



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:32 AM UTC

PDB ID : 3E20 / pdb_00003e20
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

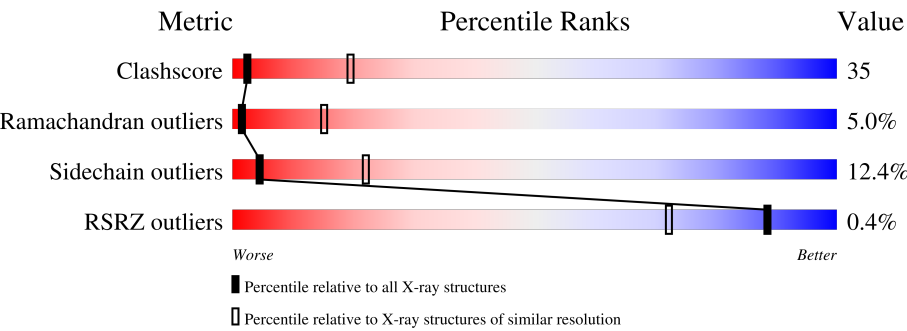
1 Overall quality at a glance i

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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	% 22% 14% 60%

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
1	A	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	D	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	E	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	J	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			

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 2088	C 1321	N 347	O 405	S 15	0	0	0
2	B	261	Total 2088	C 1321	N 347	O 405	S 15	0	0	0
2	H	175	Total 1412	C 900	N 225	O 277	S 10	0	0	0
2	K	175	Total 1412	C 900	N 225	O 277	S 10	0	0	0

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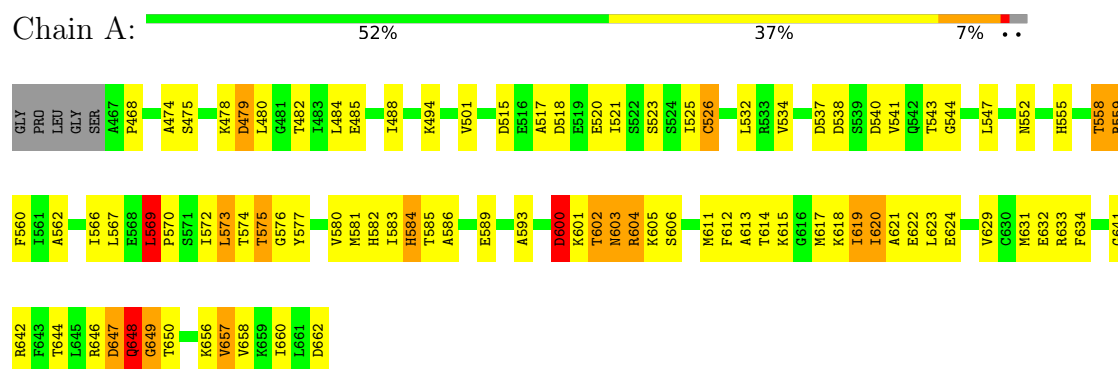
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Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P79063
K	0	MET	-	expression tag	UNP P79063

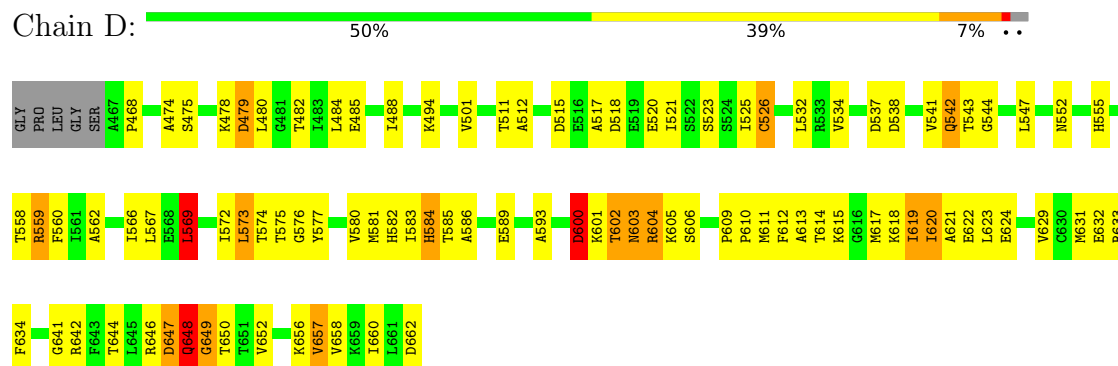
3 Residue-property plots

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.

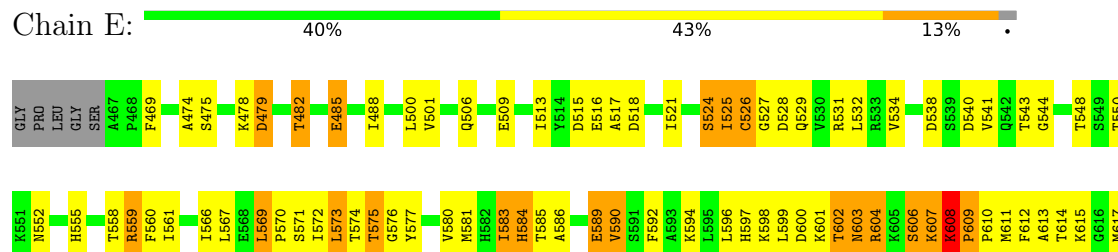
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit



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



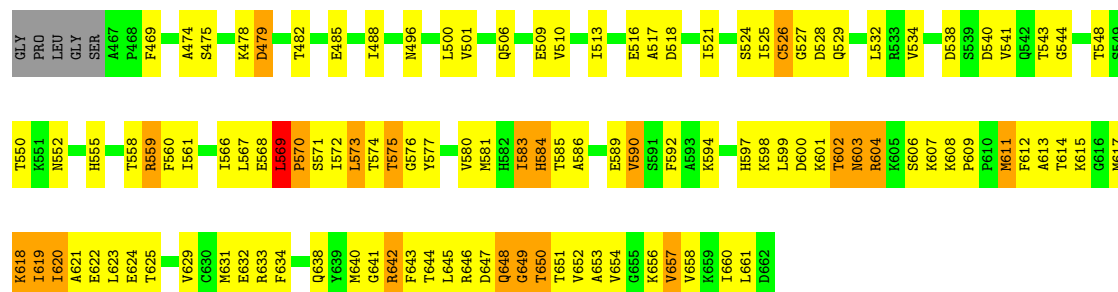
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit





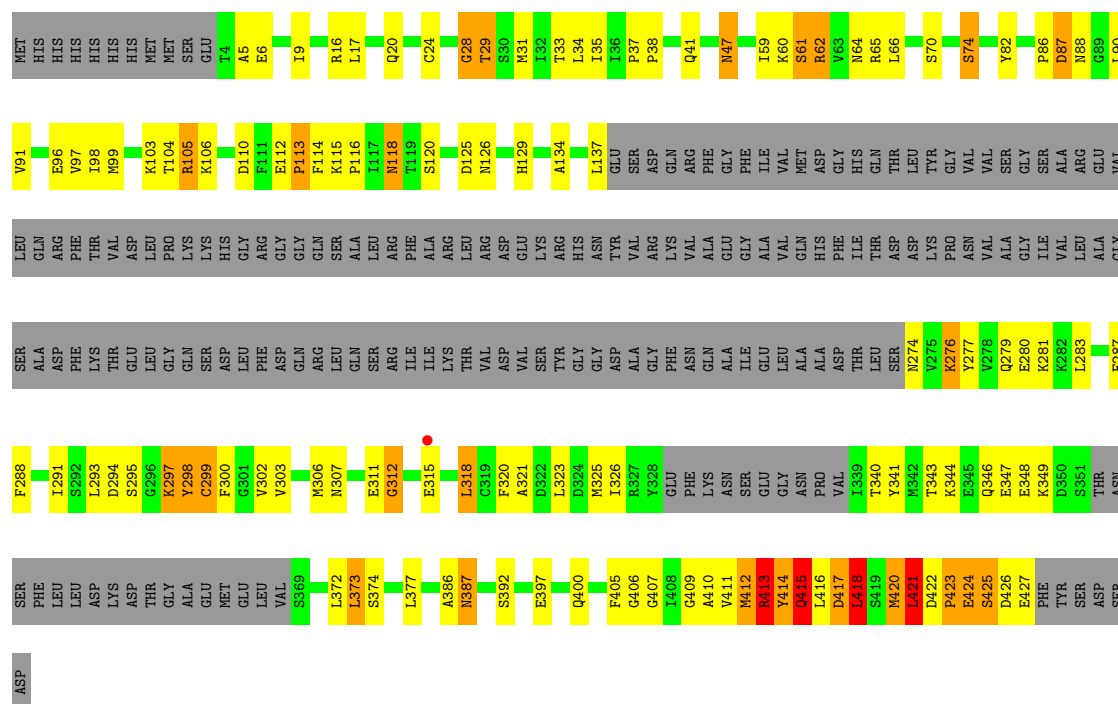
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit

Chain J: 41% 46% 10%



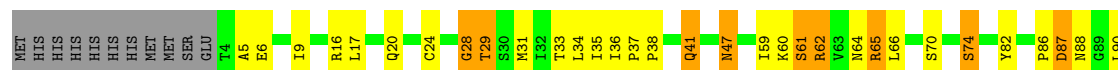
- Molecule 2: Eukaryotic peptide chain release factor subunit 1

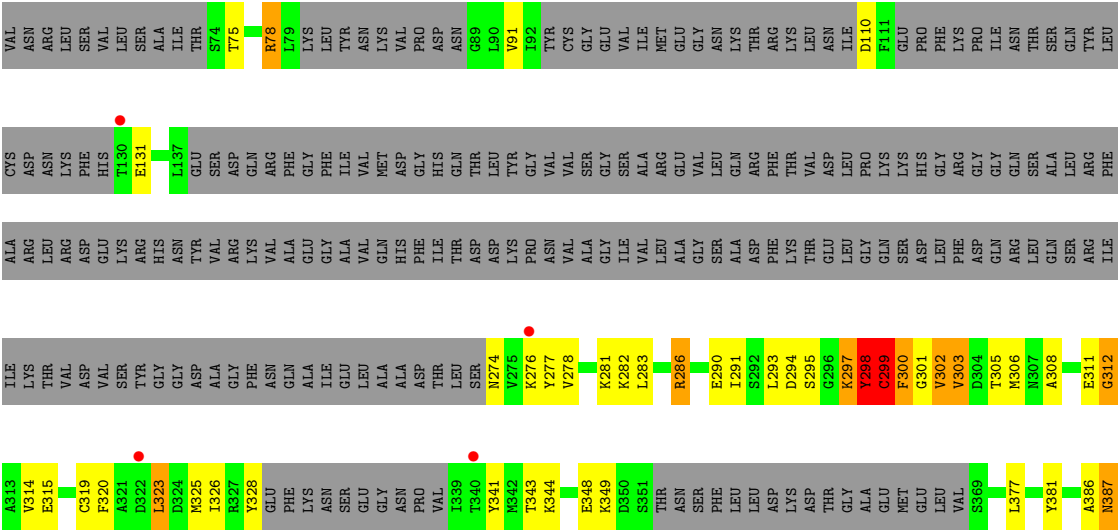
Chain C: 32% 21% 6% 41%



- Molecule 2: Eukaryotic peptide chain release factor subunit 1

Chain B: 30% 22% 6% 41%





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 30.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.50) 99.7 (30.00-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.258 , 0.280 0.277 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	123.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 178.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13096	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage'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

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	0.46	0/1547	0.85	4/2089 (0.2%)
1	D	0.46	0/1547	0.84	3/2089 (0.1%)
1	E	0.61	2/1547 (0.1%)	0.98	6/2089 (0.3%)
1	J	0.58	0/1547	0.97	7/2089 (0.3%)
2	B	0.40	0/2119	0.87	6/2848 (0.2%)
2	C	0.41	0/2119	0.85	6/2848 (0.2%)
2	H	0.40	0/1425	0.76	0/1901
2	K	0.40	0/1425	0.78	2/1901 (0.1%)
All	All	0.47	2/13276 (0.0%)	0.87	34/17854 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	609	PRO	CA-C	6.40	1.58	1.52
1	E	608	LYS	N-CA	-5.98	1.37	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	608	LYS	CA-C-N	10.89	131.60	120.38
1	E	608	LYS	C-N-CA	10.89	131.60	120.38
2	B	105	ARG	CG-CD-NE	8.02	129.65	112.00
1	E	609	PRO	N-CA-C	-7.90	101.06	110.70
1	D	600	ASP	N-CA-C	7.70	115.09	108.78
1	A	570	PRO	N-CA-C	-7.33	97.38	112.47
1	E	649	GLY	N-CA-C	-7.13	103.64	112.77
1	A	600	ASP	N-CA-C	7.12	114.62	108.78
2	B	413	ARG	N-CA-C	-7.11	95.66	110.80
2	B	414	TYR	N-CA-CB	-7.10	99.96	111.24
2	C	413	ARG	N-CA-C	-7.09	95.70	110.80
2	C	414	TYR	N-CA-CB	-6.75	100.50	111.24
1	J	609	PRO	CA-C-N	6.71	126.75	119.90
1	J	609	PRO	C-N-CA	6.71	126.75	119.90
1	J	569	LEU	CA-C-N	-6.65	111.53	119.84
1	J	569	LEU	C-N-CA	-6.65	111.53	119.84
2	K	413	ARG	NE-CZ-NH2	6.65	125.18	119.20
1	A	649	GLY	N-CA-C	-6.61	104.50	112.49
1	D	649	GLY	N-CA-C	-6.54	104.58	112.49
2	B	343	THR	CB-CA-C	-6.12	108.25	117.07
2	C	65	ARG	CB-CG-CD	-6.09	97.28	111.30
2	C	343	THR	CB-CA-C	-6.09	108.30	117.07
1	A	569	LEU	N-CA-C	6.02	122.24	108.81
2	B	105	ARG	CB-CG-CD	-5.96	97.58	111.30
1	J	649	GLY	N-CA-C	-5.79	105.36	112.77
2	K	299	CYS	N-CA-C	-5.74	98.57	110.80
1	E	608	LYS	CB-CG-CD	-5.62	98.38	111.30
1	E	527	GLY	N-CA-C	-5.45	108.50	115.42
2	C	105	ARG	CG-CD-NE	5.33	123.73	112.00
1	J	527	GLY	N-CA-C	-5.29	108.70	115.42
1	J	607	LYS	N-CA-C	-5.28	101.11	109.76
1	D	542	GLN	CB-CG-CD	-5.17	103.81	112.60
2	B	343	THR	CA-C-O	5.09	120.89	117.94
2	C	343	THR	CA-C-O	5.05	120.87	117.94

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

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Mol	Chain	Res	Type	Group
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	91	0
1	D	1524	0	1569	93	0
1	E	1524	0	1569	123	0
1	J	1524	0	1569	106	0
2	B	2088	0	2077	155	0
2	C	2088	0	2077	143	0
2	H	1412	0	1388	121	0
2	K	1412	0	1388	92	0
All	All	13096	0	13206	920	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 35.

All (920) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:325:MET:HE1	2:H:341:TYR:HB3	1.17	1.13
2:H:420:MET:HA	2:H:421:LEU:CB	1.76	1.13
1:D:572:ILE:HD11	1:D:612:PHE:CB	1.79	1.11
2:C:423:PRO:HA	2:C:424:GLU:C	1.73	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:B:423:PRO:HA	2:B:424:GLU:C	1.72	1.10
2:K:418:LEU:H	2:K:418:LEU:HD22	1.06	1.10
2:K:423:PRO:HA	2:K:424:GLU:C	1.74	1.10
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:325:MET:HE1	2:K:341:TYR:HB3	1.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:423:PRO:HA	2:H:424:GLU:C	1.74	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: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: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: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
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
1:E:613:ALA:HA	1:E:617:MET:HE1	1.45	0.98
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:386:ALA:CA	2:H:387:ASN:HB2	1.95	0.95
1:J:560:PHE:HZ	1:J:581:MET:HE1	1.31	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:560:PHE:HZ	1:E:581:MET:HE1	1.30	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:B:325:MET:HE1	2:B:341:TYR:HB3	1.50	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: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
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
1:E:560:PHE:CZ	1:E:581:MET:HE1	2.05	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
1:D:560:PHE:CZ	1:D:581:MET:HE1	2.05	0.91
2:H:418:LEU:CD2	2:H:418:LEU:H	1.82	0.91
1:A:560:PHE:CZ	1:A:581:MET:HE1	2.05	0.91
2:B:413:ARG:O	2:B:414:TYR:CD1	2.24	0.90
1:J:613:ALA:HA	1:J:617:MET:HE1	1.51	0.90
2:C:325:MET:HE1	2:C:341:TYR:HB3	1.50	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
1:J:560:PHE:CZ	1:J:581:MET:HE1	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:298:TYR:H	2:C:412:MET:HE2	1.40	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: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:414:TYR:CD2	2:C:416:LEU:HD11	2.13	0.84
1:D:560:PHE:HZ	1:D:581:MET:HE1	1.43	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:298:TYR:H	2:B:412:MET:HE2	1.44	0.82
2:B:386:ALA:HA	2:B:387:ASN:CB	2.06	0.82
2:C:47:ASN:HD22	2:C:47:ASN:C	1.86	0.82
2:B:414:TYR:CD2	2:B:416:LEU:HD11	2.14	0.82
1:A:560:PHE:HZ	1:A:581:MET:HE1	1.42	0.81
2:B:47:ASN:C	2:B:47:ASN:HD22	1.86	0.81
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
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: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:298:TYR:H	2:B:412:MET:CE	1.95	0.78
2:B:425:SER:HB2	2:B:426:ASP:C	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:425:SER:HB2	2:C:426:ASP:C	2.09	0.78
2:H:301:GLY:O	2:H:305:THR:OG1	2.02	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:C:417:ASP:C	2:C:418:LEU:HD22	2.09	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
2:B:306:MET:HE2	2:B:306:MET:HA	1.66	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:423:PRO:CA	2:K:424:GLU:C	2.57	0.77
1:E:574:THR:O	1:E:576:GLY:N	2.18	0.76
2:B:417:ASP:C	2:B:418:LEU:HD22	2.10	0.76
1:E:589:GLU:OE2	1:E:626:GLN:HG2	1.86	0.76
2:C:306:MET:HE2	2:C:306:MET:HA	1.66	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
2:H:425:SER:HB2	2:H:426:ASP:C	2.11	0.75
2:C:325:MET:CE	2:C:341:TYR:HB3	2.15	0.75
2:C:420:MET:HA	2:C:421:LEU:HB3	0.86	0.75
2:C:298:TYR:N	2:C:412:MET:HE2	2.00	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:H:417:ASP:C	2:H:418:LEU:HD22	2.12	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:425:SER:HB2	2:K:426:ASP:C	2.12	0.74
1:D:478:LYS:O	1:D:479:ASP:HB2	1.87	0.74
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:B:423:PRO:CA	2:B:424:GLU:C	2.58	0.73
2:H:411:VAL:O	2:H:411:VAL:HG23	1.88	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:H:414:TYR:O	2:H:416:LEU:CD1	2.35	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: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
1:J:478:LYS:O	1:J:479:ASP:HB2	1.89	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:C:415:GLN:C	2:C:416:LEU:HD12	2.15	0.71
2:H:423:PRO:CA	2:H:424:GLU:C	2.57	0.71
2:B:59:ILE:HG22	2:B:61:SER:H	1.56	0.71
2:B:415:GLN:C	2:B:416:LEU:HD12	2.16	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
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
1:J:576:GLY:HA3	2:K:400:GLN:HA	1.73	0.70
1:J:572:ILE:HG13	1:J:612:PHE:HD1	1.55	0.70
2:C:423:PRO:CA	2:C:424:GLU:C	2.58	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:B:298:TYR:N	2:B:412:MET:HE2	2.07	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
1:J:517:ALA:O	1:J:518:ASP:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:421:LEU:HD22	2:H:421:LEU:C	2.17	0.69
2:K:421:LEU:HD22	2:K:421:LEU:C	2.17	0.68
1:D:572:ILE:CD1	1:D:612:PHE:CD1	2.76	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:613:ALA:HA	1:D:617:MET:HE1	1.75	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:A:613:ALA:HA	1:A:617:MET:HE1	1.75	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:325:MET:HE1	2:H:341:TYR:CB	2.11	0.67
2:H:377:LEU:O	2:H:381:TYR: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: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
2:C:425:SER:HG	2:C:426:ASP:HA	1.58	0.66
1:D:602:THR:HG23	1:D:604:ARG:HD2	1.75	0.66
2:B:421:LEU:HD22	2:B:421:LEU:C	2.21	0.66
2:C:315:GLU:HB2	2:C:413:ARG:HG2	1.77	0.65
2:B:306:MET:HE1	2:B:377:LEU:HD21	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:B:293:LEU:O	2:B:294:ASP:HB3	1.94	0.64
2:C:344:LYS:HA	2:C:346:GLN:HE21	1.63	0.64
2:B:411:VAL:HG23	2:B:411:VAL:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:306:MET:HE1	2:C:377:LEU:HD21	1.78	0.64
1:E:572:ILE:CD1	1:E:612:PHE:HB2	2.26	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:H:299:CYS:SG	2:H:412:MET:HE3	2.38	0.64
2:C:421:LEU:HD22	2:C:421:LEU:C	2.21	0.64
2:C:423:PRO:HA	2:C:424:GLU:O	1.94	0.64
2:B:414:TYR:O	2:B:415:GLN:C	2.41	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:K:301:GLY:O	2:K:305:THR:OG1	2.15	0.63
2:B:344:LYS:HA	2:B:346:GLN:HE21	1.63	0.63
1:E:646:ARG:HD3	1:E:648:GLN:CD	2.22	0.63
2:C:298:TYR:N	2:C:412:MET:CE	2.59	0.63
2:C:414:TYR:O	2:C:415:GLN:C	2.42	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
2:B:99:MET:HE3	2:B:105:ARG:HD2	1.80	0.62
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
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
1:D:573:LEU:CD2	1:D:577:TYR:CG	2.83	0.61
1:J:573:LEU:HD13	1:J:573:LEU:C	2.25	0.61
2:K:306:MET:HA	2:K:306:MET:HE2	1.82	0.61
1:A:573:LEU:CD2	1:A:577:TYR:CG	2.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:306:MET:HE2	2:H:306:MET:HA	1.82	0.61
1:A:573:LEU:C	1:A:573:LEU:HD13	2.26	0.61
1:D:573:LEU:C	1:D:573:LEU:HD13	2.26	0.61
1:A:475:SER:HB2	1:A:485:GLU:CG	2.30	0.61
1:E:573:LEU:HD13	1:E:573:LEU:C	2.25	0.61
2:C:414:TYR:CD2	2:C:416:LEU:CD1	2.82	0.61
1:E:516:GLU:OE2	1:E:529:GLN:HB3	2.01	0.61
2:C:426:ASP:C	2:C:427:GLU:OE1	2.44	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:415:GLN:C	2:H:416:LEU:HD12	2.25	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
2:C:416:LEU:C	2:C:417:ASP:OD1	2.45	0.60
1:A:631:MET:HG3	1:A:660:ILE:HD11	1.84	0.60
2:B:426:ASP:C	2:B:427:GLU:OE1	2.44	0.60
1:A:559:ARG:CG	1:A:559:ARG:NH1	2.41	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:B:294:ASP:O	2:B:295:SER:C	2.44	0.59
1:E:478:LYS:HE3	1:E:482:THR:OG1	2.02	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
2:B:416:LEU:C	2:B:417:ASP:OD1	2.46	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: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
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:B:422:ASP:CB	2:B:423:PRO:HD2	2.34	0.58
2:C:47:ASN:C	2:C:47:ASN:ND2	2.59	0.58
1:J:488:ILE:HD12	1:J:525:ILE:O	2.03	0.58
1:E:647:ASP:C	1:E:649:GLY:H	2.04	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:K:426:ASP:C	2:K:427:GLU:OE1	2.47	0.58
2:B:300:PHE:N	2:B:409:GLY:HA2	2.16	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:299:CYS:SG	2:K:412:MET:HE3	2.44	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
2:K:306:MET:HE1	2:K:377:LEU:HD21	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
2:H:416:LEU:O	2:H:417:ASP:C	2.47	0.57
2:H:426:ASP:C	2:H:427:GLU:OE1	2.46	0.57
2:C:415:GLN:C	2:C:416:LEU:CD1	2.77	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
1:A:560:PHE:HZ	1:A:581:MET:CE	2.14	0.57
2:C:423:PRO:CA	2:C:424:GLU:O	2.53	0.57
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
2:C:311:GLU:O	2:C:312:GLY:C	2.48	0.56
1:D:478:LYS:O	1:D:479:ASP:CB	2.49	0.56
1:D:560:PHE:HZ	1:D:581:MET:CE	2.15	0.56
2:B:415:GLN:C	2:B:416:LEU:CD1	2.78	0.56
1:E:572:ILE:CG1	1:E:612:PHE:HB2	2.36	0.56
1:E:634:PHE:CE1	1:E:638:GLN:HG2	2.41	0.56
1:J:538:ASP:C	1:J:540:ASP:H	2.13	0.56
2:K:417:ASP:OD1	2:K:417:ASP:C	2.47	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: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:H:423:PRO:HA	2:H:424:GLU:O	2.03	0.56
2:C:6:GLU:O	2:C:9:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:6:GLU:O	2:B:9:ILE:HG22	2.06	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:134:ALA:HA	2:B:137:LEU:HD12	1.86	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: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
2:H:425:SER:HG	2:H:426:ASP:HA	1.63	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:B:311:GLU:O	2:B:312:GLY:C	2.48	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
1:E:538:ASP:C	1:E:540:ASP:H	2.14	0.54
2:K:418:LEU:H	2:K:418:LEU:HD23	1.60	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:647:ASP:C	1:J:649:GLY:H	2.08	0.54
2:K:311:GLU:O	2:K:312:GLY:C	2.51	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:125:ASP:CG	2:B:126:ASN:H	2.16	0.53
2:B:86:PRO:O	2:B:87:ASP:C	2.50	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
2:C:422:ASP:O	2:C:423:PRO:C	2.51	0.53
1:J:572:ILE:CD1	1:J:612:PHE:CG	2.92	0.53
2:K:5:ALA:C	2:K:7:LYS:H	2.16	0.53
2:C:37:PRO:HD3	2:C:120:SER:HA	1.91	0.53
2:H:421:LEU:O	2:H:422:ASP:CG	2.52	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
2:C:86:PRO:O	2:C:87:ASP:C	2.51	0.53
1:J:513:ILE:HG13	1:J:532:LEU:CD2	2.39	0.53
2:K:421:LEU:O	2:K:422:ASP:CG	2.52	0.53
1:A:633:ARG:HA	1:A:657:VAL:HG22	1.91	0.53
1:E:613:ALA:HA	1:E:617:MET:CE	2.28	0.53
1:A:573:LEU:CD2	1:A:577:TYR:CD1	2.92	0.53
2:H:422:ASP:O	2:H:423:PRO:C	2.51	0.53
2:C:125:ASP:CG	2:C:126:ASN:H	2.17	0.53
2:C:325:MET:HE1	2:C:341:TYR:CB	2.33	0.53
1:E:597:HIS:HB2	1:E:620:ILE:HG23	1.91	0.53
2:K:422:ASP:CB	2:K:423:PRO:HD2	2.39	0.53
2:C:413:ARG:C	2:C:414:TYR:CD1	2.87	0.52
2:B:299:CYS:HA	2:B:300:PHE:HB3	1.91	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
2:K:422:ASP:O	2:K:423:PRO:C	2.51	0.52
1:D:573:LEU:CD2	1:D:577:TYR:CD1	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:LEU:O	2:C:294:ASP:C	2.53	0.52
2:C:294:ASP:CG	2:C:294:ASP:O	2.50	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
2:H:414:TYR:CD2	2:H:414:TYR:C	2.87	0.52
2:H:422:ASP:CB	2:H:423:PRO:HD2	2.40	0.52
2:B:31:MET:HG3	2:B:126:ASN:C	2.35	0.52
2:C:347:GLU:CD	2:C:347:GLU:H	2.18	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
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:47:ASN:C	2:B:47:ASN:ND2	2.59	0.52
2:B:422:ASP:O	2:B:423:PRO:C	2.52	0.52
1:A:647:ASP:C	1:A:649:GLY:H	2.11	0.52
2:H:306:MET:HE1	2:H:377:LEU:HD21	1.92	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:D:633:ARG:HA	1:D:657:VAL:HG22	1.91	0.51
2:B:413:ARG:C	2:B:414:TYR:CD1	2.88	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:298:TYR:N	2:B:412:MET:CE	2.69	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:C:99:MET:HE3	2:C:105:ARG:HB3	1.93	0.51
2:H:414:TYR:CD2	2:H:414:TYR:O	2.64	0.51
2:K:325:MET:HE1	2:K:341:TYR:CB	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:311:GLU:O	2:H:312:GLY:C	2.54	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
1:E:573:LEU:C	1:E:573:LEU:CD1	2.84	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:421:LEU:O	2:C:422:ASP:CG	2.55	0.50
2:B:347:GLU:CD	2:B:347:GLU:H	2.18	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:31:MET:HG3	2:C:126:ASN:C	2.36	0.50
1:D:619:ILE:HG12	1:D:620:ILE:N	2.25	0.50
2:C:91:VAL:O	2:C:110:ASP:HA	2.12	0.50
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
1:D:573:LEU:C	1:D:573:LEU:CD1	2.85	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:H:417:ASP:C	2:H:417:ASP:OD1	2.55	0.50
2:C:417:ASP:O	2:C:418:LEU:C	2.55	0.49
2:B:59:ILE:O	2:B:60:LYS:HB2	2.10	0.49
1:E:538:ASP:C	1:E:540:ASP:N	2.70	0.49
1:E:572:ILE:HG12	1:E:573:LEU:N	2.26	0.49
2:B:300:PHE:H	2:B:409:GLY:HA3	1.73	0.49
1:J:538:ASP:C	1:J:540:ASP:N	2.68	0.49
1:J:573:LEU:C	1:J:573:LEU:CD1	2.85	0.49
1:A:573:LEU:C	1:A:573:LEU:CD1	2.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:425:SER:OG	2:H:426:ASP:CA	2.32	0.49
1:E:646:ARG:HD3	1:E:648:GLN:OE1	2.13	0.49
1:J:584:HIS:C	1:J:586:ALA:H	2.21	0.49
2:C:62:ARG:HB3	2:C:62:ARG:NH1	2.28	0.48
2:B:421:LEU:O	2:B:422:ASP:CG	2.55	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: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
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:B:306:MET:HA	2:B:306:MET:CE	2.41	0.48
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: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
1:J:574:THR:HG22	1:J:612:PHE:HA	1.94	0.48
1:J:613:ALA:HA	1:J:617:MET:CE	2.32	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
2:B:417:ASP:O	2:B:418:LEU:C	2.55	0.48
1:E:589:GLU:O	1:E:589:GLU:HG3	2.12	0.48
2:H:421:LEU:C	2:H:421:LEU:CD2	2.86	0.48
2:B:62:ARG:NH1	2:B:62:ARG:HB3	2.28	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
1:D:647:ASP:C	1:D:649:GLY:H	2.11	0.48
2:B:417:ASP:C	2:B:418:LEU:CD2	2.85	0.48
1:E:613:ALA:CA	1:E:617:MET:HE1	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASP:C	1:A:515:ASP:OD1	2.56	0.47
2:C:70:SER:O	2:C:74:SER:HB2	2.14	0.47
2:C:280:GLU:CD	2:C:392:SER:H	2.23	0.47
2:B:325:MET:HE1	2:B:341:TYR:CB	2.34	0.47
2:H:302:VAL:HG23	2:H:303:VAL:H	1.79	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
1:J:602:THR:O	1:J:603:ASN:C	2.56	0.47
2:K:294:ASP:O	2:K:294:ASP:CG	2.56	0.47
1:E:572:ILE:CD1	1:E:612:PHE:CG	2.95	0.47
1:D:515:ASP:OD1	1:D:515:ASP:C	2.55	0.47
2:H:75:THR:O	2:H:75:THR:HG22	2.14	0.47
2:C:61:SER:O	2:C:62:ARG:C	2.58	0.47
2:C:96:GLU:HB3	2:C:106:LYS:HG3	1.95	0.47
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: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
2:K:421:LEU:C	2:K:421:LEU:CD2	2.86	0.47
1:A:478:LYS:HE2	1:A:482:THR:OG1	2.15	0.47
2:C:306:MET:HA	2:C:306:MET:CE	2.41	0.47
1:D:479:ASP:O	1:D:480:LEU:C	2.58	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:E:646:ARG:HG2	1:E:648:GLN:HG2	1.95	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:61:SER:O	2:B:62:ARG:C	2.58	0.47
2:C:34:LEU:C	2:C:35:ILE:HD12	2.39	0.46
2:C:300:PHE:CD1	2:C:300:PHE:C	2.92	0.46
1:D:517:ALA:O	1:D:518:ASP:HB2	2.15	0.46
2:B:34:LEU:C	2:B:35:ILE:HD12	2.40	0.46
2:B:99:MET:HE3	2:B:105:ARG:HB3	1.96	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:C:421:LEU:C	2:C:421:LEU:CD2	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LEU:O	2:B:20:GLN:HG2	2.15	0.46
2:B:421:LEU:C	2:B:421:LEU:CD2	2.87	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
1:D:572:ILE:HG13	1:D:612:PHE:HD1	1.79	0.46
2:B:280:GLU:CD	2:B:392:SER:H	2.23	0.46
1:E:647:ASP:C	1:E:649:GLY:N	2.67	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
1:A:479:ASP:O	1:A:480:LEU:C	2.58	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
2:K:425:SER:HG	2:K:426:ASP:HA	1.66	0.46
1:A:517:ALA:O	1:A:518:ASP:HB2	2.15	0.46
2:C:297:LYS:HA	2:C:412:MET:HE3	1.96	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:E:602:THR:O	1:E:603:ASN:C	2.59	0.46
1:J:500:LEU:HB2	1:J:550:THR:HG22	1.96	0.46
1:J:647:ASP:C	1:J:649:GLY:N	2.71	0.46
1:J:581:MET:SD	1:J:583:ILE:HG13	2.56	0.46
1:D:647:ASP:C	1:D:649:GLY:N	2.73	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
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
2:B:62:ARG:HB3	2:B:62:ARG:CZ	2.46	0.46
2:B:300:PHE:CD1	2:B:300:PHE:C	2.93	0.46
1:E:641:GLY:HA2	1:E:657:VAL:HG13	1.98	0.46
1:A:537:ASP:OD2	1:A:537:ASP:C	2.59	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
1:D:602:THR:O	1:D:603:ASN:C	2.59	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
2:H:5:ALA:C	2:H:7:LYS:H	2.23	0.46
1:J:561:ILE:O	1:J:658:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:THR:O	1:A:624:GLU:HA	2.16	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
1:D:537:ASP:C	1:D:537:ASP:OD2	2.59	0.45
1:D:613:ALA:HA	1:D:617:MET:CE	2.43	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
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:A:602:THR:O	1:A:603:ASN:C	2.59	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: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
2:B:414:TYR:CD2	2:B:414:TYR:C	2.94	0.45
1:D:474:ALA:HA	1:D:585:THR:OG1	2.16	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: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
1:A:582:HIS:N	1:A:582:HIS:CD2	2.84	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:B:372:LEU:O	2:B:373:LEU:C	2.59	0.45
1:E:584:HIS:C	1:E:586:ALA:H	2.25	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
2:C:372:LEU:O	2:C:373:LEU:C	2.60	0.45
1:J:634:PHE:CB	1:J:656:LYS:HB2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:526:CYS:C	1:J:528:ASP:H	2.24	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:J:581:MET:HE2	1:J:643:PHE:CG	2.53	0.44
1:A:559:ARG:HG2	1:A:624:GLU:HG2	1.98	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
2:H:386:ALA:HB1	2:H:387:ASN:C	2.43	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
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
1:A:484:LEU:HD12	1:A:534:VAL:HG11	2.00	0.44
1:A:584:HIS:HD2	1:A:586:ALA:N	2.16	0.44
2:C:414:TYR:CD2	2:C:414:TYR:C	2.96	0.44
1:D:580:VAL:HG21	1:D:648:GLN:HG3	1.99	0.44
2:B:28:GLY:O	2:B:29:THR:C	2.61	0.44
2:B:291:ILE:HG12	2:B:298:TYR:CD1	2.53	0.44
2:H:294:ASP:O	2:H:294:ASP:CG	2.60	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
1:A:574:THR:O	1:A:575:THR:C	2.61	0.43
2:B:420:MET:HG3	2:B:421:LEU:HD12	1.87	0.43
1:A:580:VAL:HG21	1:A:648:GLN:HG3	2.00	0.43
1:A:602:THR:O	1:A:602:THR:OG1	2.36	0.43
2:C:276:LYS:HD3	2:C:276:LYS:N	2.32	0.43
2:H:300:PHE:CD1	2:H:300:PHE:C	2.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:PHE:HE1	2:B:405:PHE:CE2	2.35	0.43
1:E:584:HIS:C	1:E:586:ALA:N	2.75	0.43
1:E:646:ARG:C	1:E:648:GLN:N	2.76	0.43
1:J:572:ILE:HG12	1:J:573:LEU:H	1.83	0.43
2:C:28:GLY:O	2:C:29:THR:C	2.62	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
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
2:H:298:TYR:CD2	2:H:298:TYR:C	2.95	0.43
1:J:598:LYS:HB3	1:J:598:LYS:HE2	1.78	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
2:B:320:PHE:O	2:B:321:ALA:C	2.61	0.43
2:B:405:PHE:C	2:B:407:GLY:H	2.27	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:584:HIS:C	1:J:586:ALA:N	2.75	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
2:H:320:PHE:HA	2:H:391:VAL:O	2.19	0.43
2:K:298:TYR:C	2:K:299:CYS:SG	3.02	0.43
1:A:488:ILE:HB	1:A:526:CYS:HA	2.00	0.42
2:C:320:PHE:O	2:C:321:ALA:C	2.62	0.42
2:C:417:ASP:C	2:C:418:LEU:CD2	2.85	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:C:405:PHE:C	2:C:407:GLY:H	2.26	0.42
1:E:649:GLY:C	1:E:650:THR:HG22	2.43	0.42
1:J:634:PHE:HE1	1:J:642:ARG:HH11	1.66	0.42
1:D:537:ASP:OD2	1:D:538:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:537:ASP:OD2	1:A:538:ASP:N	2.53	0.42
2:K:320:PHE:HA	2:K:391:VAL:O	2.20	0.42
1:E:526:CYS:C	1:E:528:ASP:H	2.28	0.42
1:A:593:ALA:HB2	1:A:624:GLU:HG3	2.00	0.42
1:A:605:LYS:O	1:A:606:SER:C	2.62	0.42
2:B:287:PHE:CD2	2:B:287:PHE:C	2.97	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:298:TYR:HA	2:C:410:ALA:O	2.20	0.42
2:H:421:LEU:O	2:H:422:ASP:CB	2.66	0.42
1:J:574:THR:O	1:J:575:THR:C	2.63	0.42
2:C:98:ILE:HA	2:C:104:THR:HG22	2.02	0.42
1:J:614:THR:HG22	1:J:617:MET:SD	2.59	0.42
1:A:538:ASP:C	1:A:540:ASP:N	2.78	0.42
2:C:287:PHE:CD2	2:C:287:PHE:C	2.98	0.42
2:C:412:MET:HE3	2:C:412:MET:HB2	1.84	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
1:J:611:MET:HE2	1:J:611:MET:HA	2.02	0.42
2:B:425:SER:HG	2:B:426:ASP:HA	1.71	0.41
1:J:649:GLY:C	1:J:650:THR:HG22	2.44	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
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:574:THR:O	1:E:575:THR:C	2.63	0.41
2:H:315:GLU:O	2:H:387:ASN:HB3	2.20	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
2:B:297:LYS:HA	2:B:412:MET:HE3	2.02	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:J:559:ARG:HB3	1:J:661:LEU:HD12	2.01	0.41
2:K:405:PHE:C	2:K:407:GLY:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ASN:ND2	2:B:420:MET:O	2.54	0.41
2:K:281:LYS:O	2:K:282:LYS:C	2.63	0.41
2:K:300:PHE:CD1	2:K:300:PHE:C	2.99	0.41
1:A:573:LEU:HD22	1:A:577:TYR:CD2	2.56	0.41
1:D:584:HIS:CD2	1:D:585:THR:HG22	2.56	0.41
1:E:609:PRO:O	1:E:610:PRO:C	2.63	0.41
1:E:646:ARG:HG2	1:E:648:GLN:N	2.35	0.41
1:A:600:ASP:HB3	1:A:601:LYS:H	1.60	0.41
1:D:605:LYS:O	1:D:606:SER:C	2.63	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
1:E:515:ASP:OD1	1:E:515:ASP:C	2.62	0.41
1:E:509:GLU:O	1:E:534:VAL:HA	2.21	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: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
2:B:98:ILE:HA	2:B:104:THR:HG22	2.03	0.41
2:K:5:ALA:C	2:K:7:LYS:N	2.79	0.41
2:C:125:ASP:CG	2:C:126:ASN:N	2.79	0.40
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:125:ASP:CG	2:B:126:ASN:N	2.79	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
2:K:417:ASP:C	2:K:418:LEU:HD22	2.33	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
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
1:E:572:ILE:CD1	1:E:612:PHE:CD1	3.04	0.40
2:H:392:SER:OG	2:H:394:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:343:THR:OG1	2:K:344:LYS:N	2.52	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:H:299:CYS:HA	2:H:300:PHE:C	2.45	0.40
2:K:274:ASN:HB2	2:K:278:VAL:HG13	2.04	0.40
2:K:308:ALA:HB2	2:K:412:MET:HE3	2.03	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%)	5	31
1	D	194/201 (96%)	170 (88%)	20 (10%)	4 (2%)	5	31
1	E	194/201 (96%)	164 (84%)	23 (12%)	7 (4%)	2	22
1	J	194/201 (96%)	166 (86%)	23 (12%)	5 (3%)	4	27
2	B	253/441 (57%)	201 (79%)	33 (13%)	19 (8%)	1	9
2	C	253/441 (57%)	203 (80%)	31 (12%)	19 (8%)	1	9
2	H	155/441 (35%)	113 (73%)	30 (19%)	12 (8%)	1	8
2	K	155/441 (35%)	114 (74%)	31 (20%)	10 (6%)	1	11
All	All	1592/2568 (62%)	1301 (82%)	211 (13%)	80 (5%)	1	15

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
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

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Mol	Chain	Res	Type
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
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

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%)	150 (87%)	22 (13%)	4	21
1	D	172/175 (98%)	149 (87%)	23 (13%)	4	20
1	E	172/175 (98%)	142 (83%)	30 (17%)	2	11
1	J	172/175 (98%)	144 (84%)	28 (16%)	2	14
2	B	232/383 (61%)	206 (89%)	26 (11%)	6	25
2	C	232/383 (61%)	208 (90%)	24 (10%)	7	28
2	H	154/383 (40%)	141 (92%)	13 (8%)	10	34
2	K	154/383 (40%)	139 (90%)	15 (10%)	8	30
All	All	1460/2232 (65%)	1279 (88%)	181 (12%)	4	22

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	526	CYS
1	A	543	THR
1	A	558	THR
1	A	559	ARG
1	A	573	LEU
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	611	MET
1	A	619	ILE
1	A	620	ILE
1	A	623	LEU
1	A	629	VAL
1	A	644	THR
1	A	648	GLN
1	A	650	THR
1	A	656	LYS
1	A	657	VAL
1	A	662	ASP
2	C	41	GLN

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Mol	Chain	Res	Type
2	C	47	ASN
2	C	61	SER
2	C	62	ARG
2	C	66	LEU
2	C	74	SER
2	C	118	ASN
2	C	276	LYS
2	C	279	GLN
2	C	297	LYS
2	C	302	VAL
2	C	303	VAL
2	C	318	LEU
2	C	323	LEU
2	C	326	ILE
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
1	D	543	THR
1	D	559	ARG
1	D	569	LEU
1	D	573	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	611	MET
1	D	619	ILE
1	D	620	ILE
1	D	623	LEU
1	D	629	VAL
1	D	644	THR
1	D	648	GLN

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Mol	Chain	Res	Type
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	65	ARG
2	B	66	LEU
2	B	74	SER
2	B	105	ARG
2	B	107	LEU
2	B	118	ASN
2	B	276	LYS
2	B	279	GLN
2	B	297	LYS
2	B	302	VAL
2	B	303	VAL
2	B	323	LEU
2	B	326	ILE
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
2	B	425	SER
1	E	475	SER
1	E	482	THR
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

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Mol	Chain	Res	Type
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	618	LYS
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	293	LEU
2	H	297	LYS
2	H	302	VAL
2	H	303	VAL
2	H	314	VAL
2	H	315	GLU
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
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

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Mol	Chain	Res	Type
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	618	LYS
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	293	LEU
2	K	297	LYS
2	K	302	VAL
2	K	303	VAL
2	K	314	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 (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	ASN
1	A	552	ASN
1	A	555	HIS
1	A	563	GLN
1	A	584	HIS
1	A	597	HIS

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Mol	Chain	Res	Type
2	C	41	GLN
2	C	47	ASN
2	C	88	ASN
2	C	108	ASN
2	C	118	ASN
2	C	121	GLN
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	542	GLN
1	D	555	HIS
1	D	563	GLN
1	D	584	HIS
1	D	597	HIS
2	B	41	GLN
2	B	47	ASN
2	B	88	ASN
2	B	108	ASN
2	B	118	ASN
2	B	121	GLN
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	542	GLN
1	E	555	HIS
1	E	563	GLN
1	E	584	HIS
1	E	597	HIS
2	H	310	GLN
2	H	396	GLN
2	H	400	GLN
1	J	496	ASN
1	J	542	GLN
1	J	555	HIS

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Mol	Chain	Res	Type
1	J	563	GLN
1	J	584	HIS
1	J	597	HIS
2	K	310	GLN
2	K	396	GLN
2	K	400	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.92	0	100 100	69, 77, 80, 82	0
1	D	196/201 (97%)	-0.94	0	100 100	69, 77, 80, 82	0
1	E	196/201 (97%)	-1.08	0	100 100	49, 58, 67, 72	0
1	J	196/201 (97%)	-1.06	0	100 100	49, 58, 67, 72	0
2	B	261/441 (59%)	-0.69	1 (0%)	88 72	66, 79, 83, 83	0
2	C	261/441 (59%)	-0.70	1 (0%)	88 72	66, 79, 83, 83	0
2	H	175/441 (39%)	-0.35	1 (0%)	85 65	66, 83, 116, 122	0
2	K	175/441 (39%)	-0.25	4 (2%)	61 37	66, 83, 118, 138	0
All	All	1656/2568 (64%)	-0.76	7 (0%)	88 72	49, 77, 98, 138	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	340	THR	4.9
2	K	276	LYS	3.2
2	K	130	THR	3.1
2	H	340	THR	2.2
2	K	322	ASP	2.1
2	B	423	PRO	2.1
2	C	315	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.