



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:09 AM UTC

PDB ID : 7YSG / pdb_00007ysg
EMDB ID : EMD-34074
Title : Cryo-EM structure of human FcmR bound to sIgM
Authors : Li, Y.; Shen, H.; Xiao, J.
Deposited on : 2022-08-12
Resolution : 3.18 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

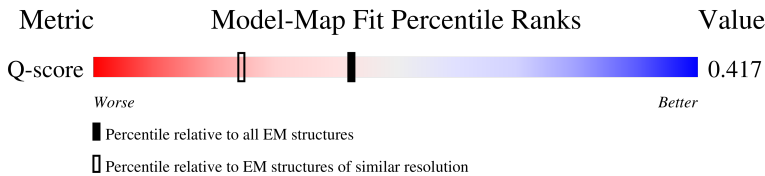
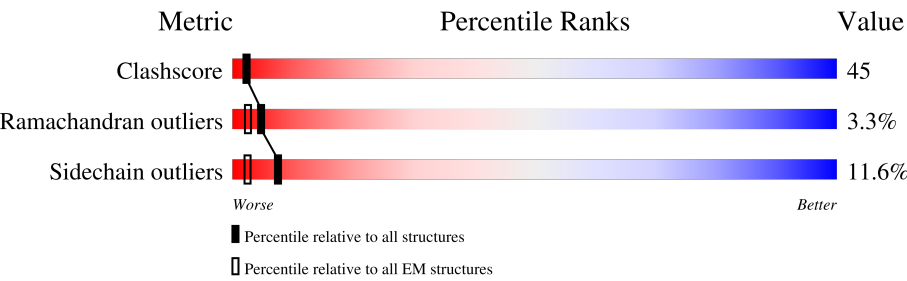
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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	14470 (2.68 - 3.68)

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	232	 22% 41% 36% 18% 5%
1	B	232	 21% 36% 36% 22% . .
1	C	232	 31% 48% 36% 9% 5% .
1	D	232	 23% 56% 34% 5% .

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Mol	Chain	Length	Quality of chain
1	E	232	
1	F	232	
1	G	232	
1	H	232	
1	K	232	
1	L	232	
2	J	136	
3	P	541	
4	R	107	
4	S	107	
4	U	107	
4	V	107	
5	I	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25676 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	231	Total	C	N	O	S	0	0
			1786	1123	303	351	9		
1	B	228	Total	C	N	O	S	0	0
			1769	1114	300	347	8		
1	C	227	Total	C	N	O	S	0	0
			1763	1111	299	345	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	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
1	K	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
1	L	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		

- Molecule 2 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

- Molecule 3 is a protein called Secretory component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	495	Total	C	N	O	S	0	0
			3851	2431	670	731	19		

- Molecule 4 is a protein called Fas apoptotic inhibitory molecule 3.

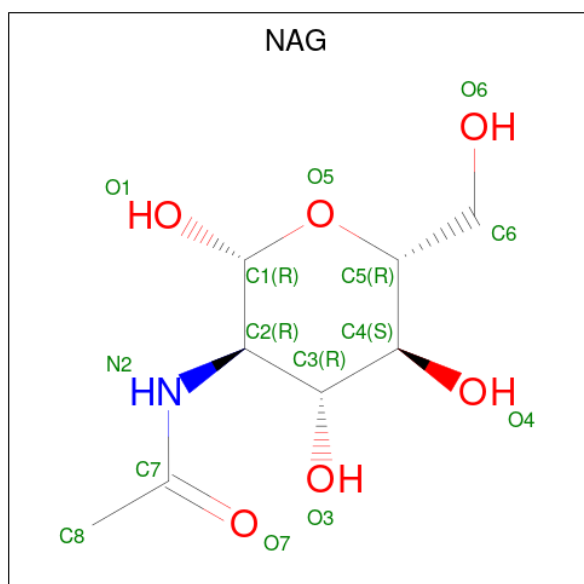
Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	101	Total	C	N	O	S	0	0
			766	480	132	147	7		
4	S	103	Total	C	N	O	S	0	0
			785	492	137	149	7		
4	U	101	Total	C	N	O	S	0	0
			766	480	132	147	7		
4	V	106	Total	C	N	O	S	0	0
			805	504	140	154	7		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	

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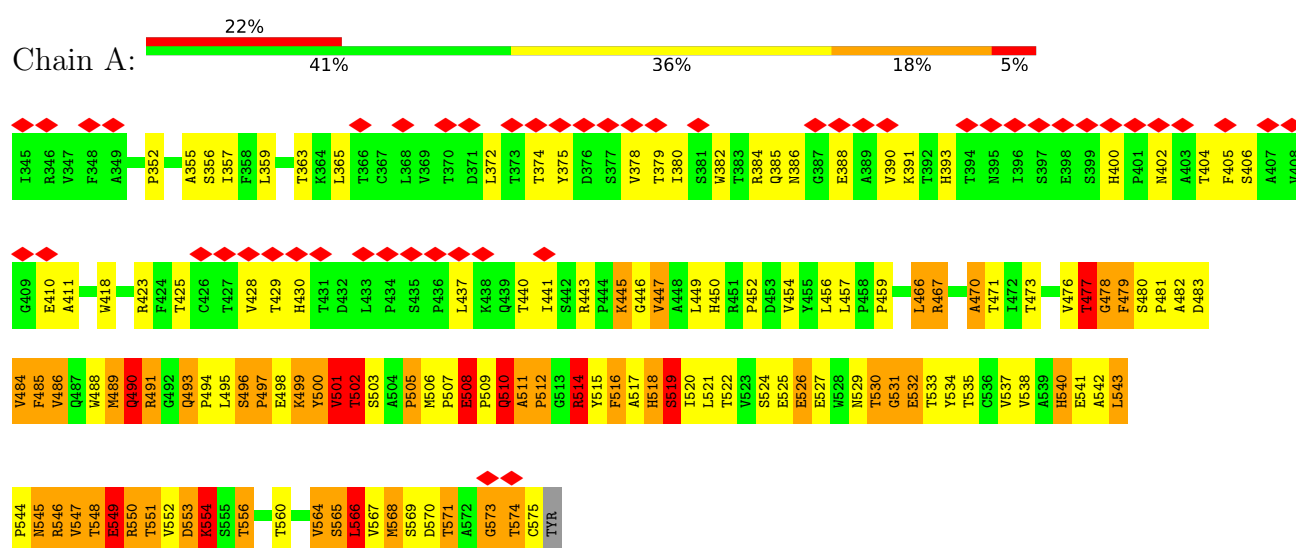
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Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	G	1	Total	C	N	O	0
			15	8	1	6	
6	H	1	Total	C	N	O	0
			14	8	1	5	
6	K	1	Total	C	N	O	0
			14	8	1	5	
6	L	1	Total	C	N	O	0
			14	8	1	5	

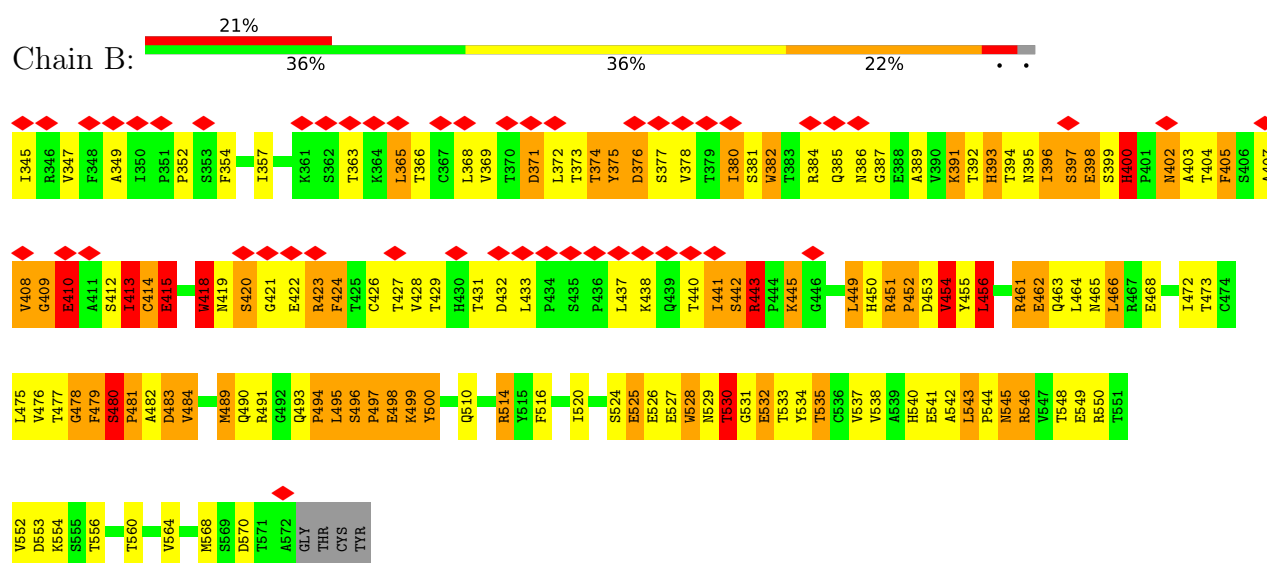
3 Residue-property plots

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.

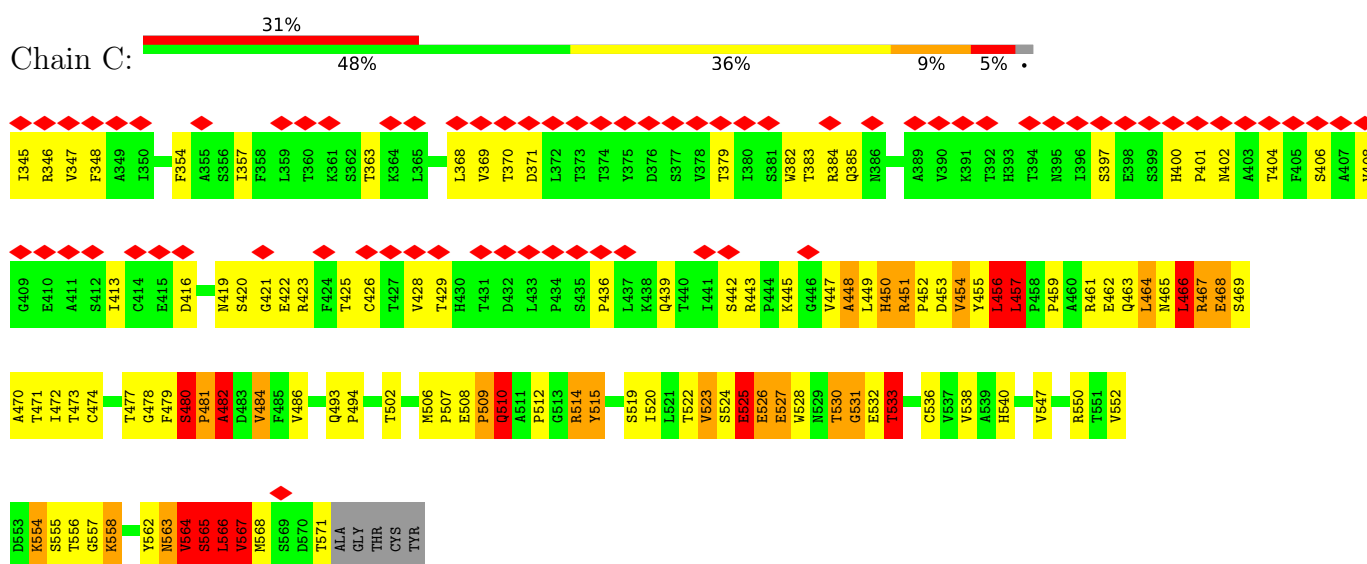
• Molecule 1: Immunoglobulin heavy constant mu



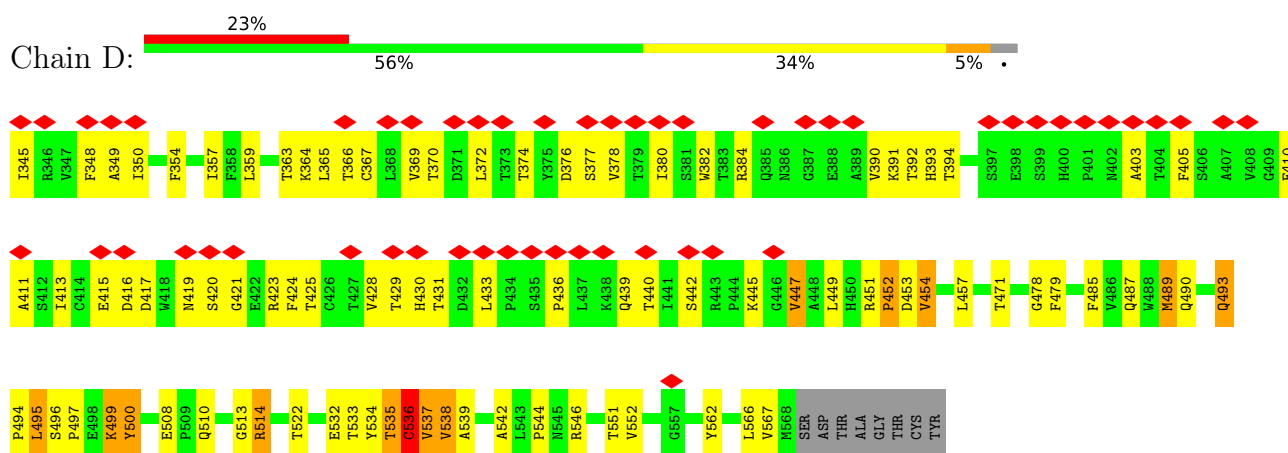
• Molecule 1: Immunoglobulin heavy constant mu



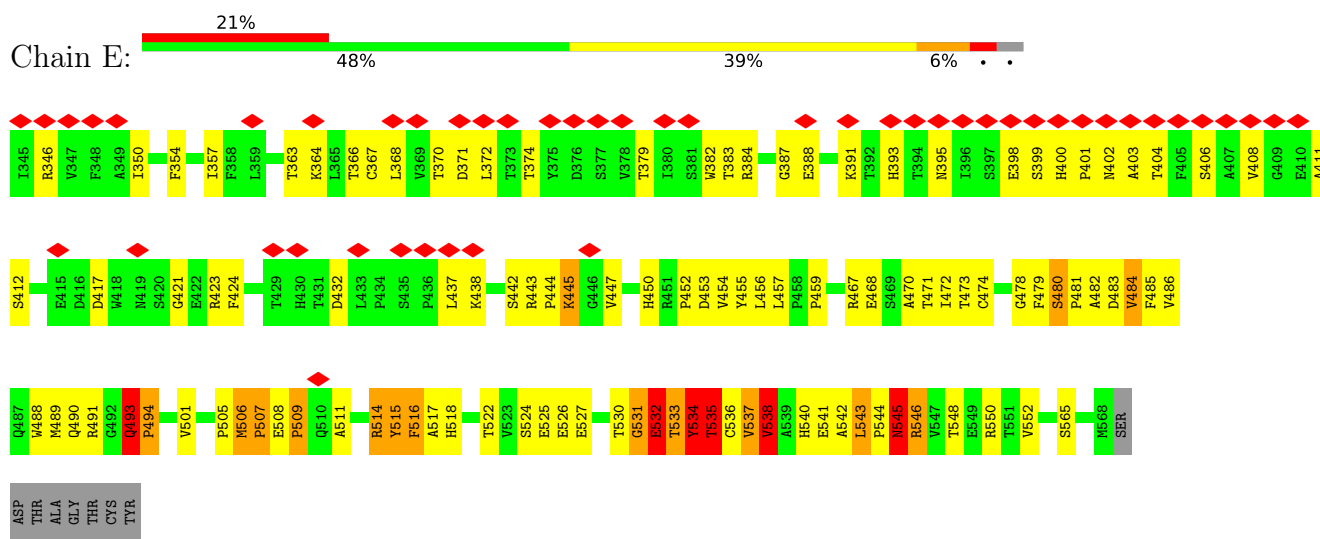
• Molecule 1: Immunoglobulin heavy constant mu



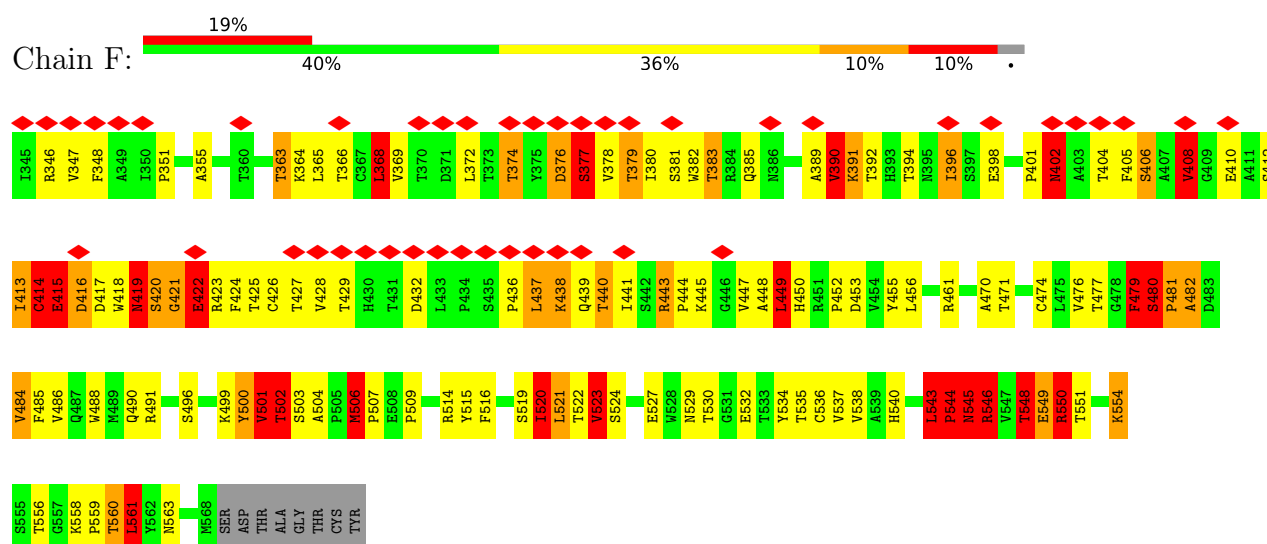
• Molecule 1: Immunoglobulin heavy constant mu



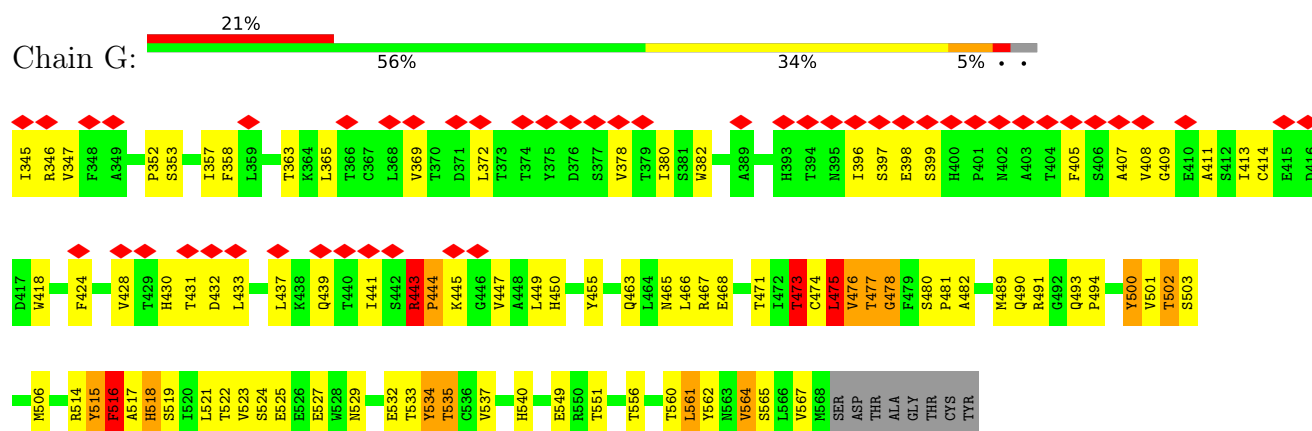
• Molecule 1: Immunoglobulin heavy constant mu



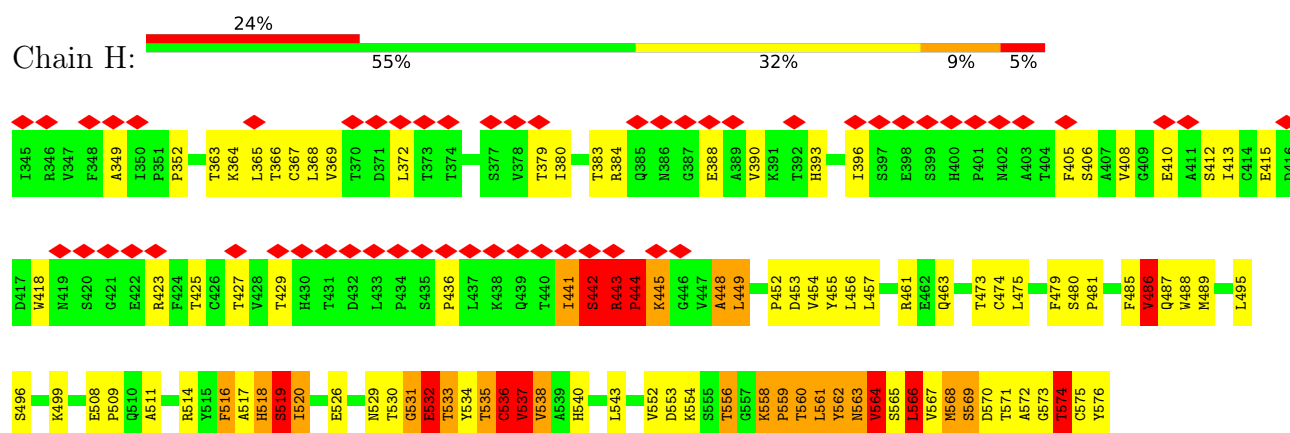
• Molecule 1: Immunoglobulin heavy constant mu



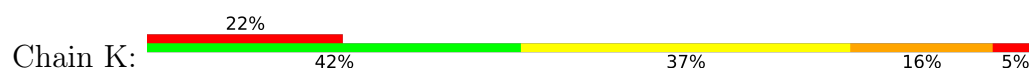
• Molecule 1: Immunoglobulin heavy constant mu

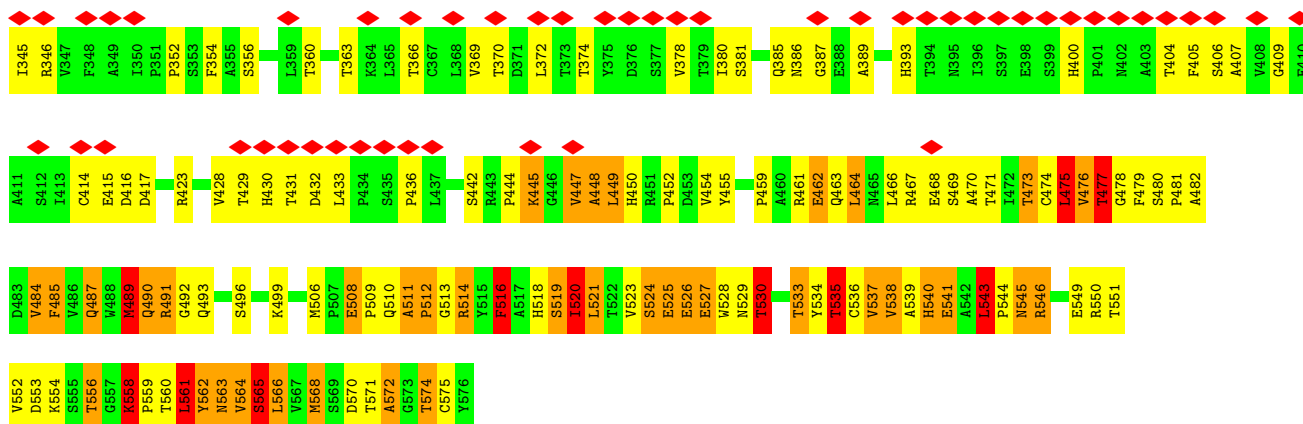


• Molecule 1: Immunoglobulin heavy constant mu

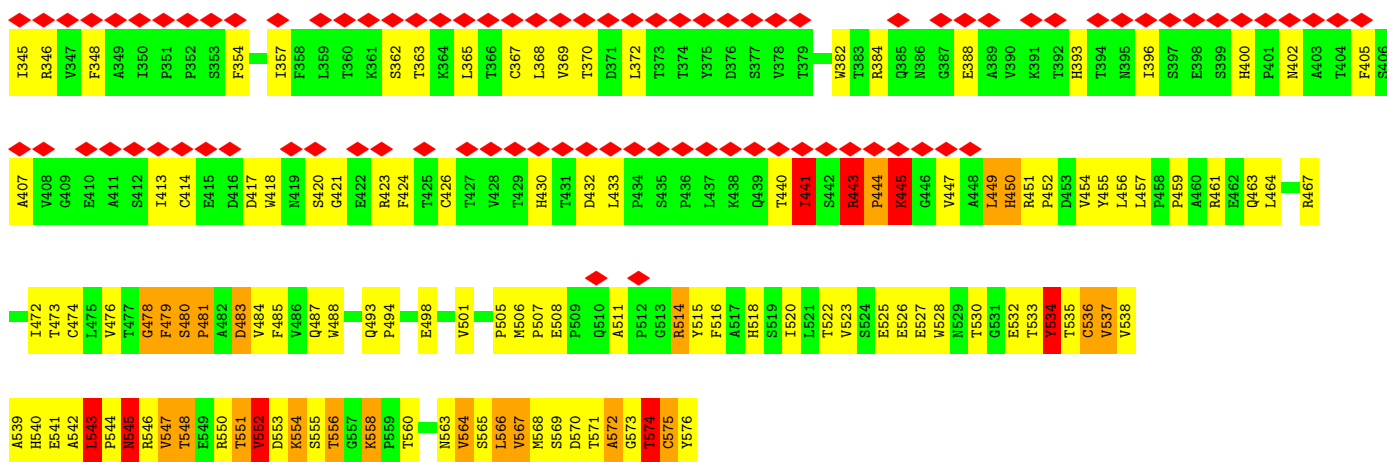
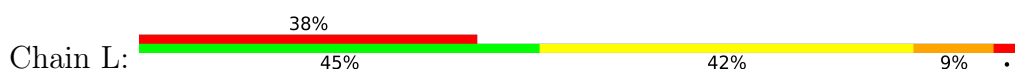


• Molecule 1: Immunoglobulin heavy constant mu

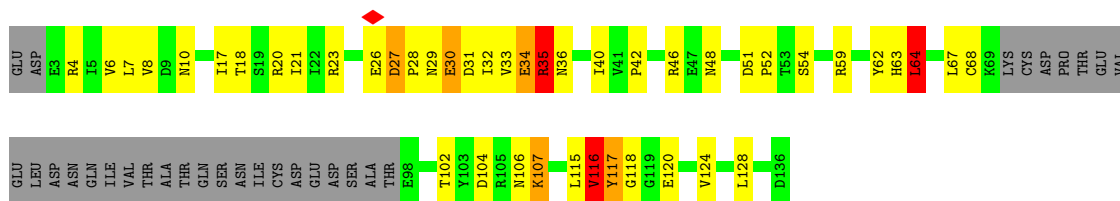




• Molecule 1: Immunoglobulin heavy constant mu

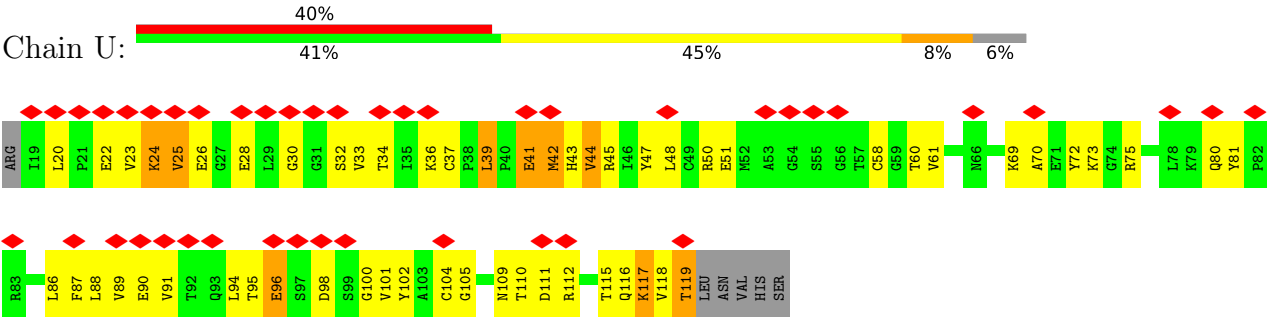


• Molecule 2: Immunoglobulin J chain

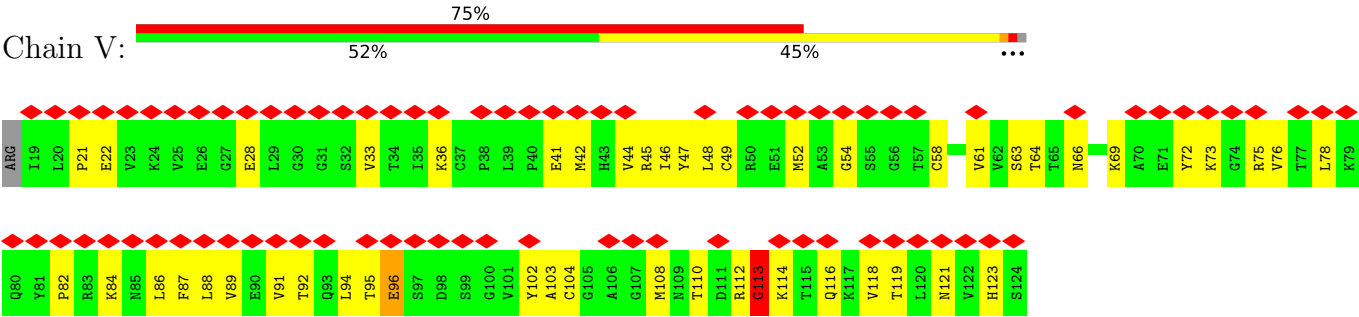


• Molecule 3: Secretory component

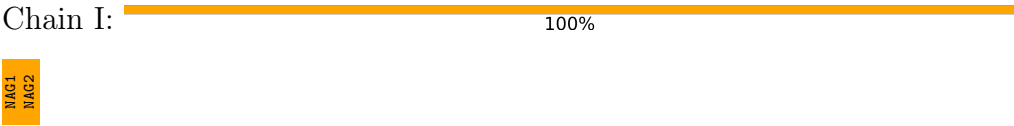




• Molecule 4: Fas apoptotic inhibitory molecule 3



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	297136	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.308	Depositor
Minimum map value	-1.208	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.27	Depositor
Map size ($\text{\AA}$)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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	1.75	61/1831 (3.3%)	1.28	27/2508 (1.1%)
1	B	1.65	53/1814 (2.9%)	1.47	37/2485 (1.5%)
1	C	1.17	18/1808 (1.0%)	1.05	17/2476 (0.7%)
1	D	0.80	9/1788 (0.5%)	0.83	7/2449 (0.3%)
1	E	0.99	20/1788 (1.1%)	1.07	17/2449 (0.7%)
1	F	1.16	21/1788 (1.2%)	1.34	32/2449 (1.3%)
1	G	1.09	25/1787 (1.4%)	0.90	11/2447 (0.4%)
1	H	1.19	26/1844 (1.4%)	0.97	14/2526 (0.6%)
1	K	1.35	34/1844 (1.8%)	1.21	22/2526 (0.9%)
1	L	0.96	13/1844 (0.7%)	1.15	23/2526 (0.9%)
2	J	0.96	8/864 (0.9%)	0.93	8/1173 (0.7%)
3	P	0.75	13/3935 (0.3%)	1.02	34/5333 (0.6%)
4	R	0.44	0/776	0.83	3/1046 (0.3%)
4	S	0.57	0/795	0.92	4/1071 (0.4%)
4	U	0.46	0/776	0.92	4/1046 (0.4%)
4	V	0.30	0/816	0.53	1/1101 (0.1%)
All	All	1.10	301/26098 (1.2%)	1.09	261/35611 (0.7%)

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	3
1	E	0	1
1	H	0	1
3	P	0	2
All	All	0	7

All (301) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	404	GLY	C-N	13.60	1.52	1.33
1	H	536	CYS	C-O	-9.95	1.12	1.24
1	L	567	VAL	C-O	-9.77	1.13	1.24
1	G	562	TYR	C-O	-9.72	1.13	1.23
1	B	477	THR	CA-C	-9.70	1.40	1.52
1	K	564	VAL	C-O	-9.56	1.14	1.24
1	H	537	VAL	C-O	-9.54	1.13	1.24
1	A	477	THR	CA-C	-9.46	1.41	1.52
1	K	475	LEU	C-O	-9.42	1.13	1.24
1	G	475	LEU	C-O	-9.37	1.12	1.24
1	H	517	ALA	C-O	-9.34	1.12	1.23
1	B	455	TYR	C-O	-8.83	1.12	1.24
1	K	565	SER	CA-C	-8.73	1.43	1.53
1	H	487	GLN	C-O	-8.71	1.13	1.23
1	A	516	PHE	C-O	-8.69	1.13	1.24
1	L	565	SER	C-O	-8.68	1.13	1.24
1	A	515	TYR	C-O	-8.65	1.15	1.24
1	G	474	CYS	C-O	-8.64	1.13	1.24
1	L	564	VAL	C-O	-8.54	1.14	1.24
1	H	562	TYR	C-O	-8.53	1.13	1.24
1	K	538	VAL	C-O	-8.44	1.15	1.24
1	F	501	VAL	C-O	-8.43	1.15	1.24
1	K	565	SER	C-O	-8.42	1.13	1.23
1	L	574	THR	C-O	-8.38	1.14	1.23
1	F	548	THR	C-O	-8.31	1.13	1.24
1	H	538	VAL	C-O	-8.18	1.15	1.24
1	C	567	VAL	C-O	-8.18	1.15	1.24
1	H	486	VAL	C-O	-8.14	1.15	1.24
1	C	455	TYR	C-O	-8.10	1.14	1.24
1	G	473	THR	C-O	-8.08	1.14	1.23
1	A	546	ARG	C-O	-8.05	1.13	1.24
1	A	486	VAL	C-O	-8.04	1.14	1.24
1	H	516	PHE	C-O	-7.87	1.14	1.23
1	A	490	GLN	CA-C	-7.86	1.42	1.52
1	F	520	ILE	C-O	-7.78	1.15	1.24
1	A	479	PHE	C-O	-7.78	1.13	1.23
1	H	536	CYS	CA-C	-7.71	1.43	1.52
3	P	59	LYS	C-O	-7.68	1.15	1.23
1	L	574	THR	CA-C	-7.67	1.45	1.53
1	A	485	PHE	C-O	-7.66	1.14	1.24
1	H	564	VAL	C-O	-7.64	1.15	1.24
1	D	535	THR	C-O	-7.63	1.15	1.23
1	H	518	HIS	C-O	-7.62	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	489	MET	CA-C	-7.56	1.43	1.52
1	A	519	SER	C-O	-7.54	1.15	1.24
1	K	519	SER	CA-C	-7.49	1.42	1.52
1	A	550	ARG	C-O	-7.46	1.15	1.24
1	H	520	ILE	C-O	-7.45	1.16	1.24
1	B	484	VAL	C-O	-7.43	1.16	1.24
1	K	475	LEU	CA-C	-7.43	1.44	1.52
1	A	568	MET	C-O	-7.40	1.14	1.23
1	C	456	LEU	CA-C	-7.34	1.44	1.52
1	B	535	THR	C-O	-7.33	1.14	1.23
1	H	519	SER	C-O	-7.31	1.15	1.24
1	F	548	THR	CA-C	-7.29	1.44	1.52
1	C	566	LEU	C-O	-7.29	1.15	1.23
1	F	521	LEU	CA-C	-7.28	1.44	1.52
3	P	56	VAL	C-O	-7.28	1.16	1.23
1	D	536	CYS	C-O	-7.28	1.15	1.24
1	A	479	PHE	CA-C	-7.26	1.43	1.53
1	F	503	SER	C-O	-7.24	1.15	1.23
1	K	539	ALA	CA-C	-7.24	1.44	1.52
1	A	507	PRO	C-O	-7.23	1.14	1.24
2	J	35	ARG	C-O	-7.23	1.14	1.23
1	A	502	THR	CA-C	-7.22	1.43	1.52
1	F	549	GLU	C-O	-7.21	1.14	1.23
1	B	466	LEU	CA-C	-7.18	1.42	1.52
1	A	501	VAL	C-O	-7.14	1.15	1.24
1	B	527	GLU	C-O	-7.13	1.15	1.24
1	F	520	ILE	CA-C	-7.11	1.44	1.52
1	F	500	TYR	C-O	-7.11	1.15	1.23
1	A	549	GLU	CA-C	-7.08	1.43	1.52
1	A	449	LEU	CA-C	-7.05	1.45	1.53
1	B	525	GLU	CA-C	-7.05	1.43	1.52
1	H	517	ALA	CA-C	-7.00	1.44	1.52
1	B	461	ARG	CA-C	-6.99	1.43	1.52
1	G	562	TYR	CA-C	-6.99	1.44	1.52
1	K	537	VAL	CA-CB	-6.98	1.45	1.53
1	L	566	LEU	C-O	-6.96	1.15	1.24
1	G	475	LEU	CA-C	-6.96	1.44	1.52
1	C	565	SER	C-O	-6.94	1.17	1.23
3	P	99	ARG	C-O	-6.94	1.15	1.24
1	B	480	SER	C-O	-6.90	1.15	1.24
1	B	455	TYR	CA-C	-6.87	1.44	1.52
1	C	564	VAL	C-O	-6.86	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	561	LEU	C-O	-6.82	1.15	1.24
1	B	452	PRO	C-O	-6.81	1.16	1.23
1	B	544	PRO	CA-C	-6.79	1.42	1.52
1	F	546	ARG	C-O	-6.77	1.15	1.24
1	B	524	SER	C-O	-6.75	1.15	1.23
1	A	508	GLU	CA-C	-6.72	1.45	1.53
1	A	477	THR	C-O	-6.66	1.15	1.24
1	A	542	ALA	CA-C	-6.65	1.44	1.52
1	B	524	SER	CA-C	-6.62	1.44	1.52
1	B	534	TYR	CA-C	-6.59	1.44	1.52
1	A	496	SER	CA-C	-6.58	1.44	1.53
1	A	515	TYR	CA-CB	-6.57	1.44	1.53
1	D	536	CYS	CA-C	-6.56	1.44	1.52
1	A	542	ALA	C-O	-6.54	1.15	1.24
1	A	506	MET	C-O	-6.53	1.15	1.25
3	P	99	ARG	CA-C	-6.53	1.43	1.52
1	K	566	LEU	C-O	-6.51	1.14	1.23
1	E	518	HIS	C-O	-6.48	1.16	1.23
1	C	493	GLN	C-O	-6.47	1.19	1.25
1	G	503	SER	C-O	-6.47	1.15	1.23
1	A	548	THR	C-O	-6.44	1.15	1.23
1	E	505	PRO	C-O	-6.44	1.16	1.23
1	A	552	VAL	C-O	-6.43	1.17	1.23
1	A	489	MET	CA-C	-6.39	1.45	1.52
1	B	454	VAL	C-O	-6.39	1.17	1.24
1	E	536	CYS	C-O	-6.39	1.16	1.24
1	C	484	VAL	C-O	-6.38	1.17	1.24
1	A	566	LEU	C-O	-6.36	1.16	1.23
1	B	496	SER	CA-C	-6.34	1.45	1.52
1	B	463	GLN	CA-C	-6.33	1.44	1.52
1	B	532	GLU	CA-C	-6.33	1.44	1.52
2	J	62	TYR	C-O	-6.29	1.16	1.24
1	K	564	VAL	CA-C	-6.27	1.45	1.52
1	C	524	SER	CA-C	-6.25	1.45	1.52
1	H	520	ILE	CA-CB	-6.24	1.46	1.54
1	C	479	PHE	CA-C	-6.23	1.45	1.52
1	B	463	GLN	C-O	-6.23	1.15	1.24
1	A	507	PRO	CA-C	-6.22	1.43	1.52
1	B	479	PHE	C-O	-6.20	1.15	1.23
1	D	453	ASP	C-O	-6.20	1.16	1.24
1	G	502	THR	C-O	-6.19	1.16	1.23
1	A	553	ASP	C-O	-6.18	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	486	VAL	C-O	-6.18	1.17	1.24
1	K	473	THR	C-O	-6.18	1.17	1.24
1	A	505	PRO	C-O	-6.17	1.16	1.23
1	B	494	PRO	CA-C	-6.17	1.44	1.52
1	B	483	ASP	CA-C	-6.17	1.46	1.52
1	G	515	TYR	C-O	-6.15	1.17	1.24
1	H	562	TYR	CA-C	-6.15	1.44	1.52
1	B	525	GLU	C-O	-6.14	1.16	1.24
1	L	554	LYS	CA-C	-6.13	1.44	1.52
1	A	517	ALA	C-O	-6.12	1.15	1.24
3	P	40	GLN	N-CA	-6.10	1.38	1.46
1	A	484	VAL	CA-CB	-6.09	1.46	1.55
1	C	515	TYR	CA-CB	-6.09	1.45	1.53
1	K	520	ILE	C-O	-6.08	1.17	1.24
1	A	506	MET	CA-C	-6.08	1.46	1.53
1	C	563	ASN	CG-ND2	-6.08	1.20	1.33
1	K	561	LEU	CA-C	-6.08	1.45	1.52
1	B	495	LEU	CA-C	-6.07	1.45	1.52
1	B	528	TRP	C-O	-6.07	1.16	1.24
1	A	549	GLU	C-O	-6.06	1.16	1.23
3	P	40	GLN	CA-C	-6.06	1.45	1.52
1	A	505	PRO	CA-C	-6.05	1.45	1.52
1	C	455	TYR	CA-C	-6.02	1.45	1.52
1	A	502	THR	C-O	-6.02	1.16	1.23
1	G	533	THR	CA-C	-6.02	1.44	1.52
1	B	480	SER	CA-C	-6.02	1.45	1.52
1	G	518	HIS	C-O	-6.01	1.16	1.23
1	C	456	LEU	C-O	-6.01	1.16	1.24
1	H	563	ASN	C-O	-6.00	1.15	1.24
1	E	518	HIS	CA-C	-6.00	1.45	1.52
1	A	489	MET	C-O	-5.99	1.16	1.24
1	F	481	PRO	CA-C	-5.99	1.45	1.52
1	B	453	ASP	C-O	-5.94	1.16	1.24
1	K	538	VAL	CA-C	-5.93	1.46	1.52
2	J	63	HIS	C-O	-5.92	1.16	1.23
1	G	517	ALA	C-O	-5.92	1.16	1.23
1	H	485	PHE	C-O	-5.90	1.17	1.23
1	L	575	CYS	C-O	-5.90	1.16	1.24
1	C	455	TYR	CB-CG	-5.89	1.38	1.51
1	B	534	TYR	C-O	-5.89	1.17	1.24
1	G	518	HIS	CA-C	-5.89	1.45	1.52
1	B	500	TYR	C-O	-5.88	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	489	MET	CA-C	-5.88	1.45	1.52
1	B	493	GLN	C-O	-5.87	1.17	1.24
1	A	519	SER	CA-C	-5.86	1.45	1.52
1	G	535	THR	C-O	-5.85	1.16	1.23
1	B	465	ASN	C-O	-5.85	1.17	1.24
1	B	527	GLU	CA-C	-5.84	1.45	1.52
1	C	563	ASN	C-O	-5.81	1.15	1.23
1	B	462	GLU	C-O	-5.80	1.16	1.24
1	E	505	PRO	CA-C	-5.80	1.44	1.52
1	L	571	THR	CA-C	-5.77	1.46	1.53
1	G	465	ASN	C-O	-5.77	1.16	1.24
1	K	516	PHE	C-O	-5.76	1.17	1.23
1	K	539	ALA	C-O	-5.76	1.17	1.24
1	A	498	GLU	C-O	-5.75	1.17	1.24
1	E	536	CYS	CA-C	-5.74	1.45	1.52
1	G	561	LEU	C-O	-5.74	1.16	1.24
1	G	500	TYR	C-O	-5.73	1.16	1.23
1	E	533	THR	C-O	-5.72	1.16	1.24
1	L	565	SER	CA-C	-5.72	1.45	1.52
1	K	476	VAL	C-O	-5.71	1.16	1.23
1	B	478	GLY	C-O	-5.71	1.16	1.24
1	G	534	TYR	C-O	-5.70	1.16	1.24
1	A	564	VAL	CA-CB	-5.69	1.46	1.54
1	K	563	ASN	C-O	-5.69	1.16	1.24
1	A	564	VAL	C-O	-5.68	1.17	1.24
1	G	565	SER	CA-C	-5.68	1.45	1.52
1	A	498	GLU	CA-C	-5.68	1.45	1.52
1	K	519	SER	C-O	-5.67	1.16	1.24
1	A	499	LYS	C-O	-5.67	1.16	1.24
1	K	536	CYS	C-O	-5.67	1.17	1.24
1	A	500	TYR	C-O	-5.67	1.16	1.23
1	B	500	TYR	CA-C	-5.66	1.45	1.53
1	E	486	VAL	CA-C	-5.66	1.46	1.52
1	A	485	PHE	CA-C	-5.66	1.46	1.52
1	K	485	PHE	C-O	-5.66	1.17	1.23
1	K	538	VAL	N-CA	-5.66	1.39	1.46
1	B	499	LYS	CA-C	-5.66	1.46	1.52
1	H	534	TYR	C-O	-5.65	1.16	1.24
1	D	452	PRO	C-O	-5.65	1.17	1.23
1	F	521	LEU	C-O	-5.65	1.17	1.24
1	G	534	TYR	CA-C	-5.64	1.45	1.52
1	E	485	PHE	C-O	-5.64	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	520	ILE	CA-CB	-5.64	1.47	1.54
1	E	507	PRO	C-O	-5.61	1.16	1.24
1	L	575	CYS	CA-C	-5.61	1.45	1.52
1	F	480	SER	C-O	-5.61	1.17	1.24
1	A	569	SER	C-O	-5.61	1.16	1.23
1	H	443	ARG	N-CA	5.61	1.54	1.46
1	K	562	TYR	CA-CB	-5.60	1.45	1.53
3	P	100	GLY	CA-C	-5.59	1.44	1.51
1	G	474	CYS	CA-C	-5.58	1.44	1.52
1	B	466	LEU	C-O	-5.57	1.17	1.24
1	D	454	VAL	C-O	-5.56	1.16	1.23
2	J	34	GLU	CA-CB	-5.54	1.45	1.53
2	J	33	VAL	CA-CB	-5.53	1.47	1.54
1	K	564	VAL	CA-CB	-5.53	1.47	1.54
1	E	538	VAL	C-O	-5.52	1.17	1.24
1	F	550	ARG	C-O	-5.52	1.17	1.23
1	G	533	THR	C-O	-5.51	1.17	1.24
1	C	469	SER	C-O	-5.50	1.17	1.23
1	A	541	GLU	CA-C	-5.50	1.44	1.52
1	K	487	GLN	C-O	-5.50	1.17	1.23
1	K	527	GLU	C-O	-5.50	1.17	1.24
1	B	464	LEU	C-O	-5.49	1.17	1.24
1	E	506	MET	C-O	-5.49	1.17	1.24
1	B	452	PRO	CA-C	-5.49	1.45	1.52
1	A	514	ARG	C-O	-5.48	1.16	1.23
1	B	461	ARG	C-O	-5.48	1.17	1.24
1	A	547	VAL	C-O	-5.47	1.17	1.23
1	A	490	GLN	C-O	-5.47	1.17	1.24
3	P	404	GLY	C-O	-5.46	1.18	1.24
1	H	519	SER	CA-C	-5.43	1.46	1.52
1	K	525	GLU	C-O	-5.42	1.17	1.24
1	B	491	ARG	CA-C	-5.41	1.48	1.53
1	K	524	SER	CA-C	-5.40	1.45	1.52
1	F	479	PHE	CA-C	-5.39	1.45	1.52
1	F	549	GLU	CA-C	-5.38	1.46	1.52
1	H	566	LEU	C-O	-5.38	1.17	1.24
1	D	537	VAL	C-O	-5.38	1.17	1.24
1	A	503	SER	C-O	-5.37	1.17	1.24
1	B	477	THR	C-O	-5.35	1.18	1.23
1	A	568	MET	CA-CB	-5.35	1.45	1.53
3	P	40	GLN	C-O	-5.35	1.17	1.24
1	H	443	ARG	CA-C	-5.34	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	561	LEU	C-O	-5.34	1.17	1.24
1	L	572	ALA	CA-C	-5.33	1.45	1.52
1	K	540	HIS	CA-C	-5.33	1.45	1.52
1	E	518	HIS	C-N	-5.29	1.26	1.33
1	K	534	TYR	C-O	-5.29	1.17	1.24
1	H	561	LEU	C-O	-5.29	1.17	1.24
1	E	532	GLU	C-O	-5.28	1.20	1.23
1	G	476	VAL	C-O	-5.28	1.15	1.23
1	A	511	ALA	C-O	-5.27	1.18	1.24
1	G	516	PHE	C-O	-5.27	1.17	1.23
1	F	481	PRO	C-O	-5.26	1.17	1.23
1	E	535	THR	C-O	-5.25	1.16	1.23
1	D	489	MET	CA-C	-5.25	1.46	1.52
1	E	484	VAL	C-O	-5.24	1.18	1.23
1	H	518	HIS	CA-C	-5.24	1.46	1.53
1	E	546	ARG	C-O	-5.23	1.17	1.24
1	A	478	GLY	C-O	-5.22	1.16	1.24
1	G	564	VAL	C-O	-5.21	1.18	1.24
1	B	482	ALA	C-O	-5.20	1.17	1.24
1	E	517	ALA	C-O	-5.18	1.17	1.23
1	H	535	THR	C-O	-5.18	1.17	1.23
1	B	534	TYR	CA-CB	-5.16	1.44	1.53
2	J	34	GLU	C-O	-5.16	1.17	1.23
1	L	573	GLY	C-O	-5.16	1.17	1.23
1	B	533	THR	C-O	-5.16	1.17	1.23
1	A	551	THR	C-O	-5.15	1.17	1.23
1	A	565	SER	C-O	-5.14	1.17	1.24
1	B	484	VAL	CA-CB	-5.13	1.48	1.54
1	B	466	LEU	N-CA	-5.12	1.39	1.46
1	A	486	VAL	CA-CB	-5.11	1.48	1.54
1	C	523	VAL	N-CA	-5.11	1.40	1.46
1	A	541	GLU	C-O	-5.11	1.16	1.24
1	E	516	PHE	C-O	-5.11	1.17	1.23
1	D	500	TYR	CA-C	-5.09	1.46	1.52
1	B	528	TRP	CA-C	-5.09	1.45	1.52
2	J	116	VAL	C-O	-5.07	1.18	1.23
3	P	98	SER	CA-C	-5.07	1.44	1.52
1	A	470	ALA	CA-C	-5.06	1.46	1.52
1	F	549	GLU	CA-CB	-5.05	1.45	1.53
1	B	489	MET	C-O	-5.04	1.17	1.23
1	B	545	ASN	CA-CB	-5.03	1.46	1.53
3	P	100	GLY	C-O	-5.02	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	550	ARG	CA-C	-5.02	1.46	1.52
2	J	35	ARG	CA-CB	-5.01	1.44	1.53
1	K	535	THR	C-O	-5.00	1.17	1.23
3	P	289	SER	CA-C	-5.00	1.48	1.53
1	B	454	VAL	CA-C	-5.00	1.46	1.52
1	F	506	MET	C-O	-5.00	1.17	1.24

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	493	GLN	CA-C-N	18.52	142.99	119.84
1	E	493	GLN	C-N-CA	18.52	142.99	119.84
1	L	551	THR	N-CA-C	16.42	136.17	109.40
3	P	404	GLY	CA-C-N	14.64	149.50	121.54
3	P	404	GLY	C-N-CA	14.64	149.50	121.54
1	B	496	SER	CA-C-N	14.20	137.59	119.84
1	B	496	SER	C-N-CA	14.20	137.59	119.84
1	L	552	VAL	N-CA-C	13.67	125.56	108.06
1	L	543	LEU	CA-C-N	13.02	134.16	119.32
1	L	543	LEU	C-N-CA	13.02	134.16	119.32
1	F	558	LYS	CA-C-N	12.77	135.81	119.84
1	F	558	LYS	C-N-CA	12.77	135.81	119.84
1	C	564	VAL	CB-CA-C	-12.39	97.57	111.45
1	F	448	ALA	N-CA-C	12.32	126.76	112.72
1	B	414	CYS	N-CA-C	12.04	129.35	109.24
1	A	480	SER	C-N-CD	-11.81	94.61	120.60
1	E	537	VAL	N-CA-C	11.42	122.64	106.53
1	K	543	LEU	CA-C-N	11.25	133.91	119.84
1	K	543	LEU	C-N-CA	11.25	133.91	119.84
3	P	272	ALA	CA-C-N	11.18	131.46	119.05
3	P	272	ALA	C-N-CA	11.18	131.46	119.05
1	K	477	THR	N-CA-C	11.18	126.63	108.41
1	L	552	VAL	CB-CA-C	-11.12	94.68	111.80
1	K	537	VAL	N-CA-C	11.06	124.31	106.72
1	G	443	ARG	CA-C-N	11.06	133.67	119.84
1	G	443	ARG	C-N-CA	11.06	133.67	119.84
1	A	493	GLN	CA-C-N	11.03	133.63	119.84
1	A	493	GLN	C-N-CA	11.03	133.63	119.84
3	P	404	GLY	CA-C-O	-10.82	106.23	120.29
1	F	506	MET	CA-C-N	10.59	133.08	119.84
1	F	506	MET	C-N-CA	10.59	133.08	119.84
1	D	496	SER	CA-C-N	10.31	132.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	496	SER	C-N-CA	10.31	132.73	119.84
3	P	448	VAL	CA-C-N	9.86	130.64	119.99
3	P	448	VAL	C-N-CA	9.86	130.64	119.99
1	C	493	GLN	CA-C-N	9.80	132.09	119.84
1	C	493	GLN	C-N-CA	9.80	132.09	119.84
1	A	480	SER	CA-C-N	9.78	150.47	127.00
1	A	480	SER	C-N-CA	9.78	150.47	127.00
1	B	479	PHE	N-CA-C	9.71	123.16	110.43
1	A	498	GLU	N-CA-C	-9.60	99.69	111.40
4	S	39	LEU	CA-C-N	9.54	131.76	119.84
4	S	39	LEU	C-N-CA	9.54	131.76	119.84
1	A	511	ALA	CA-C-N	9.52	131.74	119.84
1	A	511	ALA	C-N-CA	9.52	131.74	119.84
1	E	533	THR	N-CA-C	9.39	130.80	110.80
1	F	543	LEU	CA-C-N	9.18	131.31	119.84
1	F	543	LEU	C-N-CA	9.18	131.31	119.84
1	L	533	THR	N-CA-C	9.17	123.72	112.54
1	F	414	CYS	N-CA-C	9.12	124.29	112.26
4	R	66	ASN	N-CA-C	8.90	129.76	110.80
1	F	417	ASP	N-CA-C	-8.78	99.94	113.02
1	F	406	SER	N-CA-C	-8.73	100.31	112.45
1	B	381	SER	N-CA-C	-8.73	93.68	107.73
1	B	385	GLN	N-CA-C	-8.68	101.82	111.28
1	K	449	LEU	N-CA-C	8.64	129.21	110.80
1	H	443	ARG	N-CA-CB	8.55	125.60	110.37
1	A	530	THR	N-CA-C	-8.51	101.95	111.14
1	L	443	ARG	CA-C-N	8.49	130.45	119.84
1	L	443	ARG	C-N-CA	8.49	130.45	119.84
1	B	514	ARG	N-CA-C	8.48	121.26	110.33
1	C	480	SER	CA-C-N	8.38	130.32	119.84
1	C	480	SER	C-N-CA	8.38	130.32	119.84
1	E	543	LEU	CA-C-N	8.37	130.30	119.84
1	E	543	LEU	C-N-CA	8.37	130.30	119.84
1	G	478	GLY	N-CA-C	8.32	132.90	113.18
1	K	566	LEU	N-CA-C	8.27	123.46	108.17
1	A	506	MET	CA-C-N	8.26	130.17	119.84
1	A	506	MET	C-N-CA	8.26	130.17	119.84
1	D	493	GLN	CA-C-N	8.21	130.10	119.84
1	D	493	GLN	C-N-CA	8.21	130.10	119.84
1	A	479	PHE	N-CA-C	8.07	120.95	110.53
1	L	564	VAL	CB-CA-C	-8.00	99.42	111.33
1	B	443	ARG	N-CA-C	-7.98	94.33	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	LYS	N-CA-C	-7.92	102.58	112.72
1	B	418	TRP	N-CA-C	-7.86	94.05	110.80
4	U	24	LYS	N-CA-C	7.82	121.33	107.80
1	K	537	VAL	CB-CA-C	-7.72	101.98	111.32
1	A	496	SER	CA-C-N	7.66	129.42	119.84
1	A	496	SER	C-N-CA	7.66	129.42	119.84
2	J	34	GLU	N-CA-C	7.63	121.69	110.17
1	G	476	VAL	N-CA-CB	-7.45	104.14	111.89
3	P	58	SER	N-CA-C	-7.35	103.20	111.14
1	K	564	VAL	CB-CA-C	-7.32	99.66	111.59
1	B	398	GLU	N-CA-C	7.30	120.41	110.55
1	B	400	HIS	N-CA-C	7.30	121.03	109.64
1	A	554	LYS	N-CA-C	7.30	126.34	110.80
2	J	118	GLY	N-CA-C	-7.29	95.91	113.18
1	H	441	ILE	CA-C-N	7.27	135.43	121.54
1	H	441	ILE	C-N-CA	7.27	135.43	121.54
3	P	448	VAL	N-CA-C	7.26	124.57	108.88
1	D	538	VAL	CB-CA-C	-7.18	100.00	110.63
1	F	428	VAL	N-CA-C	7.15	118.16	107.51
1	K	473	THR	N-CA-C	7.11	120.67	108.02
1	K	566	LEU	N-CA-CB	-7.08	100.41	110.46
1	C	482	ALA	N-CA-C	7.08	125.87	110.80
1	A	445	LYS	N-CA-C	7.05	118.94	110.19
1	K	476	VAL	N-CA-CB	-7.02	103.18	111.60
1	H	448	ALA	N-CA-C	-7.01	102.02	108.75
1	E	534	TYR	N-CA-C	6.97	125.65	110.80
1	F	520	ILE	CB-CA-C	-6.95	100.47	110.83
1	G	565	SER	N-CA-C	-6.94	99.94	110.14
1	F	419	ASN	N-CA-C	-6.94	96.02	110.80
1	L	572	ALA	N-CA-C	-6.92	96.06	110.80
1	H	443	ARG	CA-C-N	6.88	128.44	119.84
1	H	443	ARG	C-N-CA	6.88	128.44	119.84
1	K	476	VAL	N-CA-C	6.88	117.33	106.88
1	A	486	VAL	CB-CA-C	-6.86	101.52	110.84
1	B	543	LEU	CA-C-N	6.81	128.35	119.84
1	B	543	LEU	C-N-CA	6.81	128.35	119.84
1	E	546	ARG	N-CA-C	6.77	125.23	110.80
1	B	493	GLN	CA-C-N	6.76	126.52	119.76
1	B	493	GLN	C-N-CA	6.76	126.52	119.76
1	A	447	VAL	CB-CA-C	-6.76	100.20	111.29
3	P	404	GLY	N-CA-C	6.76	123.34	113.48
1	K	546	ARG	N-CA-C	6.74	123.97	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	563	ASN	CB-CA-C	6.74	121.48	111.17
1	G	476	VAL	N-CA-C	6.73	117.16	106.32
1	G	477	THR	N-CA-C	6.72	119.62	110.35
1	F	394	THR	N-CA-C	-6.69	99.40	110.17
1	A	556	THR	N-CA-C	-6.68	104.77	113.12
1	B	371	ASP	N-CA-C	6.67	120.74	112.47
3	P	532	HIS	N-CA-C	-6.66	103.72	110.97
1	B	409	GLY	N-CA-C	-6.65	97.41	113.18
1	C	525	GLU	N-CA-C	6.63	124.93	110.80
1	B	397	SER	N-CA-C	6.62	119.07	110.53
1	B	382	TRP	N-CA-C	-6.60	96.31	107.99
3	P	353	CYS	CB-CA-C	-6.60	103.64	110.17
1	B	415	GLU	N-CA-C	6.54	124.74	110.80
1	K	527	GLU	N-CA-C	-6.54	104.07	111.14
1	H	520	ILE	CB-CA-C	-6.54	100.95	110.63
2	J	33	VAL	CB-CA-C	-6.53	102.81	110.91
3	P	447	LYS	N-CA-C	6.52	119.57	109.60
1	F	504	ALA	CA-C-N	6.51	126.49	119.78
1	F	504	ALA	C-N-CA	6.51	126.49	119.78
1	L	547	VAL	CB-CA-C	-6.51	105.62	111.74
3	P	99	ARG	N-CA-C	6.50	123.81	114.39
1	F	482	ALA	N-CA-C	6.49	119.81	108.52
1	L	537	VAL	N-CA-C	6.47	117.23	108.17
1	F	449	LEU	N-CA-C	6.45	124.53	110.80
1	H	564	VAL	CB-CA-C	-6.44	100.72	111.29
1	C	449	LEU	N-CA-C	6.41	117.89	107.32
1	A	505	PRO	CA-C-O	-6.41	114.38	121.23
1	L	545	ASN	O-C-N	6.38	129.72	122.20
3	P	310	HIS	N-CA-C	-6.38	97.22	110.80
1	E	493	GLN	N-CA-C	6.30	118.38	108.55
1	B	525	GLU	N-CA-C	6.28	118.93	111.71
1	D	452	PRO	CB-CA-C	-6.27	101.95	110.60
1	B	432	ASP	N-CA-C	-6.23	105.50	113.23
3	P	57	SER	N-CA-C	6.22	124.05	110.80
1	F	479	PHE	N-CA-CB	6.20	119.10	110.17
1	F	379	THR	N-CA-C	6.20	119.20	109.96
3	P	311	SER	N-CA-C	6.20	124.00	110.80
1	B	375	TYR	N-CA-C	-6.12	97.76	110.80
1	F	479	PHE	N-CA-C	6.12	119.13	110.50
1	E	532	GLU	N-CA-C	6.10	121.75	113.21
3	P	480	TRP	N-CA-C	6.10	118.55	109.59
4	U	95	THR	N-CA-C	-6.08	104.93	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	27	ASP	CA-C-N	6.07	127.40	120.85
2	J	27	ASP	C-N-CA	6.07	127.40	120.85
2	J	34	GLU	CB-CA-C	-6.01	99.57	111.60
1	G	473	THR	N-CA-C	5.98	121.18	107.48
1	K	530	THR	N-CA-C	-5.97	104.46	110.97
1	L	558	LYS	CA-C-N	5.94	126.44	120.14
1	L	558	LYS	C-N-CA	5.94	126.44	120.14
1	K	558	LYS	CA-C-N	5.93	125.95	119.90
1	K	558	LYS	C-N-CA	5.93	125.95	119.90
2	J	116	VAL	CB-CA-C	-5.92	104.84	111.23
1	C	467	ARG	N-CA-C	5.89	123.34	110.80
1	A	514	ARG	CB-CA-C	-5.89	99.88	110.36
1	F	502	THR	N-CA-C	5.87	117.97	108.41
1	H	538	VAL	CB-CA-C	-5.86	102.10	110.83
3	P	353	CYS	N-CA-C	5.82	119.16	108.69
1	H	532	GLU	N-CA-C	5.81	118.86	109.86
4	S	99	SER	N-CA-C	5.80	118.12	109.59
1	K	538	VAL	CB-CA-C	-5.79	103.57	111.33
1	E	515	TYR	CB-CA-C	-5.78	102.00	113.45
1	B	481	PRO	N-CA-C	-5.75	100.62	112.47
1	K	519	SER	N-CA-C	-5.74	98.58	110.80
1	G	478	GLY	CA-C-N	5.73	131.09	123.00
1	G	478	GLY	C-N-CA	5.73	131.09	123.00
1	G	518	HIS	CB-CA-C	-5.71	98.04	109.35
1	F	560	THR	N-CA-C	5.70	122.95	110.80
1	E	531	GLY	N-CA-C	-5.68	99.73	113.18
1	F	398	GLU	N-CA-C	5.67	118.91	110.52
1	A	510	GLN	N-CA-C	5.66	119.39	111.30
3	P	398	LEU	N-CA-C	5.66	117.23	110.44
1	F	366	THR	N-CA-C	5.65	117.60	108.34
1	A	477	THR	CB-CA-C	-5.64	98.59	109.37
1	B	483	ASP	N-CA-C	-5.64	97.80	107.61
1	C	531	GLY	N-CA-C	5.64	126.54	113.18
3	P	288	GLY	N-CA-C	-5.62	99.86	113.18
1	K	448	ALA	N-CA-C	5.62	115.98	108.23
3	P	277	GLY	CA-C-N	5.62	132.27	121.54
3	P	277	GLY	C-N-CA	5.62	132.27	121.54
1	A	489	MET	CB-CG-SD	-5.60	95.89	112.70
1	F	402	ASN	N-CA-C	-5.58	103.61	110.65
1	L	553	ASP	O-C-N	5.58	129.38	123.42
1	B	489	MET	CB-CA-C	-5.57	98.64	109.68
1	K	536	CYS	N-CA-CB	-5.56	101.18	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	486	VAL	CB-CA-C	-5.55	102.38	110.81
3	P	537	THR	N-CA-C	5.55	118.72	109.96
1	L	483	ASP	N-CA-C	5.54	122.60	110.80
1	F	415	GLU	N-CA-C	5.52	122.55	110.80
4	U	39	LEU	CA-C-N	5.50	125.17	119.56
4	U	39	LEU	C-N-CA	5.50	125.17	119.56
1	H	442	SER	N-CA-C	5.49	122.50	110.80
4	V	113	GLY	N-CA-C	5.49	126.19	113.18
2	J	64	LEU	N-CA-C	5.48	122.48	110.80
1	E	537	VAL	CB-CA-C	-5.48	105.23	111.59
1	H	533	THR	N-CA-C	5.47	119.96	112.68
1	L	440	THR	O-C-N	5.46	129.45	123.22
3	P	9	GLU	CB-CA-C	-5.46	104.66	111.43
3	P	476	TYR	N-CA-C	5.46	118.16	109.81
3	P	156	VAL	N-CA-C	-5.45	102.02	109.37
1	F	422	GLU	CB-CA-C	-5.44	107.60	114.40
1	C	566	LEU	CB-CA-C	-5.42	100.59	109.53
3	P	413	LEU	N-CA-C	5.39	122.28	110.80
3	P	361	LYS	N-CA-C	5.37	118.07	110.50
1	B	365	LEU	N-CA-C	5.37	118.91	107.70
1	E	538	VAL	N-CA-C	5.37	120.50	109.34
3	P	407	THR	CB-CA-C	-5.36	103.62	111.23
1	B	452	PRO	CA-C-O	-5.35	114.89	121.31
1	B	494	PRO	CB-CA-C	-5.35	104.10	111.21
1	E	545	ASN	N-CA-C	-5.33	104.05	110.44
1	A	540	HIS	O-C-N	-5.32	117.10	123.27
1	F	484	VAL	N-CA-CB	-5.32	101.70	111.91
1	L	440	THR	CA-C-N	5.31	131.53	121.97
1	L	440	THR	C-N-CA	5.31	131.53	121.97
1	H	564	VAL	N-CA-C	5.31	120.38	109.34
4	R	20	LEU	CA-C-N	5.27	126.43	119.84
4	R	20	LEU	C-N-CA	5.27	126.43	119.84
1	A	526	GLU	O-C-N	5.25	127.69	122.12
3	P	60	TYR	N-CA-CB	5.25	120.10	112.28
1	B	477	THR	CB-CA-C	-5.24	100.48	109.65
1	A	486	VAL	N-CA-C	5.24	115.85	108.36
3	P	431	TRP	N-CA-C	-5.23	101.94	110.20
1	B	373	THR	N-CA-C	5.21	117.44	110.35
1	E	533	THR	CA-C-O	-5.21	113.06	120.51
1	C	533	THR	CB-CA-C	5.20	118.93	110.24
1	B	414	CYS	CA-CB-SG	-5.20	102.44	114.40
1	C	454	VAL	CB-CA-C	-5.20	102.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	THR	N-CA-C	-5.19	106.53	112.92
4	S	97	SER	N-CA-C	-5.17	98.49	107.49
1	L	445	LYS	N-CA-C	-5.17	106.82	113.23
1	D	452	PRO	CA-C-O	-5.16	115.72	122.12
3	P	344	VAL	N-CA-C	5.16	116.34	109.37
1	F	368	LEU	N-CA-C	-5.14	102.03	109.59
1	C	524	SER	N-CA-C	-5.12	99.92	108.32
1	K	473	THR	CB-CA-C	-5.12	102.89	110.62
1	C	566	LEU	N-CA-C	5.08	118.50	109.96
1	F	545	ASN	N-CA-C	-5.06	104.37	110.44
1	B	452	PRO	CB-CA-C	-5.05	104.49	111.21
1	L	567	VAL	N-CA-C	5.05	116.19	109.37
1	B	402	ASN	N-CA-C	-5.04	106.72	112.92
1	F	408	VAL	N-CA-C	5.02	116.43	109.45
3	P	9	GLU	N-CA-C	5.01	115.72	107.20
1	B	456	LEU	N-CA-CB	-5.01	102.70	110.57
1	C	457	LEU	CA-C-N	5.01	125.54	120.38
1	C	457	LEU	C-N-CA	5.01	125.54	120.38
1	L	575	CYS	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	452	PRO	Mainchain
1	C	464	LEU	Mainchain
1	C	480	SER	Peptide
1	E	480	SER	Peptide
1	H	441	ILE	Mainchain
3	P	376	ARG	Mainchain
3	P	400	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1786	0	1741	177	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1769	0	1729	167	0
1	C	1763	0	1724	140	0
1	D	1743	0	1708	95	0
1	E	1743	0	1710	143	0
1	F	1743	0	1706	154	0
1	G	1742	0	1709	93	0
1	H	1798	0	1751	108	0
1	K	1798	0	1753	200	0
1	L	1798	0	1751	274	0
2	J	851	0	842	82	0
3	P	3851	0	3755	535	0
4	R	766	0	784	93	0
4	S	785	0	808	93	0
4	U	766	0	784	60	0
4	V	805	0	821	53	0
5	I	28	0	25	6	0
6	A	14	0	13	1	0
6	B	14	0	13	1	0
6	C	14	0	13	2	0
6	D	14	0	13	0	0
6	E	14	0	13	1	0
6	F	14	0	13	1	0
6	G	15	0	15	0	0
6	H	14	0	13	3	0
6	K	14	0	13	4	0
6	L	14	0	13	0	0
All	All	25676	0	25233	2288	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 45.

All (2288) 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:F:482:ALA:HB2	1:F:515:TYR:CD2	1.29	1.63
4:R:20:LEU:HD21	4:R:117:LYS:CG	1.17	1.62
1:A:359:LEU:HD12	2:J:117:TYR:CD2	1.09	1.58
4:R:20:LEU:CD2	4:R:117:LYS:HG3	1.16	1.57
3:P:395:LEU:CD1	3:P:410:LEU:HD13	1.29	1.56
1:L:540:HIS:CB	1:L:543:LEU:HD21	1.18	1.56
3:P:395:LEU:HD13	3:P:410:LEU:CD1	1.36	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:131:THR:CG2	3:P:188:VAL:HG22	1.23	1.54
1:L:450:HIS:H	1:L:480:SER:CB	1.19	1.54
1:A:359:LEU:CD1	2:J:117:TYR:HD2	1.14	1.53
3:P:131:THR:HG21	3:P:188:VAL:CG2	1.34	1.53
3:P:466:PHE:CE2	3:P:507:ARG:HG3	1.39	1.51
1:L:540:HIS:CA	1:L:543:LEU:CD2	1.86	1.51
1:F:482:ALA:CB	1:F:515:TYR:CD2	1.92	1.51
1:C:563:ASN:ND2	6:C:601:NAG:C1	1.70	1.50
4:S:31:GLY:C	4:S:94:LEU:HD23	1.09	1.49
4:S:39:LEU:HD13	4:S:87:PHE:CD1	1.46	1.49
3:P:278:ARG:O	3:P:422:TRP:CZ2	1.66	1.45
1:F:535:THR:HG22	1:F:551:THR:CG2	1.43	1.45
3:P:448:VAL:HB	3:P:449:PRO:CD	1.14	1.45
3:P:477:TRP:CH2	3:P:524:TYR:CD1	2.02	1.45
1:L:540:HIS:CB	1:L:543:LEU:CD2	1.95	1.45
3:P:345:ALA:C	3:P:413:LEU:HD12	1.34	1.45
1:L:540:HIS:HB3	1:L:543:LEU:CD2	1.46	1.43
3:P:446:LEU:CA	3:P:465:HIS:O	1.66	1.43
1:K:450:HIS:CD2	1:K:514:ARG:HH12	1.36	1.43
1:K:464:LEU:CD1	1:K:525:GLU:OE2	1.64	1.43
1:L:511:ALA:HB3	1:L:514:ARG:CD	1.51	1.41
1:L:540:HIS:N	1:L:543:LEU:HD23	1.35	1.40
4:S:31:GLY:C	4:S:94:LEU:CD2	1.95	1.40
1:H:554:LYS:HZ3	1:H:558:LYS:NZ	1.03	1.38
1:E:489:MET:SD	1:E:494:PRO:HD3	1.65	1.37
1:H:554:LYS:NZ	1:H:558:LYS:NZ	1.71	1.37
1:L:424:PHE:N	1:L:441:ILE:HD11	1.36	1.36
3:P:477:TRP:HH2	3:P:524:TYR:CD1	1.36	1.36
1:L:424:PHE:CB	1:L:441:ILE:HD11	1.54	1.35
1:F:560:THR:O	1:G:560:THR:HG22	1.25	1.35
3:P:131:THR:CG2	3:P:188:VAL:CG2	1.97	1.35
1:E:450:HIS:CG	1:E:514:ARG:NH2	1.95	1.34
3:P:340:VAL:CG1	3:P:436:GLU:HB3	1.54	1.34
4:S:39:LEU:CD1	4:S:87:PHE:CE1	2.08	1.34
3:P:346:GLY:N	3:P:413:LEU:CG	1.88	1.34
1:L:421:GLY:O	1:L:443:ARG:NH1	1.59	1.33
1:A:356:SER:CA	2:J:117:TYR:OH	1.77	1.32
1:F:482:ALA:CB	1:F:515:TYR:HD2	1.29	1.32
3:P:446:LEU:HD21	3:P:537:THR:O	1.17	1.32
3:P:368:LEU:N	3:P:378:PRO:HD2	1.46	1.31
1:L:424:PHE:CB	1:L:441:ILE:CD1	2.09	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:450:HIS:N	1:L:480:SER:CB	1.94	1.30
1:L:424:PHE:HB2	1:L:441:ILE:CD1	1.61	1.30
1:L:511:ALA:HB3	1:L:514:ARG:CG	1.60	1.30
3:P:448:VAL:CB	3:P:449:PRO:CD	2.01	1.30
1:E:450:HIS:ND1	1:E:514:ARG:NH2	1.75	1.30
3:P:446:LEU:CD2	3:P:537:THR:O	1.79	1.30
3:P:466:PHE:HE2	3:P:507:ARG:CG	1.46	1.29
4:S:31:GLY:O	4:S:94:LEU:HD23	1.25	1.29
1:L:424:PHE:CA	1:L:441:ILE:HD11	1.62	1.29
1:L:540:HIS:C	1:L:543:LEU:CD2	2.05	1.28
3:P:251:PHE:CE1	3:P:308:GLY:O	1.86	1.28
1:C:508:GLU:HG2	1:C:509:PRO:CD	1.61	1.28
3:P:477:TRP:CZ2	3:P:524:TYR:HB3	1.67	1.27
1:D:421:GLY:HA2	1:D:445:LYS:CE	1.66	1.26
1:L:424:PHE:N	1:L:441:ILE:CD1	1.99	1.26
3:P:261:CYS:CB	3:P:315:LEU:HD23	1.66	1.25
4:S:29:LEU:CD2	4:S:95:THR:HG23	1.66	1.24
3:P:447:LYS:HG2	3:P:465:HIS:CB	1.68	1.23
1:G:523:VAL:HG21	1:G:534:TYR:OH	1.32	1.22
1:L:450:HIS:HB2	1:L:480:SER:OG	1.07	1.22
1:L:450:HIS:CB	1:L:480:SER:OG	1.87	1.22
1:L:479:PHE:CB	1:L:515:TYR:O	1.87	1.22
3:P:278:ARG:O	3:P:422:TRP:HZ2	0.94	1.22
1:F:535:THR:CG2	1:F:551:THR:HG22	1.69	1.22
1:L:456:LEU:HD23	1:L:552:VAL:CG2	1.68	1.22
4:S:39:LEU:CD1	4:S:87:PHE:CD1	2.22	1.21
1:A:356:SER:CB	2:J:117:TYR:OH	1.87	1.21
1:K:509:PRO:CG	1:L:501:VAL:HG21	1.69	1.21
1:L:479:PHE:HB2	1:L:515:TYR:O	1.05	1.20
3:P:345:ALA:C	3:P:413:LEU:CD1	2.13	1.20
4:S:37:CYS:CB	4:S:116:GLN:OE1	1.88	1.20
3:P:448:VAL:CB	3:P:449:PRO:HD2	1.64	1.20
1:L:540:HIS:C	1:L:543:LEU:HD22	1.63	1.20
1:D:490:GLN:OE1	1:D:532:GLU:HB3	1.41	1.20
1:L:540:HIS:N	1:L:543:LEU:CD2	1.94	1.20
1:C:461:ARG:NH1	1:C:465:ASN:HD21	1.40	1.19
2:J:21:ILE:CD1	1:L:555:SER:HB3	1.71	1.19
1:K:463:GLN:HB2	1:L:455:TYR:CZ	1.77	1.18
3:P:466:PHE:CE2	3:P:507:ARG:CG	2.24	1.17
1:K:354:PHE:HE1	1:K:541:GLU:N	1.42	1.16
3:P:261:CYS:SG	3:P:315:LEU:HD23	0.64	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:421:TYR:CE1	3:P:437:ILE:HD12	1.79	1.16
4:S:37:CYS:HA	4:S:116:GLN:OE1	1.45	1.16
3:P:368:LEU:H	3:P:378:PRO:CD	1.59	1.16
1:B:413:ILE:CD1	1:B:414:CYS:H	1.58	1.15
1:E:493:GLN:HB2	1:E:494:PRO:HD2	1.20	1.15
1:L:540:HIS:CA	1:L:543:LEU:HD21	1.59	1.15
1:L:511:ALA:HB3	1:L:514:ARG:HD2	1.26	1.15
1:K:511:ALA:HB1	1:K:512:PRO:CD	1.72	1.15
1:B:414:CYS:SG	1:C:416:ASP:HB2	1.87	1.14
1:B:461:ARG:HH21	1:L:570:ASP:CG	1.54	1.14
3:P:261:CYS:SG	3:P:315:LEU:CG	2.35	1.14
1:B:413:ILE:HD13	1:B:414:CYS:N	1.62	1.14
1:F:482:ALA:CB	1:F:515:TYR:CE2	2.30	1.13
1:L:424:PHE:H	1:L:441:ILE:CD1	1.58	1.13
1:E:543:LEU:HD23	1:E:544:PRO:HD3	1.30	1.13
1:K:509:PRO:HG3	1:L:501:VAL:HG21	1.17	1.13
3:P:450:GLY:HA3	3:P:540:VAL:HG12	1.29	1.13
1:B:480:SER:OG	1:B:481:PRO:HD3	1.47	1.12
1:A:514:ARG:HB3	1:A:514:ARG:HH11	1.11	1.12
4:S:37:CYS:CA	4:S:116:GLN:OE1	1.97	1.12
1:D:420:SER:C	1:D:445:LYS:HZ2	1.56	1.11
1:G:506:MET:HE3	1:G:516:PHE:HE2	1.09	1.11
3:P:345:ALA:HA	3:P:413:LEU:HB2	1.17	1.11
3:P:261:CYS:SG	3:P:315:LEU:CD2	1.19	1.11
1:C:508:GLU:HG2	1:C:509:PRO:HD3	1.33	1.10
3:P:250:LYS:HG2	3:P:309:ALA:HB2	1.33	1.10
3:P:346:GLY:N	3:P:413:LEU:CB	2.14	1.10
4:R:75:ARG:NH2	4:R:95:THR:OG1	1.84	1.10
1:F:524:SER:HG	1:F:527:GLU:HB2	1.16	1.10
1:K:464:LEU:HD12	1:K:525:GLU:OE2	1.44	1.10
4:U:22:GLU:HB2	4:U:119:THR:O	1.51	1.10
1:A:478:GLY:O	1:A:514:ARG:NH1	1.83	1.10
1:L:540:HIS:H	1:L:543:LEU:CD2	1.57	1.10
3:P:411:ASN:HB3	3:P:537:THR:OG1	1.47	1.10
3:P:445:ASN:O	3:P:466:PHE:HA	1.51	1.10
4:R:116:GLN:HE22	4:R:118:VAL:CG2	1.64	1.10
3:P:475:LYS:HB2	3:P:507:ARG:HD2	1.20	1.09
1:A:493:GLN:HB2	1:A:494:PRO:HD2	1.25	1.09
1:K:464:LEU:HD11	1:K:525:GLU:OE2	1.47	1.09
1:A:356:SER:HB2	2:J:117:TYR:OH	1.44	1.09
1:C:508:GLU:HG2	1:C:509:PRO:HD2	1.27	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:563:ASN:HD21	6:K:601:NAG:C1	1.63	1.09
4:R:61:VAL:HG21	4:R:72:TYR:CD2	1.87	1.08
1:B:480:SER:HG	1:B:481:PRO:HD3	1.00	1.08
1:L:540:HIS:O	1:L:543:LEU:CD2	2.01	1.08
3:P:448:VAL:CG2	3:P:449:PRO:HD2	1.82	1.08
3:P:447:LYS:HG2	3:P:465:HIS:HB3	1.30	1.08
1:K:450:HIS:CD2	1:K:514:ARG:NH1	2.20	1.07
3:P:131:THR:HG23	3:P:188:VAL:HA	1.32	1.07
4:R:61:VAL:HG21	4:R:72:TYR:HD2	1.11	1.07
1:D:421:GLY:CA	1:D:445:LYS:CE	2.33	1.07
3:P:251:PHE:CD1	3:P:308:GLY:O	2.07	1.07
4:S:39:LEU:HD13	4:S:87:PHE:CE1	1.82	1.07
1:L:450:HIS:N	1:L:480:SER:HB2	1.58	1.07
1:F:482:ALA:HB2	1:F:515:TYR:CE2	1.88	1.07
4:R:22:GLU:HA	4:R:117:LYS:O	1.54	1.07
1:A:356:SER:HA	2:J:117:TYR:OH	1.55	1.07
1:E:421:GLY:HA3	1:E:445:LYS:HE3	1.36	1.07
1:F:482:ALA:HB1	1:F:515:TYR:HD2	1.16	1.06
1:L:511:ALA:CB	1:L:514:ARG:CD	2.31	1.06
1:K:527:GLU:HA	1:K:530:THR:OG1	1.55	1.06
1:L:450:HIS:N	1:L:480:SER:OG	1.85	1.06
1:L:424:PHE:H	1:L:441:ILE:CG1	1.69	1.06
4:R:50:ARG:HD2	4:R:72:TYR:OH	1.56	1.06
1:K:354:PHE:CE1	1:K:541:GLU:N	2.24	1.06
3:P:340:VAL:CG1	3:P:436:GLU:CB	2.34	1.06
1:E:454:VAL:HG21	1:E:538:VAL:HG21	1.37	1.05
1:E:450:HIS:CG	1:E:514:ARG:HH22	1.68	1.05
1:E:508:GLU:OE1	1:E:509:PRO:HD2	1.55	1.05
1:K:454:VAL:CG2	1:K:538:VAL:HG21	1.85	1.05
1:L:511:ALA:CB	1:L:514:ARG:HD2	1.86	1.05
3:P:243:PRO:O	3:P:246:ALA:CB	2.04	1.05
3:P:261:CYS:SG	3:P:315:LEU:HD21	1.91	1.05
1:F:450:HIS:HD2	1:F:514:ARG:CZ	1.68	1.05
1:L:443:ARG:N	1:L:444:PRO:HD3	1.67	1.04
3:P:477:TRP:CZ2	3:P:524:TYR:CB	2.40	1.04
1:C:508:GLU:CG	1:C:509:PRO:HD3	1.87	1.04
1:L:456:LEU:CD2	1:L:552:VAL:CG2	2.34	1.04
1:E:450:HIS:CE1	1:E:514:ARG:HH12	1.75	1.04
3:P:448:VAL:HB	3:P:449:PRO:HD2	1.07	1.04
3:P:345:ALA:CA	3:P:413:LEU:HB2	1.87	1.03
2:J:21:ILE:HD11	1:L:555:SER:HB3	1.08	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:395:LEU:HB2	3:P:410:LEU:HD11	1.40	1.03
3:P:346:GLY:H	3:P:413:LEU:CB	1.69	1.03
4:R:22:GLU:OE1	4:R:101:VAL:HG13	1.57	1.03
4:R:46:ILE:H	4:R:64:THR:CG2	1.72	1.03
1:B:478:GLY:O	1:B:514:ARG:HG3	1.59	1.02
1:K:509:PRO:CG	1:L:501:VAL:CG2	2.35	1.02
1:L:456:LEU:CD2	1:L:552:VAL:HG22	1.89	1.02
1:E:489:MET:SD	1:E:494:PRO:CD	2.47	1.02
1:E:543:LEU:HD23	1:E:544:PRO:CD	1.89	1.02
1:C:566:LEU:H	1:C:566:LEU:HD12	1.23	1.02
3:P:368:LEU:H	3:P:378:PRO:HD2	0.89	1.02
3:P:368:LEU:HB2	3:P:378:PRO:CG	1.90	1.02
4:R:116:GLN:NE2	4:R:118:VAL:HG23	1.74	1.02
1:C:451:ARG:HB3	1:C:451:ARG:HH11	1.20	1.02
1:G:501:VAL:HG21	1:H:509:PRO:HD3	1.42	1.01
2:J:27:ASP:HB2	2:J:28:PRO:CD	1.90	1.01
3:P:418:ALA:HB2	3:P:439:ILE:HD13	1.43	1.01
3:P:462:VAL:HG12	3:P:540:VAL:HG11	1.36	1.01
1:F:524:SER:OG	1:F:527:GLU:HB2	1.61	1.01
3:P:340:VAL:HG12	3:P:436:GLU:O	1.60	1.01
1:K:354:PHE:HZ	1:K:546:ARG:HD3	1.26	1.01
1:L:421:GLY:O	1:L:443:ARG:CZ	2.06	1.01
4:S:29:LEU:HD23	4:S:95:THR:HG23	1.42	1.01
1:C:461:ARG:NH1	1:C:465:ASN:ND2	2.08	1.01
2:J:115:LEU:HD12	2:J:124:VAL:HG21	1.38	1.01
1:K:509:PRO:HG2	1:L:501:VAL:CG2	1.90	1.01
3:P:446:LEU:CD2	3:P:538:ALA:HB2	1.89	1.01
1:E:450:HIS:CD2	1:E:514:ARG:NH1	2.29	1.00
1:F:450:HIS:CD2	1:F:514:ARG:CZ	2.42	1.00
1:K:484:VAL:HG23	1:K:540:HIS:HB2	1.43	1.00
1:K:511:ALA:HB1	1:K:512:PRO:HD3	1.01	1.00
4:R:20:LEU:CD2	4:R:117:LYS:CG	1.96	1.00
3:P:447:LYS:H	3:P:465:HIS:H	1.03	1.00
1:L:424:PHE:CG	1:L:441:ILE:HD11	1.96	1.00
1:A:456:LEU:HD11	1:A:550:ARG:O	1.59	1.00
3:P:414:THR:OG1	3:P:417:ASP:OD2	1.80	1.00
3:P:447:LYS:HG2	3:P:465:HIS:HB2	1.42	1.00
1:C:457:LEU:HD12	1:C:473:THR:OG1	1.62	1.00
3:P:391:TYR:OH	3:P:416:ARG:NH1	1.95	0.99
3:P:450:GLY:CA	3:P:540:VAL:HG12	1.92	0.99
3:P:131:THR:CG2	3:P:188:VAL:HA	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ARG:HG2	1:B:542:ALA:O	1.60	0.99
1:K:527:GLU:O	1:K:530:THR:OG1	1.80	0.99
1:D:421:GLY:HA2	1:D:445:LYS:HE2	1.42	0.99
1:E:421:GLY:HA3	1:E:445:LYS:CE	1.91	0.99
1:K:527:GLU:C	1:K:530:THR:HG1	1.70	0.99
1:E:493:GLN:CB	1:E:494:PRO:HD2	1.77	0.99
1:L:424:PHE:CG	1:L:441:ILE:CD1	2.46	0.99
1:B:413:ILE:HD13	1:B:414:CYS:H	0.82	0.99
1:D:421:GLY:CA	1:D:445:LYS:NZ	2.26	0.99
1:L:456:LEU:HD23	1:L:552:VAL:HG22	1.01	0.99
1:E:450:HIS:CG	1:E:514:ARG:CZ	2.46	0.98
3:P:131:THR:HG23	3:P:188:VAL:HG22	1.42	0.98
4:S:29:LEU:HD22	4:S:95:THR:HG23	1.43	0.98
1:C:508:GLU:CG	1:C:509:PRO:CD	2.40	0.98
1:E:508:GLU:OE1	1:E:509:PRO:CD	2.11	0.98
1:K:511:ALA:CB	1:K:512:PRO:HD3	1.89	0.98
3:P:447:LYS:CG	3:P:465:HIS:HB3	1.92	0.98
1:C:482:ALA:HB2	1:C:515:TYR:CD1	1.97	0.98
1:B:450:HIS:O	1:B:542:ALA:CB	2.12	0.98
1:D:421:GLY:N	1:D:445:LYS:NZ	2.12	0.98
1:A:502:THR:HB	1:A:519:SER:HB2	1.46	0.97
4:R:116:GLN:HE22	4:R:118:VAL:HG23	1.23	0.97
3:P:446:LEU:HA	3:P:465:HIS:C	1.88	0.97
1:H:526:GLU:O	1:H:530:THR:HG23	1.64	0.97
3:P:368:LEU:HB2	3:P:378:PRO:CD	1.94	0.97
3:P:447:LYS:H	3:P:465:HIS:N	1.62	0.97
1:A:355:ALA:O	2:J:117:TYR:HE2	1.48	0.97
1:K:527:GLU:CA	1:K:530:THR:OG1	2.12	0.97
2:J:21:ILE:HD11	1:L:555:SER:CB	1.93	0.97
4:S:31:GLY:HA3	4:S:94:LEU:HD21	1.47	0.97
1:K:450:HIS:CG	1:K:514:ARG:HH12	1.82	0.96
3:P:340:VAL:HG13	3:P:436:GLU:CB	1.92	0.96
3:P:243:PRO:O	3:P:246:ALA:HB3	1.63	0.96
4:U:50:ARG:NH1	4:U:100:GLY:HA3	1.79	0.96
3:P:395:LEU:CD1	3:P:410:LEU:CD1	2.13	0.96
1:E:450:HIS:CE1	1:E:514:ARG:HH22	1.83	0.96
3:P:345:ALA:O	3:P:413:LEU:HD12	1.65	0.95
3:P:477:TRP:CH2	3:P:524:TYR:HD1	1.62	0.95
3:P:342:LYS:HB3	3:P:438:LYS:HB3	1.45	0.95
3:P:445:ASN:O	3:P:467:PRO:HD3	1.66	0.95
4:R:61:VAL:CG2	4:R:72:TYR:HD2	1.77	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:VAL:CG2	1:E:538:VAL:HG21	1.96	0.95
1:E:450:HIS:NE2	1:E:514:ARG:NH1	2.13	0.95
4:U:22:GLU:CG	4:U:119:THR:HG23	1.96	0.95
1:K:510:GLN:CG	1:L:522:THR:HG21	1.97	0.95
1:L:543:LEU:HB2	1:L:546:ARG:HA	1.46	0.95
3:P:477:TRP:CZ2	3:P:524:TYR:CG	2.54	0.95
3:P:477:TRP:CZ2	3:P:524:TYR:CD1	2.54	0.94
1:D:420:SER:C	1:D:445:LYS:NZ	2.26	0.94
1:L:487:GLN:O	1:L:537:VAL:HG12	1.66	0.94
1:B:451:ARG:HG2	1:B:542:ALA:C	1.93	0.94
1:L:540:HIS:O	1:L:543:LEU:HD23	1.67	0.94
4:S:29:LEU:CD2	4:S:95:THR:CG2	2.44	0.94
1:F:450:HIS:HD2	1:F:514:ARG:NH2	1.64	0.94
1:L:424:PHE:HB2	1:L:441:ILE:HD13	1.46	0.94
3:P:366:TRP:CE2	3:P:408:VAL:HG21	2.03	0.94
3:P:450:GLY:HA3	3:P:540:VAL:CG1	1.97	0.94
3:P:340:VAL:HG13	3:P:436:GLU:HB3	0.96	0.94
1:A:355:ALA:C	2:J:117:TYR:HE2	1.75	0.93
1:L:443:ARG:H	1:L:444:PRO:HD3	1.34	0.93
1:C:526:GLU:O	1:C:530:THR:HG23	1.67	0.93
1:G:506:MET:HE3	1:G:516:PHE:CE2	2.01	0.93
1:K:563:ASN:ND2	6:K:601:NAG:C1	2.31	0.93
1:K:454:VAL:HG21	1:K:538:VAL:HG21	1.47	0.93
1:C:457:LEU:CD1	1:C:473:THR:OG1	2.17	0.93
1:E:450:HIS:HD1	1:E:514:ARG:HH22	1.11	0.93
3:P:446:LEU:HA	3:P:465:HIS:O	0.75	0.93
3:P:477:TRP:HZ2	3:P:524:TYR:CB	1.81	0.93
1:C:461:ARG:HH12	1:C:465:ASN:ND2	1.63	0.93
4:S:31:GLY:CA	4:S:94:LEU:CD2	2.47	0.92
3:P:278:ARG:O	3:P:422:TRP:CH2	2.21	0.92
3:P:446:LEU:H	3:P:446:LEU:HD12	1.33	0.92
1:B:450:HIS:O	1:B:542:ALA:HB3	1.68	0.92
4:R:111:ASP:O	4:R:114:LYS:CE	2.18	0.92
4:S:39:LEU:CD1	4:S:87:PHE:HE1	1.77	0.92
1:A:359:LEU:CD1	2:J:117:TYR:CD2	2.04	0.92
1:H:554:LYS:NZ	1:H:558:LYS:HZ2	1.50	0.92
1:K:516:PHE:CE2	1:L:520:ILE:HD13	2.04	0.92
1:L:424:PHE:H	1:L:441:ILE:HG13	1.32	0.92
4:R:116:GLN:NE2	4:R:118:VAL:CG2	2.32	0.92
1:A:359:LEU:HD13	2:J:117:TYR:HB3	1.50	0.92
3:P:448:VAL:HB	3:P:449:PRO:HD3	0.92	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:479:LYS:HG2	3:P:524:TYR:CE1	2.05	0.91
1:L:479:PHE:CZ	1:L:484:VAL:HG11	2.05	0.91
1:L:540:HIS:O	1:L:543:LEU:HD22	1.65	0.91
4:S:39:LEU:HD12	4:S:87:PHE:CE1	2.04	0.91
1:K:510:GLN:HG2	1:L:522:THR:HG21	1.52	0.91
3:P:131:THR:HG23	3:P:188:VAL:CA	1.99	0.91
3:P:278:ARG:C	3:P:422:TRP:HZ2	1.78	0.91
3:P:529:LYS:CE	3:P:534:TYR:HE2	1.82	0.91
3:P:411:ASN:ND2	3:P:525:TRP:CZ2	2.39	0.91
1:B:414:CYS:SG	1:C:416:ASP:CB	2.58	0.91
1:F:502:THR:OG1	1:F:519:SER:CB	2.18	0.91
2:J:28:PRO:HG3	1:L:467:ARG:CZ	1.99	0.91
1:E:482:ALA:CB	1:E:515:TYR:HE2	1.83	0.90
4:S:31:GLY:CA	4:S:94:LEU:HD23	2.01	0.90
1:K:445:LYS:HA	1:K:445:LYS:CE	2.02	0.90
3:P:475:LYS:CB	3:P:507:ARG:HD2	2.00	0.90
4:R:46:ILE:H	4:R:64:THR:HG23	1.35	0.90
1:K:450:HIS:CG	1:K:514:ARG:NH1	2.38	0.90
1:L:450:HIS:H	1:L:480:SER:HB2	0.76	0.90
1:B:461:ARG:NH2	1:L:570:ASP:OD2	2.05	0.90
3:P:346:GLY:N	3:P:413:LEU:HB2	1.86	0.90
1:G:450:HIS:HD2	1:G:514:ARG:NH2	1.68	0.90
1:L:424:PHE:HB2	1:L:441:ILE:CG1	2.01	0.90
3:P:448:VAL:CB	3:P:449:PRO:HD3	1.81	0.90
4:U:22:GLU:CB	4:U:119:THR:HG23	2.01	0.90
1:L:540:HIS:HB3	1:L:543:LEU:HD21	0.90	0.90
3:P:477:TRP:HH2	3:P:524:TYR:CE1	1.89	0.89
1:H:554:LYS:CE	1:H:558:LYS:HZ2	1.85	0.89
3:P:395:LEU:HB2	3:P:410:LEU:CD1	2.02	0.89
3:P:445:ASN:OD1	3:P:467:PRO:HG2	1.71	0.89
1:E:526:GLU:O	1:E:530:THR:HG23	1.73	0.89
4:R:25:VAL:HG11	4:R:33:VAL:HG13	1.54	0.89
1:K:511:ALA:CB	1:K:512:PRO:CD	2.46	0.89
4:S:117:LYS:HD3	4:S:117:LYS:N	1.87	0.89
3:P:447:LYS:HB2	3:P:464:CYS:C	1.98	0.89
3:P:529:LYS:HG3	3:P:534:TYR:CE2	2.08	0.89
1:F:450:HIS:ND1	1:F:480:SER:CB	2.30	0.88
1:K:510:GLN:HG3	1:L:522:THR:CG2	2.03	0.88
1:L:540:HIS:H	1:L:543:LEU:HD23	0.84	0.88
1:F:482:ALA:HB3	1:F:515:TYR:CE2	2.08	0.88
1:K:510:GLN:CG	1:L:522:THR:CG2	2.50	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:366:TRP:CZ3	3:P:380:LEU:HD12	2.08	0.88
1:B:481:PRO:HD2	1:B:540:HIS:NE2	1.89	0.88
1:L:511:ALA:CB	1:L:514:ARG:CG	2.50	0.88
3:P:345:ALA:CA	3:P:413:LEU:HD12	1.98	0.88
1:A:356:SER:HB2	2:J:117:TYR:HH	1.37	0.87
1:E:527:GLU:O	1:E:530:THR:OG1	1.92	0.87
1:A:554:LYS:O	1:A:554:LYS:NZ	2.08	0.87
1:B:545:ASN:O	1:B:545:ASN:ND2	2.06	0.87
3:P:529:LYS:NZ	3:P:534:TYR:CE2	2.43	0.87
1:H:554:LYS:CE	1:H:558:LYS:NZ	2.37	0.87
3:P:357:ARG:NH2	3:P:403:ASN:HD22	1.72	0.87
3:P:470:PHE:HE2	3:P:528:VAL:HG11	1.39	0.87
4:S:39:LEU:HD11	4:S:87:PHE:HE1	1.38	0.87
3:P:131:THR:CG2	3:P:188:VAL:CA	2.52	0.87
4:S:39:LEU:HD13	4:S:87:PHE:HD1	1.07	0.87
1:A:493:GLN:OE1	1:A:493:GLN:N	2.07	0.87
1:F:450:HIS:CD2	1:F:514:ARG:NH1	2.43	0.87
4:S:37:CYS:HB2	4:S:116:GLN:OE1	1.72	0.87
1:A:493:GLN:CB	1:A:494:PRO:HD2	1.94	0.87
1:C:564:VAL:HG21	1:H:566:LEU:HD21	1.55	0.87
1:L:545:ASN:ND2	1:L:545:ASN:O	2.07	0.87
1:L:540:HIS:CA	1:L:543:LEU:HD23	1.74	0.87
1:K:445:LYS:HA	1:K:445:LYS:HE3	1.57	0.86
1:F:480:SER:HB2	1:F:481:PRO:HD2	1.56	0.86
3:P:411:ASN:ND2	3:P:525:TRP:CE2	2.42	0.86
3:P:529:LYS:HG3	3:P:534:TYR:CD2	2.09	0.86
1:F:535:THR:CG2	1:F:551:THR:CG2	2.37	0.86
3:P:418:ALA:HB2	3:P:439:ILE:CD1	2.03	0.86
1:A:355:ALA:C	2:J:117:TYR:CE2	2.53	0.86
1:F:363:THR:HG21	1:F:419:ASN:HB2	1.57	0.86
1:G:357:ILE:HD12	1:G:363:THR:HG22	1.57	0.86
3:P:412:GLN:NE2	3:P:412:GLN:O	2.08	0.86
3:P:357:ARG:HH21	3:P:403:ASN:HD22	1.20	0.86
1:B:451:ARG:CG	1:B:542:ALA:O	2.24	0.86
1:C:451:ARG:HH11	1:C:451:ARG:CB	1.87	0.86
3:P:418:ALA:HA	3:P:439:ILE:HD11	1.56	0.86
3:P:446:LEU:HD22	3:P:538:ALA:HB2	1.56	0.86
1:E:506:MET:HG2	1:E:507:PRO:HD2	1.58	0.85
1:K:354:PHE:CZ	1:K:546:ARG:HD3	2.10	0.85
4:R:111:ASP:O	4:R:114:LYS:HE3	1.76	0.85
3:P:264:VAL:HG13	3:P:275:PHE:CD2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:471:SER:O	3:P:475:LYS:NZ	2.09	0.85
3:P:395:LEU:HD12	3:P:409:ILE:O	1.76	0.85
1:A:456:LEU:CD1	1:A:550:ARG:O	2.25	0.85
1:E:511:ALA:HB1	1:E:514:ARG:HG3	1.57	0.85
1:B:478:GLY:O	1:B:514:ARG:CG	2.25	0.85
3:P:253:CYS:SG	3:P:315:LEU:HB3	2.16	0.85
3:P:357:ARG:HH21	3:P:403:ASN:ND2	1.74	0.85
1:K:516:PHE:CE2	1:L:520:ILE:CD1	2.59	0.85
1:C:482:ALA:HB2	1:C:515:TYR:CE1	2.11	0.84
1:C:525:GLU:N	1:C:525:GLU:OE1	2.10	0.84
1:K:527:GLU:C	1:K:530:THR:OG1	2.17	0.84
6:H:601:NAG:H61	6:K:601:NAG:H61	1.58	0.84
1:D:421:GLY:CA	1:D:445:LYS:HE3	2.07	0.84
1:E:493:GLN:HB2	1:E:494:PRO:CD	2.08	0.84
1:G:443:ARG:O	1:G:443:ARG:NE	2.09	0.84
1:H:554:LYS:NZ	1:H:558:LYS:HZ1	1.53	0.84
1:G:525:GLU:OE2	1:G:529:ASN:ND2	2.10	0.84
2:J:27:ASP:HB2	2:J:28:PRO:HD3	1.57	0.84
1:K:463:GLN:HB2	1:L:455:TYR:CE2	2.13	0.84
1:F:502:THR:OG1	1:F:519:SER:HA	1.77	0.84
1:D:421:GLY:N	1:D:445:LYS:HZ1	1.76	0.84
4:R:29:LEU:O	4:R:94:LEU:O	1.96	0.84
1:E:491:ARG:HD3	4:V:44:VAL:HG11	1.59	0.83
1:H:475:LEU:HD13	1:H:518:HIS:CE1	2.13	0.83
1:L:479:PHE:HZ	1:L:484:VAL:HG11	1.43	0.83
1:A:518:HIS:HE1	1:B:520:ILE:CG2	1.91	0.83
1:A:491:ARG:HH11	1:A:491:ARG:HG2	1.42	0.83
1:C:480:SER:O	1:C:540:HIS:CE1	2.31	0.83
1:E:421:GLY:CA	1:E:445:LYS:HE2	2.09	0.83
1:L:540:HIS:HB2	1:L:543:LEU:HD21	1.57	0.83
1:L:511:ALA:HB3	1:L:514:ARG:HG3	1.59	0.83
3:P:131:THR:HG21	3:P:188:VAL:HG23	1.57	0.83
1:K:509:PRO:HG2	1:L:501:VAL:HG23	1.60	0.83
3:P:439:ILE:H	3:P:439:ILE:HD12	1.42	0.83
1:L:443:ARG:N	1:L:444:PRO:CD	2.42	0.82
1:L:540:HIS:HB3	1:L:543:LEU:HD22	1.60	0.82
3:P:395:LEU:CB	3:P:410:LEU:CD1	2.55	0.82
1:K:509:PRO:HG3	1:L:501:VAL:CG2	2.01	0.82
1:C:526:GLU:O	1:C:530:THR:CG2	2.27	0.82
1:K:516:PHE:CD2	1:L:520:ILE:HD13	2.15	0.82
4:R:20:LEU:HD23	4:R:117:LYS:CG	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ARG:HH11	1:A:514:ARG:CB	1.91	0.82
1:B:443:ARG:H	1:B:443:ARG:HD3	1.44	0.82
1:B:443:ARG:HG2	1:B:443:ARG:HH11	1.43	0.82
1:L:481:PRO:HD2	1:L:540:HIS:HE2	1.45	0.82
1:C:527:GLU:O	1:C:532:GLU:HG2	1.80	0.82
3:P:475:LYS:CE	3:P:475:LYS:H	1.93	0.82
1:A:356:SER:N	2:J:117:TYR:OH	2.13	0.82
2:J:27:ASP:CB	2:J:28:PRO:CD	2.55	0.82
3:P:366:TRP:CE3	3:P:380:LEU:HD12	2.15	0.82
1:L:450:HIS:HB2	1:L:480:SER:HG	0.85	0.81
1:B:451:ARG:NH1	1:B:451:ARG:HB2	1.95	0.81
3:P:525:TRP:CZ3	3:P:537:THR:HG21	2.14	0.81
1:F:480:SER:HB2	1:F:481:PRO:CD	2.10	0.81
3:P:446:LEU:HD23	3:P:538:ALA:HB2	1.62	0.81
3:P:523:TRP:CZ3	3:P:539:ALA:HB1	2.14	0.81
3:P:529:LYS:HE2	3:P:534:TYR:HE2	1.43	0.81
1:E:421:GLY:CA	1:E:445:LYS:CE	2.58	0.81
1:B:449:LEU:HA	1:B:480:SER:OG	1.81	0.81
3:P:344:VAL:HG22	3:P:413:LEU:CD1	2.10	0.81
3:P:345:ALA:HA	3:P:413:LEU:CB	2.06	0.81
1:F:535:THR:HG22	1:F:551:THR:HG21	1.58	0.81
1:K:510:GLN:HG3	1:L:522:THR:HG23	1.63	0.81
1:L:479:PHE:O	1:L:515:TYR:HB2	1.81	0.81
3:P:525:TRP:CE3	3:P:537:THR:HG21	2.16	0.81
4:R:46:ILE:H	4:R:64:THR:HG21	1.46	0.81
1:D:493:GLN:OE1	1:D:493:GLN:N	2.14	0.81
1:E:543:LEU:CD2	1:E:544:PRO:HD2	2.11	0.81
1:E:543:LEU:CD2	1:E:544:PRO:CD	2.58	0.81
1:F:523:VAL:HG11	1:F:534:TYR:CZ	2.15	0.81
1:K:454:VAL:HG22	1:K:538:VAL:HG21	1.61	0.81
1:A:533:THR:HA	1:A:553:ASP:HB3	1.62	0.81
1:F:450:HIS:CD2	1:F:514:ARG:NH2	2.47	0.81
3:P:462:VAL:HB	3:P:509:VAL:HB	1.62	0.81
1:D:421:GLY:HA2	1:D:445:LYS:NZ	1.93	0.81
4:S:39:LEU:HD11	4:S:87:PHE:CE1	2.10	0.81
1:A:482:ALA:O	1:A:505:PRO:HG2	1.79	0.80
3:P:345:ALA:C	3:P:413:LEU:CG	2.47	0.80
3:P:446:LEU:HD23	3:P:537:THR:O	1.79	0.80
3:P:412:GLN:HE22	3:P:414:THR:HG23	1.47	0.80
4:R:61:VAL:CG2	4:R:72:TYR:CD2	2.59	0.80
1:A:510:GLN:NE2	1:A:510:GLN:H	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:27:ASP:HB2	2:J:28:PRO:HD2	1.61	0.80
1:F:524:SER:OG	1:F:527:GLU:CB	2.29	0.80
1:K:563:ASN:HB3	1:L:563:ASN:HA	1.64	0.80
1:A:356:SER:HA	2:J:117:TYR:CZ	2.15	0.80
3:P:411:ASN:HB3	3:P:537:THR:CB	2.12	0.80
3:P:418:ALA:CA	3:P:439:ILE:HD11	2.12	0.80
3:P:479:LYS:CG	3:P:524:TYR:CE1	2.65	0.80
1:B:461:ARG:NH2	1:L:570:ASP:CG	2.38	0.80
1:L:479:PHE:CZ	1:L:484:VAL:CG1	2.64	0.80
3:P:261:CYS:SG	3:P:315:LEU:HD22	1.36	0.80
4:S:32:SER:N	4:S:94:LEU:HD23	1.95	0.80
3:P:348:SER:CB	3:P:537:THR:OG1	2.30	0.80
1:B:480:SER:CB	1:B:481:PRO:HD3	2.12	0.79
1:G:450:HIS:CD2	1:G:514:ARG:CZ	2.65	0.79
1:L:450:HIS:CA	1:L:480:SER:OG	2.29	0.79
1:L:479:PHE:HB3	1:L:515:TYR:CB	2.12	0.79
3:P:131:THR:HG22	3:P:187:VAL:O	1.81	0.79
1:A:514:ARG:HB3	1:A:514:ARG:NH1	1.95	0.79
1:L:424:PHE:CB	1:L:441:ILE:HD13	2.07	0.79
1:L:443:ARG:H	1:L:444:PRO:CD	1.93	0.79
3:P:248:VAL:CG1	3:P:311:SER:H	1.95	0.79
1:B:382:TRP:CZ3	1:B:441:ILE:HD11	2.18	0.79
1:E:482:ALA:HB2	1:E:515:TYR:HE2	1.46	0.78
3:P:355:TYR:CE1	3:P:405:THR:N	2.51	0.78
1:A:489:MET:HE1	1:A:537:VAL:HG21	1.65	0.78
1:E:454:VAL:HG21	1:E:538:VAL:CG2	2.13	0.78
3:P:131:THR:HG23	3:P:188:VAL:CB	2.12	0.78
3:P:340:VAL:HG12	3:P:436:GLU:C	2.07	0.78
1:G:501:VAL:CG2	1:H:509:PRO:HD3	2.13	0.78
1:K:543:LEU:HD12	1:K:543:LEU:H	1.48	0.78
3:P:475:LYS:H	3:P:475:LYS:CD	1.96	0.78
1:B:354:PHE:HZ	1:B:546:ARG:HG2	1.46	0.78
1:B:461:ARG:NH2	1:L:570:ASP:OD1	2.17	0.78
1:A:535:THR:HG22	1:A:551:THR:HB	1.65	0.78
1:L:479:PHE:HB3	1:L:515:TYR:HB2	1.64	0.78
3:P:342:LYS:CE	3:P:438:LYS:HE2	2.14	0.78
4:S:75:ARG:O	4:S:92:THR:HG23	1.84	0.78
1:A:359:LEU:CD1	2:J:117:TYR:HB3	2.13	0.78
1:B:454:VAL:HG22	1:B:550:ARG:HG3	1.66	0.78
1:G:450:HIS:HD2	1:G:514:ARG:CZ	1.95	0.78
6:H:601:NAG:H83	6:H:601:NAG:O3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:413:LEU:HD23	3:P:413:LEU:H	1.49	0.77
3:P:471:SER:HA	3:P:475:LYS:HZ3	1.49	0.77
1:L:479:PHE:CZ	1:L:484:VAL:HB	2.19	0.77
3:P:287:ASP:OD1	3:P:287:ASP:N	2.17	0.77
3:P:479:LYS:CG	3:P:524:TYR:HE1	1.96	0.77
1:G:523:VAL:CG2	1:G:534:TYR:OH	2.26	0.77
3:P:346:GLY:N	3:P:413:LEU:CD1	2.41	0.77
4:R:20:LEU:HD21	4:R:117:LYS:CB	2.14	0.77
4:S:31:GLY:CA	4:S:94:LEU:HD21	2.13	0.77
1:L:540:HIS:C	1:L:543:LEU:HD23	1.88	0.77
3:P:131:THR:CG2	3:P:188:VAL:CB	2.63	0.77
3:P:346:GLY:H	3:P:413:LEU:HB2	1.45	0.77
3:P:446:LEU:HD22	3:P:538:ALA:CB	2.15	0.77
3:P:348:SER:OG	3:P:537:THR:OG1	2.02	0.77
3:P:361:LYS:HG2	3:P:364:LYS:HE2	1.64	0.77
1:F:396:ILE:HA	1:F:408:VAL:HG22	1.67	0.77
3:P:132:ILE:HD13	3:P:187:VAL:HG23	1.66	0.77
3:P:529:LYS:CE	3:P:534:TYR:CE2	2.67	0.77
1:A:491:ARG:NH1	1:A:491:ARG:O	2.19	0.77
3:P:134:CYS:HB2	3:P:185:PHE:HD2	1.50	0.77
1:E:346:ARG:HE	1:E:371:ASP:HB2	1.49	0.76
1:E:516:PHE:CZ	1:F:520:ILE:HD11	2.20	0.76
1:H:365:LEU:HD11	1:H:418:TRP:HZ2	1.50	0.76
1:K:510:GLN:HG2	1:L:522:THR:CG2	2.12	0.76
1:D:364:LYS:HD2	1:D:410:GLU:HG3	1.65	0.76
1:L:514:ARG:HB3	1:L:514:ARG:HH11	1.48	0.76
3:P:348:SER:HB3	3:P:536:GLU:HB2	1.66	0.76
1:L:424:PHE:N	1:L:441:ILE:CG1	2.42	0.76
4:R:20:LEU:CD2	4:R:117:LYS:CB	2.63	0.76
3:P:466:PHE:CD2	3:P:507:ARG:HG3	2.16	0.76
3:P:425:THR:O	3:P:430:LEU:HD21	1.85	0.76
4:R:23:VAL:HB	4:R:118:VAL:HG13	1.66	0.76
1:L:514:ARG:HH11	1:L:514:ARG:CB	1.98	0.76
3:P:450:GLY:N	3:P:540:VAL:HG12	2.00	0.76
1:E:450:HIS:CE1	1:E:514:ARG:NH1	2.49	0.76
1:F:450:HIS:HE2	1:F:514:ARG:HH12	1.34	0.76
3:P:43:ARG:HG2	3:P:43:ARG:HH11	1.50	0.76
1:G:471:THR:HG22	1:G:522:THR:HG22	1.67	0.76
1:F:348:PHE:H	1:F:369:VAL:HG13	1.51	0.75
1:A:550:ARG:HG2	1:A:550:ARG:HH11	1.51	0.75
3:P:243:PRO:HA	3:P:246:ALA:HB2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:GLY:HA3	1:D:445:LYS:HE3	1.67	0.75
1:H:554:LYS:HZ3	1:H:558:LYS:HZ3	1.26	0.75
3:P:462:VAL:CG2	3:P:509:VAL:O	2.35	0.75
1:L:467:ARG:NH1	1:L:525:GLU:OE1	2.20	0.75
3:P:368:LEU:N	3:P:378:PRO:CD	2.28	0.75
3:P:525:TRP:CE3	3:P:537:THR:CG2	2.68	0.75
1:A:524:SER:OG	1:A:527:GLU:HB2	1.87	0.75
1:L:450:HIS:HB2	1:L:480:SER:CB	2.15	0.75
1:L:532:GLU:HB2	1:L:534:TYR:CE2	2.22	0.75
4:S:71:GLU:N	4:S:71:GLU:OE1	2.19	0.75
1:G:537:VAL:HG22	1:G:549:GLU:HG2	1.68	0.75
1:H:554:LYS:HZ3	1:H:558:LYS:HZ1	0.76	0.75
1:A:355:ALA:O	2:J:117:TYR:CE2	2.39	0.75
3:P:357:ARG:NH2	3:P:403:ASN:ND2	2.32	0.75
1:A:359:LEU:HD12	2:J:117:TYR:CG	2.07	0.75
1:E:483:ASP:O	1:E:540:HIS:ND1	2.19	0.75
1:F:449:LEU:HA	1:F:481:PRO:HD3	1.67	0.75
1:F:502:THR:OG1	1:F:519:SER:CA	2.35	0.75
4:S:29:LEU:HD23	4:S:95:THR:CG2	2.14	0.75
1:F:560:THR:O	1:G:560:THR:CG2	2.21	0.74
3:P:131:THR:HG22	3:P:187:VAL:C	2.12	0.74
3:P:411:ASN:CB	3:P:537:THR:OG1	2.32	0.74
1:B:454:VAL:HG11	1:B:538:VAL:HG11	1.68	0.74
1:E:471:THR:HG22	1:E:522:THR:HG22	1.68	0.74
4:S:31:GLY:O	4:S:94:LEU:CD2	2.17	0.74
4:S:37:CYS:HB3	4:S:116:GLN:OE1	1.84	0.74
5:I:1:NAG:C1	5:I:1:NAG:H82	2.18	0.74
1:L:424:PHE:CG	1:L:441:ILE:HD13	2.18	0.74
3:P:361:LYS:O	3:P:361:LYS:HE3	1.87	0.74
3:P:450:GLY:CA	3:P:540:VAL:CG1	2.61	0.74
3:P:466:PHE:HE2	3:P:507:ARG:CB	2.00	0.74
5:I:1:NAG:O4	5:I:1:NAG:N2	2.17	0.74
1:B:466:LEU:HB3	1:B:468:GLU:HG3	1.70	0.74
1:K:463:GLN:CB	1:L:455:TYR:CZ	2.67	0.74
3:P:43:ARG:HG2	3:P:43:ARG:NH1	2.01	0.74
1:B:443:ARG:H	1:B:443:ARG:CD	2.01	0.74
1:D:514:ARG:HH11	4:V:66:ASN:ND2	1.85	0.74
1:E:450:HIS:CD2	1:E:514:ARG:CZ	2.68	0.74
3:P:342:LYS:HB3	3:P:438:LYS:CB	2.18	0.74
1:L:424:PHE:HB2	1:L:441:ILE:HG12	1.69	0.74
3:P:446:LEU:CD2	3:P:538:ALA:CB	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:477:TRP:HZ2	3:P:524:TYR:CG	1.96	0.74
1:K:464:LEU:CD1	1:K:525:GLU:CD	2.59	0.73
3:P:264:VAL:HG12	3:P:265:VAL:HG23	1.69	0.73
3:P:395:LEU:HA	3:P:410:LEU:HD12	1.70	0.73
3:P:446:LEU:HD21	3:P:537:THR:C	2.12	0.73
4:V:21:PRO:HD2	4:V:116:GLN:HG3	1.69	0.73
1:E:450:HIS:CB	1:E:514:ARG:NH2	2.51	0.73
3:P:368:LEU:CB	3:P:378:PRO:CD	2.66	0.73
4:R:25:VAL:HG11	4:R:33:VAL:CG1	2.16	0.73
3:P:243:PRO:O	3:P:246:ALA:HB2	1.84	0.73
1:F:482:ALA:HB3	1:F:515:TYR:HE2	1.50	0.73
1:L:479:PHE:HZ	1:L:484:VAL:CG1	1.99	0.73
3:P:281:LEU:HD11	3:P:290:PHE:HE2	1.52	0.73
3:P:446:LEU:HD12	3:P:446:LEU:N	2.03	0.73
1:L:421:GLY:O	1:L:443:ARG:NH2	2.22	0.73
3:P:361:LYS:HG2	3:P:364:LYS:CE	2.17	0.73
1:F:450:HIS:NE2	1:F:514:ARG:NH1	2.35	0.73
3:P:348:SER:HB2	3:P:537:THR:OG1	1.88	0.73
1:A:485:PHE:HE2	2:J:115:LEU:HD22	1.53	0.73
1:B:490:GLN:HG3	1:B:490:GLN:O	1.88	0.73
1:K:518:HIS:CE1	1:L:518:HIS:ND1	2.57	0.73
3:P:265:VAL:HG21	3:P:279:ILE:HG21	1.71	0.73
4:R:31:GLY:O	4:R:94:LEU:HD13	1.88	0.73
1:C:456:LEU:HD12	1:C:550:ARG:HB2	1.71	0.73
1:D:514:ARG:HD3	1:D:514:ARG:N	2.02	0.73
1:D:514:ARG:NH2	1:D:514:ARG:HG2	2.02	0.73
1:E:543:LEU:HD22	1:E:544:PRO:HD2	1.70	0.73
3:P:398:LEU:HD11	3:P:409:ILE:HG13	1.69	0.73
4:R:75:ARG:HG2	4:R:75:ARG:O	1.89	0.73
4:S:35:ILE:HG12	4:S:118:VAL:HG21	1.70	0.73
1:B:480:SER:OG	1:B:481:PRO:CD	2.34	0.73
1:C:467:ARG:HD3	1:C:467:ARG:N	2.03	0.73
3:P:345:ALA:C	3:P:413:LEU:HB2	2.13	0.73
4:S:72:TYR:HB3	4:S:76:VAL:HG21	1.70	0.73
1:F:535:THR:HG22	1:F:551:THR:HG22	0.75	0.72
3:P:342:LYS:HE2	3:P:438:LYS:HE2	1.69	0.72
3:P:471:SER:CA	3:P:475:LYS:HZ3	2.02	0.72
1:C:461:ARG:HH12	1:C:465:ASN:HD21	0.78	0.72
1:E:493:GLN:NE2	1:E:493:GLN:H	1.87	0.72
3:P:244:GLU:H	3:P:244:GLU:CD	1.97	0.72
1:L:479:PHE:CZ	1:L:484:VAL:CB	2.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:LYS:O	1:C:554:LYS:HG2	1.89	0.72
4:S:71:GLU:CD	4:S:71:GLU:H	1.95	0.72
1:C:421:GLY:O	1:C:423:ARG:NH2	2.23	0.72
1:C:454:VAL:HG22	1:C:538:VAL:HG21	1.71	0.72
2:J:64:LEU:HD22	2:J:64:LEU:N	2.04	0.72
3:P:479:LYS:HG2	3:P:524:TYR:CD1	2.24	0.72
4:S:32:SER:N	4:S:94:LEU:CD2	2.51	0.72
1:L:540:HIS:N	1:L:543:LEU:HD21	1.85	0.72
3:P:450:GLY:N	3:P:540:VAL:CG1	2.53	0.72
4:U:22:GLU:O	4:U:22:GLU:HG2	1.89	0.72
1:A:554:LYS:HZ2	1:A:554:LYS:C	1.96	0.72
1:K:471:THR:HG23	1:K:520:ILE:HG13	1.71	0.72
3:P:132:ILE:N	3:P:132:ILE:HD12	2.05	0.71
4:S:39:LEU:HD22	4:S:86:LEU:N	2.04	0.71
1:B:450:HIS:C	1:B:542:ALA:CB	2.63	0.71
3:P:439:ILE:HD12	3:P:439:ILE:N	2.05	0.71
3:P:447:LYS:HB2	3:P:465:HIS:N	2.04	0.71
1:E:506:MET:CG	1:E:507:PRO:HD2	2.19	0.71
1:K:484:VAL:HG23	1:K:540:HIS:CB	2.20	0.71
4:V:76:VAL:HG12	4:V:91:VAL:HG22	1.72	0.71
1:L:527:GLU:HB3	1:L:534:TYR:OH	1.89	0.71
1:L:479:PHE:HZ	1:L:484:VAL:CB	2.03	0.71
1:G:430:HIS:CD2	1:G:431:THR:H	2.09	0.71
1:H:365:LEU:HD22	1:H:413:ILE:HD13	1.73	0.71
1:K:553:ASP:OD2	1:K:554:LYS:N	2.23	0.71
1:C:371:ASP:H	1:C:404:THR:HG23	1.55	0.71
1:G:428:VAL:H	1:G:437:LEU:HB3	1.55	0.71
3:P:340:VAL:HG12	3:P:436:GLU:CB	2.20	0.71
1:B:421:GLY:H	1:B:443:ARG:HH21	1.37	0.71
1:C:568:MET:HE2	1:H:562:TYR:CD1	2.26	0.71
1:K:540:HIS:O	1:K:543:LEU:HD12	1.91	0.71
3:P:418:ALA:CB	3:P:439:ILE:CD1	2.69	0.71
1:K:354:PHE:CE1	1:K:541:GLU:HB3	2.26	0.71
1:D:478:GLY:HA2	1:D:514:ARG:HB3	1.72	0.70
1:F:449:LEU:HA	1:F:481:PRO:CD	2.20	0.70
1:L:456:LEU:HG	1:L:552:VAL:HG21	1.73	0.70
1:A:356:SER:HA	2:J:117:TYR:CE2	2.26	0.70
1:A:550:ARG:HG2	1:A:550:ARG:NH1	2.03	0.70
4:U:22:GLU:CB	4:U:119:THR:CG2	2.68	0.70
1:A:357:ILE:HG12	1:A:363:THR:HG22	1.73	0.70
1:B:454:VAL:HG11	1:B:538:VAL:CG1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:368:LEU:HD12	3:P:378:PRO:HG2	1.72	0.70
3:P:529:LYS:CG	3:P:534:TYR:CE2	2.73	0.70
1:E:372:LEU:HD12	1:E:432:ASP:HB3	1.74	0.70
3:P:421:TYR:CD1	3:P:437:ILE:HD12	2.26	0.70
4:U:37:CYS:HB3	4:U:87:PHE:HB3	1.73	0.70
1:F:543:LEU:HD23	1:F:544:PRO:HD2	1.71	0.70
3:P:466:PHE:CD2	3:P:507:ARG:CG	2.74	0.70
4:S:99:SER:HB2	4:S:120:LEU:O	1.91	0.70
1:H:418:TRP:HB3	1:H:443:ARG:HB2	1.72	0.70
2:J:21:ILE:HD13	1:L:554:LYS:HG2	1.74	0.70
3:P:529:LYS:HE2	3:P:534:TYR:CE2	2.26	0.70
1:C:566:LEU:HD12	1:C:566:LEU:N	2.01	0.70
1:F:550:ARG:HG2	1:F:550:ARG:NH1	2.05	0.70
3:P:134:CYS:HB2	3:P:185:PHE:CD2	2.26	0.70
3:P:471:SER:HB2	3:P:475:LYS:NZ	2.07	0.70
1:B:374:THR:HB	1:B:399:SER:HA	1.72	0.70
1:K:381:SER:HB3	1:K:389:ALA:HB1	1.74	0.70
3:P:479:LYS:HB2	3:P:488:LEU:HD13	1.74	0.70
1:G:532:GLU:OE1	1:G:532:GLU:HA	1.90	0.70
1:C:566:LEU:HD13	1:D:566:LEU:HD23	1.74	0.69
3:P:247:ASN:OD1	3:P:247:ASN:N	2.24	0.69
4:V:45:ARG:NH2	4:V:110:THR:OG1	2.25	0.69
3:P:418:ALA:CA	3:P:439:ILE:CD1	2.69	0.69
3:P:471:SER:CA	3:P:475:LYS:NZ	2.55	0.69
1:A:356:SER:CB	2:J:117:TYR:HH	1.97	0.69
3:P:306:LEU:HD22	3:P:321:ILE:HD12	1.74	0.69
4:U:22:GLU:HG3	4:U:119:THR:HG23	1.72	0.69
4:U:33:VAL:HG12	4:U:94:LEU:HD11	1.75	0.69
3:P:413:LEU:HD23	3:P:413:LEU:N	2.06	0.69
1:L:354:PHE:HA	1:L:357:ILE:HG12	1.75	0.69
1:L:508:GLU:OE1	1:L:508:GLU:HA	1.92	0.69
4:R:116:GLN:HE22	4:R:118:VAL:HG22	1.53	0.69
1:E:508:GLU:OE1	1:E:509:PRO:HD3	1.93	0.69
4:S:61:VAL:CG1	4:S:72:TYR:CD1	2.76	0.69
3:P:446:LEU:HB3	3:P:466:PHE:CD1	2.27	0.69
3:P:462:VAL:HB	3:P:509:VAL:O	1.92	0.69
4:R:47:TYR:HE2	4:R:49:CYS:HB2	1.57	0.69
1:C:564:VAL:CG2	1:H:566:LEU:HD21	2.23	0.69
3:P:149:LYS:HD2	3:P:151:ILE:CG2	2.22	0.69
3:P:340:VAL:HG12	3:P:436:GLU:HB3	1.69	0.69
3:P:447:LYS:CG	3:P:465:HIS:CB	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:ARG:HB3	1:C:451:ARG:NH1	2.03	0.69
1:H:456:LEU:HD22	1:H:552:VAL:HB	1.75	0.68
4:S:61:VAL:HG11	4:S:72:TYR:CD1	2.27	0.68
1:B:443:ARG:HH11	1:B:443:ARG:CG	2.06	0.68
2:J:30:GLU:OE1	2:J:30:GLU:HA	1.92	0.68
4:S:72:TYR:HB3	4:S:76:VAL:CG2	2.24	0.68
1:C:457:LEU:HD13	1:D:457:LEU:HD23	1.75	0.68
1:K:454:VAL:HG21	1:K:538:VAL:CG2	2.21	0.68
1:L:424:PHE:O	1:L:441:ILE:HG12	1.93	0.68
1:K:566:LEU:HD23	1:K:566:LEU:O	1.94	0.68
4:R:75:ARG:HH22	4:R:95:THR:HG1	1.36	0.68
1:L:487:GLN:HB3	1:L:537:VAL:CG1	2.24	0.68
3:P:476:TYR:CD1	3:P:527:GLY:O	2.46	0.68
2:J:64:LEU:HD22	2:J:64:LEU:H	1.59	0.68
1:K:509:PRO:HG2	1:L:501:VAL:HG21	1.54	0.68
1:K:561:LEU:HG	1:K:561:LEU:O	1.93	0.68
1:F:543:LEU:HD13	1:F:548:THR:HG22	1.75	0.68
3:P:526:CYS:O	3:P:538:ALA:CB	2.42	0.68
4:S:76:VAL:HG22	4:S:91:VAL:HG22	1.75	0.68
1:E:357:ILE:HG22	1:E:363:THR:HA	1.76	0.67
1:F:549:GLU:O	1:F:549:GLU:HG2	1.94	0.67
3:P:149:LYS:HD2	3:P:151:ILE:HG22	1.75	0.67
3:P:151:ILE:C	3:P:151:ILE:HD12	2.19	0.67
1:A:518:HIS:CE1	1:B:520:ILE:CG2	2.76	0.67
1:L:384:ARG:HD3	1:L:388:GLU:HB3	1.77	0.67
1:L:511:ALA:HB3	1:L:514:ARG:HG2	1.71	0.67
3:P:344:VAL:HG22	3:P:413:LEU:HD11	1.74	0.67
4:U:41:GLU:C	4:U:43:HIS:H	2.02	0.67
4:U:70:ALA:HA	4:U:73:LYS:HE2	1.76	0.67
1:E:452:PRO:HD2	1:E:543:LEU:HG	1.76	0.67
1:L:540:HIS:CB	1:L:543:LEU:HD22	2.08	0.67
3:P:526:CYS:O	3:P:538:ALA:HB3	1.94	0.67
1:C:480:SER:O	1:C:540:HIS:NE2	2.26	0.67
3:P:395:LEU:CG	3:P:410:LEU:CD1	2.71	0.67
4:V:28:GLU:C	4:V:96:GLU:OE1	2.37	0.67
1:A:471:THR:HG22	1:A:522:THR:HG22	1.75	0.67
6:A:601:NAG:H5	6:B:601:NAG:H4	1.76	0.67
1:C:456:LEU:CD1	1:C:550:ARG:HB2	2.25	0.67
2:J:4:ARG:HG2	2:J:20:ARG:HD3	1.76	0.67
3:P:261:CYS:SG	3:P:315:LEU:CB	2.82	0.67
3:P:342:LYS:CB	3:P:438:LYS:O	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:346:GLY:H	3:P:413:LEU:CA	2.08	0.67
3:P:348:SER:HB3	3:P:537:THR:H	1.57	0.67
1:G:450:HIS:CD2	1:G:514:ARG:NH2	2.59	0.67
1:G:516:PHE:CE1	1:H:520:ILE:HD12	2.30	0.67
3:P:135:PRO:O	3:P:204:ALA:HB3	1.94	0.67
1:F:450:HIS:HB2	1:F:480:SER:N	2.10	0.67
3:P:131:THR:CG2	3:P:188:VAL:HG23	2.18	0.67
1:G:524:SER:HB3	1:G:527:GLU:HG3	1.75	0.66
4:U:102:TYR:HB2	4:U:118:VAL:HG23	1.77	0.66
3:P:352:LEU:HD23	3:P:406:PHE:O	1.96	0.66
3:P:395:LEU:CG	3:P:410:LEU:HD13	2.22	0.66
1:B:382:TRP:HZ3	1:B:441:ILE:HD11	1.59	0.66
1:L:473:THR:HG22	1:L:520:ILE:HG22	1.75	0.66
3:P:261:CYS:SG	3:P:315:LEU:HB3	2.34	0.66
1:C:345:ILE:N	1:C:370:THR:O	2.29	0.66
1:L:479:PHE:CE2	1:L:484:VAL:HG11	2.30	0.66
3:P:480:TRP:CH2	3:P:482:ASN:HB3	2.31	0.66
1:B:354:PHE:CZ	1:B:546:ARG:HG2	2.28	0.66
3:P:368:LEU:HB2	3:P:378:PRO:HG2	1.76	0.66
4:U:22:GLU:HB3	4:U:119:THR:CG2	2.26	0.66
1:C:466:LEU:HD21	4:V:45:ARG:NE	2.11	0.66
3:P:132:ILE:HD12	3:P:132:ILE:H	1.60	0.66
1:A:538:VAL:CG2	1:A:548:THR:CG2	2.74	0.66
3:P:475:LYS:H	3:P:475:LYS:HE2	1.59	0.66
1:H:368:LEU:HB2	1:H:406:SER:HB2	1.76	0.66
1:F:374:THR:H	1:F:401:PRO:HB3	1.61	0.66
1:F:502:THR:OG1	1:F:519:SER:OG	2.06	0.66
1:B:564:VAL:HG22	1:C:564:VAL:HA	1.78	0.65
1:E:482:ALA:HB2	1:E:515:TYR:CE2	2.29	0.65
1:E:482:ALA:HA	1:E:515:TYR:CE2	2.30	0.65
4:U:94:LEU:C	4:U:96:GLU:H	2.04	0.65
1:G:380:ILE:HD13	1:G:409:GLY:HA3	1.78	0.65
3:P:368:LEU:CA	3:P:378:PRO:CD	2.74	0.65
1:K:535:THR:HG22	1:K:551:THR:OG1	1.96	0.65
1:A:483:ASP:O	1:A:540:HIS:HD2	1.79	0.65
1:B:451:ARG:HA	1:B:542:ALA:HB3	1.77	0.65
1:C:568:MET:CE	1:H:562:TYR:HD1	2.09	0.65
1:E:545:ASN:OD1	1:E:545:ASN:N	2.25	0.65
1:F:523:VAL:CG1	1:F:534:TYR:CZ	2.80	0.65
2:J:21:ILE:CG1	1:L:555:SER:HB3	2.25	0.65
1:A:564:VAL:HG11	1:L:568:MET:HE1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:ARG:HG2	1:D:514:ARG:HH21	1.62	0.65
1:L:443:ARG:HD3	1:L:443:ARG:C	2.21	0.65
1:B:480:SER:CB	1:B:481:PRO:CD	2.70	0.65
3:P:529:LYS:CG	3:P:534:TYR:CD2	2.79	0.65
1:E:421:GLY:CA	1:E:445:LYS:HE3	2.21	0.65
1:F:347:VAL:HG13	1:F:437:LEU:HB3	1.77	0.65
1:L:424:PHE:O	1:L:441:ILE:CG1	2.45	0.65
3:P:368:LEU:CA	3:P:378:PRO:HD2	2.25	0.65
3:P:462:VAL:CG1	3:P:540:VAL:HG11	2.21	0.65
3:P:477:TRP:CE2	3:P:524:TYR:HB3	2.30	0.65
3:P:471:SER:C	3:P:475:LYS:HZ1	2.05	0.65
1:B:397:SER:HB2	1:B:408:VAL:HG12	1.78	0.65
1:D:391:LYS:NZ	1:D:392:THR:O	2.29	0.65
1:C:508:GLU:HG3	1:C:509:PRO:HD3	1.79	0.64
1:L:546:ARG:HG2	1:L:546:ARG:O	1.97	0.64
3:P:340:VAL:CG1	3:P:436:GLU:CG	2.74	0.64
4:U:22:GLU:HB2	4:U:119:THR:N	2.12	0.64
1:A:540:HIS:HB3	1:A:543:LEU:HD12	1.78	0.64
1:G:397:SER:HB3	1:G:408:VAL:HG23	1.79	0.64
3:P:394:ARG:NH1	3:P:414:THR:OG1	2.30	0.64
3:P:462:VAL:HG23	3:P:509:VAL:O	1.96	0.64
4:S:39:LEU:CD2	4:S:85:ASN:HA	2.27	0.64
4:U:22:GLU:HA	4:U:118:VAL:HA	1.77	0.64
1:B:347:VAL:HG11	1:B:428:VAL:HG21	1.79	0.64
1:B:568:MET:HE2	1:K:562:TYR:CD2	2.32	0.64
1:A:459:PRO:CG	1:A:470:ALA:HB1	2.28	0.64
1:F:546:ARG:HH11	1:F:546:ARG:CG	2.10	0.64
1:H:372:LEU:HD11	1:H:405:PHE:HB2	1.80	0.64
2:J:27:ASP:CB	2:J:28:PRO:HD2	2.26	0.64
3:P:264:VAL:CG2	3:P:275:PHE:HE2	2.10	0.64
3:P:470:PHE:HE2	3:P:528:VAL:CG1	2.10	0.64
1:E:450:HIS:CE1	1:E:514:ARG:NH2	2.54	0.64
1:G:346:ARG:NH1	1:G:347:VAL:O	2.31	0.64
1:G:556:THR:O	1:H:461:ARG:NH2	2.30	0.64
1:K:464:LEU:HD13	1:K:525:GLU:OE2	1.91	0.64
3:P:471:SER:HB2	3:P:475:LYS:HZ2	1.62	0.64
1:F:383:THR:HA	1:F:389:ALA:HA	1.79	0.64
1:K:452:PRO:HG3	1:K:479:PHE:HB3	1.78	0.64
1:K:518:HIS:ND1	1:L:518:HIS:ND1	2.45	0.64
3:P:448:VAL:HG23	3:P:449:PRO:HD2	1.75	0.64
4:U:22:GLU:CB	4:U:119:THR:O	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:ALA:HA	1:E:515:TYR:CD2	2.33	0.64
1:L:367:CYS:HB2	1:L:382:TRP:HE3	1.63	0.64
3:P:526:CYS:HB3	3:P:538:ALA:HB3	1.79	0.64
1:B:413:ILE:CD1	1:B:414:CYS:N	2.40	0.64
1:L:527:GLU:O	1:L:530:THR:OG1	2.15	0.64
4:U:50:ARG:HH12	4:U:100:GLY:HA3	1.62	0.64
1:A:485:PHE:HE2	2:J:115:LEU:CD2	2.11	0.64
1:E:516:PHE:CE2	1:F:520:ILE:HD11	2.33	0.64
1:F:482:ALA:HB1	1:F:515:TYR:CD2	1.99	0.64
1:K:521:LEU:HD23	1:K:521:LEU:O	1.97	0.64
3:P:314:GLN:CA	3:P:314:GLN:HE21	2.09	0.64
4:R:48:LEU:HD11	4:R:102:TYR:HB3	1.79	0.64
1:C:419:ASN:O	1:C:443:ARG:NH1	2.30	0.63
1:K:516:PHE:CD2	1:L:520:ILE:CD1	2.79	0.63
3:P:250:LYS:HG2	3:P:309:ALA:CB	2.20	0.63
1:L:537:VAL:HA	1:L:548:THR:O	1.99	0.63
3:P:525:TRP:HA	3:P:538:ALA:O	1.98	0.63
4:R:21:PRO:O	4:R:117:LYS:O	2.14	0.63
4:R:46:ILE:HG22	4:R:64:THR:CG2	2.28	0.63
5:I:2:NAG:O7	5:I:2:NAG:O3	2.12	0.63
1:H:384:ARG:HH21	1:H:390:VAL:HG22	1.61	0.63
1:K:469:SER:CA	1:K:525:GLU:HB2	2.29	0.63
1:L:451:ARG:NH1	1:L:544:PRO:HG3	2.13	0.63
1:A:566:LEU:HD13	1:A:566:LEU:N	2.13	0.63
3:P:494:GLY:O	3:P:507:ARG:NH2	2.30	0.63
1:A:502:THR:HA	1:A:519:SER:HA	1.80	0.63
1:C:457:LEU:HD11	1:C:473:THR:OG1	1.98	0.63
1:D:471:THR:HG22	1:D:522:THR:HG22	1.79	0.63
1:C:369:VAL:O	1:C:406:SER:HA	1.99	0.63
1:K:518:HIS:ND1	1:L:518:HIS:CE1	2.66	0.63
1:K:540:HIS:O	1:K:543:LEU:CD1	2.47	0.63
3:P:131:THR:HG21	3:P:188:VAL:HG22	0.63	0.63
1:F:346:ARG:HH21	1:F:348:PHE:HA	1.64	0.63
1:A:493:GLN:HB2	1:A:494:PRO:CD	2.15	0.63
2:J:35:ARG:HG2	2:J:35:ARG:HH11	1.64	0.63
1:L:511:ALA:CB	1:L:514:ARG:NE	2.62	0.63
3:P:131:THR:HG23	3:P:188:VAL:CG2	2.02	0.63
3:P:264:VAL:HG22	3:P:275:PHE:HE2	1.64	0.63
3:P:334:ILE:HG23	3:P:431:TRP:CZ3	2.34	0.63
1:L:538:VAL:HG13	1:L:548:THR:OG1	1.98	0.62
3:P:345:ALA:CA	3:P:413:LEU:CB	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:41:GLU:HA	4:S:41:GLU:OE2	1.99	0.62
2:J:10:ASN:HD22	2:J:67:LEU:HD22	1.65	0.62
3:P:398:LEU:N	3:P:398:LEU:HD12	2.13	0.62
4:R:20:LEU:CD2	4:R:117:LYS:HG2	2.20	0.62
4:U:25:VAL:HG23	4:U:25:VAL:O	1.99	0.62
1:C:451:ARG:HH11	1:C:451:ARG:CG	2.11	0.62
1:A:537:VAL:HG22	1:A:549:GLU:HB3	1.81	0.62
1:A:570:ASP:HB2	4:R:112:ARG:HH22	1.64	0.62
1:C:568:MET:CE	1:H:562:TYR:CD1	2.81	0.62
1:F:449:LEU:HD22	1:F:449:LEU:H	1.64	0.62
3:P:361:LYS:CG	3:P:364:LYS:HE2	2.30	0.62
1:D:354:PHE:HA	1:D:357:ILE:HG22	1.81	0.62
1:F:543:LEU:HD22	1:F:548:THR:CG2	2.28	0.62
3:P:43:ARG:HH11	3:P:43:ARG:CG	2.13	0.62
3:P:464:CYS:O	3:P:507:ARG:O	2.17	0.62
3:P:466:PHE:CE2	3:P:507:ARG:CB	2.79	0.62
1:E:482:ALA:CB	1:E:515:TYR:CE2	2.76	0.62
1:H:560:THR:HB	1:K:560:THR:O	1.99	0.62
1:C:454:VAL:CG2	1:C:538:VAL:HG21	2.29	0.62
1:A:538:VAL:HG23	1:A:548:THR:HG22	1.80	0.62
1:F:450:HIS:ND1	1:F:480:SER:HB3	2.11	0.62
1:F:545:ASN:HB3	1:G:358:PHE:HZ	1.64	0.62
1:K:378:VAL:HG12	1:K:431:THR:HG23	1.81	0.62
1:A:566:LEU:HD13	1:A:566:LEU:H	1.64	0.62
1:C:563:ASN:HD22	6:C:601:NAG:C1	2.03	0.62
1:K:521:LEU:HD23	1:K:521:LEU:C	2.25	0.62
3:P:471:SER:CB	3:P:475:LYS:NZ	2.63	0.62
1:B:345:ILE:HA	1:B:372:LEU:HB2	1.82	0.62
1:E:450:HIS:HB3	1:E:514:ARG:NH2	2.15	0.62
1:L:543:LEU:HD22	1:L:543:LEU:H	1.64	0.62
4:R:111:ASP:O	4:R:114:LYS:CD	2.47	0.62
3:P:398:LEU:HD11	3:P:409:ILE:CG1	2.30	0.61
4:R:86:LEU:HD23	4:R:88:LEU:HD21	1.82	0.61
2:J:8:VAL:HG11	2:J:68:CYS:HA	1.81	0.61
3:P:366:TRP:NE1	3:P:408:VAL:HG21	2.14	0.61
3:P:418:ALA:CB	3:P:439:ILE:HD13	2.25	0.61
1:B:354:PHE:HA	1:B:357:ILE:HG22	1.82	0.61
1:B:418:TRP:CE2	1:B:443:ARG:HB3	2.35	0.61
1:K:469:SER:N	1:K:525:GLU:HB2	2.15	0.61
3:P:529:LYS:HG3	3:P:534:TYR:HD2	1.65	0.61
4:S:31:GLY:HA3	4:S:94:LEU:CD2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:22:GLU:HB2	4:U:119:THR:C	2.22	0.61
1:A:508:GLU:HG2	1:A:509:PRO:HD2	1.80	0.61
1:B:445:LYS:CA	1:B:445:LYS:HZ3	2.13	0.61
3:P:529:LYS:HG3	3:P:534:TYR:HE2	1.62	0.61
1:E:459:PRO:HG3	1:E:470:ALA:HB1	1.82	0.61
4:R:46:ILE:O	4:R:64:THR:HG23	2.00	0.61
4:R:76:VAL:HG12	4:R:91:VAL:HG22	1.82	0.61
1:H:481:PRO:HB2	1:H:540:HIS:HE2	1.66	0.61
2:J:6:VAL:HA	2:J:18:THR:HG22	1.83	0.61
1:E:483:ASP:O	1:E:540:HIS:CE1	2.54	0.61
1:E:491:ARG:CD	4:V:44:VAL:HG11	2.29	0.61
1:C:566:LEU:HD21	1:H:564:VAL:HG11	1.81	0.61
3:P:264:VAL:HG13	3:P:275:PHE:CE2	2.35	0.61
3:P:462:VAL:HB	3:P:509:VAL:CB	2.30	0.61
3:P:466:PHE:CD1	3:P:470:PHE:CZ	2.83	0.61
1:A:356:SER:CA	2:J:117:TYR:CZ	2.76	0.61
1:A:518:HIS:CE1	1:B:520:ILE:HG21	2.36	0.61
2:J:106:ASN:HA	3:P:29:VAL:HG21	1.83	0.61
3:P:342:LYS:HA	3:P:438:LYS:O	2.00	0.61
3:P:342:LYS:HE3	3:P:438:LYS:HE2	1.82	0.61
1:B:510:GLN:HA	1:B:510:GLN:OE1	2.01	0.61
1:K:540:HIS:HB3	1:K:543:LEU:HD11	1.83	0.61
3:P:418:ALA:HA	3:P:439:ILE:CD1	2.27	0.61
1:A:490:GLN:HB3	1:A:495:LEU:HD21	1.83	0.60
1:A:518:HIS:HE1	1:B:520:ILE:HG21	1.63	0.60
1:B:363:THR:HG23	1:B:415:GLU:HA	1.82	0.60
1:H:384:ARG:HE	1:H:390:VAL:HG22	1.66	0.60
2:J:115:LEU:HD12	2:J:124:VAL:CG2	2.24	0.60
3:P:286:LYS:C	3:P:286:LYS:HD3	2.26	0.60
4:V:112:ARG:HB3	4:V:112:ARG:CZ	2.31	0.60
1:A:567:VAL:O	1:A:567:VAL:HG12	2.02	0.60
3:P:276:GLU:OE1	3:P:372:ALA:HB2	2.01	0.60
4:S:49:CYS:N	4:S:103:ALA:O	2.33	0.60
1:C:467:ARG:HD3	1:C:467:ARG:H	1.66	0.60
1:C:482:ALA:HB2	1:C:515:TYR:CG	2.35	0.60
1:F:524:SER:OG	1:F:527:GLU:CG	2.50	0.60
1:G:352:PRO:HB2	1:G:357:ILE:HD11	1.83	0.60
1:K:484:VAL:CG2	1:K:540:HIS:HB2	2.25	0.60
3:P:471:SER:C	3:P:475:LYS:NZ	2.59	0.60
4:R:20:LEU:HD22	4:R:20:LEU:C	2.26	0.60
1:K:546:ARG:O	1:K:546:ARG:HG2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:537:VAL:HG23	1:L:548:THR:O	2.01	0.60
4:U:39:LEU:O	4:U:39:LEU:HD23	2.02	0.60
1:D:493:GLN:H	1:D:493:GLN:CD	2.09	0.60
1:H:532:GLU:O	1:H:553:ASP:CB	2.49	0.60
1:L:538:VAL:CG1	1:L:548:THR:OG1	2.50	0.60
1:E:447:VAL:O	1:E:447:VAL:HG13	2.01	0.60
1:F:490:GLN:NE2	1:F:532:GLU:OE1	2.33	0.60
1:G:467:ARG:HH11	1:G:467:ARG:HG3	1.67	0.60
1:G:516:PHE:C	1:G:516:PHE:CD2	2.80	0.60
1:H:418:TRP:O	1:H:442:SER:O	2.18	0.60
3:P:466:PHE:HE2	3:P:507:ARG:HG3	0.72	0.60
1:A:516:PHE:CE1	1:B:520:ILE:HD11	2.37	0.60
1:L:479:PHE:CE2	1:L:484:VAL:CG1	2.85	0.60
3:P:462:VAL:CB	3:P:509:VAL:O	2.49	0.60
1:C:347:VAL:O	1:C:439:GLN:NE2	2.34	0.60
1:C:471:THR:HG22	1:C:522:THR:HG22	1.82	0.60
1:H:529:ASN:C	1:H:531:GLY:H	2.10	0.60
1:L:424:PHE:CA	1:L:441:ILE:CG1	2.78	0.60
1:L:480:SER:CB	1:L:481:PRO:HD3	2.32	0.60
1:L:543:LEU:CB	1:L:546:ARG:HA	2.27	0.60
3:P:366:TRP:O	3:P:379:LEU:HA	2.02	0.60
4:R:21:PRO:O	4:R:117:LYS:HB2	2.01	0.60
4:U:81:TYR:HD1	4:U:86:LEU:HB2	1.65	0.60
1:D:449:LEU:HB3	1:D:542:ALA:HB2	1.82	0.60
1:L:423:ARG:NH2	1:L:444:PRO:HB3	2.17	0.60
4:S:39:LEU:HD12	4:S:87:PHE:CD1	2.31	0.60
1:E:399:SER:HB3	1:E:403:ALA:HA	1.82	0.60
1:F:480:SER:CB	1:F:481:PRO:CD	2.80	0.60
1:L:417:ASP:OD2	1:L:418:TRP:N	2.35	0.60
2:J:48:ASN:HB3	2:J:51:ASP:HB3	1.84	0.59
1:L:484:VAL:HG13	1:L:484:VAL:O	2.00	0.59
3:P:348:SER:CB	3:P:537:THR:H	2.15	0.59
1:A:489:MET:HE1	1:A:537:VAL:CG2	2.31	0.59
1:A:491:ARG:HG2	1:A:491:ARG:NH1	2.14	0.59
4:S:61:VAL:HG11	4:S:72:TYR:HD1	1.67	0.59
1:A:532:GLU:O	1:A:553:ASP:HB2	2.02	0.59
3:P:391:TYR:HH	3:P:416:ARG:HH12	1.42	0.59
3:P:447:LYS:N	3:P:465:HIS:H	1.86	0.59
4:U:50:ARG:HH11	4:U:100:GLY:HA3	1.65	0.59
1:E:493:GLN:H	1:E:493:GLN:HE21	1.50	0.59
3:P:122:TYR:CE2	3:P:132:ILE:HG23	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:131:THR:HG22	3:P:188:VAL:HA	1.83	0.59
3:P:341:VAL:HG23	3:P:341:VAL:O	2.01	0.59
1:E:478:GLY:HA2	1:E:514:ARG:HB3	1.83	0.59
1:H:568:MET:O	1:H:569:SER:C	2.45	0.59
1:K:571:THR:O	1:K:572:ALA:C	2.45	0.59
3:P:128:ARG:HE	3:P:320:PRO:HB3	1.67	0.59
3:P:248:VAL:HG12	3:P:311:SER:H	1.66	0.59
4:V:95:THR:HG22	4:V:95:THR:O	2.02	0.59
1:A:551:THR:HG23	1:A:551:THR:O	2.02	0.59
1:D:421:GLY:N	1:D:445:LYS:HZ2	1.80	0.59
1:F:543:LEU:CD2	1:F:548:THR:HG21	2.32	0.59
2:J:42:PRO:HG3	2:J:102:THR:HG22	1.85	0.59
1:L:574:THR:HG23	1:L:574:THR:O	2.01	0.59
3:P:281:LEU:HD11	3:P:290:PHE:CE2	2.35	0.59
3:P:342:LYS:HE2	3:P:438:LYS:CE	2.32	0.59
3:P:342:LYS:CA	3:P:438:LYS:O	2.51	0.59
3:P:523:TRP:CH2	3:P:539:ALA:HB1	2.37	0.59
1:B:384:ARG:HB3	1:B:387:GLY:H	1.68	0.59
1:C:567:VAL:O	1:C:567:VAL:HG22	2.03	0.59
1:F:550:ARG:HG2	1:F:550:ARG:HH11	1.66	0.59
1:K:464:LEU:HD11	1:K:525:GLU:CD	2.24	0.59
3:P:132:ILE:CD1	3:P:187:VAL:HG23	2.33	0.59
1:B:443:ARG:HD3	1:B:443:ARG:O	2.02	0.59
1:E:374:THR:OG1	1:E:398:GLU:O	2.18	0.59
1:E:493:GLN:CB	1:E:494:PRO:CD	2.64	0.59
1:L:537:VAL:HG13	1:L:537:VAL:O	2.02	0.59
3:P:43:ARG:HG2	3:P:43:ARG:O	2.03	0.59
3:P:361:LYS:CB	3:P:364:LYS:HE2	2.33	0.59
3:P:446:LEU:C	3:P:465:HIS:O	2.41	0.59
4:V:28:GLU:CA	4:V:96:GLU:OE1	2.51	0.59
1:A:493:GLN:CB	1:A:494:PRO:CD	2.73	0.59
1:L:363:THR:HG21	1:L:418:TRP:HB2	1.85	0.59
4:S:23:VAL:HB	4:S:35:ILE:HD13	1.85	0.59
4:U:101:VAL:O	4:U:101:VAL:HG13	2.02	0.59
1:E:456:LEU:HD23	1:E:552:VAL:HG12	1.83	0.58
1:G:468:GLU:HG2	4:S:60:THR:HG21	1.85	0.58
2:J:40:ILE:HD13	1:K:574:THR:HG21	1.83	0.58
3:P:159:ILE:HD11	3:P:173:ILE:HG21	1.85	0.58
4:R:20:LEU:CD2	4:R:117:LYS:HB2	2.33	0.58
4:V:94:LEU:HD23	4:V:96:GLU:HG2	1.84	0.58
1:C:368:LEU:HD11	1:C:406:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:565:SER:HB3	6:E:601:NAG:H62	1.85	0.58
1:F:545:ASN:HB3	1:G:358:PHE:CZ	2.38	0.58
3:P:149:LYS:O	3:P:155:PRO:HA	2.03	0.58
1:C:565:SER:O	1:C:565:SER:OG	2.17	0.58
1:E:354:PHE:HA	1:E:357:ILE:HG12	1.85	0.58
1:G:467:ARG:HH11	1:G:467:ARG:CG	2.16	0.58
3:P:445:ASN:O	3:P:467:PRO:CD	2.48	0.58
3:P:35:LYS:HB2	3:P:52:SER:HB2	1.85	0.58
3:P:122:TYR:HE2	3:P:132:ILE:HG23	1.68	0.58
3:P:131:THR:HG22	3:P:188:VAL:CA	2.33	0.58
3:P:528:VAL:HG13	3:P:535:GLY:HA3	1.85	0.58
4:R:20:LEU:CG	4:R:117:LYS:HG3	2.22	0.58
4:R:111:ASP:O	4:R:114:LYS:HD2	2.03	0.58
4:S:94:LEU:HD12	4:S:94:LEU:O	2.02	0.58
1:B:451:ARG:HB2	1:B:451:ARG:HH11	1.68	0.58
1:G:378:VAL:HG21	1:G:405:PHE:CE2	2.38	0.58
3:P:398:LEU:CD1	3:P:407:THR:O	2.52	0.58
4:R:45:ARG:NH2	4:R:110:THR:OG1	2.37	0.58
4:U:104:CYS:HB2	4:U:116:GLN:HG2	1.84	0.58
1:L:400:HIS:CE1	1:L:405:PHE:HA	2.38	0.58
3:P:189:ILE:HG23	3:P:192:LEU:HD11	1.85	0.58
3:P:476:TYR:CD1	3:P:529:LYS:HB2	2.38	0.58
1:F:372:LEU:H	1:F:404:THR:HA	1.69	0.58
1:F:449:LEU:HA	1:F:480:SER:HB2	1.84	0.58
1:H:562:TYR:CD2	1:H:562:TYR:N	2.71	0.58
1:K:520:ILE:O	1:K:520:ILE:HG23	2.03	0.58
1:L:430:HIS:CE1	1:L:432:ASP:HB3	2.37	0.58
4:U:41:GLU:OE1	4:U:41:GLU:HA	2.03	0.58
4:V:22:GLU:HA	4:V:118:VAL:HA	1.84	0.58
1:A:393:HIS:HA	1:A:410:GLU:HB3	1.84	0.58
1:B:454:VAL:HB	1:B:476:VAL:HG12	1.85	0.58
1:C:459:PRO:HD3	1:C:472:ILE:HG12	1.85	0.58
1:F:563:ASN:OD1	6:F:601:NAG:N2	2.36	0.58
1:G:523:VAL:HG21	1:G:534:TYR:HH	1.63	0.58
2:J:31:ASP:HB2	1:L:554:LYS:NZ	2.19	0.58
1:K:545:ASN:ND2	1:K:545:ASN:H	2.00	0.58
1:L:424:PHE:CA	1:L:441:ILE:CD1	2.45	0.58
1:L:540:HIS:ND1	1:L:542:ALA:HB3	2.18	0.58
1:A:356:SER:N	2:J:117:TYR:HH	2.00	0.58
1:E:537:VAL:O	1:E:537:VAL:HG12	2.03	0.58
1:H:393:HIS:HB2	1:H:396:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:448:ALA:HB1	1:K:481:PRO:HG3	1.85	0.58
3:P:314:GLN:HE21	3:P:314:GLN:HA	1.69	0.58
4:R:47:TYR:CE2	4:R:49:CYS:HB2	2.38	0.58
4:S:99:SER:CB	4:S:120:LEU:HB3	2.34	0.58
4:V:84:LYS:HE3	4:V:86:LEU:HD23	1.86	0.58
1:C:567:VAL:HB	1:D:567:VAL:HG13	1.86	0.57
2:J:116:VAL:O	2:J:116:VAL:HG22	2.04	0.57
1:K:354:PHE:CE1	1:K:541:GLU:CA	2.87	0.57
1:L:367:CYS:HB2	1:L:382:TRP:CE3	2.38	0.57
1:L:450:HIS:CA	1:L:480:SER:CB	2.81	0.57
1:L:450:HIS:NE2	4:R:65:THR:HG22	2.18	0.57
3:P:398:LEU:HD13	3:P:407:THR:O	2.03	0.57
1:B:450:HIS:O	1:B:542:ALA:HB2	2.03	0.57
1:F:351:PRO:HB3	1:F:443:ARG:HD2	1.85	0.57
1:H:445:LYS:HA	1:H:445:LYS:HE3	1.86	0.57
3:P:314:GLN:HE21	3:P:314:GLN:N	2.02	0.57
4:R:46:ILE:N	4:R:64:THR:HG21	2.18	0.57
1:B:423:ARG:HA	1:B:442:SER:HB2	1.85	0.57
1:E:524:SER:OG	1:E:527:GLU:OE1	2.22	0.57
1:E:535:THR:CG2	1:E:550:ARG:O	2.52	0.57
1:H:364:LYS:HE3	1:H:410:GLU:HB3	1.87	0.57
1:D:349:ALA:HB2	1:D:439:GLN:HG3	1.85	0.57
2:J:36:ASN:ND2	1:L:563:ASN:OD1	2.37	0.57
3:P:340:VAL:HG11	3:P:436:GLU:CD	2.29	0.57
4:U:102:TYR:HB2	4:U:118:VAL:CG2	2.34	0.57
2:J:52:PRO:HG3	2:J:128:LEU:HD21	1.86	0.57
1:L:540:HIS:ND1	1:L:542:ALA:CB	2.67	0.57
1:K:366:THR:HG23	1:K:409:GLY:H	1.69	0.57
1:K:476:VAL:O	1:K:476:VAL:HG12	2.04	0.57
1:A:491:ARG:HG2	1:A:491:ARG:O	2.04	0.57
3:P:475:LYS:HE2	3:P:475:LYS:N	2.20	0.57
1:A:488:TRP:NE1	1:A:519:SER:OG	2.24	0.57
1:A:491:ARG:HH11	1:A:491:ARG:CG	2.16	0.57
1:B:568:MET:HE1	1:L:564:VAL:HG21	1.86	0.57
1:D:534:TYR:N	1:D:534:TYR:CD1	2.73	0.57
1:E:400:HIS:HB3	1:E:404:THR:H	1.69	0.57
1:L:543:LEU:HD13	1:L:543:LEU:N	2.19	0.57
3:P:201:LEU:HD13	3:P:214:ASN:HA	1.86	0.57
3:P:541:TYR:N	3:P:541:TYR:CD1	2.73	0.57
1:A:501:VAL:HG13	1:A:501:VAL:O	2.04	0.57
1:F:452:PRO:HD2	1:F:543:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:GLU:HG3	1:G:399:SER:H	1.70	0.57
1:G:475:LEU:HG	1:G:475:LEU:O	2.04	0.57
1:L:534:TYR:CD2	1:L:534:TYR:N	2.73	0.57
3:P:147:LEU:HB3	3:P:159:ILE:HB	1.86	0.57
3:P:368:LEU:HB2	3:P:378:PRO:HD3	1.83	0.57
4:S:39:LEU:CD2	4:S:85:ASN:C	2.78	0.57
1:A:359:LEU:CD1	2:J:117:TYR:CB	2.82	0.57
1:A:489:MET:CE	1:A:537:VAL:CG2	2.83	0.57
1:C:566:LEU:H	1:C:566:LEU:CD1	2.01	0.57
1:F:548:THR:HG23	1:F:548:THR:O	2.05	0.57
1:D:374:THR:HG22	1:D:403:ALA:HB1	1.85	0.56
1:G:363:THR:HG21	1:G:418:TRP:HB3	1.86	0.56
4:V:108:MET:HA	4:V:108:MET:HE3	1.85	0.56
1:A:520:ILE:HD13	1:B:475:LEU:HD11	1.87	0.56
1:C:383:THR:HG1	1:C:425:THR:HG1	1.53	0.56
1:D:454:VAL:HG21	1:D:538:VAL:HG21	1.87	0.56
1:E:489:MET:SD	1:E:493:GLN:HA	2.45	0.56
1:H:568:MET:O	1:H:570:ASP:N	2.38	0.56
1:K:452:PRO:HD2	1:K:543:LEU:HG	1.86	0.56
5:I:2:NAG:O6	5:I:2:NAG:O4	2.02	0.56
1:B:484:VAL:HG13	1:B:484:VAL:O	2.05	0.56
1:E:364:LYS:NZ	1:E:412:SER:OG	2.31	0.56
1:K:477:THR:HG22	1:K:516:PHE:HB2	1.86	0.56
3:P:523:TRP:HZ3	3:P:539:ALA:HB1	1.68	0.56
4:R:35:ILE:HD12	4:R:118:VAL:HG11	1.87	0.56
4:S:72:TYR:HD2	4:S:72:TYR:N	2.03	0.56
4:U:22:GLU:HB3	4:U:119:THR:HG22	1.86	0.56
4:U:118:VAL:HG23	4:U:118:VAL:O	2.04	0.56
1:A:501:VAL:O	1:A:501:VAL:HG22	2.03	0.56
1:C:486:VAL:HG22	1:C:538:VAL:HG22	1.87	0.56
1:E:437:LEU:HG	1:E:438:LYS:H	1.69	0.56
1:G:396:ILE:HD11	1:G:407:ALA:HB1	1.88	0.56
1:G:467:ARG:O	4:S:60:THR:HG22	2.06	0.56
1:H:456:LEU:HD12	1:H:536:CYS:HB3	1.86	0.56
3:P:149:LYS:CD	3:P:151:ILE:HG22	2.34	0.56
3:P:361:LYS:HD2	3:P:361:LYS:C	2.30	0.56
1:H:479:PHE:HB2	1:H:540:HIS:CE1	2.41	0.56
1:K:478:GLY:HA2	1:K:514:ARG:HB3	1.86	0.56
1:C:508:GLU:CG	1:C:509:PRO:HD2	2.17	0.56
1:C:556:THR:O	1:C:556:THR:HG22	2.04	0.56
1:D:367:CYS:HB3	1:D:382:TRP:CZ2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:452:PRO:HD2	1:H:543:LEU:HG	1.88	0.56
1:K:560:THR:O	1:K:560:THR:HG23	2.05	0.56
3:P:407:THR:O	3:P:407:THR:HG22	2.06	0.56
1:B:564:VAL:CG2	1:C:564:VAL:HA	2.35	0.56
1:D:369:VAL:HG11	1:D:378:VAL:HG21	1.87	0.56
1:D:429:THR:HB	1:D:436:PRO:HA	1.87	0.56
1:E:367:CYS:H	1:E:382:TRP:HH2	1.52	0.56
4:U:51:GLU:HA	4:U:58:CYS:HA	1.88	0.56
1:A:450:HIS:N	1:A:450:HIS:CD2	2.72	0.56
1:A:489:MET:CE	1:A:537:VAL:HG21	2.33	0.56
1:G:501:VAL:O	1:G:501:VAL:HG12	2.06	0.56
1:G:502:THR:HG23	1:G:502:THR:O	2.04	0.56
2:J:64:LEU:H	2:J:64:LEU:CD2	2.18	0.56
3:P:366:TRP:CZ2	3:P:408:VAL:HG21	2.41	0.56
3:P:431:TRP:N	3:P:431:TRP:CD1	2.72	0.56
3:P:462:VAL:CB	3:P:509:VAL:HB	2.34	0.56
4:R:91:VAL:HG12	4:R:93:GLN:O	2.06	0.56
1:D:380:ILE:HD12	1:D:393:HIS:CD2	2.41	0.56
1:K:510:GLN:CG	1:L:522:THR:HG23	2.27	0.56
1:L:487:GLN:HB3	1:L:537:VAL:HG11	1.88	0.56
4:S:34:THR:HB	4:S:88:LEU:HD11	1.88	0.56
1:A:564:VAL:HG22	1:B:564:VAL:HA	1.88	0.56
1:K:535:THR:HA	1:K:550:ARG:O	2.06	0.56
1:L:452:PRO:HB3	1:L:479:PHE:HD1	1.71	0.56
2:J:21:ILE:CD1	1:L:555:SER:CB	2.65	0.55
3:P:250:LYS:HA	3:P:309:ALA:HA	1.87	0.55
4:S:61:VAL:HG13	4:S:72:TYR:CD1	2.41	0.55
1:B:449:LEU:HA	1:B:480:SER:HG	1.72	0.55
1:G:516:PHE:C	1:G:516:PHE:HD2	2.14	0.55
1:H:532:GLU:O	1:H:553:ASP:HB3	2.05	0.55
2:J:17:ILE:HD11	2:J:64:LEU:HD12	1.87	0.55
1:K:380:ILE:HB	1:K:393:HIS:HD2	1.71	0.55
1:K:496:SER:HG	1:K:499:LYS:HZ3	1.48	0.55
3:P:421:TYR:CZ	3:P:437:ILE:HD12	2.37	0.55
1:B:451:ARG:CB	1:B:451:ARG:CZ	2.84	0.55
1:C:478:GLY:HA2	1:C:514:ARG:HG2	1.89	0.55
1:E:491:ARG:HG2	4:V:44:VAL:HG11	1.88	0.55
1:H:443:ARG:N	1:H:444:PRO:HD3	2.22	0.55
1:H:554:LYS:HE2	1:H:558:LYS:NZ	2.21	0.55
3:P:469:LYS:HG2	3:P:469:LYS:O	2.05	0.55
4:R:61:VAL:HG21	4:R:72:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:116:VAL:O	2:J:116:VAL:HG13	2.05	0.55
1:L:369:VAL:HG12	1:L:372:LEU:HD21	1.88	0.55
3:P:317:GLU:N	3:P:317:GLU:OE2	2.39	0.55
3:P:491:GLN:HE22	3:P:510:SER:HB2	1.72	0.55
1:B:553:ASP:OD1	1:B:554:LYS:N	2.36	0.55
3:P:395:LEU:CA	3:P:410:LEU:HD12	2.35	0.55
4:S:23:VAL:HG22	4:S:25:VAL:HG23	1.89	0.55
1:A:356:SER:N	2:J:117:TYR:CE2	2.75	0.55
1:A:574:THR:HA	1:K:461:ARG:NH1	2.21	0.55
1:B:461:ARG:CZ	1:L:570:ASP:OD2	2.55	0.55
1:C:423:ARG:HE	1:C:442:SER:HB3	1.71	0.55
2:J:21:ILE:CD1	1:L:554:LYS:HG2	2.37	0.55
1:L:424:PHE:N	1:L:441:ILE:HG13	2.10	0.55
1:L:424:PHE:CD2	1:L:441:ILE:HD13	2.41	0.55
1:L:450:HIS:CB	1:L:480:SER:CB	2.78	0.55
1:L:511:ALA:O	1:L:514:ARG:CG	2.55	0.55
3:P:38:CYS:SG	3:P:91:LYS:HB2	2.47	0.55
3:P:315:LEU:HG	3:P:315:LEU:O	2.05	0.55
3:P:450:GLY:H	3:P:540:VAL:HG12	1.67	0.55
1:B:454:VAL:CG1	1:B:538:VAL:HG11	2.36	0.55
1:H:443:ARG:N	1:H:444:PRO:CD	2.68	0.55
1:L:508:GLU:CG	1:L:514:ARG:HB2	2.36	0.55
1:L:508:GLU:HG3	1:L:514:ARG:HB2	1.89	0.55
1:L:511:ALA:CB	1:L:514:ARG:HG2	2.34	0.55
3:P:249:ALA:O	3:P:309:ALA:HA	2.06	0.55
3:P:371:GLY:H	3:P:375:GLY:HA2	1.72	0.55
1:A:516:PHE:C	1:A:516:PHE:CD2	2.85	0.55
1:B:420:SER:CB	1:B:422:GLU:OE1	2.54	0.55
1:B:445:LYS:HZ3	1:B:445:LYS:N	2.05	0.55
1:D:384:ARG:NH1	1:D:390:VAL:HA	2.22	0.55
4:S:72:TYR:N	4:S:72:TYR:CD2	2.72	0.55
1:A:423:ARG:HE	1:A:440:THR:HG23	1.71	0.55
1:C:454:VAL:HG13	1:C:474:CYS:SG	2.46	0.55
1:D:369:VAL:HB	1:D:428:VAL:HG11	1.89	0.55
1:E:450:HIS:CE1	1:E:514:ARG:CZ	2.90	0.55
1:F:520:ILE:O	1:F:520:ILE:HG13	2.05	0.55
1:K:563:ASN:HB3	1:L:563:ASN:CA	2.35	0.55
3:P:30:ASN:O	3:P:35:LYS:NZ	2.34	0.55
3:P:39:ARG:HB2	3:P:49:LEU:HD11	1.87	0.55
5:I:1:NAG:C1	5:I:1:NAG:C8	2.85	0.55
1:B:380:ILE:HB	1:B:393:HIS:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:454:VAL:HG21	1:H:538:VAL:HG21	1.89	0.55
2:J:35:ARG:HH11	2:J:35:ARG:CG	2.19	0.55
1:K:354:PHE:CE1	1:K:541:GLU:CB	2.90	0.55
3:P:464:CYS:O	3:P:507:ARG:C	2.50	0.55
1:F:537:VAL:HG22	1:F:549:GLU:HB3	1.89	0.54
1:K:535:THR:CG2	1:K:551:THR:OG1	2.54	0.54
1:A:400:HIS:ND1	1:A:402:ASN:OD1	2.39	0.54
1:G:476:VAL:O	1:G:476:VAL:HG12	2.06	0.54
4:S:39:LEU:O	4:S:39:LEU:HD23	2.07	0.54
1:A:391:LYS:HA	1:A:391:LYS:HE3	1.90	0.54
1:E:454:VAL:HG22	1:E:538:VAL:HG21	1.87	0.54
1:E:479:PHE:HB2	1:E:540:HIS:CE1	2.41	0.54
2:J:31:ASP:HB2	1:L:554:LYS:HZ1	1.72	0.54
1:B:393:HIS:CD2	1:B:409:GLY:HA3	2.43	0.54
1:B:568:MET:HE2	1:K:562:TYR:CE2	2.42	0.54
1:C:346:ARG:HG2	1:C:371:ASP:OD1	2.08	0.54
1:D:500:TYR:C	1:D:500:TYR:CD1	2.85	0.54
1:F:500:TYR:CD1	1:F:500:TYR:C	2.84	0.54
1:G:463:GLN:HG2	1:H:455:TYR:CZ	2.42	0.54
2:J:117:TYR:CD1	2:J:117:TYR:C	2.85	0.54
1:K:481:PRO:HG2	1:K:541:GLU:OE2	2.06	0.54
3:P:290:PHE:CD1	3:P:290:PHE:C	2.85	0.54
3:P:425:THR:O	3:P:430:LEU:CD2	2.54	0.54
1:C:419:ASN:OD1	1:C:420:SER:N	2.40	0.54
1:L:523:VAL:HG11	1:L:534:TYR:HE1	1.71	0.54
3:P:361:LYS:HB3	3:P:364:LYS:HE2	1.90	0.54
3:P:369:TRP:CD1	3:P:420:PHE:H	2.26	0.54
3:P:447:LYS:N	3:P:465:HIS:N	2.46	0.54
3:P:450:GLY:H	3:P:540:VAL:CG1	2.20	0.54
4:R:99:SER:HB2	4:R:120:LEU:HB2	1.89	0.54
1:B:369:VAL:HG23	1:B:407:ALA:HB2	1.89	0.54
1:B:400:HIS:HB3	1:B:403:ALA:HA	1.90	0.54
1:K:512:PRO:HD2	1:K:514:ARG:HG2	1.90	0.54
1:L:354:PHE:CD2	1:L:546:ARG:NH2	2.75	0.54
1:L:414:CYS:SG	3:P:497:LYS:NZ	2.75	0.54
3:P:263:VAL:HG21	3:P:314:GLN:NE2	2.23	0.54
3:P:399:GLU:O	3:P:406:PHE:HA	2.08	0.54
3:P:450:GLY:HA2	3:P:463:PRO:HD2	1.90	0.54
4:R:116:GLN:NE2	4:R:116:GLN:O	2.41	0.54
1:A:566:LEU:N	1:A:566:LEU:CD1	2.70	0.54
1:B:476:VAL:HG23	1:B:479:PHE:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LYS:HA	1:D:411:ALA:O	2.08	0.54
1:E:482:ALA:CA	1:E:515:TYR:CE2	2.91	0.54
1:L:481:PRO:HD2	1:L:540:HIS:NE2	2.20	0.54
3:P:289:SER:O	3:P:289:SER:OG	2.20	0.54
4:V:61:VAL:HA	4:V:69:LYS:HB2	1.90	0.54
1:F:486:VAL:HG22	1:F:538:VAL:HG22	1.90	0.54
1:L:456:LEU:CG	1:L:552:VAL:HG21	2.35	0.54
3:P:462:VAL:HG11	3:P:509:VAL:CG1	2.37	0.54
1:A:524:SER:HG	1:A:527:GLU:HB2	1.70	0.54
1:B:443:ARG:HD3	1:B:443:ARG:N	2.15	0.54
1:D:454:VAL:CG2	1:D:538:VAL:HG21	2.38	0.54
3:P:473:TYR:CD2	3:P:473:TYR:N	2.76	0.54
1:B:531:GLY:HA2	1:B:554:LYS:HB2	1.90	0.54
1:C:448:ALA:O	1:C:481:PRO:HD3	2.08	0.54
1:L:456:LEU:CG	1:L:552:VAL:CG2	2.85	0.54
3:P:314:GLN:HA	3:P:314:GLN:NE2	2.23	0.54
1:D:487:GLN:NE2	1:D:494:PRO:HB3	2.22	0.53
1:K:354:PHE:HE1	1:K:540:HIS:C	2.13	0.53
1:B:473:THR:HG22	1:B:520:ILE:HG22	1.90	0.53
1:F:502:THR:O	1:F:502:THR:HG22	2.08	0.53
1:H:445:LYS:HA	1:H:445:LYS:CE	2.38	0.53
1:L:346:ARG:HG2	1:L:370:THR:H	1.73	0.53
3:P:264:VAL:HG13	3:P:275:PHE:HD2	1.66	0.53
3:P:264:VAL:CG1	3:P:275:PHE:CE2	2.91	0.53
3:P:366:TRP:CZ3	3:P:380:LEU:CD1	2.87	0.53
4:R:22:GLU:HG3	4:R:119:THR:HG22	1.90	0.53
1:A:538:VAL:HG22	1:A:548:THR:CG2	2.38	0.53
1:C:457:LEU:CD1	1:D:457:LEU:HD23	2.38	0.53
1:K:463:GLN:HB2	1:L:455:TYR:CE1	2.37	0.53
3:P:445:ASN:OD1	3:P:467:PRO:CG	2.51	0.53
3:P:121:VAL:HA	3:P:216:ASP:HB3	1.90	0.53
3:P:541:TYR:N	3:P:541:TYR:HD1	2.06	0.53
4:U:105:GLY:HA2	4:U:115:THR:HG23	1.90	0.53
3:P:24:TYR:CD2	3:P:30:ASN:HB3	2.43	0.53
3:P:355:TYR:CD1	3:P:405:THR:HA	2.44	0.53
3:P:447:LYS:HE2	3:P:465:HIS:CG	2.44	0.53
1:A:384:ARG:NH1	1:A:388:GLU:OE2	2.42	0.53
1:A:483:ASP:O	1:A:540:HIS:CD2	2.62	0.53
1:B:421:GLY:N	1:B:443:ARG:HH21	2.04	0.53
1:C:473:THR:HG22	1:C:520:ILE:HG22	1.91	0.53
1:D:377:SER:O	1:D:431:THR:OG1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:562:TYR:N	1:K:562:TYR:HD1	2.06	0.53
3:P:37:TRP:HB3	3:P:50:ILE:HG22	1.89	0.53
3:P:134:CYS:O	3:P:185:PHE:HB3	2.09	0.53
3:P:197:ALA:HB2	3:P:219:VAL:HG13	1.91	0.53
3:P:477:TRP:HD1	3:P:526:CYS:HB2	1.74	0.53
1:C:457:LEU:CD1	1:C:473:THR:HG1	2.21	0.53
1:E:383:THR:HB	1:E:387:GLY:HA2	1.91	0.53
1:E:482:ALA:CA	1:E:515:TYR:HE2	2.22	0.53
3:P:355:TYR:HE1	3:P:405:THR:O	1.92	0.53
1:C:477:THR:OG1	1:C:508:GLU:OE2	2.26	0.53
1:G:482:ALA:HB2	1:G:515:TYR:CE2	2.44	0.53
1:K:491:ARG:O	1:K:493:GLN:N	2.41	0.53
3:P:447:LYS:CD	3:P:465:HIS:HB3	2.37	0.53
1:C:506:MET:HG3	1:C:507:PRO:HD2	1.91	0.53
1:K:480:SER:HB2	1:K:481:PRO:HD3	1.91	0.53
3:P:479:LYS:HG3	3:P:524:TYR:HE1	1.73	0.53
1:A:459:PRO:HG2	1:A:470:ALA:HB1	1.90	0.53
1:A:538:VAL:CG2	1:A:548:THR:HG22	2.38	0.53
1:F:471:THR:HG22	1:F:522:THR:HG23	1.91	0.53
4:R:46:ILE:N	4:R:64:THR:HG23	2.15	0.53
1:B:489:MET:HG2	1:B:494:PRO:HA	1.91	0.52
1:C:426:CYS:HB3	1:C:439:GLN:HB2	1.91	0.52
1:E:480:SER:O	1:E:480:SER:OG	2.25	0.52
1:G:481:PRO:HD2	1:G:540:HIS:CE1	2.44	0.52
1:G:482:ALA:HB2	1:G:515:TYR:CZ	2.44	0.52
1:L:511:ALA:HB2	1:L:514:ARG:HD2	1.81	0.52
3:P:8:GLU:OE1	3:P:8:GLU:N	2.42	0.52
3:P:446:LEU:CD2	3:P:537:THR:C	2.75	0.52
3:P:463:PRO:HA	3:P:508:LEU:HD12	1.91	0.52
4:R:22:GLU:OE1	4:R:101:VAL:CG1	2.44	0.52
4:S:75:ARG:HG3	4:S:91:VAL:HG13	1.90	0.52
4:U:36:LYS:HA	4:U:88:LEU:HD23	1.90	0.52
1:A:466:LEU:N	1:A:466:LEU:CD1	2.72	0.52
1:A:489:MET:HG2	1:A:494:PRO:HA	1.91	0.52
1:A:538:VAL:HG22	1:A:548:THR:HG23	1.91	0.52
1:B:384:ARG:HA	1:B:424:PHE:CE2	2.45	0.52
1:E:535:THR:HG22	1:E:550:ARG:O	2.10	0.52
1:K:356:SER:O	1:K:360:THR:OG1	2.25	0.52
1:K:508:GLU:HG3	1:K:514:ARG:HB2	1.89	0.52
1:K:562:TYR:N	1:K:562:TYR:CD1	2.71	0.52
3:P:27:THR:OG1	3:P:30:ASN:OD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:GLU:HG2	1:A:509:PRO:CD	2.40	0.52
1:F:456:LEU:HD11	1:F:536:CYS:HB3	1.91	0.52
1:K:480:SER:HA	1:K:513:GLY:O	2.09	0.52
1:L:449:LEU:HA	1:L:480:SER:HB3	1.89	0.52
1:B:568:MET:HE2	1:K:562:TYR:HD2	1.75	0.52
1:C:466:LEU:HD21	4:V:45:ARG:CZ	2.39	0.52
1:L:556:THR:O	1:L:556:THR:HG23	2.10	0.52
3:P:196:ASP:O	3:P:200:TYR:OH	2.25	0.52
3:P:344:VAL:HG21	3:P:444:PRO:HA	1.92	0.52
3:P:470:PHE:CZ	3:P:528:VAL:HB	2.43	0.52
3:P:491:GLN:NE2	3:P:510:SER:HB2	2.24	0.52
4:R:52:MET:CE	4:R:69:LYS:HZ2	2.22	0.52
1:F:449:LEU:N	1:F:449:LEU:CD2	2.73	0.52
1:F:453:ASP:OD2	1:F:455:TYR:OH	2.21	0.52
2:J:35:ARG:CG	2:J:35:ARG:NH1	2.70	0.52
1:L:430:HIS:HE1	1:L:432:ASP:HB3	1.74	0.52
4:U:48:LEU:HB2	4:U:89:VAL:HG11	1.91	0.52
1:K:558:LYS:NZ	1:L:461:ARG:HE	2.06	0.52
1:L:505:PRO:O	1:L:506:MET:HE2	2.10	0.52
4:R:37:CYS:HA	4:R:116:GLN:HG3	1.91	0.52
1:A:510:GLN:H	1:A:510:GLN:CD	2.18	0.52
1:B:420:SER:HB2	1:B:422:GLU:OE1	2.10	0.52
1:F:414:CYS:HB3	1:G:414:CYS:SG	2.50	0.52
1:L:456:LEU:CD2	1:L:552:VAL:HG21	2.32	0.52
4:R:25:VAL:HB	4:R:120:LEU:HG	1.91	0.52
4:R:95:THR:C	4:R:97:SER:H	2.17	0.52
1:B:454:VAL:HG22	1:B:550:ARG:CG	2.38	0.52
1:C:451:ARG:NH1	1:C:451:ARG:CG	2.72	0.52
1:L:450:HIS:CE1	4:R:65:THR:HG22	2.45	0.52
3:P:261:CYS:O	3:P:263:VAL:N	2.43	0.52
2:J:40:ILE:CD1	1:K:574:THR:HG21	2.39	0.52
1:K:565:SER:O	1:K:565:SER:OG	2.19	0.52
4:U:22:GLU:CB	4:U:119:THR:N	2.72	0.52
4:U:22:GLU:CD	4:U:119:THR:HG23	2.33	0.52
1:E:493:GLN:NE2	1:E:493:GLN:N	2.58	0.52
1:F:449:LEU:HD22	1:F:449:LEU:N	2.25	0.52
1:L:526:GLU:O	1:L:530:THR:HG23	2.10	0.52
1:A:356:SER:CA	2:J:117:TYR:CE2	2.92	0.51
1:E:368:LEU:HD21	1:E:406:SER:HB2	1.92	0.51
1:F:474:CYS:HB2	1:F:488:TRP:CZ2	2.45	0.51
1:K:450:HIS:NE2	1:K:514:ARG:NH1	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:227:VAL:HG23	3:P:326:LEU:HA	1.92	0.51
1:A:518:HIS:HE1	1:B:520:ILE:HG23	1.70	0.51
1:A:535:THR:HG22	1:A:551:THR:CB	2.37	0.51
1:C:526:GLU:H	1:C:526:GLU:CD	2.17	0.51
1:E:467:ARG:HD3	1:E:525:GLU:HG3	1.92	0.51
1:L:354:PHE:HD2	1:L:546:ARG:HH21	1.55	0.51
3:P:63:ARG:NH2	3:P:86:ASP:OD2	2.41	0.51
3:P:355:TYR:CE1	3:P:405:THR:CA	2.93	0.51
3:P:525:TRP:CE3	3:P:537:THR:HG22	2.44	0.51
4:S:79:LYS:HD3	4:S:80:GLN:H	1.75	0.51
1:A:564:VAL:CG2	1:B:564:VAL:HA	2.40	0.51
1:C:429:THR:HG22	1:C:436:PRO:HB3	1.92	0.51
1:H:495:LEU:HD22	1:H:499:LYS:HE3	1.92	0.51
1:K:518:HIS:ND1	1:L:518:HIS:CG	2.78	0.51
1:A:467:ARG:HG3	1:A:525:GLU:OE1	2.11	0.51
1:C:466:LEU:CD2	4:V:45:ARG:CZ	2.88	0.51
1:D:562:TYR:CE1	1:H:568:MET:SD	3.04	0.51
3:P:361:LYS:HG2	3:P:364:LYS:HE3	1.91	0.51
3:P:450:GLY:N	3:P:540:VAL:HG13	2.26	0.51
1:F:543:LEU:HD22	1:F:548:THR:HG21	1.92	0.51
1:G:518:HIS:NE2	1:H:520:ILE:HD11	2.25	0.51
3:P:295:THR:HG22	3:P:432:ARG:HB2	1.93	0.51
3:P:525:TRP:CZ3	3:P:537:THR:CG2	2.92	0.51
4:V:112:ARG:CB	4:V:112:ARG:NH1	2.73	0.51
1:C:482:ALA:CB	1:C:515:TYR:CE1	2.91	0.51
1:F:546:ARG:CG	1:F:546:ARG:NH1	2.72	0.51
2:J:28:PRO:HG3	1:L:467:ARG:NH2	2.24	0.51
1:K:423:ARG:HG3	1:K:442:SER:HB2	1.93	0.51
3:P:127:GLY:N	3:P:192:LEU:O	2.35	0.51
4:U:39:LEU:HD23	4:U:39:LEU:C	2.35	0.51
1:B:445:LYS:CB	1:B:445:LYS:NZ	2.72	0.51
1:B:498:GLU:O	1:B:498:GLU:HG2	2.11	0.51
1:H:453:ASP:OD1	1:H:455:TYR:OH	2.18	0.51
1:K:510:GLN:OE1	1:K:510:GLN:HA	2.09	0.51
3:P:368:LEU:CD1	3:P:378:PRO:HG2	2.39	0.51
1:A:380:ILE:H	1:A:393:HIS:CD2	2.29	0.51
1:G:352:PRO:HD3	1:G:365:LEU:HD13	1.92	0.51
3:P:132:ILE:HD12	3:P:187:VAL:O	2.11	0.51
3:P:239:CYS:HB2	3:P:290:PHE:CE1	2.46	0.51
3:P:248:VAL:HG12	3:P:311:SER:N	2.26	0.51
1:F:427:THR:HG23	1:F:438:LYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:514:ARG:CA	1:L:514:ARG:NH1	2.73	0.51
3:P:60:TYR:HB3	3:P:64:ALA:HB3	1.93	0.51
3:P:368:LEU:CG	3:P:378:PRO:HG2	2.40	0.51
3:P:391:TYR:N	3:P:391:TYR:CD1	2.79	0.51
4:S:29:LEU:HD22	4:S:95:THR:CG2	2.27	0.51
4:U:72:TYR:HA	4:U:75:ARG:HD3	1.92	0.51
1:A:400:HIS:HD2	1:A:406:SER:HB2	1.76	0.51
1:L:365:LEU:HD23	1:L:413:ILE:HD11	1.93	0.51
3:P:314:GLN:CA	3:P:314:GLN:NE2	2.72	0.51
1:D:393:HIS:CD2	1:D:393:HIS:H	2.27	0.50
1:G:502:THR:HA	1:G:519:SER:HA	1.93	0.50
1:L:523:VAL:HG11	1:L:534:TYR:CE1	2.46	0.50
1:L:540:HIS:HB3	1:L:543:LEU:CG	2.32	0.50
3:P:446:LEU:CD2	3:P:538:ALA:CA	2.90	0.50
3:P:470:PHE:O	3:P:473:TYR:CE2	2.64	0.50
1:G:443:ARG:C	1:G:443:ARG:CD	2.84	0.50
1:K:537:VAL:HG12	1:K:549:GLU:HG2	1.93	0.50
3:P:253:CYS:HB2	3:P:306:LEU:HB2	1.93	0.50
4:U:41:GLU:C	4:U:43:HIS:N	2.69	0.50
1:A:477:THR:HG22	1:A:508:GLU:OE2	2.12	0.50
1:G:450:HIS:CD2	1:G:514:ARG:NH1	2.80	0.50
2:J:21:ILE:CG1	1:L:555:SER:CB	2.90	0.50
1:K:516:PHE:CD1	1:K:516:PHE:C	2.88	0.50
3:P:243:PRO:CA	3:P:246:ALA:HB2	2.37	0.50
3:P:368:LEU:C	3:P:378:PRO:HD3	2.36	0.50
3:P:529:LYS:CG	3:P:534:TYR:HE2	2.17	0.50
4:R:28:GLU:HG3	4:R:29:LEU:H	1.76	0.50
4:U:48:LEU:HD22	4:U:89:VAL:HG21	1.93	0.50
1:C:384:ARG:NH2	1:C:422:GLU:O	2.44	0.50
1:D:421:GLY:CA	1:D:445:LYS:HZ1	2.11	0.50
1:E:484:VAL:O	1:E:484:VAL:HG13	2.12	0.50
1:F:523:VAL:CG1	1:F:534:TYR:OH	2.60	0.50
1:H:365:LEU:HD11	1:H:418:TRP:CZ2	2.40	0.50
1:K:477:THR:CG2	1:K:516:PHE:HB2	2.41	0.50
3:P:414:THR:HG1	3:P:417:ASP:CG	2.10	0.50
1:A:384:ARG:HG2	1:A:385:GLN:H	1.77	0.50
1:A:459:PRO:CB	1:A:470:ALA:HB1	2.41	0.50
4:S:97:SER:O	4:S:97:SER:OG	2.29	0.50
1:F:545:ASN:N	1:F:545:ASN:ND2	2.58	0.50
1:K:430:HIS:CD2	1:K:432:ASP:HB2	2.47	0.50
1:K:490:GLN:O	1:K:490:GLN:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:448:VAL:HG23	3:P:463:PRO:CG	2.41	0.50
3:P:470:PHE:O	3:P:473:TYR:CD2	2.64	0.50
4:V:48:LEU:HD21	4:V:102:TYR:CG	2.47	0.50
1:A:560:THR:O	1:B:560:THR:N	2.43	0.50
1:L:511:ALA:O	1:L:514:ARG:HG2	2.11	0.50
3:P:148:TYR:HD2	3:P:202:CYS:HA	1.77	0.50
3:P:478:CYS:HA	3:P:487:ALA:HA	1.93	0.50
1:A:402:ASN:OD1	1:A:404:THR:OG1	2.22	0.50
1:F:427:THR:HG22	1:F:436:PRO:HB2	1.94	0.50
2:J:115:LEU:CD1	2:J:124:VAL:HG21	2.25	0.50
3:P:245:VAL:HG11	3:P:320:PRO:HG2	1.93	0.50
3:P:351:VAL:HG11	3:P:435:VAL:HG11	1.94	0.50
1:B:445:LYS:HZ3	1:B:445:LYS:CB	2.25	0.50
1:D:514:ARG:HH11	4:V:66:ASN:HD21	1.60	0.50
3:P:526:CYS:O	3:P:538:ALA:HB2	2.11	0.50
4:R:36:LYS:HE2	4:R:86:LEU:HG	1.93	0.50
1:A:359:LEU:CD1	2:J:117:TYR:CG	2.81	0.49
1:C:456:LEU:HD11	1:C:536:CYS:HB3	1.93	0.49
1:G:467:ARG:HD3	1:G:525:GLU:OE1	2.12	0.49
1:K:510:GLN:HG3	1:L:522:THR:HG21	1.72	0.49
3:P:476:TYR:O	3:P:527:GLY:N	2.45	0.49
1:C:484:VAL:O	1:C:484:VAL:HG13	2.11	0.49
1:H:480:SER:HB3	1:H:481:PRO:HD3	1.94	0.49
1:K:464:LEU:HD13	1:K:525:GLU:CG	2.42	0.49
1:K:473:THR:O	1:K:473:THR:HG22	2.12	0.49
1:K:479:PHE:HB2	1:K:540:HIS:CE1	2.47	0.49
3:P:24:TYR:HD2	3:P:30:ASN:HB3	1.75	0.49
3:P:368:LEU:CA	3:P:378:PRO:HD3	2.42	0.49
4:U:34:THR:HG22	4:U:90:GLU:HG3	1.94	0.49
1:A:489:MET:HB2	1:A:535:THR:OG1	2.13	0.49
1:F:449:LEU:CA	1:F:480:SER:HB2	2.37	0.49
1:K:459:PRO:HG3	1:K:470:ALA:HB1	1.95	0.49
4:R:81:TYR:HB2	4:R:86:LEU:HB2	1.95	0.49
1:A:485:PHE:CE2	2:J:115:LEU:HD22	2.41	0.49
1:L:484:VAL:HA	1:L:539:ALA:O	2.12	0.49
3:P:466:PHE:CE2	3:P:507:ARG:HB2	2.47	0.49
1:A:457:LEU:HB2	1:A:473:THR:CG2	2.42	0.49
1:B:496:SER:HB2	1:B:497:PRO:HD2	1.95	0.49
1:C:480:SER:O	1:C:540:HIS:HE1	1.93	0.49
1:K:566:LEU:HD23	1:K:566:LEU:C	2.37	0.49
3:P:310:HIS:CE1	3:P:316:GLN:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:50:ARG:NH1	4:U:100:GLY:CA	2.64	0.49
1:B:543:LEU:HD11	1:B:548:THR:HG22	1.95	0.49
1:E:514:ARG:NH1	1:E:514:ARG:HG2	2.27	0.49
1:G:489:MET:HA	1:G:494:PRO:HA	1.94	0.49
1:L:514:ARG:CB	1:L:514:ARG:NH1	2.72	0.49
3:P:351:VAL:HB	3:P:408:VAL:HG22	1.95	0.49
3:P:361:LYS:C	3:P:361:LYS:CD	2.85	0.49
4:V:78:LEU:HB2	4:V:87:PHE:CE1	2.47	0.49
1:H:573:GLY:O	1:H:574:THR:C	2.56	0.49
1:K:463:GLN:O	1:K:463:GLN:HG2	2.09	0.49
4:R:50:ARG:NH1	4:R:51:GLU:O	2.45	0.49
4:S:46:ILE:HD13	4:S:87:PHE:CD2	2.47	0.49
4:V:75:ARG:NH2	4:V:95:THR:H	2.11	0.49
1:C:363:THR:OG1	1:C:413:ILE:O	2.30	0.49
1:C:502:THR:HA	1:C:519:SER:HA	1.94	0.49
1:D:376:ASP:HB3	1:D:430:HIS:NE2	2.28	0.49
1:D:376:ASP:OD1	1:D:377:SER:N	2.45	0.49
1:E:514:ARG:HG2	1:E:514:ARG:HH11	1.78	0.49
1:G:378:VAL:HG21	1:G:405:PHE:HE2	1.77	0.49
1:K:380:ILE:HB	1:K:393:HIS:CD2	2.48	0.49
4:U:32:SER:HA	4:U:91:VAL:O	2.13	0.49
1:A:423:ARG:CZ	1:A:425:THR:HB	2.43	0.49
1:B:481:PRO:HD2	1:B:540:HIS:CE1	2.48	0.49
1:B:537:VAL:HG12	1:B:549:GLU:HG2	1.95	0.49
1:C:463:GLN:O	1:C:466:LEU:HB2	2.12	0.49
1:E:511:ALA:CB	1:E:514:ARG:HG3	2.38	0.49
3:P:99:ARG:HG3	3:P:99:ARG:O	2.11	0.49
3:P:340:VAL:HG11	3:P:436:GLU:CG	2.43	0.49
3:P:368:LEU:CB	3:P:378:PRO:CG	2.78	0.49
3:P:400:GLU:HA	3:P:402:GLY:N	2.27	0.49
4:U:94:LEU:C	4:U:96:GLU:N	2.69	0.49
1:B:354:PHE:CZ	1:B:546:ARG:CG	2.96	0.49
1:F:554:LYS:C	1:F:554:LYS:CD	2.85	0.49
1:K:533:THR:HG22	1:K:551:THR:CG2	2.43	0.49
4:R:20:LEU:CD2	4:R:20:LEU:C	2.86	0.49
1:K:346:ARG:O	1:K:370:THR:OG1	2.24	0.48
1:K:487:GLN:HB3	1:K:537:VAL:HG23	1.95	0.48
3:P:263:VAL:HG21	3:P:314:GLN:HE22	1.78	0.48
3:P:286:LYS:C	3:P:286:LYS:CD	2.85	0.48
1:F:561:LEU:HD12	1:F:561:LEU:HA	1.52	0.48
1:H:572:ALA:HB3	1:H:574:THR:HG22	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:463:GLN:HA	1:K:466:LEU:HD23	1.93	0.48
4:S:50:ARG:N	4:S:59:GLY:O	2.45	0.48
1:C:481:PRO:O	1:C:481:PRO:HG2	2.13	0.48
1:D:510:GLN:OE1	1:D:510:GLN:HA	2.14	0.48
1:K:386:ASN:OD1	1:K:387:GLY:N	2.46	0.48
1:K:545:ASN:ND2	1:K:545:ASN:N	2.60	0.48
3:P:29:VAL:O	3:P:33:THR:HG23	2.13	0.48
3:P:395:LEU:CB	3:P:410:LEU:HD11	2.20	0.48
3:P:411:ASN:ND2	3:P:525:TRP:CH2	2.81	0.48
4:S:39:LEU:HD23	4:S:85:ASN:HA	1.94	0.48
4:S:49:CYS:HB3	4:S:58:CYS:HB2	1.44	0.48
1:A:428:VAL:HG22	1:A:437:LEU:H	1.78	0.48
1:B:389:ALA:C	1:B:391:LYS:H	2.21	0.48
1:E:459:PRO:HD3	1:E:472:ILE:HG13	1.96	0.48
1:G:491:ARG:HD2	4:U:44:VAL:HG11	1.95	0.48
1:L:538:VAL:HG12	1:L:548:THR:HB	1.94	0.48
3:P:251:PHE:CZ	3:P:308:GLY:O	2.58	0.48
4:U:50:ARG:HH12	4:U:100:GLY:CA	2.24	0.48
1:B:414:CYS:SG	1:C:416:ASP:HB3	2.49	0.48
1:F:470:ALA:HB3	1:F:523:VAL:HG23	1.95	0.48
1:F:554:LYS:O	1:F:554:LYS:HD3	2.13	0.48
1:L:540:HIS:HB3	1:L:543:LEU:CD1	2.44	0.48
4:U:37:CYS:HB3	4:U:87:PHE:O	2.13	0.48
4:V:86:LEU:HD12	4:V:87:PHE:H	1.79	0.48
1:C:562:TYR:CD2	1:H:568:MET:HE2	2.48	0.48
1:C:566:LEU:HD13	1:D:566:LEU:CD2	2.43	0.48
1:E:508:GLU:HB2	1:E:514:ARG:O	2.14	0.48
3:P:366:TRP:O	3:P:380:LEU:N	2.45	0.48
1:E:367:CYS:N	1:E:382:TRP:HH2	2.11	0.48
1:F:414:CYS:HB2	1:F:418:TRP:CD1	2.49	0.48
1:G:467:ARG:CG	1:G:467:ARG:NH1	2.72	0.48
1:K:467:ARG:NH2	4:R:111:ASP:OD1	2.46	0.48
1:L:487:GLN:C	1:L:537:VAL:HG12	2.37	0.48
3:P:243:PRO:C	3:P:246:ALA:HB2	2.39	0.48
3:P:447:LYS:HB2	3:P:464:CYS:CA	2.44	0.48
1:E:491:ARG:CG	4:V:44:VAL:HG11	2.44	0.48
1:H:565:SER:HB3	1:K:565:SER:HB2	1.96	0.48
1:L:345:ILE:HA	1:L:433:LEU:HD11	1.96	0.48
1:L:576:TYR:HD2	1:L:576:TYR:N	2.10	0.48
4:R:22:GLU:HA	4:R:117:LYS:C	2.35	0.48
4:U:20:LEU:HG	4:U:117:LYS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:80:GLN:OE1	4:U:87:PHE:HD1	1.95	0.48
1:D:514:ARG:HH21	1:D:514:ARG:CG	2.23	0.48
1:H:514:ARG:HH12	4:S:65:THR:HG23	1.79	0.48
1:H:554:LYS:HZ2	1:H:558:LYS:HZ2	1.52	0.48
1:H:554:LYS:HZ2	1:H:558:LYS:NZ	1.94	0.48
4:S:78:LEU:HD11	4:S:87:PHE:HD2	1.78	0.48
4:V:47:TYR:OH	4:V:113:GLY:HA3	2.14	0.48
1:A:531:GLY:HA2	1:A:554:LYS:HB2	1.96	0.48
1:B:461:ARG:HH22	1:K:570:ASP:HB3	1.79	0.48
1:B:472:ILE:HG21	1:B:552:VAL:HG11	1.96	0.48
1:D:348:PHE:HD2	1:D:370:THR:HB	1.79	0.48
1:K:521:LEU:C	1:K:521:LEU:CD2	2.85	0.48
1:B:476:VAL:HG11	1:B:538:VAL:HG21	1.96	0.47
1:C:379:THR:HB	1:C:429:THR:OG1	2.14	0.47
1:D:535:THR:HG22	1:D:551:THR:HB	1.96	0.47
4:R:47:TYR:OH	4:R:110:THR:O	2.32	0.47
4:R:62:VAL:HG12	4:R:68:ILE:HG22	1.94	0.47
1:B:384:ARG:HB3	1:B:387:GLY:N	2.29	0.47
1:D:384:ARG:HH11	1:D:390:VAL:HA	1.79	0.47
1:E:457:LEU:HB2	1:E:473:THR:CG2	2.44	0.47
1:E:489:MET:SD	1:E:494:PRO:N	2.87	0.47
1:L:449:LEU:CA	1:L:480:SER:HB3	2.44	0.47
3:P:120:LYS:O	3:P:216:ASP:N	2.47	0.47
3:P:286:LYS:HD3	3:P:286:LYS:O	2.12	0.47
3:P:445:ASN:CB	3:P:536:GLU:OE2	2.62	0.47
4:R:46:ILE:HG22	4:R:64:THR:HG21	1.95	0.47
4:S:105:GLY:HA3	4:S:114:LYS:HA	1.95	0.47
1:D:359:LEU:HD21	1:D:485:PHE:CZ	2.48	0.47
1:K:445:LYS:CE	1:K:445:LYS:CA	2.84	0.47
3:P:466:PHE:CD2	3:P:466:PHE:N	2.82	0.47
1:B:347:VAL:HG22	1:B:369:VAL:HG13	1.95	0.47
1:B:363:THR:HG21	1:B:418:TRP:HB2	1.96	0.47
1:C:382:TRP:CH2	1:C:426:CYS:HB2	2.50	0.47
3:P:431:TRP:CD1	3:P:431:TRP:H	2.31	0.47
4:V:75:ARG:HG3	4:V:76:VAL:HG13	1.97	0.47
1:D:493:GLN:HA	1:D:494:PRO:HD2	1.45	0.47
1:F:524:SER:OG	1:F:527:GLU:CD	2.58	0.47
2:J:42:PRO:HG3	2:J:102:THR:CG2	2.43	0.47
1:K:529:ASN:HA	1:K:554:LYS:HD3	1.97	0.47
1:K:556:THR:HG23	1:K:556:THR:O	2.14	0.47
1:L:424:PHE:CD1	1:L:441:ILE:HD11	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:452:PRO:HB3	1:L:479:PHE:CD1	2.48	0.47
1:L:480:SER:HB2	1:L:481:PRO:HD3	1.97	0.47
1:A:466:LEU:N	1:A:466:LEU:HD13	2.29	0.47
1:E:490:GLN:HB3	1:E:534:TYR:HA	1.96	0.47
1:F:545:ASN:CB	1:G:358:PHE:HZ	2.27	0.47
1:G:443:ARG:HA	1:G:444:PRO:HD2	1.52	0.47
1:G:473:THR:O	1:G:473:THR:OG1	2.23	0.47
1:H:379:THR:HG21	1:H:429:THR:OG1	2.15	0.47
1:K:489:MET:HE2	1:K:489:MET:HB2	1.58	0.47
1:K:526:GLU:HA	1:K:529:ASN:OD1	2.14	0.47
1:L:417:ASP:O	1:L:420:SER:OG	2.31	0.47
4:S:39:LEU:HD23	4:S:85:ASN:C	2.39	0.47
1:A:491:ARG:NH1	1:A:491:ARG:CG	2.73	0.47
1:B:451:ARG:NH1	1:B:451:ARG:CB	2.72	0.47
1:C:533:THR:O	1:C:552:VAL:O	2.33	0.47
1:G:468:GLU:O	1:G:525:GLU:HB2	2.15	0.47
1:H:516:PHE:CD2	1:H:516:PHE:C	2.93	0.47
1:K:416:ASP:OD1	1:K:417:ASP:N	2.47	0.47
3:P:56:VAL:O	3:P:56:VAL:HG23	2.14	0.47
3:P:445:ASN:HB2	3:P:536:GLU:OE2	2.14	0.47
3:P:530:GLN:NE2	3:P:530:GLN:C	2.73	0.47
4:S:81:TYR:HB3	4:S:84:LYS:HB2	1.96	0.47
1:E:489:MET:O	1:E:535:THR:CB	2.63	0.47
1:H:552:VAL:HG13	1:H:556:THR:HG21	1.95	0.47
2:J:21:ILE:HD11	1:L:555:SER:CA	2.44	0.47
3:P:462:VAL:HB	3:P:509:VAL:C	2.38	0.47
3:P:526:CYS:CB	3:P:538:ALA:HB3	2.44	0.47
4:S:39:LEU:HD21	4:S:41:GLU:HG2	1.97	0.47
1:E:350:ILE:HB	1:E:366:THR:HB	1.96	0.47
1:E:453:ASP:OD2	1:E:455:TYR:OH	2.27	0.47
1:F:452:PRO:HD3	1:F:540:HIS:HD2	1.79	0.47
1:H:364:LYS:HB3	1:H:410:GLU:HB3	1.96	0.47
1:K:558:LYS:O	1:K:558:LYS:HG2	2.15	0.47
3:P:462:VAL:HG11	3:P:509:VAL:HG12	1.97	0.47
3:P:466:PHE:CD1	3:P:470:PHE:HZ	2.31	0.47
1:G:413:ILE:HD13	1:G:424:PHE:HZ	1.79	0.47
1:H:384:ARG:HD2	1:H:388:GLU:HB2	1.97	0.47
1:K:537:VAL:CG1	1:K:549:GLU:HG2	2.44	0.47
3:P:143:LYS:O	3:P:145:LYS:HG3	2.14	0.47
4:S:105:GLY:HA2	4:S:115:THR:HG23	1.96	0.47
4:V:121:ASN:HD21	4:V:123:HIS:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ARG:HH11	1:A:514:ARG:CG	2.28	0.46
1:B:410:GLU:H	1:B:410:GLU:HG3	1.47	0.46
1:F:546:ARG:HH11	1:F:546:ARG:HG3	1.79	0.46
1:G:493:GLN:HG2	4:U:42:MET:O	2.15	0.46
1:G:521:LEU:HD21	1:G:534:TYR:CE2	2.50	0.46
1:H:474:CYS:HB2	1:H:488:TRP:CZ2	2.50	0.46
1:K:528:TRP:HH2	1:K:552:VAL:HG22	1.79	0.46
1:L:423:ARG:HH21	1:L:444:PRO:HB3	1.80	0.46
1:L:445:LYS:H	1:L:445:LYS:HG3	1.48	0.46
3:P:412:GLN:NE2	3:P:412:GLN:C	2.73	0.46
3:P:462:VAL:O	3:P:509:VAL:N	2.47	0.46
4:R:116:GLN:NE2	4:R:116:GLN:C	2.73	0.46
1:C:461:ARG:NH1	1:C:465:ASN:CG	2.69	0.46
1:E:423:ARG:HA	1:E:442:SER:HB3	1.96	0.46
1:E:467:ARG:NH1	4:U:111:ASP:OD2	2.48	0.46
1:K:464:LEU:HD13	1:K:464:LEU:HA	1.60	0.46
3:P:224:PRO:HG3	3:P:304:ARG:HH12	1.80	0.46
3:P:352:LEU:HD21	3:P:401:PRO:HG2	1.97	0.46
1:C:526:GLU:CD	1:C:526:GLU:N	2.73	0.46
1:E:468:GLU:OE2	4:U:45:ARG:NH1	2.43	0.46
1:F:449:LEU:HA	1:F:481:PRO:HD2	1.97	0.46
1:L:478:GLY:O	1:L:515:TYR:N	2.39	0.46
3:P:38:CYS:HB2	3:P:46:CYS:HB3	1.52	0.46
4:R:45:ARG:HA	4:R:64:THR:OG1	2.16	0.46
4:S:79:LYS:HD3	4:S:80:GLN:N	2.30	0.46
1:B:450:HIS:C	1:B:542:ALA:HB1	2.39	0.46
1:D:391:LYS:NZ	1:D:394:THR:OG1	2.42	0.46
1:G:363:THR:OG1	1:G:413:ILE:HG13	2.15	0.46
1:K:414:CYS:SG	1:K:415:GLU:N	2.88	0.46
4:S:39:LEU:CD2	4:S:85:ASN:CA	2.94	0.46
1:E:535:THR:HG23	1:E:550:ARG:O	2.15	0.46
1:G:382:TRP:CG	1:G:411:ALA:HB2	2.50	0.46
1:H:532:GLU:O	1:H:553:ASP:HB2	2.14	0.46
3:P:365:TYR:CE1	3:P:379:LEU:HD13	2.50	0.46
3:P:395:LEU:CB	3:P:410:LEU:HD12	2.41	0.46
4:R:22:GLU:CG	4:R:119:THR:HG22	2.45	0.46
1:A:575:CYS:CB	2:J:7:LEU:HD23	2.46	0.46
1:F:479:PHE:CD1	1:F:479:PHE:N	2.84	0.46
1:F:506:MET:O	1:F:516:PHE:CE2	2.68	0.46
1:G:535:THR:HG22	1:G:551:THR:OG1	2.15	0.46
1:H:571:THR:O	1:H:572:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:484:VAL:HG23	1:K:540:HIS:CG	2.49	0.46
1:L:451:ARG:HH12	1:L:544:PRO:HG3	1.80	0.46
4:V:36:LYS:HG2	4:V:86:LEU:CD1	2.46	0.46
4:V:47:TYR:HA	4:V:63:SER:HA	1.97	0.46
4:V:86:LEU:HG	4:V:88:LEU:HD22	1.97	0.46
1:A:510:GLN:CD	1:A:510:GLN:C	2.84	0.46
1:B:570:ASP:HB2	1:C:571:THR:HA	1.97	0.46
1:D:421:GLY:CA	1:D:445:LYS:HZ2	2.10	0.46
1:F:413:ILE:HG13	1:F:414:CYS:H	1.80	0.46
1:F:496:SER:OG	1:F:499:LYS:NZ	2.48	0.46
1:F:502:THR:OG1	1:F:519:SER:HB2	2.08	0.46
1:H:352:PRO:HD2	1:H:418:TRP:CH2	2.51	0.46
1:K:574:THR:OG1	1:K:575:CYS:N	2.49	0.46
3:P:344:VAL:HG21	3:P:443:GLU:O	2.16	0.46
1:A:390:VAL:HG13	1:A:391:LYS:N	2.31	0.46
1:D:423:ARG:HD3	1:D:440:THR:HG23	1.98	0.46
1:G:372:LEU:HD11	1:G:433:LEU:HB2	1.97	0.46
1:H:554:LYS:CE	1:H:558:LYS:HZ1	2.14	0.46
1:L:457:LEU:HB2	1:L:473:THR:OG1	2.15	0.46
3:P:351:VAL:CG1	3:P:435:VAL:HG11	2.46	0.46
3:P:368:LEU:HB2	3:P:378:PRO:HG3	1.89	0.46
3:P:450:GLY:HA2	3:P:462:VAL:HA	1.97	0.46
4:V:28:GLU:O	4:V:94:LEU:HB3	2.15	0.46
1:D:382:TRP:CZ3	1:D:424:PHE:HB3	2.51	0.46
1:E:443:ARG:HG3	1:E:444:PRO:HD2	1.97	0.46
1:E:481:PRO:HD2	1:E:540:HIS:CE1	2.51	0.46
1:E:509:PRO:HG3	1:F:501:VAL:HG12	1.97	0.46
1:G:443:ARG:NE	1:G:443:ARG:C	2.73	0.46
1:H:554:LYS:NZ	1:H:558:LYS:HZ3	1.90	0.46
1:K:470:ALA:HB3	1:K:523:VAL:HG12	1.97	0.46
1:K:481:PRO:CG	1:K:541:GLU:OE2	2.63	0.46
1:L:506:MET:HB3	1:L:507:PRO:HD2	1.97	0.46
3:P:275:PHE:HB3	3:P:279:ILE:HD12	1.98	0.46
4:R:35:ILE:HB	4:R:89:VAL:HB	1.98	0.46
4:S:39:LEU:HG	4:S:41:GLU:HG2	1.98	0.46
4:V:72:TYR:HA	4:V:75:ARG:HD3	1.97	0.46
1:D:363:THR:OG1	1:D:413:ILE:O	2.30	0.46
1:H:486:VAL:HG11	1:H:519:SER:OG	2.16	0.46
1:K:528:TRP:CD1	1:K:528:TRP:O	2.69	0.46
1:L:424:PHE:O	1:L:441:ILE:HG13	2.14	0.46
1:L:543:LEU:HA	1:L:544:PRO:HD3	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:237:PHE:O	3:P:291:SER:HA	2.16	0.46
4:S:61:VAL:HG13	4:S:72:TYR:CG	2.51	0.46
1:A:478:GLY:C	1:A:514:ARG:HH12	2.17	0.45
1:A:510:GLN:CD	1:A:510:GLN:N	2.73	0.45
1:E:400:HIS:CD2	1:E:402:ASN:H	2.34	0.45
1:F:500:TYR:CD1	1:F:500:TYR:O	2.69	0.45
1:L:540:HIS:CE1	1:L:542:ALA:HB2	2.51	0.45
3:P:271:ARG:HB2	3:P:372:ALA:HB3	1.97	0.45
4:R:46:ILE:HG22	4:R:64:THR:HG22	1.99	0.45
1:A:352:PRO:HD3	1:A:365:LEU:HD23	1.97	0.45
1:C:555:SER:HA	1:C:558:LYS:HD2	1.96	0.45
1:F:415:GLU:O	1:F:416:ASP:C	2.59	0.45
1:H:572:ALA:C	1:H:574:THR:H	2.23	0.45
1:K:378:VAL:HG23	1:K:380:ILE:HG12	1.97	0.45
1:K:568:MET:HE3	1:K:568:MET:HB2	1.62	0.45
1:L:382:TRP:CZ3	1:L:426:CYS:HB2	2.51	0.45
3:P:368:LEU:CB	3:P:378:PRO:HG2	2.43	0.45
4:S:36:LYS:HD3	4:S:86:LEU:HD13	1.98	0.45
4:S:102:TYR:N	4:S:118:VAL:O	2.34	0.45
1:A:356:SER:N	2:J:117:TYR:CZ	2.84	0.45
1:A:400:HIS:HB3	1:A:404:THR:H	1.82	0.45
1:A:476:VAL:O	1:A:516:PHE:HA	2.16	0.45
1:A:516:PHE:CD2	1:A:516:PHE:O	2.69	0.45
1:A:565:SER:HB2	2:J:59:ARG:HA	1.99	0.45
1:A:573:GLY:O	1:A:574:THR:C	2.59	0.45
1:B:349:ALA:HB1	1:B:382:TRP:CZ3	2.51	0.45
1:E:501:VAL:HG21	1:F:509:PRO:HD3	1.99	0.45
1:F:363:THR:HG23	1:F:415:GLU:HG2	1.97	0.45
1:F:477:THR:HG22	1:F:516:PHE:HB2	1.98	0.45
1:F:481:PRO:HG2	1:F:481:PRO:O	2.16	0.45
1:H:418:TRP:HE3	1:H:443:ARG:HB2	1.80	0.45
1:L:372:LEU:HG	1:L:407:ALA:HB3	1.96	0.45
3:P:94:LEU:HB2	3:P:101:LEU:HD23	1.99	0.45
4:V:48:LEU:HD13	4:V:89:VAL:HG11	1.97	0.45
1:E:379:THR:HB	1:E:393:HIS:HB3	1.99	0.45
1:K:558:LYS:HZ1	1:L:461:ARG:HE	1.64	0.45
1:L:456:LEU:HD11	1:L:488:TRP:CH2	2.52	0.45
1:L:493:GLN:NE2	1:L:494:PRO:O	2.49	0.45
1:L:514:ARG:HH11	1:L:514:ARG:CA	2.30	0.45
1:L:514:ARG:NH1	1:L:514:ARG:HA	2.31	0.45
3:P:491:GLN:O	3:P:507:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:TYR:CD2	1:A:500:TYR:C	2.94	0.45
1:C:526:GLU:O	1:C:530:THR:HG21	2.15	0.45
1:D:363:THR:OG1	1:D:363:THR:O	2.34	0.45
1:E:489:MET:CE	1:E:494:PRO:HD3	2.44	0.45
1:F:382:TRP:HB2	1:F:392:THR:HA	1.98	0.45
1:F:438:LYS:HE2	1:F:438:LYS:HB2	1.36	0.45
1:H:454:VAL:CG2	1:H:538:VAL:HG21	2.47	0.45
4:S:47:TYR:CZ	4:S:110:THR:HA	2.51	0.45
4:V:112:ARG:CZ	4:V:112:ARG:CB	2.94	0.45
1:A:378:VAL:HG12	1:A:393:HIS:NE2	2.32	0.45
1:C:566:LEU:HD22	1:H:564:VAL:HG21	1.99	0.45
1:D:493:GLN:N	1:D:493:GLN:CD	2.71	0.45
1:F:420:SER:HB2	1:F:421:GLY:H	1.50	0.45
1:G:365:LEU:HB2	1:G:411:ALA:HB3	1.98	0.45
1:G:490:GLN:NE2	1:G:532:GLU:OE2	2.30	0.45
1:H:383:THR:HA	1:H:390:VAL:HG23	1.99	0.45
1:K:516:PHE:CE2	1:L:520:ILE:HD11	2.46	0.45
3:P:136:PHE:O	3:P:136:PHE:CD2	2.70	0.45
3:P:413:LEU:H	3:P:413:LEU:CD2	2.07	0.45
1:A:485:PHE:CD2	1:A:485:PHE:O	2.70	0.45
1:A:510:GLN:H	1:A:510:GLN:HE21	1.63	0.45
1:B:528:TRP:O	1:B:528:TRP:CG	2.69	0.45
1:F:365:LEU:HD23	1:F:365:LEU:HA	1.84	0.45
1:G:481:PRO:HD2	1:G:540:HIS:HE1	1.81	0.45
1:K:485:PHE:O	1:K:485:PHE:CD1	2.70	0.45
1:L:372:LEU:HB2	1:L:405:PHE:O	2.17	0.45
3:P:272:ALA:HA	3:P:273:PRO:HD3	1.57	0.45
3:P:382:ASP:OD1	3:P:386:TRP:N	2.48	0.45
1:B:345:ILE:HG22	1:B:372:LEU:HD13	1.98	0.45
1:B:365:LEU:HB3	1:B:382:TRP:NE1	2.31	0.45
1:D:416:ASP:OD2	1:D:417:ASP:N	2.50	0.45
1:F:449:LEU:CA	1:F:480:SER:CB	2.93	0.45
1:F:523:VAL:HG11	1:F:534:TYR:OH	2.16	0.45
1:F:543:LEU:CD2	1:F:548:THR:CG2	2.94	0.45
1:K:468:GLU:HA	4:R:67:PHE:CE2	2.51	0.45
3:P:290:PHE:CD1	3:P:290:PHE:O	2.69	0.45
1:A:545:ASN:C	1:A:547:VAL:H	2.24	0.45
1:C:525:GLU:N	1:C:525:GLU:CD	2.72	0.45
1:D:495:LEU:HD22	1:D:495:LEU:HA	1.70	0.45
1:H:560:THR:CB	1:K:560:THR:O	2.65	0.45
3:P:448:VAL:HG23	3:P:463:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:35:ILE:O	4:R:88:LEU:HA	2.17	0.45
1:A:500:TYR:HA	1:A:520:ILE:O	2.17	0.45
1:E:384:ARG:HD3	1:E:388:GLU:HB3	1.99	0.45
1:E:543:LEU:HD13	1:E:548:THR:OG1	2.15	0.45
1:F:536:CYS:O	1:F:549:GLU:HB2	2.17	0.45
1:K:485:PHE:O	1:K:485:PHE:CG	2.69	0.45
3:P:99:ARG:HA	3:P:99:ARG:HD3	1.58	0.45
3:P:173:ILE:HD13	3:P:189:ILE:HB	1.99	0.45
3:P:243:PRO:O	3:P:246:ALA:N	2.50	0.45
3:P:345:ALA:CA	3:P:413:LEU:CD1	2.74	0.45
4:V:36:LYS:HG2	4:V:86:LEU:HD11	1.98	0.45
1:B:404:THR:O	1:B:405:PHE:C	2.59	0.44
1:B:500:TYR:HA	1:B:520:ILE:O	2.17	0.44
1:C:384:ARG:HG3	1:C:385:GLN:N	2.32	0.44
1:C:568:MET:CE	1:K:564:VAL:HG21	2.47	0.44
1:G:372:LEU:HD21	1:G:433:LEU:HD12	1.97	0.44
1:G:480:SER:OG	1:G:481:PRO:HD3	2.16	0.44
3:P:127:GLY:HA2	3:P:191:GLN:HA	1.99	0.44
3:P:149:LYS:HG2	3:P:200:TYR:CE1	2.52	0.44
3:P:526:CYS:HB3	3:P:538:ALA:CB	2.45	0.44
1:B:451:ARG:HB2	1:B:451:ARG:CZ	2.45	0.44
1:B:528:TRP:O	1:B:528:TRP:CD2	2.70	0.44
1:C:509:PRO:HG2	1:D:522:THR:HG21	1.98	0.44
1:F:471:THR:CG2	1:F:522:THR:HG23	2.47	0.44
1:G:363:THR:OG1	1:G:414:CYS:O	2.29	0.44
2:J:117:TYR:CG	2:J:117:TYR:O	2.69	0.44
3:P:149:LYS:HD2	3:P:151:ILE:HG21	1.99	0.44
3:P:310:HIS:O	3:P:310:HIS:CG	2.70	0.44
4:U:47:TYR:CE2	4:U:110:THR:HG23	2.53	0.44
1:A:514:ARG:CD	1:A:514:ARG:N	2.78	0.44
1:B:461:ARG:NE	1:L:570:ASP:OD2	2.51	0.44
1:D:423:ARG:HH11	1:D:425:THR:HB	1.83	0.44
1:E:540:HIS:CD2	1:E:542:ALA:H	2.34	0.44
1:G:500:TYR:CD1	1:G:500:TYR:C	2.95	0.44
1:K:476:VAL:HG12	1:K:479:PHE:CD1	2.53	0.44
3:P:439:ILE:CD1	3:P:439:ILE:H	2.22	0.44
3:P:480:TRP:C	3:P:480:TRP:CD2	2.93	0.44
4:V:104:CYS:HB2	4:V:116:GLN:HB3	1.98	0.44
1:A:372:LEU:HD21	1:A:405:PHE:HD2	1.83	0.44
1:A:386:ASN:OD1	1:A:388:GLU:HG2	2.17	0.44
1:D:452:PRO:HG3	1:D:479:PHE:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ASP:HB3	1:E:424:PHE:CZ	2.52	0.44
1:F:456:LEU:HD13	1:F:550:ARG:HB2	1.99	0.44
1:H:367:CYS:HB2	1:H:380:ILE:HG13	1.99	0.44
1:K:345:ILE:HG22	1:K:372:LEU:HD21	1.98	0.44
1:K:428:VAL:HG12	1:K:430:HIS:HB2	2.00	0.44
1:L:511:ALA:O	1:L:514:ARG:HG3	2.16	0.44
3:P:31:ARG:HD2	3:P:70:PRO:HB3	1.98	0.44
3:P:287:ASP:HB2	3:P:288:GLY:H	1.47	0.44
3:P:368:LEU:CB	3:P:378:PRO:HD2	2.43	0.44
3:P:411:ASN:HD22	3:P:537:THR:HG21	1.83	0.44
3:P:414:THR:OG1	3:P:417:ASP:CG	2.56	0.44
3:P:418:ALA:N	3:P:439:ILE:HD11	2.31	0.44
4:S:99:SER:HB2	4:S:120:LEU:HB3	1.98	0.44
4:U:22:GLU:HB2	4:U:119:THR:CA	2.47	0.44
1:C:454:VAL:CG1	1:C:474:CYS:SG	3.05	0.44
1:C:459:PRO:HG3	1:C:470:ALA:HB1	2.00	0.44
1:D:350:ILE:HB	1:D:366:THR:OG1	2.17	0.44
1:E:391:LYS:HG3	1:E:412:SER:H	1.82	0.44
1:G:347:VAL:HG22	1:G:369:VAL:HG13	1.99	0.44
1:H:575:CYS:HB2	1:K:575:CYS:HB3	1.61	0.44
3:P:471:SER:HA	3:P:475:LYS:NZ	2.22	0.44
1:B:421:GLY:H	1:B:443:ARG:NH2	2.11	0.44
1:C:371:ASP:N	1:C:404:THR:HG23	2.29	0.44
1:C:447:VAL:HG11	1:C:481:PRO:HB3	1.99	0.44
1:F:491:ARG:HE	1:F:491:ARG:HB2	1.58	0.44
1:K:493:GLN:HG3	4:S:44:VAL:HG22	2.00	0.44
3:P:526:CYS:C	3:P:538:ALA:HB3	2.42	0.44
1:B:393:HIS:CG	1:B:409:GLY:HA3	2.53	0.44
1:F:501:VAL:O	1:F:501:VAL:HG22	2.17	0.44
4:S:28:GLU:O	4:S:94:LEU:HG	2.18	0.44
4:V:112:ARG:NH1	4:V:112:ARG:HB2	2.33	0.44
1:C:346:ARG:HH21	1:C:348:PHE:HB2	1.82	0.44
1:D:447:VAL:O	1:D:447:VAL:HG22	2.18	0.44
1:E:511:ALA:HB1	1:E:514:ARG:CG	2.39	0.44
1:E:541:GLU:C	1:E:543:LEU:H	2.25	0.44
1:F:365:LEU:HG	1:F:413:ILE:HG21	2.00	0.44
1:H:562:TYR:H	1:H:562:TYR:HD2	1.64	0.44
1:K:462:GLU:HB3	1:L:455:TYR:HE1	1.83	0.44
4:V:41:GLU:OE1	4:V:82:PRO:HB3	2.18	0.44
1:A:390:VAL:O	1:A:391:LYS:HD2	2.18	0.44
1:B:426:CYS:O	1:B:438:LYS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ASN:ND2	1:B:545:ASN:C	2.75	0.44
1:F:385:GLN:HG2	1:F:422:GLU:HB2	1.99	0.44
1:B:352:PRO:HG2	1:B:418:TRP:CZ2	2.53	0.43
1:D:345:ILE:HB	1:D:372:LEU:HD13	2.00	0.43
1:E:530:THR:HG1	1:E:531:GLY:H	1.66	0.43
1:H:558:LYS:HA	1:H:559:PRO:HD3	1.79	0.43
1:K:385:GLN:HE21	1:K:423:ARG:H	1.66	0.43
3:P:47:ILE:HG13	3:P:47:ILE:O	2.17	0.43
4:R:36:LYS:O	4:R:116:GLN:HG3	2.18	0.43
4:R:46:ILE:N	4:R:64:THR:CG2	2.57	0.43
4:S:96:GLU:CD	4:S:96:GLU:C	2.86	0.43
1:A:418:TRP:CD1	1:A:443:ARG:HE	2.36	0.43
1:B:478:GLY:O	1:B:514:ARG:HG2	2.14	0.43
1:B:481:PRO:CD	1:B:540:HIS:NE2	2.72	0.43
1:E:382:TRP:CD2	1:E:411:ALA:HB2	2.53	0.43
1:F:364:LYS:HB3	1:F:364:LYS:HE3	1.80	0.43
3:P:151:ILE:HD12	3:P:152:GLY:N	2.32	0.43
4:S:19:ILE:HG22	4:S:21:PRO:HD3	2.00	0.43
4:S:37:CYS:HA	4:S:116:GLN:CD	2.32	0.43
4:V:49:CYS:HB3	4:V:103:ALA:HB3	2.00	0.43
1:A:514:ARG:NH1	1:A:514:ARG:CG	2.77	0.43
1:B:396:ILE:H	1:B:396:ILE:HG13	1.38	0.43
1:F:424:PHE:O	1:F:440:THR:HA	2.18	0.43
1:G:450:HIS:ND1	1:G:450:HIS:N	2.66	0.43
1:K:374:THR:HA	1:K:405:PHE:HB2	1.99	0.43
1:K:380:ILE:CG2	1:K:409:GLY:HA2	2.49	0.43
1:G:516:PHE:CZ	1:H:520:ILE:HD12	2.54	0.43
3:P:149:LYS:H	3:P:155:PRO:HB3	1.84	0.43
4:R:50:ARG:HG2	4:R:50:ARG:HH11	1.82	0.43
1:A:352:PRO:HD2	1:A:418:TRP:CH2	2.53	0.43
1:A:499:LYS:HB3	1:A:521:LEU:HD12	2.01	0.43
1:C:466:LEU:HD13	1:C:468:GLU:CD	2.43	0.43
1:C:508:GLU:CB	1:C:509:PRO:CD	2.90	0.43
1:E:354:PHE:HD1	1:E:357:ILE:HD11	1.84	0.43
1:F:390:VAL:HB	1:F:391:LYS:H	1.72	0.43
1:F:402:ASN:HD22	1:F:402:ASN:HA	1.49	0.43
1:F:450:HIS:HE2	1:F:514:ARG:NH1	1.99	0.43
1:H:457:LEU:HB2	1:H:473:THR:OG1	2.19	0.43
1:K:490:GLN:OE1	1:K:491:ARG:N	2.51	0.43
1:L:569:SER:HB3	1:L:572:ALA:HB2	1.99	0.43
3:P:345:ALA:O	3:P:413:LEU:CD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD12	1:A:550:ARG:O	2.15	0.43
1:B:443:ARG:CG	1:B:443:ARG:NH1	2.73	0.43
1:E:534:TYR:CD2	1:E:534:TYR:N	2.85	0.43
1:L:430:HIS:CE1	1:L:432:ASP:CB	3.01	0.43
3:P:477:TRP:CD1	3:P:526:CYS:HB2	2.52	0.43
1:A:374:THR:HG22	1:A:405:PHE:HB2	2.01	0.43
1:A:467:ARG:HE	1:A:467:ARG:HB2	1.38	0.43
1:B:400:HIS:CE1	1:B:404:THR:HG22	2.53	0.43
1:D:451:ARG:HH12	1:D:544:PRO:HD3	1.83	0.43
6:H:601:NAG:C6	6:K:601:NAG:H61	2.37	0.43
2:J:32:ILE:HG23	1:L:560:THR:HB	2.00	0.43
2:J:46:ARG:HD2	2:J:54:SER:O	2.19	0.43
1:K:405:PHE:CE2	1:K:407:ALA:HB2	2.53	0.43
1:L:450:HIS:CA	1:L:480:SER:HB2	2.40	0.43
3:P:253:CYS:SG	3:P:315:LEU:CB	2.99	0.43
1:B:384:ARG:HG2	1:B:386:ASN:H	1.83	0.43
1:B:454:VAL:HG22	1:B:454:VAL:O	2.18	0.43
1:B:496:SER:CB	1:B:497:PRO:HD2	2.42	0.43
1:B:541:GLU:C	1:B:543:LEU:H	2.27	0.43
1:B:549:GLU:O	1:B:550:ARG:NH1	2.42	0.43
1:D:380:ILE:HD12	1:D:393:HIS:CG	2.54	0.43
1:D:384:ARG:HD3	1:D:390:VAL:HG22	2.01	0.43
1:F:447:VAL:HG21	1:F:481:PRO:HB3	2.01	0.43
1:G:353:SER:O	1:G:357:ILE:HG12	2.18	0.43
2:J:29:ASN:HD21	1:L:464:LEU:C	2.26	0.43
3:P:148:TYR:HB3	3:P:155:PRO:HB3	2.01	0.43
3:P:150:GLN:OE1	3:P:201:LEU:HD23	2.18	0.43
3:P:466:PHE:CE2	3:P:475:LYS:HB3	2.53	0.43
1:B:418:TRP:HE3	1:B:419:ASN:HB2	1.83	0.43
1:B:552:VAL:HG23	1:B:556:THR:HG21	2.00	0.43
1:C:450:HIS:ND1	1:C:450:HIS:N	2.67	0.43
1:D:485:PHE:HB3	1:D:539:ALA:HB3	2.00	0.43
1:F:382:TRP:HZ3	1:F:424:PHE:O	2.02	0.43
1:F:535:THR:CG2	1:F:551:THR:HG21	2.30	0.43
1:H:520:ILE:HG21	1:H:520:ILE:HD13	1.59	0.43
3:P:128:ARG:HD3	3:P:128:ARG:HA	1.77	0.43
3:P:410:LEU:HD12	3:P:410:LEU:HA	1.88	0.43
3:P:480:TRP:O	3:P:480:TRP:CE3	2.72	0.43
1:A:526:GLU:O	1:A:530:THR:N	2.52	0.43
1:B:456:LEU:C	1:B:456:LEU:HD12	2.43	0.43
1:C:451:ARG:O	1:C:451:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:HIS:CG	1:E:401:PRO:HD2	2.54	0.43
1:F:529:ASN:OD1	1:F:530:THR:N	2.52	0.43
1:G:347:VAL:HG22	1:G:369:VAL:HA	2.00	0.43
1:G:443:ARG:C	1:G:443:ARG:HE	2.18	0.43
1:K:455:TYR:CZ	1:L:463:GLN:HB3	2.54	0.43
3:P:298:ARG:NH2	3:P:300:GLU:OE2	2.52	0.43
4:R:52:MET:CE	4:R:69:LYS:NZ	2.81	0.43
1:A:571:THR:HG21	1:B:568:MET:HE3	2.00	0.42
1:B:530:THR:O	1:B:530:THR:CG2	2.67	0.42
1:E:526:GLU:HG2	1:E:527:GLU:OE1	2.19	0.42
1:F:355:ALA:HA	1:F:485:PHE:HB2	2.00	0.42
1:K:450:HIS:CE1	1:K:514:ARG:NH1	2.87	0.42
1:L:550:ARG:HD3	1:L:550:ARG:HA	1.61	0.42
3:P:290:PHE:H	3:P:290:PHE:HD1	1.66	0.42
4:R:46:ILE:CG2	4:R:64:THR:CG2	2.96	0.42
1:A:496:SER:O	1:A:496:SER:OG	2.28	0.42
1:C:466:LEU:CD2	4:V:45:ARG:NH2	2.82	0.42
1:E:395:ASN:HB3	1:E:408:VAL:HB	2.00	0.42
1:F:376:ASP:O	1:F:377:SER:C	2.62	0.42
1:F:543:LEU:HD21	1:F:548:THR:HG21	1.99	0.42
1:H:448:ALA:HB3	1:H:480:SER:OG	2.19	0.42
1:H:529:ASN:C	1:H:531:GLY:N	2.73	0.42
2:J:21:ILE:HG13	1:L:555:SER:CB	2.48	0.42
1:K:429:THR:HA	1:K:436:PRO:HB3	2.01	0.42
1:K:475:LEU:O	1:K:475:LEU:HG	2.19	0.42
1:K:554:LYS:HB3	1:K:554:LYS:HE3	1.81	0.42
4:S:39:LEU:HD22	4:S:85:ASN:C	2.40	0.42
4:U:28:GLU:HG3	4:U:30:GLY:H	1.84	0.42
1:B:452:PRO:HG2	1:B:452:PRO:O	2.19	0.42
1:B:478:GLY:HA2	1:B:514:ARG:HG2	2.00	0.42
1:E:457:LEU:HB2	1:E:473:THR:HG23	2.02	0.42
3:P:334:ILE:HG23	3:P:431:TRP:CE3	2.54	0.42
1:B:414:CYS:SG	1:B:415:GLU:N	2.92	0.42
1:C:347:VAL:HG22	1:C:369:VAL:HG23	2.01	0.42
1:E:474:CYS:HB2	1:E:488:TRP:CZ2	2.54	0.42
1:E:543:LEU:HD23	1:E:543:LEU:HA	1.61	0.42
1:F:449:LEU:H	1:F:449:LEU:CD2	2.30	0.42
1:H:445:LYS:HE2	1:H:445:LYS:HB3	1.56	0.42
1:H:481:PRO:HD2	1:H:540:HIS:CE1	2.55	0.42
4:R:48:LEU:HD22	4:R:89:VAL:HG21	2.01	0.42
1:A:520:ILE:HD12	1:B:516:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:TRP:HB3	1:B:419:ASN:H	1.48	0.42
1:B:540:HIS:O	1:B:543:LEU:HB2	2.19	0.42
1:C:459:PRO:HD2	1:C:528:TRP:CZ2	2.54	0.42
1:D:508:GLU:HB3	1:D:514:ARG:O	2.19	0.42
1:G:413:ILE:HD13	1:G:424:PHE:CZ	2.54	0.42
1:G:561:LEU:HA	1:G:561:LEU:HD23	1.76	0.42
2:J:107:LYS:HB3	2:J:107:LYS:HE3	1.54	0.42
1:K:479:PHE:CD2	1:K:482:ALA:HA	2.55	0.42
1:L:476:VAL:O	1:L:516:PHE:HA	2.20	0.42
3:P:357:ARG:HG2	3:P:404:GLY:HA3	2.01	0.42
3:P:447:LYS:HD3	3:P:447:LYS:HA	1.37	0.42
4:S:19:ILE:HG22	4:S:21:PRO:CD	2.49	0.42
4:S:39:LEU:HD23	4:S:85:ASN:CA	2.49	0.42
1:A:375:TYR:HD2	1:A:430:HIS:CE1	2.38	0.42
1:A:375:TYR:HB2	1:A:430:HIS:NE2	2.35	0.42
1:A:511:ALA:HA	1:A:512:PRO:HD2	1.59	0.42
1:A:532:GLU:O	1:A:553:ASP:CB	2.67	0.42
1:B:466:LEU:O	3:P:34:ARG:NH1	2.51	0.42
1:C:400:HIS:CG	1:C:401:PRO:HD2	2.54	0.42
1:D:423:ARG:HA	1:D:442:SER:HB2	2.02	0.42
1:D:429:THR:OG1	1:D:433:LEU:O	2.38	0.42
1:F:449:LEU:N	1:F:481:PRO:HD3	2.34	0.42
1:F:506:MET:O	1:F:516:PHE:CD2	2.73	0.42
1:H:415:GLU:O	1:H:418:TRP:HB2	2.20	0.42
1:H:558:LYS:HB2	1:K:559:PRO:HG2	2.00	0.42
1:K:518:HIS:CE1	1:L:518:HIS:CG	3.08	0.42
3:P:345:ALA:C	3:P:413:LEU:CB	2.71	0.42
3:P:377:CYS:O	3:P:377:CYS:SG	2.78	0.42
3:P:395:LEU:CD1	3:P:410:LEU:HD12	2.35	0.42
1:D:513:GLY:C	1:D:514:ARG:HD3	2.45	0.42
1:E:493:GLN:NE2	4:V:42:MET:HE3	2.35	0.42
1:E:527:GLU:C	1:E:530:THR:HG1	2.21	0.42
1:K:464:LEU:CD1	1:K:525:GLU:CG	2.97	0.42
1:L:474:CYS:HB2	1:L:488:TRP:CZ2	2.55	0.42
3:P:264:VAL:HG22	3:P:275:PHE:CE2	2.49	0.42
3:P:471:SER:HB2	3:P:475:LYS:HZ3	1.83	0.42
4:R:111:ASP:O	4:R:114:LYS:HE2	2.15	0.42
4:U:61:VAL:HG12	4:U:69:LYS:HD2	2.02	0.42
1:B:479:PHE:CD1	1:B:479:PHE:N	2.86	0.42
1:B:543:LEU:HA	1:B:543:LEU:HD23	1.40	0.42
1:E:370:THR:HG22	1:E:371:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:384:ARG:HE	1:H:390:VAL:CG2	2.31	0.42
1:H:566:LEU:O	1:H:567:VAL:C	2.63	0.42
1:K:405:PHE:HE2	1:K:407:ALA:HB2	1.85	0.42
1:K:476:VAL:O	1:K:479:PHE:HE1	2.02	0.42
1:L:400:HIS:HE1	1:L:405:PHE:HA	1.82	0.42
1:L:445:LYS:HB2	1:L:445:LYS:HE2	1.70	0.42
3:P:317:GLU:CD	3:P:317:GLU:H	2.25	0.42
3:P:526:CYS:CA	3:P:538:ALA:HB3	2.50	0.42
4:U:37:CYS:CB	4:U:87:PHE:O	2.68	0.42
4:V:52:MET:HE3	4:V:54:GLY:H	1.84	0.42
1:B:376:ASP:HB2	1:B:377:SER:H	1.61	0.42
1:B:568:MET:HB3	1:C:568:MET:HG2	2.02	0.42
1:C:466:LEU:HD23	4:V:45:ARG:NH2	2.34	0.42
1:E:515:TYR:CD1	1:E:515:TYR:N	2.83	0.42
1:F:461:ARG:HD3	1:F:461:ARG:HA	1.79	0.42
1:K:400:HIS:HB3	1:K:404:THR:O	2.20	0.42
4:V:86:LEU:HD12	4:V:87:PHE:N	2.35	0.42
1:A:484:VAL:O	1:A:484:VAL:HG13	2.16	0.42
1:A:486:VAL:HG22	1:A:538:VAL:HG12	2.02	0.42
1:A:496:SER:HA	1:A:497:PRO:HD3	1.75	0.42
1:A:543:LEU:HD23	1:A:544:PRO:HD2	2.02	0.42
1:B:500:TYR:CD1	1:B:500:TYR:N	2.86	0.42
1:F:523:VAL:HB	1:F:524:SER:H	1.41	0.42
1:H:423:ARG:HH11	1:H:425:THR:HB	1.85	0.42
1:L:372:LEU:HD23	1:L:407:ALA:H	1.85	0.42
1:B:445:LYS:CA	1:B:445:LYS:NZ	2.82	0.41
1:C:454:VAL:CG2	1:C:538:VAL:CG2	2.98	0.41
1:D:489:MET:HB2	1:D:489:MET:HE2	1.83	0.41
1:F:536:CYS:O	1:F:549:GLU:HA	2.20	0.41
1:H:427:THR:OG1	1:H:436:PRO:HB3	2.20	0.41
1:K:369:VAL:O	1:K:406:SER:HA	2.21	0.41
3:P:148:TYR:CE2	3:P:203:GLN:HG2	2.55	0.41
4:S:49:CYS:HB2	4:S:103:ALA:HB3	2.01	0.41
4:U:104:CYS:O	4:U:115:THR:N	2.33	0.41
1:A:382:TRP:CD1	1:A:411:ALA:HB2	2.54	0.41
1:G:365:LEU:HG	1:G:424:PHE:CD2	2.55	0.41
1:H:568:MET:HB3	1:H:568:MET:HE3	1.50	0.41
4:U:81:TYR:OH	4:U:88:LEU:HD12	2.20	0.41
4:V:75:ARG:O	4:V:92:THR:N	2.53	0.41
1:A:379:THR:H	1:A:429:THR:HB	1.84	0.41
1:A:495:LEU:CD1	1:A:521:LEU:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ARG:HG3	1:B:424:PHE:CZ	2.55	0.41
1:B:525:GLU:O	1:B:525:GLU:CG	2.68	0.41
1:C:423:ARG:HE	1:C:442:SER:CB	2.33	0.41
1:C:462:GLU:O	1:C:465:ASN:HB2	2.20	0.41
1:C:467:ARG:N	1:C:467:ARG:CD	2.72	0.41
1:G:489:MET:SD	1:G:537:VAL:HG21	2.60	0.41
4:V:33:VAL:HG22	4:V:91:VAL:HB	2.01	0.41
1:B:483:ASP:O	1:B:540:HIS:HD2	2.03	0.41
1:D:533:THR:HA	1:D:552:VAL:O	2.21	0.41
1:E:370:THR:HG22	1:E:371:ASP:H	1.86	0.41
1:E:467:ARG:O	4:U:60:THR:HB	2.20	0.41
1:E:481:PRO:HD2	1:E:540:HIS:NE2	2.35	0.41
1:E:532:GLU:HB3	1:E:534:TYR:CE2	2.56	0.41
1:G:439:GLN:HG3	1:G:441:ILE:HG23	2.01	0.41
2:J:104:ASP:HB3	2:J:107:LYS:HB2	2.03	0.41
1:L:354:PHE:CG	1:L:541:GLU:HB3	2.55	0.41
1:L:400:HIS:CD2	1:L:402:ASN:HB2	2.55	0.41
1:L:528:TRP:CH2	1:L:554:LYS:HA	2.55	0.41
1:L:556:THR:O	1:L:556:THR:CG2	2.69	0.41
3:P:25:PRO:HB3	3:P:329:ASN:HD21	1.86	0.41
3:P:479:LYS:CE	3:P:524:TYR:HE1	2.34	0.41
4:S:39:LEU:CD2	4:S:41:GLU:HG2	2.51	0.41
1:C:466:LEU:CD2	1:C:466:LEU:O	2.69	0.41
1:E:421:GLY:N	1:E:445:LYS:HE2	2.35	0.41
1:F:449:LEU:CA	1:F:481:PRO:HD3	2.44	0.41
1:F:546:ARG:NH1	1:F:546:ARG:HG2	2.35	0.41
1:G:432:ASP:OD1	1:G:433:LEU:N	2.53	0.41
1:K:558:LYS:HA	1:K:559:PRO:HD3	1.87	0.41
1:L:348:PHE:HB3	1:L:368:LEU:HB2	2.02	0.41
1:L:393:HIS:ND1	1:L:396:ILE:HD13	2.36	0.41
3:P:315:LEU:CG	3:P:315:LEU:O	2.69	0.41
3:P:388:LYS:HD2	3:P:388:LYS:HA	1.61	0.41
3:P:446:LEU:C	3:P:446:LEU:CD1	2.93	0.41
4:R:48:LEU:HD22	4:R:89:VAL:HG11	2.02	0.41
1:A:490:GLN:HB2	1:A:534:TYR:HE1	1.85	0.41
1:C:397:SER:H	1:C:408:VAL:HG22	1.85	0.41
1:C:509:PRO:HG2	1:D:522:THR:CG2	2.50	0.41
1:D:514:ARG:N	1:D:514:ARG:CD	2.77	0.41
1:F:348:PHE:N	1:F:369:VAL:HG13	2.29	0.41
1:F:484:VAL:O	1:F:484:VAL:HG13	2.18	0.41
1:H:352:PRO:HD2	1:H:418:TRP:HH2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:450:HIS:HB3	1:K:514:ARG:NH2	2.36	0.41
1:L:488:TRP:CE2	1:L:536:CYS:HB2	2.55	0.41
1:L:532:GLU:O	1:L:534:TYR:CE2	2.74	0.41
3:P:131:THR:HG22	3:P:188:VAL:N	2.36	0.41
3:P:295:THR:CG2	3:P:432:ARG:HB2	2.49	0.41
3:P:340:VAL:HG11	3:P:436:GLU:OE1	2.20	0.41
4:U:109:ASN:HD22	4:U:112:ARG:NH2	2.19	0.41
1:A:525:GLU:O	1:A:529:ASN:N	2.54	0.41
1:B:495:LEU:HA	1:B:495:LEU:HD23	1.60	0.41
1:D:449:LEU:H	1:D:449:LEU:HG	1.44	0.41
1:D:539:ALA:HA	1:D:546:ARG:O	2.20	0.41
1:E:450:HIS:HB3	1:E:514:ARG:HH21	1.85	0.41
1:F:368:LEU:HD12	1:F:408:VAL:HA	2.03	0.41
1:F:545:ASN:ND2	1:F:545:ASN:H	2.19	0.41
1:H:489:MET:SD	1:H:537:VAL:HG11	2.61	0.41
1:K:509:PRO:O	1:L:498:GLU:OE2	2.39	0.41
1:L:362:SER:OG	1:L:363:THR:N	2.53	0.41
1:L:485:PHE:CE2	1:L:487:GLN:HB2	2.56	0.41
3:P:148:TYR:HB3	3:P:155:PRO:CG	2.51	0.41
3:P:245:VAL:CG2	3:P:309:ALA:HB3	2.51	0.41
3:P:466:PHE:CD2	3:P:507:ARG:HG2	2.55	0.41
1:A:548:THR:OG1	1:A:549:GLU:N	2.54	0.41
1:B:545:ASN:HD21	1:C:547:VAL:HG21	1.85	0.41
1:C:400:HIS:HD2	1:C:402:ASN:CG	2.29	0.41
1:C:400:HIS:ND1	1:C:401:PRO:HD2	2.35	0.41
1:D:367:CYS:SG	1:D:382:TRP:NE1	2.93	0.41
1:F:481:PRO:O	1:F:540:HIS:HE1	2.04	0.41
1:G:455:TYR:CZ	1:H:463:GLN:HG3	2.56	0.41
1:L:354:PHE:HD2	1:L:546:ARG:NH2	2.16	0.41
3:P:25:PRO:HA	3:P:26:PRO:HD3	1.89	0.41
1:A:454:VAL:HG21	1:A:538:VAL:HG21	2.02	0.41
1:C:564:VAL:H	1:C:564:VAL:HG23	1.56	0.41
1:D:536:CYS:O	1:D:536:CYS:SG	2.78	0.41
1:G:365:LEU:HD11	1:G:418:TRP:CZ3	2.55	0.41
1:H:496:SER:HB3	1:H:499:LYS:HZ3	1.85	0.41
1:K:463:GLN:HA	1:L:455:TYR:OH	2.21	0.41
1:K:564:VAL:H	1:K:564:VAL:HG23	1.59	0.41
1:L:454:VAL:HG13	1:L:550:ARG:HB2	2.02	0.41
1:L:459:PRO:HD3	1:L:472:ILE:HG12	2.02	0.41
3:P:140:ASN:ND2	3:P:143:LYS:HB2	2.35	0.41
3:P:239:CYS:HB2	3:P:290:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:462:VAL:CG1	3:P:509:VAL:HB	2.51	0.41
3:P:480:TRP:HH2	3:P:482:ASN:HB3	1.82	0.41
4:R:24:LYS:HD3	4:R:119:THR:HG23	2.03	0.41
4:R:45:ARG:HD3	4:R:108:MET:HE2	2.03	0.41
4:V:22:GLU:HB2	4:V:119:THR:H	1.85	0.41
1:B:456:LEU:HG	1:B:552:VAL:HB	2.02	0.41
1:C:532:GLU:OE2	1:C:532:GLU:HA	2.21	0.41
1:D:369:VAL:HG13	1:D:405:PHE:CD2	2.56	0.41
1:F:381:SER:O	1:F:426:CYS:HA	2.21	0.41
1:K:352:PRO:HG2	1:K:363:THR:HG23	2.02	0.41
1:K:430:HIS:HD2	1:K:433:LEU:H	1.69	0.41
1:K:526:GLU:C	1:K:526:GLU:CD	2.89	0.41
1:L:511:ALA:HB1	1:L:514:ARG:NE	2.36	0.41
3:P:340:VAL:HG12	3:P:436:GLU:CA	2.51	0.41
4:V:69:LYS:O	4:V:73:LYS:HG2	2.21	0.41
4:V:112:ARG:HB2	4:V:112:ARG:HH11	1.85	0.41
1:A:502:THR:CB	1:A:519:SER:HB2	2.33	0.40
1:C:354:PHE:HD1	1:C:357:ILE:HD12	1.85	0.40
1:C:428:VAL:O	1:C:436:PRO:HA	2.21	0.40
1:D:382:TRP:HZ3	1:D:424:PHE:HB3	1.86	0.40
1:D:415:GLU:O	1:D:419:ASN:ND2	2.34	0.40
1:F:476:VAL:O	1:F:516:PHE:HA	2.21	0.40
1:F:523:VAL:HG12	1:F:534:TYR:OH	2.21	0.40
1:H:508:GLU:HB3	1:H:511:ALA:HB3	2.03	0.40
1:L:367:CYS:O	1:L:369:VAL:HG23	2.21	0.40
3:P:172:ARG:HD2	3:P:190:ASN:O	2.21	0.40
4:V:58:CYS:SG	4:V:110:THR:HG22	2.61	0.40
1:A:441:ILE:HD12	1:A:441:ILE:HA	1.90	0.40
1:B:456:LEU:HD11	1:B:472:ILE:HG22	2.03	0.40
1:B:510:GLN:OE1	1:B:510:GLN:CA	2.69	0.40
1:F:438:LYS:H	1:F:438:LYS:HG3	1.72	0.40
1:F:523:VAL:HG11	1:F:534:TYR:CE2	2.56	0.40
1:H:408:VAL:HG13	1:H:408:VAL:O	2.21	0.40
1:K:506:MET:HB2	1:K:516:PHE:HE1	1.85	0.40
4:R:52:MET:HE3	4:R:69:LYS:HZ2	1.86	0.40
1:A:390:VAL:HG13	1:A:391:LYS:H	1.86	0.40
1:A:452:PRO:HG3	1:A:479:PHE:HB3	2.02	0.40
1:A:545:ASN:O	1:A:547:VAL:N	2.52	0.40
1:E:543:LEU:HA	1:E:544:PRO:HD3	1.84	0.40
3:P:11:ASN:HA	3:P:108:GLU:O	2.21	0.40
3:P:317:GLU:N	3:P:317:GLU:CD	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:20:LEU:HD23	4:R:117:LYS:HG2	1.92	0.40
4:R:95:THR:C	4:R:97:SER:N	2.80	0.40
4:V:46:ILE:H	4:V:64:THR:HG1	1.63	0.40
1:C:510:GLN:OE1	1:C:510:GLN:CA	2.70	0.40
1:F:476:VAL:HG12	1:F:479:PHE:CE1	2.56	0.40
1:H:349:ALA:HA	1:H:366:THR:O	2.22	0.40
1:H:567:VAL:HG21	1:H:576:TYR:OH	2.21	0.40
1:K:385:GLN:NE2	1:K:423:ARG:H	2.20	0.40
3:P:354:PRO:HA	3:P:405:THR:HB	2.03	0.40
3:P:471:SER:CB	3:P:475:LYS:HZ3	2.29	0.40
4:S:93:GLN:OE1	4:S:93:GLN:CA	2.70	0.40
5:I:2:NAG:O3	5:I:2:NAG:C7	2.70	0.40
1:B:481:PRO:O	1:B:481:PRO:CG	2.69	0.40
1:B:498:GLU:O	1:B:498:GLU:CG	2.69	0.40
1:B:546:ARG:HE	1:B:546:ARG:HB2	1.47	0.40
1:C:464:LEU:O	1:C:466:LEU:N	2.55	0.40
1:D:365:LEU:HD23	1:D:365:LEU:H	1.86	0.40
1:D:367:CYS:SG	1:D:393:HIS:HE1	2.45	0.40
1:D:499:LYS:HB3	1:D:499:LYS:HE2	1.71	0.40
1:E:364:LYS:HD3	1:E:411:ALA:O	2.21	0.40
1:G:363:THR:OG1	1:G:413:ILE:O	2.40	0.40
1:H:363:THR:O	1:H:412:SER:HA	2.22	0.40
1:H:369:VAL:HG12	1:H:372:LEU:HD23	2.02	0.40
3:P:25:PRO:HB3	3:P:329:ASN:ND2	2.36	0.40
3:P:377:CYS:HA	3:P:378:PRO:HD3	1.97	0.40
3:P:447:LYS:H	3:P:465:HIS:CA	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/232 (99%)	195 (85%)	24 (10%)	10 (4%)	2	13
1	B	226/232 (97%)	192 (85%)	27 (12%)	7 (3%)	3	19
1	C	225/232 (97%)	188 (84%)	26 (12%)	11 (5%)	1	12
1	D	222/232 (96%)	204 (92%)	16 (7%)	2 (1%)	14	45
1	E	222/232 (96%)	198 (89%)	19 (9%)	5 (2%)	5	26
1	F	222/232 (96%)	185 (83%)	23 (10%)	14 (6%)	1	7
1	G	222/232 (96%)	205 (92%)	15 (7%)	2 (1%)	14	45
1	H	230/232 (99%)	202 (88%)	19 (8%)	9 (4%)	2	15
1	K	230/232 (99%)	202 (88%)	19 (8%)	9 (4%)	2	15
1	L	230/232 (99%)	193 (84%)	29 (13%)	8 (4%)	3	17
2	J	102/136 (75%)	92 (90%)	8 (8%)	2 (2%)	6	28
3	P	481/541 (89%)	408 (85%)	54 (11%)	19 (4%)	2	15
4	R	99/107 (92%)	80 (81%)	17 (17%)	2 (2%)	6	28
4	S	101/107 (94%)	88 (87%)	11 (11%)	2 (2%)	6	28
4	U	99/107 (92%)	88 (89%)	8 (8%)	3 (3%)	3	20
4	V	104/107 (97%)	97 (93%)	6 (6%)	1 (1%)	12	43
All	All	3244/3425 (95%)	2817 (87%)	321 (10%)	106 (3%)	5	18

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	ARG
1	A	554	LYS
1	B	415	GLU
1	B	418	TRP
1	B	480	SER
1	C	482	ALA
1	E	494	PRO
1	E	533	THR
1	E	546	ARG
1	F	444	PRO
1	F	480	SER
1	F	546	ARG
1	G	444	PRO
1	H	442	SER
1	H	569	SER
1	H	574	THR

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Mol	Chain	Res	Type
1	K	447	VAL
1	K	492	GLY
1	K	511	ALA
1	K	512	PRO
1	K	541	GLU
1	L	441	ILE
1	L	443	ARG
1	L	481	PRO
3	P	101	LEU
3	P	259	GLU
3	P	261	CYS
3	P	262	ASP
3	P	311	SER
3	P	379	LEU
3	P	399	GLU
3	P	413	LEU
3	P	448	VAL
4	R	66	ASN
4	S	53	ALA
4	S	98	ASP
4	U	96	GLU
1	A	446	GLY
1	B	405	PHE
1	B	410	GLU
1	B	497	PRO
1	C	531	GLY
1	E	534	TYR
1	F	390	VAL
1	F	419	ASN
1	F	421	GLY
1	F	449	LEU
1	F	507	PRO
1	F	523	VAL
1	G	478	GLY
1	H	531	GLY
1	H	564	VAL
2	J	64	LEU
1	L	478	GLY
1	L	534	TYR
3	P	310	HIS
3	P	403	ASN
3	P	416	ARG

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Mol	Chain	Res	Type
1	A	491	ARG
1	A	512	PRO
1	C	448	ALA
1	C	509	PRO
1	C	510	GLN
1	C	512	PRO
1	D	497	PRO
1	F	415	GLU
1	H	444	PRO
1	H	449	LEU
1	H	559	PRO
2	J	120	GLU
1	K	572	ALA
1	L	444	PRO
1	L	447	VAL
3	P	155	PRO
3	P	378	PRO
3	P	473	TYR
4	U	98	ASP
1	A	497	PRO
1	A	573	GLY
1	C	481	PRO
1	C	523	VAL
1	C	557	GLY
1	D	447	VAL
1	E	509	PRO
1	F	377	SER
1	F	544	PRO
1	H	560	THR
1	K	519	SER
1	K	544	PRO
1	L	483	ASP
3	P	57	SER
3	P	287	ASP
4	R	96	GLU
4	V	113	GLY
1	C	466	LEU
1	C	558	LYS
3	P	157	LEU
1	A	501	VAL
1	F	559	PRO
4	U	42	MET

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Mol	Chain	Res	Type
1	K	444	PRO
1	A	531	GLY
1	B	413	ILE
1	F	413	ILE
3	P	288	GLY
1	A	481	PRO

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	205/206 (100%)	183 (89%)	22 (11%)	6	25
1	B	203/206 (98%)	155 (76%)	48 (24%)	1	4
1	C	203/206 (98%)	181 (89%)	22 (11%)	6	24
1	D	200/206 (97%)	195 (98%)	5 (2%)	42	66
1	E	200/206 (97%)	193 (96%)	7 (4%)	32	61
1	F	200/206 (97%)	151 (76%)	49 (24%)	1	3
1	G	200/206 (97%)	188 (94%)	12 (6%)	17	46
1	H	206/206 (100%)	187 (91%)	19 (9%)	8	31
1	K	206/206 (100%)	176 (85%)	30 (15%)	3	14
1	L	206/206 (100%)	183 (89%)	23 (11%)	6	23
2	J	100/128 (78%)	92 (92%)	8 (8%)	11	37
3	P	423/461 (92%)	365 (86%)	58 (14%)	3	16
4	R	86/92 (94%)	76 (88%)	10 (12%)	5	22
4	S	88/92 (96%)	75 (85%)	13 (15%)	3	14
4	U	86/92 (94%)	78 (91%)	8 (9%)	8	30
4	V	91/92 (99%)	89 (98%)	2 (2%)	45	68
All	All	2903/3017 (96%)	2567 (88%)	336 (12%)	7	22

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	LYS
1	A	447	VAL
1	A	466	LEU
1	A	467	ARG
1	A	477	THR
1	A	490	GLN
1	A	502	THR
1	A	508	GLU
1	A	510	GLN
1	A	514	ARG
1	A	518	HIS
1	A	519	SER
1	A	532	GLU
1	A	543	LEU
1	A	545	ASN
1	A	549	GLU
1	A	554	LYS
1	A	556	THR
1	A	566	LEU
1	A	568	MET
1	A	571	THR
1	A	574	THR
1	B	366	THR
1	B	368	LEU
1	B	371	ASP
1	B	374	THR
1	B	375	TYR
1	B	376	ASP
1	B	378	VAL
1	B	380	ILE
1	B	391	LYS
1	B	392	THR
1	B	393	HIS
1	B	394	THR
1	B	395	ASN
1	B	396	ILE
1	B	398	GLU
1	B	400	HIS
1	B	402	ASN
1	B	408	VAL
1	B	410	GLU
1	B	412	SER
1	B	413	ILE

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Mol	Chain	Res	Type
1	B	420	SER
1	B	423	ARG
1	B	424	PHE
1	B	427	THR
1	B	429	THR
1	B	431	THR
1	B	433	LEU
1	B	437	LEU
1	B	440	THR
1	B	441	ILE
1	B	442	SER
1	B	443	ARG
1	B	445	LYS
1	B	449	LEU
1	B	451	ARG
1	B	454	VAL
1	B	456	LEU
1	B	462	GLU
1	B	480	SER
1	B	498	GLU
1	B	499	LYS
1	B	526	GLU
1	B	529	ASN
1	B	530	THR
1	B	532	GLU
1	B	535	THR
1	B	546	ARG
1	C	445	LYS
1	C	450	HIS
1	C	451	ARG
1	C	453	ASP
1	C	456	LEU
1	C	457	LEU
1	C	466	LEU
1	C	468	GLU
1	C	480	SER
1	C	494	PRO
1	C	510	GLN
1	C	514	ARG
1	C	525	GLU
1	C	526	GLU
1	C	527	GLU

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Mol	Chain	Res	Type
1	C	530	THR
1	C	533	THR
1	C	554	LYS
1	C	564	VAL
1	C	565	SER
1	C	566	LEU
1	C	567	VAL
1	D	495	LEU
1	D	499	LYS
1	D	514	ARG
1	D	536	CYS
1	D	537	VAL
1	E	445	LYS
1	E	493	GLN
1	E	514	ARG
1	E	532	GLU
1	E	535	THR
1	E	538	VAL
1	E	545	ASN
1	F	363	THR
1	F	368	LEU
1	F	374	THR
1	F	376	ASP
1	F	377	SER
1	F	378	VAL
1	F	379	THR
1	F	380	ILE
1	F	383	THR
1	F	390	VAL
1	F	391	LYS
1	F	396	ILE
1	F	402	ASN
1	F	405	PHE
1	F	406	SER
1	F	408	VAL
1	F	410	GLU
1	F	412	SER
1	F	414	CYS
1	F	416	ASP
1	F	420	SER
1	F	422	GLU
1	F	423	ARG

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Mol	Chain	Res	Type
1	F	425	THR
1	F	429	THR
1	F	432	ASP
1	F	437	LEU
1	F	438	LYS
1	F	439	GLN
1	F	440	THR
1	F	441	ILE
1	F	443	ARG
1	F	445	LYS
1	F	479	PHE
1	F	501	VAL
1	F	502	THR
1	F	506	MET
1	F	520	ILE
1	F	521	LEU
1	F	523	VAL
1	F	543	LEU
1	F	544	PRO
1	F	545	ASN
1	F	546	ARG
1	F	548	THR
1	F	550	ARG
1	F	554	LYS
1	F	556	THR
1	F	561	LEU
1	G	345	ILE
1	G	443	ARG
1	G	445	LYS
1	G	447	VAL
1	G	449	LEU
1	G	466	LEU
1	G	473	THR
1	G	475	LEU
1	G	477	THR
1	G	516	PHE
1	G	564	VAL
1	G	567	VAL
1	H	442	SER
1	H	443	ARG
1	H	444	PRO
1	H	445	LYS

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Mol	Chain	Res	Type
1	H	449	LEU
1	H	486	VAL
1	H	519	SER
1	H	532	GLU
1	H	533	THR
1	H	535	THR
1	H	536	CYS
1	H	537	VAL
1	H	556	THR
1	H	558	LYS
1	H	561	LEU
1	H	563	ASN
1	H	566	LEU
1	H	568	MET
1	H	574	THR
2	J	23	ARG
2	J	26	GLU
2	J	30	GLU
2	J	34	GLU
2	J	35	ARG
2	J	107	LYS
2	J	116	VAL
2	J	117	TYR
1	K	445	LYS
1	K	447	VAL
1	K	449	LEU
1	K	462	GLU
1	K	464	LEU
1	K	474	CYS
1	K	475	LEU
1	K	477	THR
1	K	484	VAL
1	K	489	MET
1	K	490	GLN
1	K	491	ARG
1	K	508	GLU
1	K	514	ARG
1	K	516	PHE
1	K	520	ILE
1	K	521	LEU
1	K	524	SER
1	K	526	GLU

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Mol	Chain	Res	Type
1	K	530	THR
1	K	533	THR
1	K	535	THR
1	K	543	LEU
1	K	545	ASN
1	K	556	THR
1	K	558	LYS
1	K	561	LEU
1	K	565	SER
1	K	568	MET
1	K	574	THR
1	L	441	ILE
1	L	443	ARG
1	L	445	LYS
1	L	449	LEU
1	L	450	HIS
1	L	479	PHE
1	L	480	SER
1	L	514	ARG
1	L	534	TYR
1	L	535	THR
1	L	536	CYS
1	L	543	LEU
1	L	545	ASN
1	L	547	VAL
1	L	548	THR
1	L	551	THR
1	L	552	VAL
1	L	556	THR
1	L	558	LYS
1	L	566	LEU
1	L	567	VAL
1	L	574	THR
1	L	575	CYS
3	P	10	VAL
3	P	43	ARG
3	P	60	TYR
3	P	99	ARG
3	P	131	THR
3	P	132	ILE
3	P	151	ILE
3	P	245	VAL

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Mol	Chain	Res	Type
3	P	247	ASN
3	P	257	SER
3	P	259	GLU
3	P	260	ASN
3	P	275	PHE
3	P	287	ASP
3	P	290	PHE
3	P	314	GLN
3	P	315	LEU
3	P	316	GLN
3	P	317	GLU
3	P	340	VAL
3	P	342	LYS
3	P	344	VAL
3	P	349	VAL
3	P	358	LYS
3	P	361	LYS
3	P	379	LEU
3	P	387	VAL
3	P	388	LYS
3	P	390	GLN
3	P	392	GLU
3	P	398	LEU
3	P	399	GLU
3	P	400	GLU
3	P	403	ASN
3	P	405	THR
3	P	409	ILE
3	P	412	GLN
3	P	413	LEU
3	P	414	THR
3	P	430	LEU
3	P	431	TRP
3	P	432	ARG
3	P	439	ILE
3	P	446	LEU
3	P	447	LYS
3	P	462	VAL
3	P	464	CYS
3	P	466	PHE
3	P	469	LYS
3	P	470	PHE

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Mol	Chain	Res	Type
3	P	473	TYR
3	P	475	LYS
3	P	478	CYS
3	P	533	PHE
3	P	536	GLU
3	P	537	THR
3	P	540	VAL
3	P	541	TYR
4	R	20	LEU
4	R	24	LYS
4	R	55	SER
4	R	65	THR
4	R	93	GLN
4	R	94	LEU
4	R	95	THR
4	R	96	GLU
4	R	115	THR
4	R	116	GLN
4	S	39	LEU
4	S	42	MET
4	S	71	GLU
4	S	72	TYR
4	S	73	LYS
4	S	92	THR
4	S	93	GLN
4	S	94	LEU
4	S	96	GLU
4	S	115	THR
4	S	116	GLN
4	S	117	LYS
4	S	118	VAL
4	U	23	VAL
4	U	24	LYS
4	U	25	VAL
4	U	26	GLU
4	U	41	GLU
4	U	44	VAL
4	U	117	LYS
4	U	119	THR
4	V	96	GLU
4	V	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	GLN
1	A	540	HIS
1	B	385	GLN
1	B	393	HIS
1	B	400	HIS
1	B	450	HIS
1	B	529	ASN
1	B	545	ASN
1	C	400	HIS
1	C	465	ASN
1	D	393	HIS
1	E	400	HIS
1	E	493	GLN
1	E	529	ASN
1	F	402	ASN
1	F	439	GLN
1	F	540	HIS
1	F	545	ASN
1	G	563	ASN
1	H	419	ASN
1	H	430	HIS
1	H	439	GLN
1	K	430	HIS
1	K	487	GLN
1	K	545	ASN
1	K	563	ASN
1	L	430	HIS
1	L	463	GLN
1	L	490	GLN
1	L	545	ASN
3	P	40	GLN
3	P	199	GLN
3	P	260	ASN
3	P	310	HIS
3	P	314	GLN
3	P	322	GLN
3	P	390	GLN
3	P	403	ASN
3	P	411	ASN
3	P	412	GLN
3	P	481	ASN
3	P	530	GLN

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Mol	Chain	Res	Type
3	P	532	HIS
4	R	93	GLN
4	R	116	GLN
4	U	109	ASN
4	V	66	ASN
4	V	121	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 ⓘ

2 monosaccharides 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$
5	NAG	I	1	5,2	14,14,15	3.36	2 (14%)	17,19,21	2.89	7 (41%)
5	NAG	I	2	5	14,14,15	1.10	0	17,19,21	3.40	7 (41%)

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
5	NAG	I	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	NAG	C1-C2	11.05	1.67	1.52
5	I	1	NAG	O5-C1	-4.27	1.36	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	C2-N2-C7	-10.40	108.97	122.90
5	I	1	NAG	O5-C5-C6	-5.41	97.13	107.66
5	I	1	NAG	C1-O5-C5	5.36	119.37	112.19
5	I	2	NAG	C1-O5-C5	5.17	119.11	112.19
5	I	1	NAG	C4-C3-C2	-4.59	104.29	111.02
5	I	2	NAG	C3-C4-C5	-4.30	102.44	110.23
5	I	2	NAG	C4-C3-C2	-4.22	104.84	111.02
5	I	1	NAG	O4-C4-C3	-3.40	102.35	110.38
5	I	1	NAG	C1-C2-N2	3.39	115.78	110.43
5	I	1	NAG	O5-C1-C2	-3.29	106.20	111.29
5	I	1	NAG	O3-C3-C2	-2.76	103.68	109.40
5	I	2	NAG	C1-C2-N2	2.23	113.95	110.43
5	I	2	NAG	O5-C1-C2	2.21	114.72	111.29
5	I	2	NAG	O3-C3-C2	-2.17	104.88	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

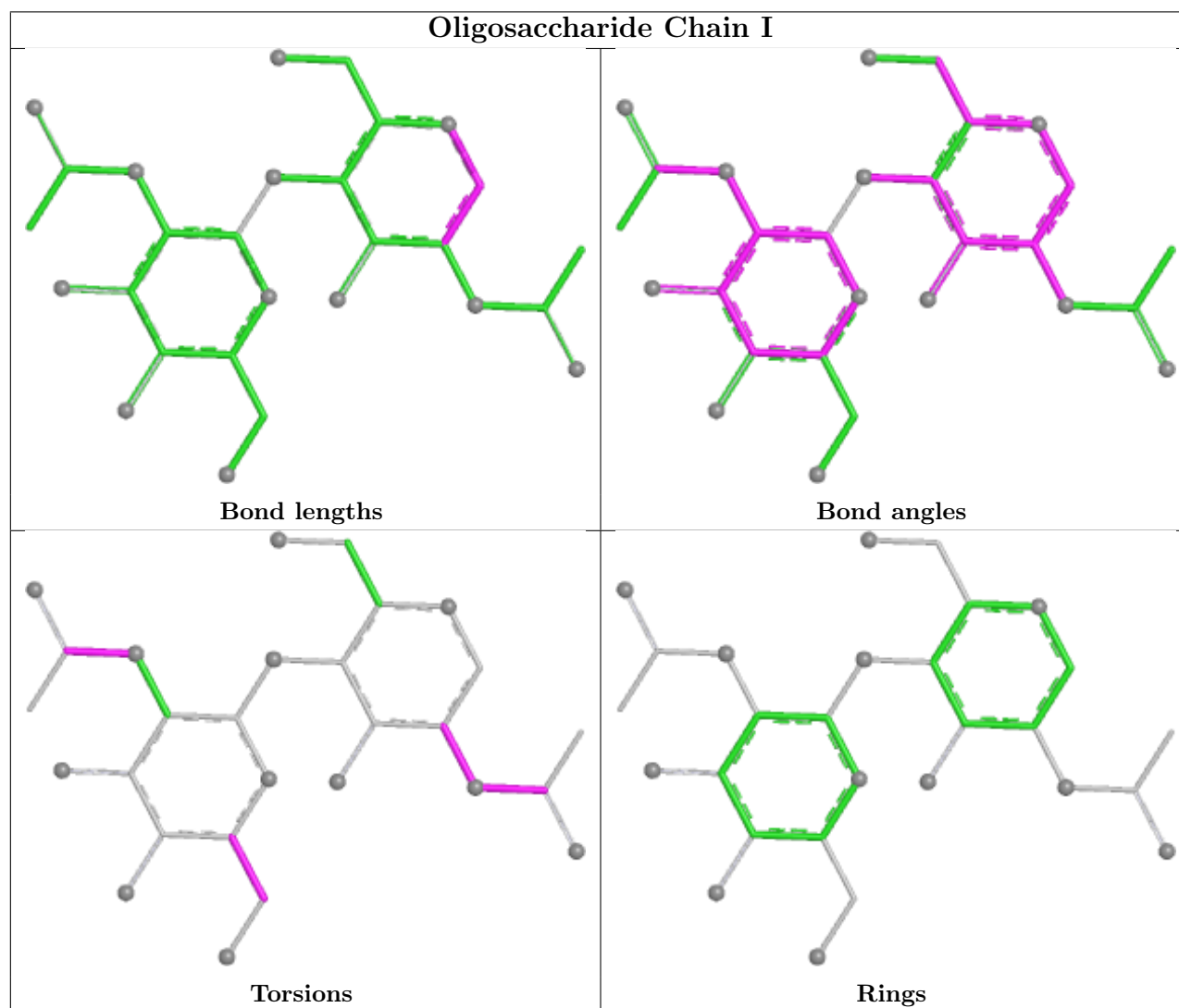
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	I	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C1-C2-N2-C7
5	I	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	3	0
5	I	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
6	NAG	G	601	-	15,15,15	0.46	0	21,21,21	1.54	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	F	601	1	14,14,15	0.37	0	17,19,21	0.50	0
6	NAG	K	601	-	14,14,15	0.26	0	17,19,21	0.35	0
6	NAG	A	601	1	14,14,15	0.27	0	17,19,21	0.37	0
6	NAG	D	601	1	14,14,15	0.20	0	17,19,21	0.44	0
6	NAG	H	601	1	14,14,15	2.76	3 (21%)	17,19,21	3.90	7 (41%)
6	NAG	L	601	1	14,14,15	0.28	0	17,19,21	0.53	0
6	NAG	C	601	-	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	E	601	1	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	B	601	1	14,14,15	0.21	0	17,19,21	0.43	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
6	NAG	G	601	-	-	4/6/26/26	0/1/1/1
6	NAG	F	601	1	-	1/6/23/26	0/1/1/1
6	NAG	K	601	-	-	4/6/23/26	0/1/1/1
6	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	NAG	D	601	1	-	2/6/23/26	0/1/1/1
6	NAG	H	601	1	-	4/6/23/26	0/1/1/1
6	NAG	L	601	1	-	2/6/23/26	0/1/1/1
6	NAG	C	601	-	-	4/6/23/26	0/1/1/1
6	NAG	E	601	1	-	2/6/23/26	0/1/1/1
6	NAG	B	601	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	601	NAG	C1-C2	8.50	1.63	1.52
6	H	601	NAG	C2-N2	-4.18	1.39	1.46
6	H	601	NAG	C3-C2	-2.17	1.48	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	601	NAG	C1-C2-N2	-10.77	93.46	110.43
6	H	601	NAG	C4-C3-C2	-8.07	99.20	111.02
6	H	601	NAG	O5-C1-C2	-5.97	102.05	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	601	NAG	O5-C1-C2	4.53	114.07	109.52
6	H	601	NAG	C2-N2-C7	-3.36	118.39	122.90
6	H	601	NAG	C3-C4-C5	-3.33	104.20	110.23
6	G	601	NAG	C1-O5-C5	3.25	119.94	113.65
6	H	601	NAG	O4-C4-C5	2.42	115.28	109.32
6	H	601	NAG	O3-C3-C2	2.33	114.24	109.40

There are no chirality outliers.

All (25) torsion outliers are listed below:

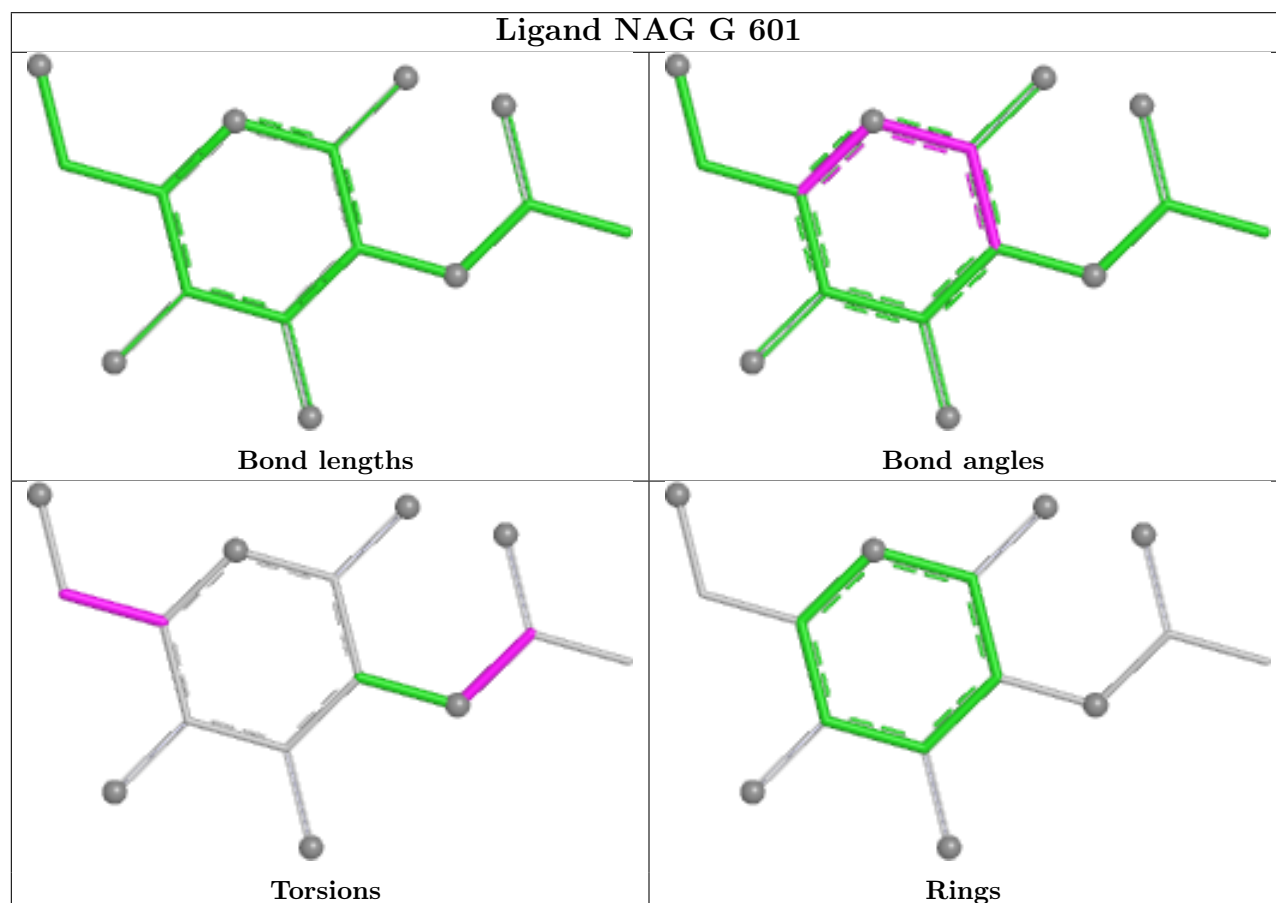
Mol	Chain	Res	Type	Atoms
6	G	601	NAG	C8-C7-N2-C2
6	G	601	NAG	O7-C7-N2-C2
6	H	601	NAG	C8-C7-N2-C2
6	H	601	NAG	O7-C7-N2-C2
6	C	601	NAG	C4-C5-C6-O6
6	H	601	NAG	C4-C5-C6-O6
6	D	601	NAG	O5-C5-C6-O6
6	K	601	NAG	C4-C5-C6-O6
6	K	601	NAG	O5-C5-C6-O6
6	D	601	NAG	C4-C5-C6-O6
6	B	601	NAG	O5-C5-C6-O6
6	C	601	NAG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

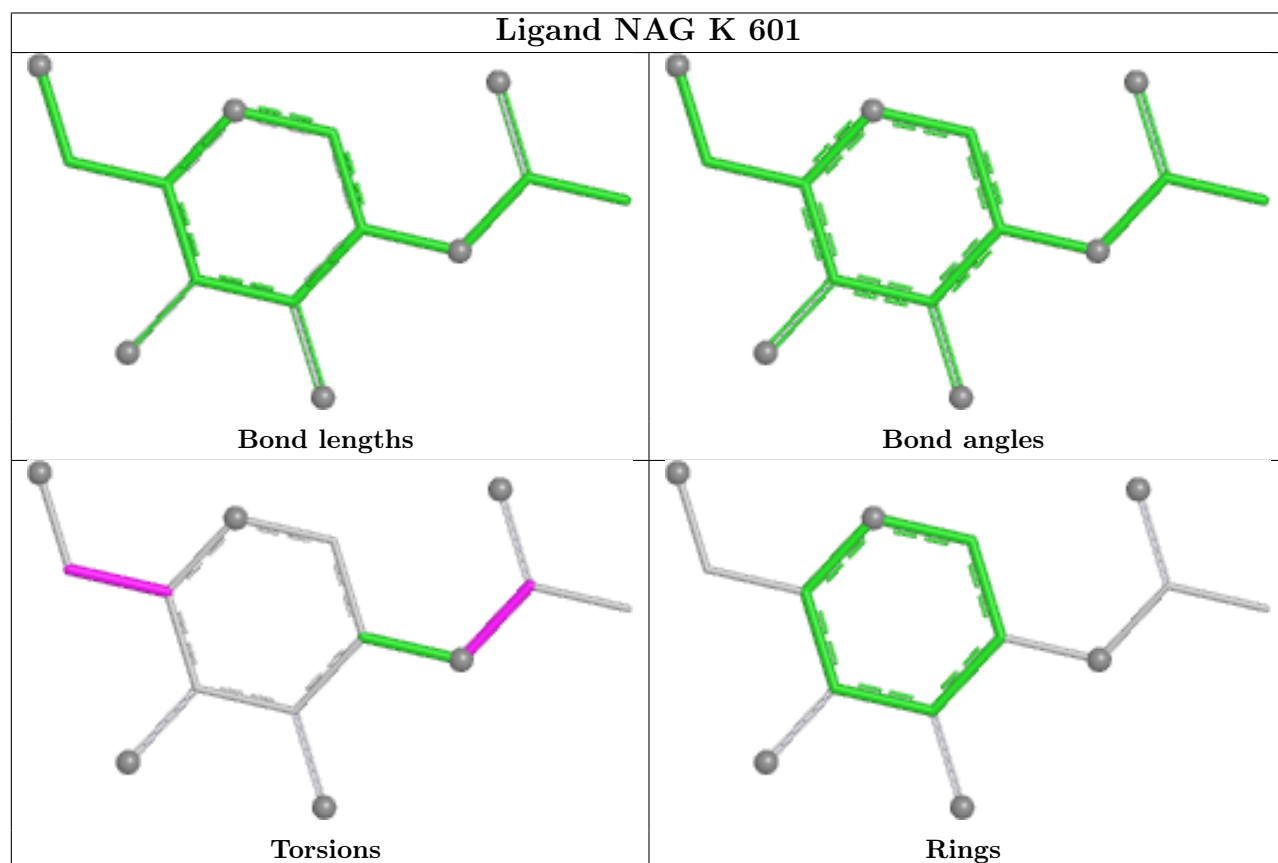
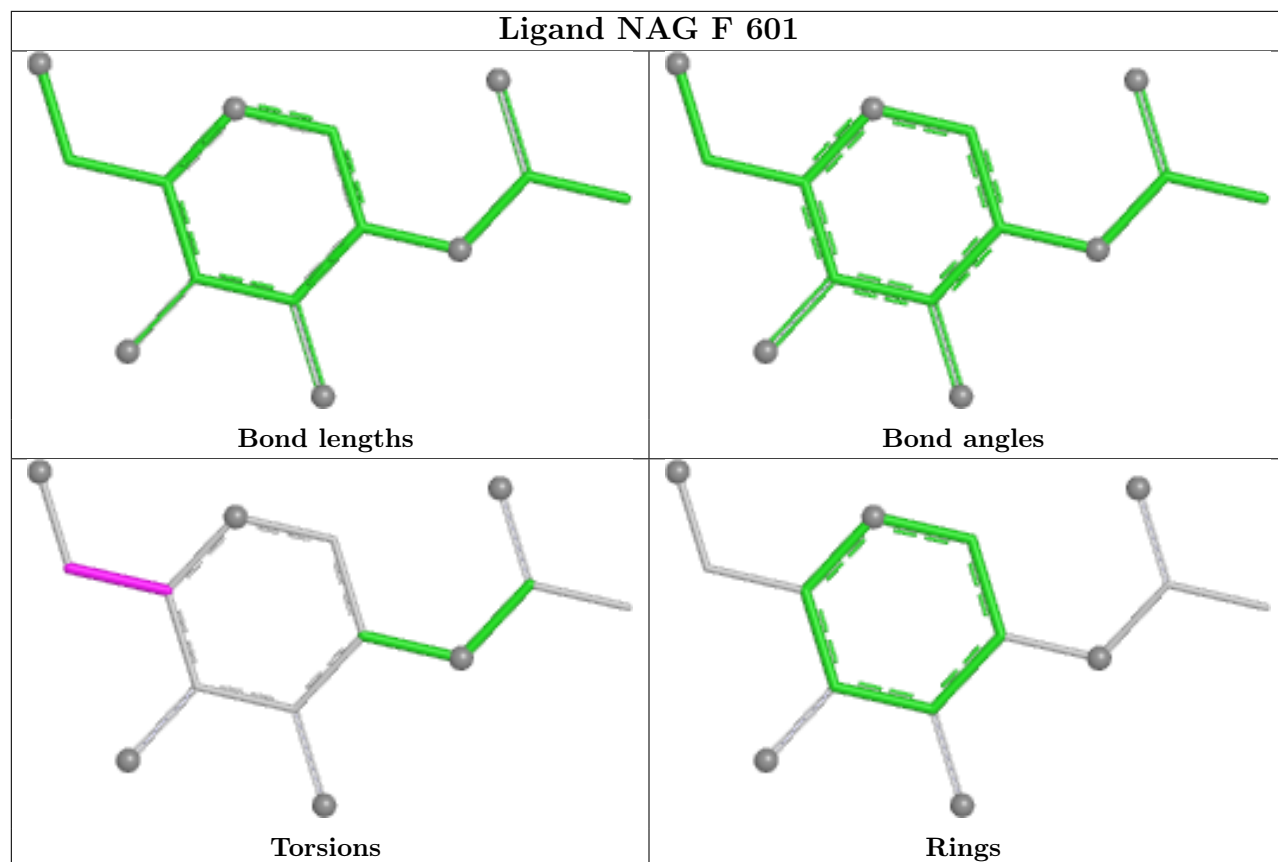
There are no ring outliers.

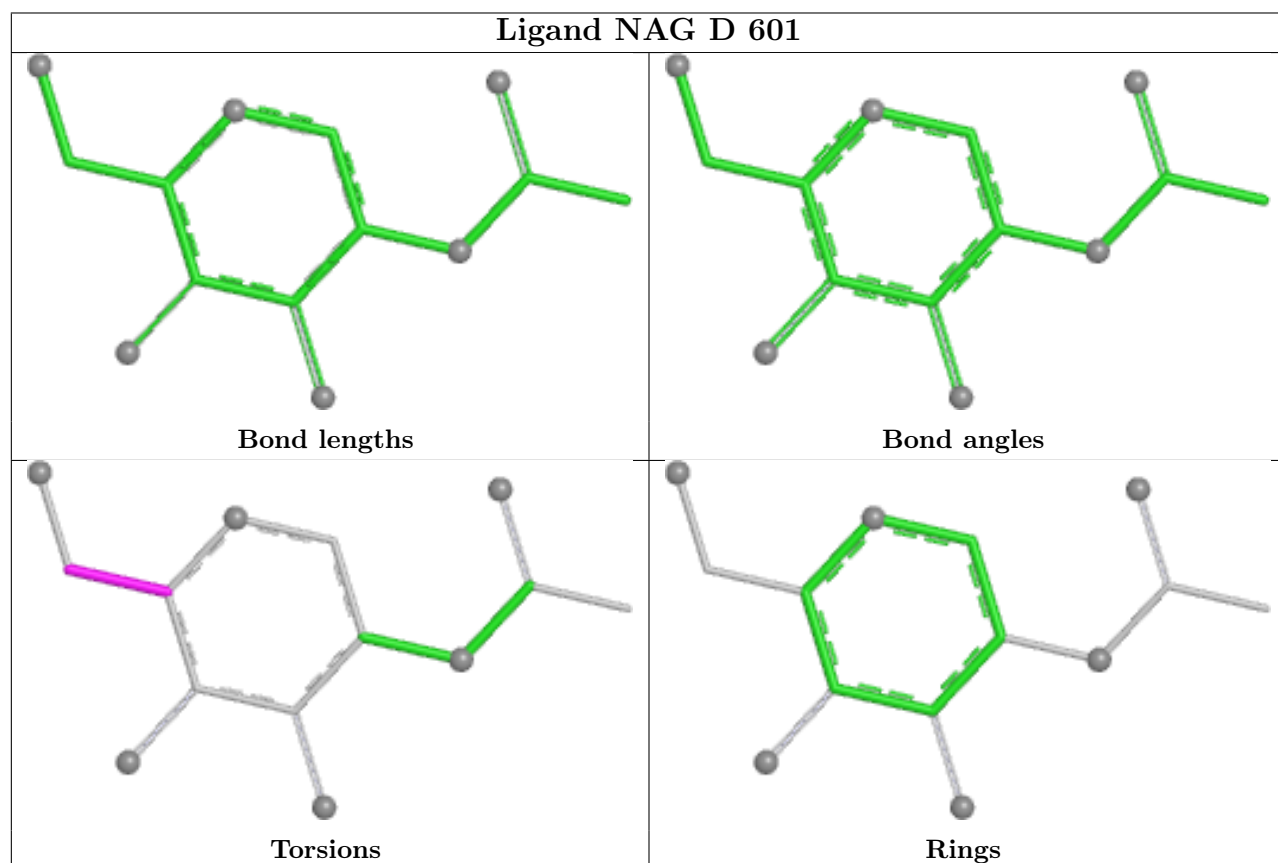
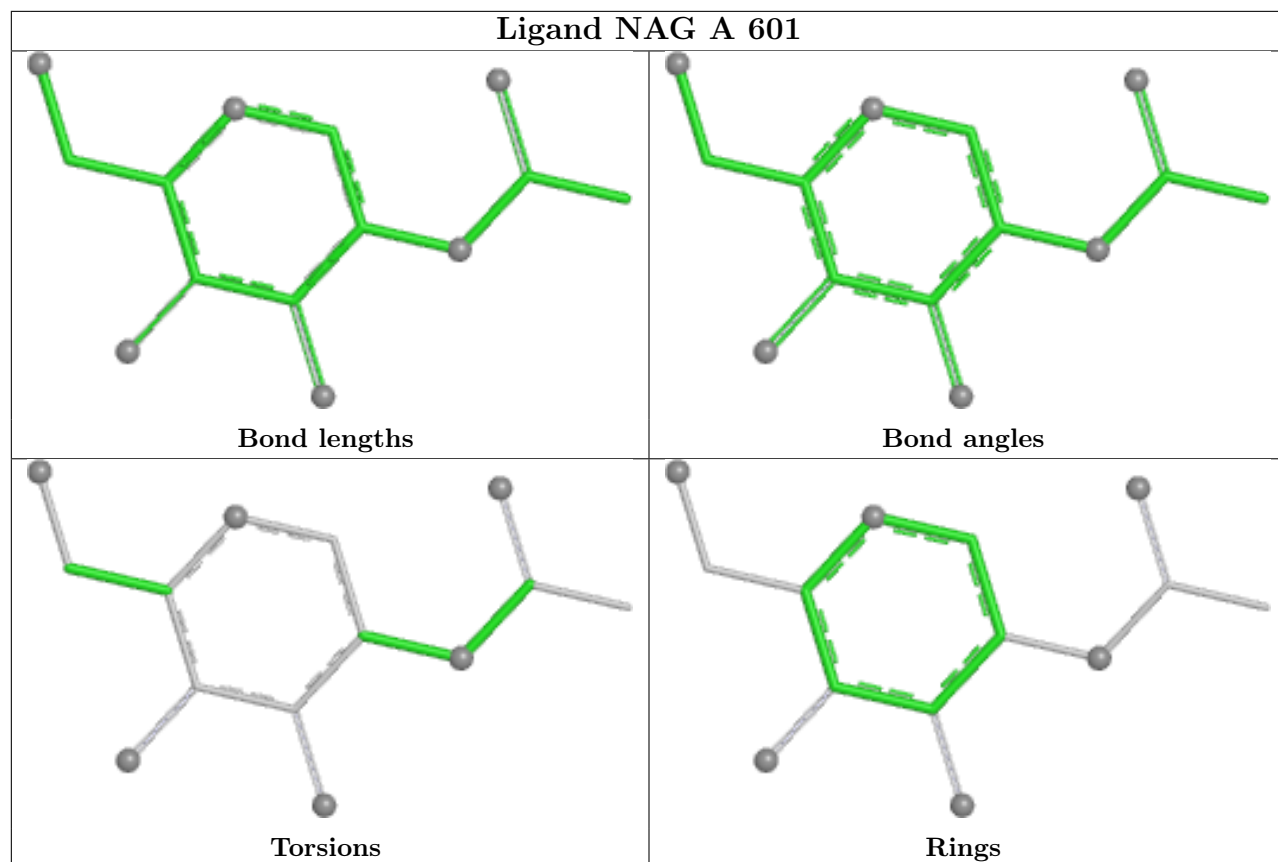
7 monomers are involved in 10 short contacts:

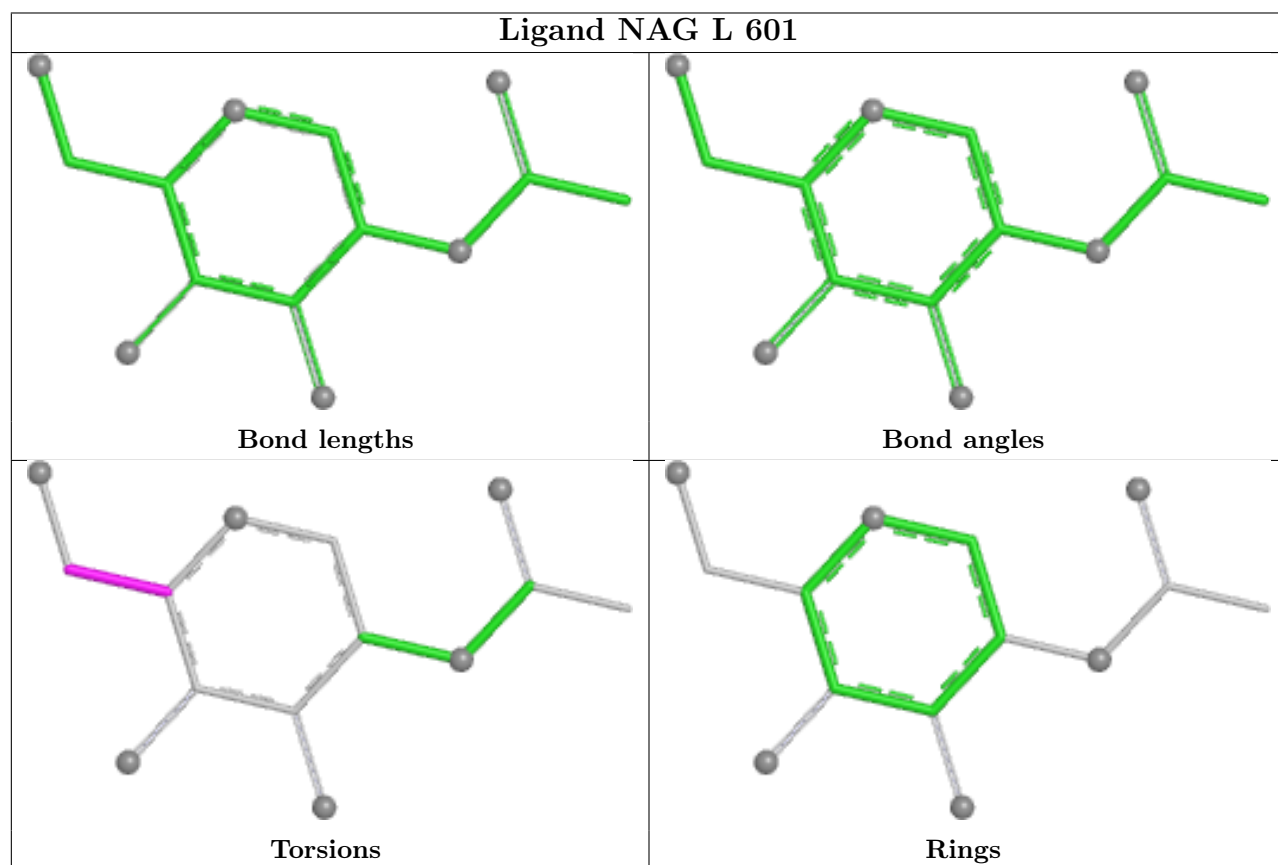
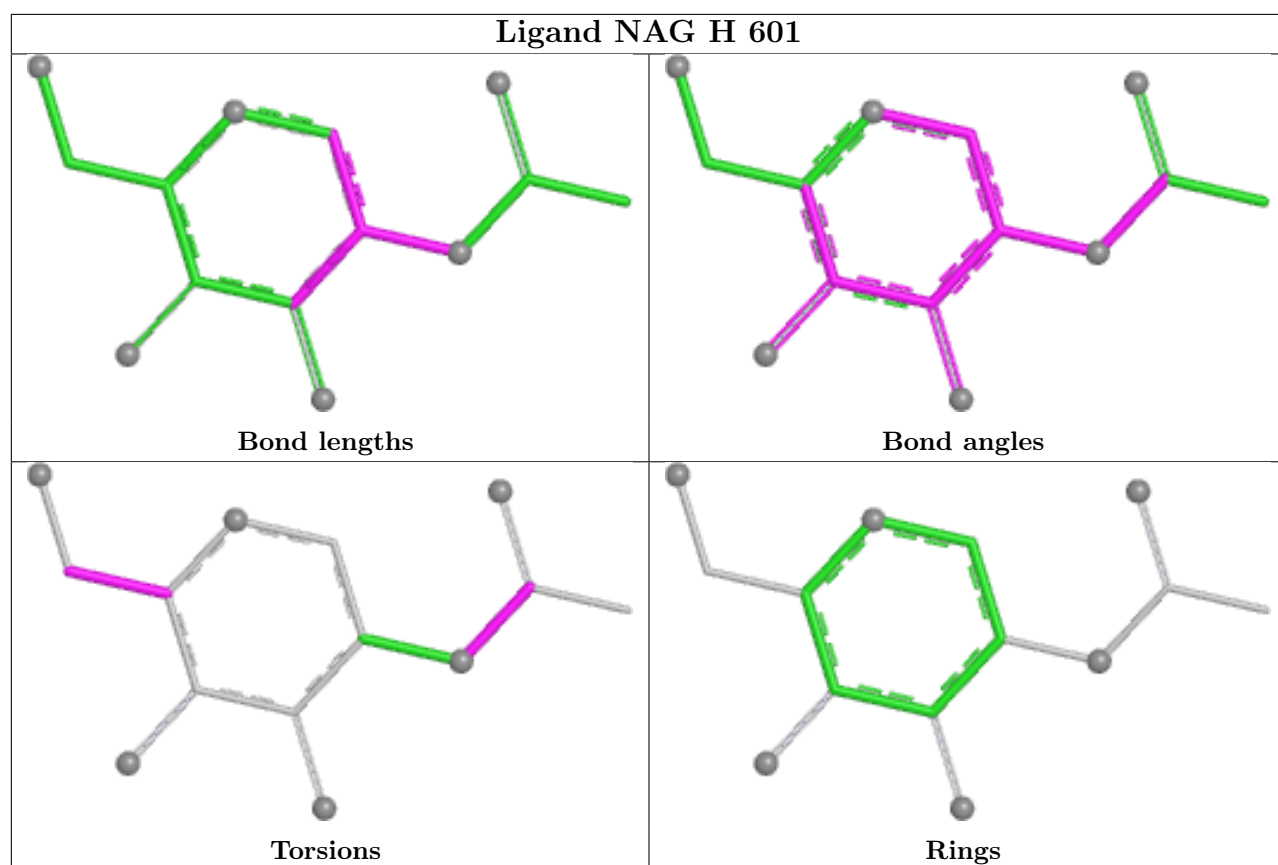
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	601	NAG	1	0
6	K	601	NAG	4	0
6	A	601	NAG	1	0
6	H	601	NAG	3	0
6	C	601	NAG	2	0
6	E	601	NAG	1	0
6	B	601	NAG	1	0

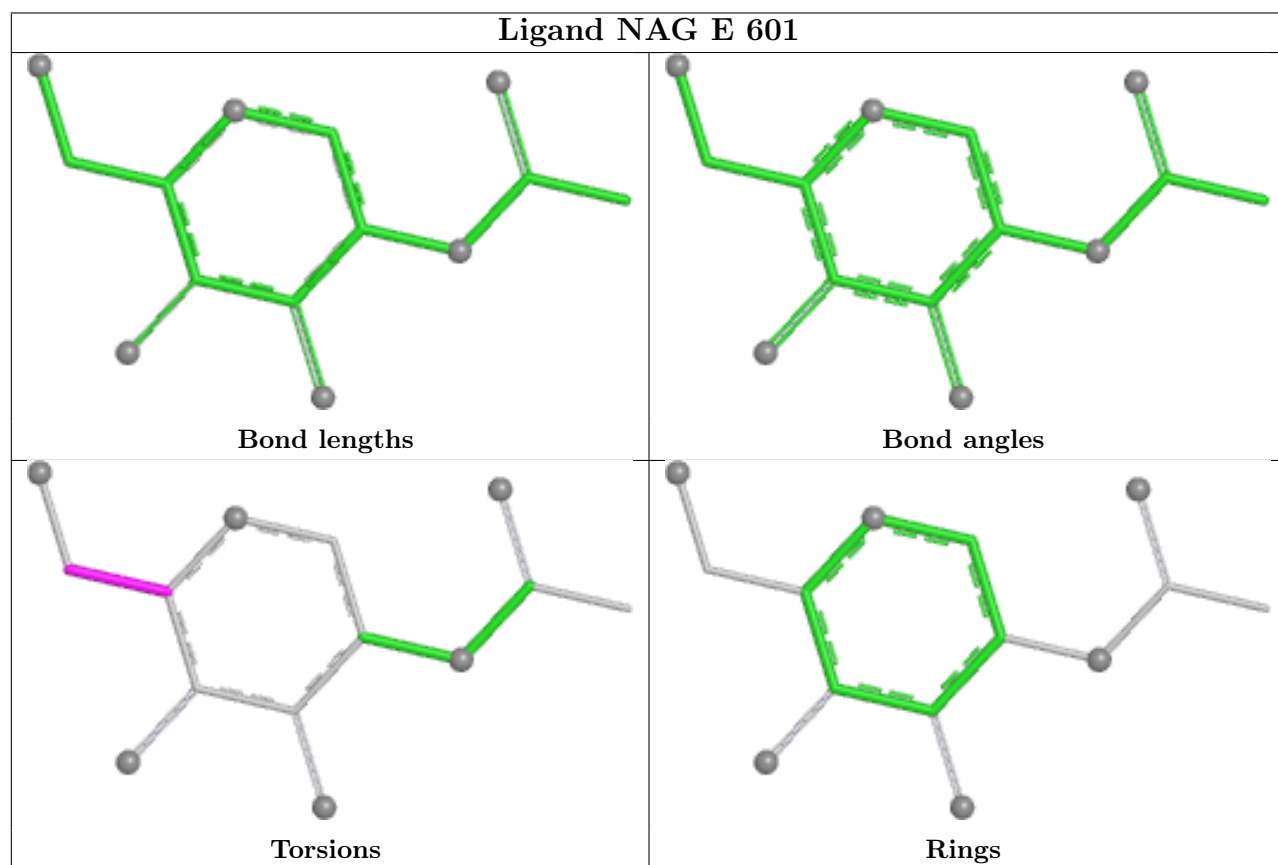
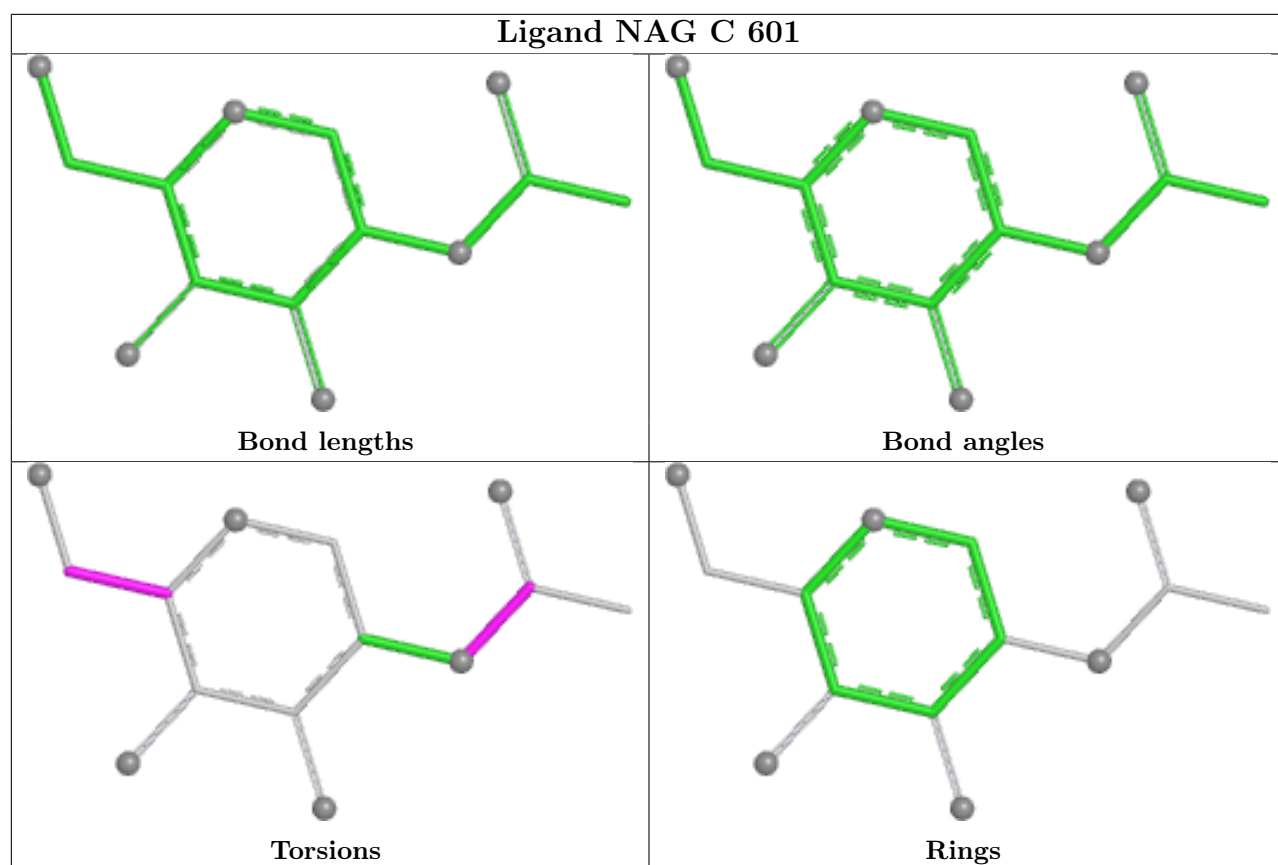
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

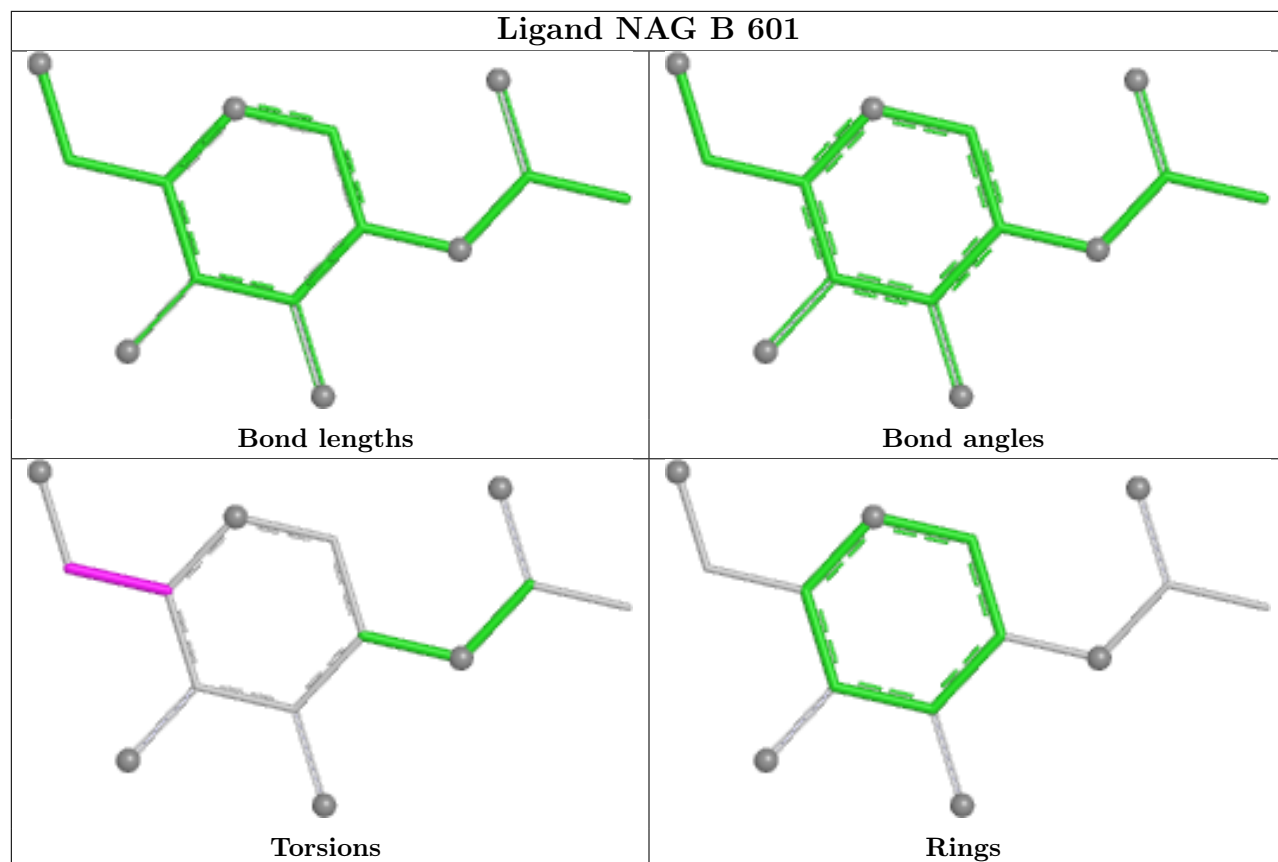












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

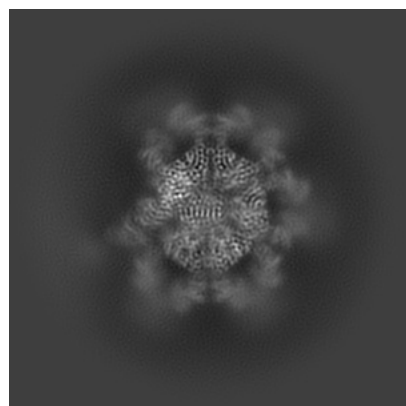
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34074. These allow visual inspection of the internal detail of the map and identification of artifacts.

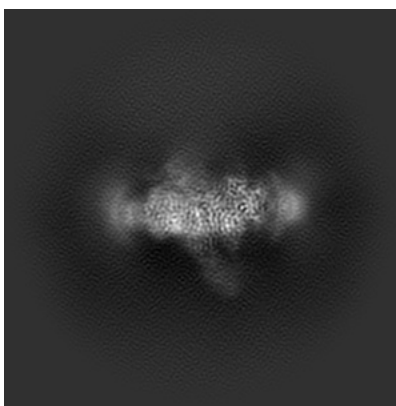
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

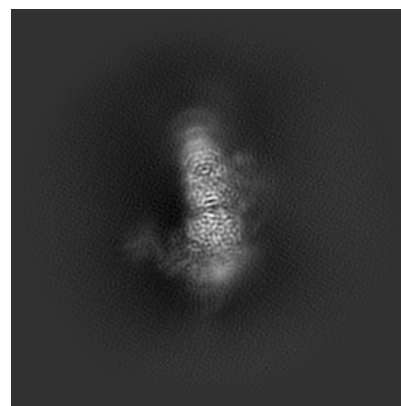
6.1.1 Primary map



X

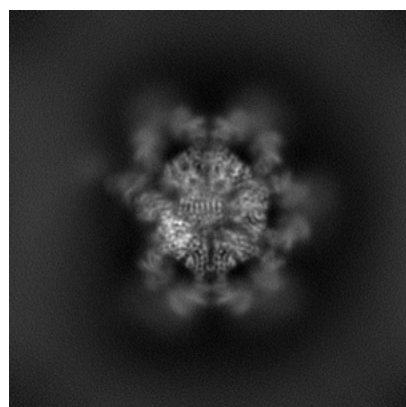


Y

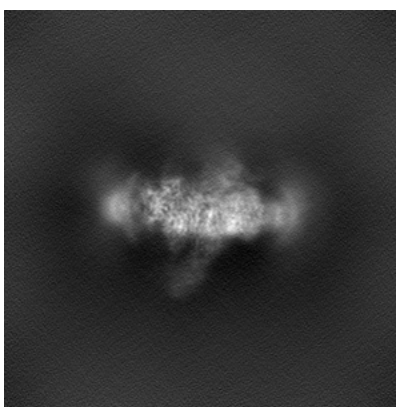


Z

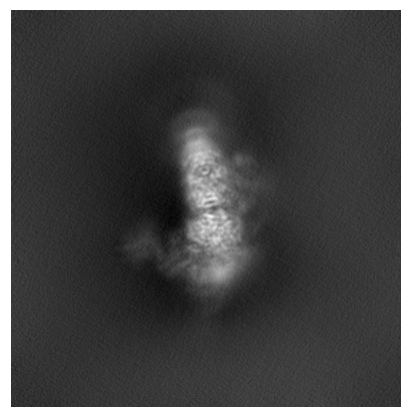
6.1.2 Raw map



X



Y

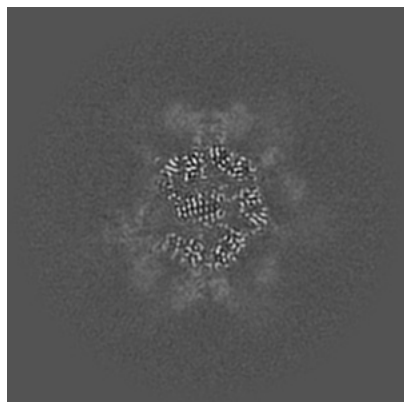


Z

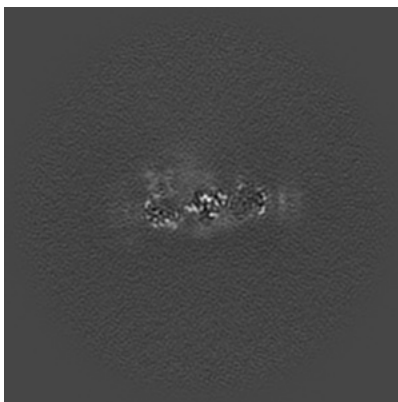
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

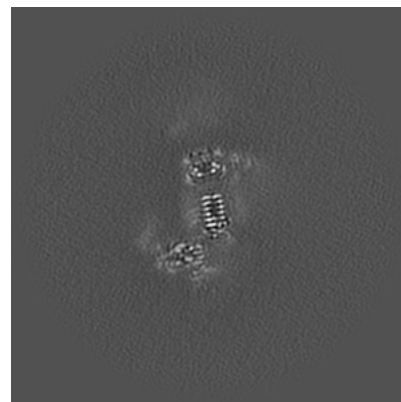
6.2.1 Primary map



X Index: 160

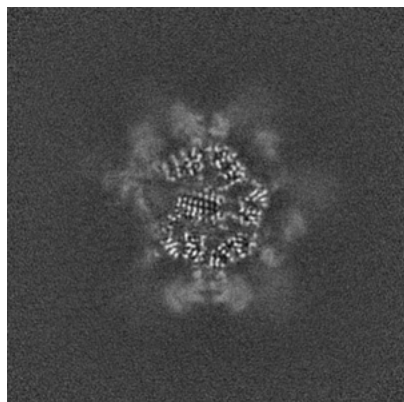


Y Index: 160

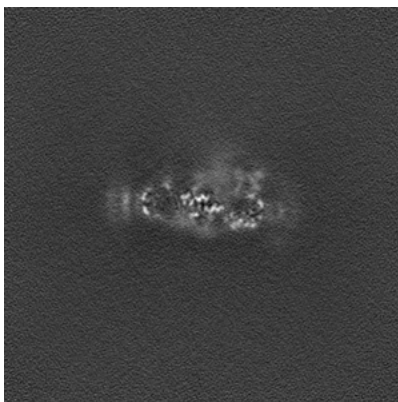


Z Index: 160

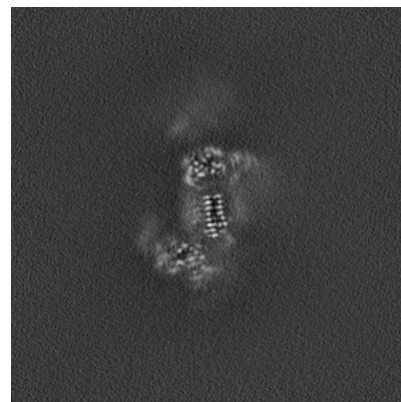
6.2.2 Raw map



X Index: 160



Y Index: 160

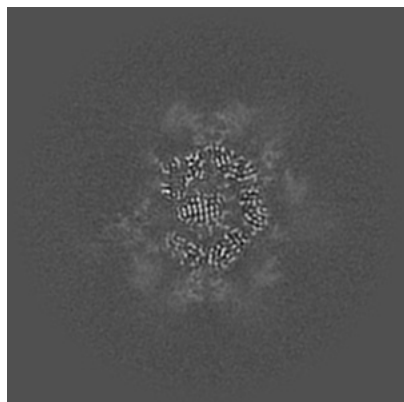


Z Index: 160

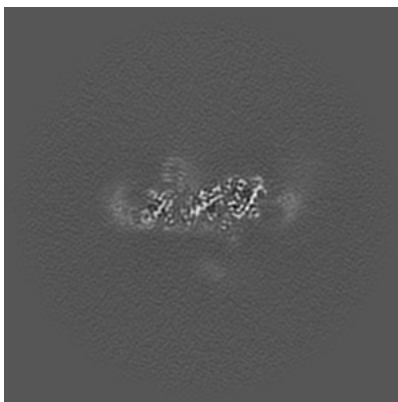
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

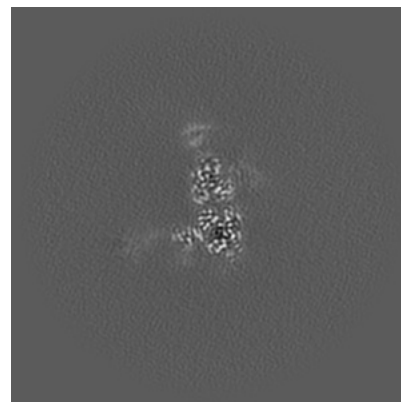
6.3.1 Primary map



X Index: 158

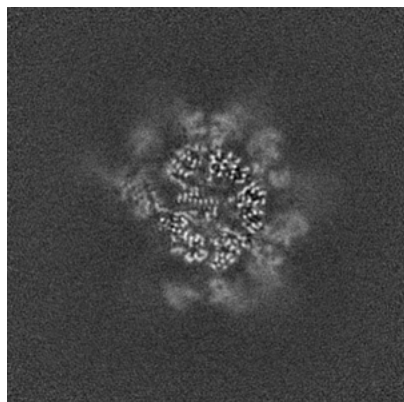


Y Index: 146

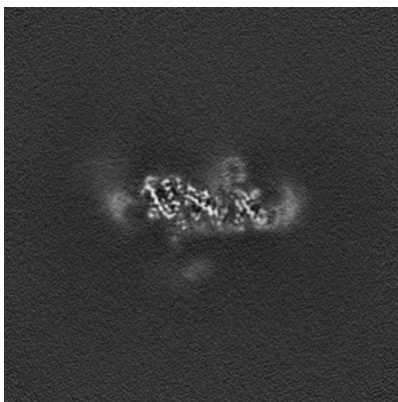


Z Index: 187

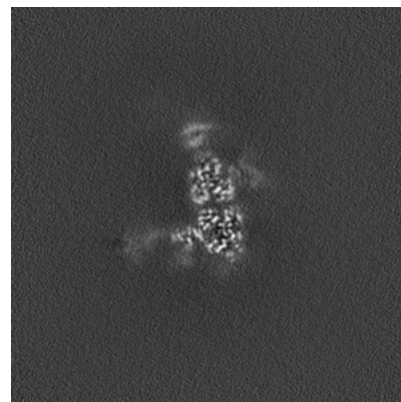
6.3.2 Raw map



X Index: 153



Y Index: 146

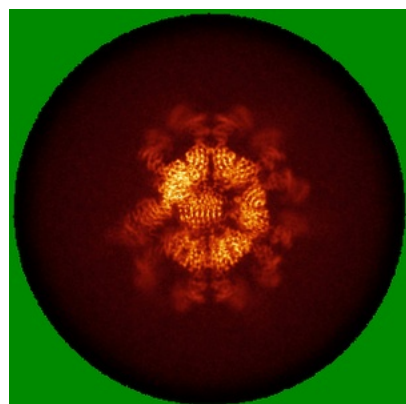


Z Index: 132

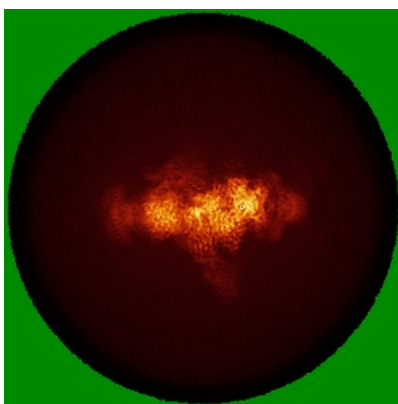
The images above show the largest variance slices of the map in three orthogonal directions.

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

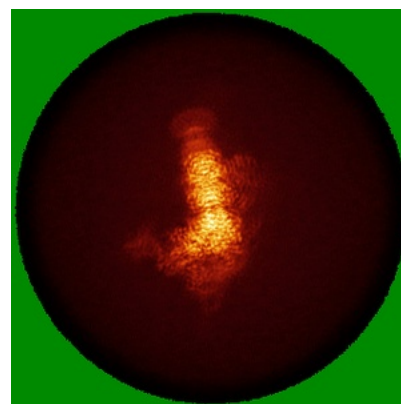
6.4.1 Primary map



X

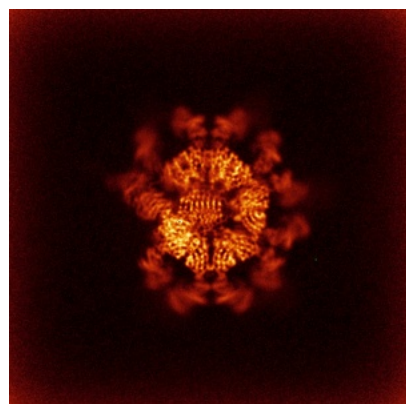


Y

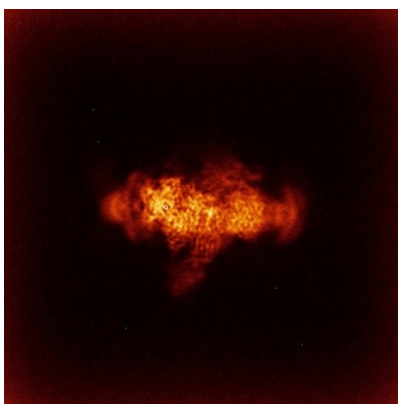


Z

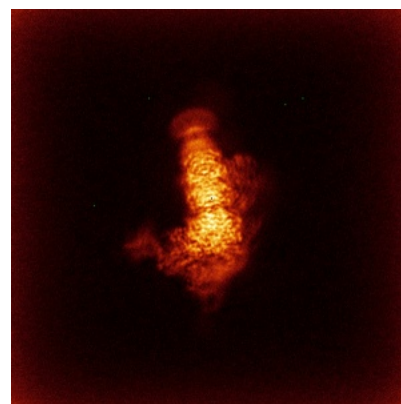
6.4.2 Raw map



X



Y

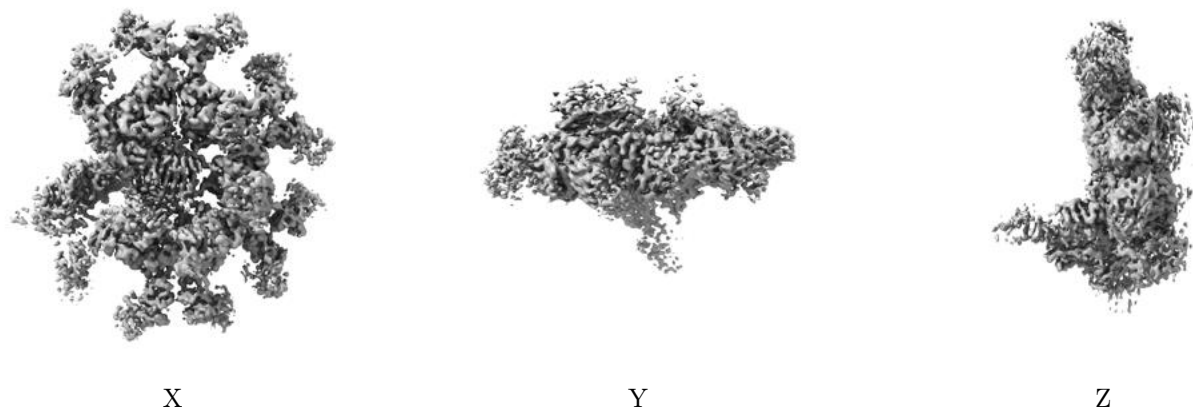


Z

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.

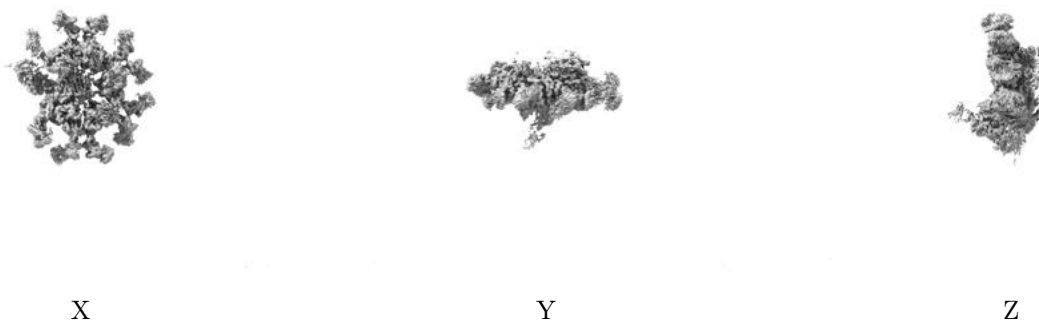
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.27. 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.

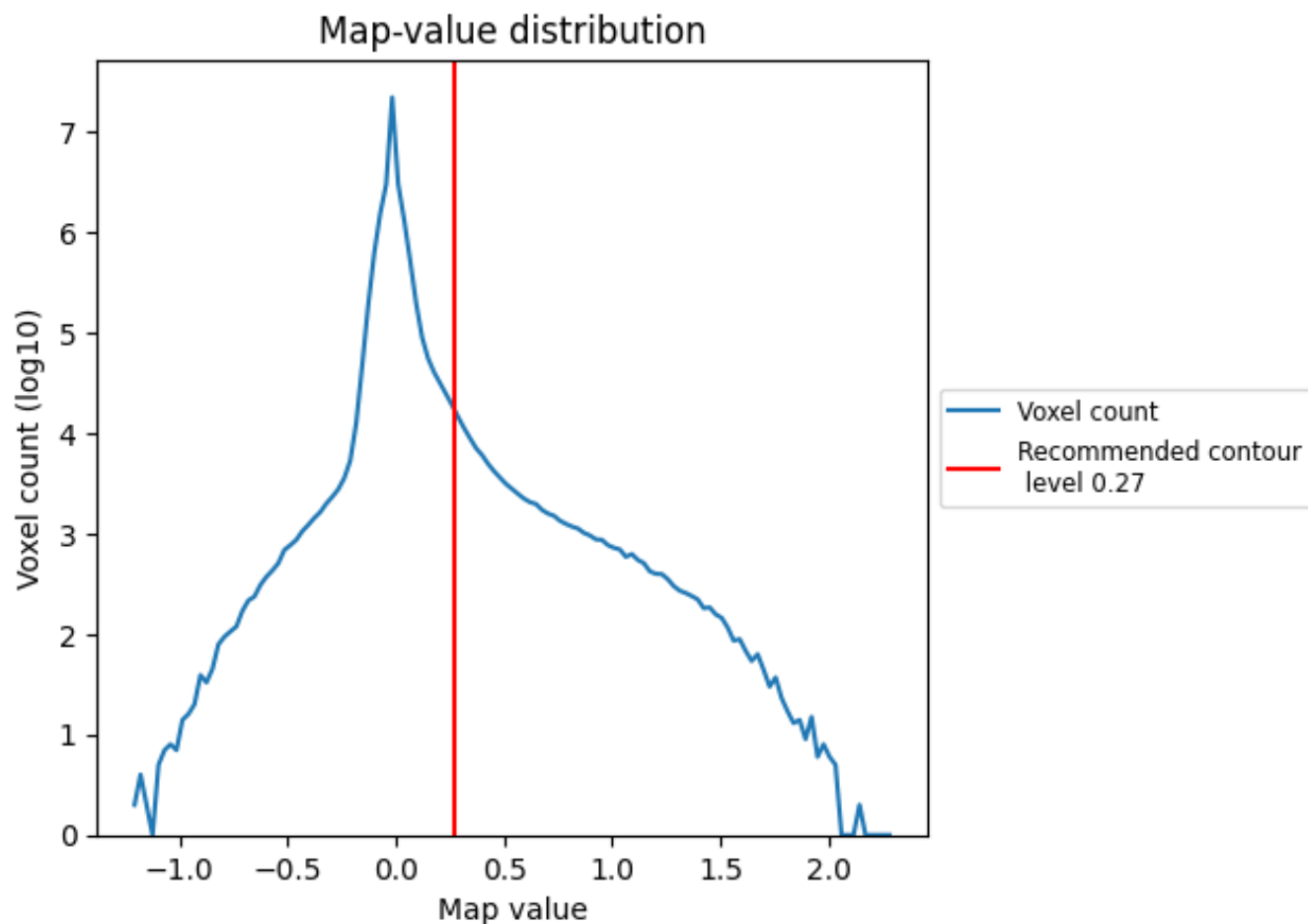
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

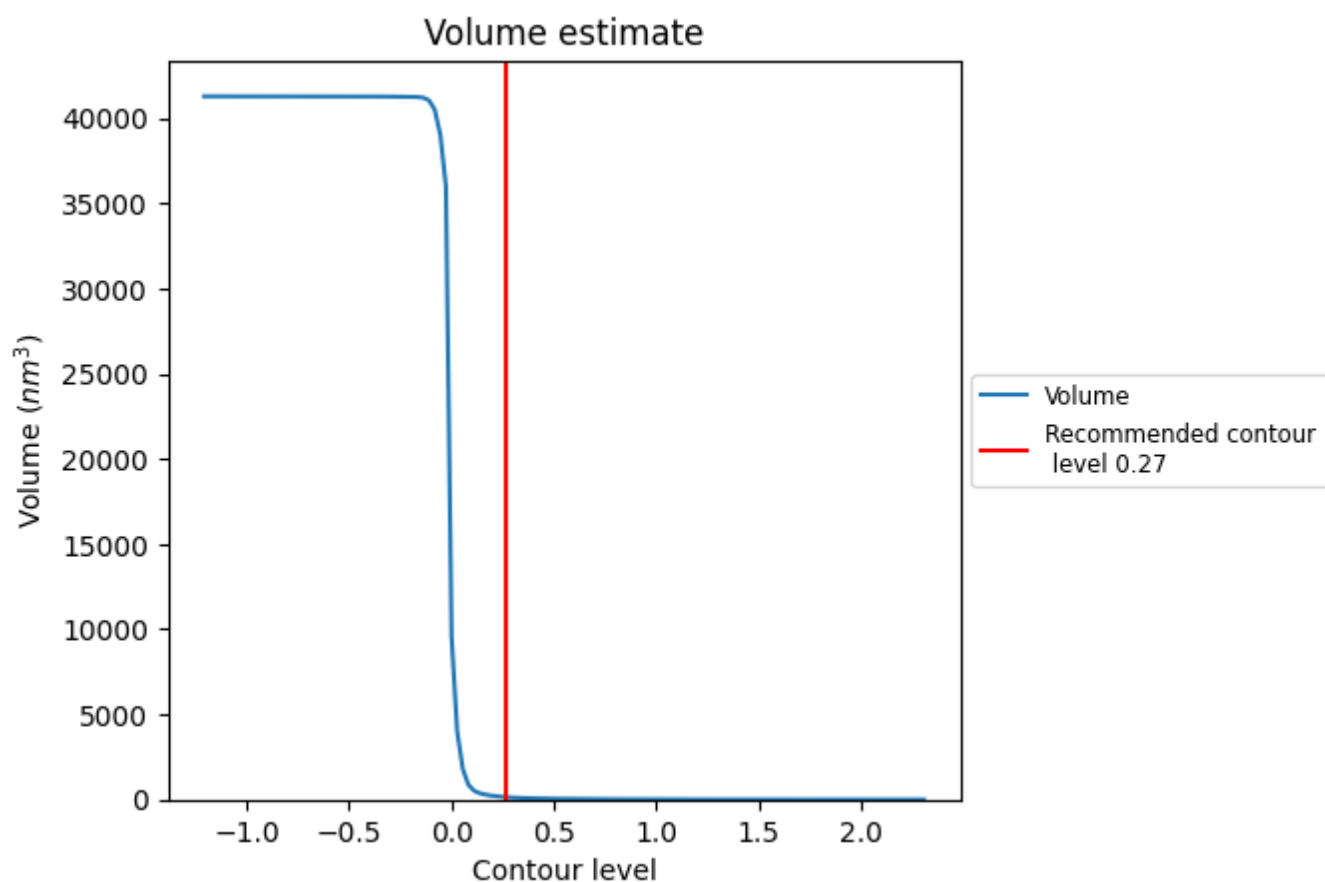
This section contains the results of statistical analysis of the map.

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.

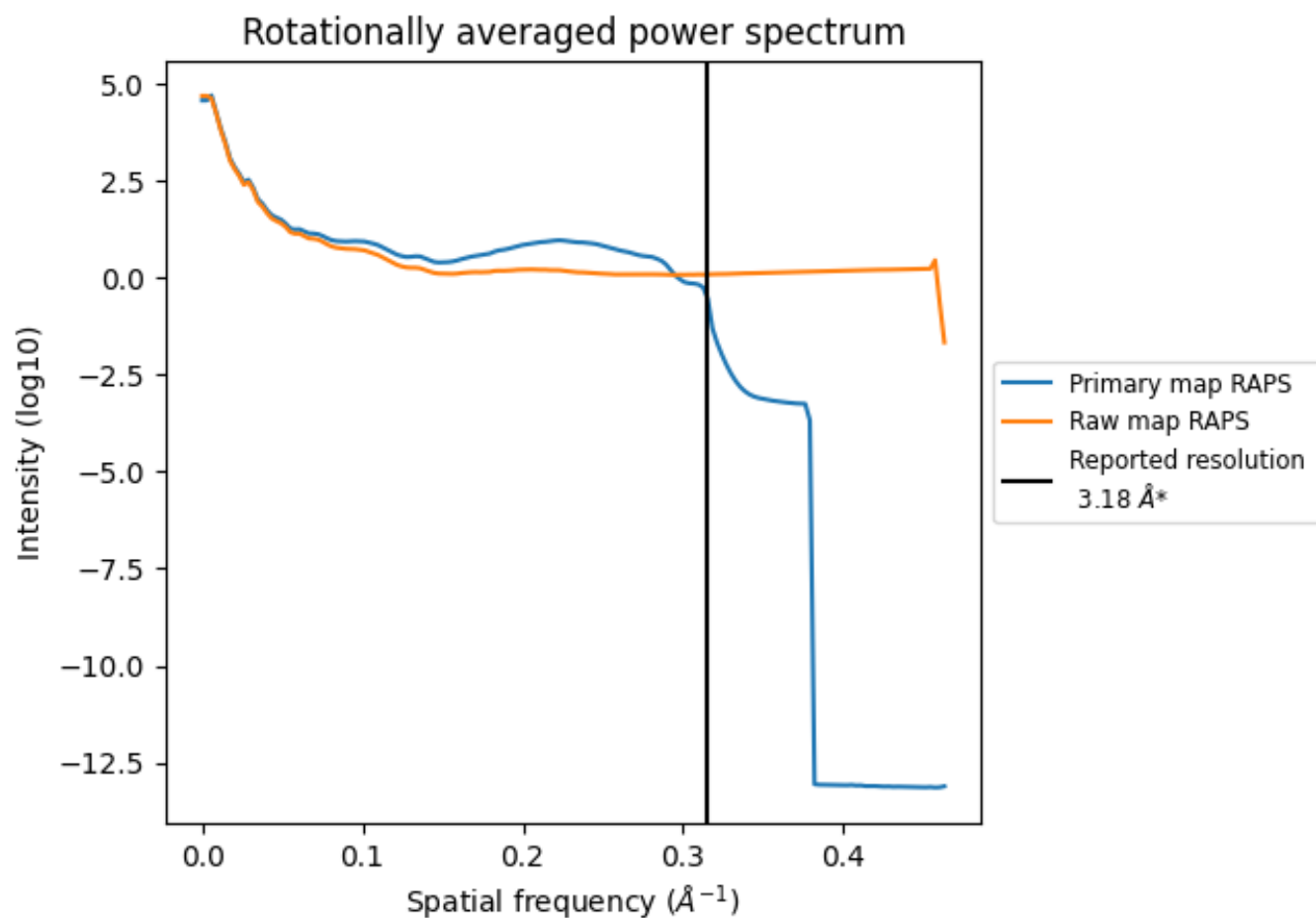
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 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 ⓘ

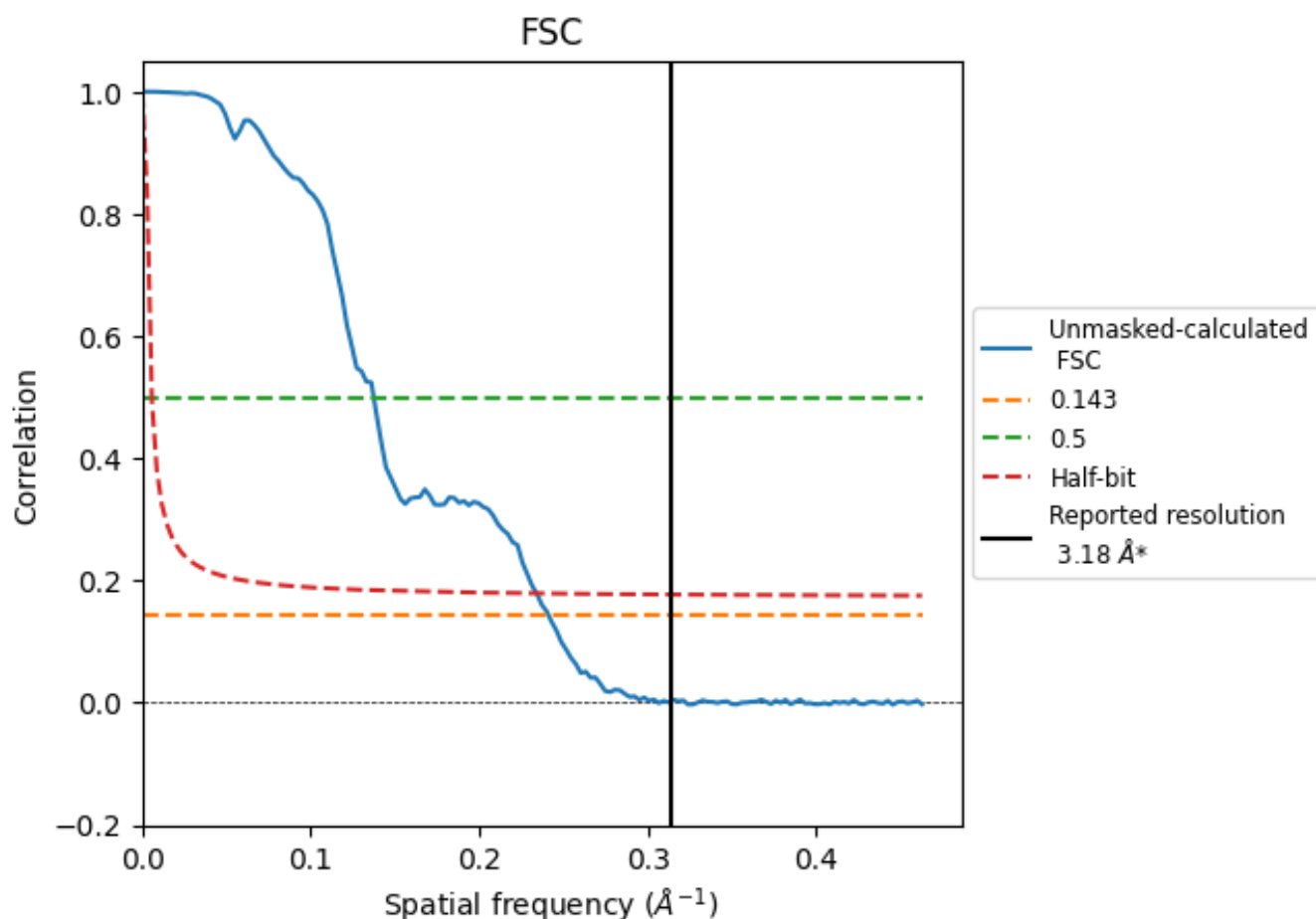


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

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 $0.314 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

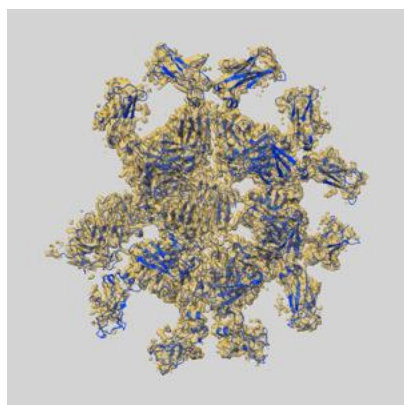
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	7.28	4.27

*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 4.15 differs from the reported value 3.18 by more than 10 %

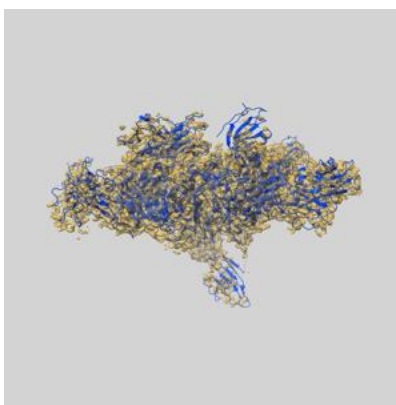
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34074 and PDB model 7YSG. Per-residue inclusion information can be found in section 3 on page 7.

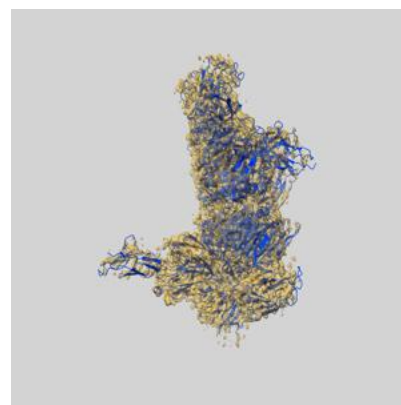
9.1 Map-model overlay [i](#)



X



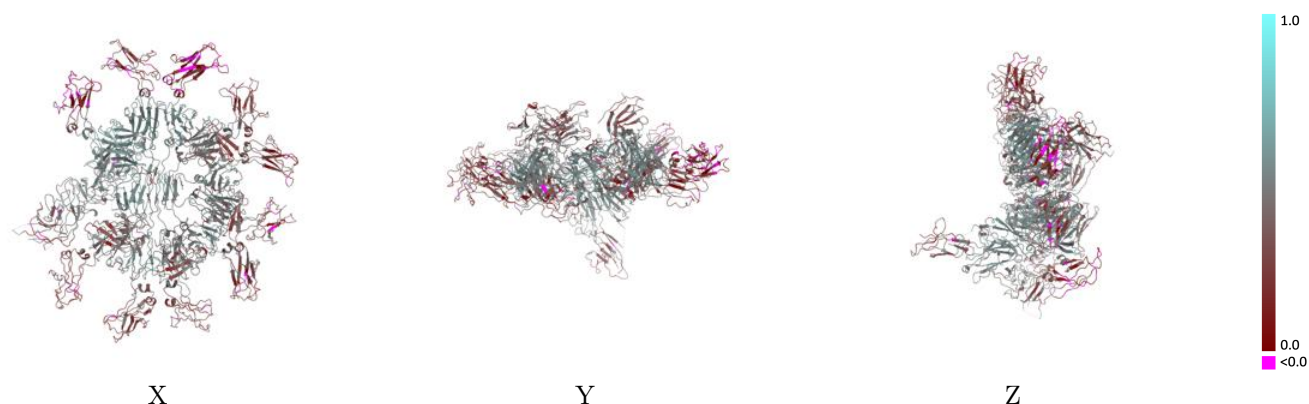
Y



Z

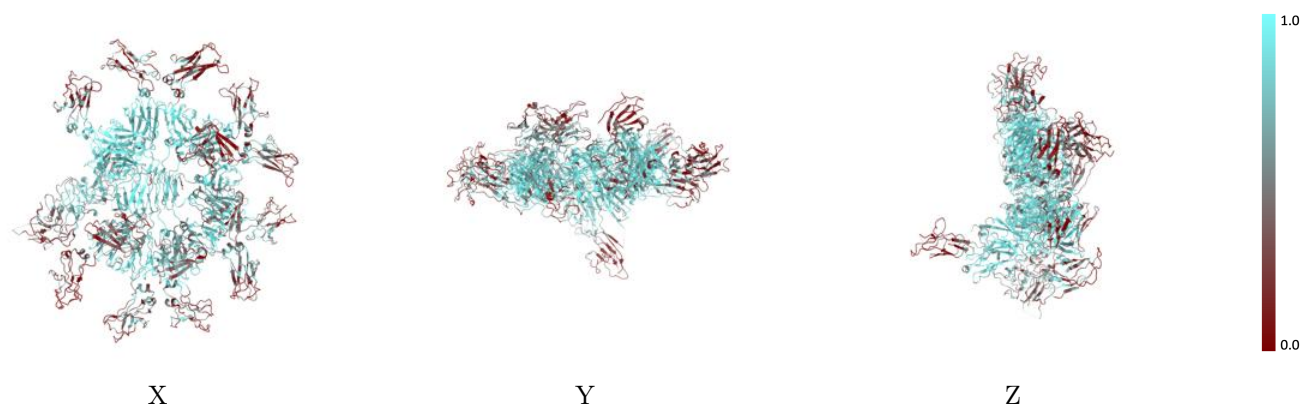
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



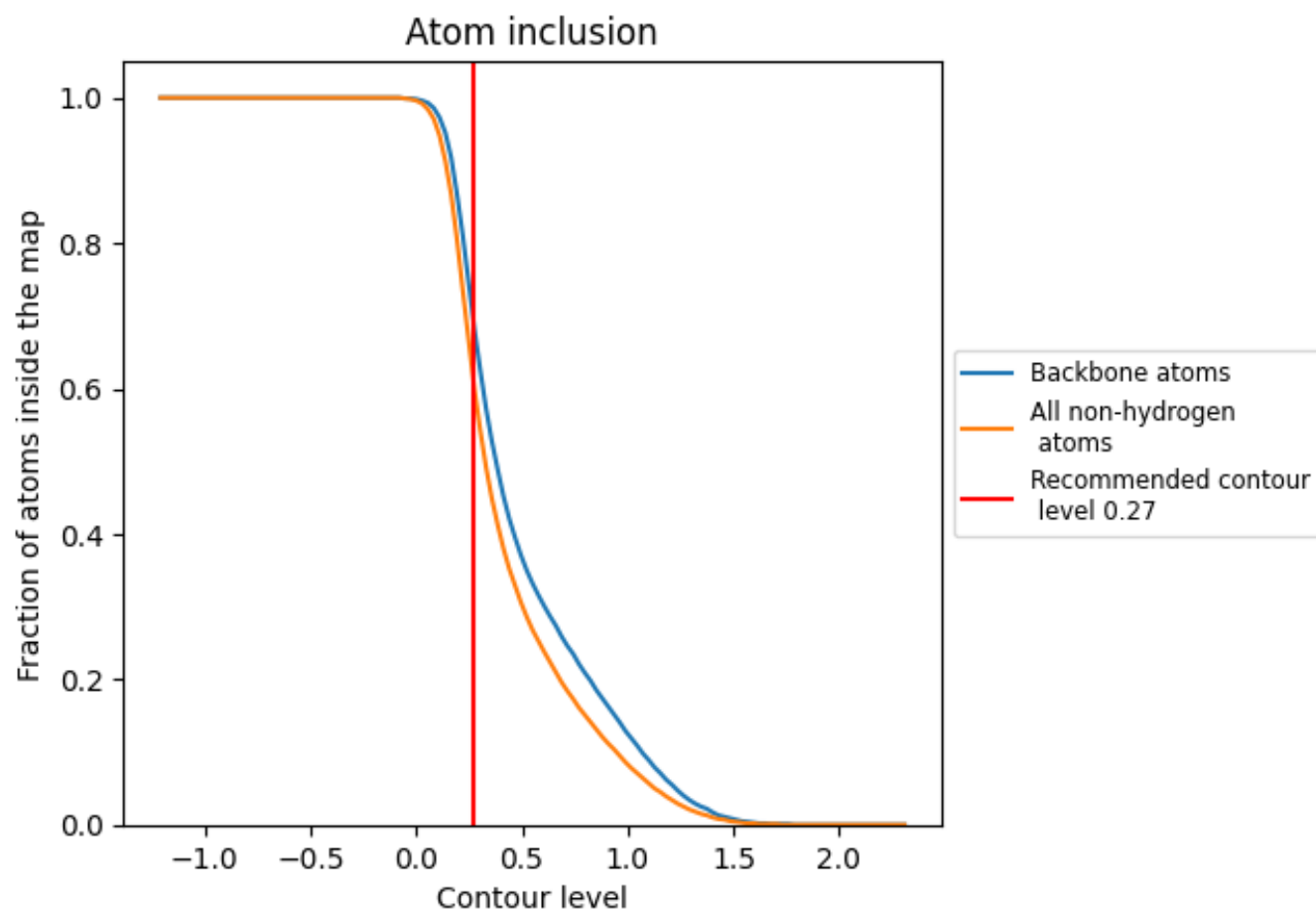
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 61% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6130	 0.4170
A	 0.7060	 0.4120
B	 0.6740	 0.4140
C	 0.6330	 0.3630
D	 0.6710	 0.4220
E	 0.6530	 0.4120
F	 0.6720	 0.4230
G	 0.6590	 0.4200
H	 0.6520	 0.4220
I	 0.8570	 0.5310
J	 0.8730	 0.5460
K	 0.6670	 0.4280
L	 0.5250	 0.3900
P	 0.5720	 0.4370
R	 0.3350	 0.3800
S	 0.4800	 0.4030
U	 0.4590	 0.4160
V	 0.2330	 0.3610

