



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 1FSK / pdb_00001fsk
Title : COMPLEX FORMATION BETWEEN A FAB FRAGMENT OF A MONO-CLONAL IGG ANTIBODY AND THE MAJOR ALLERGEN FROM BIRCH POLLEN BET V 1
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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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

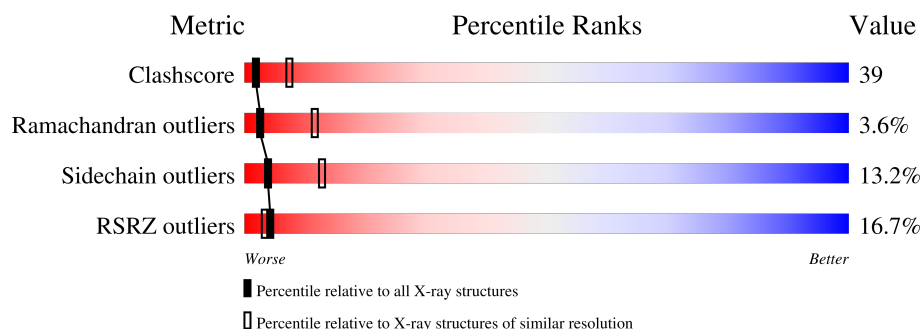
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	159	10% 45% 44% 11%
1	D	159	12% 45% 43% 11%
1	G	159	34% 44% 45% 11%
1	J	159	52% 43% 46% 11%
2	B	214	10% 35% 52% 12%
2	E	214	7% 37% 51% 12%
2	H	214	41% 36% 51% 12%

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Mol	Chain	Length	Quality of chain
2	K	214	15% 37% 50% 12%
3	C	220	5% 44% 44% 11%
3	F	220	6% 42% 45% 12%
3	I	220	10% 41% 47% 11%
3	L	220	8% 42% 45% 12%

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

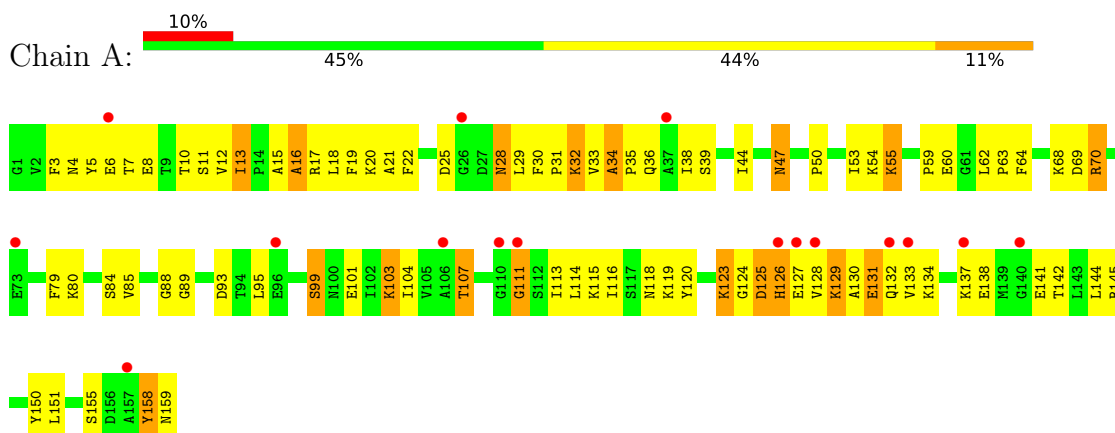
- Molecule 3 is a protein called ANTIBODY HEAVY CHAIN FAB.

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

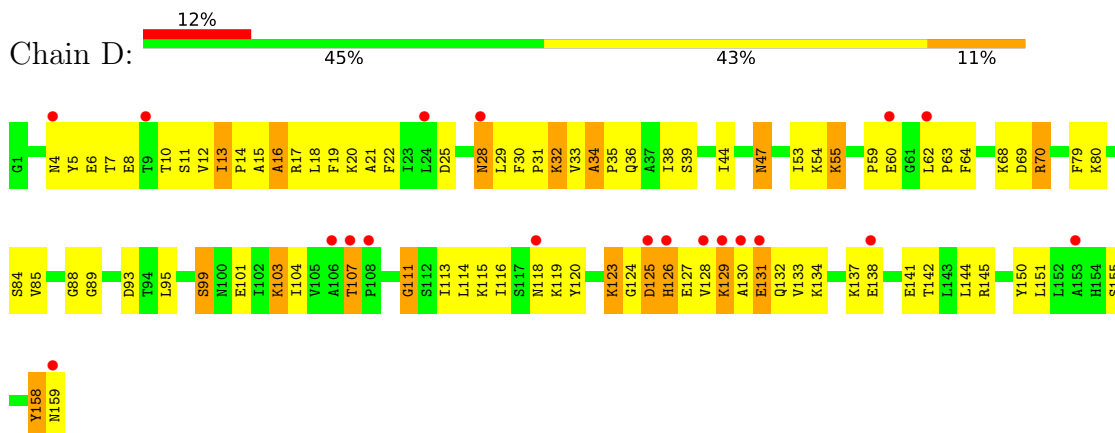
3 Residue-property plots

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.

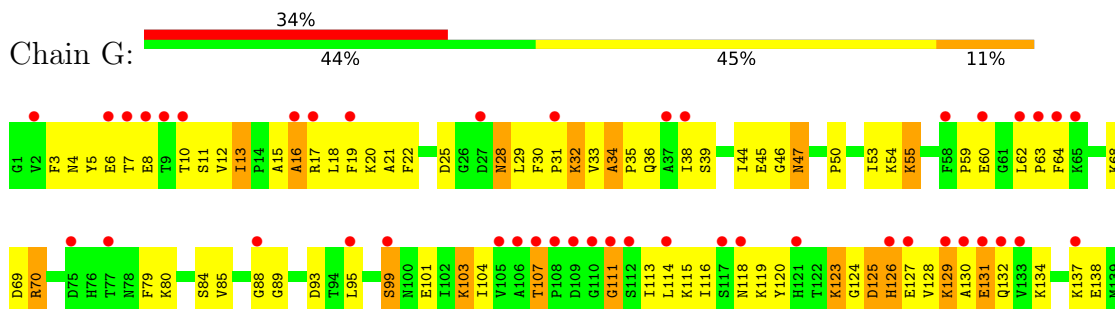
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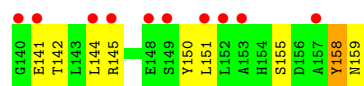


• Molecule 1: MAJOR POLLEN ALLERGEN BET V 1-A

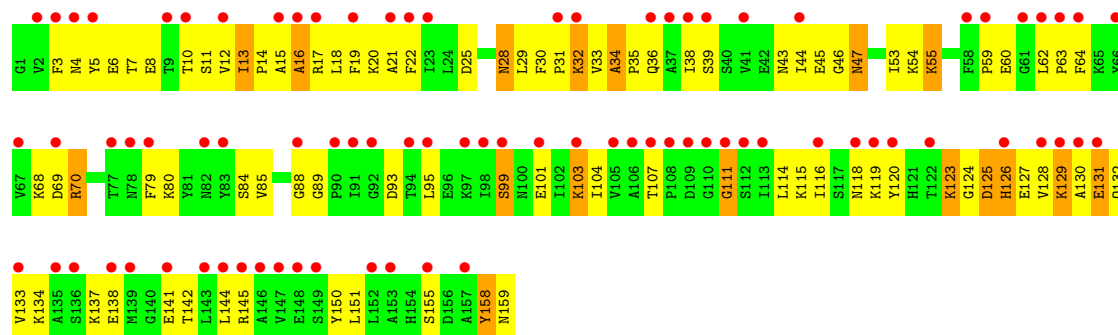


• Molecule 1: MAJOR POLLEN ALLERGEN BET V 1-A

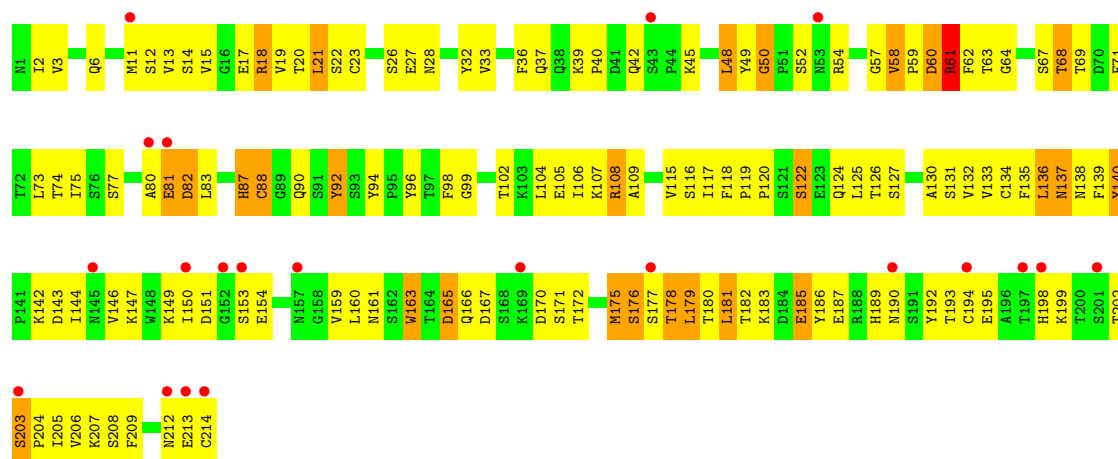




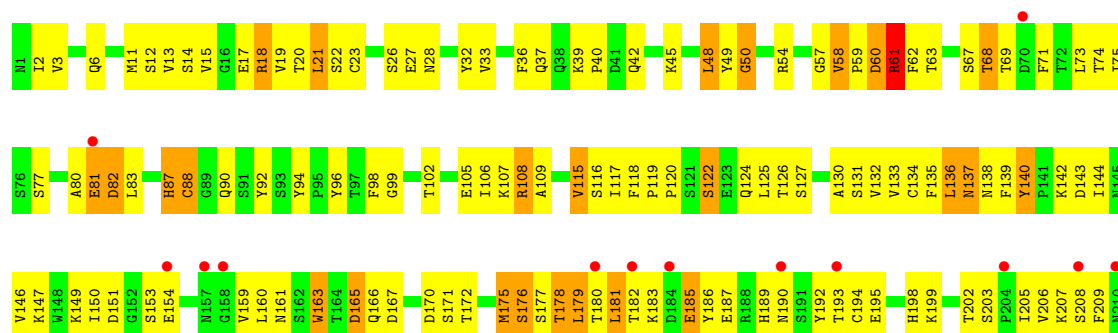
● Molecule 1: MAJOR POLLEN ALLERGEN BET V 1-A



● Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN

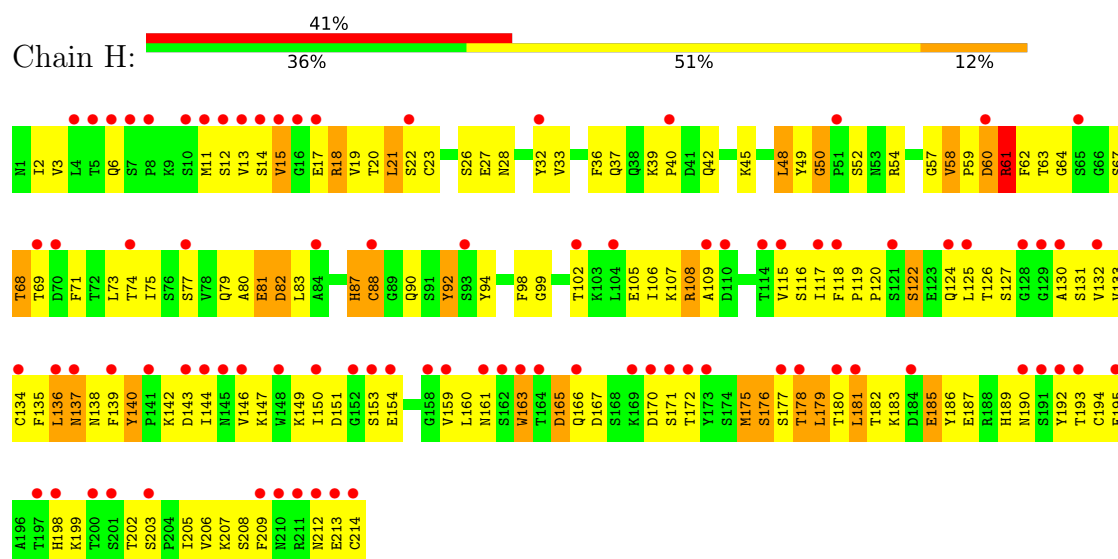


● Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN

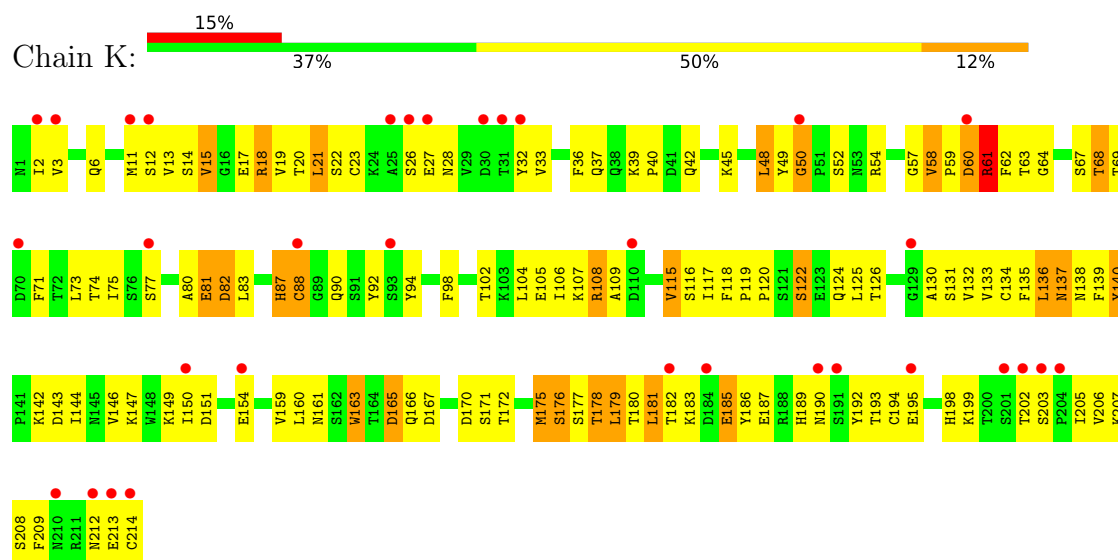




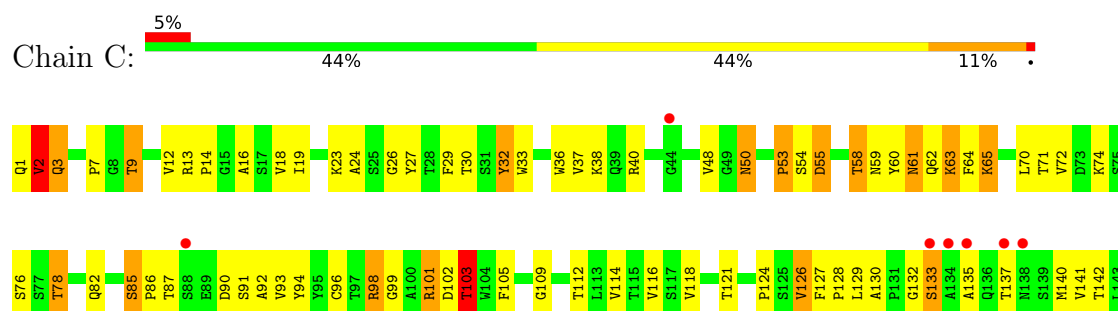
• Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN

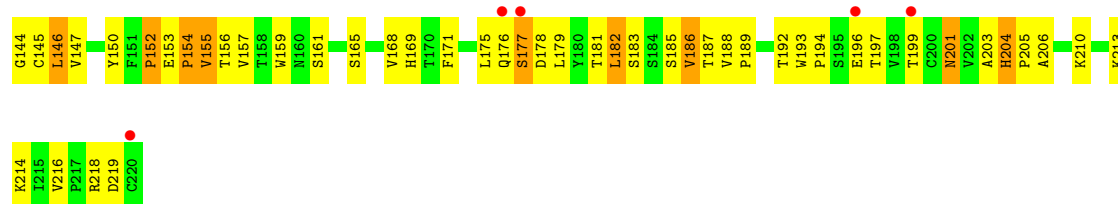


• Molecule 2: IMMUNOGLOBULIN KAPPA LIGHT CHAIN

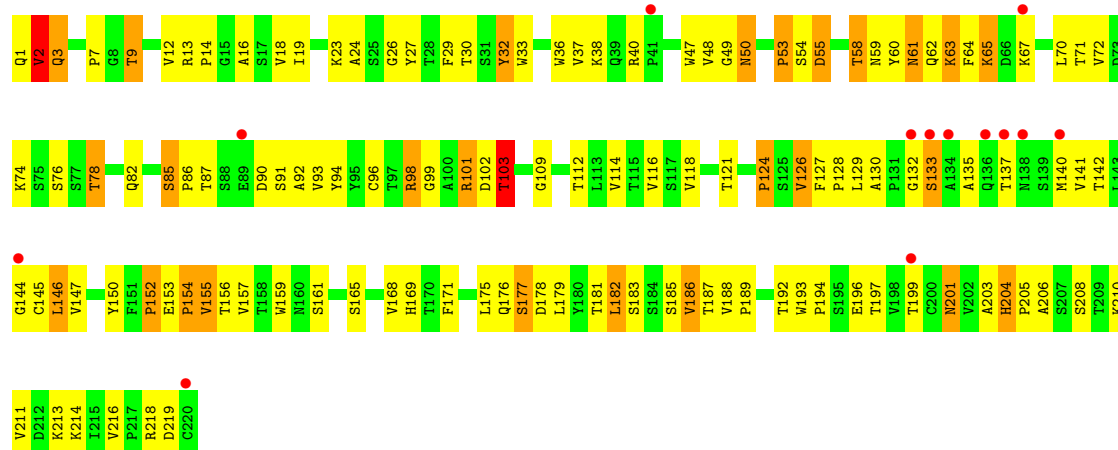


• Molecule 3: ANTIBODY HEAVY CHAIN FAB

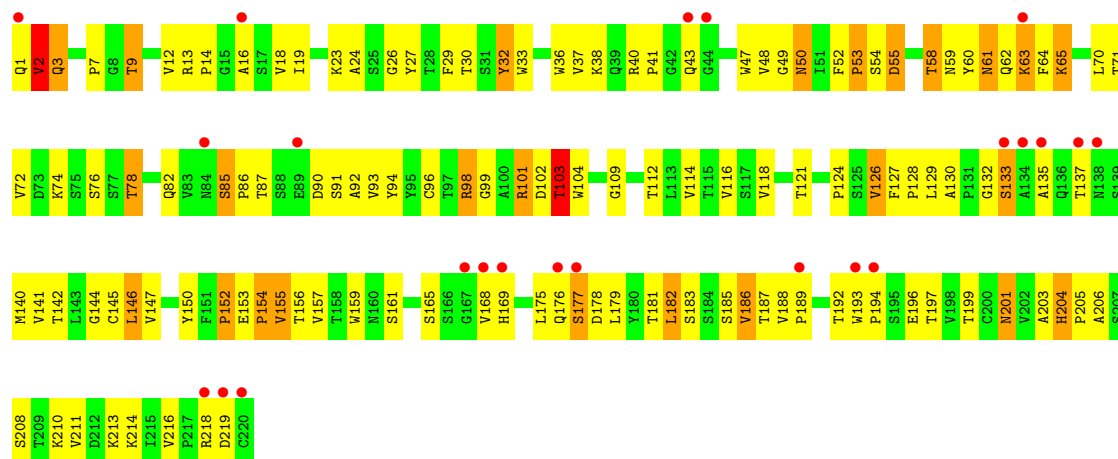




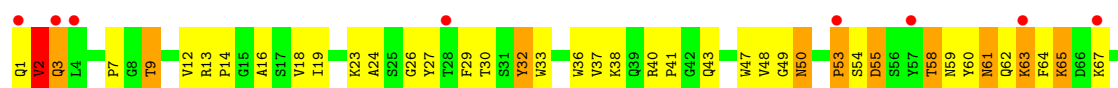
• Molecule 3: ANTIBODY HEAVY CHAIN FAB

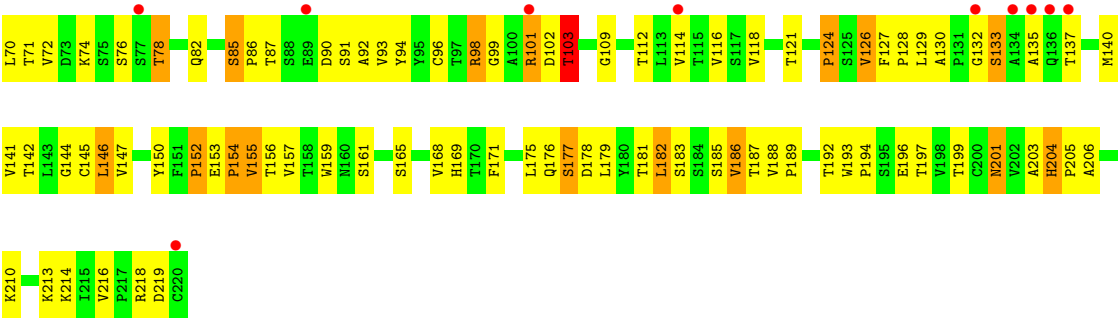


• Molecule 3: ANTIBODY HEAVY CHAIN FAB



• Molecule 3: ANTIBODY HEAVY CHAIN FAB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	53.1	Xtrriage
Anisotropy	0.271	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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	0.56	0/1255	1.06	8/1696 (0.5%)
1	D	0.57	0/1255	1.06	8/1696 (0.5%)
1	G	0.57	0/1255	1.06	8/1696 (0.5%)
1	J	0.57	0/1255	1.06	8/1696 (0.5%)
2	B	0.58	0/1707	1.10	9/2319 (0.4%)
2	E	0.58	0/1707	1.10	10/2319 (0.4%)
2	H	0.57	0/1707	1.09	8/2319 (0.3%)
2	K	0.58	0/1707	1.10	8/2319 (0.3%)
3	C	0.62	0/1727	1.12	12/2368 (0.5%)
3	F	0.62	0/1727	1.12	12/2368 (0.5%)
3	I	0.61	0/1727	1.12	12/2368 (0.5%)
3	L	0.62	0/1727	1.12	12/2368 (0.5%)
All	All	0.59	0/18756	1.09	115/25532 (0.5%)

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	94	TYR	N-CA-C	-11.39	94.59	110.31
2	E	94	TYR	N-CA-C	-11.08	95.02	110.31
2	H	94	TYR	N-CA-C	-10.95	95.20	110.31
2	B	94	TYR	N-CA-C	-10.92	95.23	110.31
3	I	61	ASN	N-CA-C	-8.08	99.10	110.50
3	C	61	ASN	N-CA-C	-8.03	99.18	110.50
3	F	61	ASN	N-CA-C	-7.98	99.25	110.50
3	L	61	ASN	N-CA-C	-7.95	99.29	110.50
1	A	34	ALA	CA-C-N	7.45	129.16	119.84
1	A	34	ALA	C-N-CA	7.45	129.16	119.84
1	D	34	ALA	CA-C-N	7.43	129.13	119.84
1	D	34	ALA	C-N-CA	7.43	129.13	119.84
1	G	34	ALA	CA-C-N	7.41	129.11	119.84
1	G	34	ALA	C-N-CA	7.41	129.11	119.84
1	J	34	ALA	CA-C-N	7.38	129.06	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	34	ALA	C-N-CA	7.38	129.06	119.84
2	H	87	HIS	N-CA-C	6.71	120.45	109.85
2	E	87	HIS	N-CA-C	6.70	120.43	109.85
3	I	133	SER	N-CA-C	-6.68	104.00	111.28
3	F	133	SER	N-CA-C	-6.65	104.03	111.28
2	K	87	HIS	N-CA-C	6.63	120.32	109.85
3	L	133	SER	N-CA-C	-6.63	104.06	111.28
3	C	133	SER	N-CA-C	-6.62	104.06	111.28
3	L	96	CYS	N-CA-C	-6.62	98.90	109.76
3	I	96	CYS	N-CA-C	-6.61	98.92	109.76
2	B	87	HIS	N-CA-C	6.61	120.29	109.85
3	L	85	SER	CA-C-N	6.58	126.96	119.92
3	L	85	SER	C-N-CA	6.58	126.96	119.92
3	C	85	SER	CA-C-N	6.56	126.94	119.92
3	C	85	SER	C-N-CA	6.56	126.94	119.92
3	I	85	SER	CA-C-N	6.54	126.92	119.92
3	I	85	SER	C-N-CA	6.54	126.92	119.92
3	F	85	SER	CA-C-N	6.51	126.89	119.92
3	F	85	SER	C-N-CA	6.51	126.89	119.92
3	C	96	CYS	N-CA-C	-6.50	99.10	109.76
3	F	96	CYS	N-CA-C	-6.43	99.22	109.76
2	B	137	ASN	N-CA-C	6.41	119.90	109.59
2	E	137	ASN	N-CA-C	6.35	119.81	109.59
2	K	137	ASN	N-CA-C	6.35	119.81	109.59
2	H	137	ASN	N-CA-C	6.33	119.78	109.59
3	C	103	THR	CB-CA-C	-6.15	99.24	111.91
2	B	203	SER	CA-C-N	6.15	126.16	119.89
2	B	203	SER	C-N-CA	6.15	126.16	119.89
3	L	103	THR	CB-CA-C	-6.15	99.25	111.91
2	K	203	SER	CA-C-N	6.14	126.15	119.89
2	K	203	SER	C-N-CA	6.14	126.15	119.89
2	E	203	SER	CA-C-N	6.13	126.15	119.89
2	E	203	SER	C-N-CA	6.13	126.15	119.89
3	F	103	THR	CB-CA-C	-6.11	99.33	111.91
2	H	203	SER	CA-C-N	6.09	126.10	119.89
2	H	203	SER	C-N-CA	6.09	126.10	119.89
3	I	103	THR	CB-CA-C	-6.09	99.37	111.91
3	I	2	VAL	N-CA-C	-5.83	97.20	109.34
3	F	2	VAL	N-CA-C	-5.82	97.25	109.34
3	L	2	VAL	N-CA-C	-5.81	97.25	109.34
3	C	2	VAL	N-CA-C	-5.80	97.28	109.34
3	L	3	GLN	N-CA-C	5.79	118.64	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	GLN	N-CA-C	5.72	118.53	109.50
3	F	3	GLN	N-CA-C	5.70	118.51	109.50
3	I	3	GLN	N-CA-C	5.67	118.45	109.50
1	D	85	VAL	N-CA-C	-5.62	101.47	108.89
1	J	85	VAL	N-CA-C	-5.58	101.52	108.89
1	A	85	VAL	N-CA-C	-5.57	101.54	108.89
1	G	85	VAL	N-CA-C	-5.49	101.64	108.89
1	J	22	PHE	N-CA-C	5.47	117.95	111.33
2	B	61	ARG	N-CA-C	-5.47	106.11	112.89
3	F	109	GLY	N-CA-C	-5.46	104.15	112.51
2	H	61	ARG	N-CA-C	-5.44	106.14	112.89
1	D	22	PHE	N-CA-C	5.43	117.91	111.33
2	E	61	ARG	N-CA-C	-5.43	106.15	112.89
2	K	61	ARG	N-CA-C	-5.41	106.18	112.89
1	G	22	PHE	N-CA-C	5.41	117.88	111.33
1	G	28	ASN	N-CA-C	-5.40	106.56	114.39
3	C	204	HIS	CA-C-N	5.40	124.86	119.24
3	C	204	HIS	C-N-CA	5.40	124.86	119.24
3	L	204	HIS	CA-C-N	5.39	124.85	119.24
3	L	204	HIS	C-N-CA	5.39	124.85	119.24
3	C	109	GLY	N-CA-C	-5.39	104.27	112.51
3	L	109	GLY	N-CA-C	-5.38	104.28	112.51
1	J	28	ASN	N-CA-C	-5.37	106.60	114.39
2	K	92	TYR	N-CA-C	-5.37	104.31	111.24
2	B	92	TYR	N-CA-C	-5.36	104.32	111.24
1	A	22	PHE	N-CA-C	5.36	117.81	111.33
2	H	92	TYR	N-CA-C	-5.35	104.34	111.24
3	I	204	HIS	CA-C-N	5.35	124.80	119.24
3	I	204	HIS	C-N-CA	5.35	124.80	119.24
3	I	109	GLY	N-CA-C	-5.34	104.34	112.51
1	D	28	ASN	N-CA-C	-5.34	106.65	114.39
1	A	28	ASN	N-CA-C	-5.31	106.69	114.39
2	E	92	TYR	N-CA-C	-5.29	104.42	111.24
3	F	204	HIS	CA-C-N	5.29	124.74	119.24
3	F	204	HIS	C-N-CA	5.29	124.74	119.24
1	A	126	HIS	N-CA-C	-5.23	103.58	110.33
1	J	126	HIS	N-CA-C	-5.23	103.59	110.33
3	L	32	TYR	N-CA-C	5.20	117.71	109.50
1	G	126	HIS	N-CA-C	-5.18	103.65	110.33
3	F	32	TYR	N-CA-C	5.16	117.65	109.50
3	C	32	TYR	N-CA-C	5.15	117.64	109.50
1	D	126	HIS	N-CA-C	-5.15	103.69	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	32	TYR	N-CA-C	5.13	117.61	109.50
2	B	99	GLY	N-CA-C	-5.09	105.80	112.82
1	G	107	THR	CA-C-N	5.08	125.37	119.47
1	G	107	THR	C-N-CA	5.08	125.37	119.47
2	E	99	GLY	N-CA-C	-5.07	105.82	112.82
1	J	107	THR	CA-C-N	5.06	125.34	119.47
1	J	107	THR	C-N-CA	5.06	125.34	119.47
1	D	107	THR	CA-C-N	5.05	125.33	119.47
1	D	107	THR	C-N-CA	5.05	125.33	119.47
2	B	96	TYR	N-CA-C	-5.05	102.81	110.28
2	K	115	VAL	N-CA-C	5.04	116.51	109.55
2	H	99	GLY	N-CA-C	-5.04	105.86	112.82
2	E	96	TYR	N-CA-C	-5.03	102.83	110.28
2	E	115	VAL	N-CA-C	5.02	116.47	109.55
1	A	107	THR	CA-C-N	5.01	125.28	119.47
1	A	107	THR	C-N-CA	5.01	125.28	119.47

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	78	0
1	D	1230	0	1221	79	0
1	G	1230	0	1221	82	0
1	J	1230	0	1221	87	0
2	B	1668	0	1592	162	0
2	E	1668	0	1592	162	0
2	H	1668	0	1592	161	0
2	K	1668	0	1592	156	0
3	C	1679	0	1635	117	0
3	F	1679	0	1635	117	0
3	I	1679	0	1635	116	0
3	L	1679	0	1635	130	0
All	All	18308	0	17792	1398	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 39.

All (1398) 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
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
3:L:76:SER:O	3:L:78:THR:HG22	1.73	0.89
2:B:134:CYS:HG	2:B:194:CYS:HG	0.94	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:134:CYS:HG	2:H:194:CYS:HG	0.95	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
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
1:G:25:ASP:CG	1:G:28:ASN:HD21	1.91	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
1:D:25:ASP:CG	1:D:28:ASN:HD21	1.91	0.78
3:I:12:VAL:HG22	3:I:16:ALA:HB3	1.65	0.77
1:J:25:ASP:CG	1:J:28:ASN:HD21	1.92	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
1:A:25:ASP:CG	1:A:28:ASN:HD21	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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
1:G:80:LYS:HE3	1:G:101:GLU:CD	2.15	0.72
2:H:120:PRO:HD3	2:H:132:VAL:HG22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:80:LYS:HE3	1:A:101:GLU:CD	2.14	0.71
1:J:80:LYS:HE3	1:J:101:GLU:CD	2.15	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
1:D:80:LYS:HE3	1:D:101:GLU:CD	2.15	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:J:33:VAL:C	1:J:35:PRO:HD3	2.17	0.70
1:A:33:VAL:C	1:A:35:PRO:HD3	2.17	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
1:G:33:VAL:C	1:G:35:PRO:HD3	2.17	0.69
2:H:134:CYS:CB	2:H:194:CYS:HG	2.05	0.69
2:K:134:CYS:CB	2:K:194:CYS:HG	2.05	0.69
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
1:D:33:VAL:C	1:D:35:PRO:HD3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:L:182:LEU:C	3:L:182:LEU:HD12	2.20	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:ASN:HB3	2:H:212:ASN:ND2	2.10	0.66
3:I:182:LEU:C	3:I:182:LEU:HD12	2.20	0.66
3:C:182:LEU:HD12	3:C:182:LEU:C	2.20	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
3:F:182:LEU:C	3:F:182:LEU:HD12	2.20	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: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: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
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: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
2:E:165:ASP:O	2:E:166:GLN:C	2.41	0.64
2:K:163:TRP:CZ2	2:K:175:MET:HE2	2.33	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
2:B:163:TRP:CZ2	2:B:175:MET:HE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:165:ASP:O	2:K:166:GLN:C	2.41	0.63
2:H:163:TRP:CZ2	2:H:175:MET:HE2	2.33	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:E:163:TRP:CZ2	2:E:175:MET:HE2	2.33	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
2:H:165:ASP:O	2:H:166:GLN:C	2.41	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
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:E:23:CYS:CB	2:E:88:CYS:HG	2.11	0.62
2:H:61:ARG:HH11	2:H:61:ARG:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:ASP:OD1	1:J:28:ASN:ND2	2.32	0.62
3:L:18:VAL:C	3:L:19:ILE:HD12	2.25	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
2:K:81:GLU:C	2:K:83:LEU:H	2.08	0.62
1:A:11:SER:OG	1:A:13:ILE:HG12	1.99	0.62
2:B:81:GLU:C	2:B:83:LEU:H	2.08	0.62
2:B:165:ASP:O	2:B:166:GLN:C	2.41	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
2:E:195:GLU:OE2	2:E:206:VAL:HG22	1.99	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:18:VAL:C	3:F:19:ILE:HD12	2.25	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:18:VAL:C	3:C:19:ILE:HD12	2.25	0.61
3:C:101:ARG:O	3:C:102:ASP:HB2	2.00	0.61
2:E:81:GLU:C	2:E:83:LEU:H	2.08	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
3:I:18:VAL:C	3:I:19:ILE:HD12	2.25	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:81:GLU:C	2:H:83:LEU:H	2.08	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
1:G:129:LYS:C	1:G:131:GLU:N	2.61	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: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
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:A:129:LYS:C	1:A:131:GLU:N	2.61	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
2:K:198:HIS:C	2:K:199:LYS:HG3	2.29	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
2:H:170:ASP:CG	2:H:172:THR:HG23	2.30	0.57
3:I:159:TRP:CE2	3:I:186:VAL:HG22	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:C	1:D:131:GLU:N	2.61	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:H:198:HIS:C	2:H:199:LYS:HG3	2.29	0.57
1:A:20:LYS:NZ	1:A:159:ASN:HD22	2.03	0.57
2:B:170:ASP:CG	2:B:172:THR:HG23	2.30	0.57
2:B:198:HIS:C	2:B:199:LYS:HG3	2.29	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
2:E:170:ASP:CG	2:E:172:THR:HG23	2.30	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
2:H:81:GLU:CD	2:H:81:GLU:H	2.13	0.57
3:I:23:LYS:HA	3:I:78:THR:HB	1.87	0.57
2:K:170:ASP:CG	2:K:172:THR:HG23	2.29	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
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
2:E:198:HIS:C	2:E:199:LYS:HG3	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:129:LYS:C	1:G:131:GLU:H	2.14	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
2:E:81:GLU:H	2:E:81:GLU:CD	2.14	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:81:GLU:CD	2:K:81:GLU:H	2.14	0.56
2:B:81:GLU:H	2:B:81:GLU:CD	2.14	0.56
3:C:176:GLN:O	3:C:177:SER:C	2.48	0.56
2:K:175:MET:HG2	2:K:176:SER:N	2.20	0.56
3:L:176:GLN:O	3:L:177:SER:C	2.48	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
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:176:GLN:O	3:I:177:SER:C	2.48	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
1:A:129:LYS:C	1:A:131:GLU:H	2.14	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
1:A:36:GLN:CD	1:A:36:GLN:H	2.14	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
1:G:36:GLN:H	1:G:36:GLN:CD	2.15	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
1:J:129:LYS:C	1:J:131:GLU:H	2.14	0.56
2:K:108:ARG:HG3	2:K:140:TYR:CE2	2.41	0.56
3:L:58:THR:HG1	3:L:60:TYR:HE2	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:LYS:O	2:E:193:THR:HG22	2.06	0.55
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:F:64:PHE:O	3:F:65:LYS:C	2.50	0.55
2:B:187:GLU:C	2:B:189:HIS:H	2.15	0.55
3:C:192:THR:O	3:C:196:GLU:HB2	2.07	0.55
1:D:129:LYS:C	1:D:131:GLU:H	2.14	0.55
1:J:36:GLN:CD	1:J:36:GLN:H	2.15	0.55
3:L:64:PHE:O	3:L:65:LYS:C	2.50	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:64:PHE:O	3:C:65:LYS:C	2.50	0.55
2:H:187:GLU:C	2:H:189:HIS:H	2.15	0.55
3:I:64:PHE:O	3:I:65:LYS:C	2.50	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
2:E:187:GLU:C	2:E:189:HIS:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:36:GLN:H	1:D:36:GLN:CD	2.15	0.54
2:E:81:GLU:N	2:E:81:GLU:CD	2.66	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
2:B:81:GLU:N	2:B:81:GLU:CD	2.66	0.54
1:D:131:GLU:O	1:D:134:LYS:HB3	2.06	0.54
3:F:93:VAL:HA	3:F:112:THR:O	2.07	0.54
3:F:176:GLN:O	3:F:177:SER:C	2.48	0.54
2:K:81:GLU:N	2:K:81:GLU:CD	2.66	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
2:K:187:GLU:C	2:K:189:HIS:H	2.15	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
2:H:81:GLU:N	2:H:81:GLU:CD	2.66	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:J:129:LYS:C	1:J: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:87:THR:C	3:I:116:VAL:HG21	2.34	0.53
2:K:136:LEU:HD21	2:K:146:VAL:CG2	2.39	0.53
3:L:87:THR:C	3:L:116:VAL:HG21	2.34	0.53
2:E:68:THR:HG22	2:E:69:THR:N	2.23	0.53
3:F:87:THR:C	3:F:116:VAL:HG21	2.34	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
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
3:C:87:THR:C	3:C:116:VAL:HG21	2.34	0.53
2:E:149:LYS:HB2	2:E:193:THR:CG2	2.38	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:J:20:LYS:HZ2	1:J:159:ASN:HB2	1.74	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
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
3:L:168:VAL:O	3:L:169:HIS:HD2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:LEU:HD21	2:H:146:VAL:CG2	2.39	0.52
2:B:21:LEU:HD12	2:B:102:THR:CG2	2.40	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
1:G:20:LYS:HZ2	1:G:159:ASN:HB2	1.75	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
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:D:7:THR:CG2	1:D:8:GLU:N	2.73	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
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
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
3:F:1:GLN:C	3:F:2:VAL:HG12	2.36	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
2:E:68:THR:HG22	2:E:69:THR:HG22	1.93	0.51
2:E:150:ILE:O	2:E:151:ASP:HB2	2.09	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
3:I:116:VAL:HG23	3:I:116:VAL:O	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:GLN:HE22	3:C:65:LYS:HE2	1.76	0.51
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
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
3:L:1:GLN:CG	3:L:2:VAL:N	2.71	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
2:B:139:PHE:O	2:B:140:TYR:HB2	2.11	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
3:L:1:GLN:C	3:L:2:VAL:HG12	2.36	0.50
1:A:15:ALA:O	1:A:16:ALA:C	2.55	0.50
2:H:68:THR:HG22	2:H:69:THR:HG22	1.93	0.50
2:K:175:MET:HG2	2:K:176:SER:H	1.77	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
3:L:116:VAL:HG23	3:L:116:VAL:O	2.10	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: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
1:J:15:ALA:O	1:J:16:ALA:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:GLN:C	3:I:2:VAL:HG12	2.36	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
3:C:1:GLN:C	3:C:2:VAL:HG12	2.36	0.50
2:E:137:ASN:HB3	2:E:138:ASN:ND2	2.27	0.50
3:F:61:ASN:OD1	3:F:63:LYS:HE2	2.12	0.50
2:H:61:ARG:HH22	2:H:82:ASP:CG	2.20	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
1:D:15:ALA:O	1:D:16:ALA:C	2.55	0.49
1:D:20:LYS:NZ	1:D:159:ASN:HB2	2.27	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:E:49:TYR:O	2:E:49:TYR:CD1	2.65	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:204:HIS:CE1	3:F:206:ALA:HB3	2.48	0.49
2:H:81:GLU:C	2:H:83:LEU:N	2.69	0.49
3:I:132:GLY:CA	3:I:218:ARG:HD3	2.33	0.49
2:K:68:THR:HG22	2:K:69:THR:HG22	1.93	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
2:B:81:GLU:C	2:B:83:LEU:N	2.69	0.49
1:G:15:ALA:O	1:G:16:ALA:C	2.55	0.49
2:H:19:VAL:HG12	2:H:20:THR:N	2.28	0.49
3:I:38:LYS:HB2	3:I:94:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:61:ARG:HH22	2:B:82:ASP:CG	2.20	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
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
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: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:182:LEU:HD12	3:L:183:SER:N	2.28	0.48
3:C:24:ALA:HB1	3:C:27:TYR:CE1	2.49	0.48
2:E:61:ARG:HH22	2:E:82:ASP:CG	2.20	0.48
2:E:71:PHE:N	2:E:71:PHE:CD2	2.80	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
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
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
2:K:61:ARG:HH22	2:K:82:ASP:CG	2.20	0.48
2:E:19:VAL:HG12	2:E:20:THR:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:81:GLU:C	2:K:83:LEU:N	2.69	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
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
2:E:187:GLU:C	2:E:189:HIS:N	2.72	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
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
2:K:187:GLU:C	2:K:189:HIS:N	2.73	0.47
3:L:24:ALA:HB1	3:L:27:TYR:CE1	2.49	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
3:C:182:LEU:HD12	3:C:183:SER:N	2.28	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
2:H:187:GLU:C	2:H:189:HIS:N	2.72	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
1:A:25:ASP:CG	1:A:28:ASN:ND2	2.68	0.47
3:F:54:SER:OG	3:F:55:ASP:N	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
2:E:142:LYS:HD3	2:E:142:LYS:C	2.40	0.47
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
1:G:150:TYR:C	1:G:150:TYR:CD2	2.93	0.47
2:H:142:LYS:HD3	2:H:142:LYS:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:150:TYR:C	1:A:150:TYR:CD2	2.93	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
2:B:142:LYS:C	2:B:142:LYS:HD3	2.40	0.47
1:D:150:TYR:C	1:D:150:TYR:CD2	2.93	0.47
1:G:25:ASP:CG	1:G:28:ASN:ND2	2.68	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
2:K:142:LYS:HD3	2:K:142:LYS:C	2.40	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
2:E:170:ASP:OD2	2:E:170:ASP:C	2.58	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
3:L:2:VAL:C	3:L:3:GLN:HG3	2.39	0.46
1:A:17:ARG:NH2	1:A:151:LEU:O	2.48	0.46
3:C:70:LEU:C	3:C:71:THR:HG23	2.41	0.46
3:F:2:VAL:C	3:F:3:GLN:HG3	2.39	0.46
2:K:57:GLY:O	2:K:58:VAL:C	2.58	0.46
2:K:179:LEU:HD13	2:K:180:THR:N	2.30	0.46
3:L:182:LEU:C	3:L:182:LEU:CD1	2.88	0.46
1:A:20:LYS:HZ2	1:A:159:ASN:HD22	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:GLN:HE22	2:E:87:HIS:HA	1.81	0.46
2:E:57:GLY:O	2:E:58:VAL:C	2.58	0.46
2:H:26:SER:O	2:H:27:GLU:HG3	2.16	0.46
3:I:2:VAL:C	3:I:3:GLN:HG3	2.39	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
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:150:ILE:O	2:H:150:ILE:HG13	2.15	0.46
3:C:2:VAL:C	3:C:3:GLN:HG3	2.39	0.46
1:D:15:ALA:HB1	1:D:104:ILE:HG22	1.98	0.46
1:D:34:ALA:N	1:D:35:PRO:CD	2.79	0.46
1:D:132:GLN:C	1:D:134:LYS:N	2.73	0.46
1:G:62:LEU:N	1:G:62:LEU:HD12	2.31	0.46
3:I:70:LEU:C	3:I:71:THR:HG23	2.41	0.46
1:J:150:TYR:C	1:J:150:TYR:CD2	2.93	0.46
2:K:11:MET:HE1	2:K:19:VAL:HG13	1.98	0.46
2:K:170:ASP:OD2	2:K:170:ASP:C	2.58	0.46
3:L:12:VAL:CG1	3:L:116:VAL:HG12	2.45	0.46
1:A:132:GLN:C	1:A:134:LYS:N	2.73	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
3:F:70:LEU:C	3:F:71:THR:HG23	2.41	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
3:L:70:LEU:C	3:L:71:THR:HG23	2.41	0.46
1:A:69:ASP:HA	1:A:84:SER:O	2.15	0.46
3:C:13:ARG:O	3:C:14:PRO:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:170:ASP:OD2	2:B:170:ASP:C	2.58	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:57:GLY:O	2:B:58:VAL:C	2.58	0.45
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:11:MET:HE1	2:H:19:VAL:HG13	1.98	0.45
2:H:33:VAL:O	2:H:50:GLY:HA2	2.16	0.45
2:H:170:ASP:OD2	2:H:170:ASP:C	2.58	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
2:K:26:SER:C	2:K:27:GLU:HG3	2.41	0.45
3:L:188:VAL:HB	3:L:189:PRO:CD	2.46	0.45
3:C:98:ARG:HD2	3:C:99:GLY:O	2.16	0.45
3:C:133:SER:C	3:C:135:ALA:H	2.24	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: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
1:J:25:ASP:CG	1:J:28:ASN:ND2	2.68	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:HE1	2:E:19:VAL:HG13	1.98	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:98:ARG:HD2	3:I:99:GLY:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:26:SER:C	2:H:27:GLU:HG3	2.41	0.45
2:H:57:GLY:O	2:H:58:VAL:C	2.58	0.45
3:I:133:SER:C	3:I:135:ALA:H	2.24	0.45
3:I:188:VAL:HB	3:I:189:PRO:CD	2.46	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:13:ARG:O	3:I:14:PRO:C	2.59	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
2:B:183:LYS:O	2:B:186:TYR:HB3	2.17	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
2:B:187:GLU:C	2:B:189:HIS:N	2.73	0.45
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:26:SER:C	2:E:27:GLU:HG3	2.41	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:11:MET:HE1	2:B:19:VAL:HG13	1.99	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
2:K:21:LEU:N	2:K:21:LEU:HD22	2.32	0.44
2:B:26:SER:C	2:B:27:GLU:HG3	2.41	0.44
2:B:167:ASP:OD2	2:B:167:ASP:C	2.60	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
2:E:81:GLU:C	2:E:83:LEU:N	2.69	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
3:F:133:SER:C	3:F:135:ALA:H	2.24	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
1:J:132:GLN:C	1:J:134:LYS:N	2.74	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
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
1:G:132:GLN:C	1:G:134:LYS:N	2.73	0.44
2:H:186:TYR:HE1	2:H:192:TYR:CE2	2.33	0.44
3:L:86:PRO:C	3:L:87:THR:CG2	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:PRO:C	3:C:87:THR:CG2	2.90	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:86:PRO:C	3:F:87:THR:CG2	2.90	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:144:ILE:CG2	2:K:175:MET:HE3	2.48	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
1:D:20:LYS:HZ3	1:D:159:ASN:HD22	1.64	0.44
2:E:160:LEU:O	2:E:177:SER:HA	2.16	0.44
3:F:13:ARG:O	3:F:14:PRO:C	2.59	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:45:GLU:CD	3:L:32:TYR:HD1	2.26	0.44
3:L:133:SER:C	3:L:135:ALA:H	2.24	0.44
3:L:175:LEU:C	3:L:175:LEU:HD13	2.43	0.44
1:A:29:LEU:O	1:A:32:LYS:HB3	2.17	0.44
1:D:114:LEU:HD22	1:D:144:LEU:HD22	2.00	0.44
2:E:144:ILE:CG2	2:E:175:MET:HE3	2.48	0.44
2:E:186:TYR:O	2:E:192:TYR:OH	2.34	0.44
3:C:182:LEU:C	3:C:182:LEU:CD1	2.89	0.43
2:E:167:ASP:OD2	2:E:167:ASP:C	2.60	0.43
3:I:182:LEU:C	3:I:182:LEU:CD1	2.89	0.43
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
3:I:33:TRP:CZ3	3:I:50:ASN:CG	2.97	0.43
3:I:86:PRO:C	3:I:87:THR:CG2	2.91	0.43
2:K:11:MET:SD	2:K:19:VAL:CG1	3.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:ARG:HD3	2:H:62:PHE:O	2.18	0.43
2:H:167:ASP:C	2:H:167:ASP:OD2	2.60	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
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
2:B:144:ILE:CG2	2:B:175:MET:HE3	2.48	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
2:H:144:ILE:CG2	2:H:175:MET:HE3	2.48	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
3:I:175:LEU:C	3:I:175:LEU:HD13	2.43	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
3:C:33:TRP:CZ3	3:C:50:ASN:CG	2.97	0.43
3:C:175:LEU:HD13	3:C:175:LEU:C	2.44	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: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
3:L:13:ARG:O	3:L:14:PRO:C	2.59	0.43
3:L:128:PRO:O	3:L:129:LEU:HD23	2.19	0.43
1:A:115:LYS:C	1:A:116:ILE:HG13	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:175:LEU:HD13	3:F:175:LEU:C	2.43	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
1:G:115:LYS:C	1:G:116:ILE:HG13	2.44	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
3:F:33:TRP:CZ3	3:F:50:ASN:CG	2.96	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LYS:C	1:D:116:ILE:HG13	2.44	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
1:D:25:ASP:CG	1:D:28:ASN:ND2	2.68	0.42
2:E:125:LEU:C	2:E:127:SER:H	2.28	0.42
2:K:167:ASP:OD2	2:K:167:ASP:C	2.60	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
2:H:115:VAL:HG12	2:H:116:SER:N	2.34	0.42
2:H:125:LEU:C	2:H:127:SER:H	2.28	0.42
1:J:132:GLN:O	1:J:133:VAL:C	2.62	0.42
2:K:163:TRP:HE3	2:K:163:TRP:H	1.67	0.42
1:A:132:GLN:O	1:A:133:VAL:C	2.62	0.42
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.54	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:33:TRP:CZ3	3:L:50:ASN:CG	2.96	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
2:B:58:VAL:HA	2:B:59:PRO:HD2	1.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:119:PRO:O	2:K:120:PRO:C	2.63	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
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: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
3:L:36:TRP:O	3:L:48:VAL:HB	2.20	0.42
1:A:20:LYS:HZ3	1:A:159:ASN:HB2	1.85	0.42
1:A:62:LEU:HD12	1:A:62:LEU:H	1.84	0.42
3:C:155:VAL:HG23	3:C:204:HIS:CD2	2.55	0.42
2:E:23:CYS:CB	2:E:88:CYS:SG	3.06	0.42
2:E:59:PRO:C	2:E:61:ARG:H	2.28	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
2:B:119:PRO:O	2:B:120:PRO:C	2.63	0.42
2:E:13:VAL:HB	2:E:17:GLU:OE2	2.20	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
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:62:PHE:C	2:H:63:THR:HG23	2.45	0.41
2:H:119:PRO:O	2:H:120:PRO:C	2.63	0.41
2:H:133:VAL:HG12	2:H:178:THR:HB	2.03	0.41
3:I:54:SER:HA	3:I:74:LYS:HE3	2.01	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
2:B:13:VAL:HG11	2:B:19:VAL:CG2	2.50	0.41
2:B:125:LEU:C	2:B:127:SER:H	2.28	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: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
1:J:115:LYS:C	1:J:116:ILE:HG13	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLN:O	2:B:45:LYS:HE2	2.20	0.41
2:B:59:PRO:C	2:B:61:ARG:H	2.28	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
2:K:62:PHE:C	2:K:63:THR:HG23	2.46	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: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
2:K:133:VAL:HG12	2:K:178:THR:HB	2.03	0.41
1:A:4:ASN:CG	1:A:5:TYR:N	2.79	0.41
2:B:133:VAL:HG12	2:B:178:THR:HB	2.03	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
1:G:107:THR:CG2	1:G:113:ILE:HD11	2.51	0.41
2:H:59:PRO:C	2:H:61:ARG:H	2.28	0.41
2:H:198:HIS:CG	2:H:199:LYS:N	2.89	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: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
1:D:4:ASN:CG	1:D:5:TYR:N	2.79	0.41
1:D:116:ILE:O	1:D:116:ILE:HG22	2.20	0.41
2:E:23:CYS:SG	2:E:88:CYS:HB3	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:THR:CA	2:H:208:SER:HB3	2.48	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
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
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:62:PHE:C	2:E:63:THR:HG23	2.46	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
1:J:4:ASN:CG	1:J:5:TYR:N	2.79	0.41
2:K:15:VAL:O	2:K:15:VAL:HG22	2.21	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
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:B:62:PHE:C	2:B:63:THR:HG23	2.46	0.40
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: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:62:PHE:O	2:H:63:THR:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:126:VAL:HG13	3:I:211:VAL:HG11	2.03	0.40
1:J:14:PRO:O	1:J:15:ALA:C	2.64	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
1:D:14:PRO:O	1:D:15:ALA:C	2.64	0.40
2:E:119:PRO:O	2:E:120:PRO:C	2.63	0.40
2:H:52:SER:CB	2:H:64:GLY:O	2.70	0.40
2:H:163:TRP:CE2	2:H:175:MET:HE2	2.57	0.40
2:H:205:ILE:HD12	2:H:205:ILE:H	1.87	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: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
2:K:59:PRO:C	2:K:61:ARG:H	2.28	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
2:E:62:PHE:O	2:E:63:THR:CG2	2.69	0.40
2:E:163:TRP:CE2	2:E:175:MET:HE2	2.57	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
3:I:52:PHE:C	3:I:53:PRO:O	2.65	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:D:132:GLN:O	1:D:133:VAL:C	2.62	0.40
1:G:4:ASN:CG	1:G:5:TYR:N	2.79	0.40
1:G:114:LEU:HD12	1:G:114:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:CYS:SG	2:H:88:CYS:HB3	2.61	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	15
2	E	212/214 (99%)	177 (84%)	29 (14%)	6 (3%)	4	15
2	H	212/214 (99%)	176 (83%)	30 (14%)	6 (3%)	4	15
2	K	212/214 (99%)	176 (83%)	30 (14%)	6 (3%)	4	15
3	C	218/220 (99%)	192 (88%)	20 (9%)	6 (3%)	4	15
3	F	218/220 (99%)	192 (88%)	20 (9%)	6 (3%)	4	15
3	I	218/220 (99%)	193 (88%)	19 (9%)	6 (3%)	4	15
3	L	218/220 (99%)	192 (88%)	20 (9%)	6 (3%)	4	15
All	All	2348/2372 (99%)	1955 (83%)	309 (13%)	84 (4%)	2	11

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
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

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Mol	Chain	Res	Type
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
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%)	119 (89%)	15 (11%)	6	19
1	D	134/134 (100%)	119 (89%)	15 (11%)	6	19
1	G	134/134 (100%)	119 (89%)	15 (11%)	6	19
1	J	134/134 (100%)	119 (89%)	15 (11%)	6	19
2	B	193/193 (100%)	169 (88%)	24 (12%)	4	15
2	E	193/193 (100%)	169 (88%)	24 (12%)	4	15
2	H	193/193 (100%)	169 (88%)	24 (12%)	4	15
2	K	193/193 (100%)	169 (88%)	24 (12%)	4	15
3	C	192/192 (100%)	163 (85%)	29 (15%)	3	10
3	F	192/192 (100%)	162 (84%)	30 (16%)	2	9
3	I	192/192 (100%)	163 (85%)	29 (15%)	3	10
3	L	192/192 (100%)	162 (84%)	30 (16%)	2	9
All	All	2076/2076 (100%)	1802 (87%)	274 (13%)	4	13

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	13	ILE
1	A	32	LYS
1	A	47	ASN
1	A	55	LYS
1	A	60	GLU
1	A	70	ARG
1	A	95	LEU
1	A	99	SER
1	A	103	LYS
1	A	123	LYS
1	A	125	ASP
1	A	129	LYS
1	A	131	GLU

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Mol	Chain	Res	Type
1	A	145	ARG
2	B	15	VAL
2	B	18	ARG
2	B	21	LEU
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	136	LEU
2	B	143	ASP
2	B	154	GLU
2	B	163	TRP
2	B	165	ASP
2	B	175	MET
2	B	176	SER
2	B	178	THR
2	B	179	LEU
2	B	181	LEU
2	B	185	GLU
2	B	202	THR
2	B	214	CYS
3	C	2	VAL
3	C	7	PRO
3	C	9	THR
3	C	37	VAL
3	C	50	ASN
3	C	55	ASP
3	C	58	THR
3	C	72	VAL
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

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Mol	Chain	Res	Type
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	182	LEU
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	32	LYS
1	D	47	ASN
1	D	55	LYS
1	D	60	GLU
1	D	70	ARG
1	D	95	LEU
1	D	99	SER
1	D	103	LYS
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	21	LEU
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
2	E	136	LEU
2	E	143	ASP
2	E	154	GLU
2	E	163	TRP

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Mol	Chain	Res	Type
2	E	165	ASP
2	E	175	MET
2	E	176	SER
2	E	178	THR
2	E	179	LEU
2	E	181	LEU
2	E	185	GLU
2	E	202	THR
2	E	214	CYS
3	F	2	VAL
3	F	7	PRO
3	F	9	THR
3	F	37	VAL
3	F	50	ASN
3	F	55	ASP
3	F	58	THR
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	182	LEU
3	F	186	VAL
3	F	197	THR
3	F	199	THR
3	F	201	ASN
3	F	219	ASP
1	G	10	THR
1	G	13	ILE
1	G	32	LYS

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Mol	Chain	Res	Type
1	G	47	ASN
1	G	55	LYS
1	G	60	GLU
1	G	70	ARG
1	G	95	LEU
1	G	99	SER
1	G	103	LYS
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	21	LEU
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	136	LEU
2	H	143	ASP
2	H	154	GLU
2	H	163	TRP
2	H	165	ASP
2	H	175	MET
2	H	176	SER
2	H	178	THR
2	H	179	LEU
2	H	181	LEU
2	H	185	GLU
2	H	202	THR
2	H	214	CYS
3	I	2	VAL
3	I	7	PRO
3	I	9	THR
3	I	37	VAL
3	I	50	ASN
3	I	55	ASP

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Mol	Chain	Res	Type
3	I	58	THR
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	182	LEU
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	32	LYS
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	103	LYS
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	21	LEU
2	K	22	SER

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Mol	Chain	Res	Type
2	K	48	LEU
2	K	60	ASP
2	K	61	ARG
2	K	81	GLU
2	K	88	CYS
2	K	108	ARG
2	K	122	SER
2	K	136	LEU
2	K	143	ASP
2	K	154	GLU
2	K	163	TRP
2	K	165	ASP
2	K	175	MET
2	K	176	SER
2	K	178	THR
2	K	179	LEU
2	K	181	LEU
2	K	185	GLU
2	K	202	THR
2	K	214	CYS
3	L	2	VAL
3	L	7	PRO
3	L	9	THR
3	L	37	VAL
3	L	50	ASN
3	L	55	ASP
3	L	58	THR
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

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Mol	Chain	Res	Type
3	L	157	VAL
3	L	181	THR
3	L	182	LEU
3	L	186	VAL
3	L	197	THR
3	L	199	THR
3	L	201	ASN
3	L	219	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) 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	37	GLN
2	B	38	GLN
2	B	87	HIS
2	B	138	ASN
2	B	156	GLN
2	B	210	ASN
2	B	212	ASN
3	C	39	GLN
3	C	50	ASN
3	C	59	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	28	ASN
1	D	47	ASN
1	D	118	ASN
1	D	121	HIS
1	D	132	GLN
1	D	159	ASN

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Mol	Chain	Res	Type
2	E	6	GLN
2	E	28	ASN
2	E	37	GLN
2	E	87	HIS
2	E	138	ASN
2	E	198	HIS
2	E	210	ASN
2	E	212	ASN
3	F	50	ASN
3	F	59	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	28	ASN
1	G	47	ASN
1	G	76	HIS
1	G	118	ASN
1	G	121	HIS
1	G	132	GLN
1	G	159	ASN
2	H	6	GLN
2	H	28	ASN
2	H	37	GLN
2	H	87	HIS
2	H	138	ASN
2	H	190	ASN
2	H	210	ASN
2	H	212	ASN
3	I	1	GLN
3	I	3	GLN
3	I	50	ASN
3	I	59	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	28	ASN

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Mol	Chain	Res	Type
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	37	GLN
2	K	87	HIS
2	K	138	ASN
2	K	198	HIS
2	K	210	ASN
2	K	212	ASN
3	L	1	GLN
3	L	3	GLN
3	L	50	ASN
3	L	59	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 [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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	159/159 (100%)	0.84	16 (10%) 12 10	22, 56, 89, 124	0
1	D	159/159 (100%)	0.96	19 (11%) 9 7	18, 55, 92, 109	0
1	G	159/159 (100%)	1.57	54 (33%) 1 1	27, 76, 108, 128	0
1	J	159/159 (100%)	2.19	83 (52%) 0 0	27, 89, 116, 133	0
2	B	214/214 (100%)	0.67	21 (9%) 13 11	19, 52, 92, 137	0
2	E	214/214 (100%)	0.84	16 (7%) 20 16	19, 56, 93, 132	0
2	H	214/214 (100%)	1.87	88 (41%) 0 0	41, 86, 119, 153	0
2	K	214/214 (100%)	1.09	33 (15%) 5 4	32, 62, 91, 132	0
3	C	220/220 (100%)	0.36	12 (5%) 30 24	18, 44, 84, 123	0
3	F	220/220 (100%)	0.49	13 (5%) 28 22	14, 49, 86, 121	0
3	I	220/220 (100%)	0.86	23 (10%) 11 10	33, 60, 106, 134	0
3	L	220/220 (100%)	0.88	18 (8%) 17 14	25, 56, 93, 123	0
All	All	2372/2372 (100%)	1.02	396 (16%) 4 3	14, 59, 105, 153	0

All (396) 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	6.6
3	L	134	ALA	6.4
1	G	106	ALA	6.2
2	H	154	GLU	5.8
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	4.9
1	J	112	SER	4.8
1	A	157	ALA	4.8
3	I	134	ALA	4.8
1	G	112	SER	4.7
1	J	106	ALA	4.7
1	G	107	THR	4.7
2	H	190	ASN	4.6
1	J	3	PHE	4.5
2	H	198	HIS	4.4
3	L	132	GLY	4.4
2	H	16	GLY	4.4
1	J	37	ALA	4.3
1	G	118	ASN	4.3
2	H	125	LEU	4.3
1	G	111	GLY	4.3
1	J	149	SER	4.2
3	I	89	GLU	4.2
1	J	122	THR	4.2
1	J	135	ALA	4.2
1	J	67	VAL	4.1
2	H	145	ASN	4.1
2	H	162	SER	4.1
3	L	137	THR	4.0
1	J	94	THR	4.0
2	H	13	VAL	4.0
1	J	138	GLU	4.0
1	G	144	LEU	3.9
1	J	95	LEU	3.9
2	H	11	MET	3.9
1	G	153	ALA	3.9
3	C	137	THR	3.9
1	J	19	PHE	3.9
1	J	21	ALA	3.9
2	H	153	SER	3.9
1	J	146	ALA	3.8
2	K	70	ASP	3.8
2	H	134	CYS	3.8
1	J	4	ASN	3.8
1	G	140	GLY	3.8
1	J	91	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	127	GLU	3.7
1	J	62	LEU	3.6
3	L	1	GLN	3.6
3	I	194	PRO	3.6
2	H	210	ASN	3.6
1	D	107	THR	3.6
2	H	4	LEU	3.6
2	B	198	HIS	3.6
3	I	176	GLN	3.6
2	B	213	GLU	3.6
2	B	203	SER	3.5
2	H	12	SER	3.5
2	H	129	GLY	3.5
1	A	26	GLY	3.5
1	G	110	GLY	3.5
1	J	31	PRO	3.5
2	K	210	ASN	3.5
1	G	148	GLU	3.4
2	H	121	SER	3.4
1	J	131	GLU	3.3
1	J	98	ILE	3.3
1	J	79	PHE	3.3
2	B	152	GLY	3.3
2	K	50	GLY	3.3
2	K	32	TYR	3.3
2	K	27	GLU	3.3
1	D	106	ALA	3.3
1	J	143	LEU	3.3
2	H	69	THR	3.2
2	H	102	THR	3.2
3	F	137	THR	3.2
1	G	132	GLN	3.2
3	I	1	GLN	3.2
2	H	93	SER	3.2
1	G	64	PHE	3.2
1	G	75	ASP	3.1
1	J	64	PHE	3.1
1	G	17	ARG	3.1
1	G	37	ALA	3.1
2	H	6	GLN	3.1
2	K	202	THR	3.1
1	G	99	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	105	VAL	3.1
2	H	159	VAL	3.1
1	G	6	GLU	3.1
1	J	99	SER	3.1
2	H	141	PRO	3.1
2	H	195	GLU	3.1
1	J	22	PHE	3.0
2	K	77	SER	3.0
2	K	184	ASP	3.0
1	J	36	GLN	3.0
1	G	145	ARG	3.0
2	H	181	LEU	3.0
1	J	83	TYR	3.0
2	H	14	SER	3.0
1	G	88	GLY	3.0
2	B	214	CYS	3.0
3	L	220	CYS	3.0
2	H	118	PHE	3.0
2	H	170	ASP	3.0
2	H	191	SER	3.0
2	K	30	ASP	3.0
3	C	176	GLN	3.0
1	G	9	THR	3.0
2	H	209	PHE	3.0
1	A	111	GLY	3.0
2	H	70	ASP	3.0
2	H	184	ASP	3.0
1	J	148	GLU	3.0
1	J	128	VAL	3.0
3	L	101	ARG	2.9
1	J	88	GLY	2.9
2	B	169	LYS	2.9
2	E	213	GLU	2.9
2	B	190	ASN	2.9
1	G	149	SER	2.9
2	H	143	ASP	2.9
2	H	130	ALA	2.9
1	G	77	THR	2.9
2	H	172	THR	2.9
3	F	220	CYS	2.9
2	H	136	LEU	2.9
1	G	27	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	157	ASN	2.9
3	F	138	ASN	2.9
2	K	25	ALA	2.9
3	L	67	LYS	2.9
2	H	104	LEU	2.9
2	H	213	GLU	2.9
1	J	129	LYS	2.9
2	E	157	ASN	2.9
1	A	126	HIS	2.9
3	I	137	THR	2.9
2	H	163	TRP	2.8
3	F	41	PRO	2.8
2	H	60	ASP	2.8
1	J	113	ILE	2.8
1	G	108	PRO	2.8
1	A	137	LYS	2.8
2	H	32	TYR	2.8
1	J	16	ALA	2.8
1	G	109	ASP	2.8
2	H	139	PHE	2.8
1	D	159	ASN	2.8
2	E	214	CYS	2.8
1	G	127	GLU	2.8
3	I	193	TRP	2.8
1	J	5	TYR	2.8
1	J	120	TYR	2.8
1	G	129	LYS	2.8
1	J	9	THR	2.8
3	L	63	LYS	2.8
1	J	155	SER	2.8
3	I	63	LYS	2.7
1	D	125	ASP	2.7
1	J	92	GLY	2.7
1	J	59	PRO	2.7
3	C	196	GLU	2.7
1	D	128	VAL	2.7
2	H	148	TRP	2.7
3	C	220	CYS	2.7
1	J	108	PRO	2.7
3	I	189	PRO	2.7
2	H	77	SER	2.7
2	H	203	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	K	195	GLU	2.7
1	A	106	ALA	2.7
2	B	201	SER	2.7
2	K	93	SER	2.7
3	L	89	GLU	2.7
3	F	134	ALA	2.7
1	J	107	THR	2.7
1	J	105	VAL	2.7
3	L	77	SER	2.7
1	J	63	PRO	2.6
2	K	204	PRO	2.6
2	H	166	GLN	2.6
2	K	60	ASP	2.6
1	G	16	ALA	2.6
1	J	15	ALA	2.6
1	J	153	ALA	2.6
3	I	16	ALA	2.6
1	J	147	VAL	2.6
2	H	115	VAL	2.6
1	J	139	MET	2.6
2	K	26	SER	2.6
2	K	214	CYS	2.6
2	H	193	THR	2.6
1	J	69	ASP	2.6
2	E	70	ASP	2.6
1	G	137	LYS	2.6
1	A	110	GLY	2.6
1	J	116	ILE	2.6
1	D	131	GLU	2.6
2	E	81	GLU	2.6
1	D	130	ALA	2.6
2	E	204	PRO	2.5
1	J	144	LEU	2.5
1	J	41	VAL	2.5
2	E	180	THR	2.5
3	C	199	THR	2.5
1	G	19	PHE	2.5
2	H	137	ASN	2.5
2	H	171	SER	2.5
1	G	31	PRO	2.5
2	H	150	ILE	2.5
2	K	182	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	I	135	ALA	2.5
1	J	17	ARG	2.5
3	C	177	SER	2.5
1	G	152	LEU	2.5
2	H	51	PRO	2.5
2	H	192	TYR	2.5
1	A	6	GLU	2.5
1	A	73	GLU	2.5
2	H	5	THR	2.5
1	J	32	LYS	2.5
1	J	82	ASN	2.5
2	K	88	CYS	2.5
2	H	177	SER	2.5
3	L	53	PRO	2.5
1	A	128	VAL	2.5
1	J	157	ALA	2.5
2	E	193	THR	2.5
2	H	164	THR	2.5
2	K	31	THR	2.5
1	J	12	VAL	2.4
2	E	158	GLY	2.4
2	H	128	GLY	2.4
2	K	12	SER	2.4
2	K	191	SER	2.4
2	K	154	GLU	2.4
2	H	173	TYR	2.4
1	J	10	THR	2.4
1	D	4	ASN	2.4
1	J	133	VAL	2.4
2	H	152	GLY	2.4
2	H	10	SER	2.4
1	D	60	GLU	2.4
1	G	141	GLU	2.4
1	D	24	LEU	2.4
3	I	44	GLY	2.4
1	A	96	GLU	2.4
2	K	201	SER	2.4
1	A	37	ALA	2.4
3	L	135	ALA	2.4
3	F	199	THR	2.4
1	J	126	HIS	2.4
2	H	211	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	110	ASP	2.4
1	J	141	GLU	2.4
3	C	134	ALA	2.4
2	B	153	SER	2.4
2	H	144	ILE	2.4
2	K	150	ILE	2.4
1	J	145	ARG	2.3
2	H	161	ASN	2.3
2	K	129	GLY	2.3
3	I	218	ARG	2.3
1	J	130	ALA	2.3
3	C	88	SER	2.3
2	H	114	THR	2.3
2	H	169	LYS	2.3
2	K	3	VAL	2.3
2	H	110	ASP	2.3
1	D	62	LEU	2.3
2	H	158	GLY	2.3
3	C	138	ASN	2.3
1	D	153	ALA	2.3
2	E	184	ASP	2.3
2	H	214	CYS	2.3
1	J	119	LYS	2.3
2	B	43	SER	2.3
3	F	133	SER	2.3
2	H	180	THR	2.3
1	J	78	ASN	2.3
1	G	131	GLU	2.3
2	H	17	GLU	2.3
3	C	135	ALA	2.3
2	K	2	ILE	2.3
3	I	169	HIS	2.3
3	F	144	GLY	2.3
1	D	138	GLU	2.2
1	G	60	GLU	2.2
1	G	133	VAL	2.2
3	C	133	SER	2.2
3	I	177	SER	2.2
3	L	57	TYR	2.2
2	K	11	MET	2.2
1	G	65	LYS	2.2
3	F	67	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	117	ILE	2.2
1	D	9	THR	2.2
2	B	197	THR	2.2
2	H	15	VAL	2.2
3	L	114	VAL	2.2
1	J	61	GLY	2.2
1	J	58	PHE	2.2
1	G	8	GLU	2.2
1	J	152	LEU	2.2
2	B	81	GLU	2.2
1	J	44	ILE	2.2
3	I	43	GLN	2.2
1	G	63	PRO	2.2
2	H	40	PRO	2.2
2	H	132	VAL	2.2
1	J	136	SER	2.2
2	H	7	SER	2.2
1	J	97	LYS	2.2
1	G	62	LEU	2.2
1	G	95	LEU	2.2
2	K	213	GLU	2.2
1	G	38	ILE	2.2
3	I	84	ASN	2.2
3	L	3	GLN	2.2
1	D	126	HIS	2.2
2	B	11	MET	2.2
3	I	220	CYS	2.2
1	G	151	LEU	2.2
2	E	208	SER	2.2
2	H	65	SER	2.2
2	H	201	SER	2.2
3	I	133	SER	2.2
1	G	157	ALA	2.2
1	J	101	GLU	2.2
2	H	84	ALA	2.2
3	F	89	GLU	2.2
2	H	124	GLN	2.1
1	A	133	VAL	2.1
1	G	2	VAL	2.1
3	I	219	ASP	2.1
2	H	74	THR	2.1
1	J	39	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	38	ILE	2.1
3	F	136	GLN	2.1
1	G	121	HIS	2.1
1	D	118	ASN	2.1
2	B	53	ASN	2.1
1	D	108	PRO	2.1
1	J	2	VAL	2.1
1	J	90	PRO	2.1
3	I	168	VAL	2.1
1	G	58	PHE	2.1
1	D	28	ASN	2.1
1	D	129	LYS	2.1
2	B	212	ASN	2.1
1	G	114	LEU	2.1
3	L	4	LEU	2.1
2	H	197	THR	2.1
2	H	200	THR	2.1
1	G	130	ALA	2.1
1	J	23	ILE	2.1
1	G	117	SER	2.1
1	A	132	GLN	2.1
1	J	103	LYS	2.1
3	F	140	MET	2.1
3	F	132	GLY	2.1
2	H	178	THR	2.1
2	E	154	GLU	2.1
2	B	177	SER	2.0
2	H	22	SER	2.0
2	B	194	CYS	2.0
2	H	88	CYS	2.0
3	L	136	GLN	2.0
2	H	146	VAL	2.0
2	B	145	ASN	2.0
1	A	140	GLY	2.0
3	C	44	GLY	2.0
2	B	80	ALA	2.0
1	J	66	TYR	2.0
1	G	126	HIS	2.0
2	K	203	SER	2.0
2	H	8	PRO	2.0
3	I	138	ASN	2.0
3	I	167	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	150	ILE	2.0
1	G	7	THR	2.0
1	G	10	THR	2.0
1	J	77	THR	2.0
2	E	182	THR	2.0
3	L	28	THR	2.0
1	J	109	ASP	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.