Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2025 – 12:08 PM JST

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:

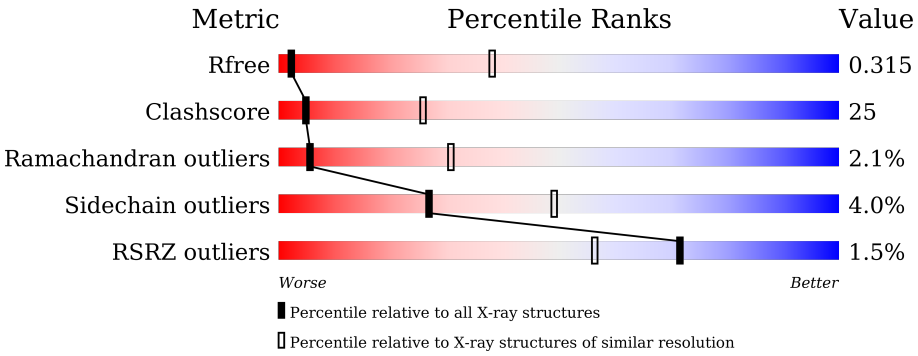
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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}	164625	1028 (4.72-3.86)
Clashscore	180529	1030 (4.70-3.90)
Ramachandran outliers	177936	1014 (4.76-3.84)
Sidechain outliers	177891	1022 (4.76-3.82)
RSRZ outliers	164620	1026 (4.72-3.86)

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 <=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% 51% 30% • 15%
1	M	264	39% 35% • 22%
1	X	264	% 41% 28% • 28%
2	B	264	2% 41% 35% • • 19%
2	F	433	% 48% 27% • 23%
2	K	433	% 38% 35% • • 24%

2 Entry composition (i)

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			

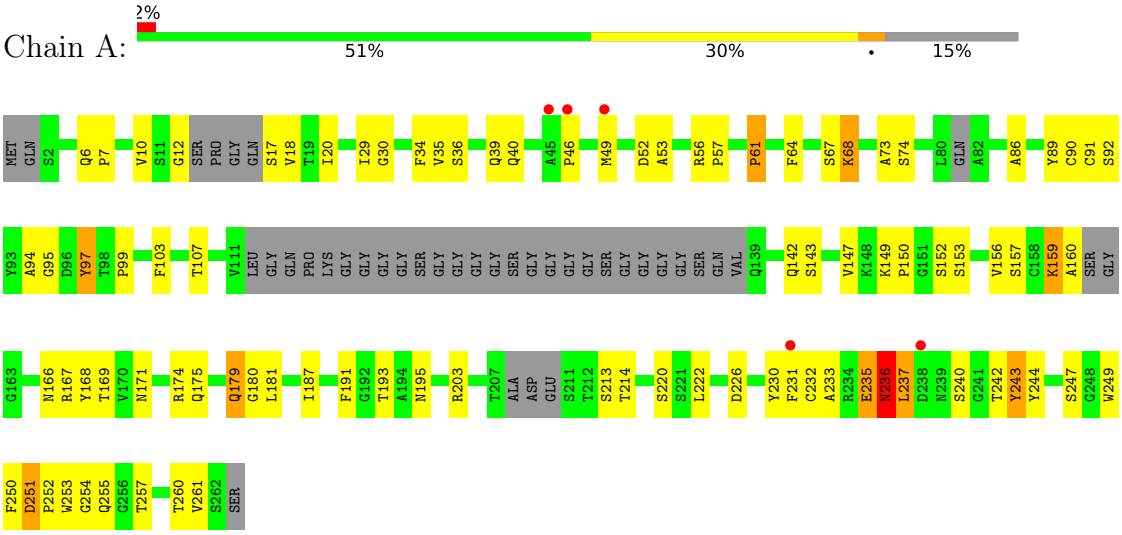
- Molecule 2 is a protein called RABV-G-ecto.

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			

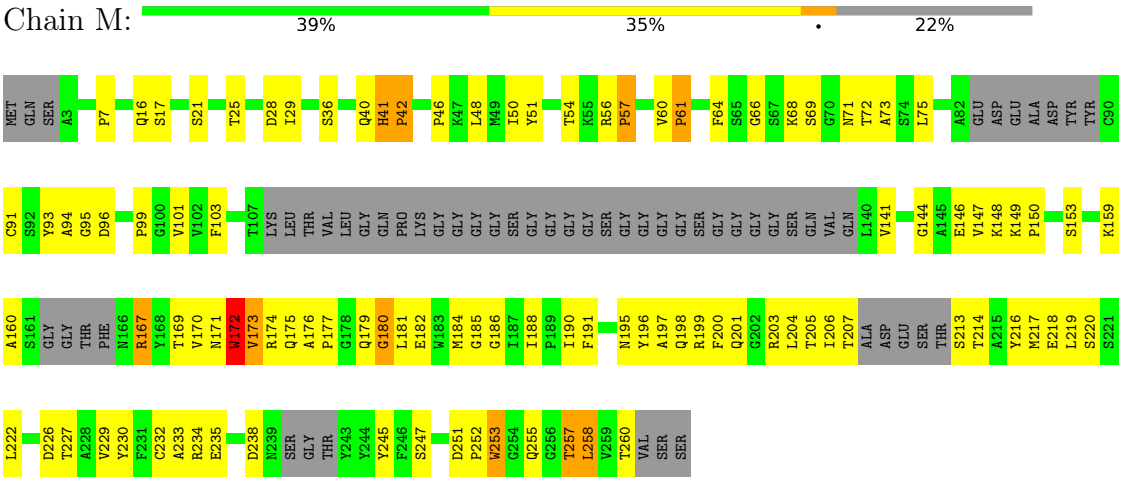
3 Residue-property plots (i)

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

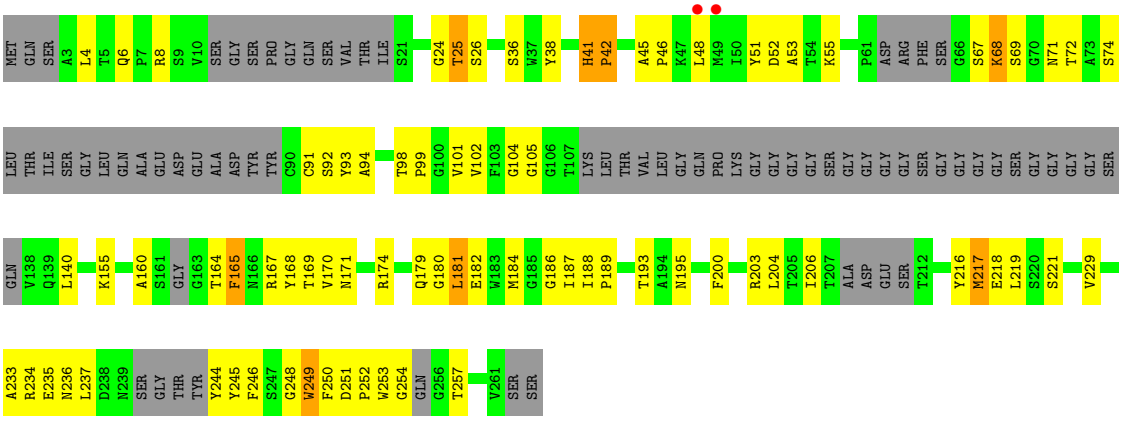
• Molecule 1: NM57-scFv light chain, NM57-scFv heavy chain



• Molecule 1: NM57-scFv light chain, NM57-scFv heavy chain

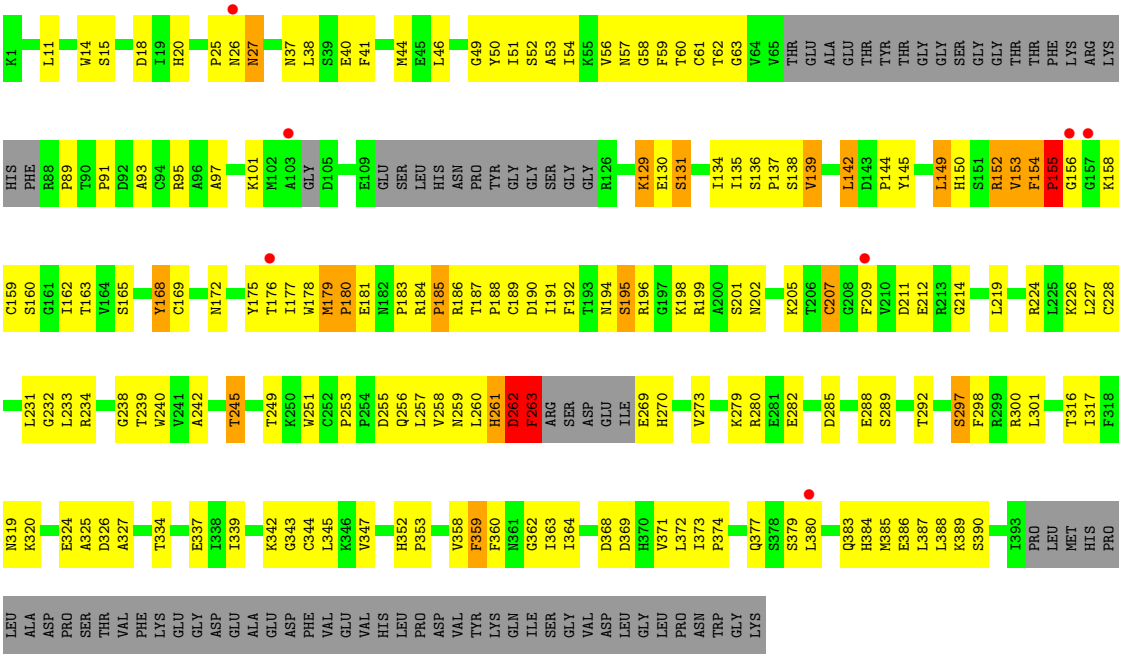


• Molecule 1: NM57-scFv light chain, NM57-scFv heavy chain



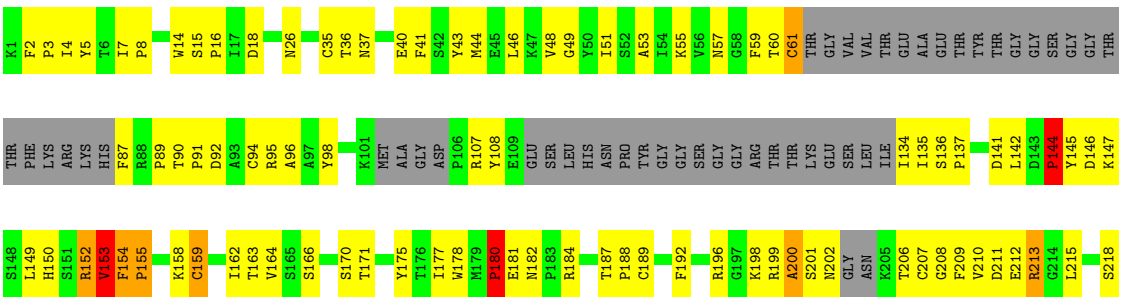
• Molecule 2: RABV-G-ecto

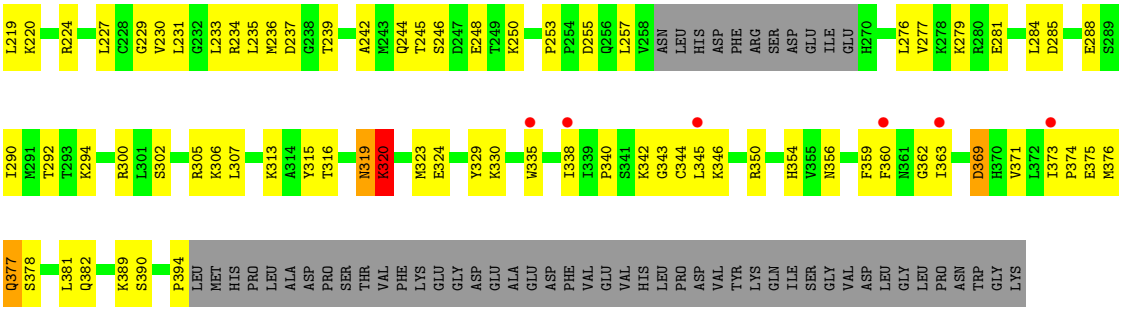
Chain B:



• Molecule 2: RABV-G-ecto

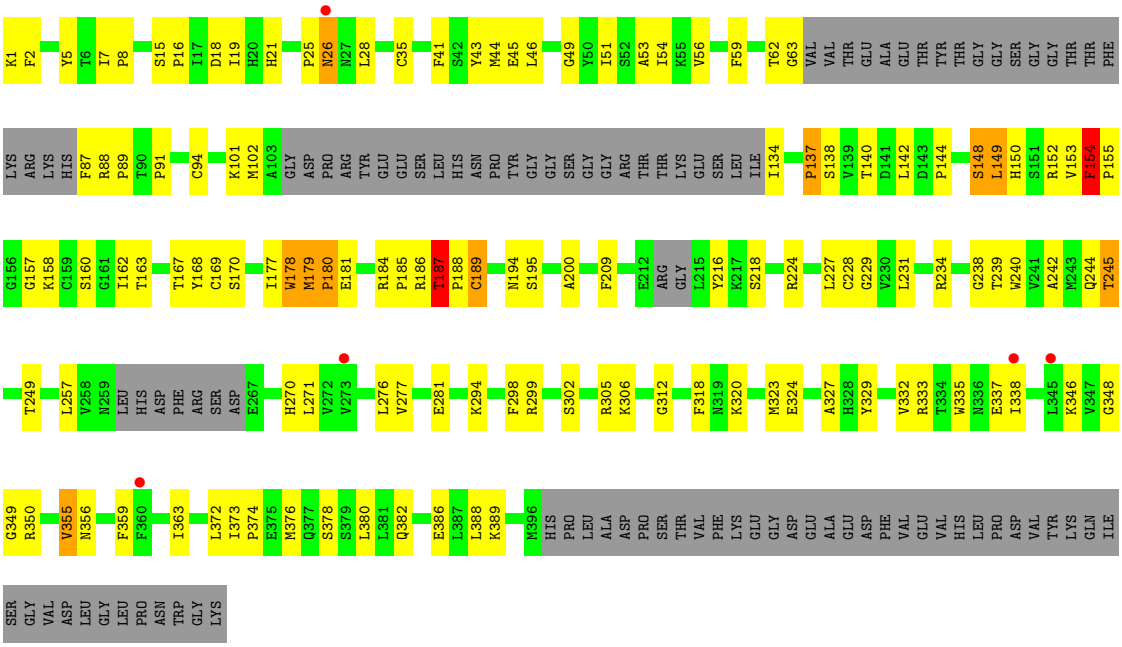
Chain K:





- Molecule 2: RABV-G-ecto

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	902 reflections (4.60%)	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 , 339.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/1733	0.77	6/2348 (0.3%)
1	M	0.39	0/1598	0.97	9/2164 (0.4%)
1	X	0.31	0/1469	0.74	8/1985 (0.4%)
2	B	0.32	0/2813	0.81	16/3808 (0.4%)
2	F	0.31	0/2681	0.80	13/3630 (0.4%)
2	K	0.32	0/2653	0.92	22/3590 (0.6%)
All	All	0.32	0/12947	0.84	74/17525 (0.4%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	94	ALA	CB-CA-C	-17.24	84.23	110.10
1	M	173	VAL	N-CA-C	12.16	143.83	111.00
2	B	153	VAL	CB-CA-C	11.34	132.94	111.40
1	M	173	VAL	N-CA-CB	-11.30	86.63	111.50
2	B	358	VAL	CB-CA-C	9.89	130.19	111.40
2	B	153	VAL	N-CA-C	-9.79	84.58	111.00
2	K	181	GLU	N-CA-CB	-9.76	93.03	110.60
2	K	153	VAL	N-CA-C	8.90	135.03	111.00
2	K	180	PRO	CB-CA-C	-8.71	90.23	112.00
1	A	236	ASN	N-CA-CB	-8.66	95.02	110.60
2	K	319	ASN	CB-CA-C	-8.38	93.63	110.40
1	A	237	LEU	N-CA-CB	8.29	126.97	110.40
2	B	26	ASN	N-CA-C	-7.98	89.47	111.00
2	K	144	PRO	N-CA-CB	-7.91	93.81	103.30
2	K	152	ARG	CB-CA-C	-7.74	94.92	110.40
2	F	153	VAL	CB-CA-C	7.68	125.98	111.40
2	K	320	LYS	N-CA-CB	7.65	124.37	110.60
1	M	94	ALA	N-CA-C	-7.64	90.38	111.00
1	A	153	SER	N-CA-CB	-7.57	99.14	110.50
2	F	26	ASN	CB-CA-C	7.53	125.45	110.40
1	X	179	GLN	CB-CA-C	-7.52	95.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	153	VAL	N-CA-CB	-7.17	95.73	111.50
2	F	355	VAL	CB-CA-C	-7.02	98.06	111.40
2	B	257	LEU	CB-CA-C	-6.87	97.15	110.20
2	B	359	PHE	N-CA-C	-6.87	92.46	111.00
2	F	26	ASN	N-CA-C	-6.84	92.53	111.00
1	X	218	GLU	N-CA-C	-6.66	93.02	111.00
2	F	149	LEU	N-CA-CB	6.49	123.38	110.40
2	F	148	SER	N-CA-C	-6.41	93.69	111.00
2	K	377	GLN	N-CA-C	-6.33	93.90	111.00
2	K	180	PRO	N-CA-C	-6.26	95.83	112.10
2	B	27	ASN	N-CA-CB	6.25	121.84	110.60
2	K	108	TYR	N-CA-CB	6.21	121.79	110.60
1	M	257	THR	N-CA-C	-6.17	94.34	111.00
1	X	180	GLY	N-CA-C	6.17	128.52	113.10
2	F	270	HIS	N-CA-C	6.14	127.59	111.00
2	B	154	PHE	N-CA-C	-6.14	94.43	111.00
2	K	320	LYS	CB-CA-C	6.11	122.61	110.40
1	M	153	SER	N-CA-CB	6.10	119.66	110.50
1	A	235	GLU	CB-CA-C	-6.10	98.20	110.40
1	M	258	LEU	N-CA-C	-6.08	94.59	111.00
2	B	359	PHE	CB-CA-C	-6.04	98.31	110.40
1	A	179	GLN	N-CA-C	-6.04	94.69	111.00
2	K	320	LYS	N-CA-C	-6.02	94.74	111.00
2	F	270	HIS	CB-CA-C	-5.96	98.47	110.40
2	K	26	ASN	CB-CA-C	5.91	122.22	110.40
2	B	358	VAL	N-CA-C	-5.88	95.11	111.00
2	B	262	ASP	N-CA-C	-5.88	95.12	111.00
1	X	218	GLU	N-CA-CB	5.81	121.06	110.60
2	K	96	ALA	N-CA-CB	-5.76	102.03	110.10
2	B	263	PHE	N-CA-CB	5.75	120.95	110.60
2	K	182	ASN	N-CA-C	-5.65	95.75	111.00
2	K	26	ASN	N-CA-C	-5.59	95.91	111.00
2	F	154	PHE	N-CA-CB	5.52	120.53	110.60
2	B	26	ASN	CB-CA-C	5.50	121.40	110.40
2	K	369	ASP	CB-CG-OD1	5.47	123.22	118.30
2	F	153	VAL	N-CA-C	-5.46	96.25	111.00
1	M	227	THR	N-CA-C	-5.41	96.39	111.00
2	B	27	ASN	N-CA-C	-5.40	96.42	111.00
1	M	172	TRP	N-CA-C	5.39	125.57	111.00
2	F	257	LEU	CA-CB-CG	5.36	127.62	115.30
2	F	356	ASN	N-CA-C	-5.33	96.60	111.00
2	K	378	SER	N-CA-CB	5.29	118.44	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	245	THR	N-CA-C	-5.25	96.83	111.00
2	B	262	ASP	CB-CA-C	5.23	120.86	110.40
1	X	26	SER	N-CA-CB	5.23	118.34	110.50
1	X	26	SER	N-CA-C	-5.17	97.05	111.00
1	X	217	MET	CB-CA-C	5.16	120.71	110.40
2	K	107	ARG	N-CA-C	-5.14	97.12	111.00
2	B	359	PHE	N-CA-CB	5.06	119.70	110.60
2	K	378	SER	N-CA-C	-5.05	97.36	111.00
1	A	180	GLY	N-CA-C	5.02	125.64	113.10
2	K	356	ASN	N-CA-C	-5.00	97.49	111.00
1	X	25	THR	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	70	0
1	M	1562	0	1490	99	0
1	X	1438	0	1367	66	0
2	B	2749	0	2720	155	0
2	F	2619	0	2594	106	0
2	K	2590	0	2565	147	0
All	All	12653	0	12346	620	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 25.

All (620) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:37:ASN:O	2:K:200:ALA:HA	1.86	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
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
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
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:152:ARG:O	2:B:153:VAL:C	2.32	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:155:PRO:HG2	2:K:158:LYS:C	2.16	0.66
2:K:284:LEU:HD21	2:F:382:GLN:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:305:ARG:HG2	2:K:306:LYS:O	1.95	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:K:285:ASP:OD1	2:F:299:ARG:NH1	2.32	0.63
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:PRO:HG2	2:B:172:ASN:CG	2.20	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: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:368:ASP:CG	2:B:369:ASP:H	2.06	0.58
2:B:25:PRO:HG2	2:B:27:ASN:HD21	1.68	0.58
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:154:PHE:O	2:B:155:PRO:C	2.41	0.58
2:K:319:ASN:OD1	2:K:319:ASN:C	2.40	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
2:K:201:SER:HB3	2:K:206:THR:C	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:59:PHE:CG	2:K:60:THR:N	2.69	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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:218:SER:C	2:K:220:LYS:H	2.14	0.51
1:X:36:SER:O	1:X:91:CYS:N	2.43	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
1:X:184:MET:HE1	1:X:219:LEU:HD22	1.92	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
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
1:X:186:GLY:HA3	1:X:246:PHE:HE1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:237:LEU:HB3	1:A:249:TRP:CZ3	2.48	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:180:PRO:O	2:K:180:PRO:HD2	2.12	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
1:A:231:PHE:CD2	1:A:255:GLN:HA	2.49	0.48
2:B:52:SER:HB3	2:B:259:ASN:CG	2.34	0.48
2:K:220:LYS:O	2:K:236:MET:HE2	2.13	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
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: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
1:M:217:MET:CE	1:M:219:LEU:HB2	2.44	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
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:14:TRP:CH2	2:B:316:THR:HG22	2.49	0.47
2:B:58:GLY:HA3	2:B:179:MET:HE3	1.97	0.47
2:B:319:ASN:OD1	2:B:320:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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:B:253:PRO:C	2:B:255:ASP:H	2.18	0.46
2:K:354:HIS:ND1	2:K:354:HIS:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:179:GLN:HG3	1:M:180:GLY:H	1.80	0.46
2:B:368:ASP:CG	2:B:369:ASP:N	2.70	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
2:F:376:MET:C	2:F:378:SER:H	2.19	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:51:ILE:C	2:F:53:ALA:H	2.20	0.44
2:F:59:PHE:O	2:F:179:MET:HB3	2.17	0.44
2:B:60:THR:OG1	2:B:137:PRO:O	2.23	0.44
2:B:279:LYS:HD2	2:B:279:LYS:HA	1.79	0.44
2:K:201:SER:O	2:K:202:ASN:C	2.56	0.44
1:X:45:ALA:HB2	1:X:254:GLY:C	2.38	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
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:K:320:LYS:HZ2	2:K:390:SER:HB2	1.82	0.44
2:F:8:PRO:HG3	2:F:329:TYR:HE1	1.82	0.44
2:K:338:ILE:HD11	2:K:376:MET:HE1	1.99	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:384:HIS:O	2:B:384:HIS:CG	2.71	0.44
1:M:28:ASP:HB2	1:M:96:ASP:CG	2.37	0.44
2:F:187:THR:C	2:F:189:CYS:N	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
1:X:24:GLY:O	1:X:25:THR:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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
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: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
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
2:B:386:GLU:C	2:B:387:LEU:HD22	2.39	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: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
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
1:X:6:GLN:HG3	1:X:104:GLY:CA	2.48	0.43
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
2:B:260:LEU:O	2:B:261:HIS:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:305:ARG:CG	2:K:306:LYS:O	2.64	0.42
1:M:173:VAL:HG13	1:M:174:ARG:N	2.34	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
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: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:K:14:TRP:HB3	2:K:323:MET:HE2	2.01	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
1:M:207:THR:C	1:M:216:TYR:H	2.22	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: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: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:B:142:LEU:HD22	2:B:179:MET:HE2	2.01	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
1:A:95:GLY:HA2	2:B:226:LYS:NZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:345:LEU:HD23	2:K:345:LEU:HA	1.95	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:F:244:GLN:O	2:F:245:THR:C	2.58	0.41
1:A:169:THR:O	1:A:171:ASN:ND2	2.54	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
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
2:B:95:ARG:NE	2:B:183:PRO:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 50
1	M	195/264 (74%)	158 (81%)	31 (16%)	6 (3%)	3 23
1	X	172/264 (65%)	146 (85%)	23 (13%)	3 (2%)	7 36
2	B	339/433 (78%)	276 (81%)	56 (16%)	7 (2%)	5 31
2	F	324/433 (75%)	267 (82%)	50 (15%)	7 (2%)	5 30
2	K	316/433 (73%)	261 (83%)	47 (15%)	8 (2%)	4 27
All	All	1558/2091 (74%)	1287 (83%)	238 (15%)	33 (2%)	5 31

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
2	B	180	PRO

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	182/202 (90%)	175 (96%)	7 (4%)	28 50
1	M	167/202 (83%)	165 (99%)	2 (1%)	67 79
1	X	153/202 (76%)	148 (97%)	5 (3%)	33 55
2	B	313/381 (82%)	291 (93%)	22 (7%)	12 33
2	F	298/381 (78%)	288 (97%)	10 (3%)	32 54
2	K	295/381 (77%)	284 (96%)	11 (4%)	29 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1408/1749 (80%)	1351 (96%)	57 (4%)	27 49

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	68	LYS
1	A	90	CYS
1	A	97	TYR
1	A	159	LYS
1	A	236	ASN
1	A	243	TYR
2	B	15	SER
2	B	20	HIS
2	B	129	LYS
2	B	131	SER
2	B	142	LEU
2	B	145	TYR
2	B	149	LEU
2	B	152	ARG
2	B	155	PRO
2	B	168	TYR
2	B	169	CYS
2	B	179	MET
2	B	189	CYS
2	B	195	SER
2	B	207	CYS
2	B	261	HIS
2	B	262	ASP
2	B	263	PHE
2	B	269	GLU
2	B	297	SER
2	B	326	ASP
2	B	344	CYS
2	K	35	CYS
2	K	41	PHE
2	K	43	TYR
2	K	61	CYS
2	K	87	PHE
2	K	144	PRO
2	K	159	CYS
2	K	213	ARG

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Mol	Chain	Res	Type
2	K	294	LYS
2	K	344	CYS
2	K	350	ARG
1	M	167	ARG
1	M	172	TRP
2	F	1	LYS
2	F	41	PHE
2	F	88	ARG
2	F	102	MET
2	F	154	PHE
2	F	178	TRP
2	F	179	MET
2	F	187	THR
2	F	189	CYS
2	F	218	SER
1	X	8	ARG
1	X	68	LYS
1	X	181	LEU
1	X	195	ASN
1	X	249	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
2	B	27	ASN
2	B	256	GLN
2	B	259	ASN
2	B	370	HIS
1	M	201	GLN
1	X	171	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, 95^{th} 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%)	-0.10	5 (2%) 62 46	152, 209, 248, 262	0
1	M	207/264 (78%)	-0.16	0 100 100	163, 242, 276, 300	0
1	X	190/264 (71%)	-0.07	2 (1%) 77 62	186, 241, 274, 283	0
2	B	349/433 (80%)	-0.07	7 (2%) 64 49	132, 198, 257, 298	0
2	F	334/433 (77%)	-0.15	5 (1%) 71 56	133, 209, 266, 290	0
2	K	328/433 (75%)	-0.03	6 (1%) 67 51	133, 197, 252, 282	0
All	All	1632/2091 (78%)	-0.09	25 (1%) 71 56	132, 213, 266, 300	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	3.0
2	B	176	THR	2.9
2	F	345	LEU	2.8
2	B	157	GLY	2.8
2	F	273	VAL	2.7
2	K	373	ILE	2.6
2	K	345	LEU	2.6
1	A	46	PRO	2.4
2	B	26	ASN	2.4
2	B	380	LEU	2.4
2	K	360	PHE	2.3
2	K	335	TRP	2.3
1	A	231	PHE	2.3
2	F	26	ASN	2.2
2	K	338	ILE	2.2
1	A	238	ASP	2.2
2	B	103	ALA	2.1
2	B	156	GLY	2.1
2	K	363	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	48	LEU	2.1
2	B	209	PHE	2.0
2	F	360	PHE	2.0
1	X	49	MET	2.0
1	A	49	MET	2.0
2	F	338	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.