Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2023 – 02:13 PM JST

PDB ID	:	8J6V
Title	:	Structure of yeast Arginyl-tRNA-protein transferase 1
Authors	:	Yashiro, Y.; Tomita, K.
Deposited on	:	2023-04-26
Resolution	:	3.40 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:

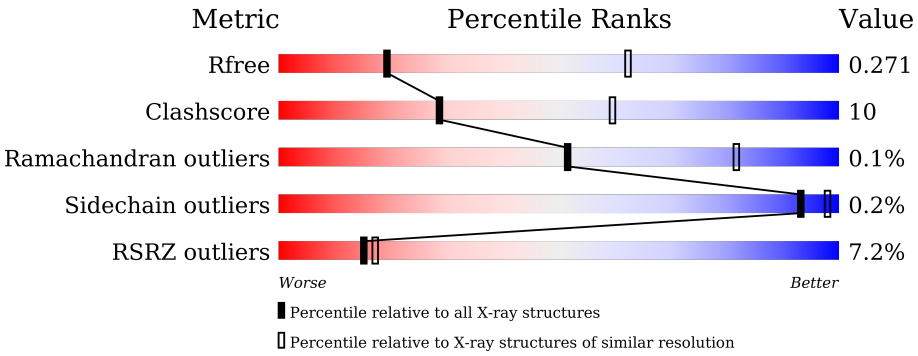
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	511	7% 70% 22% 8%
1	B	511	5% 66% 25% 9%
1	C	511	6% 70% 22% 8%
1	D	511	5% 72% 19% 10%
1	E	511	6% 66% 25% 9%
1	F	511	5% 69% 22% 9%

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Mol	Chain	Length	Quality of chain
1	G	511	10% 69% 21% 10%
1	H	511	5% 70% 21% 9%
1	I	511	5% 69% 21% 10%
1	J	511	5% 64% 26% 9%
1	K	511	8% 71% 20% 9%
1	L	511	10% 69% 22% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 45256 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 arginyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3817	2455	630	705	27			
1	B	465	Total	C	N	O	S	0	0	0
			3778	2431	622	698	27			
1	D	462	Total	C	N	O	S	0	0	0
			3748	2412	616	693	27			
1	F	464	Total	C	N	O	S	0	0	0
			3764	2424	618	696	26			
1	E	464	Total	C	N	O	S	0	0	0
			3768	2425	619	697	27			
1	L	465	Total	C	N	O	S	0	0	0
			3778	2431	622	698	27			
1	H	464	Total	C	N	O	S	0	0	0
			3760	2421	618	696	25			
1	G	462	Total	C	N	O	S	0	0	0
			3752	2416	616	694	26			
1	C	469	Total	C	N	O	S	0	0	0
			3812	2455	627	703	27			
1	K	465	Total	C	N	O	S	0	0	0
			3774	2429	621	698	26			
1	I	461	Total	C	N	O	S	0	0	0
			3746	2414	616	690	26			
1	J	463	Total	C	N	O	S	0	0	0
			3759	2421	618	694	26			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
A	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
A	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
A	504	LEU	-	expression tag	UNP A0A8H4C2T6
A	505	GLU	-	expression tag	UNP A0A8H4C2T6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	506	HIS	-	expression tag	UNP A0A8H4C2T6
A	507	HIS	-	expression tag	UNP A0A8H4C2T6
A	508	HIS	-	expression tag	UNP A0A8H4C2T6
A	509	HIS	-	expression tag	UNP A0A8H4C2T6
A	510	HIS	-	expression tag	UNP A0A8H4C2T6
A	511	HIS	-	expression tag	UNP A0A8H4C2T6
B	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
B	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
B	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
B	504	LEU	-	expression tag	UNP A0A8H4C2T6
B	505	GLU	-	expression tag	UNP A0A8H4C2T6
B	506	HIS	-	expression tag	UNP A0A8H4C2T6
B	507	HIS	-	expression tag	UNP A0A8H4C2T6
B	508	HIS	-	expression tag	UNP A0A8H4C2T6
B	509	HIS	-	expression tag	UNP A0A8H4C2T6
B	510	HIS	-	expression tag	UNP A0A8H4C2T6
B	511	HIS	-	expression tag	UNP A0A8H4C2T6
D	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
D	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
D	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
D	504	LEU	-	expression tag	UNP A0A8H4C2T6
D	505	GLU	-	expression tag	UNP A0A8H4C2T6
D	506	HIS	-	expression tag	UNP A0A8H4C2T6
D	507	HIS	-	expression tag	UNP A0A8H4C2T6
D	508	HIS	-	expression tag	UNP A0A8H4C2T6
D	509	HIS	-	expression tag	UNP A0A8H4C2T6
D	510	HIS	-	expression tag	UNP A0A8H4C2T6
D	511	HIS	-	expression tag	UNP A0A8H4C2T6
F	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
F	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
F	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
F	504	LEU	-	expression tag	UNP A0A8H4C2T6
F	505	GLU	-	expression tag	UNP A0A8H4C2T6
F	506	HIS	-	expression tag	UNP A0A8H4C2T6
F	507	HIS	-	expression tag	UNP A0A8H4C2T6
F	508	HIS	-	expression tag	UNP A0A8H4C2T6
F	509	HIS	-	expression tag	UNP A0A8H4C2T6
F	510	HIS	-	expression tag	UNP A0A8H4C2T6
F	511	HIS	-	expression tag	UNP A0A8H4C2T6
E	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
E	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
E	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	504	LEU	-	expression tag	UNP A0A8H4C2T6
E	505	GLU	-	expression tag	UNP A0A8H4C2T6
E	506	HIS	-	expression tag	UNP A0A8H4C2T6
E	507	HIS	-	expression tag	UNP A0A8H4C2T6
E	508	HIS	-	expression tag	UNP A0A8H4C2T6
E	509	HIS	-	expression tag	UNP A0A8H4C2T6
E	510	HIS	-	expression tag	UNP A0A8H4C2T6
E	511	HIS	-	expression tag	UNP A0A8H4C2T6
L	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
L	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
L	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
L	504	LEU	-	expression tag	UNP A0A8H4C2T6
L	505	GLU	-	expression tag	UNP A0A8H4C2T6
L	506	HIS	-	expression tag	UNP A0A8H4C2T6
L	507	HIS	-	expression tag	UNP A0A8H4C2T6
L	508	HIS	-	expression tag	UNP A0A8H4C2T6
L	509	HIS	-	expression tag	UNP A0A8H4C2T6
L	510	HIS	-	expression tag	UNP A0A8H4C2T6
L	511	HIS	-	expression tag	UNP A0A8H4C2T6
H	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
H	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
H	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
H	504	LEU	-	expression tag	UNP A0A8H4C2T6
H	505	GLU	-	expression tag	UNP A0A8H4C2T6
H	506	HIS	-	expression tag	UNP A0A8H4C2T6
H	507	HIS	-	expression tag	UNP A0A8H4C2T6
H	508	HIS	-	expression tag	UNP A0A8H4C2T6
H	509	HIS	-	expression tag	UNP A0A8H4C2T6
H	510	HIS	-	expression tag	UNP A0A8H4C2T6
H	511	HIS	-	expression tag	UNP A0A8H4C2T6
G	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
G	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
G	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
G	504	LEU	-	expression tag	UNP A0A8H4C2T6
G	505	GLU	-	expression tag	UNP A0A8H4C2T6
G	506	HIS	-	expression tag	UNP A0A8H4C2T6
G	507	HIS	-	expression tag	UNP A0A8H4C2T6
G	508	HIS	-	expression tag	UNP A0A8H4C2T6
G	509	HIS	-	expression tag	UNP A0A8H4C2T6
G	510	HIS	-	expression tag	UNP A0A8H4C2T6
G	511	HIS	-	expression tag	UNP A0A8H4C2T6
C	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
C	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
C	504	LEU	-	expression tag	UNP A0A8H4C2T6
C	505	GLU	-	expression tag	UNP A0A8H4C2T6
C	506	HIS	-	expression tag	UNP A0A8H4C2T6
C	507	HIS	-	expression tag	UNP A0A8H4C2T6
C	508	HIS	-	expression tag	UNP A0A8H4C2T6
C	509	HIS	-	expression tag	UNP A0A8H4C2T6
C	510	HIS	-	expression tag	UNP A0A8H4C2T6
C	511	HIS	-	expression tag	UNP A0A8H4C2T6
K	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
K	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
K	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
K	504	LEU	-	expression tag	UNP A0A8H4C2T6
K	505	GLU	-	expression tag	UNP A0A8H4C2T6
K	506	HIS	-	expression tag	UNP A0A8H4C2T6
K	507	HIS	-	expression tag	UNP A0A8H4C2T6
K	508	HIS	-	expression tag	UNP A0A8H4C2T6
K	509	HIS	-	expression tag	UNP A0A8H4C2T6
K	510	HIS	-	expression tag	UNP A0A8H4C2T6
K	511	HIS	-	expression tag	UNP A0A8H4C2T6
I	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
I	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
I	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
I	504	LEU	-	expression tag	UNP A0A8H4C2T6
I	505	GLU	-	expression tag	UNP A0A8H4C2T6
I	506	HIS	-	expression tag	UNP A0A8H4C2T6
I	507	HIS	-	expression tag	UNP A0A8H4C2T6
I	508	HIS	-	expression tag	UNP A0A8H4C2T6
I	509	HIS	-	expression tag	UNP A0A8H4C2T6
I	510	HIS	-	expression tag	UNP A0A8H4C2T6
I	511	HIS	-	expression tag	UNP A0A8H4C2T6
J	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
J	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
J	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
J	504	LEU	-	expression tag	UNP A0A8H4C2T6
J	505	GLU	-	expression tag	UNP A0A8H4C2T6
J	506	HIS	-	expression tag	UNP A0A8H4C2T6
J	507	HIS	-	expression tag	UNP A0A8H4C2T6
J	508	HIS	-	expression tag	UNP A0A8H4C2T6
J	509	HIS	-	expression tag	UNP A0A8H4C2T6
J	510	HIS	-	expression tag	UNP A0A8H4C2T6

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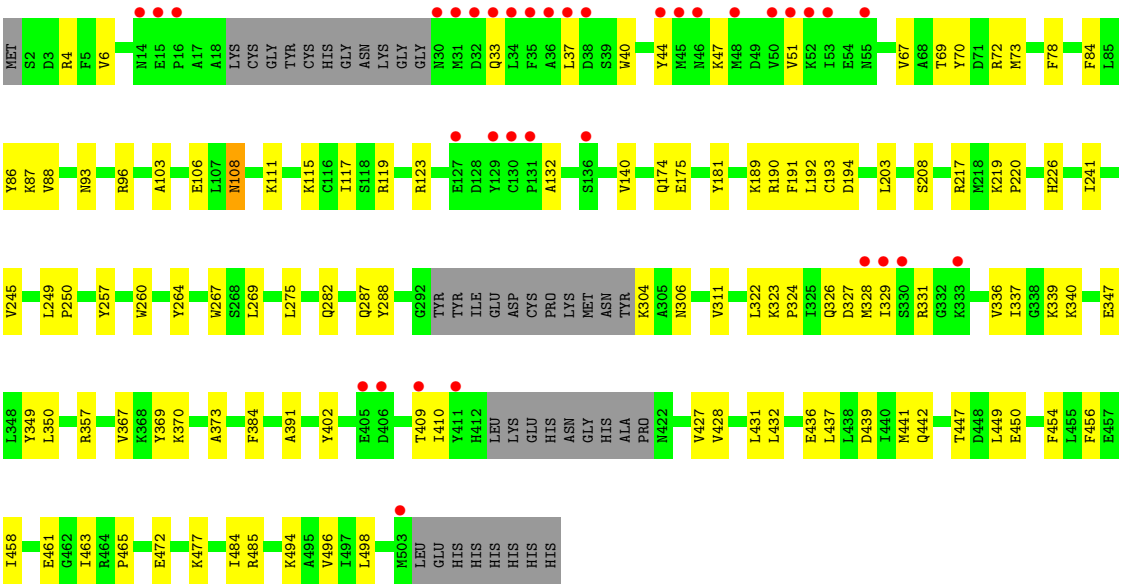
Chain	Residue	Modelled	Actual	Comment	Reference
J	511	HIS	-	expression tag	UNP A0A8H4C2T6

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.

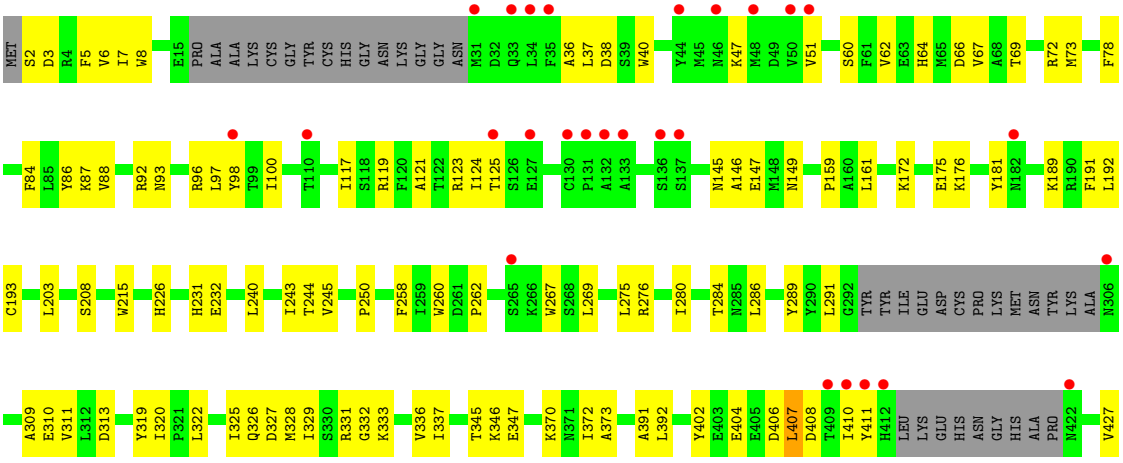
• Molecule 1: arginyltransferase

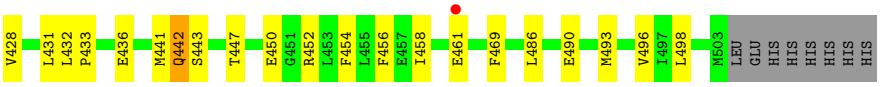
Chain A:



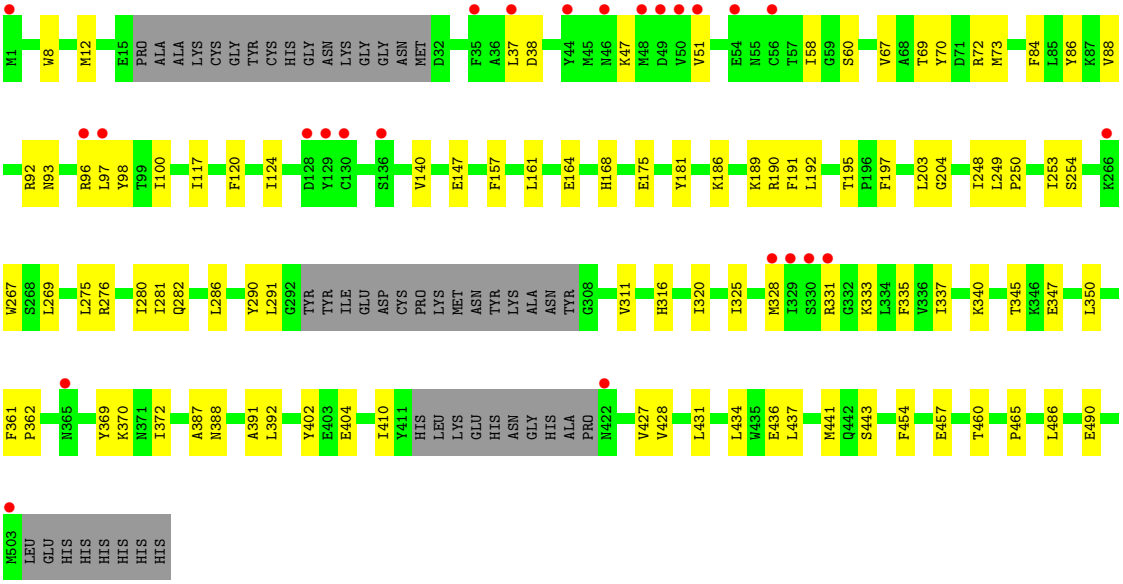
• Molecule 1: arginyltransferase

Chain B:

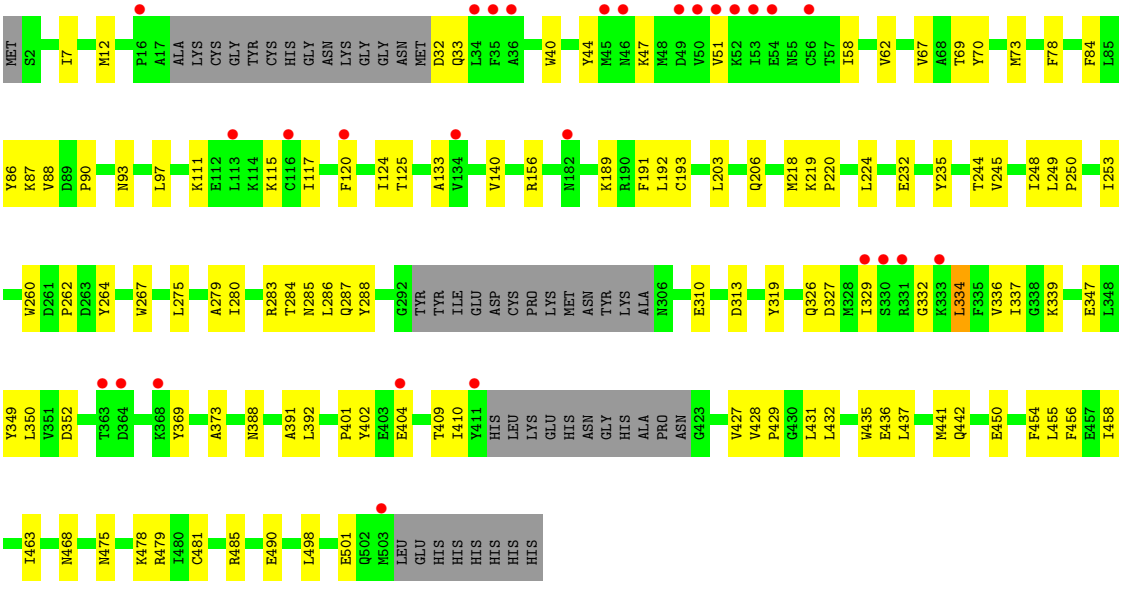




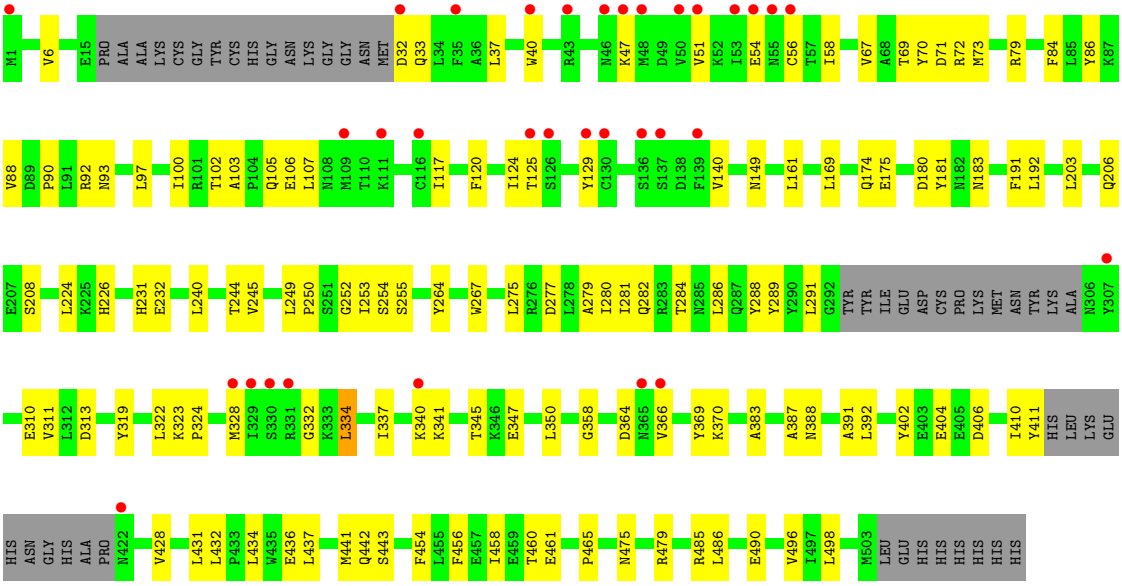
• Molecule 1: arginyltransferase



• Molecule 1: arginyltransferase

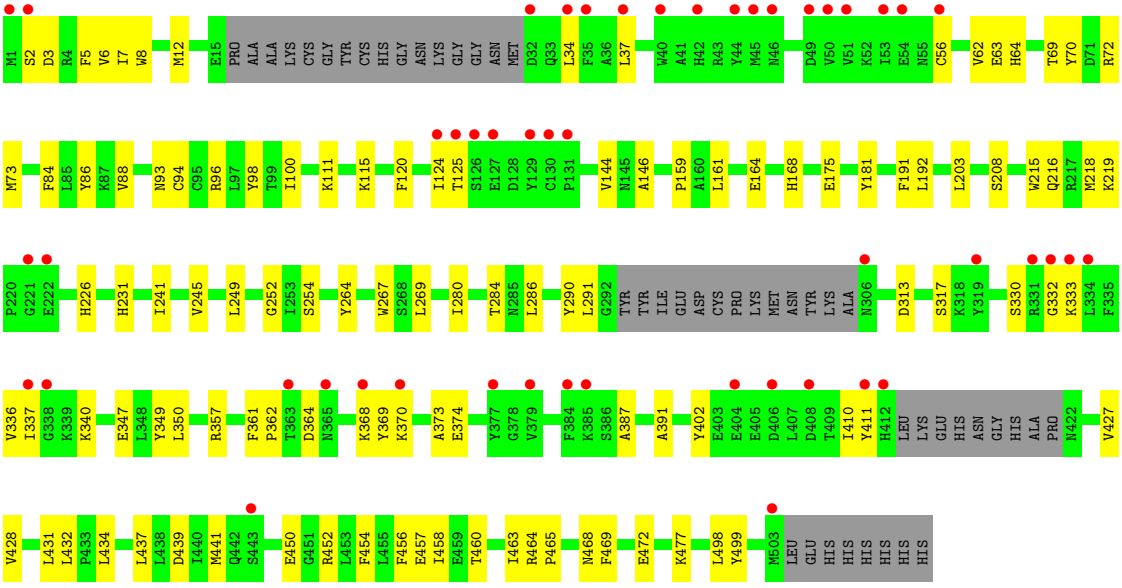


• Molecule 1: arginyltransferase



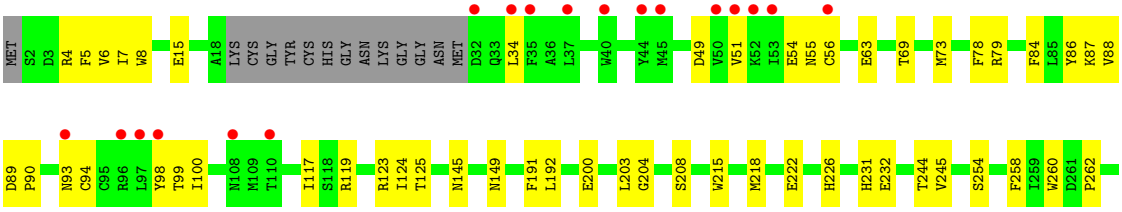
• Molecule 1: arginyltransferase

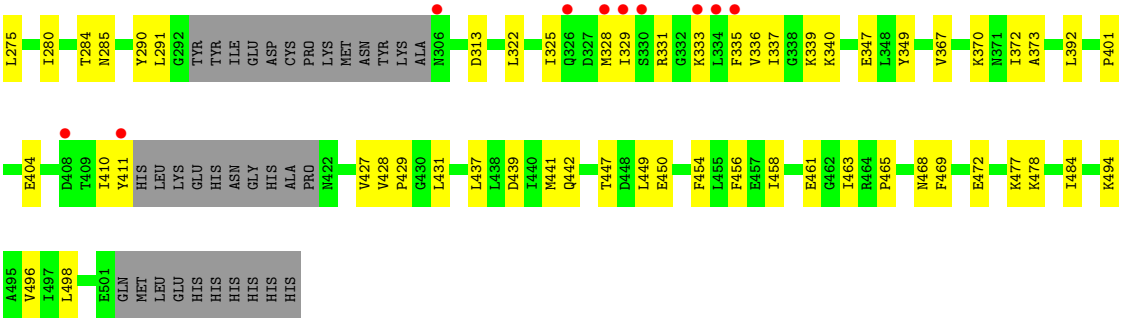
Chain L:



• Molecule 1: arginyltransferase

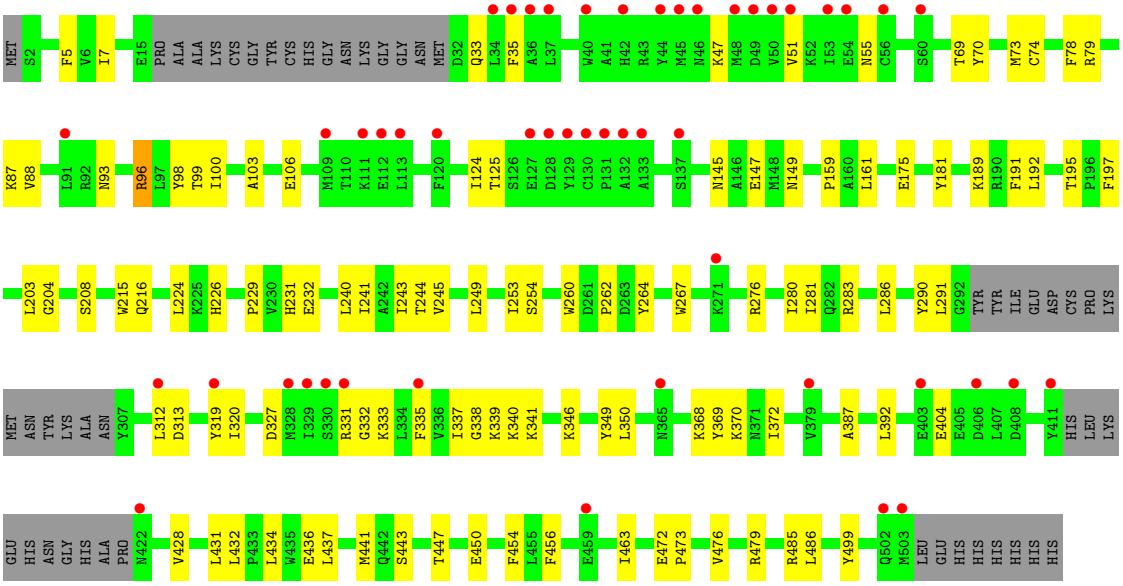
Chain H:





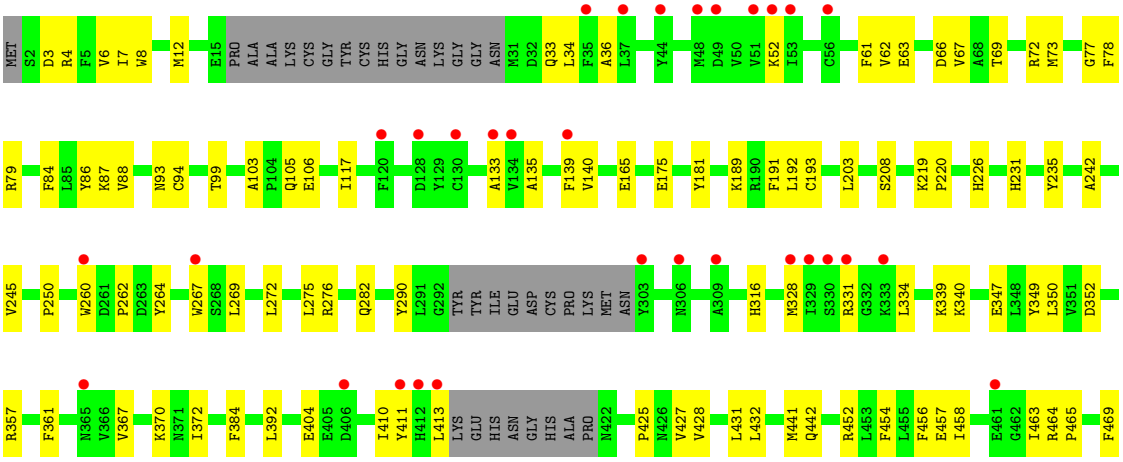
• Molecule 1: arginyltransferase

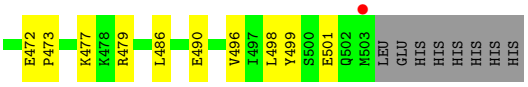
Chain G:



• Molecule 1: arginyltransferase

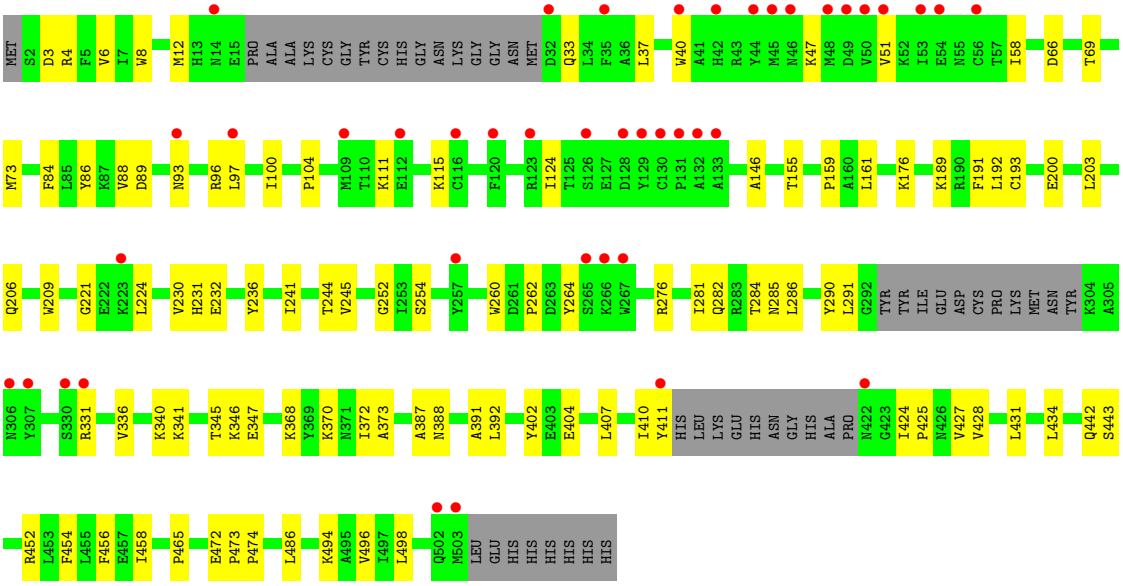
Chain C:





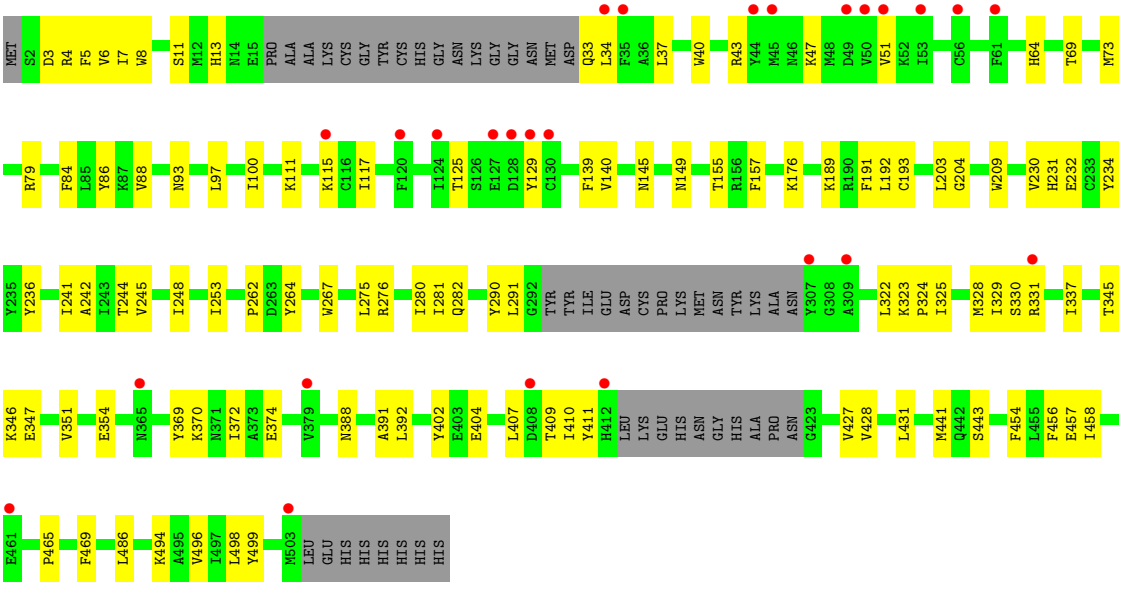
• Molecule 1: arginyltransferase

Chain K:



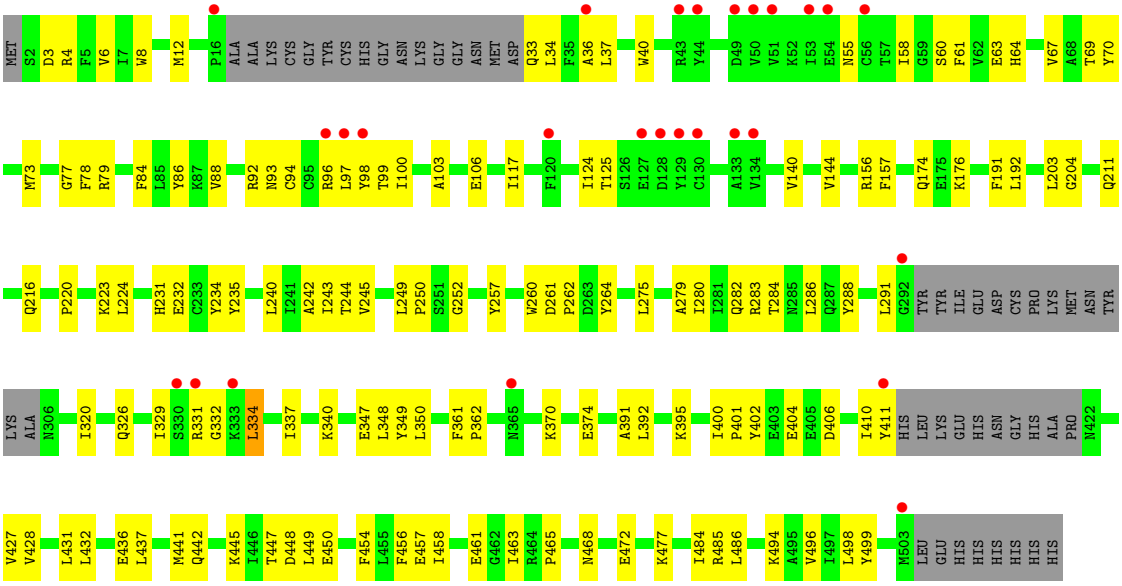
• Molecule 1: arginyltransferase

Chain I:



• Molecule 1: arginyltransferase

Chain J:


MET S2 D3 R4 F5 V6 I7 W8 M12 P16 ALA ALA LYS CYS GLY TYR CYS HIS GLY ASN LYS GLY GLY ASN MET ASP Q33 L34 F35 A36 L37 W40 R43 Y44 D49 V50 V51 K52 I53 E54 N55 C56 T57 I58 G59 S60 F61 V62 E63 H64 V67 A68 T69 Y70
M73 G77 F78 R79 F84 L85 Y86 K87 V88 R92 N93 C94 C95 R96 L97 Y98 T99 I100 A103 E106 I117 F120 I124 T125 S126 E127 D128 Y129 C130 A133 V134 V140 V144 R156 F157 Q174 E175 K176 F191 L192 L203 G204 Q211
Q216 P220 K223 L224 H231 E232 C233 Y234 Y235 L240 I241 A242 I243 T244 V245 L249 P250 S251 G252 Y257 W260 D261 P262 D263 Y264 L275 A279 I280 I281 Q282 R283 T284 N285 L286 Q287 Y288 L291 G292 TYR TYR ILE GLU ASP CYS PRO LYS MET ASN TYR
LYS ALA N306 I320 Q326 I329 S330 R331 G332 K333 L334 I337 K340 E347 L348 Y349 L350 F361 P362 N365 K370 E374 A391 L392 K395 I400 P401 Y402 E403 E404 E405 D406 I410 Y411 HIS LEU LYS GLU HIS ASN GLY HIS ALA PRO N422
V427 V428 L431 L432 E436 L437 M441 Q442 K445 I446 T447 D448 L449 E450 F454 L455 F456 E457 I458 E461 G462 I463 R464 P465 N468 E472 K477 I484 R485 L486 K494 A495 V496 I497 L498 Y499 N503 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	235.66Å 235.66Å 171.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 3.40 48.56 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.56-3.40) 99.9 (48.56-3.40)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.238 , 0.270 0.239 , 0.271	Depositor DCC
R_{free} test set	6441 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	82.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	45256	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.27	0/3909	0.48	0/5279
1	B	0.26	0/3869	0.50	0/5224
1	C	0.26	0/3904	0.47	0/5271
1	D	0.26	0/3837	0.48	0/5180
1	E	0.26	0/3858	0.49	0/5209
1	F	0.26	0/3855	0.48	0/5207
1	G	0.26	0/3842	0.48	0/5188
1	H	0.27	0/3851	0.50	0/5203
1	I	0.26	0/3837	0.48	0/5181
1	J	0.27	0/3850	0.48	0/5200
1	K	0.26	0/3864	0.47	0/5217
1	L	0.25	0/3869	0.48	0/5224
All	All	0.26	0/46345	0.48	0/62583

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	3817	0	3775	72	0
1	B	3778	0	3734	97	0
1	C	3812	0	3772	74	0
1	D	3748	0	3715	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3768	0	3730	87	0
1	F	3764	0	3724	73	0
1	G	3752	0	3712	77	0
1	H	3760	0	3718	81	0
1	I	3746	0	3709	74	0
1	J	3759	0	3721	96	0
1	K	3774	0	3736	76	0
1	L	3778	0	3737	75	0
All	All	45256	0	44783	872	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 10.

All (872) 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:98:TYR:CZ	1:B:328:MET:HG2	1.83	1.13
1:K:340:LYS:HG2	1:K:370:LYS:HD3	1.52	0.91
1:F:220:PRO:HB3	1:C:219:LYS:HD3	1.54	0.90
1:B:98:TYR:CE1	1:B:328:MET:HG2	2.08	0.87
1:D:340:LYS:HG2	1:D:370:LYS:HD3	1.57	0.84
1:B:98:TYR:OH	1:B:332:GLY:HA2	1.79	0.83
1:H:336:VAL:H	1:H:373:ALA:HB2	1.44	0.83
1:L:349:TYR:HB3	1:G:443:SER:HB3	1.61	0.82
1:H:15:GLU:N	1:H:55:ASN:HD21	1.76	0.82
1:L:219:LYS:HD3	1:J:220:PRO:HB3	1.61	0.81
1:B:98:TYR:CE1	1:B:328:MET:CG	2.64	0.80
1:E:311:VAL:HG13	1:E:322:LEU:HD11	1.62	0.80
1:E:79:ARG:HH12	1:E:254:SER:HB2	1.47	0.79
1:B:320:ILE:HD12	1:B:337:ILE:HD12	1.65	0.78
1:G:340:LYS:HG2	1:G:370:LYS:HD3	1.66	0.78
1:I:43:ARG:HH22	1:I:409:THR:HG22	1.49	0.77
1:C:52:LYS:HE3	1:C:413:LEU:HD12	1.65	0.76
1:H:100:ILE:HD11	1:H:291:LEU:HD12	1.68	0.76
1:K:284:THR:HG22	1:K:285:ASN:H	1.52	0.75
1:G:96:ARG:HH21	1:G:332:GLY:H	1.35	0.74
1:G:350:LEU:N	1:G:436:GLU:OE2	2.20	0.74
1:K:12:MET:HG2	1:K:58:ILE:HG12	1.67	0.74
1:E:284:THR:HG23	1:E:286:LEU:HD23	1.69	0.74
1:A:220:PRO:HB3	1:F:219:LYS:HD3	1.70	0.73
1:C:340:LYS:HG2	1:C:370:LYS:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:TYR:CE2	1:B:328:MET:HG2	2.22	0.72
1:K:96:ARG:NH2	1:K:331:ARG:O	2.21	0.72
1:J:33:GLN:HB3	1:J:331:ARG:HG2	1.72	0.71
1:E:100:ILE:HG23	1:E:291:LEU:HB2	1.72	0.71
1:K:33:GLN:HB3	1:K:331:ARG:HG3	1.73	0.71
1:K:391:ALA:HB1	1:K:402:TYR:HB3	1.72	0.71
1:A:442:GLN:HB3	1:B:345:THR:HB	1.73	0.71
1:F:284:THR:HG23	1:F:286:LEU:HD23	1.72	0.71
1:H:15:GLU:H	1:H:55:ASN:HD21	1.38	0.70
1:F:349:TYR:HB3	1:E:443:SER:HB3	1.72	0.70
1:K:442:GLN:HE22	1:J:348:LEU:HA	1.56	0.70
1:K:224:LEU:HG	1:K:284:THR:HG21	1.72	0.70
1:I:33:GLN:HG3	1:I:34:LEU:H	1.56	0.69
1:J:350:LEU:N	1:J:436:GLU:OE2	2.26	0.69
1:H:322:LEU:HD21	1:H:329:ILE:HD12	1.74	0.69
1:J:392:LEU:HD11	1:J:404:GLU:OE2	1.92	0.69
1:D:100:ILE:HG23	1:D:291:LEU:HB2	1.75	0.69
1:A:349:TYR:HB3	1:B:443:SER:HB3	1.75	0.69
1:E:310:GLU:HG2	1:E:319:TYR:HB3	1.74	0.68
1:A:456:PHE:HD2	1:A:498:LEU:HG	1.59	0.68
1:E:350:LEU:N	1:E:436:GLU:OE2	2.26	0.68
1:E:174:GLN:HG2	1:E:183:ASN:HD21	1.59	0.67
1:E:277:ASP:O	1:E:281:ILE:HD12	1.93	0.67
1:H:442:GLN:HB3	1:I:345:THR:HB	1.76	0.67
1:E:174:GLN:HG3	1:E:180:ASP:HB3	1.76	0.67
1:K:443:SER:HB3	1:J:349:TYR:HB3	1.76	0.67
1:F:336:VAL:H	1:F:373:ALA:HB2	1.60	0.67
1:C:33:GLN:HG3	1:C:331:ARG:HB3	1.76	0.66
1:L:468:ASN:HD21	1:G:341:LYS:HD2	1.60	0.66
1:J:456:PHE:HD2	1:J:498:LEU:HG	1.61	0.66
1:F:280:ILE:O	1:F:284:THR:HG22	1.96	0.65
1:E:431:LEU:HD22	1:E:486:LEU:HA	1.77	0.65
1:H:4:ARG:HD2	1:H:496:VAL:HG23	1.78	0.65
1:A:340:LYS:HG2	1:A:370:LYS:HD2	1.77	0.65
1:K:8:TRP:HH2	1:K:458:ILE:HD11	1.61	0.65
1:K:345:THR:HB	1:J:442:GLN:HB3	1.78	0.65
1:D:431:LEU:HD22	1:D:486:LEU:HA	1.78	0.65
1:C:189:LYS:HA	1:C:193:CYS:HB2	1.78	0.65
1:B:98:TYR:OH	1:B:332:GLY:CA	2.45	0.65
1:B:313:ASP:OD2	1:B:337:ILE:HG22	1.97	0.65
1:F:442:GLN:HB3	1:E:345:THR:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:TRP:CH2	1:C:458:ILE:HD11	2.32	0.65
1:J:326:GLN:O	1:J:329:ILE:HG12	1.97	0.65
1:D:350:LEU:N	1:D:436:GLU:OE2	2.30	0.64
1:G:387:ALA:HB1	1:G:434:LEU:HD12	1.79	0.64
1:J:320:ILE:HD12	1:J:337:ILE:HD12	1.79	0.64
1:L:340:LYS:HG2	1:L:370:LYS:HD3	1.79	0.64
1:L:452:ARG:NH1	1:K:206:GLN:OE1	2.30	0.64
1:J:284:THR:HG23	1:J:286:LEU:HD23	1.78	0.64
1:H:454:PHE:HD2	1:G:203:LEU:HD13	1.63	0.64
1:K:8:TRP:CH2	1:K:458:ILE:HD11	2.33	0.64
1:K:336:VAL:H	1:K:373:ALA:HB2	1.63	0.64
1:J:88:VAL:HG11	1:J:97:LEU:HD13	1.79	0.64
1:C:392:LEU:HD11	1:C:404:GLU:OE2	1.98	0.63
1:A:175:GLU:HB2	1:A:181:TYR:CE1	2.33	0.63
1:A:391:ALA:HB1	1:A:402:TYR:HB3	1.79	0.63
1:F:224:LEU:HG	1:F:284:THR:OG1	1.98	0.63
1:F:334:LEU:HD11	1:F:429:PRO:HG2	1.80	0.63
1:G:327:ASP:HB2	1:G:333:LYS:HD2	1.80	0.63
1:A:103:ALA:HB3	1:A:106:GLU:HG2	1.80	0.63
1:B:432:LEU:HG	1:B:436:GLU:OE2	1.99	0.62
1:E:224:LEU:HG	1:E:284:THR:OG1	1.99	0.62
1:D:391:ALA:HB1	1:D:402:TYR:HB3	1.81	0.62
1:L:456:PHE:HD2	1:L:498:LEU:HG	1.63	0.62
1:H:340:LYS:HG2	1:H:370:LYS:HD3	1.80	0.62
1:C:4:ARG:NH1	1:C:452:ARG:O	2.32	0.62
1:C:456:PHE:HD2	1:C:498:LEU:HG	1.65	0.62
1:K:111:LYS:HE2	1:K:115:LYS:HE3	1.81	0.62
1:I:330:SER:O	1:I:331:ARG:HG2	2.00	0.62
1:E:280:ILE:O	1:E:284:THR:HG22	2.00	0.62
1:H:449:LEU:HD11	1:H:484:ILE:HD11	1.82	0.62
1:D:392:LEU:HD11	1:D:404:GLU:OE2	2.00	0.61
1:B:336:VAL:H	1:B:373:ALA:HB2	1.65	0.61
1:F:12:MET:HG2	1:F:58:ILE:HG12	1.81	0.61
1:L:96:ARG:HH21	1:L:332:GLY:HA3	1.64	0.61
1:C:88:VAL:HB	1:C:93:ASN:HD22	1.64	0.61
1:H:222:GLU:O	1:H:285:ASN:ND2	2.30	0.61
1:H:313:ASP:OD2	1:H:337:ILE:HG22	2.00	0.61
1:K:189:LYS:HA	1:K:193:CYS:HB2	1.82	0.61
1:J:103:ALA:HB3	1:J:106:GLU:HG2	1.82	0.61
1:B:392:LEU:HD11	1:B:404:GLU:OE2	2.00	0.61
1:E:90:PRO:HB2	1:E:334:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:ARG:HD2	1:I:496:VAL:HG23	1.83	0.61
1:A:203:LEU:HD13	1:D:454:PHE:HD2	1.65	0.61
1:J:449:LEU:HD11	1:J:484:ILE:HD11	1.83	0.61
1:A:339:LYS:HE2	1:A:367:VAL:HG11	1.83	0.60
1:G:96:ARG:HE	1:G:332:GLY:HA3	1.64	0.60
1:K:3:ASP:HB2	1:K:66:ASP:HB3	1.83	0.60
1:G:208:SER:HB2	1:G:226:HIS:HB2	1.83	0.60
1:H:208:SER:HB2	1:H:226:HIS:HB2	1.83	0.60
1:C:103:ALA:HB3	1:C:106:GLU:HG2	1.84	0.60
1:K:252:GLY:HA2	1:K:286:LEU:HB3	1.83	0.60
1:I:325:ILE:HG23	1:I:328:MET:HB3	1.83	0.60
1:B:2:SER:N	1:B:66:ASP:OD2	2.34	0.60
1:K:370:LYS:HE3	1:K:372:ILE:HG22	1.84	0.60
1:A:350:LEU:N	1:A:436:GLU:OE2	2.35	0.60
1:F:350:LEU:N	1:F:436:GLU:OE2	2.33	0.60
1:C:117:ILE:HD11	1:C:275:LEU:HD13	1.84	0.60
1:A:322:LEU:HD21	1:A:329:ILE:HD13	1.85	0.59
1:B:88:VAL:HB	1:B:93:ASN:HD22	1.67	0.59
1:E:454:PHE:HD2	1:C:203:LEU:HD13	1.68	0.59
1:A:117:ILE:HD11	1:A:275:LEU:HD13	1.83	0.59
1:I:410:ILE:HG23	1:I:411:TYR:CD2	2.37	0.59
1:B:452:ARG:NE	1:F:206:GLN:OE1	2.36	0.59
1:H:328:MET:SD	1:H:335:PHE:HB3	2.42	0.59
1:J:3:ASP:OD2	1:J:64:HIS:NE2	2.25	0.59
1:F:310:GLU:HG2	1:F:319:TYR:HB3	1.84	0.59
1:K:392:LEU:HD11	1:K:404:GLU:OE2	2.03	0.59
1:L:8:TRP:HH2	1:L:458:ILE:HD11	1.66	0.59
1:D:72:ARG:NH2	1:D:490:GLU:OE2	2.36	0.59
1:J:88:VAL:HG21	1:J:97:LEU:H	1.68	0.59
1:G:88:VAL:HB	1:G:93:ASN:HD22	1.66	0.58
1:J:117:ILE:HD11	1:J:275:LEU:HD13	1.84	0.58
1:A:347:GLU:OE2	1:A:427:VAL:HG13	2.03	0.58
1:B:447:THR:O	1:B:450:GLU:HG2	2.02	0.58
1:K:124:ILE:HD11	1:K:146:ALA:HB1	1.84	0.58
1:I:117:ILE:HD11	1:I:275:LEU:HD13	1.85	0.58
1:D:96:ARG:NH1	1:D:331:ARG:O	2.36	0.58
1:E:92:ARG:NH2	1:E:406:ASP:OD2	2.37	0.58
1:E:117:ILE:HD11	1:E:275:LEU:HD13	1.84	0.58
1:L:347:GLU:OE2	1:L:427:VAL:HG13	2.03	0.58
1:C:8:TRP:HH2	1:C:458:ILE:HD11	1.68	0.58
1:J:447:THR:O	1:J:450:GLU:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:TRP:O	1:B:60:SER:OG	2.21	0.58
1:D:328:MET:SD	1:D:328:MET:N	2.76	0.58
1:F:117:ILE:HD11	1:F:275:LEU:HD13	1.86	0.58
1:C:3:ASP:OD2	1:C:66:ASP:HB3	2.04	0.58
1:J:96:ARG:NH2	1:J:331:ARG:O	2.37	0.58
1:G:103:ALA:HB3	1:G:106:GLU:HG2	1.84	0.58
1:J:280:ILE:O	1:J:284:THR:HG22	2.03	0.58
1:A:6:VAL:HG22	1:A:496:VAL:HB	1.85	0.58
1:H:347:GLU:OE2	1:H:427:VAL:HG13	2.04	0.58
1:F:44:TYR:OH	1:F:409:THR:OG1	2.22	0.57
1:K:346:LYS:NZ	1:J:442:GLN:OE1	2.36	0.57
1:J:12:MET:HE2	1:J:58:ILE:HG12	1.86	0.57
1:B:98:TYR:CZ	1:B:328:MET:CG	2.73	0.57
1:G:240:LEU:HD21	1:G:243:ILE:HD11	1.86	0.57
1:A:447:THR:O	1:A:450:GLU:HG2	2.04	0.57
1:L:457:GLU:HB3	1:L:499:TYR:CE2	2.39	0.57
1:H:54:GLU:HG2	1:H:55:ASN:N	2.19	0.57
1:K:387:ALA:HB1	1:K:434:LEU:HD12	1.86	0.57
1:D:88:VAL:HG21	1:D:97:LEU:H	1.69	0.57
1:K:340:LYS:HG3	1:K:368:LYS:HE3	1.85	0.57
1:I:8:TRP:CH2	1:I:458:ILE:HD11	2.40	0.57
1:H:8:TRP:HH2	1:H:458:ILE:HD11	1.70	0.57
1:A:463:ILE:HG23	1:D:161:LEU:HD22	1.87	0.57
1:D:88:VAL:HG11	1:D:97:LEU:HD13	1.86	0.56
1:H:231:HIS:CD2	1:H:245:VAL:HG22	2.40	0.56
1:B:232:GLU:HG2	1:B:244:THR:HB	1.86	0.56
1:B:310:GLU:HG2	1:B:319:TYR:HB3	1.87	0.56
1:B:100:ILE:HG23	1:B:291:LEU:HB2	1.86	0.56
1:G:313:ASP:OD2	1:G:337:ILE:HG22	2.05	0.56
1:G:428:VAL:HB	1:G:431:LEU:HD12	1.86	0.56
1:L:284:THR:O	1:L:286:LEU:N	2.31	0.56
1:I:454:PHE:CE2	1:J:203:LEU:HD22	2.41	0.56
1:J:78:PHE:O	1:J:79:ARG:NH1	2.35	0.56
1:D:337:ILE:HD11	1:D:361:PHE:CE1	2.40	0.56
1:B:145:ASN:OD1	1:B:149:ASN:ND2	2.38	0.56
1:K:221:GLY:C	1:K:285:ASN:HD21	2.09	0.56
1:D:69:THR:O	1:D:73:MET:HG2	2.05	0.56
1:F:192:LEU:HD22	1:F:245:VAL:HG21	1.86	0.56
1:L:2:SER:HB3	1:L:64:HIS:NE2	2.21	0.56
1:E:392:LEU:HD11	1:E:404:GLU:OE2	2.06	0.56
1:B:203:LEU:HD13	1:F:454:PHE:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:431:LEU:HD22	1:K:486:LEU:HA	1.86	0.55
1:B:124:ILE:HD11	1:B:146:ALA:HB1	1.89	0.55
1:B:311:VAL:HG13	1:B:322:LEU:HD13	1.88	0.55
1:E:391:ALA:HB1	1:E:402:TYR:HB3	1.87	0.55
1:L:203:LEU:HD22	1:K:454:PHE:CE2	2.41	0.55
1:B:88:VAL:HG21	1:B:97:LEU:H	1.71	0.55
1:H:392:LEU:HD11	1:H:404:GLU:OE2	2.06	0.55
1:K:6:VAL:HG22	1:K:496:VAL:HB	1.88	0.55
1:J:260:TRP:CZ3	1:J:262:PRO:HA	2.42	0.55
1:A:4:ARG:NH2	1:D:204:GLY:O	2.40	0.55
1:A:174:GLN:OE1	1:A:257:TYR:OH	2.22	0.55
1:K:192:LEU:HD22	1:K:245:VAL:HG21	1.87	0.55
1:I:351:VAL:HG13	1:I:354:GLU:HB2	1.88	0.55
1:A:88:VAL:HB	1:A:93:ASN:HD22	1.71	0.55
1:B:325:ILE:HG23	1:B:327:ASP:OD1	2.07	0.55
1:G:472:GLU:OE2	1:G:476:VAL:HG11	2.07	0.55
1:C:339:LYS:HE2	1:C:367:VAL:HG11	1.89	0.55
1:C:472:GLU:HG3	1:C:473:PRO:HD2	1.89	0.55
1:D:12:MET:HG2	1:D:58:ILE:HG12	1.89	0.55
1:C:352:ASP:OD2	1:C:490:GLU:HG3	2.07	0.55
1:C:410:ILE:HG22	1:C:411:TYR:H	1.72	0.54
1:H:339:LYS:HG2	1:H:367:VAL:HG11	1.89	0.54
1:H:463:ILE:HG23	1:G:161:LEU:HD22	1.89	0.54
1:I:204:GLY:O	1:J:4:ARG:NH1	2.39	0.54
1:E:340:LYS:HG2	1:E:370:LYS:HD2	1.88	0.54
1:E:313:ASP:OD2	1:E:337:ILE:HG22	2.06	0.54
1:L:12:MET:HE2	1:L:56:CYS:HB3	1.89	0.54
1:C:72:ARG:NH1	1:C:357:ARG:HE	2.06	0.54
1:J:224:LEU:HG	1:J:284:THR:OG1	2.07	0.54
1:D:195:THR:HB	1:D:197:PHE:HD2	1.73	0.54
1:D:345:THR:HB	1:C:442:GLN:HB3	1.89	0.54
1:F:327:ASP:O	1:F:332:GLY:N	2.31	0.54
1:E:58:ILE:HG22	1:E:486:LEU:HD11	1.90	0.54
1:F:347:GLU:OE2	1:F:427:VAL:HG13	2.08	0.54
1:F:391:ALA:HB1	1:F:402:TYR:HB3	1.89	0.54
1:L:428:VAL:HB	1:L:431:LEU:HD12	1.89	0.54
1:H:4:ARG:NH2	1:G:204:GLY:O	2.40	0.54
1:I:325:ILE:HG22	1:I:329:ILE:HG23	1.90	0.54
1:G:145:ASN:OD1	1:G:149:ASN:ND2	2.41	0.54
1:I:3:ASP:OD2	1:I:64:HIS:NE2	2.41	0.54
1:A:449:LEU:HD11	1:A:484:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:PHE:CD2	1:A:498:LEU:HG	2.41	0.54
1:B:147:GLU:OE2	1:B:276:ARG:NE	2.36	0.54
1:D:325:ILE:HD12	1:D:328:MET:HE1	1.90	0.54
1:D:362:PRO:HB3	1:E:206:GLN:HE21	1.73	0.54
1:A:111:LYS:HE2	1:A:115:LYS:HE3	1.90	0.53
1:G:73:MET:HB3	1:G:78:PHE:HD2	1.74	0.53
1:J:432:LEU:HB3	1:J:485:ARG:HA	1.89	0.53
1:J:437:LEU:O	1:J:441:MET:HG2	2.08	0.53
1:E:69:THR:O	1:E:73:MET:HG2	2.08	0.53
1:E:208:SER:HB2	1:E:226:HIS:HB2	1.90	0.53
1:A:454:PHE:HD2	1:D:203:LEU:HD13	1.72	0.53
1:H:325:ILE:CG2	1:H:328:MET:HG2	2.38	0.53
1:I:391:ALA:HB1	1:I:402:TYR:HB3	1.89	0.53
1:E:328:MET:HA	1:E:332:GLY:HA2	1.90	0.53
1:B:88:VAL:HG11	1:B:97:LEU:HD13	1.89	0.53
1:B:117:ILE:HD11	1:B:275:LEU:HD13	1.90	0.53
1:I:454:PHE:HE2	1:J:203:LEU:HD22	1.73	0.53
1:A:4:ARG:HD3	1:A:494:LYS:O	2.08	0.53
1:A:72:ARG:HH12	1:A:357:ARG:NE	2.06	0.53
1:C:242:ALA:HB2	1:C:269:LEU:HD13	1.89	0.53
1:L:454:PHE:HD2	1:K:203:LEU:HD13	1.74	0.53
1:F:189:LYS:HA	1:F:193:CYS:HB2	1.89	0.53
1:I:125:THR:HG21	1:I:129:TYR:CD1	2.44	0.53
1:B:336:VAL:N	1:B:373:ALA:HB2	2.24	0.53
1:F:388:ASN:HB3	1:F:404:GLU:HG2	1.91	0.53
1:A:69:THR:O	1:A:73:MET:HG2	2.09	0.53
1:B:370:LYS:HE3	1:B:372:ILE:HG22	1.91	0.53
1:J:395:LYS:HD3	1:J:401:PRO:HA	1.90	0.53
1:B:69:THR:O	1:B:73:MET:HG2	2.09	0.52
1:G:33:GLN:HA	1:G:331:ARG:HE	1.73	0.52
1:K:191:PHE:HD2	1:K:192:LEU:HG	1.74	0.52
1:D:88:VAL:HB	1:D:93:ASN:HD22	1.73	0.52
1:A:119:ARG:HB3	1:A:123:ARG:NH1	2.25	0.52
1:B:78:PHE:CE1	1:B:87:LYS:HD2	2.44	0.52
1:L:364:ASP:OD1	1:L:369:TYR:OH	2.24	0.52
1:L:457:GLU:HA	1:L:499:TYR:O	2.09	0.52
1:C:34:LEU:HD22	1:C:94:CYS:HB2	1.90	0.52
1:B:84:PHE:CE2	1:B:86:TYR:HB3	2.44	0.52
1:F:133:ALA:HB1	1:C:133:ALA:HB3	1.91	0.52
1:G:100:ILE:HG23	1:G:291:LEU:HB2	1.90	0.52
1:G:264:TYR:HB3	1:G:267:TRP:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:VAL:HB	1:F:93:ASN:HD22	1.75	0.52
1:H:325:ILE:HG21	1:H:328:MET:HG2	1.90	0.52
1:C:78:PHE:CE1	1:C:87:LYS:HD2	2.44	0.52
1:K:104:PRO:HB2	1:K:282:GLN:HB2	1.92	0.52
1:A:428:VAL:HB	1:A:431:LEU:HD12	1.91	0.52
1:B:454:PHE:CE2	1:F:203:LEU:HD22	2.45	0.52
1:L:69:THR:O	1:L:73:MET:HG2	2.10	0.52
1:C:347:GLU:OE2	1:C:427:VAL:HG13	2.09	0.52
1:K:454:PHE:CD1	1:K:465:PRO:HA	2.45	0.52
1:F:285:ASN:OD1	1:C:219:LYS:NZ	2.40	0.52
1:E:125:THR:HG21	1:E:129:TYR:CD1	2.45	0.52
1:I:203:LEU:HD13	1:J:454:PHE:HD2	1.73	0.52
1:F:326:GLN:HA	1:F:329:ILE:HD13	1.91	0.52
1:H:56:CYS:SG	1:H:89:ASP:HB3	2.50	0.52
1:K:100:ILE:HG23	1:K:291:LEU:HB2	1.91	0.52
1:I:191:PHE:CD2	1:I:192:LEU:HG	2.45	0.52
1:G:472:GLU:CD	1:G:473:PRO:HD2	2.30	0.52
1:J:191:PHE:CD2	1:J:192:LEU:HG	2.45	0.52
1:L:218:MET:SD	1:L:284:THR:HG22	2.50	0.51
1:G:232:GLU:HG2	1:G:244:THR:HB	1.91	0.51
1:C:6:VAL:HG22	1:C:496:VAL:HB	1.90	0.51
1:C:410:ILE:HG22	1:C:411:TYR:N	2.25	0.51
1:A:219:LYS:HD2	1:C:220:PRO:HB3	1.91	0.51
1:B:456:PHE:HD2	1:B:498:LEU:HG	1.75	0.51
1:L:100:ILE:HG23	1:L:291:LEU:HB2	1.92	0.51
1:H:191:PHE:HD2	1:H:192:LEU:HG	1.75	0.51
1:H:192:LEU:HD22	1:H:245:VAL:HG21	1.92	0.51
1:C:69:THR:O	1:C:73:MET:HG2	2.11	0.51
1:B:172:LYS:HE3	1:B:176:LYS:NZ	2.26	0.51
1:H:69:THR:O	1:H:73:MET:HG2	2.11	0.51
1:H:90:PRO:HG2	1:H:429:PRO:HB2	1.92	0.51
1:A:70:TYR:HD2	1:A:249:LEU:HD21	1.76	0.51
1:E:88:VAL:HB	1:E:93:ASN:HD22	1.75	0.51
1:C:192:LEU:HD22	1:C:245:VAL:HG21	1.92	0.51
1:I:111:LYS:HG2	1:I:115:LYS:HE3	1.92	0.51
1:I:392:LEU:HD11	1:I:404:GLU:OE2	2.11	0.51
1:J:79:ARG:HH22	1:J:99:THR:HG23	1.75	0.51
1:B:96:ARG:NH2	1:B:331:ARG:O	2.43	0.51
1:B:309:ALA:HB3	1:B:322:LEU:HD22	1.93	0.51
1:E:231:HIS:CD2	1:E:245:VAL:HG22	2.45	0.51
1:H:447:THR:O	1:H:450:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:337:ILE:HG23	1:I:369:TYR:HB3	1.91	0.51
1:D:70:TYR:HD2	1:D:249:LEU:HD21	1.75	0.51
1:L:387:ALA:HB1	1:L:434:LEU:HD12	1.93	0.51
1:J:458:ILE:H	1:J:458:ILE:HD12	1.75	0.51
1:D:267:TRP:HE3	1:D:269:LEU:HD21	1.76	0.51
1:F:392:LEU:HD11	1:F:404:GLU:OE2	2.11	0.51
1:E:232:GLU:CG	1:E:244:THR:HB	2.41	0.51
1:B:98:TYR:CD1	1:B:328:MET:HG3	2.46	0.50
1:B:327:ASP:OD1	1:B:327:ASP:N	2.42	0.50
1:J:231:HIS:CD2	1:J:245:VAL:HG22	2.46	0.50
1:J:400:ILE:HD11	1:J:441:MET:HE2	1.93	0.50
1:E:387:ALA:HB1	1:E:434:LEU:HD12	1.93	0.50
1:L:252:GLY:HA2	1:L:286:LEU:HB3	1.93	0.50
1:C:472:GLU:O	1:C:477:LYS:HE3	2.11	0.50
1:I:157:PHE:HZ	1:I:280:ILE:HD13	1.76	0.50
1:I:370:LYS:NZ	1:I:372:ILE:HG22	2.27	0.50
1:B:37:LEU:HB2	1:B:40:TRP:HD1	1.75	0.50
1:E:337:ILE:HG13	1:E:369:TYR:HB3	1.93	0.50
1:G:350:LEU:HD12	1:G:432:LEU:HA	1.93	0.50
1:I:4:ARG:HD3	1:I:494:LYS:O	2.10	0.50
1:I:69:THR:O	1:I:73:MET:HG2	2.12	0.50
1:I:88:VAL:HB	1:I:93:ASN:HD22	1.75	0.50
1:A:67:VAL:HG12	1:A:250:PRO:HD3	1.93	0.50
1:E:388:ASN:HB3	1:E:404:GLU:HG2	1.94	0.50
1:H:454:PHE:CD1	1:H:465:PRO:HA	2.47	0.50
1:G:192:LEU:HD22	1:G:245:VAL:HG21	1.93	0.50
1:E:264:TYR:HB3	1:E:267:TRP:CD1	2.47	0.50
1:L:37:LEU:HD13	1:L:374:GLU:HG2	1.94	0.50
1:L:254:SER:HA	1:L:290:TYR:HB2	1.94	0.50
1:C:431:LEU:HD22	1:C:486:LEU:HA	1.94	0.50
1:C:231:HIS:CD2	1:C:245:VAL:HG22	2.47	0.50
1:A:132:ALA:HB2	1:C:135:ALA:HB2	1.94	0.50
1:L:464:ARG:NH2	1:L:472:GLU:OE1	2.44	0.50
1:G:370:LYS:HE3	1:G:372:ILE:HG22	1.93	0.50
1:A:4:ARG:HD2	1:A:496:VAL:HG23	1.92	0.50
1:A:33:GLN:OE1	1:A:331:ARG:NH2	2.44	0.50
1:A:327:ASP:OD1	1:A:328:MET:N	2.45	0.50
1:B:98:TYR:OH	1:B:332:GLY:C	2.49	0.50
1:E:125:THR:HG23	1:E:149:ASN:O	2.12	0.50
1:L:144:VAL:HG13	1:L:216:GLN:HB3	1.94	0.50
1:K:232:GLU:CG	1:K:244:THR:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:THR:O	1:J:73:MET:HG2	2.11	0.50
1:E:454:PHE:CD1	1:E:465:PRO:HA	2.47	0.50
1:H:232:GLU:CG	1:H:244:THR:HB	2.42	0.50
1:G:195:THR:HB	1:G:197:PHE:HD2	1.77	0.50
1:I:428:VAL:HB	1:I:431:LEU:HD12	1.93	0.50
1:G:78:PHE:CE1	1:G:87:LYS:HD2	2.47	0.49
1:C:316:HIS:CG	1:C:361:PHE:HZ	2.30	0.49
1:K:336:VAL:N	1:K:373:ALA:HB2	2.27	0.49
1:J:391:ALA:HB1	1:J:402:TYR:HB3	1.93	0.49
1:D:191:PHE:CD2	1:D:192:LEU:HG	2.47	0.49
1:F:70:TYR:HD2	1:F:249:LEU:HD21	1.76	0.49
1:F:69:THR:O	1:F:73:MET:HG2	2.11	0.49
1:L:175:GLU:HB2	1:L:181:TYR:CE1	2.48	0.49
1:K:89:ASP:H	1:K:93:ASN:ND2	2.10	0.49
1:B:175:GLU:HB2	1:B:181:TYR:CE1	2.47	0.49
1:F:388:ASN:HD22	1:F:404:GLU:HA	1.78	0.49
1:E:432:LEU:HB3	1:E:485:ARG:HA	1.93	0.49
1:C:12:MET:SD	1:C:425:PRO:HD3	2.52	0.49
1:J:261:ASP:HB3	1:J:264:TYR:HD2	1.78	0.49
1:D:67:VAL:HG12	1:D:250:PRO:HD3	1.94	0.49
1:H:4:ARG:HD3	1:H:494:LYS:O	2.13	0.49
1:K:4:ARG:NH1	1:K:452:ARG:O	2.43	0.49
1:J:347:GLU:OE2	1:J:427:VAL:HG13	2.12	0.49
1:A:461:GLU:O	1:D:189:LYS:HD2	2.13	0.49
1:G:224:LEU:HD12	1:G:286:LEU:HD21	1.94	0.49
1:D:370:LYS:HE3	1:D:372:ILE:HG22	1.95	0.49
1:F:352:ASP:OD2	1:F:490:GLU:HG3	2.12	0.49
1:E:105:GLN:OE1	1:E:282:GLN:NE2	2.46	0.49
1:K:88:VAL:HG21	1:K:97:LEU:H	1.78	0.49
1:K:159:PRO:HB2	1:K:161:LEU:HG	1.95	0.49
1:I:431:LEU:HD22	1:I:486:LEU:HA	1.94	0.49
1:H:215:TRP:CD2	1:H:280:ILE:HG12	2.48	0.49
1:C:464:ARG:NH2	1:C:472:GLU:OE2	2.40	0.49
1:J:92:ARG:NH2	1:J:406:ASP:OD2	2.39	0.49
1:B:232:GLU:CG	1:B:244:THR:HB	2.43	0.49
1:B:322:LEU:HD11	1:B:328:MET:CE	2.43	0.49
1:C:479:ARG:HH22	1:C:501:GLU:HA	1.77	0.49
1:B:119:ARG:HB3	1:B:123:ARG:NH1	2.28	0.48
1:L:454:PHE:CE2	1:K:203:LEU:HD22	2.47	0.48
1:G:74:CYS:SG	1:G:79:ARG:NH1	2.87	0.48
1:B:98:TYR:CE1	1:B:328:MET:HG3	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:TYR:OH	1:B:332:GLY:O	2.31	0.48
1:F:90:PRO:HB2	1:F:334:LEU:HD12	1.94	0.48
1:K:88:VAL:HG11	1:K:97:LEU:HD13	1.95	0.48
1:B:231:HIS:CD2	1:B:245:VAL:HG22	2.49	0.48
1:E:37:LEU:HB2	1:E:40:TRP:HD1	1.78	0.48
1:K:84:PHE:CE2	1:K:86:TYR:HB3	2.48	0.48
1:E:203:LEU:HD22	1:C:454:PHE:CE2	2.49	0.48
1:G:232:GLU:CG	1:G:244:THR:HB	2.44	0.48
1:B:36:ALA:O	1:B:333:LYS:HB2	2.13	0.48
1:H:428:VAL:HB	1:H:431:LEU:HD12	1.96	0.48
1:C:165:GLU:OE2	1:C:235:TYR:OH	2.29	0.48
1:C:370:LYS:HE3	1:C:372:ILE:HG22	1.95	0.48
1:J:454:PHE:CD1	1:J:465:PRO:HA	2.49	0.48
1:B:410:ILE:HD11	1:B:411:TYR:CE2	2.48	0.48
1:L:164:GLU:HG3	1:L:168:HIS:NE2	2.29	0.48
1:H:6:VAL:HG12	1:H:63:GLU:HB3	1.96	0.48
1:C:72:ARG:HH12	1:C:357:ARG:HE	1.60	0.48
1:I:47:LYS:O	1:I:51:VAL:HG23	2.13	0.48
1:I:88:VAL:HG21	1:I:97:LEU:H	1.79	0.48
1:D:311:VAL:HG21	1:D:328:MET:HE1	1.95	0.48
1:F:428:VAL:HB	1:F:431:LEU:HD12	1.95	0.48
1:E:437:LEU:O	1:E:441:MET:HG2	2.14	0.48
1:L:340:LYS:HA	1:L:370:LYS:HE2	1.96	0.48
1:A:191:PHE:CD2	1:A:192:LEU:HG	2.49	0.48
1:A:203:LEU:HD22	1:D:454:PHE:CE2	2.49	0.48
1:A:458:ILE:HD12	1:A:458:ILE:H	1.79	0.48
1:F:456:PHE:HD2	1:F:498:LEU:HG	1.79	0.48
1:L:5:PHE:CE2	1:L:7:ILE:HD13	2.49	0.48
1:H:328:MET:SD	1:H:333:LYS:HB2	2.53	0.48
1:J:340:LYS:HA	1:J:370:LYS:HE2	1.95	0.48
1:B:47:LYS:O	1:B:51:VAL:HG23	2.14	0.48
1:E:456:PHE:HD2	1:E:498:LEU:HG	1.78	0.48
1:H:401:PRO:HG2	1:H:478:LYS:HD2	1.96	0.48
1:G:254:SER:HA	1:G:290:TYR:HB2	1.95	0.48
1:G:260:TRP:CZ3	1:G:262:PRO:HA	2.49	0.48
1:G:320:ILE:HD11	1:G:335:PHE:CE2	2.48	0.48
1:K:4:ARG:HG3	1:K:494:LYS:O	2.14	0.48
1:I:176:LYS:HB2	1:I:262:PRO:HG2	1.94	0.48
1:J:410:ILE:HG13	1:J:411:TYR:CD2	2.49	0.48
1:A:337:ILE:HG23	1:A:369:TYR:HB3	1.95	0.47
1:C:441:MET:HE1	1:C:469:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:8:TRP:CD1	1:J:61:PHE:HD2	2.32	0.47
1:A:439:ASP:OD1	1:B:346:LYS:NZ	2.39	0.47
1:B:407:LEU:HD12	1:B:408:ASP:H	1.78	0.47
1:D:47:LYS:O	1:D:51:VAL:HG23	2.14	0.47
1:H:370:LYS:HE3	1:H:372:ILE:HG22	1.95	0.47
1:I:236:TYR:HB3	1:I:241:ILE:HG21	1.96	0.47
1:J:156:ARG:NH2	1:J:235:TYR:OH	2.47	0.47
1:D:186:LYS:HE3	1:D:190:ARG:HH21	1.78	0.47
1:D:437:LEU:O	1:D:441:MET:HG2	2.15	0.47
1:L:72:ARG:HH12	1:L:357:ARG:HE	1.62	0.47
1:H:232:GLU:HG2	1:H:244:THR:HB	1.95	0.47
1:G:447:THR:O	1:G:450:GLU:HG2	2.14	0.47
1:H:8:TRP:CH2	1:H:458:ILE:HD11	2.49	0.47
1:D:316:HIS:CG	1:D:361:PHE:HZ	2.33	0.47
1:H:331:ARG:HG2	1:H:333:LYS:NZ	2.29	0.47
1:H:456:PHE:HD2	1:H:498:LEU:HG	1.79	0.47
1:G:392:LEU:HD11	1:G:404:GLU:OE2	2.14	0.47
1:K:284:THR:HG22	1:K:285:ASN:N	2.24	0.47
1:I:84:PHE:CE2	1:I:86:TYR:HB3	2.49	0.47
1:J:77:GLY:HA2	1:J:99:THR:OG1	2.14	0.47
1:J:428:VAL:HB	1:J:431:LEU:HD12	1.97	0.47
1:A:33:GLN:HE22	1:A:331:ARG:HG2	1.80	0.47
1:B:6:VAL:HG22	1:B:496:VAL:HB	1.95	0.47
1:B:260:TRP:CZ3	1:B:262:PRO:HA	2.50	0.47
1:F:218:MET:O	1:F:283:ARG:NH1	2.46	0.47
1:E:456:PHE:CD2	1:E:498:LEU:HG	2.50	0.47
1:H:191:PHE:CD2	1:H:192:LEU:HG	2.49	0.47
1:C:175:GLU:HB2	1:C:181:TYR:CE1	2.50	0.47
1:K:254:SER:HA	1:K:290:TYR:HB2	1.97	0.47
1:I:4:ARG:NH2	1:J:204:GLY:O	2.47	0.47
1:E:47:LYS:O	1:E:51:VAL:HG23	2.15	0.47
1:H:15:GLU:H	1:H:55:ASN:ND2	2.09	0.47
1:H:88:VAL:HB	1:H:93:ASN:HD22	1.79	0.47
1:H:335:PHE:CG	1:H:335:PHE:O	2.66	0.47
1:K:388:ASN:HB3	1:K:404:GLU:HG2	1.97	0.47
1:K:428:VAL:HB	1:K:431:LEU:HD12	1.96	0.47
1:J:211:GLN:NE2	1:J:223:LYS:O	2.33	0.47
1:E:252:GLY:HA3	1:E:288:TYR:O	2.15	0.47
1:L:203:LEU:HD22	1:K:454:PHE:HE2	1.80	0.47
1:G:216:GLN:O	1:G:283:ARG:NH2	2.48	0.47
1:J:4:ARG:HD2	1:J:496:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:PHE:CD1	1:D:465:PRO:HA	2.50	0.47
1:L:391:ALA:HB1	1:L:402:TYR:HB3	1.97	0.47
1:G:70:TYR:HD2	1:G:249:LEU:HD21	1.80	0.47
1:I:264:TYR:HB3	1:I:267:TRP:CD1	2.50	0.47
1:J:67:VAL:HG12	1:J:250:PRO:HD3	1.97	0.47
1:B:189:LYS:HA	1:B:193:CYS:HB2	1.97	0.47
1:F:78:PHE:HD1	1:F:87:LYS:HB3	1.80	0.47
1:F:339:LYS:HE2	1:F:369:TYR:HE1	1.79	0.47
1:E:253:ILE:HB	1:E:281:ILE:HD11	1.96	0.47
1:H:49:ASP:OD1	1:H:49:ASP:N	2.48	0.47
1:G:253:ILE:HB	1:G:281:ILE:HD11	1.97	0.47
1:C:67:VAL:HG12	1:C:250:PRO:HD3	1.97	0.47
1:J:70:TYR:HD2	1:J:249:LEU:HD21	1.80	0.47
1:J:100:ILE:HG23	1:J:291:LEU:HB2	1.97	0.47
1:B:191:PHE:CD2	1:B:192:LEU:HG	2.50	0.46
1:B:244:THR:HG1	1:B:258:PHE:HD1	1.62	0.46
1:E:103:ALA:HB3	1:E:106:GLU:HG2	1.97	0.46
1:L:203:LEU:HD12	1:K:4:ARG:HD2	1.96	0.46
1:H:119:ARG:HB3	1:H:123:ARG:NH1	2.30	0.46
1:C:428:VAL:HB	1:C:431:LEU:HD12	1.97	0.46
1:A:349:TYR:H	1:B:442:GLN:HE22	1.62	0.46
1:A:454:PHE:CD1	1:A:465:PRO:HA	2.50	0.46
1:F:32:ASP:OD1	1:F:33:GLN:N	2.48	0.46
1:F:47:LYS:O	1:F:51:VAL:HG23	2.15	0.46
1:F:435:TRP:CZ2	1:E:442:GLN:NE2	2.83	0.46
1:E:255:SER:HG	1:E:289:TYR:HH	1.62	0.46
1:L:6:VAL:HG12	1:L:63:GLU:HB3	1.96	0.46
1:L:8:TRP:CH2	1:L:458:ILE:HD11	2.49	0.46
1:C:140:VAL:HG21	1:C:282:GLN:OE1	2.15	0.46
1:K:472:GLU:HG3	1:K:473:PRO:HD2	1.97	0.46
1:B:391:ALA:HB1	1:B:402:TYR:HB3	1.97	0.46
1:B:428:VAL:HB	1:B:431:LEU:HD12	1.98	0.46
1:D:84:PHE:CE2	1:D:86:TYR:HB3	2.50	0.46
1:H:124:ILE:HG13	1:H:125:THR:HG23	1.98	0.46
1:G:191:PHE:CD2	1:G:192:LEU:HG	2.50	0.46
1:G:437:LEU:O	1:G:441:MET:HG2	2.15	0.46
1:C:73:MET:HB3	1:C:78:PHE:HD2	1.80	0.46
1:K:12:MET:SD	1:K:425:PRO:HD3	2.56	0.46
1:K:176:LYS:HB2	1:K:262:PRO:HG2	1.98	0.46
1:B:92:ARG:NH2	1:B:406:ASP:OD2	2.48	0.46
1:L:7:ILE:HG22	1:L:62:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:284:THR:CG2	1:J:286:LEU:HD23	2.46	0.46
1:B:431:LEU:HD22	1:B:486:LEU:HA	1.96	0.46
1:D:254:SER:HA	1:D:290:TYR:HB2	1.97	0.46
1:F:111:LYS:HE2	1:F:115:LYS:HE3	1.97	0.46
1:H:34:LEU:HD22	1:H:94:CYS:HB2	1.96	0.46
1:I:441:MET:HE1	1:I:469:PHE:HE2	1.80	0.46
1:J:457:GLU:HA	1:J:499:TYR:O	2.15	0.46
1:F:84:PHE:CE2	1:F:86:TYR:HB3	2.51	0.46
1:E:88:VAL:HG21	1:E:97:LEU:H	1.80	0.46
1:H:78:PHE:CE1	1:H:87:LYS:HD2	2.51	0.46
1:G:241:ILE:HB	1:G:264:TYR:HD2	1.81	0.46
1:I:11:SER:OG	1:I:13:HIS:NE2	2.49	0.46
1:I:234:TYR:HB2	1:I:242:ALA:HB3	1.97	0.46
1:B:458:ILE:HD12	1:B:458:ILE:H	1.81	0.46
1:E:460:THR:O	1:E:461:GLU:HG3	2.15	0.46
1:L:472:GLU:O	1:L:477:LYS:HE3	2.16	0.46
1:J:144:VAL:HG13	1:J:216:GLN:HB3	1.98	0.46
1:A:260:TRP:HB2	1:A:269:LEU:HD12	1.98	0.46
1:F:7:ILE:HG22	1:F:62:VAL:HA	1.96	0.46
1:F:260:TRP:CZ3	1:F:262:PRO:HA	2.50	0.46
1:L:98:TYR:OH	1:L:333:LYS:O	2.32	0.46
1:H:472:GLU:O	1:H:477:LYS:HE3	2.15	0.46
1:I:40:TRP:CZ3	1:I:410:ILE:HG22	2.50	0.46
1:B:5:PHE:CE2	1:B:7:ILE:HD13	2.51	0.46
1:D:175:GLU:HB2	1:D:181:TYR:CE1	2.51	0.46
1:E:140:VAL:HG22	1:E:279:ALA:HA	1.98	0.46
1:E:458:ILE:HD12	1:E:458:ILE:H	1.81	0.46
1:C:77:GLY:HA2	1:C:99:THR:OG1	2.16	0.46
1:K:33:GLN:OE1	1:K:331:ARG:NE	2.48	0.46
1:K:410:ILE:HG13	1:K:411:TYR:CD2	2.50	0.46
1:J:252:GLY:HA3	1:J:288:TYR:O	2.15	0.46
1:A:264:TYR:HB3	1:A:267:TRP:CD1	2.51	0.45
1:F:475:ASN:O	1:F:479:ARG:HG3	2.17	0.45
1:L:88:VAL:HB	1:L:93:ASN:HD22	1.80	0.45
1:L:313:ASP:O	1:L:317:SER:N	2.49	0.45
1:L:410:ILE:HG13	1:L:411:TYR:CD2	2.52	0.45
1:H:461:GLU:O	1:G:189:LYS:HD2	2.16	0.45
1:G:175:GLU:HG3	1:G:181:TYR:CZ	2.51	0.45
1:K:37:LEU:HB2	1:K:40:TRP:HD1	1.81	0.45
1:J:8:TRP:O	1:J:60:SER:OG	2.34	0.45
1:L:231:HIS:CD2	1:L:245:VAL:HG22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:267:TRP:HE3	1:L:269:LEU:HD21	1.80	0.45
1:G:432:LEU:HB3	1:G:485:ARG:HA	1.99	0.45
1:K:260:TRP:CZ3	1:K:262:PRO:HA	2.51	0.45
1:J:84:PHE:CE2	1:J:86:TYR:HB3	2.51	0.45
1:L:203:LEU:HD13	1:K:454:PHE:HD2	1.79	0.45
1:L:361:PHE:CG	1:L:362:PRO:HD2	2.51	0.45
1:G:147:GLU:OE2	1:G:276:ARG:NH2	2.49	0.45
1:C:264:TYR:HB3	1:C:267:TRP:CD1	2.51	0.45
1:I:232:GLU:HG2	1:I:244:THR:HB	1.98	0.45
1:A:44:TYR:OH	1:A:409:THR:HG23	2.16	0.45
1:A:287:GLN:HG3	1:A:288:TYR:CD2	2.52	0.45
1:D:157:PHE:HZ	1:D:280:ILE:HD13	1.82	0.45
1:E:350:LEU:HD12	1:E:432:LEU:HA	1.99	0.45
1:L:215:TRP:CD2	1:L:280:ILE:HG12	2.51	0.45
1:L:313:ASP:OD2	1:L:337:ILE:HG22	2.16	0.45
1:L:454:PHE:CD1	1:L:465:PRO:HA	2.51	0.45
1:H:437:LEU:O	1:H:441:MET:HG2	2.17	0.45
1:J:79:ARG:NH2	1:J:99:THR:HG23	2.30	0.45
1:F:432:LEU:HB3	1:F:485:ARG:HA	1.98	0.45
1:L:111:LYS:HE2	1:L:115:LYS:HE3	1.98	0.45
1:A:304:LYS:O	1:A:329:ILE:HD11	2.16	0.45
1:F:437:LEU:O	1:F:441:MET:HG2	2.16	0.45
1:H:454:PHE:CE2	1:G:203:LEU:HD22	2.51	0.45
1:C:84:PHE:CE2	1:C:86:TYR:HB3	2.51	0.45
1:J:6:VAL:HG22	1:J:496:VAL:HB	1.99	0.45
1:E:461:GLU:O	1:C:189:LYS:HD2	2.16	0.45
1:L:191:PHE:CD2	1:L:192:LEU:HG	2.50	0.45
1:L:208:SER:HB2	1:L:226:HIS:HB2	1.99	0.45
1:G:5:PHE:CE2	1:G:7:ILE:HD13	2.51	0.45
1:C:79:ARG:HH22	1:C:290:TYR:HB3	1.82	0.45
1:K:368:LYS:HE2	1:K:368:LYS:HB3	1.63	0.45
1:I:454:PHE:CD2	1:J:203:LEU:HD13	2.52	0.45
1:K:69:THR:O	1:K:73:MET:HG2	2.17	0.45
1:B:72:ARG:NH2	1:B:490:GLU:OE2	2.50	0.45
1:L:34:LEU:HD22	1:L:94:CYS:HB2	1.97	0.45
1:L:437:LEU:O	1:L:441:MET:HG2	2.17	0.45
1:L:456:PHE:CD1	1:L:463:ILE:HG22	2.52	0.45
1:G:312:LEU:HB2	1:G:319:TYR:CE1	2.52	0.45
1:C:454:PHE:CD1	1:C:465:PRO:HA	2.52	0.45
1:J:456:PHE:HB2	1:J:463:ILE:HG12	1.98	0.45
1:A:437:LEU:O	1:A:441:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HD11	1:B:322:LEU:HD22	1.99	0.45
1:F:437:LEU:HD21	1:F:481:CYS:HB3	1.99	0.45
1:I:388:ASN:HB3	1:I:404:GLU:HG2	1.97	0.45
1:E:475:ASN:O	1:E:479:ARG:HG3	2.17	0.44
1:C:6:VAL:HG12	1:C:63:GLU:HB3	1.98	0.44
1:B:3:ASP:OD2	1:B:64:HIS:NE2	2.49	0.44
1:B:347:GLU:OE2	1:B:427:VAL:HG13	2.17	0.44
1:H:254:SER:HA	1:H:290:TYR:HB2	2.00	0.44
1:G:215:TRP:CD2	1:G:280:ILE:HG12	2.53	0.44
1:I:454:PHE:CD1	1:I:465:PRO:HA	2.52	0.44
1:B:322:LEU:HD11	1:B:328:MET:HE2	2.00	0.44
1:B:326:GLN:O	1:B:329:ILE:HG12	2.17	0.44
1:B:452:ARG:HB3	1:B:493:MET:O	2.17	0.44
1:E:102:THR:HG21	1:E:107:LEU:HD12	1.99	0.44
1:E:428:VAL:HB	1:E:431:LEU:HD12	1.98	0.44
1:G:195:THR:HG21	1:G:229:PRO:HG3	1.99	0.44
1:K:224:LEU:HG	1:K:284:THR:CG2	2.44	0.44
1:J:140:VAL:HG21	1:J:282:GLN:OE1	2.17	0.44
1:A:84:PHE:CE2	1:A:86:TYR:HB3	2.53	0.44
1:B:215:TRP:CD2	1:B:280:ILE:HG12	2.53	0.44
1:D:37:LEU:HA	1:D:333:LYS:HZ2	1.82	0.44
1:E:161:LEU:HD22	1:C:463:ILE:HG23	2.00	0.44
1:H:441:MET:HE1	1:H:469:PHE:HE2	1.82	0.44
1:G:340:LYS:HA	1:G:370:LYS:HE2	1.98	0.44
1:K:340:LYS:HA	1:K:370:LYS:HE2	1.98	0.44
1:D:387:ALA:HB1	1:D:434:LEU:HD12	1.99	0.44
1:G:253:ILE:HD12	1:G:281:ILE:HG13	1.99	0.44
1:K:47:LYS:O	1:K:51:VAL:HG23	2.16	0.44
1:I:117:ILE:HD13	1:I:139:PHE:HB2	1.99	0.44
1:B:267:TRP:HE3	1:B:269:LEU:HD21	1.82	0.44
1:B:280:ILE:O	1:B:284:THR:HG22	2.17	0.44
1:D:140:VAL:HG21	1:D:282:GLN:OE1	2.18	0.44
1:F:156:ARG:NH2	1:F:235:TYR:OH	2.51	0.44
1:E:203:LEU:HD13	1:C:454:PHE:HD2	1.82	0.44
1:E:232:GLU:HG2	1:E:244:THR:HB	1.98	0.44
1:I:232:GLU:CG	1:I:244:THR:HB	2.47	0.44
1:J:4:ARG:HD3	1:J:494:LYS:O	2.18	0.44
1:D:320:ILE:HD12	1:D:335:PHE:HE2	1.82	0.44
1:D:320:ILE:HD13	1:D:337:ILE:HG21	1.98	0.44
1:D:347:GLU:OE2	1:D:427:VAL:HG13	2.18	0.44
1:J:340:LYS:HG2	1:J:370:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:TRP:O	1:D:60:SER:OG	2.35	0.44
1:E:328:MET:SD	1:E:328:MET:N	2.86	0.44
1:L:120:PHE:O	1:L:124:ILE:HG12	2.17	0.44
1:L:330:SER:HB3	1:L:333:LYS:HB2	1.99	0.44
1:B:98:TYR:OH	1:B:328:MET:HA	2.17	0.44
1:L:159:PRO:HB2	1:L:161:LEU:HG	2.00	0.44
1:H:340:LYS:HA	1:H:370:LYS:HE2	2.00	0.44
1:G:35:PHE:O	1:G:331:ARG:NH1	2.51	0.44
1:G:124:ILE:HG13	1:G:125:THR:HG23	2.00	0.44
1:C:384:PHE:CE1	1:C:410:ILE:HD11	2.53	0.44
1:E:70:TYR:HD2	1:E:249:LEU:HD21	1.83	0.43
1:E:79:ARG:NH1	1:E:254:SER:HB2	2.25	0.43
1:E:347:GLU:OE2	1:E:383:ALA:HB1	2.18	0.43
1:E:364:ASP:OD1	1:E:366:VAL:HG22	2.17	0.43
1:L:350:LEU:HD12	1:L:432:LEU:HA	2.00	0.43
1:L:450:GLU:OE1	1:G:339:LYS:HE3	2.18	0.43
1:H:322:LEU:HD11	1:H:329:ILE:HB	1.98	0.43
1:I:8:TRP:HH2	1:I:458:ILE:HD11	1.82	0.43
1:I:140:VAL:HG21	1:I:282:GLN:OE1	2.18	0.43
1:I:6:VAL:HG22	1:I:496:VAL:HB	1.98	0.43
1:B:461:GLU:HA	1:F:189:LYS:HZ1	1.83	0.43
1:F:264:TYR:HB3	1:F:267:TRP:CD1	2.54	0.43
1:E:175:GLU:HB2	1:E:181:TYR:CE1	2.52	0.43
1:L:457:GLU:HG2	1:L:460:THR:OG1	2.17	0.43
1:H:260:TRP:CZ3	1:H:262:PRO:HA	2.54	0.43
1:D:117:ILE:HD11	1:D:275:LEU:HD13	1.99	0.43
1:F:73:MET:HB3	1:F:78:PHE:HD2	1.82	0.43
1:F:336:VAL:N	1:F:373:ALA:HB2	2.31	0.43
1:H:203:LEU:HD22	1:G:454:PHE:CZ	2.53	0.43
1:G:472:GLU:HG3	1:G:476:VAL:HB	2.01	0.43
1:C:33:GLN:CD	1:C:331:ARG:HD2	2.39	0.43
1:J:6:VAL:HG12	1:J:63:GLU:HB3	1.99	0.43
1:J:232:GLU:CG	1:J:244:THR:HB	2.48	0.43
1:A:241:ILE:HG22	1:A:264:TYR:HE2	1.84	0.43
1:E:323:LYS:HG3	1:E:324:PRO:HD3	2.01	0.43
1:H:145:ASN:OD1	1:H:149:ASN:ND2	2.51	0.43
1:G:479:ARG:NH1	1:G:499:TYR:HB2	2.34	0.43
1:C:208:SER:HB2	1:C:226:HIS:HB2	2.01	0.43
1:I:370:LYS:HZ2	1:I:372:ILE:HG22	1.84	0.43
1:B:98:TYR:CD1	1:B:328:MET:CG	2.99	0.43
1:E:6:VAL:HG22	1:E:496:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:340:LYS:HE3	1:L:368:LYS:O	2.19	0.43
1:G:231:HIS:CD2	1:G:245:VAL:HG22	2.53	0.43
1:E:454:PHE:CE2	1:C:203:LEU:HD22	2.54	0.43
1:G:98:TYR:OH	1:G:332:GLY:O	2.32	0.43
1:K:209:TRP:CH2	1:K:230:VAL:HG12	2.53	0.43
1:I:145:ASN:OD1	1:I:149:ASN:ND2	2.51	0.43
1:I:209:TRP:CH2	1:I:230:VAL:HG12	2.53	0.43
1:J:176:LYS:HD2	1:J:262:PRO:HG2	2.01	0.43
1:B:67:VAL:HG12	1:B:250:PRO:HD3	2.01	0.43
1:F:67:VAL:HG12	1:F:250:PRO:HD3	2.01	0.43
1:I:189:LYS:HA	1:I:193:CYS:HB2	2.01	0.43
1:I:322:LEU:HD11	1:I:329:ILE:HD13	2.00	0.43
1:J:234:TYR:CD2	1:J:242:ALA:HB3	2.53	0.43
1:A:208:SER:HB2	1:A:226:HIS:HB2	1.99	0.43
1:L:468:ASN:ND2	1:G:341:LYS:HD2	2.30	0.43
1:H:56:CYS:SG	1:H:93:ASN:HB2	2.59	0.43
1:H:218:MET:SD	1:H:284:THR:HG22	2.59	0.43
1:G:456:PHE:HD1	1:G:463:ILE:HB	1.84	0.43
1:C:7:ILE:HG22	1:C:62:VAL:HG22	2.01	0.43
1:I:347:GLU:OE2	1:I:427:VAL:HG13	2.19	0.43
1:A:189:LYS:HA	1:A:193:CYS:HB2	2.00	0.43
1:A:349:TYR:CD1	1:A:436:GLU:OE2	2.72	0.43
1:F:401:PRO:HG2	1:F:478:LYS:HD2	2.00	0.43
1:E:191:PHE:CD2	1:E:192:LEU:HG	2.54	0.43
1:E:284:THR:CG2	1:E:286:LEU:HD23	2.45	0.43
1:L:336:VAL:H	1:L:373:ALA:HB2	1.83	0.43
1:K:155:THR:HG21	1:K:276:ARG:CZ	2.48	0.43
1:I:203:LEU:HD22	1:J:454:PHE:CE2	2.54	0.43
1:A:217:ARG:HD3	1:C:105:GLN:OE1	2.19	0.42
1:D:120:PHE:O	1:D:124:ILE:HG12	2.18	0.42
1:L:439:ASP:OD1	1:G:346:LYS:NZ	2.37	0.42
1:H:5:PHE:CE2	1:H:7:ILE:HD13	2.54	0.42
1:H:79:ARG:HH22	1:H:99:THR:HG23	1.84	0.42
1:H:244:THR:HG1	1:H:258:PHE:HD1	1.67	0.42
1:K:236:TYR:HB3	1:K:241:ILE:HG21	2.01	0.42
1:J:232:GLU:HG2	1:J:244:THR:HB	2.00	0.42
1:J:361:PHE:CG	1:J:362:PRO:HD2	2.53	0.42
1:A:326:GLN:O	1:A:329:ILE:HG22	2.19	0.42
1:D:281:ILE:HG23	1:D:286:LEU:HB2	2.01	0.42
1:D:388:ASN:HB3	1:D:404:GLU:HG2	2.01	0.42
1:E:323:LYS:CG	1:E:324:PRO:HD3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:TRP:HD1	1:C:61:PHE:O	2.03	0.42
1:C:350:LEU:HD12	1:C:432:LEU:HA	2.01	0.42
1:J:192:LEU:HD22	1:J:245:VAL:HG21	2.01	0.42
1:B:289:TYR:HE2	1:B:291:LEU:HD23	1.84	0.42
1:D:362:PRO:HG2	1:D:369:TYR:OH	2.20	0.42
1:F:232:GLU:CG	1:F:244:THR:HB	2.49	0.42
1:F:475:ASN:ND2	1:F:501:GLU:OE2	2.52	0.42
1:E:54:GLU:HG3	1:E:56:CYS:SG	2.59	0.42
1:E:337:ILE:HD11	1:E:369:TYR:CG	2.55	0.42
1:L:124:ILE:HG13	1:L:125:THR:HG23	2.02	0.42
1:G:337:ILE:HG13	1:G:369:TYR:HB3	2.02	0.42
1:K:456:PHE:CD2	1:K:498:LEU:HG	2.54	0.42
1:J:279:ALA:O	1:J:283:ARG:HG2	2.19	0.42
1:J:431:LEU:HD22	1:J:486:LEU:HA	2.01	0.42
1:B:203:LEU:HD22	1:F:454:PHE:CE2	2.55	0.42
1:D:443:SER:HB3	1:C:349:TYR:HB3	2.01	0.42
1:E:140:VAL:HG21	1:E:282:GLN:OE1	2.19	0.42
1:L:84:PHE:CE2	1:L:86:TYR:HB3	2.53	0.42
1:L:241:ILE:HG22	1:L:264:TYR:HE2	1.83	0.42
1:G:69:THR:O	1:G:73:MET:HG2	2.19	0.42
1:I:248:ILE:HD13	1:I:253:ILE:HG12	2.01	0.42
1:J:98:TYR:OH	1:J:332:GLY:O	2.24	0.42
1:A:78:PHE:CE1	1:A:87:LYS:HD2	2.55	0.42
1:B:98:TYR:HH	1:B:332:GLY:C	2.21	0.42
1:E:169:LEU:HD22	1:E:240:LEU:HG	2.00	0.42
1:H:84:PHE:CE2	1:H:86:TYR:HB3	2.54	0.42
1:H:439:ASP:OD1	1:I:346:LYS:NZ	2.40	0.42
1:I:231:HIS:CD2	1:I:245:VAL:HG22	2.54	0.42
1:I:456:PHE:CD2	1:I:498:LEU:HG	2.53	0.42
1:J:34:LEU:HD22	1:J:94:CYS:HB2	2.02	0.42
1:A:73:MET:HB3	1:A:78:PHE:HD2	1.85	0.42
1:B:433:PRO:HD2	1:B:436:GLU:OE2	2.19	0.42
1:B:454:PHE:HD2	1:F:203:LEU:HD13	1.84	0.42
1:H:331:ARG:HE	1:H:333:LYS:HE2	1.83	0.42
1:K:12:MET:SD	1:K:424:ILE:HA	2.59	0.42
1:I:5:PHE:CE2	1:I:7:ILE:HD13	2.55	0.42
1:J:36:ALA:HB1	1:J:334:LEU:HD22	2.01	0.42
1:F:40:TRP:CZ2	1:F:410:ILE:HD13	2.53	0.42
1:K:241:ILE:HG22	1:K:264:TYR:HE2	1.85	0.42
1:K:341:LYS:HD3	1:J:468:ASN:ND2	2.34	0.42
1:K:456:PHE:HD2	1:K:498:LEU:HG	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:406:ASP:CG	1:J:410:ILE:HG22	2.40	0.42
1:A:311:VAL:HG13	1:A:322:LEU:HD12	2.01	0.42
1:A:336:VAL:H	1:A:373:ALA:HB2	1.84	0.42
1:A:432:LEU:HB3	1:A:485:ARG:HA	2.01	0.42
1:C:191:PHE:CD2	1:C:192:LEU:HG	2.54	0.42
1:C:272:LEU:O	1:C:276:ARG:HG3	2.20	0.42
1:I:100:ILE:HG23	1:I:291:LEU:HB3	2.02	0.42
1:I:457:GLU:HG2	1:I:499:TYR:CE2	2.55	0.42
1:J:156:ARG:O	1:J:232:GLU:HA	2.19	0.42
1:J:240:LEU:HD21	1:J:243:ILE:HD11	2.02	0.42
1:A:384:PHE:CE1	1:A:410:ILE:HD12	2.55	0.42
1:B:124:ILE:HG13	1:B:125:THR:HG23	2.02	0.42
1:D:147:GLU:OE2	1:D:276:ARG:NH2	2.53	0.42
1:G:431:LEU:HD22	1:G:486:LEU:HA	2.01	0.42
1:J:400:ILE:HG12	1:J:477:LYS:HB3	2.01	0.42
1:B:7:ILE:HG22	1:B:62:VAL:HG22	2.01	0.42
1:F:124:ILE:HG13	1:F:125:THR:HG23	2.02	0.42
1:F:313:ASP:OD2	1:F:337:ILE:HG22	2.20	0.42
1:L:96:ARG:NH2	1:L:332:GLY:HA3	2.33	0.42
1:H:349:TYR:HB3	1:I:443:SER:HB3	2.02	0.42
1:F:450:GLU:OE2	1:F:468:ASN:HA	2.20	0.41
1:F:458:ILE:HD12	1:F:458:ILE:H	1.85	0.41
1:H:73:MET:HB3	1:H:78:PHE:HD2	1.84	0.41
1:K:347:GLU:OE2	1:K:427:VAL:HG13	2.20	0.41
1:A:140:VAL:HG21	1:A:282:GLN:OE1	2.20	0.41
1:D:92:ARG:HG2	1:D:410:ILE:HD13	2.01	0.41
1:D:248:ILE:HD13	1:D:253:ILE:HG12	2.03	0.41
1:L:70:TYR:HD2	1:L:249:LEU:HD21	1.85	0.41
1:L:124:ILE:HD11	1:L:146:ALA:HB1	2.01	0.41
1:H:200:GLU:O	1:H:204:GLY:N	2.50	0.41
1:G:159:PRO:HB2	1:G:161:LEU:HG	2.02	0.41
1:K:231:HIS:CD2	1:K:245:VAL:HG22	2.54	0.41
1:J:445:LYS:HD2	1:J:448:ASP:OD2	2.19	0.41
1:A:37:LEU:HB2	1:A:40:TRP:HD1	1.86	0.41
1:B:121:ALA:O	1:B:125:THR:OG1	2.31	0.41
1:B:159:PRO:HB2	1:B:161:LEU:HG	2.01	0.41
1:L:3:ASP:HB2	1:K:200:GLU:OE1	2.20	0.41
1:L:441:MET:HE1	1:L:469:PHE:HE2	1.86	0.41
1:J:224:LEU:HD12	1:J:286:LEU:HD21	2.02	0.41
1:E:67:VAL:HG12	1:E:250:PRO:HD3	2.02	0.41
1:E:72:ARG:NH2	1:E:490:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:ILE:HG22	1:E:411:TYR:N	2.36	0.41
1:G:312:LEU:HD13	1:G:319:TYR:CZ	2.55	0.41
1:I:79:ARG:HH22	1:I:290:TYR:HB3	1.85	0.41
1:B:38:ASP:OD2	1:B:333:LYS:NZ	2.53	0.41
1:F:287:GLN:HG3	1:F:288:TYR:CD2	2.56	0.41
1:H:78:PHE:HD1	1:H:87:LYS:HB3	1.85	0.41
1:H:98:TYR:CE1	1:H:335:PHE:HE1	2.38	0.41
1:C:260:TRP:CZ3	1:C:262:PRO:HA	2.56	0.41
1:B:441:MET:HE1	1:B:469:PHE:CE2	2.54	0.41
1:D:325:ILE:HD12	1:D:328:MET:CE	2.51	0.41
1:E:319:TYR:HE2	1:E:358:GLY:HA2	1.85	0.41
1:K:281:ILE:HG23	1:K:286:LEU:HB2	2.03	0.41
1:I:8:TRP:CZ3	1:I:458:ILE:HD11	2.56	0.41
1:J:472:GLU:O	1:J:477:LYS:HE3	2.19	0.41
1:C:457:GLU:HA	1:C:499:TYR:O	2.21	0.41
1:F:120:PHE:O	1:F:124:ILE:HG12	2.20	0.41
1:I:37:LEU:HD22	1:I:374:GLU:OE2	2.20	0.41
1:A:47:LYS:O	1:A:51:VAL:HG23	2.21	0.41
1:A:192:LEU:HD22	1:A:245:VAL:HG21	2.02	0.41
1:A:323:LYS:HB3	1:A:324:PRO:HD3	2.03	0.41
1:B:240:LEU:HD21	1:B:243:ILE:HD11	2.03	0.41
1:B:284:THR:HG23	1:B:286:LEU:HG	2.03	0.41
1:D:164:GLU:O	1:D:168:HIS:ND1	2.47	0.41
1:D:428:VAL:HB	1:D:431:LEU:HD12	2.03	0.41
1:F:455:LEU:O	1:F:463:ILE:HG13	2.20	0.41
1:E:32:ASP:OD1	1:E:33:GLN:N	2.53	0.41
1:E:84:PHE:CE2	1:E:86:TYR:HB3	2.56	0.41
1:G:79:ARG:HH22	1:G:99:THR:HG23	1.86	0.41
1:I:253:ILE:HD12	1:I:281:ILE:HG13	2.02	0.41
1:I:324:PRO:HG2	1:I:325:ILE:HG12	2.03	0.41
1:J:157:PHE:HZ	1:J:280:ILE:HD13	1.85	0.41
1:A:472:GLU:O	1:A:477:LYS:HE3	2.21	0.41
1:H:117:ILE:HD11	1:H:275:LEU:HD13	2.03	0.41
1:G:175:GLU:HG3	1:G:181:TYR:CE1	2.56	0.41
1:G:349:TYR:HA	1:G:436:GLU:OE2	2.20	0.41
1:J:174:GLN:OE1	1:J:257:TYR:OH	2.31	0.41
1:D:457:GLU:O	1:D:460:THR:OG1	2.27	0.40
1:F:140:VAL:HG22	1:F:279:ALA:HA	2.02	0.40
1:F:191:PHE:CD2	1:F:192:LEU:HG	2.56	0.40
1:E:71:ASP:HA	1:E:249:LEU:HD13	2.02	0.40
1:H:333:LYS:HA	1:H:333:LYS:HD3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:410:ILE:HG22	1:H:411:TYR:N	2.35	0.40
1:I:191:PHE:HD2	1:I:192:LEU:HG	1.86	0.40
1:J:37:LEU:HD22	1:J:374:GLU:OE2	2.21	0.40
1:J:124:ILE:HG13	1:J:125:THR:HG23	2.03	0.40
1:A:190:ARG:HA	1:A:194:ASP:OD2	2.21	0.40
1:D:98:TYR:CE2	1:D:328:MET:HG3	2.56	0.40
1:I:189:LYS:NZ	1:J:461:GLU:O	2.40	0.40
1:I:323:LYS:HG3	1:I:324:PRO:HD3	2.03	0.40
1:J:88:VAL:HB	1:J:93:ASN:HD22	1.86	0.40
1:F:88:VAL:HG11	1:F:97:LEU:HD13	2.04	0.40
1:H:203:LEU:HD13	1:G:454:PHE:CD2	2.56	0.40
1:H:450:GLU:OE1	1:H:468:ASN:HA	2.22	0.40
1:G:338:GLY:HA3	1:G:372:ILE:HD13	2.03	0.40
1:C:36:ALA:O	1:C:334:LEU:N	2.47	0.40
1:C:117:ILE:HD13	1:C:139:PHE:HB2	2.03	0.40
1:K:473:PRO:HA	1:K:474:PRO:HD3	1.97	0.40
1:A:108:ASN:OD1	1:A:306:ASN:ND2	2.55	0.40
1:F:248:ILE:HD13	1:F:253:ILE:HG12	2.03	0.40
1:E:120:PHE:CZ	1:E:124:ILE:HD13	2.55	0.40
1:I:155:THR:HG21	1:I:276:ARG:CZ	2.50	0.40
1:I:441:MET:HE1	1:I:469:PHE:CE2	2.56	0.40
1:B:208:SER:HB2	1:B:226:HIS:HB2	2.04	0.40
1:D:38:ASP:H	1:D:333:LYS:NZ	2.19	0.40
1:D:337:ILE:HD11	1:D:361:PHE:CZ	2.57	0.40
1:F:468:ASN:ND2	1:E:341:LYS:HD2	2.37	0.40
1:G:47:LYS:O	1:G:51:VAL:HG23	2.22	0.40
1:J:37:LEU:HB2	1:J:40:TRP:HD1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/511 (91%)	437 (94%)	26 (6%)	0	100	100
1	B	457/511 (89%)	437 (96%)	20 (4%)	0	100	100
1	C	461/511 (90%)	439 (95%)	22 (5%)	0	100	100
1	D	454/511 (89%)	432 (95%)	22 (5%)	0	100	100
1	E	456/511 (89%)	438 (96%)	17 (4%)	1 (0%)	47	78
1	F	456/511 (89%)	438 (96%)	17 (4%)	1 (0%)	47	78
1	G	454/511 (89%)	440 (97%)	14 (3%)	0	100	100
1	H	456/511 (89%)	431 (94%)	25 (6%)	0	100	100
1	I	453/511 (89%)	442 (98%)	10 (2%)	1 (0%)	47	78
1	J	455/511 (89%)	435 (96%)	19 (4%)	1 (0%)	47	78
1	K	457/511 (89%)	433 (95%)	23 (5%)	1 (0%)	47	78
1	L	457/511 (89%)	435 (95%)	22 (5%)	0	100	100
All	All	5479/6132 (89%)	5237 (96%)	237 (4%)	5 (0%)	51	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	334	LEU
1	E	334	LEU
1	K	407	LEU
1	J	334	LEU
1	I	407	LEU

5.3.2 Protein sidechains (i)

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	419/453 (92%)	417 (100%)	2 (0%)	88	94
1	B	416/453 (92%)	414 (100%)	2 (0%)	88	94
1	C	419/453 (92%)	418 (100%)	1 (0%)	93	98
1	D	413/453 (91%)	413 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	415/453 (92%)	415 (100%)	0	100	100
1	F	414/453 (91%)	414 (100%)	0	100	100
1	G	413/453 (91%)	410 (99%)	3 (1%)	84	92
1	H	413/453 (91%)	412 (100%)	1 (0%)	93	98
1	I	412/453 (91%)	412 (100%)	0	100	100
1	J	414/453 (91%)	413 (100%)	1 (0%)	93	98
1	K	415/453 (92%)	415 (100%)	0	100	100
1	L	416/453 (92%)	416 (100%)	0	100	100
All	All	4979/5436 (92%)	4969 (100%)	10 (0%)	93	98

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	108	ASN
1	B	407	LEU
1	B	442	GLN
1	H	51	VAL
1	G	55	ASN
1	G	96	ARG
1	G	368	LYS
1	C	328	MET
1	J	55	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	183	ASN
1	H	55	ASN
1	H	149	ASN
1	G	55	ASN
1	G	149	ASN
1	I	149	ASN
1	J	55	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	471/511 (92%)	0.33	35 (7%)	14	16	39, 69, 132, 165	0
1	B	465/511 (90%)	0.37	28 (6%)	21	23	42, 77, 142, 179	0
1	C	469/511 (91%)	0.43	32 (6%)	17	19	43, 77, 140, 171	0
1	D	462/511 (90%)	0.29	25 (5%)	25	26	39, 71, 134, 170	0
1	E	464/511 (90%)	0.48	33 (7%)	16	18	48, 80, 142, 167	0
1	F	464/511 (90%)	0.40	28 (6%)	21	23	43, 77, 136, 161	0
1	G	462/511 (90%)	0.63	49 (10%)	6	7	55, 103, 157, 175	0
1	H	464/511 (90%)	0.41	28 (6%)	21	23	42, 79, 140, 174	0
1	I	461/511 (90%)	0.30	26 (5%)	24	25	38, 70, 131, 175	0
1	J	463/511 (90%)	0.30	27 (5%)	23	24	37, 69, 133, 165	0
1	K	465/511 (90%)	0.54	42 (9%)	9	11	52, 87, 154, 191	0
1	L	465/511 (90%)	0.67	49 (10%)	6	7	54, 101, 149, 172	0
All	All	5575/6132 (90%)	0.43	402 (7%)	15	17	37, 79, 143, 191	0

All (402) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	330	SER	7.0
1	E	422	ASN	6.5
1	H	329	ILE	6.4
1	J	51	VAL	6.2
1	L	411	TYR	6.2
1	K	130	CYS	5.9
1	D	330	SER	5.7
1	I	503	MET	5.5
1	C	365	ASN	5.4
1	K	133	ALA	5.4
1	G	109	MET	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	329	ILE	5.2
1	K	132	ALA	5.1
1	K	116	CYS	5.1
1	D	329	ILE	5.0
1	B	411	TYR	4.8
1	F	329	ILE	4.8
1	J	49	ASP	4.7
1	I	130	CYS	4.7
1	E	56	CYS	4.7
1	J	330	SER	4.7
1	I	129	TYR	4.6
1	K	35	PHE	4.6
1	D	1	MET	4.6
1	K	330	SER	4.6
1	G	403	GLU	4.5
1	D	328	MET	4.5
1	L	44	TYR	4.4
1	C	328	MET	4.3
1	K	120	PHE	4.3
1	A	51	VAL	4.3
1	G	411	TYR	4.3
1	K	32	ASP	4.3
1	K	503	MET	4.3
1	A	329	ILE	4.2
1	J	129	TYR	4.2
1	A	330	SER	4.2
1	F	51	VAL	4.2
1	L	406	ASP	4.2
1	L	331	ARG	4.1
1	K	265	SER	4.1
1	F	330	SER	4.0
1	L	56	CYS	4.0
1	H	53	ILE	4.0
1	D	54	GLU	4.0
1	A	46	ASN	4.0
1	E	331	ARG	4.0
1	A	16	PRO	4.0
1	B	131	PRO	4.0
1	H	411	TYR	3.9
1	L	384	PHE	3.9
1	D	51	VAL	3.9
1	B	130	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	K	128	ASP	3.9
1	B	409	THR	3.9
1	C	306	ASN	3.9
1	L	332	GLY	3.9
1	I	35	PHE	3.8
1	A	53	ILE	3.8
1	F	50	VAL	3.8
1	J	133	ALA	3.8
1	E	54	GLU	3.8
1	C	330	SER	3.8
1	B	46	ASN	3.8
1	K	50	VAL	3.8
1	C	49	ASP	3.8
1	G	51	VAL	3.8
1	B	110	THR	3.8
1	A	129	TYR	3.8
1	F	46	ASN	3.7
1	A	503	MET	3.7
1	L	130	CYS	3.7
1	C	503	MET	3.7
1	B	31	MET	3.7
1	L	40	TRP	3.7
1	K	131	PRO	3.7
1	E	130	CYS	3.7
1	G	129	TYR	3.6
1	G	34	LEU	3.6
1	C	331	ARG	3.6
1	L	129	TYR	3.6
1	B	136	SER	3.6
1	D	49	ASP	3.6
1	G	56	CYS	3.6
1	H	333	LYS	3.6
1	J	50	VAL	3.6
1	H	32	ASP	3.6
1	L	306	ASN	3.6
1	G	422	ASN	3.6
1	B	306	ASN	3.6
1	G	365	ASN	3.5
1	A	127	GLU	3.5
1	F	411	TYR	3.5
1	I	307	TYR	3.5
1	K	126	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	53	ILE	3.5
1	K	93	ASN	3.4
1	G	112	GLU	3.4
1	F	34	LEU	3.4
1	B	35	PHE	3.4
1	L	408	ASP	3.4
1	L	35	PHE	3.4
1	L	54	GLU	3.4
1	B	127	GLU	3.4
1	D	365	ASN	3.4
1	G	330	SER	3.4
1	J	97	LEU	3.4
1	E	365	ASN	3.3
1	A	45	MET	3.3
1	H	51	VAL	3.3
1	K	51	VAL	3.3
1	D	128	ASP	3.3
1	L	50	VAL	3.3
1	I	115	LYS	3.3
1	B	51	VAL	3.3
1	E	329	ILE	3.3
1	H	306	ASN	3.3
1	E	50	VAL	3.3
1	J	134	VAL	3.3
1	B	132	ALA	3.3
1	F	35	PHE	3.3
1	H	326	GLN	3.2
1	D	331	ARG	3.2
1	L	126	SER	3.2
1	J	16	PRO	3.2
1	B	412	HIS	3.2
1	J	292	GLY	3.2
1	D	129	TYR	3.2
1	H	330	SER	3.2
1	G	53	ILE	3.2
1	I	51	VAL	3.2
1	K	48	MET	3.2
1	G	271	LYS	3.2
1	F	182	ASN	3.2
1	L	32	ASP	3.2
1	A	31	MET	3.2
1	L	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	365	ASN	3.2
1	E	328	MET	3.1
1	L	365	ASN	3.1
1	D	97	LEU	3.1
1	D	96	ARG	3.1
1	H	335	PHE	3.1
1	C	120	PHE	3.1
1	F	16	PRO	3.1
1	E	46	ASN	3.1
1	G	328	MET	3.1
1	L	379	VAL	3.1
1	E	109	MET	3.1
1	B	422	ASN	3.1
1	G	137	SER	3.1
1	I	124	ILE	3.0
1	K	411	TYR	3.0
1	G	406	ASP	3.0
1	B	133	ALA	3.0
1	K	331	ARG	3.0
1	D	35	PHE	3.0
1	A	411	TYR	3.0
1	G	50	VAL	3.0
1	L	49	ASP	3.0
1	C	412	HIS	3.0
1	B	33	GLN	3.0
1	L	127	GLU	3.0
1	K	46	ASN	3.0
1	K	266	LYS	3.0
1	F	53	ILE	2.9
1	G	128	ASP	2.9
1	L	404	GLU	2.9
1	L	412	HIS	2.9
1	J	331	ARG	2.9
1	K	97	LEU	2.9
1	F	49	ASP	2.9
1	E	1	MET	2.9
1	B	182	ASN	2.9
1	A	52	LYS	2.9
1	C	411	TYR	2.9
1	I	412	HIS	2.9
1	K	306	ASN	2.9
1	G	45	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	53	ILE	2.8
1	F	113	LEU	2.8
1	I	127	GLU	2.8
1	F	36	ALA	2.8
1	L	338	GLY	2.8
1	D	48	MET	2.8
1	K	267	TRP	2.8
1	B	137	SER	2.8
1	L	131	PRO	2.8
1	G	502	GLN	2.8
1	G	111	LYS	2.8
1	H	52	LYS	2.8
1	G	503	MET	2.8
1	K	54	GLU	2.8
1	G	44	TYR	2.8
1	K	44	TYR	2.8
1	H	334	LEU	2.8
1	F	54	GLU	2.7
1	L	221	GLY	2.7
1	E	53	ILE	2.7
1	C	56	CYS	2.7
1	K	14	ASN	2.7
1	C	44	TYR	2.7
1	I	331	ARG	2.7
1	G	48	MET	2.7
1	A	130	CYS	2.7
1	J	44	TYR	2.7
1	L	385	LYS	2.7
1	G	132	ALA	2.7
1	F	331	ARG	2.7
1	A	30	ASN	2.7
1	A	38	ASP	2.7
1	L	124	ILE	2.7
1	B	98	TYR	2.7
1	H	97	LEU	2.7
1	D	130	CYS	2.6
1	C	134	VAL	2.6
1	G	131	PRO	2.6
1	F	134	VAL	2.6
1	L	37	LEU	2.6
1	A	15	GLU	2.6
1	F	56	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	335	PHE	2.6
1	L	503	MET	2.6
1	I	50	VAL	2.6
1	I	128	ASP	2.6
1	I	365	ASN	2.6
1	D	44	TYR	2.6
1	E	129	TYR	2.6
1	A	44	TYR	2.6
1	L	337	ILE	2.6
1	J	130	CYS	2.6
1	A	406	ASP	2.6
1	F	368	LYS	2.6
1	L	51	VAL	2.6
1	G	35	PHE	2.6
1	I	309	ALA	2.6
1	F	404	GLU	2.6
1	K	123	ARG	2.6
1	K	53	ILE	2.6
1	J	53	ILE	2.6
1	L	370	LYS	2.6
1	H	50	VAL	2.6
1	C	128	ASP	2.6
1	J	127	GLU	2.5
1	A	35	PHE	2.5
1	E	40	TRP	2.5
1	E	35	PHE	2.5
1	E	51	VAL	2.5
1	G	312	LEU	2.5
1	G	127	GLU	2.5
1	D	422	ASN	2.5
1	H	98	TYR	2.5
1	G	36	ALA	2.5
1	B	34	LEU	2.5
1	L	333	LYS	2.5
1	H	44	TYR	2.5
1	K	129	TYR	2.5
1	A	32	ASP	2.5
1	A	48	MET	2.5
1	B	410	ILE	2.5
1	L	222	GLU	2.5
1	I	461	GLU	2.5
1	E	125	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	50	VAL	2.4
1	D	56	CYS	2.4
1	K	49	ASP	2.4
1	E	340	LYS	2.4
1	G	49	ASP	2.4
1	G	133	ALA	2.4
1	G	331	ARG	2.4
1	E	55	ASN	2.4
1	G	46	ASN	2.4
1	D	50	VAL	2.4
1	C	406	ASP	2.4
1	L	319	TYR	2.4
1	J	411	TYR	2.4
1	L	53	ILE	2.4
1	A	328	MET	2.4
1	I	49	ASP	2.4
1	A	36	ALA	2.4
1	A	131	PRO	2.4
1	E	47	LYS	2.4
1	C	333	LYS	2.4
1	K	40	TRP	2.4
1	L	2	SER	2.4
1	C	130	CYS	2.4
1	J	56	CYS	2.4
1	C	52	LYS	2.4
1	E	366	VAL	2.4
1	E	48	MET	2.4
1	H	328	MET	2.4
1	G	130	CYS	2.4
1	H	108	ASN	2.4
1	E	32	ASP	2.4
1	D	136	SER	2.3
1	J	98	TYR	2.3
1	H	37	LEU	2.3
1	H	110	THR	2.3
1	L	368	LYS	2.3
1	L	377	TYR	2.3
1	C	413	LEU	2.3
1	K	56	CYS	2.3
1	D	503	MET	2.3
1	H	408	ASP	2.3
1	H	35	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	55	ASN	2.3
1	L	46	ASN	2.3
1	C	461	GLU	2.3
1	J	503	MET	2.3
1	F	116	CYS	2.3
1	C	35	PHE	2.3
1	A	333	LYS	2.3
1	C	260	TRP	2.3
1	G	329	ILE	2.3
1	A	136	SER	2.3
1	E	43	ARG	2.3
1	F	45	MET	2.3
1	G	91	LEU	2.3
1	D	46	ASN	2.3
1	C	51	VAL	2.3
1	G	459	GLU	2.3
1	K	42	HIS	2.3
1	B	50	VAL	2.3
1	A	33	GLN	2.3
1	I	120	PHE	2.3
1	A	405	GLU	2.2
1	K	45	MET	2.2
1	J	120	PHE	2.2
1	G	37	LEU	2.2
1	J	333	LYS	2.2
1	I	45	MET	2.2
1	E	139	PHE	2.2
1	E	307	TYR	2.2
1	G	40	TRP	2.2
1	L	45	MET	2.2
1	G	379	VAL	2.2
1	B	48	MET	2.2
1	G	319	TYR	2.2
1	F	333	LYS	2.2
1	E	137	SER	2.2
1	H	40	TRP	2.2
1	H	96	ARG	2.2
1	F	52	LYS	2.2
1	K	223	LYS	2.2
1	F	503	MET	2.2
1	L	363	THR	2.2
1	C	139	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	34	LEU	2.2
1	L	334	LEU	2.2
1	C	309	ALA	2.2
1	I	56	CYS	2.2
1	G	120	PHE	2.2
1	C	133	ALA	2.1
1	E	126	SER	2.1
1	D	266	LYS	2.1
1	F	364	ASP	2.1
1	G	54	GLU	2.1
1	K	109	MET	2.1
1	K	112	GLU	2.1
1	J	128	ASP	2.1
1	D	37	LEU	2.1
1	F	363	THR	2.1
1	K	422	ASN	2.1
1	I	34	LEU	2.1
1	L	125	THR	2.1
1	H	93	ASN	2.1
1	E	111	LYS	2.1
1	G	60	SER	2.1
1	A	14	ASN	2.1
1	C	267	TRP	2.1
1	G	113	LEU	2.1
1	C	37	LEU	2.1
1	J	36	ALA	2.1
1	H	34	LEU	2.1
1	E	136	SER	2.1
1	I	44	TYR	2.1
1	G	408	ASP	2.1
1	I	379	VAL	2.1
1	B	125	THR	2.1
1	H	45	MET	2.1
1	B	44	TYR	2.1
1	L	443	SER	2.1
1	J	96	ARG	2.1
1	G	42	HIS	2.1
1	K	502	GLN	2.1
1	I	61	PHE	2.1
1	C	303	TYR	2.1
1	J	43	ARG	2.1
1	E	116	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	408	ASP	2.1
1	A	409	THR	2.1
1	H	56	CYS	2.0
1	J	54	GLU	2.0
1	B	265	SER	2.0
1	F	120	PHE	2.0
1	C	48	MET	2.0
1	K	257	TYR	2.0
1	L	42	HIS	2.0
1	A	37	LEU	2.0
1	K	307	TYR	2.0
1	B	461	GLU	2.0
1	A	34	LEU	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 monosaccharides 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.