



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 07:59 PM EDT

PDB ID : 3E20
Title : Crystal structure of S.pombe eRF1/eRF3 complex
Authors : Cheng, Z.; Lim, M.; Kong, C.; Song, H.
Deposited on : 2008-08-05
Resolution : 3.50 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
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

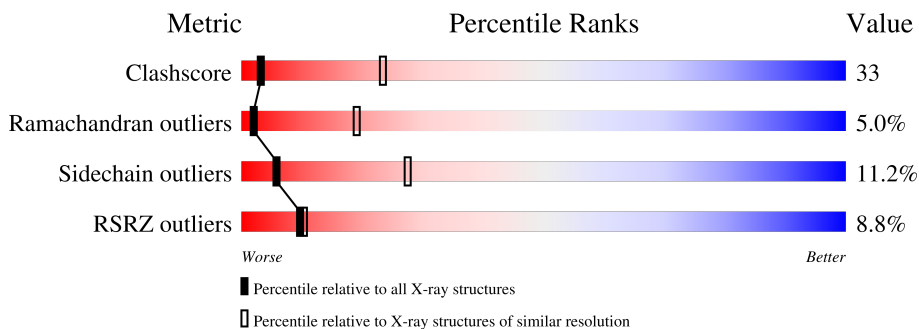
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



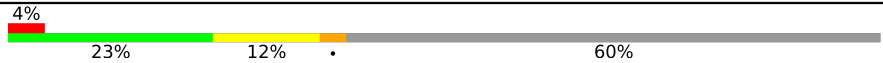
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	201	
1	D	201	
1	E	201	
1	J	201	
2	B	441	
2	C	441	
2	H	441	

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Mol	Chain	Length	Quality of chain
2	K	441	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '4%', followed by a green segment labeled '23%', a yellow segment labeled '12%', and a large grey segment at the end labeled '60%'. A small black dot is located on the boundary between the yellow and grey segments.</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13096 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 Eukaryotic peptide chain release factor GTP-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	196	1524	965	256	293	10	0	0	0
1	D	196	1524	965	256	293	10	0	0	0
1	E	196	1524	965	256	293	10	0	0	0
1	J	196	1524	965	256	293	10	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	462	GLY	-	expression tag	UNP O74718
A	463	PRO	-	expression tag	UNP O74718
A	464	LEU	-	expression tag	UNP O74718
A	465	GLY	-	expression tag	UNP O74718
A	466	SER	-	expression tag	UNP O74718
D	462	GLY	-	expression tag	UNP O74718
D	463	PRO	-	expression tag	UNP O74718
D	464	LEU	-	expression tag	UNP O74718
D	465	GLY	-	expression tag	UNP O74718
D	466	SER	-	expression tag	UNP O74718
E	462	GLY	-	expression tag	UNP O74718
E	463	PRO	-	expression tag	UNP O74718
E	464	LEU	-	expression tag	UNP O74718
E	465	GLY	-	expression tag	UNP O74718
E	466	SER	-	expression tag	UNP O74718
J	462	GLY	-	expression tag	UNP O74718
J	463	PRO	-	expression tag	UNP O74718
J	464	LEU	-	expression tag	UNP O74718
J	465	GLY	-	expression tag	UNP O74718
J	466	SER	-	expression tag	UNP O74718

- Molecule 2 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	261	Total	C	N	O	S	0	0	0
			2088	1321	347	405	15			
2	B	261	Total	C	N	O	S	0	0	0
			2088	1321	347	405	15			
2	H	175	Total	C	N	O	S	0	0	0
			1412	900	225	277	10			
2	K	175	Total	C	N	O	S	0	0	0
			1412	900	225	277	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	expression tag	UNP P79063
C	-6	HIS	-	expression tag	UNP P79063
C	-5	HIS	-	expression tag	UNP P79063
C	-4	HIS	-	expression tag	UNP P79063
C	-3	HIS	-	expression tag	UNP P79063
C	-2	HIS	-	expression tag	UNP P79063
C	-1	HIS	-	expression tag	UNP P79063
C	0	MET	-	expression tag	UNP P79063
B	-7	MET	-	expression tag	UNP P79063
B	-6	HIS	-	expression tag	UNP P79063
B	-5	HIS	-	expression tag	UNP P79063
B	-4	HIS	-	expression tag	UNP P79063
B	-3	HIS	-	expression tag	UNP P79063
B	-2	HIS	-	expression tag	UNP P79063
B	-1	HIS	-	expression tag	UNP P79063
B	0	MET	-	expression tag	UNP P79063
H	-7	MET	-	expression tag	UNP P79063
H	-6	HIS	-	expression tag	UNP P79063
H	-5	HIS	-	expression tag	UNP P79063
H	-4	HIS	-	expression tag	UNP P79063
H	-3	HIS	-	expression tag	UNP P79063
H	-2	HIS	-	expression tag	UNP P79063
H	-1	HIS	-	expression tag	UNP P79063
H	0	MET	-	expression tag	UNP P79063
K	-7	MET	-	expression tag	UNP P79063
K	-6	HIS	-	expression tag	UNP P79063
K	-5	HIS	-	expression tag	UNP P79063
K	-4	HIS	-	expression tag	UNP P79063
K	-3	HIS	-	expression tag	UNP P79063
K	-2	HIS	-	expression tag	UNP P79063

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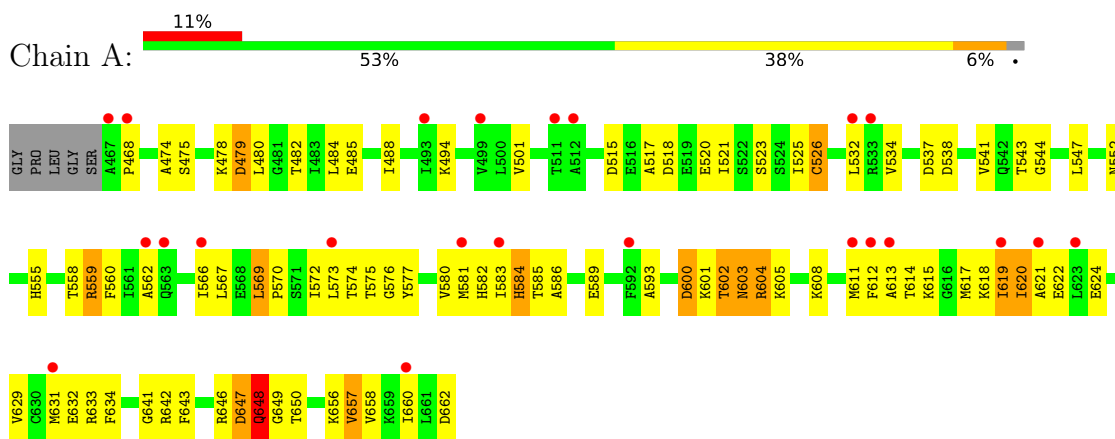
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Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P79063
K	0	MET	-	expression tag	UNP P79063

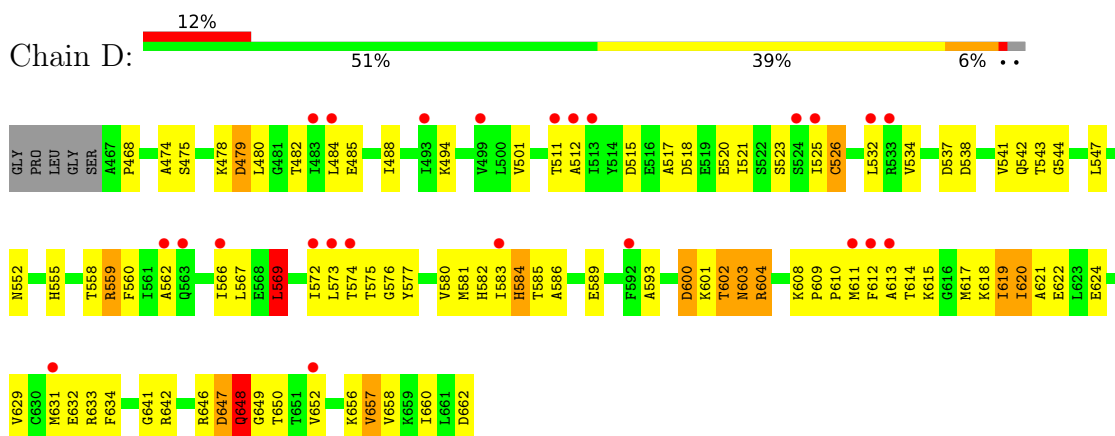
3 Residue-property plots [i](#)

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.

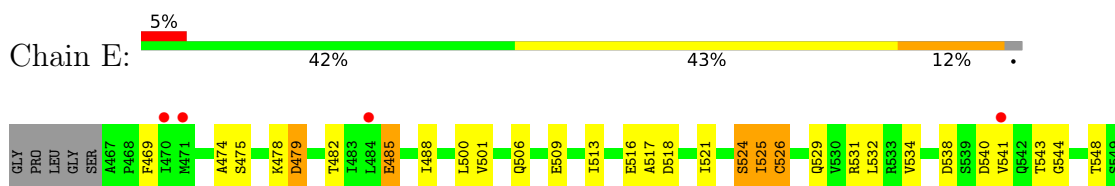
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit

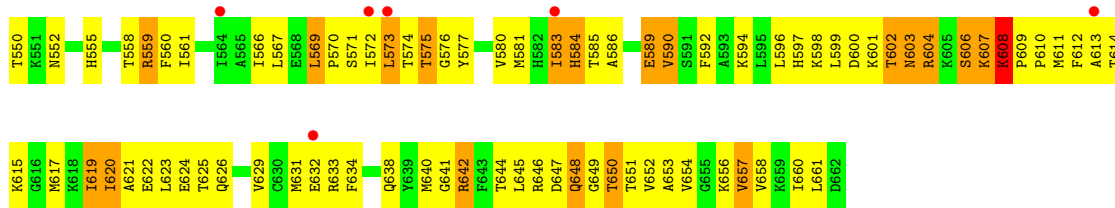


- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit

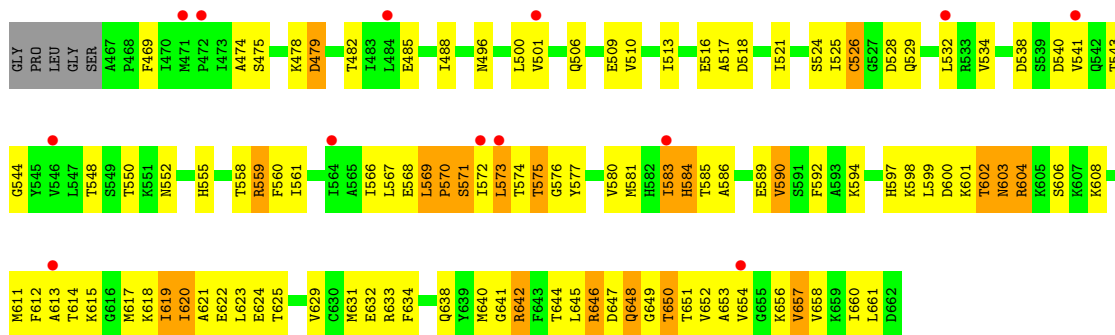


- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit

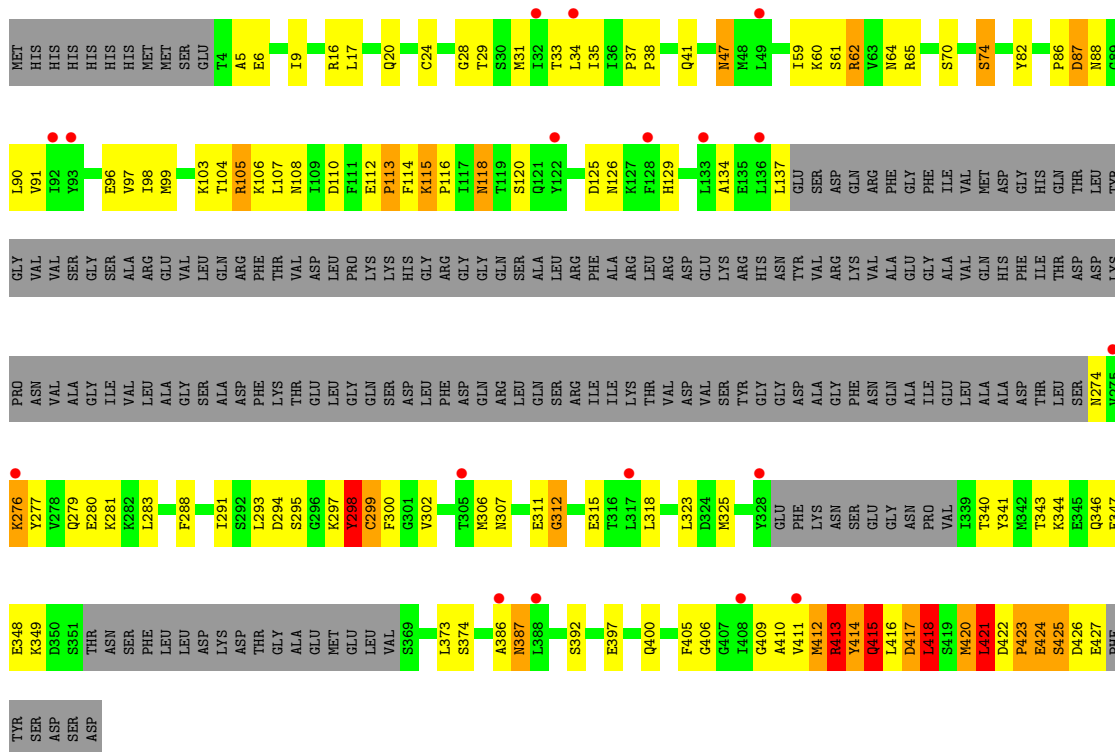
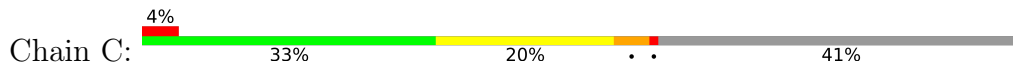




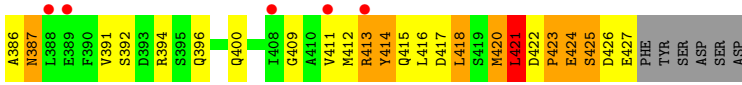
● Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit



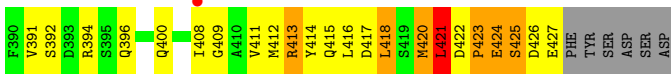
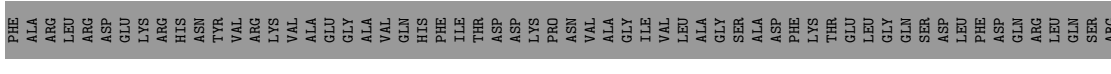
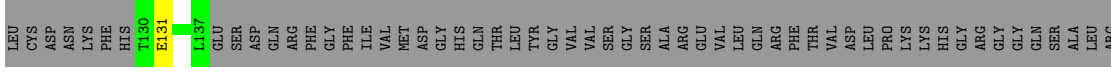
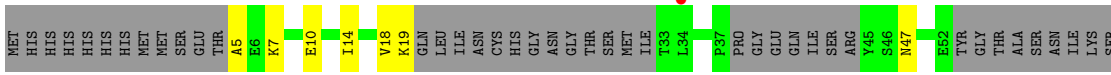
● Molecule 2: Eukaryotic peptide chain release factor subunit 1



● Molecule 2: Eukaryotic peptide chain release factor subunit 1



● Molecule 2: Eukaryotic peptide chain release factor subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	129.85Å 129.85Å 332.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 88.51 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.50) 99.7 (88.51-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.49Å)	Xtrriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.258 , 0.280 0.283 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	123.7	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 115.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13096	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.36	0/1547	0.57	1/2089 (0.0%)
1	D	0.36	0/1547	0.55	0/2089
1	E	0.49	0/1547	0.63	1/2089 (0.0%)
1	J	0.48	1/1547 (0.1%)	0.65	1/2089 (0.0%)
2	B	0.34	0/2119	0.61	6/2848 (0.2%)
2	C	0.34	0/2119	0.63	7/2848 (0.2%)
2	H	0.34	0/1425	0.55	1/1901 (0.1%)
2	K	0.34	0/1425	0.56	1/1901 (0.1%)
All	All	0.38	1/13276 (0.0%)	0.60	18/17854 (0.1%)

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	A	0	2
1	D	0	2
1	E	0	3
1	J	0	1
2	B	0	1
2	C	0	1
2	H	0	1
2	K	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	646	ARG	CB-CG	-5.26	1.38	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	413	ARG	NE-CZ-NH2	9.76	125.18	120.30
2	B	105	ARG	CG-CD-NE	8.50	129.65	111.80
2	C	413	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	C	413	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	B	413	ARG	NE-CZ-NH1	-7.29	116.66	120.30
2	C	65	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	B	413	ARG	NE-CZ-NH2	6.53	123.57	120.30
2	H	413	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	B	414	TYR	N-CA-CB	-5.91	99.96	110.60
2	C	105	ARG	CG-CD-NE	5.68	123.73	111.80
2	B	413	ARG	N-CA-C	-5.68	95.66	111.00
2	C	413	ARG	N-CA-C	-5.67	95.70	111.00
1	A	570	PRO	N-CA-C	-5.66	97.38	112.10
2	C	414	TYR	N-CA-CB	-5.61	100.50	110.60
2	C	65	ARG	CB-CG-CD	-5.51	97.28	111.60
2	B	105	ARG	CB-CG-CD	-5.39	97.58	111.60
1	J	571	SER	N-CA-CB	-5.21	102.68	110.50
1	E	608	LYS	CB-CG-CD	-5.08	98.38	111.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	569	LEU	Peptide
1	A	647	ASP	Peptide
2	B	413	ARG	Peptide
2	C	413	ARG	Peptide
1	D	569	LEU	Peptide
1	D	647	ASP	Peptide
1	E	570	PRO	Peptide
1	E	607	LYS	Peptide
1	E	608	LYS	Peptide
2	H	298	TYR	Peptide
1	J	570	PRO	Peptide
2	K	298	TYR	Peptide

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	1524	0	1569	89	0
1	D	1524	0	1569	92	0
1	E	1524	0	1569	117	0
1	J	1524	0	1569	104	0
2	B	2088	0	2077	144	0
2	C	2088	0	2077	133	0
2	H	1412	0	1388	117	0
2	K	1412	0	1388	86	0
All	All	13096	0	13206	878	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 33.

All (878) 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)
2:B:425:SER:CB	2:B:426:ASP:HA	1.52	1.38
2:H:414:TYR:CE2	2:H:416:LEU:HD11	1.60	1.36
2:C:425:SER:CB	2:C:426:ASP:HA	1.52	1.34
2:H:425:SER:CB	2:H:426:ASP:HA	1.51	1.29
2:K:425:SER:CB	2:K:426:ASP:HA	1.52	1.23
2:K:425:SER:OG	2:K:426:ASP:HA	1.38	1.22
2:C:420:MET:HG2	2:C:421:LEU:HD12	1.24	1.20
2:H:425:SER:OG	2:H:426:ASP:HA	1.37	1.19
2:C:425:SER:OG	2:C:426:ASP:HA	1.40	1.18
2:C:386:ALA:HA	2:C:387:ASN:HB2	1.18	1.17
2:B:425:SER:OG	2:B:426:ASP:HA	1.40	1.17
2:B:420:MET:HA	2:B:421:LEU:CB	1.73	1.17
2:H:418:LEU:HD22	2:H:418:LEU:N	1.54	1.17
2:B:386:ALA:HA	2:B:387:ASN:HB2	1.18	1.16
2:B:420:MET:HG2	2:B:421:LEU:HD12	1.24	1.15
2:K:418:LEU:H	2:K:418:LEU:CD2	1.54	1.15
2:C:420:MET:HA	2:C:421:LEU:CB	1.74	1.14
2:H:421:LEU:O	2:H:421:LEU:HD22	1.47	1.14
2:H:420:MET:HA	2:H:421:LEU:CB	1.76	1.13
2:H:325:MET:HE1	2:H:341:TYR:HB3	1.28	1.12
1:D:572:ILE:HD11	1:D:612:PHE:CB	1.79	1.11
2:K:421:LEU:HD22	2:K:421:LEU:O	1.49	1.11
1:A:572:ILE:HD11	1:A:612:PHE:CB	1.79	1.11
2:B:414:TYR:CE2	2:B:416:LEU:HD11	1.84	1.11
2:B:420:MET:CA	2:B:421:LEU:HB3	1.82	1.10
2:K:418:LEU:H	2:K:418:LEU:HD22	1.06	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:414:TYR:CE2	2:C:416:LEU:HD11	1.84	1.10
2:C:38:PRO:HB3	2:C:88:ASN:HA	1.21	1.10
2:H:414:TYR:CD2	2:H:416:LEU:HD11	1.87	1.10
2:C:420:MET:CA	2:C:421:LEU:HB3	1.82	1.09
2:B:421:LEU:HD22	2:B:421:LEU:O	1.51	1.09
2:K:420:MET:HA	2:K:421:LEU:CB	1.76	1.09
2:B:38:PRO:HB3	2:B:88:ASN:HA	1.20	1.09
2:H:425:SER:CB	2:H:426:ASP:CA	2.31	1.08
2:C:423:PRO:HA	2:C:424:GLU:C	1.73	1.08
2:C:421:LEU:O	2:C:421:LEU:HD22	1.51	1.08
2:B:425:SER:CB	2:B:426:ASP:CA	2.32	1.08
2:B:425:SER:HB2	2:B:426:ASP:CA	1.84	1.08
1:E:646:ARG:CD	1:E:648:GLN:HG2	1.82	1.08
2:C:425:SER:CB	2:C:426:ASP:CA	2.32	1.07
2:C:425:SER:HB2	2:C:426:ASP:CA	1.85	1.07
1:E:646:ARG:HG2	1:E:648:GLN:HA	1.36	1.07
1:J:572:ILE:HD11	1:J:612:PHE:CB	1.84	1.07
1:E:646:ARG:HD3	1:E:648:GLN:CG	1.84	1.06
2:K:420:MET:CA	2:K:421:LEU:HB3	1.84	1.06
2:K:423:PRO:HA	2:K:424:GLU:C	1.74	1.06
2:K:425:SER:CB	2:K:426:ASP:CA	2.32	1.06
1:E:646:ARG:HD3	1:E:648:GLN:HG2	1.08	1.06
2:H:420:MET:CG	2:H:421:LEU:HD12	1.86	1.06
2:K:420:MET:CG	2:K:421:LEU:HD12	1.85	1.06
2:B:423:PRO:HA	2:B:424:GLU:C	1.72	1.06
2:K:418:LEU:HD22	2:K:418:LEU:N	1.53	1.06
1:E:559:ARG:HH11	1:E:559:ARG:CG	1.69	1.05
2:K:325:MET:HE1	2:K:341:TYR:HB3	1.35	1.05
2:H:420:MET:CA	2:H:421:LEU:HB3	1.84	1.05
2:H:425:SER:HB2	2:H:426:ASP:CA	1.86	1.05
2:K:425:SER:HB2	2:K:426:ASP:HA	1.39	1.05
2:H:297:LYS:O	2:H:298:TYR:HB3	1.54	1.05
1:J:559:ARG:HH11	1:J:559:ARG:CG	1.71	1.04
2:K:386:ALA:HA	2:K:387:ASN:HB2	1.06	1.04
2:H:420:MET:HG2	2:H:421:LEU:HD12	1.06	1.03
2:H:423:PRO:HA	2:H:424:GLU:C	1.74	1.03
2:H:425:SER:HB2	2:H:426:ASP:HA	1.39	1.03
2:K:425:SER:HB2	2:K:426:ASP:CA	1.87	1.03
1:A:559:ARG:HH11	1:A:559:ARG:CG	1.71	1.03
1:D:559:ARG:HH11	1:D:559:ARG:CG	1.72	1.03
2:H:386:ALA:HA	2:H:387:ASN:HB2	1.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:ILE:HD11	1:D:612:PHE:CG	1.95	1.02
1:A:572:ILE:HD11	1:A:612:PHE:CG	1.94	1.02
2:C:420:MET:CG	2:C:421:LEU:HD12	1.90	1.02
2:B:425:SER:HB2	2:B:426:ASP:HA	1.37	1.01
2:K:420:MET:HG2	2:K:421:LEU:HD12	1.05	1.01
2:H:418:LEU:N	2:H:418:LEU:CD2	2.21	1.01
1:D:559:ARG:HG3	1:D:559:ARG:NH1	1.61	1.00
2:B:420:MET:CG	2:B:421:LEU:HD12	1.90	1.00
1:A:559:ARG:HG3	1:A:559:ARG:NH1	1.61	1.00
2:H:414:TYR:O	2:H:416:LEU:HD12	1.60	1.00
2:C:425:SER:HB2	2:C:426:ASP:HA	1.37	1.00
1:E:572:ILE:HD11	1:E:612:PHE:CB	1.91	0.99
1:J:559:ARG:HG3	1:J:559:ARG:NH1	1.61	0.99
2:H:414:TYR:CE2	2:H:416:LEU:CD1	2.46	0.98
2:K:297:LYS:O	2:K:298:TYR:HB3	1.59	0.97
1:A:572:ILE:HD11	1:A:612:PHE:HB2	1.44	0.97
1:D:572:ILE:HD11	1:D:612:PHE:HB2	1.43	0.97
2:B:24:CYS:HB2	2:B:97:VAL:HG21	1.47	0.96
1:A:559:ARG:HH11	1:A:559:ARG:HG3	0.79	0.96
2:C:24:CYS:HB2	2:C:97:VAL:HG21	1.48	0.96
2:B:418:LEU:N	2:B:418:LEU:HD22	1.80	0.96
2:H:386:ALA:CA	2:H:387:ASN:HB2	1.95	0.95
1:E:647:ASP:O	1:E:649:GLY:N	1.99	0.95
2:K:386:ALA:CA	2:K:387:ASN:HB2	1.95	0.95
2:C:413:ARG:O	2:C:414:TYR:CD1	2.20	0.94
2:K:420:MET:HG2	2:K:421:LEU:CD1	1.98	0.94
1:D:559:ARG:HH11	1:D:559:ARG:HG3	0.80	0.94
2:C:418:LEU:HD22	2:C:418:LEU:N	1.81	0.94
1:E:589:GLU:OE2	1:E:626:GLN:HG3	1.68	0.94
1:E:589:GLU:OE2	1:E:626:GLN:CG	2.16	0.93
1:E:559:ARG:HH11	1:E:559:ARG:HG3	0.78	0.93
1:J:572:ILE:HD11	1:J:612:PHE:HB2	1.49	0.93
2:K:325:MET:CE	2:K:341:TYR:HB3	1.98	0.93
2:B:297:LYS:O	2:B:298:TYR:HB3	1.69	0.93
2:C:297:LYS:O	2:C:298:TYR:HB3	1.67	0.93
2:H:420:MET:HG2	2:H:421:LEU:CD1	1.99	0.92
1:A:647:ASP:O	1:A:649:GLY:N	2.03	0.92
2:B:105:ARG:HH12	2:B:107:LEU:HD12	1.34	0.92
1:E:613:ALA:HA	1:E:617:MET:HE1	1.52	0.92
1:J:544:GLY:HA2	1:J:585:THR:HG23	1.52	0.92
1:J:559:ARG:HH11	1:J:559:ARG:HG3	0.80	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:325:MET:CE	2:H:341:TYR:HB3	2.00	0.92
2:B:415:GLN:O	2:B:416:LEU:HD12	1.71	0.92
1:J:647:ASP:O	1:J:649:GLY:N	2.03	0.91
2:C:415:GLN:O	2:C:416:LEU:HD12	1.70	0.91
2:B:86:PRO:HB2	2:B:112:GLU:OE1	1.70	0.91
1:E:544:GLY:HA2	1:E:585:THR:HG23	1.50	0.91
1:E:559:ARG:HG3	1:E:559:ARG:NH1	1.59	0.91
2:H:418:LEU:CD2	2:H:418:LEU:H	1.82	0.91
2:B:413:ARG:O	2:B:414:TYR:CD1	2.24	0.90
1:A:600:ASP:O	1:A:618:LYS:NZ	2.05	0.90
2:H:315:GLU:HB2	2:H:413:ARG:HG3	1.54	0.90
1:D:647:ASP:O	1:D:649:GLY:N	2.04	0.90
1:D:600:ASP:O	1:D:618:LYS:NZ	2.05	0.89
2:C:86:PRO:HB2	2:C:112:GLU:OE1	1.72	0.89
2:C:400:GLN:HA	1:D:576:GLY:HA3	1.54	0.89
2:H:386:ALA:HA	2:H:387:ASN:CB	1.97	0.89
2:C:298:TYR:H	2:C:412:MET:CE	1.86	0.88
1:A:576:GLY:HA3	2:B:400:GLN:HA	1.56	0.87
2:H:414:TYR:CD2	2:H:416:LEU:CD1	2.57	0.86
1:E:602:THR:HG23	1:E:604:ARG:HD2	1.55	0.85
1:A:572:ILE:HG12	1:A:573:LEU:H	1.39	0.85
2:B:105:ARG:NH1	2:B:107:LEU:HD12	1.91	0.85
2:B:298:TYR:H	2:B:412:MET:HE2	1.41	0.85
2:C:386:ALA:HA	2:C:387:ASN:CB	2.06	0.84
2:C:386:ALA:CA	2:C:387:ASN:HB2	2.04	0.84
2:C:298:TYR:N	2:C:412:MET:HE2	1.92	0.84
2:C:414:TYR:CD2	2:C:416:LEU:HD11	2.13	0.84
1:E:572:ILE:HD11	1:E:612:PHE:HB2	1.57	0.84
1:D:572:ILE:HG12	1:D:573:LEU:H	1.40	0.83
1:E:646:ARG:HG2	1:E:648:GLN:CA	2.08	0.83
2:B:386:ALA:CA	2:B:387:ASN:HB2	2.04	0.83
2:B:425:SER:HG	2:B:426:ASP:HA	1.44	0.82
2:B:386:ALA:HA	2:B:387:ASN:CB	2.06	0.82
2:B:414:TYR:CD2	2:B:416:LEU:HD11	2.14	0.82
2:B:59:ILE:HB	2:B:65:ARG:HG3	1.62	0.81
2:K:420:MET:HA	2:K:421:LEU:HB3	0.89	0.81
1:A:573:LEU:HD22	1:A:577:TYR:CG	2.16	0.81
2:H:420:MET:HA	2:H:421:LEU:HB3	0.89	0.81
2:C:300:PHE:H	2:C:409:GLY:HA2	1.45	0.80
2:C:414:TYR:HE2	2:C:416:LEU:HD11	1.46	0.80
1:D:573:LEU:HD22	1:D:577:TYR:CG	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:298:TYR:H	2:C:412:MET:HE2	1.44	0.80
2:B:325:MET:HE1	2:B:341:TYR:HB3	1.63	0.80
2:H:18:VAL:HG23	2:H:19:LYS:H	1.46	0.79
1:J:573:LEU:HD22	1:J:577:TYR:CG	2.17	0.79
2:C:47:ASN:HD22	2:C:47:ASN:C	1.86	0.79
2:B:298:TYR:N	2:B:412:MET:HE2	1.95	0.79
2:C:114:PHE:O	2:C:115:LYS:HB2	1.82	0.79
2:B:414:TYR:HE2	2:B:416:LEU:HD11	1.46	0.79
1:E:573:LEU:HD22	1:E:577:TYR:CG	2.18	0.79
2:B:47:ASN:C	2:B:47:ASN:HD22	1.86	0.78
2:B:298:TYR:H	2:B:412:MET:CE	1.95	0.78
2:B:300:PHE:H	2:B:409:GLY:CA	1.97	0.78
2:B:300:PHE:H	2:B:409:GLY:HA2	1.46	0.78
2:H:300:PHE:H	2:H:409:GLY:HA3	1.48	0.78
2:K:386:ALA:HA	2:K:387:ASN:CB	1.97	0.78
2:B:114:PHE:O	2:B:115:LYS:HB2	1.82	0.78
2:B:420:MET:HA	2:B:421:LEU:HB3	0.86	0.78
2:B:414:TYR:O	2:B:416:LEU:HD13	1.83	0.77
2:C:386:ALA:HB1	2:C:387:ASN:O	1.85	0.77
2:C:414:TYR:O	2:C:416:LEU:HD13	1.83	0.77
2:B:386:ALA:HB1	2:B:387:ASN:O	1.85	0.77
2:K:18:VAL:HG23	2:K:19:LYS:H	1.50	0.77
1:J:572:ILE:HD11	1:J:612:PHE:CG	2.19	0.77
1:J:574:THR:O	1:J:576:GLY:N	2.18	0.77
2:C:300:PHE:H	2:C:409:GLY:CA	1.96	0.77
1:A:494:LYS:HG2	1:A:523:SER:HB3	1.67	0.77
1:A:574:THR:O	1:A:576:GLY:N	2.18	0.77
2:K:425:SER:HG	2:K:426:ASP:HA	1.50	0.77
1:D:560:PHE:HZ	1:D:581:MET:HE3	1.51	0.76
1:E:574:THR:O	1:E:576:GLY:N	2.18	0.76
1:E:589:GLU:OE2	1:E:626:GLN:HG2	1.86	0.76
2:C:325:MET:CE	2:C:341:TYR:HB3	2.15	0.76
2:B:414:TYR:CD2	2:B:414:TYR:O	2.39	0.76
1:J:602:THR:HG23	1:J:604:ARG:HD2	1.68	0.76
1:A:478:LYS:O	1:A:479:ASP:HB2	1.86	0.76
1:D:494:LYS:HG2	1:D:523:SER:HB3	1.67	0.76
1:D:574:THR:O	1:D:576:GLY:N	2.18	0.76
1:E:646:ARG:CG	1:E:648:GLN:HG2	2.15	0.76
2:B:325:MET:CE	2:B:341:TYR:HB3	2.16	0.75
2:C:33:THR:HG21	2:C:129:HIS:H	1.52	0.75
2:B:33:THR:HG21	2:B:129:HIS:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:MET:HA	2:C:421:LEU:HB3	0.86	0.75
2:C:325:MET:HE1	2:C:341:TYR:HB3	1.67	0.75
1:J:580:VAL:HG21	1:J:648:GLN:HG3	1.69	0.75
2:K:411:VAL:HG23	2:K:411:VAL:O	1.87	0.75
2:C:414:TYR:CD2	2:C:414:TYR:O	2.40	0.74
1:A:572:ILE:HD11	1:A:612:PHE:CD1	2.22	0.74
2:B:414:TYR:O	2:B:416:LEU:CD1	2.36	0.74
1:D:478:LYS:O	1:D:479:ASP:HB2	1.87	0.74
2:B:425:SER:HB2	2:B:426:ASP:C	2.09	0.73
1:E:572:ILE:HD11	1:E:612:PHE:CG	2.23	0.73
2:H:91:VAL:O	2:H:110:ASP:HA	1.89	0.73
1:D:572:ILE:CD1	1:D:612:PHE:HB2	2.19	0.73
2:C:425:SER:HB2	2:C:426:ASP:C	2.09	0.73
2:H:411:VAL:O	2:H:411:VAL:HG23	1.88	0.73
1:J:613:ALA:HA	1:J:617:MET:HE1	1.69	0.73
2:C:413:ARG:O	2:C:414:TYR:HD1	1.72	0.73
1:E:607:LYS:O	1:E:608:LYS:HB2	1.88	0.73
2:C:417:ASP:C	2:C:418:LEU:HD22	2.09	0.72
2:H:414:TYR:O	2:H:416:LEU:CD1	2.35	0.72
2:H:301:GLY:O	2:H:305:THR:OG1	2.02	0.72
2:H:415:GLN:O	2:H:416:LEU:HD12	1.90	0.72
2:H:425:SER:HB2	2:H:427:GLU:OE1	1.89	0.72
2:C:425:SER:HB2	2:C:427:GLU:OE1	1.90	0.72
2:H:425:SER:HG	2:H:426:ASP:HA	1.52	0.72
2:K:423:PRO:CA	2:K:424:GLU:C	2.57	0.72
2:C:414:TYR:O	2:C:416:LEU:CD1	2.37	0.72
1:A:572:ILE:CD1	1:A:612:PHE:HB2	2.19	0.72
1:J:572:ILE:CD1	1:J:612:PHE:HB2	2.20	0.71
1:D:501:VAL:HG11	1:D:541:VAL:HG22	1.72	0.71
1:D:572:ILE:HD11	1:D:612:PHE:CD1	2.24	0.71
2:B:417:ASP:C	2:B:418:LEU:HD22	2.10	0.71
1:J:478:LYS:O	1:J:479:ASP:HB2	1.89	0.71
2:C:425:SER:HG	2:C:426:ASP:HA	1.55	0.71
1:D:475:SER:HB2	1:D:485:GLU:HG3	1.73	0.71
1:A:572:ILE:CD1	1:A:612:PHE:CD1	2.74	0.71
2:B:59:ILE:HG22	2:B:61:SER:H	1.56	0.71
1:J:555:HIS:HD2	1:J:632:GLU:OE2	1.74	0.71
1:J:634:PHE:CZ	1:J:638:GLN:HG2	2.26	0.71
1:A:501:VAL:HG11	1:A:541:VAL:HG22	1.72	0.71
1:A:475:SER:HB2	1:A:485:GLU:HG3	1.73	0.70
2:B:420:MET:HG2	2:B:421:LEU:CD1	2.13	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:PHE:HZ	1:A:581:MET:HE3	1.55	0.70
2:C:59:ILE:HG22	2:C:61:SER:H	1.56	0.70
1:A:602:THR:HG23	1:A:604:ARG:HD2	1.73	0.70
2:H:425:SER:HB2	2:H:426:ASP:C	2.11	0.70
1:J:576:GLY:HA3	2:K:400:GLN:HA	1.73	0.70
1:E:560:PHE:HZ	1:E:581:MET:HE3	1.54	0.70
1:J:572:ILE:HG13	1:J:612:PHE:HD1	1.55	0.70
2:H:417:ASP:C	2:H:418:LEU:HD22	2.12	0.70
1:E:517:ALA:O	1:E:518:ASP:HB2	1.90	0.70
1:A:544:GLY:HA2	1:A:585:THR:HG23	1.73	0.69
2:K:425:SER:HB2	2:K:426:ASP:C	2.12	0.69
1:D:544:GLY:HA2	1:D:585:THR:HG23	1.75	0.69
1:E:576:GLY:HA3	2:H:400:GLN:HA	1.75	0.69
2:C:423:PRO:CA	2:C:424:GLU:C	2.58	0.69
1:J:517:ALA:O	1:J:518:ASP:HB2	1.93	0.69
2:K:425:SER:HB2	2:K:427:GLU:OE1	1.92	0.69
1:D:572:ILE:HG12	1:D:573:LEU:N	2.08	0.69
1:D:572:ILE:CD1	1:D:612:PHE:CD1	2.76	0.68
2:H:423:PRO:CA	2:H:424:GLU:C	2.57	0.68
1:A:572:ILE:HG12	1:A:573:LEU:N	2.08	0.68
1:A:614:THR:HG22	1:A:617:MET:SD	2.34	0.68
1:E:572:ILE:HG13	1:E:612:PHE:HD1	1.58	0.68
1:D:614:THR:HG22	1:D:617:MET:SD	2.34	0.68
2:B:425:SER:HB2	2:B:427:GLU:OE1	1.94	0.68
1:J:646:ARG:HB3	1:J:648:GLN:HG2	1.75	0.68
1:E:572:ILE:HG13	1:E:612:PHE:CD1	2.29	0.68
2:C:420:MET:HG2	2:C:421:LEU:CD1	2.14	0.68
1:E:646:ARG:CG	1:E:648:GLN:HA	2.19	0.68
1:E:634:PHE:CZ	1:E:638:GLN:HG2	2.29	0.67
2:B:423:PRO:HA	2:B:424:GLU:O	1.95	0.67
2:H:377:LEU:O	2:H:381:TYR:HB3	1.94	0.67
2:B:293:LEU:O	2:B:294:ASP:HB3	1.94	0.67
2:H:297:LYS:O	2:H:298:TYR:CB	2.38	0.67
1:E:478:LYS:O	1:E:479:ASP:HB2	1.93	0.67
2:C:415:GLN:C	2:C:416:LEU:HD12	2.15	0.66
2:B:411:VAL:HG23	2:B:411:VAL:O	1.96	0.66
2:B:415:GLN:C	2:B:416:LEU:HD12	2.16	0.66
2:H:413:ARG:O	2:H:414:TYR:HB3	1.94	0.66
1:J:488:ILE:HB	1:J:526:CYS:HA	1.77	0.66
1:J:572:ILE:HG13	1:J:612:PHE:CD1	2.30	0.66
1:D:602:THR:HG23	1:D:604:ARG:HD2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:PRO:HA	2:C:424:GLU:O	1.94	0.66
2:C:315:GLU:HB2	2:C:413:ARG:HG2	1.77	0.65
1:E:559:ARG:CG	1:E:559:ARG:NH1	2.39	0.65
1:A:559:ARG:HD3	1:A:622:GLU:OE2	1.96	0.65
2:C:411:VAL:O	2:C:411:VAL:HG23	1.97	0.65
2:B:61:SER:HB2	2:B:64:ASN:HB3	1.79	0.65
1:E:488:ILE:HD12	1:E:525:ILE:O	1.95	0.65
1:E:575:THR:O	1:E:592:PHE:O	2.14	0.65
2:B:283:LEU:HD21	2:B:318:LEU:HD22	1.79	0.65
2:K:377:LEU:O	2:K:381:TYR:HB3	1.97	0.65
2:C:344:LYS:HA	2:C:346:GLN:HE21	1.63	0.64
2:C:283:LEU:HD21	2:C:318:LEU:HD22	1.79	0.64
1:J:516:GLU:OE2	1:J:529:GLN:HB3	1.97	0.64
1:E:572:ILE:CD1	1:E:612:PHE:HB2	2.26	0.64
2:H:421:LEU:HD22	2:H:421:LEU:C	2.17	0.64
1:J:559:ARG:HD3	1:J:622:GLU:OE2	1.97	0.64
2:C:61:SER:HB2	2:C:64:ASN:HB3	1.80	0.64
1:D:559:ARG:HD3	1:D:622:GLU:OE2	1.98	0.64
2:K:421:LEU:HD22	2:K:421:LEU:C	2.17	0.64
1:J:478:LYS:HE3	1:J:482:THR:OG1	1.97	0.63
1:J:573:LEU:CD2	1:J:577:TYR:CG	2.81	0.63
2:B:413:ARG:O	2:B:414:TYR:HD1	1.76	0.63
2:B:422:ASP:HB3	2:B:423:PRO:HD2	1.80	0.63
1:E:555:HIS:HD2	1:E:632:GLU:OE2	1.80	0.63
2:B:414:TYR:CD2	2:B:416:LEU:CD1	2.82	0.63
2:B:344:LYS:HA	2:B:346:GLN:HE21	1.63	0.63
2:K:418:LEU:CD2	2:K:418:LEU:N	2.21	0.63
2:C:422:ASP:HB3	2:C:423:PRO:HD2	1.80	0.63
1:D:567:LEU:O	1:D:615:LYS:HG3	1.99	0.63
1:E:488:ILE:HB	1:E:526:CYS:HA	1.79	0.62
1:D:559:ARG:CG	1:D:559:ARG:NH1	2.42	0.62
1:J:501:VAL:HG11	1:J:541:VAL:HG22	1.80	0.62
1:J:559:ARG:CG	1:J:559:ARG:NH1	2.40	0.62
1:E:559:ARG:HD3	1:E:622:GLU:OE2	1.99	0.62
2:H:348:GLU:HG3	2:H:349:LYS:H	1.65	0.62
2:B:423:PRO:CA	2:B:424:GLU:C	2.58	0.62
1:E:599:LEU:HD11	1:E:620:ILE:HG22	1.80	0.62
1:D:475:SER:HB2	1:D:485:GLU:CG	2.30	0.62
1:A:478:LYS:O	1:A:479:ASP:CB	2.48	0.62
1:A:567:LEU:O	1:A:615:LYS:HG3	2.00	0.62
2:K:348:GLU:HG3	2:K:349:LYS:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:LEU:CD2	1:D:577:TYR:CG	2.83	0.61
1:A:573:LEU:CD2	1:A:577:TYR:CG	2.82	0.61
2:C:418:LEU:N	2:C:418:LEU:CD2	2.55	0.61
2:B:418:LEU:N	2:B:418:LEU:CD2	2.54	0.61
1:E:613:ALA:HA	1:E:617:MET:CE	2.28	0.61
1:A:475:SER:HB2	1:A:485:GLU:CG	2.30	0.61
2:C:414:TYR:CD2	2:C:416:LEU:CD1	2.82	0.61
2:B:421:LEU:HD22	2:B:421:LEU:C	2.21	0.61
1:E:516:GLU:OE2	1:E:529:GLN:HB3	2.01	0.61
1:E:573:LEU:CD2	1:E:577:TYR:CG	2.84	0.61
1:J:575:THR:O	1:J:592:PHE:O	2.18	0.61
2:H:414:TYR:HE2	2:H:416:LEU:HD21	1.65	0.60
2:K:300:PHE:H	2:K:409:GLY:HA3	1.66	0.60
1:A:560:PHE:HZ	1:A:581:MET:CE	2.14	0.60
1:J:560:PHE:HZ	1:J:581:MET:HE3	1.66	0.60
1:A:631:MET:HG3	1:A:660:ILE:HD11	1.84	0.60
1:A:559:ARG:CG	1:A:559:ARG:NH1	2.41	0.59
1:D:560:PHE:HZ	1:D:581:MET:CE	2.15	0.59
2:C:300:PHE:N	2:C:409:GLY:HA2	2.16	0.59
1:J:569:LEU:HD22	1:J:652:VAL:HB	1.83	0.59
1:E:580:VAL:HG21	1:E:648:GLN:HG3	1.84	0.59
2:C:295:SER:OG	2:C:297:LYS:HG2	2.02	0.59
2:H:415:GLN:O	2:H:416:LEU:CD1	2.50	0.59
2:C:421:LEU:HD22	2:C:421:LEU:C	2.21	0.59
1:E:478:LYS:HE3	1:E:482:THR:OG1	2.02	0.59
2:B:414:TYR:O	2:B:415:GLN:C	2.41	0.59
2:H:414:TYR:HE2	2:H:416:LEU:CG	2.15	0.59
1:D:572:ILE:CG1	1:D:573:LEU:H	2.12	0.59
1:J:633:ARG:HA	1:J:657:VAL:HG22	1.85	0.59
2:B:74:SER:OG	2:B:106:LYS:HE2	2.02	0.59
2:B:281:LYS:HE3	2:B:397:GLU:OE1	2.03	0.59
1:J:613:ALA:HA	1:J:617:MET:CE	2.32	0.59
1:J:634:PHE:CE1	1:J:638:GLN:HG2	2.38	0.59
1:E:633:ARG:HA	1:E:657:VAL:HG22	1.86	0.58
1:E:646:ARG:HD3	1:E:648:GLN:CD	2.22	0.58
2:C:281:LYS:HE3	2:C:397:GLU:OE1	2.03	0.58
1:D:631:MET:HG3	1:D:660:ILE:HD11	1.85	0.58
2:C:414:TYR:O	2:C:415:GLN:C	2.42	0.58
2:B:422:ASP:CB	2:B:423:PRO:HD2	2.34	0.58
1:J:488:ILE:HD12	1:J:525:ILE:O	2.03	0.58
2:K:411:VAL:O	2:K:411:VAL:CG2	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:PHE:N	2:B:409:GLY:HA2	2.16	0.58
2:H:423:PRO:HA	2:H:424:GLU:O	2.03	0.58
2:C:422:ASP:CB	2:C:423:PRO:HD2	2.34	0.57
1:E:558:THR:O	1:E:624:GLU:HA	2.03	0.57
2:K:319:CYS:SG	2:K:323:LEU:HD12	2.43	0.57
2:H:386:ALA:HB1	2:H:387:ASN:O	2.04	0.57
2:K:75:THR:HA	2:K:78:ARG:HG3	1.85	0.57
1:A:572:ILE:CG1	1:A:573:LEU:H	2.12	0.57
1:A:584:HIS:HD2	1:A:586:ALA:H	1.51	0.57
1:D:584:HIS:HD2	1:D:586:ALA:H	1.50	0.57
2:B:423:PRO:CA	2:B:424:GLU:O	2.52	0.57
1:E:560:PHE:HZ	1:E:581:MET:CE	2.18	0.57
2:B:70:SER:O	2:B:74:SER:HB2	2.05	0.57
2:K:300:PHE:H	2:K:409:GLY:CA	2.18	0.57
2:C:423:PRO:CA	2:C:424:GLU:O	2.53	0.57
1:J:573:LEU:HD13	1:J:573:LEU:C	2.25	0.57
1:A:573:LEU:C	1:A:573:LEU:HD13	2.26	0.56
1:D:573:LEU:C	1:D:573:LEU:HD13	2.26	0.56
2:K:308:ALA:CB	2:K:412:MET:HE3	2.35	0.56
2:C:134:ALA:HA	2:C:137:LEU:HD12	1.87	0.56
2:H:290:GLU:OE1	2:H:295:SER:OG	2.20	0.56
1:D:478:LYS:O	1:D:479:ASP:CB	2.49	0.56
2:C:426:ASP:C	2:C:427:GLU:OE1	2.44	0.56
1:E:572:ILE:CG1	1:E:612:PHE:HB2	2.36	0.56
2:H:415:GLN:C	2:H:416:LEU:HD12	2.25	0.56
1:E:573:LEU:HD13	1:E:573:LEU:C	2.25	0.56
1:E:634:PHE:CE1	1:E:638:GLN:HG2	2.41	0.56
2:H:415:GLN:O	2:H:416:LEU:CG	2.54	0.56
2:H:418:LEU:H	2:H:418:LEU:HD23	1.70	0.56
2:K:423:PRO:HA	2:K:424:GLU:O	2.03	0.56
2:H:415:GLN:O	2:H:416:LEU:HG	2.06	0.56
2:C:416:LEU:CD1	2:C:416:LEU:N	2.69	0.56
2:C:416:LEU:C	2:C:417:ASP:OD1	2.45	0.56
2:C:417:ASP:OD1	2:C:417:ASP:N	2.37	0.56
2:B:113:PRO:HG2	2:B:116:PRO:HG3	1.88	0.56
2:H:326:ILE:HD12	2:H:328:TYR:CE2	2.41	0.56
2:H:411:VAL:O	2:H:411:VAL:CG2	2.53	0.56
2:C:6:GLU:O	2:C:9:ILE:HG22	2.06	0.56
1:D:560:PHE:CZ	1:D:581:MET:HE3	2.37	0.56
1:E:602:THR:CG2	1:E:604:ARG:HD2	2.33	0.56
1:E:607:LYS:O	1:E:608:LYS:CB	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:613:ALA:HA	1:D:617:MET:HE1	1.87	0.55
2:B:6:GLU:O	2:B:9:ILE:HG22	2.06	0.55
2:B:294:ASP:O	2:B:295:SER:C	2.44	0.55
1:E:631:MET:HG3	1:E:660:ILE:HD11	1.88	0.55
2:H:300:PHE:H	2:H:409:GLY:CA	2.17	0.55
2:K:326:ILE:HD12	2:K:328:TYR:CE2	2.41	0.55
2:B:426:ASP:C	2:B:427:GLU:OE1	2.44	0.55
2:B:134:ALA:HA	2:B:137:LEU:HD12	1.86	0.55
1:J:560:PHE:HZ	1:J:581:MET:CE	2.19	0.55
2:B:24:CYS:CB	2:B:97:VAL:HG21	2.30	0.55
1:J:634:PHE:HB2	1:J:656:LYS:HB2	1.89	0.55
1:J:567:LEU:CD1	1:J:654:VAL:HG13	2.37	0.55
1:J:572:ILE:HD11	1:J:612:PHE:HB3	1.83	0.55
1:A:525:ILE:HG13	1:A:526:CYS:O	2.06	0.55
2:C:113:PRO:HG2	2:C:116:PRO:HG3	1.89	0.55
1:J:572:ILE:CG1	1:J:612:PHE:HB2	2.36	0.55
2:K:290:GLU:OE1	2:K:297:LYS:HG3	2.07	0.55
1:D:525:ILE:HG13	1:D:526:CYS:O	2.07	0.55
1:E:501:VAL:HG11	1:E:541:VAL:HG22	1.89	0.55
1:D:572:ILE:CD1	1:D:612:PHE:CG	2.81	0.55
1:E:559:ARG:HG2	1:E:624:GLU:HG2	1.89	0.55
2:H:308:ALA:CB	2:H:412:MET:HE3	2.37	0.55
2:H:348:GLU:HG3	2:H:349:LYS:N	2.22	0.55
1:J:558:THR:O	1:J:624:GLU:HA	2.07	0.55
2:K:386:ALA:HB1	2:K:387:ASN:O	2.07	0.55
2:B:417:ASP:OD1	2:B:417:ASP:N	2.37	0.54
2:H:290:GLU:OE1	2:H:297:LYS:HG3	2.07	0.54
2:H:414:TYR:CE2	2:H:416:LEU:CG	2.90	0.54
2:H:414:TYR:HD2	2:H:415:GLN:O	1.90	0.54
1:J:566:ILE:HG22	1:J:615:LYS:HA	1.90	0.54
2:K:297:LYS:O	2:K:298:TYR:CB	2.39	0.54
2:K:301:GLY:HA2	2:K:408:ILE:O	2.07	0.54
1:J:521:ILE:HD11	1:J:524:SER:OG	2.08	0.54
2:H:423:PRO:CA	2:H:424:GLU:O	2.56	0.54
1:J:567:LEU:O	1:J:615:LYS:HG3	2.07	0.54
1:J:572:ILE:HG12	1:J:573:LEU:N	2.21	0.54
2:K:348:GLU:HG3	2:K:349:LYS:N	2.22	0.54
2:K:423:PRO:CA	2:K:424:GLU:O	2.56	0.54
2:B:416:LEU:C	2:B:417:ASP:OD1	2.46	0.54
2:K:301:GLY:O	2:K:305:THR:OG1	2.15	0.54
2:K:418:LEU:H	2:K:418:LEU:HD23	1.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:TYR:CE1	2:B:90:LEU:HD21	2.42	0.54
2:B:315:GLU:HB2	2:B:413:ARG:HG2	1.89	0.54
1:E:634:PHE:HB2	1:E:656:LYS:HB2	1.90	0.54
1:J:569:LEU:CD2	1:J:652:VAL:HB	2.37	0.54
1:E:567:LEU:O	1:E:615:LYS:HG3	2.08	0.53
1:E:602:THR:HG23	1:E:604:ARG:CD	2.33	0.53
1:J:559:ARG:HG2	1:J:624:GLU:HG2	1.91	0.53
2:K:291:ILE:HG12	2:K:298:TYR:CE1	2.43	0.53
1:A:619:ILE:HG12	1:A:620:ILE:N	2.23	0.53
2:B:295:SER:OG	2:B:297:LYS:HG2	2.08	0.53
2:C:82:TYR:CE1	2:C:90:LEU:HD21	2.42	0.53
2:C:420:MET:HG3	2:C:421:LEU:HD12	1.87	0.53
1:E:647:ASP:C	1:E:649:GLY:H	2.04	0.53
1:J:572:ILE:CD1	1:J:612:PHE:CG	2.92	0.53
2:C:37:PRO:HD3	2:C:120:SER:HA	1.91	0.53
1:J:469:PHE:O	1:J:548:THR:HA	2.08	0.53
1:J:590:VAL:HG23	1:J:625:THR:HG22	1.91	0.53
1:J:513:ILE:HG13	1:J:532:LEU:CD2	2.39	0.53
1:A:633:ARG:HA	1:A:657:VAL:HG22	1.91	0.53
1:A:573:LEU:CD2	1:A:577:TYR:CD1	2.92	0.53
1:E:597:HIS:HB2	1:E:620:ILE:HG23	1.91	0.53
2:H:416:LEU:O	2:H:417:ASP:C	2.47	0.53
2:K:422:ASP:CB	2:K:423:PRO:HD2	2.39	0.53
2:C:415:GLN:C	2:C:416:LEU:CD1	2.77	0.52
2:B:299:CYS:HA	2:B:300:PHE:HB3	1.91	0.52
2:H:426:ASP:C	2:H:427:GLU:OE1	2.46	0.52
2:K:426:ASP:C	2:K:427:GLU:OE1	2.47	0.52
1:A:634:PHE:HE1	1:A:642:ARG:HH11	1.57	0.52
2:C:24:CYS:CB	2:C:97:VAL:HG21	2.31	0.52
2:B:38:PRO:HB3	2:B:88:ASN:CA	2.14	0.52
1:E:513:ILE:HG13	1:E:532:LEU:CD2	2.39	0.52
1:J:597:HIS:HB2	1:J:620:ILE:HG23	1.92	0.52
1:D:573:LEU:CD2	1:D:577:TYR:CD1	2.93	0.52
2:K:417:ASP:OD1	2:K:417:ASP:C	2.47	0.52
1:D:634:PHE:HE1	1:D:642:ARG:HH11	1.57	0.52
2:B:416:LEU:CD1	2:B:416:LEU:N	2.71	0.52
1:A:560:PHE:CZ	1:A:581:MET:CE	2.92	0.52
2:C:47:ASN:C	2:C:47:ASN:ND2	2.59	0.52
2:H:422:ASP:CB	2:H:423:PRO:HD2	2.40	0.52
2:B:37:PRO:HD3	2:B:120:SER:HA	1.91	0.52
2:H:422:ASP:O	2:H:423:PRO:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:295:SER:O	2:K:415:GLN:NE2	2.43	0.52
1:D:520:GLU:HG3	1:D:521:ILE:N	2.25	0.52
2:B:415:GLN:C	2:B:416:LEU:CD1	2.78	0.52
2:C:311:GLU:O	2:C:312:GLY:C	2.48	0.52
2:B:288:PHE:HE1	2:B:405:PHE:HE2	1.57	0.51
2:C:299:CYS:HA	2:C:300:PHE:HB3	1.92	0.51
2:K:290:GLU:OE1	2:K:295:SER:OG	2.25	0.51
2:K:425:SER:OG	2:K:426:ASP:CA	2.33	0.51
2:C:422:ASP:O	2:C:423:PRO:O	2.28	0.51
2:H:15:ARG:HG2	2:H:137:LEU:HD13	1.93	0.51
2:H:414:TYR:HE2	2:H:416:LEU:CD2	2.22	0.51
1:J:474:ALA:HA	1:J:585:THR:OG1	2.09	0.51
1:J:538:ASP:C	1:J:540:ASP:H	2.13	0.51
1:D:633:ARG:HA	1:D:657:VAL:HG22	1.91	0.51
1:J:567:LEU:HD11	1:J:654:VAL:HG13	1.92	0.51
2:C:288:PHE:HE1	2:C:405:PHE:HE2	1.57	0.51
1:E:631:MET:HG3	1:E:660:ILE:CD1	2.40	0.51
2:K:422:ASP:O	2:K:423:PRO:O	2.29	0.51
2:C:38:PRO:HB3	2:C:88:ASN:CA	2.14	0.51
2:B:414:TYR:O	2:B:414:TYR:HD2	1.92	0.51
2:B:422:ASP:O	2:B:423:PRO:O	2.29	0.51
2:C:59:ILE:O	2:C:60:LYS:HB2	2.11	0.51
2:H:414:TYR:CD2	2:H:414:TYR:O	2.64	0.51
1:D:560:PHE:CZ	1:D:581:MET:CE	2.93	0.51
2:B:47:ASN:C	2:B:47:ASN:ND2	2.59	0.51
2:B:91:VAL:O	2:B:110:ASP:HA	2.11	0.51
1:E:614:THR:HG22	1:E:617:MET:SD	2.51	0.51
1:A:602:THR:HG23	1:A:604:ARG:CD	2.41	0.51
2:C:99:MET:HE3	2:C:105:ARG:HB3	1.93	0.51
1:D:619:ILE:HG12	1:D:620:ILE:N	2.25	0.51
2:K:299:CYS:HA	2:K:300:PHE:O	2.11	0.51
1:E:566:ILE:HG22	1:E:615:LYS:HA	1.93	0.50
2:H:92:ILE:HG12	2:H:110:ASP:HB3	1.93	0.50
2:H:295:SER:O	2:H:415:GLN:NE2	2.43	0.50
2:H:319:CYS:SG	2:H:323:LEU:HD12	2.50	0.50
2:H:414:TYR:HE2	2:H:416:LEU:CD1	2.17	0.50
2:H:421:LEU:O	2:H:421:LEU:CD2	2.40	0.50
2:C:306:MET:HA	2:C:306:MET:CE	2.41	0.50
2:H:414:TYR:CE2	2:H:416:LEU:HD21	2.45	0.50
1:A:520:GLU:HG3	1:A:521:ILE:N	2.26	0.50
2:C:91:VAL:O	2:C:110:ASP:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:LEU:HD23	1:D:652:VAL:CG1	2.42	0.50
1:E:573:LEU:HD22	1:E:577:TYR:CD2	2.47	0.50
2:C:414:TYR:O	2:C:414:TYR:HD2	1.93	0.50
2:B:306:MET:HA	2:B:306:MET:CE	2.41	0.50
1:E:469:PHE:O	1:E:548:THR:HA	2.12	0.50
1:E:474:ALA:HA	1:E:585:THR:OG1	2.11	0.50
1:E:596:LEU:O	1:E:609:PRO:HB3	2.11	0.50
2:B:59:ILE:O	2:B:60:LYS:HB2	2.10	0.49
1:E:572:ILE:HG12	1:E:573:LEU:N	2.26	0.49
2:B:311:GLU:O	2:B:312:GLY:C	2.48	0.49
2:B:300:PHE:H	2:B:409:GLY:HA3	1.73	0.49
2:C:294:ASP:CG	2:C:294:ASP:O	2.50	0.49
1:E:538:ASP:C	1:E:540:ASP:H	2.14	0.49
1:J:580:VAL:CG2	1:J:648:GLN:HG3	2.38	0.49
1:A:613:ALA:HA	1:A:617:MET:CE	2.43	0.49
1:D:613:ALA:HA	1:D:617:MET:CE	2.43	0.49
1:J:573:LEU:HD22	1:J:577:TYR:CD2	2.47	0.49
1:J:631:MET:HG3	1:J:660:ILE:CD1	2.42	0.49
1:D:584:HIS:CD2	1:D:586:ALA:H	2.30	0.49
2:B:315:GLU:HB3	2:B:411:VAL:O	2.13	0.49
1:E:521:ILE:HD11	1:E:524:SER:OG	2.12	0.49
1:E:590:VAL:HG23	1:E:625:THR:HG22	1.95	0.49
1:A:572:ILE:CD1	1:A:612:PHE:CG	2.80	0.49
2:H:425:SER:OG	2:H:426:ASP:CA	2.32	0.49
1:J:647:ASP:C	1:J:649:GLY:H	2.08	0.49
1:E:646:ARG:HD3	1:E:648:GLN:OE1	2.13	0.49
2:K:311:GLU:O	2:K:312:GLY:C	2.51	0.49
2:B:86:PRO:O	2:B:87:ASP:C	2.50	0.49
2:B:125:ASP:CG	2:B:126:ASN:H	2.16	0.49
2:C:62:ARG:HB3	2:C:62:ARG:NH1	2.28	0.48
2:B:99:MET:HE3	2:B:105:ARG:HB3	1.94	0.48
2:H:10:GLU:O	2:H:14:ILE:HG12	2.13	0.48
1:J:631:MET:HG3	1:J:660:ILE:HD11	1.94	0.48
2:K:5:ALA:C	2:K:7:LYS:H	2.16	0.48
2:K:274:ASN:HB3	2:K:277:TYR:HB2	1.94	0.48
1:A:468:PRO:HB3	1:A:552:ASN:HB2	1.95	0.48
1:A:572:ILE:HG13	1:A:612:PHE:HD1	1.78	0.48
2:C:422:ASP:O	2:C:423:PRO:C	2.51	0.48
1:D:468:PRO:HB3	1:D:552:ASN:HB2	1.95	0.48
1:D:574:THR:HG22	1:D:612:PHE:HA	1.95	0.48
2:C:125:ASP:CG	2:C:126:ASN:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:300:PHE:H	2:C:409:GLY:HA3	1.73	0.48
1:D:566:ILE:HG22	1:D:615:LYS:HA	1.96	0.48
1:E:572:ILE:HD11	1:E:612:PHE:HB3	1.87	0.48
2:H:315:GLU:HA	2:H:413:ARG:HE	1.78	0.48
2:C:86:PRO:O	2:C:87:ASP:C	2.51	0.48
2:B:274:ASN:HB3	2:B:277:TYR:HB2	1.96	0.48
1:E:632:GLU:HB2	1:E:640:MET:HB2	1.96	0.48
1:E:650:THR:OG1	1:E:651:THR:N	2.47	0.48
2:H:315:GLU:CB	2:H:413:ARG:HE	2.26	0.48
2:H:421:LEU:O	2:H:422:ASP:CG	2.52	0.48
1:J:574:THR:HG22	1:J:612:PHE:HA	1.94	0.48
2:K:294:ASP:O	2:K:294:ASP:OD2	2.31	0.48
2:C:274:ASN:HB3	2:C:277:TYR:HB2	1.95	0.48
1:E:589:GLU:O	1:E:589:GLU:HG3	2.12	0.48
2:H:422:ASP:O	2:H:423:PRO:C	2.51	0.48
2:B:62:ARG:NH1	2:B:62:ARG:HB3	2.28	0.48
2:K:421:LEU:O	2:K:422:ASP:CG	2.52	0.48
1:A:555:HIS:HD2	1:A:632:GLU:OE2	1.97	0.48
2:C:315:GLU:HB3	2:C:411:VAL:O	2.13	0.48
2:H:34:LEU:HD23	2:H:92:ILE:HD12	1.96	0.48
2:C:17:LEU:O	2:C:20:GLN:HG2	2.14	0.48
2:C:413:ARG:C	2:C:414:TYR:CD1	2.87	0.48
2:H:414:TYR:CD2	2:H:414:TYR:C	2.87	0.48
1:A:569:LEU:CD2	1:A:573:LEU:HB2	2.44	0.47
1:A:574:THR:HG22	1:A:612:PHE:HA	1.95	0.47
2:B:417:ASP:O	2:B:418:LEU:O	2.32	0.47
1:E:574:THR:HG22	1:E:612:PHE:HA	1.96	0.47
1:E:598:LYS:HB2	1:E:610:PRO:HG3	1.95	0.47
2:K:422:ASP:O	2:K:423:PRO:C	2.51	0.47
2:C:70:SER:O	2:C:74:SER:HB2	2.14	0.47
2:H:302:VAL:HG23	2:H:303:VAL:H	1.79	0.47
2:C:293:LEU:O	2:C:294:ASP:C	2.53	0.47
1:D:569:LEU:HD11	1:D:573:LEU:HB2	1.96	0.47
1:J:568:GLU:O	1:J:652:VAL:HG12	2.14	0.47
2:B:422:ASP:O	2:B:423:PRO:C	2.52	0.47
1:E:572:ILE:CD1	1:E:612:PHE:CG	2.95	0.47
2:C:347:GLU:CD	2:C:347:GLU:H	2.18	0.47
2:B:31:MET:HG3	2:B:126:ASN:C	2.35	0.47
2:H:75:THR:O	2:H:75:THR:HG22	2.14	0.47
1:A:560:PHE:CZ	1:A:581:MET:HE3	2.43	0.47
2:C:96:GLU:HB3	2:C:106:LYS:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:ILE:HG12	2:C:298:TYR:CE1	2.50	0.47
1:D:602:THR:HG23	1:D:604:ARG:CD	2.42	0.47
2:B:291:ILE:HG12	2:B:298:TYR:CE1	2.50	0.47
1:J:602:THR:O	1:J:602:THR:OG1	2.29	0.47
1:J:632:GLU:HB2	1:J:640:MET:HB2	1.96	0.47
1:J:646:ARG:HD3	1:J:648:GLN:HG2	1.97	0.47
1:A:478:LYS:HE2	1:A:482:THR:OG1	2.15	0.47
1:D:569:LEU:HD23	1:D:652:VAL:HB	1.97	0.47
1:D:609:PRO:HA	1:D:610:PRO:HD3	1.82	0.47
1:D:646:ARG:HB3	1:D:648:GLN:HG2	1.97	0.47
1:E:569:LEU:HD22	1:E:652:VAL:HB	1.95	0.47
1:J:619:ILE:HD11	1:J:621:ALA:HB2	1.97	0.47
1:D:517:ALA:O	1:D:518:ASP:HB2	2.15	0.47
1:E:646:ARG:HG2	1:E:648:GLN:HG2	1.95	0.47
2:K:308:ALA:HB2	2:K:412:MET:HE3	1.96	0.47
2:K:416:LEU:O	2:K:418:LEU:HD22	2.15	0.47
2:C:16:ARG:HA	2:C:16:ARG:HD2	1.71	0.47
2:B:413:ARG:C	2:B:414:TYR:CD1	2.88	0.46
1:J:555:HIS:CD2	1:J:632:GLU:OE2	2.62	0.46
2:K:283:LEU:O	2:K:286:ARG:HB3	2.15	0.46
2:C:411:VAL:O	2:C:411:VAL:CG2	2.63	0.46
2:B:17:LEU:O	2:B:20:GLN:HG2	2.15	0.46
1:E:580:VAL:CG2	1:E:648:GLN:HG3	2.45	0.46
1:J:572:ILE:CD1	1:J:612:PHE:CD1	2.98	0.46
2:K:308:ALA:HB1	2:K:412:MET:HE3	1.97	0.46
1:D:572:ILE:HG13	1:D:612:PHE:HD1	1.79	0.46
1:J:573:LEU:CD2	1:J:577:TYR:CD1	2.99	0.46
2:K:291:ILE:HG12	2:K:298:TYR:CD1	2.51	0.46
2:C:417:ASP:O	2:C:418:LEU:O	2.32	0.46
1:J:478:LYS:O	1:J:479:ASP:CB	2.59	0.46
1:A:517:ALA:O	1:A:518:ASP:HB2	2.15	0.46
1:D:555:HIS:HD2	1:D:632:GLU:OE2	1.98	0.46
1:D:562:ALA:HA	1:D:658:VAL:HG12	1.97	0.46
1:E:500:LEU:HB2	1:E:550:THR:HG22	1.97	0.46
1:J:500:LEU:HB2	1:J:550:THR:HG22	1.96	0.46
1:J:581:MET:SD	1:J:583:ILE:HG13	2.56	0.46
2:B:16:ARG:HD2	2:B:16:ARG:HA	1.72	0.46
1:E:600:ASP:HB3	1:E:601:LYS:H	1.62	0.46
2:H:311:GLU:O	2:H:312:GLY:C	2.54	0.46
1:J:566:ILE:N	1:J:566:ILE:HD12	2.30	0.46
1:A:562:ALA:HA	1:A:658:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ARG:HB3	2:B:62:ARG:CZ	2.46	0.46
1:E:573:LEU:C	1:E:573:LEU:CD1	2.84	0.46
1:E:641:GLY:HA2	1:E:657:VAL:HG13	1.98	0.46
1:A:566:ILE:HG22	1:A:615:LYS:HA	1.98	0.46
2:C:348:GLU:HG3	2:C:349:LYS:N	2.31	0.46
1:D:569:LEU:HD23	1:D:652:VAL:HG11	1.97	0.46
2:B:347:GLU:H	2:B:347:GLU:CD	2.18	0.46
1:J:650:THR:OG1	1:J:651:THR:N	2.49	0.46
2:K:91:VAL:O	2:K:110:ASP:HA	2.15	0.46
1:A:641:GLY:HA2	1:A:657:VAL:CG1	2.46	0.46
1:D:478:LYS:HE2	1:D:482:THR:OG1	2.16	0.46
1:J:561:ILE:O	1:J:658:VAL:HG12	2.16	0.46
1:A:558:THR:O	1:A:624:GLU:HA	2.16	0.45
2:C:31:MET:HG3	2:C:126:ASN:C	2.36	0.45
1:J:602:THR:HG23	1:J:604:ARG:CD	2.44	0.45
2:K:392:SER:OG	2:K:394:ARG:HG2	2.16	0.45
2:B:276:LYS:HD3	2:B:276:LYS:N	2.32	0.45
2:B:417:ASP:CA	2:B:418:LEU:HD22	2.46	0.45
2:B:421:LEU:O	2:B:421:LEU:CD2	2.43	0.45
2:C:421:LEU:O	2:C:422:ASP:CG	2.55	0.45
1:D:641:GLY:HA2	1:D:657:VAL:CG1	2.46	0.45
2:B:411:VAL:O	2:B:411:VAL:CG2	2.62	0.45
1:A:584:HIS:CD2	1:A:586:ALA:H	2.31	0.45
1:D:631:MET:HG3	1:D:660:ILE:CD1	2.46	0.45
1:E:634:PHE:HA	1:E:641:GLY:HA3	1.98	0.45
2:H:315:GLU:CA	2:H:413:ARG:HE	2.30	0.45
1:A:613:ALA:HA	1:A:617:MET:HE1	1.97	0.45
1:A:631:MET:HG3	1:A:660:ILE:CD1	2.46	0.45
2:C:99:MET:HB3	2:C:103:LYS:O	2.17	0.45
2:B:99:MET:HB3	2:B:103:LYS:O	2.17	0.45
1:J:538:ASP:C	1:J:540:ASP:N	2.68	0.45
1:D:474:ALA:HA	1:D:585:THR:OG1	2.16	0.45
1:D:515:ASP:OD1	1:D:515:ASP:C	2.55	0.45
1:D:573:LEU:C	1:D:573:LEU:CD1	2.85	0.45
1:E:538:ASP:C	1:E:540:ASP:N	2.70	0.45
2:H:131:GLU:HA	2:H:134:ALA:HB3	1.99	0.45
2:H:283:LEU:O	2:H:286:ARG:HB3	2.16	0.45
2:H:417:ASP:C	2:H:417:ASP:OD1	2.55	0.45
2:K:302:VAL:HG23	2:K:303:VAL:H	1.82	0.45
2:K:315:GLU:O	2:K:387:ASN:CB	2.65	0.45
1:A:474:ALA:HA	1:A:585:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:HIS:N	1:A:582:HIS:CD2	2.84	0.45
2:C:417:ASP:O	2:C:418:LEU:C	2.55	0.45
1:D:582:HIS:CD2	1:D:582:HIS:N	2.85	0.45
2:B:348:GLU:HG3	2:B:349:LYS:N	2.32	0.45
2:H:315:GLU:O	2:H:387:ASN:CB	2.64	0.45
1:A:602:THR:CG2	1:A:604:ARG:HD2	2.42	0.45
2:C:134:ALA:HA	2:C:137:LEU:CD1	2.47	0.45
1:J:573:LEU:C	1:J:573:LEU:CD1	2.85	0.45
1:J:634:PHE:CB	1:J:656:LYS:HB2	2.47	0.45
1:A:573:LEU:C	1:A:573:LEU:CD1	2.85	0.45
2:B:421:LEU:O	2:B:422:ASP:CG	2.55	0.45
2:H:308:ALA:HB2	2:H:412:MET:HE3	1.97	0.45
2:C:295:SER:OG	2:C:297:LYS:CG	2.66	0.44
1:D:558:THR:O	1:D:624:GLU:HA	2.16	0.44
1:D:559:ARG:HG2	1:D:624:GLU:HG2	2.00	0.44
1:D:602:THR:CG2	1:D:604:ARG:HD2	2.45	0.44
1:E:485:GLU:O	1:E:485:GLU:HG3	2.17	0.44
1:E:567:LEU:CD1	1:E:654:VAL:HG13	2.47	0.44
1:J:538:ASP:O	1:J:540:ASP:N	2.50	0.44
2:C:62:ARG:HB3	2:C:62:ARG:CZ	2.47	0.44
2:B:134:ALA:HA	2:B:137:LEU:CD1	2.47	0.44
1:A:559:ARG:HG2	1:A:624:GLU:HG2	1.98	0.44
2:C:421:LEU:O	2:C:421:LEU:CD2	2.43	0.44
1:E:555:HIS:CD2	1:E:632:GLU:OE2	2.67	0.44
2:H:274:ASN:HB3	2:H:277:TYR:HB2	1.98	0.44
2:H:291:ILE:HG12	2:H:298:TYR:CE1	2.51	0.44
2:C:417:ASP:CA	2:C:418:LEU:HD22	2.47	0.44
1:D:488:ILE:CG2	1:D:526:CYS:HA	2.48	0.44
1:D:593:ALA:HB2	1:D:624:GLU:HG3	1.99	0.44
1:E:581:MET:SD	1:E:583:ILE:HG13	2.58	0.44
1:J:584:HIS:C	1:J:586:ALA:H	2.21	0.44
1:E:560:PHE:CZ	1:E:581:MET:CE	3.00	0.44
1:E:561:ILE:O	1:E:658:VAL:HG12	2.17	0.44
2:H:308:ALA:O	2:H:311:GLU:O	2.35	0.44
1:J:594:LYS:O	1:J:621:ALA:HB1	2.18	0.44
2:K:421:LEU:O	2:K:422:ASP:CB	2.65	0.44
1:D:484:LEU:HD12	1:D:534:VAL:HG11	1.99	0.44
2:B:41:GLN:HE21	2:B:41:GLN:HB2	1.68	0.44
2:B:113:PRO:HG2	2:B:116:PRO:CG	2.46	0.44
2:B:416:LEU:HD12	2:B:416:LEU:N	2.32	0.44
1:E:559:ARG:HB3	1:E:661:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:634:PHE:CB	1:E:656:LYS:HB2	2.48	0.44
2:H:18:VAL:HG23	2:H:19:LYS:N	2.23	0.44
2:H:308:ALA:HB1	2:H:412:MET:HE3	1.99	0.44
1:A:484:LEU:HD12	1:A:534:VAL:HG11	2.00	0.44
1:A:515:ASP:C	1:A:515:ASP:OD1	2.56	0.44
1:A:584:HIS:HD2	1:A:586:ALA:N	2.16	0.44
1:D:580:VAL:HG21	1:D:648:GLN:HG3	1.99	0.44
2:B:291:ILE:HG12	2:B:298:TYR:CD1	2.53	0.44
2:H:343:THR:OG1	2:H:344:LYS:N	2.51	0.44
1:E:619:ILE:HD11	1:E:621:ALA:HB2	1.99	0.44
1:J:618:LYS:HB2	1:J:618:LYS:HE2	1.76	0.44
2:B:420:MET:HG3	2:B:421:LEU:HD12	1.87	0.43
1:J:602:THR:O	1:J:603:ASN:C	2.56	0.43
1:A:580:VAL:HG21	1:A:648:GLN:HG3	2.00	0.43
2:C:276:LYS:HD3	2:C:276:LYS:N	2.32	0.43
2:B:306:MET:HA	2:B:306:MET:HE2	1.99	0.43
1:E:613:ALA:HB1	1:E:617:MET:HE2	2.00	0.43
2:B:288:PHE:HE1	2:B:405:PHE:CE2	2.35	0.43
1:J:572:ILE:HG12	1:J:573:LEU:H	1.83	0.43
2:C:288:PHE:HE1	2:C:405:PHE:CE2	2.35	0.43
1:D:532:LEU:HD12	1:D:547:LEU:CD1	2.48	0.43
2:B:417:ASP:O	2:B:418:LEU:C	2.55	0.43
1:A:532:LEU:HD12	1:A:547:LEU:CD1	2.49	0.43
2:C:113:PRO:HG2	2:C:116:PRO:CG	2.47	0.43
1:D:572:ILE:CG1	1:D:573:LEU:N	2.75	0.43
2:H:274:ASN:HB2	2:H:278:VAL:HG13	2.01	0.43
1:J:598:LYS:HB3	1:J:598:LYS:HE2	1.78	0.43
2:K:421:LEU:O	2:K:421:LEU:CD2	2.42	0.43
2:B:96:GLU:HA	2:B:106:LYS:HA	2.01	0.43
1:A:619:ILE:HG12	1:A:620:ILE:H	1.83	0.43
1:E:594:LYS:O	1:E:621:ALA:HB1	2.19	0.43
1:J:569:LEU:HB3	1:J:571:SER:O	2.18	0.43
2:B:294:ASP:O	2:B:296:GLY:N	2.52	0.43
2:H:294:ASP:O	2:H:294:ASP:OD2	2.36	0.43
2:H:349:LYS:NZ	2:H:350:ASP:O	2.52	0.43
2:H:422:ASP:HB3	2:H:423:PRO:HD2	2.01	0.43
1:J:600:ASP:HB3	1:J:601:LYS:H	1.63	0.43
2:K:326:ILE:HD12	2:K:328:TYR:HE2	1.82	0.43
2:H:417:ASP:OD1	2:H:418:LEU:N	2.52	0.43
2:C:291:ILE:HG12	2:C:298:TYR:CD1	2.53	0.43
1:E:569:LEU:HB3	1:E:571:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:320:PHE:HA	2:H:391:VAL:O	2.19	0.43
2:K:294:ASP:O	2:K:294:ASP:CG	2.56	0.43
1:A:488:ILE:HB	1:A:526:CYS:HA	2.00	0.42
1:E:598:LYS:HB3	1:E:598:LYS:HE2	1.76	0.42
1:A:488:ILE:CG2	1:A:526:CYS:HA	2.49	0.42
1:A:619:ILE:HD11	1:A:621:ALA:HB2	2.00	0.42
2:H:421:LEU:C	2:H:421:LEU:CD2	2.86	0.42
1:J:634:PHE:HE1	1:J:642:ARG:HH11	1.66	0.42
2:C:61:SER:O	2:C:62:ARG:C	2.58	0.42
2:C:306:MET:HA	2:C:306:MET:HE2	2.00	0.42
1:D:537:ASP:OD2	1:D:538:ASP:N	2.53	0.42
1:D:619:ILE:HD11	1:D:621:ALA:HB2	2.01	0.42
1:E:634:PHE:HE1	1:E:642:ARG:HH11	1.65	0.42
2:K:421:LEU:C	2:K:421:LEU:CD2	2.86	0.42
1:A:537:ASP:OD2	1:A:538:ASP:N	2.53	0.42
1:J:560:PHE:CZ	1:J:581:MET:CE	3.01	0.42
2:K:320:PHE:HA	2:K:391:VAL:O	2.20	0.42
1:D:479:ASP:O	1:D:480:LEU:C	2.58	0.42
1:A:593:ALA:HB2	1:A:624:GLU:HG3	2.00	0.42
2:C:416:LEU:HD12	2:C:416:LEU:N	2.30	0.42
1:J:567:LEU:HD12	1:J:653:ALA:HA	2.02	0.42
1:J:634:PHE:HA	1:J:641:GLY:HA3	2.02	0.42
2:K:422:ASP:HB3	2:K:423:PRO:HD2	2.01	0.42
2:C:34:LEU:C	2:C:35:ILE:HD12	2.39	0.42
2:C:298:TYR:HA	2:C:410:ALA:O	2.20	0.42
2:B:61:SER:O	2:B:62:ARG:C	2.58	0.42
2:H:421:LEU:O	2:H:422:ASP:CB	2.66	0.42
2:C:98:ILE:HA	2:C:104:THR:HG22	2.02	0.42
2:C:300:PHE:CD1	2:C:300:PHE:C	2.92	0.42
1:J:614:THR:HG22	1:J:617:MET:SD	2.59	0.42
1:A:560:PHE:CZ	1:A:581:MET:HE1	2.55	0.42
2:B:112:GLU:HA	2:B:113:PRO:HD3	1.75	0.42
1:E:573:LEU:CD2	1:E:577:TYR:CD1	3.03	0.42
2:H:326:ILE:HD12	2:H:328:TYR:HE2	1.83	0.42
2:B:280:GLU:CD	2:B:392:SER:H	2.23	0.41
2:K:10:GLU:O	2:K:14:ILE:HG12	2.20	0.41
2:K:315:GLU:O	2:K:387:ASN:HB3	2.20	0.41
1:A:569:LEU:HD21	1:A:573:LEU:HB2	2.02	0.41
1:A:618:LYS:HE2	1:A:618:LYS:HB2	1.84	0.41
1:D:488:ILE:HB	1:D:526:CYS:HA	2.01	0.41
2:B:34:LEU:C	2:B:35:ILE:HD12	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:ALA:O	1:E:518:ASP:CB	2.64	0.41
1:E:567:LEU:HD11	1:E:654:VAL:HG13	2.01	0.41
1:E:647:ASP:C	1:E:649:GLY:N	2.67	0.41
2:H:315:GLU:O	2:H:387:ASN:HB3	2.20	0.41
1:A:479:ASP:O	1:A:480:LEU:C	2.58	0.41
1:A:600:ASP:O	1:A:618:LYS:CE	2.67	0.41
1:A:605:LYS:HB2	1:A:605:LYS:HE2	1.78	0.41
1:E:518:ASP:OD1	1:E:531:ARG:NH2	2.52	0.41
1:E:567:LEU:HD12	1:E:653:ALA:HA	2.01	0.41
1:E:602:THR:O	1:E:603:ASN:C	2.59	0.41
1:J:647:ASP:C	1:J:649:GLY:N	2.71	0.41
2:K:325:MET:HE2	2:K:341:TYR:HB3	1.94	0.41
1:A:602:THR:O	1:A:603:ASN:C	2.59	0.41
2:C:325:MET:HE3	2:C:341:TYR:HB3	2.00	0.41
1:J:559:ARG:HB3	1:J:661:LEU:HD12	2.01	0.41
1:D:647:ASP:C	1:D:649:GLY:N	2.73	0.41
2:B:307:ASN:ND2	2:B:420:MET:O	2.54	0.41
1:A:537:ASP:OD2	1:A:537:ASP:C	2.59	0.41
1:A:573:LEU:HD22	1:A:577:TYR:CD2	2.56	0.41
2:C:343:THR:OG1	2:C:344:LYS:N	2.53	0.41
1:D:584:HIS:CD2	1:D:585:THR:HG22	2.56	0.41
2:B:300:PHE:CD1	2:B:300:PHE:C	2.93	0.41
1:E:646:ARG:HG2	1:E:648:GLN:N	2.35	0.41
2:H:325:MET:HB3	2:H:325:MET:HE3	1.89	0.41
1:A:600:ASP:HB3	1:A:601:LYS:H	1.60	0.41
2:C:280:GLU:CD	2:C:392:SER:H	2.23	0.41
1:D:619:ILE:HG12	1:D:620:ILE:H	1.85	0.41
2:B:36:ILE:HA	2:B:37:PRO:HD2	1.95	0.41
2:B:93:TYR:HD1	2:B:128:PHE:CD1	2.38	0.41
2:B:421:LEU:C	2:B:421:LEU:CD2	2.87	0.41
1:J:526:CYS:C	1:J:528:ASP:H	2.24	0.41
1:D:602:THR:O	1:D:603:ASN:C	2.59	0.41
1:E:509:GLU:O	1:E:534:VAL:HA	2.21	0.41
2:H:5:ALA:C	2:H:7:LYS:H	2.23	0.41
2:C:96:GLU:HA	2:C:106:LYS:HA	2.03	0.41
2:C:307:ASN:ND2	2:C:420:MET:O	2.54	0.41
1:D:537:ASP:OD2	1:D:537:ASP:C	2.59	0.41
1:D:600:ASP:O	1:D:618:LYS:CE	2.67	0.41
1:E:572:ILE:CD1	1:E:612:PHE:CB	2.80	0.41
2:H:386:ALA:CA	2:H:387:ASN:CB	2.75	0.41
2:B:38:PRO:CB	2:B:88:ASN:HA	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ILE:HA	2:B:104:THR:HG22	2.03	0.41
1:D:511:THR:O	1:D:512:ALA:HB2	2.22	0.40
1:D:584:HIS:HD2	1:D:586:ALA:N	2.16	0.40
2:B:325:MET:HE1	2:B:341:TYR:CB	2.43	0.40
1:E:538:ASP:O	1:E:540:ASP:N	2.54	0.40
1:E:572:ILE:CG1	1:E:612:PHE:CD1	3.03	0.40
1:J:613:ALA:HB1	1:J:617:MET:HE2	2.03	0.40
2:K:343:THR:OG1	2:K:344:LYS:N	2.52	0.40
1:A:581:MET:HE2	1:A:643:PHE:CD1	2.56	0.40
1:A:646:ARG:CB	1:A:648:GLN:HG2	2.51	0.40
2:B:117:ILE:O	2:B:119:THR:N	2.54	0.40
2:B:343:THR:OG1	2:B:344:LYS:N	2.53	0.40
1:J:496:ASN:HA	1:J:510:VAL:O	2.21	0.40
1:J:544:GLY:HA2	1:J:585:THR:CG2	2.36	0.40
1:D:641:GLY:HA2	1:D:657:VAL:HG13	2.02	0.40
2:B:414:TYR:CD1	2:B:414:TYR:N	2.81	0.40
1:E:584:HIS:C	1:E:586:ALA:H	2.25	0.40
2:H:424:GLU:OE1	2:H:424:GLU:N	2.35	0.40
1:J:509:GLU:O	1:J:534:VAL:HA	2.21	0.40
2:C:421:LEU:O	2:C:422:ASP:CB	2.70	0.40
2:B:372:LEU:O	2:B:373:LEU:C	2.59	0.40
1:E:572:ILE:CD1	1:E:612:PHE:CD1	3.04	0.40
2:H:300:PHE:C	2:H:300:PHE:CD1	2.94	0.40
2:H:392:SER:OG	2:H:394:ARG:HG2	2.22	0.40
1:J:599:LEU:HD11	1:J:620:ILE:HG22	2.02	0.40
1:J:641:GLY:HA2	1:J:657:VAL:HG13	2.03	0.40
1:A:584:HIS:CD2	1:A:585:THR:HG22	2.56	0.40
1:D:600:ASP:HB3	1:D:601:LYS:H	1.61	0.40
1:D:646:ARG:CB	1:D:648:GLN:HG2	2.51	0.40
2:B:94:CYS:HA	2:B:107:LEU:O	2.21	0.40
2:K:274:ASN:HB2	2:K:278:VAL:HG13	2.04	0.40
2:K:414:TYR:CE2	2:K:416:LEU:HD11	2.57	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	194/201 (96%)	170 (88%)	20 (10%)	4 (2%)	7	38
1	D	194/201 (96%)	170 (88%)	20 (10%)	4 (2%)	7	38
1	E	194/201 (96%)	164 (84%)	23 (12%)	7 (4%)	3	26
1	J	194/201 (96%)	166 (86%)	23 (12%)	5 (3%)	5	33
2	B	253/441 (57%)	201 (79%)	33 (13%)	19 (8%)	1	11
2	C	253/441 (57%)	203 (80%)	31 (12%)	19 (8%)	1	11
2	H	155/441 (35%)	113 (73%)	30 (19%)	12 (8%)	1	10
2	K	155/441 (35%)	114 (74%)	31 (20%)	10 (6%)	1	14
All	All	1592/2568 (62%)	1301 (82%)	211 (13%)	80 (5%)	2	19

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	575	THR
1	A	648	GLN
2	C	87	ASP
2	C	299	CYS
2	C	413	ARG
2	C	423	PRO
1	D	479	ASP
1	D	575	THR
1	D	648	GLN
2	B	87	ASP
2	B	299	CYS
2	B	413	ARG
2	B	423	PRO
1	E	479	ASP
1	E	575	THR
1	E	648	GLN
2	H	298	TYR
2	H	423	PRO
1	J	479	ASP
1	J	575	THR
1	J	648	GLN
2	K	299	CYS

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Mol	Chain	Res	Type
2	K	423	PRO
2	C	29	THR
2	C	113	PRO
2	C	312	GLY
2	C	418	LEU
2	B	5	ALA
2	B	29	THR
2	B	113	PRO
2	B	312	GLY
2	B	418	LEU
2	H	7	LYS
2	H	76	ARG
2	H	420	MET
2	K	298	TYR
2	K	420	MET
2	C	5	ALA
2	C	28	GLY
2	C	298	TYR
2	C	420	MET
2	C	424	GLU
2	B	28	GLY
2	B	298	TYR
2	B	420	MET
2	B	424	GLU
1	E	606	SER
1	E	608	LYS
2	H	312	GLY
2	H	387	ASN
2	H	424	GLU
1	J	570	PRO
1	J	603	ASN
2	K	47	ASN
2	K	300	PHE
2	K	312	GLY
2	K	387	ASN
2	K	424	GLU
1	A	603	ASN
2	C	387	ASN
2	C	415	GLN
1	D	603	ASN
2	B	387	ASN
2	B	415	GLN

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Mol	Chain	Res	Type
1	E	603	ASN
2	H	46	SER
2	H	421	LEU
2	K	421	LEU
2	C	118	ASN
2	C	412	MET
2	C	421	LEU
2	B	118	ASN
2	B	412	MET
2	B	421	LEU
2	H	414	TYR
2	B	406	GLY
2	H	47	ASN
2	C	406	GLY
1	E	525	ILE

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	172/175 (98%)	153 (89%)	19 (11%)	6	29
1	D	172/175 (98%)	151 (88%)	21 (12%)	5	23
1	E	172/175 (98%)	144 (84%)	28 (16%)	2	13
1	J	172/175 (98%)	145 (84%)	27 (16%)	2	15
2	B	232/383 (61%)	208 (90%)	24 (10%)	7	32
2	C	232/383 (61%)	210 (90%)	22 (10%)	8	34
2	H	154/383 (40%)	144 (94%)	10 (6%)	17	50
2	K	154/383 (40%)	141 (92%)	13 (8%)	11	40
All	All	1460/2232 (65%)	1296 (89%)	164 (11%)	6	27

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	526	CYS
1	A	543	THR
1	A	559	ARG
1	A	583	ILE
1	A	584	HIS
1	A	589	GLU
1	A	600	ASP
1	A	602	THR
1	A	604	ARG
1	A	608	LYS
1	A	611	MET
1	A	619	ILE
1	A	620	ILE
1	A	629	VAL
1	A	648	GLN
1	A	650	THR
1	A	656	LYS
1	A	657	VAL
1	A	662	ASP
2	C	41	GLN
2	C	47	ASN
2	C	62	ARG
2	C	74	SER
2	C	107	LEU
2	C	108	ASN
2	C	115	LYS
2	C	118	ASN
2	C	276	LYS
2	C	279	GLN
2	C	298	TYR
2	C	302	VAL
2	C	323	LEU
2	C	340	THR
2	C	373	LEU
2	C	374	SER
2	C	413	ARG
2	C	415	GLN
2	C	417	ASP
2	C	418	LEU
2	C	421	LEU
2	C	425	SER
1	D	526	CYS
1	D	542	GLN

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Mol	Chain	Res	Type
1	D	543	THR
1	D	559	ARG
1	D	569	LEU
1	D	583	ILE
1	D	584	HIS
1	D	589	GLU
1	D	600	ASP
1	D	602	THR
1	D	604	ARG
1	D	608	LYS
1	D	611	MET
1	D	619	ILE
1	D	620	ILE
1	D	629	VAL
1	D	648	GLN
1	D	650	THR
1	D	656	LYS
1	D	657	VAL
1	D	662	ASP
2	B	41	GLN
2	B	47	ASN
2	B	61	SER
2	B	62	ARG
2	B	74	SER
2	B	105	ARG
2	B	107	LEU
2	B	108	ASN
2	B	115	LYS
2	B	118	ASN
2	B	276	LYS
2	B	279	GLN
2	B	298	TYR
2	B	302	VAL
2	B	323	LEU
2	B	340	THR
2	B	373	LEU
2	B	374	SER
2	B	413	ARG
2	B	415	GLN
2	B	417	ASP
2	B	418	LEU
2	B	421	LEU

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Mol	Chain	Res	Type
2	B	425	SER
1	E	475	SER
1	E	485	GLU
1	E	506	GLN
1	E	524	SER
1	E	526	CYS
1	E	543	THR
1	E	552	ASN
1	E	559	ARG
1	E	569	LEU
1	E	573	LEU
1	E	583	ILE
1	E	584	HIS
1	E	589	GLU
1	E	590	VAL
1	E	602	THR
1	E	604	ARG
1	E	606	SER
1	E	608	LYS
1	E	611	MET
1	E	619	ILE
1	E	620	ILE
1	E	623	LEU
1	E	629	VAL
1	E	642	ARG
1	E	644	THR
1	E	645	LEU
1	E	650	THR
1	E	657	VAL
2	H	276	LYS
2	H	286	ARG
2	H	298	TYR
2	H	302	VAL
2	H	303	VAL
2	H	323	LEU
2	H	396	GLN
2	H	418	LEU
2	H	421	LEU
2	H	425	SER
1	J	475	SER
1	J	485	GLU
1	J	506	GLN

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Mol	Chain	Res	Type
1	J	526	CYS
1	J	543	THR
1	J	552	ASN
1	J	559	ARG
1	J	569	LEU
1	J	573	LEU
1	J	583	ILE
1	J	584	HIS
1	J	589	GLU
1	J	590	VAL
1	J	602	THR
1	J	604	ARG
1	J	606	SER
1	J	608	LYS
1	J	611	MET
1	J	619	ILE
1	J	620	ILE
1	J	623	LEU
1	J	629	VAL
1	J	642	ARG
1	J	644	THR
1	J	645	LEU
1	J	650	THR
1	J	657	VAL
2	K	78	ARG
2	K	131	GLU
2	K	276	LYS
2	K	286	ARG
2	K	298	TYR
2	K	302	VAL
2	K	303	VAL
2	K	323	LEU
2	K	396	GLN
2	K	413	ARG
2	K	418	LEU
2	K	421	LEU
2	K	425	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	ASN

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Mol	Chain	Res	Type
1	A	552	ASN
1	A	555	HIS
1	A	563	GLN
1	A	584	HIS
2	C	25	HIS
2	C	41	GLN
2	C	47	ASN
2	C	88	ASN
2	C	108	ASN
2	C	118	ASN
2	C	285	GLN
2	C	310	GLN
2	C	346	GLN
2	C	396	GLN
2	C	400	GLN
2	C	415	GLN
1	D	496	ASN
1	D	552	ASN
1	D	555	HIS
1	D	563	GLN
1	D	584	HIS
2	B	41	GLN
2	B	47	ASN
2	B	88	ASN
2	B	108	ASN
2	B	118	ASN
2	B	285	GLN
2	B	310	GLN
2	B	346	GLN
2	B	396	GLN
2	B	400	GLN
2	B	415	GLN
1	E	496	ASN
1	E	555	HIS
1	E	563	GLN
1	E	584	HIS
2	H	310	GLN
1	J	542	GLN
1	J	555	HIS
1	J	563	GLN
1	J	584	HIS
2	K	310	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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, 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	196/201 (97%)	0.80	23 (11%) 4 5	69, 77, 80, 82	0
1	D	196/201 (97%)	0.86	24 (12%) 4 5	69, 77, 80, 82	0
1	E	196/201 (97%)	0.71	10 (5%) 28 25	49, 58, 67, 72	0
1	J	196/201 (97%)	0.72	13 (6%) 18 17	49, 58, 67, 72	0
2	B	261/441 (59%)	0.51	18 (6%) 16 16	66, 79, 83, 83	0
2	C	261/441 (59%)	0.56	18 (6%) 16 16	66, 79, 83, 83	0
2	H	175/441 (39%)	0.60	22 (12%) 3 5	66, 83, 116, 122	0
2	K	175/441 (39%)	0.56	17 (9%) 7 8	66, 83, 118, 138	0
All	All	1656/2568 (64%)	0.66	145 (8%) 10 10	49, 77, 98, 138	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	339	ILE	5.2
2	H	389	GLU	4.5
2	K	388	LEU	3.9
2	K	340	THR	3.9
2	H	388	LEU	3.9
2	H	319	CYS	3.6
2	K	275	VAL	3.5
2	B	411	VAL	3.5
2	C	32	ILE	3.5
2	H	317	LEU	3.3
2	C	122	TYR	3.3
2	H	318	LEU	3.3
2	B	32	ILE	3.3
2	K	389	GLU	3.3
1	D	611	MET	3.2
2	K	341	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	411	VAL	3.2
2	H	275	VAL	3.1
2	B	275	VAL	3.1
1	E	573	LEU	3.1
2	H	34	LEU	3.1
2	H	306	MET	3.0
2	H	339	ILE	3.0
1	A	631	MET	3.0
2	K	306	MET	3.0
1	D	513	ILE	3.0
2	K	34	LEU	3.0
2	B	133	LEU	3.0
2	H	408	ILE	2.9
2	K	408	ILE	2.9
1	A	611	MET	2.9
2	B	45	TYR	2.9
1	J	573	LEU	2.9
2	B	122	TYR	2.9
1	A	512	ALA	2.9
2	C	275	VAL	2.8
1	D	532	LEU	2.8
2	H	340	THR	2.8
2	C	276	LYS	2.8
2	C	34	LEU	2.8
2	C	317	LEU	2.7
2	C	388	LEU	2.7
1	E	572	ILE	2.7
2	C	386	ALA	2.7
2	C	133	LEU	2.7
2	K	325	MET	2.7
1	D	612	PHE	2.6
1	E	583	ILE	2.6
1	A	613	ALA	2.6
1	D	562	ALA	2.6
1	D	613	ALA	2.6
2	H	276	LYS	2.6
1	A	532	LEU	2.6
2	H	341	TYR	2.6
1	A	573	LEU	2.6
1	J	541	VAL	2.6
2	H	413	ARG	2.6
1	A	581	MET	2.6

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Mol	Chain	Res	Type	RSRZ
2	K	328	TYR	2.6
1	A	583	ILE	2.5
1	D	566	ILE	2.5
1	D	511	THR	2.5
1	J	613	ALA	2.5
1	J	583	ILE	2.5
2	B	276	LYS	2.5
1	A	563	GLN	2.5
2	H	323	LEU	2.5
1	D	533	ARG	2.5
2	H	91	VAL	2.5
2	B	34	LEU	2.5
1	E	613	ALA	2.4
2	C	128	PHE	2.4
1	D	573	LEU	2.4
2	C	136	LEU	2.4
2	K	137	LEU	2.4
2	C	92	ILE	2.4
1	E	484	LEU	2.4
1	A	566	ILE	2.4
1	D	631	MET	2.4
1	D	512	ALA	2.4
1	D	493	ILE	2.4
2	H	325	MET	2.3
1	J	472	PRO	2.3
2	B	30	SER	2.3
1	D	499	VAL	2.3
1	D	583	ILE	2.3
2	K	276	LYS	2.3
1	A	511	THR	2.3
1	D	484	LEU	2.3
1	J	471	MET	2.3
2	H	90	LEU	2.3
2	C	93	TYR	2.3
1	E	471	MET	2.3
1	A	623	LEU	2.3
2	K	91	VAL	2.3
2	C	305	THR	2.3
1	E	541	VAL	2.2
1	A	592	PHE	2.2
1	A	612	PHE	2.2
1	A	660	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	405	PHE	2.2
1	A	621	ALA	2.2
1	A	533	ARG	2.2
1	J	572	ILE	2.2
2	H	302	VAL	2.2
1	D	524	SER	2.2
2	B	328	TYR	2.2
2	C	408	ILE	2.2
1	D	592	PHE	2.2
1	A	468	PRO	2.2
2	K	323	LEU	2.2
1	D	574	THR	2.1
2	B	377	LEU	2.1
1	J	546	VAL	2.1
1	A	499	VAL	2.1
1	D	652	VAL	2.1
1	J	564	ILE	2.1
2	B	287	PHE	2.1
1	D	483	ILE	2.1
1	E	564	ILE	2.1
1	A	493	ILE	2.1
1	J	484	LEU	2.1
1	E	470	ILE	2.1
2	C	328	TYR	2.1
1	A	467	ALA	2.1
1	J	654	VAL	2.1
2	C	49	LEU	2.1
1	D	525	ILE	2.1
1	D	572	ILE	2.1
2	B	341	TYR	2.1
1	J	501	VAL	2.1
2	B	90	LEU	2.1
2	H	411	VAL	2.1
2	K	317	LEU	2.1
1	A	619	ILE	2.0
2	H	33	THR	2.0
1	J	532	LEU	2.0
2	H	292	SER	2.0
1	D	563	GLN	2.0
2	B	128	PHE	2.0
2	B	92	ILE	2.0
1	A	562	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	K	318	LEU	2.0
1	E	632	GLU	2.0
2	B	93	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 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.