



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:52 PM UTC

PDB ID : 9KFB / pdb_00009kfb
Title : RABV-G-ecto/NM57-scFv complex
Authors : Lu, G.; Yang, F.; Lin, S.
Deposited on : 2024-11-05
Resolution : 4.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

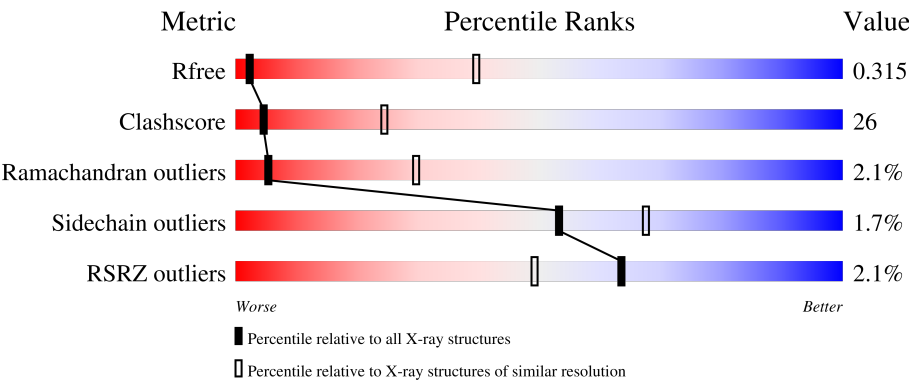
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	264	2% 50% 32% • 15%
1	M	264	37% 37% 5% 22%
1	X	264	% 43% 27% • 28%
2	B	433	2% 40% 36% • • 19%
2	F	433	2% 47% 27% • • 23%

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Mol	Chain	Length	Quality of chain
2	K	433	2% 36% 36% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12653 atoms, of which 0 are hydrogens and 0 are deuteriums.

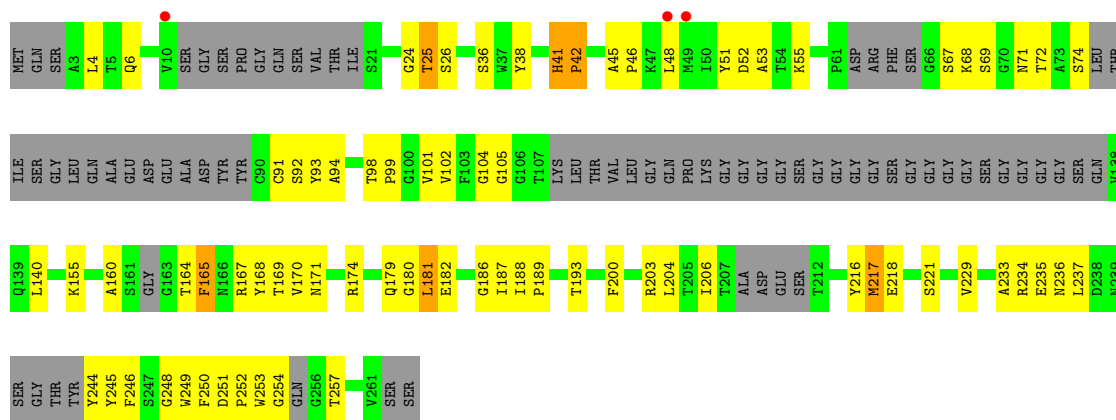
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NM57-scFv light chain, NM57-scFv heavy chain.

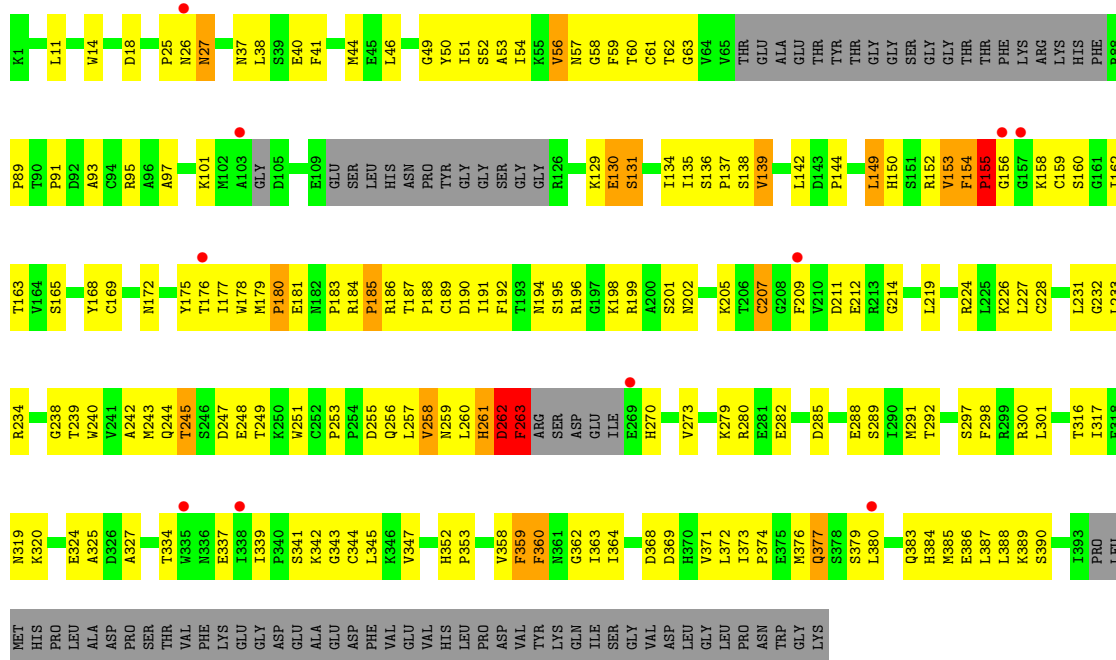
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1695	1068	284	335	8			
1	M	207	Total	C	N	O	S	0	0	0
			1562	984	267	303	8			
1	X	190	Total	C	N	O	S	0	0	0
			1438	909	245	276	8			

- Molecule 2 is a protein called RABV-G-ecto.

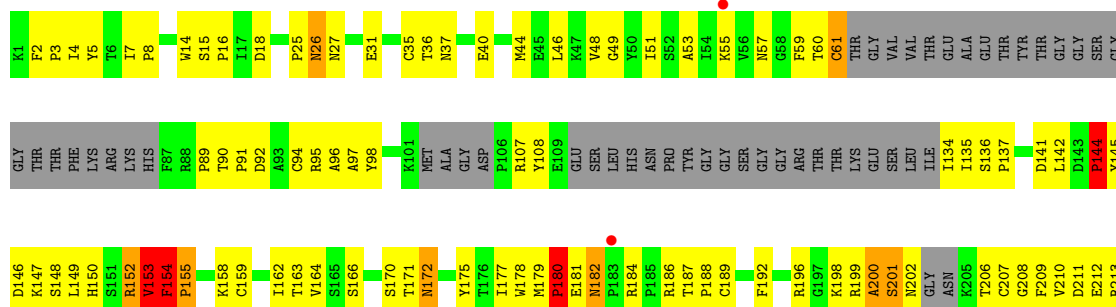
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	349	Total	C	N	O	S	0	0	0
			2749	1741	476	509	23			
2	K	328	Total	C	N	O	S	0	0	0
			2590	1647	447	474	22			
2	F	334	Total	C	N	O	S	0	0	0
			2619	1664	449	482	24			



• Molecule 2: RABV-G-ecto



• Molecule 2: RABV-G-ecto



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.62Å 157.62Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.64 – 4.30 36.64 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.64-4.30) 99.5 (36.64-4.30)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 4.27Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.261 , 0.314 0.264 , 0.315	Depositor DCC
R_{free} test set	910 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	175.9	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 342.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12653	wwPDB-VP
Average B, all atoms (Å ²)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/1733	0.82	13/2348 (0.6%)
1	M	0.32	0/1598	1.19	14/2164 (0.6%)
1	X	0.23	0/1469	0.76	10/1985 (0.5%)
2	B	0.30	0/2813	0.97	22/3808 (0.6%)
2	F	0.26	0/2681	0.96	31/3630 (0.9%)
2	K	0.27	0/2653	1.09	38/3590 (1.1%)
All	All	0.27	0/12947	0.98	128/17525 (0.7%)

There are no bond length outliers.

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	173	VAL	N-CA-C	30.12	143.83	111.00
2	B	153	VAL	N-CA-C	-18.87	84.58	109.30
1	M	94	ALA	CB-CA-C	-15.69	84.23	111.22
1	M	173	VAL	N-CA-CB	-14.33	86.63	110.56
2	B	26	ASN	N-CA-C	-13.85	89.47	110.10
2	B	153	VAL	CB-CA-C	13.44	132.94	111.71
2	B	358	VAL	CB-CA-C	13.40	130.19	110.90
2	K	180	PRO	CB-CA-C	-12.93	90.23	111.56
2	K	153	VAL	N-CA-C	12.35	135.03	109.34
2	F	355	VAL	N-CA-C	12.14	122.25	111.81
2	F	26	ASN	N-CA-C	-11.79	92.53	110.10
2	F	355	VAL	CB-CA-C	-11.73	98.06	111.55
2	B	27	ASN	N-CA-C	-11.72	96.42	112.94
1	X	180	GLY	N-CA-C	11.38	128.52	112.82
2	K	181	GLU	N-CA-CB	-11.37	93.03	110.42
2	K	97	ALA	N-CA-C	-11.19	99.18	113.72
2	F	356	ASN	N-CA-C	-11.16	96.60	110.88
2	B	359	PHE	N-CA-C	-11.08	92.46	108.96
1	A	179	GLN	N-CA-C	-10.92	94.69	108.45
2	K	378	SER	N-CA-C	-10.60	97.36	110.61
2	K	377	GLN	N-CA-C	-10.48	93.90	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	319	ASN	CB-CA-C	-10.13	93.63	109.34
2	F	27	ASN	N-CA-C	-10.01	99.89	113.30
2	F	26	ASN	CB-CA-C	9.97	125.45	109.90
2	B	262	ASP	N-CA-C	-9.96	95.12	109.96
2	K	26	ASN	N-CA-C	-9.75	95.91	110.24
2	B	257	LEU	N-CA-C	9.47	121.69	111.36
2	F	153	VAL	N-CA-C	-9.39	96.25	108.93
2	K	153	VAL	N-CA-CB	-9.39	95.73	111.23
2	F	245	THR	N-CA-C	-9.31	96.83	110.42
1	A	236	ASN	N-CA-CB	-9.21	95.02	110.95
1	A	153	SER	N-CA-C	9.20	124.09	110.48
1	X	218	GLU	N-CA-C	-9.18	93.02	108.26
1	A	237	LEU	N-CA-CB	9.17	126.97	111.66
2	F	153	VAL	CB-CA-C	9.16	125.98	111.69
1	M	258	LEU	N-CA-C	-9.04	94.59	108.96
2	K	144	PRO	N-CA-CB	-8.99	93.81	103.25
2	B	358	VAL	N-CA-C	-8.89	95.11	108.99
1	M	94	ALA	N-CA-C	-8.75	90.38	107.62
1	M	257	THR	N-CA-C	-8.74	94.34	108.41
1	X	25	THR	N-CA-C	-8.67	97.49	110.24
2	K	152	ARG	CB-CA-C	-8.67	94.92	110.36
1	X	25	THR	CB-CA-C	8.48	122.55	109.84
2	K	152	ARG	N-CA-C	-8.39	97.80	110.14
2	K	107	ARG	N-CA-C	-8.35	97.12	109.15
2	K	26	ASN	CB-CA-C	8.26	122.22	109.84
2	K	320	LYS	N-CA-CB	8.21	124.37	110.49
2	B	360	PHE	N-CA-C	8.15	121.10	110.43
2	K	180	PRO	N-CA-C	-8.08	95.83	112.47
2	B	257	LEU	CB-CA-C	-8.06	97.15	110.85
2	B	130	GLU	N-CA-C	-8.02	98.02	109.96
1	M	152	SER	N-CA-C	7.96	123.21	111.34
1	A	180	GLY	N-CA-C	7.94	125.64	112.30
2	F	270	HIS	N-CA-C	7.88	127.59	110.80
2	F	345	LEU	N-CA-C	-7.74	98.86	110.24
2	K	27	ASN	N-CA-C	-7.71	103.19	112.59
2	K	320	LYS	N-CA-C	-7.54	94.74	110.80
2	K	318	PHE	N-CA-C	7.45	122.26	112.72
2	B	262	ASP	CB-CA-C	7.43	120.86	110.16
2	F	378	SER	N-CA-C	-7.40	101.44	111.87
1	A	25	THR	N-CA-C	-7.37	99.11	110.10
2	B	26	ASN	CB-CA-C	7.37	121.40	109.90
2	F	306	LYS	N-CA-C	-7.35	99.43	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	SER	N-CA-CB	-7.33	99.14	110.29
2	K	238	GLY	N-CA-C	7.31	122.71	114.67
2	B	258	VAL	N-CA-C	-7.24	105.95	112.90
2	F	148	SER	N-CA-C	-7.15	93.69	107.57
2	F	246	SER	N-CA-C	-7.06	98.86	109.94
2	F	149	LEU	N-CA-CB	7.03	123.38	111.57
2	K	182	ASN	N-CA-C	-6.99	95.75	109.10
2	K	306	LYS	N-CA-C	-6.98	99.98	110.24
2	B	154	PHE	N-CA-C	-6.96	94.43	109.81
1	M	172	TRP	N-CA-C	6.93	125.57	110.80
1	X	179	GLN	CB-CA-C	-6.79	95.36	111.65
2	F	245	THR	CB-CA-C	6.74	119.07	109.71
2	F	277	VAL	CB-CA-C	-6.71	103.38	111.97
2	F	163	THR	N-CA-C	-6.65	101.60	110.24
2	K	272	VAL	N-CA-C	6.60	118.15	110.62
2	B	27	ASN	N-CA-CB	6.58	121.84	110.98
2	F	277	VAL	N-CA-C	6.54	116.70	110.42
2	F	307	LEU	N-CA-C	-6.50	104.98	113.17
2	K	201	SER	N-CA-C	6.47	120.13	107.57
1	M	182	GLU	N-CA-C	6.41	124.44	110.80
2	F	377	GLN	N-CA-C	-6.40	100.78	110.70
1	A	235	GLU	CB-CA-C	-6.35	98.20	109.70
1	X	218	GLU	N-CA-CB	6.31	121.06	110.77
2	F	345	LEU	CB-CA-C	6.25	119.22	109.84
2	K	356	ASN	N-CA-C	-6.25	97.49	110.80
2	K	96	ALA	N-CA-CB	-6.23	102.03	111.19
2	B	263	PHE	N-CA-CB	6.14	120.95	110.50
2	K	307	LEU	N-CA-C	-6.14	105.44	113.17
2	K	320	LYS	CB-CA-C	6.13	122.61	110.42
2	K	108	TYR	N-CA-CB	6.10	121.79	110.99
1	A	152	SER	N-CA-C	-6.09	97.83	110.80
1	M	226	ASP	N-CA-C	-6.07	97.97	108.52
2	F	306	LYS	CB-CA-C	6.03	118.89	109.84
2	F	270	HIS	CB-CA-C	-6.00	98.47	110.42
1	X	217	MET	N-CA-C	-5.94	98.15	110.80
2	B	130	GLU	CB-CA-C	5.94	118.71	110.16
1	M	172	TRP	CA-C-N	-5.89	111.12	120.55
1	M	172	TRP	C-N-CA	-5.89	111.12	120.55
2	K	154	PHE	N-CA-C	5.78	122.57	109.81
1	A	25	THR	CB-CA-C	5.75	118.87	109.90
2	K	172	ASN	N-CA-C	-5.74	98.58	110.80
2	K	96	ALA	CB-CA-C	-5.73	103.25	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	154	PHE	N-CA-CB	5.71	120.53	110.37
2	B	359	PHE	CB-CA-C	-5.63	98.31	111.09
2	K	148	SER	N-CA-C	5.58	119.39	111.92
2	K	144	PRO	CB-CA-C	-5.54	102.42	111.56
1	A	237	LEU	N-CA-C	-5.53	100.66	109.07
2	K	321	THR	N-CA-C	5.43	118.51	110.48
2	F	147	LYS	N-CA-C	-5.43	102.85	110.50
1	A	179	GLN	CB-CA-C	-5.38	100.70	113.02
2	K	306	LYS	CB-CA-C	5.36	117.87	109.84
2	F	32	ASP	N-CA-CB	5.33	119.47	110.79
2	B	377	GLN	N-CA-C	-5.28	106.81	113.20
2	F	278	LYS	N-CA-C	-5.24	106.66	113.16
2	F	155	PRO	N-CA-C	-5.24	101.68	112.47
2	F	271	LEU	N-CA-C	-5.23	106.16	112.54
1	M	153	SER	N-CA-CB	5.22	119.66	111.56
2	K	31	GLU	CB-CA-C	-5.21	102.03	110.79
1	X	217	MET	CB-CA-C	5.17	120.71	110.42
2	B	359	PHE	N-CA-CB	5.16	119.70	111.56
2	K	181	GLU	CB-CA-C	-5.13	101.09	109.56
1	A	235	GLU	N-CA-C	5.12	117.42	108.76
1	X	218	GLU	CB-CA-C	5.10	118.00	110.14
1	M	27	SER	CB-CA-C	5.08	118.72	109.83
1	X	26	SER	N-CA-C	-5.08	97.05	107.67

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	1695	0	1610	72	0
1	M	1562	0	1490	104	0
1	X	1438	0	1367	65	0
2	B	2749	0	2720	163	0
2	F	2619	0	2594	112	0
2	K	2590	0	2565	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12653	0	12346	651	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 26.

All (651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:O	1:A:222:LEU:CD1	1.96	1.14
2:K:180:PRO:CG	2:K:180:PRO:O	1.83	1.11
2:K:180:PRO:O	2:K:180:PRO:HG2	1.32	1.07
1:A:152:SER:O	1:A:222:LEU:HD13	1.55	1.03
2:K:201:SER:HB3	2:K:206:THR:HA	1.39	1.02
2:F:148:SER:O	2:F:149:LEU:HD23	1.60	1.00
2:F:244:GLN:HG2	2:F:245:THR:O	1.59	1.00
1:M:173:VAL:HG11	1:M:184:MET:HB2	1.46	0.98
2:K:335:TRP:HE1	2:K:376:MET:HB3	1.31	0.96
2:F:187:THR:H	2:F:188:PRO:HD2	1.28	0.96
2:K:59:PHE:HB3	2:K:180:PRO:HD2	1.51	0.93
1:X:93:TYR:HA	1:X:101:VAL:HG12	1.52	0.91
2:K:60:THR:HA	2:K:177:ILE:HG23	1.54	0.89
2:B:54:ILE:O	2:B:144:PRO:HD3	1.72	0.89
1:M:46:PRO:HB2	1:M:253:TRP:CZ2	2.08	0.89
1:X:41:HIS:HB2	1:X:42:PRO:HD3	1.56	0.88
1:X:167:ARG:HB2	1:X:237:LEU:HB3	1.56	0.87
2:K:224:ARG:NH2	1:M:198:GLN:OE1	2.10	0.84
2:K:180:PRO:O	2:K:180:PRO:CD	2.25	0.84
1:X:174:ARG:NH2	1:X:182:GLU:OE2	2.11	0.84
2:B:211:ASP:OD1	2:B:212:GLU:N	2.12	0.83
2:K:187:THR:O	2:K:189:CYS:N	2.13	0.81
2:K:199:ARG:HD3	2:K:206:THR:HG21	1.62	0.81
2:B:152:ARG:HD3	2:B:153:VAL:H	1.46	0.80
2:F:154:PHE:HB2	2:F:155:PRO:HD3	1.62	0.80
2:K:201:SER:HB3	2:K:206:THR:CA	2.10	0.80
1:M:181:LEU:HD13	1:M:199:ARG:HH12	1.47	0.80
1:M:46:PRO:HB2	1:M:253:TRP:CH2	2.17	0.80
2:K:319:ASN:OD1	2:K:319:ASN:O	2.00	0.79
1:X:45:ALA:HB1	1:X:253:TRP:HB3	1.66	0.78
2:K:152:ARG:HD3	2:K:153:VAL:HG13	1.65	0.78
2:K:246:SER:HA	1:M:201:GLN:HE21	1.49	0.78
1:M:175:GLN:O	1:M:229:VAL:N	2.11	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:HB3	1:A:157:SER:H	1.47	0.77
1:M:251:ASP:HB3	1:M:252:PRO:HD3	1.67	0.77
1:A:67:SER:HB2	1:A:74:SER:HB2	1.66	0.77
2:F:149:LEU:HD12	2:F:158:LYS:HD3	1.67	0.77
2:K:211:ASP:OD1	2:K:212:GLU:N	2.18	0.76
1:M:150:PRO:HD2	1:M:222:LEU:HD12	1.68	0.76
1:M:203:ARG:HB3	1:M:220:SER:HB2	1.65	0.76
1:A:168:TYR:HA	1:A:235:GLU:O	1.85	0.76
2:B:219:LEU:HD23	2:B:233:LEU:HD12	1.67	0.76
1:M:50:ILE:HG13	1:M:75:LEU:HD13	1.68	0.76
2:B:234:ARG:HD2	2:B:256:GLN:HE21	1.51	0.76
2:K:37:ASN:O	2:K:200:ALA:HA	1.86	0.76
1:M:217:MET:HE1	1:M:219:LEU:HB2	1.68	0.76
2:K:319:ASN:O	2:K:320:LYS:HG3	1.86	0.75
2:F:187:THR:H	2:F:188:PRO:CD	2.00	0.75
2:K:224:ARG:HG2	2:K:245:THR:HG21	1.67	0.75
1:X:203:ARG:HD2	1:X:221:SER:HB2	1.68	0.74
1:A:167:ARG:HB2	1:A:237:LEU:O	1.90	0.72
2:B:129:LYS:HE2	2:B:131:SER:HB2	1.69	0.72
1:M:229:VAL:HG22	1:M:258:LEU:HD13	1.70	0.72
2:B:152:ARG:O	2:B:153:VAL:C	2.32	0.71
1:A:167:ARG:O	1:A:236:ASN:HA	1.90	0.71
2:B:44:MET:HB2	2:B:242:ALA:HB3	1.72	0.71
1:M:147:VAL:HG13	1:M:260:THR:HB	1.72	0.71
2:K:155:PRO:HG2	2:K:158:LYS:C	2.16	0.71
1:X:168:TYR:HB2	1:X:189:PRO:HD2	1.72	0.71
1:A:152:SER:O	1:A:222:LEU:HD12	1.91	0.70
1:M:41:HIS:HB3	1:M:42:PRO:HD2	1.72	0.70
1:M:57:PRO:HD2	1:M:60:VAL:HG21	1.73	0.70
2:B:155:PRO:CB	2:B:172:ASN:HB3	2.21	0.70
1:A:99:PRO:HB3	2:B:231:LEU:HD22	1.74	0.70
2:F:224:ARG:HD2	2:F:231:LEU:HG	1.73	0.69
1:A:147:VAL:HG13	1:A:260:THR:HB	1.74	0.69
2:B:187:THR:HG23	2:B:191:ILE:HG21	1.75	0.69
2:B:298:PHE:HB2	2:B:386:GLU:HB3	1.75	0.69
2:F:320:LYS:H	2:F:389:LYS:HE3	1.58	0.69
1:A:160:ALA:HB3	1:A:213:SER:HB3	1.74	0.69
2:K:40:GLU:HG2	2:K:198:LYS:HG2	1.75	0.69
2:B:155:PRO:HB2	2:B:172:ASN:HB3	1.75	0.68
1:X:52:ASP:OD1	1:X:53:ALA:N	2.20	0.68
2:B:155:PRO:HG2	2:B:172:ASN:ND2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:GLU:OE2	2:K:300:ARG:NE	2.25	0.68
2:K:18:ASP:HB3	2:K:394:PRO:HD2	1.75	0.68
2:F:229:GLY:HA3	1:X:245:TYR:HB2	1.76	0.68
1:X:165:PHE:HB3	1:X:237:LEU:HD22	1.75	0.68
1:X:67:SER:HB3	1:X:74:SER:HB2	1.74	0.68
2:B:95:ARG:HB2	2:B:178:TRP:HZ3	1.59	0.68
2:K:244:GLN:NE2	1:M:196:TYR:O	2.27	0.68
1:M:173:VAL:HG13	1:M:174:ARG:HG2	1.76	0.67
2:B:150:HIS:ND1	2:B:160:SER:O	2.27	0.67
2:B:260:LEU:O	2:B:262:ASP:O	2.11	0.67
1:M:93:TYR:HA	1:M:101:VAL:HG12	1.76	0.67
2:K:284:LEU:HD21	2:F:382:GLN:HG2	1.77	0.66
2:K:305:ARG:HG2	2:K:306:LYS:O	1.95	0.66
2:B:155:PRO:HG2	2:B:172:ASN:CG	2.20	0.66
1:X:234:ARG:HB3	1:X:252:PRO:HB2	1.78	0.66
2:K:150:HIS:O	2:K:158:LYS:HA	1.96	0.66
1:A:149:LYS:HB2	1:A:150:PRO:HD3	1.76	0.65
2:F:91:PRO:HG3	2:F:168:TYR:HD1	1.61	0.65
1:A:52:ASP:OD2	1:A:242:THR:HG22	1.95	0.65
2:K:40:GLU:OE1	2:K:196:ARG:NE	2.27	0.65
1:M:172:TRP:HB2	1:M:232:CYS:HA	1.77	0.65
2:K:320:LYS:HA	2:K:390:SER:OG	1.96	0.65
2:B:159:CYS:SG	2:B:160:SER:N	2.69	0.65
2:B:202:ASN:HD21	2:B:205:LYS:HD2	1.60	0.65
1:X:69:SER:HB3	1:X:72:THR:HB	1.78	0.65
2:B:40:GLU:HG2	2:B:198:LYS:HG2	1.79	0.64
2:F:63:GLY:HA2	2:F:134:ILE:HD13	1.78	0.64
2:K:171:THR:OG1	2:K:177:ILE:HB	1.96	0.64
2:F:149:LEU:HB2	2:F:158:LYS:HE2	1.79	0.64
1:M:41:HIS:ND1	1:M:42:PRO:HD3	2.13	0.64
1:M:174:ARG:HH12	1:M:226:ASP:HA	1.61	0.64
2:F:163:THR:HG23	2:F:186:ARG:HD3	1.79	0.64
2:K:199:ARG:O	2:K:200:ALA:HB2	1.98	0.64
2:B:154:PHE:O	2:B:156:GLY:N	2.31	0.64
2:K:345:LEU:HD11	2:K:363:ILE:HG21	1.79	0.64
1:M:176:ALA:HB1	1:M:177:PRO:HD2	1.80	0.64
2:F:142:LEU:HD13	2:F:150:HIS:HB3	1.78	0.64
2:F:277:VAL:O	2:F:281:GLU:HB2	1.98	0.63
2:B:154:PHE:O	2:B:155:PRO:C	2.41	0.63
2:K:285:ASP:OD1	2:F:299:ARG:NH1	2.32	0.63
2:K:319:ASN:OD1	2:K:319:ASN:C	2.40	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:PRO:HB3	2:F:134:ILE:HD12	1.79	0.63
2:K:335:TRP:NE1	2:K:376:MET:HB3	2.09	0.63
2:F:101:LYS:HE3	2:F:137:PRO:HA	1.80	0.63
1:M:16:GLN:HG2	1:M:17:SER:H	1.63	0.63
1:M:48:LEU:HD21	1:M:51:TYR:HB3	1.81	0.63
2:B:51:ILE:HG13	2:B:259:ASN:HD21	1.64	0.62
2:B:339:ILE:HD11	2:B:373:ILE:HG13	1.81	0.62
2:B:368:ASP:CG	2:B:369:ASP:H	2.06	0.62
2:F:179:MET:SD	2:F:179:MET:N	2.72	0.62
2:B:253:PRO:HG2	2:B:255:ASP:HB2	1.80	0.62
2:K:201:SER:HB3	2:K:206:THR:C	2.23	0.62
2:K:244:GLN:OE1	1:M:196:TYR:N	2.25	0.62
2:F:167:THR:HG22	2:F:178:TRP:CZ3	2.33	0.62
2:F:167:THR:HG22	2:F:178:TRP:HZ3	1.65	0.62
2:F:44:MET:HB2	2:F:242:ALA:HB3	1.82	0.62
2:B:163:THR:HG23	2:B:165:SER:H	1.64	0.62
1:M:188:ILE:HG22	1:M:190:ILE:HG22	1.81	0.62
1:X:6:GLN:HG3	1:X:104:GLY:HA3	1.82	0.62
1:M:93:TYR:CZ	1:M:95:GLY:HA3	2.35	0.61
2:B:178:TRP:CD1	2:B:179:MET:H	2.18	0.61
2:F:51:ILE:HD12	2:F:238:GLY:O	2.00	0.61
1:X:155:LYS:HA	1:X:217:MET:O	2.00	0.61
2:K:147:LYS:HG3	1:M:29:ILE:HG12	1.80	0.61
1:X:181:LEU:HD12	1:X:181:LEU:H	1.66	0.61
1:X:250:PHE:O	1:X:253:TRP:NE1	2.34	0.61
2:K:90:THR:HG22	2:K:92:ASP:HB3	1.83	0.61
2:B:54:ILE:O	2:B:144:PRO:CD	2.46	0.61
1:M:172:TRP:CH2	1:M:217:MET:HB2	2.36	0.61
2:K:255:ASP:HB2	2:K:257:LEU:HD23	1.83	0.60
1:M:176:ALA:HB3	1:M:179:GLN:HB2	1.81	0.60
1:M:69:SER:N	1:M:72:THR:O	2.35	0.60
1:A:97:TYR:O	1:A:97:TYR:HD1	1.83	0.60
2:B:243:MET:HE3	2:B:244:GLN:OE1	2.01	0.60
2:K:359:PHE:HB2	2:K:363:ILE:HB	1.84	0.60
2:K:201:SER:CB	2:K:206:THR:HA	2.22	0.59
2:F:91:PRO:HA	2:F:94:CYS:HB2	1.84	0.59
2:F:187:THR:N	2:F:188:PRO:HD2	2.10	0.59
2:B:343:GLY:HA2	2:B:371:VAL:HG23	1.82	0.59
1:A:56:ARG:NH2	1:A:61:PRO:HG2	2.17	0.59
1:M:167:ARG:HH21	1:M:238:ASP:H	1.51	0.59
2:B:25:PRO:HG2	2:B:27:ASN:HD21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:HIS:O	2:B:273:VAL:HG22	2.03	0.58
1:X:169:THR:O	1:X:171:ASN:ND2	2.35	0.58
2:B:298:PHE:HD1	2:B:362:GLY:HA2	1.67	0.58
2:B:372:LEU:HB2	2:B:377:GLN:HG3	1.86	0.58
2:K:152:ARG:HD3	2:K:153:VAL:H	1.68	0.58
2:K:149:LEU:HD13	2:K:158:LYS:HD3	1.84	0.58
1:A:35:VAL:HG23	1:A:53:ALA:HA	1.84	0.58
1:M:172:TRP:CZ2	1:M:217:MET:HB2	2.39	0.58
1:X:251:ASP:HB3	1:X:252:PRO:HD3	1.86	0.58
2:K:171:THR:HG21	2:K:177:ILE:HG12	1.86	0.58
2:B:385:MET:SD	2:B:385:MET:N	2.76	0.58
1:A:57:PRO:HG2	1:A:61:PRO:HB3	1.86	0.57
1:A:56:ARG:HD2	1:A:64:PHE:HA	1.85	0.57
2:K:36:THR:HB	2:K:200:ALA:O	2.04	0.57
2:F:148:SER:O	2:F:149:LEU:CD2	2.44	0.57
2:B:297:SER:HB2	2:B:387:LEU:HA	1.85	0.57
1:M:93:TYR:CE1	1:M:95:GLY:HA3	2.39	0.57
2:K:342:LYS:NZ	2:K:369:ASP:OD1	2.29	0.57
2:F:349:GLY:O	2:F:350:ARG:HG2	2.04	0.57
1:M:46:PRO:O	1:M:253:TRP:NE1	2.37	0.57
1:X:204:LEU:HD11	1:X:217:MET:HG2	1.86	0.57
2:F:16:PRO:HA	2:F:323:MET:HA	1.86	0.57
1:A:10:VAL:HG21	1:A:20:ILE:HG12	1.87	0.56
2:K:219:LEU:HA	2:K:235:LEU:HD22	1.87	0.56
2:K:44:MET:HB2	2:K:242:ALA:HB3	1.87	0.56
2:K:152:ARG:HB3	2:K:154:PHE:CE2	2.40	0.56
1:A:6:GLN:HB3	1:A:107:THR:CG2	2.35	0.56
2:B:18:ASP:OD1	2:B:18:ASP:N	2.38	0.56
2:F:306:LYS:HB2	2:F:329:TYR:CD2	2.40	0.56
2:K:59:PHE:CG	2:K:60:THR:N	2.69	0.56
2:K:218:SER:C	2:K:220:LYS:H	2.14	0.56
1:M:181:LEU:HD13	1:M:199:ARG:NH1	2.19	0.56
2:F:224:ARG:HG3	2:F:249:THR:HB	1.87	0.56
1:X:140:LEU:HD23	1:X:160:ALA:HB2	1.88	0.56
2:B:201:SER:HA	2:B:207:CYS:HB2	1.88	0.56
2:B:56:VAL:O	2:B:142:LEU:HD21	2.06	0.56
2:K:142:LEU:HD21	2:K:179:MET:HE3	1.87	0.56
1:M:41:HIS:CB	1:M:42:PRO:HD2	2.34	0.56
1:M:170:VAL:O	1:M:186:GLY:HA2	2.06	0.56
1:M:41:HIS:ND1	1:M:42:PRO:CD	2.69	0.55
1:M:148:LYS:HB2	1:M:150:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:ASN:HB2	2:F:28:LEU:HG	1.88	0.55
2:F:306:LYS:HB2	2:F:329:TYR:CE2	2.42	0.55
1:A:226:ASP:O	1:A:230:TYR:OH	2.21	0.55
2:B:301:LEU:HD21	2:B:316:THR:HA	1.89	0.55
2:K:389:LYS:HD2	2:K:390:SER:H	1.71	0.55
2:B:186:ARG:O	2:B:190:ASP:HB3	2.07	0.55
2:B:282:GLU:HA	2:B:285:ASP:HB2	1.87	0.55
2:K:51:ILE:HD11	2:K:234:ARG:HE	1.72	0.55
2:B:53:ALA:O	2:B:54:ILE:HG12	2.07	0.55
2:B:60:THR:OG1	2:B:137:PRO:O	2.23	0.55
2:F:318:PHE:CZ	2:F:355:VAL:HG21	2.42	0.55
1:X:164:THR:O	1:X:165:PHE:HB2	2.06	0.55
1:X:234:ARG:NE	1:X:235:GLU:O	2.40	0.55
2:F:305:ARG:HG2	2:F:306:LYS:O	2.07	0.54
2:B:363:ILE:HG12	2:B:374:PRO:HD2	1.88	0.54
2:K:46:LEU:HB3	2:K:48:VAL:O	2.08	0.54
1:X:51:TYR:CZ	1:X:55:LYS:HB3	2.42	0.54
2:B:185:PRO:HB3	2:B:188:PRO:HG2	1.89	0.54
2:K:207:CYS:SG	2:K:208:GLY:N	2.80	0.54
2:K:152:ARG:HG3	2:K:153:VAL:HG22	1.90	0.54
2:F:227:LEU:O	2:F:229:GLY:N	2.40	0.54
2:K:199:ARG:HH11	2:K:206:THR:HG21	1.73	0.54
1:M:184:MET:O	1:M:197:ALA:N	2.41	0.54
2:B:187:THR:H	2:B:188:PRO:HD2	1.71	0.54
2:K:44:MET:HE2	1:M:191:PHE:CD2	2.43	0.54
2:K:59:PHE:HE2	2:K:61:CYS:SG	2.30	0.54
2:F:373:ILE:HB	2:F:376:MET:HB3	1.90	0.54
2:B:168:TYR:HA	2:B:178:TRP:CD1	2.42	0.54
1:X:4:LEU:HD11	1:X:92:SER:H	1.73	0.53
2:B:62:THR:O	2:B:89:PRO:HB3	2.08	0.53
2:K:320:LYS:NZ	2:K:390:SER:HB2	2.23	0.53
2:B:54:ILE:HB	2:B:144:PRO:HG3	1.91	0.53
2:B:224:ARG:NH2	2:B:249:THR:OG1	2.41	0.53
2:K:373:ILE:O	2:K:377:GLN:N	2.39	0.53
1:M:46:PRO:HB2	1:M:253:TRP:CE2	2.42	0.53
1:X:167:ARG:O	1:X:234:ARG:NH2	2.41	0.53
2:F:150:HIS:O	2:F:158:LYS:HA	2.09	0.53
1:X:229:VAL:HA	1:X:257:THR:O	2.08	0.53
2:B:342:LYS:HG3	2:B:369:ASP:HB3	1.91	0.53
2:K:14:TRP:CH2	2:K:316:THR:HG22	2.44	0.53
2:K:253:PRO:HG2	2:K:255:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:53:ALA:O	2:K:55:LYS:HD3	2.08	0.53
2:K:90:THR:CG2	2:K:92:ASP:HB3	2.38	0.53
2:B:58:GLY:HA2	2:B:180:PRO:O	2.08	0.53
2:B:178:TRP:CE2	2:B:180:PRO:HG3	2.43	0.53
2:K:60:THR:HA	2:K:177:ILE:CG2	2.34	0.53
2:B:52:SER:HB3	2:B:259:ASN:CG	2.34	0.53
2:B:129:LYS:HG2	2:B:130:GLU:O	2.09	0.53
2:K:95:ARG:O	2:K:98:TYR:HE1	1.92	0.53
1:M:48:LEU:HG	1:M:57:PRO:HG3	1.90	0.53
1:M:219:LEU:HD21	1:M:226:ASP:OD2	2.10	0.52
2:B:139:VAL:HG12	2:B:139:VAL:O	2.08	0.52
2:K:219:LEU:HD11	2:K:233:LEU:HD12	1.91	0.52
2:K:302:SER:HB3	2:K:375:GLU:HG3	1.91	0.52
2:K:316:THR:HB	2:K:360:PHE:O	2.10	0.52
2:K:359:PHE:HD2	2:K:363:ILE:HG22	1.74	0.52
2:B:95:ARG:HB2	2:B:178:TRP:CZ3	2.43	0.52
1:M:159:LYS:NZ	1:M:213:SER:O	2.42	0.52
1:M:204:LEU:HD21	1:M:206:ILE:HG13	1.91	0.52
2:B:38:LEU:HD13	2:B:198:LYS:HD2	1.91	0.52
1:A:231:PHE:HD2	1:A:255:GLN:HA	1.75	0.52
1:A:12:GLY:HA3	1:A:18:VAL:HG21	1.90	0.52
2:K:343:GLY:HA2	2:K:371:VAL:HG23	1.90	0.52
1:M:159:LYS:HB2	1:M:214:THR:HG21	1.91	0.52
2:K:207:CYS:O	2:K:219:LEU:HB3	2.09	0.52
2:B:316:THR:HB	2:B:360:PHE:HA	1.91	0.52
2:K:229:GLY:HA3	1:M:245:TYR:O	2.09	0.52
2:K:248:GLU:OE1	2:K:248:GLU:N	2.43	0.51
2:K:146:ASP:O	2:K:147:LYS:HB2	2.09	0.51
1:M:40:GLN:HB3	1:M:46:PRO:HA	1.91	0.51
1:A:230:TYR:HB2	1:A:257:THR:HB	1.91	0.51
1:A:237:LEU:HD21	1:A:243:TYR:CD1	2.45	0.51
2:K:3:PRO:HD2	2:K:307:LEU:O	2.10	0.51
1:X:36:SER:O	1:X:91:CYS:N	2.43	0.51
2:K:44:MET:HE3	1:M:193:THR:HG21	1.92	0.51
2:B:40:GLU:HA	2:B:198:LYS:HA	1.93	0.51
2:K:149:LEU:HD22	2:K:158:LYS:HD2	1.91	0.51
2:B:51:ILE:HG23	2:B:240:TRP:HB2	1.90	0.51
2:F:181:GLU:HG2	2:F:184:ARG:HD2	1.93	0.51
1:M:217:MET:SD	1:M:218:GLU:N	2.83	0.51
2:B:231:LEU:HD11	2:B:251:TRP:CH2	2.45	0.51
1:A:237:LEU:HD11	1:A:243:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ARG:HD2	2:B:256:GLN:NE2	2.23	0.51
2:B:388:LEU:O	2:B:389:LYS:HE2	2.10	0.51
2:F:376:MET:C	2:F:378:SER:H	2.19	0.51
1:X:186:GLY:HA3	1:X:246:PHE:HE1	1.76	0.51
2:B:253:PRO:C	2:B:255:ASP:H	2.18	0.51
2:K:16:PRO:HA	2:K:323:MET:HA	1.93	0.51
1:M:91:CYS:HB2	1:M:103:PHE:CD1	2.45	0.50
1:M:230:TYR:N	1:M:257:THR:O	2.44	0.50
2:F:179:MET:N	2:F:180:PRO:HD3	2.27	0.50
2:K:60:THR:OG1	2:K:137:PRO:HD2	2.11	0.50
2:K:170:SER:HB3	2:K:175:TYR:CE1	2.46	0.50
1:X:235:GLU:OE2	1:X:248:GLY:O	2.28	0.50
1:A:20:ILE:HG21	1:A:107:THR:HG21	1.93	0.50
2:B:62:THR:HG22	2:B:176:THR:HG22	1.94	0.50
2:K:152:ARG:HB3	2:K:154:PHE:CD2	2.47	0.50
2:F:137:PRO:HD2	2:F:138:SER:H	1.76	0.50
2:K:362:GLY:O	2:K:374:PRO:HG2	2.12	0.50
1:X:167:ARG:HE	1:X:245:TYR:HE1	1.55	0.50
2:B:154:PHE:O	2:B:156:GLY:O	2.30	0.50
1:M:169:THR:O	1:M:234:ARG:HA	2.11	0.50
1:X:51:TYR:CE2	1:X:55:LYS:HB3	2.46	0.50
1:X:167:ARG:HH22	1:X:244:TYR:HB2	1.76	0.50
1:M:171:ASN:O	1:M:233:ALA:HB3	2.12	0.50
1:X:169:THR:OG1	1:X:235:GLU:HB2	2.11	0.50
1:A:49:MET:O	1:A:57:PRO:HD3	2.11	0.50
2:B:51:ILE:HD13	2:B:234:ARG:HG3	1.93	0.50
1:M:141:VAL:HB	1:M:159:LYS:O	2.12	0.50
1:M:149:LYS:HE3	1:M:260:THR:HG22	1.93	0.50
2:B:232:GLY:O	2:B:233:LEU:HD23	2.12	0.49
1:M:48:LEU:HD21	1:M:51:TYR:CB	2.41	0.49
1:A:237:LEU:HB3	1:A:249:TRP:HZ3	1.77	0.49
2:B:154:PHE:CE1	2:B:179:MET:HG3	2.48	0.49
2:B:258:VAL:HG13	2:B:260:LEU:H	1.77	0.49
2:K:359:PHE:CD2	2:K:363:ILE:HG22	2.48	0.49
1:A:222:LEU:HD23	1:A:261:VAL:HG22	1.93	0.49
2:B:178:TRP:CG	2:B:180:PRO:HD3	2.47	0.49
2:K:5:TYR:HB2	2:K:376:MET:SD	2.52	0.49
2:K:290:ILE:HD11	2:K:300:ARG:HD2	1.95	0.49
2:F:229:GLY:CA	1:X:245:TYR:HB2	2.41	0.49
1:M:234:ARG:HG2	1:M:252:PRO:HD2	1.93	0.49
2:F:35:CYS:HA	2:F:200:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:6:GLN:HB2	1:X:105:GLY:H	1.76	0.49
1:X:187:ILE:HG13	1:X:193:THR:O	2.13	0.49
2:B:152:ARG:HD3	2:B:153:VAL:HG12	1.95	0.49
2:B:155:PRO:CG	2:B:172:ASN:ND2	2.75	0.49
2:B:184:ARG:HG3	2:B:185:PRO:HD2	1.95	0.49
2:B:187:THR:N	2:B:188:PRO:HD2	2.28	0.49
2:K:171:THR:HG21	2:K:177:ILE:CG1	2.43	0.49
1:A:232:CYS:O	1:A:254:GLY:N	2.35	0.49
2:B:317:ILE:HD13	2:B:389:LYS:HG2	1.95	0.49
2:B:347:VAL:HG21	2:B:352:HIS:ND1	2.28	0.49
2:F:46:LEU:HD12	2:F:240:TRP:HB3	1.95	0.49
2:F:51:ILE:C	2:F:53:ALA:H	2.20	0.49
1:A:237:LEU:HB3	1:A:249:TRP:CZ3	2.48	0.49
2:K:201:SER:O	2:K:202:ASN:C	2.56	0.49
2:F:187:THR:O	2:F:189:CYS:N	2.46	0.49
2:F:7:ILE:HG13	2:F:338:ILE:HG21	1.95	0.49
1:X:45:ALA:HB2	1:X:254:GLY:C	2.38	0.49
2:F:18:ASP:OD1	2:F:21:HIS:CE1	2.66	0.48
2:F:231:LEU:HD22	1:X:99:PRO:HB3	1.95	0.48
2:B:368:ASP:CG	2:B:369:ASP:N	2.70	0.48
2:K:320:LYS:HZ2	2:K:390:SER:HB2	1.77	0.48
2:B:51:ILE:HG12	2:B:238:GLY:O	2.13	0.48
2:B:179:MET:N	2:B:180:PRO:HD3	2.28	0.48
2:B:192:PHE:HZ	2:B:227:LEU:HB3	1.78	0.48
2:K:59:PHE:HE1	2:K:136:SER:HB2	1.78	0.48
2:K:180:PRO:O	2:K:180:PRO:HD2	2.12	0.48
1:M:28:ASP:HB2	1:M:96:ASP:CG	2.37	0.48
1:A:236:ASN:OD1	1:A:236:ASN:N	2.43	0.48
2:B:194:ASN:OD1	2:B:195:SER:N	2.46	0.48
2:K:145:TYR:CG	2:K:145:TYR:O	2.66	0.48
1:X:170:VAL:HA	1:X:233:ALA:O	2.13	0.48
2:K:8:PRO:HG3	2:K:329:TYR:CE1	2.49	0.48
2:K:340:PRO:HG3	2:K:346:LYS:HG3	1.94	0.48
1:A:171:ASN:N	1:A:233:ALA:O	2.41	0.48
2:B:63:GLY:HA3	2:B:89:PRO:HD3	1.94	0.48
2:K:201:SER:HB3	2:K:207:CYS:N	2.29	0.48
1:M:159:LYS:HG2	1:M:160:ALA:N	2.29	0.48
2:B:342:LYS:HG3	2:B:369:ASP:CB	2.44	0.48
1:M:7:PRO:HD2	1:M:21:SER:O	2.14	0.48
1:M:172:TRP:N	1:M:172:TRP:CD1	2.80	0.48
2:F:154:PHE:HB2	2:F:155:PRO:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:CD2	1:A:255:GLN:HA	2.49	0.48
2:K:233:LEU:HA	2:K:233:LEU:HD23	1.65	0.48
1:M:48:LEU:HD11	1:M:51:TYR:HA	1.95	0.48
1:M:234:ARG:HD3	1:M:252:PRO:HG2	1.96	0.48
2:F:187:THR:C	2:F:189:CYS:N	2.71	0.48
1:A:36:SER:N	1:A:91:CYS:O	2.40	0.48
1:A:103:PHE:CD2	1:A:181:LEU:HB2	2.49	0.48
2:B:386:GLU:C	2:B:387:LEU:HD22	2.39	0.48
2:K:250:LYS:HA	2:K:250:LYS:HD3	1.62	0.48
2:B:280:ARG:NH2	2:K:382:GLN:HB2	2.30	0.47
2:K:210:VAL:HA	2:K:215:LEU:O	2.14	0.47
2:K:306:LYS:HB2	2:K:329:TYR:CD2	2.49	0.47
2:K:7:ILE:O	2:K:330:LYS:N	2.42	0.47
2:F:51:ILE:HD13	2:F:234:ARG:HG3	1.96	0.47
2:F:59:PHE:HA	2:F:140:THR:H	1.79	0.47
2:B:41:PHE:CE1	2:B:199:ARG:HB2	2.49	0.47
2:F:373:ILE:HB	2:F:376:MET:HE2	1.96	0.47
1:A:6:GLN:HE22	1:A:89:TYR:HA	1.79	0.47
2:B:50:TYR:CE1	2:B:239:THR:HG23	2.50	0.47
2:K:198:LYS:O	2:K:209:PHE:HA	2.15	0.47
1:M:174:ARG:O	1:M:182:GLU:OE2	2.32	0.47
2:F:51:ILE:HD11	2:F:240:TRP:HB2	1.95	0.47
2:F:169:CYS:SG	2:F:170:SER:N	2.87	0.47
2:B:260:LEU:O	2:B:261:HIS:C	2.58	0.47
2:B:14:TRP:CH2	2:B:316:THR:HG22	2.49	0.47
2:B:319:ASN:OD1	2:B:320:LYS:HG3	2.15	0.47
2:B:364:ILE:HG12	2:B:372:LEU:HD11	1.96	0.47
2:F:194:ASN:OD1	2:F:195:SER:N	2.48	0.47
2:F:305:ARG:CG	2:F:306:LYS:O	2.63	0.47
1:X:169:THR:HG22	1:X:188:ILE:HG13	1.97	0.47
2:B:57:ASN:O	2:B:181:GLU:HB2	2.14	0.47
2:B:389:LYS:HG3	2:B:390:SER:H	1.79	0.47
2:F:87:PHE:CD1	2:F:134:ILE:HD11	2.50	0.47
2:B:93:ALA:O	2:B:97:ALA:N	2.47	0.47
2:B:372:LEU:HD22	2:B:383:GLN:OE1	2.15	0.47
1:M:68:LYS:HA	1:M:73:ALA:HA	1.97	0.47
2:F:94:CYS:HB3	2:F:178:TRP:HE1	1.79	0.47
1:X:101:VAL:HG13	1:X:246:PHE:O	2.15	0.47
2:K:305:ARG:NE	2:K:375:GLU:OE2	2.42	0.47
1:M:255:GLN:OE1	1:M:255:GLN:N	2.48	0.47
2:B:59:PHE:CZ	2:B:180:PRO:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:192:PHE:CE1	2:K:227:LEU:HD13	2.50	0.46
1:M:159:LYS:HG2	1:M:160:ALA:H	1.79	0.46
1:M:207:THR:C	1:M:216:TYR:H	2.22	0.46
2:F:8:PRO:HB3	2:F:327:ALA:HB1	1.96	0.46
2:F:19:ILE:HD11	2:F:294:LYS:HE2	1.96	0.46
2:F:25:PRO:HB3	2:F:306:LYS:HD2	1.96	0.46
2:F:43:TYR:HE1	2:F:45:GLU:HB2	1.80	0.46
2:K:230:VAL:HA	1:M:195:ASN:OD1	2.15	0.46
2:F:298:PHE:HB2	2:F:386:GLU:OE1	2.14	0.46
1:X:45:ALA:HB1	1:X:253:TRP:CB	2.39	0.46
1:A:237:LEU:HD21	1:A:243:TYR:CG	2.50	0.46
2:F:8:PRO:HG3	2:F:329:TYR:CE1	2.50	0.46
1:M:174:ARG:NH1	1:M:230:TYR:OH	2.48	0.46
1:X:46:PRO:HB2	1:X:253:TRP:CD1	2.51	0.46
1:A:175:GLN:OE1	1:A:179:GLN:O	2.33	0.46
2:B:62:THR:O	2:B:134:ILE:HG23	2.15	0.46
2:B:373:ILE:H	2:B:376:MET:HE2	1.81	0.46
1:M:36:SER:N	1:M:91:CYS:O	2.46	0.46
1:M:46:PRO:CB	1:M:253:TRP:CH2	2.96	0.46
2:F:62:THR:O	2:F:89:PRO:HG3	2.16	0.46
2:F:306:LYS:HD3	2:F:312:GLY:HA3	1.96	0.46
1:X:24:GLY:O	1:X:25:THR:C	2.56	0.46
1:X:236:ASN:HB2	1:X:249:TRP:CZ3	2.51	0.46
2:B:62:THR:HB	2:B:175:TYR:CD2	2.51	0.46
2:K:44:MET:HB2	2:K:242:ALA:CB	2.46	0.46
2:K:89:PRO:HB2	2:K:94:CYS:SG	2.55	0.46
1:X:186:GLY:HA3	1:X:246:PHE:CE1	2.50	0.46
2:K:354:HIS:ND1	2:K:354:HIS:O	2.49	0.46
1:M:179:GLN:HG3	1:M:180:GLY:H	1.80	0.46
1:A:94:ALA:O	2:B:226:LYS:NZ	2.41	0.45
2:K:95:ARG:O	2:K:98:TYR:CE1	2.68	0.45
2:F:271:LEU:HD12	2:F:271:LEU:O	2.16	0.45
1:X:68:LYS:HD3	1:X:69:SER:O	2.16	0.45
2:F:149:LEU:HD22	2:F:160:SER:HA	1.99	0.45
1:M:234:ARG:CD	1:M:252:PRO:HG2	2.46	0.45
2:F:244:GLN:O	2:F:245:THR:C	2.58	0.45
2:F:363:ILE:HG12	2:F:374:PRO:HD2	1.97	0.45
1:A:167:ARG:HH11	1:A:243:TYR:HE2	1.64	0.45
1:A:250:PHE:O	1:A:253:TRP:NE1	2.48	0.45
2:K:57:ASN:HA	2:K:141:ASP:HB3	1.99	0.45
2:F:5:TYR:HB3	2:F:332:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:SER:O	2:F:324:GLU:N	2.38	0.45
2:B:37:ASN:HB2	2:B:201:SER:O	2.17	0.45
2:K:89:PRO:HB3	2:K:134:ILE:HD12	1.99	0.45
1:M:147:VAL:HA	1:M:260:THR:H	1.82	0.45
2:F:49:GLY:O	2:F:239:THR:HG22	2.16	0.45
2:F:51:ILE:N	2:F:238:GLY:O	2.46	0.45
2:F:299:ARG:O	2:F:302:SER:OG	2.34	0.45
1:A:244:TYR:CE2	2:B:228:CYS:HA	2.52	0.45
1:A:251:ASP:HB3	1:A:252:PRO:HD3	1.99	0.45
2:K:95:ARG:NH2	2:K:166:SER:OG	2.49	0.45
1:A:244:TYR:O	1:A:247:SER:HB2	2.16	0.45
2:B:387:LEU:O	2:B:388:LEU:HD23	2.16	0.45
2:K:220:LYS:O	2:K:236:MET:HE2	2.17	0.45
2:F:18:ASP:OD1	2:F:21:HIS:ND1	2.49	0.45
1:X:38:TYR:OH	1:X:250:PHE:N	2.47	0.45
2:B:49:GLY:O	2:B:239:THR:HA	2.16	0.45
1:M:40:GLN:HB3	1:M:46:PRO:CA	2.45	0.45
2:F:277:VAL:O	2:F:281:GLU:CB	2.64	0.45
2:K:288:GLU:O	2:K:292:THR:HG23	2.16	0.45
2:F:46:LEU:HD13	2:F:54:ILE:HD11	1.99	0.45
2:F:346:LYS:HE3	2:F:348:GLY:O	2.17	0.45
1:A:68:LYS:HA	1:A:73:ALA:HA	1.99	0.45
1:A:159:LYS:HD3	1:A:214:THR:OG1	2.17	0.45
2:B:61:CYS:HA	2:B:136:SER:HA	1.99	0.45
2:B:178:TRP:CD1	2:B:180:PRO:HD3	2.52	0.45
2:B:261:HIS:HB2	2:B:262:ASP:H	1.59	0.45
2:K:164:VAL:HG13	2:K:184:ARG:NH1	2.32	0.45
1:M:25:THR:O	1:M:71:ASN:HA	2.16	0.45
1:M:54:THR:HB	1:M:66:GLY:HA3	1.97	0.45
1:A:166:ASN:O	1:A:168:TYR:HD1	2.00	0.44
2:B:177:ILE:HG23	2:B:178:TRP:N	2.32	0.44
2:B:256:GLN:HA	2:B:261:HIS:CE1	2.52	0.44
2:K:338:ILE:HD11	2:K:376:MET:HE1	1.98	0.44
2:F:209:PHE:O	2:F:216:TYR:HA	2.17	0.44
1:X:71:ASN:OD1	1:X:71:ASN:N	2.50	0.44
2:K:135:ILE:HD12	2:K:135:ILE:H	1.82	0.44
1:M:172:TRP:CB	1:M:232:CYS:HA	2.46	0.44
2:F:2:PHE:HZ	2:F:276:LEU:HD23	1.82	0.44
1:A:34:PHE:O	1:A:92:SER:HA	2.17	0.44
2:B:149:LEU:O	2:B:150:HIS:CG	2.71	0.44
2:K:276:LEU:HD23	2:F:380:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:359:PHE:N	2:K:363:ILE:O	2.44	0.44
1:M:199:ARG:HD2	1:M:200:PHE:CD2	2.51	0.44
1:A:203:ARG:HA	1:A:220:SER:HB2	1.99	0.44
2:B:384:HIS:O	2:B:387:LEU:HD23	2.17	0.44
2:F:59:PHE:O	2:F:179:MET:HB3	2.17	0.44
2:F:187:THR:O	2:F:188:PRO:C	2.59	0.44
2:B:279:LYS:HD2	2:B:279:LYS:HA	1.79	0.44
1:A:240:SER:HA	1:A:243:TYR:HB3	2.00	0.44
2:F:152:ARG:O	2:F:157:GLY:HA2	2.17	0.44
2:F:187:THR:N	2:F:188:PRO:CD	2.75	0.44
2:F:227:LEU:HA	2:F:227:LEU:HD23	1.66	0.44
2:F:305:ARG:O	2:F:306:LYS:C	2.60	0.44
1:X:41:HIS:HB2	1:X:42:PRO:CD	2.39	0.44
2:B:177:ILE:HG23	2:B:178:TRP:H	1.82	0.44
2:F:8:PRO:HG3	2:F:329:TYR:HE1	1.82	0.44
2:F:51:ILE:CG1	2:F:240:TRP:HB2	2.48	0.44
2:F:335:TRP:CZ3	2:F:376:MET:HB2	2.53	0.44
2:B:158:LYS:HE2	2:B:158:LYS:HB3	1.74	0.44
2:B:253:PRO:C	2:B:255:ASP:N	2.76	0.44
2:B:384:HIS:O	2:B:384:HIS:CG	2.71	0.44
1:A:7:PRO:O	1:A:107:THR:HG22	2.17	0.43
2:K:142:LEU:HD22	2:K:150:HIS:HB3	1.99	0.43
2:K:220:LYS:HA	2:K:220:LYS:HD2	1.70	0.43
2:B:231:LEU:HD12	2:B:231:LEU:HA	1.72	0.43
2:B:292:THR:HG21	2:K:300:ARG:HH21	1.82	0.43
2:K:244:GLN:CD	1:M:196:TYR:H	2.19	0.43
1:A:142:GLN:HG2	1:A:143:SER:N	2.33	0.43
2:B:46:LEU:HD23	2:B:46:LEU:HA	1.90	0.43
2:B:50:TYR:HD1	2:B:238:GLY:C	2.27	0.43
2:B:136:SER:O	2:B:136:SER:OG	2.34	0.43
2:B:152:ARG:O	2:B:154:PHE:N	2.50	0.43
2:K:231:LEU:HD22	1:M:99:PRO:HB3	2.00	0.43
1:X:4:LEU:HG	1:X:102:VAL:HG23	2.00	0.43
2:B:379:SER:O	2:B:380:LEU:HB2	2.18	0.43
2:K:355:VAL:O	2:K:356:ASN:C	2.61	0.43
2:F:396:MET:HE3	2:F:396:MET:HB2	1.93	0.43
1:A:235:GLU:OE2	1:A:249:TRP:N	2.51	0.43
2:B:138:SER:OG	2:B:139:VAL:N	2.51	0.43
2:K:218:SER:C	2:K:220:LYS:N	2.76	0.43
2:K:292:THR:HA	2:F:388:LEU:HD22	2.00	0.43
1:M:196:TYR:CZ	1:M:205:THR:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:PRO:HG2	2:B:27:ASN:ND2	2.32	0.43
2:B:142:LEU:HA	2:B:152:ARG:HB2	1.99	0.43
2:B:142:LEU:HD22	2:B:179:MET:HE2	2.00	0.43
2:K:8:PRO:HG3	2:K:329:TYR:HE1	1.84	0.43
2:K:135:ILE:HG22	2:K:137:PRO:HD3	2.01	0.43
2:K:149:LEU:C	2:K:150:HIS:ND1	2.76	0.43
1:A:56:ARG:CZ	1:A:61:PRO:HG2	2.49	0.43
1:A:236:ASN:ND2	1:A:236:ASN:O	2.52	0.43
2:B:135:ILE:HG23	2:B:137:PRO:HD3	2.01	0.43
1:A:187:ILE:HD12	1:A:193:THR:O	2.19	0.43
2:K:46:LEU:HD23	2:K:46:LEU:HA	1.85	0.43
2:K:186:ARG:O	2:K:187:THR:C	2.62	0.43
2:K:201:SER:HB2	2:K:207:CYS:SG	2.59	0.43
1:X:38:TYR:OH	1:X:249:TRP:N	2.52	0.43
1:A:29:ILE:HG13	1:A:30:GLY:H	1.84	0.43
2:B:162:ILE:HG23	2:B:162:ILE:O	2.19	0.43
2:K:376:MET:C	2:K:378:SER:H	2.26	0.43
1:M:217:MET:CE	1:M:219:LEU:HB2	2.44	0.43
1:X:94:ALA:HB1	1:X:98:THR:OG1	2.19	0.43
2:B:154:PHE:HE1	2:B:179:MET:HG3	1.83	0.43
2:K:4:ILE:HD12	2:K:376:MET:SD	2.59	0.43
2:K:49:GLY:O	2:K:239:THR:HA	2.19	0.43
2:K:162:ILE:HD11	2:K:179:MET:HE1	2.01	0.43
1:X:6:GLN:HG3	1:X:104:GLY:CA	2.48	0.43
2:K:171:THR:O	2:K:172:ASN:C	2.59	0.42
1:A:160:ALA:N	1:A:213:SER:O	2.51	0.42
2:B:129:LYS:H	2:B:129:LYS:HD3	1.84	0.42
2:K:2:PHE:HE2	2:K:279:LYS:HG3	1.85	0.42
1:M:181:LEU:HD22	1:M:199:ARG:NH2	2.34	0.42
1:M:235:GLU:OE2	1:M:247:SER:O	2.37	0.42
1:X:187:ILE:HA	1:X:193:THR:O	2.19	0.42
1:A:33:ASN:CG	1:A:68:LYS:HZ3	2.27	0.42
2:B:334:THR:O	2:B:337:GLU:HG2	2.19	0.42
2:K:213:ARG:HA	2:K:213:ARG:HD3	1.89	0.42
2:K:305:ARG:CG	2:K:306:LYS:O	2.64	0.42
2:F:44:MET:HB2	2:F:242:ALA:CB	2.49	0.42
2:F:178:TRP:HB2	2:F:180:PRO:HD3	2.01	0.42
1:X:233:ALA:HA	1:X:252:PRO:O	2.18	0.42
1:M:144:GLY:O	1:M:257:THR:HG23	2.19	0.42
1:M:206:ILE:HG23	1:M:216:TYR:O	2.19	0.42
2:F:231:LEU:HD12	2:F:231:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:167:ARG:HD2	1:X:236:ASN:O	2.19	0.42
1:A:156:VAL:HG22	1:A:257:THR:HG21	2.02	0.42
1:A:237:LEU:HD13	1:A:242:THR:OG1	2.20	0.42
2:B:187:THR:HG23	2:B:191:ILE:CG2	2.48	0.42
2:K:277:VAL:O	2:K:281:GLU:N	2.50	0.42
2:F:224:ARG:NH1	2:F:249:THR:OG1	2.52	0.42
2:F:363:ILE:HG23	2:F:372:LEU:O	2.19	0.42
1:X:48:LEU:HD22	1:X:251:ASP:HB2	2.02	0.42
2:K:60:THR:C	2:K:177:ILE:HD12	2.44	0.42
2:F:46:LEU:HD23	2:F:46:LEU:HA	1.95	0.42
2:F:162:ILE:HG22	2:F:167:THR:HA	2.01	0.42
1:A:142:GLN:OE1	1:A:142:GLN:N	2.53	0.42
2:B:51:ILE:CG2	2:B:240:TRP:HB2	2.49	0.42
2:B:247:ASP:C	2:B:248:GLU:HG3	2.45	0.42
1:A:49:MET:HE3	1:A:49:MET:HB3	1.96	0.42
2:K:155:PRO:HG3	2:K:159:CYS:HB3	2.02	0.42
2:K:198:LYS:HE2	2:K:210:VAL:HG11	2.00	0.42
1:A:39:GLN:O	1:A:46:PRO:HA	2.20	0.42
2:B:345:LEU:HA	2:B:345:LEU:HD23	1.81	0.42
2:F:163:THR:N	2:F:186:ARG:HG3	2.35	0.42
1:M:173:VAL:CG1	1:M:184:MET:HB2	2.33	0.42
1:A:191:PHE:CD1	2:B:194:ASN:HB2	2.55	0.41
2:B:195:SER:OG	2:B:196:ARG:N	2.52	0.41
2:B:341:SER:O	2:B:342:LYS:C	2.63	0.41
2:K:15:SER:N	2:K:324:GLU:O	2.53	0.41
2:K:163:THR:O	2:K:166:SER:HB3	2.20	0.41
2:K:237:ASP:OD1	2:K:239:THR:OG1	2.24	0.41
2:K:313:LYS:HB3	2:K:315:TYR:CE1	2.55	0.41
1:M:173:VAL:HG13	1:M:174:ARG:N	2.34	0.41
1:X:206:ILE:HG23	1:X:216:TYR:O	2.20	0.41
1:X:236:ASN:HB2	1:X:249:TRP:CE3	2.55	0.41
2:K:36:THR:HG22	2:K:37:ASN:N	2.35	0.41
1:M:56:ARG:HA	1:M:57:PRO:HD3	1.95	0.41
1:M:185:GLY:HA2	1:M:195:ASN:O	2.20	0.41
2:F:291:MET:HE2	2:F:291:MET:HB3	1.93	0.41
1:A:95:GLY:HA2	2:B:226:LYS:NZ	2.34	0.41
1:A:174:ARG:NH1	1:A:226:ASP:HA	2.35	0.41
2:B:352:HIS:CD2	2:B:353:PRO:HD2	2.56	0.41
2:K:381:LEU:HD23	2:K:381:LEU:HA	1.75	0.41
2:F:162:ILE:HD13	2:F:180:PRO:HB3	2.03	0.41
2:F:89:PRO:HG2	2:F:177:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:51:TYR:N	1:X:55:LYS:O	2.44	0.41
1:X:174:ARG:HH21	1:X:200:PHE:HZ	1.69	0.41
1:A:195:ASN:HD22	1:A:195:ASN:HA	1.66	0.41
2:B:209:PHE:CE1	2:B:219:LEU:HD11	2.56	0.41
2:B:289:SER:HB3	2:B:300:ARG:NH1	2.36	0.41
1:M:41:HIS:CB	1:M:42:PRO:CD	2.98	0.41
2:B:154:PHE:C	2:B:156:GLY:N	2.78	0.41
1:M:46:PRO:O	1:M:253:TRP:CD1	2.74	0.41
1:M:171:ASN:CA	1:M:172:TRP:HD1	2.33	0.41
1:M:52:ASP:CG	1:M:53:ALA:H	2.29	0.41
1:M:144:GLY:O	1:M:146:GLU:HG3	2.21	0.41
2:F:56:VAL:HG22	2:F:142:LEU:HD11	2.02	0.41
2:B:224:ARG:NE	2:B:245:THR:HG22	2.35	0.41
2:B:380:LEU:HD13	2:B:380:LEU:HA	1.91	0.41
1:M:41:HIS:CG	1:M:42:PRO:HD2	2.56	0.41
2:F:359:PHE:HB2	2:F:363:ILE:O	2.21	0.41
1:A:40:GLN:O	1:A:86:ALA:HB1	2.21	0.41
2:B:38:LEU:HD23	2:B:38:LEU:HA	1.86	0.41
2:B:324:GLU:HG2	2:B:325:ALA:N	2.36	0.41
2:B:359:PHE:N	2:B:363:ILE:O	2.50	0.41
2:K:25:PRO:O	2:K:26:ASN:C	2.60	0.41
2:K:345:LEU:HD23	2:K:345:LEU:HA	1.95	0.41
2:K:376:MET:C	2:K:378:SER:N	2.79	0.41
1:M:190:ILE:HG23	1:M:191:PHE:H	1.86	0.41
2:B:152:ARG:CD	2:B:153:VAL:HG12	2.51	0.41
2:B:227:LEU:HD12	2:B:240:TRP:CD2	2.56	0.41
2:B:260:LEU:HA	2:B:263:PHE:CG	2.56	0.41
2:B:291:MET:HE3	2:K:384:HIS:NE2	2.36	0.41
1:A:169:THR:O	1:A:171:ASN:ND2	2.54	0.40
2:F:51:ILE:HD12	2:F:238:GLY:C	2.46	0.40
2:F:333:ARG:HB3	2:F:337:GLU:OE1	2.21	0.40
1:X:46:PRO:HB2	1:X:253:TRP:NE1	2.35	0.40
1:X:204:LEU:HG	1:X:206:ILE:HG13	2.03	0.40
2:K:91:PRO:HG3	2:K:178:TRP:NE1	2.37	0.40
2:K:199:ARG:O	2:K:200:ALA:CB	2.63	0.40
2:B:11:LEU:HD23	2:B:327:ALA:HB2	2.04	0.40
2:K:243:MET:HE2	2:K:243:MET:HB3	1.72	0.40
1:M:61:PRO:HD2	1:M:64:PHE:CD1	2.57	0.40
2:F:7:ILE:HD13	2:F:7:ILE:HA	1.94	0.40
2:B:101:LYS:HA	2:B:101:LYS:HD2	1.96	0.40
2:K:162:ILE:H	2:K:162:ILE:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ARG:NE	2:B:183:PRO:HB3	2.36	0.40
2:B:202:ASN:OD1	2:B:205:LYS:HB2	2.22	0.40
2:K:5:TYR:OH	2:K:363:ILE:HD11	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/264 (80%)	179 (84%)	31 (15%)	2 (1%)	14	49
1	M	195/264 (74%)	158 (81%)	31 (16%)	6 (3%)	3	22
1	X	172/264 (65%)	146 (85%)	23 (13%)	3 (2%)	7	35
2	B	339/433 (78%)	276 (81%)	56 (16%)	7 (2%)	5	30
2	F	324/433 (75%)	267 (82%)	50 (15%)	7 (2%)	5	29
2	K	316/433 (73%)	261 (83%)	47 (15%)	8 (2%)	4	26
All	All	1558/2091 (74%)	1287 (83%)	238 (15%)	33 (2%)	5	30

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	144	PRO
2	K	153	VAL
2	K	155	PRO
2	F	154	PHE
2	F	187	THR
1	X	42	PRO
1	X	165	PHE
1	A	61	PRO
2	B	155	PRO

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Mol	Chain	Res	Type
2	B	180	PRO
2	K	180	PRO
2	K	200	ALA
2	F	228	CYS
2	B	245	THR
1	M	41	HIS
1	M	57	PRO
2	B	185	PRO
2	K	188	PRO
1	M	42	PRO
2	F	137	PRO
2	F	144	PRO
2	B	91	PRO
2	K	320	LYS
2	F	180	PRO
1	M	253	TRP
1	X	41	HIS
2	B	139	VAL
1	M	61	PRO
1	A	251	ASP
2	K	154	PHE
2	B	214	GLY
1	M	180	GLY
2	F	185	PRO

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	182/202 (90%)	180 (99%)	2 (1%)	65	74
1	M	167/202 (83%)	166 (99%)	1 (1%)	78	80
1	X	153/202 (76%)	152 (99%)	1 (1%)	76	79
2	B	313/381 (82%)	302 (96%)	11 (4%)	32	54
2	F	298/381 (78%)	294 (99%)	4 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	K	295/381 (77%)	290 (98%)	5 (2%)	53 67
All	All	1408/1749 (80%)	1384 (98%)	24 (2%)	53 67

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	CYS
1	A	236	ASN
2	B	56	VAL
2	B	131	SER
2	B	149	LEU
2	B	155	PRO
2	B	169	CYS
2	B	189	CYS
2	B	207	CYS
2	B	261	HIS
2	B	262	ASP
2	B	263	PHE
2	B	344	CYS
2	K	35	CYS
2	K	61	CYS
2	K	144	PRO
2	K	182	ASN
2	K	344	CYS
1	M	227	THR
2	F	187	THR
2	F	189	CYS
2	F	271	LEU
2	F	346	LYS
1	X	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	175	GLN
2	B	27	ASN
2	B	256	GLN
2	B	259	ASN
2	B	336	ASN
2	B	370	HIS

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Mol	Chain	Res	Type
2	K	21	HIS
1	M	201	GLN
1	M	239	ASN
2	F	256	GLN
2	F	328	HIS
2	F	370	HIS
2	F	377	GLN
2	F	383	GLN
1	X	142	GLN
1	X	236	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/264 (84%)	0.03	6 (2%) 56 43	152, 209, 248, 262	0
1	M	207/264 (78%)	-0.03	0 100 100	163, 242, 276, 300	0
1	X	190/264 (71%)	0.06	3 (1%) 70 55	186, 241, 274, 283	0
2	B	349/433 (80%)	0.07	10 (2%) 53 41	132, 198, 257, 298	0
2	F	334/433 (77%)	-0.02	7 (2%) 63 49	133, 209, 266, 290	0
2	K	328/433 (75%)	0.11	9 (2%) 56 43	133, 197, 252, 282	0
All	All	1632/2091 (78%)	0.04	35 (2%) 63 49	132, 213, 266, 300	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	3.4
2	B	176	THR	3.4
2	B	157	GLY	3.1
2	F	273	VAL	3.1
2	F	345	LEU	3.1
2	K	345	LEU	2.9
2	K	373	ILE	2.9
1	A	46	PRO	2.8
2	B	380	LEU	2.7
2	B	26	ASN	2.7
2	K	360	PHE	2.6
2	K	335	TRP	2.5
1	A	231	PHE	2.5
1	A	238	ASP	2.5
2	B	103	ALA	2.5
2	K	338	ILE	2.4
2	B	156	GLY	2.4
2	F	26	ASN	2.4
2	K	363	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	X	48	LEU	2.4
1	X	49	MET	2.3
2	B	209	PHE	2.3
2	F	360	PHE	2.3
2	F	19	ILE	2.3
2	F	338	ILE	2.3
1	A	49	MET	2.3
2	K	243	MET	2.2
2	B	269	GLU	2.2
1	A	206	ILE	2.1
2	F	160	SER	2.1
2	B	338	ILE	2.1
2	K	183	PRO	2.1
2	K	55	LYS	2.0
2	B	335	TRP	2.0
1	X	10	VAL	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.