



## Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 03:06 PM JST

PDB ID : 7YTC / pdb\_00007ytc  
EMDB ID : EMD-34085  
Title : Cryo-EM structure of human FcmR bound to IgM-Fc/J  
Authors : Li, Y.; Shen, H.; Xiao, J.  
Deposited on : 2022-08-14  
Resolution : 3.39 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

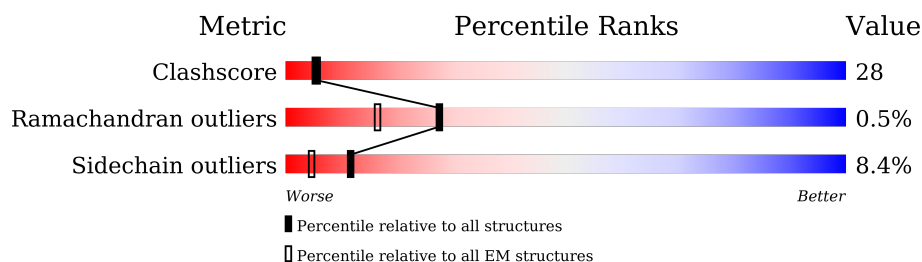
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.39 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.






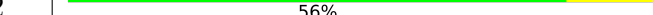
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	232	<div> <div>22%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	B	232	<div> <div>20%</div> <div>60%</div> <div>29%</div> <div>7%</div> <div>..</div> </div>
1	C	232	<div> <div>14%</div> <div>51%</div> <div>34%</div> <div>9%</div> <div>..</div> </div>
1	D	232	<div> <div>19%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	E	232	<div> <div>17%</div> <div>65%</div> <div>27%</div> <div>..</div> </div>
1	F	232	<div> <div>19%</div> <div>62%</div> <div>30%</div> <div>..</div> </div>
1	G	232	<div> <div>19%</div> <div>66%</div> <div>26%</div> <div>..</div> </div>
1	H	232	<div> <div>19%</div> <div>69%</div> <div>23%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	232	
1	L	232	
2	J	136	
3	R	107	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19328 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 Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1780	1120	302	350	8		
1	B	228	Total	C	N	O	S	0	0
			1769	1114	300	347	8		
1	C	225	Total	C	N	O	S	0	0
			1748	1103	297	340	8		
1	D	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	E	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	F	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	G	224	Total	C	N	O	S	0	0
			1742	1100	296	338	8		
1	H	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	K	225	Total	C	N	O	S	0	0
			1749	1103	297	341	8		
1	L	228	Total	C	N	O	S	0	0
			1773	1116	299	349	9		

- Molecule 2 is a protein called Immunoglobulin J chain.

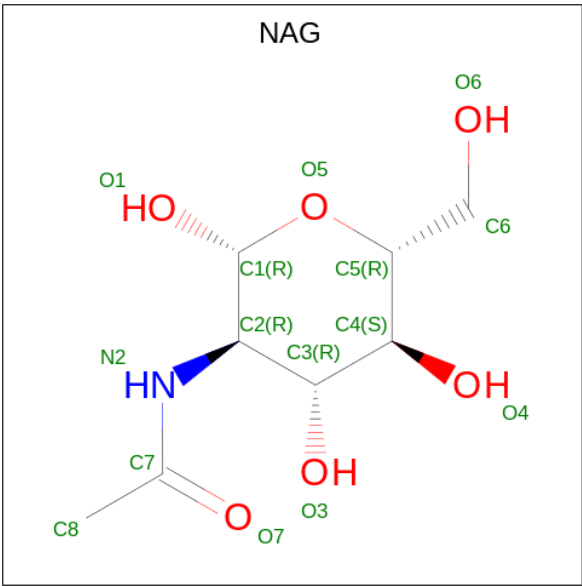
Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	103	Total	C	N	O	S	0	0
			825	513	146	159	7		

- Molecule 3 is a protein called Fas apoptotic inhibitory molecule 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	107	Total	C	N	O	S	0	0
			816	510	144	155	7		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

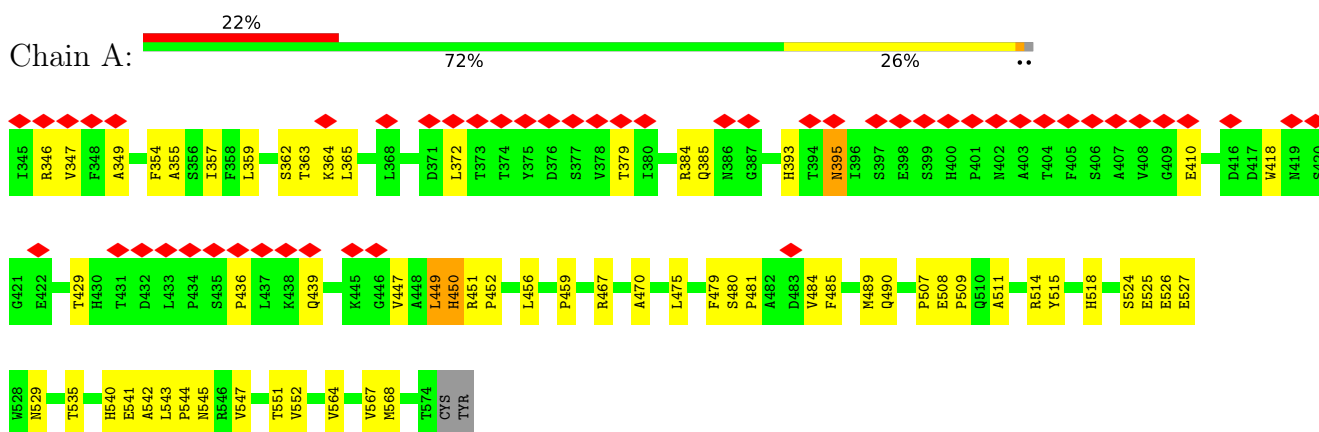


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	H	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	L	1	Total	C	N	O	0
			14	8	1	5	

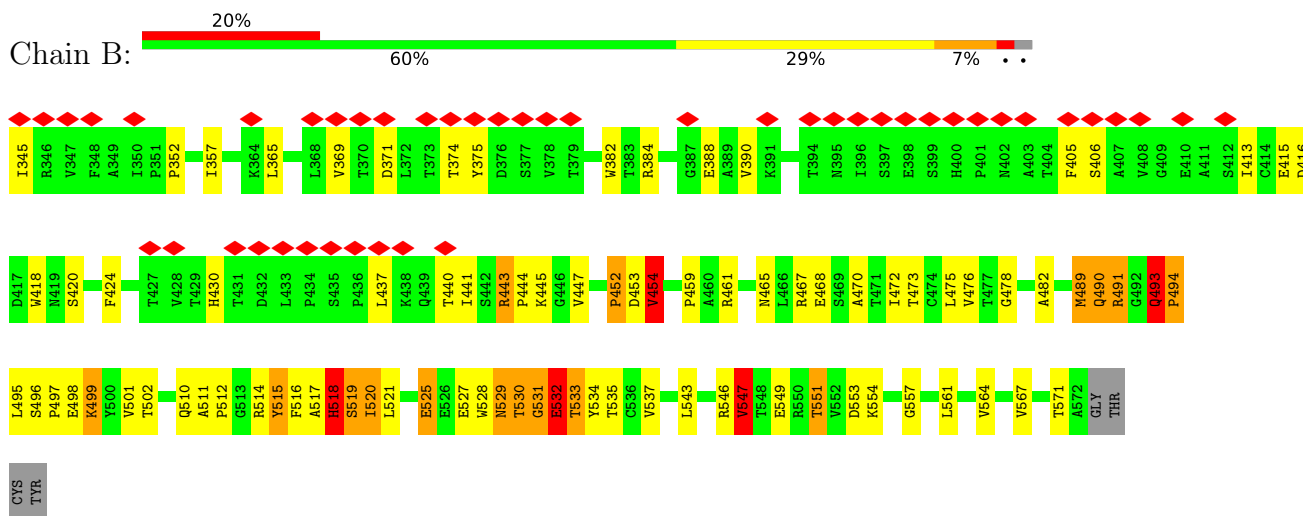
### 3 Residue-property plots

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: Immunoglobulin heavy constant mu

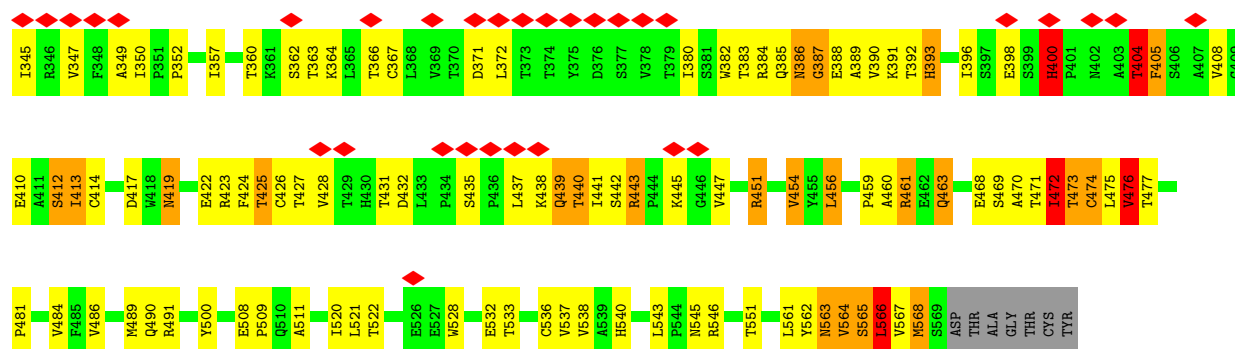


- Molecule 1: Immunoglobulin heavy constant mu

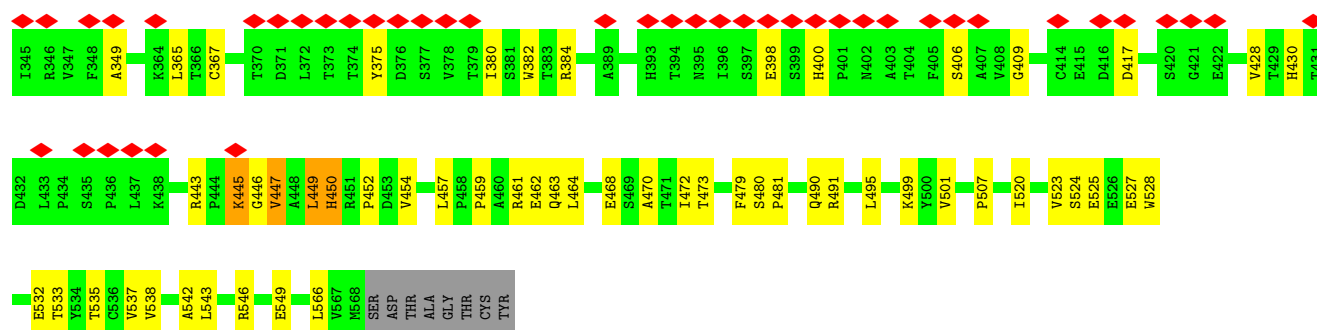


- Molecule 1: Immunoglobulin heavy constant mu

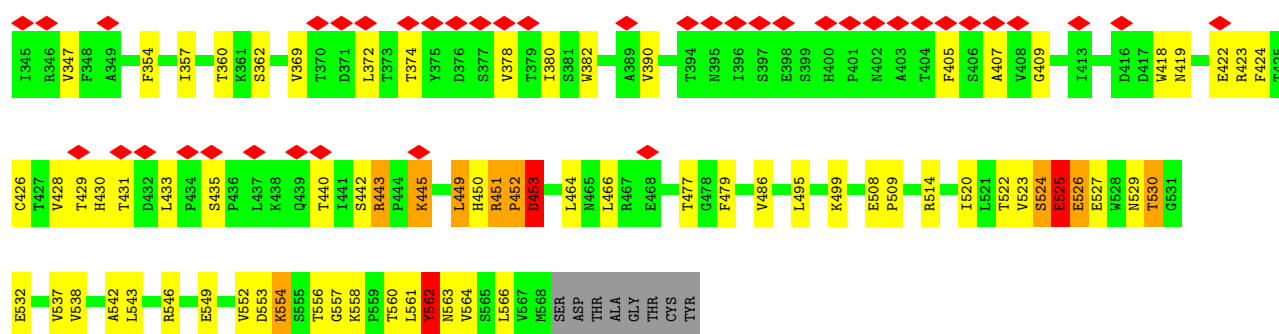




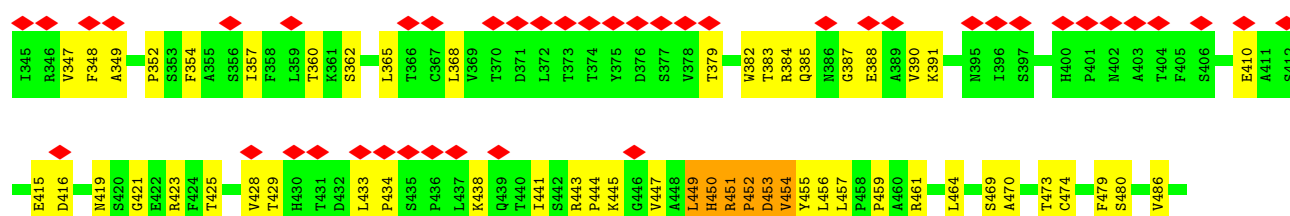
• Molecule 1: Immunoglobulin heavy constant mu

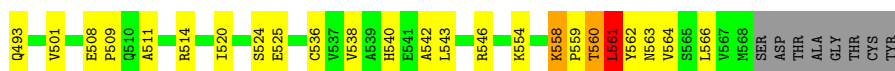


• Molecule 1: Immunoglobulin heavy constant mu

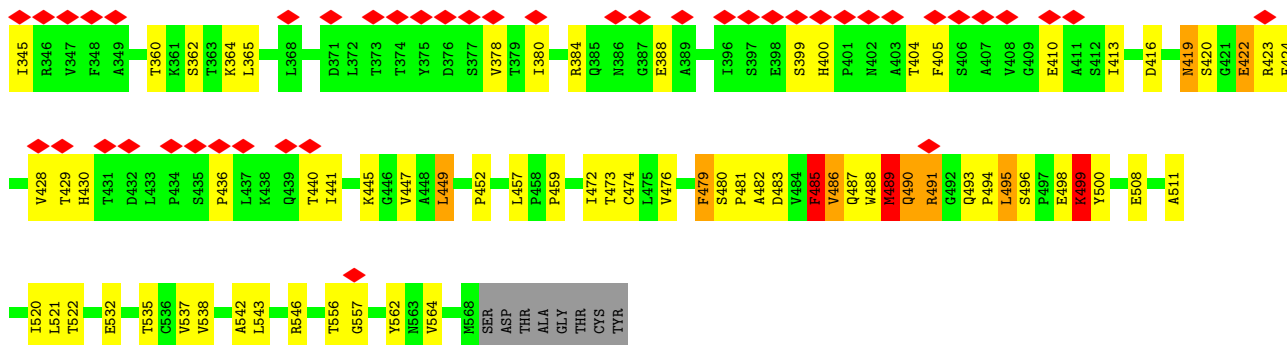


• Molecule 1: Immunoglobulin heavy constant mu

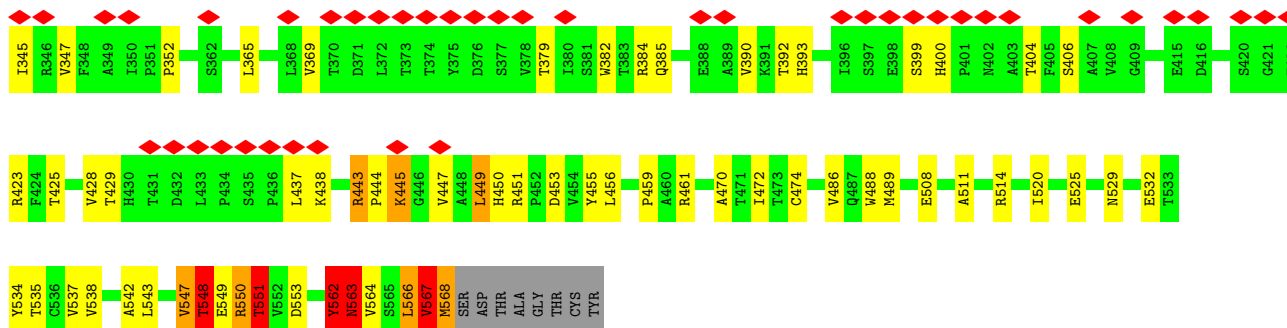




• Molecule 1: Immunoglobulin heavy constant mu



• Molecule 1: Immunoglobulin heavy constant mu



• Molecule 1: Immunoglobulin heavy constant mu



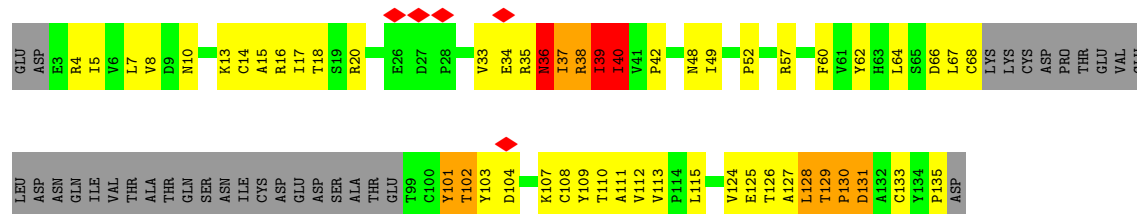
• Molecule 1: Immunoglobulin heavy constant mu



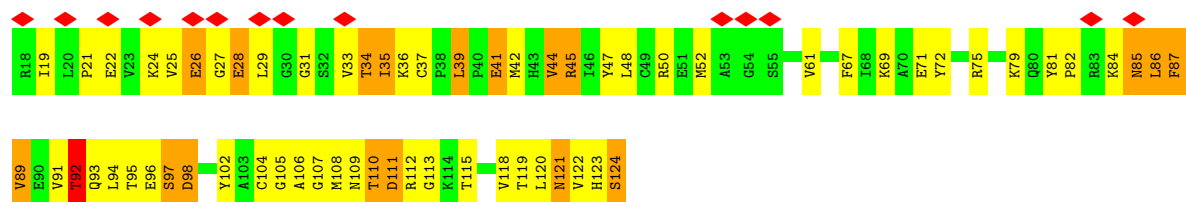




• Molecule 2: Immunoglobulin J chain



• Molecule 3: Fas apoptotic inhibitory molecule 3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	515815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.272	Depositor
Minimum map value	-1.543	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	264.96, 264.96, 264.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82799995, 0.82799995, 0.82799995	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.34	0/1825	0.45	0/2500
1	B	1.10	18/1814 (1.0%)	1.22	21/2485 (0.8%)
1	C	0.89	11/1793 (0.6%)	0.93	11/2455 (0.4%)
1	D	0.43	2/1788 (0.1%)	0.54	4/2449 (0.2%)
1	E	0.62	3/1788 (0.2%)	0.73	3/2449 (0.1%)
1	F	0.66	7/1788 (0.4%)	0.81	7/2449 (0.3%)
1	G	0.81	7/1787 (0.4%)	0.81	10/2447 (0.4%)
1	H	0.72	8/1788 (0.4%)	0.73	7/2449 (0.3%)
1	K	0.65	5/1794 (0.3%)	0.81	7/2457 (0.3%)
1	L	0.61	0/1818	1.08	15/2490 (0.6%)
2	J	1.00	5/838 (0.6%)	1.02	8/1139 (0.7%)
3	R	0.66	0/827	1.06	4/1115 (0.4%)
All	All	0.73	66/19648 (0.3%)	0.86	97/26884 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	563	ASN	CA-C	-10.33	1.39	1.52
1	H	563	ASN	C-O	-10.11	1.11	1.23
1	B	517	ALA	CA-C	-9.51	1.41	1.52
2	J	39	ILE	C-O	-9.48	1.14	1.24
1	B	520	ILE	C-O	-9.27	1.12	1.23
1	C	564	VAL	C-O	-9.27	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	452	PRO	CA-C	-8.45	1.42	1.52
1	B	517	ALA	C-O	-8.29	1.13	1.23
2	J	37	ILE	C-O	-8.26	1.15	1.24
1	K	519	SER	C-O	-8.18	1.14	1.23
1	H	548	THR	C-O	-7.95	1.13	1.23
1	F	454	VAL	C-O	-7.88	1.15	1.23
1	G	479	PHE	C-O	-7.72	1.14	1.23
1	G	486	VAL	C-O	-7.72	1.15	1.24
1	B	519	SER	C-O	-7.65	1.14	1.23
1	G	479	PHE	CA-C	-7.61	1.43	1.52
1	G	482	ALA	CA-C	-7.54	1.49	1.53
1	G	485	PHE	C-O	-7.44	1.15	1.24
1	F	454	VAL	N-CA	-7.39	1.38	1.46
2	J	40	ILE	C-O	-7.31	1.16	1.24
1	B	518	HIS	CA-C	-7.25	1.43	1.52
1	K	519	SER	CA-C	-7.11	1.44	1.52
1	C	564	VAL	CA-C	-6.95	1.44	1.52
1	E	452	PRO	C-O	-6.92	1.15	1.23
1	K	535	THR	C-O	-6.91	1.15	1.24
1	C	566	LEU	C-O	-6.64	1.16	1.23
1	B	515	TYR	C-O	-6.64	1.16	1.23
1	B	521	LEU	C-O	-6.54	1.16	1.24
1	B	521	LEU	CA-C	-6.46	1.44	1.52
1	H	562	TYR	C-O	-6.42	1.16	1.24
1	F	561	LEU	C-O	-6.42	1.15	1.24
1	D	463	GLN	CA-C	-6.37	1.44	1.52
1	B	549	GLU	C-O	-6.33	1.16	1.23
1	B	519	SER	CA-C	-6.24	1.45	1.52
1	C	474	CYS	CA-C	-6.23	1.44	1.52
1	B	496	SER	CA-C	-6.17	1.45	1.52
1	H	549	GLU	C-O	-6.12	1.16	1.23
1	C	563	ASN	CG-ND2	-6.10	1.20	1.33
1	B	489	MET	CA-C	-6.09	1.46	1.52
1	F	452	PRO	C-O	-5.93	1.17	1.23
1	C	476	VAL	C-O	-5.89	1.18	1.24
2	J	38	ARG	C-O	-5.89	1.16	1.23
1	K	516	PHE	C-O	-5.84	1.17	1.23
1	B	489	MET	N-CA	-5.80	1.39	1.46
1	F	453	ASP	CB-CG	-5.75	1.37	1.52
1	B	518	HIS	C-O	-5.75	1.16	1.23
1	F	453	ASP	C-O	-5.68	1.17	1.24
1	B	534	TYR	CB-CG	-5.67	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	37	ILE	CA-CB	-5.63	1.47	1.54
1	G	480	SER	CA-C	-5.61	1.46	1.52
1	C	476	VAL	CA-C	-5.60	1.46	1.52
1	H	567	VAL	C-O	-5.59	1.17	1.24
1	E	452	PRO	CA-C	-5.54	1.46	1.52
1	B	547	VAL	C-O	-5.39	1.18	1.23
1	D	462	GLU	C-O	-5.38	1.17	1.24
1	G	489	MET	CA-C	-5.34	1.46	1.52
1	E	453	ASP	C-O	-5.32	1.17	1.23
1	H	551	THR	C-O	-5.30	1.17	1.23
1	K	517	ALA	C-O	-5.26	1.18	1.23
1	B	520	ILE	CA-CB	-5.17	1.46	1.54
1	H	547	VAL	C-O	-5.16	1.18	1.24
1	B	527	GLU	C-O	-5.12	1.17	1.23
1	C	473	THR	C-O	-5.12	1.18	1.24
1	C	463	GLN	CA-C	-5.05	1.46	1.52
1	C	454	VAL	CA-C	-5.04	1.46	1.52
1	C	566	LEU	CA-C	-5.03	1.46	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	THR	N-CA-C	20.15	133.25	111.28
1	K	533	THR	N-CA-C	14.61	127.21	111.28
1	L	496	SER	CA-C-N	13.92	134.35	119.87
1	L	496	SER	C-N-CA	13.92	134.35	119.87
1	F	558	LYS	CA-C-N	13.70	134.25	119.05
1	F	558	LYS	C-N-CA	13.70	134.25	119.05
1	B	452	PRO	N-CA-C	13.07	130.83	113.84
1	L	506	MET	CA-C-N	12.63	135.63	119.84
1	L	506	MET	C-N-CA	12.63	135.63	119.84
1	L	442	SER	N-CA-C	11.01	124.52	108.34
1	B	496	SER	CA-C-N	10.99	133.57	119.84
1	B	496	SER	C-N-CA	10.99	133.57	119.84
1	B	493	GLN	CA-C-N	10.95	133.53	119.84
1	B	493	GLN	C-N-CA	10.95	133.53	119.84
1	H	562	TYR	N-CA-C	10.22	125.48	107.80
1	L	508	GLU	CA-C-N	10.14	130.31	119.05
1	L	508	GLU	C-N-CA	10.14	130.31	119.05
1	F	454	VAL	N-CA-C	9.69	122.62	107.98
1	B	454	VAL	CB-CA-C	-9.25	101.24	111.23
1	B	534	TYR	N-CA-C	8.99	122.25	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	LYS	N-CA-C	-8.90	103.01	114.04
1	F	561	LEU	N-CA-C	-8.71	92.25	110.80
1	G	499	LYS	N-CA-C	8.60	120.66	111.28
1	G	496	SER	CA-C-N	8.21	128.17	119.05
1	G	496	SER	C-N-CA	8.21	128.17	119.05
1	B	520	ILE	CB-CA-C	-8.12	99.20	110.90
1	E	562	TYR	N-CA-C	8.10	122.42	109.79
1	F	454	VAL	N-CA-CB	-7.93	102.19	111.39
1	G	480	SER	C-N-CD	-7.83	103.37	120.60
1	B	519	SER	CA-C-O	-7.47	112.72	121.46
2	J	102	THR	N-CA-C	7.44	121.40	110.17
1	L	453	ASP	N-CA-C	7.38	121.20	110.28
1	G	419	ASN	N-CA-C	-7.24	104.25	113.23
1	B	520	ILE	N-CA-C	7.06	120.00	108.99
1	F	454	VAL	CB-CA-C	-6.93	103.75	111.23
1	C	404	THR	N-CA-C	-6.81	98.93	109.76
1	B	531	GLY	N-CA-C	-6.78	97.10	113.18
3	R	31	GLY	N-CA-C	6.77	119.28	111.36
1	G	480	SER	CA-C-N	6.74	143.18	127.00
1	G	480	SER	C-N-CA	6.74	143.18	127.00
1	L	443	ARG	N-CA-C	6.72	121.11	109.82
1	L	493	GLN	CA-C-N	6.67	126.63	119.76
1	L	493	GLN	C-N-CA	6.67	126.63	119.76
1	K	449	LEU	N-CA-C	6.64	119.38	110.88
1	K	443	ARG	CA-C-N	6.51	127.98	119.84
1	K	443	ARG	C-N-CA	6.51	127.98	119.84
1	B	515	TYR	N-CA-C	6.49	119.91	109.79
1	D	507	PRO	CA-C-N	6.49	129.70	120.49
1	D	507	PRO	C-N-CA	6.49	129.70	120.49
2	J	66	ASP	N-CA-C	-6.47	103.72	112.26
1	B	530	THR	N-CA-C	-6.44	104.61	113.18
3	R	121	ASN	N-CA-C	6.42	119.19	109.23
1	B	453	ASP	N-CA-C	6.40	124.43	110.80
1	B	532	GLU	CA-C-N	6.38	128.83	120.28
1	B	532	GLU	C-N-CA	6.38	128.83	120.28
1	K	556	THR	N-CA-C	6.36	120.90	113.20
1	C	474	CYS	N-CA-C	-6.32	101.59	110.50
1	C	387	GLY	N-CA-C	-6.26	102.49	113.76
2	J	37	ILE	CB-CA-C	-6.06	101.71	111.59
1	H	567	VAL	N-CA-C	6.05	119.34	109.78
1	C	564	VAL	CB-CA-C	-6.05	102.25	111.69
2	J	38	ARG	N-CA-C	6.03	117.80	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	130	PRO	O-C-N	6.01	129.83	123.10
1	H	562	TYR	CB-CA-C	-6.00	101.85	110.62
1	B	443	ARG	N-CA-C	-5.96	100.61	109.42
3	R	92	THR	N-CA-C	5.91	117.40	111.07
1	D	449	LEU	N-CA-C	5.86	118.80	109.24
1	E	452	PRO	CA-C-O	-5.84	114.98	121.23
1	H	549	GLU	CB-CA-C	-5.78	99.83	111.17
1	F	560	THR	N-CA-C	5.73	123.01	110.80
1	C	400	HIS	N-CA-C	5.70	117.95	110.08
1	G	483	ASP	N-CA-C	5.68	119.27	111.54
1	H	568	MET	CB-CG-SD	-5.66	95.71	112.70
1	B	418	TRP	N-CA-C	-5.64	105.12	112.23
1	C	405	PHE	N-CA-C	-5.63	99.95	108.67
1	L	505	PRO	N-CA-C	5.59	119.98	111.15
1	C	473	THR	N-CA-C	5.56	117.47	108.41
1	C	385	GLN	N-CA-C	-5.51	105.66	112.38
1	C	435	SER	CA-C-N	-5.46	113.93	119.83
1	C	435	SER	C-N-CA	-5.46	113.93	119.83
1	K	535	THR	CA-C-N	5.45	129.87	122.19
1	K	535	THR	C-N-CA	5.45	129.87	122.19
1	C	472	ILE	N-CA-C	-5.45	100.57	108.36
1	L	508	GLU	N-CA-C	5.34	117.68	110.31
1	E	525	GLU	N-CA-C	5.32	117.07	111.28
1	G	486	VAL	CB-CA-C	-5.30	102.78	110.63
3	R	85	ASN	N-CA-C	5.30	118.70	111.39
1	L	518	HIS	N-CA-CB	-5.21	101.82	111.52
2	J	36	ASN	N-CA-C	5.19	121.85	110.80
2	J	39	ILE	CA-C-O	-5.18	115.12	121.13
1	B	529	ASN	N-CA-C	-5.18	104.25	110.88
1	L	516	PHE	N-CA-C	5.13	118.09	110.14
1	D	446	GLY	N-CA-C	5.09	122.60	115.43
1	H	563	ASN	CB-CA-C	-5.02	101.06	109.65
2	J	130	PRO	CA-C-O	-5.01	115.32	121.03
1	H	547	VAL	CB-CA-C	-5.00	103.08	111.29
1	G	482	ALA	CB-CA-C	-5.00	109.86	117.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	562	TYR	Mainchain

## 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	1780	0	1739	57	0
1	B	1769	0	1729	78	0
1	C	1748	0	1710	98	0
1	D	1743	0	1707	47	0
1	E	1743	0	1707	99	0
1	F	1743	0	1707	85	0
1	G	1742	0	1707	59	0
1	H	1743	0	1706	86	0
1	K	1749	0	1712	128	0
1	L	1773	0	1719	188	0
2	J	825	0	820	101	0
3	R	816	0	835	141	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	2	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	2	0
4	G	14	0	13	1	0
4	H	14	0	13	0	0
4	J	14	0	13	1	0
4	K	14	0	13	0	0
4	L	14	0	13	1	0
All	All	19328	0	18941	1068	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 28.

All (1068) 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)
2:J:49:ILE:HG13	2:J:103:TYR:CE1	1.34	1.62
1:E:418:TRP:CD2	1:E:443:ARG:CD	1.81	1.61
1:E:418:TRP:CD2	1:E:443:ARG:HD2	1.09	1.60
1:E:418:TRP:CE2	1:E:443:ARG:HD2	1.18	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:TRP:CE2	1:E:443:ARG:CD	1.86	1.54
1:L:488:TRP:CD2	1:L:521:LEU:CD2	1.90	1.54
1:L:452:PRO:CG	1:L:479:PHE:CA	1.81	1.54
1:C:564:VAL:HG21	1:H:566:LEU:CD2	1.34	1.53
1:L:452:PRO:HG3	1:L:479:PHE:CA	1.09	1.53
1:E:418:TRP:CZ2	1:E:443:ARG:CG	1.87	1.52
1:C:563:ASN:ND2	4:C:601:NAG:C1	1.68	1.51
1:C:384:ARG:CB	1:C:388:GLU:HB2	1.38	1.51
1:L:452:PRO:HG2	1:L:479:PHE:CB	1.38	1.50
1:E:418:TRP:CH2	1:E:443:ARG:HG2	1.47	1.47
2:J:49:ILE:CG1	2:J:103:TYR:HE1	1.24	1.47
1:C:384:ARG:HB2	1:C:388:GLU:CB	1.43	1.46
1:E:418:TRP:CZ2	1:E:443:ARG:HG2	0.94	1.45
1:C:384:ARG:NE	1:C:388:GLU:CB	1.77	1.44
1:F:450:HIS:ND1	1:F:514:ARG:NE	1.66	1.43
3:R:96:GLU:HG2	3:R:122:VAL:CG2	1.48	1.42
1:C:564:VAL:CG2	1:H:566:LEU:HD21	1.50	1.42
3:R:35:ILE:O	3:R:88:LEU:CD1	1.68	1.41
1:K:516:PHE:CE2	1:L:520:ILE:HD11	1.55	1.39
3:R:35:ILE:O	3:R:88:LEU:CD2	1.68	1.37
1:F:450:HIS:ND1	1:F:514:ARG:CZ	1.87	1.36
1:L:452:PRO:HB3	1:L:478:GLY:C	1.50	1.36
1:C:384:ARG:CD	1:C:388:GLU:HB3	1.57	1.35
1:C:384:ARG:CZ	1:C:388:GLU:HB3	1.57	1.33
1:L:452:PRO:CG	1:L:479:PHE:CB	2.01	1.32
1:E:418:TRP:CG	1:E:443:ARG:HD2	1.64	1.32
1:K:516:PHE:CE2	1:L:520:ILE:CD1	2.12	1.32
1:E:418:TRP:CH2	1:E:443:ARG:CG	2.08	1.31
1:F:450:HIS:CE1	1:F:514:ARG:CD	2.14	1.31
1:F:450:HIS:CE1	1:F:514:ARG:HD3	1.68	1.29
1:C:384:ARG:NE	1:C:388:GLU:HB3	0.99	1.29
1:F:450:HIS:CE1	1:F:514:ARG:NE	1.99	1.29
2:J:49:ILE:CG1	2:J:103:TYR:CE1	2.03	1.28
1:L:443:ARG:HD3	1:L:444:PRO:CD	1.63	1.28
1:K:422:GLU:O	1:K:443:ARG:NH1	1.64	1.28
1:K:526:GLU:C	1:K:529:ASN:OD1	1.77	1.26
3:R:75:ARG:O	3:R:92:THR:HG22	1.34	1.25
1:E:418:TRP:CE2	1:E:443:ARG:HG2	1.69	1.25
1:E:423:ARG:HG3	1:E:442:SER:OG	1.36	1.25
1:L:452:PRO:CG	1:L:479:PHE:HA	1.54	1.25
1:K:516:PHE:HE2	1:L:520:ILE:CD1	1.49	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:488:TRP:CE3	1:L:521:LEU:HD23	1.75	1.21
1:L:488:TRP:CG	1:L:521:LEU:HD21	1.76	1.21
1:L:488:TRP:CE2	1:L:521:LEU:HD22	1.76	1.20
3:R:34:THR:OG1	3:R:88:LEU:HD12	1.35	1.20
1:E:418:TRP:CE2	1:E:443:ARG:CG	2.13	1.20
1:K:526:GLU:O	1:K:529:ASN:OD1	1.56	1.19
1:B:535:THR:HG22	1:B:551:THR:OG1	1.42	1.19
1:C:384:ARG:CD	1:C:388:GLU:CB	2.18	1.18
1:F:450:HIS:CE1	1:F:514:ARG:CZ	2.25	1.18
1:G:490:GLN:OE1	1:G:532:GLU:HG3	1.42	1.17
1:L:452:PRO:CG	1:L:479:PHE:HB3	1.69	1.16
1:L:452:PRO:HB2	1:L:477:THR:O	1.44	1.16
1:L:488:TRP:O	1:L:495:LEU:HB2	1.41	1.16
1:B:490:GLN:O	1:B:493:GLN:OE1	1.63	1.15
1:E:423:ARG:CG	1:E:442:SER:OG	1.94	1.15
3:R:35:ILE:O	3:R:88:LEU:CG	1.94	1.14
3:R:35:ILE:O	3:R:88:LEU:HD22	1.41	1.14
3:R:96:GLU:CG	3:R:122:VAL:CG2	2.24	1.14
1:L:452:PRO:CG	1:L:479:PHE:N	2.09	1.14
1:L:452:PRO:HG3	1:L:479:PHE:N	1.63	1.14
2:J:39:ILE:HD13	2:J:62:TYR:CE1	1.83	1.13
3:R:35:ILE:O	3:R:88:LEU:HD13	1.41	1.13
1:L:452:PRO:CB	1:L:478:GLY:C	2.19	1.13
1:K:526:GLU:CA	1:K:529:ASN:OD1	1.97	1.12
3:R:36:LYS:HB3	3:R:86:LEU:CD1	1.79	1.12
1:L:488:TRP:CG	1:L:521:LEU:CD2	2.29	1.11
3:R:96:GLU:CG	3:R:122:VAL:HG21	1.80	1.11
1:D:450:HIS:CE1	1:D:480:SER:OG	2.04	1.11
2:J:39:ILE:CD1	2:J:62:TYR:CD1	2.32	1.11
2:J:49:ILE:CD1	2:J:103:TYR:CE1	2.33	1.10
1:L:478:GLY:HA2	1:L:514:ARG:HG3	1.11	1.09
1:L:491:ARG:HB3	1:L:493:GLN:NE2	1.68	1.09
1:C:383:THR:HA	1:C:388:GLU:O	1.52	1.09
2:J:39:ILE:HD11	2:J:62:TYR:CD1	1.88	1.09
1:K:535:THR:HG22	1:K:551:THR:HB	1.35	1.08
1:K:526:GLU:HA	1:K:529:ASN:OD1	1.52	1.08
1:L:491:ARG:CB	1:L:493:GLN:HE22	1.64	1.08
1:L:488:TRP:CD2	1:L:521:LEU:HD22	1.79	1.07
1:L:443:ARG:CD	1:L:444:PRO:HD3	1.84	1.07
1:E:418:TRP:NE1	1:E:443:ARG:HD2	1.70	1.07
1:L:491:ARG:HB3	1:L:493:GLN:HE22	0.91	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:TRP:HB2	1:C:390:VAL:HG21	1.31	1.06
3:R:34:THR:OG1	3:R:88:LEU:CD1	2.03	1.06
1:E:418:TRP:CD1	1:E:443:ARG:HD2	1.90	1.05
3:R:36:LYS:CB	3:R:86:LEU:HD11	1.85	1.05
1:H:443:ARG:HE	1:H:443:ARG:HA	1.20	1.04
1:H:535:THR:HG22	1:H:551:THR:OG1	1.58	1.04
1:H:543:LEU:HD13	1:H:548:THR:HG22	1.38	1.04
2:J:39:ILE:HD11	2:J:62:TYR:CG	1.92	1.03
1:C:384:ARG:HB2	1:C:388:GLU:CG	1.88	1.03
3:R:26:GLU:HB3	3:R:124:SER:HA	1.39	1.02
1:L:443:ARG:CD	1:L:444:PRO:CD	2.36	1.02
3:R:27:GLY:HA3	3:R:94:LEU:CD2	1.90	1.01
1:L:443:ARG:CG	1:L:444:PRO:HD2	1.91	1.01
1:C:384:ARG:HE	1:C:388:GLU:CG	1.73	1.00
1:E:418:TRP:CD2	1:E:443:ARG:HD3	1.96	1.00
1:L:488:TRP:CD2	1:L:521:LEU:HD21	1.86	1.00
3:R:26:GLU:HB3	3:R:124:SER:CA	1.92	1.00
1:E:418:TRP:CH2	1:E:443:ARG:HG3	1.94	0.99
1:D:449:LEU:HD21	1:D:481:PRO:HD3	1.43	0.99
1:C:384:ARG:NE	1:C:388:GLU:CG	2.24	0.99
1:K:535:THR:HG22	1:K:551:THR:CB	1.91	0.99
3:R:22:GLU:HA	3:R:118:VAL:HG23	1.41	0.99
3:R:96:GLU:HG2	3:R:122:VAL:HG23	1.45	0.99
1:K:516:PHE:CE2	1:L:520:ILE:HD13	1.95	0.98
1:K:463:GLN:CG	1:L:455:TYR:CE2	2.47	0.98
2:J:39:ILE:CD1	2:J:62:TYR:CG	2.45	0.98
1:K:422:GLU:O	1:K:443:ARG:CZ	2.11	0.97
1:C:459:PRO:HD3	1:C:472:ILE:HG23	1.43	0.97
1:L:508:GLU:HG2	1:L:509:PRO:HD2	1.45	0.97
3:R:27:GLY:HA3	3:R:94:LEU:HD22	1.44	0.96
1:L:488:TRP:CE3	1:L:521:LEU:CD2	2.40	0.95
1:L:452:PRO:HB3	1:L:478:GLY:O	1.65	0.95
1:E:418:TRP:CE3	1:E:443:ARG:CD	2.49	0.94
1:L:488:TRP:CE2	1:L:521:LEU:CD2	2.42	0.94
1:C:382:TRP:HB2	1:C:390:VAL:CG2	1.98	0.94
1:K:514:ARG:HG3	1:K:514:ARG:HH11	1.30	0.94
1:D:450:HIS:ND1	1:D:480:SER:OG	1.96	0.93
1:L:488:TRP:CD2	1:L:521:LEU:HD23	1.82	0.93
1:A:450:HIS:ND1	1:A:480:SER:HB3	1.83	0.93
1:E:418:TRP:CZ3	1:E:443:ARG:HG3	2.04	0.92
1:L:478:GLY:CA	1:L:514:ARG:HG3	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ARG:CG	1:C:388:GLU:HB2	1.99	0.92
1:C:384:ARG:HE	1:C:388:GLU:HG3	1.34	0.92
1:L:506:MET:O	1:L:515:TYR:HB3	1.69	0.91
3:R:45:ARG:HD3	3:R:107:GLY:O	1.70	0.91
1:L:508:GLU:CG	1:L:509:PRO:HD2	1.99	0.91
1:E:418:TRP:CZ3	1:E:443:ARG:CG	2.53	0.91
1:D:443:ARG:NH2	1:D:445:LYS:HD3	1.85	0.91
3:R:39:LEU:H	3:R:39:LEU:HD12	1.36	0.91
1:L:443:ARG:HD3	1:L:444:PRO:HD3	0.92	0.91
1:C:564:VAL:CG2	1:H:566:LEU:CD2	2.25	0.91
3:R:22:GLU:HA	3:R:118:VAL:CG2	2.01	0.90
3:R:96:GLU:HG2	3:R:122:VAL:HG22	1.52	0.90
1:D:449:LEU:CD2	1:D:481:PRO:HD3	2.01	0.90
1:K:516:PHE:HZ	1:L:501:VAL:HG11	1.36	0.90
1:L:443:ARG:CB	1:L:444:PRO:HD2	2.00	0.90
3:R:96:GLU:CB	3:R:122:VAL:HG21	2.01	0.90
2:J:34:GLU:HG3	2:J:36:ASN:OD1	1.71	0.89
1:H:443:ARG:HA	1:H:443:ARG:NE	1.81	0.89
2:J:49:ILE:HD11	2:J:103:TYR:CE1	2.07	0.89
1:L:500:TYR:HB2	1:L:521:LEU:HD13	1.54	0.89
1:E:450:HIS:NE2	1:E:514:ARG:NH1	2.21	0.88
1:E:443:ARG:HB2	1:E:443:ARG:CZ	2.02	0.88
1:A:450:HIS:CE1	1:A:480:SER:HB3	2.10	0.87
1:F:452:PRO:HB3	1:F:479:PHE:HB3	1.57	0.87
1:H:449:LEU:HD12	1:H:542:ALA:HB2	1.56	0.87
1:E:418:TRP:O	1:E:443:ARG:HD3	1.74	0.86
2:J:39:ILE:HD13	2:J:62:TYR:CD1	2.05	0.86
1:K:501:VAL:HG11	1:L:516:PHE:CZ	2.10	0.86
3:R:75:ARG:O	3:R:92:THR:CG2	2.22	0.86
1:H:543:LEU:HD13	1:H:548:THR:CG2	2.05	0.86
1:H:384:ARG:HD2	1:H:385:GLN:H	1.41	0.86
2:J:49:ILE:CG1	2:J:103:TYR:CD1	2.58	0.86
1:K:463:GLN:CB	1:L:455:TYR:CE2	2.52	0.86
1:D:449:LEU:HD21	1:D:481:PRO:CD	2.05	0.85
1:E:423:ARG:CB	1:E:442:SER:OG	2.24	0.85
1:H:543:LEU:CD1	1:H:548:THR:HG22	2.06	0.85
1:H:562:TYR:HD1	1:K:562:TYR:HD2	1.25	0.85
1:B:475:LEU:HD13	1:B:518:HIS:CD2	2.12	0.84
1:B:518:HIS:O	1:B:518:HIS:ND1	2.11	0.84
3:R:37:CYS:O	3:R:87:PHE:N	2.09	0.84
3:R:35:ILE:HD12	3:R:35:ILE:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:422:GLU:O	1:K:443:ARG:NH2	2.10	0.83
1:E:418:TRP:O	1:E:443:ARG:CZ	2.27	0.83
1:A:449:LEU:HD22	1:A:480:SER:O	1.78	0.83
1:K:463:GLN:HG3	1:L:455:TYR:CE2	2.13	0.83
1:K:516:PHE:CZ	1:L:520:ILE:HD11	2.14	0.83
1:K:563:ASN:HB3	1:L:563:ASN:HB3	1.60	0.83
1:L:443:ARG:CD	1:L:444:PRO:HD2	2.07	0.83
3:R:33:VAL:HG13	3:R:91:VAL:CG2	2.09	0.83
2:J:39:ILE:CD1	2:J:62:TYR:CE1	2.58	0.83
1:D:449:LEU:CD2	1:D:481:PRO:CD	2.57	0.82
1:C:349:ALA:HB2	1:C:439:GLN:HG3	1.62	0.82
3:R:28:GLU:HA	3:R:28:GLU:OE1	1.79	0.82
3:R:33:VAL:O	3:R:91:VAL:HG22	1.80	0.82
1:L:443:ARG:HG2	1:L:443:ARG:HH11	1.45	0.82
3:R:33:VAL:CG1	3:R:91:VAL:CG2	2.58	0.81
3:R:35:ILE:O	3:R:88:LEU:HD11	1.80	0.81
1:F:450:HIS:HE1	1:F:514:ARG:HD3	1.40	0.81
1:H:443:ARG:NE	1:H:444:PRO:HD2	1.96	0.81
1:L:452:PRO:CG	1:L:478:GLY:C	2.51	0.81
3:R:36:LYS:HB3	3:R:86:LEU:HD11	0.90	0.81
3:R:75:ARG:C	3:R:92:THR:HG22	2.05	0.80
2:J:49:ILE:O	2:J:103:TYR:OH	1.99	0.80
1:L:421:GLY:HA2	1:L:443:ARG:NH1	1.97	0.80
1:H:543:LEU:CD1	1:H:548:THR:CG2	2.59	0.80
1:C:384:ARG:CZ	1:C:388:GLU:CB	2.38	0.80
1:E:418:TRP:CG	1:E:443:ARG:CD	2.40	0.80
3:R:26:GLU:HB3	3:R:124:SER:C	2.07	0.79
1:C:384:ARG:CG	1:C:388:GLU:CB	2.58	0.79
3:R:111:ASP:OD1	3:R:111:ASP:N	2.15	0.79
1:K:450:HIS:CB	1:K:514:ARG:HH21	1.95	0.79
3:R:75:ARG:HA	3:R:92:THR:HG21	1.64	0.79
1:K:501:VAL:HG11	1:L:516:PHE:HZ	1.47	0.79
1:E:453:ASP:OD2	1:E:477:THR:CG2	2.31	0.79
3:R:27:GLY:CA	3:R:94:LEU:HD22	2.13	0.79
1:E:418:TRP:O	1:E:443:ARG:CD	2.31	0.79
3:R:35:ILE:C	3:R:88:LEU:CD1	2.56	0.79
1:C:384:ARG:HD3	1:C:388:GLU:HB3	1.63	0.78
1:H:456:LEU:HD13	1:H:550:ARG:HB3	1.66	0.78
1:L:452:PRO:CB	1:L:477:THR:O	2.30	0.78
1:L:456:LEU:HD22	1:L:552:VAL:HB	1.65	0.78
3:R:33:VAL:CG1	3:R:91:VAL:HG21	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:563:ASN:OD1	1:H:563:ASN:N	2.09	0.77
1:C:384:ARG:HB2	1:C:388:GLU:HB2	0.79	0.77
1:F:452:PRO:HG3	1:F:540:HIS:CB	2.14	0.77
1:E:453:ASP:OD2	1:E:477:THR:HG23	1.84	0.77
1:C:400:HIS:HB2	1:C:404:THR:O	1.85	0.77
1:K:520:ILE:HD12	1:L:516:PHE:CZ	2.20	0.77
1:E:450:HIS:O	1:E:542:ALA:HB3	1.85	0.76
1:F:450:HIS:ND1	1:F:514:ARG:NH2	2.33	0.76
1:E:443:ARG:HB2	1:E:443:ARG:NH1	2.01	0.76
1:A:568:MET:HE1	2:J:37:ILE:HG21	1.67	0.76
1:L:452:PRO:HB3	1:L:478:GLY:CA	2.14	0.76
1:C:364:LYS:HG2	1:C:412:SER:HA	1.65	0.76
1:H:543:LEU:HD22	1:H:548:THR:CG2	2.16	0.76
1:C:384:ARG:H	1:C:388:GLU:N	1.83	0.76
1:K:535:THR:CG2	1:K:551:THR:HB	2.15	0.76
1:L:452:PRO:HG2	1:L:479:PHE:HB3	0.76	0.76
1:F:384:ARG:HH21	1:F:388:GLU:HG3	1.50	0.75
3:R:41:GLU:OE1	3:R:82:PRO:HB3	1.86	0.75
1:B:475:LEU:HD13	1:B:518:HIS:HD2	1.52	0.75
1:C:352:PRO:HB2	1:C:357:ILE:HD11	1.68	0.75
1:L:443:ARG:HG2	1:L:443:ARG:NH1	2.00	0.75
1:L:452:PRO:CB	1:L:479:PHE:N	2.44	0.75
1:B:465:ASN:HD21	1:L:571:THR:CG2	2.00	0.75
1:E:450:HIS:NE2	1:E:514:ARG:CZ	2.49	0.75
1:B:495:LEU:HD12	1:B:495:LEU:H	1.52	0.75
1:F:450:HIS:CE1	1:F:514:ARG:NH1	2.53	0.75
1:L:452:PRO:HG3	1:L:478:GLY:C	2.10	0.75
1:K:422:GLU:C	1:K:443:ARG:NH1	2.44	0.74
1:E:537:VAL:HG12	1:E:549:GLU:HG2	1.68	0.74
1:F:454:VAL:HG22	1:F:538:VAL:HG21	1.68	0.74
2:J:113:VAL:CG1	2:J:126:THR:HB	2.17	0.74
1:K:451:ARG:NH1	1:K:451:ARG:HB2	2.01	0.74
1:C:566:LEU:HD12	1:C:566:LEU:O	1.87	0.74
1:H:425:THR:HG21	1:H:438:LYS:HG3	1.68	0.74
1:C:384:ARG:NH1	1:C:389:ALA:N	2.34	0.74
1:E:423:ARG:HB2	1:E:442:SER:HG	1.51	0.74
1:E:451:ARG:NH1	1:E:451:ARG:HB2	2.02	0.74
1:B:475:LEU:HA	1:B:518:HIS:HB3	1.68	0.74
1:E:418:TRP:O	1:E:443:ARG:NE	2.20	0.74
2:J:36:ASN:OD1	2:J:36:ASN:N	2.19	0.73
2:J:15:ALA:CB	2:J:67:LEU:HD21	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:ARG:HG2	1:E:440:THR:HG22	1.70	0.73
3:R:35:ILE:HD12	3:R:35:ILE:N	2.01	0.73
3:R:45:ARG:HG3	3:R:45:ARG:HH11	1.52	0.73
1:C:380:ILE:HG22	1:C:428:VAL:HA	1.71	0.73
1:E:450:HIS:CD2	1:E:514:ARG:CZ	2.72	0.73
1:C:563:ASN:HD22	4:C:601:NAG:C1	1.98	0.73
1:H:562:TYR:CD1	1:K:562:TYR:HD2	2.07	0.73
1:B:502:THR:HA	1:B:519:SER:HB3	1.69	0.73
2:J:39:ILE:HD13	2:J:62:TYR:CZ	2.23	0.73
2:J:113:VAL:HG22	2:J:124:VAL:O	1.89	0.73
3:R:112:ARG:HG3	3:R:112:ARG:HH11	1.54	0.73
1:E:382:TRP:HB2	1:E:390:VAL:HG21	1.69	0.73
1:E:450:HIS:CD2	1:E:514:ARG:NH2	2.57	0.72
3:R:37:CYS:O	3:R:87:PHE:HB3	1.88	0.72
1:F:450:HIS:O	1:F:542:ALA:HB3	1.89	0.72
1:H:543:LEU:CD2	1:H:548:THR:CG2	2.68	0.72
1:F:449:LEU:O	1:F:449:LEU:HD12	1.89	0.72
1:E:450:HIS:O	1:E:542:ALA:CB	2.36	0.72
1:G:490:GLN:HE22	1:G:532:GLU:HA	1.55	0.72
1:K:450:HIS:CG	1:K:514:ARG:HE	2.08	0.72
1:C:384:ARG:HD3	1:C:388:GLU:CB	2.14	0.72
1:B:502:THR:HA	1:B:519:SER:CB	2.20	0.71
1:K:514:ARG:HG3	1:K:514:ARG:NH1	1.99	0.71
1:C:372:LEU:HB2	1:C:405:PHE:HB3	1.72	0.71
1:C:473:THR:HG22	1:C:520:ILE:HG22	1.72	0.71
1:C:384:ARG:CA	1:C:388:GLU:HB2	2.18	0.71
1:E:418:TRP:CD1	1:E:443:ARG:CD	2.68	0.71
1:G:499:LYS:HG2	1:G:521:LEU:HD11	1.73	0.71
1:K:463:GLN:HB2	1:L:455:TYR:CE2	1.92	0.71
1:K:501:VAL:CG1	1:L:516:PHE:HZ	2.04	0.71
1:L:488:TRP:NE1	1:L:521:LEU:HD22	2.06	0.71
1:F:451:ARG:NH1	1:F:451:ARG:HB2	2.06	0.70
1:H:566:LEU:HD23	1:K:568:MET:HE1	1.72	0.70
1:F:453:ASP:OD1	1:F:453:ASP:N	2.22	0.70
1:L:488:TRP:CB	1:L:521:LEU:HD21	2.21	0.70
1:L:488:TRP:CD1	1:L:521:LEU:HD22	2.25	0.70
3:R:33:VAL:HG21	3:R:120:LEU:HD23	1.72	0.70
2:J:52:PRO:HD3	2:J:128:LEU:CD1	2.22	0.70
1:G:487:GLN:O	1:G:537:VAL:HG22	1.92	0.70
3:R:105:GLY:HA2	3:R:115:THR:HG23	1.71	0.70
1:H:347:VAL:HG22	1:H:369:VAL:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:7:LEU:HD23	2:J:8:VAL:HG23	1.72	0.69
1:D:524:SER:OG	1:D:527:GLU:OE1	2.10	0.69
1:K:443:ARG:CD	1:K:443:ARG:H	2.04	0.69
1:K:463:GLN:CG	1:L:455:TYR:HE2	2.00	0.69
1:L:487:GLN:O	1:L:537:VAL:HG12	1.93	0.69
1:L:488:TRP:CG	1:L:521:LEU:HD22	2.14	0.69
1:B:473:THR:HG22	1:B:520:ILE:HG22	1.74	0.69
1:E:418:TRP:CE3	1:E:443:ARG:HD3	2.23	0.69
1:G:490:GLN:O	1:G:490:GLN:HG3	1.91	0.69
1:B:493:GLN:OE1	1:B:493:GLN:N	2.25	0.69
1:B:520:ILE:HG13	1:B:520:ILE:O	1.92	0.69
2:J:113:VAL:HG11	2:J:126:THR:HB	1.73	0.69
1:L:506:MET:O	1:L:515:TYR:CB	2.40	0.69
3:R:75:ARG:HB2	3:R:92:THR:HG23	1.75	0.69
1:C:486:VAL:HG22	1:C:538:VAL:HG22	1.75	0.68
1:H:384:ARG:HD2	1:H:385:GLN:N	2.07	0.68
2:J:49:ILE:HG13	2:J:103:TYR:HE1	0.53	0.68
3:R:84:LYS:O	3:R:84:LYS:HG2	1.93	0.68
2:J:20:ARG:HH12	4:L:601:NAG:H5	1.59	0.68
1:A:451:ARG:O	1:A:451:ARG:HG3	1.94	0.68
2:J:39:ILE:HD12	2:J:62:TYR:CD2	2.29	0.68
1:L:488:TRP:CZ3	1:L:521:LEU:HD23	2.28	0.68
3:R:22:GLU:CA	3:R:118:VAL:HG23	2.19	0.68
1:L:443:ARG:CB	1:L:444:PRO:CD	2.71	0.68
1:K:392:THR:HG22	1:K:393:HIS:H	1.59	0.68
1:L:452:PRO:HG3	1:L:479:PHE:HA	0.68	0.68
1:F:360:THR:HG23	1:F:362:SER:H	1.58	0.68
1:F:554:LYS:O	1:F:554:LYS:HG2	1.92	0.68
1:K:422:GLU:C	1:K:443:ARG:HH12	1.97	0.68
1:A:544:PRO:O	2:J:135:PRO:HG3	1.94	0.67
1:B:382:TRP:HB2	1:B:390:VAL:HG21	1.77	0.67
1:E:418:TRP:CE3	1:E:443:ARG:CG	2.77	0.67
3:R:33:VAL:HG13	3:R:91:VAL:HG22	1.76	0.67
1:H:543:LEU:HD22	1:H:548:THR:HG22	1.74	0.67
2:J:49:ILE:HD11	2:J:103:TYR:CD1	2.30	0.67
3:R:39:LEU:HD12	3:R:39:LEU:N	2.07	0.67
3:R:41:GLU:CD	3:R:82:PRO:HB3	2.19	0.67
1:C:384:ARG:CB	1:C:388:GLU:CB	2.24	0.67
3:R:34:THR:HG1	3:R:88:LEU:HD12	1.55	0.67
3:R:35:ILE:C	3:R:88:LEU:HD11	2.19	0.67
1:L:433:LEU:HD12	1:L:434:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:453:ASP:N	1:L:453:ASP:OD1	2.16	0.67
1:K:516:PHE:CZ	1:L:501:VAL:HG11	2.25	0.67
3:R:28:GLU:O	3:R:94:LEU:HB2	1.95	0.67
1:B:475:LEU:HA	1:B:518:HIS:CB	2.25	0.66
2:J:39:ILE:CD1	2:J:62:TYR:CD2	2.77	0.66
1:C:345:ILE:N	1:C:371:ASP:O	2.28	0.66
2:J:42:PRO:HG3	2:J:102:THR:HG22	1.76	0.66
1:K:451:ARG:HG3	1:K:451:ARG:HH11	1.60	0.66
1:K:488:TRP:HE1	1:K:519:SER:HG	1.41	0.66
2:J:37:ILE:HD12	1:L:564:VAL:HG22	1.77	0.66
1:C:350:ILE:HB	1:C:366:THR:HB	1.76	0.66
1:E:524:SER:HB2	1:E:527:GLU:HG3	1.76	0.66
1:H:400:HIS:CE1	1:H:406:SER:HB3	2.29	0.66
1:C:384:ARG:CB	1:C:388:GLU:CG	2.67	0.66
1:B:535:THR:CG2	1:B:551:THR:OG1	2.33	0.66
1:F:452:PRO:HG3	1:F:540:HIS:HB3	1.77	0.66
1:A:449:LEU:HD13	1:A:542:ALA:HB2	1.76	0.66
1:F:450:HIS:O	1:F:542:ALA:CB	2.44	0.66
1:K:516:PHE:CD2	1:L:520:ILE:HD13	2.31	0.66
1:K:558:LYS:HD2	1:K:559:PRO:HD2	1.77	0.66
1:A:452:PRO:HB3	1:A:479:PHE:HB3	1.78	0.66
1:L:373:THR:OG1	1:L:430:HIS:NE2	2.28	0.66
1:G:459:PRO:HD3	1:G:472:ILE:HG13	1.77	0.65
1:H:443:ARG:NE	1:H:444:PRO:CD	2.59	0.65
1:H:562:TYR:HD1	1:K:562:TYR:CD2	2.12	0.65
1:D:384:ARG:NH2	1:D:417:ASP:OD2	2.28	0.65
1:K:451:ARG:HH11	1:K:451:ARG:CG	2.09	0.65
1:B:502:THR:HG23	1:B:519:SER:HB3	1.77	0.65
1:C:400:HIS:CB	1:C:404:THR:O	2.44	0.65
1:F:450:HIS:HE1	1:F:514:ARG:NH1	1.93	0.65
1:F:473:THR:HG22	1:F:520:ILE:HG22	1.77	0.65
2:J:113:VAL:HG13	2:J:126:THR:CG2	2.26	0.65
3:R:33:VAL:HG12	3:R:91:VAL:CG2	2.26	0.65
3:R:41:GLU:OE1	3:R:82:PRO:CB	2.45	0.65
1:E:449:LEU:HD12	1:E:542:ALA:HB2	1.78	0.65
1:A:393:HIS:HB3	1:A:410:GLU:H	1.60	0.65
1:F:459:PRO:HG3	1:F:470:ALA:HB1	1.79	0.65
2:J:17:ILE:HD11	2:J:64:LEU:HD22	1.78	0.65
1:K:553:ASP:H	1:K:556:THR:HB	1.62	0.65
2:J:103:TYR:HB2	1:L:574:THR:HG22	1.79	0.65
1:L:452:PRO:CD	1:L:479:PHE:HA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:75:ARG:CA	3:R:92:THR:CG2	2.75	0.64
2:J:52:PRO:HD3	2:J:128:LEU:HD11	1.79	0.64
3:R:34:THR:C	3:R:88:LEU:HD11	2.22	0.64
1:H:443:ARG:CZ	1:H:444:PRO:CD	2.76	0.64
1:L:351:PRO:HA	1:L:365:LEU:HD13	1.79	0.64
1:K:516:PHE:HE2	1:L:520:ILE:HD13	1.36	0.64
1:G:489:MET:HG2	1:G:535:THR:OG1	1.98	0.64
1:A:346:ARG:NH1	1:A:347:VAL:O	2.31	0.63
1:C:566:LEU:HD11	1:D:566:LEU:HB3	1.80	0.63
3:R:61:VAL:HG12	3:R:69:LYS:HD3	1.80	0.63
1:C:384:ARG:CD	1:C:388:GLU:HB2	2.04	0.63
1:K:346:ARG:O	1:K:370:THR:OG1	2.15	0.63
1:A:551:THR:HG21	2:J:52:PRO:HB2	1.81	0.63
1:E:380:ILE:HG21	1:E:409:GLY:HA3	1.81	0.63
1:L:506:MET:O	1:L:516:PHE:N	2.31	0.63
1:B:525:GLU:OE2	1:B:525:GLU:HA	1.99	0.62
1:F:558:LYS:HB3	1:F:559:PRO:HD2	1.81	0.62
1:K:451:ARG:HB2	1:K:451:ARG:CZ	2.29	0.62
3:R:91:VAL:HG23	3:R:91:VAL:O	1.99	0.62
3:R:120:LEU:N	3:R:120:LEU:HD12	2.14	0.62
1:E:451:ARG:HH11	1:E:451:ARG:CG	2.13	0.62
1:K:423:ARG:HD2	1:K:440:THR:HA	1.81	0.62
1:K:450:HIS:CD2	1:K:514:ARG:HE	2.17	0.62
1:A:354:PHE:HA	1:A:357:ILE:HG22	1.82	0.62
3:R:48:LEU:HD11	3:R:102:TYR:HB3	1.82	0.62
3:R:39:LEU:HG	3:R:87:PHE:HB2	1.82	0.62
1:L:433:LEU:HD23	1:L:437:LEU:HD11	1.82	0.61
1:E:451:ARG:HH11	1:E:451:ARG:HG3	1.65	0.61
1:E:418:TRP:NE1	1:E:443:ARG:CD	2.42	0.61
1:B:495:LEU:HD12	1:B:495:LEU:N	2.15	0.61
1:H:451:ARG:NH1	1:H:451:ARG:HG3	2.15	0.61
1:C:508:GLU:HG2	1:C:511:ALA:HB3	1.82	0.61
1:C:566:LEU:CD2	1:H:564:VAL:HG11	2.30	0.61
1:F:563:ASN:OD1	4:F:601:NAG:N2	2.33	0.61
1:K:365:LEU:HD21	1:K:418:TRP:HZ3	1.66	0.61
1:K:463:GLN:HG3	1:L:455:TYR:HE2	1.62	0.61
1:L:488:TRP:O	1:L:495:LEU:CB	2.33	0.61
3:R:21:PRO:O	3:R:118:VAL:HG23	2.00	0.61
3:R:28:GLU:OE1	3:R:96:GLU:HG3	2.01	0.61
1:C:567:VAL:HG12	1:C:567:VAL:O	1.99	0.61
2:J:34:GLU:CG	2:J:36:ASN:OD1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:ARG:HB2	1:E:451:ARG:CZ	2.31	0.61
1:K:347:VAL:HG23	1:K:369:VAL:HA	1.83	0.61
1:K:442:SER:HA	1:K:443:ARG:HD2	1.82	0.61
1:K:450:HIS:HB3	1:K:514:ARG:HH21	1.66	0.61
1:A:357:ILE:HG13	1:A:363:THR:HB	1.83	0.60
1:F:347:VAL:HG21	1:F:428:VAL:HG21	1.82	0.60
1:L:351:PRO:HD3	1:L:441:ILE:HG12	1.83	0.60
1:L:451:ARG:CG	1:L:451:ARG:HH21	2.14	0.60
1:A:545:ASN:ND2	2:J:125:GLU:O	2.35	0.60
1:D:495:LEU:HD23	1:D:499:LYS:HD2	1.81	0.60
1:H:543:LEU:CD2	1:H:548:THR:HG22	2.31	0.60
1:K:556:THR:HG23	1:K:556:THR:O	2.00	0.60
1:B:475:LEU:HD12	1:B:518:HIS:HB3	1.83	0.60
2:J:38:ARG:HG2	2:J:38:ARG:O	2.02	0.60
2:J:102:THR:HB	1:L:575:CYS:H	1.66	0.60
3:R:37:CYS:N	3:R:87:PHE:O	2.33	0.60
1:B:459:PRO:HG3	1:B:470:ALA:HB1	1.83	0.60
1:B:475:LEU:CD1	1:B:518:HIS:CD2	2.85	0.60
1:B:490:GLN:H	1:B:495:LEU:HD11	1.67	0.60
1:G:499:LYS:HG2	1:G:521:LEU:CD1	2.31	0.60
1:L:369:VAL:HG21	1:L:428:VAL:HG11	1.84	0.60
3:R:21:PRO:O	3:R:118:VAL:CG2	2.49	0.60
1:E:418:TRP:O	1:E:443:ARG:NH1	2.33	0.60
1:F:447:VAL:HG13	1:F:447:VAL:O	2.02	0.60
1:F:454:VAL:CG2	1:F:538:VAL:HG21	2.32	0.60
1:C:384:ARG:NH1	1:C:388:GLU:C	2.58	0.60
3:R:29:LEU:C	3:R:29:LEU:HD23	2.26	0.60
1:B:547:VAL:HG21	1:C:545:ASN:OD1	2.01	0.59
1:H:525:GLU:OE2	1:H:529:ASN:ND2	2.35	0.59
1:C:568:MET:SD	1:K:564:VAL:HG21	2.41	0.59
1:L:488:TRP:C	1:L:495:LEU:HB2	2.23	0.59
1:E:354:PHE:HA	1:E:357:ILE:HG12	1.85	0.59
1:G:489:MET:HE2	1:G:494:PRO:HG3	1.84	0.59
2:J:128:LEU:N	2:J:128:LEU:HD23	2.17	0.59
3:R:93:GLN:HE22	3:R:95:THR:HG22	1.67	0.59
3:R:112:ARG:HG3	3:R:112:ARG:NH1	2.18	0.59
1:H:535:THR:CG2	1:H:551:THR:OG1	2.44	0.59
1:C:371:ASP:H	1:C:404:THR:HG23	1.66	0.59
1:E:423:ARG:CB	1:E:442:SER:HG	2.11	0.59
1:E:562:TYR:HE2	1:F:566:LEU:HD21	1.68	0.59
1:F:452:PRO:HG3	1:F:540:HIS:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:103:TYR:H	1:L:574:THR:HA	1.67	0.59
1:B:375:TYR:HB2	1:B:430:HIS:HE1	1.67	0.59
1:B:461:ARG:NH2	1:B:557:GLY:O	2.35	0.59
1:L:451:ARG:HH21	1:L:451:ARG:HG2	1.65	0.59
1:L:533:THR:O	1:L:551:THR:OG1	2.21	0.58
3:R:19:ILE:HG22	3:R:21:PRO:HD3	1.85	0.58
3:R:71:GLU:O	3:R:75:ARG:NH1	2.36	0.58
1:B:467:ARG:HA	1:B:525:GLU:HG3	1.85	0.58
1:H:443:ARG:CZ	1:H:444:PRO:HD2	2.34	0.58
1:E:452:PRO:HB3	1:E:479:PHE:HB3	1.85	0.58
1:H:385:GLN:OE1	1:H:423:ARG:N	2.37	0.58
1:H:543:LEU:HD22	1:H:548:THR:HG21	1.85	0.58
1:L:452:PRO:CD	1:L:479:PHE:CB	2.77	0.58
3:R:112:ARG:HD2	3:R:112:ARG:O	2.04	0.58
1:L:443:ARG:HG3	1:L:444:PRO:HD2	1.84	0.58
1:L:503:SER:OG	1:L:518:HIS:N	2.34	0.58
1:B:490:GLN:O	1:B:490:GLN:HG2	2.02	0.58
1:K:450:HIS:CG	1:K:514:ARG:HH21	2.22	0.58
1:K:488:TRP:NE1	1:K:519:SER:OG	2.27	0.58
3:R:96:GLU:CD	3:R:122:VAL:HG21	2.29	0.58
1:D:447:VAL:O	1:D:447:VAL:HG22	2.03	0.58
1:K:351:PRO:HB3	1:K:418:TRP:CH2	2.39	0.58
3:R:45:ARG:HG3	3:R:45:ARG:NH1	2.19	0.58
1:B:501:VAL:O	1:B:519:SER:HB2	2.04	0.58
1:F:452:PRO:CB	1:F:479:PHE:HB3	2.30	0.58
1:H:443:ARG:CZ	1:H:444:PRO:HD3	2.34	0.58
1:H:547:VAL:O	1:H:547:VAL:HG12	2.02	0.58
1:K:351:PRO:HB3	1:K:418:TRP:HH2	1.69	0.58
1:A:449:LEU:HD21	1:A:481:PRO:HD3	1.84	0.58
1:A:525:GLU:OE2	1:A:529:ASN:ND2	2.37	0.58
1:G:429:THR:HG22	1:G:436:PRO:HB3	1.86	0.58
3:R:36:LYS:CB	3:R:86:LEU:CD1	2.64	0.58
1:D:473:THR:HG22	1:D:520:ILE:HG22	1.86	0.57
1:E:562:TYR:CE2	1:F:566:LEU:HD21	2.38	0.57
1:L:421:GLY:HA2	1:L:443:ARG:HH12	1.68	0.57
1:E:495:LEU:HD23	1:E:499:LYS:HD3	1.86	0.57
1:B:493:GLN:O	1:B:493:GLN:HG2	2.04	0.57
3:R:96:GLU:CD	3:R:122:VAL:CG2	2.76	0.57
1:L:485:PHE:HB3	1:L:539:ALA:HB3	1.86	0.57
1:G:486:VAL:HG22	1:G:538:VAL:HG22	1.87	0.57
2:J:101:TYR:N	2:J:101:TYR:CD1	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:VAL:HG11	1:E:428:VAL:HG11	1.86	0.57
1:E:557:GLY:HA2	1:F:461:ARG:NH2	2.19	0.57
1:K:363:THR:OG1	1:K:413:ILE:O	2.22	0.57
1:L:451:ARG:HD2	1:L:451:ARG:C	2.30	0.57
3:R:75:ARG:HA	3:R:92:THR:CG2	2.34	0.57
1:F:451:ARG:CB	1:F:451:ARG:CZ	2.83	0.57
1:H:543:LEU:CD1	1:H:548:THR:HG23	2.33	0.57
3:R:75:ARG:HB2	3:R:92:THR:CG2	2.34	0.57
2:J:113:VAL:HG23	2:J:113:VAL:O	2.05	0.57
3:R:50:ARG:NH1	3:R:72:TYR:OH	2.36	0.57
2:J:113:VAL:HG13	2:J:126:THR:HB	1.86	0.57
1:B:512:PRO:O	1:B:514:ARG:N	2.38	0.56
1:A:564:VAL:HG21	1:L:568:MET:HE1	1.88	0.56
1:D:447:VAL:HG21	1:D:481:PRO:HB3	1.87	0.56
1:F:486:VAL:HG22	1:F:538:VAL:HG22	1.87	0.56
1:H:352:PRO:HD3	1:H:365:LEU:HB3	1.86	0.56
1:K:510:GLN:OE1	1:L:522:THR:HG21	2.05	0.56
1:L:500:TYR:CB	1:L:521:LEU:HD13	2.31	0.56
1:D:459:PRO:HG3	1:D:470:ALA:HB1	1.87	0.56
1:H:379:THR:HB	1:H:429:THR:HB	1.87	0.56
1:K:449:LEU:HA	1:K:480:SER:O	2.06	0.56
1:L:574:THR:O	1:L:574:THR:OG1	2.19	0.56
1:A:508:GLU:HB3	1:A:511:ALA:HB3	1.86	0.56
1:C:545:ASN:O	1:C:545:ASN:ND2	2.39	0.56
2:J:38:ARG:HH12	2:J:40:ILE:HD11	1.70	0.56
1:B:532:GLU:OE1	1:B:532:GLU:HA	2.05	0.56
1:C:417:ASP:HB3	1:C:424:PHE:HZ	1.71	0.56
1:F:449:LEU:CB	1:F:480:SER:O	2.54	0.56
1:G:473:THR:HG22	1:G:520:ILE:HG22	1.87	0.56
1:K:450:HIS:CD2	1:K:514:ARG:NE	2.74	0.56
3:R:26:GLU:CB	3:R:124:SER:HA	2.27	0.56
1:D:543:LEU:HB2	1:D:546:ARG:HA	1.88	0.56
1:B:564:VAL:HG23	1:C:564:VAL:HA	1.87	0.55
1:F:383:THR:HG23	1:F:387:GLY:HA2	1.88	0.55
1:F:421:GLY:O	1:F:423:ARG:NH1	2.38	0.55
2:J:49:ILE:HG12	2:J:103:TYR:CD1	2.40	0.55
1:K:459:PRO:HB3	1:K:471:THR:H	1.70	0.55
1:L:423:ARG:HG3	1:L:442:SER:OG	2.07	0.55
3:R:29:LEU:O	3:R:93:GLN:HG2	2.05	0.55
1:A:349:ALA:HB2	1:A:439:GLN:HB3	1.88	0.55
1:D:449:LEU:CD2	1:D:481:PRO:HD2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:ASP:OD2	1:E:477:THR:HG22	2.04	0.55
1:G:380:ILE:HG22	1:G:428:VAL:HG22	1.89	0.55
1:G:479:PHE:CD1	1:G:479:PHE:C	2.83	0.55
1:L:365:LEU:HB2	1:L:411:ALA:HB3	1.89	0.55
1:L:516:PHE:C	1:L:516:PHE:CD2	2.84	0.55
3:R:96:GLU:OE2	3:R:122:VAL:CG2	2.54	0.55
1:B:465:ASN:HD21	1:L:571:THR:HG22	1.72	0.55
1:C:347:VAL:HG12	1:C:439:GLN:HG2	1.89	0.55
1:C:384:ARG:H	1:C:388:GLU:H	1.55	0.55
3:R:33:VAL:HG13	3:R:91:VAL:HG21	1.77	0.55
1:C:360:THR:HG22	1:C:362:SER:HB2	1.88	0.55
2:J:104:ASP:HB3	2:J:107:LYS:HB2	1.88	0.55
1:B:490:GLN:N	1:B:495:LEU:HD11	2.21	0.55
3:R:87:PHE:C	3:R:87:PHE:CD1	2.85	0.55
1:F:450:HIS:N	1:F:450:HIS:CD2	2.72	0.55
1:L:452:PRO:CB	1:L:478:GLY:O	2.42	0.55
1:E:451:ARG:CZ	1:E:451:ARG:CB	2.85	0.55
1:F:560:THR:O	1:F:560:THR:HG22	2.04	0.55
3:R:34:THR:OG1	3:R:88:LEU:HD11	2.01	0.55
1:G:543:LEU:HB2	1:G:546:ARG:HA	1.88	0.54
3:R:28:GLU:OE1	3:R:96:GLU:CG	2.55	0.54
3:R:75:ARG:C	3:R:92:THR:CG2	2.74	0.54
1:L:443:ARG:CG	1:L:443:ARG:HH11	2.15	0.54
1:E:526:GLU:O	1:E:530:THR:HG23	2.07	0.54
1:K:391:LYS:HD2	1:K:392:THR:N	2.22	0.54
1:B:489:MET:CE	1:B:537:VAL:HG11	2.37	0.54
1:C:384:ARG:HB2	1:C:388:GLU:HG2	1.83	0.54
2:J:39:ILE:O	1:L:566:LEU:HA	2.08	0.54
1:K:398:GLU:O	1:K:406:SER:OG	2.25	0.54
1:C:393:HIS:HB3	1:C:410:GLU:H	1.71	0.54
1:C:564:VAL:HG21	1:H:566:LEU:HD21	0.58	0.54
1:K:535:THR:HG22	1:K:551:THR:OG1	2.07	0.54
1:L:506:MET:HB2	1:L:516:PHE:O	2.08	0.54
2:J:131:ASP:HB2	3:R:44:VAL:HG13	1.90	0.54
1:L:425:THR:HB	1:L:438:LYS:HE2	1.90	0.54
1:L:452:PRO:HB2	1:L:477:THR:C	2.29	0.54
1:K:352:PRO:HD3	1:K:365:LEU:HA	1.89	0.54
1:C:484:VAL:HG23	1:C:540:HIS:HB2	1.89	0.54
3:R:96:GLU:HB3	3:R:122:VAL:HG21	1.86	0.54
1:B:384:ARG:HB3	1:B:424:PHE:CE1	2.43	0.53
1:H:382:TRP:HB2	1:H:390:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:508:GLU:HG2	1:H:511:ALA:H	1.72	0.53
1:K:385:GLN:HB2	1:K:423:ARG:HB3	1.88	0.53
1:C:489:MET:HE3	1:C:537:VAL:HG11	1.89	0.53
1:D:454:VAL:HG21	1:D:538:VAL:HG11	1.90	0.53
1:K:378:VAL:HG12	1:K:430:HIS:HD2	1.72	0.53
1:D:400:HIS:CD2	1:D:406:SER:HB3	2.43	0.53
1:G:490:GLN:NE2	1:G:532:GLU:HA	2.21	0.53
1:L:384:ARG:HD3	1:L:388:GLU:HB2	1.90	0.53
1:B:553:ASP:OD1	1:B:554:LYS:N	2.39	0.53
1:L:498:GLU:OE2	1:L:498:GLU:HA	2.09	0.53
1:B:465:ASN:HD21	1:L:571:THR:HG21	1.71	0.53
1:C:565:SER:O	1:C:565:SER:OG	2.10	0.53
1:F:382:TRP:HB2	1:F:390:VAL:HG21	1.90	0.53
1:K:456:LEU:HD23	1:K:552:VAL:HG13	1.90	0.53
3:R:37:CYS:C	3:R:87:PHE:HB3	2.32	0.53
3:R:79:LYS:HE3	3:R:81:TYR:HE2	1.73	0.53
1:A:395:ASN:C	1:A:395:ASN:HD22	2.17	0.53
1:D:464:LEU:HD11	1:D:528:TRP:CE3	2.43	0.53
1:H:543:LEU:CD2	1:H:548:THR:HG21	2.38	0.53
1:A:490:GLN:NE2	1:A:527:GLU:OE2	2.41	0.53
2:J:40:ILE:HG12	1:L:567:VAL:HG22	1.91	0.53
1:K:425:THR:HG23	1:K:439:GLN:H	1.73	0.53
1:B:515:TYR:CD1	1:B:515:TYR:N	2.71	0.53
1:H:443:ARG:NH2	1:H:444:PRO:HD3	2.23	0.53
2:J:113:VAL:CG1	2:J:126:THR:CG2	2.86	0.53
2:J:113:VAL:CG1	2:J:126:THR:CB	2.85	0.53
1:K:461:ARG:NH1	1:K:461:ARG:HB2	2.23	0.53
1:C:508:GLU:HG3	1:C:509:PRO:HD2	1.90	0.53
2:J:13:LYS:HZ3	2:J:101:TYR:HE1	1.56	0.53
1:L:421:GLY:HA2	1:L:443:ARG:HH11	1.73	0.53
1:F:564:VAL:HA	1:G:564:VAL:O	2.09	0.52
1:G:400:HIS:ND1	1:G:404:THR:O	2.42	0.52
1:B:454:VAL:HG13	1:B:476:VAL:HG22	1.90	0.52
1:D:380:ILE:HG22	1:D:428:VAL:HG22	1.92	0.52
1:K:463:GLN:HG2	1:L:455:TYR:CE2	2.42	0.52
1:A:359:LEU:HD13	2:J:115:LEU:CD1	2.39	0.52
1:D:490:GLN:HG2	1:D:491:ARG:HG3	1.90	0.52
1:G:499:LYS:O	1:G:499:LYS:HG3	2.02	0.52
1:A:450:HIS:CE1	1:A:480:SER:CB	2.89	0.52
1:A:459:PRO:HG3	1:A:470:ALA:HB1	1.92	0.52
1:D:490:GLN:NE2	1:D:532:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:520:ILE:HG13	1:L:520:ILE:O	2.10	0.52
1:L:382:TRP:HB2	1:L:390:VAL:HG21	1.89	0.52
1:L:488:TRP:CD1	1:L:500:TYR:CD2	2.98	0.52
3:R:75:ARG:CA	3:R:92:THR:HG21	2.33	0.52
1:A:449:LEU:CD2	1:A:481:PRO:HD3	2.40	0.52
1:A:509:PRO:HG3	1:B:501:VAL:HG23	1.91	0.52
1:E:380:ILE:HD11	1:E:407:ALA:HB1	1.91	0.52
3:R:52:MET:HA	3:R:52:MET:HE3	1.91	0.52
1:C:384:ARG:N	1:C:388:GLU:HB2	2.24	0.52
1:F:354:PHE:O	1:F:357:ILE:HG22	2.10	0.52
1:F:425:THR:HG21	1:F:438:LYS:HB3	1.92	0.52
1:F:508:GLU:HG3	1:F:509:PRO:HD2	1.92	0.52
1:H:543:LEU:HD11	1:H:548:THR:HG23	1.90	0.52
3:R:120:LEU:N	3:R:120:LEU:CD1	2.73	0.52
1:E:509:PRO:HB3	1:F:501:VAL:HG13	1.91	0.52
1:H:347:VAL:HG23	1:H:437:LEU:HD22	1.92	0.52
1:H:562:TYR:N	1:H:562:TYR:CD2	2.73	0.52
2:J:115:LEU:C	2:J:115:LEU:HD12	2.35	0.52
1:E:526:GLU:O	1:E:530:THR:CG2	2.58	0.52
2:J:49:ILE:CD1	2:J:103:TYR:HE1	1.87	0.52
1:A:449:LEU:HD21	1:A:481:PRO:CD	2.40	0.51
3:R:45:ARG:HH11	3:R:45:ARG:CG	2.18	0.51
1:A:456:LEU:HD23	1:A:552:VAL:HG13	1.92	0.51
1:A:484:VAL:HG23	1:A:540:HIS:HB2	1.92	0.51
1:G:499:LYS:CG	1:G:521:LEU:CD1	2.88	0.51
1:C:384:ARG:H	1:C:388:GLU:CA	2.23	0.51
1:E:564:VAL:HG21	1:F:564:VAL:HG21	1.92	0.51
1:B:529:ASN:HA	1:B:554:LYS:HD3	1.92	0.51
1:G:365:LEU:HG	1:G:424:PHE:HD1	1.75	0.51
2:J:110:THR:HG22	2:J:127:ALA:HA	1.93	0.51
1:A:364:LYS:HD2	1:A:410:GLU:HG3	1.92	0.51
1:A:450:HIS:ND1	1:A:450:HIS:N	2.58	0.51
1:F:543:LEU:HB2	1:F:546:ARG:HA	1.92	0.51
1:L:443:ARG:HB3	1:L:444:PRO:HD2	1.86	0.51
1:B:516:PHE:CD1	1:B:516:PHE:C	2.89	0.51
1:C:367:CYS:HB2	1:C:382:TRP:CZ2	2.46	0.51
3:R:48:LEU:HD13	3:R:104:CYS:SG	2.51	0.51
1:H:443:ARG:CD	1:H:444:PRO:HD2	2.40	0.51
1:L:516:PHE:C	1:L:516:PHE:HD2	2.19	0.51
3:R:96:GLU:HA	3:R:122:VAL:HG23	1.93	0.51
1:C:459:PRO:HD2	1:C:528:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:VAL:CG2	1:D:481:PRO:HD3	2.41	0.51
1:F:457:LEU:HB2	1:F:473:THR:OG1	2.12	0.51
1:G:413:ILE:HD13	1:G:424:PHE:CE1	2.46	0.51
1:K:443:ARG:CD	1:K:443:ARG:N	2.72	0.51
1:H:451:ARG:HG3	1:H:451:ARG:HH11	1.75	0.50
2:J:39:ILE:CD1	2:J:62:TYR:CZ	2.90	0.50
1:L:420:SER:OG	1:L:422:GLU:OE1	2.22	0.50
1:L:470:ALA:O	1:L:523:VAL:HG23	2.11	0.50
1:K:498:GLU:OE2	1:L:509:PRO:O	2.30	0.50
1:K:567:VAL:HG21	1:L:567:VAL:HG12	1.94	0.50
1:L:471:THR:HA	1:L:521:LEU:O	2.11	0.50
1:L:532:GLU:O	1:L:533:THR:HG22	2.12	0.50
1:A:362:SER:O	1:A:364:LYS:N	2.40	0.50
1:F:416:ASP:N	1:F:416:ASP:OD1	2.44	0.50
1:L:491:ARG:HB3	1:L:493:GLN:CD	2.33	0.50
1:L:383:THR:OG1	1:L:438:LYS:NZ	2.44	0.50
1:B:518:HIS:HD1	1:B:518:HIS:H	1.59	0.50
1:B:535:THR:HG22	1:B:551:THR:HG1	1.70	0.50
1:H:543:LEU:HD13	1:H:548:THR:N	2.27	0.50
1:K:430:HIS:CD2	1:K:431:THR:H	2.29	0.50
1:E:450:HIS:NE2	1:E:514:ARG:NH2	2.57	0.50
1:G:500:TYR:C	1:G:500:TYR:CD2	2.88	0.50
1:K:516:PHE:CD2	1:L:520:ILE:CD1	2.83	0.50
3:R:41:GLU:OE1	3:R:82:PRO:HG3	2.11	0.50
3:R:98:ASP:OD1	3:R:98:ASP:N	2.44	0.50
1:D:449:LEU:HD22	1:D:480:SER:O	2.12	0.50
1:H:451:ARG:HH11	1:H:451:ARG:CG	2.24	0.50
1:B:493:GLN:H	1:B:493:GLN:CD	2.18	0.50
1:G:413:ILE:HG21	1:G:424:PHE:CZ	2.47	0.50
1:G:487:GLN:O	1:G:537:VAL:CG2	2.59	0.50
1:G:384:ARG:HG3	1:G:388:GLU:HB3	1.94	0.49
1:G:416:ASP:HA	1:G:419:ASN:HB2	1.93	0.49
2:J:49:ILE:HD13	2:J:101:TYR:O	2.12	0.49
3:R:45:ARG:NH1	3:R:45:ARG:CG	2.72	0.49
1:H:345:ILE:HG22	1:H:437:LEU:HD21	1.94	0.49
1:C:419:ASN:HA	1:C:443:ARG:HE	1.78	0.49
2:J:5:ILE:O	2:J:18:THR:OG1	2.24	0.49
1:K:451:ARG:NH1	1:K:451:ARG:CG	2.71	0.49
1:A:384:ARG:HG2	1:A:385:GLN:H	1.78	0.49
1:D:470:ALA:N	1:D:523:VAL:O	2.45	0.49
1:C:500:TYR:HB3	1:C:521:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:451:ARG:NH1	1:K:451:ARG:CB	2.72	0.49
1:K:506:MET:HB2	1:K:516:PHE:CE1	2.48	0.49
1:A:467:ARG:HA	1:A:525:GLU:HG3	1.94	0.49
1:E:452:PRO:O	1:E:452:PRO:HG2	2.13	0.49
1:G:399:SER:HA	1:G:405:PHE:HA	1.93	0.49
1:H:474:CYS:HB2	1:H:488:TRP:CZ2	2.48	0.49
1:K:488:TRP:NE1	1:K:519:SER:HG	2.06	0.49
1:A:568:MET:HE1	2:J:37:ILE:HD13	1.95	0.49
1:E:423:ARG:CD	1:E:442:SER:OG	2.60	0.49
1:E:486:VAL:HG22	1:E:538:VAL:HG22	1.94	0.49
1:E:419:ASN:HA	1:E:443:ARG:NH2	2.28	0.49
3:R:27:GLY:HA3	3:R:94:LEU:HD23	1.89	0.49
3:R:35:ILE:H	3:R:35:ILE:CD1	2.21	0.49
1:F:508:GLU:HB3	1:F:511:ALA:HB3	1.94	0.49
1:K:366:THR:HA	1:K:409:GLY:O	2.12	0.49
1:K:443:ARG:H	1:K:443:ARG:HD3	1.75	0.48
1:K:562:TYR:HD1	1:L:562:TYR:HB2	1.77	0.48
1:B:478:GLY:O	1:B:514:ARG:NH2	2.46	0.48
3:R:21:PRO:C	3:R:118:VAL:HG23	2.37	0.48
2:J:35:ARG:HB2	1:L:562:TYR:HA	1.96	0.48
1:E:451:ARG:NH1	1:E:451:ARG:CB	2.73	0.48
1:L:506:MET:CB	1:L:507:PRO:HD2	2.42	0.48
1:L:552:VAL:HG13	1:L:556:THR:HG23	1.95	0.48
1:B:489:MET:HE3	1:B:537:VAL:HG11	1.95	0.48
1:B:493:GLN:N	1:B:493:GLN:CD	2.71	0.48
1:C:456:LEU:HD21	1:C:536:CYS:HB3	1.95	0.48
2:J:13:LYS:NZ	2:J:101:TYR:HE1	2.12	0.48
2:J:113:VAL:HG11	2:J:126:THR:CB	2.43	0.48
1:K:452:PRO:HB3	1:K:479:PHE:HB3	1.95	0.48
1:F:562:TYR:HB3	1:G:562:TYR:HB2	1.96	0.48
1:G:490:GLN:OE1	1:G:532:GLU:CG	2.36	0.48
1:L:451:ARG:C	1:L:451:ARG:CD	2.86	0.48
1:C:447:VAL:HG21	1:C:481:PRO:HB3	1.95	0.48
1:L:478:GLY:HA2	1:L:514:ARG:CG	2.07	0.48
1:G:449:LEU:HD12	1:G:449:LEU:HA	1.56	0.48
1:H:562:TYR:HB3	1:K:562:TYR:HB2	1.96	0.48
3:R:35:ILE:N	3:R:35:ILE:CD1	2.73	0.48
1:F:451:ARG:NH1	1:F:451:ARG:CB	2.77	0.48
1:B:459:PRO:HD3	1:B:472:ILE:HG12	1.96	0.47
1:B:518:HIS:ND1	1:B:518:HIS:N	2.60	0.47
1:C:491:ARG:HG3	1:C:491:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:374:THR:HA	1:K:405:PHE:HB2	1.95	0.47
1:F:452:PRO:O	1:F:452:PRO:HG2	2.14	0.47
2:J:131:ASP:HB2	3:R:44:VAL:CG1	2.44	0.47
1:L:506:MET:N	1:L:516:PHE:O	2.46	0.47
3:R:34:THR:HA	3:R:89:VAL:O	2.13	0.47
3:R:42:MET:HG3	3:R:44:VAL:CG2	2.44	0.47
1:D:537:VAL:HG12	1:D:549:GLU:HG2	1.95	0.47
1:E:360:THR:HG23	1:E:362:SER:H	1.79	0.47
1:H:459:PRO:HD3	1:H:472:ILE:HG13	1.96	0.47
2:J:113:VAL:HG13	2:J:126:THR:CB	2.43	0.47
1:D:375:TYR:HD2	1:D:430:HIS:HE1	1.61	0.47
1:D:452:PRO:HB3	1:D:479:PHE:HB3	1.96	0.47
1:A:507:PRO:HA	1:A:515:TYR:HD1	1.79	0.47
1:F:454:VAL:HG13	1:F:474:CYS:SG	2.55	0.47
1:H:543:LEU:HD13	1:H:548:THR:H	1.80	0.47
1:K:443:ARG:HA	1:K:444:PRO:HD2	1.63	0.47
1:K:526:GLU:HA	1:K:529:ASN:CG	2.34	0.47
3:R:33:VAL:HG12	3:R:91:VAL:HG21	1.90	0.47
3:R:86:LEU:CD1	3:R:88:LEU:HD23	2.45	0.47
1:A:475:LEU:HD13	1:A:518:HIS:CE1	2.50	0.47
1:D:398:GLU:O	1:D:406:SER:OG	2.29	0.47
1:G:489:MET:CG	1:G:535:THR:OG1	2.62	0.47
1:C:490:GLN:NE2	1:C:532:GLU:OE1	2.27	0.47
1:E:347:VAL:HG12	1:E:369:VAL:HG12	1.97	0.47
1:E:374:THR:HA	1:E:405:PHE:HB2	1.96	0.47
1:E:529:ASN:HA	1:E:554:LYS:HG3	1.97	0.47
1:H:449:LEU:CD1	1:H:542:ALA:HB2	2.38	0.47
1:L:451:ARG:CG	1:L:451:ARG:NH2	2.73	0.47
1:D:449:LEU:HD22	1:D:481:PRO:HD2	1.97	0.46
1:G:489:MET:O	1:G:535:THR:OG1	2.27	0.46
1:H:456:LEU:CD1	1:H:550:ARG:HB3	2.39	0.46
1:K:498:GLU:O	1:L:509:PRO:HB2	2.15	0.46
3:R:96:GLU:CG	3:R:122:VAL:HG22	2.24	0.46
1:E:466:LEU:CD2	1:G:491:ARG:NH1	2.78	0.46
1:H:566:LEU:HD23	1:K:568:MET:CE	2.40	0.46
3:R:39:LEU:HD11	3:R:85:ASN:HA	1.97	0.46
1:G:479:PHE:CD1	1:G:479:PHE:O	2.68	0.46
2:J:39:ILE:CD1	2:J:62:TYR:CE2	2.99	0.46
2:J:67:LEU:HG	2:J:67:LEU:O	2.15	0.46
3:R:112:ARG:NH1	3:R:112:ARG:CG	2.73	0.46
1:E:418:TRP:CD2	1:E:443:ARG:CG	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:LEU:HA	1:F:480:SER:O	2.16	0.46
4:F:601:NAG:H61	4:G:601:NAG:H4	1.97	0.46
1:H:399:SER:OG	1:H:404:THR:O	2.34	0.46
1:H:449:LEU:HD12	1:H:542:ALA:CB	2.37	0.46
3:R:96:GLU:OE2	3:R:122:VAL:HG21	2.14	0.46
3:R:96:GLU:HA	3:R:122:VAL:CG2	2.45	0.46
1:L:372:LEU:HD23	1:L:430:HIS:CG	2.51	0.46
1:L:486:VAL:O	1:L:500:TYR:OH	2.25	0.46
1:C:533:THR:HB	1:C:551:THR:HG23	1.97	0.46
1:H:567:VAL:HG22	1:K:567:VAL:HG13	1.98	0.46
1:A:567:VAL:HG12	1:B:567:VAL:HB	1.97	0.46
1:B:369:VAL:HB	1:B:406:SER:HA	1.98	0.46
1:B:516:PHE:O	1:B:516:PHE:CG	2.68	0.46
1:E:449:LEU:HA	1:E:449:LEU:HD13	1.63	0.46
2:J:39:ILE:HD12	2:J:62:TYR:CE2	2.51	0.46
1:A:355:ALA:HB2	1:A:485:PHE:HB2	1.96	0.46
1:F:379:THR:HB	1:F:429:THR:OG1	2.15	0.46
1:G:485:PHE:CD2	1:G:485:PHE:O	2.68	0.46
1:L:506:MET:C	1:L:515:TYR:HB3	2.39	0.46
1:F:357:ILE:HD11	1:F:415:GLU:HG2	1.97	0.46
1:H:449:LEU:HD13	1:H:449:LEU:HA	1.48	0.46
2:J:52:PRO:CD	2:J:128:LEU:HD11	2.44	0.46
1:K:351:PRO:HG3	1:K:441:ILE:HG23	1.97	0.46
1:K:354:PHE:HA	1:K:357:ILE:HG12	1.98	0.46
3:R:96:GLU:CD	3:R:122:VAL:HG22	2.41	0.46
1:C:460:ALA:HB2	1:D:457:LEU:CD2	2.46	0.45
1:D:464:LEU:HD22	1:D:525:GLU:HG2	1.97	0.45
1:E:429:THR:HA	1:E:433:LEU:HD21	1.97	0.45
1:C:425:THR:HG23	1:C:440:THR:HG23	1.98	0.45
1:G:556:THR:O	1:H:461:ARG:NH2	2.49	0.45
2:J:113:VAL:CG1	2:J:126:THR:HG21	2.46	0.45
1:A:365:LEU:HB3	1:A:418:TRP:CH2	2.51	0.45
1:D:457:LEU:HB2	1:D:473:THR:OG1	2.16	0.45
1:F:454:VAL:CG2	1:F:538:VAL:CG2	2.94	0.45
2:J:14:CYS:SG	2:J:40:ILE:HB	2.56	0.45
3:R:25:VAL:HG11	3:R:33:VAL:HG23	1.98	0.45
1:F:449:LEU:CA	1:F:480:SER:O	2.64	0.45
1:L:354:PHE:HA	1:L:357:ILE:HG12	1.99	0.45
3:R:34:THR:C	3:R:88:LEU:CD1	2.90	0.45
1:B:365:LEU:H	1:B:365:LEU:HD23	1.81	0.45
1:C:384:ARG:N	1:C:388:GLU:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:ARG:NH1	1:E:451:ARG:CG	2.72	0.45
1:L:452:PRO:HG3	1:L:478:GLY:O	2.16	0.45
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.81	0.45
1:A:544:PRO:HB2	2:J:135:PRO:CD	2.47	0.45
1:B:482:ALA:HB2	1:B:515:TYR:HE2	1.81	0.45
2:J:108:CYS:HB2	2:J:133:CYS:HB3	1.62	0.45
1:K:448:ALA:HB1	1:K:450:HIS:CE1	2.52	0.45
1:K:475:LEU:HG	1:K:477:THR:HG23	1.98	0.45
1:C:451:ARG:HE	1:C:451:ARG:HB2	1.54	0.45
1:C:564:VAL:CG2	1:H:566:LEU:HD23	2.39	0.45
1:A:547:VAL:HG11	2:J:113:VAL:HG21	1.99	0.45
1:A:564:VAL:HB	1:B:564:VAL:HA	1.99	0.45
1:D:464:LEU:CD1	1:D:528:TRP:CZ3	2.99	0.45
1:E:520:ILE:O	1:E:520:ILE:HG13	2.16	0.45
2:J:10:ASN:HD22	2:J:67:LEU:CD1	2.30	0.45
2:J:131:ASP:OD2	3:R:107:GLY:HA2	2.17	0.45
3:R:22:GLU:HA	3:R:118:VAL:HG22	1.92	0.45
1:E:423:ARG:CG	1:E:442:SER:HG	2.23	0.45
1:E:464:LEU:HD23	1:E:525:GLU:OE1	2.17	0.45
1:H:568:MET:HB2	1:H:568:MET:HE2	1.52	0.45
1:K:501:VAL:HG11	1:L:516:PHE:CE1	2.50	0.45
1:A:372:LEU:H	1:A:372:LEU:HD23	1.82	0.45
1:B:528:TRP:CE3	1:B:528:TRP:O	2.69	0.45
1:G:452:PRO:HB3	1:G:479:PHE:HB3	1.99	0.45
2:J:48:ASN:HB3	4:J:201:NAG:O5	2.17	0.45
1:K:526:GLU:O	1:K:529:ASN:CG	2.48	0.45
1:B:518:HIS:O	1:B:518:HIS:CG	2.70	0.44
1:E:450:HIS:HD2	1:E:514:ARG:NH2	2.13	0.44
1:F:456:LEU:HD11	1:F:536:CYS:SG	2.57	0.44
1:F:348:PHE:CE1	1:F:368:LEU:HB3	2.52	0.44
1:F:349:ALA:HB3	1:F:441:ILE:HG21	1.99	0.44
1:G:499:LYS:HG3	1:G:521:LEU:HD12	1.98	0.44
1:K:421:GLY:HA2	1:K:443:ARG:HD3	1.98	0.44
1:B:531:GLY:O	1:B:553:ASP:OD1	2.36	0.44
1:K:460:ALA:HB2	1:L:457:LEU:HD23	2.00	0.44
1:L:488:TRP:HD1	1:L:500:TYR:CD2	2.35	0.44
1:A:449:LEU:HD22	1:A:449:LEU:HA	1.70	0.44
1:C:383:THR:HB	1:C:387:GLY:HA2	1.98	0.44
1:C:470:ALA:O	1:C:522:THR:HA	2.18	0.44
1:D:449:LEU:HB3	1:D:542:ALA:HB2	1.98	0.44
1:E:566:LEU:HD11	1:F:562:TYR:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ILE:N	1:B:371:ASP:HB3	2.33	0.44
1:B:365:LEU:HD12	1:B:441:ILE:HD13	2.00	0.44
1:B:374:THR:HG23	1:B:405:PHE:HD2	1.82	0.44
1:D:459:PRO:HD3	1:D:472:ILE:HG12	1.99	0.44
1:K:380:ILE:HG12	1:K:428:VAL:HG12	1.99	0.44
1:C:382:TRP:CE2	1:C:426:CYS:HB2	2.53	0.44
1:D:443:ARG:CZ	1:D:445:LYS:HD3	2.45	0.44
1:D:445:LYS:HD2	1:D:445:LYS:HA	1.45	0.44
1:E:443:ARG:CZ	1:E:443:ARG:CB	2.85	0.44
2:J:33:VAL:HB	1:L:559:PRO:HA	2.00	0.44
1:K:459:PRO:HG3	1:K:470:ALA:HB1	1.99	0.44
1:F:354:PHE:HA	1:F:357:ILE:HG22	2.00	0.44
1:F:433:LEU:HD12	1:F:434:PRO:HD2	1.99	0.44
1:G:499:LYS:CG	1:G:521:LEU:HD11	2.43	0.44
1:E:418:TRP:CD1	1:E:443:ARG:NE	2.86	0.44
1:F:391:LYS:NZ	1:F:410:GLU:O	2.45	0.44
1:L:495:LEU:HA	1:L:495:LEU:HD23	1.40	0.44
1:L:347:VAL:HG22	1:L:369:VAL:HG13	1.99	0.43
1:L:347:VAL:HG13	1:L:369:VAL:HG22	2.00	0.43
1:L:559:PRO:HG2	1:L:562:TYR:CZ	2.53	0.43
1:B:352:PRO:HG2	1:B:357:ILE:HD11	2.00	0.43
1:H:445:LYS:H	1:H:445:LYS:HG2	1.45	0.43
2:J:16:ARG:HD3	2:J:16:ARG:O	2.18	0.43
1:L:506:MET:HB3	1:L:507:PRO:HD2	2.00	0.43
3:R:35:ILE:N	3:R:88:LEU:HD11	2.33	0.43
1:C:543:LEU:HB2	1:C:546:ARG:HA	2.00	0.43
1:F:561:LEU:HD23	1:F:561:LEU:HA	1.51	0.43
1:G:508:GLU:HG2	1:G:511:ALA:HB3	2.00	0.43
1:K:464:LEU:O	1:K:467:ARG:NH1	2.49	0.43
1:K:567:VAL:HB	1:L:567:VAL:HA	2.00	0.43
3:R:29:LEU:C	3:R:29:LEU:CD2	2.91	0.43
1:A:429:THR:HG23	1:A:436:PRO:HG3	2.01	0.43
1:A:489:MET:HB2	1:A:535:THR:OG1	2.18	0.43
1:B:561:LEU:HB2	1:C:561:LEU:O	2.17	0.43
1:F:455:TYR:C	1:F:456:LEU:HD12	2.43	0.43
1:G:474:CYS:HB2	1:G:488:TRP:CZ2	2.53	0.43
2:J:67:LEU:HA	2:J:67:LEU:HD12	1.85	0.43
1:K:345:ILE:HA	1:K:372:LEU:HG	2.01	0.43
1:C:475:LEU:O	1:C:476:VAL:C	2.60	0.43
1:L:479:PHE:CD1	1:L:515:TYR:O	2.71	0.43
3:R:95:THR:OG1	3:R:97:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:75:ARG:CB	3:R:92:THR:CG2	2.96	0.43
1:A:379:THR:HB	1:A:429:THR:HB	1.99	0.43
1:D:382:TRP:NE1	1:D:409:GLY:O	2.51	0.43
1:E:419:ASN:HA	1:E:443:ARG:CZ	2.49	0.43
1:K:450:HIS:ND1	1:K:450:HIS:N	2.59	0.43
1:L:346:ARG:HB3	1:L:370:THR:O	2.19	0.43
1:B:564:VAL:CG2	1:C:564:VAL:HA	2.48	0.43
1:G:495:LEU:HD12	1:G:495:LEU:HA	1.79	0.43
1:H:392:THR:HG22	1:H:393:HIS:N	2.33	0.43
1:L:391:LYS:NZ	1:L:392:THR:HG22	2.34	0.43
3:R:21:PRO:O	3:R:118:VAL:HG21	2.18	0.43
3:R:41:GLU:OE1	3:R:82:PRO:CG	2.67	0.43
1:G:489:MET:HE3	1:G:489:MET:HB3	1.86	0.43
1:H:489:MET:HE3	1:H:489:MET:HB2	1.88	0.43
1:H:532:GLU:HB3	1:H:534:TYR:CE2	2.53	0.43
3:R:86:LEU:HA	3:R:86:LEU:HD22	1.40	0.43
2:J:20:ARG:HH11	2:J:34:GLU:HG2	1.84	0.43
2:J:109:TYR:H	2:J:129:THR:HG21	1.84	0.43
3:R:45:ARG:O	3:R:106:ALA:HA	2.19	0.43
1:E:378:VAL:HG11	1:E:407:ALA:HB2	2.01	0.42
1:E:382:TRP:CE3	1:E:426:CYS:HB3	2.54	0.42
1:H:392:THR:HG22	1:H:393:HIS:H	1.84	0.42
1:H:486:VAL:HG13	1:H:538:VAL:HG12	2.00	0.42
1:K:501:VAL:CG1	1:L:516:PHE:CZ	2.85	0.42
1:C:363:THR:HG23	1:C:413:ILE:O	2.18	0.42
1:C:461:ARG:H	1:C:461:ARG:HG2	1.57	0.42
1:D:349:ALA:HA	1:D:367:CYS:HA	2.00	0.42
1:F:558:LYS:HB3	1:F:559:PRO:CD	2.48	0.42
1:K:351:PRO:HG3	1:K:441:ILE:HD12	2.00	0.42
1:A:359:LEU:HD13	2:J:115:LEU:HD13	2.00	0.42
1:C:491:ARG:HG3	1:C:491:ARG:NH1	2.35	0.42
1:C:509:PRO:HB3	1:D:501:VAL:HG23	2.02	0.42
1:F:419:ASN:HA	1:F:443:ARG:HH11	1.85	0.42
1:G:364:LYS:HE3	1:G:410:GLU:C	2.44	0.42
1:G:424:PHE:O	1:G:440:THR:HA	2.19	0.42
1:G:457:LEU:HB2	1:G:473:THR:OG1	2.19	0.42
1:G:557:GLY:HA2	1:H:461:ARG:HH21	1.85	0.42
2:J:130:PRO:HG2	2:J:130:PRO:O	2.19	0.42
1:K:514:ARG:NH1	1:K:514:ARG:CG	2.72	0.42
1:L:367:CYS:HB2	1:L:382:TRP:CZ2	2.55	0.42
3:R:33:VAL:HG21	3:R:120:LEU:CD2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:47:TYR:CE2	3:R:110:THR:HG23	2.55	0.42
1:A:568:MET:HE3	2:J:64:LEU:HD21	2.00	0.42
1:B:482:ALA:HB2	1:B:515:TYR:CE2	2.54	0.42
1:E:433:LEU:HD13	1:E:435:SER:C	2.44	0.42
1:F:464:LEU:HD22	1:F:525:GLU:HG2	2.01	0.42
3:R:37:CYS:HB2	3:R:87:PHE:CG	2.54	0.42
3:R:112:ARG:HH11	3:R:112:ARG:CG	2.22	0.42
1:F:452:PRO:HD3	1:F:540:HIS:ND1	2.35	0.42
1:G:365:LEU:HG	1:G:424:PHE:CD1	2.53	0.42
1:K:393:HIS:HB2	1:K:410:GLU:H	1.84	0.42
1:K:532:GLU:HA	1:K:532:GLU:OE1	2.19	0.42
1:L:501:VAL:HG12	1:L:520:ILE:HG13	2.01	0.42
1:A:547:VAL:HG21	2:J:124:VAL:HG11	2.02	0.42
1:B:543:LEU:HB2	1:B:546:ARG:HA	2.01	0.42
1:D:365:LEU:H	1:D:365:LEU:HD23	1.85	0.42
1:D:468:GLU:OE1	1:D:468:GLU:HA	2.19	0.42
1:G:499:LYS:HD2	1:G:522:THR:O	2.20	0.42
2:J:101:TYR:N	2:J:101:TYR:HD1	2.15	0.42
3:R:33:VAL:CG2	3:R:120:LEU:HD23	2.46	0.42
1:A:511:ALA:HB1	1:A:514:ARG:HD3	2.01	0.42
1:F:454:VAL:HG21	1:F:538:VAL:CG2	2.50	0.42
1:H:520:ILE:O	1:H:520:ILE:HG13	2.19	0.42
1:H:537:VAL:HG23	1:H:548:THR:O	2.20	0.42
1:K:364:LYS:HG2	1:K:412:SER:HA	2.02	0.42
1:K:445:LYS:HB2	1:K:445:LYS:HE2	1.75	0.42
1:A:449:LEU:CD2	1:A:480:SER:O	2.60	0.42
1:B:510:GLN:NE2	1:B:511:ALA:HB2	2.35	0.42
1:C:568:MET:HE3	1:C:568:MET:HB3	1.64	0.42
1:H:453:ASP:OD2	1:H:455:TYR:OH	2.31	0.42
2:J:49:ILE:CD1	2:J:103:TYR:CD1	2.86	0.42
2:J:111:ALA:O	2:J:125:GLU:HA	2.20	0.42
1:L:451:ARG:HA	1:L:452:PRO:HD3	1.88	0.42
1:L:510:GLN:OE1	1:L:510:GLN:N	2.39	0.42
1:F:469:SER:HA	1:F:524:SER:HA	2.01	0.42
1:G:378:VAL:HG12	1:G:430:HIS:CD2	2.54	0.42
1:L:500:TYR:HB2	1:L:521:LEU:CD1	2.37	0.42
1:D:449:LEU:HA	1:D:449:LEU:HD23	1.59	0.41
1:F:379:THR:HB	1:F:429:THR:HG1	1.85	0.41
1:L:480:SER:HB3	1:L:514:ARG:HA	2.02	0.41
1:H:450:HIS:CE1	1:H:514:ARG:HE	2.39	0.41
3:R:96:GLU:OE2	3:R:122:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLU:HG2	3:R:67:PHE:CD2	2.55	0.41
1:E:430:HIS:CD2	1:E:431:THR:H	2.38	0.41
2:J:68:CYS:O	2:J:68:CYS:SG	2.79	0.41
1:A:568:MET:CE	2:J:37:ILE:HD13	2.51	0.41
1:G:476:VAL:HG12	1:G:479:PHE:HD2	1.84	0.41
1:L:488:TRP:CD1	1:L:521:LEU:CD2	2.87	0.41
3:R:34:THR:CB	3:R:88:LEU:HD12	2.42	0.41
1:B:475:LEU:HA	1:B:518:HIS:HB2	2.01	0.41
1:C:384:ARG:C	1:C:386:ASN:N	2.77	0.41
1:E:543:LEU:HB2	1:E:546:ARG:HA	2.03	0.41
2:J:60:PHE:HB3	2:J:62:TYR:CE2	2.55	0.41
2:J:102:THR:CB	1:L:575:CYS:H	2.31	0.41
1:L:381:SER:HB2	1:L:427:THR:HB	2.02	0.41
1:F:443:ARG:HA	1:F:444:PRO:HD3	1.94	0.41
1:F:452:PRO:HB3	1:F:479:PHE:CB	2.40	0.41
1:F:493:GLN:OE1	1:F:493:GLN:HA	2.21	0.41
1:H:543:LEU:CG	1:H:548:THR:HG22	2.51	0.41
1:H:562:TYR:CB	1:K:562:TYR:HB2	2.51	0.41
1:K:477:THR:HG22	1:K:516:PHE:HB2	2.03	0.41
1:E:372:LEU:HD21	1:E:430:HIS:CD2	2.55	0.41
1:E:508:GLU:HG3	1:E:509:PRO:HD2	2.01	0.41
1:F:385:GLN:OE1	1:F:385:GLN:HA	2.21	0.41
1:G:422:GLU:HB3	1:G:424:PHE:CE2	2.56	0.41
1:K:413:ILE:HG22	1:K:414:CYS:N	2.35	0.41
1:A:524:SER:OG	1:A:526:GLU:OE1	2.39	0.41
1:B:384:ARG:NH1	1:B:388:GLU:HB3	2.36	0.41
1:C:384:ARG:CZ	1:C:388:GLU:C	2.93	0.41
1:F:352:PRO:HD3	1:F:365:LEU:HD23	2.03	0.41
1:G:520:ILE:O	1:G:520:ILE:HG13	2.21	0.41
1:B:533:THR:O	1:B:533:THR:HG22	2.16	0.41
1:D:450:HIS:HE1	1:D:480:SER:OG	1.88	0.41
1:E:445:LYS:HD3	1:E:445:LYS:C	2.46	0.41
1:F:449:LEU:HA	1:F:480:SER:OG	2.20	0.41
1:H:532:GLU:HB3	1:H:534:TYR:CD2	2.56	0.41
1:H:553:ASP:OD1	1:H:553:ASP:N	2.54	0.41
2:J:109:TYR:H	2:J:129:THR:CG2	2.33	0.41
1:K:463:GLN:HG2	1:L:455:TYR:HE2	1.79	0.41
1:K:505:PRO:HA	1:K:516:PHE:O	2.20	0.41
1:L:467:ARG:HA	1:L:525:GLU:HG3	2.02	0.41
1:B:465:ASN:ND2	1:L:571:THR:HG21	2.36	0.41
1:F:452:PRO:CA	1:F:479:PHE:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:8:VAL:HG12	2:J:10:ASN:H	1.85	0.41
2:J:20:ARG:NH1	2:J:34:GLU:HG2	2.36	0.41
1:K:451:ARG:CZ	1:K:451:ARG:CB	2.95	0.41
1:K:461:ARG:HB2	1:K:461:ARG:HH11	1.85	0.41
1:L:470:ALA:O	1:L:523:VAL:CG2	2.69	0.41
3:R:24:LYS:HD3	3:R:24:LYS:HA	1.95	0.41
1:C:463:GLN:HE21	1:C:463:GLN:HB2	1.66	0.40
1:G:360:THR:HG23	1:G:362:SER:HB3	2.03	0.40
1:G:485:PHE:CD2	1:G:485:PHE:C	2.97	0.40
1:H:428:VAL:HB	1:H:437:LEU:HB2	2.03	0.40
1:L:352:PRO:HD3	1:L:365:LEU:HD22	2.03	0.40
1:L:443:ARG:HD3	1:L:443:ARG:HA	1.67	0.40
1:L:488:TRP:O	1:L:495:LEU:N	2.54	0.40
1:B:437:LEU:HD23	1:B:437:LEU:H	1.86	0.40
1:B:502:THR:HA	1:B:519:SER:HB2	1.98	0.40
1:F:451:ARG:HB2	1:F:451:ARG:HH11	1.84	0.40
1:H:459:PRO:HG3	1:H:470:ALA:HB1	2.03	0.40
1:H:535:THR:HA	1:H:551:THR:OG1	2.21	0.40
2:J:4:ARG:HG2	2:J:20:ARG:HD2	2.03	0.40
1:L:490:GLN:O	1:L:493:GLN:CD	2.65	0.40
1:L:543:LEU:HB2	1:L:546:ARG:HA	2.02	0.40
3:R:35:ILE:N	3:R:88:LEU:CD1	2.84	0.40
1:B:525:GLU:CD	1:B:525:GLU:O	2.65	0.40
1:C:454:VAL:H	1:C:454:VAL:HG23	1.58	0.40
1:D:533:THR:HB	1:D:535:THR:HG23	2.04	0.40
1:G:449:LEU:HG	1:G:542:ALA:HB2	2.03	0.40
1:K:432:ASP:OD1	1:K:433:LEU:N	2.53	0.40
1:L:531:GLY:C	1:L:533:THR:H	2.29	0.40
1:A:540:HIS:H	1:A:543:LEU:HD12	1.86	0.40
1:G:489:MET:CG	1:G:489:MET:O	2.69	0.40
1:K:506:MET:O	1:K:516:PHE:HD1	2.04	0.40
1:L:506:MET:CB	1:L:507:PRO:CD	2.94	0.40
1:C:384:ARG:N	1:C:388:GLU:N	2.60	0.40
1:E:422:GLU:HB3	1:E:424:PHE:HE2	1.87	0.40
1:G:364:LYS:HD2	1:G:364:LYS:HA	1.91	0.40
2:J:40:ILE:HG12	1:L:567:VAL:CG2	2.51	0.40
1:K:520:ILE:HD12	1:L:516:PHE:CE1	2.56	0.40
1:L:354:PHE:CZ	1:L:541:GLU:HB3	2.56	0.40
3:R:33:VAL:H	3:R:91:VAL:HG23	1.87	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	228/232 (98%)	213 (93%)	15 (7%)	0	100	100
1	B	226/232 (97%)	192 (85%)	29 (13%)	5 (2%)	5	24
1	C	223/232 (96%)	198 (89%)	25 (11%)	0	100	100
1	D	222/232 (96%)	207 (93%)	15 (7%)	0	100	100
1	E	222/232 (96%)	205 (92%)	16 (7%)	1 (0%)	25	54
1	F	222/232 (96%)	206 (93%)	16 (7%)	0	100	100
1	G	222/232 (96%)	193 (87%)	28 (13%)	1 (0%)	25	54
1	H	222/232 (96%)	202 (91%)	20 (9%)	0	100	100
1	K	223/232 (96%)	204 (92%)	18 (8%)	1 (0%)	30	60
1	L	224/232 (97%)	205 (92%)	16 (7%)	3 (1%)	10	33
2	J	99/136 (73%)	82 (83%)	16 (16%)	1 (1%)	13	39
3	R	105/107 (98%)	98 (93%)	6 (6%)	1 (1%)	13	39
All	All	2438/2563 (95%)	2205 (90%)	220 (9%)	13 (0%)	27	54

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	532	GLU
1	B	494	PRO
1	B	497	PRO
1	B	491	ARG
1	L	452	PRO
1	L	575	CYS
1	E	563	ASN
1	G	481	PRO
2	J	36	ASN
1	K	532	GLU
3	R	113	GLY
1	B	444	PRO

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Mol	Chain	Res	Type
1	L	523	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	204/206 (99%)	199 (98%)	5 (2%)	42 65
1	B	203/206 (98%)	181 (89%)	22 (11%)	5 20
1	C	201/206 (98%)	161 (80%)	40 (20%)	1 3
1	D	200/206 (97%)	196 (98%)	4 (2%)	50 70
1	E	200/206 (97%)	180 (90%)	20 (10%)	6 22
1	F	200/206 (97%)	195 (98%)	5 (2%)	42 65
1	G	200/206 (97%)	184 (92%)	16 (8%)	10 31
1	H	200/206 (97%)	189 (94%)	11 (6%)	18 44
1	K	201/206 (98%)	188 (94%)	13 (6%)	14 39
1	L	204/206 (99%)	186 (91%)	18 (9%)	8 28
2	J	97/128 (76%)	88 (91%)	9 (9%)	7 25
3	R	92/92 (100%)	69 (75%)	23 (25%)	0 1
All	All	2202/2280 (97%)	2016 (92%)	186 (8%)	11 29

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	ASN
1	A	447	VAL
1	A	449	LEU
1	A	450	HIS
1	A	541	GLU
1	B	413	ILE
1	B	415	GLU
1	B	416	ASP
1	B	420	SER

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Mol	Chain	Res	Type
1	B	440	THR
1	B	443	ARG
1	B	445	LYS
1	B	447	VAL
1	B	452	PRO
1	B	454	VAL
1	B	490	GLN
1	B	491	ARG
1	B	493	GLN
1	B	494	PRO
1	B	498	GLU
1	B	499	LYS
1	B	518	HIS
1	B	525	GLU
1	B	530	THR
1	B	547	VAL
1	B	551	THR
1	B	571	THR
1	C	386	ASN
1	C	391	LYS
1	C	392	THR
1	C	393	HIS
1	C	396	ILE
1	C	398	GLU
1	C	400	HIS
1	C	404	THR
1	C	408	VAL
1	C	412	SER
1	C	413	ILE
1	C	414	CYS
1	C	419	ASN
1	C	422	GLU
1	C	423	ARG
1	C	425	THR
1	C	427	THR
1	C	431	THR
1	C	432	ASP
1	C	437	LEU
1	C	438	LYS
1	C	439	GLN
1	C	440	THR
1	C	441	ILE

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Mol	Chain	Res	Type
1	C	442	SER
1	C	443	ARG
1	C	445	LYS
1	C	451	ARG
1	C	456	LEU
1	C	461	ARG
1	C	468	GLU
1	C	469	SER
1	C	471	THR
1	C	472	ILE
1	C	474	CYS
1	C	476	VAL
1	C	477	THR
1	C	565	SER
1	C	566	LEU
1	C	568	MET
1	D	445	LYS
1	D	447	VAL
1	D	450	HIS
1	D	461	ARG
1	E	443	ARG
1	E	445	LYS
1	E	449	LEU
1	E	451	ARG
1	E	453	ASP
1	E	522	THR
1	E	523	VAL
1	E	524	SER
1	E	525	GLU
1	E	526	GLU
1	E	530	THR
1	E	532	GLU
1	E	552	VAL
1	E	553	ASP
1	E	554	LYS
1	E	556	THR
1	E	558	LYS
1	E	560	THR
1	E	561	LEU
1	E	562	TYR
1	F	445	LYS
1	F	449	LEU

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Mol	Chain	Res	Type
1	F	450	HIS
1	F	451	ARG
1	F	561	LEU
1	G	345	ILE
1	G	420	SER
1	G	422	GLU
1	G	423	ARG
1	G	441	ILE
1	G	445	LYS
1	G	447	VAL
1	G	449	LEU
1	G	485	PHE
1	G	489	MET
1	G	490	GLN
1	G	491	ARG
1	G	493	GLN
1	G	495	LEU
1	G	498	GLU
1	G	499	LYS
1	H	443	ARG
1	H	445	LYS
1	H	447	VAL
1	H	449	LEU
1	H	548	THR
1	H	550	ARG
1	H	551	THR
1	H	562	TYR
1	H	563	ASN
1	H	566	LEU
1	H	567	VAL
2	J	36	ASN
2	J	39	ILE
2	J	40	ILE
2	J	57	ARG
2	J	101	TYR
2	J	112	VAL
2	J	128	LEU
2	J	129	THR
2	J	131	ASP
1	K	443	ARG
1	K	449	LEU
1	K	450	HIS

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Mol	Chain	Res	Type
1	K	451	ARG
1	K	514	ARG
1	K	516	PHE
1	K	518	HIS
1	K	529	ASN
1	K	530	THR
1	K	532	GLU
1	K	555	SER
1	K	556	THR
1	K	558	LYS
1	L	443	ARG
1	L	450	HIS
1	L	451	ARG
1	L	455	TYR
1	L	484	VAL
1	L	486	VAL
1	L	496	SER
1	L	498	GLU
1	L	499	LYS
1	L	500	TYR
1	L	501	VAL
1	L	502	THR
1	L	514	ARG
1	L	516	PHE
1	L	518	HIS
1	L	521	LEU
1	L	523	VAL
1	L	571	THR
3	R	26	GLU
3	R	28	GLU
3	R	34	THR
3	R	35	ILE
3	R	39	LEU
3	R	41	GLU
3	R	44	VAL
3	R	45	ARG
3	R	86	LEU
3	R	87	PHE
3	R	88	LEU
3	R	89	VAL
3	R	92	THR
3	R	97	SER

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Mol	Chain	Res	Type
3	R	98	ASP
3	R	108	MET
3	R	109	ASN
3	R	110	THR
3	R	111	ASP
3	R	119	THR
3	R	121	ASN
3	R	123	HIS
3	R	124	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	GLN
1	B	465	ASN
1	B	510	GLN
1	C	400	HIS
1	C	450	HIS
1	C	463	GLN
1	D	463	GLN
1	E	463	GLN
1	G	430	HIS
1	G	439	GLN
1	H	400	HIS
1	H	430	HIS
1	K	395	ASN
1	K	430	HIS
1	K	463	GLN
1	K	518	HIS
1	L	518	HIS
3	R	80	GLN
3	R	85	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 ligands 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	$\# Z  > 2$
4	NAG	B	601	1	14,14,15	0.22	0	17,19,21	0.54	0
4	NAG	K	601	1	14,14,15	0.36	0	17,19,21	0.34	0
4	NAG	L	601	1	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	D	601	1	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	G	601	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	C	601	-	14,14,15	0.16	0	17,19,21	0.50	0
4	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.38	0
4	NAG	H	601	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
4	NAG	J	201	2	14,14,15	0.52	0	17,19,21	0.38	0
4	NAG	E	601	1	14,14,15	0.21	0	17,19,21	0.37	0
4	NAG	F	601	1	14,14,15	0.38	0	17,19,21	0.55	0

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
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	K	601	1	-	4/6/23/26	0/1/1/1
4	NAG	L	601	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	2/6/23/26	0/1/1/1
4	NAG	G	601	1	-	1/6/23/26	0/1/1/1
4	NAG	C	601	-	-	4/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	601	1	-	0/6/23/26	0/1/1/1
4	NAG	J	201	2	-	2/6/23/26	0/1/1/1
4	NAG	E	601	1	-	1/6/23/26	0/1/1/1
4	NAG	F	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	601	NAG	C1-O5-C5	2.15	115.11	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	NAG	C4-C5-C6-O6
4	L	601	NAG	O5-C5-C6-O6
4	C	601	NAG	O5-C5-C6-O6
4	K	601	NAG	O5-C5-C6-O6
4	J	201	NAG	C4-C5-C6-O6
4	L	601	NAG	C4-C5-C6-O6
4	D	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
4	K	601	NAG	C4-C5-C6-O6
4	F	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2
4	K	601	NAG	C8-C7-N2-C2
4	K	601	NAG	O7-C7-N2-C2
4	B	601	NAG	C4-C5-C6-O6
4	J	201	NAG	O5-C5-C6-O6
4	D	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	E	601	NAG	O5-C5-C6-O6
4	G	601	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	601	NAG	1	0
4	G	601	NAG	1	0
4	C	601	NAG	2	0
4	J	201	NAG	1	0
4	F	601	NAG	2	0

## 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.

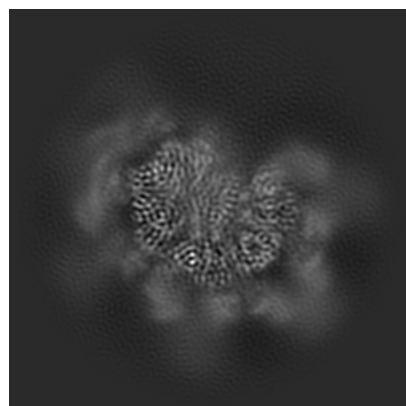
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34085. These allow visual inspection of the internal detail of the map and identification of artifacts.

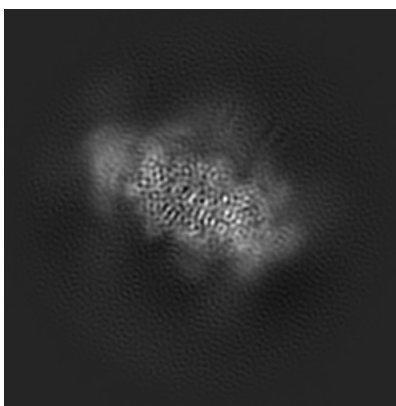
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

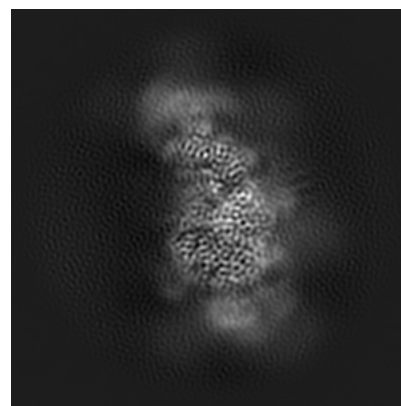
#### 6.1.1 Primary map



X

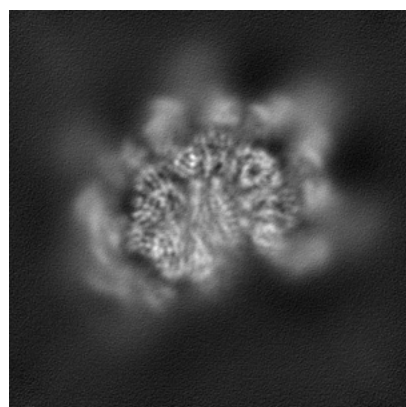


Y

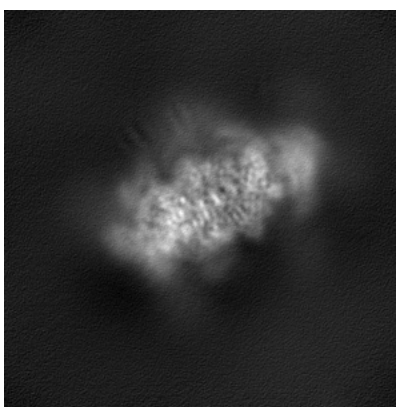


Z

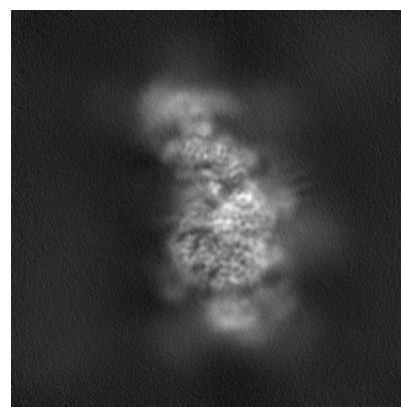
#### 6.1.2 Raw map



X



Y

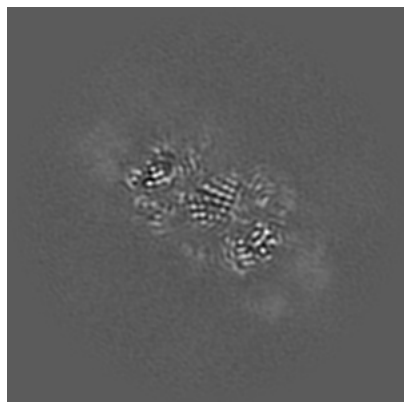


Z

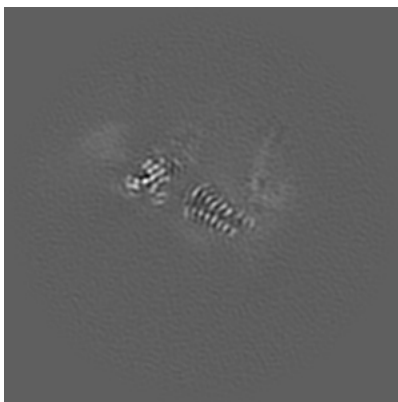
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

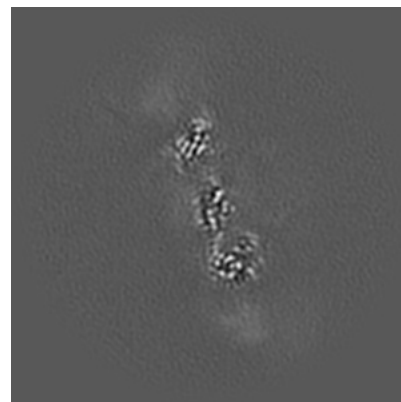
### 6.2.1 Primary map



X Index: 160

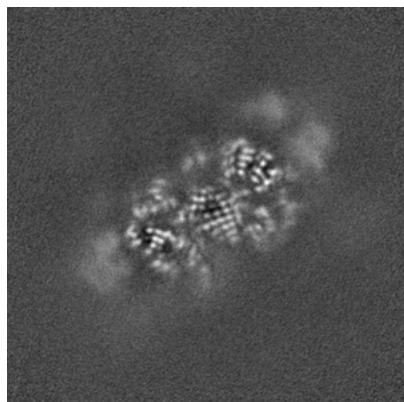


Y Index: 160

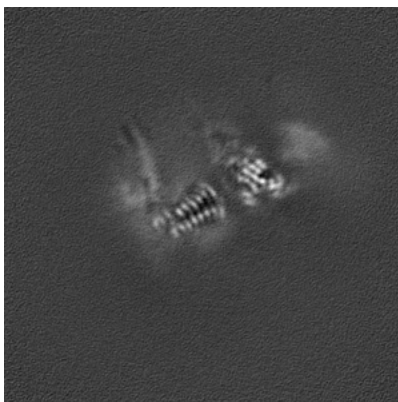


Z Index: 160

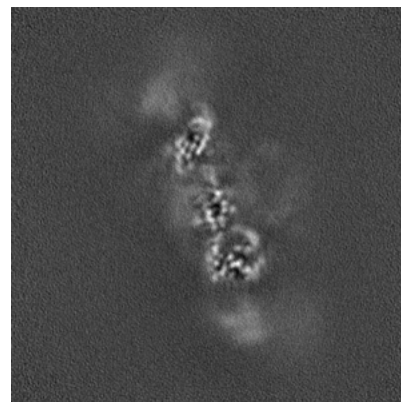
### 6.2.2 Raw map



X Index: 160



Y Index: 160

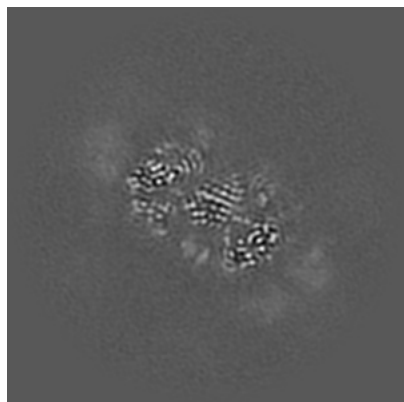


Z Index: 160

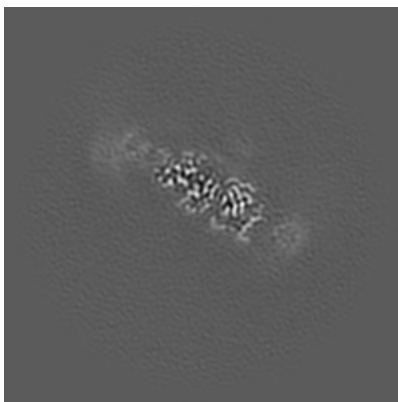
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

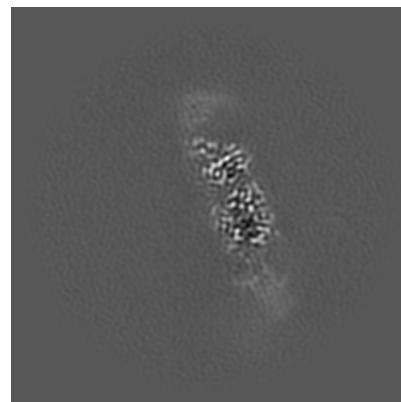
### 6.3.1 Primary map



X Index: 162

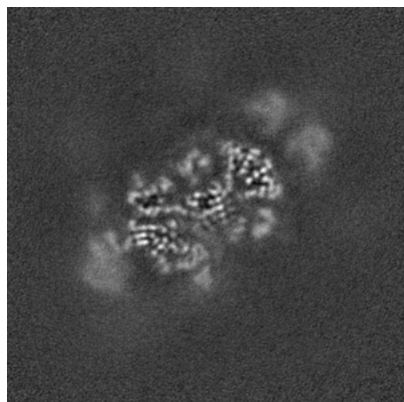


Y Index: 117

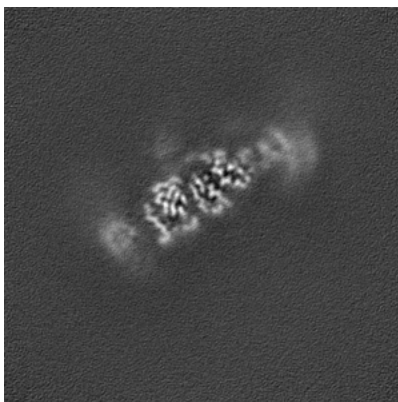


Z Index: 120

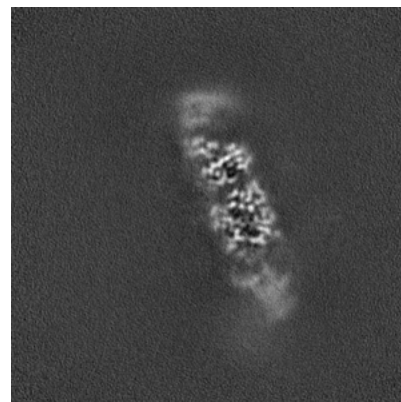
### 6.3.2 Raw map



X Index: 166



Y Index: 117



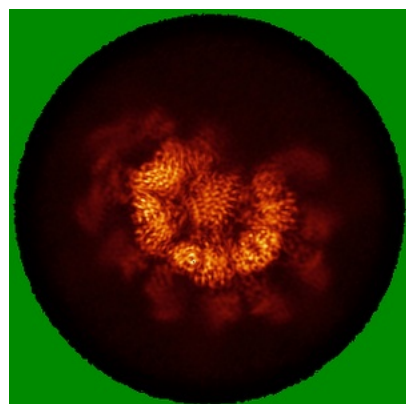
Z Index: 199

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

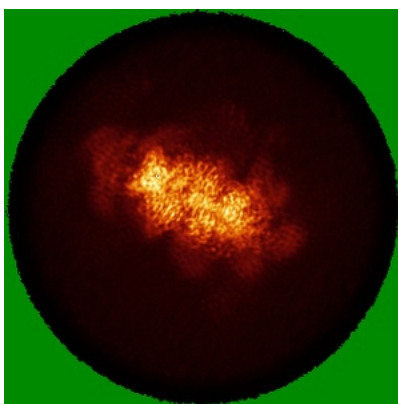


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

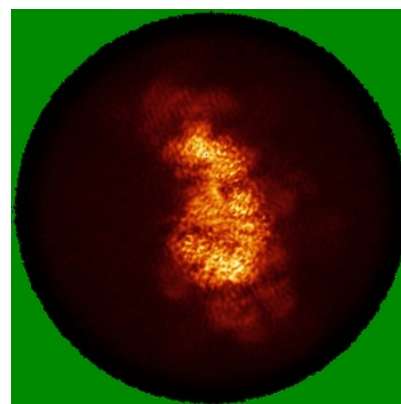
### 6.4.1 Primary map



X

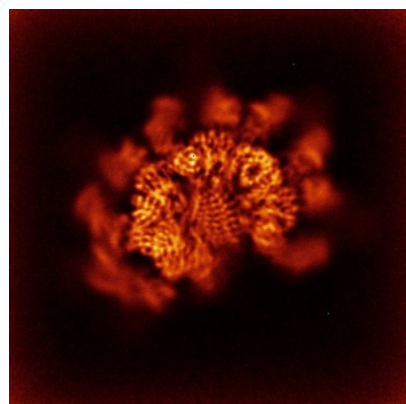


Y



Z

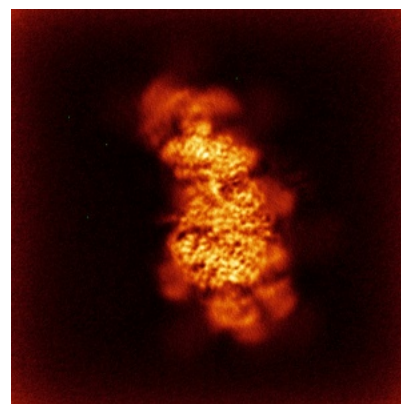
### 6.4.2 Raw map



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.



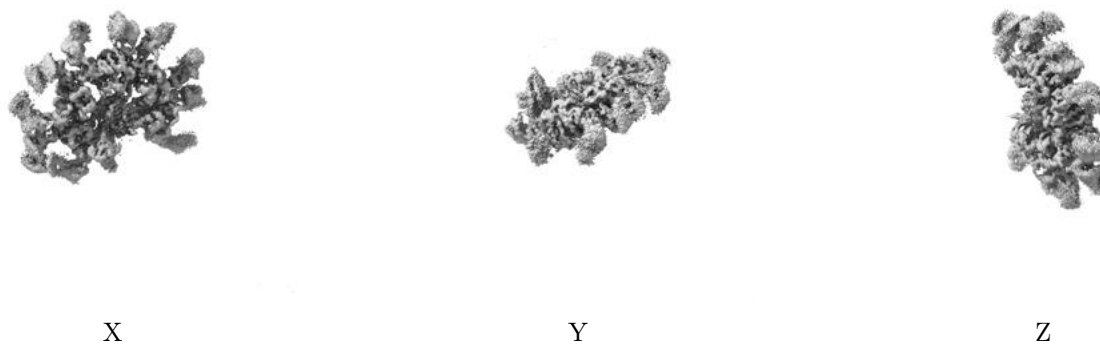
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

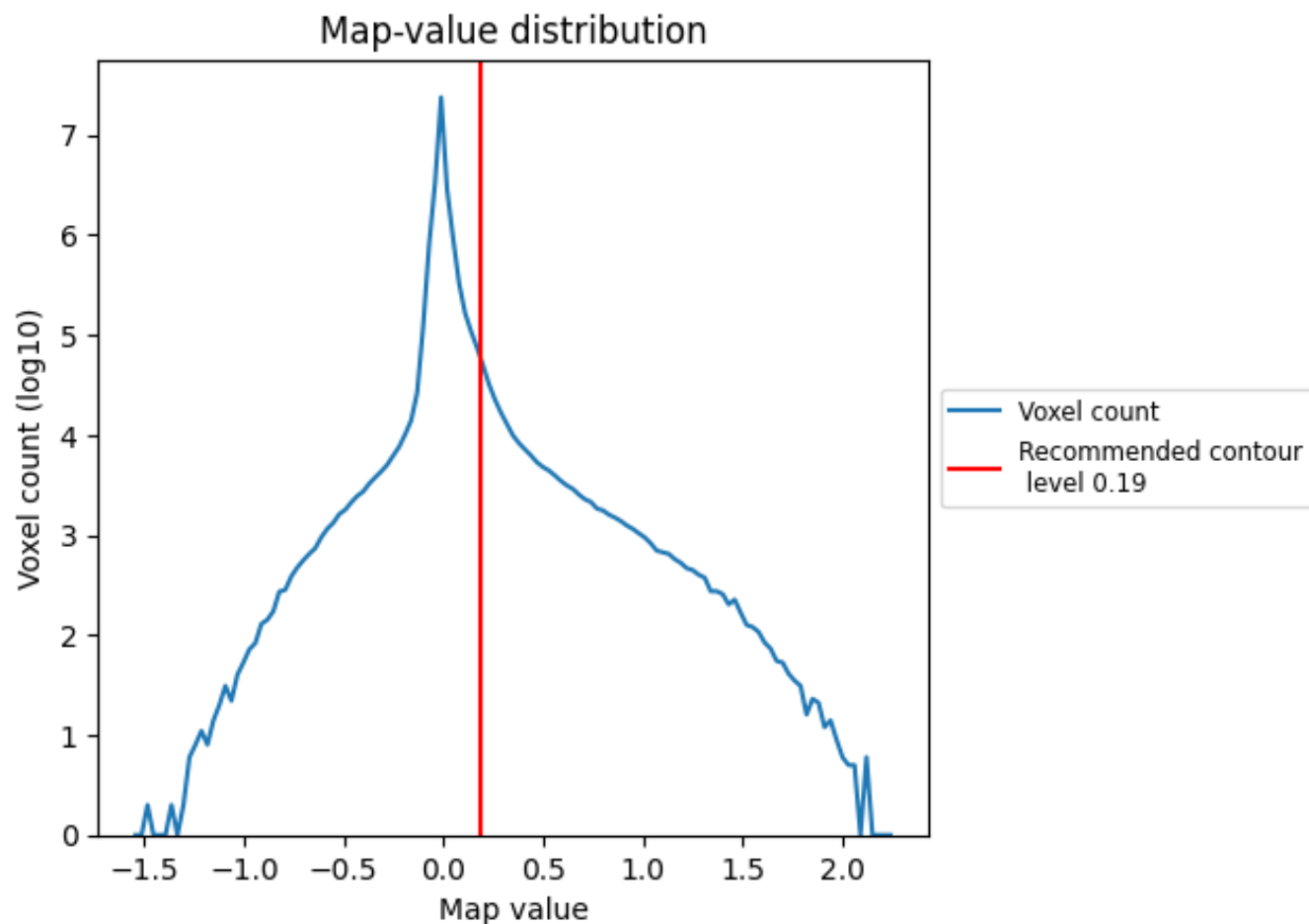
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

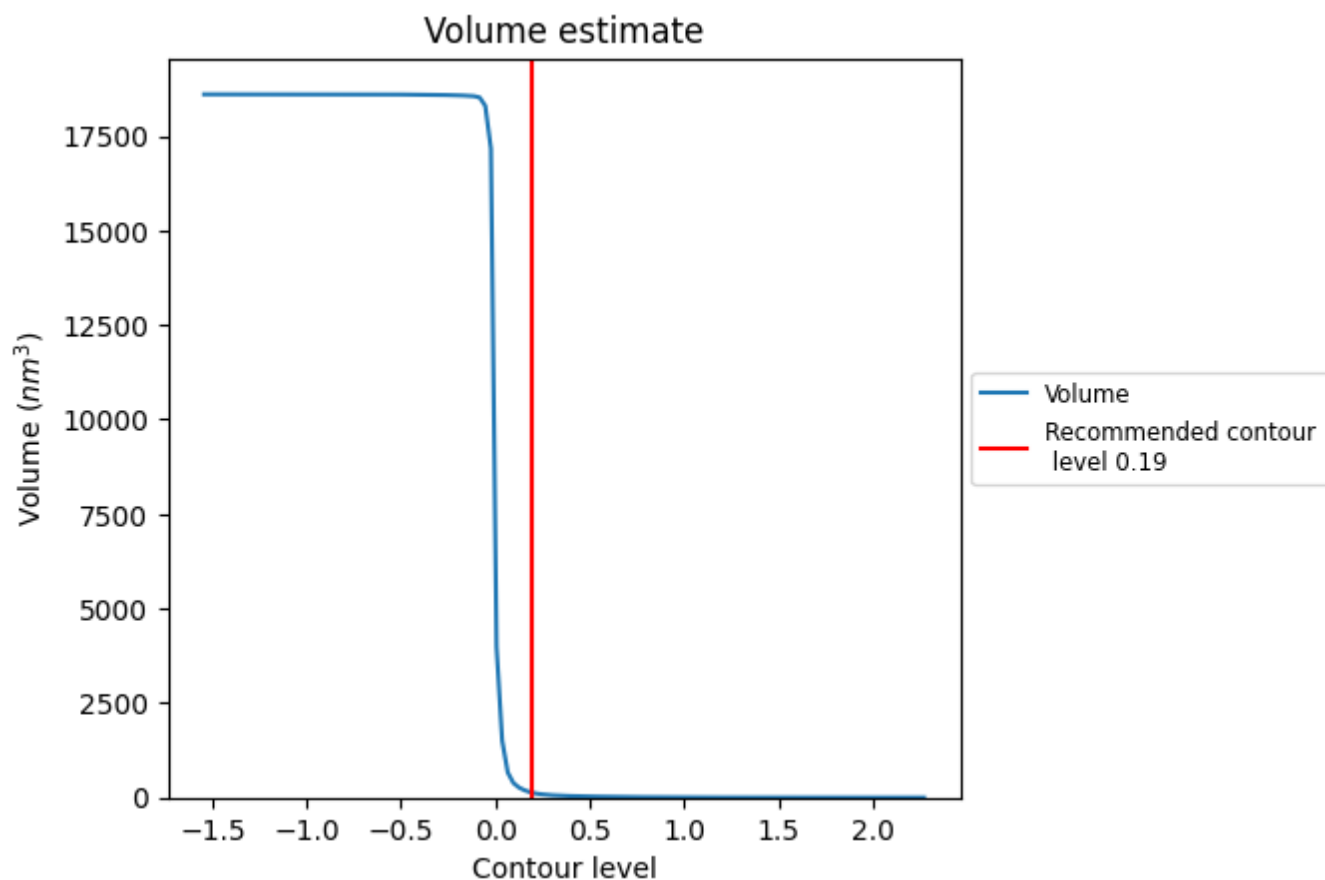
This section contains the results of statistical analysis of the map.

### 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.

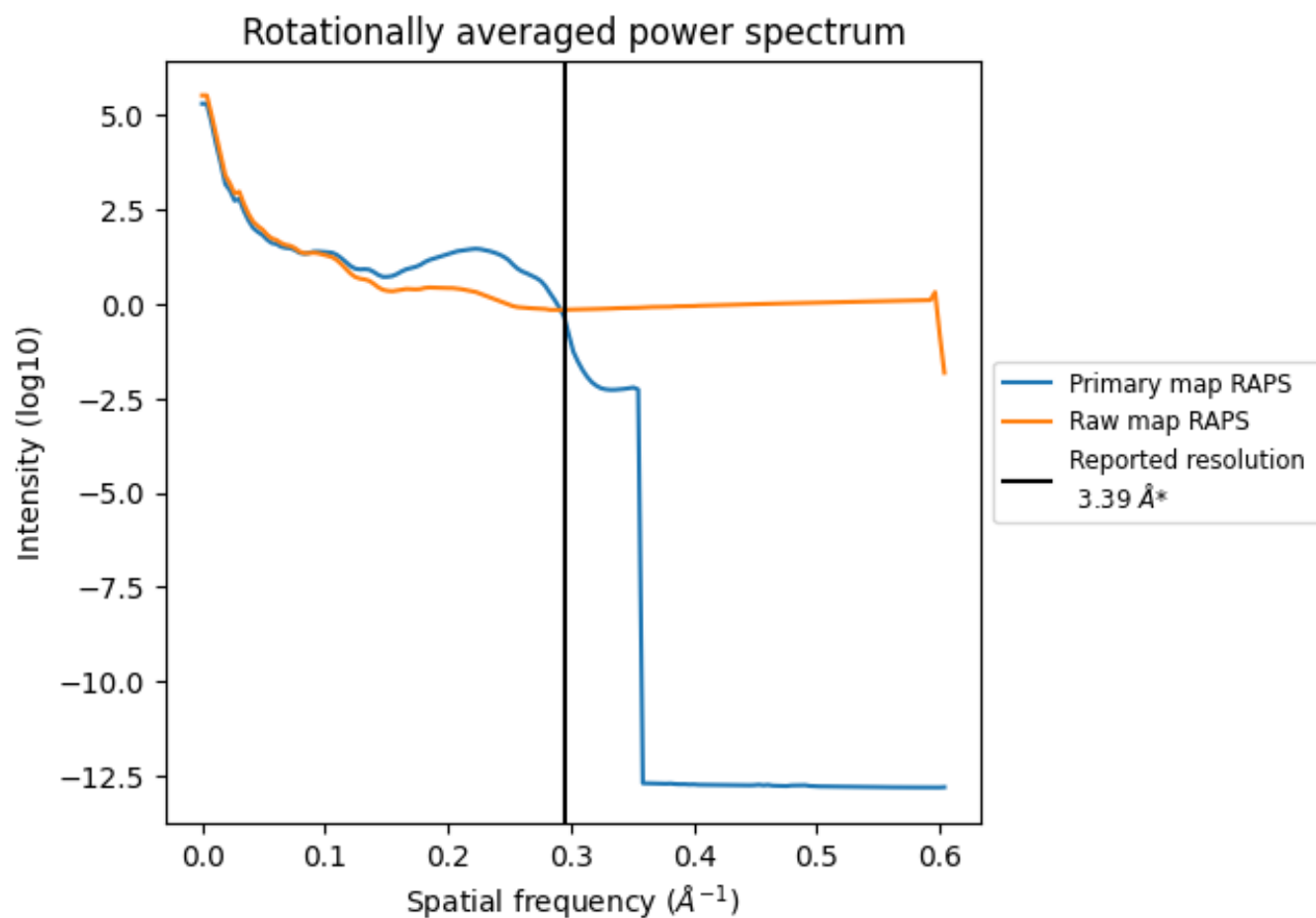
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137  $\text{nm}^3$ ; this corresponds to an approximate mass of 124 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 ⓘ

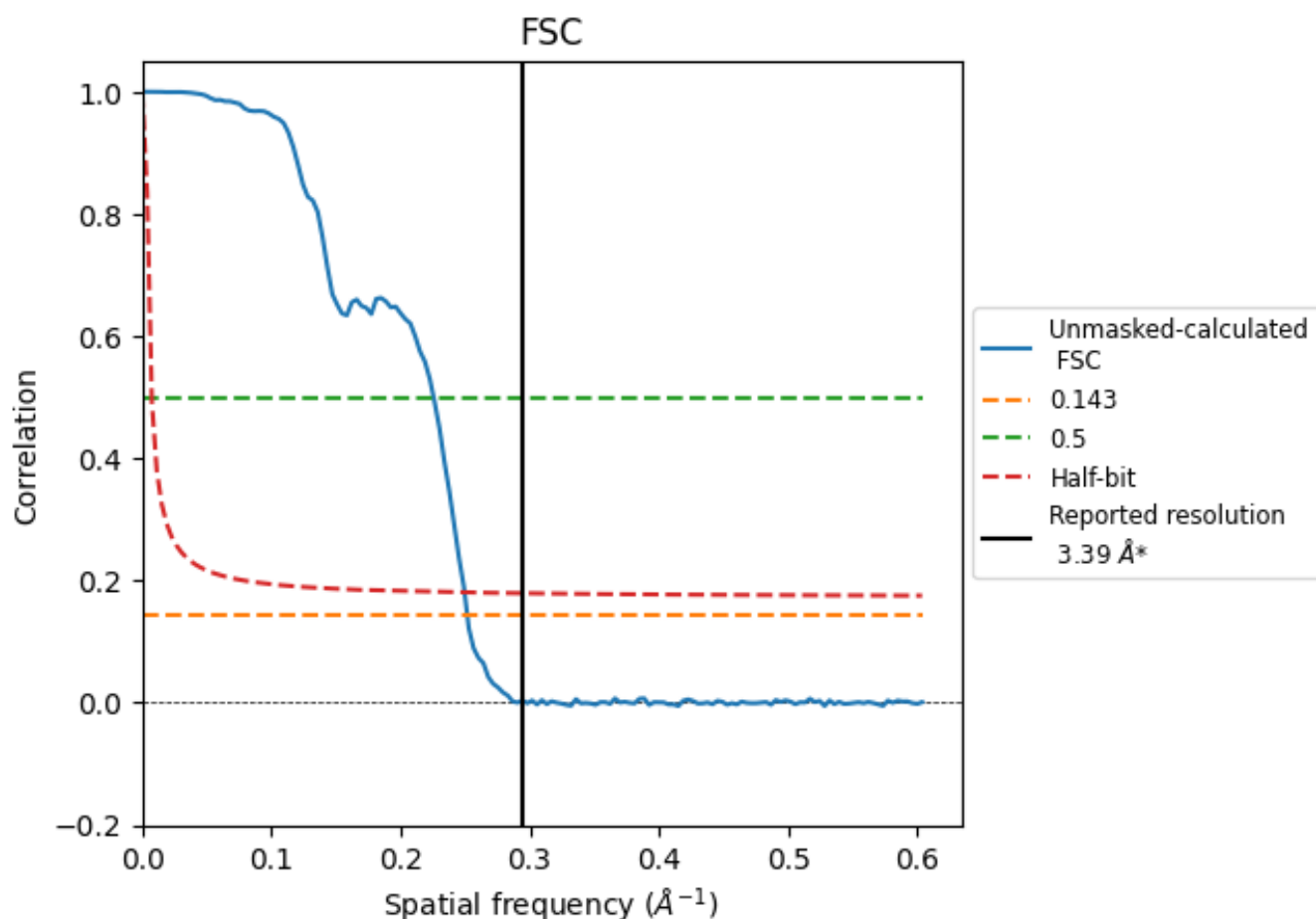


\*Reported resolution corresponds to spatial frequency of 0.295 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.295  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

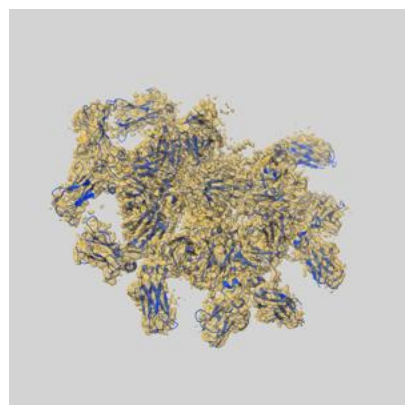
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	4.43	4.01

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 3.39 by more than 10 %

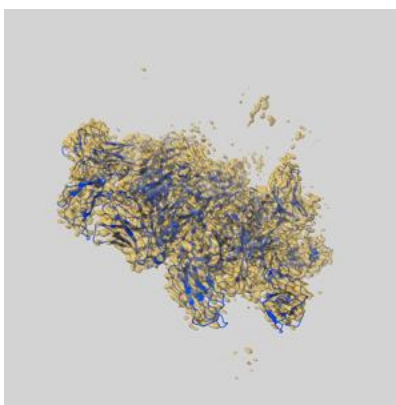
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34085 and PDB model 7YTC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

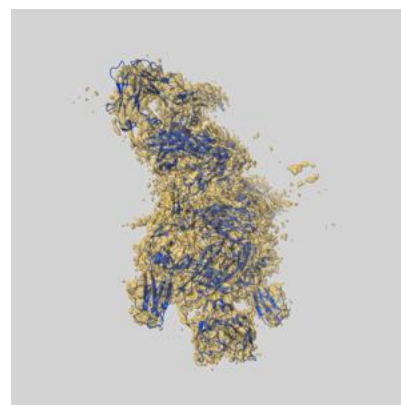
### 9.1 Map-model overlay [i](#)



X



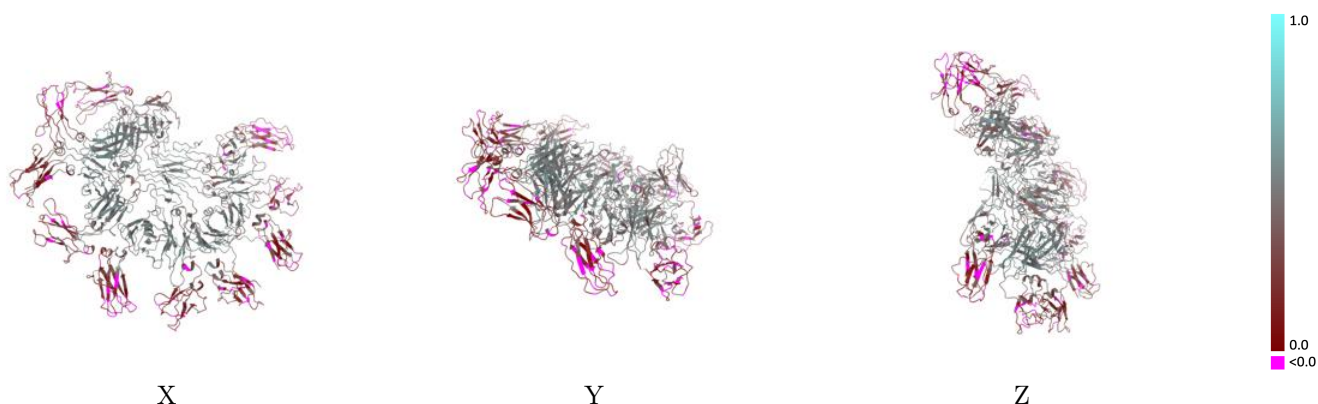
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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.

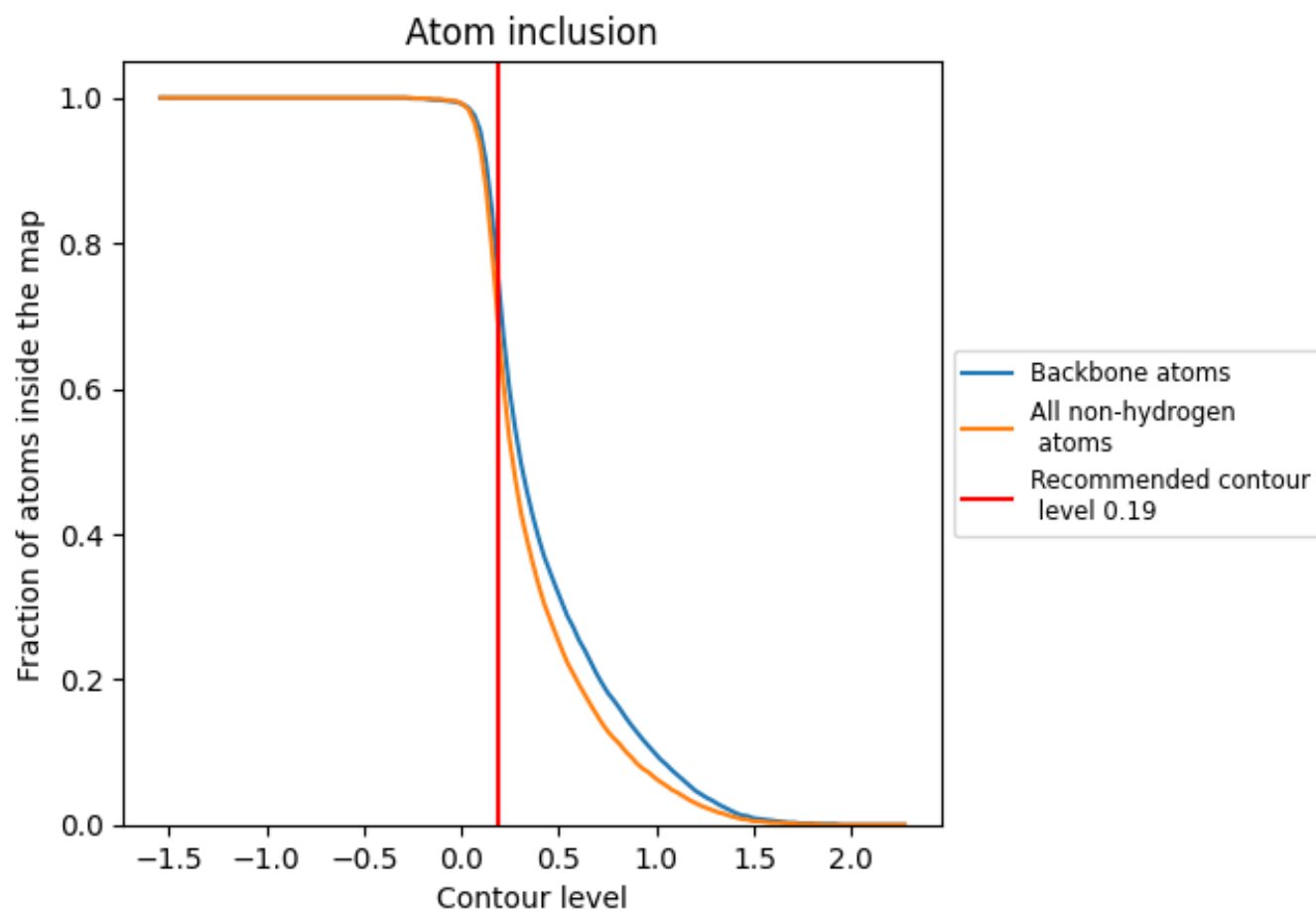
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.19).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6830	<div></div> 0.3670
A	<div></div> 0.6600	<div></div> 0.3460
B	<div></div> 0.7060	<div></div> 0.3700
C	<div></div> 0.7240	<div></div> 0.4040
D	<div></div> 0.6920	<div></div> 0.3820
E	<div></div> 0.6950	<div></div> 0.3590
F	<div></div> 0.6850	<div></div> 0.3660
G	<div></div> 0.6910	<div></div> 0.3680
H	<div></div> 0.7060	<div></div> 0.3640
J	<div></div> 0.8200	<div></div> 0.4610
K	<div></div> 0.6380	<div></div> 0.3290
L	<div></div> 0.5630	<div></div> 0.3100
R	<div></div> 0.6950	<div></div> 0.4200

1.0

0.0

<0.0