



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:48 PM UTC

PDB ID : 5LP3 / pdb_00005lp3
EMDB ID : EMD-4094
Title : Three tetrameric rings of Isoaspartyl Dipeptidase fitted in an EM volume.
Authors : Garcia-Seisdedos, H.; Empereur-Mot, C.; Elad, N.; Levy, E.D.
Deposited on : 2016-08-11
Resolution : 10.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

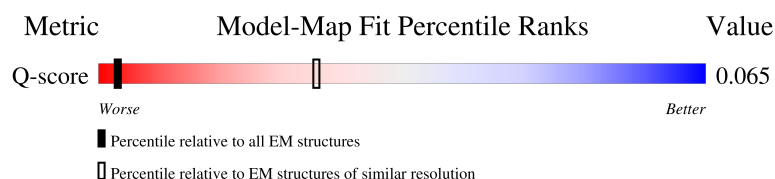
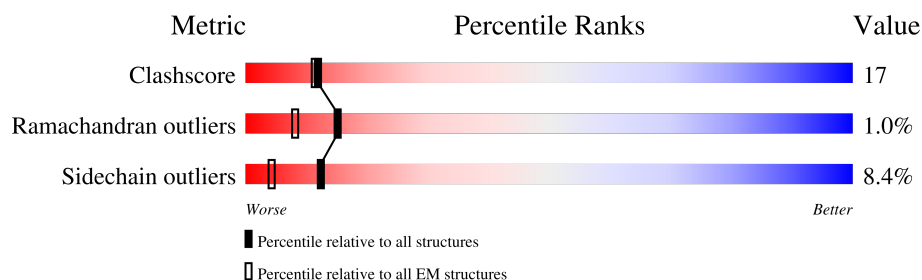
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 10.50 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	126 (10.00 - 11.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	
1	B	390	
1	C	390	
1	D	390	

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Mol	Chain	Length	Quality of chain
1	E	390	
1	F	390	
1	G	390	
1	H	390	
1	I	390	
1	J	390	
1	K	390	
1	L	390	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33200 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

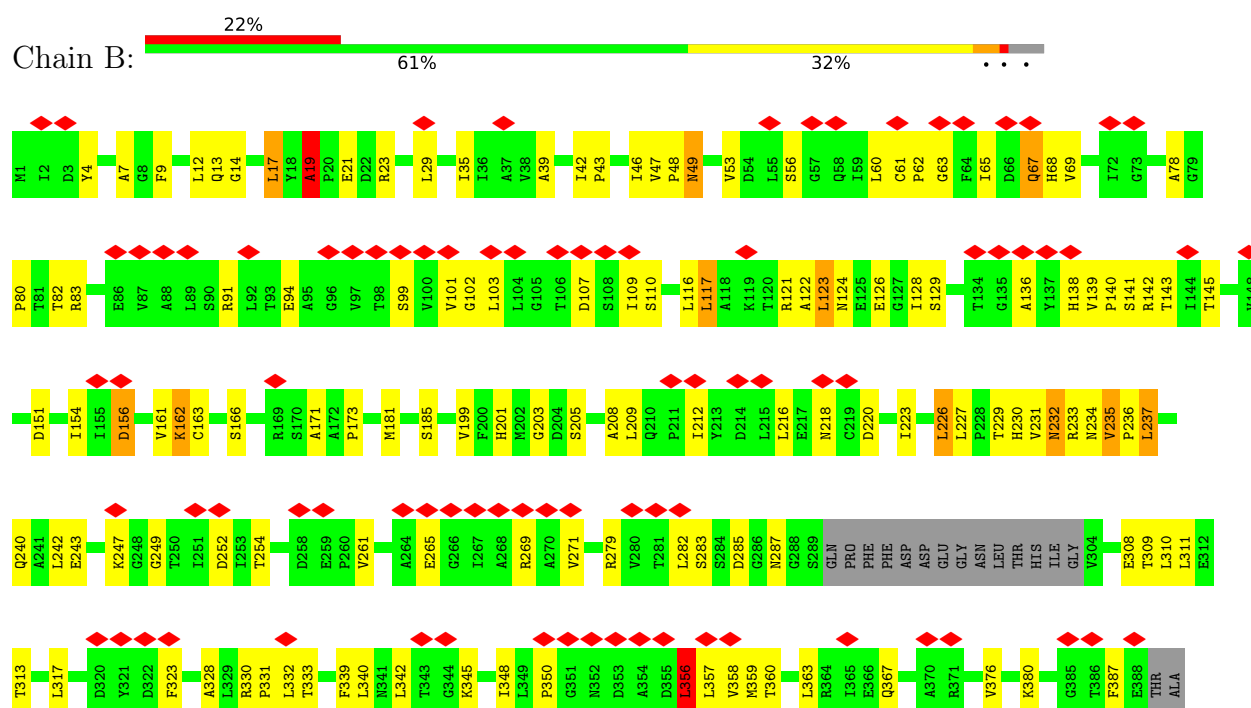
- Molecule 1 is a protein called Isoaspartyl dipeptidase.

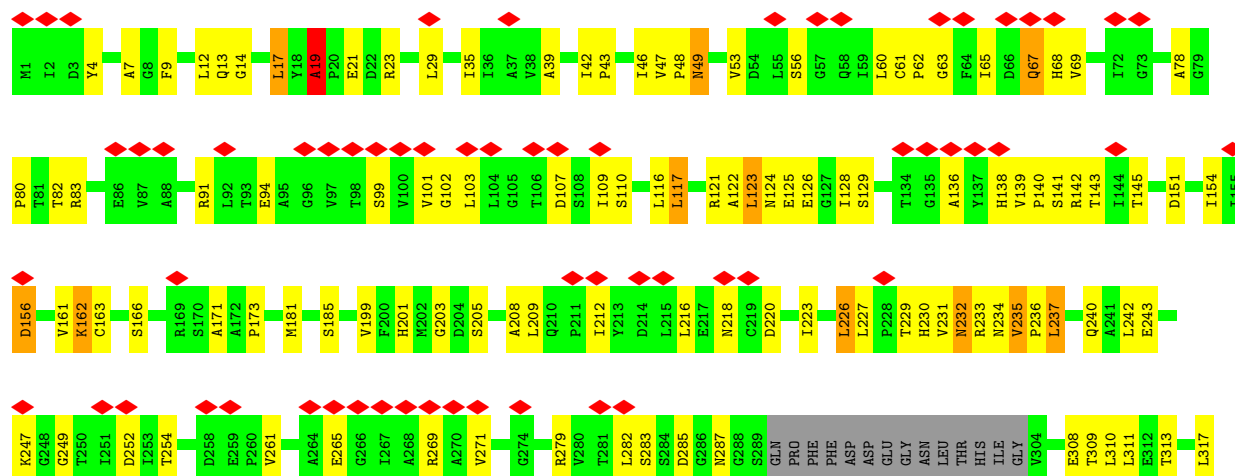
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	C	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	D	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	E	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	A	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	F	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	G	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	H	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	I	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		
1	J	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		
1	K	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		
1	L	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		

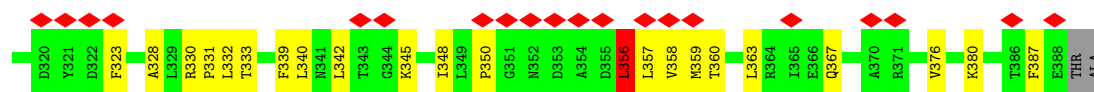
3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

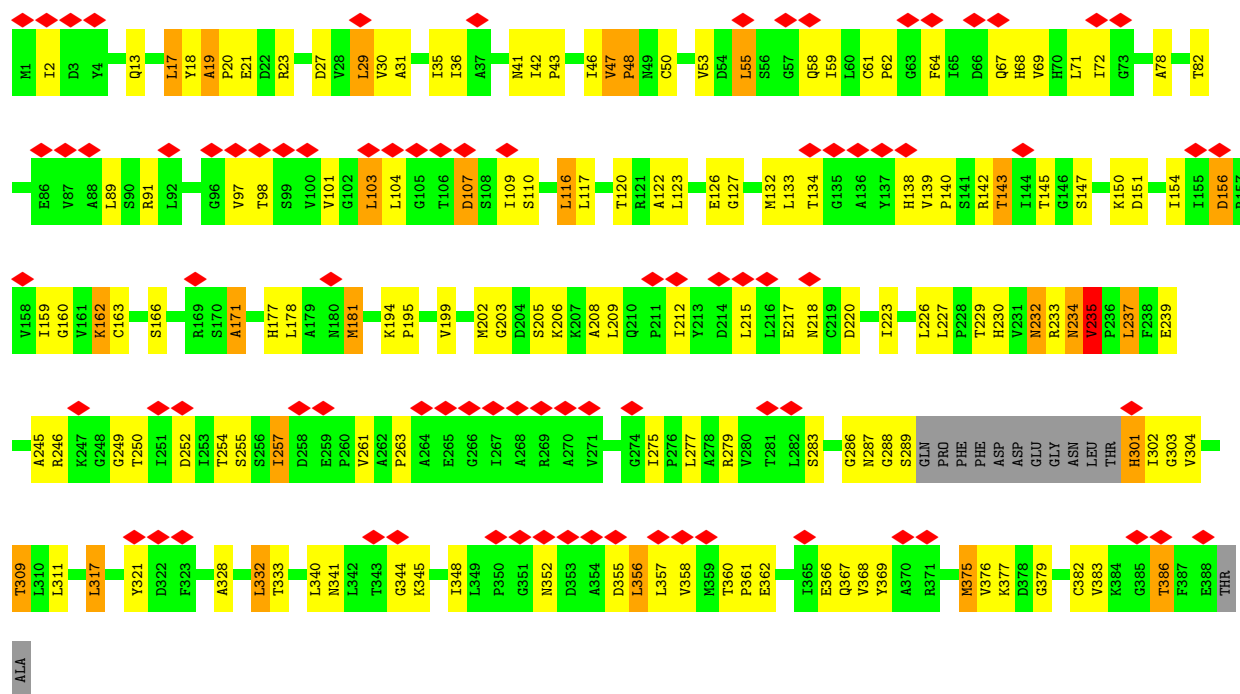
• Molecule 1: Isoaspartyl dipeptidase



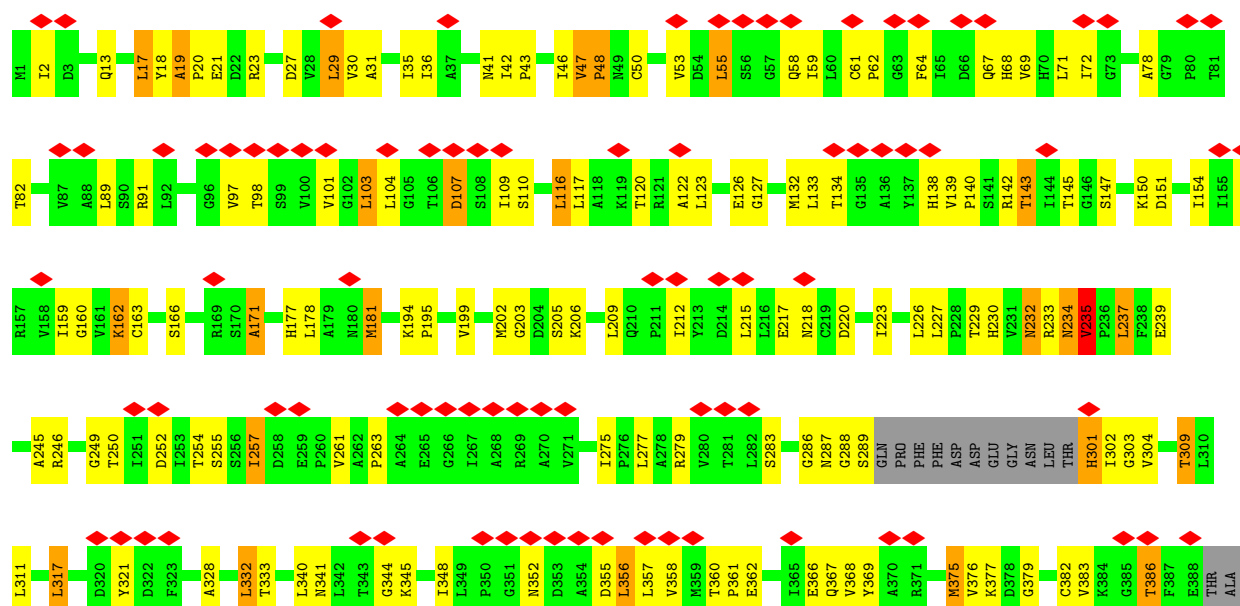




• Molecule 1: Isoaspartyl dipeptidase



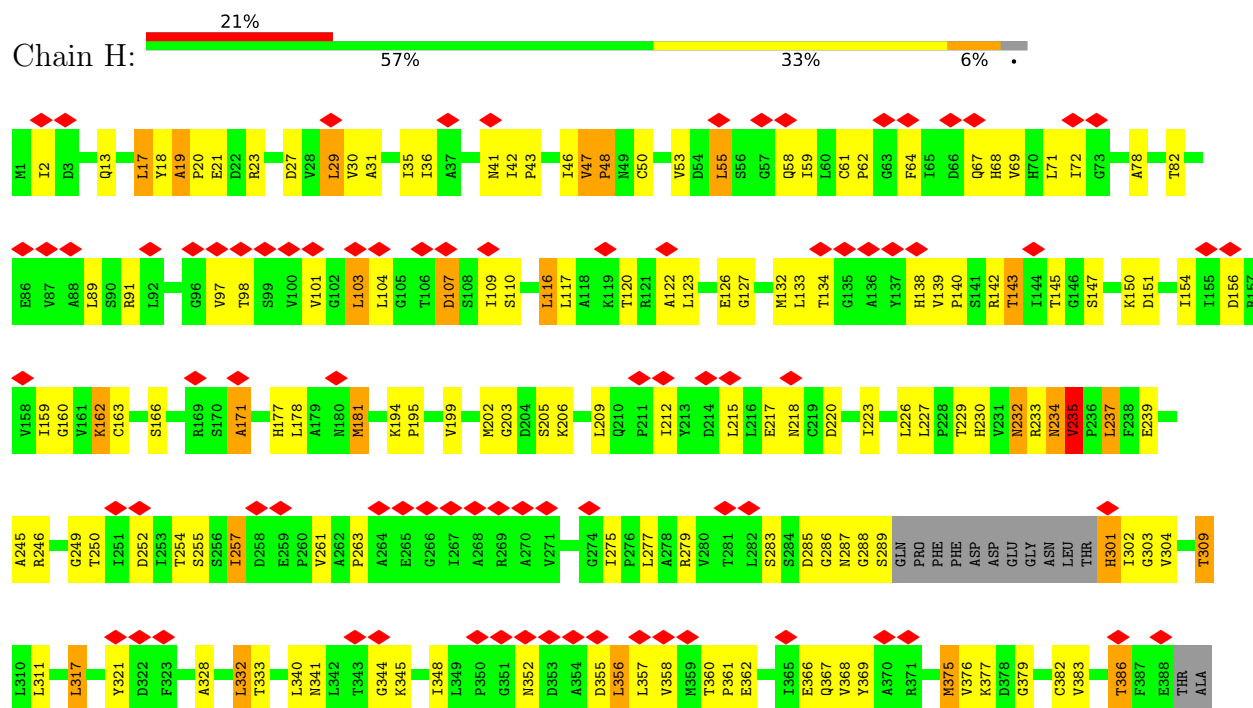
• Molecule 1: Isoaspartyl dipeptidase



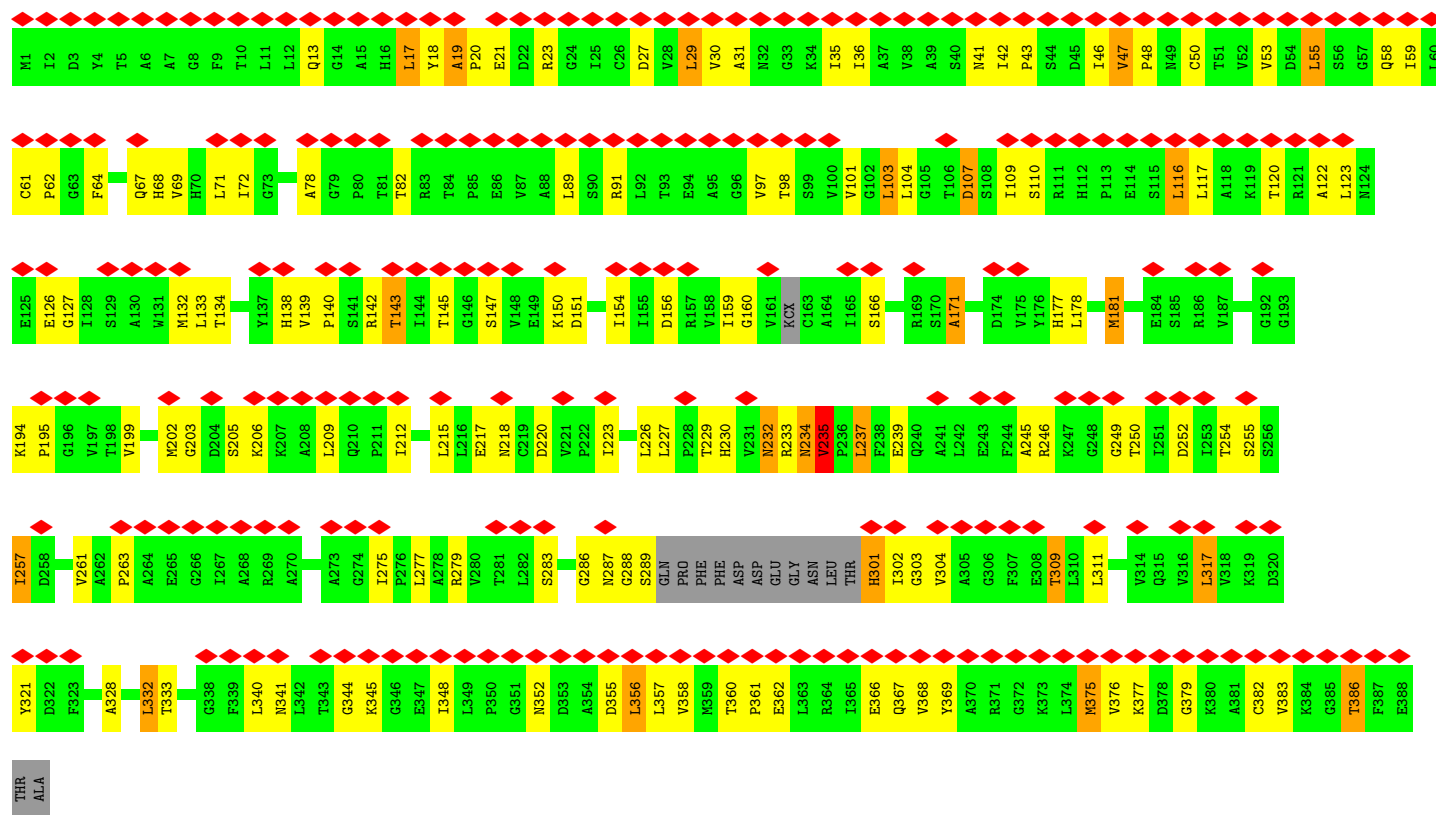
Chain G:



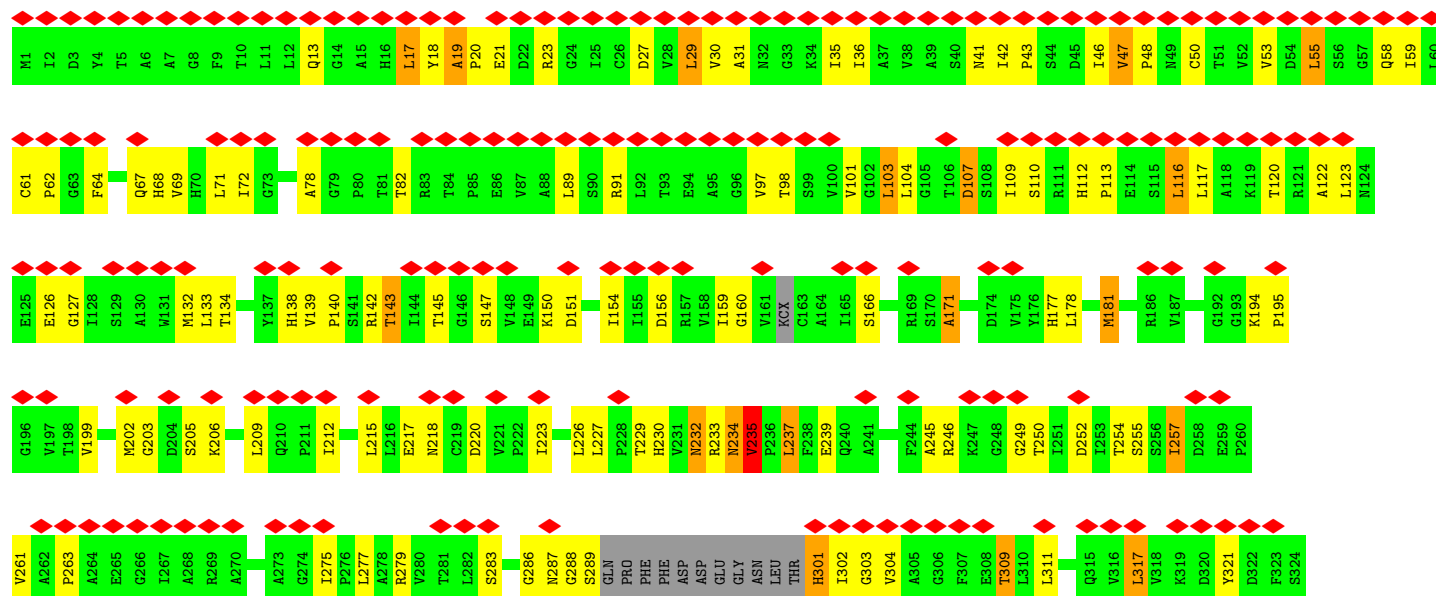
Chain H:



- Molecule 1: Isoaspartyl dipeptidase

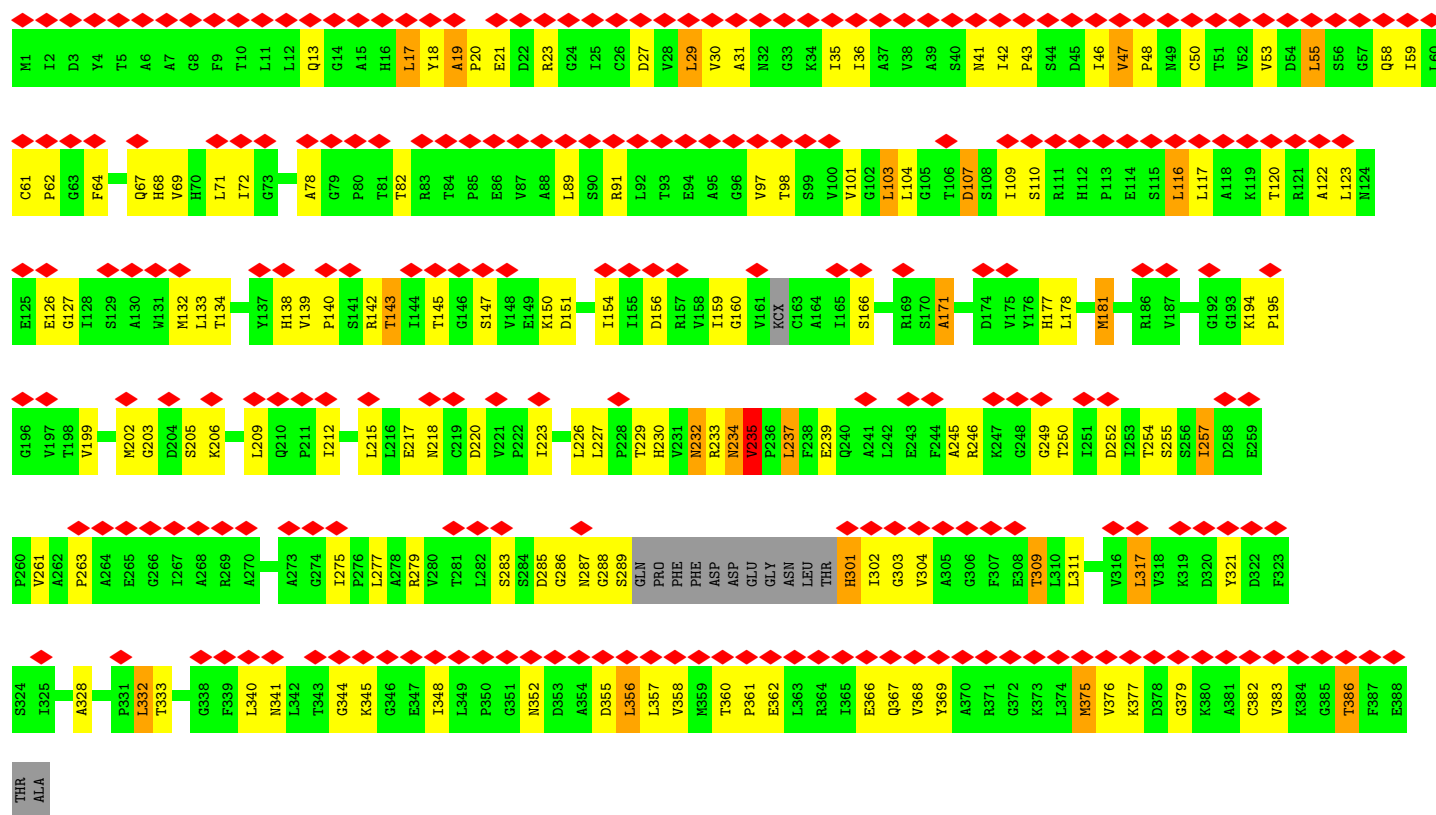


• Molecule 1: Isoaspartyl dipeptidase

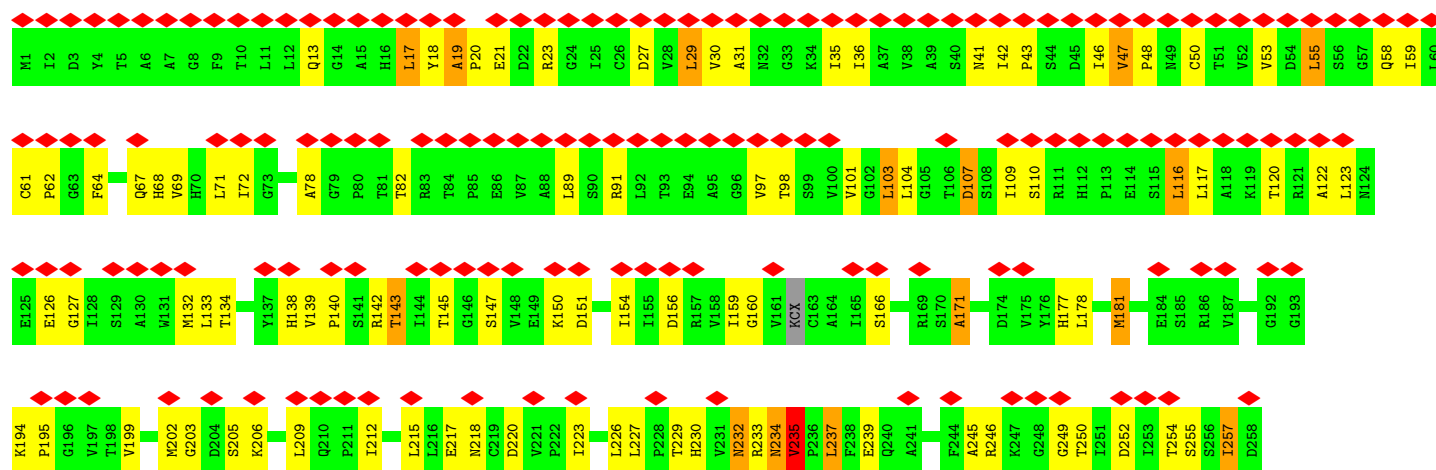


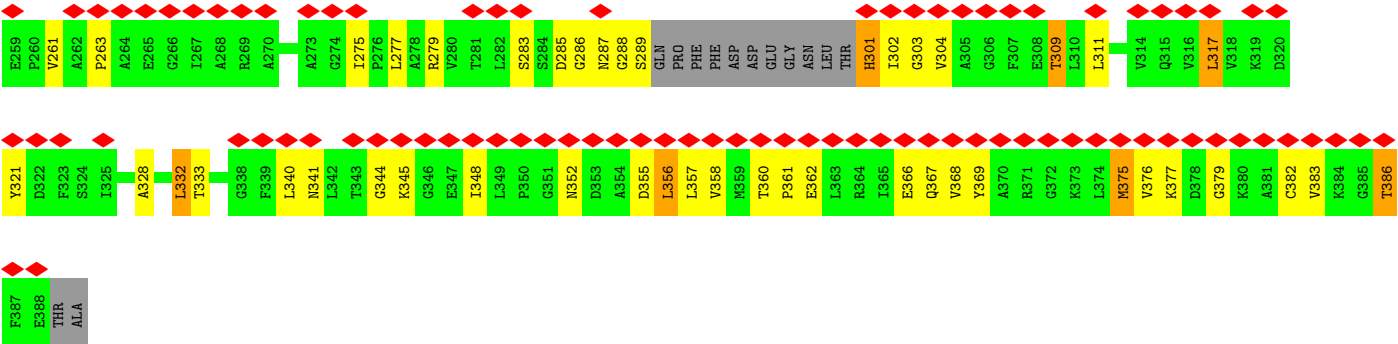


• Molecule 1: Isoaspartyl dipeptidase



• Molecule 1: Isoaspartyl dipeptidase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	17277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0338	Depositor
Map size (Å)	270.08, 270.08, 270.08	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.11, 2.11, 2.11	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX

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	0.47	0/2811	1.06	22/3825 (0.6%)
1	B	0.44	0/2788	1.00	18/3794 (0.5%)
1	C	0.44	0/2788	1.00	17/3794 (0.4%)
1	D	0.45	0/2788	1.00	17/3794 (0.4%)
1	E	0.44	0/2788	1.00	18/3794 (0.5%)
1	F	0.47	0/2811	1.06	21/3825 (0.5%)
1	G	0.47	0/2811	1.06	21/3825 (0.5%)
1	H	0.47	0/2811	1.06	22/3825 (0.6%)
1	I	0.47	0/2811	1.06	21/3825 (0.5%)
1	J	0.47	0/2811	1.06	21/3825 (0.5%)
1	K	0.47	0/2811	1.06	22/3825 (0.6%)
1	L	0.47	0/2811	1.06	22/3825 (0.6%)
All	All	0.46	0/33640	1.04	242/45776 (0.5%)

There are no bond length outliers.

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	321	TYR	N-CA-C	-9.19	95.44	109.41
1	F	321	TYR	N-CA-C	-9.17	95.47	109.41
1	G	321	TYR	N-CA-C	-9.17	95.48	109.41
1	L	321	TYR	N-CA-C	-9.14	95.52	109.41
1	A	321	TYR	N-CA-C	-9.13	95.53	109.41
1	H	321	TYR	N-CA-C	-9.12	95.54	109.41
1	K	321	TYR	N-CA-C	-9.12	95.55	109.41
1	I	321	TYR	N-CA-C	-9.11	95.57	109.41
1	H	23	ARG	N-CA-C	-7.25	97.48	109.80
1	G	23	ARG	N-CA-C	-7.25	97.48	109.80
1	K	23	ARG	N-CA-C	-7.24	97.49	109.80
1	L	23	ARG	N-CA-C	-7.24	97.49	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	23	ARG	N-CA-C	-7.23	97.51	109.80
1	B	154	ILE	N-CA-C	7.23	122.11	113.22
1	F	23	ARG	N-CA-C	-7.23	97.52	109.80
1	E	154	ILE	N-CA-C	7.22	122.10	113.22
1	A	23	ARG	N-CA-C	-7.22	97.53	109.80
1	D	154	ILE	N-CA-C	7.21	122.09	113.22
1	C	154	ILE	N-CA-C	7.21	122.09	113.22
1	J	23	ARG	N-CA-C	-7.20	97.55	109.80
1	F	379	GLY	N-CA-C	-7.05	105.59	115.32
1	L	379	GLY	N-CA-C	-7.05	105.59	115.32
1	J	154	ILE	N-CA-C	7.04	121.88	113.22
1	A	154	ILE	N-CA-C	7.04	121.88	113.22
1	G	379	GLY	N-CA-C	-7.04	105.61	115.32
1	J	379	GLY	N-CA-C	-7.04	105.60	115.32
1	K	379	GLY	N-CA-C	-7.04	105.60	115.32
1	H	379	GLY	N-CA-C	-7.04	105.61	115.32
1	F	154	ILE	N-CA-C	7.03	121.87	113.22
1	I	154	ILE	N-CA-C	7.03	121.86	113.22
1	I	379	GLY	N-CA-C	-7.03	105.62	115.32
1	A	379	GLY	N-CA-C	-7.02	105.63	115.32
1	H	154	ILE	N-CA-C	7.01	121.85	113.22
1	G	154	ILE	N-CA-C	6.99	121.81	113.22
1	K	154	ILE	N-CA-C	6.96	121.78	113.22
1	L	154	ILE	N-CA-C	6.96	121.78	113.22
1	I	142	ARG	N-CA-C	-6.80	98.85	109.25
1	G	142	ARG	N-CA-C	-6.77	98.89	109.25
1	A	142	ARG	N-CA-C	-6.77	98.89	109.25
1	F	142	ARG	N-CA-C	-6.76	98.91	109.25
1	H	142	ARG	N-CA-C	-6.75	98.92	109.25
1	J	142	ARG	N-CA-C	-6.75	98.92	109.25
1	K	142	ARG	N-CA-C	-6.74	98.93	109.25
1	L	142	ARG	N-CA-C	-6.74	98.93	109.25
1	C	23	ARG	N-CA-C	-6.61	99.56	109.94
1	B	23	ARG	N-CA-C	-6.61	99.56	109.94
1	E	19	ALA	N-CA-C	6.60	124.39	109.81
1	C	19	ALA	N-CA-C	6.59	124.37	109.81
1	B	19	ALA	N-CA-C	6.59	124.36	109.81
1	D	19	ALA	N-CA-C	6.57	124.32	109.81
1	D	23	ARG	N-CA-C	-6.54	99.67	109.94
1	E	23	ARG	N-CA-C	-6.51	99.72	109.94
1	J	127	GLY	N-CA-C	6.44	122.14	114.48
1	E	138	HIS	N-CA-C	6.43	119.61	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	GLN	N-CA-C	6.43	120.17	109.95
1	F	127	GLY	N-CA-C	6.42	122.11	114.48
1	B	13	GLN	N-CA-C	6.41	120.14	109.95
1	C	138	HIS	N-CA-C	6.41	119.57	109.96
1	E	13	GLN	N-CA-C	6.41	120.14	109.95
1	B	138	HIS	N-CA-C	6.40	119.56	109.96
1	I	127	GLY	N-CA-C	6.39	122.08	114.48
1	G	127	GLY	N-CA-C	6.38	122.08	114.48
1	H	127	GLY	N-CA-C	6.36	122.05	114.48
1	D	13	GLN	N-CA-C	6.36	120.06	109.95
1	K	127	GLY	N-CA-C	6.36	122.05	114.48
1	L	127	GLY	N-CA-C	6.36	122.05	114.48
1	A	127	GLY	N-CA-C	6.34	122.03	114.48
1	D	138	HIS	N-CA-C	6.32	119.44	109.96
1	I	109	ILE	N-CA-C	-6.25	106.84	111.90
1	A	109	ILE	N-CA-C	-6.19	106.89	111.90
1	L	109	ILE	N-CA-C	-6.18	106.89	111.90
1	D	141	SER	N-CA-C	6.16	119.39	110.28
1	H	109	ILE	N-CA-C	-6.16	106.91	111.90
1	F	109	ILE	N-CA-C	-6.16	106.91	111.90
1	J	109	ILE	N-CA-C	-6.16	106.91	111.90
1	G	109	ILE	N-CA-C	-6.14	106.92	111.90
1	K	109	ILE	N-CA-C	-6.14	106.92	111.90
1	E	109	ILE	N-CA-C	-6.12	106.98	112.12
1	J	19	ALA	N-CA-C	6.12	123.34	109.81
1	F	19	ALA	N-CA-C	6.12	123.33	109.81
1	K	19	ALA	N-CA-C	6.11	123.31	109.81
1	L	19	ALA	N-CA-C	6.11	123.31	109.81
1	G	19	ALA	N-CA-C	6.10	123.30	109.81
1	H	19	ALA	N-CA-C	6.10	123.30	109.81
1	I	19	ALA	N-CA-C	6.10	123.29	109.81
1	A	19	ALA	N-CA-C	6.09	123.28	109.81
1	E	141	SER	N-CA-C	6.09	119.29	110.28
1	D	109	ILE	N-CA-C	-6.08	107.01	112.12
1	B	141	SER	N-CA-C	6.08	119.28	110.28
1	C	141	SER	N-CA-C	6.07	119.27	110.28
1	B	109	ILE	N-CA-C	-6.05	107.04	112.12
1	C	109	ILE	N-CA-C	-6.05	107.04	112.12
1	E	156	ASP	N-CA-C	5.88	119.28	111.75
1	B	156	ASP	N-CA-C	5.88	119.27	111.75
1	C	156	ASP	N-CA-C	5.88	119.27	111.75
1	J	171	ALA	N-CA-C	-5.87	105.43	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	171	ALA	N-CA-C	-5.87	105.44	113.30
1	D	156	ASP	N-CA-C	5.86	119.25	111.75
1	H	171	ALA	N-CA-C	-5.85	105.46	113.30
1	K	171	ALA	N-CA-C	-5.85	105.46	113.30
1	I	171	ALA	N-CA-C	-5.77	105.44	112.88
1	G	171	ALA	N-CA-C	-5.76	105.45	112.88
1	L	171	ALA	N-CA-C	-5.74	105.48	112.88
1	A	171	ALA	N-CA-C	-5.73	105.49	112.88
1	F	97	VAL	N-CA-C	5.70	115.75	108.12
1	J	97	VAL	N-CA-C	5.68	115.73	108.12
1	K	97	VAL	N-CA-C	5.67	115.72	108.12
1	I	97	VAL	N-CA-C	5.67	115.71	108.12
1	A	97	VAL	N-CA-C	5.66	115.71	108.12
1	G	97	VAL	N-CA-C	5.66	115.70	108.12
1	H	97	VAL	N-CA-C	5.65	115.70	108.12
1	L	97	VAL	N-CA-C	5.64	115.68	108.12
1	E	218	ASN	N-CA-C	5.60	119.98	113.20
1	C	218	ASN	N-CA-C	5.58	119.95	113.20
1	D	218	ASN	N-CA-C	5.55	119.92	113.20
1	B	218	ASN	N-CA-C	5.54	119.90	113.20
1	G	218	ASN	N-CA-C	5.54	119.03	112.72
1	K	235	VAL	CB-CA-C	-5.54	108.44	113.70
1	L	235	VAL	CB-CA-C	-5.54	108.44	113.70
1	A	235	VAL	CB-CA-C	-5.52	108.45	113.70
1	G	235	VAL	CB-CA-C	-5.52	108.45	113.70
1	F	235	VAL	CB-CA-C	-5.51	108.46	113.70
1	I	235	VAL	CB-CA-C	-5.51	108.46	113.70
1	H	218	ASN	N-CA-C	5.51	119.00	112.72
1	H	235	VAL	CB-CA-C	-5.51	108.47	113.70
1	K	218	ASN	N-CA-C	5.50	118.98	112.72
1	L	218	ASN	N-CA-C	5.49	118.98	112.72
1	J	235	VAL	CB-CA-C	-5.48	108.49	113.70
1	A	218	ASN	N-CA-C	5.47	118.96	112.72
1	I	218	ASN	N-CA-C	5.47	118.95	112.72
1	J	143	THR	N-CA-C	5.47	117.57	109.69
1	J	218	ASN	N-CA-C	5.47	118.96	112.72
1	I	143	THR	N-CA-C	5.47	117.56	109.69
1	G	143	THR	N-CA-C	5.46	117.56	109.69
1	H	143	THR	N-CA-C	5.46	117.56	109.69
1	K	143	THR	N-CA-C	5.46	117.56	109.69
1	L	143	THR	N-CA-C	5.46	117.56	109.69
1	F	218	ASN	N-CA-C	5.46	118.95	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	THR	N-CA-C	5.46	117.55	109.69
1	F	143	THR	N-CA-C	5.44	117.53	109.69
1	F	286	GLY	N-CA-C	5.42	118.17	111.93
1	J	286	GLY	N-CA-C	5.39	118.13	111.93
1	G	286	GLY	N-CA-C	5.38	118.11	111.93
1	K	286	GLY	N-CA-C	5.37	118.11	111.93
1	L	286	GLY	N-CA-C	5.37	118.11	111.93
1	H	286	GLY	N-CA-C	5.36	118.10	111.93
1	C	387	PHE	N-CA-C	5.35	117.73	110.88
1	H	41	ASN	N-CA-C	5.35	117.17	110.91
1	F	386	THR	N-CA-C	5.34	119.28	112.34
1	E	285	ASP	N-CA-C	-5.34	105.41	112.24
1	B	387	PHE	N-CA-C	5.33	117.70	110.88
1	D	387	PHE	N-CA-C	5.33	117.70	110.88
1	K	386	THR	N-CA-C	5.33	119.27	112.34
1	E	387	PHE	N-CA-C	5.32	117.69	110.88
1	J	386	THR	N-CA-C	5.32	119.26	112.34
1	A	386	THR	N-CA-C	5.32	119.25	112.34
1	L	386	THR	N-CA-C	5.32	119.25	112.34
1	K	41	ASN	N-CA-C	5.31	117.12	110.91
1	L	41	ASN	N-CA-C	5.31	117.12	110.91
1	B	285	ASP	N-CA-C	-5.30	105.46	112.24
1	C	285	ASP	N-CA-C	-5.30	105.46	112.24
1	D	285	ASP	N-CA-C	-5.29	105.47	112.24
1	H	107	ASP	N-CA-C	5.29	116.87	108.67
1	G	41	ASN	N-CA-C	5.29	117.10	110.91
1	I	386	THR	N-CA-C	5.29	119.21	112.34
1	G	386	THR	N-CA-C	5.28	119.21	112.34
1	K	107	ASP	N-CA-C	5.28	116.86	108.67
1	I	286	GLY	N-CA-C	5.28	118.00	111.93
1	H	386	THR	N-CA-C	5.27	119.20	112.34
1	L	107	ASP	N-CA-C	5.27	116.84	108.67
1	A	286	GLY	N-CA-C	5.27	117.99	111.93
1	A	107	ASP	N-CA-C	5.26	116.83	108.67
1	E	171	ALA	N-CA-C	-5.26	106.10	112.88
1	G	107	ASP	N-CA-C	5.26	116.82	108.67
1	B	171	ALA	N-CA-C	-5.25	106.10	112.88
1	C	171	ALA	N-CA-C	-5.25	106.10	112.88
1	I	107	ASP	N-CA-C	5.25	116.81	108.67
1	F	107	ASP	N-CA-C	5.25	116.81	108.67
1	D	171	ALA	N-CA-C	-5.24	106.12	112.88
1	J	107	ASP	N-CA-C	5.23	116.78	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASN	N-CA-C	5.23	117.03	110.91
1	D	67	GLN	N-CA-C	5.23	118.48	112.57
1	F	41	ASN	N-CA-C	5.23	117.03	110.91
1	I	41	ASN	N-CA-C	5.21	117.01	110.91
1	J	41	ASN	N-CA-C	5.19	116.98	110.91
1	F	47	VAL	CA-C-N	5.18	126.32	119.84
1	F	47	VAL	C-N-CA	5.18	126.32	119.84
1	J	47	VAL	CA-C-N	5.18	126.31	119.84
1	J	47	VAL	C-N-CA	5.18	126.31	119.84
1	B	67	GLN	N-CA-C	5.17	118.41	112.57
1	C	67	GLN	N-CA-C	5.17	118.41	112.57
1	J	13	GLN	N-CA-C	5.17	117.66	109.50
1	E	17	LEU	N-CA-C	5.16	117.17	109.59
1	D	17	LEU	N-CA-C	5.16	117.17	109.59
1	B	145	THR	CA-C-N	-5.15	117.84	123.30
1	B	145	THR	C-N-CA	-5.15	117.84	123.30
1	C	145	THR	CA-C-N	-5.15	117.84	123.30
1	C	145	THR	C-N-CA	-5.15	117.84	123.30
1	C	17	LEU	N-CA-C	5.15	117.16	109.59
1	F	13	GLN	N-CA-C	5.14	117.63	109.50
1	B	17	LEU	N-CA-C	5.14	117.15	109.59
1	I	13	GLN	N-CA-C	5.14	117.62	109.50
1	K	13	GLN	N-CA-C	5.14	117.62	109.50
1	E	67	GLN	N-CA-C	5.14	118.38	112.57
1	G	13	GLN	N-CA-C	5.13	117.61	109.50
1	H	13	GLN	N-CA-C	5.13	117.61	109.50
1	E	145	THR	CA-C-N	-5.13	117.86	123.30
1	E	145	THR	C-N-CA	-5.13	117.86	123.30
1	A	13	GLN	N-CA-C	5.12	117.59	109.50
1	L	235	VAL	N-CA-C	5.12	119.07	112.67
1	J	235	VAL	N-CA-C	5.12	119.07	112.67
1	L	13	GLN	N-CA-C	5.12	117.58	109.50
1	G	235	VAL	N-CA-C	5.11	119.06	112.67
1	K	47	VAL	CA-C-N	5.11	126.22	119.84
1	K	47	VAL	C-N-CA	5.11	126.22	119.84
1	K	235	VAL	N-CA-C	5.10	119.05	112.67
1	F	235	VAL	N-CA-C	5.10	119.05	112.67
1	B	360	THR	N-CA-C	-5.09	104.27	110.13
1	L	47	VAL	CA-C-N	5.09	126.21	119.84
1	L	47	VAL	C-N-CA	5.09	126.21	119.84
1	A	47	VAL	CA-C-N	5.09	126.21	119.84
1	A	47	VAL	C-N-CA	5.09	126.21	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	THR	N-CA-C	-5.09	104.28	110.13
1	H	47	VAL	CA-C-N	5.09	126.20	119.84
1	H	47	VAL	C-N-CA	5.09	126.20	119.84
1	A	235	VAL	N-CA-C	5.08	119.02	112.67
1	H	235	VAL	N-CA-C	5.08	119.02	112.67
1	G	47	VAL	CA-C-N	5.08	126.19	119.84
1	G	47	VAL	C-N-CA	5.08	126.19	119.84
1	I	235	VAL	N-CA-C	5.08	119.02	112.67
1	I	47	VAL	CA-C-N	5.07	126.18	119.84
1	I	47	VAL	C-N-CA	5.07	126.18	119.84
1	E	360	THR	N-CA-C	-5.05	104.32	110.13
1	D	145	THR	CA-C-N	-5.05	117.95	123.30
1	D	145	THR	C-N-CA	-5.05	117.95	123.30
1	D	360	THR	N-CA-C	-5.03	104.35	110.13
1	H	285	ASP	N-CA-C	-5.02	104.97	111.74
1	K	285	ASP	N-CA-C	-5.02	104.96	111.74
1	E	356	LEU	N-CA-C	5.02	117.30	109.52
1	B	356	LEU	N-CA-C	5.01	117.29	109.52
1	L	285	ASP	N-CA-C	-5.01	104.98	111.74
1	A	156	ASP	N-CA-C	5.00	119.63	111.37

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	2778	0	2800	107	0
1	B	2756	0	2779	96	0
1	C	2756	0	2779	90	0
1	D	2756	0	2779	93	0
1	E	2756	0	2779	98	0
1	F	2778	0	2800	104	0
1	G	2778	0	2800	102	0
1	H	2778	0	2800	105	0
1	I	2766	0	2789	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2766	0	2789	103	0
1	K	2766	0	2789	101	0
1	L	2766	0	2789	101	0
All	All	33200	0	33472	1160	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 17.

All (1160) 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:D:234:ASN:HD22	1:D:236:PRO:HD2	1.35	0.91
1:E:234:ASN:HD22	1:E:236:PRO:HD2	1.35	0.91
1:C:234:ASN:HD22	1:C:236:PRO:HD2	1.35	0.90
1:C:235:VAL:HG13	1:C:236:PRO:HD3	1.53	0.90
1:B:235:VAL:HG13	1:B:236:PRO:HD3	1.52	0.90
1:B:234:ASN:HD22	1:B:236:PRO:HD2	1.35	0.90
1:A:232:ASN:H	1:A:232:ASN:HD22	1.19	0.89
1:L:232:ASN:HD22	1:L:232:ASN:H	1.19	0.89
1:D:235:VAL:HG13	1:D:236:PRO:HD3	1.52	0.89
1:E:235:VAL:HG13	1:E:236:PRO:HD3	1.52	0.88
1:I:232:ASN:HD22	1:I:232:ASN:H	1.19	0.88
1:H:232:ASN:H	1:H:232:ASN:HD22	1.19	0.88
1:G:232:ASN:HD22	1:G:232:ASN:H	1.19	0.86
1:J:232:ASN:HD22	1:J:232:ASN:H	1.19	0.86
1:F:232:ASN:H	1:F:232:ASN:HD22	1.19	0.86
1:K:232:ASN:H	1:K:232:ASN:HD22	1.19	0.86
1:C:232:ASN:H	1:C:232:ASN:HD22	1.29	0.80
1:E:232:ASN:HD22	1:E:232:ASN:H	1.29	0.80
1:B:232:ASN:HD22	1:B:232:ASN:H	1.29	0.78
1:D:232:ASN:HD22	1:D:232:ASN:H	1.29	0.78
1:G:375:MET:HE3	1:G:383:VAL:HG11	1.67	0.76
1:K:375:MET:HE3	1:K:383:VAL:HG11	1.67	0.76
1:F:78:ALA:HB3	1:F:82:THR:HG21	1.68	0.76
1:I:375:MET:HE3	1:I:383:VAL:HG11	1.67	0.76
1:J:78:ALA:HB3	1:J:82:THR:HG21	1.68	0.76
1:A:78:ALA:HB3	1:A:82:THR:HG21	1.68	0.76
1:F:375:MET:HE3	1:F:383:VAL:HG11	1.67	0.76
1:G:62:PRO:HG2	1:G:333:THR:HG21	1.68	0.76
1:I:62:PRO:HG2	1:I:333:THR:HG21	1.68	0.76
1:I:78:ALA:HB3	1:I:82:THR:HG21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ILE:HB	1:G:195:PRO:HD2	1.69	0.75
1:K:62:PRO:HG2	1:K:333:THR:HG21	1.68	0.75
1:J:159:ILE:HB	1:J:195:PRO:HD2	1.69	0.75
1:K:159:ILE:HB	1:K:195:PRO:HD2	1.69	0.75
1:K:78:ALA:HB3	1:K:82:THR:HG21	1.68	0.75
1:L:78:ALA:HB3	1:L:82:THR:HG21	1.68	0.75
1:A:62:PRO:HG2	1:A:333:THR:HG21	1.68	0.75
1:A:375:MET:HE3	1:A:383:VAL:HG11	1.68	0.75
1:F:62:PRO:HG2	1:F:333:THR:HG21	1.68	0.75
1:F:159:ILE:HB	1:F:195:PRO:HD2	1.69	0.75
1:L:62:PRO:HG2	1:L:333:THR:HG21	1.68	0.75
1:D:123:LEU:HG	1:D:128:ILE:HD11	1.68	0.75
1:A:159:ILE:HB	1:A:195:PRO:HD2	1.69	0.75
1:H:78:ALA:HB3	1:H:82:THR:HG21	1.68	0.75
1:I:159:ILE:HB	1:I:195:PRO:HD2	1.69	0.75
1:J:375:MET:HE3	1:J:383:VAL:HG11	1.67	0.75
1:G:78:ALA:HB3	1:G:82:THR:HG21	1.68	0.74
1:H:159:ILE:HB	1:H:195:PRO:HD2	1.69	0.74
1:B:123:LEU:HG	1:B:128:ILE:HD11	1.68	0.74
1:J:62:PRO:HG2	1:J:333:THR:HG21	1.67	0.74
1:E:123:LEU:HG	1:E:128:ILE:HD11	1.68	0.74
1:L:159:ILE:HB	1:L:195:PRO:HD2	1.69	0.74
1:H:62:PRO:HG2	1:H:333:THR:HG21	1.68	0.74
1:C:123:LEU:HG	1:C:128:ILE:HD11	1.68	0.74
1:H:375:MET:HE3	1:H:383:VAL:HG11	1.67	0.74
1:L:375:MET:HE3	1:L:383:VAL:HG11	1.67	0.73
1:G:360:THR:HG22	1:G:366:GLU:OE1	1.89	0.73
1:K:360:THR:HG22	1:K:366:GLU:OE1	1.89	0.73
1:C:78:ALA:HB3	1:C:82:THR:HG21	1.71	0.73
1:F:360:THR:HG22	1:F:366:GLU:OE1	1.89	0.73
1:I:360:THR:HG22	1:I:366:GLU:OE1	1.89	0.73
1:J:360:THR:HG22	1:J:366:GLU:OE1	1.89	0.73
1:L:360:THR:HG22	1:L:366:GLU:OE1	1.89	0.73
1:A:360:THR:HG22	1:A:366:GLU:OE1	1.89	0.72
1:H:360:THR:HG22	1:H:366:GLU:OE1	1.89	0.72
1:E:63:GLY:HA2	1:E:357:LEU:HG	1.72	0.72
1:D:63:GLY:HA2	1:D:357:LEU:HG	1.72	0.72
1:E:78:ALA:HB3	1:E:82:THR:HG21	1.71	0.72
1:J:232:ASN:HD22	1:J:232:ASN:N	1.87	0.71
1:J:246:ARG:HG2	1:J:275:ILE:HD11	1.72	0.71
1:B:63:GLY:HA2	1:B:357:LEU:HG	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ALA:HB3	1:B:82:THR:HG21	1.71	0.71
1:C:63:GLY:HA2	1:C:357:LEU:HG	1.72	0.71
1:K:232:ASN:HD22	1:K:232:ASN:N	1.87	0.71
1:A:202:MET:HE2	1:A:209:LEU:HD23	1.73	0.71
1:D:235:VAL:HG22	1:L:246:ARG:NH2	2.05	0.71
1:F:246:ARG:HG2	1:F:275:ILE:HD11	1.72	0.71
1:B:235:VAL:HG22	1:I:246:ARG:NH2	2.05	0.71
1:A:246:ARG:HG2	1:A:275:ILE:HD11	1.72	0.71
1:I:246:ARG:HG2	1:I:275:ILE:HD11	1.72	0.71
1:H:202:MET:HE2	1:H:209:LEU:HD23	1.73	0.70
1:J:202:MET:HE2	1:J:209:LEU:HD23	1.73	0.70
1:L:202:MET:HE2	1:L:209:LEU:HD23	1.73	0.70
1:I:202:MET:HE2	1:I:209:LEU:HD23	1.73	0.70
1:E:235:VAL:HG22	1:K:246:ARG:NH2	2.06	0.70
1:H:246:ARG:HG2	1:H:275:ILE:HD11	1.72	0.70
1:K:202:MET:HE2	1:K:209:LEU:HD23	1.73	0.70
1:D:78:ALA:HB3	1:D:82:THR:HG21	1.71	0.70
1:F:202:MET:HE2	1:F:209:LEU:HD23	1.73	0.70
1:K:246:ARG:HG2	1:K:275:ILE:HD11	1.72	0.70
1:F:232:ASN:HD22	1:F:232:ASN:N	1.87	0.70
1:G:166:SER:HB3	1:G:205:SER:HB3	1.74	0.70
1:J:29:LEU:HD13	1:J:36:ILE:HD11	1.74	0.70
1:K:166:SER:HB3	1:K:205:SER:HB3	1.74	0.70
1:C:235:VAL:HG22	1:J:246:ARG:NH2	2.06	0.70
1:K:29:LEU:HD13	1:K:36:ILE:HD11	1.74	0.70
1:G:202:MET:HE2	1:G:209:LEU:HD23	1.73	0.70
1:G:246:ARG:HG2	1:G:275:ILE:HD11	1.72	0.69
1:L:246:ARG:HG2	1:L:275:ILE:HD11	1.72	0.69
1:F:29:LEU:HD13	1:F:36:ILE:HD11	1.74	0.69
1:G:29:LEU:HD13	1:G:36:ILE:HD11	1.74	0.69
1:I:166:SER:HB3	1:I:205:SER:HB3	1.74	0.69
1:G:232:ASN:HD22	1:G:232:ASN:N	1.87	0.69
1:D:17:LEU:HD23	1:D:60:LEU:HD23	1.74	0.69
1:L:232:ASN:HD22	1:L:232:ASN:N	1.87	0.69
1:F:166:SER:HB3	1:F:205:SER:HB3	1.74	0.69
1:H:29:LEU:HD13	1:H:36:ILE:HD11	1.74	0.69
1:A:166:SER:HB3	1:A:205:SER:HB3	1.74	0.68
1:C:17:LEU:HD23	1:C:60:LEU:HD23	1.74	0.68
1:E:62:PRO:HG2	1:E:333:THR:HG21	1.75	0.68
1:A:233:ARG:HA	1:A:257:ILE:CD1	2.24	0.68
1:H:232:ASN:HD22	1:H:232:ASN:N	1.87	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:233:ARG:HA	1:I:257:ILE:CD1	2.24	0.68
1:L:166:SER:HB3	1:L:205:SER:HB3	1.74	0.68
1:E:17:LEU:HD23	1:E:60:LEU:HD23	1.74	0.68
1:A:29:LEU:HD13	1:A:36:ILE:HD11	1.74	0.68
1:H:233:ARG:HA	1:H:257:ILE:CD1	2.24	0.68
1:L:233:ARG:HA	1:L:257:ILE:CD1	2.24	0.68
1:C:62:PRO:HG2	1:C:333:THR:HG21	1.75	0.68
1:D:62:PRO:HG2	1:D:333:THR:HG21	1.75	0.68
1:J:166:SER:HB3	1:J:205:SER:HB3	1.74	0.68
1:I:29:LEU:HD13	1:I:36:ILE:HD11	1.74	0.68
1:L:29:LEU:HD13	1:L:36:ILE:HD11	1.74	0.68
1:B:17:LEU:HD23	1:B:60:LEU:HD23	1.74	0.68
1:G:233:ARG:HA	1:G:257:ILE:CD1	2.24	0.67
1:H:166:SER:HB3	1:H:205:SER:HB3	1.74	0.67
1:J:233:ARG:HA	1:J:257:ILE:CD1	2.24	0.67
1:K:233:ARG:HA	1:K:257:ILE:CD1	2.24	0.67
1:F:233:ARG:HA	1:F:257:ILE:CD1	2.24	0.67
1:B:62:PRO:HG2	1:B:333:THR:HG21	1.75	0.67
1:B:61:CYS:HB2	1:B:62:PRO:HD2	1.78	0.66
1:E:61:CYS:HB2	1:E:62:PRO:HD2	1.78	0.66
1:I:232:ASN:HD22	1:I:232:ASN:N	1.87	0.66
1:C:229:THR:HG23	1:C:252:ASP:OD1	1.96	0.66
1:E:229:THR:HG23	1:E:252:ASP:OD1	1.96	0.66
1:D:61:CYS:HB2	1:D:62:PRO:HD2	1.78	0.66
1:C:61:CYS:HB2	1:C:62:PRO:HD2	1.78	0.66
1:H:17:LEU:HD23	1:H:18:TYR:N	2.12	0.65
1:B:229:THR:HG23	1:B:252:ASP:OD1	1.96	0.65
1:A:17:LEU:HD23	1:A:18:TYR:N	2.12	0.65
1:F:17:LEU:HD23	1:F:18:TYR:N	2.12	0.65
1:H:68:HIS:HD1	1:H:229:THR:HG21	1.62	0.65
1:K:17:LEU:HD23	1:K:18:TYR:N	2.12	0.65
1:F:68:HIS:HA	1:F:103:LEU:HD11	1.80	0.64
1:I:17:LEU:HD23	1:I:18:TYR:N	2.12	0.64
1:L:17:LEU:HD23	1:L:18:TYR:N	2.12	0.64
1:G:17:LEU:HD23	1:G:18:TYR:N	2.12	0.64
1:K:68:HIS:HA	1:K:103:LEU:HD11	1.80	0.64
1:A:68:HIS:HD1	1:A:229:THR:HG21	1.62	0.64
1:F:68:HIS:HD1	1:F:229:THR:HG21	1.62	0.64
1:H:68:HIS:HA	1:H:103:LEU:HD11	1.80	0.64
1:J:68:HIS:HA	1:J:103:LEU:HD11	1.80	0.64
1:L:68:HIS:HA	1:L:103:LEU:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:THR:HG23	1:D:252:ASP:OD1	1.96	0.64
1:J:17:LEU:HD23	1:J:18:TYR:N	2.12	0.64
1:L:232:ASN:H	1:L:232:ASN:ND2	1.94	0.64
1:A:68:HIS:HA	1:A:103:LEU:HD11	1.80	0.63
1:G:68:HIS:HA	1:G:103:LEU:HD11	1.80	0.63
1:B:162:KCX:HD2	1:B:163:CYS:N	2.13	0.63
1:H:232:ASN:H	1:H:232:ASN:ND2	1.94	0.63
1:I:68:HIS:HA	1:I:103:LEU:HD11	1.80	0.63
1:A:232:ASN:HD22	1:A:232:ASN:N	1.87	0.63
1:E:162:KCX:HD2	1:E:163:CYS:N	2.14	0.63
1:G:43:PRO:HG2	1:G:46:ILE:HB	1.80	0.63
1:J:43:PRO:HG2	1:J:46:ILE:HB	1.80	0.63
1:K:206:LYS:NZ	1:K:206:LYS:HB3	2.14	0.63
1:C:162:KCX:HD2	1:C:163:CYS:N	2.13	0.63
1:G:68:HIS:HD1	1:G:229:THR:HG21	1.62	0.63
1:H:43:PRO:HG2	1:H:46:ILE:HB	1.80	0.63
1:I:206:LYS:NZ	1:I:206:LYS:HB3	2.14	0.62
1:J:206:LYS:NZ	1:J:206:LYS:HB3	2.14	0.62
1:G:206:LYS:HB3	1:G:206:LYS:NZ	2.14	0.62
1:A:206:LYS:NZ	1:A:206:LYS:HB3	2.14	0.62
1:F:43:PRO:HG2	1:F:46:ILE:HB	1.80	0.62
1:F:206:LYS:NZ	1:F:206:LYS:HB3	2.14	0.62
1:I:43:PRO:HG2	1:I:46:ILE:HB	1.80	0.62
1:J:229:THR:HG23	1:J:252:ASP:OD1	2.00	0.62
1:A:43:PRO:HG2	1:A:46:ILE:HB	1.80	0.62
1:H:206:LYS:NZ	1:H:206:LYS:HB3	2.14	0.62
1:K:43:PRO:HG2	1:K:46:ILE:HB	1.80	0.62
1:L:206:LYS:NZ	1:L:206:LYS:HB3	2.14	0.62
1:F:229:THR:HG23	1:F:252:ASP:OD1	2.00	0.62
1:L:43:PRO:HG2	1:L:46:ILE:HB	1.80	0.62
1:L:229:THR:HG23	1:L:252:ASP:OD1	2.00	0.62
1:D:162:KCX:HD2	1:D:163:CYS:N	2.13	0.62
1:G:229:THR:HG23	1:G:252:ASP:OD1	2.00	0.61
1:A:229:THR:HG23	1:A:252:ASP:OD1	2.00	0.61
1:B:35:ILE:O	1:B:350:PRO:HA	2.01	0.61
1:D:35:ILE:O	1:D:350:PRO:HA	2.01	0.61
1:I:138:HIS:HA	1:I:171:ALA:HB2	1.82	0.61
1:E:35:ILE:O	1:E:350:PRO:HA	2.01	0.61
1:E:232:ASN:H	1:E:232:ASN:ND2	1.98	0.61
1:K:229:THR:HG23	1:K:252:ASP:OD1	2.00	0.61
1:C:35:ILE:O	1:C:350:PRO:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LEU:HB2	1:D:339:PHE:CZ	2.36	0.61
1:A:229:THR:HG22	1:A:230:HIS:N	2.16	0.61
1:E:227:LEU:HB2	1:E:339:PHE:CZ	2.36	0.61
1:L:229:THR:HG22	1:L:230:HIS:N	2.16	0.61
1:H:229:THR:HG23	1:H:252:ASP:OD1	2.00	0.61
1:B:227:LEU:HB2	1:B:339:PHE:CZ	2.36	0.61
1:A:138:HIS:HA	1:A:171:ALA:HB2	1.82	0.60
1:G:17:LEU:HD23	1:G:18:TYR:H	1.66	0.60
1:C:227:LEU:HB2	1:C:339:PHE:CZ	2.36	0.60
1:A:17:LEU:HD23	1:A:18:TYR:H	1.66	0.60
1:I:229:THR:HG23	1:I:252:ASP:OD1	2.00	0.60
1:L:17:LEU:HD23	1:L:18:TYR:H	1.66	0.60
1:K:17:LEU:HD23	1:K:18:TYR:H	1.66	0.60
1:F:229:THR:HG22	1:F:230:HIS:N	2.16	0.60
1:J:138:HIS:HA	1:J:171:ALA:HB2	1.82	0.60
1:K:229:THR:HG22	1:K:230:HIS:N	2.16	0.60
1:G:229:THR:HG22	1:G:230:HIS:N	2.16	0.60
1:H:17:LEU:HD23	1:H:18:TYR:H	1.66	0.60
1:I:17:LEU:HD23	1:I:18:TYR:H	1.66	0.60
1:I:67:GLN:HA	1:I:101:VAL:HB	1.84	0.60
1:C:232:ASN:H	1:C:232:ASN:ND2	1.98	0.60
1:F:138:HIS:HA	1:F:171:ALA:HB2	1.82	0.60
1:G:138:HIS:HA	1:G:171:ALA:HB2	1.82	0.60
1:H:138:HIS:HA	1:H:171:ALA:HB2	1.82	0.60
1:A:67:GLN:HA	1:A:101:VAL:HB	1.84	0.60
1:B:4:TYR:HB2	1:B:49:ASN:HD22	1.67	0.60
1:L:67:GLN:HA	1:L:101:VAL:HB	1.84	0.60
1:L:138:HIS:HA	1:L:171:ALA:HB2	1.82	0.60
1:D:282:LEU:HD23	1:D:332:LEU:HD13	1.84	0.59
1:E:4:TYR:HB2	1:E:49:ASN:HD22	1.67	0.59
1:I:232:ASN:H	1:I:232:ASN:ND2	1.94	0.59
1:C:282:LEU:HD23	1:C:332:LEU:HD13	1.84	0.59
1:F:67:GLN:HA	1:F:101:VAL:HB	1.83	0.59
1:A:232:ASN:H	1:A:232:ASN:ND2	1.94	0.59
1:I:229:THR:HG22	1:I:230:HIS:N	2.16	0.59
1:A:233:ARG:HA	1:A:257:ILE:HD11	1.85	0.59
1:G:67:GLN:HA	1:G:101:VAL:HB	1.83	0.59
1:H:229:THR:HG22	1:H:230:HIS:N	2.16	0.59
1:K:138:HIS:HA	1:K:171:ALA:HB2	1.82	0.59
1:C:199:VAL:HG22	1:C:227:LEU:HD23	1.84	0.59
1:J:17:LEU:HD23	1:J:18:TYR:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:GLN:HA	1:J:101:VAL:HB	1.83	0.59
1:K:288:GLY:O	1:K:289:SER:HB2	2.02	0.59
1:G:288:GLY:O	1:G:289:SER:HB2	2.02	0.59
1:H:67:GLN:HA	1:H:101:VAL:HB	1.83	0.59
1:J:229:THR:HG22	1:J:230:HIS:N	2.16	0.59
1:J:288:GLY:O	1:J:289:SER:HB2	2.02	0.59
1:D:232:ASN:H	1:D:232:ASN:ND2	1.98	0.59
1:B:199:VAL:HG22	1:B:227:LEU:HD23	1.84	0.59
1:D:199:VAL:HG22	1:D:227:LEU:HD23	1.84	0.59
1:B:271:VAL:HG21	1:B:323:PHE:CE1	2.38	0.59
1:C:4:TYR:HB2	1:C:49:ASN:HD22	1.67	0.59
1:F:288:GLY:O	1:F:289:SER:HB2	2.02	0.59
1:H:233:ARG:HA	1:H:257:ILE:HD11	1.85	0.59
1:E:271:VAL:HG21	1:E:323:PHE:CE1	2.38	0.58
1:G:233:ARG:HA	1:G:257:ILE:HD11	1.85	0.58
1:K:67:GLN:HA	1:K:101:VAL:HB	1.84	0.58
1:D:4:TYR:HB2	1:D:49:ASN:HD22	1.67	0.58
1:H:288:GLY:O	1:H:289:SER:HB2	2.02	0.58
1:I:233:ARG:HA	1:I:257:ILE:HD11	1.85	0.58
1:E:199:VAL:HG22	1:E:227:LEU:HD23	1.84	0.58
1:F:17:LEU:HD23	1:F:18:TYR:H	1.66	0.58
1:L:227:LEU:HD11	1:L:252:ASP:HB2	1.86	0.58
1:B:12:LEU:HD11	1:B:356:LEU:HD13	1.86	0.58
1:B:232:ASN:H	1:B:232:ASN:ND2	1.98	0.58
1:B:282:LEU:HD23	1:B:332:LEU:HD13	1.84	0.58
1:A:227:LEU:HD11	1:A:252:ASP:HB2	1.86	0.58
1:H:227:LEU:HD11	1:H:252:ASP:HB2	1.86	0.58
1:D:12:LEU:HD11	1:D:356:LEU:HD13	1.86	0.58
1:D:271:VAL:HG21	1:D:323:PHE:CE1	2.38	0.58
1:A:288:GLY:O	1:A:289:SER:HB2	2.02	0.58
1:I:288:GLY:O	1:I:289:SER:HB2	2.02	0.58
1:C:271:VAL:HG21	1:C:323:PHE:CE1	2.38	0.58
1:L:233:ARG:HA	1:L:257:ILE:HD11	1.85	0.58
1:L:288:GLY:O	1:L:289:SER:HB2	2.02	0.58
1:E:282:LEU:HD23	1:E:332:LEU:HD13	1.84	0.57
1:I:227:LEU:HD11	1:I:252:ASP:HB2	1.86	0.57
1:J:358:VAL:HB	1:J:367:GLN:HB2	1.86	0.57
1:F:233:ARG:HA	1:F:257:ILE:HD11	1.85	0.57
1:H:358:VAL:HB	1:H:367:GLN:HB2	1.87	0.57
1:B:235:VAL:CG2	1:I:246:ARG:NH2	2.67	0.57
1:K:233:ARG:HA	1:K:257:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:358:VAL:HB	1:K:367:GLN:HB2	1.86	0.57
1:E:12:LEU:HD11	1:E:356:LEU:HD13	1.86	0.57
1:F:227:LEU:HD11	1:F:252:ASP:HB2	1.86	0.57
1:F:358:VAL:HB	1:F:367:GLN:HB2	1.86	0.57
1:J:227:LEU:HD11	1:J:252:ASP:HB2	1.86	0.57
1:D:235:VAL:CG2	1:L:246:ARG:NH2	2.68	0.57
1:E:234:ASN:ND2	1:E:237:LEU:H	2.03	0.57
1:G:227:LEU:HD11	1:G:252:ASP:HB2	1.86	0.57
1:B:235:VAL:HG22	1:I:246:ARG:HH22	1.68	0.57
1:D:212:ILE:O	1:D:216:LEU:HD13	2.05	0.57
1:D:234:ASN:ND2	1:D:237:LEU:H	2.03	0.57
1:E:235:VAL:HG22	1:K:246:ARG:HH22	1.69	0.57
1:F:47:VAL:HG23	1:F:50:CYS:HB2	1.87	0.57
1:C:12:LEU:HD11	1:C:356:LEU:HD13	1.86	0.56
1:D:229:THR:HG22	1:D:230:HIS:H	1.70	0.56
1:J:317:LEU:HD23	1:J:328:ALA:HA	1.87	0.56
1:K:227:LEU:HD11	1:K:252:ASP:HB2	1.86	0.56
1:B:234:ASN:ND2	1:B:237:LEU:H	2.03	0.56
1:A:47:VAL:HG23	1:A:50:CYS:HB2	1.87	0.56
1:A:317:LEU:HD23	1:A:328:ALA:HA	1.87	0.56
1:J:47:VAL:HG23	1:J:50:CYS:HB2	1.87	0.56
1:J:233:ARG:HA	1:J:257:ILE:HD11	1.85	0.56
1:L:317:LEU:HD23	1:L:328:ALA:HA	1.88	0.56
1:C:229:THR:HG22	1:C:230:HIS:H	1.70	0.56
1:C:234:ASN:ND2	1:C:237:LEU:H	2.03	0.56
1:D:35:ILE:HD13	1:D:348:ILE:HG23	1.88	0.56
1:D:249:GLY:O	1:D:279:ARG:HD2	2.05	0.56
1:E:46:ILE:HD11	1:F:48:PRO:HG3	1.87	0.56
1:F:317:LEU:HD23	1:F:328:ALA:HA	1.87	0.56
1:G:47:VAL:HG23	1:G:50:CYS:HB2	1.87	0.56
1:I:47:VAL:HG23	1:I:50:CYS:HB2	1.87	0.56
1:K:47:VAL:HG23	1:K:50:CYS:HB2	1.87	0.56
1:L:47:VAL:HG23	1:L:50:CYS:HB2	1.87	0.56
1:L:139:VAL:HA	1:L:140:PRO:C	2.31	0.56
1:C:212:ILE:O	1:C:216:LEU:HD13	2.05	0.56
1:G:358:VAL:HB	1:G:367:GLN:HB2	1.86	0.56
1:H:47:VAL:HG23	1:H:50:CYS:HB2	1.87	0.56
1:I:358:VAL:HB	1:I:367:GLN:HB2	1.87	0.56
1:B:205:SER:HB2	1:D:220:ASP:OD2	2.06	0.56
1:H:317:LEU:HD23	1:H:328:ALA:HA	1.88	0.56
1:D:235:VAL:HG22	1:L:246:ARG:HH22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:317:LEU:HD23	1:I:328:ALA:HA	1.87	0.56
1:B:35:ILE:HD13	1:B:348:ILE:HG23	1.88	0.56
1:C:220:ASP:OD2	1:D:205:SER:HB2	2.05	0.56
1:C:249:GLY:O	1:C:279:ARG:HD2	2.05	0.56
1:A:139:VAL:HA	1:A:140:PRO:C	2.31	0.56
1:B:220:ASP:OD2	1:E:205:SER:HB2	2.05	0.56
1:C:46:ILE:HD11	1:H:48:PRO:HG3	1.87	0.56
1:H:139:VAL:HA	1:H:140:PRO:C	2.30	0.56
1:E:229:THR:HG22	1:E:230:HIS:H	1.70	0.56
1:E:235:VAL:CG2	1:K:246:ARG:NH2	2.68	0.56
1:K:232:ASN:H	1:K:232:ASN:ND2	1.94	0.56
1:B:249:GLY:O	1:B:279:ARG:HD2	2.05	0.56
1:E:212:ILE:O	1:E:216:LEU:HD13	2.05	0.55
1:K:317:LEU:HD23	1:K:328:ALA:HA	1.88	0.55
1:G:317:LEU:HD23	1:G:328:ALA:HA	1.87	0.55
1:B:46:ILE:HD11	1:G:48:PRO:HG3	1.87	0.55
1:C:235:VAL:HG22	1:J:246:ARG:HH22	1.69	0.55
1:D:46:ILE:HD11	1:A:48:PRO:HG3	1.87	0.55
1:G:139:VAL:HA	1:G:140:PRO:C	2.31	0.55
1:I:139:VAL:HA	1:I:140:PRO:C	2.30	0.55
1:A:358:VAL:HB	1:A:367:GLN:HB2	1.87	0.55
1:G:223:ILE:HA	1:G:226:LEU:HD23	1.89	0.55
1:C:35:ILE:HD13	1:C:348:ILE:HG23	1.88	0.55
1:C:205:SER:HB2	1:E:220:ASP:OD2	2.05	0.55
1:E:143:THR:HB	1:E:151:ASP:OD1	2.06	0.55
1:J:139:VAL:HA	1:J:140:PRO:C	2.30	0.55
1:K:61:CYS:HB2	1:K:62:PRO:HD2	1.89	0.55
1:L:358:VAL:HB	1:L:367:GLN:HB2	1.86	0.55
1:B:229:THR:HG22	1:B:230:HIS:H	1.70	0.55
1:E:310:LEU:HD22	1:E:332:LEU:HD11	1.89	0.55
1:A:145:THR:OG1	1:A:150:LYS:HB3	2.07	0.55
1:F:61:CYS:HB2	1:F:62:PRO:HD2	1.89	0.55
1:K:223:ILE:HA	1:K:226:LEU:HD23	1.89	0.55
1:L:358:VAL:CG2	1:L:367:GLN:HB2	2.37	0.55
1:B:143:THR:HB	1:B:151:ASP:OD1	2.06	0.55
1:B:310:LEU:HD22	1:B:332:LEU:HD11	1.89	0.55
1:E:35:ILE:HD13	1:E:348:ILE:HG23	1.88	0.55
1:H:358:VAL:CG2	1:H:367:GLN:HB2	2.37	0.55
1:C:143:THR:HB	1:C:151:ASP:OD1	2.06	0.55
1:C:310:LEU:HD22	1:C:332:LEU:HD11	1.89	0.55
1:I:145:THR:OG1	1:I:150:LYS:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:THR:OG1	1:J:150:LYS:HB3	2.07	0.55
1:B:12:LEU:HD23	1:B:53:VAL:CG1	2.37	0.55
1:B:212:ILE:O	1:B:216:LEU:HD13	2.05	0.55
1:D:143:THR:HB	1:D:151:ASP:OD1	2.06	0.55
1:E:249:GLY:O	1:E:279:ARG:HD2	2.06	0.55
1:G:232:ASN:H	1:G:232:ASN:ND2	1.94	0.55
1:J:61:CYS:HB2	1:J:62:PRO:HD2	1.89	0.55
1:K:133:LEU:HD11	1:K:199:VAL:HG21	1.89	0.55
1:E:12:LEU:HD23	1:E:53:VAL:CG1	2.37	0.54
1:F:139:VAL:HA	1:F:140:PRO:C	2.30	0.54
1:D:12:LEU:HD23	1:D:53:VAL:CG1	2.37	0.54
1:A:358:VAL:CG2	1:A:367:GLN:HB2	2.37	0.54
1:F:145:THR:OG1	1:F:150:LYS:HB3	2.07	0.54
1:G:61:CYS:HB2	1:G:62:PRO:HD2	1.89	0.54
1:G:133:LEU:HD11	1:G:199:VAL:HG21	1.89	0.54
1:I:223:ILE:HA	1:I:226:LEU:HD23	1.89	0.54
1:A:223:ILE:HA	1:A:226:LEU:HD23	1.89	0.54
1:K:145:THR:OG1	1:K:150:LYS:HB3	2.07	0.54
1:C:235:VAL:CG2	1:J:246:ARG:NH2	2.69	0.54
1:C:65:ILE:HG12	1:C:99:SER:HB2	1.89	0.54
1:C:227:LEU:HD11	1:C:252:ASP:HB2	1.90	0.54
1:K:139:VAL:HA	1:K:140:PRO:C	2.31	0.54
1:K:358:VAL:CG2	1:K:367:GLN:HB2	2.37	0.54
1:F:133:LEU:HD11	1:F:199:VAL:HG21	1.89	0.54
1:F:223:ILE:HA	1:F:226:LEU:HD23	1.89	0.54
1:G:145:THR:OG1	1:G:150:LYS:HB3	2.07	0.54
1:J:358:VAL:CG2	1:J:367:GLN:HB2	2.37	0.54
1:C:12:LEU:HD23	1:C:53:VAL:HG11	1.90	0.54
1:C:43:PRO:HB2	1:C:46:ILE:HB	1.90	0.54
1:D:166:SER:HB3	1:D:205:SER:HB3	1.90	0.54
1:H:61:CYS:HB2	1:H:62:PRO:HD2	1.89	0.54
1:H:133:LEU:HD11	1:H:199:VAL:HG21	1.89	0.54
1:J:232:ASN:H	1:J:232:ASN:ND2	1.94	0.54
1:K:230:HIS:CD2	1:K:254:THR:HG21	2.43	0.54
1:L:61:CYS:HB2	1:L:62:PRO:HD2	1.89	0.54
1:D:227:LEU:HD11	1:D:252:ASP:HB2	1.90	0.54
1:A:230:HIS:CD2	1:A:254:THR:HG21	2.43	0.54
1:G:358:VAL:CG2	1:G:367:GLN:HB2	2.37	0.54
1:H:145:THR:OG1	1:H:150:LYS:HB3	2.07	0.54
1:J:230:HIS:CD2	1:J:254:THR:HG21	2.43	0.54
1:L:230:HIS:CD2	1:L:254:THR:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:THR:HG22	1:B:230:HIS:N	2.23	0.54
1:D:310:LEU:HD22	1:D:332:LEU:HD11	1.89	0.54
1:A:61:CYS:HB2	1:A:62:PRO:HD2	1.89	0.54
1:J:223:ILE:HA	1:J:226:LEU:HD23	1.89	0.54
1:B:166:SER:HB3	1:B:205:SER:HB3	1.90	0.54
1:I:61:CYS:HB2	1:I:62:PRO:HD2	1.89	0.54
1:I:230:HIS:CD2	1:I:254:THR:HG21	2.43	0.54
1:I:358:VAL:CG2	1:I:367:GLN:HB2	2.37	0.54
1:B:65:ILE:HG12	1:B:99:SER:HB2	1.89	0.53
1:D:12:LEU:HD23	1:D:53:VAL:HG11	1.90	0.53
1:G:230:HIS:CD2	1:G:254:THR:HG21	2.43	0.53
1:J:133:LEU:HD11	1:J:199:VAL:HG21	1.89	0.53
1:C:166:SER:HB3	1:C:205:SER:HB3	1.90	0.53
1:F:230:HIS:CD2	1:F:254:THR:HG21	2.43	0.53
1:F:358:VAL:CG2	1:F:367:GLN:HB2	2.37	0.53
1:H:223:ILE:HA	1:H:226:LEU:HD23	1.89	0.53
1:C:12:LEU:HD23	1:C:53:VAL:CG1	2.37	0.53
1:L:145:THR:OG1	1:L:150:LYS:HB3	2.07	0.53
1:B:227:LEU:HD11	1:B:252:ASP:HB2	1.90	0.53
1:E:65:ILE:HG12	1:E:99:SER:HB2	1.89	0.53
1:C:330:ARG:HB2	1:C:331:PRO:HD3	1.91	0.53
1:E:12:LEU:HD23	1:E:53:VAL:HG11	1.90	0.53
1:E:43:PRO:HB2	1:E:46:ILE:HB	1.90	0.53
1:E:80:PRO:O	1:E:83:ARG:HG3	2.08	0.53
1:E:229:THR:HG22	1:E:230:HIS:N	2.23	0.53
1:L:223:ILE:HA	1:L:226:LEU:HD23	1.89	0.53
1:B:14:GLY:O	1:B:56:SER:HA	2.09	0.53
1:D:330:ARG:HB2	1:D:331:PRO:HD3	1.90	0.53
1:H:230:HIS:CD2	1:H:254:THR:HG21	2.43	0.53
1:C:14:GLY:O	1:C:56:SER:HA	2.09	0.53
1:E:14:GLY:O	1:E:56:SER:HA	2.09	0.53
1:I:133:LEU:HD11	1:I:199:VAL:HG21	1.89	0.53
1:C:80:PRO:O	1:C:83:ARG:HG3	2.08	0.53
1:D:43:PRO:HB2	1:D:46:ILE:HB	1.90	0.53
1:E:227:LEU:HD11	1:E:252:ASP:HB2	1.90	0.53
1:A:133:LEU:HD11	1:A:199:VAL:HG21	1.89	0.53
1:B:12:LEU:HD23	1:B:53:VAL:HG11	1.90	0.53
1:B:80:PRO:O	1:B:83:ARG:HG3	2.08	0.53
1:C:229:THR:HG22	1:C:230:HIS:N	2.23	0.53
1:D:122:ALA:O	1:D:126:GLU:HG3	2.08	0.53
1:D:229:THR:HG22	1:D:230:HIS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASP:OD1	1:B:110:SER:OG	2.27	0.53
1:B:330:ARG:HB2	1:B:331:PRO:HD3	1.90	0.53
1:D:80:PRO:O	1:D:83:ARG:HG3	2.08	0.53
1:L:133:LEU:HD11	1:L:199:VAL:HG21	1.89	0.53
1:B:122:ALA:O	1:B:126:GLU:HG3	2.09	0.52
1:D:14:GLY:O	1:D:56:SER:HA	2.09	0.52
1:E:166:SER:HB3	1:E:205:SER:HB3	1.90	0.52
1:B:43:PRO:HB2	1:B:46:ILE:HB	1.90	0.52
1:D:65:ILE:HG12	1:D:99:SER:HB2	1.89	0.52
1:A:68:HIS:ND1	1:A:229:THR:HG21	2.25	0.52
1:E:122:ALA:O	1:E:126:GLU:HG3	2.09	0.52
1:A:107:ASP:OD1	1:A:110:SER:OG	2.28	0.52
1:G:206:LYS:HB3	1:G:206:LYS:HZ3	1.74	0.52
1:H:68:HIS:ND1	1:H:229:THR:HG21	2.25	0.52
1:K:68:HIS:ND1	1:K:229:THR:HG21	2.25	0.52
1:L:68:HIS:ND1	1:L:229:THR:HG21	2.25	0.52
1:C:122:ALA:O	1:C:126:GLU:HG3	2.09	0.52
1:G:107:ASP:OD1	1:G:110:SER:OG	2.28	0.52
1:E:107:ASP:OD1	1:E:110:SER:OG	2.27	0.52
1:F:68:HIS:ND1	1:F:229:THR:HG21	2.25	0.52
1:G:72:ILE:HD11	1:G:104:LEU:HD21	1.92	0.52
1:G:301:HIS:O	1:G:302:ILE:HD13	2.10	0.52
1:A:301:HIS:O	1:A:302:ILE:HD13	2.10	0.52
1:F:72:ILE:HD11	1:F:104:LEU:HD21	1.92	0.52
1:F:232:ASN:H	1:F:232:ASN:ND2	1.94	0.52
1:G:55:LEU:O	1:G:58:GLN:HB2	2.10	0.52
1:G:250:THR:HG23	1:G:279:ARG:HA	1.92	0.52
1:I:55:LEU:O	1:I:58:GLN:HB2	2.10	0.52
1:J:72:ILE:HD11	1:J:104:LEU:HD21	1.92	0.52
1:K:72:ILE:HD11	1:K:104:LEU:HD21	1.92	0.52
1:I:250:THR:HG23	1:I:279:ARG:HA	1.92	0.52
1:E:330:ARG:HB2	1:E:331:PRO:HD3	1.90	0.52
1:J:68:HIS:ND1	1:J:229:THR:HG21	2.25	0.52
1:K:250:THR:HG23	1:K:279:ARG:HA	1.92	0.52
1:L:107:ASP:OD1	1:L:110:SER:OG	2.28	0.52
1:G:345:LYS:NZ	1:G:355:ASP:OD2	2.43	0.51
1:I:68:HIS:ND1	1:I:229:THR:HG21	2.25	0.51
1:H:301:HIS:O	1:H:302:ILE:HD13	2.10	0.51
1:H:348:ILE:HD13	1:H:356:LEU:HD23	1.92	0.51
1:I:107:ASP:OD1	1:I:110:SER:OG	2.28	0.51
1:K:55:LEU:O	1:K:58:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:345:LYS:NZ	1:K:355:ASP:OD2	2.43	0.51
1:K:348:ILE:HD13	1:K:356:LEU:HD23	1.92	0.51
1:L:72:ILE:HD11	1:L:104:LEU:HD21	1.92	0.51
1:L:301:HIS:O	1:L:302:ILE:HD13	2.10	0.51
1:C:208:ALA:HB1	1:C:237:LEU:HD23	1.93	0.51
1:E:208:ALA:HB1	1:E:237:LEU:HD23	1.93	0.51
1:A:55:LEU:O	1:A:58:GLN:HB2	2.10	0.51
1:A:250:THR:HG23	1:A:279:ARG:HA	1.92	0.51
1:A:348:ILE:HD13	1:A:356:LEU:HD23	1.92	0.51
1:F:250:THR:HG23	1:F:279:ARG:HA	1.92	0.51
1:F:345:LYS:NZ	1:F:355:ASP:OD2	2.43	0.51
1:H:72:ILE:HD11	1:H:104:LEU:HD21	1.92	0.51
1:I:301:HIS:O	1:I:302:ILE:HD13	2.10	0.51
1:L:348:ILE:HD13	1:L:356:LEU:HD23	1.92	0.51
1:B:68:HIS:HB2	1:B:283:SER:HB2	1.93	0.51
1:F:301:HIS:O	1:F:302:ILE:HD13	2.10	0.51
1:F:348:ILE:HD13	1:F:356:LEU:HD23	1.92	0.51
1:J:107:ASP:OD1	1:J:110:SER:OG	2.28	0.51
1:J:55:LEU:O	1:J:58:GLN:HB2	2.10	0.51
1:C:107:ASP:OD1	1:C:110:SER:OG	2.27	0.51
1:D:68:HIS:HB2	1:D:283:SER:HB2	1.93	0.51
1:G:68:HIS:ND1	1:G:229:THR:HG21	2.25	0.51
1:I:345:LYS:NZ	1:I:355:ASP:OD2	2.43	0.51
1:J:348:ILE:HD13	1:J:356:LEU:HD23	1.92	0.51
1:K:311:LEU:O	1:K:311:LEU:HD23	2.11	0.51
1:L:250:THR:HG23	1:L:279:ARG:HA	1.92	0.51
1:F:55:LEU:O	1:F:58:GLN:HB2	2.10	0.51
1:A:72:ILE:HD11	1:A:104:LEU:HD21	1.92	0.51
1:G:311:LEU:HD23	1:G:311:LEU:O	2.11	0.51
1:H:250:THR:HG23	1:H:279:ARG:HA	1.92	0.51
1:J:250:THR:HG23	1:J:279:ARG:HA	1.93	0.51
1:K:301:HIS:O	1:K:302:ILE:HD13	2.10	0.51
1:A:311:LEU:O	1:A:311:LEU:HD23	2.11	0.51
1:A:345:LYS:NZ	1:A:355:ASP:OD2	2.43	0.51
1:F:107:ASP:OD1	1:F:110:SER:OG	2.28	0.51
1:H:311:LEU:O	1:H:311:LEU:HD23	2.11	0.51
1:I:72:ILE:HD11	1:I:104:LEU:HD21	1.92	0.51
1:J:301:HIS:O	1:J:302:ILE:HD13	2.10	0.51
1:K:107:ASP:OD1	1:K:110:SER:OG	2.28	0.51
1:H:107:ASP:OD1	1:H:110:SER:OG	2.28	0.50
1:H:206:LYS:HB3	1:H:206:LYS:HZ2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:LEU:O	1:L:58:GLN:HB2	2.10	0.50
1:C:142:ARG:HG2	1:C:142:ARG:HH11	1.76	0.50
1:H:55:LEU:O	1:H:58:GLN:HB2	2.10	0.50
1:I:348:ILE:HD13	1:I:356:LEU:HD23	1.93	0.50
1:J:311:LEU:HD23	1:J:311:LEU:O	2.11	0.50
1:L:345:LYS:NZ	1:L:355:ASP:OD2	2.43	0.50
1:I:311:LEU:HD23	1:I:311:LEU:O	2.11	0.50
1:B:208:ALA:HB1	1:B:237:LEU:HD23	1.93	0.50
1:D:367:GLN:HA	1:D:376:VAL:O	2.12	0.50
1:E:142:ARG:HH11	1:E:142:ARG:HG2	1.76	0.50
1:I:226:LEU:HD22	1:I:226:LEU:N	2.27	0.50
1:K:209:LEU:HD22	1:K:212:ILE:HD12	1.94	0.50
1:L:311:LEU:HD23	1:L:311:LEU:O	2.11	0.50
1:B:19:ALA:HA	1:B:348:ILE:HD12	1.94	0.50
1:C:367:GLN:HA	1:C:376:VAL:O	2.12	0.50
1:L:68:HIS:HD2	1:L:103:LEU:HD21	1.77	0.50
1:B:142:ARG:HH11	1:B:142:ARG:HG2	1.76	0.50
1:C:9:PHE:HB2	1:C:49:ASN:O	2.12	0.50
1:D:142:ARG:HG2	1:D:142:ARG:HH11	1.76	0.50
1:D:208:ALA:HB1	1:D:237:LEU:HD23	1.93	0.50
1:G:348:ILE:HD13	1:G:356:LEU:HD23	1.92	0.50
1:H:345:LYS:NZ	1:H:355:ASP:OD2	2.43	0.50
1:J:209:LEU:HD22	1:J:212:ILE:HD12	1.94	0.50
1:D:19:ALA:HA	1:D:348:ILE:HD12	1.94	0.50
1:G:226:LEU:HD22	1:G:226:LEU:N	2.27	0.50
1:H:226:LEU:N	1:H:226:LEU:HD22	2.27	0.50
1:I:68:HIS:HD2	1:I:103:LEU:HD21	1.77	0.50
1:K:68:HIS:HD2	1:K:103:LEU:HD21	1.77	0.50
1:F:68:HIS:HD2	1:F:103:LEU:HD21	1.77	0.50
1:F:311:LEU:O	1:F:311:LEU:HD23	2.11	0.50
1:L:255:SER:HB2	1:L:309:THR:HB	1.94	0.50
1:C:68:HIS:HB2	1:C:283:SER:HB2	1.93	0.49
1:E:68:HIS:HB2	1:E:283:SER:HB2	1.93	0.49
1:F:226:LEU:N	1:F:226:LEU:HD22	2.27	0.49
1:H:232:ASN:HB2	1:H:261:VAL:HB	1.94	0.49
1:H:255:SER:HB2	1:H:309:THR:HB	1.94	0.49
1:J:226:LEU:N	1:J:226:LEU:HD22	2.27	0.49
1:J:345:LYS:NZ	1:J:355:ASP:OD2	2.43	0.49
1:I:209:LEU:HD22	1:I:212:ILE:HD12	1.94	0.49
1:L:232:ASN:HB2	1:L:261:VAL:HB	1.94	0.49
1:D:282:LEU:HB3	1:D:332:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:226:LEU:N	1:K:226:LEU:HD22	2.27	0.49
1:K:255:SER:HB2	1:K:309:THR:HB	1.94	0.49
1:L:209:LEU:HD22	1:L:212:ILE:HD12	1.94	0.49
1:B:223:ILE:HA	1:B:226:LEU:CD2	2.43	0.49
1:C:223:ILE:HA	1:C:226:LEU:CD2	2.43	0.49
1:A:255:SER:HB2	1:A:309:THR:HB	1.94	0.49
1:F:255:SER:HB2	1:F:309:THR:HB	1.94	0.49
1:K:232:ASN:HB2	1:K:261:VAL:HB	1.94	0.49
1:D:223:ILE:HA	1:D:226:LEU:CD2	2.43	0.49
1:A:232:ASN:HB2	1:A:261:VAL:HB	1.94	0.49
1:F:232:ASN:HB2	1:F:261:VAL:HB	1.94	0.49
1:G:209:LEU:HD22	1:G:212:ILE:HD12	1.94	0.49
1:J:68:HIS:HD2	1:J:103:LEU:HD21	1.77	0.49
1:B:282:LEU:HB3	1:B:332:LEU:HD13	1.95	0.49
1:D:9:PHE:HB2	1:D:49:ASN:O	2.12	0.49
1:A:68:HIS:HD2	1:A:103:LEU:HD21	1.77	0.49
1:I:255:SER:HB2	1:I:309:THR:HB	1.94	0.49
1:L:206:LYS:HB3	1:L:206:LYS:HZ3	1.75	0.49
1:H:68:HIS:HD2	1:H:103:LEU:HD21	1.77	0.49
1:I:195:PRO:HG3	1:I:340:LEU:O	2.13	0.49
1:G:255:SER:HB2	1:G:309:THR:HB	1.94	0.49
1:B:367:GLN:HA	1:B:376:VAL:O	2.12	0.49
1:C:282:LEU:HB3	1:C:332:LEU:HD13	1.95	0.49
1:E:282:LEU:HB3	1:E:332:LEU:HD13	1.95	0.49
1:L:195:PRO:HG3	1:L:340:LEU:O	2.13	0.49
1:B:9:PHE:HB2	1:B:49:ASN:O	2.12	0.49
1:B:124:ASN:HA	1:B:128:ILE:O	2.13	0.49
1:E:9:PHE:HB2	1:E:49:ASN:O	2.12	0.49
1:E:19:ALA:HA	1:E:348:ILE:HD12	1.94	0.49
1:E:367:GLN:HA	1:E:376:VAL:O	2.12	0.49
1:F:209:LEU:HD22	1:F:212:ILE:HD12	1.94	0.49
1:F:255:SER:HA	1:F:263:PRO:HG3	1.95	0.49
1:G:68:HIS:HD2	1:G:103:LEU:HD21	1.77	0.49
1:G:195:PRO:HG3	1:G:340:LEU:O	2.13	0.49
1:H:230:HIS:HD2	1:H:254:THR:HG21	1.78	0.49
1:J:232:ASN:HB2	1:J:261:VAL:HB	1.94	0.49
1:C:124:ASN:HA	1:C:128:ILE:O	2.13	0.48
1:D:124:ASN:HA	1:D:128:ILE:O	2.13	0.48
1:E:42:ILE:HG12	1:F:2:ILE:HD13	1.95	0.48
1:E:223:ILE:HA	1:E:226:LEU:CD2	2.43	0.48
1:A:226:LEU:N	1:A:226:LEU:HD22	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:HIS:HD2	1:F:254:THR:HG21	1.78	0.48
1:I:255:SER:HA	1:I:263:PRO:HG3	1.95	0.48
1:K:255:SER:HA	1:K:263:PRO:HG3	1.95	0.48
1:A:230:HIS:HD2	1:A:254:THR:HG21	1.78	0.48
1:G:232:ASN:HB2	1:G:261:VAL:HB	1.94	0.48
1:H:195:PRO:HG3	1:H:340:LEU:O	2.13	0.48
1:I:232:ASN:HB2	1:I:261:VAL:HB	1.94	0.48
1:L:145:THR:HB	1:L:150:LYS:HD3	1.96	0.48
1:L:226:LEU:N	1:L:226:LEU:HD22	2.27	0.48
1:L:230:HIS:HD2	1:L:254:THR:HG21	1.78	0.48
1:C:19:ALA:HA	1:C:348:ILE:HD12	1.94	0.48
1:E:282:LEU:HB3	1:E:332:LEU:CD1	2.44	0.48
1:A:195:PRO:HG3	1:A:340:LEU:O	2.13	0.48
1:G:344:GLY:HA2	1:G:352:ASN:OD1	2.14	0.48
1:I:145:THR:HB	1:I:150:LYS:HD3	1.96	0.48
1:L:232:ASN:N	1:L:232:ASN:ND2	2.58	0.48
1:B:39:ALA:HB3	1:G:2:ILE:HG23	1.96	0.48
1:E:39:ALA:HB3	1:F:2:ILE:HG23	1.96	0.48
1:E:234:ASN:HD22	1:E:236:PRO:CD	2.17	0.48
1:A:145:THR:HB	1:A:150:LYS:HD3	1.96	0.48
1:A:209:LEU:HD22	1:A:212:ILE:HD12	1.94	0.48
1:G:234:ASN:ND2	1:G:237:LEU:H	2.11	0.48
1:G:255:SER:HA	1:G:263:PRO:HG3	1.96	0.48
1:H:209:LEU:HD22	1:H:212:ILE:HD12	1.94	0.48
1:H:344:GLY:HA2	1:H:352:ASN:OD1	2.14	0.48
1:I:230:HIS:HD2	1:I:254:THR:HG21	1.78	0.48
1:I:232:ASN:N	1:I:232:ASN:ND2	2.58	0.48
1:I:344:GLY:HA2	1:I:352:ASN:OD1	2.14	0.48
1:J:255:SER:HA	1:J:263:PRO:HG3	1.95	0.48
1:J:255:SER:HB2	1:J:309:THR:HB	1.94	0.48
1:L:344:GLY:HA2	1:L:352:ASN:OD1	2.14	0.48
1:A:255:SER:HA	1:A:263:PRO:HG3	1.95	0.48
1:H:145:THR:HB	1:H:150:LYS:HD3	1.96	0.48
1:H:255:SER:HA	1:H:263:PRO:HG3	1.95	0.48
1:K:195:PRO:HG3	1:K:340:LEU:O	2.13	0.48
1:L:255:SER:HA	1:L:263:PRO:HG3	1.95	0.48
1:C:282:LEU:HB3	1:C:332:LEU:CD1	2.44	0.48
1:E:124:ASN:HA	1:E:128:ILE:O	2.13	0.48
1:F:234:ASN:ND2	1:F:237:LEU:H	2.11	0.48
1:D:42:ILE:HG12	1:A:2:ILE:HD13	1.95	0.48
1:D:308:GLU:HG2	1:D:309:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:GLY:HA2	1:F:352:ASN:OD1	2.14	0.48
1:H:234:ASN:ND2	1:H:237:LEU:H	2.11	0.48
1:C:308:GLU:HG2	1:C:309:THR:N	2.29	0.48
1:F:145:THR:HB	1:F:150:LYS:HD3	1.96	0.48
1:G:367:GLN:HA	1:G:376:VAL:O	2.14	0.48
1:J:230:HIS:HD2	1:J:254:THR:HG21	1.78	0.48
1:B:42:ILE:HG12	1:G:2:ILE:HD13	1.95	0.48
1:G:145:THR:HB	1:G:150:LYS:HD3	1.96	0.48
1:G:230:HIS:HD2	1:G:254:THR:HG21	1.78	0.48
1:J:145:THR:HB	1:J:150:LYS:HD3	1.96	0.48
1:K:145:THR:HB	1:K:150:LYS:HD3	1.96	0.48
1:K:367:GLN:HA	1:K:376:VAL:O	2.14	0.48
1:E:203:GLY:O	1:E:233:ARG:HD3	2.14	0.47
1:A:35:ILE:HD13	1:A:348:ILE:HG23	1.96	0.47
1:A:234:ASN:ND2	1:A:237:LEU:H	2.11	0.47
1:F:206:LYS:HB3	1:F:206:LYS:HZ2	1.79	0.47
1:J:344:GLY:HA2	1:J:352:ASN:OD1	2.14	0.47
1:K:230:HIS:HD2	1:K:254:THR:HG21	1.78	0.47
1:K:344:GLY:HA2	1:K:352:ASN:OD1	2.14	0.47
1:J:206:LYS:HB3	1:J:206:LYS:HZ2	1.79	0.47
1:K:234:ASN:ND2	1:K:237:LEU:H	2.11	0.47
1:L:234:ASN:ND2	1:L:237:LEU:H	2.11	0.47
1:B:282:LEU:HB3	1:B:332:LEU:CD1	2.44	0.47
1:C:12:LEU:CD1	1:C:356:LEU:HD13	2.44	0.47
1:D:282:LEU:HB3	1:D:332:LEU:CD1	2.44	0.47
1:I:234:ASN:ND2	1:I:237:LEU:H	2.11	0.47
1:B:234:ASN:HD22	1:B:236:PRO:CD	2.17	0.47
1:C:42:ILE:HG12	1:H:2:ILE:HD13	1.95	0.47
1:E:308:GLU:HG2	1:E:309:THR:N	2.29	0.47
1:J:178:LEU:HD12	1:J:181:MET:CE	2.45	0.47
1:B:203:GLY:O	1:B:233:ARG:HD3	2.15	0.47
1:B:313:THR:O	1:B:317:LEU:HB2	2.15	0.47
1:E:12:LEU:CD1	1:E:356:LEU:HD13	2.44	0.47
1:A:178:LEU:HD12	1:A:181:MET:CE	2.45	0.47
1:I:35:ILE:HD13	1:I:348:ILE:HG23	1.96	0.47
1:C:231:VAL:HA	1:C:237:LEU:CD1	2.45	0.47
1:C:243:GLU:OE1	1:C:247:LYS:HE3	2.15	0.47
1:D:232:ASN:HD21	1:D:254:THR:H	1.62	0.47
1:E:231:VAL:HA	1:E:237:LEU:CD1	2.45	0.47
1:F:35:ILE:HD13	1:F:348:ILE:HG23	1.96	0.47
1:F:367:GLN:HA	1:F:376:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:LEU:HD12	1:G:181:MET:CE	2.45	0.47
1:B:161:VAL:HG12	1:B:185:SER:HB2	1.97	0.47
1:B:308:GLU:HG2	1:B:309:THR:N	2.29	0.47
1:C:39:ALA:HB3	1:H:2:ILE:HG23	1.96	0.47
1:C:313:THR:O	1:C:317:LEU:HB2	2.15	0.47
1:D:203:GLY:O	1:D:233:ARG:HD3	2.15	0.47
1:D:313:THR:O	1:D:317:LEU:HB2	2.15	0.47
1:E:161:VAL:HG12	1:E:185:SER:HB2	1.97	0.47
1:E:313:THR:O	1:E:317:LEU:HB2	2.15	0.47
1:A:367:GLN:HA	1:A:376:VAL:O	2.14	0.47
1:F:195:PRO:HG3	1:F:340:LEU:O	2.13	0.47
1:F:220:ASP:OD2	1:G:205:SER:HB2	2.15	0.47
1:H:68:HIS:CD2	1:H:103:LEU:HD21	2.50	0.47
1:H:178:LEU:HD12	1:H:181:MET:CE	2.45	0.47
1:I:367:GLN:HA	1:I:376:VAL:O	2.14	0.47
1:J:68:HIS:CD2	1:J:103:LEU:HD21	2.50	0.47
1:J:234:ASN:ND2	1:J:237:LEU:H	2.11	0.47
1:J:367:GLN:HA	1:J:376:VAL:O	2.14	0.47
1:K:35:ILE:HD13	1:K:348:ILE:HG23	1.96	0.47
1:L:178:LEU:HD12	1:L:181:MET:CE	2.45	0.47
1:D:39:ALA:HB3	1:A:2:ILE:HG23	1.96	0.47
1:D:234:ASN:HD22	1:D:236:PRO:CD	2.17	0.47
1:D:243:GLU:OE1	1:D:247:LYS:HE3	2.15	0.47
1:A:205:SER:HB2	1:G:220:ASP:OD2	2.15	0.47
1:A:344:GLY:HA2	1:A:352:ASN:OD1	2.14	0.47
1:F:68:HIS:CD2	1:F:103:LEU:HD21	2.50	0.47
1:I:178:LEU:HD12	1:I:181:MET:CE	2.45	0.47
1:I:205:SER:HB2	1:K:220:ASP:OD2	2.15	0.47
1:J:35:ILE:HD13	1:J:348:ILE:HG23	1.96	0.47
1:K:68:HIS:CD2	1:K:103:LEU:HD21	2.50	0.47
1:D:107:ASP:OD1	1:D:110:SER:OG	2.27	0.47
1:H:367:GLN:HA	1:H:376:VAL:O	2.14	0.47
1:B:232:ASN:HD21	1:B:254:THR:H	1.62	0.47
1:G:116:LEU:HD13	1:G:132:MET:HB2	1.97	0.47
1:L:68:HIS:CD2	1:L:103:LEU:HD21	2.50	0.47
1:L:355:ASP:HA	1:L:369:TYR:O	2.15	0.47
1:B:139:VAL:HA	1:B:140:PRO:C	2.40	0.46
1:C:46:ILE:HG23	1:C:47:VAL:HG22	1.97	0.46
1:C:203:GLY:O	1:C:233:ARG:HD3	2.15	0.46
1:C:232:ASN:HD21	1:C:254:THR:H	1.62	0.46
1:E:243:GLU:OE1	1:E:247:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:CD2	1:A:103:LEU:HD21	2.50	0.46
1:A:355:ASP:HA	1:A:369:TYR:O	2.15	0.46
1:G:35:ILE:HD13	1:G:348:ILE:HG23	1.96	0.46
1:I:116:LEU:HD13	1:I:132:MET:HB2	1.98	0.46
1:J:116:LEU:HD13	1:J:132:MET:HB2	1.97	0.46
1:J:195:PRO:HG3	1:J:340:LEU:O	2.13	0.46
1:K:116:LEU:HD13	1:K:132:MET:HB2	1.97	0.46
1:B:231:VAL:HA	1:B:237:LEU:CD1	2.45	0.46
1:A:255:SER:HA	1:A:263:PRO:CG	2.46	0.46
1:A:301:HIS:HD1	1:A:301:HIS:N	2.14	0.46
1:I:255:SER:HA	1:I:263:PRO:CG	2.46	0.46
1:J:220:ASP:OD2	1:K:205:SER:HB2	2.15	0.46
1:J:301:HIS:N	1:J:301:HIS:HD1	2.14	0.46
1:K:178:LEU:HD12	1:K:181:MET:CE	2.45	0.46
1:B:12:LEU:CD1	1:B:356:LEU:HD13	2.44	0.46
1:D:161:VAL:HG12	1:D:185:SER:HB2	1.97	0.46
1:E:232:ASN:HD21	1:E:254:THR:H	1.62	0.46
1:A:116:LEU:HD13	1:A:132:MET:HB2	1.97	0.46
1:F:64:PHE:CE1	1:F:332:LEU:HD23	2.51	0.46
1:F:116:LEU:HD13	1:F:132:MET:HB2	1.97	0.46
1:G:27:ASP:HB2	1:G:42:ILE:HG13	1.98	0.46
1:G:68:HIS:CD2	1:G:103:LEU:HD21	2.50	0.46
1:H:64:PHE:CE1	1:H:332:LEU:HD23	2.51	0.46
1:H:355:ASP:HA	1:H:369:TYR:O	2.15	0.46
1:I:68:HIS:CD2	1:I:103:LEU:HD21	2.50	0.46
1:I:355:ASP:HA	1:I:369:TYR:O	2.16	0.46
1:L:35:ILE:HD13	1:L:348:ILE:HG23	1.96	0.46
1:B:223:ILE:HA	1:B:226:LEU:HD23	1.98	0.46
1:E:46:ILE:HG23	1:E:47:VAL:HG22	1.98	0.46
1:F:178:LEU:HD12	1:F:181:MET:CE	2.45	0.46
1:I:27:ASP:HB2	1:I:42:ILE:HG13	1.98	0.46
1:L:301:HIS:N	1:L:301:HIS:HD1	2.14	0.46
1:C:161:VAL:HG12	1:C:185:SER:HB2	1.97	0.46
1:D:12:LEU:CD1	1:D:356:LEU:HD13	2.44	0.46
1:G:301:HIS:N	1:G:301:HIS:HD1	2.14	0.46
1:I:203:GLY:O	1:I:233:ARG:HD3	2.16	0.46
1:I:301:HIS:N	1:I:301:HIS:HD1	2.14	0.46
1:K:355:ASP:HA	1:K:369:TYR:O	2.15	0.46
1:D:223:ILE:HA	1:D:226:LEU:HD23	1.98	0.46
1:I:206:LYS:HB3	1:I:206:LYS:HZ3	1.77	0.46
1:K:301:HIS:HD1	1:K:301:HIS:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ILE:HA	1:C:226:LEU:HD23	1.98	0.46
1:D:231:VAL:HA	1:D:237:LEU:CD1	2.45	0.46
1:F:203:GLY:O	1:F:233:ARG:HD3	2.16	0.46
1:F:205:SER:HB2	1:H:220:ASP:OD2	2.15	0.46
1:F:301:HIS:HD1	1:F:301:HIS:N	2.13	0.46
1:G:64:PHE:CE1	1:G:332:LEU:HD23	2.51	0.46
1:G:203:GLY:O	1:G:233:ARG:HD3	2.16	0.46
1:H:116:LEU:HD13	1:H:132:MET:HB2	1.97	0.46
1:C:99:SER:OG	1:C:345:LYS:HD3	2.16	0.46
1:A:203:GLY:O	1:A:233:ARG:HD3	2.16	0.46
1:H:35:ILE:HD13	1:H:348:ILE:HG23	1.96	0.46
1:H:134:THR:HG22	1:H:160:GLY:O	2.16	0.46
1:I:220:ASP:OD2	1:L:205:SER:HB2	2.15	0.46
1:J:205:SER:HB2	1:L:220:ASP:OD2	2.15	0.46
1:J:245:ALA:HA	1:J:249:GLY:O	2.16	0.46
1:J:355:ASP:HA	1:J:369:TYR:O	2.15	0.46
1:K:27:ASP:HB2	1:K:42:ILE:HG13	1.98	0.46
1:L:367:GLN:HA	1:L:376:VAL:O	2.14	0.46
1:D:63:GLY:HA2	1:D:357:LEU:CG	2.45	0.46
1:A:27:ASP:HB2	1:A:42:ILE:HG13	1.98	0.46
1:H:255:SER:HA	1:H:263:PRO:CG	2.46	0.46
1:I:64:PHE:CE1	1:I:332:LEU:HD23	2.51	0.46
1:J:203:GLY:O	1:J:233:ARG:HD3	2.16	0.46
1:F:27:ASP:HB2	1:F:42:ILE:HG13	1.98	0.46
1:G:245:ALA:HA	1:G:249:GLY:O	2.16	0.46
1:J:27:ASP:HB2	1:J:42:ILE:HG13	1.98	0.46
1:J:134:THR:HG22	1:J:160:GLY:O	2.16	0.46
1:K:64:PHE:CE1	1:K:332:LEU:HD23	2.51	0.46
1:K:245:ALA:HA	1:K:249:GLY:O	2.16	0.46
1:L:64:PHE:CE1	1:L:332:LEU:HD23	2.51	0.46
1:L:116:LEU:HD13	1:L:132:MET:HB2	1.97	0.46
1:L:245:ALA:HA	1:L:249:GLY:O	2.16	0.46
1:D:46:ILE:HG23	1:D:47:VAL:HG22	1.97	0.45
1:D:139:VAL:HA	1:D:140:PRO:C	2.40	0.45
1:E:139:VAL:HA	1:E:140:PRO:C	2.40	0.45
1:A:143:THR:HB	1:A:151:ASP:OD1	2.17	0.45
1:G:255:SER:HA	1:G:263:PRO:CG	2.46	0.45
1:J:250:THR:HG23	1:J:279:ARG:C	2.42	0.45
1:L:255:SER:HA	1:L:263:PRO:CG	2.46	0.45
1:B:46:ILE:HG23	1:B:47:VAL:HG22	1.97	0.45
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:SER:OG	1:D:345:LYS:HD3	2.16	0.45
1:A:245:ALA:HA	1:A:249:GLY:O	2.16	0.45
1:G:134:THR:HG22	1:G:160:GLY:O	2.16	0.45
1:G:143:THR:HB	1:G:151:ASP:OD1	2.17	0.45
1:G:250:THR:HG23	1:G:279:ARG:C	2.42	0.45
1:H:203:GLY:O	1:H:233:ARG:HD3	2.16	0.45
1:H:250:THR:HG23	1:H:279:ARG:C	2.41	0.45
1:H:301:HIS:HD1	1:H:301:HIS:N	2.14	0.45
1:K:134:THR:HG22	1:K:160:GLY:O	2.16	0.45
1:L:143:THR:HB	1:L:151:ASP:OD1	2.17	0.45
1:E:223:ILE:HA	1:E:226:LEU:HD23	1.98	0.45
1:F:134:THR:HG22	1:F:160:GLY:O	2.16	0.45
1:G:355:ASP:HA	1:G:369:TYR:O	2.15	0.45
1:H:143:THR:HB	1:H:151:ASP:OD1	2.17	0.45
1:K:203:GLY:O	1:K:233:ARG:HD3	2.16	0.45
1:L:203:GLY:O	1:L:233:ARG:HD3	2.16	0.45
1:I:245:ALA:HA	1:I:249:GLY:O	2.16	0.45
1:J:64:PHE:CE1	1:J:332:LEU:HD23	2.51	0.45
1:E:139:VAL:HB	1:E:173:PRO:HB3	1.98	0.45
1:A:134:THR:HG22	1:A:160:GLY:O	2.16	0.45
1:A:250:THR:HG23	1:A:279:ARG:C	2.41	0.45
1:F:143:THR:HB	1:F:151:ASP:OD1	2.17	0.45
1:G:215:LEU:HD23	1:G:215:LEU:C	2.42	0.45
1:J:255:SER:HA	1:J:263:PRO:CG	2.46	0.45
1:K:143:THR:HB	1:K:151:ASP:OD1	2.17	0.45
1:L:250:THR:HG23	1:L:279:ARG:C	2.42	0.45
1:B:243:GLU:OE1	1:B:247:LYS:HE3	2.15	0.45
1:A:215:LEU:C	1:A:215:LEU:HD23	2.42	0.45
1:C:139:VAL:HA	1:C:140:PRO:C	2.40	0.45
1:A:64:PHE:CE1	1:A:332:LEU:HD23	2.51	0.45
1:A:162:KCX:HG2	1:A:163:CYS:N	2.31	0.45
1:A:220:ASP:OD2	1:H:205:SER:HB2	2.15	0.45
1:I:215:LEU:HD23	1:I:215:LEU:C	2.42	0.45
1:I:340:LEU:O	1:I:341:ASN:C	2.60	0.45
1:J:143:THR:HB	1:J:151:ASP:OD1	2.17	0.45
1:C:234:ASN:HD22	1:C:236:PRO:CD	2.17	0.45
1:F:245:ALA:HA	1:F:249:GLY:O	2.16	0.45
1:F:355:ASP:HA	1:F:369:TYR:O	2.15	0.45
1:H:27:ASP:HB2	1:H:42:ILE:HG13	1.98	0.45
1:I:143:THR:HB	1:I:151:ASP:OD1	2.17	0.45
1:K:215:LEU:C	1:K:215:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:255:SER:HA	1:K:263:PRO:CG	2.46	0.45
1:L:134:THR:HG22	1:L:160:GLY:O	2.16	0.45
1:G:18:TYR:C	1:G:20:PRO:HA	2.42	0.45
1:G:162:KCX:HG2	1:G:163:CYS:N	2.31	0.45
1:G:340:LEU:O	1:G:341:ASN:C	2.60	0.45
1:H:245:ALA:HA	1:H:249:GLY:O	2.16	0.45
1:I:18:TYR:C	1:I:20:PRO:HA	2.42	0.45
1:I:134:THR:HG22	1:I:160:GLY:O	2.16	0.45
1:L:27:ASP:HB2	1:L:42:ILE:HG13	1.98	0.45
1:B:99:SER:OG	1:B:345:LYS:HD3	2.16	0.45
1:F:250:THR:HG23	1:F:279:ARG:C	2.42	0.45
1:F:255:SER:HA	1:F:263:PRO:CG	2.46	0.45
1:H:18:TYR:C	1:H:20:PRO:HA	2.42	0.45
1:K:250:THR:HG23	1:K:279:ARG:C	2.42	0.45
1:C:17:LEU:HD11	1:C:19:ALA:HB2	1.99	0.44
1:E:99:SER:OG	1:E:345:LYS:HD3	2.16	0.44
1:J:215:LEU:C	1:J:215:LEU:HD23	2.42	0.44
1:C:358:VAL:HB	1:C:367:GLN:HB2	2.00	0.44
1:E:271:VAL:HG21	1:E:323:PHE:HE1	1.82	0.44
1:A:18:TYR:C	1:A:20:PRO:HA	2.42	0.44
1:A:340:LEU:O	1:A:341:ASN:C	2.60	0.44
1:F:215:LEU:C	1:F:215:LEU:HD23	2.42	0.44
1:H:162:KCX:HG2	1:H:163:CYS:N	2.31	0.44
1:J:202:MET:HB3	1:J:237:LEU:HD11	2.00	0.44
1:B:232:ASN:HB2	1:B:261:VAL:HB	1.99	0.44
1:C:340:LEU:HB2	1:C:342:LEU:HG	1.99	0.44
1:D:232:ASN:HB2	1:D:261:VAL:HB	2.00	0.44
1:D:340:LEU:HB2	1:D:342:LEU:HG	1.99	0.44
1:K:18:TYR:C	1:K:20:PRO:HA	2.42	0.44
1:L:215:LEU:C	1:L:215:LEU:HD23	2.42	0.44
1:B:17:LEU:HD11	1:B:19:ALA:HB2	1.99	0.44
1:D:358:VAL:HB	1:D:367:GLN:HB2	1.99	0.44
1:E:340:LEU:HB2	1:E:342:LEU:HG	1.99	0.44
1:F:18:TYR:C	1:F:20:PRO:HA	2.42	0.44
1:K:340:LEU:O	1:K:341:ASN:C	2.60	0.44
1:D:139:VAL:HB	1:D:173:PRO:HB3	1.98	0.44
1:E:17:LEU:HD11	1:E:19:ALA:HB2	1.99	0.44
1:F:162:KCX:HG2	1:F:163:CYS:N	2.31	0.44
1:F:202:MET:HB3	1:F:237:LEU:HD11	2.00	0.44
1:F:340:LEU:O	1:F:341:ASN:C	2.60	0.44
1:H:215:LEU:C	1:H:215:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:THR:HG23	1:I:279:ARG:C	2.41	0.44
1:L:69:VAL:HG12	1:L:71:LEU:HD12	2.00	0.44
1:B:358:VAL:HB	1:B:367:GLN:HB2	1.99	0.44
1:J:340:LEU:O	1:J:341:ASN:C	2.60	0.44
1:K:202:MET:HB3	1:K:237:LEU:HD11	2.00	0.44
1:A:69:VAL:HG12	1:A:71:LEU:HD12	2.00	0.44
1:I:69:VAL:HG12	1:I:71:LEU:HD12	2.00	0.44
1:L:18:TYR:C	1:L:20:PRO:HA	2.42	0.44
1:B:208:ALA:HB3	1:B:240:GLN:OE1	2.18	0.44
1:H:69:VAL:HG12	1:H:71:LEU:HD12	2.00	0.44
1:B:340:LEU:HB2	1:B:342:LEU:HG	1.99	0.44
1:E:358:VAL:HB	1:E:367:GLN:HB2	1.99	0.44
1:I:377:LYS:HB2	1:I:382:CYS:SG	2.58	0.44
1:K:377:LYS:HB2	1:K:382:CYS:SG	2.58	0.44
1:B:139:VAL:HB	1:B:173:PRO:HB3	1.98	0.43
1:C:208:ALA:HB3	1:C:240:GLN:OE1	2.18	0.43
1:G:202:MET:HB3	1:G:237:LEU:HD11	2.00	0.43
1:H:202:MET:HB3	1:H:237:LEU:HD11	2.00	0.43
1:C:139:VAL:HB	1:C:173:PRO:HB3	1.98	0.43
1:C:232:ASN:HB2	1:C:261:VAL:HB	1.99	0.43
1:D:17:LEU:HD11	1:D:19:ALA:HB2	1.99	0.43
1:D:19:ALA:CB	1:D:348:ILE:HB	2.49	0.43
1:D:208:ALA:HB3	1:D:240:GLN:OE1	2.18	0.43
1:E:94:GLU:OE1	1:E:380:LYS:HA	2.19	0.43
1:A:59:ILE:CD1	1:A:361:PRO:HA	2.49	0.43
1:H:340:LEU:O	1:H:341:ASN:C	2.60	0.43
1:I:301:HIS:N	1:I:301:HIS:ND1	2.66	0.43
1:L:59:ILE:CD1	1:L:361:PRO:HA	2.48	0.43
1:L:340:LEU:O	1:L:341:ASN:C	2.60	0.43
1:L:377:LYS:HB2	1:L:382:CYS:SG	2.58	0.43
1:B:63:GLY:HA2	1:B:357:LEU:CG	2.45	0.43
1:E:162:KCX:OQ2	1:E:201:HIS:HB2	2.19	0.43
1:L:202:MET:HB3	1:L:237:LEU:HD11	2.00	0.43
1:C:19:ALA:CB	1:C:348:ILE:HB	2.49	0.43
1:D:94:GLU:OE1	1:D:380:LYS:HA	2.18	0.43
1:E:227:LEU:HB2	1:E:339:PHE:HZ	1.84	0.43
1:E:232:ASN:HB2	1:E:261:VAL:HB	1.99	0.43
1:G:59:ILE:CD1	1:G:361:PRO:HA	2.49	0.43
1:G:69:VAL:HG12	1:G:71:LEU:HD12	2.00	0.43
1:G:156:ASP:O	1:G:194:LYS:HE2	2.19	0.43
1:J:229:THR:CG2	1:J:230:HIS:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:377:LYS:HB2	1:J:382:CYS:SG	2.58	0.43
1:K:30:VAL:HG12	1:K:31:ALA:N	2.33	0.43
1:K:156:ASP:O	1:K:194:LYS:HE2	2.18	0.43
1:D:162:KCX:OQ2	1:D:201:HIS:HB2	2.19	0.43
1:D:234:ASN:HD21	1:D:237:LEU:H	1.67	0.43
1:A:229:THR:CG2	1:A:230:HIS:N	2.82	0.43
1:A:377:LYS:HB2	1:A:382:CYS:SG	2.58	0.43
1:F:377:LYS:HB2	1:F:382:CYS:SG	2.58	0.43
1:G:30:VAL:HG12	1:G:31:ALA:N	2.33	0.43
1:G:377:LYS:HB2	1:G:382:CYS:SG	2.58	0.43
1:H:377:LYS:HB2	1:H:382:CYS:SG	2.58	0.43
1:J:59:ILE:CD1	1:J:361:PRO:HA	2.49	0.43
1:J:69:VAL:HG12	1:J:71:LEU:HD12	2.00	0.43
1:K:301:HIS:N	1:K:301:HIS:ND1	2.66	0.43
1:C:162:KCX:OQ2	1:C:201:HIS:HB2	2.19	0.43
1:D:271:VAL:HG21	1:D:323:PHE:HE1	1.82	0.43
1:A:202:MET:HB3	1:A:237:LEU:HD11	1.99	0.43
1:G:301:HIS:N	1:G:301:HIS:ND1	2.66	0.43
1:I:156:ASP:O	1:I:194:LYS:HE2	2.19	0.43
1:L:156:ASP:O	1:L:194:LYS:HE2	2.18	0.43
1:L:229:THR:CG2	1:L:230:HIS:N	2.82	0.43
1:A:30:VAL:HG12	1:A:31:ALA:N	2.33	0.43
1:A:156:ASP:O	1:A:194:LYS:HE2	2.19	0.43
1:F:59:ILE:CD1	1:F:361:PRO:HA	2.48	0.43
1:I:59:ILE:CD1	1:I:361:PRO:HA	2.49	0.43
1:I:202:MET:HB3	1:I:237:LEU:HD11	2.00	0.43
1:J:18:TYR:C	1:J:20:PRO:HA	2.42	0.43
1:J:30:VAL:HG12	1:J:31:ALA:N	2.33	0.43
1:B:94:GLU:OE1	1:B:380:LYS:HA	2.19	0.43
1:B:227:LEU:HB2	1:B:339:PHE:HZ	1.84	0.43
1:H:59:ILE:CD1	1:H:361:PRO:HA	2.49	0.43
1:C:94:GLU:OE1	1:C:380:LYS:HA	2.19	0.43
1:E:19:ALA:CB	1:E:348:ILE:HB	2.49	0.43
1:A:301:HIS:N	1:A:301:HIS:ND1	2.66	0.43
1:F:69:VAL:HG12	1:F:71:LEU:HD12	2.00	0.43
1:F:156:ASP:O	1:F:194:LYS:HE2	2.19	0.43
1:H:301:HIS:N	1:H:301:HIS:ND1	2.66	0.43
1:B:19:ALA:CB	1:B:348:ILE:HB	2.49	0.43
1:B:162:KCX:OQ2	1:B:201:HIS:HB2	2.19	0.43
1:B:234:ASN:HD21	1:B:237:LEU:H	1.67	0.43
1:A:232:ASN:N	1:A:232:ASN:ND2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:VAL:HG12	1:F:31:ALA:N	2.33	0.43
1:F:301:HIS:N	1:F:301:HIS:ND1	2.66	0.43
1:F:357:LEU:HD23	1:F:368:VAL:HG13	2.01	0.43
1:J:357:LEU:HD23	1:J:368:VAL:HG13	2.01	0.43
1:L:72:ILE:HD11	1:L:104:LEU:CD2	2.49	0.43
1:C:359:MET:HE2	1:C:363:LEU:C	2.44	0.42
1:D:359:MET:HE2	1:D:363:LEU:C	2.44	0.42
1:E:208:ALA:HB3	1:E:240:GLN:OE1	2.18	0.42
1:A:72:ILE:HD11	1:A:104:LEU:CD2	2.49	0.42
1:A:147:SER:OG	1:A:150:LYS:HB2	2.20	0.42
1:I:147:SER:OG	1:I:150:LYS:HB2	2.19	0.42
1:J:301:HIS:N	1:J:301:HIS:ND1	2.66	0.42
1:K:69:VAL:HG12	1:K:71:LEU:HD12	2.00	0.42
1:B:117:LEU:HD22	1:B:121:ARG:HD2	2.01	0.42
1:C:209:LEU:HD22	1:C:212:ILE:HD12	2.01	0.42
1:D:117:LEU:HD22	1:D:121:ARG:HD2	2.01	0.42
1:A:206:LYS:HB3	1:A:206:LYS:HZ3	1.81	0.42
1:F:229:THR:HG22	1:F:230:HIS:H	1.84	0.42
1:H:72:ILE:HD11	1:H:104:LEU:CD2	2.49	0.42
1:H:357:LEU:HD23	1:H:368:VAL:HG13	2.01	0.42
1:L:301:HIS:N	1:L:301:HIS:ND1	2.66	0.42
1:F:229:THR:CG2	1:F:230:HIS:N	2.82	0.42
1:H:156:ASP:O	1:H:194:LYS:HE2	2.18	0.42
1:L:235:VAL:O	1:L:239:GLU:HG2	2.19	0.42
1:C:234:ASN:HD21	1:C:237:LEU:H	1.67	0.42
1:E:209:LEU:HD22	1:E:212:ILE:HD12	2.01	0.42
1:A:235:VAL:O	1:A:239:GLU:HG2	2.19	0.42
1:K:59:ILE:CD1	1:K:361:PRO:HA	2.48	0.42
1:L:147:SER:OG	1:L:150:LYS:HB2	2.20	0.42
1:B:209:LEU:HD22	1:B:212:ILE:HD12	2.01	0.42
1:B:271:VAL:HG21	1:B:323:PHE:HE1	1.82	0.42
1:H:30:VAL:HG12	1:H:31:ALA:N	2.33	0.42
1:I:30:VAL:HG12	1:I:31:ALA:N	2.33	0.42
1:I:229:THR:CG2	1:I:230:HIS:N	2.82	0.42
1:I:235:VAL:O	1:I:239:GLU:HG2	2.19	0.42
1:K:147:SER:OG	1:K:150:LYS:HB2	2.20	0.42
1:L:30:VAL:HG12	1:L:31:ALA:N	2.33	0.42
1:C:67:GLN:HA	1:C:101:VAL:HB	2.02	0.42
1:E:359:MET:HE2	1:E:363:LEU:C	2.45	0.42
1:A:358:VAL:CB	1:A:367:GLN:HB2	2.50	0.42
1:I:254:THR:HA	1:I:283:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:156:ASP:O	1:J:194:LYS:HE2	2.19	0.42
1:D:227:LEU:HB2	1:D:339:PHE:HZ	1.84	0.42
1:E:67:GLN:HA	1:E:101:VAL:HB	2.02	0.42
1:G:235:VAL:O	1:G:239:GLU:HG2	2.19	0.42
1:G:254:THR:HA	1:G:283:SER:O	2.20	0.42
1:H:181:MET:HE3	1:H:181:MET:HB3	1.87	0.42
1:H:254:THR:HA	1:H:283:SER:O	2.20	0.42
1:K:229:THR:CG2	1:K:230:HIS:N	2.82	0.42
1:B:359:MET:HE2	1:B:363:LEU:C	2.44	0.42
1:F:147:SER:OG	1:F:150:LYS:HB2	2.20	0.42
1:F:254:THR:HA	1:F:283:SER:O	2.20	0.42
1:F:358:VAL:CB	1:F:367:GLN:HB2	2.49	0.42
1:G:147:SER:OG	1:G:150:LYS:HB2	2.20	0.42
1:I:72:ILE:HD11	1:I:104:LEU:CD2	2.49	0.42
1:J:72:ILE:HD11	1:J:104:LEU:CD2	2.49	0.42
1:L:358:VAL:CB	1:L:367:GLN:HB2	2.49	0.42
1:C:265:GLU:HG3	1:C:269:ARG:HD2	2.02	0.42
1:A:254:THR:HA	1:A:283:SER:O	2.20	0.42
1:K:254:THR:HA	1:K:283:SER:O	2.20	0.42
1:K:357:LEU:HD23	1:K:368:VAL:HG13	2.01	0.42
1:D:67:GLN:HA	1:D:101:VAL:HB	2.02	0.42
1:G:229:THR:CG2	1:G:230:HIS:N	2.82	0.42
1:H:235:VAL:O	1:H:239:GLU:HG2	2.19	0.42
1:J:122:ALA:O	1:J:126:GLU:HG3	2.20	0.42
1:K:72:ILE:HD11	1:K:104:LEU:CD2	2.49	0.42
1:L:357:LEU:HD23	1:L:368:VAL:HG13	2.01	0.42
1:C:271:VAL:HG21	1:C:323:PHE:HE1	1.82	0.41
1:E:63:GLY:HA2	1:E:357:LEU:CG	2.45	0.41
1:E:234:ASN:HD21	1:E:237:LEU:H	1.66	0.41
1:A:68:HIS:HA	1:A:103:LEU:CD1	2.50	0.41
1:A:357:LEU:HD23	1:A:368:VAL:HG13	2.02	0.41
1:F:122:ALA:O	1:F:126:GLU:HG3	2.20	0.41
1:G:357:LEU:HD23	1:G:368:VAL:HG13	2.02	0.41
1:I:122:ALA:O	1:I:126:GLU:HG3	2.20	0.41
1:K:206:LYS:HB3	1:K:206:LYS:HZ2	1.85	0.41
1:B:65:ILE:HA	1:B:99:SER:O	2.21	0.41
1:C:63:GLY:HA2	1:C:357:LEU:CG	2.45	0.41
1:C:163:CYS:SG	1:C:181:MET:HE1	2.60	0.41
1:D:265:GLU:HG3	1:D:269:ARG:HD2	2.02	0.41
1:F:72:ILE:HD11	1:F:104:LEU:CD2	2.49	0.41
1:G:72:ILE:HD11	1:G:104:LEU:CD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:358:VAL:CB	1:G:367:GLN:HB2	2.49	0.41
1:J:235:VAL:O	1:J:239:GLU:HG2	2.19	0.41
1:J:254:THR:HA	1:J:283:SER:O	2.20	0.41
1:L:68:HIS:CD2	1:L:103:LEU:HD11	2.56	0.41
1:B:7:ALA:HB2	1:G:36:ILE:HB	2.02	0.41
1:C:7:ALA:HB2	1:H:36:ILE:HB	2.02	0.41
1:C:117:LEU:HD22	1:C:121:ARG:HD2	2.01	0.41
1:E:117:LEU:HD22	1:E:121:ARG:HD2	2.01	0.41
1:A:68:HIS:CD2	1:A:103:LEU:HD11	2.56	0.41
1:H:68:HIS:CD2	1:H:103:LEU:HD11	2.56	0.41
1:H:122:ALA:O	1:H:126:GLU:HG3	2.20	0.41
1:H:147:SER:OG	1:H:150:LYS:HB2	2.20	0.41
1:J:147:SER:OG	1:J:150:LYS:HB2	2.20	0.41
1:K:358:VAL:CB	1:K:367:GLN:HB2	2.49	0.41
1:B:67:GLN:HA	1:B:101:VAL:HB	2.02	0.41
1:D:209:LEU:HD22	1:D:212:ILE:HD12	2.01	0.41
1:E:7:ALA:HB2	1:F:36:ILE:HB	2.02	0.41
1:E:265:GLU:HG3	1:E:269:ARG:HD2	2.02	0.41
1:A:166:SER:O	1:A:203:GLY:HA3	2.21	0.41
1:F:229:THR:HG22	1:F:230:HIS:CD2	2.56	0.41
1:G:122:ALA:O	1:G:126:GLU:HG3	2.20	0.41
1:I:68:HIS:CD2	1:I:103:LEU:HD11	2.56	0.41
1:J:166:SER:O	1:J:203:GLY:HA3	2.20	0.41
1:K:235:VAL:O	1:K:239:GLU:HG2	2.19	0.41
1:L:254:THR:HA	1:L:283:SER:O	2.20	0.41
1:D:163:CYS:SG	1:D:181:MET:HE1	2.60	0.41
1:E:69:VAL:O	1:E:102:GLY:HA2	2.21	0.41
1:F:226:LEU:HD22	1:F:226:LEU:H	1.86	0.41
1:G:177:HIS:O	1:G:181:MET:HB2	2.21	0.41
1:B:69:VAL:O	1:B:102:GLY:HA2	2.21	0.41
1:C:65:ILE:HA	1:C:99:SER:O	2.21	0.41
1:D:7:ALA:HB2	1:A:36:ILE:HB	2.02	0.41
1:D:136:ALA:O	1:D:163:CYS:HA	2.21	0.41
1:E:136:ALA:O	1:E:163:CYS:HA	2.21	0.41
1:E:231:VAL:HA	1:E:237:LEU:HD13	2.03	0.41
1:G:166:SER:O	1:G:203:GLY:HA3	2.21	0.41
1:G:229:THR:HG22	1:G:230:HIS:CD2	2.56	0.41
1:I:177:HIS:O	1:I:181:MET:HB2	2.21	0.41
1:J:68:HIS:CD2	1:J:103:LEU:HD11	2.56	0.41
1:K:122:ALA:O	1:K:126:GLU:HG3	2.20	0.41
1:B:136:ALA:O	1:B:163:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:CYS:SG	1:B:181:MET:HE1	2.60	0.41
1:B:265:GLU:HG3	1:B:269:ARG:HD2	2.02	0.41
1:A:234:ASN:ND2	1:A:234:ASN:C	2.79	0.41
1:H:177:HIS:O	1:H:181:MET:HB2	2.21	0.41
1:H:229:THR:CG2	1:H:230:HIS:N	2.82	0.41
1:I:357:LEU:HD23	1:I:368:VAL:HG13	2.01	0.41
1:J:112:HIS:HA	1:J:113:PRO:HD3	1.97	0.41
1:J:358:VAL:CB	1:J:367:GLN:HB2	2.50	0.41
1:K:206:LYS:HB3	1:K:206:LYS:HZ3	1.81	0.41
1:L:177:HIS:O	1:L:181:MET:HB2	2.21	0.41
1:L:229:THR:HG22	1:L:230:HIS:CD2	2.56	0.41
1:D:65:ILE:HA	1:D:99:SER:O	2.21	0.41
1:E:65:ILE:HA	1:E:99:SER:O	2.21	0.41
1:F:234:ASN:ND2	1:F:234:ASN:C	2.79	0.41
1:F:235:VAL:O	1:F:239:GLU:HG2	2.19	0.41
1:G:68:HIS:CD2	1:G:103:LEU:HD11	2.56	0.41
1:H:229:THR:HG22	1:H:230:HIS:CD2	2.56	0.41
1:H:358:VAL:CB	1:H:367:GLN:HB2	2.50	0.41
1:H:166:SER:O	1:H:203:GLY:HA3	2.21	0.41
1:I:229:THR:HG22	1:I:230:HIS:CD2	2.56	0.41
1:L:122:ALA:O	1:L:126:GLU:HG3	2.20	0.41
1:L:234:ASN:ND2	1:L:234:ASN:C	2.79	0.41
1:J:181:MET:HE3	1:J:181:MET:HB3	1.87	0.41
1:K:166:SER:O	1:K:203:GLY:HA3	2.21	0.41
1:E:129:SER:CB	1:E:345:LYS:HE3	2.51	0.40
1:G:234:ASN:ND2	1:G:234:ASN:C	2.79	0.40
1:J:226:LEU:HD22	1:J:226:LEU:H	1.86	0.40
1:J:229:THR:HG22	1:J:230:HIS:CD2	2.56	0.40
1:B:129:SER:CB	1:B:345:LYS:HE3	2.51	0.40
1:C:69:VAL:O	1:C:102:GLY:HA2	2.21	0.40
1:D:72:ILE:HG22	1:D:119:LYS:HB2	2.03	0.40
1:E:121:ARG:O	1:E:125:GLU:HG3	2.21	0.40
1:E:163:CYS:SG	1:E:181:MET:HE1	2.60	0.40
1:A:122:ALA:O	1:A:126:GLU:HG3	2.20	0.40
1:A:177:HIS:O	1:A:181:MET:HB2	2.21	0.40
1:F:166:SER:O	1:F:203:GLY:HA3	2.21	0.40
1:K:177:HIS:O	1:K:181:MET:HB2	2.21	0.40
1:L:166:SER:O	1:L:203:GLY:HA3	2.21	0.40
1:E:21:GLU:CD	1:E:21:GLU:H	2.29	0.40
1:E:271:VAL:HG21	1:E:323:PHE:CZ	2.57	0.40
1:I:166:SER:O	1:I:203:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:MET:HB3	1:I:181:MET:HE3	1.87	0.40
1:I:226:LEU:HD22	1:I:226:LEU:H	1.85	0.40
1:J:234:ASN:ND2	1:J:234:ASN:C	2.79	0.40
1:B:328:ALA:O	1:B:331:PRO:HD2	2.22	0.40
1:F:177:HIS:O	1:F:181:MET:HB2	2.21	0.40
1:H:234:ASN:ND2	1:H:234:ASN:C	2.79	0.40
1:J:177:HIS:O	1:J:181:MET:HB2	2.21	0.40
1:K:229:THR:HG22	1:K:230:HIS:CD2	2.56	0.40
1:K:234:ASN:ND2	1:K:234:ASN:C	2.79	0.40
1:B:21:GLU:CD	1:B:21:GLU:H	2.29	0.40
1:D:121:ARG:O	1:D:125:GLU:HG3	2.21	0.40
1:E:328:ALA:O	1:E:331:PRO:HD2	2.22	0.40
1:A:202:MET:HE1	1:A:208:ALA:O	2.22	0.40
1:A:206:LYS:HB3	1:A:206:LYS:HZ2	1.85	0.40
1:A:229:THR:HG22	1:A:230:HIS:CD2	2.56	0.40
1:A:230:HIS:O	1:A:233:ARG:HG2	2.22	0.40
1:F:230:HIS:O	1:F:233:ARG:HG2	2.22	0.40
1:H:226:LEU:HD22	1:H:226:LEU:H	1.85	0.40
1:H:230:HIS:O	1:H:233:ARG:HG2	2.22	0.40
1:J:230:HIS:O	1:J:233:ARG:HG2	2.22	0.40
1:K:68:HIS:CD2	1:K:103:LEU:HD11	2.56	0.40
1:K:230:HIS:O	1:K:233:ARG:HG2	2.22	0.40
1:L:230:HIS:O	1:L:233:ARG:HG2	2.22	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 PDB entries followed by that with respect to all EM entries.

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	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	11 46
1	B	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	16 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	16	54
1	D	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	16	54
1	E	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	16	54
1	F	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	11	46
1	G	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	11	46
1	H	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	11	46
1	I	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	11	46
1	J	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	11	46
1	K	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	11	46
1	L	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	11	46
All	All	4444/4680 (95%)	4076 (92%)	324 (7%)	44 (1%)	15	49

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	PRO
1	C	48	PRO
1	D	48	PRO
1	E	48	PRO
1	A	48	PRO
1	A	303	GLY
1	F	48	PRO
1	F	303	GLY
1	G	48	PRO
1	G	303	GLY
1	H	48	PRO
1	H	303	GLY
1	I	48	PRO
1	I	303	GLY
1	J	48	PRO
1	J	303	GLY
1	K	48	PRO
1	K	303	GLY
1	L	48	PRO
1	L	303	GLY
1	B	49	ASN
1	C	49	ASN
1	D	49	ASN

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Mol	Chain	Res	Type
1	E	49	ASN
1	A	309	THR
1	F	309	THR
1	G	309	THR
1	H	309	THR
1	I	309	THR
1	J	309	THR
1	K	309	THR
1	L	309	THR
1	A	19	ALA
1	F	19	ALA
1	G	19	ALA
1	H	19	ALA
1	I	19	ALA
1	J	19	ALA
1	K	19	ALA
1	L	19	ALA
1	B	19	ALA
1	C	19	ALA
1	D	19	ALA
1	E	19	ALA

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 PDB entries followed by that with respect to all EM entries.

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	299/312 (96%)	269 (90%)	30 (10%)	7	24
1	B	297/312 (95%)	282 (95%)	15 (5%)	21	42
1	C	297/312 (95%)	282 (95%)	15 (5%)	21	42
1	D	297/312 (95%)	282 (95%)	15 (5%)	21	42
1	E	297/312 (95%)	282 (95%)	15 (5%)	21	42
1	F	299/312 (96%)	269 (90%)	30 (10%)	7	24
1	G	299/312 (96%)	269 (90%)	30 (10%)	7	24
1	H	299/312 (96%)	269 (90%)	30 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	299/312 (96%)	269 (90%)	30 (10%)	7	24
1	J	299/312 (96%)	269 (90%)	30 (10%)	7	24
1	K	299/312 (96%)	269 (90%)	30 (10%)	7	24
1	L	299/312 (96%)	269 (90%)	30 (10%)	7	24
All	All	3580/3744 (96%)	3280 (92%)	300 (8%)	12	30

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	LEU
1	B	91	ARG
1	B	103	LEU
1	B	116	LEU
1	B	117	LEU
1	B	123	LEU
1	B	156	ASP
1	B	226	LEU
1	B	232	ASN
1	B	235	VAL
1	B	237	LEU
1	B	242	LEU
1	B	287	ASN
1	B	311	LEU
1	B	356	LEU
1	C	29	LEU
1	C	91	ARG
1	C	103	LEU
1	C	116	LEU
1	C	117	LEU
1	C	123	LEU
1	C	156	ASP
1	C	226	LEU
1	C	232	ASN
1	C	235	VAL
1	C	237	LEU
1	C	242	LEU
1	C	287	ASN
1	C	311	LEU
1	C	356	LEU
1	D	29	LEU
1	D	91	ARG

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Mol	Chain	Res	Type
1	D	103	LEU
1	D	116	LEU
1	D	117	LEU
1	D	123	LEU
1	D	156	ASP
1	D	226	LEU
1	D	232	ASN
1	D	235	VAL
1	D	237	LEU
1	D	242	LEU
1	D	287	ASN
1	D	311	LEU
1	D	356	LEU
1	E	29	LEU
1	E	91	ARG
1	E	103	LEU
1	E	116	LEU
1	E	117	LEU
1	E	123	LEU
1	E	156	ASP
1	E	226	LEU
1	E	232	ASN
1	E	235	VAL
1	E	237	LEU
1	E	242	LEU
1	E	287	ASN
1	E	311	LEU
1	E	356	LEU
1	A	17	LEU
1	A	21	GLU
1	A	29	LEU
1	A	53	VAL
1	A	55	LEU
1	A	89	LEU
1	A	91	ARG
1	A	98	THR
1	A	103	LEU
1	A	116	LEU
1	A	117	LEU
1	A	120	THR
1	A	123	LEU
1	A	181	MET

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Mol	Chain	Res	Type
1	A	217	GLU
1	A	232	ASN
1	A	234	ASN
1	A	235	VAL
1	A	237	LEU
1	A	257	ILE
1	A	277	LEU
1	A	287	ASN
1	A	301	HIS
1	A	304	VAL
1	A	317	LEU
1	A	332	LEU
1	A	356	LEU
1	A	362	GLU
1	A	375	MET
1	A	386	THR
1	F	17	LEU
1	F	21	GLU
1	F	29	LEU
1	F	53	VAL
1	F	55	LEU
1	F	89	LEU
1	F	91	ARG
1	F	98	THR
1	F	103	LEU
1	F	116	LEU
1	F	117	LEU
1	F	120	THR
1	F	123	LEU
1	F	181	MET
1	F	217	GLU
1	F	232	ASN
1	F	234	ASN
1	F	235	VAL
1	F	237	LEU
1	F	257	ILE
1	F	277	LEU
1	F	287	ASN
1	F	301	HIS
1	F	304	VAL
1	F	317	LEU
1	F	332	LEU

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Mol	Chain	Res	Type
1	F	356	LEU
1	F	362	GLU
1	F	375	MET
1	F	386	THR
1	G	17	LEU
1	G	21	GLU
1	G	29	LEU
1	G	53	VAL
1	G	55	LEU
1	G	89	LEU
1	G	91	ARG
1	G	98	THR
1	G	103	LEU
1	G	116	LEU
1	G	117	LEU
1	G	120	THR
1	G	123	LEU
1	G	181	MET
1	G	217	GLU
1	G	232	ASN
1	G	234	ASN
1	G	235	VAL
1	G	237	LEU
1	G	257	ILE
1	G	277	LEU
1	G	287	ASN
1	G	301	HIS
1	G	304	VAL
1	G	317	LEU
1	G	332	LEU
1	G	356	LEU
1	G	362	GLU
1	G	375	MET
1	G	386	THR
1	H	17	LEU
1	H	21	GLU
1	H	29	LEU
1	H	53	VAL
1	H	55	LEU
1	H	89	LEU
1	H	91	ARG
1	H	98	THR

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Mol	Chain	Res	Type
1	H	103	LEU
1	H	116	LEU
1	H	117	LEU
1	H	120	THR
1	H	123	LEU
1	H	181	MET
1	H	217	GLU
1	H	232	ASN
1	H	234	ASN
1	H	235	VAL
1	H	237	LEU
1	H	257	ILE
1	H	277	LEU
1	H	287	ASN
1	H	301	HIS
1	H	304	VAL
1	H	317	LEU
1	H	332	LEU
1	H	356	LEU
1	H	362	GLU
1	H	375	MET
1	H	386	THR
1	I	17	LEU
1	I	21	GLU
1	I	29	LEU
1	I	53	VAL
1	I	55	LEU
1	I	89	LEU
1	I	91	ARG
1	I	98	THR
1	I	103	LEU
1	I	116	LEU
1	I	117	LEU
1	I	120	THR
1	I	123	LEU
1	I	181	MET
1	I	217	GLU
1	I	232	ASN
1	I	234	ASN
1	I	235	VAL
1	I	237	LEU
1	I	257	ILE

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Mol	Chain	Res	Type
1	I	277	LEU
1	I	287	ASN
1	I	301	HIS
1	I	304	VAL
1	I	317	LEU
1	I	332	LEU
1	I	356	LEU
1	I	362	GLU
1	I	375	MET
1	I	386	THR
1	J	17	LEU
1	J	21	GLU
1	J	29	LEU
1	J	53	VAL
1	J	55	LEU
1	J	89	LEU
1	J	91	ARG
1	J	98	THR
1	J	103	LEU
1	J	116	LEU
1	J	117	LEU
1	J	120	THR
1	J	123	LEU
1	J	181	MET
1	J	217	GLU
1	J	232	ASN
1	J	234	ASN
1	J	235	VAL
1	J	237	LEU
1	J	257	ILE
1	J	277	LEU
1	J	287	ASN
1	J	301	HIS
1	J	304	VAL
1	J	317	LEU
1	J	332	LEU
1	J	356	LEU
1	J	362	GLU
1	J	375	MET
1	J	386	THR
1	K	17	LEU
1	K	21	GLU

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Mol	Chain	Res	Type
1	K	29	LEU
1	K	53	VAL
1	K	55	LEU
1	K	89	LEU
1	K	91	ARG
1	K	98	THR
1	K	103	LEU
1	K	116	LEU
1	K	117	LEU
1	K	120	THR
1	K	123	LEU
1	K	181	MET
1	K	217	GLU
1	K	232	ASN
1	K	234	ASN
1	K	235	VAL
1	K	237	LEU
1	K	257	ILE
1	K	277	LEU
1	K	287	ASN
1	K	301	HIS
1	K	304	VAL
1	K	317	LEU
1	K	332	LEU
1	K	356	LEU
1	K	362	GLU
1	K	375	MET
1	K	386	THR
1	L	17	LEU
1	L	21	GLU
1	L	29	LEU
1	L	53	VAL
1	L	55	LEU
1	L	89	LEU
1	L	91	ARG
1	L	98	THR
1	L	103	LEU
1	L	116	LEU
1	L	117	LEU
1	L	120	THR
1	L	123	LEU
1	L	181	MET

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Mol	Chain	Res	Type
1	L	217	GLU
1	L	232	ASN
1	L	234	ASN
1	L	235	VAL
1	L	237	LEU
1	L	257	ILE
1	L	277	LEU
1	L	287	ASN
1	L	301	HIS
1	L	304	VAL
1	L	317	LEU
1	L	332	LEU
1	L	356	LEU
1	L	362	GLU
1	L	375	MET
1	L	386	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	ASN
1	B	41	ASN
1	B	49	ASN
1	B	67	GLN
1	B	218	ASN
1	B	232	ASN
1	B	234	ASN
1	B	367	GLN
1	C	32	ASN
1	C	41	ASN
1	C	49	ASN
1	C	67	GLN
1	C	218	ASN
1	C	232	ASN
1	C	234	ASN
1	C	367	GLN
1	D	32	ASN
1	D	41	ASN
1	D	49	ASN
1	D	67	GLN
1	D	218	ASN
1	D	232	ASN

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Mol	Chain	Res	Type
1	D	234	ASN
1	D	367	GLN
1	E	32	ASN
1	E	49	ASN
1	E	67	GLN
1	E	218	ASN
1	E	232	ASN
1	E	234	ASN
1	E	367	GLN
1	A	32	ASN
1	A	49	ASN
1	A	67	GLN
1	A	68	HIS
1	A	180	ASN
1	A	232	ASN
1	A	234	ASN
1	A	287	ASN
1	A	315	GLN
1	F	32	ASN
1	F	49	ASN
1	F	67	GLN
1	F	68	HIS
1	F	180	ASN
1	F	232	ASN
1	F	234	ASN
1	F	287	ASN
1	F	315	GLN
1	G	32	ASN
1	G	67	GLN
1	G	68	HIS
1	G	180	ASN
1	G	232	ASN
1	G	234	ASN
1	G	287	ASN
1	G	315	GLN
1	H	32	ASN
1	H	67	GLN
1	H	68	HIS
1	H	180	ASN
1	H	232	ASN
1	H	234	ASN
1	H	287	ASN

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Mol	Chain	Res	Type
1	H	315	GLN
1	I	32	ASN
1	I	49	ASN
1	I	67	GLN
1	I	68	HIS
1	I	180	ASN
1	I	230	HIS
1	I	232	ASN
1	I	234	ASN
1	I	287	ASN
1	I	315	GLN
1	J	32	ASN
1	J	49	ASN
1	J	67	GLN
1	J	68	HIS
1	J	180	ASN
1	J	230	HIS
1	J	232	ASN
1	J	234	ASN
1	J	287	ASN
1	K	32	ASN
1	K	49	ASN
1	K	67	GLN
1	K	68	HIS
1	K	180	ASN
1	K	232	ASN
1	K	234	ASN
1	K	287	ASN
1	K	315	GLN
1	L	32	ASN
1	L	67	GLN
1	L	68	HIS
1	L	180	ASN
1	L	232	ASN
1	L	234	ASN
1	L	287	ASN
1	L	315	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	F	162	1	10,11,12	0.93	1 (10%)	6,12,14	1.20	1 (16%)
1	KCX	H	162	1	10,11,12	0.94	1 (10%)	6,12,14	1.18	1 (16%)
1	KCX	E	162	1	10,11,12	1.01	1 (10%)	6,12,14	1.16	1 (16%)
1	KCX	D	162	1	10,11,12	0.99	1 (10%)	6,12,14	1.17	1 (16%)
1	KCX	A	162	1	10,11,12	0.94	1 (10%)	6,12,14	1.19	1 (16%)
1	KCX	B	162	1	10,11,12	1.02	1 (10%)	6,12,14	1.16	1 (16%)
1	KCX	C	162	1	10,11,12	1.02	1 (10%)	6,12,14	1.16	1 (16%)
1	KCX	G	162	1	10,11,12	0.94	1 (10%)	6,12,14	1.19	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	F	162	1	-	0/9/10/12	-
1	KCX	H	162	1	-	0/9/10/12	-
1	KCX	E	162	1	-	2/9/10/12	-
1	KCX	D	162	1	-	2/9/10/12	-
1	KCX	A	162	1	-	0/9/10/12	-
1	KCX	B	162	1	-	2/9/10/12	-
1	KCX	C	162	1	-	2/9/10/12	-
1	KCX	G	162	1	-	0/9/10/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	KCX	OQ1-CX	2.66	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	KCX	OQ1-CX	2.65	1.26	1.21
1	E	162	KCX	OQ1-CX	2.64	1.26	1.21
1	D	162	KCX	OQ1-CX	2.56	1.26	1.21
1	H	162	KCX	OQ1-CX	2.47	1.26	1.21
1	G	162	KCX	OQ1-CX	2.47	1.26	1.21
1	A	162	KCX	OQ1-CX	2.46	1.26	1.21
1	F	162	KCX	OQ1-CX	2.45	1.26	1.21

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	KCX	OQ1-CX-NZ	-2.35	121.35	124.92
1	E	162	KCX	OQ1-CX-NZ	-2.34	121.37	124.92
1	C	162	KCX	OQ1-CX-NZ	-2.33	121.38	124.92
1	B	162	KCX	OQ1-CX-NZ	-2.33	121.38	124.92
1	F	162	KCX	OQ1-CX-NZ	-2.31	121.42	124.92
1	A	162	KCX	OQ1-CX-NZ	-2.28	121.46	124.92
1	G	162	KCX	OQ1-CX-NZ	-2.26	121.49	124.92
1	H	162	KCX	OQ1-CX-NZ	-2.24	121.52	124.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	162	KCX	CA-CB-CG-CD
1	C	162	KCX	CA-CB-CG-CD
1	D	162	KCX	CA-CB-CG-CD
1	E	162	KCX	CA-CB-CG-CD
1	E	162	KCX	CG-CD-CE-NZ
1	B	162	KCX	CG-CD-CE-NZ
1	C	162	KCX	CG-CD-CE-NZ
1	D	162	KCX	CG-CD-CE-NZ

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	162	KCX	1	0
1	H	162	KCX	1	0
1	E	162	KCX	2	0
1	D	162	KCX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	162	KCX	1	0
1	B	162	KCX	2	0
1	C	162	KCX	2	0
1	G	162	KCX	1	0

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.

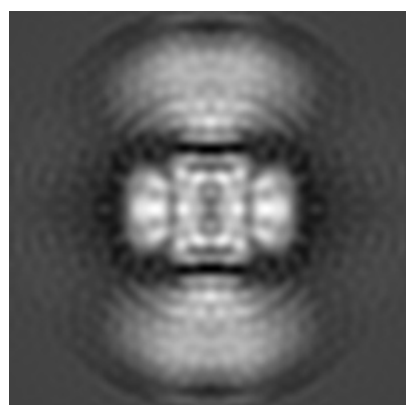
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4094. These allow visual inspection of the internal detail of the map and identification of artifacts.

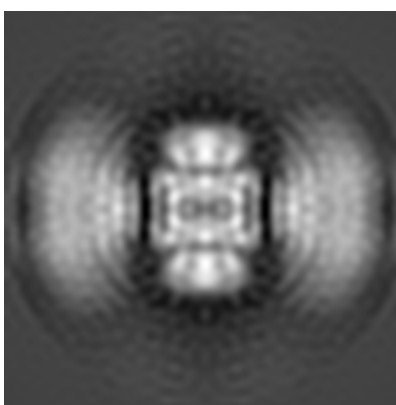
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

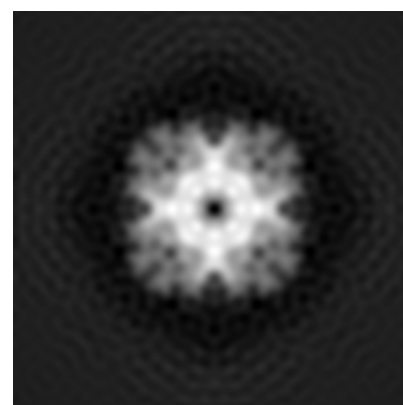
6.1.1 Primary map



X



Y

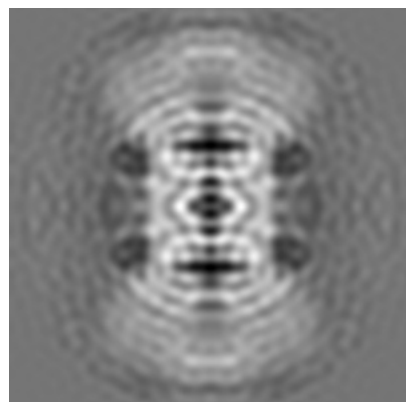


Z

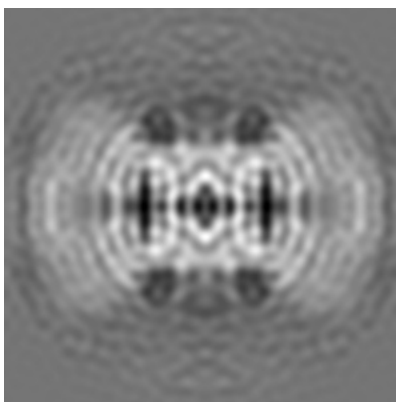
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

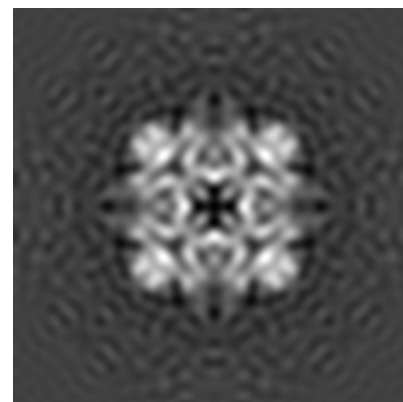
6.2.1 Primary map



X Index: 64



Y Index: 64

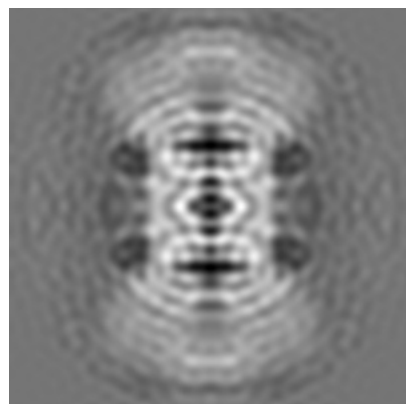


Z Index: 64

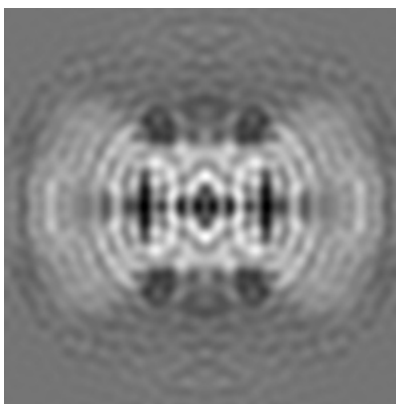
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

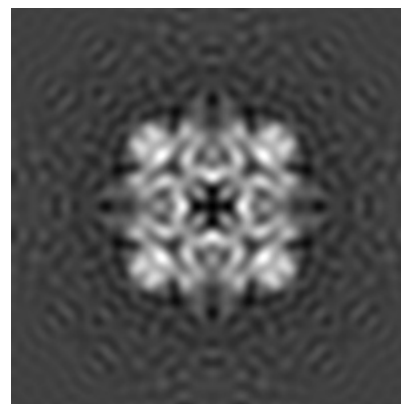
6.3.1 Primary map



X Index: 64



Y Index: 64

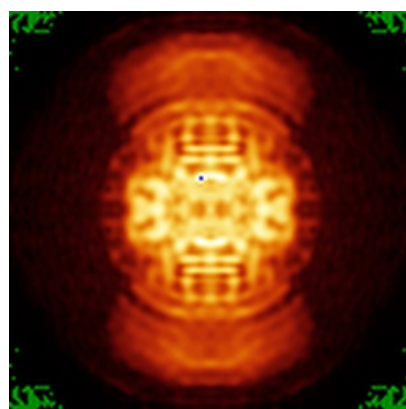


Z Index: 64

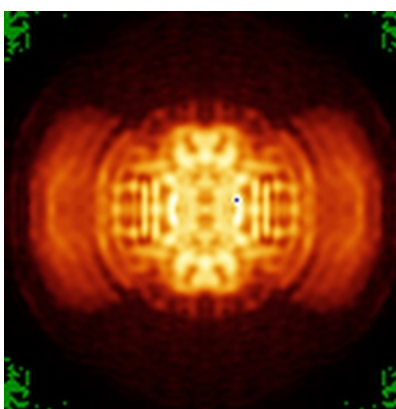
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

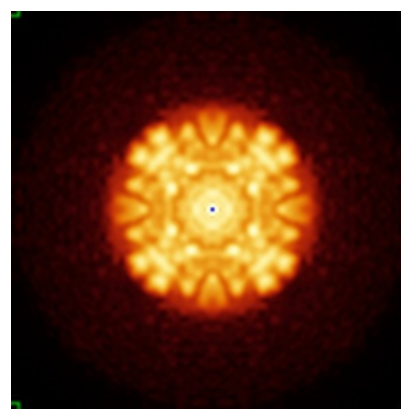
6.4.1 Primary map



X



Y



Z

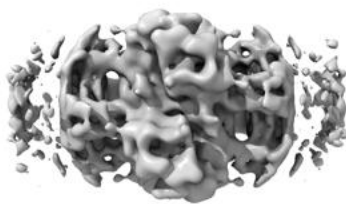
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

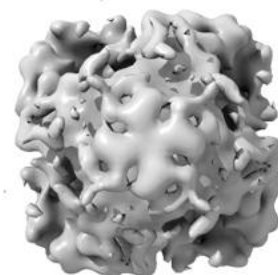
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0338. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

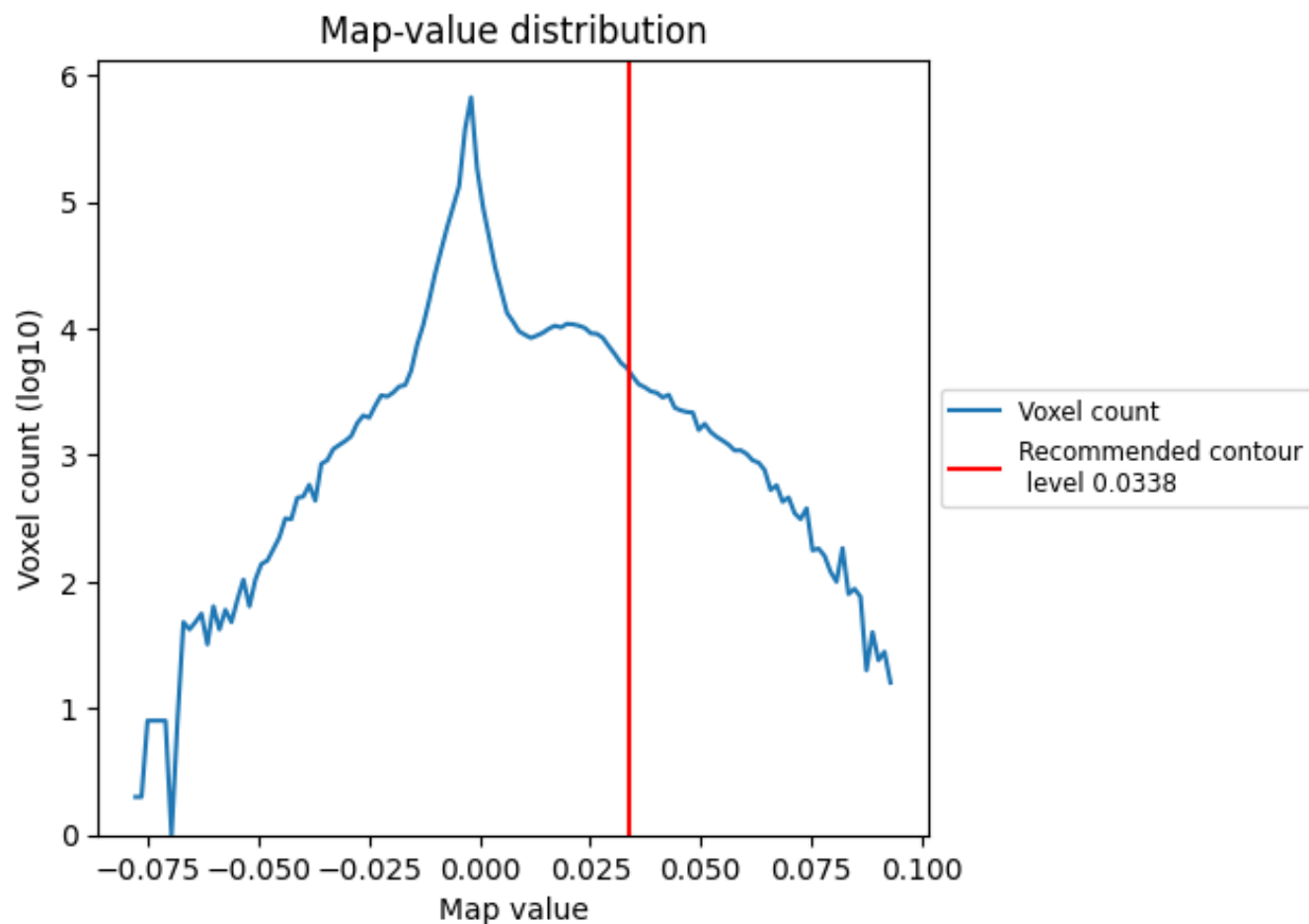
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

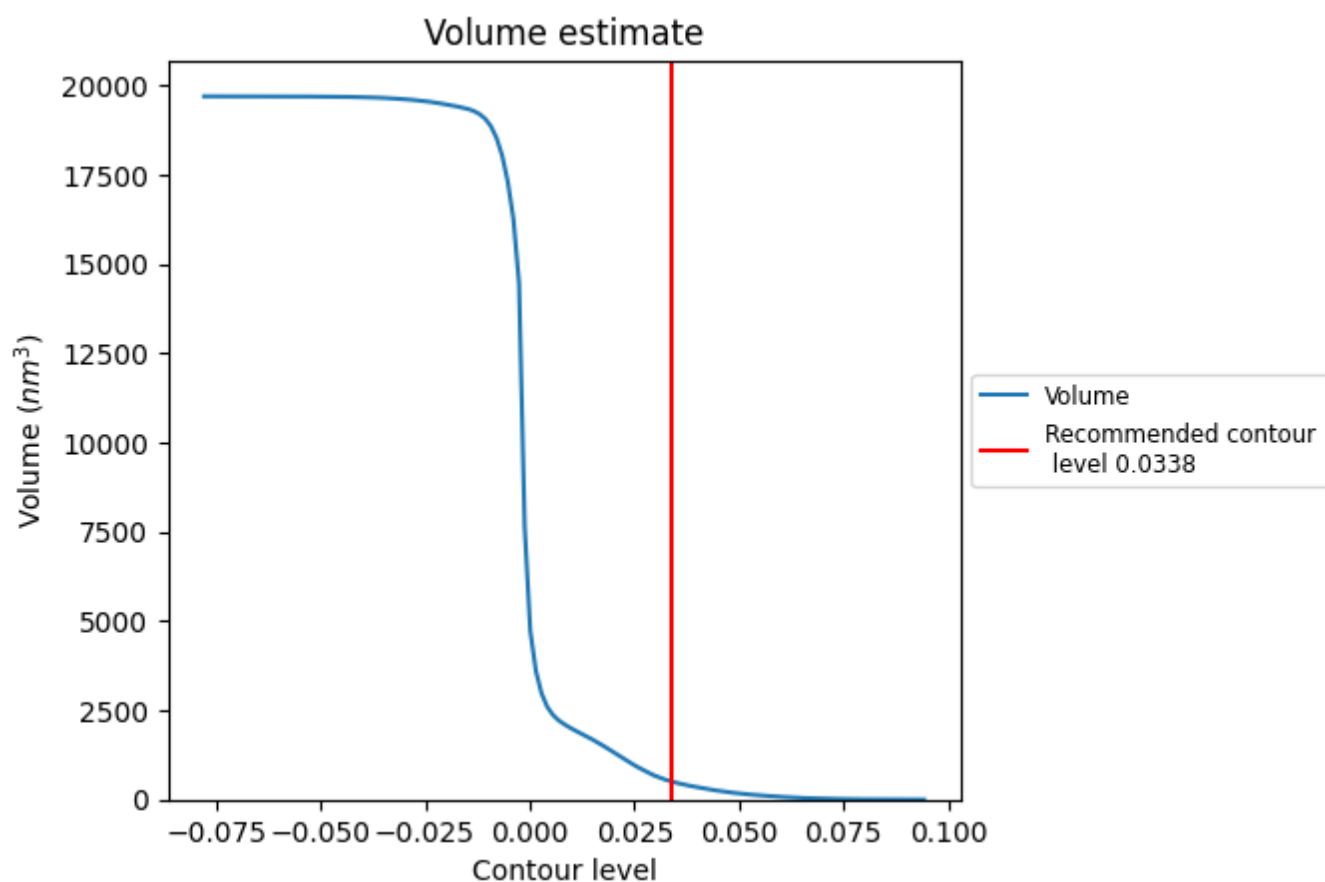
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

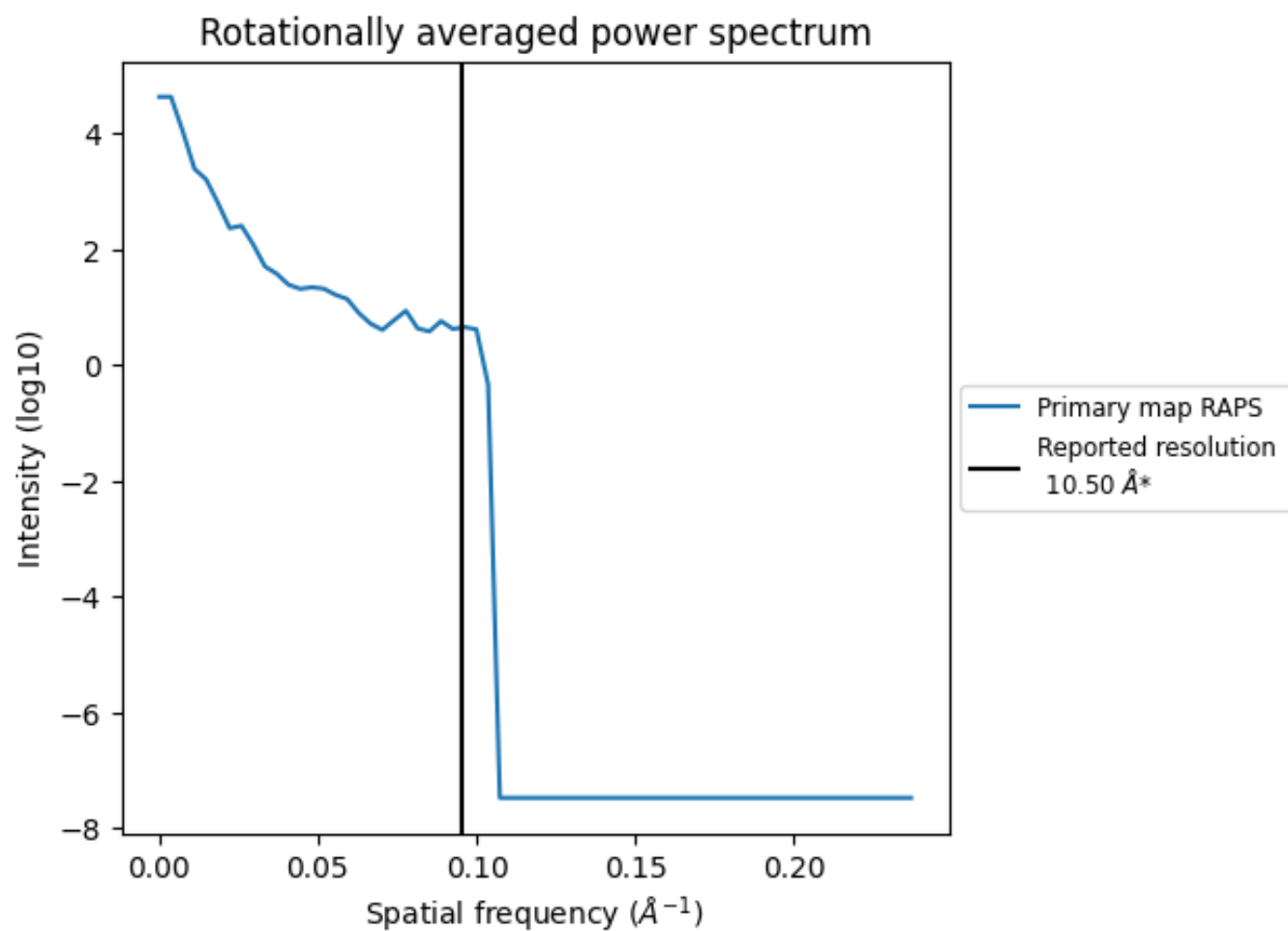
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 510 nm³; this corresponds to an approximate mass of 460 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.095 Å⁻¹

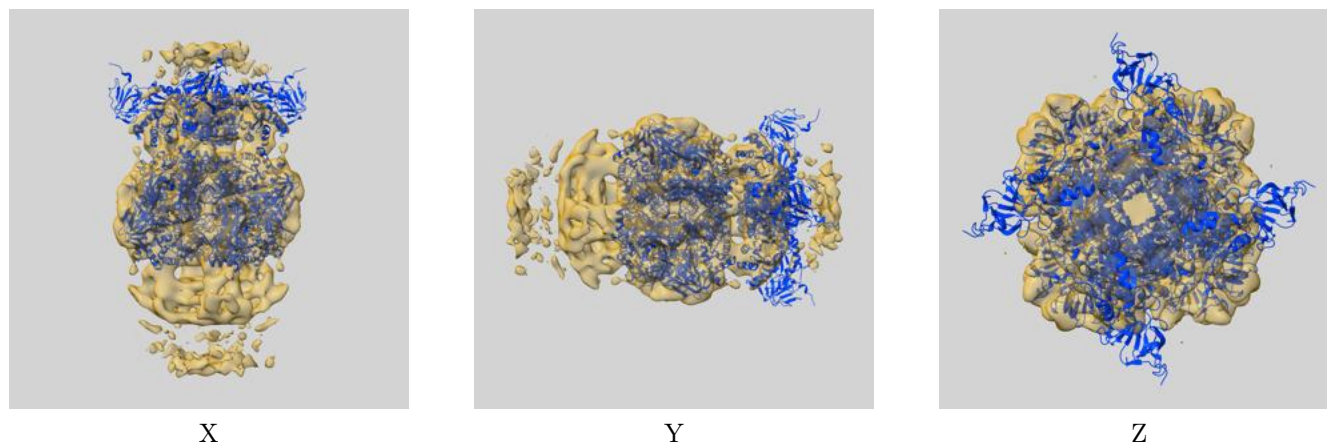
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

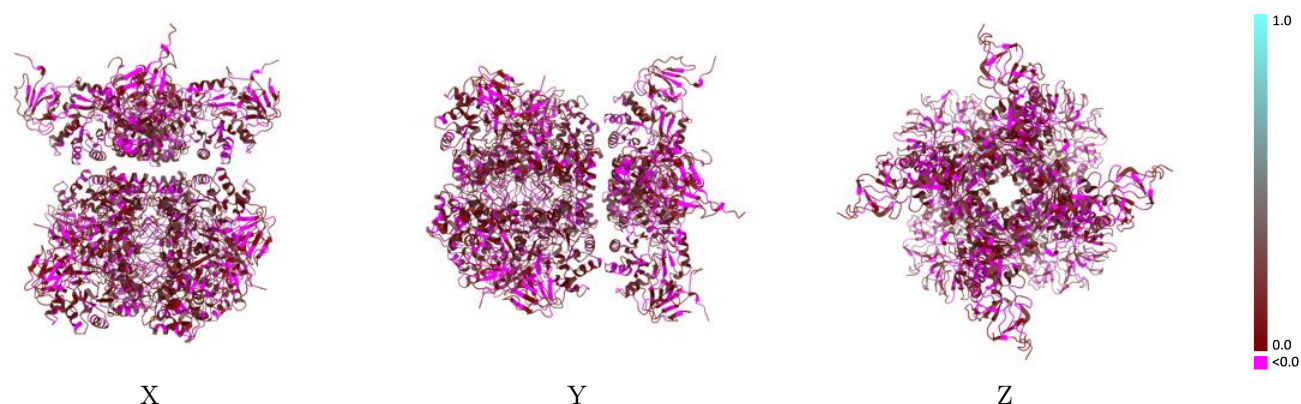
This section contains information regarding the fit between EMDB map EMD-4094 and PDB model 5LP3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



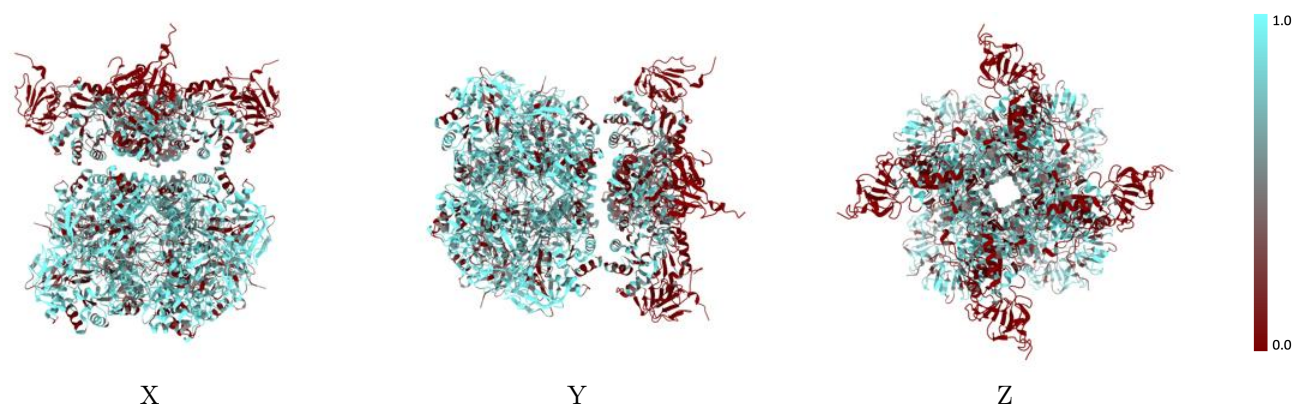
The images above show the 3D surface view of the map at the recommended contour level 0.0338 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



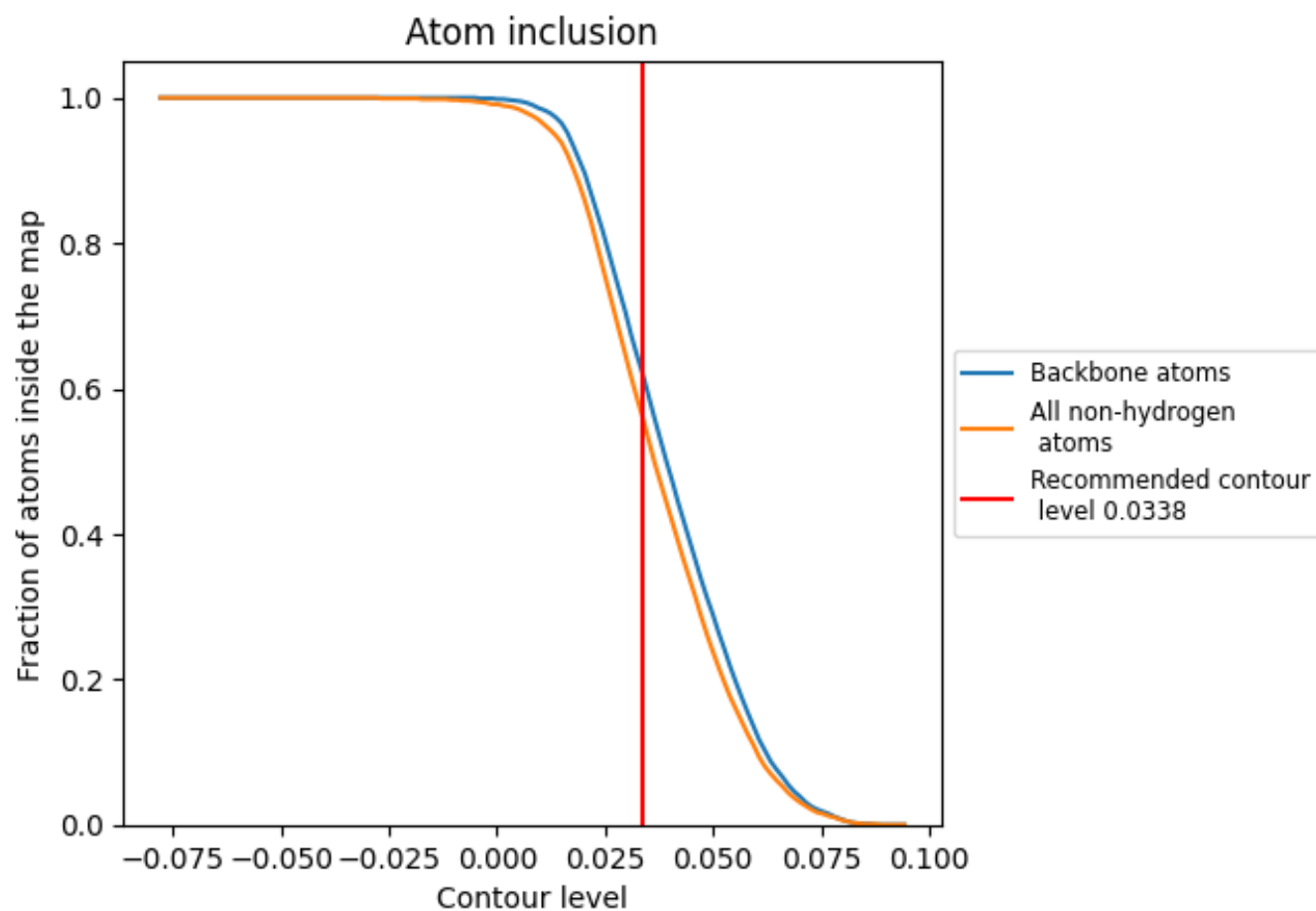
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0338).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0338) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5580	0.0650
A	0.6820	0.0690
B	0.6810	0.0680
C	0.6920	0.0740
D	0.6920	0.0720
E	0.6820	0.0700
F	0.6800	0.0700
G	0.6700	0.0650
H	0.6840	0.0730
I	0.3050	0.0550
J	0.3070	0.0560
K	0.3130	0.0560
L	0.3040	0.0560

