



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:30 PM EDT

PDB ID : 5BYV / pdb_00005byv
Title : Crystal structure of MSM-13, a putative T1-like thiolase from Mycobacterium smegmatis
Authors : Janardan, N.; Harijan, R.K.; Keima, T.R.; Wierenga, R.; Murthy, M.R.N.
Deposited on : 2015-06-11
Resolution : 2.16 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

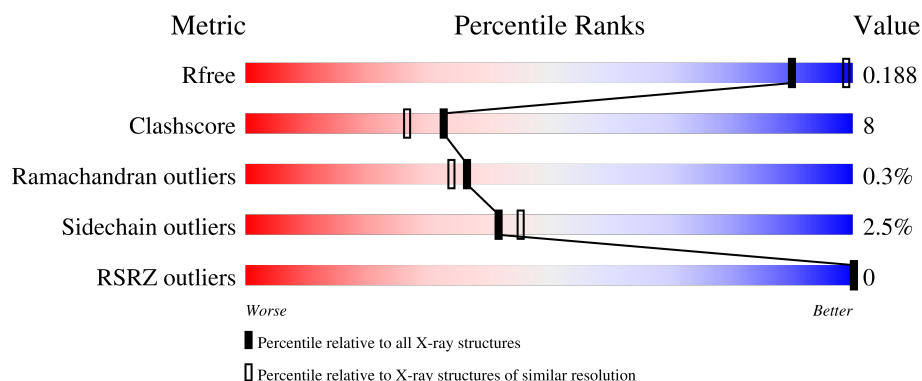
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	407	
1	B	407	
1	C	407	
1	D	407	
1	E	407	

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Mol	Chain	Length	Quality of chain
1	F	407	 81% 15% ..
1	G	407	 79% 17% ..
1	H	407	 80% 17% ..
1	J	407	 81% 16% ..
1	K	407	 85% 12% ..
1	L	407	 73% 24% ..
1	M	407	 78% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36700 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 Beta-ketothiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2895	1795	529	555	16			
1	B	398	Total	C	N	O	S	0	0	0
			2938	1819	540	563	16			
1	C	398	Total	C	N	O	S	0	0	0
			2933	1814	539	564	16			
1	D	396	Total	C	N	O	S	0	0	0
			2924	1811	538	559	16			
1	E	396	Total	C	N	O	S	0	0	0
			2925	1810	538	561	16			
1	F	399	Total	C	N	O	S	0	0	0
			2947	1824	542	565	16			
1	G	398	Total	C	N	O	S	0	0	0
			2940	1820	540	564	16			
1	H	397	Total	C	N	O	S	0	0	0
			2933	1816	540	561	16			
1	J	396	Total	C	N	O	S	0	0	0
			2925	1810	538	561	16			
1	K	399	Total	C	N	O	S	0	0	0
			2949	1825	542	566	16			
1	L	398	Total	C	N	O	S	0	0	0
			2932	1816	540	560	16			
1	M	397	Total	C	N	O	S	0	0	0
			2933	1816	540	561	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	145	Total	O	0	0
			145	145		

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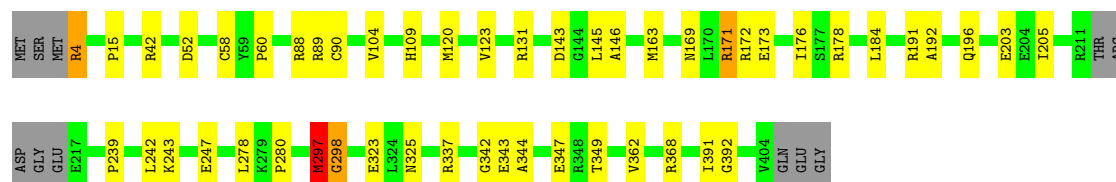
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	131	Total 131	O 131	0	0
2	D	156	Total 156	O 156	0	0
2	E	105	Total 105	O 105	0	0
2	F	129	Total 129	O 129	0	0
2	G	114	Total 114	O 114	0	0
2	H	154	Total 154	O 154	0	0
2	J	120	Total 120	O 120	0	0
2	K	142	Total 142	O 142	0	0
2	L	99	Total 99	O 99	0	0
2	M	106	Total 106	O 106	0	0

- Molecule 1: Beta-ketothiolase



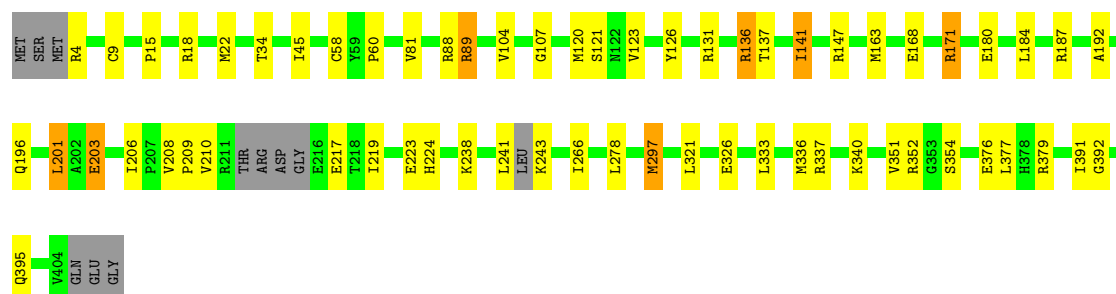
- Molecule 1: Beta-ketothiolase

Chain D: 



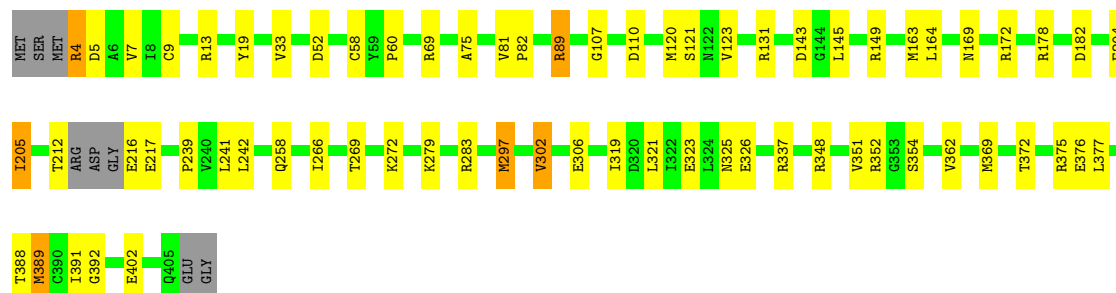
- Molecule 1: Beta-ketothiolase

Chain E: 



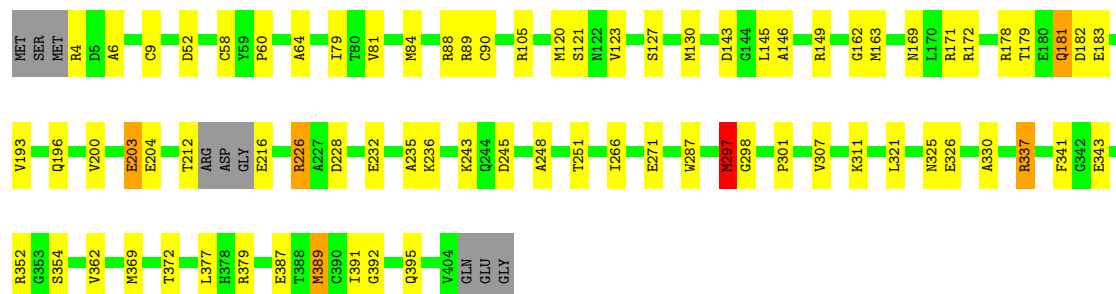
- Molecule 1: Beta-ketothiolase

Chain F: 



- Molecule 1: Beta-ketothiolase

Chain G: 



- Molecule 1: Beta-ketothiolase

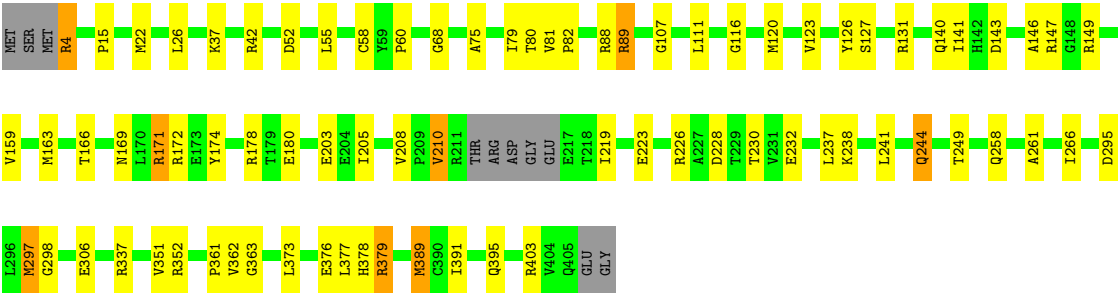
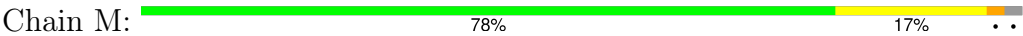
M369	E203	V208	R171
T372	E204	P209	R174
E376	I205	V210	R178
L377		R211	D182
H378	THR	ARG	V199
R379	ASP	GLY	R200
R380	GLU	E217	R203
E381		H224	R206
A382		L237	R209
T388	K243	K244	R212
M389	Q258	T249	R215
C390	V250	V251	R218
I391	T251	Q258	R221
G392	K272	K272	R224
E402	L276	K279	R227
R403	P280	P280	R230
V404	L281	L281	R233
V405	V282	V282	R236
GLU	R283	M297	R239
GLY		V302	R242
	D320	D320	R245
	L321	L321	R248
	I322	I322	R251
	E323	E323	R254
	L324	L324	R257
	N325	N325	R260
	E326	E326	R263
	R337	R337	R266
	E347	E347	R269
	V351	V351	R272
	R352	R352	R275
	G353	G353	R278
	S354	S354	R281
			R284
			R287
			R290
			R293
			R296
			R299
			R302
			R305
			R308
			R311
			R314
			R317
			R320
			R323
			R326
			R329
			R332
			R335
			R338
			R341
			R344
			R347
			R350
			R353
			R356
			R359
			R362
			R365
			R368
			R371
			R374
			R377
			R380
			R383
			R386
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			R392
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			R563
			R566
			R569
			R572
			R575
			R578
			R581
			R584
			R587
			R590
			R593
			R596
			R599
			R602
			R605
			R608
			R611
			R614
			R617
			R620
			R623
			R626
			R629
			R632
			R635
			R638
			R641
			R644
			R647
			R650
			R653

Met	S188	S354	S189	R4	C9	R42	I45	D52	C58	Y59	P60	E63	V81	M84	R88	R89	V104	G16	M120	V123	Y126	R131	T141	R147	H157	G162	M163	T166	R171	R178	T179	E180	I181	D182	E183	L184	R187
Ser	H189	V362	H190	A192	V193	Q196	V200	E203	E204	I205	R211	T18R	A18G	A18P	R88	R89	V104	G16	M120	V123	Y126	R131	T141	R147	H157	G162	M163	T166	R171	R178	T179	E180	I181	D182	E183	L184	R187
Met	S188	S354	S189	R4	C9	R42	I45	D52	C58	Y59	P60	E63	V81	M84	R88	R89	V104	G16	M120	V123	Y126	R131	T141	R147	H157	G162	M163	T166	R171	R178	T179	E180	I181	D182	E183	L184	R187

R211	R212	ARG	ASP	GLY	E216	E232	K238	S256	G257	Q258	E275	K287	G298	L321	F328	A329	A330	L333	R337	H346	T349	R352	I356	R368	T372	L377	C390	I391	Q395	Q405	GLU	GLY							
MET	SER	MET	R4	D5	A6	D52	G58	Y59	P60	R69	V81	R88	R89	V104	R105	S106	G107	D108	H109	M120	V123	Y126	A135	D143	G144	L145	R149	L164	M169	R172	R178	T179	E180	Q181	D182	V186	Q190	R191	L205

V404	M259	V159	MT
GLN	I266	M163	SR
GLU	L278	T166	MT
GLY	R279	A167	R4
	P280	E168	D5
			A6
	M297	R171	C9
		R172	E10
	I319	E173	P11
	D320		
	L321	R178	P15
		T179	
	N325	E180	R24
	E326	Q181	V33
	A327	D182	T34
	F328	E183	
	A329	L184	D52
	A330	A185	
		V186	C58
	L333		Y69
	M336	H189	P60
	R337	A192	
	H346	V193	A75
	E347		
	R348	Q196	M84
	R352	V200	R88
	G353	L201	R89
	S354	A202	C90
		E203	C91
	L358	E204	
		I205	V104
			R105
		V208	S106
			G107
		R211	D108
	R368	T212	H109
	M369	ARG	
	L370	ASP	M120
	A371	GLY	V123
	T372		
	R375	E216	S127
	E376	E217	
	L377	H224	M130
	H378		
	R379	V231	T141
	R380	E232	
			L145
	T388	L237	
	M389		R149
	C390	Q244	
	I391	E247	G153
	G392	A248	G154
		T249	K155
	Q395		F156
			H157
	P403	Q359	T352

● Molecule 1: Beta-ketothiolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	190.96Å 190.96Å 264.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.19 – 2.16 45.19 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.19-2.16) 99.9 (45.19-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.169 , 0.200 0.170 , 0.188	Depositor DCC
R_{free} test set	14680 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.226 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36700	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.40 % 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 3.1919e-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 [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	0.56	0/2939	0.91	8/3990 (0.2%)
1	B	0.56	0/2982	0.90	4/4044 (0.1%)
1	C	0.65	3/2977 (0.1%)	1.04	17/4039 (0.4%)
1	D	0.60	0/2968	0.89	3/4025 (0.1%)
1	E	0.54	0/2968	0.90	4/4023 (0.1%)
1	F	0.56	0/2991	0.90	5/4056 (0.1%)
1	G	0.56	0/2984	0.91	3/4047 (0.1%)
1	H	0.58	1/2977 (0.0%)	0.91	10/4037 (0.2%)
1	J	0.54	0/2968	0.90	4/4023 (0.1%)
1	K	0.57	0/2993	0.89	4/4059 (0.1%)
1	L	0.52	0/2976	0.93	10/4037 (0.2%)
1	M	0.54	0/2977	0.91	5/4037 (0.1%)
All	All	0.57	4/35700 (0.0%)	0.92	77/48417 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	GLU	CB-CG	11.03	1.85	1.52
1	C	216	GLU	CG-CD	8.36	1.73	1.52
1	C	216	GLU	CA-CB	6.95	1.67	1.53
1	H	389	MET	CG-SD	-5.24	1.67	1.80

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	GLU	CA-CB-CG	14.93	143.95	114.10
1	C	216	GLU	CB-CG-CD	11.62	132.36	112.60
1	C	210	VAL	CA-C-N	-9.13	106.66	122.37
1	C	210	VAL	C-N-CA	-9.13	106.66	122.37
1	C	224	HIS	CA-C-N	-8.56	111.21	119.85
1	C	224	HIS	C-N-CA	-8.56	111.21	119.85
1	A	157	HIS	CA-C-N	8.38	128.13	119.76
1	A	157	HIS	C-N-CA	8.38	128.13	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	PHE	CA-C-N	-7.93	113.41	123.16
1	A	156	PHE	C-N-CA	-7.93	113.41	123.16
1	D	297	MET	CG-SD-CE	-7.63	84.11	100.90
1	F	302	VAL	CA-C-N	-7.07	111.70	119.19
1	F	302	VAL	C-N-CA	-7.07	111.70	119.19
1	H	224	HIS	CA-C-N	-6.99	112.77	119.76
1	H	224	HIS	C-N-CA	-6.99	112.77	119.76
1	C	216	GLU	CG-CD-OE1	6.81	134.07	118.40
1	L	159	VAL	CA-C-N	6.71	126.97	119.32
1	L	159	VAL	C-N-CA	6.71	126.97	119.32
1	B	89	ARG	CB-CA-C	-6.65	108.89	116.54
1	L	181	GLN	N-CA-C	-6.48	103.72	111.69
1	F	389	MET	CA-CB-CG	-6.40	101.31	114.10
1	H	389	MET	CA-CB-CG	-6.29	101.51	114.10
1	L	205	ILE	N-CA-C	6.21	117.25	108.36
1	J	245	ASP	CA-C-N	6.21	125.95	119.05
1	J	245	ASP	C-N-CA	6.21	125.95	119.05
1	E	81	VAL	N-CA-C	6.19	113.20	107.56
1	C	216	GLU	N-CA-C	-6.12	93.86	111.00
1	K	181	GLN	N-CA-C	-6.12	104.16	111.69
1	C	216	GLU	OE1-CD-OE2	-6.10	108.26	122.90
1	C	157	HIS	CA-C-N	6.09	127.01	120.13
1	C	157	HIS	C-N-CA	6.09	127.01	120.13
1	M	81	VAL	N-CA-C	6.09	113.10	107.56
1	G	81	VAL	N-CA-C	6.02	113.04	107.56
1	A	81	VAL	N-CA-C	6.01	113.03	107.56
1	H	81	VAL	CA-C-N	6.00	125.97	120.03
1	H	81	VAL	C-N-CA	6.00	125.97	120.03
1	M	205	ILE	N-CA-C	5.88	117.48	108.71
1	J	81	VAL	N-CA-C	5.83	112.86	107.56
1	C	156	PHE	CA-C-N	-5.73	115.13	122.98
1	C	156	PHE	C-N-CA	-5.73	115.13	122.98
1	K	205	ILE	N-CA-C	5.73	116.55	108.36
1	G	64	ALA	CA-C-N	5.67	125.43	119.76
1	G	64	ALA	C-N-CA	5.67	125.43	119.76
1	H	89	ARG	CB-CA-C	-5.65	110.04	116.54
1	C	205	ILE	N-CA-C	5.59	116.35	108.36
1	L	362	VAL	N-CA-C	5.56	116.01	110.23
1	B	205	ILE	N-CA-C	5.56	116.31	108.36
1	H	302	VAL	CA-C-N	-5.55	113.31	119.19
1	H	302	VAL	C-N-CA	-5.55	113.31	119.19
1	A	159	VAL	CA-C-N	5.50	125.15	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	VAL	C-N-CA	5.50	125.15	119.05
1	H	325	ASN	CA-C-N	-5.47	114.68	122.77
1	H	325	ASN	C-N-CA	-5.47	114.68	122.77
1	E	224	HIS	CA-C-N	-5.45	114.31	119.76
1	E	224	HIS	C-N-CA	-5.45	114.31	119.76
1	F	205	ILE	N-CA-C	5.40	116.08	108.36
1	L	224	HIS	CA-C-N	-5.34	114.26	119.76
1	L	224	HIS	C-N-CA	-5.34	114.26	119.76
1	J	205	ILE	N-CA-C	5.26	115.54	108.17
1	E	89	ARG	CB-CA-C	-5.24	110.52	116.54
1	D	298	GLY	N-CA-C	-5.23	108.47	115.32
1	F	89	ARG	CB-CA-C	-5.23	110.53	116.54
1	A	205	ILE	N-CA-C	5.21	115.82	108.36
1	K	88	ARG	N-CA-C	-5.20	104.20	110.44
1	K	89	ARG	CB-CA-C	-5.16	110.60	116.54
1	M	89	ARG	CB-CA-C	-5.15	110.61	116.54
1	C	211	ARG	N-CA-C	5.13	117.79	109.06
1	D	297	MET	CA-CB-CG	-5.13	103.85	114.10
1	C	211	ARG	CB-CG-CD	-5.12	99.52	111.30
1	C	216	GLU	CB-CA-C	5.09	119.78	110.10
1	L	259	ASN	N-CA-C	5.07	116.77	109.07
1	L	208	VAL	N-CA-C	5.06	113.50	107.73
1	M	159	VAL	CA-C-N	5.05	124.65	119.05
1	M	159	VAL	C-N-CA	5.05	124.65	119.05
1	B	302	VAL	CA-C-N	-5.03	113.86	119.19
1	B	302	VAL	C-N-CA	-5.03	113.86	119.19
1	L	346	HIS	N-CA-C	-5.00	107.15	113.20

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	2895	0	2889	54	0
1	B	2938	0	2947	47	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2933	0	2932	64	0
1	D	2924	0	2939	39	1
1	E	2925	0	2933	43	0
1	F	2947	0	2955	46	0
1	G	2940	0	2952	58	0
1	H	2933	0	2947	51	0
1	J	2925	0	2933	45	0
1	K	2949	0	2960	41	0
1	L	2932	0	2944	68	0
1	M	2933	0	2947	51	0
2	A	125	0	0	2	0
2	B	145	0	0	0	0
2	C	131	0	0	2	0
2	D	156	0	0	4	0
2	E	105	0	0	1	0
2	F	129	0	0	2	0
2	G	114	0	0	7	0
2	H	154	0	0	1	0
2	J	120	0	0	1	0
2	K	142	0	0	2	0
2	L	99	0	0	2	0
2	M	106	0	0	1	0
All	All	36700	0	35278	558	1

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 8.

All (558) 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:C:216:GLU:CG	1:C:216:GLU:CB	1.85	1.49
1:E:163:MET:HG2	1:E:297:MET:HE1	1.42	0.99
1:D:297:MET:HG3	1:D:298:GLY:N	1.77	0.96
1:C:211:ARG:HD2	1:C:212:THR:H	1.33	0.93
1:B:149:ARG:NH2	1:B:258:GLN:OE1	2.04	0.90
1:G:181:GLN:NE2	1:G:330:ALA:HB2	1.89	0.87
1:M:352:ARG:HH22	1:M:379:ARG:HH21	1.16	0.87
1:K:89:ARG:HB2	1:K:391:ILE:HG23	1.57	0.87
1:G:181:GLN:HE21	1:G:330:ALA:HB2	1.41	0.85
1:C:211:ARG:NE	1:C:216:GLU:HA	1.93	0.83
1:G:163:MET:HG2	1:G:297:MET:HE1	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:149:ARG:NH2	1:M:258:GLN:OE1	2.12	0.82
1:M:163:MET:HE3	1:M:297:MET:HE1	1.61	0.81
1:B:204:GLU:OE2	1:B:352:ARG:NH1	2.14	0.81
1:D:163:MET:HG2	1:D:297:MET:HE1	1.63	0.80
1:K:297:MET:HG3	1:K:298:GLY:N	1.95	0.79
1:D:89:ARG:HB2	1:D:391:ILE:HG23	1.64	0.79
1:H:178:ARG:NH1	1:H:182:ASP:OD2	2.16	0.79
1:E:89:ARG:HB2	1:E:391:ILE:HG23	1.64	0.79
1:H:283:ARG:NH2	1:H:402:GLU:OE1	2.16	0.78
1:E:352:ARG:HH22	1:E:379:ARG:HH11	1.31	0.77
1:L:149:ARG:NH2	1:L:258:GLN:OE1	2.17	0.77
1:A:319:ILE:O	1:A:348:ARG:NH1	2.18	0.77
1:H:89:ARG:HB2	1:H:391:ILE:HG23	1.66	0.77
1:F:297:MET:HE2	1:F:392:GLY:HA2	1.65	0.77
1:G:178:ARG:HH12	1:G:235:ALA:HA	1.47	0.77
1:F:297:MET:HG3	1:F:391:ILE:O	1.86	0.76
1:L:163:MET:HG2	1:L:297:MET:SD	2.26	0.76
1:C:211:ARG:HD2	1:C:212:THR:N	2.00	0.75
1:F:149:ARG:NH2	1:F:258:GLN:OE1	2.15	0.75
1:A:52:ASP:OD1	1:B:88:ARG:NH2	2.20	0.75
1:J:89:ARG:HB2	1:J:391:ILE:HG23	1.69	0.74
1:J:88:ARG:NH2	1:K:52:ASP:OD1	2.19	0.74
1:C:89:ARG:HB2	1:C:391:ILE:HG23	1.69	0.74
1:G:326:GLU:OE1	1:G:354:SER:OG	2.04	0.74
1:C:211:ARG:NH1	1:C:212:THR:OG1	2.20	0.74
1:F:325:ASN:O	2:F:501:HOH:O	2.05	0.74
1:B:89:ARG:HB2	1:B:391:ILE:HG23	1.68	0.73
1:K:191:ARG:NH1	1:K:349:THR:O	2.21	0.72
1:L:203:GLU:OE1	1:L:379:ARG:NH2	2.23	0.72
1:L:321:LEU:HD12	1:L:377:LEU:HD12	1.71	0.72
1:F:89:ARG:HB2	1:F:391:ILE:HG23	1.71	0.72
1:F:163:MET:SD	1:F:297:MET:HE1	2.30	0.71
1:C:211:ARG:HE	1:C:216:GLU:CB	2.03	0.71
1:A:89:ARG:HB2	1:A:391:ILE:HG23	1.71	0.71
1:L:168:GLU:OE1	1:L:171:ARG:NH1	2.23	0.71
1:L:337:ARG:HH11	1:L:337:ARG:HG2	1.56	0.71
1:L:326:GLU:OE1	1:L:354:SER:OG	2.09	0.70
1:L:352:ARG:HD2	1:L:372:THR:HG23	1.73	0.70
1:E:88:ARG:NH2	1:F:52:ASP:OD1	2.19	0.70
1:M:180:GLU:OE1	1:M:337:ARG:NH2	2.25	0.70
1:E:297:MET:HE2	1:E:392:GLY:HA2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:321:LEU:HD11	1:J:380:ARG:HD2	1.73	0.69
1:G:52:ASP:OD1	1:H:88:ARG:NH2	2.26	0.69
1:G:4:ARG:N	2:G:502:HOH:O	2.26	0.69
1:J:52:ASP:OD1	1:K:88:ARG:NH2	2.24	0.69
1:L:89:ARG:HB2	1:L:391:ILE:HG23	1.74	0.69
1:G:337:ARG:HH11	1:G:337:ARG:HG2	1.57	0.68
1:L:375:ARG:HB3	1:L:379:ARG:NH1	2.09	0.68
1:D:4:ARG:NH2	1:D:104:VAL:O	2.21	0.67
1:L:181:GLN:OE1	1:L:330:ALA:HB2	1.94	0.66
1:G:379:ARG:NH1	2:G:503:HOH:O	2.26	0.66
1:L:325:ASN:O	2:L:501:HOH:O	2.14	0.66
1:G:203:GLU:OE1	2:G:501:HOH:O	2.12	0.66
1:J:58:CYS:O	1:J:89:ARG:NH2	2.28	0.66
1:B:297:MET:HG3	1:B:298:GLY:N	2.10	0.66
1:M:379:ARG:NH2	2:M:501:HOH:O	2.29	0.66
1:H:244:GLN:N	1:H:244:GLN:OE1	2.29	0.65
1:L:179:THR:O	1:L:183:GLU:HG3	1.97	0.65
1:M:89:ARG:HB2	1:M:391:ILE:HG23	1.77	0.65
1:M:297:MET:HG3	1:M:298:GLY:N	2.11	0.65
1:D:163:MET:HE3	1:D:297:MET:HE1	1.79	0.65
1:G:178:ARG:NH1	1:G:182:ASP:OD2	2.29	0.65
1:L:88:ARG:NH2	1:M:52:ASP:OD1	2.29	0.65
1:D:325:ASN:O	2:D:501:HOH:O	2.14	0.65
1:M:174:TYR:O	1:M:337:ARG:NH1	2.30	0.65
1:E:180:GLU:OE1	1:E:337:ARG:NH2	2.30	0.65
1:G:321:LEU:HD12	1:G:377:LEU:HD23	1.79	0.64
1:C:34:THR:HG21	1:C:208:VAL:HG22	1.80	0.64
1:B:352:ARG:HD2	1:B:372:THR:HG23	1.79	0.64
1:G:226:ARG:NH1	1:G:228:ASP:OD2	2.29	0.64
1:C:88:ARG:NH2	1:D:52:ASP:OD1	2.30	0.64
1:F:352:ARG:HD2	1:F:372:THR:HG23	1.80	0.64
1:L:123:VAL:HG21	1:L:145:LEU:HD21	1.78	0.64
1:A:163:MET:HG2	1:A:297:MET:HE1	1.79	0.64
1:M:241:LEU:HD22	1:M:244:GLN:HE21	1.63	0.64
1:C:169:ASN:OD1	1:C:172:ARG:NH2	2.31	0.63
1:G:88:ARG:NH2	1:H:52:ASP:OD1	2.31	0.63
1:D:347:GLU:OE1	2:D:502:HOH:O	2.15	0.63
1:D:163:MET:HG2	1:D:297:MET:CE	2.28	0.62
1:L:52:ASP:OD1	1:M:88:ARG:NH2	2.32	0.62
1:C:127:SER:HB2	1:C:141:ILE:HD13	1.81	0.62
1:K:181:GLN:NE2	1:K:330:ALA:HB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:CYS:O	1:H:89:ARG:NH2	2.32	0.62
1:D:191:ARG:NH1	1:D:349:THR:O	2.33	0.62
1:A:156:PHE:C	1:A:157:HIS:CD2	2.78	0.61
1:H:297:MET:HE2	1:H:392:GLY:N	2.15	0.61
1:J:337:ARG:HG3	1:J:337:ARG:HH11	1.66	0.61
1:C:275:GLU:OE2	2:C:501:HOH:O	2.15	0.61
1:C:297:MET:HG2	1:C:298:GLY:N	2.16	0.61
1:H:149:ARG:NH2	1:H:258:GLN:OE1	2.35	0.60
1:K:120:MET:HA	1:K:123:VAL:HG23	1.83	0.60
1:H:326:GLU:OE1	1:H:354:SER:OG	2.15	0.60
1:C:211:ARG:HH11	1:C:212:THR:H	1.47	0.60
1:E:352:ARG:NH2	1:E:379:ARG:HH11	1.97	0.60
1:J:88:ARG:HH22	1:K:52:ASP:CG	2.09	0.60
1:A:283:ARG:NH1	1:A:402:GLU:OE1	2.35	0.59
1:B:164:LEU:HD21	1:B:240:VAL:HB	1.83	0.59
1:C:60:PRO:HG2	1:D:60:PRO:HG2	1.84	0.59
1:A:326:GLU:OE1	1:A:354:SER:OG	2.15	0.59
1:L:153:GLY:O	1:L:157:HIS:HB2	2.02	0.59
1:G:89:ARG:HB2	1:G:391:ILE:HG23	1.84	0.59
1:J:326:GLU:OE1	1:J:354:SER:OG	2.15	0.59
1:L:319:ILE:O	1:L:348:ARG:NH1	2.35	0.59
1:C:52:ASP:OD1	1:D:88:ARG:NH2	2.34	0.59
1:A:178:ARG:NH2	1:A:237:LEU:O	2.36	0.59
1:L:166:THR:HG21	1:L:297:MET:HE3	1.85	0.59
1:B:326:GLU:OE1	1:B:354:SER:OG	2.14	0.59
1:A:126:TYR:OH	1:A:147:ARG:HG2	2.03	0.59
1:L:391:ILE:HB	1:L:395:GLN:HB2	1.85	0.58
1:L:52:ASP:CG	1:M:88:ARG:HH22	2.10	0.58
1:H:378:HIS:CD2	1:H:403:ARG:HG3	2.39	0.58
1:G:181:GLN:HG2	2:G:575:HOH:O	2.04	0.58
1:H:352:ARG:HD2	1:H:372:THR:HG23	1.86	0.58
1:E:203:GLU:OE1	1:E:379:ARG:NH2	2.37	0.57
1:B:244:GLN:H	1:B:244:GLN:CD	2.10	0.57
1:F:204:GLU:OE2	1:F:352:ARG:NH1	2.34	0.57
1:A:157:HIS:CD2	1:A:157:HIS:N	2.73	0.57
1:H:388:THR:C	1:H:389:MET:HG2	2.23	0.56
1:M:378:HIS:HA	1:M:403:ARG:HD2	1.86	0.56
1:G:88:ARG:HH22	1:H:52:ASP:CG	2.14	0.56
1:J:4:ARG:NH2	1:J:104:VAL:O	2.33	0.56
1:L:297:MET:SD	1:L:392:GLY:HA2	2.45	0.56
1:M:352:ARG:HH22	1:M:379:ARG:NH2	1.97	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:ARG:NH1	1:K:81:VAL:O	2.37	0.56
1:C:337:ARG:HG2	1:C:337:ARG:HH11	1.69	0.56
1:A:156:PHE:C	1:A:157:HIS:HD2	2.14	0.56
1:G:127:SER:HB3	1:G:130:MET:HE3	1.88	0.56
1:H:168:GLU:OE1	1:H:171:ARG:NE	2.38	0.56
1:C:245:ASP:HB3	1:C:248:ALA:HB2	1.88	0.56
1:H:174:TYR:O	1:H:337:ARG:NH2	2.39	0.55
1:A:297:MET:CE	1:A:392:GLY:HA2	2.36	0.55
1:E:4:ARG:NH2	1:E:104:VAL:O	2.32	0.55
1:K:180:GLU:OE2	1:K:337:ARG:NH2	2.36	0.55
1:E:321:LEU:HD12	1:E:377:LEU:HD23	1.88	0.55
1:A:52:ASP:CG	1:B:88:ARG:HH22	2.13	0.55
1:A:63:GLU:OE2	1:B:126:TYR:OH	2.22	0.55
1:D:171:ARG:NH2	1:D:247:GLU:HB2	2.21	0.55
1:K:321:LEU:HD12	1:K:377:LEU:HD23	1.88	0.55
1:G:226:ARG:HD2	1:G:228:ASP:OD1	2.07	0.55
1:L:180:GLU:OE1	1:L:337:ARG:NH2	2.39	0.55
1:E:168:GLU:OE1	1:E:171:ARG:NH2	2.36	0.55
1:J:200:VAL:HG11	1:J:379:ARG:HH11	1.72	0.55
1:L:127:SER:HB3	1:L:130:MET:HE3	1.89	0.54
1:J:60:PRO:HG2	1:K:60:PRO:HG2	1.87	0.54
1:D:323:GLU:OE1	1:D:368:ARG:NH2	2.41	0.54
1:G:149:ARG:O	1:G:162:GLY:HA2	2.07	0.54
1:L:60:PRO:HG2	1:M:60:PRO:HG2	1.89	0.54
1:C:22:MET:SD	1:C:223:GLU:HB2	2.48	0.54
1:H:297:MET:HE2	1:H:391:ILE:C	2.32	0.54
1:A:391:ILE:HB	1:A:395:GLN:HB2	1.89	0.54
1:H:321:LEU:HD12	1:H:377:LEU:HD23	1.88	0.54
1:H:34:THR:HG21	1:H:208:VAL:HG22	1.89	0.54
1:J:179:THR:O	1:J:183:GLU:HG3	2.07	0.54
1:K:178:ARG:HD2	1:K:182:ASP:OD2	2.08	0.54
1:F:321:LEU:HD12	1:F:377:LEU:HD23	1.90	0.54
1:C:184:LEU:HD12	1:C:333:LEU:HG	1.89	0.53
1:G:52:ASP:CG	1:H:88:ARG:HH22	2.14	0.53
1:J:376:GLU:O	1:J:380:ARG:HG3	2.07	0.53
1:D:58:CYS:O	1:D:89:ARG:NH2	2.41	0.53
1:D:297:MET:HE2	1:D:392:GLY:HA2	1.89	0.53
1:H:321:LEU:HD11	1:H:380:ARG:HD2	1.90	0.53
1:F:302:VAL:O	1:F:306:GLU:HG3	2.08	0.53
1:M:163:MET:HG2	1:M:297:MET:SD	2.49	0.53
1:A:88:ARG:NH2	1:B:52:ASP:OD1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:164:LEU:HD12	1:K:328:PHE:CE1	2.44	0.53
1:L:200:VAL:HB	1:L:352:ARG:NH2	2.24	0.53
1:E:22:MET:SD	1:E:223:GLU:HB2	2.49	0.53
1:G:60:PRO:HG2	1:H:60:PRO:HG2	1.91	0.53
1:L:120:MET:HA	1:L:123:VAL:HG23	1.90	0.53
1:M:178:ARG:NH2	1:M:237:LEU:O	2.40	0.53
1:C:58:CYS:O	1:C:89:ARG:NH2	2.37	0.53
1:F:279:LYS:O	1:F:279:LYS:HG3	2.08	0.53
1:E:141:ILE:HD11	1:H:141:ILE:HD11	1.90	0.52
1:A:38:GLY:HA3	1:A:206:ILE:HD12	1.91	0.52
1:E:88:ARG:HH21	1:F:82:PRO:HB2	1.74	0.52
1:J:126:TYR:OH	1:J:147:ARG:HG2	2.09	0.52
1:M:42:ARG:NH1	1:M:203:GLU:O	2.35	0.52
1:C:149:ARG:NH2	1:C:258:GLN:OE1	2.42	0.52
1:B:174:TYR:HD2	1:B:337:ARG:HD3	1.75	0.52
1:F:212:THR:HG1	1:F:216:GLU:N	2.08	0.52
1:C:319:ILE:O	1:C:348:ARG:NH1	2.41	0.52
1:D:143:ASP:HB3	1:D:146:ALA:HB3	1.91	0.52
1:H:168:GLU:HB3	1:H:171:ARG:HH21	1.73	0.52
1:B:171:ARG:HD2	1:B:249:THR:HG23	1.92	0.52
1:C:211:ARG:HE	1:C:216:GLU:HA	1.74	0.52
1:J:52:ASP:CG	1:K:88:ARG:HH22	2.17	0.52
1:L:178:ARG:NH2	1:L:237:LEU:O	2.37	0.52
1:L:375:ARG:HB3	1:L:379:ARG:HH12	1.73	0.52
1:G:212:THR:HG1	1:G:216:GLU:N	2.07	0.52
1:C:351:VAL:HG21	1:C:376:GLU:HG2	1.91	0.52
1:G:178:ARG:NH1	1:G:235:ALA:HA	2.23	0.52
1:L:352:ARG:HH22	1:L:379:ARG:CZ	2.22	0.52
1:K:191:ARG:NH2	1:K:346:HIS:O	2.43	0.52
1:A:163:MET:HG3	2:A:585:HOH:O	2.09	0.51
1:E:187:ARG:HG3	1:E:187:ARG:HH11	1.74	0.51
1:F:110:ASP:HB3	1:F:272:LYS:HD3	1.92	0.51
1:F:178:ARG:HD2	1:F:182:ASP:OD2	2.10	0.51
1:A:60:PRO:HG2	1:B:60:PRO:HG2	1.92	0.51
1:A:297:MET:HG2	1:A:298:GLY:N	2.25	0.51
1:G:179:THR:O	1:G:183:GLU:HG3	2.09	0.51
1:H:69:ARG:NH1	1:H:81:VAL:O	2.43	0.51
1:K:58:CYS:O	1:K:89:ARG:NH2	2.42	0.51
1:K:352:ARG:HD2	1:K:372:THR:HG23	1.92	0.51
1:B:120:MET:HA	1:B:123:VAL:HG23	1.92	0.51
1:F:164:LEU:HD22	1:F:241:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:TYR:OH	1:E:147:ARG:HG2	2.11	0.51
1:F:19:TYR:HB2	1:F:258:GLN:O	2.11	0.51
1:F:337:ARG:HG2	1:F:337:ARG:HH11	1.75	0.51
1:J:131:ARG:NH2	1:K:143:ASP:OD1	2.35	0.51
1:K:123:VAL:HG21	1:K:145:LEU:HD21	1.93	0.51
1:C:211:ARG:NE	1:C:216:GLU:CA	2.69	0.51
1:C:339:TRP:HB3	1:C:341:PHE:CE1	2.46	0.50
1:F:4:ARG:NH1	1:F:107:GLY:HA2	2.26	0.50
1:J:189:HIS:O	1:J:193:VAL:HG23	2.12	0.50
1:A:88:ARG:HH21	1:B:82:PRO:HB2	1.76	0.50
1:F:319:ILE:O	1:F:348:ARG:NH1	2.43	0.50
1:L:352:ARG:HH22	1:L:379:ARG:NH1	2.09	0.50
1:B:119:SER:OG	1:B:122:ASN:HB2	2.12	0.50
1:H:323:GLU:HB3	1:H:369:MET:HE2	1.93	0.50
1:E:326:GLU:OE1	1:E:354:SER:OG	2.20	0.50
1:G:193:VAL:HA	1:G:196:GLN:HG3	1.94	0.50
1:B:110:ASP:HB3	1:B:272:LYS:HD3	1.92	0.50
1:C:42:ARG:NH1	1:C:203:GLU:O	2.43	0.50
1:E:60:PRO:HG2	1:F:60:PRO:HG2	1.92	0.50
1:E:241:LEU:O	1:E:243:LYS:N	2.45	0.50
1:G:325:ASN:HB2	1:G:369:MET:SD	2.51	0.50
1:G:352:ARG:HD2	1:G:372:THR:HG23	1.94	0.50
1:H:33:VAL:HG13	1:H:75:ALA:HA	1.93	0.50
1:B:15:PRO:HD2	1:B:208:VAL:HG23	1.93	0.50
1:C:211:ARG:HE	1:C:216:GLU:CA	2.25	0.50
1:E:45:ILE:CG2	1:E:278:LEU:HD21	2.42	0.50
1:L:368:ARG:NH1	1:L:369:MET:HG3	2.27	0.50
1:B:91:GLY:HA2	1:B:389:MET:SD	2.52	0.49
1:J:187:ARG:O	1:J:191:ARG:HG3	2.11	0.49
1:L:58:CYS:O	1:L:89:ARG:NH2	2.41	0.49
1:C:84:MET:SD	1:D:88:ARG:NH1	2.86	0.49
1:D:297:MET:CE	1:D:392:GLY:HA2	2.42	0.49
1:L:91:GLY:HA2	1:L:389:MET:SD	2.53	0.49
1:B:239:PRO:HD2	1:B:242:LEU:HD22	1.95	0.49
1:F:204:GLU:HG2	1:F:375:ARG:HD2	1.93	0.49
1:C:226:ARG:HH21	1:C:228:ASP:CG	2.17	0.49
1:C:326:GLU:OE1	1:C:354:SER:OG	2.17	0.49
1:H:120:MET:HA	1:H:123:VAL:HG23	1.93	0.49
1:J:157:HIS:O	2:J:501:HOH:O	2.20	0.49
1:L:337:ARG:HH11	1:L:337:ARG:CG	2.25	0.49
1:J:178:ARG:NH2	1:J:237:LEU:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:MET:SD	1:H:88:ARG:NH1	2.85	0.49
1:J:84:MET:SD	1:K:88:ARG:NH1	2.86	0.49
1:L:181:GLN:NE2	1:L:249:THR:HB	2.27	0.49
1:C:156:PHE:C	1:C:157:HIS:ND1	2.71	0.49
1:C:166:THR:HG21	1:C:297:MET:HE3	1.93	0.49
1:A:283:ARG:NH1	1:A:285:VAL:HG22	2.28	0.49
1:B:333:LEU:HD23	1:B:336:MET:HE3	1.94	0.49
1:E:391:ILE:HB	1:E:395:GLN:HB2	1.93	0.49
1:H:90:CYS:HB3	2:H:560:HOH:O	2.13	0.49
1:M:37:LYS:HG3	1:M:75:ALA:HB1	1.94	0.49
1:F:326:GLU:OE1	1:F:354:SER:OG	2.10	0.49
1:F:351:VAL:HG21	1:F:376:GLU:HG2	1.95	0.48
1:J:141:ILE:HD11	1:M:141:ILE:HD11	1.95	0.48
1:C:187:ARG:O	1:C:191:ARG:HG3	2.13	0.48
1:G:391:ILE:HB	1:G:395:GLN:HB2	1.95	0.48
1:A:307:VAL:O	1:A:311:LYS:HG3	2.14	0.48
1:M:80:THR:O	1:M:82:PRO:HD3	2.13	0.48
1:M:228:ASP:O	1:M:230:THR:HG23	2.13	0.48
1:A:120:MET:HA	1:A:123:VAL:HG23	1.94	0.48
1:H:163:MET:SD	1:H:297:MET:HE3	2.53	0.48
1:K:391:ILE:HB	1:K:395:GLN:HB2	1.96	0.48
1:L:88:ARG:HH22	1:M:52:ASP:CG	2.21	0.48
1:A:278:LEU:O	1:A:280:PRO:HD3	2.14	0.48
1:B:352:ARG:HH21	1:B:379:ARG:NH1	2.12	0.48
1:M:120:MET:HA	1:M:123:VAL:HG23	1.94	0.48
1:M:169:ASN:OD1	1:M:172:ARG:NH2	2.45	0.48
1:G:171:ARG:HH21	1:G:172:ARG:HH11	1.62	0.48
1:M:352:ARG:NH2	1:M:379:ARG:HH21	1.97	0.48
1:G:369:MET:HE2	1:G:387:GLU:HG3	1.96	0.48
1:A:157:HIS:HB2	1:A:294:PRO:HG2	1.95	0.48
1:B:297:MET:HE2	1:B:298:GLY:HA2	1.96	0.48
1:G:123:VAL:HG21	1:G:145:LEU:HD21	1.95	0.48
1:H:279:LYS:HD2	1:H:279:LYS:C	2.39	0.48
1:A:9:CYS:HB2	1:A:266:ILE:HB	1.95	0.47
1:L:352:ARG:NH2	1:L:379:ARG:NH1	2.61	0.47
1:D:90:CYS:HB3	2:D:523:HOH:O	2.13	0.47
1:F:33:VAL:HG13	1:F:75:ALA:HA	1.96	0.47
1:G:226:ARG:HH11	1:G:228:ASP:CG	2.22	0.47
1:A:58:CYS:O	1:A:89:ARG:NH2	2.42	0.47
1:L:196:GLN:HG2	1:L:201:LEU:HD12	1.96	0.47
2:A:568:HOH:O	1:B:311:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:ARG:NH1	1:J:349:THR:O	2.48	0.47
1:K:4:ARG:CZ	1:K:107:GLY:HA2	2.45	0.47
1:B:6:ALA:HB2	1:B:105:ARG:HG3	1.96	0.47
1:G:200:VAL:HG11	1:G:379:ARG:NH1	2.29	0.47
1:J:58:CYS:HB3	1:J:89:ARG:NH2	2.29	0.47
1:C:149:ARG:HG2	2:C:600:HOH:O	2.15	0.47
1:D:120:MET:HA	1:D:123:VAL:HG23	1.97	0.47
1:G:9:CYS:HB2	1:G:266:ILE:HB	1.96	0.47
1:G:120:MET:HA	1:G:123:VAL:HG23	1.97	0.47
1:G:307:VAL:HG12	1:G:311:LYS:HE3	1.97	0.47
1:L:84:MET:SD	1:M:88:ARG:NH1	2.88	0.47
1:C:88:ARG:HH22	1:D:52:ASP:CG	2.21	0.47
1:E:192:ALA:O	1:E:196:GLN:HG3	2.15	0.47
1:M:58:CYS:O	1:M:89:ARG:NH2	2.45	0.47
1:B:161:GLY:HA3	1:B:165:GLU:HB2	1.96	0.47
1:C:203:GLU:OE1	1:C:379:ARG:NH2	2.48	0.47
1:F:169:ASN:OD1	1:F:172:ARG:NH2	2.48	0.47
1:K:6:ALA:HB2	1:K:105:ARG:HG3	1.97	0.47
1:B:320:ASP:CB	1:B:382:ALA:HB1	2.45	0.47
1:B:352:ARG:NH2	1:B:379:ARG:NH1	2.62	0.47
1:C:121:SER:O	1:D:131:ARG:HD2	2.15	0.47
1:J:192:ALA:O	1:J:196:GLN:HG3	2.15	0.47
1:B:379:ARG:CZ	1:B:379:ARG:HB2	2.45	0.46
1:F:164:LEU:HD21	2:F:527:HOH:O	2.15	0.46
1:G:245:ASP:HB3	1:G:248:ALA:HB2	1.98	0.46
1:G:297:MET:CE	1:G:392:GLY:HA2	2.44	0.46
1:A:90:CYS:O	1:A:389:MET:HE2	2.15	0.46
1:B:33:VAL:HG13	1:B:75:ALA:HA	1.97	0.46
1:B:211:ARG:HD3	1:B:216:GLU:HG3	1.96	0.46
1:C:182:ASP:O	1:C:186:VAL:HG23	2.15	0.46
1:F:69:ARG:NH1	1:F:81:VAL:O	2.47	0.46
1:L:9:CYS:HB2	1:L:266:ILE:HB	1.98	0.46
1:K:149:ARG:NH2	1:K:258:GLN:OE1	2.33	0.46
1:E:120:MET:HA	1:E:123:VAL:HG23	1.98	0.46
1:F:323:GLU:HB3	1:F:369:MET:HE2	1.98	0.46
1:H:320:ASP:CB	1:H:382:ALA:HB1	2.46	0.46
1:J:200:VAL:CG1	1:J:379:ARG:HH11	2.28	0.46
1:G:352:ARG:NH2	2:G:501:HOH:O	2.13	0.46
1:K:297:MET:HE2	1:K:390:CYS:HB2	1.96	0.46
1:K:333:LEU:O	1:K:337:ARG:HG2	2.15	0.46
1:L:11:PRO:HB2	1:L:371:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4:ARG:NH1	1:M:107:GLY:HA2	2.30	0.46
1:C:143:ASP:HB3	1:C:146:ALA:HB3	1.97	0.46
1:K:4:ARG:HD2	2:K:623:HOH:O	2.16	0.46
1:L:180:GLU:CD	1:L:337:ARG:HH22	2.24	0.46
1:L:182:ASP:O	1:L:186:VAL:HG23	2.16	0.46
1:G:6:ALA:HB2	1:G:105:ARG:HG3	1.98	0.46
1:G:127:SER:CB	1:G:130:MET:HE3	2.46	0.46
1:H:178:ARG:NH2	1:H:251:THR:HG21	2.31	0.46
1:G:301:PRO:HG3	1:G:389:MET:C	2.41	0.45
1:L:15:PRO:HD2	1:L:208:VAL:HG23	1.96	0.45
1:D:192:ALA:O	1:D:196:GLN:HG3	2.16	0.45
1:F:9:CYS:HB2	1:F:266:ILE:HB	1.98	0.45
1:H:178:ARG:HD3	1:H:249:THR:HB	1.99	0.45
1:L:378:HIS:HA	1:L:403:ARG:HD2	1.97	0.45
1:A:297:MET:HE2	1:A:392:GLY:HA2	1.99	0.45
1:B:171:ARG:NH2	1:B:172:ARG:HD3	2.31	0.45
1:B:178:ARG:HD2	1:B:182:ASP:OD2	2.16	0.45
1:B:275:GLU:O	1:G:79:ILE:HG13	2.16	0.45
1:L:184:LEU:HD21	1:L:326:GLU:CD	2.42	0.45
1:E:22:MET:HE3	1:E:219:ILE:HG21	1.97	0.45
1:L:278:LEU:O	1:L:280:PRO:HD3	2.17	0.45
1:M:15:PRO:HD2	1:M:208:VAL:HG23	1.99	0.45
1:A:106:SER:OG	1:A:108:ASP:OD2	2.30	0.45
1:C:22:MET:HG2	1:C:223:GLU:OE1	2.17	0.45
1:C:245:ASP:HA	1:C:246:PRO:HD2	1.82	0.45
1:F:5:ASP:O	1:F:269:THR:HG22	2.16	0.45
1:L:4:ARG:NH2	1:L:107:GLY:HA2	2.31	0.45
1:E:15:PRO:HD3	1:E:206:ILE:O	2.17	0.45
1:E:333:LEU:HD23	1:E:336:MET:HE3	1.99	0.45
1:L:189:HIS:O	1:L:193:VAL:HG23	2.17	0.45
1:C:157:HIS:HD2	1:C:294:PRO:HD2	1.82	0.45
1:K:105:ARG:HE	1:K:105:ARG:HB3	1.63	0.45
1:E:58:CYS:O	1:E:89:ARG:NH2	2.48	0.45
1:J:351:VAL:HG21	1:J:376:GLU:HG2	1.99	0.45
1:M:351:VAL:HG21	1:M:376:GLU:HG2	1.99	0.45
1:M:352:ARG:NH2	1:M:379:ARG:HE	2.15	0.45
1:J:379:ARG:HE	1:J:379:ARG:HB3	1.49	0.44
1:G:337:ARG:HH11	1:G:337:ARG:CG	2.27	0.44
1:J:319:ILE:O	1:J:348:ARG:NH1	2.51	0.44
1:K:256:SER:HA	1:K:356:ILE:HA	1.98	0.44
1:D:4:ARG:NH2	1:D:109:HIS:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ARG:HG3	1:E:187:ARG:NH1	2.32	0.44
1:L:358:LEU:HD13	1:L:368:ARG:HE	1.83	0.44
1:M:373:LEU:O	1:M:377:LEU:HB2	2.17	0.44
1:A:178:ARG:NH1	1:A:182:ASP:OD2	2.50	0.44
1:F:283:ARG:NH2	1:F:402:GLU:OE1	2.49	0.44
1:J:120:MET:HA	1:J:123:VAL:HG23	1.98	0.44
1:M:143:ASP:HB3	1:M:146:ALA:HB3	1.99	0.44
1:A:108:ASP:OD1	1:B:311:LYS:NZ	2.50	0.44
1:A:143:ASP:HB3	1:A:146:ALA:HB3	1.99	0.44
1:C:7:VAL:HB	1:C:280:PRO:HB3	2.00	0.44
1:C:211:ARG:HH11	1:C:212:THR:N	2.13	0.44
1:L:34:THR:HG21	1:L:208:VAL:HG22	2.00	0.44
1:C:178:ARG:HD2	1:C:182:ASP:OD2	2.17	0.44
1:F:120:MET:HA	1:F:123:VAL:HG23	1.99	0.44
1:H:178:ARG:NH2	1:H:237:LEU:O	2.50	0.44
1:H:243:LYS:HE2	1:H:243:LYS:HB2	1.82	0.44
1:C:123:VAL:HG21	1:C:145:LEU:HD21	2.00	0.44
1:C:256:SER:HB3	1:C:355:GLY:C	2.43	0.44
1:E:131:ARG:NH2	1:F:143:ASP:OD1	2.38	0.44
1:K:297:MET:HE3	1:K:391:ILE:O	2.18	0.44
1:M:22:MET:SD	1:M:223:GLU:HB2	2.56	0.44
1:C:196:GLN:HG2	1:C:201:LEU:HD12	2.00	0.44
1:J:63:GLU:OE2	1:K:126:TYR:OH	2.35	0.44
1:L:333:LEU:HA	1:L:336:MET:HE3	2.00	0.44
1:G:105:ARG:NH2	2:G:506:HOH:O	2.33	0.43
1:M:116:GLY:HA3	1:M:363:GLY:O	2.18	0.43
1:E:352:ARG:HH22	1:E:379:ARG:NH1	2.06	0.43
1:J:9:CYS:HB2	1:J:266:ILE:HB	2.00	0.43
1:K:164:LEU:HD12	1:K:328:PHE:HE1	1.82	0.43
1:B:58:CYS:O	1:B:89:ARG:NH2	2.51	0.43
1:D:178:ARG:HH21	1:D:239:PRO:HG3	1.82	0.43
1:H:182:ASP:O	1:H:186:VAL:HG23	2.18	0.43
1:A:242:LEU:O	1:A:242:LEU:HD23	2.19	0.43
1:B:5:ASP:OD2	1:B:283:ARG:HD2	2.18	0.43
1:F:7:VAL:HG12	1:F:283:ARG:HB3	2.00	0.43
1:E:121:SER:O	1:F:131:ARG:HD2	2.19	0.43
1:G:287:TRP:O	1:G:311:LYS:NZ	2.51	0.43
1:H:7:VAL:HG12	1:H:283:ARG:HB3	2.00	0.43
1:A:287:TRP:O	1:A:311:LYS:NZ	2.44	0.43
1:C:279:LYS:O	1:C:279:LYS:HG3	2.18	0.43
1:D:169:ASN:O	1:D:173:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:MET:HG2	1:G:298:GLY:N	2.22	0.43
1:J:171:ARG:HG3	1:J:249:THR:OG1	2.19	0.43
1:L:192:ALA:O	1:L:196:GLN:HG3	2.18	0.43
1:C:333:LEU:HD23	1:C:336:MET:HE3	2.00	0.43
1:E:34:THR:HG21	1:E:208:VAL:HG22	2.00	0.43
1:F:297:MET:HG3	1:F:391:ILE:C	2.43	0.43
1:J:184:LEU:HD21	1:J:326:GLU:CD	2.43	0.43
1:L:369:MET:HE1	1:L:388:THR:O	2.18	0.43
1:A:15:PRO:HD2	1:A:208:VAL:HG23	2.00	0.43
1:H:351:VAL:HG21	1:H:376:GLU:HG2	2.01	0.43
1:J:337:ARG:HG3	1:J:337:ARG:NH1	2.33	0.43
1:L:33:VAL:HG13	1:L:75:ALA:HA	2.00	0.43
1:M:4:ARG:CZ	1:M:107:GLY:HA2	2.49	0.43
1:D:342:GLY:O	1:D:344:ALA:N	2.51	0.43
1:M:127:SER:OG	1:M:140:GLN:O	2.32	0.43
1:C:211:ARG:HE	1:C:216:GLU:CG	2.32	0.42
1:J:163:MET:HG2	1:J:297:MET:HE2	2.01	0.42
1:D:171:ARG:HA	1:D:176:ILE:HD12	2.01	0.42
1:E:201:LEU:HD11	2:E:508:HOH:O	2.18	0.42
1:L:346:HIS:ND1	1:L:346:HIS:N	2.66	0.42
1:D:368:ARG:NE	2:D:507:HOH:O	2.44	0.42
1:J:245:ASP:HB3	1:J:248:ALA:HB2	2.00	0.42
1:J:42:ARG:NH1	1:J:203:GLU:O	2.45	0.42
1:J:162:GLY:O	1:J:166:THR:HG23	2.19	0.42
1:J:373:LEU:O	1:J:377:LEU:HB2	2.19	0.42
1:F:13:ARG:O	1:F:205:ILE:HA	2.19	0.42
1:H:208:VAL:HA	1:H:209:PRO:HD3	1.92	0.42
1:L:321:LEU:HD11	1:L:380:ARG:HD2	2.00	0.42
1:M:163:MET:HE3	1:M:297:MET:CE	2.41	0.42
1:A:239:PRO:HB2	1:A:242:LEU:HB2	2.02	0.42
1:A:242:LEU:HA	1:A:245:ASP:O	2.20	0.42
1:C:211:ARG:HD2	1:C:211:ARG:HA	1.57	0.42
1:C:273:ALA:HB1	1:C:278:LEU:HB2	2.02	0.42
1:H:126:TYR:OH	1:H:147:ARG:HG2	2.19	0.42
1:L:24:ARG:NH1	2:L:507:HOH:O	2.48	0.42
1:C:79:ILE:HG13	1:K:275:GLU:O	2.19	0.42
1:H:272:LYS:HE3	1:H:276:LEU:HD11	2.01	0.42
1:M:261:ALA:HB3	1:M:361:PRO:HG3	2.01	0.42
1:B:5:ASP:OD1	1:B:283:ARG:NH1	2.53	0.42
1:B:141:ILE:HD12	1:C:141:ILE:CG1	2.50	0.42
1:M:171:ARG:HD2	1:M:249:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:LEU:HD23	1:D:184:LEU:C	2.45	0.42
1:D:278:LEU:O	1:D:280:PRO:HD3	2.20	0.42
1:G:143:ASP:HB3	1:G:146:ALA:HB3	2.01	0.42
1:K:297:MET:HE3	1:K:297:MET:HB2	1.66	0.42
1:A:13:ARG:O	1:A:205:ILE:HA	2.19	0.42
1:A:171:ARG:HD2	1:A:171:ARG:C	2.45	0.42
1:B:4:ARG:NH1	1:B:107:GLY:HA2	2.34	0.42
1:C:211:ARG:CD	1:C:216:GLU:HA	2.49	0.42
1:E:141:ILE:HD13	1:E:141:ILE:HG21	1.81	0.42
1:F:239:PRO:HG2	1:F:242:LEU:HD13	2.02	0.42
1:J:339:TRP:HB3	1:J:341:PHE:CE1	2.55	0.42
1:L:104:VAL:HA	1:L:109:HIS:O	2.20	0.42
1:L:178:ARG:HD2	1:L:178:ARG:O	2.20	0.42
1:D:163:MET:CG	1:D:297:MET:HE1	2.41	0.41
1:E:9:CYS:HB2	1:E:266:ILE:HB	2.01	0.41
1:L:181:GLN:NE2	1:L:249:THR:CB	2.83	0.41
1:M:55:LEU:HD12	1:M:68:GLY:HA2	2.02	0.41
1:B:7:VAL:HB	1:B:280:PRO:HB3	2.01	0.41
1:B:149:ARG:HG2	1:B:163:MET:HG2	2.01	0.41
1:F:58:CYS:O	1:F:89:ARG:NH2	2.49	0.41
1:F:297:MET:HE3	1:F:297:MET:HB3	1.57	0.41
1:H:19:TYR:HB2	1:H:258:GLN:O	2.19	0.41
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.80	0.41
1:C:337:ARG:HG2	1:C:337:ARG:NH1	2.33	0.41
1:E:4:ARG:CZ	1:E:107:GLY:HA2	2.50	0.41
1:E:184:LEU:HD12	1:E:333:LEU:HG	2.01	0.41
1:E:209:PRO:HA	1:E:217:GLU:O	2.21	0.41
1:G:90:CYS:O	1:G:389:MET:HE2	2.20	0.41
1:K:4:ARG:NH1	1:K:107:GLY:HA2	2.36	0.41
1:L:6:ALA:HB2	1:L:105:ARG:HG3	2.02	0.41
1:B:169:ASN:OD1	1:B:172:ARG:NH2	2.53	0.41
1:D:163:MET:CE	1:D:297:MET:HE1	2.48	0.41
1:G:58:CYS:O	1:G:89:ARG:NH2	2.48	0.41
1:H:81:VAL:HA	1:H:82:PRO:HD3	1.90	0.41
1:H:163:MET:CE	1:H:297:MET:HE3	2.51	0.41
1:K:169:ASN:OD1	1:K:172:ARG:NH2	2.53	0.41
1:L:368:ARG:HH11	1:L:369:MET:HG3	1.84	0.41
1:A:11:PRO:HB2	1:A:371:ALA:HA	2.02	0.41
1:A:116:GLY:HA3	1:A:363:GLY:O	2.21	0.41
1:D:169:ASN:OD1	1:D:172:ARG:NH2	2.54	0.41
1:E:18:ARG:HG3	1:E:223:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:GLU:OE2	1:G:352:ARG:NH1	2.50	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.86	0.41
1:C:216:GLU:CG	1:C:216:GLU:HB3	2.24	0.41
1:E:131:ARG:HD2	1:F:121:SER:O	2.20	0.41
1:J:116:GLY:HA3	1:J:363:GLY:O	2.21	0.41
1:M:26:LEU:HD11	1:M:210:VAL:HG12	2.02	0.41
1:A:299:ILE:HD12	1:A:299:ILE:HA	1.92	0.41
1:C:18:ARG:HD2	1:C:223:GLU:HG2	2.02	0.41
1:D:42:ARG:NH1	1:D:203:GLU:O	2.47	0.41
1:H:163:MET:H	1:H:163:MET:HG2	1.62	0.41
1:L:167:ALA:HB2	1:L:328:PHE:CD2	2.54	0.41
1:M:226:ARG:HG2	1:M:228:ASP:OD1	2.21	0.41
1:M:378:HIS:HA	1:M:403:ARG:CD	2.51	0.41
1:A:121:SER:O	1:B:131:ARG:HD2	2.20	0.41
1:A:351:VAL:HG21	1:A:376:GLU:HG2	2.02	0.41
1:C:333:LEU:HA	1:C:336:MET:HE3	2.03	0.41
1:D:123:VAL:HG21	1:D:145:LEU:HD21	2.02	0.41
1:E:351:VAL:HG21	1:E:376:GLU:HG2	2.02	0.41
1:F:388:THR:C	1:F:389:MET:HG2	2.31	0.41
1:H:13:ARG:O	1:H:205:ILE:HA	2.21	0.41
1:J:333:LEU:HA	1:J:336:MET:HE2	2.03	0.41
1:J:391:ILE:HB	1:J:395:GLN:HB2	2.01	0.41
1:K:4:ARG:NH2	1:K:109:HIS:O	2.54	0.41
1:L:156:PHE:O	1:L:157:HIS:CD2	2.73	0.41
1:M:111:LEU:HD21	1:M:266:ILE:HD12	2.02	0.41
1:M:126:TYR:OH	1:M:147:ARG:HG2	2.21	0.41
1:M:389:MET:HE2	1:M:389:MET:HB3	1.82	0.41
1:A:189:HIS:O	1:A:193:VAL:HG23	2.21	0.41
1:A:193:VAL:HG21	1:A:227:ALA:HA	2.02	0.41
1:A:333:LEU:O	1:A:337:ARG:HG2	2.20	0.41
1:B:100:ALA:HB1	1:B:112:VAL:CG2	2.51	0.41
1:C:228:ASP:OD1	1:C:228:ASP:N	2.46	0.41
1:D:15:PRO:HD3	1:D:205:ILE:HG23	2.03	0.41
1:G:121:SER:O	1:H:131:ARG:HD2	2.21	0.41
1:M:391:ILE:HB	1:M:395:GLN:HB2	2.02	0.41
1:A:88:ARG:HG2	1:A:391:ILE:HD13	2.02	0.40
1:G:178:ARG:HH21	1:G:251:THR:HG21	1.86	0.40
1:K:186:VAL:O	1:K:190:GLN:HG3	2.21	0.40
1:L:127:SER:CB	1:L:130:MET:HE3	2.50	0.40
1:E:141:ILE:HD12	1:H:139:VAL:CG1	2.52	0.40
1:L:10:GLU:OE2	1:L:375:ARG:NH2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ARG:HG2	1:E:137:THR:HG23	2.04	0.40
1:H:281:LEU:O	1:H:378:HIS:NE2	2.54	0.40
1:K:368:ARG:NE	2:K:505:HOH:O	2.40	0.40
1:G:163:MET:HG3	2:G:566:HOH:O	2.20	0.40
1:J:286:SER:OG	1:J:308:ALA:O	2.30	0.40
1:K:135:ALA:HB2	1:M:131:ARG:O	2.22	0.40
1:A:127:SER:CB	1:A:130:MET:HE3	2.52	0.40
1:A:325:ASN:HB2	1:A:369:MET:SD	2.62	0.40
1:C:52:ASP:CG	1:D:88:ARG:HH22	2.26	0.40
1:F:4:ARG:CZ	1:F:107:GLY:HA2	2.52	0.40
1:F:123:VAL:HG21	1:F:145:LEU:HD21	2.02	0.40
1:G:163:MET:CG	1:G:297:MET:HE1	2.40	0.40
1:G:169:ASN:OD1	1:G:172:ARG:NH2	2.55	0.40
1:M:166:THR:HG22	1:M:295:ASP:HA	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:NH2	1:D:342:GLY:CA[5_554]	2.08	0.12

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	392/407 (96%)	381 (97%)	9 (2%)	2 (0%)	24	20
1	B	394/407 (97%)	382 (97%)	11 (3%)	1 (0%)	36	34
1	C	394/407 (97%)	384 (98%)	9 (2%)	1 (0%)	36	34
1	D	392/407 (96%)	380 (97%)	9 (2%)	3 (1%)	16	10
1	E	390/407 (96%)	382 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	395/407 (97%)	386 (98%)	8 (2%)	1 (0%)	36	34
1	G	394/407 (97%)	382 (97%)	10 (2%)	2 (0%)	24	20
1	H	393/407 (97%)	385 (98%)	8 (2%)	0	100	100
1	J	390/407 (96%)	378 (97%)	11 (3%)	1 (0%)	36	34
1	K	395/407 (97%)	384 (97%)	10 (2%)	1 (0%)	36	34
1	L	394/407 (97%)	381 (97%)	13 (3%)	0	100	100
1	M	393/407 (97%)	383 (98%)	8 (2%)	2 (0%)	24	20
All	All	4716/4884 (97%)	4588 (97%)	114 (2%)	14 (0%)	36	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	343	GLU
1	A	136	ARG
1	D	297	MET
1	G	297	MET
1	K	297	MET
1	M	297	MET
1	M	362	VAL
1	F	362	VAL
1	B	297	MET
1	D	362	VAL
1	G	362	VAL
1	A	362	VAL
1	C	362	VAL
1	J	362	VAL

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	294/309 (95%)	289 (98%)	5 (2%)	53	60
1	B	301/309 (97%)	295 (98%)	6 (2%)	48	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	300/309 (97%)	292 (97%)	8 (3%)	39	41
1	D	300/309 (97%)	294 (98%)	6 (2%)	48	54
1	E	300/309 (97%)	291 (97%)	9 (3%)	36	38
1	F	302/309 (98%)	299 (99%)	3 (1%)	68	75
1	G	302/309 (98%)	290 (96%)	12 (4%)	28	27
1	H	301/309 (97%)	297 (99%)	4 (1%)	61	68
1	J	300/309 (97%)	295 (98%)	5 (2%)	53	60
1	K	303/309 (98%)	296 (98%)	7 (2%)	44	49
1	L	300/309 (97%)	285 (95%)	15 (5%)	22	18
1	M	301/309 (97%)	290 (96%)	11 (4%)	30	30
All	All	3604/3708 (97%)	3513 (98%)	91 (2%)	42	45

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ILE
1	A	157	HIS
1	A	211	ARG
1	A	297	MET
1	A	389	MET
1	B	79	ILE
1	B	104	VAL
1	B	193	VAL
1	B	210	VAL
1	B	219	ILE
1	B	297	MET
1	C	155	LYS
1	C	157	HIS
1	C	216	GLU
1	C	232	GLU
1	C	279	LYS
1	C	297	MET
1	C	337	ARG
1	C	343	GLU
1	D	4	ARG
1	D	171	ARG
1	D	242	LEU
1	D	243	LYS

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Mol	Chain	Res	Type
1	D	297	MET
1	D	337	ARG
1	E	136	ARG
1	E	141	ILE
1	E	171	ARG
1	E	201	LEU
1	E	203	GLU
1	E	210	VAL
1	E	238	LYS
1	E	297	MET
1	E	340	LYS
1	F	4	ARG
1	F	217	GLU
1	F	297	MET
1	G	181	GLN
1	G	203	GLU
1	G	226	ARG
1	G	232	GLU
1	G	236	LYS
1	G	243	LYS
1	G	271	GLU
1	G	297	MET
1	G	337	ARG
1	G	341	PHE
1	G	343	GLU
1	G	389	MET
1	H	203	GLU
1	H	210	VAL
1	H	337	ARG
1	H	347	GLU
1	J	45	ILE
1	J	141	ILE
1	J	179	THR
1	J	181	GLN
1	J	377	LEU
1	K	4	ARG
1	K	104	VAL
1	K	164	LEU
1	K	211	ARG
1	K	232	GLU
1	K	238	LYS
1	K	297	MET

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Mol	Chain	Res	Type
1	L	141	ILE
1	L	155	LYS
1	L	173	GLU
1	L	181	GLN
1	L	211	ARG
1	L	216	GLU
1	L	217	GLU
1	L	231	VAL
1	L	232	GLU
1	L	244	GLN
1	L	247	GLU
1	L	297	MET
1	L	337	ARG
1	L	346	HIS
1	L	352	ARG
1	M	4	ARG
1	M	79	ILE
1	M	171	ARG
1	M	210	VAL
1	M	219	ILE
1	M	232	GLU
1	M	238	LYS
1	M	244	GLN
1	M	306	GLU
1	M	379	ARG
1	M	389	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	103	GLN
1	A	157	HIS
1	A	258	GLN
1	A	346	HIS
1	B	99	GLN
1	B	103	GLN
1	B	325	ASN
1	C	140	GLN
1	C	190	GLN
1	C	346	HIS
1	D	99	GLN

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Mol	Chain	Res	Type
1	D	103	GLN
1	D	122	ASN
1	E	99	GLN
1	E	103	GLN
1	E	122	ASN
1	F	175	HIS
1	F	346	HIS
1	G	99	GLN
1	G	103	GLN
1	G	325	ASN
1	G	346	HIS
1	J	99	GLN
1	J	103	GLN
1	K	99	GLN
1	K	103	GLN
1	K	196	GLN
1	K	346	HIS
1	L	142	HIS
1	L	157	HIS
1	L	181	GLN
1	M	157	HIS
1	M	181	GLN
1	M	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/407 (97%)	-1.36	0 100 100	16, 31, 50, 66	0
1	B	398/407 (97%)	-1.40	0 100 100	14, 27, 49, 73	0
1	C	398/407 (97%)	-1.36	0 100 100	15, 30, 53, 73	0
1	D	396/407 (97%)	-1.43	0 100 100	15, 24, 45, 62	0
1	E	396/407 (97%)	-1.35	0 100 100	17, 32, 53, 70	0
1	F	399/407 (98%)	-1.40	0 100 100	16, 28, 50, 75	0
1	G	398/407 (97%)	-1.37	0 100 100	16, 30, 54, 72	0
1	H	397/407 (97%)	-1.44	0 100 100	16, 25, 45, 67	0
1	J	396/407 (97%)	-1.36	0 100 100	15, 31, 54, 68	0
1	K	399/407 (98%)	-1.42	0 100 100	15, 26, 50, 76	0
1	L	398/407 (97%)	-1.28	0 100 100	18, 36, 56, 76	0
1	M	397/407 (97%)	-1.35	0 100 100	20, 31, 53, 73	0
All	All	4768/4884 (97%)	-1.38	0 100 100	14, 29, 52, 76	0

There are no RSRZ outliers to report.

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.