
1	M	81	SER	2.3
1	D	144	LYS	2.3
1	D	215	LYS	2.3
1	R	126	PRO	2.3
1	L	239	GLY	2.3
1	M	222	ASP	2.3
1	R	270	GLU	2.3
1	N	241	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	27	MET	2.3
1	L	78	LEU	2.3
1	P	81	SER	2.3
1	B	68	HIS	2.3
1	D	282	THR	2.3
1	F	30	ILE	2.3
1	R	282	THR	2.3
1	L	288	VAL	2.3
1	O	128	GLY	2.3
1	Q	155	GLY	2.3
1	M	75	PHE	2.3
1	I	17	ALA	2.3
1	D	87	ASP	2.3
1	H	9	ASP	2.3
1	Q	104	ASP	2.3
1	A	303	LEU	2.3
1	B	197	LEU	2.3
1	R	29	LEU	2.3
1	F	160	HIS	2.3
1	M	207	LYS	2.3
1	P	85	HIS	2.3
1	R	180	ILE	2.3
1	R	237	HIS	2.3
1	K	206	THR	2.3
1	I	210	ARG	2.3
1	P	231	TYR	2.3
1	I	79	PRO	2.3
1	I	239	GLY	2.3
1	L	154	GLY	2.3
1	L	312	GLY	2.3
1	E	232	GLU	2.3
1	H	216	ALA	2.3
1	N	94	GLU	2.3
1	N	230	ALA	2.3
1	N	222	ASP	2.3
1	C	2	LYS	2.3
1	F	207	LYS	2.3
1	G	218	LYS	2.3
1	B	51	ILE	2.3
1	N	90	ILE	2.3
1	K	199	THR	2.3
1	B	79	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	39	VAL	2.3
1	J	44	GLY	2.3
1	I	94	GLU	2.2
1	O	38	ASN	2.2
1	O	314	ALA	2.2
1	H	200	LEU	2.2
1	I	303	LEU	2.2
1	K	207	LYS	2.2
1	M	215	LYS	2.2
1	R	139	LYS	2.2
1	D	211	ASP	2.2
1	R	92	ASP	2.2
1	A	316	ILE	2.2
1	G	30	ILE	2.2
1	D	160	HIS	2.2
1	R	160	HIS	2.2
1	R	241	CYS	2.2
1	H	224	THR	2.2
1	R	224	THR	2.2
1	G	281	VAL	2.2
1	R	297	VAL	2.2
1	L	118	TYR	2.2
1	K	11	GLY	2.2
1	P	119	GLY	2.2
1	R	226	PHE	2.2
1	D	230	ALA	2.2
1	I	82	ALA	2.2
1	R	205	GLU	2.2
1	E	38	ASN	2.2
1	E	204	LYS	2.2
1	G	213	ASN	2.2
1	H	38	ASN	2.2
1	H	228	ILE	2.2
1	R	111	ILE	2.2
1	D	222	ASP	2.2
1	F	13	ASP	2.2
1	R	210	ARG	2.2
1	B	293	VAL	2.2
1	C	199	THR	2.2
1	M	202	THR	2.2
1	R	99	PRO	2.2
1	C	67	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	37	GLY	2.2
1	L	31	GLY	2.2
1	P	75	PHE	2.2
1	B	107	ALA	2.2
1	J	197	LEU	2.2
1	K	107	ALA	2.2
1	N	317	ALA	2.2
1	R	61	LYS	2.2
1	R	66	LEU	2.2
1	K	213	ASN	2.2
1	M	95	ILE	2.2
1	M	316	ILE	2.2
1	C	68	HIS	2.2
1	E	113	ASP	2.2
1	I	13	ASP	2.2
1	L	113	ASP	2.2
1	I	295	VAL	2.2
1	A	256	THR	2.2
1	K	202	THR	2.2
1	R	15	THR	2.2
1	R	52	THR	2.2
1	R	214	THR	2.2
1	G	86	GLY	2.2
1	L	2	LYS	2.2
1	C	200	LEU	2.2
1	I	201	LEU	2.2
1	R	8	LEU	2.2
1	B	94	GLU	2.2
1	L	105	GLU	2.2
1	N	216	ALA	2.2
1	P	216	ALA	2.2
1	R	105	GLU	2.2
1	K	264	ASN	2.2
1	J	244	HIS	2.2
1	D	236	PRO	2.2
1	N	123	VAL	2.2
1	I	202	THR	2.2
1	O	33	THR	2.2
1	I	207	LYS	2.2
1	K	56	GLY	2.2
1	K	161	GLY	2.2
1	L	217	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	81	SER	2.2
1	A	59	GLU	2.2
1	K	235	ALA	2.2
1	R	165	ALA	2.2
1	R	228	ILE	2.1
1	N	39	VAL	2.1
1	N	79	PRO	2.1
1	R	93	VAL	2.1
1	Q	109	ASP	2.1
1	B	189	THR	2.1
1	D	234	THR	2.1
1	E	234	THR	2.1
1	J	204	LYS	2.1
1	L	139	LYS	2.1
1	L	290	THR	2.1
1	P	139	LYS	2.1
1	J	86	GLY	2.1
1	J	220	LEU	2.1
1	M	78	LEU	2.1
1	N	200	LEU	2.1
1	G	17	ALA	2.1
1	L	136	ALA	2.1
1	Q	94	GLU	2.1
1	I	80	ILE	2.1
1	K	90	ILE	2.1
1	R	191	ILE	2.1
1	D	38	ASN	2.1
1	C	299	VAL	2.1
1	R	79	PRO	2.1
1	K	9	ASP	2.1
1	C	65	GLY	2.1
1	D	44	GLY	2.1
1	J	78	LEU	2.1
1	R	6	LEU	2.1
1	L	317	ALA	2.1
1	N	82	ALA	2.1
1	N	294	ALA	2.1
1	P	36	TYR	2.1
1	B	80	ILE	2.1
1	F	159	ILE	2.1
1	M	30	ILE	2.1
1	Q	105	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	295	VAL	2.1
1	L	77	VAL	2.1
1	B	22	LEU	2.1
1	A	199	THR	2.1
1	K	214	THR	2.1
1	L	7	ASP	2.1
1	L	286	ASP	2.1
1	M	87	ASP	2.1
1	M	201	LEU	2.1
1	R	220	LEU	2.1
1	O	256	THR	2.1
1	Q	202	THR	2.1
1	A	69	ALA	2.1
1	E	30	ILE	2.1
1	L	94	GLU	2.1
1	M	191	ILE	2.1
1	P	230	ALA	2.1
1	R	32	ILE	2.1
1	R	43	GLN	2.1
1	C	207	LYS	2.1
1	N	215	LYS	2.1
1	R	307	MET	2.1
1	J	93	VAL	2.1
1	P	288	VAL	2.1
1	M	96	PRO	2.1
1	M	285	ASN	2.1
1	D	193	LEU	2.1
1	D	200	LEU	2.1
1	R	243	LEU	2.1
1	B	89	GLY	2.1
1	D	154	GLY	2.1
1	G	279	GLY	2.1
1	Q	148	GLY	2.1
1	B	131	THR	2.1
1	K	33	THR	2.1
1	B	171	ILE	2.1
1	D	84	ILE	2.1
1	D	235	ALA	2.1
1	E	317	ALA	2.1
1	L	235	ALA	2.1
1	I	231	TYR	2.1
1	K	36	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	24	SER	2.0
1	G	24	SER	2.0
1	G	74	SER	2.0
1	L	72	LYS	2.0
1	M	85	HIS	2.0
1	N	93	VAL	2.0
1	K	38	ASN	2.0
1	M	164	ASN	2.0
1	F	275	GLY	2.0
1	M	83	PHE	2.0
1	R	11	GLY	2.0
1	R	312	GLY	2.0
1	F	33	THR	2.0
1	I	167	THR	2.0
1	J	199	THR	2.0
1	E	69	ALA	2.0
1	F	104	ASP	2.0
1	M	169	ALA	2.0
1	N	13	ASP	2.0
1	P	111	ILE	2.0
1	R	90	ILE	2.0
1	F	317	ALA	2.0
1	J	142	GLU	2.0
1	C	138	LYS	2.0
1	K	231	TYR	2.0
1	P	116	LYS	2.0
1	B	24	SER	2.0
1	P	115	VAL	2.0
1	R	57	HIS	2.0
1	R	62	VAL	2.0
1	R	114	SER	2.0
1	K	79	PRO	2.0
1	L	287	PRO	2.0
1	R	300	PRO	2.0
1	R	152	LEU	2.0
1	D	159	ILE	2.0
1	H	90	ILE	2.0
1	K	95	ILE	2.0
1	M	159	ILE	2.0
1	A	17	ALA	2.0
1	E	290	THR	2.0
1	M	135	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	94	GLU	2.0
1	D	270	GLU	2.0
1	M	76	GLU	2.0
1	Q	138	LYS	2.0
1	L	231	TYR	2.0
1	M	227	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	N	400	1/1	0.77	0.09	43,43,43,43	0
2	CA	H	400	1/1	0.80	0.07	36,36,36,36	0
2	CA	I	400	1/1	0.83	0.07	32,32,32,32	0
2	CA	R	400	1/1	0.83	0.08	46,46,46,46	0
2	CA	K	400	1/1	0.85	0.06	39,39,39,39	0
2	CA	Q	400	1/1	0.86	0.11	38,38,38,38	0
2	CA	A	400	1/1	0.86	0.07	21,21,21,21	0
2	CA	F	400	1/1	0.88	0.07	30,30,30,30	0
2	CA	M	400	1/1	0.91	0.08	32,32,32,32	0
2	CA	P	400	1/1	0.92	0.05	32,32,32,32	0
2	CA	L	400	1/1	0.93	0.06	39,39,39,39	0
2	CA	G	400	1/1	0.93	0.09	28,28,28,28	0
2	CA	D	400	1/1	0.93	0.06	29,29,29,29	0
2	CA	O	400	1/1	0.94	0.06	32,32,32,32	0
2	CA	J	400	1/1	0.96	0.08	31,31,31,31	0
2	CA	E	400	1/1	0.97	0.06	32,32,32,32	0
2	CA	B	400	1/1	0.98	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	C	400	1/1	0.99	0.07	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.