



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 04:50 PM EDT

PDB ID : 1FSK  
Title : COMPLEX FORMATION BETWEEN A FAB FRAGMENT OF A MONO-CLONAL IGG ANTIBODY AND THE MAJOR ALLERGEN FROM BIRCH POLLEN BET V 1  
Authors : Mirza, O.; Henriksen, A.; Ipsen, H.; Larsen, J.; Wissenbach, M.; Spangfort, M.; Gajhede, M.  
Deposited on : 2000-09-11  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

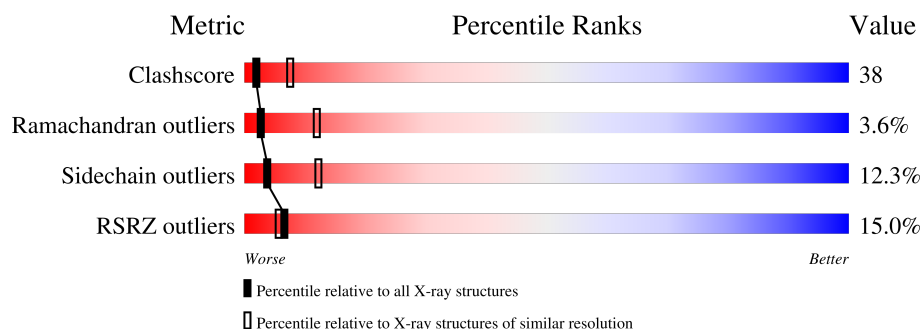
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	159	<div> <div>9%</div> <div>47%</div> <div>46%</div> <div>7%</div> </div>
1	D	159	<div> <div>11%</div> <div>48%</div> <div>45%</div> <div>7%</div> </div>
1	G	159	<div> <div>30%</div> <div>47%</div> <div>47%</div> <div>7%</div> </div>
1	J	159	<div> <div>48%</div> <div>48%</div> <div>45%</div> <div>8%</div> </div>
2	B	214	<div> <div>7%</div> <div>37%</div> <div>54%</div> <div>9%</div> </div>
2	E	214	<div> <div>7%</div> <div>40%</div> <div>51%</div> <div>9%</div> </div>
2	H	214	<div> <div>38%</div> <div>38%</div> <div>52%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	214	<div><div></div><div>15%</div><div>38%</div><div>52%</div><div>10%</div></div>
3	C	220	<div><div></div><div>5%</div><div>45%</div><div>46%</div><div>9%</div></div>
3	F	220	<div><div></div><div>5%</div><div>43%</div><div>48%</div><div>9%</div></div>
3	I	220	<div><div></div><div>10%</div><div>42%</div><div>49%</div><div>9%</div></div>
3	L	220	<div><div></div><div>7%</div><div>43%</div><div>48%</div><div>9%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18308 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 MAJOR POLLEN ALLERGEN BET V 1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1230	783	202	244	1			
1	D	159	Total	C	N	O	S	0	0	0
			1230	783	202	244	1			
1	G	159	Total	C	N	O	S	0	0	0
			1230	783	202	244	1			
1	J	159	Total	C	N	O	S	0	0	0
			1230	783	202	244	1			

- Molecule 2 is a protein called IMMUNOGLOBULIN KAPPA LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1668	1040	277	344	7			
2	E	214	Total	C	N	O	S	0	0	0
			1668	1040	277	344	7			
2	H	214	Total	C	N	O	S	0	0	0
			1668	1040	277	344	7			
2	K	214	Total	C	N	O	S	0	0	0
			1668	1040	277	344	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	LEU	MET	conflict	UNP P01837
B	13	VAL	MET	conflict	UNP P01837
B	22	SER	THR	conflict	UNP P01837
B	30	ASP	VAL	conflict	UNP P01837
B	34	PHE	SER	conflict	UNP P01837
B	36	PHE	TYR	conflict	UNP P01837
B	41	ASP	GLU	conflict	UNP P01837
B	48	LEU	ILE	conflict	UNP P01837

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Chain	Residue	Modelled	Actual	Comment	Reference
B	51	PRO	ALA	conflict	UNP P01837
B	68	THR	ALA	conflict	UNP P01837
B	91	SER	GLY	conflict	UNP P01837
B	149	LYS	ASN	conflict	UNP P01837
E	4	LEU	MET	conflict	UNP P01837
E	13	VAL	MET	conflict	UNP P01837
E	22	SER	THR	conflict	UNP P01837
E	30	ASP	VAL	conflict	UNP P01837
E	34	PHE	SER	conflict	UNP P01837
E	36	PHE	TYR	conflict	UNP P01837
E	41	ASP	GLU	conflict	UNP P01837
E	48	LEU	ILE	conflict	UNP P01837
E	51	PRO	ALA	conflict	UNP P01837
E	68	THR	ALA	conflict	UNP P01837
E	91	SER	GLY	conflict	UNP P01837
E	149	LYS	ASN	conflict	UNP P01837
H	4	LEU	MET	conflict	UNP P01837
H	13	VAL	MET	conflict	UNP P01837
H	22	SER	THR	conflict	UNP P01837
H	30	ASP	VAL	conflict	UNP P01837
H	34	PHE	SER	conflict	UNP P01837
H	36	PHE	TYR	conflict	UNP P01837
H	41	ASP	GLU	conflict	UNP P01837
H	48	LEU	ILE	conflict	UNP P01837
H	51	PRO	ALA	conflict	UNP P01837
H	68	THR	ALA	conflict	UNP P01837
H	91	SER	GLY	conflict	UNP P01837
H	149	LYS	ASN	conflict	UNP P01837
K	4	LEU	MET	conflict	UNP P01837
K	13	VAL	MET	conflict	UNP P01837
K	22	SER	THR	conflict	UNP P01837
K	30	ASP	VAL	conflict	UNP P01837
K	34	PHE	SER	conflict	UNP P01837
K	36	PHE	TYR	conflict	UNP P01837
K	41	ASP	GLU	conflict	UNP P01837
K	48	LEU	ILE	conflict	UNP P01837
K	51	PRO	ALA	conflict	UNP P01837
K	68	THR	ALA	conflict	UNP P01837
K	91	SER	GLY	conflict	UNP P01837
K	149	LYS	ASN	conflict	UNP P01837

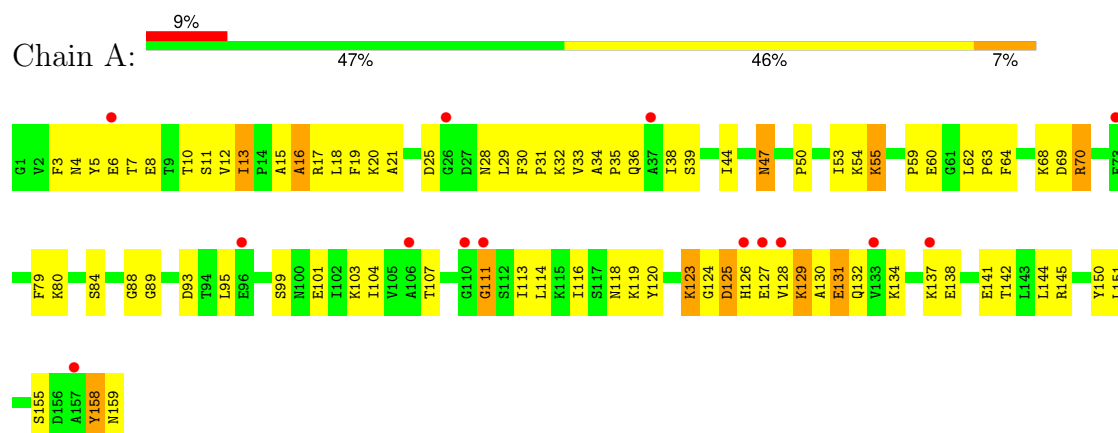
- Molecule 3 is a protein called ANTIBODY HEAVY CHAIN FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total 1679	C 1066	N 276	O 330	S 7	0	0	0
3	F	220	Total 1679	C 1066	N 276	O 330	S 7	0	0	0
3	I	220	Total 1679	C 1066	N 276	O 330	S 7	0	0	0
3	L	220	Total 1679	C 1066	N 276	O 330	S 7	0	0	0

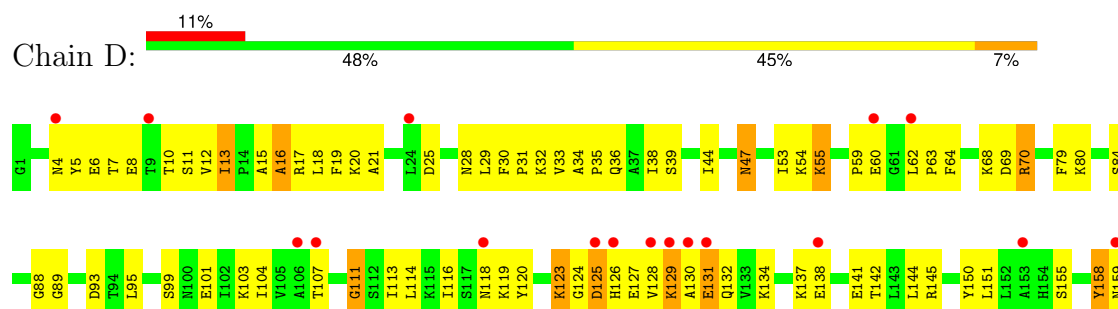
### 3 Residue-property plots [i](#)

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

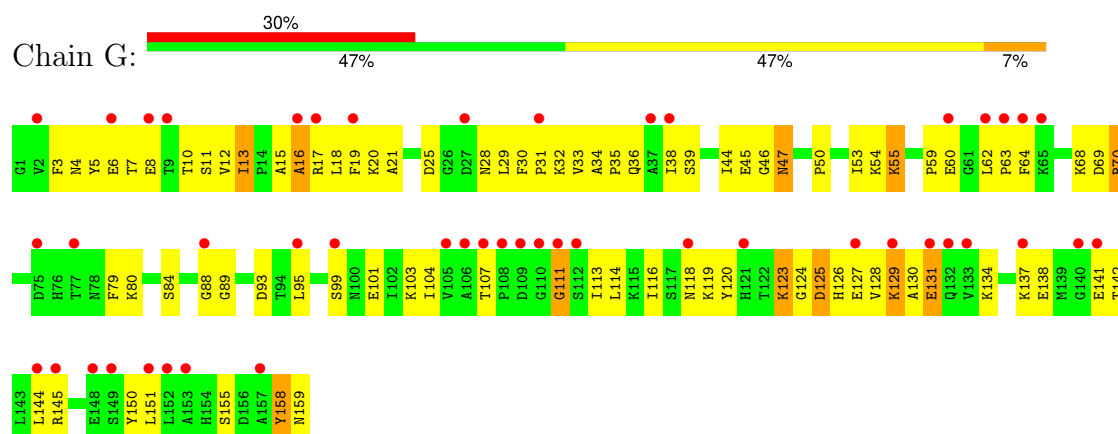
#### • Molecule 1: MAJOR POLLEN ALLERGEN BET V 1-A



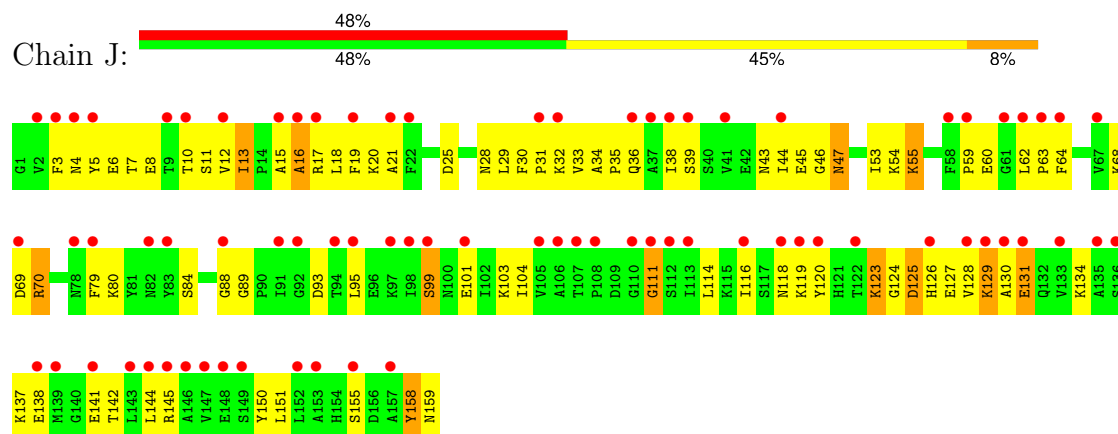
#### • Molecule 1: MAJOR POLLEN ALLERGEN BET V 1-A



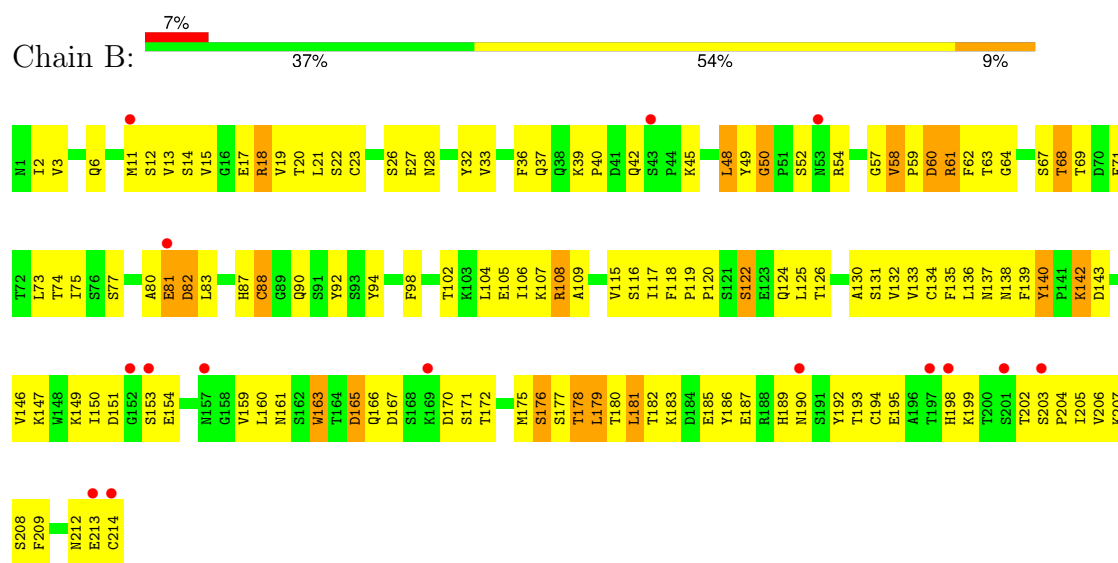
#### • Molecule 1: MAJOR POLLEN ALLERGEN BET V 1-A



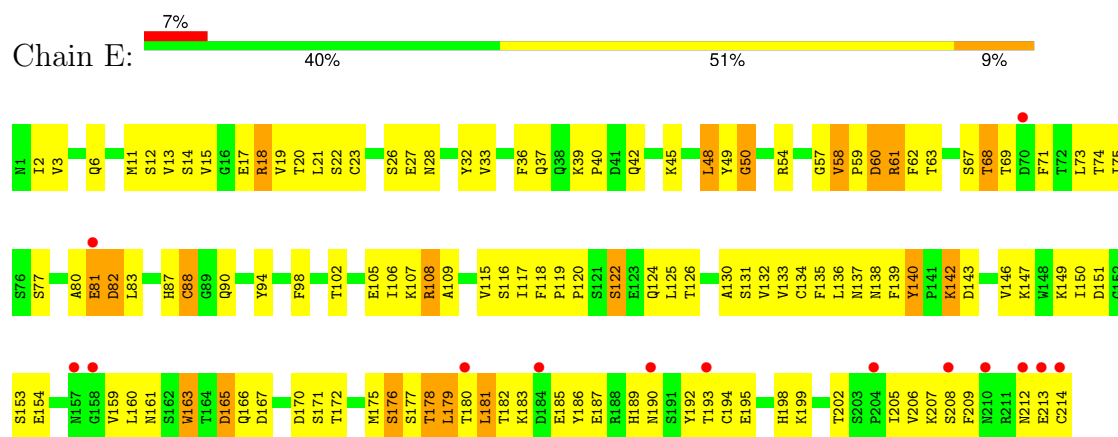
• Molecule 1: MAJOR POLLEN ALLERGEN BET V 1-A



• Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN



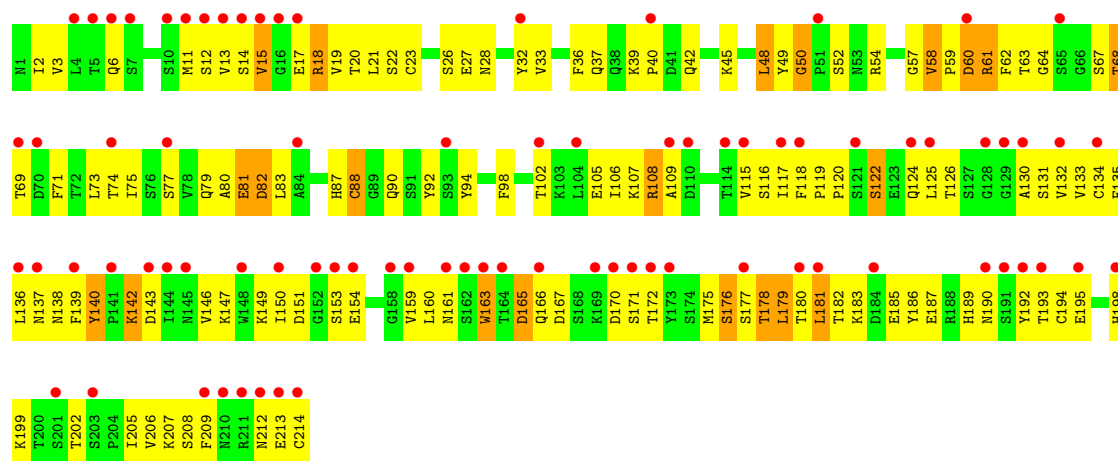
• Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN



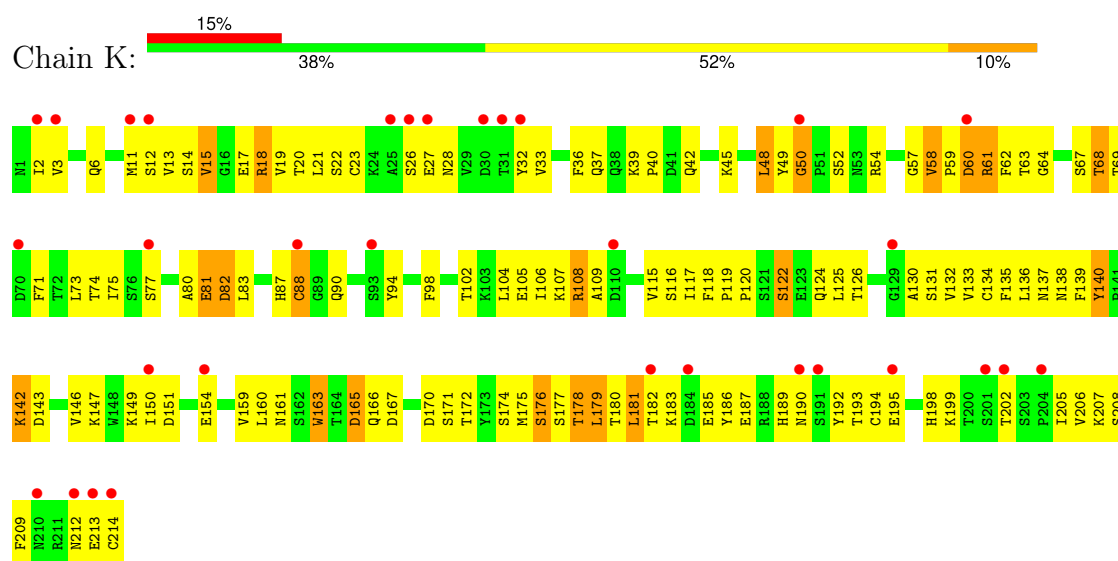
• Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN



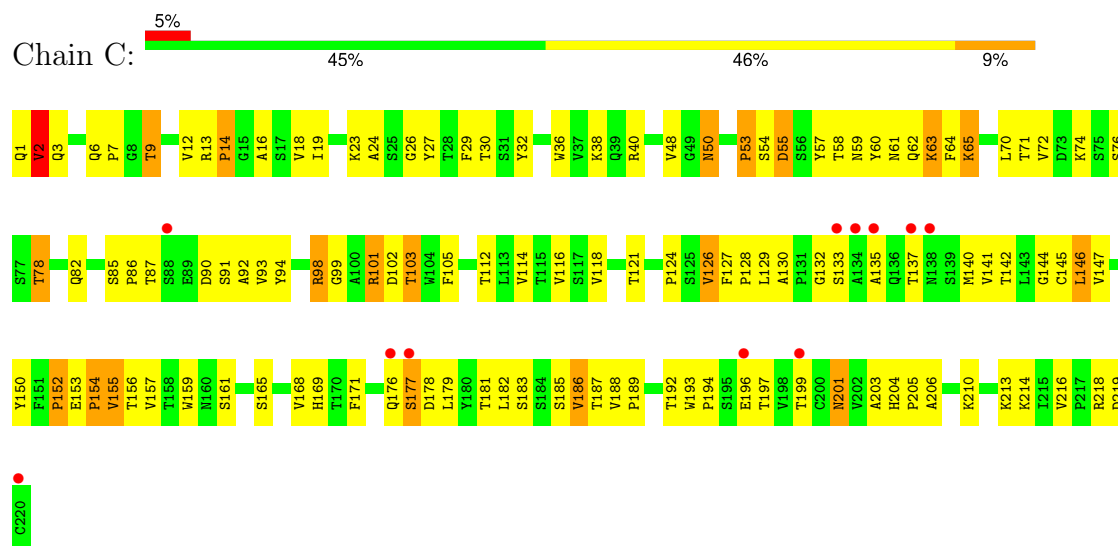




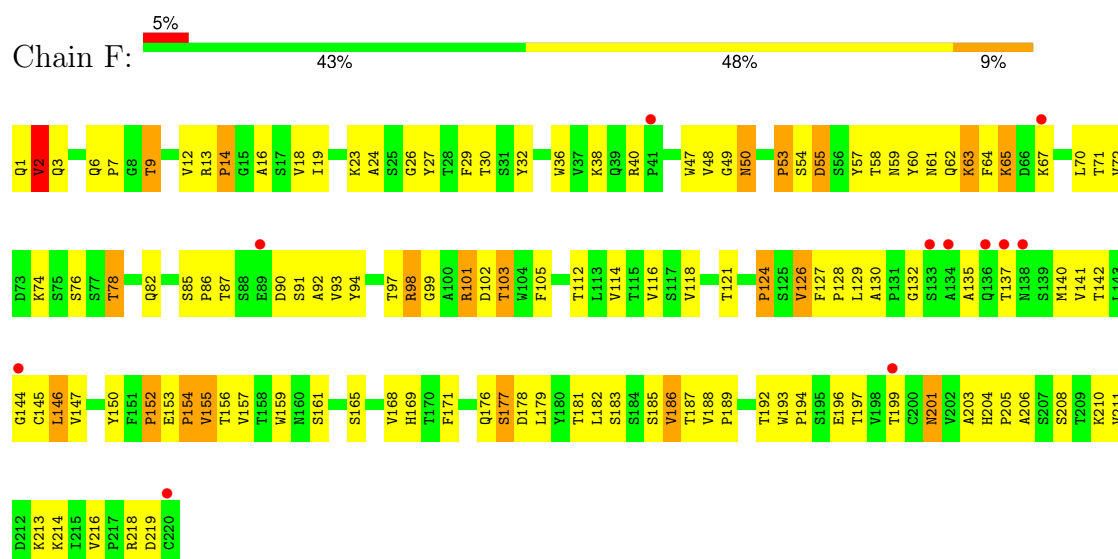
• Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN



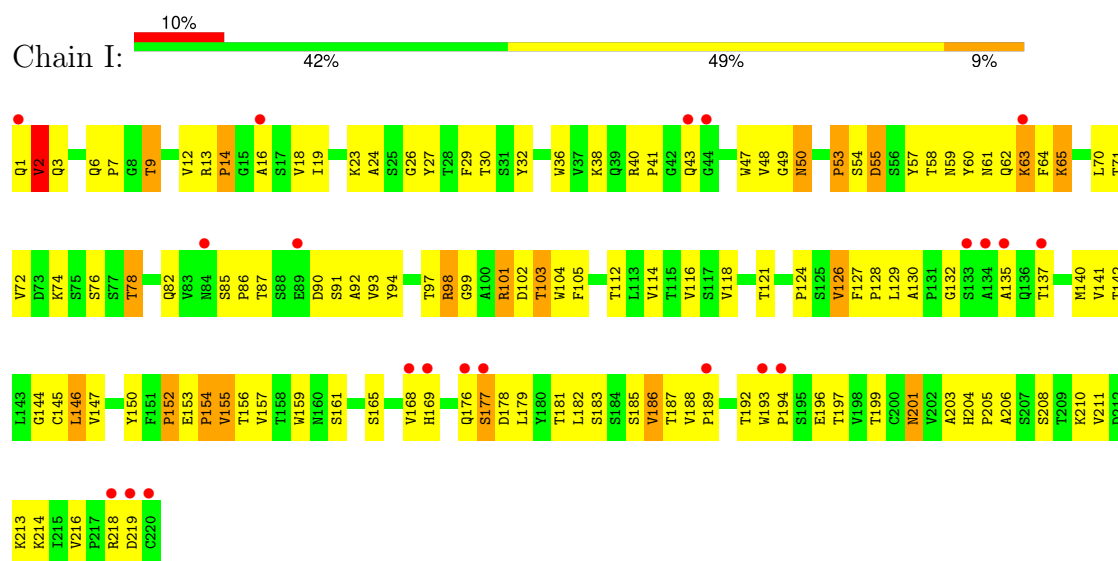
• Molecule 3: ANTIBODY HEAVY CHAIN FAB



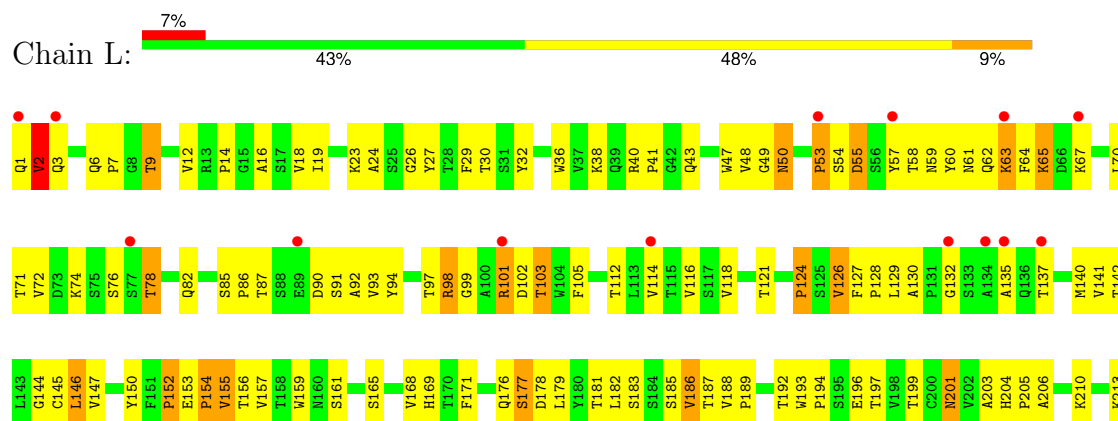
• Molecule 3: ANTIBODY HEAVY CHAIN FAB



• Molecule 3: ANTIBODY HEAVY CHAIN FAB



• Molecule 3: ANTIBODY HEAVY CHAIN FAB



K214
T215
V216
F217
R218
D219
G220

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.65Å 99.14Å 108.91Å 105.70° 98.32° 97.62°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-2.90) 82.6 (20.00-2.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.88Å)	Xtrriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.253 , 0.285 0.267 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtrriage
Anisotropy	0.271	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 77.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	18308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1592e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/1255	0.71	0/1696
1	D	0.51	0/1255	0.71	0/1696
1	G	0.51	0/1255	0.71	0/1696
1	J	0.51	0/1255	0.71	0/1696
2	B	0.51	0/1707	0.78	1/2319 (0.0%)
2	E	0.51	0/1707	0.78	1/2319 (0.0%)
2	H	0.51	0/1707	0.78	1/2319 (0.0%)
2	K	0.52	0/1707	0.78	1/2319 (0.0%)
3	C	0.54	0/1727	0.77	1/2368 (0.0%)
3	F	0.54	0/1727	0.77	1/2368 (0.0%)
3	I	0.54	0/1727	0.77	1/2368 (0.0%)
3	L	0.54	0/1727	0.77	1/2368 (0.0%)
All	All	0.52	0/18756	0.76	8/25532 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	94	TYR	N-CA-C	-6.08	94.59	111.00
2	E	94	TYR	N-CA-C	-5.92	95.02	111.00
2	H	94	TYR	N-CA-C	-5.85	95.20	111.00
2	B	94	TYR	N-CA-C	-5.84	95.23	111.00
3	I	2	VAL	N-CA-C	-5.11	97.20	111.00
3	F	2	VAL	N-CA-C	-5.09	97.25	111.00
3	L	2	VAL	N-CA-C	-5.09	97.25	111.00
3	C	2	VAL	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1230	0	1221	74	0
1	D	1230	0	1221	74	0
1	G	1230	0	1221	80	0
1	J	1230	0	1221	81	0
2	B	1668	0	1592	155	0
2	E	1668	0	1592	156	0
2	H	1668	0	1592	154	0
2	K	1668	0	1592	154	0
3	C	1679	0	1635	114	0
3	F	1679	0	1635	114	0
3	I	1679	0	1635	112	0
3	L	1679	0	1635	125	0
All	All	18308	0	17792	1344	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 38.

All (1344) 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:49:TYR:HB2	3:C:103:THR:HG21	1.26	1.16
2:E:49:TYR:HB2	3:F:103:THR:HG21	1.28	1.09
2:K:49:TYR:HB2	3:L:103:THR:HG21	1.38	1.05
2:H:49:TYR:HB2	3:I:103:THR:HG21	1.34	1.04
2:B:49:TYR:HB2	3:C:103:THR:CG2	1.92	0.99
3:L:50:ASN:HD21	3:L:59:ASN:HB2	1.27	0.98
2:E:49:TYR:HB2	3:F:103:THR:CG2	1.95	0.96
3:F:50:ASN:HD21	3:F:59:ASN:HB2	1.28	0.96
3:I:50:ASN:HD21	3:I:59:ASN:HB2	1.28	0.96
3:C:50:ASN:HD21	3:C:59:ASN:HB2	1.28	0.95
3:L:132:GLY:HA2	3:L:218:ARG:HD3	1.48	0.95
3:F:161:SER:H	3:F:201:ASN:HD21	1.13	0.95
3:L:161:SER:H	3:L:201:ASN:HD21	1.13	0.94
3:F:132:GLY:HA2	3:F:218:ARG:HD3	1.48	0.94
3:C:132:GLY:HA2	3:C:218:ARG:HD3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:132:GLY:HA2	3:I:218:ARG:HD3	1.48	0.93
3:I:161:SER:H	3:I:201:ASN:HD21	1.13	0.93
2:E:134:CYS:HG	2:E:194:CYS:HG	1.03	0.92
2:B:23:CYS:HG	2:B:88:CYS:CB	1.82	0.91
3:F:142:THR:HG22	3:F:187:THR:HG23	1.54	0.89
3:F:76:SER:O	3:F:78:THR:HG22	1.73	0.89
3:C:161:SER:H	3:C:201:ASN:HD21	1.14	0.89
3:I:76:SER:O	3:I:78:THR:HG22	1.72	0.89
3:L:142:THR:HG22	3:L:187:THR:HG23	1.54	0.89
2:B:134:CYS:HG	2:B:194:CYS:HG	0.94	0.89
3:L:76:SER:O	3:L:78:THR:HG22	1.73	0.89
3:I:142:THR:HG22	3:I:187:THR:HG23	1.54	0.88
3:C:142:THR:HG22	3:C:187:THR:HG23	1.54	0.88
3:C:76:SER:O	3:C:78:THR:HG22	1.73	0.88
2:H:49:TYR:HB2	3:I:103:THR:CG2	2.03	0.88
1:A:62:LEU:HB3	1:A:63:PRO:HD2	1.57	0.86
1:J:62:LEU:HB3	1:J:63:PRO:HD2	1.58	0.86
2:K:134:CYS:HG	2:K:194:CYS:HG	0.88	0.86
2:K:49:TYR:HB2	3:L:103:THR:CG2	2.07	0.85
1:G:62:LEU:HB3	1:G:63:PRO:HD2	1.57	0.85
1:D:62:LEU:HB3	1:D:63:PRO:HD2	1.57	0.84
2:H:3:VAL:HG22	2:H:26:SER:HB3	1.59	0.84
2:H:134:CYS:HG	2:H:194:CYS:HG	0.91	0.83
2:K:3:VAL:HG22	2:K:26:SER:HB3	1.59	0.83
2:E:3:VAL:HG22	2:E:26:SER:HB3	1.59	0.83
1:A:119:LYS:H	1:A:119:LYS:HD3	1.44	0.82
3:C:50:ASN:ND2	3:C:59:ASN:HB2	1.93	0.82
2:K:17:GLU:O	2:K:77:SER:HA	1.79	0.82
2:K:147:LYS:HB3	2:K:195:GLU:HB3	1.62	0.82
3:L:50:ASN:ND2	3:L:59:ASN:HB2	1.93	0.82
2:B:3:VAL:HG22	2:B:26:SER:HB3	1.59	0.82
3:I:50:ASN:ND2	3:I:59:ASN:HB2	1.93	0.82
1:G:119:LYS:H	1:G:119:LYS:HD3	1.44	0.82
2:H:17:GLU:O	2:H:77:SER:HA	1.79	0.82
2:E:17:GLU:O	2:E:77:SER:HA	1.80	0.82
2:B:147:LYS:HB3	2:B:195:GLU:HB3	1.62	0.81
2:E:147:LYS:HB3	2:E:195:GLU:HB3	1.62	0.81
3:I:161:SER:N	3:I:201:ASN:HD21	1.79	0.81
3:F:50:ASN:ND2	3:F:59:ASN:HB2	1.93	0.81
1:D:99:SER:HB2	1:D:119:LYS:HE2	1.63	0.81
3:F:161:SER:N	3:F:201:ASN:HD21	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:LYS:HB3	2:H:195:GLU:HB3	1.62	0.81
2:B:17:GLU:O	2:B:77:SER:HA	1.79	0.80
1:D:119:LYS:H	1:D:119:LYS:HD3	1.43	0.80
1:J:119:LYS:H	1:J:119:LYS:HD3	1.44	0.80
1:A:99:SER:HB2	1:A:119:LYS:HE2	1.63	0.80
1:J:99:SER:HB2	1:J:119:LYS:HE2	1.62	0.80
3:L:161:SER:N	3:L:201:ASN:HD21	1.78	0.80
1:G:99:SER:HB2	1:G:119:LYS:HE2	1.62	0.79
2:H:192:TYR:O	2:H:208:SER:HB2	1.83	0.79
3:C:161:SER:N	3:C:201:ASN:HD21	1.79	0.78
2:K:192:TYR:O	2:K:208:SER:HB2	1.83	0.78
2:B:192:TYR:O	2:B:208:SER:HB2	1.84	0.78
3:L:12:VAL:HG22	3:L:16:ALA:HB3	1.65	0.78
3:I:12:VAL:HG22	3:I:16:ALA:HB3	1.65	0.77
2:E:192:TYR:O	2:E:208:SER:HB2	1.83	0.77
3:C:12:VAL:HG22	3:C:16:ALA:HB3	1.66	0.77
2:K:80:ALA:HA	2:K:106:ILE:CD1	2.16	0.76
2:B:49:TYR:CB	3:C:103:THR:HG21	2.13	0.76
2:B:80:ALA:HA	2:B:106:ILE:CD1	2.16	0.76
3:F:12:VAL:HG22	3:F:16:ALA:HB3	1.66	0.76
2:K:133:VAL:HG21	3:L:129:LEU:HD13	1.66	0.76
2:E:83:LEU:HD21	2:E:166:GLN:HB3	1.68	0.75
2:H:83:LEU:HD21	2:H:166:GLN:HB3	1.68	0.75
3:C:178:ASP:O	3:C:179:LEU:HD23	1.86	0.75
2:H:80:ALA:HA	2:H:106:ILE:CD1	2.16	0.75
3:L:178:ASP:O	3:L:179:LEU:HD23	1.86	0.75
3:F:178:ASP:O	3:F:179:LEU:HD23	1.87	0.75
2:E:80:ALA:HA	2:E:106:ILE:CD1	2.16	0.74
3:F:161:SER:H	3:F:201:ASN:ND2	1.84	0.74
3:L:161:SER:H	3:L:201:ASN:ND2	1.84	0.74
3:C:161:SER:H	3:C:201:ASN:ND2	1.85	0.74
1:D:129:LYS:HE3	1:D:129:LYS:HA	1.69	0.74
3:I:50:ASN:HD22	3:I:50:ASN:H	1.35	0.74
1:J:129:LYS:HE3	1:J:129:LYS:HA	1.69	0.74
2:B:83:LEU:HD21	2:B:166:GLN:HB3	1.69	0.74
3:C:50:ASN:H	3:C:50:ASN:HD22	1.35	0.74
3:I:178:ASP:O	3:I:179:LEU:HD23	1.87	0.74
1:A:129:LYS:HE3	1:A:129:LYS:HA	1.69	0.73
1:G:25:ASP:CG	1:G:28:ASN:HD21	1.91	0.73
3:L:50:ASN:HD22	3:L:50:ASN:H	1.35	0.73
2:H:136:LEU:HD12	2:H:136:LEU:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASN:HD21	1:A:6:GLU:HG3	1.54	0.73
2:B:108:ARG:HD3	2:B:109:ALA:O	1.89	0.73
1:D:25:ASP:CG	1:D:28:ASN:HD21	1.91	0.73
2:H:108:ARG:HD3	2:H:109:ALA:O	1.89	0.73
1:J:4:ASN:HD21	1:J:6:GLU:HG3	1.54	0.73
2:K:136:LEU:N	2:K:136:LEU:HD12	2.03	0.73
3:I:161:SER:H	3:I:201:ASN:ND2	1.84	0.73
1:J:25:ASP:CG	1:J:28:ASN:HD21	1.92	0.73
2:E:108:ARG:HD3	2:E:109:ALA:O	1.89	0.72
2:E:136:LEU:HD12	2:E:136:LEU:N	2.03	0.72
1:G:129:LYS:HA	1:G:129:LYS:HE3	1.69	0.72
2:K:83:LEU:HD21	2:K:166:GLN:HB3	1.69	0.72
2:B:136:LEU:N	2:B:136:LEU:HD12	2.03	0.72
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.71	0.72
2:B:134:CYS:CB	2:B:194:CYS:HG	2.02	0.72
1:A:25:ASP:CG	1:A:28:ASN:HD21	1.92	0.72
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.72	0.72
1:D:4:ASN:HD21	1:D:6:GLU:HG3	1.54	0.72
1:A:138:GLU:O	1:A:142:THR:HG23	1.89	0.72
1:D:138:GLU:O	1:D:142:THR:HG23	1.90	0.72
2:H:120:PRO:HD3	2:H:132:VAL:HG22	1.72	0.72
3:F:50:ASN:H	3:F:50:ASN:HD22	1.36	0.71
1:G:4:ASN:HD21	1:G:6:GLU:HG3	1.54	0.71
2:K:108:ARG:HD3	2:K:109:ALA:O	1.88	0.71
1:J:138:GLU:O	1:J:142:THR:HG23	1.89	0.71
2:E:120:PRO:HD3	2:E:132:VAL:HG22	1.72	0.71
1:J:119:LYS:HD3	1:J:119:LYS:N	2.06	0.70
3:C:91:SER:OG	3:C:116:VAL:HG22	1.91	0.70
1:A:119:LYS:HD3	1:A:119:LYS:N	2.06	0.70
1:G:138:GLU:O	1:G:142:THR:HG23	1.90	0.70
1:G:119:LYS:HD3	1:G:119:LYS:N	2.06	0.70
2:E:49:TYR:CB	3:F:103:THR:HG21	2.16	0.69
3:F:91:SER:OG	3:F:116:VAL:HG22	1.91	0.69
3:F:168:VAL:HG12	3:F:186:VAL:HG13	1.73	0.69
1:D:119:LYS:HD3	1:D:119:LYS:N	2.06	0.69
1:J:119:LYS:H	1:J:119:LYS:CD	2.05	0.69
2:H:182:THR:OG1	2:H:185:GLU:HB2	1.93	0.69
3:L:91:SER:OG	3:L:116:VAL:HG22	1.92	0.69
1:D:34:ALA:N	1:D:35:PRO:HD3	2.08	0.69
2:E:23:CYS:HG	2:E:88:CYS:HG	1.29	0.69
2:K:134:CYS:CB	2:K:194:CYS:HG	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:168:VAL:HG12	3:L:186:VAL:HG13	1.73	0.69
2:B:149:LYS:HB2	2:B:193:THR:HG23	1.75	0.69
1:G:34:ALA:N	1:G:35:PRO:HD3	2.08	0.69
3:I:168:VAL:HG12	3:I:186:VAL:HG13	1.73	0.69
3:C:168:VAL:HG12	3:C:186:VAL:HG13	1.73	0.69
3:F:30:THR:HA	3:F:53:PRO:HG2	1.75	0.69
3:I:91:SER:OG	3:I:116:VAL:HG22	1.91	0.69
2:K:182:THR:OG1	2:K:185:GLU:HB2	1.93	0.69
1:A:119:LYS:H	1:A:119:LYS:CD	2.05	0.69
1:D:47:ASN:HD22	1:D:47:ASN:H	1.41	0.69
1:J:30:PHE:HB3	1:J:38:ILE:HD12	1.75	0.69
2:B:182:THR:OG1	2:B:185:GLU:HB2	1.93	0.68
1:D:119:LYS:H	1:D:119:LYS:CD	2.05	0.68
2:E:149:LYS:HB2	2:E:193:THR:HG23	1.75	0.68
3:F:208:SER:HB3	3:I:214:LYS:HB3	1.75	0.68
1:A:34:ALA:N	1:A:35:PRO:HD3	2.08	0.68
1:D:30:PHE:HB3	1:D:38:ILE:HD12	1.76	0.68
2:E:28:ASN:ND2	2:E:68:THR:HA	2.09	0.68
2:K:149:LYS:HB2	2:K:193:THR:HG23	1.75	0.68
1:A:47:ASN:HD22	1:A:47:ASN:H	1.42	0.68
2:B:118:PHE:HB2	2:B:133:VAL:HG22	1.75	0.68
2:E:182:THR:OG1	2:E:185:GLU:HB2	1.93	0.68
1:G:119:LYS:H	1:G:119:LYS:CD	2.05	0.68
3:I:30:THR:HA	3:I:53:PRO:HG2	1.75	0.68
2:B:23:CYS:HG	2:B:88:CYS:HB3	1.57	0.68
2:B:61:ARG:CB	2:B:61:ARG:HH11	2.07	0.68
2:B:80:ALA:HA	2:B:106:ILE:HD13	1.76	0.68
3:C:30:THR:HA	3:C:53:PRO:HG2	1.75	0.68
2:H:149:LYS:HB2	2:H:193:THR:HG23	1.75	0.68
1:A:80:LYS:HE3	1:A:101:GLU:CD	2.14	0.68
2:E:190:ASN:HB3	2:E:212:ASN:ND2	2.09	0.67
3:L:30:THR:HA	3:L:53:PRO:HG2	1.75	0.67
2:E:118:PHE:HB2	2:E:133:VAL:HG22	1.75	0.67
1:G:30:PHE:HB3	1:G:38:ILE:HD12	1.76	0.67
2:H:80:ALA:HA	2:H:106:ILE:HD13	1.76	0.67
2:K:28:ASN:ND2	2:K:68:THR:HA	2.09	0.67
2:K:118:PHE:HB2	2:K:133:VAL:HG22	1.74	0.67
2:B:190:ASN:HB3	2:B:212:ASN:ND2	2.10	0.67
2:E:61:ARG:HH11	2:E:61:ARG:CB	2.07	0.67
2:H:118:PHE:HB2	2:H:133:VAL:HG22	1.75	0.67
2:B:28:ASN:ND2	2:B:68:THR:HA	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:LYS:HE3	1:G:101:GLU:CD	2.15	0.67
2:H:61:ARG:CB	2:H:61:ARG:HH11	2.07	0.67
3:F:205:PRO:HG2	3:F:206:ALA:H	1.60	0.67
1:G:47:ASN:H	1:G:47:ASN:HD22	1.41	0.67
2:H:134:CYS:CB	2:H:194:CYS:HG	2.07	0.67
1:J:80:LYS:HE3	1:J:101:GLU:CD	2.15	0.67
1:A:30:PHE:HB3	1:A:38:ILE:HD12	1.76	0.67
2:K:61:ARG:CB	2:K:61:ARG:HH11	2.08	0.67
2:H:28:ASN:ND2	2:H:68:THR:HA	2.09	0.67
3:I:205:PRO:HG2	3:I:206:ALA:H	1.60	0.67
1:J:34:ALA:N	1:J:35:PRO:HD3	2.08	0.67
2:K:190:ASN:HB3	2:K:212:ASN:ND2	2.09	0.67
3:C:205:PRO:HG2	3:C:206:ALA:H	1.60	0.66
1:D:80:LYS:HE3	1:D:101:GLU:CD	2.15	0.66
2:E:23:CYS:HG	2:E:88:CYS:CB	2.08	0.66
3:L:205:PRO:HG2	3:L:206:ALA:H	1.59	0.66
1:G:131:GLU:HA	1:G:131:GLU:OE1	1.95	0.66
1:J:43:ASN:O	3:L:101:ARG:HA	1.95	0.66
1:J:131:GLU:OE1	1:J:131:GLU:HA	1.95	0.66
2:H:190:ASN:HB3	2:H:212:ASN:ND2	2.10	0.66
2:K:80:ALA:HA	2:K:106:ILE:HD13	1.76	0.66
1:J:47:ASN:H	1:J:47:ASN:HD22	1.41	0.66
1:A:12:VAL:O	1:A:111:GLY:HA2	1.96	0.66
1:A:103:LYS:HD3	1:A:104:ILE:N	2.11	0.66
2:E:206:VAL:O	2:E:207:LYS:HD3	1.96	0.66
1:D:131:GLU:OE1	1:D:131:GLU:HA	1.95	0.65
2:K:206:VAL:O	2:K:207:LYS:HD3	1.96	0.65
1:A:131:GLU:OE1	1:A:131:GLU:HA	1.96	0.65
2:E:80:ALA:HA	2:E:106:ILE:HD13	1.76	0.65
1:J:12:VAL:O	1:J:111:GLY:HA2	1.96	0.65
2:H:206:VAL:O	2:H:207:LYS:HD3	1.96	0.65
2:B:206:VAL:O	2:B:207:LYS:HD3	1.96	0.65
1:D:137:LYS:O	1:D:141:GLU:HB2	1.97	0.65
1:G:137:LYS:O	1:G:141:GLU:HB2	1.96	0.65
1:J:33:VAL:C	1:J:35:PRO:HD3	2.17	0.65
1:J:137:LYS:O	1:J:141:GLU:HB2	1.97	0.65
2:K:36:PHE:HB2	2:K:87:HIS:HB2	1.79	0.65
1:A:33:VAL:C	1:A:35:PRO:HD3	2.17	0.65
1:J:103:LYS:HD3	1:J:104:ILE:N	2.12	0.65
3:C:144:GLY:HA2	3:C:159:TRP:CZ2	2.32	0.65
2:E:23:CYS:CB	2:E:88:CYS:HG	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:144:GLY:HA2	3:L:159:TRP:CZ2	2.32	0.65
1:A:137:LYS:O	1:A:141:GLU:HB2	1.97	0.65
2:E:20:THR:HG23	2:E:74:THR:HG22	1.79	0.65
2:H:36:PHE:HB2	2:H:87:HIS:HB2	1.79	0.65
1:G:7:THR:HG22	1:G:8:GLU:N	2.13	0.64
1:G:33:VAL:C	1:G:35:PRO:HD3	2.17	0.64
1:G:103:LYS:HD3	1:G:104:ILE:N	2.12	0.64
1:J:45:GLU:OE1	3:L:32:TYR:HD1	1.80	0.64
1:D:118:ASN:O	1:D:120:TYR:HD1	1.81	0.64
2:H:12:SER:HA	2:H:105:GLU:O	1.97	0.64
3:F:153:GLU:OE2	3:F:154:PRO:HA	1.97	0.64
3:C:189:PRO:HB2	3:C:192:THR:HG23	1.80	0.64
3:I:144:GLY:HA2	3:I:159:TRP:CZ2	2.32	0.64
2:B:61:ARG:HH11	2:B:61:ARG:HB2	1.63	0.64
1:D:33:VAL:C	1:D:35:PRO:HD3	2.17	0.64
1:D:80:LYS:HE3	1:D:101:GLU:OE2	1.98	0.64
3:L:189:PRO:HB2	3:L:192:THR:HG23	1.80	0.64
2:B:20:THR:HG23	2:B:74:THR:HG22	1.79	0.64
1:D:103:LYS:HD3	1:D:104:ILE:N	2.12	0.64
1:G:118:ASN:O	1:G:120:TYR:HD1	1.81	0.64
2:B:12:SER:HA	2:B:105:GLU:O	1.97	0.63
2:B:36:PHE:HB2	2:B:87:HIS:HB2	1.79	0.63
2:E:61:ARG:HH11	2:E:61:ARG:HB2	1.63	0.63
3:I:189:PRO:HB2	3:I:192:THR:HG23	1.80	0.63
1:D:12:VAL:O	1:D:111:GLY:HA2	1.97	0.63
2:E:12:SER:HA	2:E:105:GLU:O	1.97	0.63
2:H:20:THR:HG23	2:H:74:THR:HG22	1.79	0.63
2:K:12:SER:HA	2:K:105:GLU:O	1.97	0.63
3:F:189:PRO:HB2	3:F:192:THR:HG23	1.80	0.63
2:H:190:ASN:CB	2:H:212:ASN:HD21	2.12	0.63
2:K:190:ASN:CB	2:K:212:ASN:HD21	2.12	0.63
3:I:153:GLU:OE2	3:I:154:PRO:HA	1.98	0.63
1:A:80:LYS:HE3	1:A:101:GLU:OE2	1.98	0.63
2:E:36:PHE:HB2	2:E:87:HIS:HB2	1.79	0.63
1:G:12:VAL:O	1:G:111:GLY:HA2	1.97	0.63
1:J:7:THR:HG22	1:J:8:GLU:N	2.13	0.63
3:L:153:GLU:OE2	3:L:154:PRO:HA	1.97	0.63
3:F:144:GLY:HA2	3:F:159:TRP:CZ2	2.33	0.63
1:G:99:SER:HB2	1:G:119:LYS:CE	2.29	0.63
1:J:118:ASN:O	1:J:120:TYR:HD1	1.81	0.63
3:C:153:GLU:OE2	3:C:154:PRO:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:ILE:HG22	2:H:192:TYR:CE1	2.34	0.63
2:E:190:ASN:CB	2:E:212:ASN:HD21	2.11	0.63
1:G:80:LYS:HE3	1:G:101:GLU:OE2	1.99	0.62
1:A:118:ASN:O	1:A:120:TYR:HD1	1.81	0.62
2:B:150:ILE:HG22	2:B:192:TYR:CE1	2.34	0.62
3:F:50:ASN:HD21	3:F:59:ASN:CB	2.09	0.62
2:K:20:THR:HG23	2:K:74:THR:HG22	1.79	0.62
2:E:150:ILE:HG22	2:E:192:TYR:CE1	2.34	0.62
2:B:2:ILE:HG22	2:B:3:VAL:N	2.13	0.62
2:H:2:ILE:HG22	2:H:3:VAL:N	2.14	0.62
2:K:28:ASN:HA	2:K:68:THR:O	2.00	0.62
1:D:7:THR:HG22	1:D:8:GLU:N	2.13	0.62
2:H:61:ARG:HH11	2:H:61:ARG:HB2	1.63	0.62
1:J:25:ASP:OD1	1:J:28:ASN:ND2	2.32	0.62
3:L:182:LEU:C	3:L:182:LEU:HD12	2.20	0.62
1:A:7:THR:HG22	1:A:8:GLU:N	2.13	0.62
2:K:150:ILE:HG22	2:K:192:TYR:CE1	2.34	0.62
2:E:190:ASN:HB3	2:E:212:ASN:HD21	1.64	0.62
3:F:101:ARG:O	3:F:102:ASP:HB2	1.99	0.62
2:H:18:ARG:HG3	2:H:18:ARG:HH11	1.65	0.62
1:J:11:SER:OG	1:J:13:ILE:HG12	2.00	0.62
2:K:2:ILE:HG22	2:K:3:VAL:N	2.14	0.62
1:A:11:SER:OG	1:A:13:ILE:HG12	1.99	0.62
3:C:144:GLY:HA2	3:C:159:TRP:CH2	2.35	0.62
2:B:190:ASN:HB3	2:B:212:ASN:HD21	1.65	0.62
2:B:28:ASN:HA	2:B:68:THR:O	2.00	0.62
1:D:11:SER:OG	1:D:13:ILE:HG12	1.99	0.62
1:D:99:SER:HB2	1:D:119:LYS:CE	2.29	0.62
1:G:11:SER:OG	1:G:13:ILE:HG12	2.00	0.62
2:B:18:ARG:HG3	2:B:18:ARG:HH11	1.65	0.61
1:D:25:ASP:OD1	1:D:28:ASN:ND2	2.32	0.61
3:I:182:LEU:C	3:I:182:LEU:HD12	2.20	0.61
2:E:195:GLU:OE2	2:E:206:VAL:HG22	1.99	0.61
2:K:174:SER:HG	3:L:169:HIS:CE1	2.18	0.61
1:A:64:PHE:CD1	1:A:89:GLY:HA2	2.36	0.61
3:C:129:LEU:HG	3:C:145:CYS:HA	1.83	0.61
3:C:182:LEU:HD12	3:C:182:LEU:C	2.20	0.61
2:K:119:PRO:HG2	3:L:218:ARG:CZ	2.30	0.61
3:L:101:ARG:O	3:L:102:ASP:HB2	1.99	0.61
1:A:99:SER:HB2	1:A:119:LYS:CE	2.29	0.61
2:E:2:ILE:HG22	2:E:3:VAL:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:PHE:CD1	1:J:89:GLY:HA2	2.36	0.61
2:K:2:ILE:CG2	2:K:3:VAL:N	2.63	0.61
2:K:195:GLU:OE2	2:K:206:VAL:HG22	2.00	0.61
2:E:3:VAL:HG23	2:E:3:VAL:O	2.00	0.61
2:E:18:ARG:HG3	2:E:18:ARG:HH11	1.65	0.61
3:F:182:LEU:C	3:F:182:LEU:HD12	2.20	0.61
1:J:80:LYS:HE3	1:J:101:GLU:OE2	1.99	0.61
2:E:13:VAL:HG11	2:E:19:VAL:HG22	1.83	0.61
2:E:28:ASN:HA	2:E:68:THR:O	2.00	0.61
2:E:186:TYR:CE1	2:E:192:TYR:CE2	2.89	0.61
2:H:190:ASN:HB3	2:H:212:ASN:HD21	1.65	0.61
2:H:195:GLU:OE2	2:H:206:VAL:HG22	1.99	0.61
3:I:9:THR:HG21	3:I:153:GLU:O	2.01	0.61
1:J:99:SER:HB2	1:J:119:LYS:CE	2.29	0.61
2:K:3:VAL:HG23	2:K:3:VAL:O	1.99	0.61
2:K:133:VAL:HG21	3:L:129:LEU:CD1	2.31	0.61
2:H:28:ASN:HA	2:H:68:THR:O	1.99	0.61
2:B:190:ASN:CB	2:B:212:ASN:HD21	2.12	0.61
2:B:195:GLU:OE2	2:B:206:VAL:HG22	2.00	0.61
1:G:64:PHE:CD1	1:G:89:GLY:HA2	2.36	0.61
2:H:2:ILE:CG2	2:H:3:VAL:N	2.63	0.61
2:K:18:ARG:NH1	2:K:18:ARG:HG3	2.16	0.61
2:K:193:THR:HA	2:K:208:SER:HB3	1.83	0.61
1:A:25:ASP:OD1	1:A:28:ASN:ND2	2.32	0.61
3:C:101:ARG:O	3:C:102:ASP:HB2	2.00	0.61
2:H:18:ARG:HG3	2:H:18:ARG:NH1	2.16	0.61
3:L:129:LEU:HG	3:L:145:CYS:HA	1.83	0.61
2:B:3:VAL:HG23	2:B:3:VAL:O	2.00	0.61
2:H:193:THR:HA	2:H:208:SER:CB	2.31	0.61
2:K:61:ARG:HH11	2:K:61:ARG:HB2	1.64	0.61
2:B:2:ILE:CG2	2:B:3:VAL:N	2.63	0.60
2:B:193:THR:HA	2:B:208:SER:HB3	1.83	0.60
3:F:9:THR:HG21	3:F:153:GLU:O	2.01	0.60
3:F:142:THR:HG22	3:F:187:THR:CG2	2.30	0.60
2:H:3:VAL:HG23	2:H:3:VAL:O	2.00	0.60
3:I:101:ARG:O	3:I:102:ASP:HB2	1.99	0.60
3:L:127:PHE:HB2	3:L:146:LEU:CD2	2.32	0.60
3:C:27:TYR:HE2	3:C:32:TYR:HB2	1.66	0.60
2:K:106:ILE:O	2:K:166:GLN:NE2	2.35	0.60
2:B:186:TYR:CE1	2:B:192:TYR:CE2	2.89	0.60
3:F:85:SER:N	3:F:86:PRO:HD3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ARG:HG3	2:B:18:ARG:NH1	2.16	0.60
1:D:64:PHE:CD1	1:D:89:GLY:HA2	2.36	0.60
3:F:127:PHE:HB2	3:F:146:LEU:CD2	2.32	0.60
2:H:49:TYR:CB	3:I:103:THR:HG21	2.22	0.60
2:K:186:TYR:CE1	2:K:192:TYR:CE2	2.90	0.60
2:K:190:ASN:HB3	2:K:212:ASN:HD21	1.65	0.60
3:L:144:GLY:HA2	3:L:159:TRP:CH2	2.36	0.60
2:B:193:THR:HA	2:B:208:SER:CB	2.31	0.60
2:E:2:ILE:CG2	2:E:3:VAL:N	2.64	0.60
2:E:136:LEU:HD21	2:E:146:VAL:HG22	1.83	0.60
3:F:27:TYR:HE2	3:F:32:TYR:HB2	1.67	0.60
3:I:129:LEU:HG	3:I:145:CYS:HA	1.83	0.60
2:K:18:ARG:HG3	2:K:18:ARG:HH11	1.65	0.60
3:L:27:TYR:HE2	3:L:32:TYR:HB2	1.67	0.60
1:G:25:ASP:OD1	1:G:28:ASN:ND2	2.32	0.60
3:I:144:GLY:HA2	3:I:159:TRP:CH2	2.36	0.60
2:K:193:THR:HA	2:K:208:SER:CB	2.31	0.60
3:L:124:PRO:HB2	3:L:147:VAL:HG13	1.84	0.60
3:C:124:PRO:HB2	3:C:147:VAL:HG13	1.84	0.60
2:H:23:CYS:HG	2:H:88:CYS:CB	2.14	0.60
2:H:108:ARG:O	2:H:140:TYR:HE2	1.85	0.60
2:H:193:THR:HA	2:H:208:SER:HB3	1.83	0.60
3:I:127:PHE:HB2	3:I:146:LEU:CD2	2.32	0.60
2:E:193:THR:HA	2:E:208:SER:CB	2.31	0.60
2:H:186:TYR:CE1	2:H:192:TYR:CE2	2.89	0.60
2:K:13:VAL:HG11	2:K:19:VAL:HG22	1.83	0.60
3:L:50:ASN:HD21	3:L:59:ASN:CB	2.09	0.60
3:L:142:THR:HG22	3:L:187:THR:CG2	2.31	0.60
2:E:106:ILE:O	2:E:166:GLN:NE2	2.34	0.60
2:E:193:THR:HA	2:E:208:SER:HB3	1.83	0.60
3:F:129:LEU:HG	3:F:145:CYS:HA	1.83	0.60
3:I:85:SER:N	3:I:86:PRO:HD3	2.16	0.60
1:J:44:ILE:HB	1:J:53:ILE:HG22	1.82	0.60
2:B:48:LEU:HD22	2:B:73:LEU:HD13	1.84	0.59
3:C:129:LEU:HB2	3:C:144:GLY:O	2.02	0.59
3:I:27:TYR:HE2	3:I:32:TYR:HB2	1.67	0.59
3:C:9:THR:HG21	3:C:153:GLU:O	2.01	0.59
3:C:40:ARG:HG3	3:C:92:ALA:HB2	1.84	0.59
1:D:44:ILE:HB	1:D:53:ILE:HG22	1.84	0.59
3:F:144:GLY:HA2	3:F:159:TRP:CH2	2.36	0.59
2:H:106:ILE:O	2:H:166:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:108:ARG:O	2:K:140:TYR:HE2	1.85	0.59
2:E:18:ARG:HG3	2:E:18:ARG:NH1	2.16	0.59
3:I:124:PRO:HB2	3:I:147:VAL:HG13	1.84	0.59
3:I:129:LEU:HB2	3:I:144:GLY:O	2.02	0.59
1:J:46:GLY:O	3:L:102:ASP:HA	2.02	0.59
2:B:13:VAL:HG11	2:B:19:VAL:HG22	1.83	0.59
3:C:85:SER:N	3:C:86:PRO:HD3	2.16	0.59
2:E:108:ARG:O	2:E:140:TYR:HE2	1.85	0.59
2:H:13:VAL:HG11	2:H:19:VAL:HG22	1.83	0.59
3:I:40:ARG:HG3	3:I:92:ALA:HB2	1.84	0.59
2:K:136:LEU:HD21	2:K:146:VAL:HG22	1.83	0.59
3:L:40:ARG:HG3	3:L:92:ALA:HB2	1.84	0.59
2:B:106:ILE:O	2:B:166:GLN:NE2	2.34	0.59
3:C:127:PHE:HB2	3:C:146:LEU:CD2	2.32	0.59
2:E:165:ASP:O	2:E:166:GLN:C	2.41	0.59
3:L:129:LEU:HB2	3:L:144:GLY:O	2.03	0.59
3:F:40:ARG:HG3	3:F:92:ALA:HB2	1.84	0.59
1:G:44:ILE:HB	1:G:53:ILE:HG22	1.83	0.59
2:H:48:LEU:HD22	2:H:73:LEU:HD13	1.85	0.59
2:H:136:LEU:HD21	2:H:146:VAL:HG22	1.84	0.59
3:L:58:THR:HG1	3:L:60:TYR:HE2	1.51	0.59
3:L:85:SER:N	3:L:86:PRO:HD3	2.16	0.59
3:C:142:THR:HG22	3:C:187:THR:CG2	2.31	0.59
1:D:47:ASN:HD22	1:D:47:ASN:N	1.98	0.59
2:E:48:LEU:HD22	2:E:73:LEU:HD13	1.84	0.59
3:C:50:ASN:HD21	3:C:59:ASN:CB	2.09	0.59
3:I:142:THR:HG22	3:I:187:THR:CG2	2.31	0.59
2:K:165:ASP:O	2:K:166:GLN:C	2.41	0.59
3:L:9:THR:HG21	3:L:153:GLU:O	2.02	0.59
1:A:44:ILE:HB	1:A:53:ILE:HG22	1.84	0.58
1:J:45:GLU:HB2	3:L:32:TYR:CE1	2.37	0.58
2:B:136:LEU:HD21	2:B:146:VAL:HG22	1.84	0.58
2:H:81:GLU:OE1	2:H:81:GLU:N	2.37	0.58
1:A:13:ILE:HG21	1:A:151:LEU:HD13	1.86	0.58
2:B:108:ARG:O	2:B:140:TYR:HE2	1.85	0.58
2:E:81:GLU:N	2:E:81:GLU:OE1	2.37	0.58
2:H:165:ASP:O	2:H:166:GLN:C	2.41	0.58
2:K:48:LEU:HD22	2:K:73:LEU:HD13	1.84	0.58
3:F:159:TRP:CE2	3:F:186:VAL:HG22	2.39	0.58
1:J:5:TYR:HE2	1:J:128:VAL:HG11	1.69	0.58
3:F:50:ASN:HD22	3:F:50:ASN:N	1.97	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:124:PRO:HB2	3:F:147:VAL:HG13	1.84	0.58
1:J:47:ASN:HD22	1:J:47:ASN:N	1.99	0.58
1:G:13:ILE:HG21	1:G:151:LEU:HD13	1.85	0.58
1:A:129:LYS:O	1:A:131:GLU:N	2.37	0.58
2:B:81:GLU:N	2:B:81:GLU:OE1	2.37	0.58
1:J:129:LYS:O	1:J:131:GLU:N	2.37	0.58
3:F:129:LEU:HB2	3:F:144:GLY:O	2.03	0.57
3:L:159:TRP:CE2	3:L:186:VAL:HG22	2.39	0.57
1:D:5:TYR:HE2	1:D:128:VAL:HG11	1.69	0.57
3:I:159:TRP:CE2	3:I:186:VAL:HG22	2.39	0.57
3:L:18:VAL:C	3:L:19:ILE:HD12	2.25	0.57
1:G:129:LYS:O	1:G:131:GLU:N	2.37	0.57
1:A:5:TYR:HE2	1:A:128:VAL:HG11	1.69	0.57
2:B:67:SER:O	2:B:68:THR:HB	2.04	0.57
2:E:133:VAL:HG21	3:F:129:LEU:HD13	1.86	0.57
2:K:81:GLU:C	2:K:83:LEU:H	2.08	0.57
1:A:20:LYS:NZ	1:A:159:ASN:HD22	2.03	0.57
2:B:81:GLU:C	2:B:83:LEU:H	2.08	0.57
2:B:165:ASP:O	2:B:166:GLN:C	2.41	0.57
3:C:159:TRP:CE2	3:C:186:VAL:HG22	2.39	0.57
3:I:50:ASN:HD21	3:I:59:ASN:CB	2.09	0.57
1:D:129:LYS:O	1:D:131:GLU:N	2.37	0.57
2:E:67:SER:O	2:E:68:THR:HB	2.05	0.57
2:H:67:SER:O	2:H:68:THR:HB	2.05	0.57
3:C:58:THR:HG1	3:C:60:TYR:HE2	1.52	0.57
3:C:205:PRO:HG2	3:C:206:ALA:N	2.20	0.57
2:E:3:VAL:HG22	2:E:26:SER:CB	2.33	0.57
1:J:13:ILE:HG21	1:J:151:LEU:HD13	1.85	0.57
2:K:81:GLU:N	2:K:81:GLU:OE1	2.37	0.57
3:C:91:SER:HA	3:C:114:VAL:HG23	1.87	0.57
3:F:23:LYS:HA	3:F:78:THR:HB	1.86	0.57
1:G:5:TYR:HE2	1:G:128:VAL:HG11	1.69	0.57
1:D:13:ILE:HG21	1:D:151:LEU:HD13	1.85	0.57
1:G:20:LYS:NZ	1:G:159:ASN:HD22	2.03	0.57
2:K:67:SER:O	2:K:68:THR:HB	2.05	0.57
1:D:118:ASN:O	1:D:120:TYR:CD1	2.57	0.57
2:E:23:CYS:SG	2:E:88:CYS:CB	2.93	0.57
3:I:23:LYS:HA	3:I:78:THR:HB	1.87	0.57
3:L:23:LYS:HA	3:L:78:THR:HB	1.87	0.57
1:J:20:LYS:NZ	1:J:159:ASN:HD22	2.02	0.56
2:K:21:LEU:HD12	2:K:102:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:133:VAL:CG2	3:L:129:LEU:HD13	2.35	0.56
2:B:175:MET:HG2	2:B:176:SER:N	2.21	0.56
1:A:118:ASN:O	1:A:120:TYR:CD1	2.58	0.56
1:D:20:LYS:NZ	1:D:159:ASN:HD22	2.03	0.56
3:F:18:VAL:C	3:F:19:ILE:HD12	2.25	0.56
2:H:149:LYS:O	2:H:193:THR:HG22	2.06	0.56
3:L:205:PRO:HG2	3:L:206:ALA:N	2.20	0.56
3:C:18:VAL:C	3:C:19:ILE:HD12	2.25	0.56
3:F:91:SER:HA	3:F:114:VAL:HG23	1.87	0.56
1:G:123:LYS:HA	1:G:123:LYS:HE2	1.87	0.56
3:I:91:SER:HA	3:I:114:VAL:HG23	1.87	0.56
2:K:23:CYS:SG	2:K:88:CYS:CB	2.94	0.56
1:G:47:ASN:H	1:G:47:ASN:ND2	2.03	0.56
1:G:118:ASN:O	1:G:120:TYR:CD1	2.58	0.56
1:J:118:ASN:O	1:J:120:TYR:CD1	2.57	0.56
2:K:175:MET:HG2	2:K:176:SER:N	2.20	0.56
2:B:147:LYS:HB3	2:B:195:GLU:CB	2.35	0.56
2:E:48:LEU:HD12	2:E:54:ARG:HA	1.88	0.56
3:I:18:VAL:C	3:I:19:ILE:HD12	2.25	0.56
1:J:47:ASN:H	1:J:47:ASN:ND2	2.04	0.56
3:L:91:SER:HA	3:L:114:VAL:HG23	1.87	0.56
1:D:47:ASN:H	1:D:47:ASN:ND2	2.04	0.56
1:G:47:ASN:HD22	1:G:47:ASN:N	1.98	0.56
3:I:205:PRO:HG2	3:I:206:ALA:N	2.20	0.56
1:A:47:ASN:H	1:A:47:ASN:ND2	2.04	0.56
3:C:50:ASN:HD22	3:C:50:ASN:N	1.97	0.56
2:E:21:LEU:HD12	2:E:102:THR:HG21	1.87	0.56
2:H:23:CYS:SG	2:H:88:CYS:CB	2.94	0.56
2:H:81:GLU:C	2:H:83:LEU:H	2.08	0.56
2:E:108:ARG:HG3	2:E:140:TYR:CE2	2.41	0.56
2:E:175:MET:HG2	2:E:176:SER:N	2.21	0.56
2:H:108:ARG:HG3	2:H:140:TYR:CE2	2.41	0.56
2:H:175:MET:HG2	2:H:176:SER:N	2.21	0.56
2:K:108:ARG:HG3	2:K:140:TYR:CE2	2.41	0.56
2:B:108:ARG:HG3	2:B:140:TYR:CE2	2.41	0.55
2:H:21:LEU:HD12	2:H:102:THR:HG21	1.87	0.55
2:H:48:LEU:HD12	2:H:54:ARG:HA	1.88	0.55
2:K:115:VAL:HA	2:K:135:PHE:O	2.07	0.55
1:D:123:LYS:HA	1:D:123:LYS:HE2	1.87	0.55
2:E:81:GLU:C	2:E:83:LEU:H	2.08	0.55
2:E:149:LYS:O	2:E:193:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1:GLN:HG2	3:I:26:GLY:HA3	1.88	0.55
3:L:50:ASN:HD22	3:L:50:ASN:N	1.98	0.55
2:B:3:VAL:HG22	2:B:26:SER:CB	2.33	0.55
2:E:147:LYS:HB3	2:E:195:GLU:CB	2.35	0.55
3:F:205:PRO:HG2	3:F:206:ALA:N	2.20	0.55
3:I:93:VAL:HA	3:I:112:THR:O	2.07	0.55
1:A:123:LYS:HE2	1:A:123:LYS:HA	1.87	0.55
2:B:48:LEU:HD12	2:B:54:ARG:HA	1.88	0.55
2:E:115:VAL:HA	2:E:135:PHE:O	2.06	0.55
2:H:115:VAL:HA	2:H:135:PHE:O	2.07	0.55
2:K:48:LEU:HD12	2:K:54:ARG:HA	1.88	0.55
2:B:115:VAL:HA	2:B:135:PHE:O	2.07	0.55
3:F:1:GLN:HG2	3:F:26:GLY:HA3	1.88	0.55
1:J:123:LYS:HE2	1:J:123:LYS:HA	1.87	0.55
3:L:1:GLN:HG2	3:L:26:GLY:HA3	1.88	0.55
2:B:149:LYS:O	2:B:193:THR:HG22	2.06	0.55
2:E:122:SER:HA	2:E:125:LEU:HD12	1.89	0.55
3:C:192:THR:O	3:C:196:GLU:HB2	2.07	0.55
3:L:192:THR:O	3:L:196:GLU:HB2	2.07	0.55
1:A:59:PRO:O	1:A:62:LEU:HD13	2.07	0.55
2:E:39:LYS:HB3	2:E:40:PRO:HD2	1.89	0.55
2:K:149:LYS:O	2:K:193:THR:HG22	2.06	0.55
3:C:23:LYS:HA	3:C:78:THR:HB	1.87	0.54
1:D:59:PRO:O	1:D:62:LEU:HD13	2.07	0.54
3:F:161:SER:N	3:F:201:ASN:ND2	2.51	0.54
3:I:1:GLN:CG	3:I:2:VAL:N	2.70	0.54
1:G:131:GLU:O	1:G:134:LYS:HB3	2.07	0.54
1:A:131:GLU:O	1:A:134:LYS:HB3	2.06	0.54
2:B:39:LYS:HB3	2:B:40:PRO:HD2	1.88	0.54
3:F:168:VAL:O	3:F:169:HIS:HD2	1.91	0.54
3:F:192:THR:O	3:F:196:GLU:HB2	2.07	0.54
2:H:39:LYS:HB3	2:H:40:PRO:HD2	1.89	0.54
2:H:122:SER:HA	2:H:125:LEU:HD12	1.89	0.54
1:J:45:GLU:OE1	3:L:32:TYR:CD1	2.61	0.54
2:B:21:LEU:HD12	2:B:102:THR:HG21	1.88	0.54
3:C:93:VAL:HA	3:C:112:THR:O	2.07	0.54
1:J:131:GLU:O	1:J:134:LYS:HB3	2.07	0.54
3:C:1:GLN:HG2	3:C:26:GLY:HA3	1.88	0.54
2:K:122:SER:HA	2:K:125:LEU:HD12	1.89	0.54
3:L:1:GLN:CG	3:L:2:VAL:N	2.71	0.54
1:D:131:GLU:O	1:D:134:LYS:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:93:VAL:HA	3:F:112:THR:O	2.07	0.54
2:B:122:SER:HA	2:B:125:LEU:HD12	1.89	0.54
2:E:61:ARG:HB2	2:E:61:ARG:NH1	2.23	0.54
1:G:129:LYS:C	1:G:131:GLU:N	2.61	0.54
1:J:129:LYS:C	1:J:131:GLU:N	2.61	0.54
2:H:149:LYS:HB2	2:H:193:THR:CG2	2.38	0.54
2:K:3:VAL:HG22	2:K:26:SER:CB	2.33	0.54
2:K:149:LYS:HB2	2:K:193:THR:CG2	2.38	0.54
2:B:23:CYS:SG	2:B:88:CYS:CB	2.93	0.54
3:F:16:ALA:O	3:F:86:PRO:CD	2.56	0.54
2:H:79:GLN:NE2	1:J:3:PHE:CE1	2.76	0.54
1:J:59:PRO:O	1:J:62:LEU:HD13	2.07	0.54
2:K:147:LYS:HB3	2:K:195:GLU:CB	2.35	0.54
3:L:16:ALA:O	3:L:86:PRO:CD	2.56	0.54
3:L:93:VAL:HA	3:L:112:THR:O	2.08	0.54
1:A:47:ASN:HD22	1:A:47:ASN:N	1.99	0.53
2:E:32:TYR:O	2:E:90:GLN:HA	2.09	0.53
3:C:16:ALA:O	3:C:86:PRO:CD	2.57	0.53
3:C:168:VAL:O	3:C:169:HIS:HD2	1.91	0.53
2:H:32:TYR:O	2:H:90:GLN:HA	2.08	0.53
2:H:147:LYS:HB3	2:H:195:GLU:CB	2.35	0.53
3:I:193:TRP:CD1	3:I:194:PRO:HA	2.44	0.53
1:A:129:LYS:C	1:A:131:GLU:N	2.61	0.53
2:B:68:THR:HG22	2:B:69:THR:N	2.23	0.53
3:F:58:THR:HG1	3:F:60:TYR:HE2	1.57	0.53
1:G:59:PRO:O	1:G:62:LEU:HD13	2.08	0.53
3:I:16:ALA:O	3:I:86:PRO:CD	2.56	0.53
3:I:192:THR:O	3:I:196:GLU:HB2	2.07	0.53
2:K:39:LYS:HB3	2:K:40:PRO:HD2	1.88	0.53
2:K:136:LEU:HD21	2:K:146:VAL:CG2	2.39	0.53
2:E:68:THR:HG22	2:E:69:THR:N	2.23	0.53
3:F:193:TRP:CD1	3:F:194:PRO:HA	2.44	0.53
2:H:3:VAL:HG22	2:H:26:SER:CB	2.33	0.53
2:H:61:ARG:HB2	2:H:61:ARG:NH1	2.23	0.53
2:H:198:HIS:C	2:H:199:LYS:HG3	2.29	0.53
3:C:1:GLN:CG	3:C:2:VAL:N	2.71	0.53
1:D:62:LEU:HB3	1:D:63:PRO:CD	2.35	0.53
3:F:1:GLN:CG	3:F:2:VAL:N	2.71	0.53
2:B:198:HIS:C	2:B:199:LYS:HG3	2.29	0.53
2:E:23:CYS:HG	2:E:88:CYS:HB3	1.73	0.53
2:E:149:LYS:HB2	2:E:193:THR:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:170:ASP:CG	2:H:172:THR:HG23	2.30	0.53
3:L:193:TRP:CD1	3:L:194:PRO:HA	2.44	0.53
3:C:12:VAL:HG11	3:C:18:VAL:CG2	2.39	0.53
3:I:168:VAL:O	3:I:169:HIS:HD2	1.91	0.53
1:D:129:LYS:C	1:D:131:GLU:N	2.61	0.53
2:H:68:THR:HG22	2:H:69:THR:N	2.23	0.53
1:J:70:ARG:O	1:J:70:ARG:HG2	2.08	0.53
2:K:32:TYR:O	2:K:90:GLN:HA	2.08	0.53
2:B:61:ARG:HB2	2:B:61:ARG:NH1	2.23	0.52
2:B:170:ASP:CG	2:B:172:THR:HG23	2.30	0.52
3:C:193:TRP:CD1	3:C:194:PRO:HA	2.44	0.52
2:E:21:LEU:HD12	2:E:102:THR:CG2	2.39	0.52
3:F:12:VAL:HG11	3:F:18:VAL:CG2	2.39	0.52
2:K:21:LEU:HD12	2:K:102:THR:CG2	2.39	0.52
2:K:170:ASP:OD2	2:K:172:THR:HG23	2.09	0.52
2:B:32:TYR:O	2:B:90:GLN:HA	2.08	0.52
2:E:124:GLN:HE22	2:E:131:SER:CB	2.22	0.52
2:H:21:LEU:HD12	2:H:102:THR:CG2	2.40	0.52
2:K:198:HIS:C	2:K:199:LYS:HG3	2.29	0.52
3:L:168:VAL:O	3:L:169:HIS:HD2	1.91	0.52
2:E:170:ASP:CG	2:E:172:THR:HG23	2.30	0.52
2:E:170:ASP:OD2	2:E:172:THR:HG23	2.10	0.52
1:A:7:THR:CG2	1:A:8:GLU:N	2.73	0.52
1:D:12:VAL:HG23	1:D:13:ILE:N	2.25	0.52
1:G:7:THR:CG2	1:G:8:GLU:N	2.72	0.52
3:I:12:VAL:HG11	3:I:18:VAL:CG2	2.39	0.52
3:L:161:SER:N	3:L:201:ASN:ND2	2.51	0.52
2:B:124:GLN:HE22	2:B:131:SER:CB	2.23	0.52
3:C:132:GLY:CA	3:C:218:ARG:HD3	2.33	0.52
2:E:136:LEU:HD21	2:E:146:VAL:CG2	2.39	0.52
2:H:136:LEU:HD21	2:H:146:VAL:CG2	2.39	0.52
2:K:170:ASP:CG	2:K:172:THR:HG23	2.29	0.52
2:B:21:LEU:HD12	2:B:102:THR:CG2	2.40	0.52
2:H:81:GLU:CD	2:H:81:GLU:H	2.13	0.52
2:K:61:ARG:HB2	2:K:61:ARG:NH1	2.24	0.52
2:K:124:GLN:HE22	2:K:131:SER:CB	2.23	0.52
1:D:70:ARG:O	1:D:70:ARG:HG2	2.10	0.52
2:E:198:HIS:C	2:E:199:LYS:HG3	2.29	0.52
2:K:68:THR:HG22	2:K:69:THR:N	2.24	0.52
2:B:136:LEU:HD21	2:B:146:VAL:CG2	2.39	0.52
2:B:149:LYS:HB2	2:B:193:THR:CG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ARG:O	1:G:70:ARG:HG2	2.08	0.52
1:G:158:TYR:O	1:G:159:ASN:CB	2.57	0.52
2:H:124:GLN:HE22	2:H:131:SER:CB	2.23	0.52
2:K:49:TYR:CB	3:L:103:THR:HG21	2.26	0.52
1:A:158:TYR:O	1:A:159:ASN:CB	2.58	0.51
1:G:31:PRO:HB3	1:G:39:SER:O	2.10	0.51
1:G:129:LYS:C	1:G:131:GLU:H	2.14	0.51
3:I:116:VAL:HG23	3:I:116:VAL:O	2.10	0.51
1:D:7:THR:CG2	1:D:8:GLU:N	2.73	0.51
2:E:81:GLU:H	2:E:81:GLU:CD	2.14	0.51
1:G:62:LEU:HB3	1:G:63:PRO:CD	2.35	0.51
2:H:150:ILE:O	2:H:151:ASP:HB2	2.10	0.51
1:J:31:PRO:HB3	1:J:39:SER:O	2.11	0.51
2:B:59:PRO:HB2	2:B:61:ARG:HG3	1.93	0.51
2:B:81:GLU:H	2:B:81:GLU:CD	2.14	0.51
3:C:176:GLN:O	3:C:177:SER:C	2.48	0.51
1:J:7:THR:CG2	1:J:8:GLU:N	2.73	0.51
1:J:158:TYR:O	1:J:159:ASN:CB	2.57	0.51
3:L:176:GLN:O	3:L:177:SER:C	2.48	0.51
2:B:150:ILE:O	2:B:151:ASP:HB2	2.10	0.51
1:A:62:LEU:HB3	1:A:63:PRO:CD	2.35	0.51
3:C:116:VAL:HG23	3:C:116:VAL:O	2.10	0.51
2:E:150:ILE:O	2:E:151:ASP:HB2	2.09	0.51
1:G:12:VAL:HG23	1:G:13:ILE:N	2.25	0.51
3:I:62:GLN:HE22	3:I:65:LYS:HE2	1.76	0.51
3:I:176:GLN:O	3:I:177:SER:C	2.48	0.51
1:A:129:LYS:C	1:A:131:GLU:H	2.14	0.51
2:E:68:THR:HG22	2:E:69:THR:HG22	1.93	0.51
2:H:108:ARG:HG3	2:H:140:TYR:CD2	2.46	0.51
3:I:29:PHE:O	3:I:53:PRO:HG3	2.11	0.51
3:I:76:SER:OG	3:I:78:THR:HG23	2.11	0.51
2:K:81:GLU:CD	2:K:81:GLU:H	2.14	0.51
1:A:12:VAL:HG23	1:A:13:ILE:N	2.25	0.51
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.46	0.51
2:B:170:ASP:OD2	2:B:172:THR:HG23	2.10	0.51
3:F:62:GLN:HE22	3:F:65:LYS:HE2	1.75	0.51
1:J:12:VAL:HG23	1:J:13:ILE:N	2.25	0.51
1:J:129:LYS:C	1:J:131:GLU:H	2.14	0.51
2:K:150:ILE:O	2:K:151:ASP:HB2	2.10	0.51
3:L:62:GLN:HE22	3:L:65:LYS:HE2	1.75	0.51
3:C:62:GLN:HE22	3:C:65:LYS:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:76:SER:OG	3:F:78:THR:HG23	2.11	0.51
3:F:116:VAL:HG23	3:F:116:VAL:O	2.10	0.51
1:G:36:GLN:H	1:G:36:GLN:CD	2.15	0.51
3:L:12:VAL:HG11	3:L:18:VAL:CG2	2.40	0.51
3:L:76:SER:OG	3:L:78:THR:HG23	2.11	0.51
3:C:29:PHE:O	3:C:53:PRO:HG3	2.11	0.51
2:H:139:PHE:O	2:H:140:TYR:HB2	2.11	0.51
2:H:119:PRO:HB3	2:H:209:PHE:CE2	2.46	0.51
2:K:59:PRO:HB2	2:K:61:ARG:HG3	1.93	0.51
1:D:158:TYR:O	1:D:159:ASN:CB	2.58	0.50
2:E:119:PRO:HB3	2:E:209:PHE:CE2	2.46	0.50
1:J:62:LEU:HB3	1:J:63:PRO:CD	2.35	0.50
1:A:70:ARG:O	1:A:70:ARG:HG2	2.09	0.50
1:D:31:PRO:HB3	1:D:39:SER:O	2.11	0.50
2:E:108:ARG:HG3	2:E:140:TYR:CD2	2.46	0.50
2:E:119:PRO:HG2	3:F:218:ARG:CZ	2.42	0.50
1:G:119:LYS:N	1:G:119:LYS:CD	2.72	0.50
2:B:108:ARG:HG3	2:B:140:TYR:CD2	2.46	0.50
2:H:59:PRO:HB2	2:H:61:ARG:HG3	1.92	0.50
2:H:170:ASP:OD2	2:H:172:THR:HG23	2.10	0.50
3:L:29:PHE:O	3:L:53:PRO:HG3	2.10	0.50
3:L:116:VAL:HG23	3:L:116:VAL:O	2.10	0.50
1:A:36:GLN:CD	1:A:36:GLN:H	2.14	0.50
2:B:139:PHE:O	2:B:140:TYR:HB2	2.11	0.50
3:F:64:PHE:O	3:F:65:LYS:C	2.50	0.50
3:I:61:ASN:OD1	3:I:63:LYS:HE2	2.12	0.50
2:K:119:PRO:HB3	2:K:209:PHE:CE2	2.46	0.50
2:K:136:LEU:N	2:K:136:LEU:CD1	2.75	0.50
1:D:129:LYS:C	1:D:131:GLU:H	2.14	0.50
2:H:68:THR:HG22	2:H:69:THR:HG22	1.93	0.50
1:J:36:GLN:CD	1:J:36:GLN:H	2.15	0.50
2:K:175:MET:HG2	2:K:176:SER:H	1.77	0.50
3:L:64:PHE:O	3:L:65:LYS:C	2.50	0.50
2:E:3:VAL:CG2	2:E:26:SER:HB3	2.36	0.50
2:K:108:ARG:HG3	2:K:140:TYR:CD2	2.46	0.50
3:L:61:ASN:OD1	3:L:63:LYS:HE2	2.11	0.50
1:A:31:PRO:HB3	1:A:39:SER:O	2.11	0.50
2:B:133:VAL:HG21	3:C:129:LEU:HD13	1.93	0.50
2:B:137:ASN:HB3	2:B:138:ASN:ND2	2.27	0.50
2:B:146:VAL:HA	2:B:195:GLU:O	2.12	0.50
3:C:64:PHE:O	3:C:65:LYS:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:SER:OG	3:C:78:THR:HG23	2.11	0.50
2:E:59:PRO:HB2	2:E:61:ARG:HG3	1.92	0.50
2:H:187:GLU:C	2:H:189:HIS:H	2.15	0.50
3:I:64:PHE:O	3:I:65:LYS:C	2.50	0.50
1:J:45:GLU:HB2	3:L:32:TYR:HE1	1.77	0.50
2:B:81:GLU:O	2:B:83:LEU:N	2.45	0.50
2:E:175:MET:HG2	2:E:176:SER:H	1.77	0.50
2:H:146:VAL:HA	2:H:195:GLU:O	2.12	0.50
3:I:58:THR:HG1	3:I:60:TYR:HE2	1.59	0.50
1:A:32:LYS:HE3	2:H:190:ASN:OD1	2.11	0.50
2:E:137:ASN:HB3	2:E:138:ASN:ND2	2.27	0.50
2:E:187:GLU:C	2:E:189:HIS:H	2.14	0.50
3:F:61:ASN:OD1	3:F:63:LYS:HE2	2.12	0.50
1:A:20:LYS:NZ	1:A:159:ASN:HB2	2.27	0.49
2:E:139:PHE:O	2:E:140:TYR:HB2	2.11	0.49
3:L:38:LYS:HB2	3:L:94:TYR:CE1	2.47	0.49
3:C:38:LYS:HB2	3:C:94:TYR:CE1	2.48	0.49
3:F:29:PHE:O	3:F:53:PRO:HG3	2.11	0.49
2:H:81:GLU:O	2:H:83:LEU:N	2.45	0.49
2:H:205:ILE:HD12	2:H:205:ILE:N	2.27	0.49
2:B:187:GLU:C	2:B:189:HIS:H	2.15	0.49
1:D:20:LYS:NZ	1:D:159:ASN:HB2	2.27	0.49
1:D:36:GLN:H	1:D:36:GLN:CD	2.15	0.49
2:E:81:GLU:N	2:E:81:GLU:CD	2.66	0.49
2:E:146:VAL:HA	2:E:195:GLU:O	2.12	0.49
2:H:49:TYR:CD1	2:H:49:TYR:O	2.65	0.49
2:H:107:LYS:HA	2:H:140:TYR:OH	2.13	0.49
2:H:175:MET:HG2	2:H:176:SER:H	1.77	0.49
1:J:20:LYS:NZ	1:J:159:ASN:HB2	2.27	0.49
2:K:81:GLU:O	2:K:83:LEU:N	2.46	0.49
2:K:137:ASN:HB3	2:K:138:ASN:ND2	2.27	0.49
2:K:139:PHE:O	2:K:140:TYR:HB2	2.11	0.49
2:B:81:GLU:N	2:B:81:GLU:CD	2.66	0.49
2:E:49:TYR:O	2:E:49:TYR:CD1	2.65	0.49
2:H:19:VAL:HG12	2:H:20:THR:N	2.28	0.49
2:H:23:CYS:HG	2:H:88:CYS:HB3	1.76	0.49
2:K:71:PHE:CD2	2:K:71:PHE:N	2.80	0.49
2:K:119:PRO:O	3:L:218:ARG:NH2	2.39	0.49
3:F:176:GLN:O	3:F:177:SER:C	2.48	0.49
3:F:204:HIS:CE1	3:F:206:ALA:HB3	2.48	0.49
3:I:132:GLY:CA	3:I:218:ARG:HD3	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:68:THR:HG22	2:K:69:THR:HG22	1.93	0.49
2:K:81:GLU:N	2:K:81:GLU:CD	2.66	0.49
2:K:107:LYS:HA	2:K:140:TYR:OH	2.12	0.49
2:B:68:THR:HG22	2:B:69:THR:HG22	1.93	0.49
3:I:38:LYS:HB2	3:I:94:TYR:CE1	2.48	0.49
2:K:187:GLU:C	2:K:189:HIS:H	2.15	0.49
2:B:71:PHE:CD2	2:B:71:PHE:N	2.80	0.49
3:C:203:ALA:HB2	3:C:210:LYS:HE3	1.95	0.49
2:E:19:VAL:HG12	2:E:20:THR:N	2.28	0.49
2:E:107:LYS:HA	2:E:140:TYR:OH	2.12	0.49
2:H:71:PHE:N	2:H:71:PHE:CD2	2.80	0.49
2:K:49:TYR:O	2:K:49:TYR:CD1	2.66	0.49
2:B:49:TYR:O	2:B:49:TYR:CD1	2.66	0.49
3:C:27:TYR:CE2	3:C:32:TYR:HB2	2.47	0.49
2:E:205:ILE:HD12	2:E:205:ILE:N	2.28	0.49
1:G:64:PHE:CG	1:G:89:GLY:HA2	2.48	0.49
2:H:81:GLU:N	2:H:81:GLU:CD	2.66	0.49
3:I:203:ALA:HB2	3:I:210:LYS:HE3	1.95	0.49
2:B:107:LYS:HA	2:B:140:TYR:OH	2.13	0.49
2:E:81:GLU:O	2:E:83:LEU:N	2.46	0.49
3:F:38:LYS:HB2	3:F:94:TYR:CE1	2.47	0.49
3:F:182:LEU:HD12	3:F:183:SER:N	2.28	0.49
1:G:20:LYS:NZ	1:G:159:ASN:HB2	2.27	0.49
3:L:182:LEU:HD12	3:L:183:SER:N	2.28	0.49
2:B:39:LYS:HB2	2:B:42:GLN:OE1	2.13	0.48
3:I:204:HIS:CE1	3:I:206:ALA:HB3	2.48	0.48
1:J:64:PHE:CG	1:J:89:GLY:HA2	2.48	0.48
3:C:182:LEU:HD12	3:C:183:SER:N	2.28	0.48
3:C:204:HIS:CE1	3:C:206:ALA:HB3	2.48	0.48
3:F:27:TYR:CE2	3:F:32:TYR:HB2	2.48	0.48
3:I:161:SER:N	3:I:201:ASN:ND2	2.51	0.48
3:L:87:THR:C	3:L:116:VAL:HG21	2.34	0.48
3:C:24:ALA:HB1	3:C:27:TYR:CE1	2.49	0.48
2:E:71:PHE:N	2:E:71:PHE:CD2	2.80	0.48
3:F:87:THR:C	3:F:116:VAL:HG21	2.34	0.48
3:L:204:HIS:CE1	3:L:206:ALA:HB3	2.48	0.48
2:B:175:MET:HG2	2:B:176:SER:H	1.77	0.48
3:I:87:THR:C	3:I:116:VAL:HG21	2.34	0.48
2:K:146:VAL:HA	2:K:195:GLU:O	2.12	0.48
3:L:132:GLY:CA	3:L:218:ARG:HD3	2.33	0.48
2:B:136:LEU:N	2:B:136:LEU:CD1	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ASN:OD1	3:C:63:LYS:HE2	2.12	0.48
2:H:39:LYS:HB2	2:H:42:GLN:OE1	2.13	0.48
2:K:19:VAL:HG12	2:K:20:THR:N	2.28	0.48
3:C:87:THR:C	3:C:116:VAL:HG21	2.34	0.48
2:E:39:LYS:HB2	2:E:42:GLN:OE1	2.13	0.48
3:F:62:GLN:NE2	3:F:65:LYS:HE2	2.28	0.48
2:H:137:ASN:HB3	2:H:138:ASN:ND2	2.27	0.48
3:I:50:ASN:HD22	3:I:50:ASN:N	1.98	0.48
1:A:64:PHE:CG	1:A:89:GLY:HA2	2.48	0.48
2:B:19:VAL:HG12	2:B:20:THR:N	2.28	0.48
2:E:134:CYS:HG	2:E:194:CYS:CB	2.27	0.48
2:E:163:TRP:CZ2	2:E:175:MET:HE2	2.49	0.48
3:I:205:PRO:CG	3:I:206:ALA:H	2.27	0.48
2:K:3:VAL:CG2	2:K:26:SER:HB3	2.36	0.48
2:K:205:ILE:N	2:K:205:ILE:HD12	2.28	0.48
3:L:62:GLN:NE2	3:L:65:LYS:HE2	2.28	0.48
2:B:88:CYS:O	2:B:98:PHE:HA	2.14	0.48
2:B:205:ILE:N	2:B:205:ILE:HD12	2.28	0.48
3:I:182:LEU:HD12	3:I:183:SER:N	2.28	0.48
2:K:88:CYS:O	2:K:98:PHE:HA	2.14	0.48
3:C:205:PRO:CG	3:C:206:ALA:H	2.27	0.48
2:E:88:CYS:O	2:E:98:PHE:HA	2.14	0.48
3:F:24:ALA:HB1	3:F:27:TYR:CE1	2.49	0.48
1:D:64:PHE:CG	1:D:89:GLY:HA2	2.48	0.47
3:F:97:THR:HG1	3:F:105:PHE:HD2	1.62	0.47
2:K:39:LYS:HB2	2:K:42:GLN:OE1	2.13	0.47
2:H:11:MET:SD	2:H:19:VAL:HG13	2.54	0.47
3:I:62:GLN:NE2	3:I:65:LYS:HE2	2.28	0.47
3:L:24:ALA:HB1	3:L:27:TYR:CE1	2.49	0.47
3:F:54:SER:OG	3:F:55:ASP:N	2.48	0.47
3:F:203:ALA:HB2	3:F:210:LYS:HE3	1.95	0.47
2:B:3:VAL:CG2	2:B:26:SER:HB3	2.36	0.47
2:E:179:LEU:HD13	2:E:180:THR:N	2.30	0.47
2:H:88:CYS:O	2:H:98:PHE:HA	2.14	0.47
2:H:179:LEU:HD13	2:H:180:THR:N	2.29	0.47
3:I:54:SER:OG	3:I:55:ASP:N	2.47	0.47
3:L:27:TYR:CE2	3:L:32:TYR:HB2	2.48	0.47
2:H:166:GLN:HG3	2:H:171:SER:O	2.14	0.47
2:K:108:ARG:O	2:K:140:TYR:CE2	2.67	0.47
3:C:50:ASN:ND2	3:C:50:ASN:N	2.63	0.47
3:C:62:GLN:NE2	3:C:65:LYS:HE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:132:GLY:CA	3:F:218:ARG:HD3	2.33	0.47
1:G:69:ASP:HA	1:G:84:SER:O	2.15	0.47
3:I:24:ALA:HB1	3:I:27:TYR:CE1	2.49	0.47
3:L:54:SER:OG	3:L:55:ASP:N	2.47	0.47
3:L:205:PRO:CG	3:L:206:ALA:H	2.27	0.47
2:B:150:ILE:O	2:B:150:ILE:HG13	2.15	0.47
2:B:166:GLN:HG3	2:B:171:SER:O	2.14	0.47
3:C:54:SER:OG	3:C:55:ASP:N	2.47	0.47
3:F:146:LEU:O	3:F:146:LEU:HD23	2.15	0.47
3:I:27:TYR:CE2	3:I:32:TYR:HB2	2.48	0.47
2:H:108:ARG:O	2:H:140:TYR:CE2	2.67	0.47
2:K:6:GLN:HE22	2:K:87:HIS:HA	1.80	0.47
2:K:198:HIS:CG	2:K:199:LYS:H	2.33	0.47
3:L:203:ALA:HB2	3:L:210:LYS:HE3	1.95	0.47
2:B:11:MET:SD	2:B:19:VAL:HG13	2.55	0.47
1:G:50:PRO:CD	2:H:92:TYR:O	2.63	0.47
2:K:11:MET:CE	2:K:19:VAL:HG13	2.45	0.47
1:D:69:ASP:HA	1:D:84:SER:O	2.15	0.46
2:E:166:GLN:HG3	2:E:171:SER:O	2.15	0.46
3:I:144:GLY:HA3	3:I:185:SER:HA	1.97	0.46
1:J:69:ASP:HA	1:J:84:SER:O	2.15	0.46
2:K:3:VAL:O	2:K:3:VAL:CG2	2.63	0.46
2:K:11:MET:SD	2:K:19:VAL:HG13	2.55	0.46
1:A:17:ARG:NH2	1:A:151:LEU:O	2.48	0.46
2:B:163:TRP:CZ2	2:B:175:MET:HE2	2.51	0.46
2:K:179:LEU:HD13	2:K:180:THR:N	2.30	0.46
2:B:160:LEU:O	2:B:177:SER:HA	2.16	0.46
2:E:11:MET:CE	2:E:19:VAL:HG13	2.46	0.46
3:F:12:VAL:CG1	3:F:116:VAL:HG12	2.45	0.46
3:I:12:VAL:CG1	3:I:116:VAL:HG12	2.46	0.46
2:B:108:ARG:O	2:B:140:TYR:CE2	2.67	0.46
1:D:62:LEU:HD12	1:D:62:LEU:N	2.31	0.46
2:E:6:GLN:HE22	2:E:87:HIS:HA	1.81	0.46
2:H:26:SER:O	2:H:27:GLU:HG3	2.16	0.46
1:J:34:ALA:N	1:J:35:PRO:CD	2.78	0.46
2:B:6:GLN:HE22	2:B:87:HIS:HA	1.81	0.46
2:B:11:MET:CE	2:B:19:VAL:HG13	2.46	0.46
2:B:198:HIS:CG	2:B:199:LYS:H	2.34	0.46
2:H:133:VAL:HG21	3:I:129:LEU:HD13	1.97	0.46
2:K:150:ILE:O	2:K:150:ILE:HG13	2.15	0.46
2:K:163:TRP:CE3	2:K:163:TRP:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:LEU:HD13	2:B:180:THR:N	2.30	0.46
3:F:67:LYS:HE3	3:F:67:LYS:HB3	1.85	0.46
2:H:81:GLU:C	2:H:83:LEU:N	2.69	0.46
2:H:150:ILE:O	2:H:150:ILE:HG13	2.15	0.46
1:D:15:ALA:HB1	1:D:104:ILE:HG22	1.98	0.46
1:D:20:LYS:HZ3	1:D:159:ASN:HD22	1.63	0.46
1:D:34:ALA:N	1:D:35:PRO:CD	2.79	0.46
3:F:1:GLN:C	3:F:2:VAL:HG12	2.36	0.46
1:G:20:LYS:HZ2	1:G:159:ASN:HB2	1.81	0.46
1:G:62:LEU:N	1:G:62:LEU:HD12	2.31	0.46
2:H:163:TRP:CZ2	2:H:175:MET:HE2	2.51	0.46
3:L:12:VAL:CG1	3:L:116:VAL:HG12	2.45	0.46
2:B:26:SER:O	2:B:27:GLU:HG3	2.16	0.46
3:C:144:GLY:HA3	3:C:185:SER:HA	1.97	0.46
2:E:150:ILE:O	2:E:150:ILE:HG13	2.16	0.46
2:H:11:MET:CE	2:H:19:VAL:HG13	2.45	0.46
3:I:146:LEU:HD23	3:I:146:LEU:O	2.16	0.46
1:J:129:LYS:HA	1:J:129:LYS:CE	2.44	0.46
2:K:166:GLN:HG3	2:K:171:SER:O	2.15	0.46
1:A:69:ASP:HA	1:A:84:SER:O	2.15	0.46
1:G:13:ILE:HG12	1:G:13:ILE:H	1.46	0.46
1:G:19:PHE:CD2	1:G:79:PHE:HD1	2.34	0.46
2:H:6:GLN:HE22	2:H:87:HIS:HA	1.80	0.46
1:J:62:LEU:N	1:J:62:LEU:HD12	2.31	0.46
3:L:50:ASN:ND2	3:L:50:ASN:N	2.63	0.46
1:A:62:LEU:HD12	1:A:62:LEU:N	2.31	0.46
2:B:3:VAL:O	2:B:3:VAL:CG2	2.63	0.46
3:C:146:LEU:O	3:C:146:LEU:HD23	2.16	0.46
3:F:188:VAL:HB	3:F:189:PRO:CD	2.46	0.46
1:J:19:PHE:CD2	1:J:79:PHE:HD1	2.34	0.46
2:B:163:TRP:N	2:B:163:TRP:CE3	2.84	0.45
3:C:12:VAL:CG1	3:C:116:VAL:HG12	2.46	0.45
2:E:26:SER:O	2:E:27:GLU:HG3	2.16	0.45
1:G:29:LEU:O	1:G:32:LYS:HB3	2.17	0.45
1:G:46:GLY:O	3:I:102:ASP:HA	2.16	0.45
2:H:33:VAL:O	2:H:50:GLY:HA2	2.16	0.45
1:J:15:ALA:HB1	1:J:104:ILE:HG22	1.98	0.45
1:J:46:GLY:O	3:L:102:ASP:CA	2.64	0.45
3:L:1:GLN:C	3:L:2:VAL:HG12	2.36	0.45
3:L:188:VAL:HB	3:L:189:PRO:CD	2.46	0.45
1:A:15:ALA:O	1:A:16:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:ARG:HD2	3:C:99:GLY:O	2.16	0.45
3:C:161:SER:N	3:C:201:ASN:ND2	2.52	0.45
1:D:123:LYS:O	1:D:125:ASP:N	2.49	0.45
2:E:81:GLU:C	2:E:83:LEU:N	2.69	0.45
2:E:183:LYS:O	2:E:186:TYR:HB3	2.17	0.45
1:G:15:ALA:HB1	1:G:104:ILE:HG22	1.98	0.45
1:G:17:ARG:NH2	1:G:151:LEU:O	2.49	0.45
2:K:26:SER:O	2:K:27:GLU:HG3	2.16	0.45
2:K:33:VAL:O	2:K:50:GLY:HA2	2.16	0.45
2:K:186:TYR:HE1	2:K:192:TYR:CE2	2.33	0.45
2:E:11:MET:SD	2:E:19:VAL:HG13	2.55	0.45
2:E:108:ARG:O	2:E:140:TYR:CE2	2.67	0.45
3:F:50:ASN:ND2	3:F:50:ASN:N	2.63	0.45
2:H:3:VAL:CG2	2:H:26:SER:HB3	2.37	0.45
2:H:116:SER:O	2:H:134:CYS:HA	2.17	0.45
3:I:50:ASN:ND2	3:I:50:ASN:N	2.63	0.45
3:I:98:ARG:HD2	3:I:99:GLY:O	2.16	0.45
1:J:20:LYS:HZ2	1:J:159:ASN:HB2	1.81	0.45
1:J:123:LYS:O	1:J:125:ASP:N	2.50	0.45
3:L:67:LYS:HE3	3:L:67:LYS:HB3	1.85	0.45
3:L:144:GLY:HA3	3:L:185:SER:HA	1.98	0.45
2:B:23:CYS:CB	2:B:88:CYS:HG	2.30	0.45
1:D:29:LEU:O	1:D:32:LYS:HB3	2.16	0.45
2:E:193:THR:CB	2:E:208:SER:HB3	2.47	0.45
1:G:13:ILE:HB	1:G:18:LEU:HB2	1.98	0.45
1:G:123:LYS:O	1:G:125:ASP:N	2.50	0.45
3:I:188:VAL:HB	3:I:189:PRO:CD	2.46	0.45
1:J:15:ALA:O	1:J:16:ALA:C	2.55	0.45
2:K:175:MET:CA	3:L:171:PHE:HE1	2.29	0.45
1:A:15:ALA:HB1	1:A:104:ILE:HG22	1.98	0.45
1:D:13:ILE:HB	1:D:18:LEU:HB2	1.99	0.45
2:E:163:TRP:N	2:E:163:TRP:CE3	2.84	0.45
3:F:205:PRO:CG	3:F:206:ALA:H	2.27	0.45
3:I:141:VAL:HG12	3:I:188:VAL:O	2.16	0.45
3:L:98:ARG:HD2	3:L:99:GLY:O	2.16	0.45
1:A:20:LYS:HZ2	1:A:159:ASN:HD22	1.62	0.45
2:B:183:LYS:O	2:B:186:TYR:HB3	2.17	0.45
3:C:1:GLN:C	3:C:2:VAL:HG12	2.36	0.45
3:I:1:GLN:C	3:I:2:VAL:HG12	2.36	0.45
3:L:146:LEU:HD23	3:L:146:LEU:O	2.16	0.45
2:B:33:VAL:O	2:B:50:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:SER:HA	2:B:204:PRO:HD2	1.81	0.45
1:D:19:PHE:CD2	1:D:79:PHE:HD1	2.35	0.45
2:E:116:SER:O	2:E:134:CYS:HA	2.17	0.45
2:E:186:TYR:HE1	2:E:192:TYR:CE2	2.33	0.45
3:F:86:PRO:HA	3:F:90:ASP:OD2	2.17	0.45
2:H:61:ARG:HH22	2:H:82:ASP:CG	2.20	0.45
2:H:183:LYS:O	2:H:186:TYR:HB3	2.17	0.45
2:H:198:HIS:CG	2:H:199:LYS:H	2.34	0.45
3:I:30:THR:HA	3:I:53:PRO:CG	2.46	0.45
1:J:17:ARG:NH2	1:J:151:LEU:O	2.49	0.45
1:J:29:LEU:O	1:J:32:LYS:HB3	2.16	0.45
2:K:81:GLU:C	2:K:83:LEU:N	2.69	0.45
2:K:160:LEU:O	2:K:177:SER:HA	2.17	0.45
3:L:30:THR:HA	3:L:53:PRO:CG	2.46	0.45
3:L:141:VAL:HG12	3:L:188:VAL:O	2.17	0.45
3:C:50:ASN:ND2	3:C:50:ASN:H	2.10	0.45
1:D:129:LYS:HA	1:D:129:LYS:CE	2.44	0.45
1:G:34:ALA:N	1:G:35:PRO:CD	2.78	0.45
2:K:116:SER:O	2:K:134:CYS:HA	2.17	0.45
3:L:86:PRO:HA	3:L:90:ASP:OD2	2.17	0.45
2:B:81:GLU:C	2:B:83:LEU:N	2.69	0.45
2:B:186:TYR:O	2:B:192:TYR:OH	2.35	0.45
3:C:86:PRO:HA	3:C:90:ASP:OD2	2.17	0.45
3:C:141:VAL:HG12	3:C:188:VAL:O	2.17	0.45
1:D:15:ALA:O	1:D:16:ALA:C	2.55	0.45
2:E:33:VAL:O	2:E:50:GLY:HA2	2.17	0.45
2:K:23:CYS:CB	2:K:88:CYS:SG	3.05	0.45
1:A:123:LYS:O	1:A:125:ASP:N	2.50	0.45
2:B:23:CYS:CB	2:B:88:CYS:SG	3.05	0.45
2:B:116:SER:O	2:B:134:CYS:HA	2.17	0.45
2:B:193:THR:CB	2:B:208:SER:HB3	2.47	0.45
1:D:17:ARG:NH2	1:D:151:LEU:O	2.49	0.45
2:H:163:TRP:N	2:H:163:TRP:CE3	2.84	0.45
2:H:193:THR:CB	2:H:208:SER:HB3	2.47	0.45
3:I:126:VAL:HG22	3:I:213:LYS:HG3	1.98	0.45
1:A:19:PHE:CD2	1:A:79:PHE:HD1	2.35	0.44
1:A:54:LYS:O	1:A:68:LYS:HA	2.18	0.44
3:C:188:VAL:HB	3:C:189:PRO:CD	2.47	0.44
2:E:49:TYR:HB2	3:F:103:THR:HG23	1.94	0.44
3:F:98:ARG:HD2	3:F:99:GLY:O	2.16	0.44
3:F:214:LYS:HB3	3:I:208:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:21:LEU:N	2:K:21:LEU:HD22	2.32	0.44
1:D:47:ASN:N	1:D:47:ASN:ND2	2.64	0.44
2:E:3:VAL:O	2:E:3:VAL:CG2	2.64	0.44
1:G:15:ALA:O	1:G:16:ALA:C	2.55	0.44
2:H:160:LEU:O	2:H:177:SER:HA	2.16	0.44
3:L:126:VAL:HG22	3:L:213:LYS:HG3	1.99	0.44
2:E:18:ARG:HH11	2:E:18:ARG:CG	2.30	0.44
2:H:3:VAL:O	2:H:3:VAL:CG2	2.63	0.44
2:H:21:LEU:N	2:H:21:LEU:HD22	2.32	0.44
3:I:130:ALA:O	3:I:218:ARG:NH1	2.49	0.44
2:K:183:LYS:O	2:K:186:TYR:HB3	2.16	0.44
2:B:49:TYR:O	2:B:50:GLY:O	2.36	0.44
2:B:61:ARG:HH22	2:B:82:ASP:CG	2.20	0.44
3:C:126:VAL:HG22	3:C:213:LYS:HG3	1.99	0.44
3:F:30:THR:HA	3:F:53:PRO:CG	2.46	0.44
3:F:141:VAL:HG12	3:F:188:VAL:O	2.17	0.44
3:F:144:GLY:HA3	3:F:185:SER:HA	1.98	0.44
1:G:47:ASN:O	2:H:32:TYR:HE2	1.99	0.44
2:H:186:TYR:HE1	2:H:192:TYR:CE2	2.33	0.44
2:E:21:LEU:N	2:E:21:LEU:HD22	2.31	0.44
2:E:49:TYR:O	2:E:49:TYR:CG	2.70	0.44
3:F:205:PRO:CG	3:F:206:ALA:N	2.81	0.44
2:H:49:TYR:O	2:H:49:TYR:CG	2.71	0.44
2:K:49:TYR:O	2:K:49:TYR:CG	2.71	0.44
2:K:163:TRP:CZ2	2:K:175:MET:HE2	2.52	0.44
2:H:11:MET:SD	2:H:19:VAL:CG1	3.06	0.44
2:H:23:CYS:CB	2:H:88:CYS:SG	3.05	0.44
2:K:193:THR:CB	2:K:208:SER:HB3	2.47	0.44
2:B:186:TYR:HE1	2:B:192:TYR:CE2	2.33	0.44
2:E:160:LEU:O	2:E:177:SER:HA	2.16	0.44
3:F:165:SER:O	3:F:168:VAL:HG22	2.18	0.44
3:I:86:PRO:HA	3:I:90:ASP:OD2	2.17	0.44
3:I:205:PRO:CG	3:I:206:ALA:N	2.81	0.44
1:J:13:ILE:HB	1:J:18:LEU:HB2	1.99	0.44
3:L:205:PRO:CG	3:L:206:ALA:N	2.81	0.44
1:A:13:ILE:HB	1:A:18:LEU:HB2	1.98	0.44
2:E:198:HIS:CG	2:E:199:LYS:H	2.33	0.44
3:F:126:VAL:HG22	3:F:213:LYS:HG3	1.99	0.44
1:G:5:TYR:CE2	1:G:128:VAL:HG11	2.52	0.44
1:J:20:LYS:HZ2	1:J:159:ASN:HD22	1.66	0.44
1:A:29:LEU:O	1:A:32:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LEU:HD22	1:D:144:LEU:HD22	2.00	0.44
2:E:61:ARG:HH22	2:E:82:ASP:CG	2.20	0.44
2:E:186:TYR:O	2:E:192:TYR:OH	2.34	0.44
2:K:49:TYR:O	2:K:50:GLY:O	2.36	0.43
2:K:193:THR:CA	2:K:208:SER:HB3	2.48	0.43
2:K:11:MET:SD	2:K:19:VAL:CG1	3.06	0.43
2:K:61:ARG:HH22	2:K:82:ASP:CG	2.20	0.43
2:K:130:ALA:HB3	2:K:181:LEU:O	2.18	0.43
1:G:47:ASN:O	2:H:32:TYR:CE2	2.71	0.43
2:H:54:ARG:HD3	2:H:62:PHE:O	2.18	0.43
3:L:165:SER:O	3:L:168:VAL:HG22	2.19	0.43
2:E:161:ASN:ND2	2:E:177:SER:HB3	2.33	0.43
1:G:54:LYS:O	1:G:68:LYS:HA	2.18	0.43
2:H:49:TYR:O	2:H:50:GLY:O	2.36	0.43
3:I:97:THR:HG1	3:I:105:PHE:HD2	1.64	0.43
2:K:161:ASN:ND2	2:K:177:SER:HB3	2.33	0.43
2:B:54:ARG:HD3	2:B:62:PHE:O	2.18	0.43
2:B:117:ILE:HD12	2:B:194:CYS:HB2	2.00	0.43
1:D:54:LYS:O	1:D:68:LYS:HA	2.18	0.43
3:F:19:ILE:HD12	3:F:19:ILE:N	2.33	0.43
3:F:92:ALA:O	3:F:114:VAL:HG22	2.19	0.43
1:G:114:LEU:HD22	1:G:144:LEU:HD22	2.00	0.43
3:I:19:ILE:HD12	3:I:19:ILE:N	2.34	0.43
3:I:165:SER:O	3:I:168:VAL:HG22	2.19	0.43
1:J:114:LEU:HD22	1:J:144:LEU:HD22	2.00	0.43
3:L:132:GLY:O	3:L:135:ALA:HB3	2.18	0.43
2:E:54:ARG:HD3	2:E:62:PHE:O	2.18	0.43
3:F:214:LYS:HG2	3:F:216:VAL:HG13	2.01	0.43
3:I:128:PRO:O	3:I:129:LEU:HD23	2.19	0.43
1:A:44:ILE:CG1	1:A:55:LYS:HB2	2.49	0.43
1:A:114:LEU:HD22	1:A:144:LEU:HD22	2.00	0.43
2:B:11:MET:SD	2:B:19:VAL:CG1	3.07	0.43
2:B:21:LEU:N	2:B:21:LEU:HD22	2.32	0.43
3:C:205:PRO:CG	3:C:206:ALA:N	2.81	0.43
2:E:115:VAL:HG12	2:E:116:SER:N	2.34	0.43
2:E:130:ALA:HB3	2:E:181:LEU:O	2.19	0.43
2:E:187:GLU:C	2:E:189:HIS:N	2.72	0.43
2:E:193:THR:CA	2:E:208:SER:HB3	2.48	0.43
3:F:132:GLY:O	3:F:135:ALA:HB3	2.18	0.43
2:H:117:ILE:HD12	2:H:194:CYS:HB2	2.01	0.43
2:H:161:ASN:ND2	2:H:177:SER:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:128:PRO:O	3:L:129:LEU:HD23	2.19	0.43
2:E:117:ILE:HD12	2:E:194:CYS:HB2	2.01	0.43
2:E:133:VAL:HG21	3:F:129:LEU:CD1	2.49	0.43
3:I:92:ALA:O	3:I:114:VAL:HG22	2.19	0.43
1:J:54:LYS:O	1:J:68:LYS:HA	2.18	0.43
2:B:161:ASN:ND2	2:B:177:SER:HB3	2.33	0.43
3:C:165:SER:O	3:C:168:VAL:HG22	2.19	0.43
3:C:214:LYS:HG2	3:C:216:VAL:HG13	2.01	0.43
1:D:62:LEU:HD12	1:D:62:LEU:H	1.83	0.43
2:K:186:TYR:O	2:K:192:TYR:OH	2.35	0.43
2:K:187:GLU:C	2:K:189:HIS:N	2.73	0.43
3:L:92:ALA:O	3:L:114:VAL:HG22	2.19	0.43
2:B:115:VAL:HG12	2:B:116:SER:N	2.33	0.43
2:E:119:PRO:HB3	2:E:209:PHE:CZ	2.54	0.43
3:F:140:MET:HG2	3:F:187:THR:HG22	2.01	0.43
3:F:193:TRP:CG	3:F:194:PRO:HA	2.54	0.43
2:H:130:ALA:HB3	2:H:181:LEU:O	2.19	0.43
2:H:136:LEU:N	2:H:136:LEU:CD1	2.75	0.43
3:I:152:PRO:HD2	3:I:206:ALA:HB1	2.01	0.43
1:J:5:TYR:CE2	1:J:128:VAL:HG11	2.52	0.43
2:K:37:GLN:O	2:K:45:LYS:HE2	2.19	0.43
3:L:161:SER:HA	3:L:201:ASN:ND2	2.34	0.43
3:L:214:LYS:HG2	3:L:216:VAL:HG13	2.01	0.43
2:B:48:LEU:HD12	2:B:48:LEU:HA	1.89	0.42
2:B:49:TYR:O	2:B:49:TYR:CG	2.71	0.42
2:B:130:ALA:HB3	2:B:181:LEU:O	2.19	0.42
2:E:11:MET:SD	2:E:19:VAL:CG1	3.07	0.42
2:E:37:GLN:O	2:E:45:LYS:HE2	2.19	0.42
2:E:49:TYR:O	2:E:50:GLY:O	2.37	0.42
2:E:61:ARG:O	2:E:75:ILE:HA	2.19	0.42
1:J:16:ALA:HA	1:J:79:PHE:CZ	2.54	0.42
2:K:119:PRO:HB3	2:K:209:PHE:CZ	2.54	0.42
1:D:16:ALA:HA	1:D:79:PHE:CZ	2.54	0.42
1:G:44:ILE:CG1	1:G:55:LYS:HB2	2.49	0.42
2:H:13:VAL:HB	2:H:17:GLU:OE2	2.19	0.42
2:H:61:ARG:O	2:H:75:ILE:HA	2.19	0.42
2:H:187:GLU:C	2:H:189:HIS:N	2.72	0.42
3:I:161:SER:HA	3:I:201:ASN:ND2	2.34	0.42
1:J:44:ILE:CG1	1:J:55:LYS:HB2	2.49	0.42
2:K:54:ARG:HD3	2:K:62:PHE:O	2.18	0.42
3:L:97:THR:HG1	3:L:105:PHE:HD2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:HA	1:A:79:PHE:CZ	2.54	0.42
2:B:213:GLU:O	2:B:213:GLU:HG2	2.19	0.42
3:C:124:PRO:CA	3:C:150:TYR:HB3	2.49	0.42
1:D:5:TYR:CE2	1:D:128:VAL:HG11	2.52	0.42
2:H:37:GLN:O	2:H:45:LYS:HE2	2.19	0.42
3:I:50:ASN:ND2	3:I:50:ASN:H	2.10	0.42
3:I:132:GLY:O	3:I:135:ALA:HB3	2.18	0.42
3:I:188:VAL:HB	3:I:189:PRO:HD2	2.01	0.42
2:K:117:ILE:HD12	2:K:194:CYS:HB2	2.01	0.42
2:K:213:GLU:O	2:K:213:GLU:HG2	2.19	0.42
2:B:61:ARG:O	2:B:75:ILE:HA	2.19	0.42
2:B:193:THR:CA	2:B:208:SER:HB3	2.48	0.42
2:E:142:LYS:HD3	2:E:142:LYS:C	2.40	0.42
3:F:2:VAL:C	3:F:3:GLN:HG3	2.39	0.42
2:H:142:LYS:HD3	2:H:142:LYS:C	2.40	0.42
3:L:188:VAL:HB	3:L:189:PRO:HD2	2.01	0.42
2:B:119:PRO:HG2	3:C:218:ARG:CZ	2.49	0.42
3:C:128:PRO:O	3:C:129:LEU:HD23	2.19	0.42
3:C:132:GLY:O	3:C:135:ALA:HB3	2.18	0.42
3:F:12:VAL:O	3:F:116:VAL:HA	2.20	0.42
3:F:124:PRO:CA	3:F:150:TYR:HB3	2.49	0.42
3:F:130:ALA:O	3:F:218:ARG:NH1	2.49	0.42
1:G:150:TYR:C	1:G:150:TYR:CD2	2.93	0.42
2:H:115:VAL:HG12	2:H:116:SER:N	2.34	0.42
2:K:142:LYS:HD3	2:K:142:LYS:C	2.40	0.42
2:K:163:TRP:HE3	2:K:163:TRP:H	1.67	0.42
1:A:150:TYR:C	1:A:150:TYR:CD2	2.93	0.42
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.54	0.42
1:G:25:ASP:CG	1:G:28:ASN:ND2	2.68	0.42
1:J:62:LEU:HD12	1:J:62:LEU:H	1.84	0.42
2:K:61:ARG:O	2:K:75:ILE:HA	2.19	0.42
2:K:115:VAL:HG12	2:K:116:SER:N	2.34	0.42
3:L:124:PRO:CA	3:L:150:TYR:HB3	2.49	0.42
3:L:193:TRP:CG	3:L:194:PRO:HA	2.55	0.42
1:A:25:ASP:CG	1:A:28:ASN:ND2	2.68	0.42
2:B:58:VAL:HA	2:B:59:PRO:HD2	1.93	0.42
3:C:2:VAL:C	3:C:3:GLN:HG3	2.39	0.42
3:C:92:ALA:O	3:C:114:VAL:HG22	2.19	0.42
3:C:188:VAL:HB	3:C:189:PRO:HD2	2.01	0.42
3:C:193:TRP:CG	3:C:194:PRO:HA	2.55	0.42
1:D:44:ILE:CG1	1:D:55:LYS:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:SER:HA	3:F:201:ASN:ND2	2.34	0.42
3:F:188:VAL:HB	3:F:189:PRO:HD2	2.01	0.42
1:G:116:ILE:O	1:G:116:ILE:HG22	2.20	0.42
2:H:163:TRP:HE3	2:H:163:TRP:H	1.68	0.42
3:I:155:VAL:HG23	3:I:204:HIS:CD2	2.55	0.42
3:L:152:PRO:HD2	3:L:206:ALA:HB1	2.01	0.42
3:C:30:THR:HA	3:C:53:PRO:CG	2.46	0.42
3:C:161:SER:HA	3:C:201:ASN:ND2	2.35	0.42
1:D:150:TYR:CD2	1:D:150:TYR:C	2.93	0.42
3:F:128:PRO:O	3:F:129:LEU:HD23	2.19	0.42
1:G:16:ALA:HA	1:G:79:PHE:CZ	2.55	0.42
1:G:20:LYS:HZ2	1:G:159:ASN:HD22	1.66	0.42
1:G:126:HIS:ND1	1:G:127:GLU:N	2.68	0.42
3:I:12:VAL:O	3:I:116:VAL:HA	2.19	0.42
2:K:170:ASP:OD2	2:K:170:ASP:C	2.58	0.42
3:L:36:TRP:O	3:L:48:VAL:HB	2.20	0.42
1:A:62:LEU:HD12	1:A:62:LEU:H	1.84	0.42
1:A:132:GLN:C	1:A:134:LYS:N	2.73	0.42
2:B:142:LYS:C	2:B:142:LYS:HD3	2.40	0.42
3:C:155:VAL:HG23	3:C:204:HIS:CD2	2.55	0.42
1:G:45:GLU:HG2	3:I:104:TRP:CZ3	2.54	0.42
1:G:62:LEU:HD12	1:G:62:LEU:H	1.84	0.42
3:C:70:LEU:C	3:C:71:THR:HG23	2.41	0.42
1:D:132:GLN:C	1:D:134:LYS:N	2.73	0.42
2:E:13:VAL:HB	2:E:17:GLU:OE2	2.20	0.42
2:E:170:ASP:OD2	2:E:170:ASP:C	2.58	0.42
2:E:176:SER:HB3	3:F:171:PHE:CD1	2.55	0.42
3:F:155:VAL:HG23	3:F:204:HIS:CD2	2.55	0.42
2:H:119:PRO:HB3	2:H:209:PHE:CZ	2.54	0.42
3:I:193:TRP:CG	3:I:194:PRO:HA	2.55	0.42
2:K:23:CYS:CB	2:K:88:CYS:HG	2.32	0.42
2:K:57:GLY:O	2:K:58:VAL:C	2.58	0.42
3:L:140:MET:HG2	3:L:187:THR:HG22	2.01	0.42
3:C:152:PRO:HD2	3:C:206:ALA:HB1	2.01	0.41
2:E:163:TRP:HE3	2:E:163:TRP:H	1.68	0.41
2:H:133:VAL:HG12	2:H:178:THR:HB	2.03	0.41
3:I:2:VAL:C	3:I:3:GLN:HG3	2.39	0.41
3:I:54:SER:HA	3:I:74:LYS:HE3	2.01	0.41
3:L:2:VAL:C	3:L:3:GLN:HG3	2.39	0.41
3:L:12:VAL:O	3:L:116:VAL:HA	2.20	0.41
1:A:15:ALA:CB	1:A:104:ILE:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:VAL:HG11	2:B:19:VAL:CG2	2.50	0.41
2:B:176:SER:HB3	3:C:171:PHE:CD1	2.54	0.41
3:C:130:ALA:O	3:C:218:ARG:NH1	2.49	0.41
2:E:57:GLY:O	2:E:58:VAL:C	2.58	0.41
2:E:198:HIS:CG	2:E:199:LYS:N	2.89	0.41
2:E:213:GLU:O	2:E:213:GLU:HG2	2.19	0.41
2:H:132:VAL:O	2:H:179:LEU:N	2.48	0.41
3:L:155:VAL:HG23	3:L:204:HIS:CD2	2.55	0.41
1:A:126:HIS:ND1	1:A:127:GLU:N	2.68	0.41
2:B:37:GLN:O	2:B:45:LYS:HE2	2.20	0.41
2:B:163:TRP:HE3	2:B:163:TRP:H	1.68	0.41
1:D:15:ALA:CB	1:D:104:ILE:HG22	2.50	0.41
2:H:213:GLU:HG2	2:H:213:GLU:O	2.20	0.41
3:I:140:MET:HG2	3:I:187:THR:HG22	2.01	0.41
3:L:19:ILE:HD12	3:L:19:ILE:N	2.34	0.41
2:B:13:VAL:HB	2:B:17:GLU:OE2	2.20	0.41
3:C:19:ILE:HD12	3:C:19:ILE:N	2.34	0.41
2:E:14:SER:O	2:E:17:GLU:HB2	2.21	0.41
3:F:36:TRP:O	3:F:48:VAL:HB	2.20	0.41
3:L:54:SER:HA	3:L:74:LYS:HE3	2.01	0.41
3:L:124:PRO:HB3	3:L:150:TYR:HB3	2.03	0.41
2:B:176:SER:HB3	3:C:171:PHE:CE1	2.56	0.41
1:D:114:LEU:HD12	1:D:114:LEU:N	2.36	0.41
2:E:13:VAL:HG11	2:E:19:VAL:CG2	2.50	0.41
2:E:23:CYS:CB	2:E:88:CYS:SG	3.06	0.41
2:E:134:CYS:CB	2:E:194:CYS:SG	3.08	0.41
2:H:122:SER:O	2:H:126:THR:HG23	2.21	0.41
3:I:36:TRP:O	3:I:48:VAL:HB	2.20	0.41
3:I:124:PRO:CA	3:I:150:TYR:HB3	2.50	0.41
1:J:15:ALA:CB	1:J:104:ILE:HG22	2.50	0.41
1:J:150:TYR:C	1:J:150:TYR:CD2	2.93	0.41
2:K:133:VAL:HG12	2:K:178:THR:HB	2.03	0.41
2:B:133:VAL:HG12	2:B:178:THR:HB	2.03	0.41
2:B:187:GLU:C	2:B:189:HIS:N	2.73	0.41
3:C:155:VAL:HG23	3:C:204:HIS:HD2	1.86	0.41
1:D:126:HIS:ND1	1:D:127:GLU:N	2.68	0.41
3:F:47:TRP:CH2	3:F:49:GLY:HA2	2.56	0.41
3:F:70:LEU:C	3:F:71:THR:HG23	2.41	0.41
1:G:107:THR:CG2	1:G:113:ILE:HD11	2.51	0.41
2:H:57:GLY:O	2:H:58:VAL:C	2.58	0.41
2:H:198:HIS:CG	2:H:199:LYS:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:70:LEU:C	3:L:71:THR:HG23	2.41	0.41
1:A:50:PRO:CD	2:B:92:TYR:O	2.68	0.41
2:B:14:SER:O	2:B:17:GLU:HB2	2.21	0.41
2:B:57:GLY:O	2:B:58:VAL:C	2.58	0.41
2:B:122:SER:O	2:B:126:THR:HG23	2.21	0.41
3:C:12:VAL:O	3:C:116:VAL:HA	2.20	0.41
3:C:13:ARG:O	3:C:14:PRO:C	2.59	0.41
1:D:116:ILE:O	1:D:116:ILE:HG22	2.20	0.41
3:F:152:PRO:HD2	3:F:206:ALA:HB1	2.01	0.41
2:H:18:ARG:HH11	2:H:18:ARG:CG	2.30	0.41
2:H:59:PRO:HG2	2:H:62:PHE:CD2	2.56	0.41
2:H:170:ASP:OD2	2:H:170:ASP:C	2.58	0.41
2:H:193:THR:CA	2:H:208:SER:HB3	2.48	0.41
3:I:70:LEU:C	3:I:71:THR:HG23	2.41	0.41
2:K:13:VAL:HB	2:K:17:GLU:OE2	2.20	0.41
2:K:119:PRO:HG2	3:L:218:ARG:NH2	2.34	0.41
2:B:62:PHE:O	2:B:63:THR:CG2	2.69	0.41
2:B:170:ASP:OD2	2:B:170:ASP:C	2.58	0.41
3:C:54:SER:HA	3:C:74:LYS:HE3	2.02	0.41
3:C:124:PRO:HB3	3:C:150:TYR:HB3	2.03	0.41
1:G:3:PHE:CD2	1:G:128:VAL:HG23	2.56	0.41
1:G:15:ALA:CB	1:G:104:ILE:HG22	2.50	0.41
3:I:214:LYS:HG2	3:I:216:VAL:HG13	2.01	0.41
1:A:3:PHE:CD2	1:A:128:VAL:HG23	2.56	0.41
1:A:107:THR:CG2	1:A:113:ILE:HD11	2.51	0.41
2:B:36:PHE:HZ	3:C:105:PHE:CD1	2.39	0.41
2:B:159:VAL:O	2:B:160:LEU:HD23	2.21	0.41
3:C:133:SER:C	3:C:135:ALA:H	2.24	0.41
1:D:13:ILE:HG12	1:D:13:ILE:H	1.47	0.41
2:E:58:VAL:HA	2:E:59:PRO:HD2	1.93	0.41
2:E:122:SER:O	2:E:126:THR:HG23	2.21	0.41
3:F:126:VAL:HG13	3:F:211:VAL:HG11	2.03	0.41
2:H:14:SER:O	2:H:17:GLU:HB2	2.20	0.41
3:I:70:LEU:O	3:I:71:THR:CG2	2.69	0.41
2:K:15:VAL:O	2:K:15:VAL:HG22	2.21	0.41
2:K:26:SER:C	2:K:27:GLU:HG3	2.41	0.41
2:K:122:SER:O	2:K:126:THR:HG23	2.21	0.41
3:L:47:TRP:CH2	3:L:49:GLY:HA2	2.56	0.41
3:L:70:LEU:O	3:L:71:THR:CG2	2.69	0.41
1:A:116:ILE:O	1:A:116:ILE:HG22	2.20	0.41
2:E:136:LEU:N	2:E:136:LEU:CD1	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:PHE:HB2	2:E:140:TYR:H	1.77	0.41
2:E:149:LYS:HA	2:E:153:SER:O	2.21	0.41
3:F:50:ASN:ND2	3:F:50:ASN:H	2.10	0.41
3:F:54:SER:HA	3:F:74:LYS:HE3	2.02	0.41
3:I:155:VAL:HG23	3:I:204:HIS:HD2	1.86	0.41
2:K:14:SER:O	2:K:17:GLU:HB2	2.21	0.41
2:K:62:PHE:O	2:K:63:THR:CG2	2.69	0.41
2:K:198:HIS:CG	2:K:199:LYS:N	2.89	0.41
3:C:36:TRP:O	3:C:48:VAL:HB	2.21	0.40
3:C:140:MET:HG2	3:C:187:THR:HG22	2.01	0.40
2:E:26:SER:C	2:E:27:GLU:HG3	2.41	0.40
2:E:182:THR:HG1	2:E:185:GLU:HB2	1.84	0.40
3:F:124:PRO:HB3	3:F:150:TYR:HB3	2.03	0.40
2:H:15:VAL:O	2:H:15:VAL:HG22	2.21	0.40
2:H:26:SER:C	2:H:27:GLU:HG3	2.41	0.40
2:H:62:PHE:O	2:H:63:THR:CG2	2.69	0.40
3:I:126:VAL:HG13	3:I:211:VAL:HG11	2.03	0.40
1:J:114:LEU:N	1:J:114:LEU:HD12	2.36	0.40
2:K:82:ASP:O	2:K:104:LEU:HD23	2.21	0.40
2:K:159:VAL:O	2:K:160:LEU:HD23	2.21	0.40
1:A:5:TYR:CE2	1:A:128:VAL:HG11	2.52	0.40
2:B:149:LYS:HA	2:B:153:SER:O	2.21	0.40
3:F:13:ARG:O	3:F:14:PRO:C	2.59	0.40
2:H:52:SER:CB	2:H:64:GLY:O	2.70	0.40
2:H:205:ILE:HD12	2:H:205:ILE:H	1.87	0.40
3:I:13:ARG:O	3:I:14:PRO:C	2.59	0.40
1:J:116:ILE:O	1:J:116:ILE:HG22	2.20	0.40
1:J:126:HIS:ND1	1:J:127:GLU:N	2.68	0.40
2:B:82:ASP:O	2:B:104:LEU:HD23	2.21	0.40
3:C:2:VAL:O	3:C:2:VAL:HG22	2.21	0.40
3:C:32:TYR:O	3:C:53:PRO:HD2	2.22	0.40
3:C:86:PRO:C	3:C:87:THR:CG2	2.90	0.40
3:C:87:THR:O	3:C:116:VAL:HG21	2.21	0.40
1:D:107:THR:CG2	1:D:113:ILE:HD11	2.51	0.40
2:E:133:VAL:HG12	2:E:178:THR:HB	2.03	0.40
2:E:159:VAL:O	2:E:160:LEU:HD23	2.21	0.40
2:H:159:VAL:O	2:H:160:LEU:HD23	2.21	0.40
1:J:3:PHE:CD2	1:J:128:VAL:HG23	2.56	0.40
3:L:168:VAL:O	3:L:168:VAL:HG23	2.21	0.40
2:B:198:HIS:CG	2:B:199:LYS:N	2.89	0.40
3:C:70:LEU:O	3:C:71:THR:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:PHE:O	2:E:63:THR:CG2	2.69	0.40
3:F:2:VAL:O	3:F:2:VAL:HG22	2.21	0.40
2:H:149:LYS:HA	2:H:153:SER:O	2.21	0.40
3:I:47:TRP:CH2	3:I:49:GLY:HA2	2.56	0.40
2:K:59:PRO:HG2	2:K:62:PHE:CD2	2.56	0.40
3:L:41:PRO:O	3:L:43:GLN:HG2	2.22	0.40
3:L:130:ALA:O	3:L:218:ARG:NH1	2.49	0.40
1:A:129:LYS:HA	1:A:129:LYS:CE	2.44	0.40
2:B:52:SER:CB	2:B:64:GLY:O	2.70	0.40
1:G:114:LEU:HD12	1:G:114:LEU:N	2.36	0.40
3:I:41:PRO:O	3:I:43:GLN:HG2	2.22	0.40
1:J:45:GLU:HB2	3:L:32:TYR:CD1	2.56	0.40
2:K:13:VAL:HG11	2:K:19:VAL:CG2	2.50	0.40
2:K:52:SER:CB	2:K:64:GLY:O	2.69	0.40
3:L:2:VAL:O	3:L:2:VAL:HG22	2.21	0.40
3:L:86:PRO:O	3:L:87:THR:HG22	2.21	0.40
3:L:155:VAL:HG23	3:L:204:HIS:HD2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/159 (99%)	120 (76%)	28 (18%)	9 (6%)	1	4
1	D	157/159 (99%)	120 (76%)	28 (18%)	9 (6%)	1	4
1	G	157/159 (99%)	120 (76%)	28 (18%)	9 (6%)	1	4
1	J	157/159 (99%)	120 (76%)	28 (18%)	9 (6%)	1	4
2	B	212/214 (99%)	177 (84%)	29 (14%)	6 (3%)	4	16
2	E	212/214 (99%)	177 (84%)	29 (14%)	6 (3%)	4	16
2	H	212/214 (99%)	176 (83%)	30 (14%)	6 (3%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	212/214 (99%)	176 (83%)	30 (14%)	6 (3%)	4	16
3	C	218/220 (99%)	192 (88%)	20 (9%)	6 (3%)	4	16
3	F	218/220 (99%)	192 (88%)	20 (9%)	6 (3%)	4	16
3	I	218/220 (99%)	193 (88%)	19 (9%)	6 (3%)	4	16
3	L	218/220 (99%)	192 (88%)	20 (9%)	6 (3%)	4	16
All	All	2348/2372 (99%)	1955 (83%)	309 (13%)	84 (4%)	3	12

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	2	VAL
3	F	2	VAL
3	I	2	VAL
3	L	2	VAL
1	A	130	ALA
2	B	82	ASP
2	B	140	TYR
3	C	101	ARG
1	D	130	ALA
2	E	82	ASP
2	E	140	TYR
3	F	101	ARG
1	G	130	ALA
2	H	82	ASP
2	H	140	TYR
3	I	101	ARG
1	J	130	ALA
2	K	82	ASP
2	K	140	TYR
3	L	101	ARG
1	A	16	ALA
1	A	21	ALA
1	A	111	GLY
1	A	124	GLY
1	A	155	SER
2	B	50	GLY
3	C	65	LYS
1	D	16	ALA
1	D	21	ALA
1	D	124	GLY

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Mol	Chain	Res	Type
1	D	155	SER
2	E	50	GLY
2	E	60	ASP
3	F	65	LYS
1	G	16	ALA
1	G	21	ALA
1	G	124	GLY
1	G	155	SER
2	H	50	GLY
3	I	65	LYS
1	J	16	ALA
1	J	21	ALA
1	J	124	GLY
1	J	155	SER
2	K	50	GLY
3	L	65	LYS
1	A	93	ASP
2	B	60	ASP
2	B	68	THR
3	C	177	SER
1	D	93	ASP
1	D	111	GLY
2	E	68	THR
3	F	177	SER
1	G	93	ASP
1	G	111	GLY
2	H	60	ASP
2	H	68	THR
3	I	177	SER
1	J	93	ASP
1	J	111	GLY
2	K	60	ASP
2	K	68	THR
3	L	177	SER
2	B	58	VAL
3	C	53	PRO
3	C	63	LYS
2	E	58	VAL
3	F	53	PRO
3	F	63	LYS
2	H	58	VAL
3	I	53	PRO

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Mol	Chain	Res	Type
3	I	63	LYS
2	K	58	VAL
3	L	53	PRO
3	L	63	LYS
1	A	158	TYR
1	D	158	TYR
1	G	158	TYR
1	J	158	TYR
1	A	88	GLY
1	D	88	GLY
1	G	88	GLY
1	J	88	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/134 (100%)	122 (91%)	12 (9%)	8	25
1	D	134/134 (100%)	122 (91%)	12 (9%)	8	25
1	G	134/134 (100%)	122 (91%)	12 (9%)	8	25
1	J	134/134 (100%)	121 (90%)	13 (10%)	6	22
2	B	193/193 (100%)	171 (89%)	22 (11%)	4	15
2	E	193/193 (100%)	171 (89%)	22 (11%)	4	15
2	H	193/193 (100%)	171 (89%)	22 (11%)	4	15
2	K	193/193 (100%)	171 (89%)	22 (11%)	4	15
3	C	192/192 (100%)	163 (85%)	29 (15%)	2	7
3	F	192/192 (100%)	162 (84%)	30 (16%)	2	7
3	I	192/192 (100%)	163 (85%)	29 (15%)	2	7
3	L	192/192 (100%)	162 (84%)	30 (16%)	2	7
All	All	2076/2076 (100%)	1821 (88%)	255 (12%)	4	12

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	13	ILE
1	A	47	ASN
1	A	55	LYS
1	A	60	GLU
1	A	70	ARG
1	A	95	LEU
1	A	123	LYS
1	A	125	ASP
1	A	129	LYS
1	A	131	GLU
1	A	145	ARG
2	B	15	VAL
2	B	18	ARG
2	B	22	SER
2	B	48	LEU
2	B	60	ASP
2	B	61	ARG
2	B	81	GLU
2	B	88	CYS
2	B	108	ARG
2	B	122	SER
2	B	142	LYS
2	B	143	ASP
2	B	154	GLU
2	B	163	TRP
2	B	165	ASP
2	B	167	ASP
2	B	176	SER
2	B	178	THR
2	B	179	LEU
2	B	181	LEU
2	B	202	THR
2	B	214	CYS
3	C	2	VAL
3	C	6	GLN
3	C	7	PRO
3	C	9	THR
3	C	14	PRO
3	C	50	ASN
3	C	55	ASP
3	C	57	TYR
3	C	72	VAL

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Mol	Chain	Res	Type
3	C	78	THR
3	C	82	GLN
3	C	98	ARG
3	C	103	THR
3	C	118	VAL
3	C	121	THR
3	C	126	VAL
3	C	137	THR
3	C	146	LEU
3	C	152	PRO
3	C	154	PRO
3	C	155	VAL
3	C	156	THR
3	C	157	VAL
3	C	181	THR
3	C	186	VAL
3	C	197	THR
3	C	199	THR
3	C	201	ASN
3	C	219	ASP
1	D	10	THR
1	D	13	ILE
1	D	47	ASN
1	D	55	LYS
1	D	60	GLU
1	D	70	ARG
1	D	95	LEU
1	D	123	LYS
1	D	125	ASP
1	D	129	LYS
1	D	131	GLU
1	D	145	ARG
2	E	15	VAL
2	E	18	ARG
2	E	22	SER
2	E	48	LEU
2	E	60	ASP
2	E	61	ARG
2	E	81	GLU
2	E	88	CYS
2	E	108	ARG
2	E	122	SER

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Mol	Chain	Res	Type
2	E	142	LYS
2	E	143	ASP
2	E	154	GLU
2	E	163	TRP
2	E	165	ASP
2	E	167	ASP
2	E	176	SER
2	E	178	THR
2	E	179	LEU
2	E	181	LEU
2	E	202	THR
2	E	214	CYS
3	F	2	VAL
3	F	6	GLN
3	F	7	PRO
3	F	9	THR
3	F	14	PRO
3	F	50	ASN
3	F	55	ASP
3	F	57	TYR
3	F	72	VAL
3	F	78	THR
3	F	82	GLN
3	F	98	ARG
3	F	103	THR
3	F	118	VAL
3	F	121	THR
3	F	124	PRO
3	F	126	VAL
3	F	137	THR
3	F	146	LEU
3	F	152	PRO
3	F	154	PRO
3	F	155	VAL
3	F	156	THR
3	F	157	VAL
3	F	181	THR
3	F	186	VAL
3	F	197	THR
3	F	199	THR
3	F	201	ASN
3	F	219	ASP

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Mol	Chain	Res	Type
1	G	10	THR
1	G	13	ILE
1	G	47	ASN
1	G	55	LYS
1	G	60	GLU
1	G	70	ARG
1	G	95	LEU
1	G	123	LYS
1	G	125	ASP
1	G	129	LYS
1	G	131	GLU
1	G	145	ARG
2	H	15	VAL
2	H	18	ARG
2	H	22	SER
2	H	48	LEU
2	H	60	ASP
2	H	61	ARG
2	H	81	GLU
2	H	88	CYS
2	H	108	ARG
2	H	122	SER
2	H	142	LYS
2	H	143	ASP
2	H	154	GLU
2	H	163	TRP
2	H	165	ASP
2	H	167	ASP
2	H	176	SER
2	H	178	THR
2	H	179	LEU
2	H	181	LEU
2	H	202	THR
2	H	214	CYS
3	I	2	VAL
3	I	6	GLN
3	I	7	PRO
3	I	9	THR
3	I	14	PRO
3	I	50	ASN
3	I	55	ASP
3	I	57	TYR

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Mol	Chain	Res	Type
3	I	72	VAL
3	I	78	THR
3	I	82	GLN
3	I	98	ARG
3	I	103	THR
3	I	118	VAL
3	I	121	THR
3	I	126	VAL
3	I	137	THR
3	I	146	LEU
3	I	152	PRO
3	I	154	PRO
3	I	155	VAL
3	I	156	THR
3	I	157	VAL
3	I	181	THR
3	I	186	VAL
3	I	197	THR
3	I	199	THR
3	I	201	ASN
3	I	219	ASP
1	J	10	THR
1	J	13	ILE
1	J	47	ASN
1	J	55	LYS
1	J	60	GLU
1	J	70	ARG
1	J	95	LEU
1	J	99	SER
1	J	123	LYS
1	J	125	ASP
1	J	129	LYS
1	J	131	GLU
1	J	145	ARG
2	K	15	VAL
2	K	18	ARG
2	K	22	SER
2	K	48	LEU
2	K	60	ASP
2	K	61	ARG
2	K	81	GLU
2	K	88	CYS

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Mol	Chain	Res	Type
2	K	108	ARG
2	K	122	SER
2	K	142	LYS
2	K	143	ASP
2	K	154	GLU
2	K	163	TRP
2	K	165	ASP
2	K	167	ASP
2	K	176	SER
2	K	178	THR
2	K	179	LEU
2	K	181	LEU
2	K	202	THR
2	K	214	CYS
3	L	2	VAL
3	L	6	GLN
3	L	7	PRO
3	L	9	THR
3	L	14	PRO
3	L	50	ASN
3	L	55	ASP
3	L	57	TYR
3	L	72	VAL
3	L	78	THR
3	L	82	GLN
3	L	98	ARG
3	L	103	THR
3	L	118	VAL
3	L	121	THR
3	L	124	PRO
3	L	126	VAL
3	L	137	THR
3	L	146	LEU
3	L	152	PRO
3	L	154	PRO
3	L	155	VAL
3	L	156	THR
3	L	157	VAL
3	L	181	THR
3	L	186	VAL
3	L	197	THR
3	L	199	THR

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Mol	Chain	Res	Type
3	L	201	ASN
3	L	219	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	47	ASN
1	A	118	ASN
1	A	121	HIS
1	A	132	GLN
1	A	159	ASN
2	B	6	GLN
2	B	28	ASN
2	B	138	ASN
2	B	212	ASN
3	C	50	ASN
3	C	62	GLN
3	C	82	GLN
3	C	110	GLN
3	C	169	HIS
3	C	201	ASN
1	D	4	ASN
1	D	47	ASN
1	D	118	ASN
1	D	121	HIS
1	D	132	GLN
1	D	159	ASN
2	E	6	GLN
2	E	28	ASN
2	E	138	ASN
2	E	212	ASN
3	F	50	ASN
3	F	62	GLN
3	F	82	GLN
3	F	110	GLN
3	F	169	HIS
3	F	201	ASN
1	G	4	ASN
1	G	47	ASN
1	G	118	ASN
1	G	121	HIS

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Mol	Chain	Res	Type
1	G	132	GLN
1	G	159	ASN
2	H	6	GLN
2	H	28	ASN
2	H	138	ASN
2	H	190	ASN
2	H	212	ASN
3	I	1	GLN
3	I	3	GLN
3	I	50	ASN
3	I	62	GLN
3	I	82	GLN
3	I	110	GLN
3	I	169	HIS
3	I	201	ASN
1	J	4	ASN
1	J	47	ASN
1	J	118	ASN
1	J	121	HIS
1	J	132	GLN
1	J	159	ASN
2	K	6	GLN
2	K	28	ASN
2	K	138	ASN
2	K	212	ASN
3	L	50	ASN
3	L	62	GLN
3	L	82	GLN
3	L	110	GLN
3	L	169	HIS
3	L	201	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	159/159 (100%)	0.71	14 (8%)	17	15	22, 56, 89, 124	0
1	D	159/159 (100%)	0.82	17 (10%)	12	11	18, 55, 92, 109	0
1	G	159/159 (100%)	1.45	47 (29%)	1	1	27, 76, 108, 128	0
1	J	159/159 (100%)	2.08	77 (48%)	0	0	27, 89, 116, 133	0
2	B	214/214 (100%)	0.53	15 (7%)	24	20	19, 52, 92, 137	0
2	E	214/214 (100%)	0.71	14 (6%)	26	22	19, 56, 93, 132	0
2	H	214/214 (100%)	1.75	81 (37%)	1	1	41, 86, 119, 153	0
2	K	214/214 (100%)	0.96	32 (14%)	6	6	32, 62, 91, 132	0
3	C	220/220 (100%)	0.22	11 (5%)	35	30	18, 44, 84, 123	0
3	F	220/220 (100%)	0.35	11 (5%)	35	30	14, 49, 86, 121	0
3	I	220/220 (100%)	0.73	21 (9%)	15	13	33, 60, 106, 134	0
3	L	220/220 (100%)	0.75	15 (6%)	25	21	25, 56, 93, 123	0
All	All	2372/2372 (100%)	0.89	355 (14%)	6	6	14, 59, 105, 153	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	118	ASN	7.5
1	J	110	GLY	7.4
1	J	111	GLY	6.5
3	L	134	ALA	6.4
1	G	106	ALA	6.2
2	H	154	GLU	5.9
2	H	109	ALA	5.4
2	K	190	ASN	5.3
2	E	190	ASN	5.3
2	E	212	ASN	5.3
2	H	212	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
2	K	212	ASN	5.1
2	E	210	ASN	4.8
1	J	112	SER	4.8
1	A	157	ALA	4.8
3	I	134	ALA	4.7
1	G	112	SER	4.6
1	J	106	ALA	4.6
1	G	107	THR	4.6
2	H	190	ASN	4.5
1	J	3	PHE	4.4
2	H	198	HIS	4.4
3	L	132	GLY	4.3
1	J	37	ALA	4.3
1	G	118	ASN	4.3
2	H	16	GLY	4.3
3	I	89	GLU	4.2
2	H	125	LEU	4.2
1	J	149	SER	4.2
1	G	111	GLY	4.2
1	J	122	THR	4.1
1	J	135	ALA	4.1
2	H	145	ASN	4.0
1	J	67	VAL	4.0
2	H	162	SER	4.0
3	L	137	THR	4.0
1	J	138	GLU	4.0
1	J	94	THR	3.9
2	H	13	VAL	3.9
1	G	144	LEU	3.8
1	J	95	LEU	3.8
1	G	153	ALA	3.8
3	C	137	THR	3.8
2	H	153	SER	3.8
1	J	21	ALA	3.8
2	H	11	MET	3.8
1	J	146	ALA	3.7
1	J	19	PHE	3.7
2	K	70	ASP	3.7
1	J	4	ASN	3.7
1	J	91	ILE	3.7
1	A	127	GLU	3.6
1	G	140	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	134	CYS	3.6
3	L	1	GLN	3.6
1	J	62	LEU	3.5
2	B	213	GLU	3.5
2	H	210	ASN	3.5
3	I	176	GLN	3.5
3	I	194	PRO	3.5
1	D	107	THR	3.5
2	B	198	HIS	3.5
2	B	203	SER	3.5
2	H	4	LEU	3.5
2	H	12	SER	3.5
2	H	129	GLY	3.4
2	K	210	ASN	3.4
1	G	148	GLU	3.4
1	A	26	GLY	3.4
1	G	110	GLY	3.4
1	J	31	PRO	3.3
1	J	131	GLU	3.3
2	H	121	SER	3.3
2	K	27	GLU	3.2
1	J	98	ILE	3.2
2	B	152	GLY	3.2
1	D	106	ALA	3.2
2	K	50	GLY	3.2
1	J	79	PHE	3.2
2	K	32	TYR	3.1
1	J	143	LEU	3.1
1	G	132	GLN	3.1
2	H	69	THR	3.1
2	H	102	THR	3.1
3	F	137	THR	3.1
3	I	1	GLN	3.1
1	G	17	ARG	3.1
2	H	93	SER	3.1
1	G	75	ASP	3.1
2	H	6	GLN	3.0
1	G	6	GLU	3.0
1	G	37	ALA	3.0
1	G	64	PHE	3.0
2	K	202	THR	3.0
1	G	99	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	195	GLU	3.0
1	G	105	VAL	3.0
2	H	159	VAL	3.0
1	G	145	ARG	3.0
1	J	64	PHE	3.0
1	J	99	SER	3.0
1	J	36	GLN	3.0
2	K	77	SER	3.0
2	K	184	ASP	2.9
2	H	141	PRO	2.9
2	H	14	SER	2.9
3	C	176	GLN	2.9
2	H	181	LEU	2.9
1	J	148	GLU	2.9
3	L	101	ARG	2.9
2	H	191	SER	2.9
1	J	22	PHE	2.9
1	G	88	GLY	2.9
2	H	170	ASP	2.9
2	K	30	ASP	2.9
1	J	83	TYR	2.9
1	G	9	THR	2.9
2	B	169	LYS	2.9
2	H	70	ASP	2.9
2	H	184	ASP	2.9
2	B	214	CYS	2.9
3	L	220	CYS	2.9
1	J	128	VAL	2.9
2	E	213	GLU	2.9
2	H	118	PHE	2.8
1	A	111	GLY	2.8
2	B	190	ASN	2.8
2	H	209	PHE	2.8
3	L	67	LYS	2.8
1	J	88	GLY	2.8
1	G	149	SER	2.8
2	H	143	ASP	2.8
2	H	130	ALA	2.8
1	G	77	THR	2.8
2	H	172	THR	2.8
2	H	213	GLU	2.8
1	J	129	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	157	ASN	2.8
3	F	138	ASN	2.8
1	G	27	ASP	2.8
2	K	25	ALA	2.8
2	H	136	LEU	2.8
2	E	157	ASN	2.8
1	A	137	LYS	2.8
3	F	220	CYS	2.8
3	I	137	THR	2.8
2	H	104	LEU	2.8
1	A	126	HIS	2.8
2	H	60	ASP	2.7
1	J	113	ILE	2.7
3	F	41	PRO	2.7
1	J	16	ALA	2.7
1	G	109	ASP	2.7
1	G	127	GLU	2.7
1	G	108	PRO	2.7
2	H	163	TRP	2.7
1	D	159	ASN	2.7
1	G	129	LYS	2.7
3	L	63	LYS	2.7
2	H	32	TYR	2.7
3	I	63	LYS	2.7
1	J	155	SER	2.7
3	C	196	GLU	2.7
1	J	9	THR	2.7
2	H	139	PHE	2.6
2	K	195	GLU	2.6
1	J	5	TYR	2.6
1	J	120	TYR	2.6
1	D	125	ASP	2.6
1	D	128	VAL	2.6
2	E	214	CYS	2.6
3	I	193	TRP	2.6
3	L	89	GLU	2.6
1	J	59	PRO	2.6
1	J	92	GLY	2.6
2	H	77	SER	2.6
2	H	203	SER	2.6
1	A	106	ALA	2.6
1	J	108	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	189	PRO	2.6
2	B	201	SER	2.6
2	K	93	SER	2.6
3	F	134	ALA	2.6
2	H	148	TRP	2.6
3	C	220	CYS	2.6
1	J	107	THR	2.6
1	J	105	VAL	2.6
3	L	77	SER	2.6
2	H	166	GLN	2.5
1	G	16	ALA	2.5
1	J	15	ALA	2.5
1	J	153	ALA	2.5
3	I	16	ALA	2.5
2	K	60	ASP	2.5
1	J	63	PRO	2.5
2	K	204	PRO	2.5
1	J	147	VAL	2.5
2	H	115	VAL	2.5
2	K	26	SER	2.5
1	G	137	LYS	2.5
1	D	131	GLU	2.5
2	E	81	GLU	2.5
1	J	139	MET	2.5
2	H	193	THR	2.5
1	J	69	ASP	2.5
2	E	70	ASP	2.5
1	D	130	ALA	2.5
1	J	116	ILE	2.5
1	J	17	ARG	2.4
1	A	110	GLY	2.4
1	J	41	VAL	2.4
2	K	214	CYS	2.4
2	H	137	ASN	2.4
2	E	180	THR	2.4
3	C	199	THR	2.4
2	H	171	SER	2.4
2	E	204	PRO	2.4
1	J	144	LEU	2.4
1	A	6	GLU	2.4
1	A	73	GLU	2.4
2	H	150	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	32	LYS	2.4
3	I	135	ALA	2.4
2	K	182	THR	2.4
1	G	31	PRO	2.4
3	C	177	SER	2.4
1	G	19	PHE	2.4
1	J	82	ASN	2.4
2	H	5	THR	2.4
2	H	51	PRO	2.4
1	G	152	LEU	2.4
2	H	177	SER	2.4
1	A	128	VAL	2.4
2	K	154	GLU	2.4
1	J	157	ALA	2.4
2	E	193	THR	2.4
2	H	164	THR	2.4
2	K	31	THR	2.4
2	H	192	TYR	2.3
3	L	53	PRO	2.3
1	J	12	VAL	2.3
2	K	12	SER	2.3
2	K	191	SER	2.3
1	D	60	GLU	2.3
1	G	141	GLU	2.3
1	D	4	ASN	2.3
1	J	10	THR	2.3
2	K	88	CYS	2.3
2	E	158	GLY	2.3
2	H	128	GLY	2.3
1	J	133	VAL	2.3
1	A	96	GLU	2.3
2	H	10	SER	2.3
2	H	211	ARG	2.3
2	H	173	TYR	2.3
2	H	152	GLY	2.3
1	J	141	GLU	2.3
1	A	37	ALA	2.3
2	K	201	SER	2.3
3	L	135	ALA	2.3
1	J	145	ARG	2.3
3	I	218	ARG	2.3
1	D	24	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	199	THR	2.3
1	J	126	HIS	2.3
3	I	44	GLY	2.3
3	C	134	ALA	2.3
2	B	153	SER	2.3
2	K	110	ASP	2.3
2	H	169	LYS	2.3
2	H	161	ASN	2.2
2	H	144	ILE	2.2
2	K	150	ILE	2.2
1	J	130	ALA	2.2
3	C	88	SER	2.2
2	H	114	THR	2.2
2	K	3	VAL	2.2
2	K	129	GLY	2.2
1	J	119	LYS	2.2
2	H	110	ASP	2.2
3	C	138	ASN	2.2
1	D	153	ALA	2.2
1	G	131	GLU	2.2
2	H	17	GLU	2.2
1	D	62	LEU	2.2
2	E	184	ASP	2.2
2	B	43	SER	2.2
3	F	133	SER	2.2
2	H	180	THR	2.2
2	H	158	GLY	2.2
1	J	78	ASN	2.2
3	C	135	ALA	2.2
1	D	138	GLU	2.2
1	G	60	GLU	2.2
2	K	2	ILE	2.2
3	I	169	HIS	2.1
1	G	65	LYS	2.1
3	F	67	LYS	2.1
2	H	214	CYS	2.1
1	G	133	VAL	2.1
3	C	133	SER	2.1
3	F	144	GLY	2.1
3	I	177	SER	2.1
1	G	8	GLU	2.1
2	B	81	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	117	ILE	2.1
2	H	15	VAL	2.1
3	L	114	VAL	2.1
2	K	11	MET	2.1
1	D	9	THR	2.1
2	B	197	THR	2.1
1	J	97	LYS	2.1
3	I	43	GLN	2.1
3	L	57	TYR	2.1
2	K	213	GLU	2.1
1	J	44	ILE	2.1
2	H	132	VAL	2.1
1	J	61	GLY	2.1
1	J	136	SER	2.1
1	J	152	LEU	2.1
2	H	7	SER	2.1
3	L	3	GLN	2.1
1	J	101	GLU	2.1
3	F	89	GLU	2.1
3	I	84	ASN	2.1
1	G	63	PRO	2.1
2	H	40	PRO	2.1
1	G	38	ILE	2.1
1	D	126	HIS	2.1
1	J	58	PHE	2.1
1	G	62	LEU	2.0
1	G	95	LEU	2.0
2	H	124	GLN	2.0
1	G	157	ALA	2.0
2	E	208	SER	2.0
2	H	65	SER	2.0
2	H	84	ALA	2.0
2	H	201	SER	2.0
3	I	133	SER	2.0
1	A	133	VAL	2.0
1	G	2	VAL	2.0
2	B	11	MET	2.0
1	G	151	LEU	2.0
2	H	74	THR	2.0
3	F	136	GLN	2.0
3	I	219	ASP	2.0
1	J	39	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	38	ILE	2.0
1	D	118	ASN	2.0
2	B	53	ASN	2.0
1	D	129	LYS	2.0
1	J	2	VAL	2.0
3	I	168	VAL	2.0
1	G	121	HIS	2.0
3	I	220	CYS	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.