



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 04:23 AM UTC

PDB ID : 4CHW / pdb_00004chw
EMDB ID : EMD-2527
Title : The electron crystallography structure of the cAMP-free potassium channel MloK1
Authors : Kowal, J.; Chami, M.; Baumgartner, P.; Arheit, M.; Chiu, P.L.; Rangl, M.; Scheuring, S.; Schroeder, G.F.; Nimigean, C.M.; Stahlberg, H.
Deposited on : 2013-12-04
Resolution : 7.00 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
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

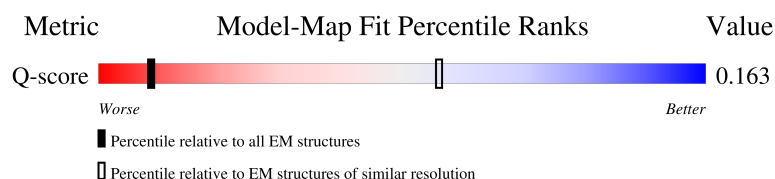
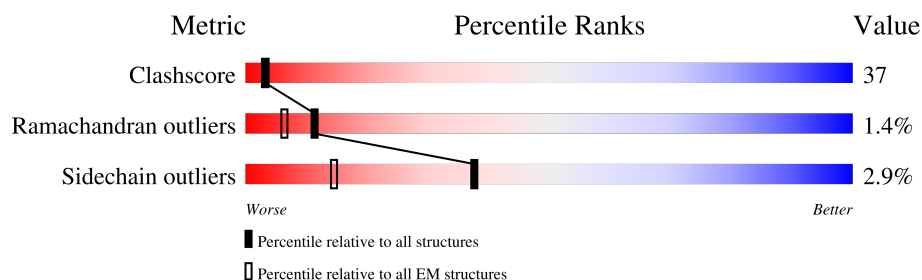
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 7.00 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	483 (6.50 - 7.50)

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	361	
1	B	361	
1	C	361	
1	D	361	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10342 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 CYCLIC NUCLEOTIDE-GATED POTASSIUM CHANNEL MLL3241.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	344	Total	C	N	O	S	0	1
			2585	1684	444	447	10		
1	B	344	Total	C	N	O	S	0	1
			2585	1684	444	447	10		
1	C	344	Total	C	N	O	S	0	1
			2585	1684	444	447	10		
1	D	344	Total	C	N	O	S	0	1
			2585	1684	444	447	10		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	HIS	-	expression tag	UNP Q98GN8
A	357	HIS	-	expression tag	UNP Q98GN8
A	358	HIS	-	expression tag	UNP Q98GN8
A	359	HIS	-	expression tag	UNP Q98GN8
A	360	HIS	-	expression tag	UNP Q98GN8
A	361	HIS	-	expression tag	UNP Q98GN8
B	356	HIS	-	expression tag	UNP Q98GN8
B	357	HIS	-	expression tag	UNP Q98GN8
B	358	HIS	-	expression tag	UNP Q98GN8
B	359	HIS	-	expression tag	UNP Q98GN8
B	360	HIS	-	expression tag	UNP Q98GN8
B	361	HIS	-	expression tag	UNP Q98GN8
C	356	HIS	-	expression tag	UNP Q98GN8
C	357	HIS	-	expression tag	UNP Q98GN8
C	358	HIS	-	expression tag	UNP Q98GN8
C	359	HIS	-	expression tag	UNP Q98GN8
C	360	HIS	-	expression tag	UNP Q98GN8
C	361	HIS	-	expression tag	UNP Q98GN8
D	356	HIS	-	expression tag	UNP Q98GN8
D	357	HIS	-	expression tag	UNP Q98GN8
D	358	HIS	-	expression tag	UNP Q98GN8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	359	HIS	-	expression tag	UNP Q98GN8
D	360	HIS	-	expression tag	UNP Q98GN8
D	361	HIS	-	expression tag	UNP Q98GN8

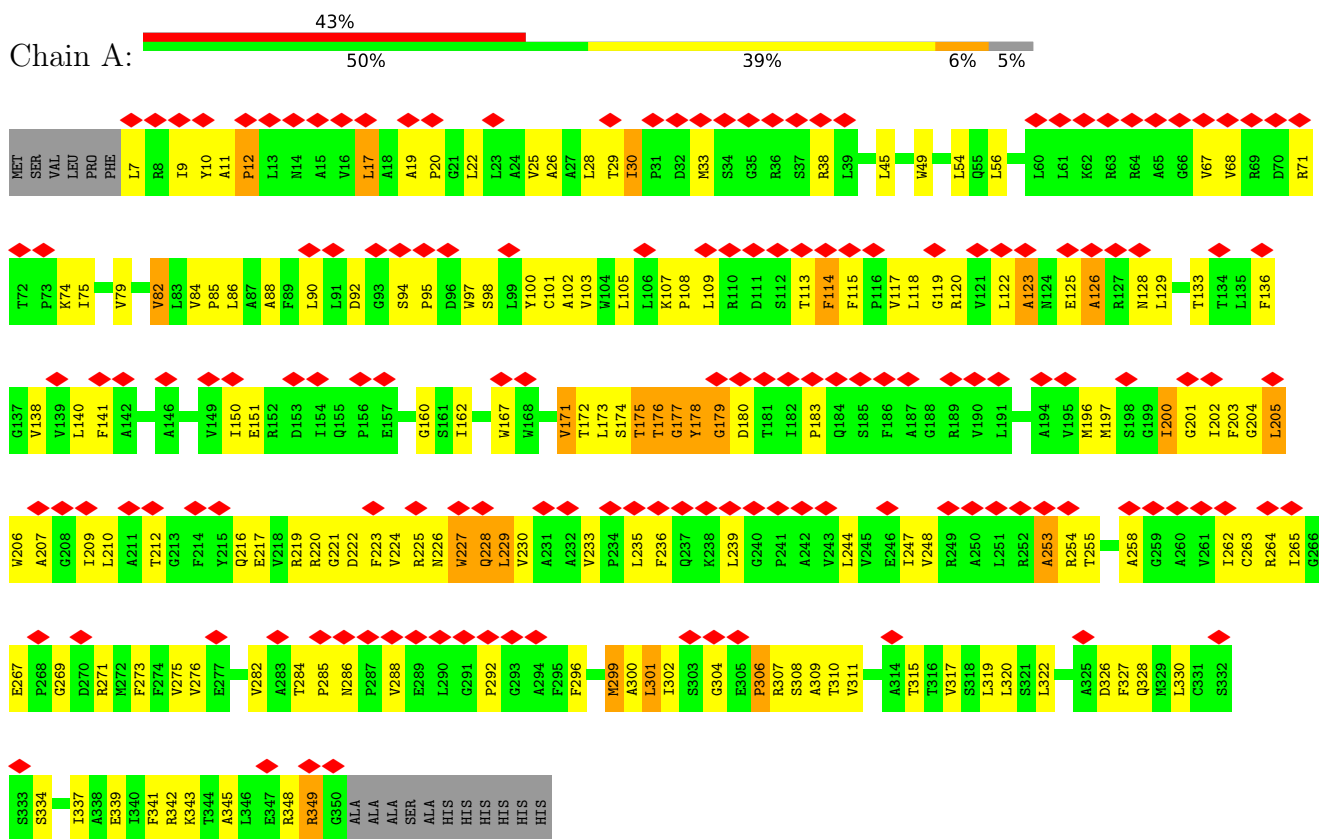
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total K 2 2	0

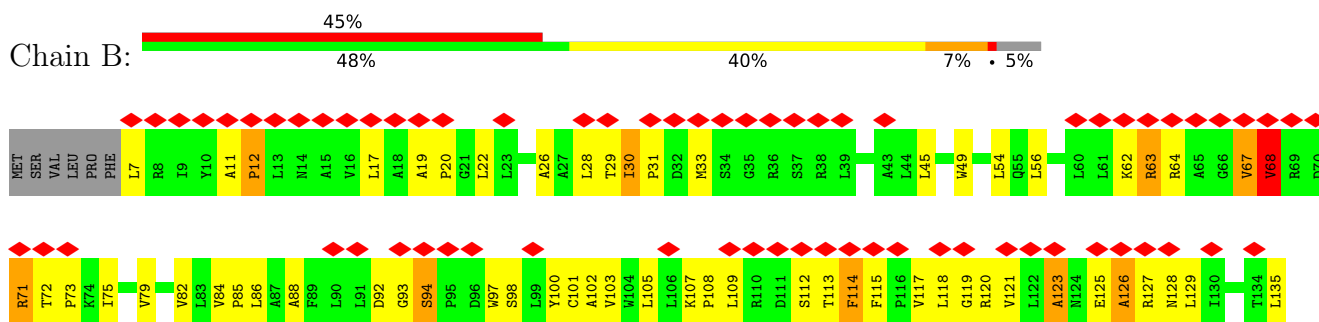
3 Residue-property plots

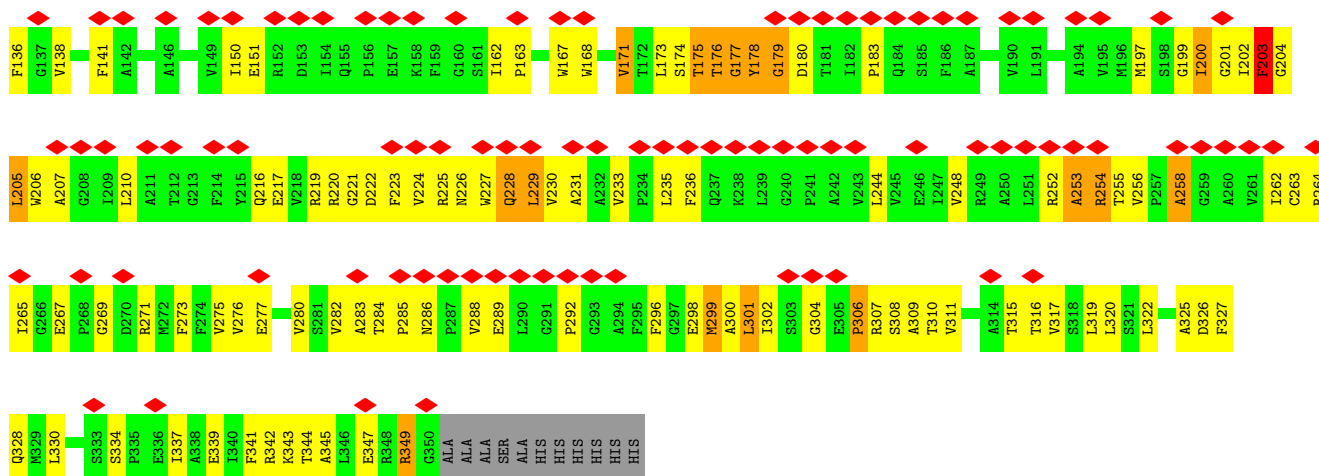
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CYCLIC NUCLEOTIDE-GATED POTASSIUM CHANNEL MLL3241

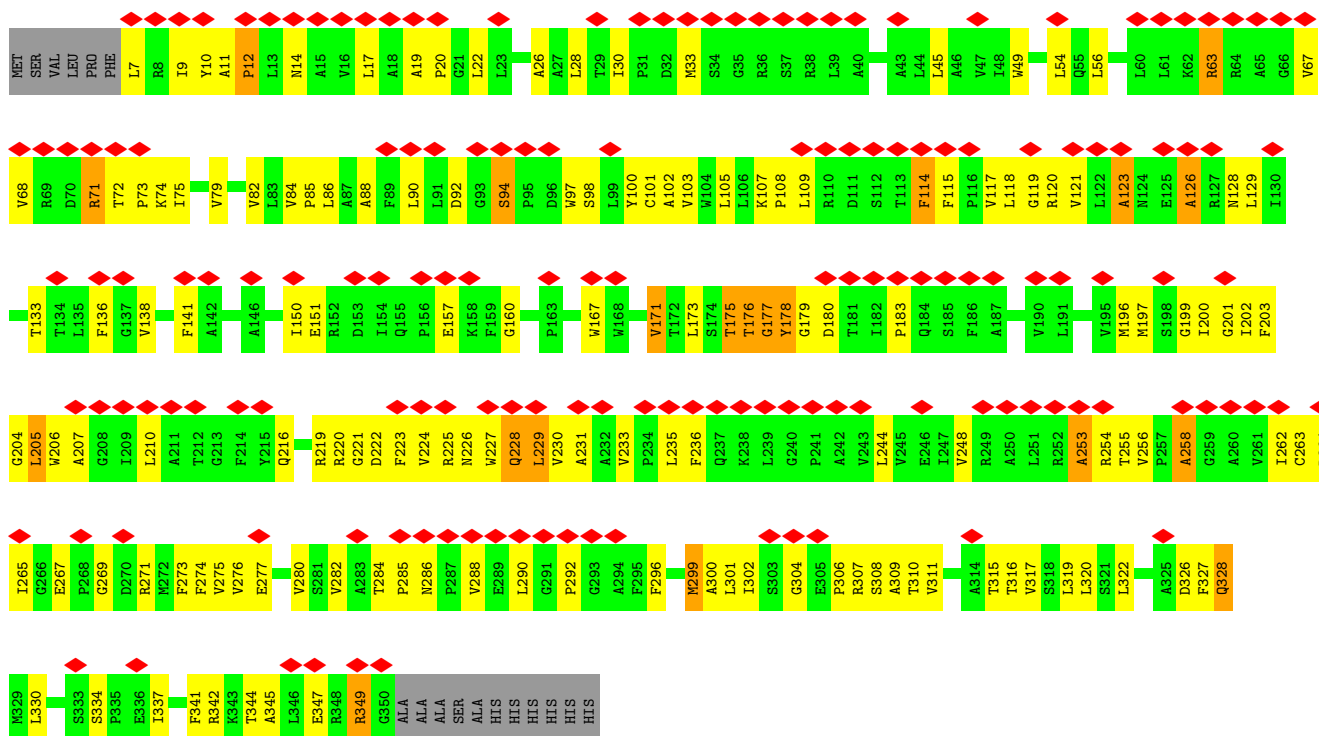
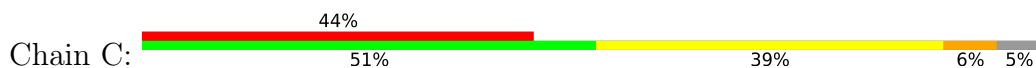


• Molecule 1: CYCLIC NUCLEOTIDE-GATED POTASSIUM CHANNEL MLL3241

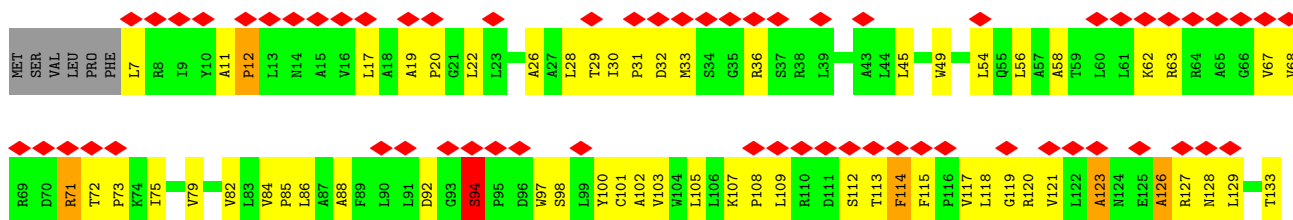
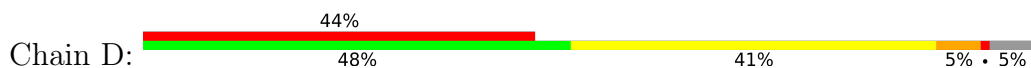


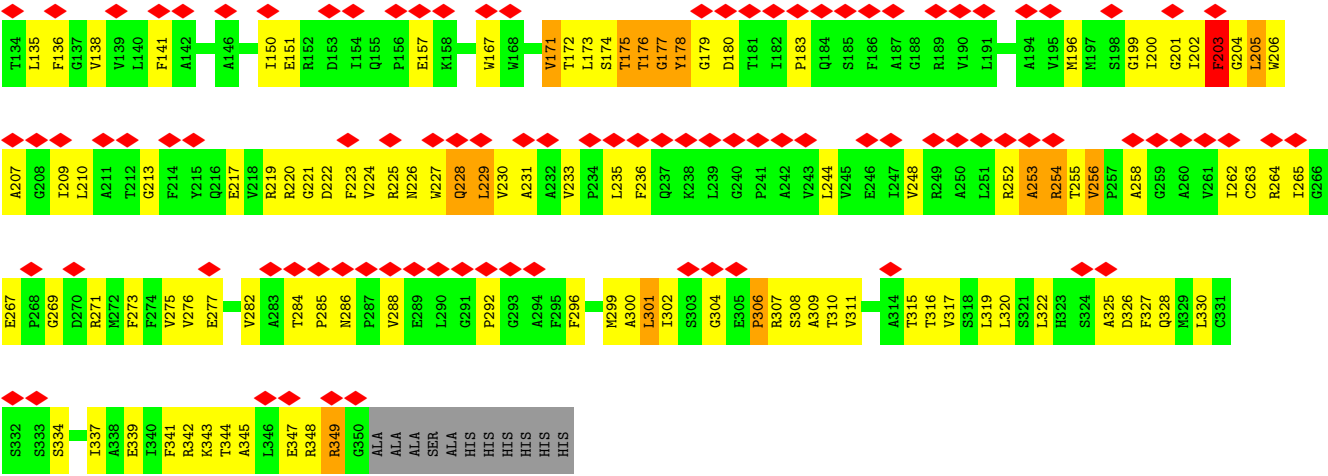


• Molecule 1: CYCLIC NUCLEOTIDE-GATED POTASSIUM CHANNEL MLL3241



• Molecule 1: CYCLIC NUCLEOTIDE-GATED POTASSIUM CHANNEL MLL3241





4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, γ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	OTHER	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	5	Depositor
Minimum defocus (nm)	655	Depositor
Maximum defocus (nm)	3077	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	4.081	Depositor
Minimum map value	-1.170	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.3	Depositor
Map size (Å)	104.325005, 104.325005, 104.325005	wwPDB
Map dimensions	107, 107, 107	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.975, 0.975, 0.975	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.87	6/2642 (0.2%)	1.28	25/3607 (0.7%)
1	B	0.87	8/2642 (0.3%)	1.28	26/3607 (0.7%)
1	C	0.86	6/2642 (0.2%)	1.25	22/3607 (0.6%)
1	D	0.87	5/2642 (0.2%)	1.27	23/3607 (0.6%)
All	All	0.87	25/10568 (0.2%)	1.27	96/14428 (0.7%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	TYR	C-O	8.45	1.34	1.24
1	C	178	TYR	C-O	8.32	1.34	1.24
1	D	178	TYR	C-O	8.22	1.33	1.24
1	B	178	TYR	C-O	7.79	1.33	1.24
1	D	178	TYR	CA-C	7.01	1.61	1.52
1	C	178	TYR	CA-C	6.60	1.61	1.52
1	A	178	TYR	CA-C	6.38	1.61	1.52
1	A	180	ASP	N-CA	6.28	1.53	1.46
1	B	180	ASP	N-CA	6.16	1.53	1.46
1	D	180	ASP	N-CA	6.14	1.53	1.46
1	B	178	TYR	CA-C	5.82	1.60	1.52
1	C	349	ARG	C-N	-5.78	1.25	1.33
1	C	180	ASP	N-CA	5.77	1.53	1.46
1	B	176	THR	CA-C	5.71	1.60	1.52
1	B	256	VAL	N-CA	-5.69	1.41	1.46
1	D	349	ARG	C-N	-5.68	1.25	1.33
1	B	349	ARG	C-N	-5.68	1.25	1.33
1	A	349	ARG	C-N	-5.66	1.25	1.33
1	B	7	LEU	C-O	5.64	1.34	1.23
1	C	7	LEU	C-O	5.63	1.34	1.23
1	D	7	LEU	C-O	5.57	1.34	1.23
1	A	7	LEU	C-O	5.37	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	GLY	C-N	-5.29	1.27	1.33
1	C	176	THR	CA-C	5.17	1.59	1.52
1	A	179	GLY	C-N	-5.12	1.27	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	PHE	N-CA-C	9.74	121.49	111.07
1	A	114	PHE	N-CA-C	9.16	120.87	111.07
1	A	207	ALA	N-CA-C	8.93	122.68	111.69
1	B	114	PHE	N-CA-C	8.81	120.50	111.07
1	D	71	ARG	N-CA-C	8.68	124.11	112.30
1	B	71	ARG	N-CA-C	8.60	123.23	111.71
1	D	114	PHE	N-CA-C	8.52	120.18	111.07
1	C	207	ALA	N-CA-C	8.29	121.88	111.69
1	C	71	ARG	N-CA-C	8.14	123.36	112.30
1	C	178	TYR	N-CA-C	7.96	120.04	111.36
1	B	178	TYR	N-CA-C	7.72	119.77	111.36
1	B	126	ALA	CA-C-N	-7.58	110.12	120.28
1	B	126	ALA	C-N-CA	-7.58	110.12	120.28
1	D	178	TYR	N-CA-C	7.48	119.51	111.36
1	C	253	ALA	N-CA-C	7.41	120.71	109.23
1	A	178	TYR	N-CA-C	7.31	119.33	111.36
1	A	253	ALA	N-CA-C	7.30	120.54	109.23
1	D	126	ALA	CA-C-N	-7.27	110.54	120.28
1	D	126	ALA	C-N-CA	-7.27	110.54	120.28
1	A	126	ALA	CA-C-N	-7.26	110.56	120.28
1	A	126	ALA	C-N-CA	-7.26	110.56	120.28
1	A	175	THR	CA-C-N	7.16	130.45	120.29
1	A	175	THR	C-N-CA	7.16	130.45	120.29
1	C	126	ALA	CA-C-N	-7.15	110.70	120.28
1	C	126	ALA	C-N-CA	-7.15	110.70	120.28
1	B	175	THR	CA-C-N	7.05	130.30	120.29
1	B	175	THR	C-N-CA	7.05	130.30	120.29
1	D	207	ALA	N-CA-C	6.96	122.12	112.45
1	A	67	VAL	N-CA-C	6.92	116.93	110.42
1	B	253	ALA	N-CA-C	6.80	120.59	109.24
1	D	253	ALA	N-CA-C	6.79	120.60	109.06
1	D	175	THR	CA-C-N	6.73	129.85	120.29
1	D	175	THR	C-N-CA	6.73	129.85	120.29
1	B	128	ASN	N-CA-C	6.72	118.68	111.36
1	C	176	THR	N-CA-C	6.63	118.58	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ILE	N-CA-C	6.45	116.61	110.42
1	C	175	THR	CA-C-N	6.43	129.41	120.29
1	C	175	THR	C-N-CA	6.43	129.41	120.29
1	B	176	THR	N-CA-C	6.42	118.35	111.36
1	D	176	THR	N-CA-C	6.23	118.15	111.36
1	B	171	VAL	N-CA-CB	-6.22	103.27	110.55
1	B	207	ALA	N-CA-C	6.22	121.04	112.90
1	B	123	ALA	N-CA-C	6.17	118.01	111.28
1	D	203	PHE	CA-CB-CG	6.14	119.94	113.80
1	A	176	THR	N-CA-C	6.10	118.01	111.36
1	A	82	VAL	N-CA-C	6.00	116.78	110.72
1	D	171	VAL	N-CA-CB	-5.96	103.58	110.55
1	D	150	ILE	N-CA-C	5.86	116.64	110.72
1	A	128	ASN	N-CA-C	5.83	117.72	111.36
1	D	172	THR	N-CA-C	5.83	117.71	111.36
1	A	123	ALA	N-CA-C	5.78	117.58	111.28
1	B	30	ILE	CA-C-N	5.77	125.68	119.85
1	B	30	ILE	C-N-CA	5.77	125.68	119.85
1	B	112	SER	N-CA-C	5.75	118.32	110.55
1	C	150	ILE	N-CA-C	5.72	116.50	110.72
1	B	180	ASP	N-CA-C	5.67	117.46	111.28
1	A	171	VAL	N-CA-CB	-5.64	103.95	110.55
1	C	17	LEU	N-CA-C	5.55	117.42	111.36
1	D	94	SER	CA-C-N	5.55	125.39	119.28
1	D	94	SER	C-N-CA	5.55	125.39	119.28
1	C	171	VAL	N-CA-CB	-5.50	104.12	110.55
1	A	150	ILE	N-CA-C	5.45	116.22	110.72
1	B	203	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	200	ILE	CB-CA-C	-5.42	105.03	111.97
1	B	200	ILE	O-C-N	5.40	127.20	121.91
1	C	128	ASN	N-CA-C	5.39	117.24	111.36
1	A	227	TRP	N-CA-C	-5.39	104.90	112.12
1	D	123	ALA	N-CA-C	5.37	117.13	111.28
1	B	93	GLY	N-CA-C	-5.33	107.35	115.66
1	D	128	ASN	N-CA-C	5.32	117.15	111.36
1	A	17	LEU	N-CA-C	5.29	117.13	111.36
1	A	301	LEU	N-CA-C	5.25	117.08	111.36
1	C	256	VAL	CA-C-N	5.24	125.14	119.85
1	C	256	VAL	C-N-CA	5.24	125.14	119.85
1	D	112	SER	N-CA-C	5.23	118.22	110.48
1	A	172	THR	N-CA-C	5.22	117.05	111.36
1	A	30	ILE	CA-C-N	5.19	125.09	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ILE	C-N-CA	5.19	125.09	119.85
1	B	258	ALA	N-CA-C	5.18	117.74	110.23
1	B	17	LEU	N-CA-C	5.17	117.00	111.36
1	C	90	LEU	N-CA-C	5.17	116.72	111.14
1	C	299	MET	CB-CA-C	-5.17	102.21	110.79
1	C	301	LEU	N-CA-C	5.17	116.99	111.36
1	A	90	LEU	N-CA-C	5.15	116.71	111.14
1	D	256	VAL	CA-C-N	5.14	125.04	119.85
1	D	256	VAL	C-N-CA	5.14	125.04	119.85
1	C	74	LYS	N-CA-C	5.13	116.96	111.36
1	B	299	MET	CB-CA-C	-5.12	102.29	110.79
1	D	301	LEU	N-CA-C	5.09	116.91	111.36
1	C	258	ALA	N-CA-C	5.08	117.60	110.23
1	C	123	ALA	N-CA-C	5.08	116.82	111.28
1	A	299	MET	CB-CA-C	-5.07	102.37	110.79
1	A	74	LYS	N-CA-C	5.05	116.86	111.36
1	B	254	ARG	N-CA-CB	5.04	120.08	111.66
1	D	254	ARG	N-CA-CB	5.01	120.03	111.66
1	B	301	LEU	N-CA-C	5.00	116.81	111.36

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	2585	0	2694	238	0
1	B	2585	0	2694	242	0
1	C	2585	0	2694	215	0
1	D	2585	0	2694	242	0
2	A	2	0	0	0	0
All	All	10342	0	10776	783	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 37.

All (783) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:O	1:A:229:LEU:HB2	1.16	1.29
1:D:230:VAL:HG13	1:D:236:PHE:CD2	1.66	1.28
1:C:230:VAL:HG13	1:C:236:PHE:CD2	1.69	1.26
1:B:230:VAL:HG13	1:B:236:PHE:CD2	1.73	1.21
1:A:229:LEU:CD1	1:A:320:LEU:HD21	1.71	1.20
1:D:229:LEU:CD2	1:D:276:VAL:HG11	1.71	1.19
1:B:229:LEU:CD2	1:B:276:VAL:HG11	1.71	1.19
1:C:229:LEU:CD2	1:C:276:VAL:HG11	1.73	1.19
1:A:299:MET:HG2	1:A:345:ALA:HB1	1.34	1.08
1:D:299:MET:HG2	1:D:345:ALA:HB1	1.36	1.07
1:A:225:ARG:O	1:A:229:LEU:CB	2.00	1.07
1:B:299:MET:HG2	1:B:345:ALA:HB1	1.37	1.07
1:A:229:LEU:HD13	1:A:320:LEU:HD21	1.34	1.06
1:C:200:ILE:HG23	1:D:206:TRP:HA	1.37	1.06
1:C:299:MET:HG2	1:C:345:ALA:HB1	1.41	1.03
1:A:225:ARG:HA	1:A:229:LEU:HG	1.42	1.02
1:D:230:VAL:HG13	1:D:236:PHE:HD2	1.22	0.99
1:A:206:TRP:HA	1:D:200:ILE:HG23	1.43	0.98
1:A:56:LEU:HD22	1:A:82:VAL:HG21	1.48	0.94
1:A:229:LEU:HD12	1:A:320:LEU:HD21	1.47	0.94
1:C:230:VAL:HG13	1:C:236:PHE:HD2	1.33	0.93
1:B:230:VAL:HG13	1:B:236:PHE:HD2	1.34	0.93
1:B:56:LEU:HD22	1:B:82:VAL:HG21	1.51	0.92
1:B:200:ILE:HG23	1:C:206:TRP:HA	1.50	0.92
1:D:56:LEU:HD22	1:D:82:VAL:HG21	1.54	0.90
1:A:229:LEU:HB3	1:A:320:LEU:HD11	1.54	0.89
1:B:229:LEU:HD21	1:B:276:VAL:HG11	1.53	0.88
1:C:56:LEU:HD22	1:C:82:VAL:HG21	1.53	0.88
1:A:210:LEU:HD12	1:D:204:GLY:HA3	1.53	0.88
1:B:173:LEU:HD12	1:B:202:ILE:HD13	1.54	0.87
1:B:258:ALA:HB2	1:B:315:THR:HA	1.56	0.87
1:C:204:GLY:HA3	1:D:210:LEU:HD12	1.55	0.86
1:C:229:LEU:HD21	1:C:276:VAL:HG11	1.55	0.85
1:B:179:GLY:HA3	1:C:178:TYR:O	1.77	0.85
1:C:179:GLY:HA3	1:D:178:TYR:O	1.77	0.84
1:A:178:TYR:O	1:D:179:GLY:HA3	1.78	0.84
1:D:229:LEU:HD21	1:D:276:VAL:HG11	1.60	0.84
1:A:126:ALA:HB3	1:B:254:ARG:HH21	1.42	0.84
1:D:229:LEU:HD22	1:D:276:VAL:HG21	1.58	0.84
1:A:126:ALA:HB3	1:B:254:ARG:NH2	1.93	0.83
1:C:258:ALA:HB2	1:C:315:THR:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ASN:CB	1:D:248:VAL:HG13	2.10	0.82
1:C:226:ASN:CB	1:C:248:VAL:HG13	2.10	0.81
1:A:299:MET:HE1	1:A:349:ARG:HD2	1.62	0.81
1:A:258:ALA:HB2	1:A:315:THR:HA	1.63	0.81
1:D:258:ALA:HB2	1:D:315:THR:HA	1.62	0.80
1:D:173:LEU:HD12	1:D:202:ILE:HD13	1.61	0.80
1:C:229:LEU:HD22	1:C:276:VAL:HG21	1.64	0.80
1:B:299:MET:HE1	1:B:349:ARG:HD2	1.64	0.80
1:B:126:ALA:HB3	1:C:254:ARG:NH2	1.97	0.79
1:C:299:MET:HG2	1:C:345:ALA:CB	2.12	0.79
1:D:299:MET:HG2	1:D:345:ALA:CB	2.11	0.79
1:A:226:ASN:CB	1:A:248:VAL:HG13	2.12	0.79
1:B:229:LEU:HD22	1:B:276:VAL:HG21	1.65	0.79
1:A:299:MET:HG2	1:A:345:ALA:CB	2.13	0.78
1:A:179:GLY:HA2	1:B:178:TYR:HB3	1.64	0.78
1:B:226:ASN:CB	1:B:248:VAL:HG13	2.14	0.78
1:A:302:ILE:HD13	1:A:342:ARG:HA	1.64	0.78
1:C:299:MET:HE1	1:C:349:ARG:HD2	1.64	0.78
1:B:204:GLY:HA3	1:C:210:LEU:HD12	1.65	0.77
1:A:224:VAL:O	1:A:228:GLN:HB2	1.85	0.77
1:B:229:LEU:HD22	1:B:276:VAL:HG11	1.67	0.77
1:C:175:THR:O	1:D:176:THR:HA	1.83	0.77
1:A:117:VAL:HA	1:A:120:ARG:NH1	2.00	0.77
1:A:176:THR:HA	1:D:175:THR:O	1.83	0.77
1:B:179:GLY:HA2	1:C:178:TYR:HB3	1.65	0.77
1:A:196:MET:SD	1:B:173:LEU:HD23	2.25	0.76
1:D:229:LEU:HD22	1:D:276:VAL:HG11	1.66	0.76
1:D:203:PHE:HA	1:D:206:TRP:CD1	2.20	0.76
1:A:200:ILE:HG23	1:B:206:TRP:HA	1.67	0.76
1:B:175:THR:O	1:C:176:THR:HA	1.86	0.76
1:C:226:ASN:HB2	1:C:248:VAL:HG13	1.68	0.76
1:A:171:VAL:HG22	1:A:178:TYR:CD1	2.21	0.75
1:C:126:ALA:HB3	1:D:254:ARG:NH2	2.00	0.75
1:B:299:MET:SD	1:B:349:ARG:HG3	2.27	0.75
1:B:171:VAL:CG1	1:B:177:GLY:HA2	2.17	0.75
1:B:126:ALA:HB3	1:C:254:ARG:HH21	1.52	0.75
1:D:226:ASN:HB2	1:D:248:VAL:HG13	1.68	0.75
1:C:179:GLY:HA2	1:D:178:TYR:HB3	1.68	0.75
1:B:203:PHE:HA	1:B:206:TRP:CD1	2.22	0.74
1:B:299:MET:HG2	1:B:345:ALA:CB	2.14	0.74
1:B:302:ILE:HD13	1:B:342:ARG:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:HA3	1:B:178:TYR:O	1.87	0.74
1:C:171:VAL:CG1	1:C:177:GLY:HA2	2.18	0.74
1:C:299:MET:SD	1:C:349:ARG:HG3	2.28	0.73
1:A:136:PHE:HE1	1:A:202:ILE:HG23	1.51	0.73
1:A:175:THR:O	1:B:176:THR:HA	1.88	0.73
1:C:229:LEU:HD22	1:C:276:VAL:HG11	1.68	0.73
1:A:254:ARG:NH2	1:D:126:ALA:HB3	2.03	0.73
1:A:254:ARG:HH21	1:D:126:ALA:HB3	1.52	0.73
1:A:299:MET:SD	1:A:349:ARG:HG3	2.28	0.73
1:A:178:TYR:HB3	1:D:179:GLY:HA2	1.68	0.73
1:C:196:MET:SD	1:D:173:LEU:HD23	2.29	0.73
1:D:102:ALA:O	1:D:105:LEU:HG	1.89	0.73
1:A:171:VAL:CG1	1:A:177:GLY:HA2	2.19	0.73
1:A:226:ASN:HB2	1:A:248:VAL:HG13	1.70	0.73
1:D:299:MET:HE1	1:D:349:ARG:HD2	1.70	0.73
1:D:299:MET:SD	1:D:349:ARG:HG3	2.28	0.73
1:B:171:VAL:HG22	1:B:178:TYR:CD2	2.24	0.73
1:C:171:VAL:HG22	1:C:178:TYR:CD1	2.24	0.73
1:D:171:VAL:HG22	1:D:178:TYR:CD1	2.24	0.72
1:B:136:PHE:HE1	1:B:202:ILE:HG23	1.54	0.72
1:D:302:ILE:HD13	1:D:342:ARG:HA	1.69	0.72
1:B:120:ARG:HD2	1:C:271:ARG:NH2	2.05	0.72
1:D:244:LEU:O	1:D:248:VAL:HG23	1.90	0.72
1:D:225:ARG:O	1:D:229:LEU:CB	2.38	0.72
1:B:225:ARG:O	1:B:229:LEU:CB	2.38	0.72
1:D:171:VAL:CG1	1:D:177:GLY:HA2	2.19	0.72
1:A:120:ARG:HA	1:A:123:ALA:HB3	1.71	0.72
1:A:105:LEU:HB3	1:D:138:VAL:HG13	1.70	0.71
1:B:226:ASN:HB2	1:B:248:VAL:HG13	1.72	0.71
1:A:244:LEU:O	1:A:248:VAL:HG23	1.91	0.71
1:C:227:TRP:CZ2	1:D:328:GLN:HG2	2.25	0.71
1:C:302:ILE:HD13	1:C:342:ARG:HA	1.72	0.70
1:D:225:ARG:O	1:D:229:LEU:HB2	1.91	0.70
1:B:171:VAL:HG22	1:B:178:TYR:HD2	1.54	0.70
1:B:117:VAL:HG22	1:B:120:ARG:HH22	1.57	0.70
1:A:203:PHE:HA	1:A:206:TRP:CD1	2.27	0.70
1:A:26:ALA:HB2	1:D:141:PHE:HE2	1.56	0.70
1:A:328:GLN:HG2	1:D:227:TRP:CZ2	2.27	0.70
1:C:230:VAL:CG1	1:C:236:PHE:CD2	2.63	0.70
1:C:225:ARG:O	1:C:229:LEU:CB	2.40	0.69
1:C:244:LEU:O	1:C:248:VAL:HG23	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LEU:CD1	1:D:202:ILE:HD13	2.21	0.69
1:B:262:ILE:HD13	1:B:319:LEU:HD11	1.74	0.69
1:B:173:LEU:CD1	1:B:202:ILE:HD13	2.23	0.69
1:B:171:VAL:HG13	1:B:177:GLY:HA2	1.73	0.69
1:D:120:ARG:HA	1:D:123:ALA:HB3	1.75	0.69
1:A:206:TRP:HB3	1:D:200:ILE:HA	1.75	0.69
1:B:138:VAL:HG13	1:C:105:LEU:HB3	1.74	0.68
1:B:229:LEU:CD2	1:B:276:VAL:CG1	2.63	0.68
1:D:229:LEU:HD23	1:D:276:VAL:HG11	1.73	0.68
1:C:262:ILE:HD13	1:C:319:LEU:HD11	1.75	0.68
1:B:244:LEU:O	1:B:248:VAL:HG23	1.92	0.68
1:D:315:THR:O	1:D:317:VAL:HG23	1.94	0.68
1:A:315:THR:O	1:A:317:VAL:HG23	1.94	0.68
1:C:315:THR:O	1:C:317:VAL:HG23	1.94	0.68
1:B:197:MET:O	1:B:200:ILE:HG12	1.94	0.68
1:D:229:LEU:CD2	1:D:276:VAL:CG1	2.63	0.67
1:A:229:LEU:HD13	1:A:320:LEU:CD2	2.18	0.67
1:C:226:ASN:HB3	1:C:248:VAL:HG13	1.75	0.67
1:A:206:TRP:HE3	1:D:199:GLY:C	2.03	0.67
1:B:315:THR:O	1:B:317:VAL:HG23	1.93	0.67
1:A:201:GLY:O	1:A:205:LEU:HD13	1.95	0.67
1:A:102:ALA:O	1:A:105:LEU:HG	1.95	0.67
1:C:229:LEU:CD2	1:C:276:VAL:CG1	2.64	0.67
1:D:226:ASN:HB3	1:D:248:VAL:HG13	1.76	0.67
1:A:141:PHE:HE2	1:B:26:ALA:HB2	1.59	0.67
1:A:262:ILE:HD13	1:A:319:LEU:HD11	1.76	0.67
1:C:49:TRP:CZ2	1:C:86:LEU:HD13	2.30	0.66
1:C:200:ILE:HD13	1:D:206:TRP:CD2	2.29	0.66
1:A:204:GLY:HA3	1:B:210:LEU:HD12	1.77	0.66
1:A:226:ASN:HB3	1:A:248:VAL:HG13	1.77	0.66
1:A:227:TRP:CZ2	1:B:328:GLN:HG2	2.31	0.66
1:C:136:PHE:HE1	1:C:202:ILE:HG23	1.60	0.66
1:D:105:LEU:O	1:D:108:PRO:HD2	1.95	0.66
1:C:126:ALA:HB3	1:D:254:ARG:HH21	1.58	0.65
1:D:262:ILE:HD13	1:D:319:LEU:HD11	1.77	0.65
1:B:225:ARG:HA	1:B:229:LEU:HB2	1.78	0.65
1:B:284:THR:HG23	1:B:309:ALA:HB2	1.79	0.65
1:A:105:LEU:O	1:A:108:PRO:HD2	1.97	0.65
1:B:225:ARG:O	1:B:229:LEU:HB2	1.97	0.64
1:B:225:ARG:O	1:B:229:LEU:HB3	1.96	0.64
1:B:226:ASN:HB3	1:B:248:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:O	1:A:227:TRP:HB2	1.97	0.64
1:B:49:TRP:CZ2	1:B:86:LEU:HD13	2.32	0.64
1:B:102:ALA:O	1:B:105:LEU:HG	1.96	0.64
1:B:284:THR:HB	1:B:285:PRO:CD	2.27	0.64
1:C:201:GLY:O	1:C:205:LEU:HD13	1.98	0.64
1:B:62:LYS:HG2	1:B:64:ARG:H	1.63	0.64
1:B:179:GLY:HA2	1:C:178:TYR:CB	2.28	0.64
1:B:284:THR:HB	1:B:285:PRO:HD2	1.80	0.64
1:C:141:PHE:HE2	1:D:26:ALA:HB2	1.62	0.64
1:B:141:PHE:HE1	1:C:26:ALA:HB2	1.61	0.64
1:B:167:TRP:O	1:B:171:VAL:HG23	1.97	0.64
1:D:229:LEU:HD22	1:D:276:VAL:CG2	2.28	0.64
1:B:201:GLY:O	1:B:205:LEU:HD13	1.98	0.63
1:C:225:ARG:O	1:C:229:LEU:HB3	1.98	0.63
1:C:284:THR:HG23	1:C:309:ALA:HB2	1.78	0.63
1:B:200:ILE:HD13	1:C:206:TRP:CD2	2.34	0.63
1:C:263:CYS:SG	1:C:311:VAL:HB	2.38	0.63
1:C:284:THR:HB	1:C:285:PRO:HD2	1.80	0.63
1:C:284:THR:HB	1:C:285:PRO:CD	2.29	0.63
1:A:200:ILE:HD13	1:B:206:TRP:CE3	2.34	0.63
1:C:9:ILE:HG22	1:C:10:TYR:CD2	2.34	0.63
1:D:171:VAL:HG12	1:D:177:GLY:HA2	1.80	0.63
1:D:230:VAL:CG1	1:D:236:PHE:CD2	2.61	0.63
1:A:49:TRP:CZ2	1:A:86:LEU:HD13	2.33	0.62
1:A:171:VAL:HG12	1:A:177:GLY:HA2	1.81	0.62
1:B:263:CYS:SG	1:B:311:VAL:HB	2.39	0.62
1:C:225:ARG:HA	1:C:229:LEU:HB2	1.81	0.62
1:A:225:ARG:O	1:A:229:LEU:CG	2.47	0.62
1:C:105:LEU:O	1:C:108:PRO:HD2	1.99	0.62
1:C:171:VAL:HG12	1:C:177:GLY:HA2	1.80	0.62
1:D:284:THR:HG23	1:D:309:ALA:HB2	1.80	0.62
1:C:225:ARG:O	1:C:229:LEU:HB2	1.98	0.62
1:C:138:VAL:HG13	1:D:105:LEU:HB3	1.81	0.62
1:D:269:GLY:H	1:D:306:PRO:HA	1.65	0.62
1:A:206:TRP:HA	1:D:200:ILE:CG2	2.25	0.62
1:D:49:TRP:CZ2	1:D:86:LEU:HD13	2.33	0.62
1:B:230:VAL:CG1	1:B:236:PHE:CD2	2.68	0.61
1:D:117:VAL:HA	1:D:120:ARG:NH1	2.14	0.61
1:D:225:ARG:HD2	1:D:253:ALA:HB3	1.82	0.61
1:A:282:VAL:HG12	1:A:284:THR:HG23	1.81	0.61
1:B:120:ARG:HA	1:B:123:ALA:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ALA:CB	1:D:315:THR:HA	2.30	0.61
1:B:225:ARG:HD2	1:B:253:ALA:HB3	1.81	0.61
1:A:9:ILE:HG22	1:A:10:TYR:CD2	2.35	0.61
1:B:258:ALA:CB	1:B:315:THR:HA	2.30	0.61
1:A:179:GLY:HA2	1:B:178:TYR:CB	2.29	0.61
1:A:225:ARG:CA	1:A:229:LEU:HG	2.22	0.61
1:C:49:TRP:CD1	1:C:85:PRO:HB2	2.35	0.60
1:C:102:ALA:O	1:C:105:LEU:HG	2.00	0.60
1:D:225:ARG:HA	1:D:229:LEU:HB2	1.82	0.60
1:A:206:TRP:CA	1:D:200:ILE:HG23	2.25	0.60
1:A:299:MET:CG	1:A:345:ALA:HB1	2.22	0.60
1:B:28:LEU:HD22	1:B:98:SER:CB	2.31	0.60
1:A:225:ARG:HD2	1:A:253:ALA:HB3	1.84	0.60
1:C:88:ALA:HB1	1:C:97:TRP:HB2	1.84	0.60
1:C:229:LEU:HD22	1:C:276:VAL:CG2	2.32	0.60
1:B:199:GLY:C	1:C:206:TRP:HE3	2.10	0.60
1:A:171:VAL:HG22	1:A:178:TYR:HD1	1.66	0.59
1:C:120:ARG:HA	1:C:123:ALA:HB3	1.84	0.59
1:D:151:GLU:OE2	1:D:183:PRO:HA	2.02	0.59
1:B:63:ARG:HA	1:B:71:ARG:NH2	2.17	0.59
1:B:151:GLU:OE2	1:B:183:PRO:HA	2.02	0.59
1:C:88:ALA:HB2	1:C:100:TYR:CG	2.38	0.59
1:B:229:LEU:HD22	1:B:276:VAL:CG2	2.33	0.59
1:C:167:TRP:O	1:C:171:VAL:HG23	2.02	0.59
1:C:171:VAL:HG13	1:C:177:GLY:HA2	1.85	0.59
1:A:230:VAL:HG13	1:A:236:PHE:CG	2.37	0.59
1:C:151:GLU:OE2	1:C:183:PRO:HA	2.03	0.59
1:A:206:TRP:CD1	1:A:206:TRP:H	2.21	0.59
1:C:179:GLY:HA2	1:D:178:TYR:CB	2.33	0.59
1:C:229:LEU:HD23	1:C:276:VAL:HG11	1.79	0.59
1:A:226:ASN:O	1:A:230:VAL:CG2	2.51	0.58
1:D:28:LEU:HD22	1:D:98:SER:CB	2.33	0.58
1:A:258:ALA:CB	1:A:315:THR:HA	2.33	0.58
1:C:258:ALA:CB	1:C:315:THR:HA	2.32	0.58
1:C:199:GLY:C	1:D:206:TRP:HE3	2.10	0.58
1:A:28:LEU:HD22	1:A:98:SER:CB	2.33	0.58
1:D:225:ARG:O	1:D:229:LEU:HB3	2.02	0.58
1:D:230:VAL:HG13	1:D:236:PHE:CG	2.35	0.58
1:A:49:TRP:CD1	1:A:85:PRO:HB2	2.38	0.58
1:C:203:PHE:HA	1:C:206:TRP:CD1	2.39	0.58
1:D:88:ALA:HB1	1:D:97:TRP:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HG22	1:C:178:TYR:HD1	1.69	0.58
1:D:302:ILE:HD13	1:D:342:ARG:CA	2.34	0.58
1:B:49:TRP:CD1	1:B:85:PRO:HB2	2.39	0.58
1:D:202:ILE:HA	1:D:205:LEU:HD22	1.86	0.58
1:A:19:ALA:HA	1:A:22:LEU:HD12	1.86	0.57
1:A:265:ILE:HB	1:A:310:THR:OG1	2.04	0.57
1:C:299:MET:HE1	1:C:349:ARG:CD	2.34	0.57
1:D:88:ALA:HB2	1:D:100:TYR:CG	2.39	0.57
1:D:229:LEU:HD22	1:D:276:VAL:CG1	2.33	0.57
1:C:28:LEU:HD22	1:C:98:SER:CB	2.35	0.57
1:B:120:ARG:HD2	1:C:271:ARG:CZ	2.34	0.57
1:A:167:TRP:O	1:A:171:VAL:HG23	2.05	0.57
1:A:227:TRP:HZ2	1:B:328:GLN:HG2	1.68	0.57
1:B:88:ALA:HB2	1:B:100:TYR:CG	2.40	0.57
1:D:233:VAL:HG12	1:D:235:LEU:HB3	1.87	0.57
1:A:171:VAL:HG13	1:A:177:GLY:HA2	1.85	0.57
1:A:179:GLY:HA2	1:B:178:TYR:CD1	2.39	0.57
1:C:299:MET:HG2	1:C:345:ALA:CA	2.35	0.57
1:A:202:ILE:O	1:A:205:LEU:HB2	2.04	0.57
1:D:171:VAL:HG13	1:D:177:GLY:HA2	1.85	0.57
1:A:302:ILE:HD13	1:A:342:ARG:CA	2.33	0.57
1:D:167:TRP:O	1:D:171:VAL:HG23	2.05	0.57
1:A:88:ALA:HB2	1:A:100:TYR:CG	2.40	0.56
1:B:203:PHE:HA	1:B:206:TRP:NE1	2.20	0.56
1:C:284:THR:HG23	1:C:309:ALA:CB	2.35	0.56
1:A:230:VAL:HG13	1:A:236:PHE:CD2	2.39	0.56
1:A:276:VAL:O	1:A:292:PRO:HB3	2.05	0.56
1:B:109:LEU:HD22	1:B:115:PHE:CE1	2.41	0.56
1:C:200:ILE:CG2	1:D:206:TRP:HA	2.26	0.56
1:D:225:ARG:C	1:D:229:LEU:HB2	2.30	0.56
1:C:119:GLY:O	1:C:123:ALA:HB2	2.06	0.56
1:C:276:VAL:O	1:C:292:PRO:HB3	2.06	0.56
1:A:308:SER:HA	1:A:349:ARG:NH2	2.21	0.56
1:B:121:VAL:HG22	1:B:216:GLN:OE1	2.05	0.56
1:B:233:VAL:HG12	1:B:235:LEU:HB3	1.88	0.56
1:B:302:ILE:HD13	1:B:342:ARG:CA	2.34	0.56
1:D:171:VAL:HG13	1:D:178:TYR:H	1.71	0.56
1:A:179:GLY:CA	1:B:178:TYR:HB3	2.35	0.56
1:B:229:LEU:HD23	1:B:276:VAL:HG11	1.79	0.56
1:B:284:THR:HG23	1:B:309:ALA:CB	2.35	0.56
1:A:200:ILE:HA	1:B:206:TRP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ILE:HD13	1:C:342:ARG:CA	2.35	0.56
1:C:120:ARG:HD2	1:D:271:ARG:NH2	2.21	0.56
1:D:284:THR:HB	1:D:285:PRO:HD2	1.87	0.56
1:A:119:GLY:O	1:A:123:ALA:HB2	2.05	0.56
1:A:233:VAL:HG12	1:A:235:LEU:HB3	1.88	0.56
1:D:171:VAL:HG22	1:D:178:TYR:HD1	1.68	0.56
1:A:151:GLU:OE2	1:A:183:PRO:HA	2.06	0.55
1:B:171:VAL:HG12	1:B:177:GLY:HA2	1.87	0.55
1:A:138:VAL:HG13	1:B:105:LEU:HB3	1.87	0.55
1:A:178:TYR:CB	1:D:179:GLY:HA2	2.33	0.55
1:B:225:ARG:C	1:B:229:LEU:HB2	2.31	0.55
1:C:229:LEU:HD22	1:C:276:VAL:CG1	2.35	0.55
1:B:308:SER:HA	1:B:349:ARG:NH2	2.22	0.55
1:B:30:ILE:HG21	1:B:33:MET:HE3	1.89	0.55
1:B:227:TRP:CZ2	1:C:328:GLN:HG2	2.41	0.55
1:C:282:VAL:HG13	1:C:309:ALA:HB3	1.89	0.55
1:D:19:ALA:HA	1:D:22:LEU:HD12	1.87	0.55
1:D:276:VAL:O	1:D:292:PRO:HB3	2.07	0.55
1:B:119:GLY:O	1:B:123:ALA:HB2	2.07	0.55
1:B:276:VAL:O	1:B:292:PRO:HB3	2.07	0.55
1:C:45:LEU:HD13	1:C:101:CYS:SG	2.46	0.55
1:C:138:VAL:CG1	1:D:105:LEU:HB3	2.35	0.55
1:A:88:ALA:O	1:A:92:ASP:HB3	2.07	0.55
1:D:136:PHE:HE1	1:D:202:ILE:HG23	1.71	0.55
1:D:263:CYS:HB2	1:D:307:ARG:HG3	1.88	0.55
1:D:119:GLY:O	1:D:123:ALA:HB2	2.07	0.54
1:D:206:TRP:CD1	1:D:206:TRP:H	2.24	0.54
1:D:255:THR:HG22	1:D:316:THR:HG22	1.88	0.54
1:B:229:LEU:HD22	1:B:276:VAL:CG1	2.34	0.54
1:A:120:ARG:HE	1:B:271:ARG:NH2	2.06	0.54
1:D:223:PHE:O	1:D:227:TRP:HB2	2.06	0.54
1:A:328:GLN:HG2	1:D:227:TRP:HZ2	1.69	0.54
1:B:28:LEU:C	1:B:28:LEU:HD23	2.32	0.54
1:C:286:ASN:O	1:C:288:VAL:HG23	2.07	0.54
1:A:224:VAL:HG13	1:A:225:ARG:H	1.73	0.54
1:B:224:VAL:HG13	1:B:225:ARG:H	1.73	0.54
1:B:216:GLN:HE21	1:B:220:ARG:NH2	2.05	0.54
1:B:286:ASN:O	1:B:288:VAL:HG23	2.08	0.54
1:C:117:VAL:HG22	1:C:120:ARG:NH2	2.22	0.54
1:C:225:ARG:C	1:C:229:LEU:HB2	2.33	0.54
1:D:203:PHE:CD1	1:D:203:PHE:C	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:VAL:HG13	1:D:225:ARG:H	1.73	0.54
1:A:138:VAL:HG13	1:B:105:LEU:HD13	1.89	0.54
1:A:176:THR:HA	1:D:175:THR:C	2.27	0.54
1:C:230:VAL:HG13	1:C:236:PHE:CG	2.35	0.54
1:D:28:LEU:C	1:D:28:LEU:HD23	2.32	0.54
1:D:30:ILE:HG21	1:D:33:MET:HE3	1.90	0.54
1:D:229:LEU:HD13	1:D:320:LEU:HD21	1.90	0.54
1:A:173:LEU:HD11	1:A:202:ILE:HG13	1.90	0.54
1:A:271:ARG:NH2	1:D:120:ARG:HH21	2.06	0.54
1:C:109:LEU:HD22	1:C:115:PHE:CE1	2.42	0.54
1:C:224:VAL:HG13	1:C:225:ARG:H	1.73	0.54
1:D:235:LEU:HD11	1:D:337:ILE:HG21	1.89	0.54
1:A:202:ILE:O	1:A:206:TRP:CD1	2.61	0.54
1:A:226:ASN:O	1:A:230:VAL:HG21	2.08	0.54
1:A:109:LEU:HD22	1:A:115:PHE:CE1	2.44	0.53
1:B:200:ILE:N	1:C:206:TRP:HE3	2.06	0.53
1:B:105:LEU:O	1:B:108:PRO:HD2	2.08	0.53
1:D:284:THR:HG23	1:D:309:ALA:CB	2.37	0.53
1:A:141:PHE:CE2	1:B:26:ALA:HB2	2.42	0.53
1:A:271:ARG:HH21	1:D:120:ARG:HH21	1.55	0.53
1:B:223:PHE:O	1:B:227:TRP:HB2	2.08	0.53
1:C:233:VAL:HG12	1:C:235:LEU:HB3	1.90	0.53
1:A:138:VAL:CG1	1:B:105:LEU:HB3	2.38	0.53
1:A:334:SER:CB	1:A:337:ILE:HD12	2.39	0.53
1:C:263:CYS:HB2	1:C:307:ARG:HG3	1.91	0.53
1:A:109:LEU:HD22	1:A:115:PHE:CZ	2.43	0.53
1:C:322:LEU:HD21	1:C:327:PHE:HA	1.90	0.53
1:D:67:VAL:HG12	1:D:68:VAL:HG23	1.91	0.53
1:A:178:TYR:CD2	1:D:179:GLY:HA2	2.44	0.53
1:A:175:THR:C	1:B:176:THR:HA	2.29	0.53
1:A:219:ARG:HD2	1:A:220:ARG:NH1	2.23	0.53
1:B:299:MET:CG	1:B:345:ALA:HB1	2.25	0.53
1:D:255:THR:CG2	1:D:316:THR:HG22	2.38	0.53
1:B:265:ILE:HB	1:B:310:THR:OG1	2.09	0.53
1:A:171:VAL:HG13	1:A:178:TYR:H	1.73	0.53
1:B:141:PHE:CE1	1:C:26:ALA:HB2	2.41	0.53
1:B:230:VAL:HG13	1:B:236:PHE:CG	2.40	0.53
1:C:28:LEU:HD23	1:C:28:LEU:C	2.34	0.53
1:A:263:CYS:HB2	1:A:307:ARG:HG3	1.90	0.53
1:D:219:ARG:HD2	1:D:220:ARG:NH1	2.24	0.53
1:A:136:PHE:CE1	1:A:202:ILE:HG23	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:HB	1:A:285:PRO:HD2	1.91	0.52
1:C:160:GLY:O	1:D:31:PRO:HG3	2.10	0.52
1:B:263:CYS:HB2	1:B:307:ARG:HG3	1.92	0.52
1:B:322:LEU:HD11	1:B:326:ASP:HB3	1.91	0.52
1:C:203:PHE:O	1:C:206:TRP:HD1	1.92	0.52
1:C:255:THR:HG22	1:C:316:THR:HG22	1.92	0.52
1:D:88:ALA:O	1:D:92:ASP:HB3	2.10	0.52
1:A:322:LEU:HD11	1:A:326:ASP:HB3	1.91	0.52
1:D:308:SER:HA	1:D:349:ARG:NH2	2.24	0.52
1:A:222:ASP:HA	1:A:226:ASN:HB2	1.92	0.52
1:C:302:ILE:HD11	1:C:341:PHE:HB3	1.91	0.52
1:A:200:ILE:CD1	1:B:206:TRP:HA	2.39	0.52
1:A:200:ILE:CA	1:B:206:TRP:HE3	2.22	0.52
1:B:72:THR:HB	1:B:73:PRO:HD3	1.91	0.52
1:B:200:ILE:HD13	1:C:206:TRP:CE3	2.45	0.52
1:D:109:LEU:HD22	1:D:115:PHE:CZ	2.43	0.52
1:D:201:GLY:O	1:D:205:LEU:HD13	2.10	0.52
1:C:255:THR:CG2	1:C:316:THR:HG22	2.40	0.52
1:C:328:GLN:HE21	1:C:328:GLN:HA	1.74	0.52
1:A:105:LEU:C	1:A:108:PRO:HD2	2.35	0.52
1:A:133:THR:O	1:A:136:PHE:HB3	2.10	0.52
1:A:286:ASN:O	1:A:288:VAL:HG23	2.09	0.52
1:C:114:PHE:CE2	1:C:118:LEU:HD22	2.45	0.52
1:C:72:THR:HB	1:C:73:PRO:HD3	1.91	0.52
1:C:229:LEU:HD13	1:C:320:LEU:HD21	1.92	0.52
1:C:282:VAL:HG12	1:C:284:THR:HG23	1.91	0.52
1:D:84:VAL:HB	1:D:85:PRO:HD3	1.92	0.52
1:A:28:LEU:C	1:A:28:LEU:HD23	2.35	0.51
1:A:88:ALA:HB1	1:A:97:TRP:HB2	1.92	0.51
1:A:299:MET:HE1	1:A:349:ARG:CD	2.38	0.51
1:B:334:SER:CB	1:B:337:ILE:HD12	2.40	0.51
1:A:206:TRP:HE3	1:D:200:ILE:N	2.07	0.51
1:B:138:VAL:CG1	1:C:105:LEU:HB3	2.39	0.51
1:B:200:ILE:HA	1:C:206:TRP:HB3	1.92	0.51
1:C:197:MET:O	1:C:200:ILE:HG12	2.10	0.51
1:C:322:LEU:HD11	1:C:326:ASP:HB3	1.92	0.51
1:A:71:ARG:O	1:A:75:ILE:HG12	2.09	0.51
1:A:84:VAL:HB	1:A:85:PRO:HD3	1.91	0.51
1:A:226:ASN:C	1:A:230:VAL:HG23	2.35	0.51
1:A:322:LEU:HD21	1:A:327:PHE:HA	1.92	0.51
1:B:264:ARG:O	1:B:267:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:VAL:HB	1:C:85:PRO:HD3	1.91	0.51
1:C:175:THR:C	1:D:176:THR:HA	2.31	0.51
1:D:334:SER:CB	1:D:337:ILE:HD12	2.39	0.51
1:A:206:TRP:CB	1:D:200:ILE:HA	2.39	0.51
1:B:84:VAL:HB	1:B:85:PRO:HD3	1.92	0.51
1:B:114:PHE:CE2	1:B:118:LEU:HD22	2.45	0.51
1:C:173:LEU:HD11	1:C:202:ILE:HG13	1.92	0.51
1:C:179:GLY:HA2	1:D:178:TYR:CD2	2.46	0.51
1:B:269:GLY:H	1:B:306:PRO:HA	1.75	0.51
1:D:114:PHE:HB2	1:D:217:GLU:OE1	2.11	0.51
1:D:299:MET:HG2	1:D:345:ALA:CA	2.40	0.51
1:C:105:LEU:C	1:C:108:PRO:HD2	2.34	0.51
1:A:38:ARG:NH2	1:A:95:PRO:HB3	2.25	0.51
1:B:175:THR:C	1:C:176:THR:HA	2.30	0.51
1:D:282:VAL:HG13	1:D:309:ALA:HB3	1.92	0.51
1:A:206:TRP:CE3	1:D:199:GLY:C	2.88	0.51
1:B:225:ARG:CA	1:B:229:LEU:HB2	2.40	0.51
1:A:178:TYR:HD2	1:D:179:GLY:HA2	1.75	0.51
1:A:221:GLY:HA3	1:A:225:ARG:HH21	1.76	0.51
1:C:92:ASP:OD1	1:C:94:SER:HB3	2.11	0.51
1:D:72:THR:HB	1:D:73:PRO:HD3	1.92	0.51
1:D:299:MET:HE1	1:D:349:ARG:CD	2.38	0.51
1:A:45:LEU:HD13	1:A:101:CYS:SG	2.50	0.51
1:A:203:PHE:O	1:A:206:TRP:HD1	1.94	0.51
1:A:263:CYS:SG	1:A:311:VAL:HB	2.50	0.51
1:C:11:ALA:HB3	1:C:12:PRO:HD3	1.93	0.51
1:C:171:VAL:HG13	1:C:178:TYR:H	1.76	0.51
1:C:200:ILE:HG23	1:D:206:TRP:CA	2.25	0.51
1:A:179:GLY:HA2	1:B:178:TYR:HD1	1.76	0.50
1:B:229:LEU:HD13	1:B:320:LEU:HD21	1.92	0.50
1:C:235:LEU:HD21	1:C:330:LEU:HD21	1.93	0.50
1:D:49:TRP:CD1	1:D:85:PRO:HB2	2.46	0.50
1:A:11:ALA:HB3	1:A:12:PRO:HD3	1.93	0.50
1:D:339:GLU:OE2	1:D:343:LYS:HE3	2.11	0.50
1:A:177:GLY:HA3	1:B:176:THR:HG22	1.93	0.50
1:B:92:ASP:OD1	1:B:94:SER:HB3	2.11	0.50
1:C:334:SER:CB	1:C:337:ILE:HD12	2.42	0.50
1:D:263:CYS:SG	1:D:307:ARG:HD2	2.51	0.50
1:A:117:VAL:HG22	1:A:120:ARG:HH12	1.75	0.50
1:C:206:TRP:CD1	1:C:206:TRP:H	2.29	0.50
1:A:26:ALA:HB2	1:D:141:PHE:CE2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD22	1:A:276:VAL:HG21	1.93	0.50
1:B:282:VAL:HG13	1:B:309:ALA:HB3	1.93	0.50
1:C:199:GLY:C	1:D:206:TRP:CE3	2.89	0.50
1:D:221:GLY:HA3	1:D:225:ARG:HH21	1.76	0.50
1:A:176:THR:HG22	1:D:177:GLY:HA3	1.93	0.50
1:A:235:LEU:HD11	1:A:337:ILE:HG21	1.93	0.50
1:B:63:ARG:H	1:B:63:ARG:HD2	1.76	0.50
1:C:225:ARG:HD2	1:C:253:ALA:HB3	1.93	0.50
1:C:179:GLY:HA3	1:D:178:TYR:C	2.36	0.50
1:D:286:ASN:O	1:D:288:VAL:HG23	2.12	0.50
1:A:235:LEU:HD21	1:A:330:LEU:HD21	1.93	0.50
1:B:45:LEU:HD13	1:B:101:CYS:SG	2.51	0.50
1:B:88:ALA:HB1	1:B:97:TRP:HB2	1.94	0.50
1:C:284:THR:CG2	1:C:309:ALA:HB2	2.41	0.50
1:A:282:VAL:HG13	1:A:309:ALA:HB3	1.93	0.49
1:C:202:ILE:HA	1:C:205:LEU:HD22	1.94	0.49
1:D:299:MET:CG	1:D:345:ALA:HB1	2.25	0.49
1:A:71:ARG:HD2	1:A:75:ILE:HD11	1.93	0.49
1:A:203:PHE:CA	1:A:206:TRP:CD1	2.95	0.49
1:C:264:ARG:O	1:C:267:GLU:HB2	2.12	0.49
1:D:219:ARG:HD2	1:D:220:ARG:HH12	1.78	0.49
1:D:322:LEU:HD11	1:D:326:ASP:HB3	1.94	0.49
1:C:177:GLY:HA3	1:D:176:THR:HG22	1.94	0.49
1:D:109:LEU:HD22	1:D:115:PHE:CE1	2.47	0.49
1:A:114:PHE:CE2	1:A:118:LEU:HD22	2.47	0.49
1:B:222:ASP:HA	1:B:226:ASN:HB2	1.95	0.49
1:B:105:LEU:C	1:B:108:PRO:HD2	2.38	0.49
1:B:302:ILE:HD11	1:B:341:PHE:HB3	1.95	0.49
1:C:269:GLY:H	1:C:306:PRO:HA	1.76	0.49
1:D:63:ARG:HA	1:D:71:ARG:NH2	2.28	0.49
1:D:264:ARG:O	1:D:267:GLU:HB2	2.11	0.49
1:D:302:ILE:HD11	1:D:341:PHE:HB3	1.95	0.49
1:A:269:GLY:H	1:A:306:PRO:HA	1.77	0.49
1:B:171:VAL:HG13	1:B:178:TYR:H	1.77	0.49
1:B:199:GLY:C	1:C:206:TRP:CE3	2.91	0.49
1:C:141:PHE:CE2	1:D:26:ALA:HB2	2.46	0.49
1:D:202:ILE:O	1:D:206:TRP:CD1	2.66	0.49
1:A:202:ILE:HG22	1:A:206:TRP:HE1	1.77	0.49
1:B:235:LEU:HD11	1:B:337:ILE:HG21	1.94	0.49
1:C:179:GLY:HA2	1:D:178:TYR:HD2	1.77	0.49
1:C:200:ILE:HD13	1:D:206:TRP:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HB2	1:A:108:PRO:HD3	1.95	0.48
1:A:203:PHE:C	1:A:206:TRP:HD1	2.21	0.48
1:A:200:ILE:N	1:B:206:TRP:HE3	2.10	0.48
1:A:125:GLU:O	1:A:129:LEU:HG	2.13	0.48
1:B:114:PHE:HB2	1:B:217:GLU:OE1	2.13	0.48
1:C:225:ARG:CA	1:C:229:LEU:HB2	2.42	0.48
1:D:120:ARG:NH2	1:D:220:ARG:NE	2.60	0.48
1:A:178:TYR:C	1:D:179:GLY:HA3	2.39	0.48
1:A:219:ARG:HD2	1:A:220:ARG:HH12	1.78	0.48
1:B:107:LYS:HB2	1:B:108:PRO:HD3	1.95	0.48
1:C:265:ILE:HB	1:C:310:THR:OG1	2.14	0.48
1:A:275:VAL:HG22	1:A:319:LEU:CD2	2.43	0.48
1:B:162:ILE:N	1:B:163:PRO:HD2	2.29	0.48
1:C:202:ILE:O	1:C:206:TRP:CD1	2.67	0.48
1:D:114:PHE:CE2	1:D:118:LEU:HD22	2.49	0.48
1:A:200:ILE:HA	1:B:206:TRP:CB	2.43	0.48
1:B:94:SER:O	1:B:97:TRP:HD1	1.96	0.48
1:A:129:LEU:HD22	1:A:209:ILE:CD1	2.44	0.48
1:D:45:LEU:HD13	1:D:101:CYS:SG	2.53	0.48
1:D:49:TRP:CH2	1:D:86:LEU:HD13	2.49	0.48
1:D:342:ARG:HD2	1:D:342:ARG:C	2.39	0.48
1:A:105:LEU:HB3	1:D:138:VAL:CG1	2.40	0.48
1:A:203:PHE:CE1	1:B:203:PHE:CE1	3.01	0.48
1:B:168:TRP:O	1:B:171:VAL:HB	2.14	0.48
1:B:255:THR:CG2	1:B:316:THR:HG22	2.44	0.48
1:C:19:ALA:HA	1:C:22:LEU:HD12	1.96	0.48
1:D:94:SER:O	1:D:97:TRP:HD1	1.97	0.48
1:D:222:ASP:HA	1:D:226:ASN:HB2	1.95	0.48
1:B:275:VAL:O	1:B:292:PRO:HA	2.14	0.47
1:C:221:GLY:HA3	1:C:225:ARG:HH21	1.78	0.47
1:D:127:ARG:HB2	1:D:127:ARG:NH1	2.29	0.47
1:A:114:PHE:HB2	1:A:217:GLU:OE1	2.14	0.47
1:A:176:THR:CG2	1:D:177:GLY:HA3	2.44	0.47
1:C:30:ILE:HG21	1:C:33:MET:HE3	1.95	0.47
1:C:227:TRP:HZ2	1:D:328:GLN:HG2	1.76	0.47
1:C:275:VAL:HG22	1:C:319:LEU:CD2	2.44	0.47
1:D:235:LEU:HD21	1:D:330:LEU:HD21	1.95	0.47
1:D:265:ILE:HB	1:D:310:THR:OG1	2.14	0.47
1:A:302:ILE:HD11	1:A:341:PHE:HB3	1.96	0.47
1:B:269:GLY:N	1:B:306:PRO:HA	2.29	0.47
1:B:299:MET:HG2	1:B:345:ALA:CA	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:SER:OG	1:B:349:ARG:HG3	2.14	0.47
1:A:226:ASN:O	1:A:230:VAL:HG23	2.14	0.47
1:B:138:VAL:HG13	1:C:105:LEU:HD13	1.96	0.47
1:B:200:ILE:HD12	1:C:206:TRP:HA	1.97	0.47
1:B:221:GLY:HA3	1:B:225:ARG:HH21	1.79	0.47
1:A:203:PHE:CZ	1:B:203:PHE:CE1	3.02	0.47
1:B:203:PHE:HZ	1:C:203:PHE:CE1	2.32	0.47
1:B:339:GLU:OE2	1:B:343:LYS:HE3	2.13	0.47
1:D:203:PHE:C	1:D:203:PHE:HD1	2.21	0.47
1:D:203:PHE:HD1	1:D:203:PHE:O	1.98	0.47
1:D:252:ARG:HH21	1:D:271:ARG:HH12	1.62	0.47
1:A:113:THR:CG2	1:A:217:GLU:HG3	2.45	0.47
1:A:203:PHE:HA	1:A:206:TRP:NE1	2.29	0.47
1:A:221:GLY:O	1:A:225:ARG:HB2	2.15	0.47
1:B:299:MET:HE1	1:B:349:ARG:CD	2.39	0.47
1:D:136:PHE:CZ	1:D:173:LEU:HD21	2.49	0.47
1:A:196:MET:O	1:B:206:TRP:HZ3	1.98	0.47
1:C:222:ASP:HA	1:C:226:ASN:HB2	1.97	0.47
1:D:17:LEU:O	1:D:20:PRO:HD2	2.15	0.47
1:D:107:LYS:HB2	1:D:108:PRO:HD3	1.97	0.47
1:D:113:THR:CG2	1:D:217:GLU:HG3	2.45	0.47
1:B:135:LEU:O	1:B:138:VAL:HB	2.15	0.47
1:D:129:LEU:HD22	1:D:209:ILE:CD1	2.45	0.47
1:C:107:LYS:HB2	1:C:108:PRO:HD3	1.95	0.46
1:A:160:GLY:O	1:B:31:PRO:HG3	2.16	0.46
1:D:308:SER:HA	1:D:349:ARG:CZ	2.45	0.46
1:A:179:GLY:HA3	1:B:178:TYR:C	2.39	0.46
1:A:284:THR:HG23	1:A:309:ALA:CB	2.46	0.46
1:A:299:MET:SD	1:A:345:ALA:O	2.73	0.46
1:B:200:ILE:HG23	1:C:206:TRP:CA	2.35	0.46
1:D:225:ARG:CA	1:D:229:LEU:HB2	2.43	0.46
1:A:301:LEU:HD13	1:A:327:PHE:CG	2.50	0.46
1:B:71:ARG:HH11	1:B:75:ILE:HD11	1.80	0.46
1:B:179:GLY:HA2	1:C:178:TYR:CD2	2.50	0.46
1:C:126:ALA:HA	1:C:129:LEU:HB3	1.98	0.46
1:D:126:ALA:HA	1:D:129:LEU:HB2	1.96	0.46
1:D:308:SER:OG	1:D:349:ARG:HG3	2.15	0.46
1:D:322:LEU:HD21	1:D:327:PHE:HA	1.98	0.46
1:B:19:ALA:HB3	1:B:20:PRO:HD3	1.97	0.46
1:B:228:GLN:O	1:B:231:ALA:HB3	2.15	0.46
1:D:221:GLY:O	1:D:225:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:NH2	1:A:220:ARG:NE	2.63	0.46
1:C:121:VAL:HG22	1:C:216:GLN:OE1	2.16	0.46
1:D:282:VAL:HG12	1:D:284:THR:HG23	1.98	0.46
1:A:299:MET:HG2	1:A:345:ALA:CA	2.45	0.46
1:B:299:MET:SD	1:B:345:ALA:O	2.73	0.46
1:C:235:LEU:HD11	1:C:337:ILE:HG21	1.97	0.46
1:C:308:SER:CB	1:C:349:ARG:HE	2.29	0.46
1:A:230:VAL:HG13	1:A:236:PHE:CB	2.46	0.46
1:B:67:VAL:O	1:B:68:VAL:HB	2.15	0.46
1:B:235:LEU:HD21	1:B:330:LEU:HD21	1.97	0.46
1:C:200:ILE:HA	1:D:206:TRP:HB3	1.96	0.46
1:C:203:PHE:C	1:C:206:TRP:HD1	2.24	0.46
1:A:263:CYS:SG	1:A:307:ARG:HD2	2.56	0.45
1:B:203:PHE:CD2	1:C:206:TRP:CB	3.00	0.45
1:D:284:THR:HB	1:D:285:PRO:CD	2.46	0.45
1:A:342:ARG:C	1:A:342:ARG:HD2	2.41	0.45
1:D:203:PHE:HA	1:D:206:TRP:NE1	2.30	0.45
1:A:282:VAL:CG1	1:A:309:ALA:HB3	2.46	0.45
1:D:105:LEU:C	1:D:108:PRO:HD2	2.40	0.45
1:B:49:TRP:CH2	1:B:86:LEU:HD13	2.52	0.45
1:D:30:ILE:CG2	1:D:33:MET:HE3	2.47	0.45
1:D:301:LEU:HD13	1:D:327:PHE:CG	2.51	0.45
1:B:203:PHE:O	1:B:206:TRP:HD1	2.00	0.45
1:B:275:VAL:HG22	1:B:319:LEU:CD2	2.47	0.45
1:C:63:ARG:HA	1:C:71:ARG:NH2	2.31	0.45
1:A:25:VAL:HG12	1:D:141:PHE:HZ	1.80	0.45
1:A:284:THR:HG21	1:A:348:ARG:O	2.17	0.45
1:A:308:SER:HA	1:A:349:ARG:HH21	1.81	0.45
1:B:117:VAL:HG13	1:B:120:ARG:NH2	2.32	0.45
1:D:203:PHE:O	1:D:206:TRP:HD1	1.98	0.45
1:A:299:MET:CE	1:A:349:ARG:HD2	2.39	0.45
1:B:203:PHE:C	1:B:203:PHE:CD1	2.94	0.45
1:B:342:ARG:HD2	1:B:342:ARG:C	2.41	0.45
1:B:301:LEU:HD13	1:B:327:PHE:CG	2.52	0.45
1:B:308:SER:HA	1:B:349:ARG:CZ	2.46	0.45
1:C:228:GLN:O	1:C:231:ALA:HB3	2.17	0.45
1:A:339:GLU:OE2	1:A:343:LYS:HE3	2.17	0.45
1:B:19:ALA:HA	1:B:22:LEU:HD12	1.99	0.45
1:B:113:THR:CG2	1:B:217:GLU:HG3	2.47	0.45
1:B:322:LEU:HD21	1:B:327:PHE:HA	1.99	0.45
1:D:299:MET:SD	1:D:345:ALA:O	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLY:HA3	1:B:176:THR:CG2	2.48	0.44
1:A:308:SER:OG	1:A:349:ARG:HG3	2.18	0.44
1:C:171:VAL:HG22	1:C:178:TYR:CE1	2.52	0.44
1:C:177:GLY:HA3	1:D:176:THR:CG2	2.47	0.44
1:B:171:VAL:CG2	1:B:178:TYR:HD2	2.28	0.44
1:C:300:ALA:O	1:C:304:GLY:N	2.51	0.44
1:D:256:VAL:O	1:D:316:THR:HA	2.18	0.44
1:D:273:PHE:HB2	1:D:296:PHE:CZ	2.51	0.44
1:C:223:PHE:O	1:C:227:TRP:HB2	2.18	0.44
1:D:11:ALA:HB3	1:D:12:PRO:HD3	1.98	0.44
1:A:200:ILE:HA	1:B:206:TRP:HE3	1.82	0.44
1:C:203:PHE:CZ	1:D:203:PHE:CE1	3.05	0.44
1:A:203:PHE:O	1:A:206:TRP:CD1	2.71	0.44
1:A:269:GLY:N	1:A:306:PRO:HA	2.32	0.44
1:B:179:GLY:HA2	1:C:178:TYR:HD2	1.83	0.44
1:C:344:THR:O	1:C:347:GLU:HB2	2.17	0.44
1:B:109:LEU:HD22	1:B:115:PHE:CZ	2.52	0.44
1:C:54:LEU:HD13	1:C:54:LEU:C	2.43	0.44
1:C:203:PHE:CZ	1:D:203:PHE:CD1	3.05	0.44
1:C:19:ALA:HB3	1:C:20:PRO:HD3	2.00	0.44
1:C:299:MET:SD	1:C:345:ALA:O	2.75	0.44
1:B:177:GLY:HA3	1:C:176:THR:HG22	2.00	0.44
1:B:203:PHE:CD2	1:C:206:TRP:HB2	2.53	0.44
1:C:133:THR:O	1:C:136:PHE:HB3	2.18	0.44
1:C:228:GLN:NE2	1:C:228:GLN:HA	2.33	0.44
1:B:71:ARG:NH1	1:B:75:ILE:HD11	2.32	0.43
1:B:299:MET:CE	1:B:349:ARG:HD2	2.41	0.43
1:A:206:TRP:CE3	1:D:200:ILE:N	2.86	0.43
1:B:228:GLN:NE2	1:B:228:GLN:HA	2.33	0.43
1:C:342:ARG:HD2	1:C:342:ARG:C	2.42	0.43
1:A:220:ARG:HH21	1:B:271:ARG:NH2	2.16	0.43
1:B:221:GLY:O	1:B:225:ARG:HB2	2.18	0.43
1:C:221:GLY:O	1:C:225:ARG:HB2	2.19	0.43
1:A:30:ILE:HG21	1:A:33:MET:HE3	2.00	0.43
1:B:11:ALA:HB3	1:B:12:PRO:HD3	1.99	0.43
1:B:125:GLU:O	1:B:129:LEU:HD13	2.18	0.43
1:C:269:GLY:N	1:C:306:PRO:HA	2.33	0.43
1:D:54:LEU:C	1:D:54:LEU:HD13	2.44	0.43
1:B:264:ARG:HB3	1:B:267:GLU:HG3	2.00	0.43
1:D:299:MET:HE1	1:D:349:ARG:HB2	2.00	0.43
1:A:206:TRP:HB2	1:D:203:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:O	1:B:75:ILE:HG13	2.18	0.43
1:C:202:ILE:HG22	1:C:206:TRP:HE1	1.82	0.43
1:D:264:ARG:HB2	1:D:267:GLU:HG3	2.01	0.43
1:B:113:THR:HG22	1:B:217:GLU:HG3	2.01	0.43
1:B:203:PHE:CD2	1:C:206:TRP:CG	3.07	0.43
1:A:30:ILE:CG2	1:A:33:MET:HE3	2.49	0.43
1:A:230:VAL:CG1	1:A:236:PHE:CB	2.97	0.43
1:B:204:GLY:HA3	1:C:210:LEU:CD1	2.44	0.43
1:C:299:MET:HE2	1:C:299:MET:HB3	1.88	0.43
1:D:277:GLU:O	1:D:317:VAL:HG13	2.18	0.43
1:A:284:THR:HB	1:A:285:PRO:CD	2.48	0.43
1:B:54:LEU:C	1:B:54:LEU:HD13	2.44	0.43
1:B:136:PHE:CZ	1:B:173:LEU:HD21	2.54	0.43
1:B:267:GLU:O	1:B:306:PRO:HB3	2.19	0.43
1:C:138:VAL:HG13	1:D:105:LEU:HD13	2.00	0.43
1:D:235:LEU:HD11	1:D:337:ILE:CG2	2.49	0.43
1:A:140:LEU:CD1	1:D:196:MET:HE1	2.49	0.42
1:A:196:MET:O	1:B:206:TRP:CZ3	2.72	0.42
1:A:235:LEU:HD11	1:A:337:ILE:CG2	2.50	0.42
1:D:203:PHE:C	1:D:206:TRP:HD1	2.27	0.42
1:A:54:LEU:C	1:A:54:LEU:HD13	2.43	0.42
1:A:75:ILE:O	1:A:79:VAL:HG23	2.20	0.42
1:A:171:VAL:HG22	1:A:178:TYR:CE1	2.53	0.42
1:A:308:SER:CB	1:A:349:ARG:HE	2.31	0.42
1:B:273:PHE:HB2	1:B:296:PHE:CZ	2.54	0.42
1:B:344:THR:O	1:B:347:GLU:HB2	2.19	0.42
1:C:264:ARG:HB3	1:C:267:GLU:HG3	2.00	0.42
1:C:204:GLY:HA3	1:D:210:LEU:CD1	2.38	0.42
1:D:135:LEU:O	1:D:138:VAL:HB	2.19	0.42
1:D:267:GLU:O	1:D:307:ARG:HG2	2.20	0.42
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.79	0.42
1:C:308:SER:OG	1:C:349:ARG:HG3	2.19	0.42
1:D:275:VAL:HG22	1:D:319:LEU:CD2	2.49	0.42
1:A:17:LEU:O	1:A:20:PRO:HD2	2.18	0.42
1:B:30:ILE:CG2	1:B:33:MET:HE3	2.49	0.42
1:D:75:ILE:O	1:D:79:VAL:HG23	2.18	0.42
1:D:275:VAL:O	1:D:292:PRO:HA	2.19	0.42
1:A:19:ALA:HB3	1:A:20:PRO:HD3	2.01	0.42
1:A:120:ARG:HA	1:A:123:ALA:CB	2.45	0.42
1:A:200:ILE:HD13	1:B:206:TRP:HA	2.01	0.42
1:A:206:TRP:CZ3	1:D:196:MET:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:TRP:HZ3	1:D:199:GLY:HA3	1.84	0.42
1:B:219:ARG:HD2	1:B:220:ARG:NH1	2.35	0.42
1:C:109:LEU:HD22	1:C:115:PHE:CZ	2.54	0.42
1:D:299:MET:HE2	1:D:299:MET:HB3	1.90	0.42
1:A:228:GLN:NE2	1:A:228:GLN:HA	2.35	0.42
1:C:136:PHE:CE1	1:C:202:ILE:HG23	2.48	0.42
1:C:275:VAL:O	1:C:292:PRO:HA	2.19	0.42
1:B:179:GLY:HA3	1:C:178:TYR:C	2.45	0.42
1:C:49:TRP:HZ2	1:C:86:LEU:HD13	1.81	0.42
1:B:75:ILE:O	1:B:79:VAL:HG23	2.20	0.41
1:B:203:PHE:O	1:B:206:TRP:CD1	2.73	0.41
1:B:219:ARG:HD2	1:B:220:ARG:HH12	1.84	0.41
1:B:235:LEU:HD11	1:B:337:ILE:CG2	2.50	0.41
1:B:300:ALA:O	1:B:304:GLY:CA	2.68	0.41
1:B:300:ALA:O	1:B:304:GLY:N	2.53	0.41
1:D:228:GLN:NE2	1:D:228:GLN:HA	2.33	0.41
1:A:175:THR:HB	1:B:174:SER:O	2.20	0.41
1:A:284:THR:HG23	1:A:309:ALA:HB2	2.02	0.41
1:B:308:SER:CB	1:B:349:ARG:HE	2.33	0.41
1:C:277:GLU:O	1:C:317:VAL:HG13	2.19	0.41
1:D:203:PHE:CA	1:D:206:TRP:CD1	2.98	0.41
1:A:113:THR:HG22	1:A:217:GLU:HG3	2.02	0.41
1:A:138:VAL:HG22	1:B:105:LEU:HD22	2.01	0.41
1:A:273:PHE:HB2	1:A:296:PHE:CZ	2.55	0.41
1:A:230:VAL:CG1	1:A:236:PHE:HB3	2.50	0.41
1:C:117:VAL:HG22	1:C:120:ARG:HH21	1.84	0.41
1:C:171:VAL:CG1	1:C:178:TYR:H	2.33	0.41
1:C:219:ARG:HH21	1:D:325:ALA:HB3	1.85	0.41
1:D:113:THR:HG22	1:D:217:GLU:HG3	2.02	0.41
1:D:284:THR:HG21	1:D:348:ARG:O	2.19	0.41
1:B:120:ARG:NH2	1:B:220:ARG:HG3	2.36	0.41
1:B:284:THR:CG2	1:B:309:ALA:HB2	2.47	0.41
1:D:120:ARG:NH2	1:D:220:ARG:HE	2.19	0.41
1:D:121:VAL:HG21	1:D:213:GLY:HA2	2.01	0.41
1:D:133:THR:O	1:D:136:PHE:HB3	2.20	0.41
1:D:171:VAL:CG1	1:D:178:TYR:H	2.32	0.41
1:D:344:THR:O	1:D:347:GLU:HB2	2.20	0.41
1:B:280:VAL:O	1:B:289:GLU:HA	2.20	0.41
1:B:296:PHE:HA	1:B:298:GLU:OE1	2.21	0.41
1:D:71:ARG:HG3	1:D:75:ILE:HD11	2.03	0.41
1:D:263:CYS:SG	1:D:311:VAL:HB	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MET:O	1:A:200:ILE:HG12	2.20	0.41
1:A:264:ARG:HB3	1:A:267:GLU:HG3	2.02	0.41
1:A:300:ALA:O	1:A:304:GLY:CA	2.68	0.41
1:D:228:GLN:O	1:D:231:ALA:HB3	2.20	0.41
1:B:123:ALA:O	1:C:254:ARG:NE	2.54	0.41
1:B:252:ARG:NH2	1:B:271:ARG:HH12	2.19	0.41
1:C:30:ILE:CG2	1:C:33:MET:HE3	2.51	0.41
1:C:175:THR:HB	1:D:174:SER:O	2.21	0.41
1:C:273:PHE:HB2	1:C:296:PHE:CZ	2.55	0.41
1:A:162:ILE:HG13	1:B:29:THR:OG1	2.21	0.41
1:A:216:GLN:HE21	1:A:220:ARG:NH2	2.18	0.41
1:C:94:SER:O	1:C:97:TRP:HD1	2.04	0.41
1:D:58:ALA:O	1:D:62:LYS:HB3	2.21	0.41
1:D:255:THR:HG22	1:D:316:THR:CG2	2.50	0.41
1:D:308:SER:CB	1:D:349:ARG:HE	2.34	0.41
1:A:174:SER:O	1:D:175:THR:HB	2.22	0.41
1:B:126:ALA:O	1:B:127:ARG:C	2.63	0.41
1:B:171:VAL:HG22	1:B:178:TYR:CE2	2.54	0.41
1:C:49:TRP:CH2	1:C:86:LEU:HD13	2.56	0.41
1:C:67:VAL:HG12	1:C:68:VAL:HG23	2.02	0.41
1:C:75:ILE:O	1:C:79:VAL:HG23	2.20	0.41
1:D:220:ARG:C	1:D:222:ASP:N	2.79	0.41
1:A:49:TRP:CH2	1:A:86:LEU:HD13	2.56	0.40
1:A:254:ARG:NE	1:D:123:ALA:O	2.54	0.40
1:B:277:GLU:O	1:B:317:VAL:HG13	2.21	0.40
1:D:117:VAL:HA	1:D:120:ARG:HH11	1.82	0.40
1:D:199:GLY:O	1:D:203:PHE:HB3	2.21	0.40
1:A:210:LEU:CD1	1:D:204:GLY:HA3	2.37	0.40
1:A:308:SER:HA	1:A:349:ARG:CZ	2.50	0.40
1:B:177:GLY:HA3	1:C:176:THR:CG2	2.51	0.40
1:B:283:ALA:O	1:B:309:ALA:HB1	2.20	0.40
1:C:216:GLN:O	1:C:220:ARG:HG2	2.21	0.40
1:A:171:VAL:CG1	1:A:178:TYR:H	2.34	0.40
1:A:200:ILE:N	1:B:206:TRP:CE3	2.89	0.40
1:A:239:LEU:HD13	1:A:247:ILE:CD1	2.51	0.40
1:B:252:ARG:HH21	1:B:271:ARG:HH12	1.68	0.40
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.80	0.40
1:A:178:TYR:HB3	1:D:179:GLY:CA	2.43	0.40
1:A:219:ARG:HH21	1:B:325:ALA:HB3	1.86	0.40
1:A:220:ARG:C	1:A:222:ASP:N	2.80	0.40
1:C:280:VAL:HG22	1:C:290:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:THR:CG2	1:D:309:ALA:HB2	2.51	0.40
1:D:300:ALA:O	1:D:304:GLY:N	2.55	0.40
1:A:300:ALA:O	1:A:304:GLY:N	2.54	0.40
1:C:274:PHE:HB2	1:C:320:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	342/361 (95%)	326 (95%)	10 (3%)	6 (2%)	6	34
1	B	342/361 (95%)	327 (96%)	10 (3%)	5 (2%)	8	40
1	C	342/361 (95%)	326 (95%)	13 (4%)	3 (1%)	14	51
1	D	342/361 (95%)	330 (96%)	7 (2%)	5 (2%)	8	40
All	All	1368/1444 (95%)	1309 (96%)	40 (3%)	19 (1%)	11	40

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLY
1	A	306	PRO
1	B	68	VAL
1	B	177	GLY
1	B	306	PRO
1	C	177	GLY
1	D	177	GLY
1	D	306	PRO
1	C	103	VAL
1	B	103	VAL
1	D	103	VAL

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Mol	Chain	Res	Type
1	A	12	PRO
1	A	103	VAL
1	B	12	PRO
1	C	12	PRO
1	D	12	PRO
1	D	29	THR
1	A	29	THR
1	A	68	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 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	266/279 (95%)	259 (97%)	7 (3%)	40	62
1	B	266/279 (95%)	258 (97%)	8 (3%)	36	57
1	C	266/279 (95%)	258 (97%)	8 (3%)	36	57
1	D	266/279 (95%)	258 (97%)	8 (3%)	36	57
All	All	1064/1116 (95%)	1033 (97%)	31 (3%)	38	58

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	SER
1	A	122	LEU
1	A	205	LEU
1	A	212	THR
1	A	228	GLN
1	A	229	LEU
1	A	255	THR
1	B	63	ARG
1	B	67	VAL
1	B	68	VAL
1	B	94	SER
1	B	203	PHE
1	B	205	LEU

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Mol	Chain	Res	Type
1	B	228	GLN
1	B	229	LEU
1	C	14	ASN
1	C	63	ARG
1	C	94	SER
1	C	157	GLU
1	C	205	LEU
1	C	228	GLN
1	C	229	LEU
1	C	328	GLN
1	D	32	ASP
1	D	36	ARG
1	D	94	SER
1	D	157	GLU
1	D	203	PHE
1	D	205	LEU
1	D	228	GLN
1	D	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	55	GLN
1	A	124	ASN
1	A	128	ASN
1	A	216	GLN
1	A	228	GLN
1	A	328	GLN
1	B	55	GLN
1	B	128	ASN
1	B	216	GLN
1	B	228	GLN
1	B	286	ASN
1	B	328	GLN
1	C	55	GLN
1	C	124	ASN
1	C	226	ASN
1	C	228	GLN
1	C	328	GLN
1	D	55	GLN
1	D	124	ASN

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Mol	Chain	Res	Type
1	D	128	ASN
1	D	226	ASN
1	D	228	GLN
1	D	328	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

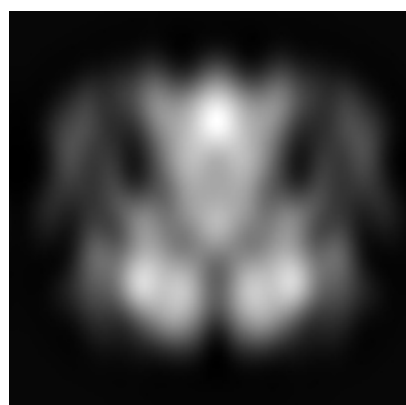
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2527. These allow visual inspection of the internal detail of the map and identification of artifacts.

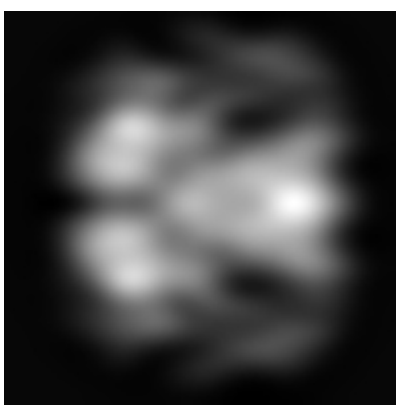
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

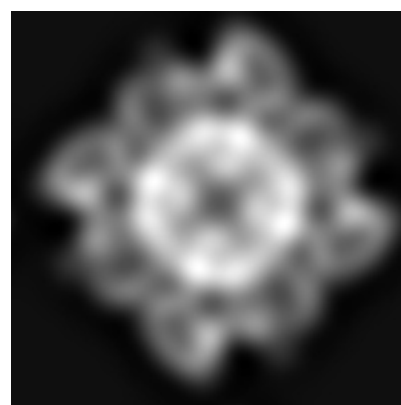
6.1.1 Primary map



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: 53



Y Index: 53



Z Index: 53

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: 61



Y Index: 61

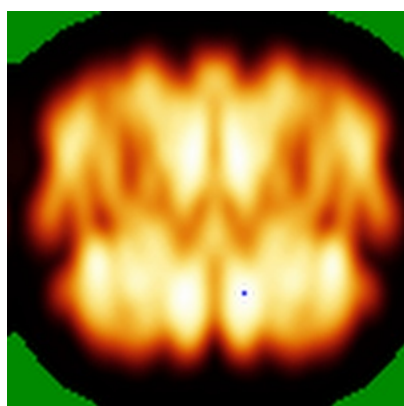


Z Index: 34

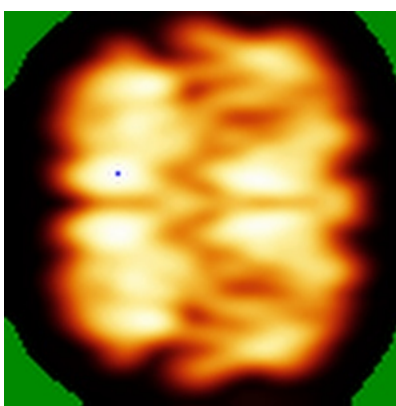
The images above show the largest variance slices of the map in three orthogonal directions.

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

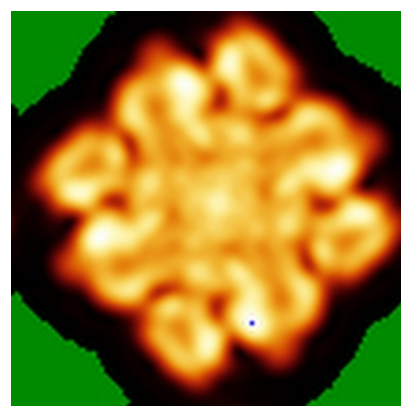
6.4.1 Primary map



X



Y

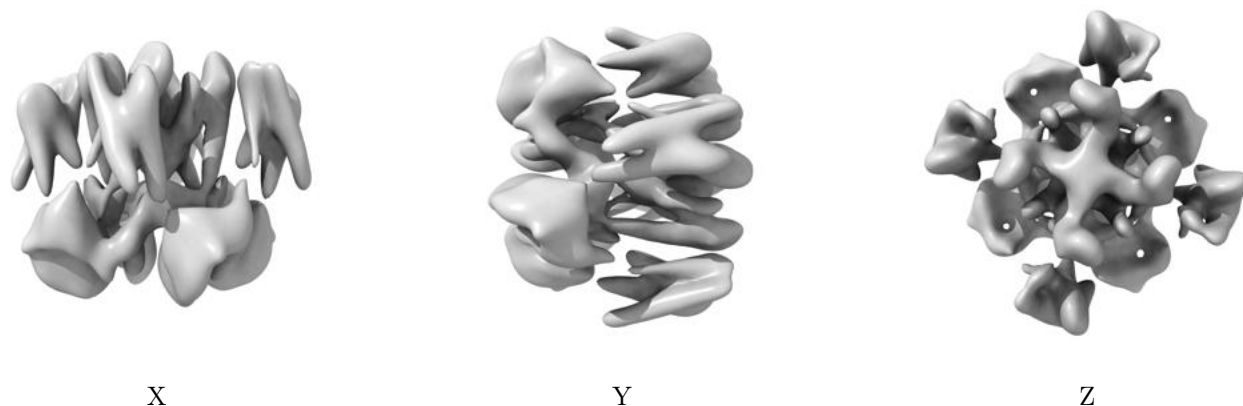


Z

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



The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

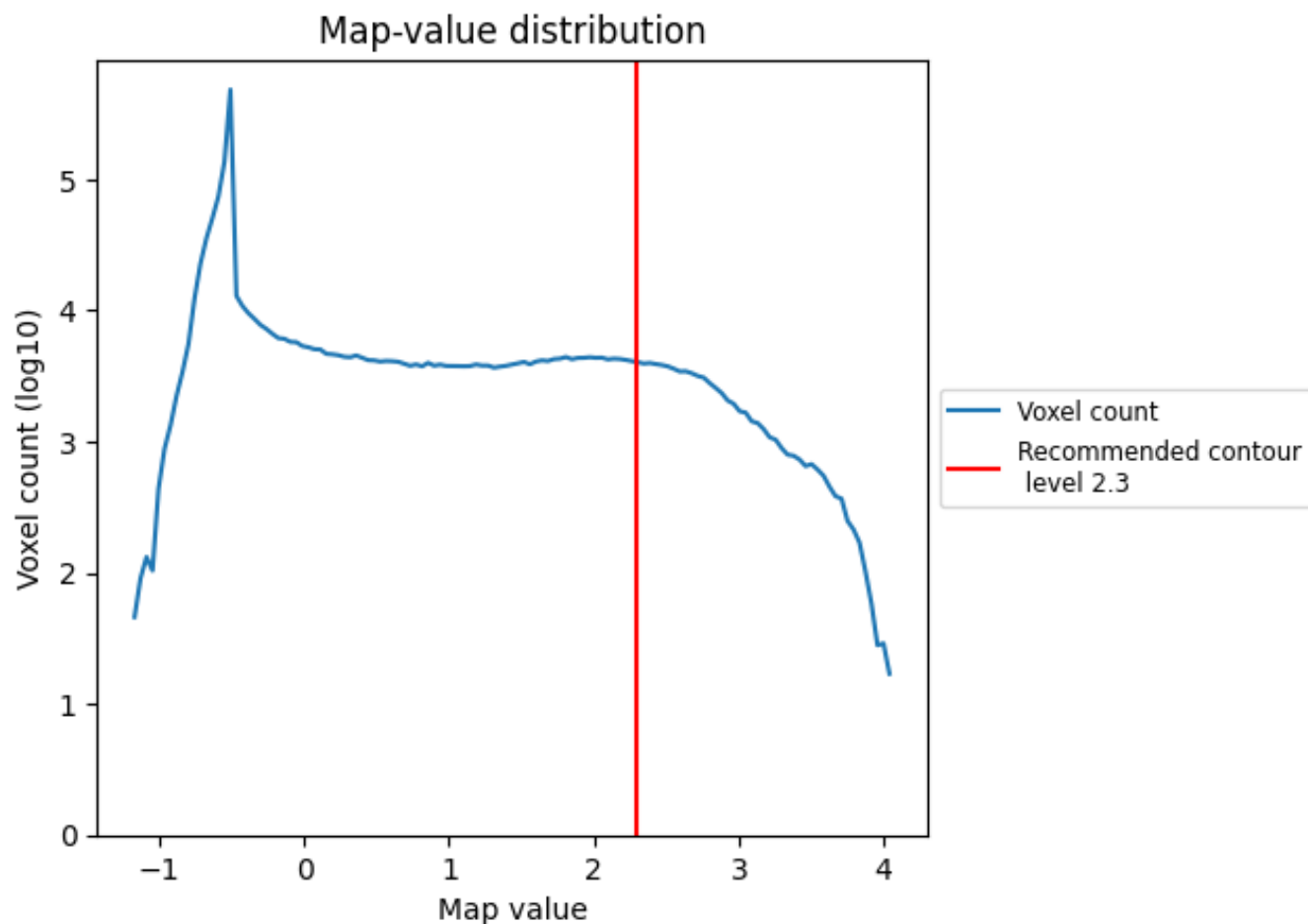
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

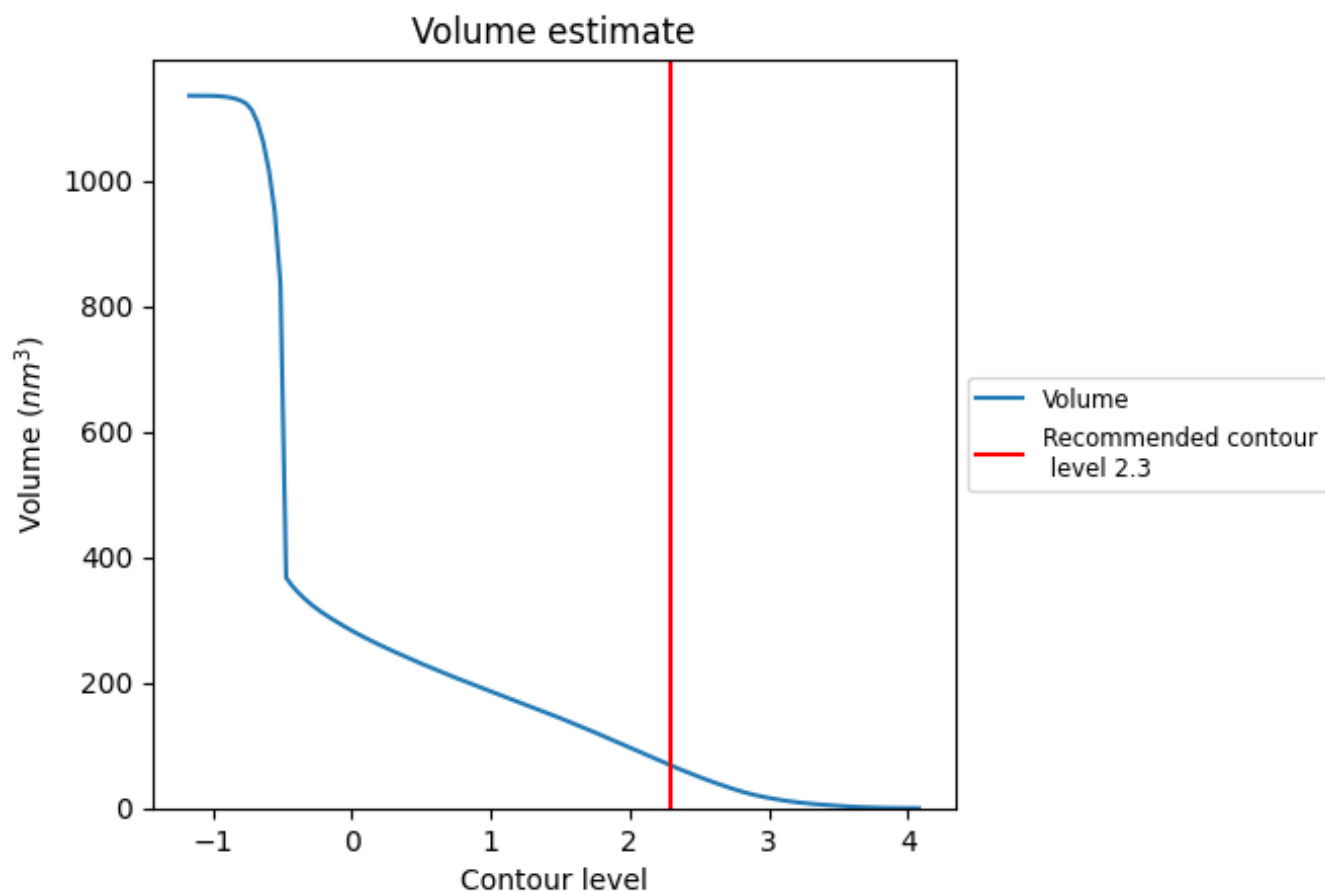
This section contains the results of statistical analysis of the map.

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.

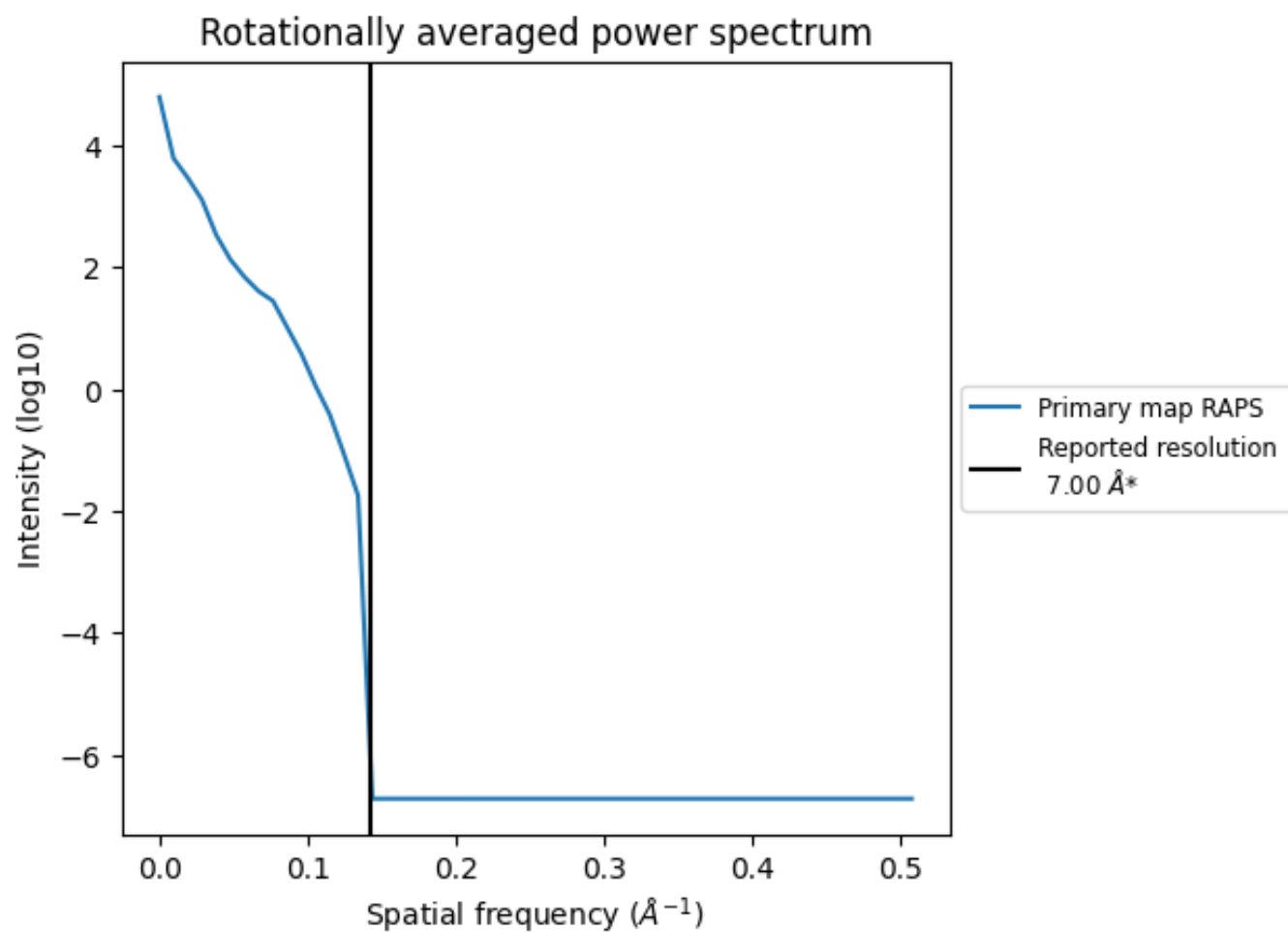
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68 nm³; this corresponds to an approximate mass of 61 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 0.143 Å⁻¹

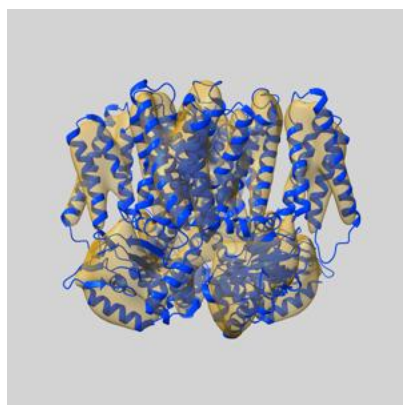
8 Fourier-Shell correlation

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

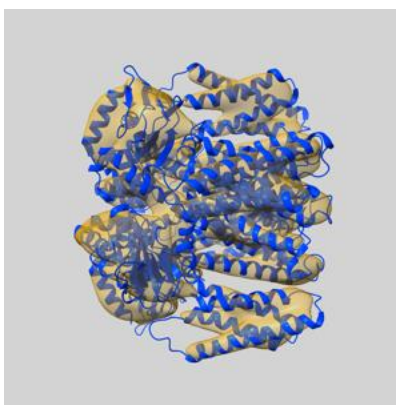
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2527 and PDB model 4CHW. Per-residue inclusion information can be found in section [3](#) on page [5](#).

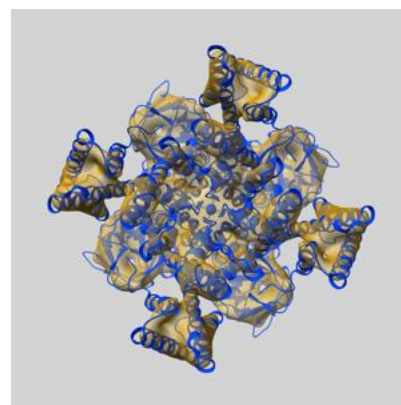
9.1 Map-model overlay [i](#)



X



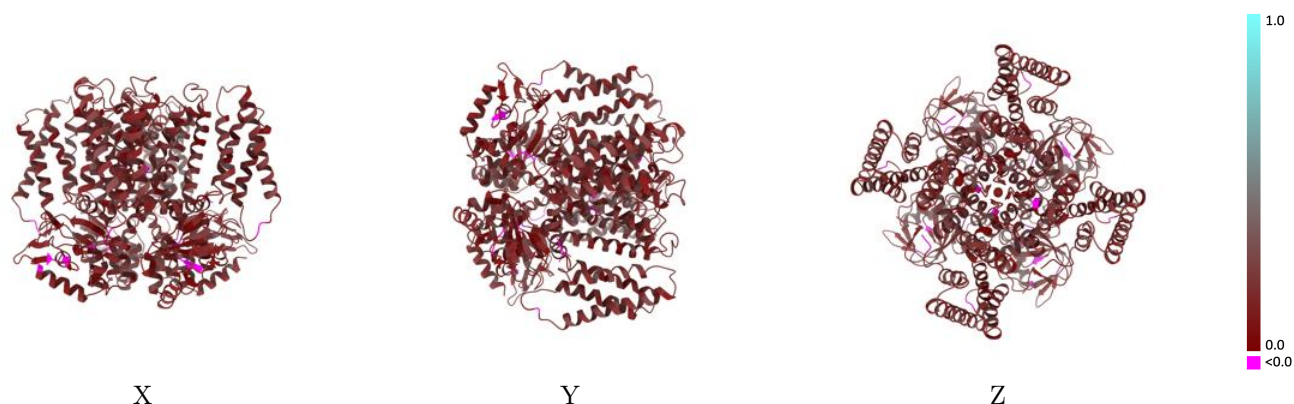
Y



Z

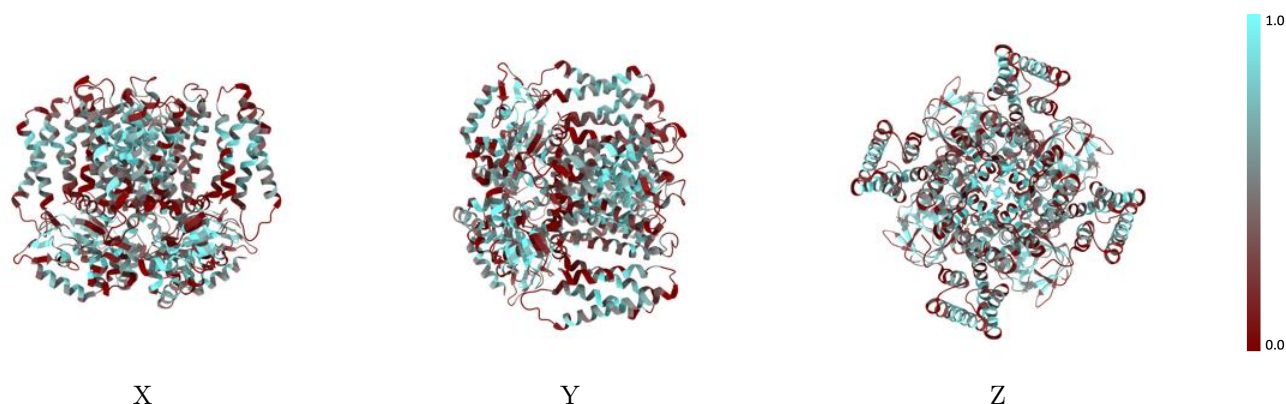
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



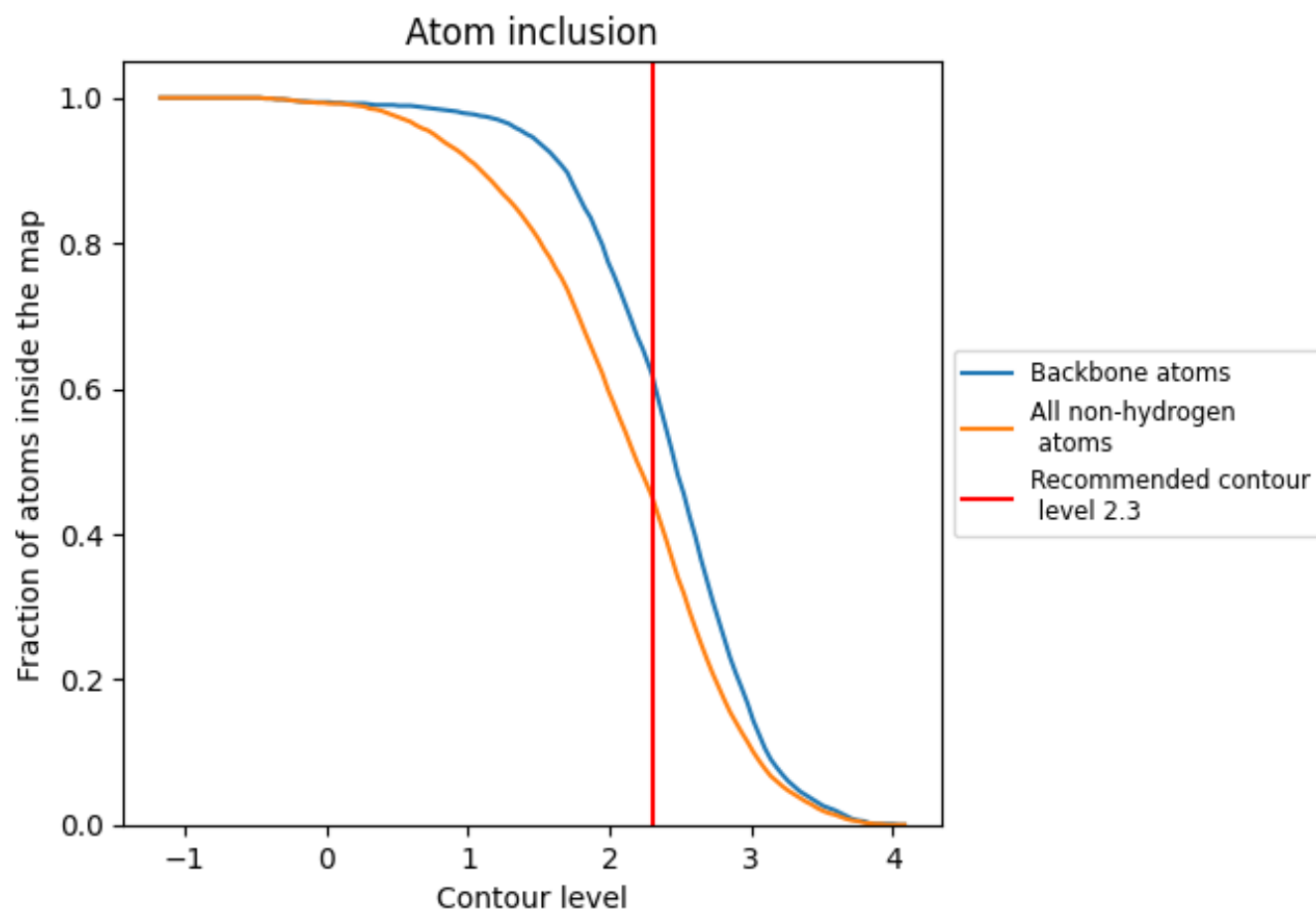
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 45% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4510	0.1630
A	0.4550	0.1630
B	0.4490	0.1610
C	0.4490	0.1620
D	0.4540	0.1640

