



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:01 PM UTC

PDB ID : 8Z3P / pdb_00008z3p
EMDB ID : EMD-39750
Title : The structure of type III CRISPR-associated deaminase in complex cA6 and ATP, fully activated
Authors : Chen, M.R.; Li, Z.X.; Xiao, Y.B.
Deposited on : 2024-04-15
Resolution : 3.40 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

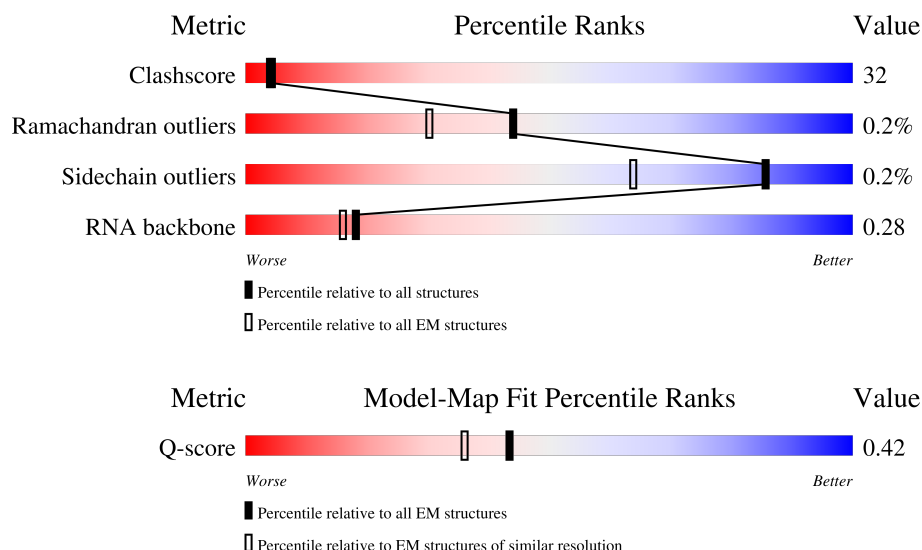
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



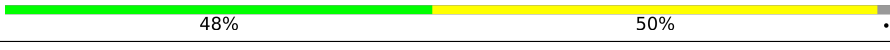
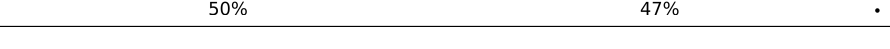
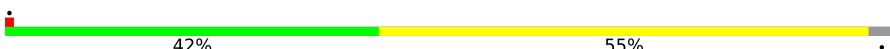
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	X	6	
1	Y	6	
1	Z	6	

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Mol	Chain	Length	Quality of chain
2	A	628	
2	B	628	
2	C	628	
2	D	628	
2	E	628	
2	F	628	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29566 atoms, of which 72 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 RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	6	Total	C	N	O	P	0	0
			132	60	30	36	6		
1	Y	6	Total	C	N	O	P	0	0
			132	60	30	36	6		
1	Z	6	Total	C	N	O	P	0	0
			132	60	30	36	6		

- Molecule 2 is a protein called Adenosine deaminase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	B	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	C	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	D	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	E	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
2	F	612	Total	C	N	O	S	0	0
			4804	3034	892	856	22		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	F	1	Total	Zn	0
			1	1	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA (5'-R(P*AP*AP*AP*AP*AP*A)-3')

Chain X: 

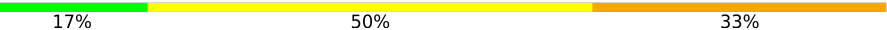


- Molecule 1: RNA (5'-R(P*AP*AP*AP*AP*AP*A)-3')

Chain Y: 



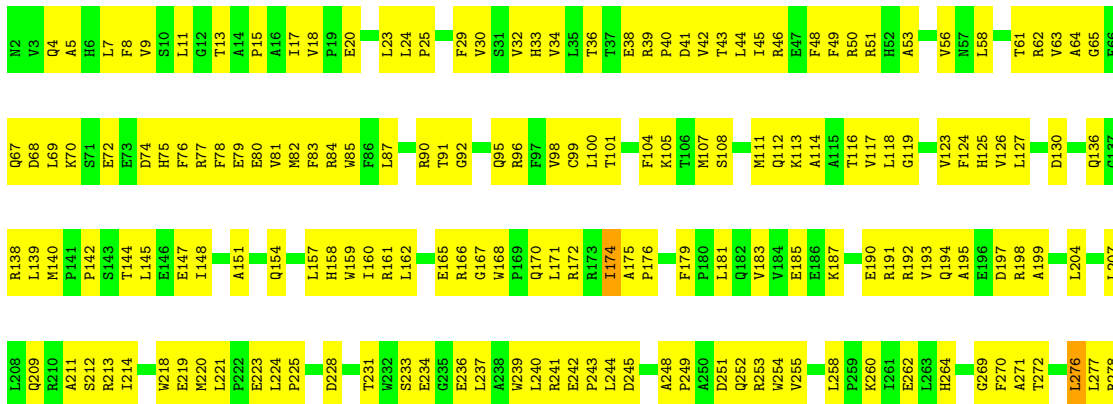
- Molecule 1: RNA (5'-R(P*AP*AP*AP*AP*AP*A)-3')

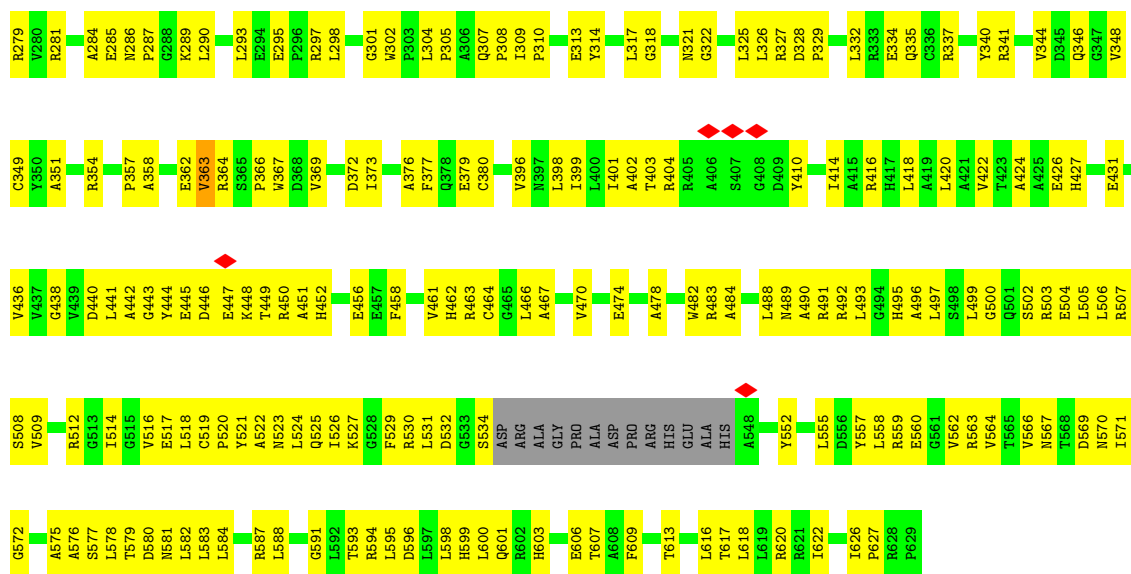
Chain Z: 



- Molecule 2: Adenosine deaminase domain-containing protein

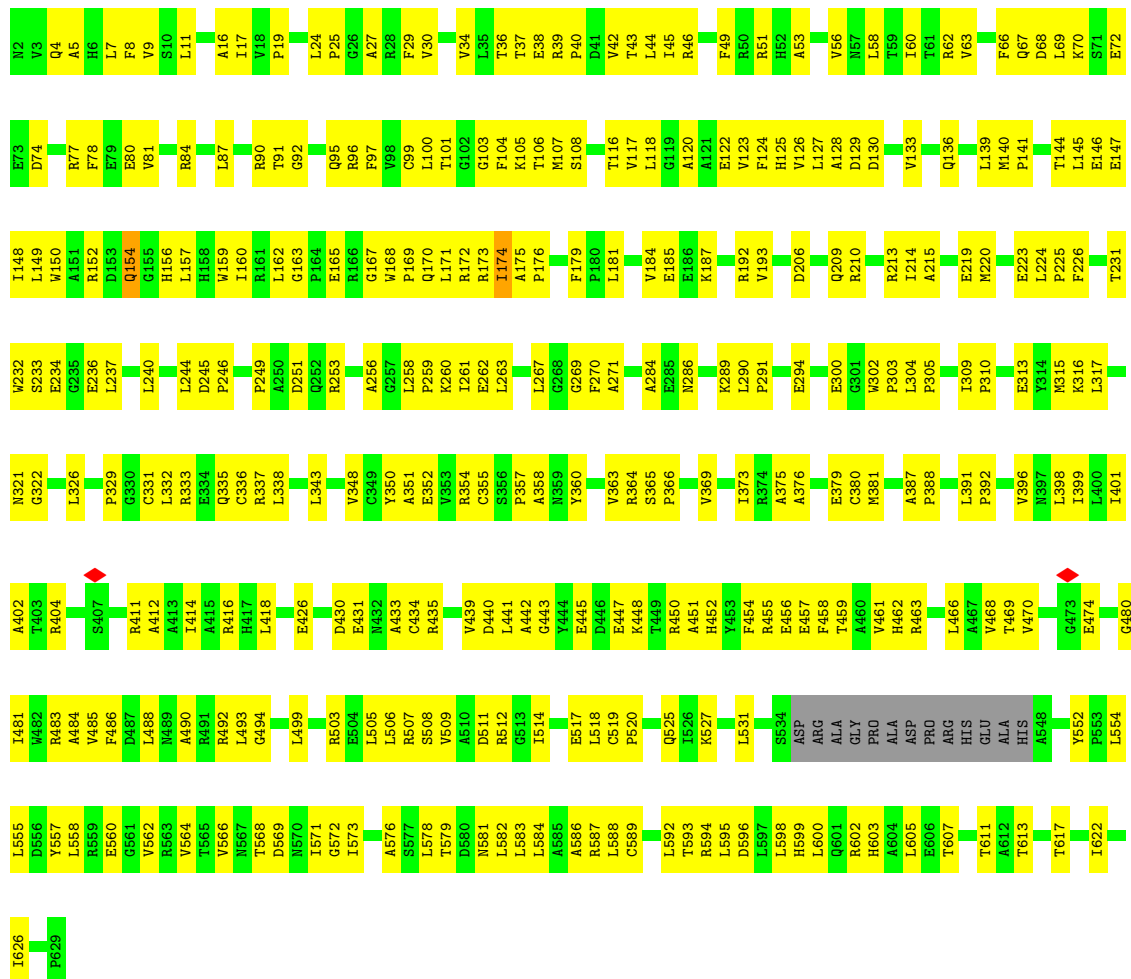
Chain A: 



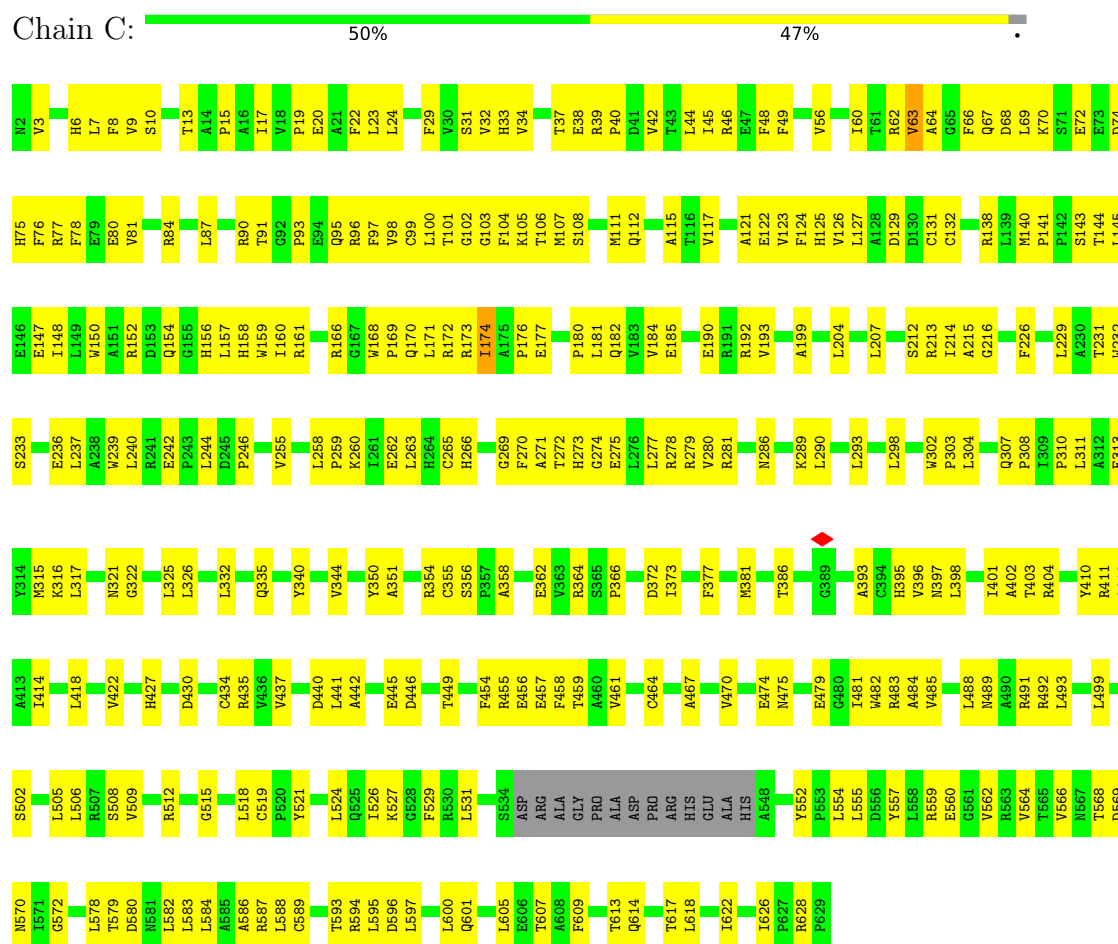


• Molecule 2: Adenosine deaminase domain-containing protein

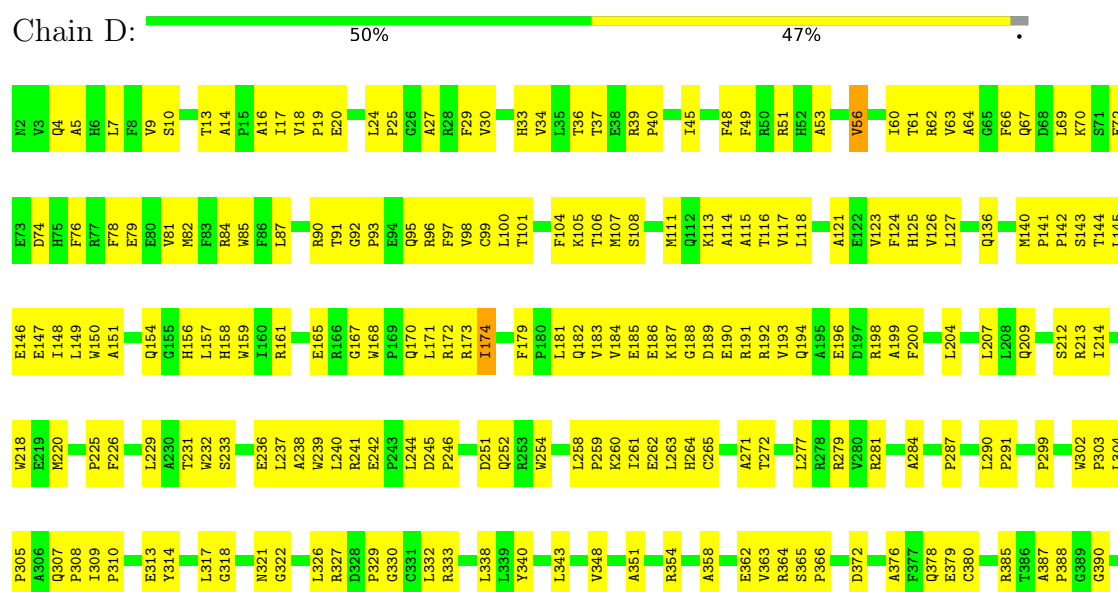
Chain B: 48% 50% .

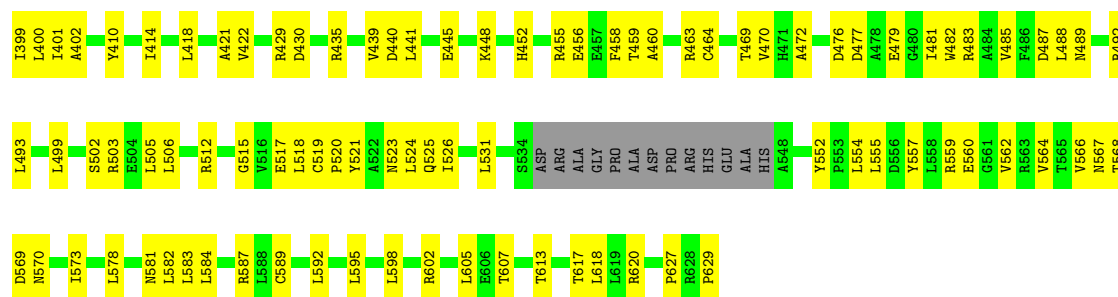


- Molecule 2: Adenosine deaminase domain-containing protein

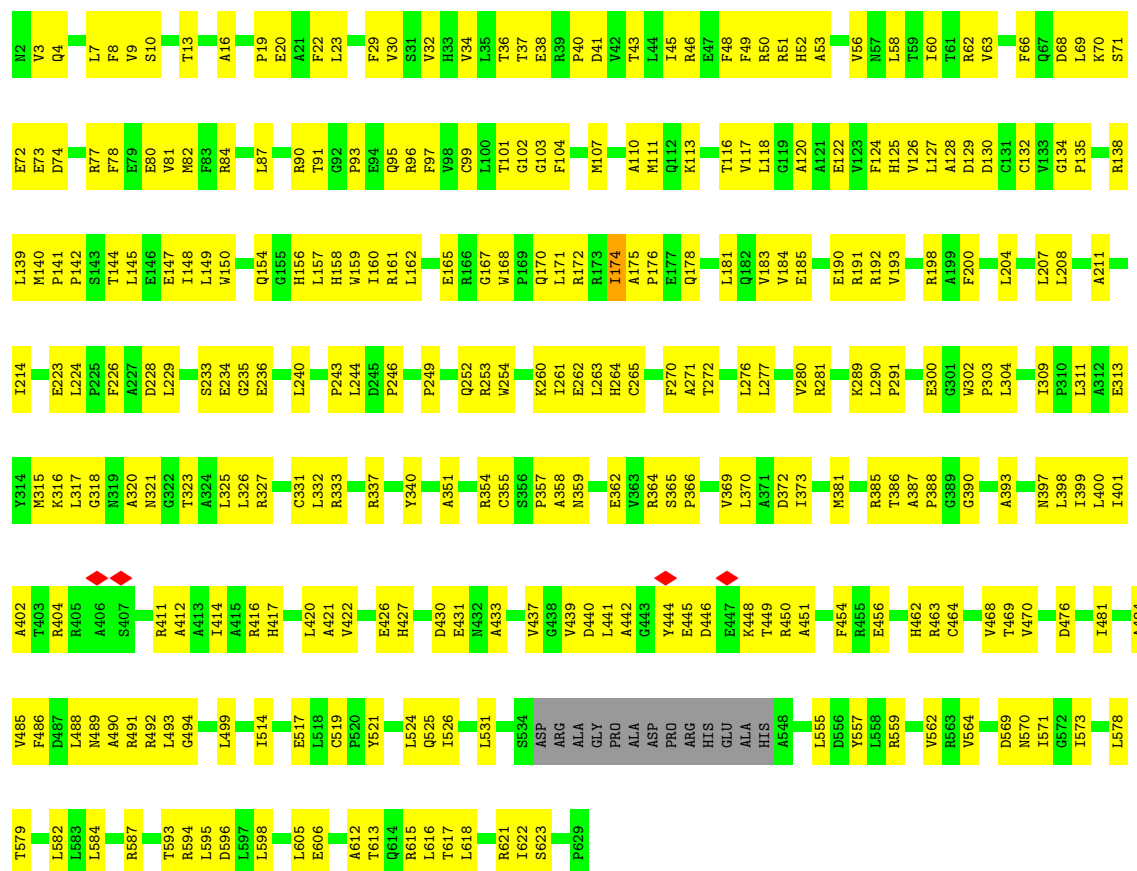


- Molecule 2: Adenosine deaminase domain-containing protein

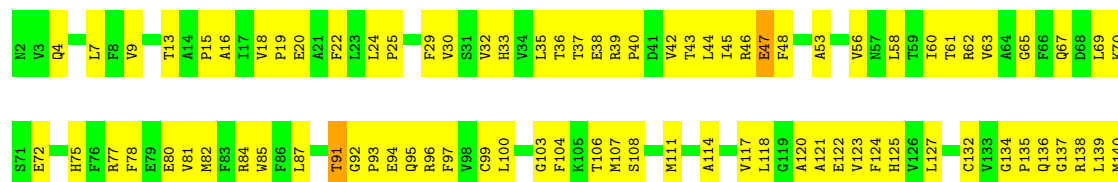




• Molecule 2: Adenosine deaminase domain-containing protein



• Molecule 2: Adenosine deaminase domain-containing protein



A586	A587	L588	G591	L592	T593	R594	L595	D596	L597	L600	Q601	R602	H603	A604	L605	E606	T607	T613	Q614	T617	L618	L619	I622	I626	P627	R628	P629																												
V516	E517	L518	C519	P520	Y521	L524	Q525	R530	L531	S534	ASP	ARG	ALA	GLY	PRO	F458	T459	A460	V461	H462	R463	C464	G465	L466	T469	V470	H471	A472	G473	E474	A478	W482	R483	A484	V485	L488	N489	R492	L493	G494	L499	S502	L505	L506	R507	S508	V509	G515							
D440	L441	A442	G443	Y444	E445	D446	E447	E448	T449	R450	A451	H452	Y453	F454	R455	E456	E457	F458	T459	A460	V461	H462	R463	C464	G465	L466	T469	V470	H471	A472	G473	E474	A478	W482	R483	A484	V485	L488	N489	R492	L493	G494	L499	S502	L505	L506	R507	S508	V509	G515					
S356	P357	A358	N359	Y360	A361	E362	V363	R364	S365	P366	V369	Q378	E379	C380	R385	T386	A387	A388	G389	G390	A393	N397	L398	I399	L400	I401	A402	T403	R404	S407	R411	A412	A413	I414	A415	R416	H417	L418	A421	V422	H427	E431	R432	A433	C434	V437	G438	V439							
Q209	R210	R213	I214	W220	E223	L224	P225	F226	L229	A230	T231	W232	S233	E236	L237	A238	W239	L240	R241	E242	P243	L244	D245	P246	R247	A248	P249	A250	D251	Q252	R253	W254	V255	L258	P259	K260	L261	E262	L263	H264	C265	H266	G269	F270	A271	T272	L276	L277	R278	R279	L280				
R281	A284	E285	N286	P287	L290	L293	E294	E295	F296	R297	L298	P299	E300	G301	W302	P303	L304	P305	A306	L311	M315	K316	L317	T323	A324	L325	L326	R327	D328	P329	G330	C331	R333	E334	Q335	C336	R337	L338	L339	Y340	R341	V344	D345	Q346	Y350	A351	E352	V353	R354	C355					
P141	P142	S143	T144	L145	E146	E147	L148	L149	W150	D153	Q154	G155	H156	L157	I160	R161	L162	G163	P164	E165	R166	G167	W168	P169	Q170	L171	R172	R173	I174	A175	P176	E177	Q178	F179	P180	L181	Q182	E185	R192	V193	Q194	A195	E196	D197	R198	A199	F200	G201	T202	P203	L204	Q205	D206	L207	L208

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55742	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.686	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	477.184, 477.184, 477.184	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ZN

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	X	0.09	0/149	0.13	0/230
1	Y	0.09	0/149	0.13	0/230
1	Z	0.08	0/149	0.14	0/230
2	A	0.17	0/4936	0.44	1/6712 (0.0%)
2	B	0.15	0/4936	0.37	1/6712 (0.0%)
2	C	0.16	0/4936	0.40	1/6712 (0.0%)
2	D	0.15	0/4936	0.38	2/6712 (0.0%)
2	E	0.16	0/4936	0.38	0/6712
2	F	0.16	0/4919	0.45	2/6687 (0.0%)
All	All	0.16	0/30046	0.40	7/40937 (0.0%)

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
2	C	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	297	ARG	CA-C-N	7.85	132.61	120.68
2	F	297	ARG	C-N-CA	7.85	132.61	120.68
2	A	363	VAL	N-CA-C	-6.50	107.54	113.71
2	B	363	VAL	N-CA-C	-6.16	107.86	113.71
2	C	177	GLU	N-CA-C	-5.37	107.73	114.56
2	D	56	VAL	CA-C-N	5.12	130.10	122.82
2	D	56	VAL	C-N-CA	5.12	130.10	122.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	63	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	132	0	67	7	0
1	Y	132	0	67	10	0
1	Z	132	0	67	7	0
2	A	4820	0	4786	367	0
2	B	4820	0	4786	310	0
2	C	4820	0	4786	281	0
2	D	4820	0	4786	316	0
2	E	4820	0	4786	286	0
2	F	4804	0	4772	386	0
3	A	31	12	12	0	0
3	B	31	12	12	1	0
3	C	31	12	12	1	0
3	D	31	12	12	1	0
3	E	31	12	12	2	0
3	F	31	12	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	29494	72	28975	1859	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 32.

All (1859) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:LEU:HA	2:B:174:ILE:HD11	1.37	1.00
2:F:142:PRO:HD2	2:F:147:GLU:HG2	1.44	0.99
2:D:104:PHE:HB2	2:D:107:MET:HG3	1.43	0.99
2:A:287:PRO:HA	2:A:290:LEU:HD13	1.45	0.98
2:A:171:LEU:HA	2:A:174:ILE:HD11	1.42	0.98
2:F:9:VAL:HG22	2:F:99:CYS:HB3	1.47	0.96
2:B:9:VAL:HG22	2:B:99:CYS:HB3	1.47	0.94
2:B:470:VAL:HG21	2:B:484:ALA:HB1	1.50	0.93
2:E:470:VAL:HG21	2:E:484:ALA:HB1	1.46	0.93
2:F:298:LEU:HD12	2:F:302:TRP:HB2	1.52	0.92
2:E:246:PRO:HG2	2:E:587:ARG:HG3	1.50	0.92
2:A:271:ALA:HB1	2:A:276:LEU:HD13	1.52	0.91
2:C:470:VAL:HG21	2:C:484:ALA:HB1	1.51	0.91
2:A:117:VAL:HG11	2:A:204:LEU:HD21	1.53	0.91
2:E:426:GLU:HG3	2:F:416:ARG:HD3	1.52	0.91
2:F:584:LEU:HA	2:F:587:ARG:HG2	1.54	0.90
2:A:127:LEU:HB2	2:A:158:HIS:HB2	1.53	0.90
2:F:171:LEU:HA	2:F:174:ILE:HD11	1.52	0.89
2:D:116:THR:HA	2:D:165:GLU:HG2	1.54	0.89
2:F:117:VAL:HG21	2:F:204:LEU:HD11	1.54	0.89
2:A:9:VAL:HG22	2:A:99:CYS:HB3	1.52	0.89
2:D:226:PHE:HB2	2:D:229:LEU:HD23	1.54	0.88
2:F:317:LEU:HB3	2:F:573:ILE:HD11	1.55	0.88
1:Y:10:A:H1'	2:C:103:GLY:HA2	1.56	0.88
2:F:80:GLU:HG3	2:F:198:ARG:HA	1.56	0.87
2:D:287:PRO:HA	2:D:290:LEU:HD23	1.55	0.87
2:E:290:LEU:HD12	2:E:291:PRO:HD2	1.57	0.86
2:F:15:PRO:HB2	2:F:44:LEU:HD12	1.58	0.86
2:D:82:MET:HG3	2:D:111:MET:HE1	1.58	0.86
2:F:84:ARG:HD2	2:F:87:LEU:HD21	1.58	0.86
2:B:402:ALA:HB1	2:B:414:ILE:HG13	1.58	0.85
2:F:18:VAL:HB	2:F:45:ILE:HD12	1.57	0.85
2:C:402:ALA:HB1	2:C:414:ILE:HD12	1.59	0.85
2:B:5:ALA:H	2:B:95:GLN:HB2	1.41	0.84
2:B:286:ASN:HB3	2:B:289:LYS:HE3	1.58	0.84
2:D:272:THR:HG21	2:D:573:ILE:HG22	1.58	0.84
2:B:605:LEU:HD12	2:B:622:ILE:HD12	1.57	0.84
2:E:144:THR:HG23	2:E:147:GLU:HB3	1.58	0.84
2:A:123:VAL:HG13	2:A:162:LEU:HB2	1.56	0.84
2:A:145:LEU:HA	2:A:148:ILE:HD13	1.60	0.84
2:F:346:GLN:HE22	2:F:579:THR:HG23	1.43	0.83
2:F:287:PRO:HA	2:F:290:LEU:HD23	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:HD13	2:B:148:ILE:HD12	1.59	0.83
2:C:605:LEU:HD12	2:C:622:ILE:HD12	1.60	0.83
2:A:18:VAL:HG22	2:A:45:ILE:HD12	1.61	0.83
2:F:93:PRO:HD3	2:F:173:ARG:HH22	1.45	0.82
2:B:258:LEU:HD12	2:B:259:PRO:HD2	1.61	0.82
2:C:270:PHE:HB3	2:C:335:GLN:HE22	1.45	0.82
2:D:19:PRO:HD3	2:D:45:ILE:HD13	1.61	0.82
2:D:515:GLY:HA3	2:D:607:THR:HG21	1.62	0.81
2:A:354:ARG:HB3	2:A:401:ILE:HD11	1.63	0.81
2:E:468:VAL:HG13	2:E:490:ALA:HA	1.62	0.81
2:F:281:ARG:HD2	2:F:293:LEU:HD13	1.61	0.81
2:E:129:ASP:HB2	2:E:156:HIS:HB3	1.63	0.80
2:C:140:MET:HG2	2:C:141:PRO:HD2	1.63	0.80
2:A:104:PHE:HB2	2:A:107:MET:HG3	1.61	0.80
2:E:605:LEU:HD12	2:E:622:ILE:HD12	1.64	0.79
2:D:24:LEU:HD12	2:D:25:PRO:HD2	1.64	0.79
2:D:151:ALA:HA	2:D:154:GLN:HE21	1.46	0.79
2:C:87:LEU:HD11	2:C:174:ILE:HD13	1.65	0.79
2:C:19:PRO:HD3	2:C:45:ILE:HG22	1.62	0.79
2:C:48:PHE:HD1	2:C:145:LEU:HD23	1.48	0.78
2:C:381:MET:HE2	2:C:395:HIS:HA	1.64	0.78
2:F:258:LEU:HD12	2:F:259:PRO:HD2	1.62	0.78
2:D:400:LEU:HD12	2:D:421:ALA:HB2	1.65	0.77
2:A:7:LEU:HB3	2:A:32:VAL:HG13	1.64	0.77
2:E:557:TYR:HB3	2:E:564:VAL:HG21	1.67	0.77
2:D:84:ARG:HB3	2:D:181:LEU:HD21	1.67	0.77
2:F:132:CYS:HB2	2:F:139:LEU:HB2	1.66	0.77
2:E:82:MET:HG3	2:E:111:MET:HE1	1.66	0.76
2:C:281:ARG:HH12	2:C:293:LEU:HA	1.49	0.76
2:C:568:THR:HG23	2:C:578:LEU:HD13	1.67	0.76
2:A:183:VAL:HG22	2:A:193:VAL:HG12	1.65	0.76
2:A:491:ARG:HD2	2:A:609:PHE:HE1	1.51	0.76
2:B:468:VAL:HG13	2:B:490:ALA:HA	1.67	0.76
2:D:5:ALA:H	2:D:95:GLN:HB2	1.50	0.76
2:D:264:HIS:HA	2:D:354:ARG:HH12	1.51	0.76
2:E:63:VAL:HG13	2:E:81:VAL:HG11	1.68	0.76
2:A:478:ALA:HB1	2:A:505:LEU:HD12	1.65	0.76
2:B:127:LEU:HD11	2:C:69:LEU:HD23	1.67	0.76
2:A:221:LEU:HA	2:A:224:LEU:HD23	1.67	0.75
2:D:557:TYR:HB3	2:D:564:VAL:HG21	1.68	0.75
2:B:19:PRO:HD3	2:B:45:ILE:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:MET:HG2	2:E:141:PRO:HD2	1.67	0.75
2:E:142:PRO:HD2	2:E:147:GLU:HG2	1.68	0.75
2:A:191:ARG:HG3	2:A:193:VAL:HG13	1.69	0.75
2:D:69:LEU:HG	2:E:127:LEU:HD11	1.69	0.74
2:B:129:ASP:HB3	2:B:156:HIS:HB3	1.69	0.74
2:B:354:ARG:HB3	2:B:401:ILE:HD11	1.68	0.74
2:D:358:ALA:HA	2:D:366:PRO:HB3	1.68	0.74
2:A:557:TYR:HB3	2:A:564:VAL:HG21	1.68	0.74
2:F:261:ILE:HD11	2:F:622:ILE:HD11	1.70	0.74
2:B:24:LEU:HD23	2:B:27:ALA:HB3	1.70	0.74
2:C:171:LEU:HD12	2:C:174:ILE:HG12	1.70	0.74
2:A:72:GLU:HA	2:F:160:ILE:HD11	1.68	0.73
2:C:515:GLY:HA3	2:C:607:THR:HG21	1.70	0.73
2:D:72:GLU:HG3	2:E:160:ILE:HG13	1.69	0.73
2:A:566:VAL:HG11	2:A:582:LEU:HD23	1.70	0.73
2:B:7:LEU:HD13	2:B:29:PHE:HE2	1.53	0.73
2:B:74:ASP:HA	2:B:77:ARG:HG2	1.70	0.73
2:F:530:ARG:HH12	2:F:551:PRO:HA	1.54	0.73
2:A:127:LEU:HD11	2:F:69:LEU:HD23	1.69	0.73
2:E:170:GLN:HE21	2:E:207:LEU:HD11	1.53	0.73
2:E:404:ARG:HH21	2:E:445:GLU:HB3	1.53	0.73
2:A:11:LEU:HD23	2:A:34:VAL:HG11	1.71	0.73
2:C:38:GLU:HA	2:C:62:ARG:HE	1.53	0.73
2:D:51:ARG:HH12	2:D:149:LEU:HD11	1.52	0.73
2:F:170:GLN:HE21	2:F:207:LEU:HD11	1.53	0.73
2:B:290:LEU:HD23	2:B:291:PRO:HD2	1.71	0.72
2:B:518:LEU:HD13	2:B:564:VAL:HG13	1.71	0.72
2:A:91:THR:HG23	2:A:96:ARG:HH21	1.54	0.72
2:B:557:TYR:HB3	2:B:564:VAL:HG21	1.72	0.72
2:A:463:ARG:HD2	2:B:411:ARG:HB2	1.71	0.72
2:B:24:LEU:HD12	2:B:25:PRO:HD2	1.71	0.71
2:A:98:VAL:HG13	2:A:123:VAL:HG23	1.71	0.71
2:F:400:LEU:HD12	2:F:421:ALA:HB2	1.72	0.71
2:A:456:GLU:HG2	2:B:459:THR:HG21	1.70	0.71
2:F:354:ARG:HD3	2:F:401:ILE:HD11	1.72	0.71
2:B:128:ALA:HA	2:B:157:LEU:HD13	1.73	0.71
2:C:354:ARG:NH1	2:C:440:ASP:OD2	2.23	0.71
2:B:84:ARG:HE	2:B:179:PHE:HB3	1.56	0.70
2:A:499:LEU:HD21	2:A:506:LEU:HA	1.73	0.70
2:B:63:VAL:HG22	2:B:81:VAL:HG11	1.72	0.70
2:C:23:LEU:HD11	2:C:152:ARG:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:446:ASP:OD2	2:A:448:LYS:NZ	2.25	0.70
2:E:66:PHE:HE1	2:E:74:ASP:HB3	1.55	0.70
2:A:416:ARG:HD3	2:B:426:GLU:HG3	1.74	0.70
2:A:160:ILE:HG23	2:F:72:GLU:HG3	1.72	0.69
2:D:246:PRO:HG2	2:D:587:ARG:HG2	1.74	0.69
2:F:586:ALA:HA	2:F:592:LEU:HD23	1.72	0.69
2:A:566:VAL:HG23	2:A:600:LEU:HD13	1.74	0.69
2:C:63:VAL:HG13	2:C:81:VAL:HG21	1.74	0.69
2:D:187:LYS:HE3	2:D:190:GLU:HB3	1.73	0.69
2:B:391:LEU:HD12	2:B:392:PRO:HD2	1.75	0.69
2:E:401:ILE:HA	2:E:440:ASP:HB3	1.74	0.69
1:Z:13:A:H61	2:F:39:ARG:HG3	1.58	0.69
2:B:354:ARG:NH1	2:B:440:ASP:OD2	2.26	0.69
2:E:7:LEU:HB3	2:E:32:VAL:HG22	1.75	0.68
2:B:447:GLU:OE1	2:B:450:ARG:NH2	2.26	0.68
2:D:140:MET:HG2	2:D:141:PRO:HD2	1.75	0.68
2:E:38:GLU:HA	2:E:62:ARG:HE	1.56	0.68
2:C:170:GLN:HE21	2:C:207:LEU:HD11	1.58	0.68
2:C:31:SER:HG	2:C:33:HIS:HE2	1.41	0.68
2:B:69:LEU:HD13	2:C:160:ILE:HG21	1.76	0.68
2:D:402:ALA:HB1	2:D:414:ILE:HG23	1.76	0.68
2:A:151:ALA:HA	2:A:154:GLN:HE21	1.59	0.68
2:A:482:TRP:HD1	2:A:505:LEU:HD21	1.58	0.68
2:B:34:VAL:HB	2:B:60:ILE:HD13	1.74	0.68
2:E:481:ILE:HG21	2:E:499:LEU:HD13	1.75	0.68
2:A:105:LYS:NZ	2:F:103:GLY:O	2.26	0.68
2:F:62:ARG:HB3	2:F:192:ARG:HA	1.76	0.67
2:F:452:HIS:HB3	2:F:483:ARG:HD2	1.75	0.67
2:C:470:VAL:HG11	2:C:488:LEU:HD23	1.77	0.67
2:C:521:TYR:HE1	2:C:584:LEU:HD13	1.60	0.67
2:F:240:LEU:HD12	2:F:594:ARG:HB2	1.77	0.67
2:A:15:PRO:HB2	2:A:44:LEU:HD21	1.77	0.67
2:A:92:GLY:H	2:A:95:GLN:HE22	1.40	0.67
2:B:91:THR:HG23	2:B:96:ARG:HH11	1.58	0.67
2:A:552:TYR:HB2	2:A:588:LEU:HD22	1.76	0.67
2:B:225:PRO:O	2:B:602:ARG:NH1	2.28	0.67
2:C:441:LEU:HD21	2:C:454:PHE:HD2	1.58	0.67
2:F:354:ARG:HB3	2:F:401:ILE:HD11	1.78	0.66
2:C:104:PHE:H	2:C:107:MET:HE2	1.61	0.66
2:D:479:GLU:OE2	2:D:483:ARG:NH1	2.28	0.66
2:F:305:PRO:HG2	2:F:524:LEU:HG	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:TRP:O	2:C:594:ARG:NH1	2.28	0.66
2:D:354:ARG:HB3	2:D:401:ILE:HD11	1.76	0.66
2:E:145:LEU:HA	2:E:148:ILE:HG22	1.76	0.66
2:E:91:THR:HG23	2:E:96:ARG:HH11	1.60	0.66
2:E:130:ASP:HB2	2:E:138:ARG:HH11	1.61	0.66
2:E:354:ARG:NH1	2:E:440:ASP:OD2	2.28	0.66
2:F:117:VAL:HG23	2:F:168:TRP:HD1	1.60	0.66
2:D:562:VAL:HG13	2:D:564:VAL:HG23	1.77	0.66
2:F:447:GLU:OE2	2:F:450:ARG:NH1	2.28	0.66
2:F:134:GLY:HA3	2:F:139:LEU:HD12	1.76	0.66
2:E:463:ARG:HG3	2:F:412:ALA:HA	1.77	0.66
2:C:418:LEU:HD22	2:C:461:VAL:HG21	1.77	0.65
2:E:281:ARG:NH2	2:E:291:PRO:O	2.25	0.65
2:F:7:LEU:HD23	2:F:32:VAL:HG13	1.78	0.65
2:F:246:PRO:O	2:F:252:GLN:NE2	2.30	0.65
2:E:385:ARG:NH1	2:E:390:GLY:O	2.28	0.65
2:E:120:ALA:N	2:E:165:GLU:OE2	2.30	0.65
2:B:506:LEU:HD21	2:B:560:GLU:HB3	1.77	0.65
2:D:170:GLN:HE21	2:D:207:LEU:HD11	1.61	0.65
2:F:401:ILE:O	2:F:417:HIS:ND1	2.29	0.65
2:D:326:LEU:HD22	2:D:332:LEU:HD13	1.77	0.65
2:E:618:LEU:HD23	2:E:621:ARG:HD3	1.77	0.65
2:E:277:LEU:HD21	2:E:320:ALA:HB1	1.78	0.65
2:C:354:ARG:HB3	2:C:401:ILE:HD11	1.78	0.65
2:E:327:ARG:HH21	2:E:362:GLU:HB3	1.60	0.65
2:F:354:ARG:HG2	2:F:399:ILE:HG23	1.78	0.65
2:A:48:PHE:HD1	2:A:145:LEU:HD13	1.61	0.65
2:E:150:TRP:O	2:E:154:GLN:NE2	2.29	0.65
2:D:220:MET:HE1	2:D:241:ARG:HH22	1.62	0.64
2:F:38:GLU:HB3	2:F:62:ARG:HD2	1.78	0.64
2:A:160:ILE:HG13	2:F:69:LEU:HD11	1.79	0.64
2:D:87:LEU:O	2:D:90:ARG:NH2	2.25	0.64
2:E:171:LEU:HA	2:E:174:ILE:HD11	1.79	0.64
2:F:224:LEU:HD12	2:F:225:PRO:HD2	1.79	0.64
2:A:5:ALA:H	2:A:95:GLN:HB2	1.62	0.64
3:D:701:ATP:O2G	3:D:701:ATP:O3'	2.15	0.64
2:E:456:GLU:HB2	2:F:456:GLU:HB2	1.80	0.64
2:E:524:LEU:HD13	2:E:584:LEU:HD21	1.79	0.64
2:B:209:GLN:O	2:B:213:ARG:HG2	1.98	0.64
2:B:80:GLU:O	2:B:84:ARG:HG2	1.98	0.64
2:A:53:ALA:HB1	2:A:56:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:271:ALA:CB	2:A:276:LEU:HD13	2.27	0.64
2:E:62:ARG:HB2	2:E:192:ARG:HG2	1.78	0.64
2:A:91:THR:OG1	2:A:95:GLN:NE2	2.30	0.64
2:D:232:TRP:O	2:D:236:GLU:HB2	1.98	0.64
2:A:228:ASP:O	2:A:231:THR:HG22	1.97	0.64
2:D:9:VAL:HG22	2:D:99:CYS:HB3	1.77	0.64
2:F:566:VAL:HG12	2:F:600:LEU:HD21	1.79	0.64
2:A:269:GLY:O	2:A:572:GLY:N	2.24	0.63
2:A:578:LEU:HA	2:A:581:ASN:HD22	1.63	0.63
2:B:246:PRO:HG2	2:B:587:ARG:HG3	1.80	0.63
2:F:521:TYR:O	2:F:525:GLN:HG2	1.99	0.63
2:B:499:LEU:HD21	2:B:506:LEU:HA	1.79	0.63
2:C:39:ARG:NH2	2:C:67:GLN:OE1	2.30	0.63
2:C:445:GLU:OE2	2:C:475:ASN:N	2.28	0.63
2:A:346:GLN:HE22	2:A:577:SER:HB2	1.64	0.63
2:E:451:ALA:HB1	2:E:488:LEU:HD22	1.79	0.63
2:E:244:LEU:HA	2:E:594:ARG:HH21	1.62	0.63
2:A:68:ASP:OD2	2:A:70:LYS:NZ	2.25	0.63
2:A:166:ARG:HD3	2:F:209:GLN:HE22	1.63	0.63
2:C:226:PHE:HB2	2:C:229:LEU:HD13	1.80	0.63
2:A:38:GLU:HA	2:A:62:ARG:HE	1.62	0.63
2:D:25:PRO:HG2	2:D:161:ARG:HH22	1.64	0.63
2:D:100:LEU:HD23	2:D:125:HIS:HB3	1.78	0.63
2:E:46:ARG:NH2	2:E:190:GLU:OE2	2.31	0.63
2:A:167:GLY:O	2:A:172:ARG:NH2	2.32	0.63
2:B:136:GLN:HG3	2:B:139:LEU:HD21	1.81	0.63
2:F:250:ALA:HA	2:F:253:ARG:HH12	1.64	0.63
2:B:80:GLU:OE2	2:B:84:ARG:NH1	2.32	0.62
2:E:233:SER:HB3	2:E:236:GLU:HG3	1.81	0.62
2:F:140:MET:HG2	2:F:141:PRO:HD2	1.81	0.62
2:C:72:GLU:HB3	2:C:76:PHE:HE2	1.62	0.62
2:A:245:ASP:OD2	2:A:248:ALA:N	2.33	0.62
2:B:232:TRP:O	2:B:236:GLU:HB2	1.99	0.62
2:E:481:ILE:HG23	2:E:493:LEU:HD13	1.81	0.62
2:F:357:PRO:HB3	2:F:369:VAL:HG13	1.80	0.62
2:B:411:ARG:HA	2:B:414:ILE:HG22	1.81	0.62
2:D:91:THR:O	2:D:96:ARG:NH2	2.32	0.62
2:F:404:ARG:HD3	2:F:454:PHE:HE2	1.63	0.62
2:E:117:VAL:HG11	2:E:204:LEU:HD11	1.80	0.62
2:A:144:THR:O	2:A:147:GLU:HG3	2.00	0.62
2:E:66:PHE:CE1	2:E:74:ASP:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:264:HIS:HD2	2:F:569:ASP:HA	1.63	0.62
2:B:103:GLY:HA3	2:B:107:MET:HE3	1.81	0.62
2:D:93:PRO:HD3	2:D:173:ARG:HH12	1.63	0.62
2:D:279:ARG:HD2	2:D:338:LEU:HD21	1.81	0.62
2:A:32:VAL:HB	2:A:58:LEU:HD13	1.81	0.62
2:A:354:ARG:HG2	2:A:399:ILE:HG13	1.82	0.62
2:A:482:TRP:CD1	2:A:505:LEU:HD21	2.35	0.62
2:B:51:ARG:HH22	2:B:145:LEU:HB2	1.64	0.62
2:F:209:GLN:O	2:F:213:ARG:HG2	2.00	0.62
2:D:181:LEU:HD12	2:D:193:VAL:HG22	1.82	0.61
2:E:7:LEU:HD22	2:E:32:VAL:HG13	1.81	0.61
2:E:370:LEU:HD22	2:E:420:LEU:HD11	1.82	0.61
2:C:232:TRP:O	2:C:236:GLU:HB2	2.00	0.61
2:F:7:LEU:HB2	2:F:29:PHE:CD2	2.35	0.61
2:F:552:TYR:HD1	2:F:553:PRO:HD2	1.65	0.61
2:D:33:HIS:HB3	2:D:85:TRP:CZ2	2.35	0.61
2:A:25:PRO:HD3	2:A:159:TRP:HZ3	1.64	0.61
2:E:113:LYS:HA	2:E:116:THR:HG22	1.81	0.61
2:F:42:VAL:HG21	2:F:60:ILE:HD12	1.82	0.61
2:D:277:LEU:O	2:D:281:ARG:N	2.34	0.61
2:D:489:ASN:HD22	2:E:486:PHE:HD2	1.48	0.61
2:E:404:ARG:HD2	2:E:449:THR:HG22	1.81	0.61
2:D:327:ARG:HH12	2:D:362:GLU:HB3	1.64	0.61
2:B:317:LEU:HD22	2:B:573:ILE:HG23	1.81	0.61
2:C:260:LYS:HA	2:C:601:GLN:NE2	2.15	0.61
2:A:7:LEU:HB2	2:A:29:PHE:CD1	2.36	0.61
2:A:270:PHE:HB3	2:A:335:GLN:NE2	2.16	0.61
2:A:519:CYS:SG	2:A:569:ASP:HB2	2.41	0.61
2:B:461:VAL:HG22	2:B:466:LEU:HB3	1.83	0.61
2:D:84:ARG:HH12	2:D:199:ALA:HB3	1.64	0.61
2:E:7:LEU:HB2	2:E:29:PHE:CD1	2.36	0.61
2:A:13:THR:HA	2:A:40:PRO:HB3	1.82	0.60
2:E:264:HIS:HD2	2:E:569:ASP:HA	1.65	0.60
2:A:526:ILE:HG13	2:A:527:LYS:HG2	1.83	0.60
2:D:72:GLU:HG2	2:E:161:ARG:O	2.02	0.60
2:C:531:LEU:HD13	2:C:588:LEU:HD23	1.84	0.60
2:D:51:ARG:HH21	2:D:145:LEU:HB3	1.67	0.60
2:F:84:ARG:HA	2:F:87:LEU:HG	1.83	0.60
2:A:507:ARG:HH21	2:A:560:GLU:HG3	1.67	0.60
2:E:167:GLY:O	2:E:172:ARG:NH2	2.34	0.60
2:D:327:ARG:NH1	2:D:362:GLU:HB3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:84:ARG:HB3	2:E:181:LEU:HD21	1.84	0.60
2:A:264:HIS:HA	2:A:354:ARG:NH1	2.17	0.60
2:B:244:LEU:HA	2:B:594:ARG:HE	1.67	0.60
2:D:258:LEU:HD12	2:D:259:PRO:HD2	1.84	0.60
2:E:22:PHE:HD2	2:E:23:LEU:HD22	1.67	0.60
2:A:452:HIS:HB3	2:A:483:ARG:HD2	1.83	0.59
2:B:69:LEU:HA	2:B:74:ASP:OD1	2.02	0.59
2:F:278:ARG:HH21	2:F:293:LEU:HD11	1.67	0.59
2:F:240:LEU:HD21	2:F:595:LEU:HD13	1.84	0.59
2:B:451:ALA:HB1	2:B:488:LEU:HD11	1.85	0.59
2:E:224:LEU:HD22	2:E:229:LEU:HD11	1.85	0.59
2:B:17:ILE:HD12	2:B:101:THR:HG22	1.84	0.59
2:C:23:LEU:HD12	2:C:152:ARG:NH1	2.18	0.59
2:C:479:GLU:O	2:C:483:ARG:HG2	2.02	0.59
2:F:366:PRO:HA	2:F:369:VAL:HG12	1.85	0.59
2:E:323:THR:HG22	2:E:359:ASN:HB3	1.84	0.59
2:F:341:ARG:NH1	2:F:341:ARG:HA	2.17	0.59
2:C:7:LEU:HB2	2:C:29:PHE:HD2	1.67	0.59
2:F:232:TRP:O	2:F:236:GLU:HB2	2.02	0.59
2:A:313:GLU:O	2:A:317:LEU:HG	2.03	0.59
2:B:101:THR:HA	2:C:105:LYS:HZ2	1.68	0.59
2:D:7:LEU:HB2	2:D:29:PHE:CD2	2.37	0.59
2:F:346:GLN:NE2	2:F:579:THR:HG23	2.14	0.59
2:B:450:ARG:HG2	2:B:451:ALA:H	1.68	0.59
2:A:63:VAL:HG21	2:A:78:PHE:HD1	1.68	0.59
2:A:255:VAL:O	2:A:260:LYS:NZ	2.28	0.59
2:B:84:ARG:HH21	2:B:179:PHE:HA	1.67	0.59
2:C:91:THR:O	2:C:96:ARG:NH1	2.35	0.59
2:D:87:LEU:HD11	2:D:200:PHE:CE2	2.38	0.59
2:E:38:GLU:HA	2:E:62:ARG:NE	2.17	0.59
2:A:506:LEU:HG	2:A:560:GLU:HG2	1.85	0.59
2:B:404:ARG:HD2	2:B:454:PHE:HE2	1.67	0.59
2:C:185:GLU:HG3	2:C:192:ARG:HB3	1.84	0.59
2:D:329:PRO:HB3	2:D:364:ARG:NH1	2.18	0.59
2:E:365:SER:CB	2:F:427:HIS:HA	2.33	0.59
2:F:65:GLY:O	2:F:77:ARG:NH2	2.36	0.59
2:F:284:ALA:HB3	2:F:290:LEU:HD21	1.84	0.59
2:E:19:PRO:HB3	2:E:48:PHE:CD1	2.37	0.58
2:E:366:PRO:HA	2:E:369:VAL:HG12	1.85	0.58
2:A:521:TYR:OH	2:A:580:ASP:HB3	2.03	0.58
2:C:23:LEU:CD1	2:C:152:ARG:HG3	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:VAL:HG11	2:D:204:LEU:HD11	1.84	0.58
2:F:271:ALA:HA	2:F:276:LEU:HD13	1.85	0.58
2:A:18:VAL:HG11	2:A:34:VAL:HG21	1.84	0.58
2:A:446:ASP:OD1	2:A:449:THR:HG22	2.03	0.58
2:B:167:GLY:O	2:B:172:ARG:NH1	2.36	0.58
2:D:213:ARG:CZ	2:D:233:SER:HB3	2.34	0.58
2:D:499:LEU:HD21	2:D:506:LEU:HA	1.84	0.58
2:F:114:ALA:HA	2:F:117:VAL:HG12	1.84	0.58
2:F:245:ASP:N	2:F:251:ASP:OD1	2.32	0.58
2:E:593:THR:OG1	2:E:596:ASP:OD1	2.11	0.58
2:F:337:ARG:O	2:F:341:ARG:HG2	2.04	0.58
2:A:65:GLY:H	2:A:77:ARG:HH12	1.51	0.58
2:C:7:LEU:HB2	2:C:29:PHE:CD2	2.38	0.58
2:D:492:ARG:HD2	2:D:607:THR:HG22	1.84	0.58
1:Y:7:A:H1'	2:B:103:GLY:HA2	1.84	0.58
2:A:99:CYS:HB2	2:A:124:PHE:CZ	2.39	0.58
2:D:48:PHE:HB2	2:D:145:LEU:HD21	1.86	0.58
2:E:125:HIS:HB3	2:E:160:ILE:CG2	2.33	0.58
2:E:404:ARG:HD2	2:E:449:THR:CG2	2.34	0.58
2:F:277:LEU:HA	2:F:280:VAL:HG12	1.86	0.58
2:A:456:GLU:HG3	2:B:456:GLU:HA	1.84	0.58
2:F:524:LEU:HD22	2:F:584:LEU:HD11	1.85	0.58
2:B:7:LEU:HG	2:B:9:VAL:HG23	1.86	0.58
2:C:170:GLN:NE2	2:C:207:LEU:HD11	2.19	0.58
2:C:397:ASN:HD22	2:C:437:VAL:HG11	1.69	0.58
2:F:255:VAL:O	2:F:260:LYS:NZ	2.31	0.58
2:F:326:LEU:HD12	2:F:332:LEU:HD13	1.85	0.58
2:A:33:HIS:HB3	2:A:85:TRP:CH2	2.39	0.58
2:A:426:GLU:OE2	2:B:416:ARG:HG2	2.03	0.58
2:F:137:GLY:O	2:F:138:ARG:HD3	2.04	0.58
2:A:190:GLU:OE1	2:A:191:ARG:N	2.37	0.57
2:A:233:SER:HB3	2:A:236:GLU:OE1	2.03	0.57
2:A:376:ALA:O	2:A:379:GLU:HG3	2.04	0.57
2:B:101:THR:OG1	2:B:125:HIS:HB2	2.03	0.57
2:C:508:SER:O	2:C:512:ARG:HG3	2.04	0.57
2:A:157:LEU:O	2:F:70:LYS:NZ	2.33	0.57
2:A:241:ARG:HE	2:A:595:LEU:HD22	1.69	0.57
2:A:272:THR:HG22	2:A:295:GLU:OE1	2.05	0.57
2:B:326:LEU:HB2	2:B:360:TYR:CE1	2.40	0.57
2:D:262:GLU:OE2	2:D:578:LEU:HD21	2.05	0.57
2:E:49:PHE:HD1	2:E:53:ALA:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:18:VAL:CG2	2:A:45:ILE:HD12	2.32	0.57
2:A:431:GLU:OE1	2:A:431:GLU:N	2.37	0.57
2:B:87:LEU:O	2:B:176:PRO:HG3	2.04	0.57
2:D:63:VAL:HG22	2:D:81:VAL:HG11	1.85	0.57
2:D:400:LEU:HD12	2:D:421:ALA:CB	2.35	0.57
2:F:7:LEU:HD13	2:F:29:PHE:HE2	1.69	0.57
2:A:114:ALA:O	2:A:118:LEU:HG	2.05	0.57
2:C:100:LEU:O	2:C:108:SER:OG	2.16	0.57
2:C:455:ARG:O	2:C:459:THR:HG23	2.04	0.57
2:A:234:GLU:N	2:A:234:GLU:OE2	2.36	0.57
2:A:260:LYS:HG2	2:A:578:LEU:HD23	1.87	0.57
2:C:277:LEU:HB3	2:C:278:ARG:NH1	2.20	0.57
2:D:69:LEU:HA	2:D:74:ASP:OD2	2.04	0.57
2:F:33:HIS:HB3	2:F:85:TRP:CZ2	2.40	0.57
2:F:134:GLY:HA3	2:F:139:LEU:CD1	2.34	0.57
2:F:213:ARG:CZ	2:F:233:SER:HB3	2.34	0.57
2:F:431:GLU:OE1	2:F:431:GLU:N	2.38	0.57
2:A:260:LYS:HB2	2:A:348:VAL:HG22	1.86	0.57
2:F:84:ARG:HA	2:F:87:LEU:CD2	2.35	0.57
2:B:141:PRO:HB3	2:B:147:GLU:OE1	2.04	0.57
2:C:236:GLU:OE2	2:C:628:ARG:HD3	2.05	0.57
2:C:482:TRP:HE3	2:C:483:ARG:HD2	1.70	0.57
2:E:41:ASP:OD1	2:E:43:THR:HG23	2.04	0.57
2:E:402:ALA:HB1	2:E:414:ILE:HG23	1.87	0.57
2:A:63:VAL:HG21	2:A:78:PHE:CD1	2.40	0.57
2:A:517:GLU:HB3	2:A:567:ASN:ND2	2.19	0.57
2:C:171:LEU:HD12	2:C:174:ILE:CG1	2.34	0.57
2:C:184:VAL:CG2	2:C:192:ARG:HG2	2.34	0.57
2:E:263:LEU:HD23	2:E:492:ARG:CZ	2.34	0.57
2:F:53:ALA:HB1	2:F:56:VAL:HG21	1.87	0.57
2:A:531:LEU:HD21	2:A:587:ARG:HD3	1.86	0.57
2:F:530:ARG:HH22	2:F:551:PRO:HB3	1.69	0.57
2:A:158:HIS:ND1	2:F:69:LEU:O	2.37	0.56
2:C:502:SER:HB2	2:C:505:LEU:HB3	1.86	0.56
2:D:168:TRP:HB2	2:D:171:LEU:HG	1.86	0.56
2:B:78:PHE:CE2	2:B:107:MET:HG2	2.40	0.56
2:B:414:ILE:HG23	2:B:457:GLU:OE1	2.05	0.56
2:C:166:ARG:HG3	2:C:172:ARG:HH12	1.69	0.56
2:D:460:ALA:HA	2:D:463:ARG:HG2	1.87	0.56
2:E:36:THR:OG1	2:E:62:ARG:HG2	2.05	0.56
2:E:135:PRO:HD2	2:E:139:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:376:ALA:O	2:D:379:GLU:HG3	2.04	0.56
2:D:503:ARG:HH22	2:D:506:LEU:HD23	1.69	0.56
2:E:260:LYS:HE2	2:E:579:THR:HG22	1.87	0.56
2:E:431:GLU:N	2:E:431:GLU:OE2	2.38	0.56
2:F:43:THR:O	2:F:46:ARG:HG2	2.05	0.56
2:F:122:GLU:OE2	2:F:161:ARG:HG3	2.05	0.56
2:F:236:GLU:HG2	2:F:628:ARG:HH21	1.70	0.56
2:A:69:LEU:HD22	2:A:104:PHE:CE1	2.41	0.56
2:A:72:GLU:CA	2:F:160:ILE:HD11	2.36	0.56
2:B:53:ALA:HB1	2:B:56:VAL:HG21	1.87	0.56
2:C:246:PRO:HB3	2:C:583:LEU:HD12	1.87	0.56
2:B:69:LEU:HD13	2:C:160:ILE:HD13	1.86	0.56
2:B:105:LYS:HB2	2:C:125:HIS:CE1	2.40	0.56
2:C:9:VAL:CG1	2:C:34:VAL:HG12	2.35	0.56
2:F:446:ASP:OD1	2:F:449:THR:HG22	2.05	0.56
1:Y:8:A:C5	2:B:140:MET:HE1	2.40	0.56
2:C:63:VAL:CG1	2:C:81:VAL:HG21	2.36	0.56
2:C:499:LEU:HD22	2:C:506:LEU:HD13	1.88	0.56
2:F:117:VAL:HG13	2:F:118:LEU:HD22	1.88	0.56
2:A:104:PHE:HB2	2:A:107:MET:CG	2.36	0.56
2:B:101:THR:HA	2:C:105:LYS:NZ	2.20	0.56
2:C:84:ARG:HB2	2:C:181:LEU:HD21	1.87	0.56
2:C:531:LEU:HD12	2:C:587:ARG:HG2	1.87	0.56
2:D:264:HIS:HA	2:D:354:ARG:NH1	2.20	0.56
2:A:304:LEU:HD11	2:A:524:LEU:HD23	1.88	0.56
2:A:332:LEU:HD21	2:A:373:ILE:HG12	1.86	0.56
2:B:440:ASP:OD1	2:B:441:LEU:N	2.38	0.56
2:B:451:ALA:HB1	2:B:488:LEU:CD1	2.35	0.56
2:C:226:PHE:HB2	2:C:229:LEU:CD1	2.35	0.56
2:C:446:ASP:OD2	2:C:449:THR:HG22	2.06	0.56
2:E:244:LEU:HA	2:E:594:ARG:NH2	2.21	0.56
2:F:354:ARG:HH21	2:F:469:THR:HG21	1.70	0.56
2:F:552:TYR:HD2	2:F:588:LEU:HD22	1.70	0.56
2:A:458:PHE:O	2:A:461:VAL:HG12	2.06	0.56
2:A:461:VAL:HG22	2:A:466:LEU:HB3	1.88	0.56
2:B:578:LEU:O	2:B:582:LEU:HG	2.06	0.56
2:E:357:PRO:HB3	2:E:369:VAL:HG13	1.88	0.56
2:F:122:GLU:OE2	2:F:124:PHE:HB3	2.06	0.56
2:F:269:GLY:HA3	2:F:570:ASN:HD22	1.70	0.56
2:F:521:TYR:OH	2:F:580:ASP:HB3	2.06	0.56
2:A:23:LEU:H	2:A:23:LEU:HD23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:75:HIS:NE2	2:A:79:GLU:OE2	2.40	0.56
2:C:66:PHE:CD1	2:C:74:ASP:HB2	2.41	0.56
2:C:74:ASP:HA	2:C:77:ARG:HD3	1.88	0.56
2:D:98:VAL:CG1	2:D:123:VAL:HG22	2.36	0.56
2:D:101:THR:OG1	2:D:125:HIS:HB2	2.06	0.56
2:D:168:TRP:CD1	2:D:171:LEU:HD21	2.41	0.56
2:A:42:VAL:HG22	2:A:45:ILE:HB	1.88	0.55
2:A:179:PHE:HE1	2:A:199:ALA:HB3	1.71	0.55
2:A:349:CYS:SG	2:A:622:ILE:HD11	2.46	0.55
2:C:263:LEU:HD23	2:C:492:ARG:CZ	2.36	0.55
2:C:274:GLY:O	2:C:278:ARG:NH1	2.40	0.55
2:B:127:LEU:HD11	2:C:69:LEU:CD2	2.36	0.55
2:C:422:VAL:HG13	2:C:464:CYS:SG	2.46	0.55
2:D:7:LEU:HG	2:D:9:VAL:HG23	1.88	0.55
2:E:126:VAL:HA	2:E:159:TRP:HD1	1.71	0.55
2:F:7:LEU:HB2	2:F:29:PHE:HD2	1.71	0.55
2:A:48:PHE:CD1	2:A:145:LEU:HD13	2.42	0.55
2:A:399:ILE:HG22	2:A:438:GLY:N	2.21	0.55
2:F:117:VAL:HG22	2:F:171:LEU:HD23	1.87	0.55
2:C:103:GLY:HA3	2:C:107:MET:CE	2.37	0.55
2:D:209:GLN:O	2:D:213:ARG:HG2	2.06	0.55
2:F:84:ARG:NH2	2:F:180:PRO:O	2.34	0.55
2:F:482:TRP:HB2	2:F:505:LEU:HD11	1.89	0.55
2:A:140:MET:O	2:A:142:PRO:HD3	2.07	0.55
2:B:263:LEU:HB3	2:B:492:ARG:NH1	2.22	0.55
2:D:105:LYS:HB3	2:E:125:HIS:CE1	2.41	0.55
2:E:99:CYS:HB2	2:E:124:PHE:CZ	2.41	0.55
2:E:178:GLN:N	2:E:178:GLN:OE1	2.39	0.55
2:A:500:GLY:HA2	2:A:503:ARG:HH22	1.71	0.55
2:B:579:THR:O	2:B:583:LEU:HG	2.06	0.55
2:D:521:TYR:O	2:D:524:LEU:HG	2.06	0.55
2:E:134:GLY:HA3	2:E:139:LEU:HD22	1.89	0.55
2:F:108:SER:HA	2:F:111:MET:HE3	1.89	0.55
2:F:361:ALA:HB1	2:F:364:ARG:O	2.07	0.55
2:B:7:LEU:HD12	2:B:97:PHE:O	2.06	0.55
2:E:400:LEU:HD12	2:E:421:ALA:HB2	1.88	0.55
2:A:233:SER:O	2:A:237:LEU:HD23	2.07	0.55
2:B:568:THR:HG23	2:B:578:LEU:HD23	1.89	0.55
2:C:38:GLU:OE2	2:C:66:PHE:N	2.40	0.55
2:D:16:ALA:C	2:D:19:PRO:HD2	2.32	0.55
2:D:281:ARG:NH2	2:D:291:PRO:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:PRO:HB3	2:F:48:PHE:CD2	2.40	0.55
2:F:37:THR:O	2:F:38:GLU:HG3	2.07	0.55
2:F:301:GLY:O	2:F:304:LEU:N	2.27	0.55
2:F:452:HIS:HB3	2:F:483:ARG:CD	2.36	0.55
2:F:493:LEU:O	2:F:517:GLU:HG2	2.07	0.55
2:A:118:LEU:HA	2:A:171:LEU:CD1	2.36	0.55
2:A:295:GLU:HB3	2:A:297:ARG:HH12	1.71	0.55
2:B:126:VAL:HG12	2:B:159:TRP:CD1	2.41	0.55
2:B:169:PRO:HA	2:B:172:ARG:HG2	1.88	0.55
2:B:431:GLU:OE2	2:B:611:THR:OG1	2.20	0.55
2:C:427:HIS:HA	2:D:365:SER:CB	2.37	0.55
2:F:402:ALA:HB1	2:F:414:ILE:HG23	1.88	0.55
2:A:518:LEU:HD23	2:A:552:TYR:HE2	1.72	0.54
2:B:130:ASP:OD1	2:B:140:MET:HB3	2.07	0.54
2:C:240:LEU:HD23	2:C:595:LEU:HB2	1.88	0.54
2:C:340:TYR:O	2:C:344:VAL:HG23	2.07	0.54
2:D:7:LEU:HB2	2:D:29:PHE:CE2	2.42	0.54
2:D:76:PHE:O	2:D:79:GLU:HG3	2.08	0.54
2:A:161:ARG:O	2:F:72:GLU:HG2	2.08	0.54
2:A:166:ARG:HD3	2:F:209:GLN:NE2	2.22	0.54
2:A:377:PHE:CE2	2:A:398:LEU:HD21	2.41	0.54
2:B:99:CYS:HA	2:B:124:PHE:O	2.06	0.54
2:B:210:ARG:NH1	2:B:214:ILE:HD11	2.22	0.54
2:B:508:SER:O	2:B:512:ARG:HG3	2.08	0.54
2:D:470:VAL:HG21	2:D:488:LEU:HD23	1.89	0.54
2:E:78:PHE:CZ	2:E:107:MET:HG2	2.42	0.54
2:E:272:THR:HG21	2:E:318:GLY:HA2	1.90	0.54
2:E:327:ARG:NH2	2:E:362:GLU:HB3	2.22	0.54
2:A:502:SER:HB3	2:A:505:LEU:HB2	1.88	0.54
2:B:223:GLU:OE1	2:B:223:GLU:N	2.40	0.54
2:B:593:THR:OG1	2:B:596:ASP:OD1	2.11	0.54
2:E:80:GLU:HG3	2:E:198:ARG:HA	1.89	0.54
2:A:25:PRO:HD3	2:A:159:TRP:CZ3	2.43	0.54
2:A:61:THR:HG22	2:A:191:ARG:HD2	1.87	0.54
2:A:118:LEU:HD12	2:A:119:GLY:O	2.08	0.54
2:A:171:LEU:HA	2:A:174:ILE:CD1	2.29	0.54
2:B:302:TRP:O	2:B:305:PRO:HD3	2.07	0.54
2:D:183:VAL:HG11	2:D:186:GLU:HB2	1.89	0.54
2:D:229:LEU:HD11	2:D:598:LEU:HD12	1.89	0.54
2:E:272:THR:O	2:E:277:LEU:HD22	2.06	0.54
2:F:263:LEU:HD23	2:F:492:ARG:CZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LEU:HD12	2:B:259:PRO:CD	2.37	0.54
2:B:531:LEU:HD11	2:B:584:LEU:HD11	1.90	0.54
2:C:87:LEU:O	2:C:176:PRO:HB3	2.07	0.54
2:E:464:CYS:SG	2:F:416:ARG:NH1	2.80	0.54
2:F:471:HIS:HB3	2:F:474:GLU:OE1	2.07	0.54
2:B:70:LYS:HA	2:C:158:HIS:HD2	1.73	0.54
2:C:185:GLU:HG2	2:C:192:ARG:NH2	2.22	0.54
2:D:100:LEU:CD2	2:D:125:HIS:HB3	2.38	0.54
2:E:7:LEU:HD21	2:E:9:VAL:HB	1.88	0.54
2:E:72:GLU:OE1	2:E:72:GLU:N	2.41	0.54
2:F:67:GLN:N	2:F:67:GLN:OE1	2.40	0.54
2:F:91:THR:HG23	2:F:96:ARG:NH2	2.22	0.54
2:F:401:ILE:HD13	2:F:440:ASP:HB3	1.90	0.54
2:F:515:GLY:HA2	2:F:563:ARG:HG3	1.90	0.54
2:A:260:LYS:HA	2:A:601:GLN:NE2	2.23	0.54
2:A:301:GLY:HA2	2:A:305:PRO:N	2.23	0.54
2:A:441:LEU:HD21	2:A:458:PHE:HE1	1.73	0.54
2:B:125:HIS:CE1	2:C:106:THR:HG22	2.43	0.54
2:B:309:ILE:HG12	2:B:525:GLN:O	2.08	0.54
2:B:430:ASP:OD2	2:B:433:ALA:HB3	2.07	0.54
2:C:72:GLU:HB3	2:C:76:PHE:CE2	2.43	0.54
2:C:150:TRP:HE1	2:C:154:GLN:HE21	1.55	0.54
2:C:506:LEU:HD21	2:C:560:GLU:HG3	1.89	0.54
2:C:555:LEU:CD1	2:C:589:CYS:HB3	2.38	0.54
2:D:226:PHE:HB2	2:D:229:LEU:CD2	2.33	0.54
2:A:603:HIS:O	2:A:607:THR:HG22	2.08	0.54
2:C:403:THR:O	2:C:414:ILE:HD11	2.08	0.54
2:C:458:PHE:CG	2:C:488:LEU:HD11	2.43	0.54
2:C:613:THR:O	2:C:617:THR:HG23	2.08	0.54
2:D:145:LEU:HA	2:D:148:ILE:HG22	1.90	0.54
2:F:264:HIS:HA	2:F:354:ARG:NH1	2.23	0.54
2:A:76:PHE:HB3	2:A:198:ARG:HD3	1.90	0.54
2:A:244:LEU:HB2	2:A:594:ARG:HG2	1.89	0.54
2:A:341:ARG:NH1	2:A:341:ARG:HA	2.22	0.54
2:B:404:ARG:H	2:B:443:GLY:HA3	1.72	0.54
2:C:39:ARG:HB3	2:C:40:PRO:HD3	1.88	0.54
2:D:84:ARG:HB3	2:D:181:LEU:CD2	2.36	0.54
2:B:92:GLY:H	2:B:95:GLN:HE22	1.55	0.54
2:B:225:PRO:HG3	2:B:599:HIS:ND1	2.22	0.54
2:B:234:GLU:OE1	2:B:234:GLU:N	2.41	0.54
2:C:332:LEU:HD21	2:C:373:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:351:ALA:O	2:C:396:VAL:HA	2.07	0.54
2:E:68:ASP:HB3	2:E:70:LYS:NZ	2.23	0.54
2:E:118:LEU:HD22	2:E:171:LEU:HD21	1.89	0.54
2:F:441:LEU:HD22	2:F:458:PHE:CZ	2.43	0.54
2:B:262:GLU:OE1	2:B:263:LEU:N	2.41	0.53
2:C:10:SER:HB3	2:C:111:MET:CE	2.38	0.53
2:C:521:TYR:CE1	2:C:584:LEU:HD13	2.43	0.53
2:F:7:LEU:HD12	2:F:97:PHE:O	2.08	0.53
2:F:100:LEU:HD23	2:F:100:LEU:H	1.73	0.53
2:F:209:GLN:HE21	2:F:213:ARG:HE	1.55	0.53
2:A:578:LEU:O	2:A:582:LEU:HG	2.08	0.53
2:C:40:PRO:O	2:C:62:ARG:NH2	2.40	0.53
2:D:64:ALA:HB3	2:D:194:GLN:NE2	2.23	0.53
2:A:95:GLN:OE1	2:A:95:GLN:N	2.41	0.53
2:A:332:LEU:HD21	2:A:373:ILE:CG1	2.38	0.53
2:B:260:LYS:HE2	2:B:579:THR:HG22	1.91	0.53
2:A:251:ASP:O	2:A:255:VAL:HG23	2.09	0.53
2:A:521:TYR:O	2:A:525:GLN:HG2	2.09	0.53
2:B:49:PHE:CE2	2:B:56:VAL:HG11	2.42	0.53
2:B:552:TYR:CE2	2:B:554:LEU:HB2	2.44	0.53
2:D:126:VAL:HG12	2:D:159:TRP:CD1	2.43	0.53
2:E:117:VAL:HG11	2:E:204:LEU:CD1	2.39	0.53
2:E:317:LEU:HD22	2:E:573:ILE:HG23	1.90	0.53
2:F:117:VAL:HG23	2:F:168:TRP:CD1	2.43	0.53
2:F:243:PRO:HA	2:F:593:THR:HA	1.90	0.53
2:B:40:PRO:O	2:B:62:ARG:NH2	2.30	0.53
2:D:99:CYS:SG	2:D:125:HIS:HA	2.49	0.53
2:D:284:ALA:CB	2:D:290:LEU:HD21	2.39	0.53
2:D:506:LEU:HD21	2:D:560:GLU:HG3	1.90	0.53
2:F:117:VAL:HG13	2:F:118:LEU:CD2	2.39	0.53
2:F:530:ARG:NH1	2:F:551:PRO:HA	2.21	0.53
2:A:32:VAL:O	2:A:58:LEU:HD12	2.08	0.53
2:C:38:GLU:HA	2:C:62:ARG:HH21	1.74	0.53
2:C:270:PHE:HB3	2:C:335:GLN:NE2	2.21	0.53
2:C:410:TYR:CE1	2:C:411:ARG:HD3	2.43	0.53
2:D:156:HIS:O	2:D:157:LEU:HD22	2.08	0.53
2:A:7:LEU:HB2	2:A:29:PHE:HD1	1.73	0.53
2:A:337:ARG:O	2:A:341:ARG:HG2	2.09	0.53
2:C:99:CYS:HB2	2:C:124:PHE:CZ	2.44	0.53
2:C:122:GLU:OE2	2:C:161:ARG:HB2	2.09	0.53
2:E:323:THR:HG23	3:E:701:ATP:O1B	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:ARG:O	2:F:87:LEU:HG	2.08	0.53
2:F:202:THR:HA	2:F:205:GLN:OE1	2.08	0.53
2:A:225:PRO:HG2	2:A:598:LEU:HB3	1.91	0.53
2:A:304:LEU:HD11	2:A:524:LEU:CD2	2.38	0.53
2:A:522:ALA:O	2:A:526:ILE:HG12	2.08	0.53
2:B:91:THR:HG23	2:B:96:ARG:NH1	2.21	0.53
2:B:391:LEU:CD1	2:B:392:PRO:HD2	2.38	0.53
2:B:512:ARG:NH2	2:C:489:ASN:O	2.35	0.53
2:C:311:LEU:O	2:C:315:MET:HG2	2.09	0.53
2:C:430:ASP:O	2:C:435:ARG:HD3	2.07	0.53
2:D:36:THR:O	2:D:62:ARG:HA	2.09	0.53
2:D:326:LEU:HD22	2:D:332:LEU:CD1	2.39	0.53
2:F:4:GLN:HB2	2:F:95:GLN:HE21	1.74	0.53
2:F:37:THR:HA	2:F:63:VAL:HG22	1.91	0.53
2:F:605:LEU:HD21	2:F:619:LEU:HB2	1.91	0.53
2:A:506:LEU:CG	2:A:560:GLU:HG2	2.39	0.53
2:B:36:THR:O	2:B:62:ARG:HA	2.08	0.53
2:B:44:LEU:HD21	2:B:145:LEU:HD21	1.91	0.53
2:C:131:CYS:HA	2:C:138:ARG:HH21	1.74	0.53
2:F:462:HIS:NE2	2:F:489:ASN:HB2	2.23	0.53
2:F:499:LEU:HB3	2:F:557:TYR:OH	2.09	0.53
2:A:249:PRO:O	2:A:252:GLN:HG3	2.08	0.53
2:C:68:ASP:HB3	2:C:70:LYS:CE	2.38	0.53
2:D:552:TYR:CE2	2:D:554:LEU:HB2	2.44	0.53
2:E:38:GLU:HA	2:E:62:ARG:HD3	1.91	0.53
2:E:411:ARG:O	2:F:463:ARG:HD3	2.09	0.53
2:A:64:ALA:HB3	2:A:77:ARG:HH22	1.73	0.52
2:B:174:ILE:HG22	2:B:175:ALA:H	1.74	0.52
2:B:352:GLU:OE1	2:B:399:ILE:HD11	2.09	0.52
2:B:485:VAL:HG13	2:B:514:ILE:CD1	2.38	0.52
2:C:38:GLU:HA	2:C:62:ARG:NE	2.21	0.52
2:C:98:VAL:CG2	2:C:123:VAL:HG22	2.39	0.52
2:C:298:LEU:HD13	2:C:302:TRP:CD1	2.44	0.52
2:D:61:THR:HG22	2:D:191:ARG:HD2	1.90	0.52
2:F:563:ARG:HD3	2:F:607:THR:HG22	1.91	0.52
2:A:101:THR:OG1	2:A:126:VAL:HG22	2.08	0.52
2:C:519:CYS:SG	2:C:569:ASP:HB2	2.50	0.52
2:D:218:TRP:CE3	2:E:214:ILE:HD11	2.45	0.52
2:E:277:LEU:O	2:E:281:ARG:HG3	2.09	0.52
2:F:123:VAL:HG12	2:F:162:LEU:HD21	1.91	0.52
2:A:84:ARG:NH2	2:A:181:LEU:HG	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LEU:HD12	2:B:174:ILE:HB	1.91	0.52
2:D:100:LEU:HD23	2:D:100:LEU:H	1.74	0.52
2:D:244:LEU:HD11	2:D:251:ASP:HB3	1.90	0.52
2:E:13:THR:HA	2:E:40:PRO:HB3	1.91	0.52
2:F:176:PRO:HG2	2:F:177:GLU:OE1	2.10	0.52
2:F:224:LEU:CD1	2:F:225:PRO:HD2	2.39	0.52
2:F:254:TRP:CZ3	2:F:627:PRO:HD2	2.44	0.52
2:A:84:ARG:HH21	2:A:181:LEU:HA	1.75	0.52
2:A:100:LEU:HD12	2:A:108:SER:OG	2.08	0.52
2:A:327:ARG:HH21	2:A:362:GLU:HB3	1.75	0.52
2:B:69:LEU:CD1	2:C:160:ILE:HD13	2.38	0.52
2:C:68:ASP:HB3	2:C:70:LYS:HE3	1.92	0.52
2:C:171:LEU:O	2:C:174:ILE:HD11	2.10	0.52
2:E:142:PRO:CD	2:E:147:GLU:HG2	2.39	0.52
2:A:185:GLU:OE2	2:A:192:ARG:NH1	2.43	0.52
2:A:244:LEU:HD13	2:A:594:ARG:HD3	1.91	0.52
2:B:430:ASP:O	2:B:435:ARG:HD3	2.10	0.52
2:E:82:MET:HG3	2:E:111:MET:CE	2.37	0.52
2:E:243:PRO:HA	2:E:593:THR:HG22	1.91	0.52
2:F:250:ALA:HA	2:F:253:ARG:NH1	2.25	0.52
2:F:566:VAL:HG22	2:F:581:ASN:HD21	1.74	0.52
2:A:427:HIS:HA	2:B:365:SER:CB	2.40	0.52
2:B:401:ILE:HA	2:B:440:ASP:HB3	1.92	0.52
2:B:586:ALA:HA	2:B:592:LEU:HD23	1.92	0.52
2:D:20:GLU:HG2	2:D:148:ILE:HD11	1.92	0.52
2:D:51:ARG:NH1	2:D:149:LEU:HD11	2.21	0.52
2:D:313:GLU:O	2:D:317:LEU:HG	2.09	0.52
2:D:455:ARG:NH1	2:D:487:ASP:O	2.43	0.52
2:F:506:LEU:HD21	2:F:560:GLU:HG2	1.91	0.52
2:A:310:PRO:HD2	2:A:313:GLU:CG	2.40	0.52
2:B:375:ALA:O	2:B:379:GLU:HG2	2.10	0.52
2:D:99:CYS:HB2	2:D:124:PHE:CZ	2.45	0.52
2:D:329:PRO:HB2	2:D:333:ARG:HH21	1.75	0.52
2:F:53:ALA:HB1	2:F:56:VAL:CG2	2.40	0.52
2:F:213:ARG:HD2	2:F:233:SER:CA	2.40	0.52
1:X:5:A:OP2	2:E:102:GLY:HA2	2.09	0.52
2:A:127:LEU:HB2	2:A:158:HIS:CB	2.35	0.52
2:B:458:PHE:O	2:B:461:VAL:HG12	2.09	0.52
2:C:509:VAL:HG12	2:C:562:VAL:HG23	1.92	0.52
2:C:521:TYR:OH	2:C:580:ASP:HB3	2.10	0.52
2:D:150:TRP:O	2:D:154:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:482:TRP:HB2	2:D:505:LEU:HD12	1.90	0.52
2:D:519:CYS:O	2:D:523:ASN:ND2	2.43	0.52
2:E:578:LEU:O	2:E:582:LEU:HG	2.09	0.52
2:F:20:GLU:HB2	2:F:157:LEU:CD2	2.39	0.52
2:F:262:GLU:OE1	2:F:351:ALA:HB1	2.10	0.52
2:F:263:LEU:HB2	2:F:567:ASN:HD21	1.75	0.52
2:F:593:THR:HG23	2:F:596:ASP:H	1.75	0.52
2:A:61:THR:HG21	2:A:85:TRP:NE1	2.25	0.52
2:A:168:TRP:HH2	2:F:208:LEU:HD11	1.74	0.52
2:A:555:LEU:O	2:A:559:ARG:HG2	2.10	0.52
2:B:494:GLY:HA2	2:B:517:GLU:CG	2.40	0.52
1:Y:10:A:N1	2:C:37:THR:HG21	2.25	0.52
2:A:616:LEU:HD11	2:A:620:ARG:HE	1.73	0.52
2:B:100:LEU:HD13	2:B:108:SER:OG	2.09	0.52
2:B:262:GLU:O	2:B:351:ALA:HA	2.10	0.52
2:B:294:GLU:N	2:B:294:GLU:OE2	2.42	0.52
2:C:166:ARG:O	2:C:172:ARG:NH1	2.43	0.52
2:C:564:VAL:HG13	2:C:600:LEU:CD2	2.39	0.52
2:D:60:ILE:HG23	2:D:190:GLU:HA	1.91	0.52
2:D:144:THR:HB	2:D:146:GLU:OE1	2.10	0.52
2:E:264:HIS:CD2	2:E:569:ASP:HA	2.45	0.52
2:F:7:LEU:HD23	2:F:32:VAL:CG1	2.39	0.52
2:F:162:LEU:H	2:F:162:LEU:HD23	1.74	0.52
2:F:185:GLU:HG3	2:F:192:ARG:HB3	1.90	0.52
2:A:64:ALA:HB2	2:A:194:GLN:HB3	1.92	0.51
2:D:252:GLN:HG2	2:D:583:LEU:CD1	2.40	0.51
2:F:278:ARG:NH2	2:F:293:LEU:HD11	2.26	0.51
1:X:1:A:O2'	2:D:13:THR:N	2.43	0.51
2:A:125:HIS:O	2:A:160:ILE:N	2.43	0.51
2:A:279:ARG:O	2:A:334:GLU:HG2	2.09	0.51
2:A:307:GLN:CD	2:A:308:PRO:HD2	2.35	0.51
2:A:327:ARG:NH2	2:A:362:GLU:HB3	2.25	0.51
2:B:122:GLU:OE2	2:B:124:PHE:HB3	2.10	0.51
2:B:170:GLN:HE22	2:C:216:GLY:HA2	1.74	0.51
2:C:91:THR:HG23	2:C:95:GLN:HB2	1.92	0.51
2:D:440:ASP:OD1	2:D:441:LEU:N	2.44	0.51
2:E:309:ILE:HG12	2:E:525:GLN:O	2.11	0.51
2:F:233:SER:O	2:F:237:LEU:HD23	2.11	0.51
2:A:422:VAL:HG13	2:A:464:CYS:SG	2.50	0.51
2:B:84:ARG:HB2	2:B:181:LEU:HD11	1.93	0.51
2:B:106:THR:HG23	2:C:125:HIS:ND1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:354:ARG:HD3	2:C:401:ILE:HD11	1.92	0.51
2:D:18:VAL:HB	2:D:45:ILE:HD13	1.91	0.51
2:D:61:THR:HG22	2:D:191:ARG:CG	2.40	0.51
2:D:84:ARG:NH1	2:D:199:ALA:HB3	2.24	0.51
2:B:452:HIS:O	2:B:455:ARG:HG3	2.10	0.51
2:D:263:LEU:HD23	2:D:492:ARG:CZ	2.41	0.51
2:E:90:ARG:CZ	2:E:176:PRO:HG2	2.41	0.51
2:F:260:LYS:HA	2:F:601:GLN:NE2	2.25	0.51
2:A:278:ARG:NH1	2:A:293:LEU:HD11	2.25	0.51
2:C:440:ASP:OD1	2:C:441:LEU:N	2.43	0.51
2:D:76:PHE:HB3	2:D:198:ARG:HH22	1.75	0.51
2:E:103:GLY:HA3	2:E:107:MET:CE	2.41	0.51
2:F:333:ARG:O	2:F:337:ARG:HG2	2.11	0.51
2:F:506:LEU:CD2	2:F:560:GLU:HG2	2.40	0.51
2:C:526:ILE:HG22	2:C:527:LYS:HG2	1.93	0.51
2:E:226:PHE:O	2:E:229:LEU:HG	2.10	0.51
2:F:4:GLN:O	2:F:30:VAL:HG22	2.11	0.51
2:F:99:CYS:HB2	2:F:124:PHE:CE1	2.46	0.51
2:F:125:HIS:HB3	2:F:160:ILE:CG2	2.41	0.51
2:F:521:TYR:CE1	2:F:584:LEU:HD13	2.46	0.51
2:F:566:VAL:HG22	2:F:581:ASN:ND2	2.26	0.51
2:A:209:GLN:HE22	2:F:166:ARG:HG2	1.75	0.51
2:A:277:LEU:O	2:A:281:ARG:HG2	2.11	0.51
2:B:70:LYS:HA	2:C:158:HIS:CD2	2.45	0.51
2:B:125:HIS:NE2	2:B:160:ILE:HD11	2.26	0.51
2:D:238:ALA:O	2:D:242:GLU:HG3	2.11	0.51
2:D:452:HIS:HB3	2:D:483:ARG:HD2	1.91	0.51
2:D:557:TYR:O	2:D:562:VAL:HG12	2.11	0.51
2:F:32:VAL:HB	2:F:58:LEU:HD12	1.92	0.51
2:F:182:GLN:OE1	2:F:194:GLN:HB3	2.11	0.51
2:F:386:THR:OG1	2:F:393:ALA:HB2	2.10	0.51
2:F:531:LEU:HD23	2:F:587:ARG:CZ	2.40	0.51
2:F:239:TRP:HA	2:F:242:GLU:OE1	2.10	0.51
2:F:519:CYS:SG	2:F:569:ASP:HB2	2.51	0.51
2:A:170:GLN:NE2	2:A:207:LEU:HD11	2.25	0.51
2:A:552:TYR:HB2	2:A:588:LEU:CD2	2.39	0.51
2:F:19:PRO:HD3	2:F:45:ILE:HD12	1.92	0.51
2:A:50:ARG:NH1	2:A:51:ARG:HA	2.26	0.51
2:A:100:LEU:HD23	2:A:100:LEU:H	1.75	0.51
2:B:81:VAL:HG21	2:B:193:VAL:HG23	1.92	0.51
2:B:116:THR:HA	2:B:165:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:ALA:N	2:D:95:GLN:HB2	2.25	0.51
2:D:69:LEU:HD22	2:D:104:PHE:CZ	2.45	0.51
2:E:450:ARG:HH12	2:E:476:ASP:HB2	1.76	0.51
2:F:167:GLY:O	2:F:172:ARG:NH2	2.44	0.51
2:A:127:LEU:O	2:A:157:LEU:HD22	2.11	0.50
2:A:557:TYR:CB	2:A:564:VAL:HG21	2.40	0.50
2:B:302:TRP:HB3	2:B:303:PRO:HD3	1.94	0.50
2:B:404:ARG:CZ	2:B:441:LEU:HG	2.41	0.50
2:C:132:CYS:SG	2:C:141:PRO:HA	2.51	0.50
2:C:307:GLN:NE2	2:C:308:PRO:HD2	2.26	0.50
2:D:69:LEU:HD22	2:D:104:PHE:CE1	2.46	0.50
2:D:76:PHE:HB3	2:D:198:ARG:NH2	2.26	0.50
2:A:4:GLN:O	2:A:30:VAL:HG22	2.10	0.50
2:A:470:VAL:HG21	2:A:484:ALA:HB1	1.93	0.50
2:B:493:LEU:O	2:B:517:GLU:HG2	2.11	0.50
2:E:51:ARG:HH21	2:E:145:LEU:HD22	1.76	0.50
2:E:63:VAL:CG1	2:E:81:VAL:HG11	2.40	0.50
2:F:144:THR:HB	2:F:146:GLU:OE1	2.11	0.50
2:F:378:GLN:HE22	2:F:433:ALA:HB1	1.77	0.50
2:A:197:ASP:OD1	2:A:198:ARG:N	2.44	0.50
2:C:313:GLU:O	2:C:317:LEU:HG	2.11	0.50
2:D:13:THR:HA	2:D:40:PRO:HB3	1.93	0.50
2:D:72:GLU:OE1	2:E:160:ILE:HA	2.12	0.50
2:E:224:LEU:HD22	2:E:229:LEU:CD1	2.41	0.50
2:E:270:PHE:CD1	2:E:571:ILE:HD12	2.47	0.50
2:F:93:PRO:HD3	2:F:173:ARG:NH2	2.21	0.50
2:F:262:GLU:O	2:F:351:ALA:HA	2.11	0.50
2:F:266:HIS:HB2	2:F:570:ASN:ND2	2.25	0.50
2:A:499:LEU:HB3	2:A:557:TYR:OH	2.11	0.50
2:B:269:GLY:O	2:B:572:GLY:N	2.38	0.50
2:C:17:ILE:HD11	2:C:101:THR:HG21	1.92	0.50
2:D:37:THR:HG22	2:D:66:PHE:HD2	1.77	0.50
2:D:67:GLN:OE1	2:D:67:GLN:N	2.44	0.50
2:E:38:GLU:HA	2:E:62:ARG:CD	2.42	0.50
2:F:225:PRO:HD3	2:F:595:LEU:HD11	1.91	0.50
2:A:242:GLU:HB2	2:A:243:PRO:HD2	1.92	0.50
2:D:72:GLU:HG3	2:E:160:ILE:CG1	2.38	0.50
2:E:3:VAL:CG1	2:E:95:GLN:HG2	2.41	0.50
2:E:170:GLN:OE1	2:E:170:GLN:N	2.44	0.50
2:E:333:ARG:HD2	2:E:337:ARG:HH21	1.76	0.50
2:A:9:VAL:O	2:A:34:VAL:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:THR:HA	2:A:442:ALA:O	2.11	0.50
2:A:474:GLU:OE2	2:A:495:HIS:HB2	2.12	0.50
2:B:95:GLN:N	2:B:95:GLN:OE1	2.44	0.50
2:B:290:LEU:HD23	2:B:291:PRO:CD	2.39	0.50
2:C:242:GLU:OE1	2:C:242:GLU:N	2.31	0.50
2:C:350:TYR:HB2	2:C:618:LEU:HD21	1.94	0.50
2:C:404:ARG:HD2	2:C:454:PHE:HE2	1.77	0.50
2:C:552:TYR:CE2	2:C:554:LEU:HB2	2.46	0.50
2:D:171:LEU:HA	2:D:174:ILE:HD11	1.93	0.50
2:D:458:PHE:CG	2:D:488:LEU:HD11	2.47	0.50
2:F:78:PHE:HA	2:F:81:VAL:HG22	1.94	0.50
2:F:458:PHE:O	2:F:461:VAL:HG12	2.12	0.50
2:A:112:GLN:O	2:A:116:THR:HG23	2.12	0.50
2:A:174:ILE:HG22	2:A:175:ALA:H	1.76	0.50
2:A:260:LYS:CB	2:A:348:VAL:HG22	2.41	0.50
2:A:276:LEU:HD12	2:A:277:LEU:N	2.27	0.50
2:B:24:LEU:HD23	2:B:27:ALA:CB	2.41	0.50
2:D:330:GLY:HA2	2:D:333:ARG:NH1	2.27	0.50
2:F:94:GLU:OE1	2:F:94:GLU:N	2.32	0.50
2:B:11:LEU:CD2	2:B:42:VAL:HG12	2.42	0.50
2:C:401:ILE:HA	2:C:440:ASP:HB3	1.94	0.50
2:D:66:PHE:HD1	2:D:74:ASP:HB2	1.77	0.50
2:D:310:PRO:HG2	2:D:313:GLU:CG	2.42	0.50
2:F:285:GLU:OE1	2:F:329:PRO:HD2	2.12	0.50
2:A:571:ILE:HG13	2:A:576:ALA:O	2.11	0.50
2:A:618:LEU:O	2:A:622:ILE:HD12	2.12	0.50
2:B:566:VAL:HG23	2:B:600:LEU:HD13	1.93	0.50
2:C:7:LEU:CD2	2:C:9:VAL:HB	2.42	0.50
2:D:45:ILE:HD11	2:D:49:PHE:HE1	1.77	0.50
2:D:93:PRO:HD3	2:D:173:ARG:NH1	2.27	0.50
2:D:170:GLN:HE21	2:D:207:LEU:HD21	1.76	0.50
2:F:32:VAL:O	2:F:58:LEU:HG	2.11	0.50
2:F:226:PHE:HB2	2:F:229:LEU:HD13	1.93	0.50
2:A:38:GLU:HA	2:A:62:ARG:NE	2.26	0.49
2:A:579:THR:O	2:A:583:LEU:HG	2.11	0.49
2:C:184:VAL:HG22	2:C:192:ARG:HG2	1.94	0.49
2:C:524:LEU:HD12	2:C:529:PHE:H	1.76	0.49
2:D:126:VAL:HG12	2:D:159:TRP:HD1	1.76	0.49
2:D:489:ASN:ND2	2:E:486:PHE:HD2	2.10	0.49
2:E:127:LEU:HB2	2:E:158:HIS:HB2	1.94	0.49
2:E:315:MET:HE2	3:E:701:ATP:O2G	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:494:GLY:HA2	2:F:517:GLU:CG	2.41	0.49
2:F:524:LEU:CD1	2:F:531:LEU:HD11	2.42	0.49
2:A:262:GLU:HB3	2:A:351:ALA:CB	2.41	0.49
2:B:39:ARG:HG3	2:B:40:PRO:HD3	1.95	0.49
2:C:332:LEU:HD21	2:C:373:ILE:CG1	2.41	0.49
2:C:356:SER:OG	2:C:401:ILE:HB	2.12	0.49
2:D:16:ALA:HA	2:D:19:PRO:HD2	1.94	0.49
2:D:472:ALA:HB3	2:D:481:ILE:HD13	1.94	0.49
2:E:91:THR:HG23	2:E:96:ARG:NH1	2.24	0.49
2:E:481:ILE:HG21	2:E:499:LEU:CD1	2.41	0.49
2:F:278:ARG:NH2	2:F:295:GLU:OE2	2.46	0.49
2:F:399:ILE:HG13	2:F:438:GLY:C	2.36	0.49
2:A:346:GLN:HE22	2:A:578:LEU:H	1.60	0.49
2:C:144:THR:HG23	2:C:147:GLU:HG2	1.93	0.49
2:C:286:ASN:ND2	2:C:289:LYS:HD2	2.28	0.49
2:C:457:GLU:OE2	2:C:457:GLU:N	2.37	0.49
2:D:354:ARG:NE	2:D:440:ASP:OD2	2.46	0.49
2:E:84:ARG:HB3	2:E:181:LEU:CD2	2.43	0.49
2:E:134:GLY:HA3	2:E:139:LEU:CD2	2.42	0.49
2:E:362:GLU:OE2	2:E:362:GLU:N	2.45	0.49
2:E:494:GLY:HA2	2:E:517:GLU:CG	2.42	0.49
2:F:125:HIS:O	2:F:160:ILE:HG22	2.12	0.49
2:F:239:TRP:O	2:F:594:ARG:NH1	2.45	0.49
2:B:118:LEU:HA	2:B:171:LEU:CD1	2.43	0.49
2:C:22:PHE:HD1	2:C:32:VAL:HG21	1.77	0.49
2:C:310:PRO:HG2	2:C:313:GLU:OE1	2.11	0.49
2:D:24:LEU:HD23	2:D:27:ALA:CB	2.43	0.49
2:D:53:ALA:HB1	2:D:56:VAL:HG21	1.93	0.49
2:D:340:TYR:CD2	2:D:380:CYS:HB3	2.47	0.49
2:D:481:ILE:HG23	2:D:493:LEU:HD23	1.95	0.49
2:E:397:ASN:ND2	2:E:437:VAL:HG11	2.27	0.49
2:E:422:VAL:HG13	2:E:464:CYS:SG	2.52	0.49
2:E:493:LEU:O	2:E:517:GLU:HG2	2.12	0.49
2:A:440:ASP:OD1	2:A:441:LEU:N	2.46	0.49
2:A:462:HIS:NE2	2:A:489:ASN:HB2	2.28	0.49
2:B:133:VAL:O	2:B:139:LEU:HD23	2.12	0.49
2:B:358:ALA:HA	2:B:366:PRO:HB3	1.93	0.49
2:C:84:ARG:HH12	2:C:180:PRO:HD2	1.78	0.49
2:C:386:THR:OG1	2:C:393:ALA:HB2	2.12	0.49
2:D:17:ILE:HA	2:D:20:GLU:OE1	2.13	0.49
2:D:161:ARG:N	2:E:72:GLU:OE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:LEU:HD21	2:F:78:PHE:HE1	1.76	0.49
2:A:7:LEU:HD12	2:A:8:PHE:H	1.77	0.49
2:A:46:ARG:HB2	2:A:46:ARG:NH1	2.27	0.49
2:A:562:VAL:HG13	2:A:564:VAL:HG23	1.94	0.49
2:E:7:LEU:HB2	2:E:29:PHE:CE1	2.47	0.49
2:B:37:THR:O	2:B:62:ARG:NE	2.43	0.49
2:B:215:ALA:HB1	2:C:170:GLN:HE22	1.76	0.49
2:B:381:MET:CE	2:B:396:VAL:H	2.26	0.49
2:B:481:ILE:HG23	2:B:493:LEU:HD13	1.95	0.49
2:C:8:PHE:HB2	2:C:98:VAL:HG12	1.93	0.49
2:C:126:VAL:HG22	2:C:159:TRP:CD1	2.47	0.49
2:C:272:THR:O	2:C:277:LEU:HD22	2.13	0.49
2:D:552:TYR:HB3	2:D:589:CYS:SG	2.53	0.49
2:E:122:GLU:OE2	2:E:161:ARG:HB2	2.12	0.49
2:E:309:ILE:HB	2:E:313:GLU:OE2	2.12	0.49
2:F:125:HIS:O	2:F:160:ILE:N	2.45	0.49
2:F:232:TRP:HB3	2:F:236:GLU:HB2	1.93	0.49
2:A:301:GLY:HA2	2:A:305:PRO:CD	2.43	0.49
2:A:461:VAL:CG2	2:A:466:LEU:HB3	2.43	0.49
2:B:462:HIS:NE2	2:B:488:LEU:O	2.42	0.49
2:C:271:ALA:O	2:C:321:ASN:ND2	2.41	0.49
2:E:50:ARG:HH21	2:E:51:ARG:HH11	1.58	0.49
2:E:485:VAL:HG13	2:E:514:ILE:CD1	2.43	0.49
2:F:33:HIS:HB3	2:F:85:TRP:HZ2	1.78	0.49
2:F:108:SER:HA	2:F:111:MET:CE	2.42	0.49
2:A:67:GLN:HG2	2:A:68:ASP:OD1	2.11	0.49
2:A:341:ARG:HA	2:A:341:ARG:CZ	2.42	0.49
2:D:314:TYR:CE2	2:D:526:ILE:HD11	2.47	0.49
2:D:439:VAL:O	2:D:469:THR:HG22	2.13	0.49
2:E:175:ALA:HB3	2:E:178:GLN:HE22	1.77	0.49
2:E:606:GLU:O	2:E:615:ARG:NH1	2.44	0.49
2:F:414:ILE:O	2:F:418:LEU:HD23	2.13	0.49
2:F:552:TYR:CD1	2:F:553:PRO:HD2	2.47	0.49
2:F:567:ASN:O	2:F:581:ASN:ND2	2.45	0.49
2:C:66:PHE:HD1	2:C:74:ASP:HB2	1.75	0.49
2:C:185:GLU:HG2	2:C:192:ARG:CZ	2.43	0.49
2:C:269:GLY:O	2:C:572:GLY:N	2.42	0.49
2:D:63:VAL:HG21	2:D:78:PHE:CD1	2.48	0.49
2:D:82:MET:HE1	2:D:114:ALA:HB2	1.94	0.49
2:D:518:LEU:HD12	2:D:564:VAL:HG13	1.95	0.49
2:E:34:VAL:HB	2:E:60:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:249:PRO:HB2	2:F:253:ARG:NH2	2.28	0.49
2:A:79:GLU:O	2:A:82:MET:HG3	2.13	0.48
2:A:285:GLU:CD	2:A:329:PRO:HD2	2.37	0.48
2:B:38:GLU:HA	2:B:62:ARG:HE	1.78	0.48
2:B:333:ARG:HG2	2:B:337:ARG:NH1	2.28	0.48
2:C:64:ALA:O	2:C:77:ARG:NH2	2.33	0.48
2:C:84:ARG:NH2	2:C:199:ALA:HB3	2.28	0.48
2:C:315:MET:HE1	3:C:701:ATP:N3	2.28	0.48
2:C:427:HIS:HA	2:D:365:SER:HB2	1.93	0.48
2:D:244:LEU:HD12	2:D:245:ASP:H	1.77	0.48
2:E:430:ASP:HB3	2:E:433:ALA:HB3	1.95	0.48
2:A:187:LYS:HA	2:A:187:LYS:HE3	1.95	0.48
2:A:252:GLN:NE2	2:A:253:ARG:HG3	2.27	0.48
2:B:123:VAL:O	2:B:162:LEU:HB2	2.14	0.48
2:B:337:ARG:HG2	2:B:380:CYS:SG	2.54	0.48
2:B:351:ALA:O	2:B:396:VAL:HA	2.12	0.48
2:D:62:ARG:NH1	2:D:190:GLU:OE1	2.45	0.48
2:E:440:ASP:OD1	2:E:441:LEU:N	2.46	0.48
2:F:334:GLU:HA	2:F:337:ARG:HG3	1.93	0.48
2:A:74:ASP:O	2:A:77:ARG:HG2	2.13	0.48
2:B:123:VAL:HG12	2:B:163:GLY:O	2.13	0.48
2:B:499:LEU:O	2:B:499:LEU:HD23	2.13	0.48
2:D:105:LYS:O	2:D:108:SER:OG	2.32	0.48
2:F:84:ARG:NE	2:F:179:PHE:HB3	2.28	0.48
2:F:276:LEU:HD12	2:F:277:LEU:HD22	1.94	0.48
2:F:613:THR:O	2:F:617:THR:HG23	2.13	0.48
2:A:41:ASP:OD1	2:A:43:THR:HG23	2.13	0.48
2:A:404:ARG:HG3	2:A:444:TYR:O	2.13	0.48
2:B:150:TRP:O	2:B:154:GLN:HG3	2.13	0.48
2:D:263:LEU:HB3	2:D:492:ARG:NH2	2.28	0.48
2:D:272:THR:C	2:D:277:LEU:HD21	2.38	0.48
2:D:302:TRP:O	2:D:305:PRO:HD3	2.13	0.48
2:E:101:THR:HG21	2:E:126:VAL:HG22	1.95	0.48
2:F:400:LEU:HD12	2:F:421:ALA:CB	2.40	0.48
1:Y:8:A:H4'	2:C:105:LYS:HE2	1.96	0.48
2:A:7:LEU:CB	2:A:32:VAL:HG13	2.38	0.48
2:A:36:THR:HG23	2:A:62:ARG:HD2	1.96	0.48
2:B:225:PRO:HG2	2:B:598:LEU:HB3	1.94	0.48
2:C:64:ALA:HB2	2:C:193:VAL:O	2.13	0.48
2:C:272:THR:HG22	2:C:321:ASN:HB3	1.95	0.48
2:C:302:TRP:HB3	2:C:303:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:ILE:HD13	2:C:440:ASP:CB	2.43	0.48
2:C:593:THR:OG1	2:C:596:ASP:OD1	2.31	0.48
2:D:307:GLN:NE2	2:D:308:PRO:HD2	2.28	0.48
2:E:412:ALA:HA	2:F:463:ARG:CG	2.43	0.48
2:F:622:ILE:O	2:F:626:ILE:HG13	2.14	0.48
2:A:78:PHE:HA	2:A:81:VAL:HG12	1.95	0.48
2:A:599:HIS:O	2:A:603:HIS:ND1	2.46	0.48
2:D:107:MET:O	2:D:111:MET:HG2	2.12	0.48
2:D:116:THR:HA	2:D:165:GLU:CG	2.36	0.48
2:D:414:ILE:O	2:D:418:LEU:HG	2.14	0.48
2:E:68:ASP:OD1	2:E:69:LEU:N	2.47	0.48
2:E:101:THR:HG21	2:E:126:VAL:CG2	2.43	0.48
2:E:521:TYR:CE2	2:E:584:LEU:HD22	2.48	0.48
2:F:245:ASP:OD2	2:F:248:ALA:N	2.46	0.48
1:Z:13:A:N3	2:F:103:GLY:HA2	2.29	0.48
2:A:39:ARG:HH21	2:A:67:GLN:HG3	1.78	0.48
2:A:127:LEU:HD11	2:F:69:LEU:CD2	2.41	0.48
2:A:145:LEU:HA	2:A:148:ILE:CD1	2.40	0.48
2:B:244:LEU:HD12	2:B:245:ASP:H	1.79	0.48
2:B:262:GLU:HB3	2:B:351:ALA:CB	2.43	0.48
2:D:92:GLY:H	2:D:95:GLN:HE22	1.62	0.48
2:D:499:LEU:O	2:D:499:LEU:HD23	2.14	0.48
2:E:562:VAL:HG13	2:E:564:VAL:CG2	2.44	0.48
2:F:145:LEU:HD13	2:F:148:ILE:HD11	1.95	0.48
2:B:315:MET:HE1	3:B:701:ATP:H2'	1.96	0.48
2:B:439:VAL:O	2:B:469:THR:HG22	2.14	0.48
2:E:262:GLU:O	2:E:351:ALA:HA	2.13	0.48
2:E:446:ASP:OD1	2:E:448:LYS:HG3	2.14	0.48
2:E:492:ARG:O	2:E:493:LEU:HD23	2.13	0.48
2:F:84:ARG:HA	2:F:87:LEU:CG	2.44	0.48
2:F:84:ARG:HB2	2:F:181:LEU:HD21	1.96	0.48
2:F:225:PRO:HG2	2:F:229:LEU:HD22	1.96	0.48
2:F:563:ARG:HD3	2:F:607:THR:CG2	2.43	0.48
2:B:187:LYS:HE2	2:B:187:LYS:HA	1.96	0.48
2:B:503:ARG:NH2	2:B:506:LEU:HD13	2.29	0.48
2:B:520:PRO:HD2	2:B:581:ASN:OD1	2.13	0.48
2:C:303:PRO:O	2:C:304:LEU:HD23	2.14	0.48
2:D:140:MET:O	2:D:142:PRO:HD3	2.13	0.48
2:D:354:ARG:HA	2:D:399:ILE:O	2.13	0.48
2:D:481:ILE:HG23	2:D:493:LEU:CD2	2.44	0.48
2:E:519:CYS:SG	2:E:569:ASP:HB2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:THR:O	2:F:15:PRO:HD3	2.14	0.48
2:F:570:ASN:HB2	2:F:573:ILE:HG22	1.94	0.48
2:A:321:ASN:OD1	2:A:325:LEU:HD23	2.14	0.48
2:A:427:HIS:HA	2:B:365:SER:OG	2.13	0.48
2:B:105:LYS:HD3	2:C:105:LYS:HG2	1.96	0.48
2:B:122:GLU:HG3	2:B:124:PHE:HD1	1.78	0.48
2:B:310:PRO:HD2	2:B:313:GLU:CG	2.44	0.48
2:C:6:HIS:O	2:C:97:PHE:HB2	2.14	0.48
2:D:24:LEU:HD23	2:D:27:ALA:HB2	1.96	0.48
2:F:24:LEU:HD11	2:F:161:ARG:HH21	1.79	0.48
2:F:39:ARG:HB2	2:F:40:PRO:HD3	1.96	0.48
2:F:264:HIS:HA	2:F:354:ARG:HH12	1.78	0.48
2:F:385:ARG:HD2	2:F:390:GLY:C	2.38	0.48
2:A:495:HIS:HE1	2:A:519:CYS:HB2	1.77	0.47
2:B:303:PRO:O	2:B:304:LEU:HD23	2.13	0.47
2:C:265:CYS:O	2:C:354:ARG:HG3	2.14	0.47
2:F:82:MET:HE1	2:F:111:MET:HA	1.96	0.47
2:F:281:ARG:CD	2:F:293:LEU:HD13	2.40	0.47
2:F:502:SER:HB3	2:F:505:LEU:HB2	1.96	0.47
2:B:271:ALA:O	2:B:321:ASN:ND2	2.36	0.47
2:C:364:ARG:HH22	2:C:372:ASP:HB2	1.78	0.47
2:D:272:THR:CG2	2:D:318:GLY:HA2	2.44	0.47
2:D:385:ARG:HD2	2:D:390:GLY:O	2.14	0.47
2:D:492:ARG:NE	2:D:517:GLU:OE2	2.33	0.47
2:D:555:LEU:O	2:D:559:ARG:HG2	2.13	0.47
2:F:196:GLU:HG3	2:F:197:ASP:CG	2.38	0.47
2:A:151:ALA:O	2:A:154:GLN:NE2	2.48	0.47
2:B:309:ILE:HB	2:B:313:GLU:OE2	2.13	0.47
2:C:145:LEU:O	2:C:148:ILE:HG22	2.14	0.47
2:C:362:GLU:N	2:C:362:GLU:OE2	2.46	0.47
2:D:512:ARG:HD3	2:E:491:ARG:HD2	1.97	0.47
2:E:446:ASP:CG	2:E:448:LYS:HG3	2.39	0.47
2:F:565:THR:OG1	2:F:604:ALA:HB2	2.15	0.47
2:A:49:PHE:CE1	2:A:56:VAL:HG11	2.49	0.47
2:C:19:PRO:HB3	2:C:48:PHE:CD2	2.49	0.47
2:D:261:ILE:HG22	2:D:263:LEU:CD1	2.45	0.47
2:A:456:GLU:OE1	2:B:456:GLU:HA	2.13	0.47
2:B:225:PRO:HG3	2:B:599:HIS:CE1	2.49	0.47
2:B:486:PHE:HD1	2:C:489:ASN:HD22	1.60	0.47
2:C:213:ARG:HD2	2:C:233:SER:N	2.29	0.47
2:C:290:LEU:HD11	2:C:325:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:SER:HA	2:E:168:TRP:CZ3	2.50	0.47
2:D:354:ARG:HB3	2:D:401:ILE:CD1	2.44	0.47
2:E:84:ARG:HB2	2:E:181:LEU:HD11	1.95	0.47
2:E:174:ILE:HG22	2:E:178:GLN:NE2	2.29	0.47
2:F:339:LEU:HD21	2:F:353:VAL:HG11	1.96	0.47
2:F:555:LEU:O	2:F:559:ARG:HG2	2.14	0.47
2:A:358:ALA:HA	2:A:366:PRO:HB3	1.96	0.47
2:B:16:ALA:HA	2:B:19:PRO:HG2	1.97	0.47
2:B:145:LEU:HD13	2:B:148:ILE:CD1	2.39	0.47
2:B:381:MET:HE2	2:B:396:VAL:H	1.79	0.47
2:C:456:GLU:HG3	2:D:459:THR:HG21	1.97	0.47
2:D:66:PHE:CD1	2:D:74:ASP:HB2	2.50	0.47
2:D:220:MET:HE1	2:D:241:ARG:NH2	2.29	0.47
2:D:329:PRO:HB3	2:D:364:ARG:HH12	1.79	0.47
2:E:107:MET:O	2:E:111:MET:HG2	2.15	0.47
2:E:170:GLN:NE2	2:E:207:LEU:HD21	2.29	0.47
2:F:520:PRO:HB3	2:F:552:TYR:CE2	2.50	0.47
2:F:521:TYR:HE1	2:F:584:LEU:HD13	1.78	0.47
1:X:2:A:O2'	1:X:3:A:H5'	2.14	0.47
1:X:3:A:H4'	1:X:4:A:C8	2.50	0.47
2:A:13:THR:O	2:A:15:PRO:HD3	2.14	0.47
2:A:15:PRO:CB	2:A:44:LEU:HD21	2.43	0.47
2:A:139:LEU:HG	2:A:140:MET:O	2.15	0.47
2:A:466:LEU:HD12	2:A:467:ALA:H	1.79	0.47
2:B:58:LEU:HD21	2:B:60:ILE:HD11	1.97	0.47
2:B:99:CYS:SG	2:B:125:HIS:HA	2.55	0.47
2:C:20:GLU:HA	2:C:23:LEU:CD2	2.44	0.47
2:C:48:PHE:CD1	2:C:145:LEU:HD23	2.38	0.47
2:C:401:ILE:HD13	2:C:440:ASP:HB3	1.97	0.47
2:D:24:LEU:CD1	2:D:25:PRO:HD2	2.39	0.47
2:D:520:PRO:HB2	2:D:584:LEU:CD2	2.45	0.47
2:E:49:PHE:CE1	2:E:56:VAL:HG21	2.50	0.47
2:E:184:VAL:HG22	2:E:192:ARG:O	2.15	0.47
2:E:262:GLU:OE2	2:E:265:CYS:HB2	2.14	0.47
2:E:355:CYS:SG	2:E:398:LEU:HD12	2.54	0.47
2:E:485:VAL:CG2	2:E:493:LEU:HD11	2.44	0.47
2:E:531:LEU:HD23	2:E:587:ARG:NH2	2.29	0.47
2:E:570:ASN:HB3	2:E:573:ILE:HD13	1.96	0.47
2:F:121:ALA:O	2:F:164:PRO:HB3	2.14	0.47
2:F:179:PHE:HD2	2:F:200:PHE:HD2	1.62	0.47
2:F:451:ALA:HB1	2:F:488:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:138:ARG:HA	2:A:138:ARG:CZ	2.44	0.47
2:A:364:ARG:NH2	2:A:372:ASP:OD1	2.48	0.47
2:A:470:VAL:HG23	2:A:490:ALA:HB2	1.95	0.47
2:D:100:LEU:HD12	2:D:108:SER:HB2	1.97	0.47
2:D:225:PRO:O	2:D:602:ARG:NH1	2.39	0.47
2:D:470:VAL:CG2	2:D:488:LEU:HD23	2.45	0.47
2:D:583:LEU:O	2:D:587:ARG:HG3	2.14	0.47
2:E:387:ALA:HB1	2:E:388:PRO:HD2	1.96	0.47
2:F:299:PRO:HG2	2:F:302:TRP:CE3	2.49	0.47
2:F:340:TYR:CD2	2:F:380:CYS:HB3	2.50	0.47
2:F:566:VAL:HG12	2:F:600:LEU:CD2	2.43	0.47
1:Z:14:A:N6	2:F:140:MET:SD	2.87	0.47
2:A:116:THR:HA	2:A:165:GLU:CD	2.39	0.47
2:A:530:ARG:HD3	2:A:534:SER:C	2.39	0.47
2:B:233:SER:O	2:B:237:LEU:HD23	2.14	0.47
2:B:518:LEU:HD13	2:B:564:VAL:CG1	2.43	0.47
2:C:499:LEU:HD21	2:C:506:LEU:HA	1.97	0.47
2:D:262:GLU:OE1	2:D:265:CYS:HB2	2.15	0.47
2:E:462:HIS:NE2	2:E:489:ASN:HB2	2.30	0.47
2:A:298:LEU:HA	2:A:302:TRP:HE1	1.81	0.47
2:B:185:GLU:OE1	2:B:192:ARG:HG3	2.14	0.47
2:C:182:GLN:HE22	2:C:184:VAL:HA	1.79	0.47
2:D:118:LEU:HA	2:D:171:LEU:CD1	2.45	0.47
2:E:10:SER:OG	2:E:101:THR:O	2.30	0.47
2:E:45:ILE:H	2:E:45:ILE:HD12	1.80	0.47
2:E:240:LEU:HG	2:E:594:ARG:HG3	1.97	0.47
1:Z:16:A:C5	2:A:13:THR:HG23	2.50	0.46
2:A:504:GLU:OE2	2:E:416:ARG:NH1	2.46	0.46
2:B:104:PHE:H	2:B:107:MET:HE3	1.79	0.46
2:B:117:VAL:O	2:B:171:LEU:HD11	2.15	0.46
2:B:267:LEU:O	2:B:335:GLN:NE2	2.48	0.46
2:D:78:PHE:CZ	2:D:107:MET:HE3	2.51	0.46
2:D:385:ARG:HD2	2:D:390:GLY:C	2.40	0.46
2:E:68:ASP:HB3	2:E:70:LYS:HZ1	1.80	0.46
2:E:117:VAL:HG12	2:E:171:LEU:HD22	1.97	0.46
2:E:211:ALA:HA	2:E:214:ILE:HG22	1.96	0.46
1:Y:11:A:O2'	1:Y:12:A:H5'	2.15	0.46
2:A:18:VAL:HG21	2:A:45:ILE:HG23	1.97	0.46
2:B:256:ALA:HA	2:B:579:THR:HG21	1.97	0.46
2:B:511:ASP:HB3	2:C:491:ARG:NH1	2.30	0.46
2:C:78:PHE:CZ	2:C:107:MET:HG2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:GLN:OE1	2:D:95:GLN:N	2.48	0.46
2:E:8:PHE:CE2	2:E:96:ARG:HG2	2.50	0.46
2:E:191:ARG:HG2	2:E:193:VAL:HG13	1.97	0.46
2:E:300:GLU:OE2	2:E:300:GLU:N	2.45	0.46
2:E:365:SER:HB3	2:F:427:HIS:HA	1.98	0.46
2:F:96:ARG:HB2	2:F:121:ALA:H	1.80	0.46
2:F:341:ARG:HH12	2:F:344:VAL:HB	1.80	0.46
2:F:485:VAL:HG22	2:F:493:LEU:HD21	1.98	0.46
1:Z:17:A:C2	2:A:17:ILE:HD11	2.50	0.46
2:A:105:LYS:HD2	2:F:108:SER:CB	2.46	0.46
2:B:38:GLU:OE2	2:B:66:PHE:N	2.47	0.46
2:B:74:ASP:HA	2:B:77:ARG:CG	2.40	0.46
2:B:622:ILE:O	2:B:626:ILE:HG13	2.14	0.46
2:C:117:VAL:HG11	2:C:204:LEU:HD11	1.96	0.46
2:D:63:VAL:HG21	2:D:78:PHE:HD1	1.80	0.46
2:F:75:HIS:CE1	2:F:106:THR:HB	2.50	0.46
2:F:326:LEU:HD12	2:F:332:LEU:CD1	2.45	0.46
2:B:441:LEU:HD11	2:B:454:PHE:CD2	2.50	0.46
2:C:445:GLU:HA	2:C:449:THR:HG23	1.96	0.46
2:C:594:ARG:HA	2:C:597:LEU:HD13	1.97	0.46
2:C:622:ILE:O	2:C:626:ILE:HG12	2.15	0.46
2:D:570:ASN:CB	2:D:573:ILE:HG12	2.45	0.46
2:E:183:VAL:HG12	2:E:191:ARG:CD	2.46	0.46
2:F:311:LEU:O	2:F:315:MET:HG3	2.16	0.46
2:A:219:GLU:OE1	2:A:219:GLU:N	2.45	0.46
2:A:492:ARG:NE	2:A:517:GLU:OE1	2.41	0.46
2:A:521:TYR:CE1	2:A:584:LEU:HD13	2.50	0.46
2:B:357:PRO:HB3	2:B:369:VAL:HG12	1.97	0.46
2:B:571:ILE:HG23	2:B:576:ALA:O	2.16	0.46
2:C:34:VAL:CG2	2:C:60:ILE:HG13	2.46	0.46
2:C:244:LEU:HD22	2:C:586:ALA:CB	2.46	0.46
2:C:557:TYR:O	2:C:562:VAL:HG12	2.16	0.46
2:D:264:HIS:HB3	2:D:567:ASN:HB2	1.97	0.46
2:E:117:VAL:HG12	2:E:171:LEU:CD2	2.46	0.46
2:E:234:GLU:HG2	2:E:235:GLY:N	2.31	0.46
2:F:96:ARG:HB2	2:F:120:ALA:HA	1.96	0.46
2:F:104:PHE:H	2:F:107:MET:CE	2.29	0.46
2:F:132:CYS:SG	2:F:141:PRO:HA	2.55	0.46
2:F:144:THR:HB	2:F:146:GLU:CD	2.41	0.46
2:F:404:ARG:HG3	2:F:442:ALA:O	2.16	0.46
2:B:329:PRO:HB3	2:B:364:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:GLU:N	2:B:445:GLU:OE2	2.49	0.46
2:C:273:HIS:CD2	2:C:298:LEU:HD11	2.49	0.46
2:D:240:LEU:HD23	2:D:595:LEU:HB2	1.96	0.46
2:E:613:THR:O	2:E:617:THR:HG23	2.15	0.46
2:F:220:MET:HB2	2:F:223:GLU:OE2	2.16	0.46
2:F:482:TRP:CD1	2:F:505:LEU:HD21	2.51	0.46
2:F:566:VAL:H	2:F:600:LEU:HD21	1.80	0.46
2:C:168:TRP:HB2	2:C:171:LEU:HB3	1.97	0.46
2:C:316:LYS:HA	2:C:316:LYS:HE2	1.98	0.46
2:C:398:LEU:HD23	2:C:434:CYS:SG	2.55	0.46
2:C:427:HIS:HA	2:D:365:SER:OG	2.16	0.46
2:D:430:ASP:O	2:D:435:ARG:HD3	2.15	0.46
2:E:229:LEU:HD22	2:E:598:LEU:HD13	1.98	0.46
2:A:505:LEU:HA	2:A:505:LEU:HD23	1.61	0.46
2:B:128:ALA:HB3	2:B:140:MET:HE2	1.98	0.46
2:B:398:LEU:HD23	2:B:434:CYS:SG	2.55	0.46
2:B:568:THR:HG23	2:B:578:LEU:CD2	2.45	0.46
2:D:4:GLN:O	2:D:30:VAL:HG12	2.16	0.46
2:D:82:MET:HE2	2:D:111:MET:HE2	1.97	0.46
2:E:326:LEU:HB3	2:E:332:LEU:HD13	1.97	0.46
2:E:411:ARG:HB2	2:F:463:ARG:NE	2.29	0.46
1:Z:13:A:C5	2:F:13:THR:HG23	2.50	0.46
2:A:271:ALA:O	2:A:321:ASN:ND2	2.49	0.46
2:A:295:GLU:HB3	2:A:297:ARG:NH1	2.31	0.46
2:A:571:ILE:O	2:A:575:ALA:N	2.45	0.46
2:B:53:ALA:HB1	2:B:56:VAL:CG2	2.45	0.46
2:B:333:ARG:HG3	2:B:376:ALA:HB2	1.98	0.46
2:D:613:THR:O	2:D:617:THR:HG23	2.16	0.46
2:F:264:HIS:HB3	2:F:567:ASN:CB	2.46	0.46
2:F:350:TYR:HB2	2:F:618:LEU:HD21	1.98	0.46
2:A:218:TRP:O	2:A:221:LEU:HB2	2.16	0.46
2:A:414:ILE:O	2:A:418:LEU:HD23	2.17	0.46
2:A:497:LEU:HD11	2:A:523:ASN:ND2	2.31	0.46
2:B:11:LEU:HD23	2:B:42:VAL:HG12	1.98	0.46
2:B:72:GLU:HG2	2:C:161:ARG:O	2.16	0.46
2:B:149:LEU:HD22	2:B:152:ARG:NH2	2.30	0.46
2:B:214:ILE:CG1	2:B:231:THR:HG22	2.46	0.46
2:B:261:ILE:HD13	2:B:350:TYR:HB3	1.98	0.46
2:C:98:VAL:HG21	2:C:115:ALA:HB2	1.98	0.46
2:C:499:LEU:HD23	2:C:499:LEU:O	2.16	0.46
2:E:228:ASP:CB	2:E:623:SER:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:340:TYR:CE1	2:E:381:MET:HG3	2.50	0.46
2:F:104:PHE:H	2:F:107:MET:HE3	1.80	0.46
2:F:213:ARG:HD2	2:F:233:SER:HA	1.98	0.46
2:A:262:GLU:HB3	2:A:351:ALA:HB2	1.97	0.45
2:B:448:LYS:HD2	2:F:447:GLU:OE1	2.15	0.45
2:B:519:CYS:SG	2:B:569:ASP:HB2	2.56	0.45
2:C:100:LEU:HB2	2:C:108:SER:OG	2.15	0.45
2:D:64:ALA:HB3	2:D:194:GLN:CD	2.41	0.45
2:D:321:ASN:OD1	2:D:322:GLY:N	2.49	0.45
2:E:97:PHE:CD2	2:E:122:GLU:HB3	2.50	0.45
2:F:94:GLU:HG2	2:F:95:GLN:OE1	2.16	0.45
2:F:578:LEU:HD23	2:F:578:LEU:HA	1.83	0.45
2:A:258:LEU:O	2:A:260:LYS:NZ	2.47	0.45
2:B:7:LEU:HB2	2:B:29:PHE:CD2	2.51	0.45
2:B:343:LEU:HD22	2:B:348:VAL:HG21	1.98	0.45
2:C:262:GLU:C	2:C:263:LEU:HD12	2.40	0.45
2:D:10:SER:HB2	2:D:107:MET:CE	2.46	0.45
2:D:98:VAL:HG11	2:D:115:ALA:HB2	1.97	0.45
2:D:254:TRP:CD1	2:D:627:PRO:HG2	2.52	0.45
2:F:4:GLN:OE1	2:F:95:GLN:NE2	2.49	0.45
2:F:62:ARG:O	2:F:193:VAL:HG22	2.16	0.45
2:A:307:GLN:OE1	2:A:308:PRO:HD2	2.16	0.45
2:A:508:SER:O	2:A:512:ARG:HG3	2.16	0.45
2:B:69:LEU:CD1	2:C:160:ILE:HG21	2.44	0.45
2:B:104:PHE:H	2:B:107:MET:CE	2.30	0.45
2:B:261:ILE:CD1	2:B:350:TYR:HB3	2.46	0.45
2:C:233:SER:O	2:C:237:LEU:HD23	2.16	0.45
2:D:143:SER:O	2:D:144:THR:OG1	2.32	0.45
2:D:554:LEU:HD12	2:D:564:VAL:HG11	1.97	0.45
2:F:22:PHE:CE1	2:F:29:PHE:HB2	2.51	0.45
2:F:145:LEU:O	2:F:149:LEU:HD23	2.15	0.45
2:F:385:ARG:HD2	2:F:390:GLY:O	2.16	0.45
2:F:520:PRO:HB3	2:F:552:TYR:HE2	1.81	0.45
1:X:3:A:H5''	2:E:104:PHE:HD2	1.82	0.45
2:A:401:ILE:HA	2:A:440:ASP:HB3	1.97	0.45
2:B:260:LYS:HE2	2:B:579:THR:CG2	2.46	0.45
2:C:579:THR:O	2:C:583:LEU:HD23	2.15	0.45
2:E:354:ARG:HA	2:E:399:ILE:O	2.16	0.45
2:E:524:LEU:CD1	2:E:531:LEU:HD11	2.47	0.45
2:F:61:THR:OG1	2:F:85:TRP:NE1	2.50	0.45
2:F:135:PRO:HG2	2:F:136:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:255:VAL:HG13	2:F:582:LEU:HD12	1.97	0.45
2:F:258:LEU:HD12	2:F:259:PRO:CD	2.38	0.45
2:A:262:GLU:OE2	2:A:264:HIS:N	2.49	0.45
2:A:304:LEU:HD12	2:A:305:PRO:CD	2.47	0.45
2:A:524:LEU:HD13	2:A:529:PHE:HB2	1.99	0.45
2:B:481:ILE:HG22	2:B:505:LEU:HD21	1.99	0.45
2:C:559:ARG:HD3	2:C:559:ARG:HA	1.70	0.45
2:D:326:LEU:CD2	2:D:332:LEU:HA	2.46	0.45
2:E:240:LEU:CD2	2:E:595:LEU:HD13	2.47	0.45
2:E:555:LEU:O	2:E:559:ARG:HG2	2.17	0.45
2:F:168:TRP:O	2:F:172:ARG:HG3	2.16	0.45
2:B:170:GLN:NE2	2:C:215:ALA:O	2.49	0.45
2:C:17:ILE:HG12	2:C:101:THR:HG22	1.98	0.45
2:C:258:LEU:HD12	2:C:259:PRO:HD2	1.98	0.45
2:D:70:LYS:HA	2:D:70:LYS:HE2	1.97	0.45
2:E:557:TYR:O	2:E:562:VAL:HG12	2.17	0.45
2:A:53:ALA:HB1	2:A:56:VAL:CG2	2.45	0.45
2:A:264:HIS:HA	2:A:354:ARG:HH12	1.79	0.45
2:A:354:ARG:HB3	2:A:401:ILE:CD1	2.42	0.45
2:B:43:THR:O	2:B:46:ARG:HB3	2.17	0.45
2:B:310:PRO:HD2	2:B:313:GLU:HG2	1.98	0.45
2:D:118:LEU:HD13	2:D:171:LEU:HD13	1.98	0.45
2:D:322:GLY:O	2:D:326:LEU:HB2	2.17	0.45
2:E:145:LEU:O	2:E:149:LEU:HD23	2.17	0.45
2:E:228:ASP:HB2	2:E:623:SER:HB3	1.99	0.45
2:F:249:PRO:HA	2:F:252:GLN:OE1	2.17	0.45
2:A:310:PRO:HD2	2:A:313:GLU:HG2	1.99	0.45
2:B:69:LEU:HD12	2:B:69:LEU:O	2.17	0.45
2:D:53:ALA:HB1	2:D:56:VAL:CG2	2.46	0.45
2:F:170:GLN:NE2	2:F:207:LEU:HD21	2.32	0.45
2:A:24:LEU:HA	2:A:25:PRO:HD3	1.82	0.45
2:A:243:PRO:HB3	2:A:591:GLY:HA2	1.99	0.45
2:A:244:LEU:HD11	2:A:251:ASP:HB3	1.98	0.45
2:A:286:ASN:OD1	2:A:289:LYS:HE3	2.17	0.45
2:A:613:THR:O	2:A:617:THR:HG23	2.17	0.45
2:E:289:LYS:NZ	2:E:327:ARG:HB2	2.32	0.45
2:E:358:ALA:HB3	2:E:417:HIS:CE1	2.51	0.45
2:E:439:VAL:O	2:E:469:THR:HG22	2.17	0.45
2:F:244:LEU:HD12	2:F:244:LEU:H	1.80	0.45
2:F:459:THR:O	2:F:463:ARG:N	2.46	0.45
2:A:285:GLU:OE2	2:A:329:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:357:PRO:HB3	2:A:369:VAL:HG12	1.99	0.45
2:B:5:ALA:N	2:B:95:GLN:HB2	2.21	0.45
2:B:168:TRP:CZ3	2:C:212:SER:HA	2.52	0.45
2:C:377:PHE:CD2	2:C:398:LEU:HD21	2.52	0.45
2:D:445:GLU:OE1	2:D:445:GLU:N	2.50	0.45
2:D:476:ASP:OD2	2:D:477:ASP:N	2.49	0.45
2:E:16:ALA:HA	2:E:19:PRO:CG	2.47	0.45
2:F:271:ALA:HA	2:F:276:LEU:CD1	2.47	0.45
2:F:330:GLY:HA2	2:F:333:ARG:NH1	2.32	0.45
2:A:113:LYS:O	2:A:117:VAL:HG22	2.17	0.44
2:A:521:TYR:HE1	2:A:584:LEU:HD13	1.82	0.44
2:B:219:GLU:OE2	2:B:219:GLU:N	2.42	0.44
2:C:358:ALA:HA	2:C:366:PRO:HB3	1.99	0.44
2:D:60:ILE:HG23	2:D:190:GLU:HG2	1.99	0.44
2:D:69:LEU:CG	2:E:127:LEU:HD11	2.43	0.44
2:E:204:LEU:O	2:E:208:LEU:HD23	2.17	0.44
2:E:246:PRO:O	2:E:252:GLN:NE2	2.50	0.44
2:E:262:GLU:C	2:E:263:LEU:HD12	2.42	0.44
2:F:145:LEU:CD1	2:F:148:ILE:HD11	2.47	0.44
2:F:261:ILE:HG22	2:F:263:LEU:CD1	2.46	0.44
2:F:461:VAL:HG22	2:F:466:LEU:HB3	1.99	0.44
2:A:225:PRO:CG	2:A:598:LEU:HB3	2.47	0.44
2:A:531:LEU:HD23	2:A:532:ASP:N	2.32	0.44
2:B:414:ILE:O	2:B:418:LEU:HD23	2.18	0.44
2:C:275:GLU:O	2:C:279:ARG:HG3	2.17	0.44
2:C:467:ALA:HB1	2:C:609:PHE:CZ	2.52	0.44
2:D:117:VAL:HG11	2:D:204:LEU:CD1	2.47	0.44
2:D:410:TYR:O	2:D:414:ILE:HG13	2.17	0.44
2:D:568:THR:HG22	2:D:581:ASN:ND2	2.32	0.44
1:Y:11:A:OP2	2:C:102:GLY:HA2	2.17	0.44
2:A:516:VAL:HG12	2:A:518:LEU:HD13	1.99	0.44
2:B:4:GLN:O	2:B:30:VAL:HG22	2.17	0.44
2:B:58:LEU:HD21	2:B:60:ILE:CD1	2.47	0.44
2:B:499:LEU:HB3	2:B:557:TYR:OH	2.16	0.44
2:C:555:LEU:HG	2:C:589:CYS:HB3	1.99	0.44
2:D:167:GLY:O	2:D:172:ARG:NH2	2.49	0.44
2:D:214:ILE:HG13	2:D:231:THR:HG22	1.99	0.44
2:D:519:CYS:SG	2:D:569:ASP:HB2	2.58	0.44
2:F:478:ALA:HB1	2:F:505:LEU:HD13	1.99	0.44
2:A:49:PHE:CD2	2:A:58:LEU:HD22	2.52	0.44
2:A:84:ARG:HH12	2:A:195:ALA:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:84:ARG:HD2	2:A:179:PHE:C	2.43	0.44
2:A:84:ARG:HG2	2:A:181:LEU:HD12	2.00	0.44
2:B:7:LEU:HB2	2:B:29:PHE:CE2	2.52	0.44
2:B:8:PHE:CE2	2:B:96:ARG:HG3	2.53	0.44
2:B:240:LEU:HD21	2:B:595:LEU:HB2	1.99	0.44
2:B:474:GLU:O	2:B:527:LYS:NZ	2.29	0.44
2:B:557:TYR:O	2:B:562:VAL:HG12	2.18	0.44
2:C:481:ILE:HG23	2:C:493:LEU:HD13	1.98	0.44
2:E:171:LEU:HD23	2:E:171:LEU:O	2.17	0.44
2:E:302:TRP:HB3	2:E:303:PRO:HD3	1.99	0.44
2:F:262:GLU:C	2:F:263:LEU:HD12	2.42	0.44
2:F:378:GLN:NE2	2:F:433:ALA:HB1	2.33	0.44
2:F:518:LEU:HD23	2:F:552:TYR:CE1	2.52	0.44
2:A:240:LEU:O	2:A:240:LEU:HD23	2.17	0.44
2:A:314:TYR:HE1	2:A:525:GLN:HB2	1.83	0.44
2:B:90:ARG:CZ	2:B:176:PRO:HG2	2.47	0.44
2:C:49:PHE:CE1	2:C:56:VAL:HG11	2.52	0.44
2:C:170:GLN:OE1	2:C:170:GLN:N	2.32	0.44
2:C:404:ARG:HG2	2:C:442:ALA:O	2.18	0.44
2:D:7:LEU:HD13	2:D:29:PHE:CE2	2.52	0.44
2:D:555:LEU:HD21	2:D:592:LEU:HD13	1.99	0.44
2:E:249:PRO:HB2	2:E:253:ARG:HH12	1.81	0.44
2:E:557:TYR:CB	2:E:564:VAL:HG21	2.41	0.44
2:F:505:LEU:O	2:F:509:VAL:HG23	2.17	0.44
2:A:427:HIS:HA	2:B:365:SER:HB2	2.00	0.44
2:A:488:LEU:HA	2:A:488:LEU:HD23	1.86	0.44
2:A:503:ARG:NE	2:A:503:ARG:HA	2.33	0.44
2:B:412:ALA:O	2:B:416:ARG:HG3	2.18	0.44
2:C:260:LYS:HA	2:C:601:GLN:HE22	1.81	0.44
2:D:187:LYS:HD2	2:D:188:GLY:O	2.16	0.44
2:D:518:LEU:O	2:D:566:VAL:HA	2.18	0.44
2:E:463:ARG:HD2	2:F:411:ARG:HB2	2.00	0.44
2:A:92:GLY:N	2:A:95:GLN:HE22	2.13	0.44
2:A:404:ARG:HA	2:A:410:TYR:CD2	2.53	0.44
2:B:450:ARG:HD2	2:B:452:HIS:CE1	2.53	0.44
2:C:173:ARG:C	2:C:174:ILE:HD12	2.43	0.44
2:D:99:CYS:HA	2:D:124:PHE:O	2.18	0.44
2:D:144:THR:O	2:D:147:GLU:N	2.50	0.44
2:E:104:PHE:O	2:E:107:MET:HB2	2.18	0.44
2:F:300:GLU:OE2	2:F:306:ALA:HB3	2.18	0.44
2:A:7:LEU:HD12	2:A:8:PHE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:ARG:HH11	2:A:50:ARG:C	2.26	0.44
2:C:42:VAL:HG23	2:C:46:ARG:HH21	1.83	0.44
2:C:381:MET:CE	2:C:396:VAL:H	2.31	0.44
2:D:127:LEU:HB2	2:D:158:HIS:HB2	1.99	0.44
2:E:260:LYS:HE2	2:E:579:THR:CG2	2.48	0.44
2:E:261:ILE:HG22	2:E:263:LEU:CD1	2.47	0.44
2:B:120:ALA:H	2:B:165:GLU:HB2	1.82	0.44
2:B:146:GLU:OE1	2:B:146:GLU:N	2.43	0.44
2:C:22:PHE:CD1	2:C:32:VAL:HG21	2.53	0.44
2:C:377:PHE:HD2	2:C:398:LEU:HD21	1.83	0.44
2:D:117:VAL:O	2:D:171:LEU:HD11	2.17	0.44
2:D:171:LEU:CA	2:D:174:ILE:HD11	2.48	0.44
2:D:429:ARG:HH11	2:D:429:ARG:HB2	1.83	0.44
2:D:552:TYR:CD2	2:D:554:LEU:HB2	2.53	0.44
2:E:37:THR:HG23	2:E:66:PHE:CD2	2.53	0.44
2:E:316:LYS:HE2	2:E:316:LYS:HA	1.99	0.44
2:E:404:ARG:HG2	2:E:442:ALA:O	2.18	0.44
2:E:615:ARG:HE	2:E:615:ARG:HB2	1.59	0.44
2:F:114:ALA:HA	2:F:117:VAL:CG1	2.48	0.44
2:F:325:LEU:O	2:F:325:LEU:HD23	2.17	0.44
2:F:578:LEU:O	2:F:582:LEU:HG	2.18	0.44
2:F:602:ARG:HH21	2:F:619:LEU:HD11	1.83	0.44
2:A:7:LEU:CG	2:A:32:VAL:HG13	2.48	0.43
2:A:233:SER:OG	2:A:234:GLU:OE2	2.35	0.43
2:A:262:GLU:O	2:A:351:ALA:HA	2.18	0.43
2:A:503:ARG:HH21	2:A:506:LEU:HD22	1.83	0.43
2:A:520:PRO:HG3	2:A:581:ASN:O	2.17	0.43
2:B:78:PHE:HA	2:B:81:VAL:HG12	1.99	0.43
2:B:355:CYS:SG	2:B:398:LEU:HD12	2.58	0.43
2:C:332:LEU:HD11	2:C:373:ILE:HG12	2.00	0.43
2:D:60:ILE:HG22	2:D:189:ASP:O	2.18	0.43
2:E:58:LEU:HD21	2:E:60:ILE:HD11	2.00	0.43
2:E:364:ARG:NH2	2:E:372:ASP:OD1	2.48	0.43
2:E:618:LEU:HA	2:E:621:ARG:HG2	2.00	0.43
2:A:497:LEU:HD21	2:A:523:ASN:ND2	2.33	0.43
2:A:563:ARG:NH1	2:A:606:GLU:HG2	2.33	0.43
2:B:226:PHE:CE2	2:B:598:LEU:HD12	2.53	0.43
2:B:461:VAL:CG2	2:B:466:LEU:HB3	2.47	0.43
2:C:410:TYR:O	2:C:414:ILE:HG12	2.18	0.43
2:D:281:ARG:HA	2:D:281:ARG:HD2	1.75	0.43
2:D:503:ARG:NH2	2:D:506:LEU:HD23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:ILE:HD12	2:E:313:GLU:OE2	2.18	0.43
2:F:36:THR:O	2:F:62:ARG:HD3	2.17	0.43
2:F:137:GLY:C	2:F:138:ARG:HD3	2.42	0.43
2:F:166:ARG:HG3	2:F:172:ARG:HH21	1.82	0.43
2:F:199:ALA:O	2:F:202:THR:HG22	2.17	0.43
2:F:269:GLY:HA3	2:F:570:ASN:ND2	2.32	0.43
2:A:322:GLY:H	2:A:326:LEU:HD23	1.83	0.43
2:B:404:ARG:N	2:B:442:ALA:O	2.50	0.43
2:C:91:THR:CG2	2:C:95:GLN:HB2	2.48	0.43
2:C:277:LEU:O	2:C:280:VAL:HG12	2.19	0.43
2:D:19:PRO:HG3	2:D:48:PHE:CD2	2.53	0.43
2:D:92:GLY:H	2:D:95:GLN:NE2	2.16	0.43
2:D:97:PHE:HE2	2:D:121:ALA:HB3	1.83	0.43
2:D:185:GLU:OE2	2:D:192:ARG:HD3	2.17	0.43
2:D:364:ARG:HH22	2:D:372:ASP:HB2	1.82	0.43
2:E:51:ARG:HG2	2:E:52:HIS:CD2	2.53	0.43
2:F:91:THR:HG23	2:F:96:ARG:HH21	1.81	0.43
2:F:236:GLU:O	2:F:239:TRP:HB3	2.17	0.43
2:F:264:HIS:CD2	2:F:569:ASP:HA	2.50	0.43
2:A:38:GLU:HA	2:A:62:ARG:HH21	1.83	0.43
2:A:212:SER:HA	2:F:168:TRP:CZ3	2.53	0.43
2:B:262:GLU:OE2	2:B:578:LEU:HD21	2.18	0.43
2:C:100:LEU:HD22	2:C:112:GLN:HB2	1.98	0.43
2:C:568:THR:HG23	2:C:578:LEU:CD1	2.44	0.43
2:D:310:PRO:HG2	2:D:313:GLU:HG3	1.99	0.43
2:E:77:ARG:HG2	2:E:198:ARG:NH2	2.33	0.43
2:E:411:ARG:HA	2:E:414:ILE:HD12	2.01	0.43
2:F:117:VAL:CG2	2:F:204:LEU:HD11	2.35	0.43
2:F:323:THR:HG22	2:F:359:ASN:HB3	2.01	0.43
2:F:340:TYR:O	2:F:344:VAL:HG23	2.17	0.43
1:Y:8:A:C4	2:B:140:MET:HE1	2.53	0.43
2:D:264:HIS:HD2	2:D:569:ASP:HA	1.82	0.43
2:E:125:HIS:HB3	2:E:160:ILE:HG23	2.00	0.43
2:F:280:VAL:HA	2:F:334:GLU:OE1	2.18	0.43
2:F:452:HIS:HB3	2:F:483:ARG:CG	2.49	0.43
1:Y:10:A:H1'	2:C:103:GLY:CA	2.37	0.43
2:A:520:PRO:HB2	2:A:584:LEU:HD22	1.99	0.43
2:B:613:THR:O	2:B:617:THR:HG23	2.18	0.43
2:C:214:ILE:HG13	2:C:231:THR:HG22	2.00	0.43
2:C:262:GLU:O	2:C:351:ALA:HA	2.19	0.43
2:C:395:HIS:CD2	2:C:614:GLN:HE22	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:418:LEU:O	2:C:422:VAL:HG23	2.19	0.43
2:D:182:GLN:OE1	2:D:196:GLU:HG3	2.19	0.43
2:D:233:SER:O	2:D:237:LEU:HD13	2.19	0.43
2:D:387:ALA:HB1	2:D:388:PRO:HD2	2.00	0.43
2:D:620:ARG:NH2	2:E:223:GLU:OE1	2.52	0.43
2:E:4:GLN:O	2:E:30:VAL:HG12	2.19	0.43
2:E:311:LEU:HD13	2:E:526:ILE:HD13	2.00	0.43
2:E:325:LEU:HG	2:E:331:CYS:SG	2.59	0.43
2:E:494:GLY:HA2	2:E:517:GLU:HG2	2.00	0.43
2:F:150:TRP:O	2:F:153:ASP:HB2	2.19	0.43
2:F:507:ARG:HH22	2:F:560:GLU:HG3	1.84	0.43
2:A:84:ARG:HE	2:A:181:LEU:HA	1.83	0.43
2:A:272:THR:HG21	2:A:318:GLY:HA2	1.99	0.43
2:A:451:ALA:HB1	2:A:488:LEU:CD1	2.49	0.43
2:C:566:VAL:HG11	2:C:582:LEU:HD23	2.00	0.43
2:D:99:CYS:HB2	2:D:124:PHE:CE2	2.53	0.43
2:D:145:LEU:O	2:D:148:ILE:HG22	2.19	0.43
2:D:271:ALA:HB3	2:D:321:ASN:ND2	2.33	0.43
2:D:422:VAL:HG13	2:D:464:CYS:SG	2.58	0.43
2:E:81:VAL:HG21	2:E:193:VAL:HG23	2.00	0.43
2:E:441:LEU:HD11	2:E:454:PHE:CE2	2.54	0.43
2:F:154:GLN:HG3	2:F:156:HIS:CE1	2.53	0.43
2:F:169:PRO:HG2	2:F:170:GLN:OE1	2.18	0.43
2:F:354:ARG:HA	2:F:399:ILE:O	2.18	0.43
1:X:1:A:C5	2:D:13:THR:HG23	2.53	0.43
2:A:69:LEU:HA	2:A:74:ASP:OD2	2.19	0.43
2:A:211:ALA:HA	2:A:214:ILE:HG22	2.00	0.43
2:A:249:PRO:HB2	2:A:253:ARG:HH12	1.84	0.43
2:A:278:ARG:HH12	2:A:293:LEU:HD11	1.82	0.43
2:B:144:THR:HB	2:B:146:GLU:OE2	2.18	0.43
2:C:281:ARG:HE	2:C:290:LEU:HD21	1.84	0.43
2:F:210:ARG:O	2:F:214:ILE:HG12	2.19	0.43
2:F:478:ALA:HB1	2:F:505:LEU:CD1	2.49	0.43
2:A:593:THR:O	2:A:596:ASP:HB2	2.19	0.43
2:B:62:ARG:O	2:B:192:ARG:HA	2.19	0.43
2:D:33:HIS:HB3	2:D:85:TRP:CH2	2.53	0.43
2:E:93:PRO:HA	2:E:96:ARG:NH2	2.34	0.43
2:E:270:PHE:HD1	2:E:571:ILE:HD12	1.83	0.43
2:E:612:ALA:O	2:E:616:LEU:HD23	2.19	0.43
2:F:460:ALA:HA	2:F:463:ARG:HB3	2.01	0.43
2:A:354:ARG:CZ	2:A:399:ILE:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:424:ALA:HB1	2:A:436:VAL:HG21	2.01	0.43
2:B:7:LEU:HD13	2:B:29:PHE:CE2	2.43	0.43
2:B:125:HIS:HE1	2:C:106:THR:HG22	1.83	0.43
2:C:255:VAL:HG11	2:C:583:LEU:CD2	2.49	0.43
2:C:355:CYS:SG	2:C:398:LEU:HD12	2.59	0.43
2:D:14:ALA:O	2:D:17:ILE:HG12	2.19	0.43
2:D:113:LYS:HA	2:D:116:THR:HG22	2.00	0.43
2:D:184:VAL:HG22	2:D:192:ARG:O	2.18	0.43
2:D:517:GLU:HB3	2:D:567:ASN:ND2	2.34	0.43
2:E:51:ARG:NH2	2:E:145:LEU:HD22	2.33	0.43
2:E:73:GLU:O	2:E:77:ARG:HG3	2.19	0.43
2:F:7:LEU:HD13	2:F:29:PHE:CE2	2.52	0.43
2:F:248:ALA:HB3	2:F:251:ASP:HB2	2.00	0.43
2:F:422:VAL:HG13	2:F:464:CYS:SG	2.59	0.43
2:F:557:TYR:HB3	2:F:564:VAL:HG11	1.99	0.43
2:A:220:MET:O	2:A:223:GLU:HG3	2.18	0.42
2:A:340:TYR:O	2:A:344:VAL:HG23	2.19	0.42
2:C:518:LEU:O	2:C:566:VAL:HA	2.19	0.42
2:D:107:MET:HE2	2:D:107:MET:HB3	1.81	0.42
2:D:429:ARG:HB2	2:D:429:ARG:NH1	2.33	0.42
2:E:7:LEU:CB	2:E:32:VAL:HG22	2.45	0.42
2:E:261:ILE:HD11	2:E:622:ILE:CD1	2.48	0.42
2:A:416:ARG:CD	2:B:426:GLU:HG3	2.47	0.42
2:B:170:GLN:NE2	2:C:216:GLY:HA2	2.33	0.42
2:B:270:PHE:HE2	2:B:338:LEU:HB3	1.83	0.42
2:D:499:LEU:HB3	2:D:557:TYR:OH	2.18	0.42
2:E:80:GLU:HG3	2:E:198:ARG:HD3	2.01	0.42
2:E:82:MET:CE	2:E:110:ALA:HB1	2.49	0.42
2:E:450:ARG:HH22	2:E:476:ASP:HB2	1.83	0.42
2:F:100:LEU:HD23	2:F:124:PHE:O	2.19	0.42
2:F:258:LEU:HG	2:F:259:PRO:O	2.19	0.42
2:F:579:THR:O	2:F:583:LEU:HG	2.19	0.42
2:A:478:ALA:HB1	2:A:505:LEU:CD1	2.43	0.42
2:B:92:GLY:H	2:B:95:GLN:NE2	2.17	0.42
2:D:146:GLU:OE2	2:D:146:GLU:N	2.43	0.42
2:D:303:PRO:C	2:D:304:LEU:HD22	2.44	0.42
2:E:303:PRO:C	2:E:304:LEU:HD22	2.44	0.42
2:F:317:LEU:HD23	2:F:573:ILE:CG1	2.50	0.42
2:F:350:TYR:CD1	2:F:618:LEU:HD21	2.54	0.42
2:F:524:LEU:HD11	2:F:531:LEU:HD11	2.02	0.42
2:A:441:LEU:HD21	2:A:458:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:566:VAL:CG1	2:A:582:LEU:HD23	2.44	0.42
2:B:160:ILE:CD1	2:C:69:LEU:HD21	2.49	0.42
2:C:7:LEU:HB3	2:C:32:VAL:HG13	2.01	0.42
2:C:44:LEU:HD22	2:C:143:SER:OG	2.18	0.42
2:E:132:CYS:SG	2:E:142:PRO:HD3	2.59	0.42
2:E:404:ARG:HG3	2:E:444:TYR:O	2.19	0.42
1:X:3:A:H5"	2:E:104:PHE:CD2	2.55	0.42
2:A:100:LEU:HA	2:A:111:MET:SD	2.59	0.42
2:A:130:ASP:OD1	2:A:140:MET:N	2.53	0.42
2:A:269:GLY:HA3	2:A:570:ASN:HA	2.01	0.42
2:A:276:LEU:H	2:A:276:LEU:HG	1.54	0.42
2:A:304:LEU:CD2	2:A:531:LEU:HD12	2.50	0.42
2:B:557:TYR:HB3	2:B:564:VAL:CG2	2.45	0.42
2:B:603:HIS:O	2:B:607:THR:HG22	2.19	0.42
2:C:3:VAL:CG1	2:C:95:GLN:HG2	2.49	0.42
2:C:74:ASP:HA	2:C:77:ARG:CD	2.49	0.42
2:C:281:ARG:HD2	2:C:325:LEU:HD13	2.01	0.42
2:D:260:LYS:HE3	2:D:582:LEU:HD12	2.01	0.42
2:D:310:PRO:HG2	2:D:313:GLU:HG2	2.01	0.42
2:D:520:PRO:HB2	2:D:584:LEU:HD22	2.01	0.42
2:D:555:LEU:HD23	2:D:589:CYS:CB	2.50	0.42
2:E:357:PRO:O	2:E:369:VAL:HG11	2.20	0.42
2:A:15:PRO:CB	2:A:44:LEU:HD11	2.50	0.42
2:A:44:LEU:HD12	2:A:45:ILE:HD13	2.02	0.42
2:A:49:PHE:CE2	2:A:58:LEU:HD22	2.54	0.42
2:B:69:LEU:HD11	2:C:127:LEU:HD11	2.02	0.42
2:B:174:ILE:HG23	2:B:174:ILE:HD12	1.78	0.42
2:B:387:ALA:HB1	2:B:388:PRO:HD2	2.02	0.42
2:C:321:ASN:OD1	2:C:322:GLY:N	2.52	0.42
2:D:39:ARG:HD3	2:D:67:GLN:O	2.20	0.42
2:D:78:PHE:HZ	2:D:107:MET:HE3	1.85	0.42
2:E:145:LEU:O	2:E:148:ILE:HG22	2.20	0.42
2:E:162:LEU:HD23	2:E:162:LEU:H	1.83	0.42
2:E:332:LEU:HD21	2:E:373:ILE:HD11	2.02	0.42
2:F:77:ARG:O	2:F:81:VAL:HG22	2.20	0.42
2:F:169:PRO:HA	2:F:172:ARG:NH1	2.34	0.42
2:F:354:ARG:NE	2:F:440:ASP:OD1	2.50	0.42
2:A:138:ARG:HA	2:A:138:ARG:NE	2.35	0.42
2:A:264:HIS:HB3	2:A:567:ASN:HD22	1.85	0.42
2:A:298:LEU:HG	2:A:302:TRP:HE1	1.85	0.42
2:A:496:ALA:O	2:A:557:TYR:OH	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:CYS:SG	2:B:373:ILE:HG23	2.59	0.42
2:B:506:LEU:HD21	2:B:560:GLU:CB	2.46	0.42
2:B:557:TYR:CB	2:B:564:VAL:HG21	2.45	0.42
2:B:562:VAL:HG13	2:B:564:VAL:CG2	2.50	0.42
2:C:213:ARG:NE	2:C:233:SER:HB3	2.34	0.42
2:D:456:GLU:O	2:D:459:THR:HG22	2.20	0.42
2:F:278:ARG:NH2	2:F:293:LEU:HD21	2.35	0.42
2:F:582:LEU:HD13	2:F:597:LEU:HD11	2.01	0.42
2:A:351:ALA:O	2:A:396:VAL:HA	2.20	0.42
2:B:284:ALA:HB2	2:B:331:CYS:SG	2.60	0.42
2:B:354:ARG:CB	2:B:401:ILE:HD11	2.44	0.42
2:B:505:LEU:O	2:B:509:VAL:HG23	2.20	0.42
2:C:13:THR:O	2:C:15:PRO:HD3	2.19	0.42
2:C:281:ARG:HD2	2:C:325:LEU:CD1	2.50	0.42
2:C:445:GLU:OE2	2:C:474:GLU:HB3	2.19	0.42
2:D:9:VAL:O	2:D:34:VAL:HA	2.20	0.42
2:D:81:VAL:CG2	2:D:193:VAL:HG13	2.50	0.42
2:D:106:THR:HG23	2:E:125:HIS:ND1	2.34	0.42
2:D:385:ARG:NH1	2:D:390:GLY:O	2.50	0.42
2:D:570:ASN:HB2	2:D:573:ILE:HG12	2.01	0.42
2:E:113:LYS:O	2:E:116:THR:HG22	2.19	0.42
2:F:62:ARG:HD3	2:F:62:ARG:HA	1.80	0.42
2:F:354:ARG:HD3	2:F:401:ILE:CD1	2.46	0.42
2:F:614:GLN:O	2:F:618:LEU:HD13	2.20	0.42
2:A:100:LEU:HD21	2:A:125:HIS:HB2	2.02	0.42
2:A:491:ARG:HD2	2:A:609:PHE:CE1	2.42	0.42
2:A:526:ILE:HD12	2:A:527:LYS:HZ1	1.84	0.42
2:B:124:PHE:HB2	2:B:160:ILE:O	2.20	0.42
2:B:354:ARG:HB3	2:B:401:ILE:CD1	2.46	0.42
2:B:402:ALA:HB1	2:B:414:ILE:CG1	2.37	0.42
2:B:450:ARG:HD3	2:B:480:GLY:HA2	2.00	0.42
2:C:354:ARG:CB	2:C:401:ILE:HD11	2.46	0.42
2:C:470:VAL:CG1	2:C:488:LEU:HD23	2.48	0.42
2:D:229:LEU:HD11	2:D:598:LEU:CD1	2.50	0.42
2:F:281:ARG:CZ	2:F:293:LEU:HB2	2.50	0.42
2:F:387:ALA:HB1	2:F:388:PRO:HD2	2.02	0.42
1:Y:12:A:N6	2:C:129:ASP:OD1	2.53	0.42
2:A:377:PHE:CD1	2:A:396:VAL:HG11	2.55	0.42
2:A:447:GLU:HG2	2:A:450:ARG:HH11	1.84	0.42
2:B:145:LEU:HA	2:B:148:ILE:HD12	2.02	0.42
2:B:316:LYS:HE3	2:B:316:LYS:HB3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:HIS:HB3	2:B:483:ARG:HD2	2.01	0.42
2:D:105:LYS:HB3	2:E:125:HIS:HE1	1.82	0.42
2:D:307:GLN:CD	2:D:308:PRO:HD2	2.44	0.42
2:D:362:GLU:HG2	2:D:363:VAL:N	2.35	0.42
2:D:400:LEU:HD12	2:D:421:ALA:CA	2.50	0.42
2:D:482:TRP:HB2	2:D:505:LEU:CD1	2.50	0.42
2:E:126:VAL:HG12	2:E:159:TRP:CD1	2.55	0.42
2:F:19:PRO:HD3	2:F:45:ILE:CD1	2.49	0.42
2:F:91:THR:OG1	2:F:92:GLY:N	2.49	0.42
2:F:558:LEU:HD23	2:F:558:LEU:HA	1.87	0.42
2:A:76:PHE:HB3	2:A:198:ARG:CD	2.50	0.41
2:A:80:GLU:HG2	2:A:198:ARG:HA	2.02	0.41
2:A:116:THR:HA	2:A:165:GLU:OE1	2.20	0.41
2:A:276:LEU:HD12	2:A:277:LEU:H	1.85	0.41
2:A:322:GLY:O	2:A:326:LEU:HB2	2.20	0.41
2:A:441:LEU:HD11	2:A:458:PHE:CE1	2.54	0.41
2:A:499:LEU:O	2:A:499:LEU:HD23	2.20	0.41
2:B:503:ARG:O	2:B:507:ARG:HG2	2.20	0.41
2:C:277:LEU:HB3	2:C:278:ARG:HH11	1.84	0.41
2:C:280:VAL:HG13	2:C:325:LEU:HD21	2.02	0.41
2:C:412:ALA:HA	2:D:463:ARG:HB3	2.02	0.41
2:D:258:LEU:HD12	2:D:259:PRO:CD	2.49	0.41
2:E:99:CYS:HB2	2:E:124:PHE:CE2	2.55	0.41
2:E:325:LEU:HD12	2:E:325:LEU:O	2.20	0.41
2:F:298:LEU:HD23	2:F:298:LEU:H	1.85	0.41
2:F:520:PRO:HD3	2:F:566:VAL:HG23	2.02	0.41
2:F:530:ARG:H	2:F:530:ARG:HD3	1.85	0.41
2:B:44:LEU:CD2	2:B:145:LEU:HD21	2.50	0.41
2:B:100:LEU:HG	2:B:125:HIS:HB3	2.00	0.41
2:B:172:ARG:C	2:B:173:ARG:HD3	2.45	0.41
2:B:225:PRO:HD3	2:B:595:LEU:HD11	2.01	0.41
2:C:74:ASP:OD1	2:C:75:HIS:N	2.53	0.41
2:C:145:LEU:HA	2:C:148:ILE:HG22	2.01	0.41
2:C:266:HIS:HB2	2:C:570:ASN:OD1	2.21	0.41
2:C:485:VAL:CG2	2:C:493:LEU:HD11	2.50	0.41
2:D:76:PHE:HB3	2:D:198:ARG:HH12	1.85	0.41
2:D:87:LEU:HD11	2:D:200:PHE:CD2	2.55	0.41
2:D:262:GLU:O	2:D:351:ALA:HA	2.20	0.41
2:E:71:SER:OG	2:E:72:GLU:OE1	2.29	0.41
2:E:174:ILE:HD12	2:E:174:ILE:HG23	1.79	0.41
2:F:462:HIS:NE2	2:F:488:LEU:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:367:TRP:HE3	2:A:420:LEU:HD12	1.86	0.41
2:A:402:ALA:HB1	2:A:414:ILE:HG23	2.02	0.41
2:A:404:ARG:HH21	2:A:445:GLU:HG3	1.86	0.41
2:B:321:ASN:OD1	2:B:322:GLY:N	2.53	0.41
2:B:555:LEU:HG	2:B:589:CYS:HB3	2.02	0.41
2:D:45:ILE:HD11	2:D:49:PHE:CE1	2.55	0.41
2:E:20:GLU:HG3	2:E:157:LEU:HD11	2.02	0.41
2:E:271:ALA:O	2:E:321:ASN:ND2	2.53	0.41
2:F:84:ARG:CZ	2:F:179:PHE:HB3	2.49	0.41
2:F:397:ASN:HD22	2:F:437:VAL:HG11	1.85	0.41
2:F:445:GLU:HA	2:F:449:THR:CG2	2.50	0.41
2:A:17:ILE:O	2:A:20:GLU:HG2	2.20	0.41
2:A:416:ARG:HD3	2:B:426:GLU:CG	2.47	0.41
2:A:500:GLY:O	2:A:503:ARG:NH1	2.47	0.41
2:A:622:ILE:O	2:A:626:ILE:HG12	2.19	0.41
2:D:92:GLY:HA2	2:D:173:ARG:HH12	1.85	0.41
2:D:557:TYR:CB	2:D:564:VAL:HG21	2.44	0.41
2:E:103:GLY:HA3	2:E:107:MET:SD	2.61	0.41
2:E:411:ARG:C	2:F:463:ARG:HD3	2.45	0.41
2:F:117:VAL:HG22	2:F:171:LEU:CD2	2.50	0.41
2:F:272:THR:C	2:F:277:LEU:HD21	2.45	0.41
2:F:355:CYS:SG	2:F:398:LEU:HD12	2.61	0.41
2:B:67:GLN:HG2	2:B:68:ASP:N	2.34	0.41
2:B:447:GLU:OE2	2:D:448:LYS:HE3	2.20	0.41
2:D:531:LEU:HD23	2:D:587:ARG:NH2	2.35	0.41
2:F:466:LEU:HD12	2:F:466:LEU:HA	1.89	0.41
1:Z:15:A:C8	2:F:127:LEU:HD12	2.56	0.41
2:A:181:LEU:HD23	2:A:193:VAL:HB	2.02	0.41
2:A:284:ALA:HB1	2:A:328:ASP:OD1	2.21	0.41
2:A:285:GLU:OE1	2:A:329:PRO:HD2	2.21	0.41
2:A:493:LEU:HD23	2:A:514:ILE:HG21	2.02	0.41
2:D:76:PHE:HB3	2:D:198:ARG:NH1	2.34	0.41
2:D:92:GLY:HA2	2:D:173:ARG:HH22	1.85	0.41
2:D:481:ILE:O	2:D:485:VAL:HG23	2.21	0.41
2:E:290:LEU:CD1	2:E:291:PRO:HD2	2.41	0.41
2:E:326:LEU:HD22	2:E:332:LEU:HD12	2.02	0.41
2:E:448:LYS:HD2	2:E:449:THR:OG1	2.21	0.41
2:F:38:GLU:HA	2:F:62:ARG:NH1	2.36	0.41
2:F:39:ARG:NH1	2:F:67:GLN:HA	2.35	0.41
2:F:104:PHE:CD2	2:F:107:MET:HE2	2.54	0.41
2:F:299:PRO:HG2	2:F:302:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:358:ALA:HB3	2:F:417:HIS:NE2	2.36	0.41
2:A:90:ARG:NH2	2:A:176:PRO:HD3	2.36	0.41
2:A:192:ARG:CZ	2:A:192:ARG:HB2	2.50	0.41
2:A:337:ARG:HG3	2:A:380:CYS:SG	2.60	0.41
2:B:206:ASP:HA	2:B:209:GLN:HB3	2.02	0.41
2:B:309:ILE:HD12	2:B:313:GLU:OE2	2.19	0.41
2:B:531:LEU:HD13	2:B:588:LEU:HD23	2.01	0.41
2:B:552:TYR:CD2	2:B:554:LEU:HB2	2.55	0.41
2:C:93:PRO:O	2:C:121:ALA:HB2	2.20	0.41
2:C:564:VAL:HG13	2:C:600:LEU:HD23	2.03	0.41
2:C:593:THR:O	2:C:596:ASP:HB2	2.20	0.41
2:D:354:ARG:CB	2:D:401:ILE:HD11	2.49	0.41
2:E:476:ASP:N	2:E:476:ASP:OD2	2.52	0.41
2:F:22:PHE:HE1	2:F:29:PHE:HB2	1.85	0.41
2:F:270:PHE:HB3	2:F:335:GLN:NE2	2.36	0.41
2:A:456:GLU:CG	2:B:456:GLU:HA	2.49	0.41
2:B:584:LEU:HD12	2:B:587:ARG:HB2	2.01	0.41
2:C:38:GLU:HA	2:C:62:ARG:NH2	2.35	0.41
2:C:39:ARG:HH22	2:C:67:GLN:HB3	1.85	0.41
2:C:98:VAL:O	2:C:123:VAL:HA	2.20	0.41
2:C:614:GLN:HG3	2:C:618:LEU:HD13	2.01	0.41
2:D:378:GLN:NE2	2:D:378:GLN:HA	2.36	0.41
2:F:24:LEU:HD12	2:F:25:PRO:HD2	2.02	0.41
2:F:140:MET:CG	2:F:141:PRO:HD2	2.48	0.41
2:F:210:ARG:NH1	2:F:231:THR:HG21	2.35	0.41
2:F:331:CYS:O	2:F:334:GLU:HG3	2.20	0.41
2:F:385:ARG:HA	2:F:385:ARG:HD3	1.75	0.41
2:A:83:PHE:O	2:A:87:LEU:HD23	2.20	0.41
2:A:236:GLU:HA	2:A:239:TRP:HB3	2.02	0.41
2:A:362:GLU:HG2	2:A:363:VAL:N	2.36	0.41
2:B:72:GLU:N	2:B:72:GLU:OE1	2.53	0.41
2:B:122:GLU:HG3	2:B:124:PHE:CD1	2.56	0.41
2:B:300:GLU:O	2:B:300:GLU:HG2	2.21	0.41
2:B:343:LEU:HD23	2:B:343:LEU:HA	1.81	0.41
2:B:404:ARG:HD2	2:B:441:LEU:HD11	2.02	0.41
2:C:23:LEU:HD12	2:C:152:ARG:CZ	2.50	0.41
2:C:62:ARG:HD2	2:C:190:GLU:OE2	2.21	0.41
2:C:156:HIS:C	2:C:157:LEU:HD12	2.45	0.41
2:C:260:LYS:HE3	2:C:579:THR:HG23	2.03	0.41
2:C:481:ILE:O	2:C:485:VAL:HG23	2.21	0.41
2:D:97:PHE:CE2	2:D:121:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:232:TRP:O	2:D:233:SER:OG	2.33	0.41
2:D:309:ILE:HG12	2:D:525:GLN:O	2.20	0.41
2:D:605:LEU:HD11	2:D:618:LEU:HB2	2.03	0.41
2:E:49:PHE:CD1	2:E:56:VAL:HG21	2.55	0.41
2:E:73:GLU:OE1	2:E:73:GLU:N	2.45	0.41
2:E:87:LEU:HD11	2:E:200:PHE:CE1	2.55	0.41
2:E:223:GLU:OE1	2:E:223:GLU:N	2.54	0.41
2:E:427:HIS:HA	2:F:365:SER:CB	2.51	0.41
2:F:124:PHE:HB2	2:F:160:ILE:O	2.21	0.41
2:F:195:ALA:HB3	2:F:198:ARG:HH21	1.85	0.41
2:F:255:VAL:HG12	2:F:579:THR:HG22	2.02	0.41
2:F:362:GLU:N	2:F:362:GLU:OE1	2.54	0.41
2:F:530:ARG:HH22	2:F:551:PRO:CB	2.34	0.41
2:A:341:ARG:HH12	2:A:344:VAL:HG21	1.86	0.41
2:A:403:THR:HG23	2:A:443:GLY:CA	2.51	0.41
2:A:474:GLU:HG3	2:A:495:HIS:CB	2.51	0.41
2:B:262:GLU:HB3	2:B:351:ALA:HB2	2.03	0.41
2:C:240:LEU:CD2	2:C:595:LEU:HB2	2.50	0.41
2:D:173:ARG:C	2:D:174:ILE:HD12	2.46	0.41
2:D:343:LEU:HD22	2:D:348:VAL:HG21	2.02	0.41
2:D:385:ARG:HD3	2:D:385:ARG:HA	1.92	0.41
2:E:20:GLU:OE2	2:E:128:ALA:HB2	2.21	0.41
2:E:276:LEU:O	2:E:280:VAL:HG23	2.21	0.41
2:F:593:THR:HG22	2:F:596:ASP:OD2	2.21	0.41
2:A:309:ILE:HB	2:A:313:GLU:OE2	2.21	0.40
2:A:558:LEU:HD23	2:A:558:LEU:HA	1.82	0.40
2:B:249:PRO:HB2	2:B:253:ARG:HH12	1.86	0.40
2:C:80:GLU:OE2	2:C:199:ALA:N	2.54	0.40
2:D:214:ILE:CG1	2:D:231:THR:HG22	2.51	0.40
2:D:271:ALA:O	2:D:321:ASN:HB2	2.22	0.40
2:E:524:LEU:HD12	2:E:531:LEU:HD11	2.03	0.40
2:F:20:GLU:HB2	2:F:157:LEU:HD21	2.04	0.40
2:F:123:VAL:O	2:F:162:LEU:HD23	2.21	0.40
2:A:260:LYS:HE2	2:A:579:THR:HG22	2.02	0.40
2:A:493:LEU:HD23	2:A:514:ILE:CG2	2.51	0.40
2:A:506:LEU:HA	2:A:509:VAL:HG12	2.03	0.40
2:B:214:ILE:HG12	2:B:231:THR:HG22	2.03	0.40
2:B:332:LEU:HD21	2:B:373:ILE:HG13	2.03	0.40
2:D:239:TRP:CZ3	2:D:629:PRO:HG3	2.56	0.40
2:D:329:PRO:HB2	2:D:333:ARG:NH2	2.35	0.40
2:D:557:TYR:HB3	2:D:564:VAL:CG2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:PRO:HB3	2:E:48:PHE:CE1	2.56	0.40
2:F:262:GLU:HB3	2:F:351:ALA:CB	2.50	0.40
2:F:441:LEU:HD21	2:F:454:PHE:HD2	1.86	0.40
2:A:130:ASP:HA	2:A:140:MET:HA	2.02	0.40
2:A:213:ARG:NH1	2:A:233:SER:HB2	2.36	0.40
2:A:254:TRP:CZ3	2:A:627:PRO:HG2	2.57	0.40
2:A:297:ARG:NE	2:A:297:ARG:HA	2.35	0.40
2:B:213:ARG:HD2	2:B:233:SER:N	2.35	0.40
2:B:220:MET:O	2:B:224:LEU:HD13	2.21	0.40
2:B:226:PHE:HE2	2:B:598:LEU:HD12	1.86	0.40
2:B:463:ARG:HA	2:B:463:ARG:HD3	1.90	0.40
2:B:518:LEU:HD22	2:B:554:LEU:HD13	2.03	0.40
2:B:558:LEU:CD2	2:B:596:ASP:HB3	2.51	0.40
2:C:24:LEU:HD21	2:C:161:ARG:CZ	2.52	0.40
2:D:61:THR:HG22	2:D:191:ARG:CD	2.51	0.40
2:D:179:PHE:CE1	2:D:199:ALA:HB1	2.56	0.40
2:D:240:LEU:CD2	2:D:595:LEU:HB2	2.51	0.40
2:D:502:SER:OG	2:D:505:LEU:HB3	2.22	0.40
2:E:224:LEU:HD13	2:E:229:LEU:HD12	2.03	0.40
2:E:386:THR:OG1	2:E:393:ALA:HB2	2.21	0.40
2:F:209:GLN:HE21	2:F:213:ARG:NE	2.19	0.40
2:F:280:VAL:HG23	2:F:334:GLU:OE1	2.22	0.40
2:F:327:ARG:HB3	2:F:362:GLU:CD	2.47	0.40
2:A:84:ARG:C	2:A:181:LEU:HD11	2.46	0.40
2:A:161:ARG:N	2:F:72:GLU:OE2	2.37	0.40
2:B:184:VAL:CG2	2:B:192:ARG:HB2	2.51	0.40
2:B:332:LEU:HD21	2:B:373:ILE:CG1	2.52	0.40
2:C:90:ARG:N	2:C:90:ARG:HD2	2.36	0.40
2:C:169:PRO:HA	2:C:172:ARG:HE	1.85	0.40
2:C:326:LEU:HD22	2:C:332:LEU:HA	2.03	0.40
2:D:182:GLN:HG2	2:D:194:GLN:O	2.22	0.40
2:D:299:PRO:HD2	2:D:302:TRP:CE3	2.56	0.40
2:E:19:PRO:O	2:E:23:LEU:HD23	2.22	0.40
2:E:49:PHE:CD1	2:E:53:ALA:HB3	2.51	0.40
2:E:141:PRO:HA	2:E:142:PRO:HD3	1.84	0.40
2:E:555:LEU:HD11	2:E:559:ARG:HH12	1.87	0.40
2:E:562:VAL:HG13	2:E:564:VAL:HG23	2.02	0.40
2:F:305:PRO:HD2	2:F:524:LEU:HD21	2.03	0.40
2:F:440:ASP:OD2	2:F:441:LEU:N	2.54	0.40
2:F:627:PRO:C	2:F:628:ARG:HD2	2.46	0.40
2:A:34:VAL:HG23	2:A:58:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:557:TYR:O	2:A:562:VAL:HG12	2.22	0.40
2:B:244:LEU:HD11	2:B:251:ASP:HB3	2.04	0.40
2:B:329:PRO:HB3	2:B:364:ARG:NH1	2.37	0.40
2:D:172:ARG:CB	2:D:173:ARG:HD2	2.51	0.40
2:D:181:LEU:HB3	2:D:193:VAL:CG2	2.51	0.40
2:E:9:VAL:CG1	2:E:34:VAL:HG22	2.51	0.40
2:E:185:GLU:OE1	2:E:192:ARG:HD3	2.22	0.40
2:E:254:TRP:CH2	2:E:594:ARG:HB2	2.56	0.40
2:F:16:ALA:HA	2:F:19:PRO:CG	2.51	0.40
2:F:47:GLU:HG2	2:F:48:PHE:N	2.37	0.40
2:F:77:ARG:O	2:F:81:VAL:HG13	2.22	0.40
2:F:94:GLU:HA	2:F:121:ALA:HB2	2.04	0.40
2:F:398:LEU:HD23	2:F:434:CYS:SG	2.62	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	
2	A	611/628 (97%)	573 (94%)	37 (6%)	1 (0%)	43	71
2	B	611/628 (97%)	570 (93%)	40 (6%)	1 (0%)	43	71
2	C	611/628 (97%)	567 (93%)	43 (7%)	1 (0%)	43	71
2	D	611/628 (97%)	568 (93%)	42 (7%)	1 (0%)	43	71
2	E	611/628 (97%)	568 (93%)	42 (7%)	1 (0%)	43	71
2	F	608/628 (97%)	561 (92%)	45 (7%)	2 (0%)	36	65
All	All	3663/3768 (97%)	3407 (93%)	249 (7%)	7 (0%)	44	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	174	ILE
2	B	174	ILE
2	F	91	THR
2	C	174	ILE
2	E	174	ILE
2	F	174	ILE
2	D	174	ILE

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	
2	A	495/504 (98%)	493 (100%)	2 (0%)	84	83
2	B	495/504 (98%)	494 (100%)	1 (0%)	87	85
2	C	495/504 (98%)	495 (100%)	0	100	100
2	D	495/504 (98%)	494 (100%)	1 (0%)	87	85
2	E	495/504 (98%)	495 (100%)	0	100	100
2	F	494/504 (98%)	493 (100%)	1 (0%)	87	85
All	All	2969/3024 (98%)	2964 (100%)	5 (0%)	85	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	136	GLN
2	A	276	LEU
2	B	154	GLN
2	D	136	GLN
2	F	47	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	95	GLN
2	A	112	GLN

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Mol	Chain	Res	Type
2	A	154	GLN
2	A	178	GLN
2	A	346	GLN
2	A	471	HIS
2	A	489	ASN
2	A	495	HIS
2	A	581	ASN
2	B	286	ASN
2	B	471	HIS
2	B	570	ASN
2	C	75	HIS
2	C	154	GLN
2	C	158	HIS
2	C	194	GLN
2	C	395	HIS
2	D	75	HIS
2	D	125	HIS
2	D	154	GLN
2	D	156	HIS
2	D	273	HIS
2	D	395	HIS
2	D	452	HIS
2	D	471	HIS
2	D	581	ASN
2	D	599	HIS
2	D	614	GLN
2	E	154	GLN
2	E	205	GLN
2	E	335	GLN
2	E	523	ASN
2	E	567	ASN
2	E	581	ASN
2	F	2	ASN
2	F	209	GLN
2	F	264	HIS
2	F	346	GLN
2	F	397	ASN
2	F	452	HIS
2	F	570	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	5/6 (83%)	4 (80%)	0
1	Y	5/6 (83%)	2 (40%)	0
1	Z	5/6 (83%)	2 (40%)	0
All	All	15/18 (83%)	8 (53%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	A
1	X	5	A
1	X	6	A
1	Y	8	A
1	Y	11	A
1	Z	14	A
1	Z	17	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	ATP	A	701	-	32,33,33	0.28	0	48,52,52	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	D	701	5	32,33,33	0.28	0	48,52,52	0.67	1 (2%)
3	ATP	C	701	5	32,33,33	0.31	0	48,52,52	0.71	0
3	ATP	E	701	-	32,33,33	0.28	0	48,52,52	0.70	0
3	ATP	B	701	-	32,33,33	0.30	0	48,52,52	0.68	0
3	ATP	F	701	-	32,33,33	0.28	0	48,52,52	0.72	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
3	ATP	A	701	-	-	7/22/38/38	0/3/3/3
3	ATP	D	701	5	-	8/22/38/38	0/3/3/3
3	ATP	C	701	5	-	3/22/38/38	0/3/3/3
3	ATP	E	701	-	-	4/22/38/38	0/3/3/3
3	ATP	B	701	-	-	0/22/38/38	0/3/3/3
3	ATP	F	701	-	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	ATP	O3'-C3'-C4'	-2.01	105.30	111.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	ATP	O4'-C4'-C5'-O5'
3	C	701	ATP	C5'-O5'-PA-O1A
3	C	701	ATP	C5'-O5'-PA-O2A
3	C	701	ATP	C5'-O5'-PA-O3A
3	D	701	ATP	C5'-O5'-PA-O1A
3	D	701	ATP	C5'-O5'-PA-O3A
3	E	701	ATP	PB-O3B-PG-O2G
3	E	701	ATP	C5'-O5'-PA-O2A
3	E	701	ATP	C5'-O5'-PA-O3A
3	D	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	C3'-C4'-C5'-O5'

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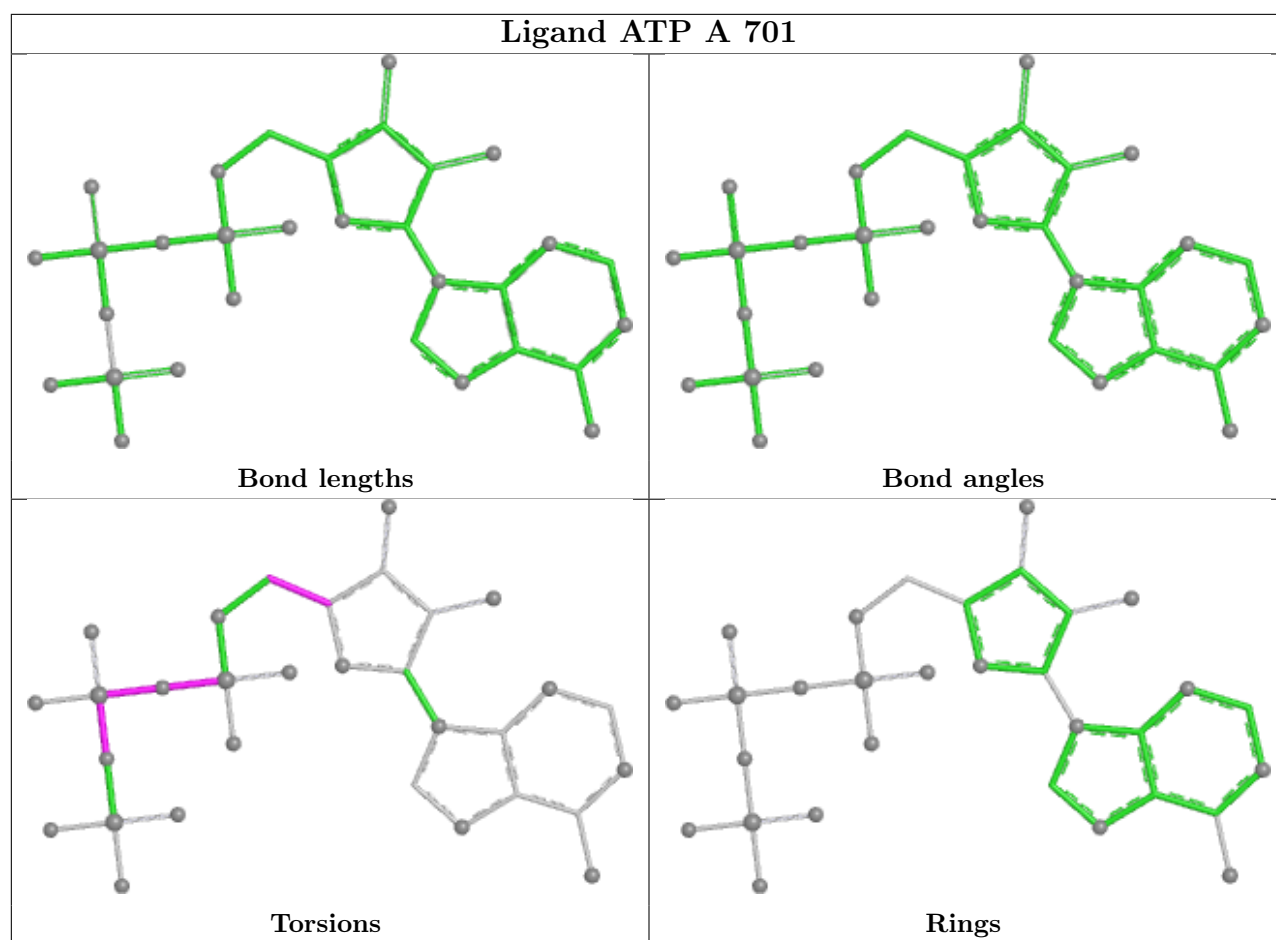
Mol	Chain	Res	Type	Atoms
3	D	701	ATP	C3'-C4'-C5'-O5'
3	E	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	PG-O3B-PB-O2B
3	A	701	ATP	PB-O3A-PA-O1A
3	D	701	ATP	C5'-O5'-PA-O2A
3	D	701	ATP	C4'-C5'-O5'-PA
3	D	701	ATP	PB-O3A-PA-O2A
3	F	701	ATP	PB-O3A-PA-O2A
3	F	701	ATP	PG-O3B-PB-O1B
3	A	701	ATP	PG-O3B-PB-O1B
3	A	701	ATP	PA-O3A-PB-O2B
3	D	701	ATP	PB-O3A-PA-O1A
3	A	701	ATP	PB-O3A-PA-O2A

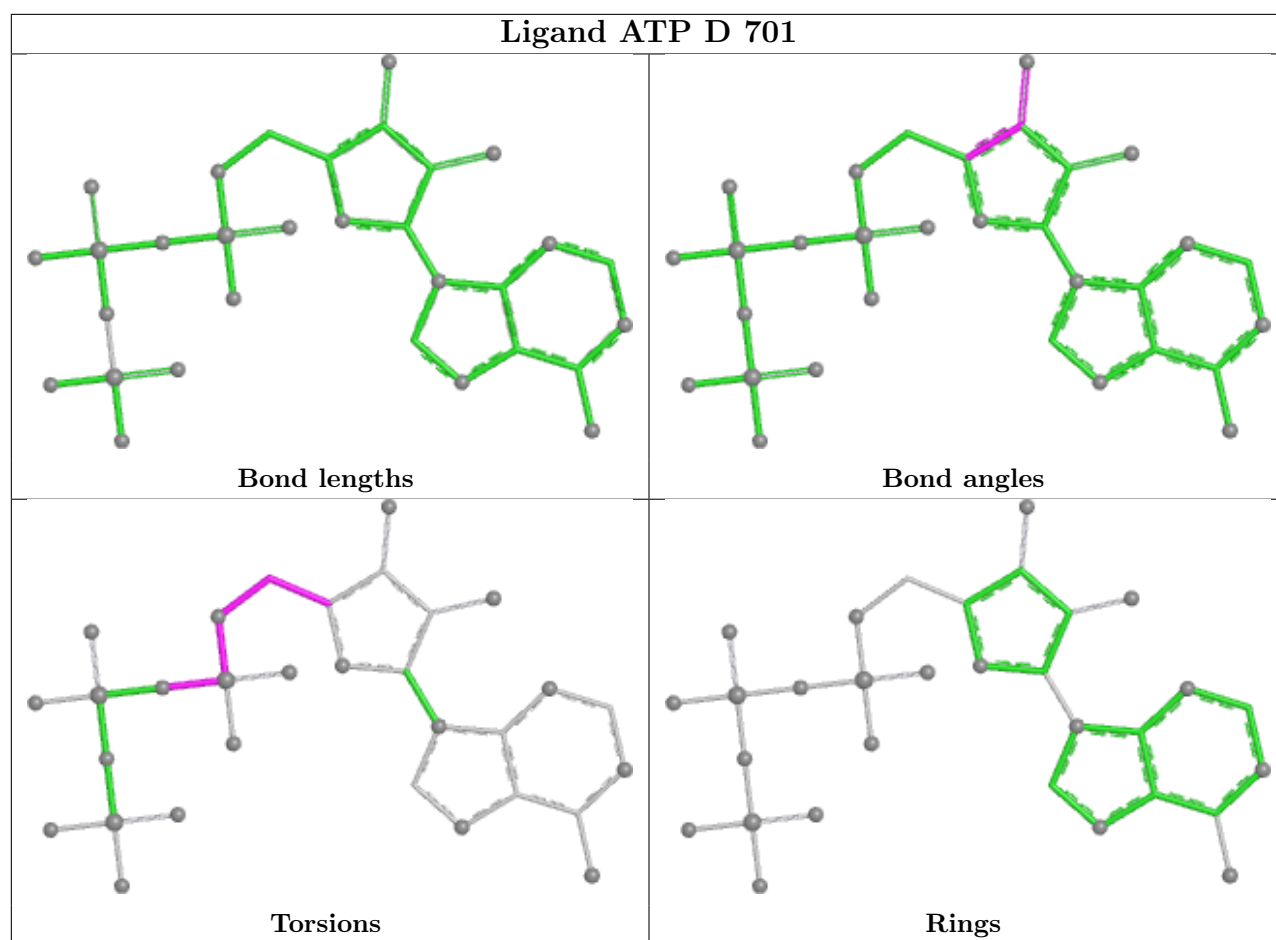
There are no ring outliers.

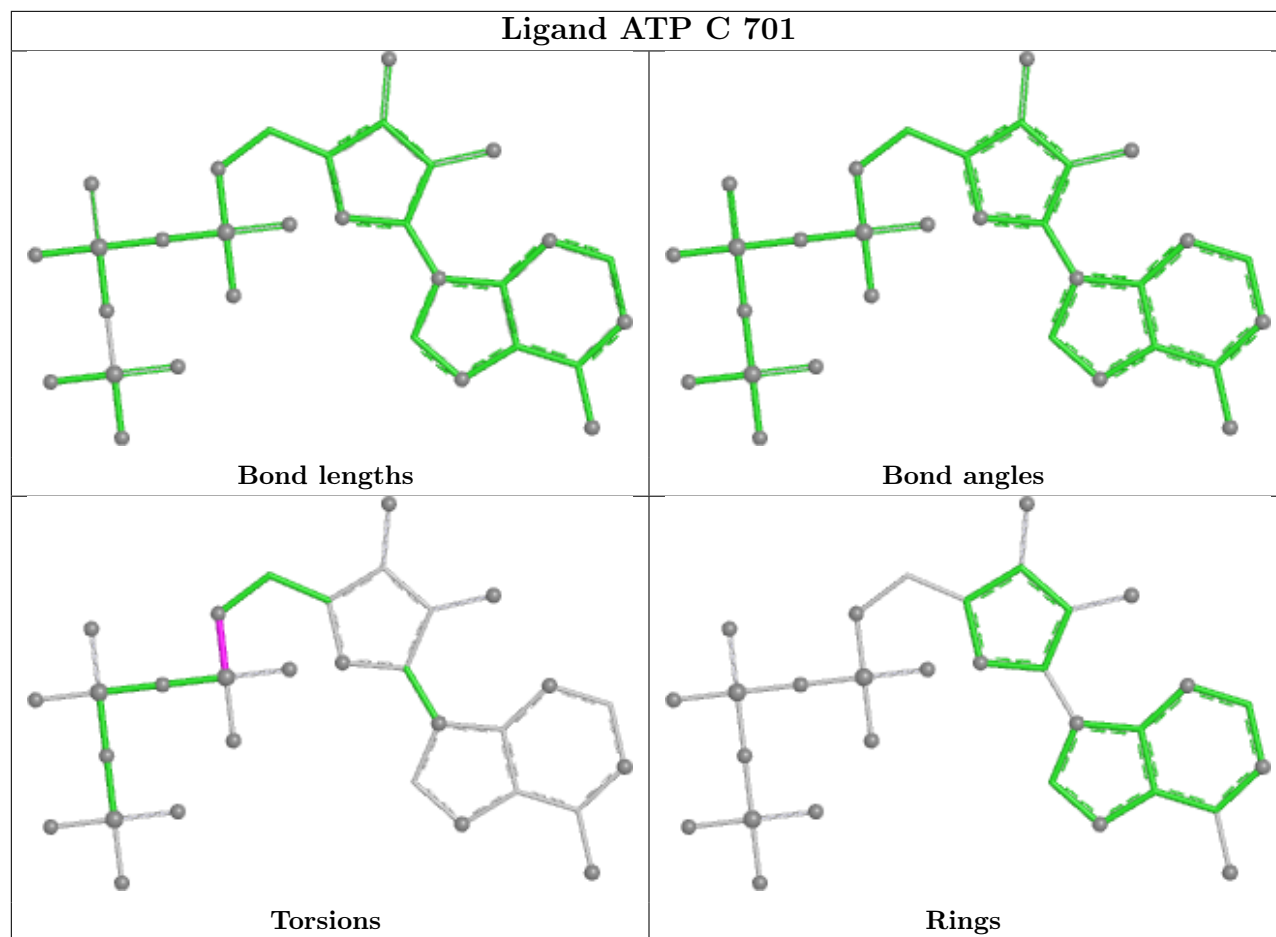
4 monomers are involved in 5 short contacts:

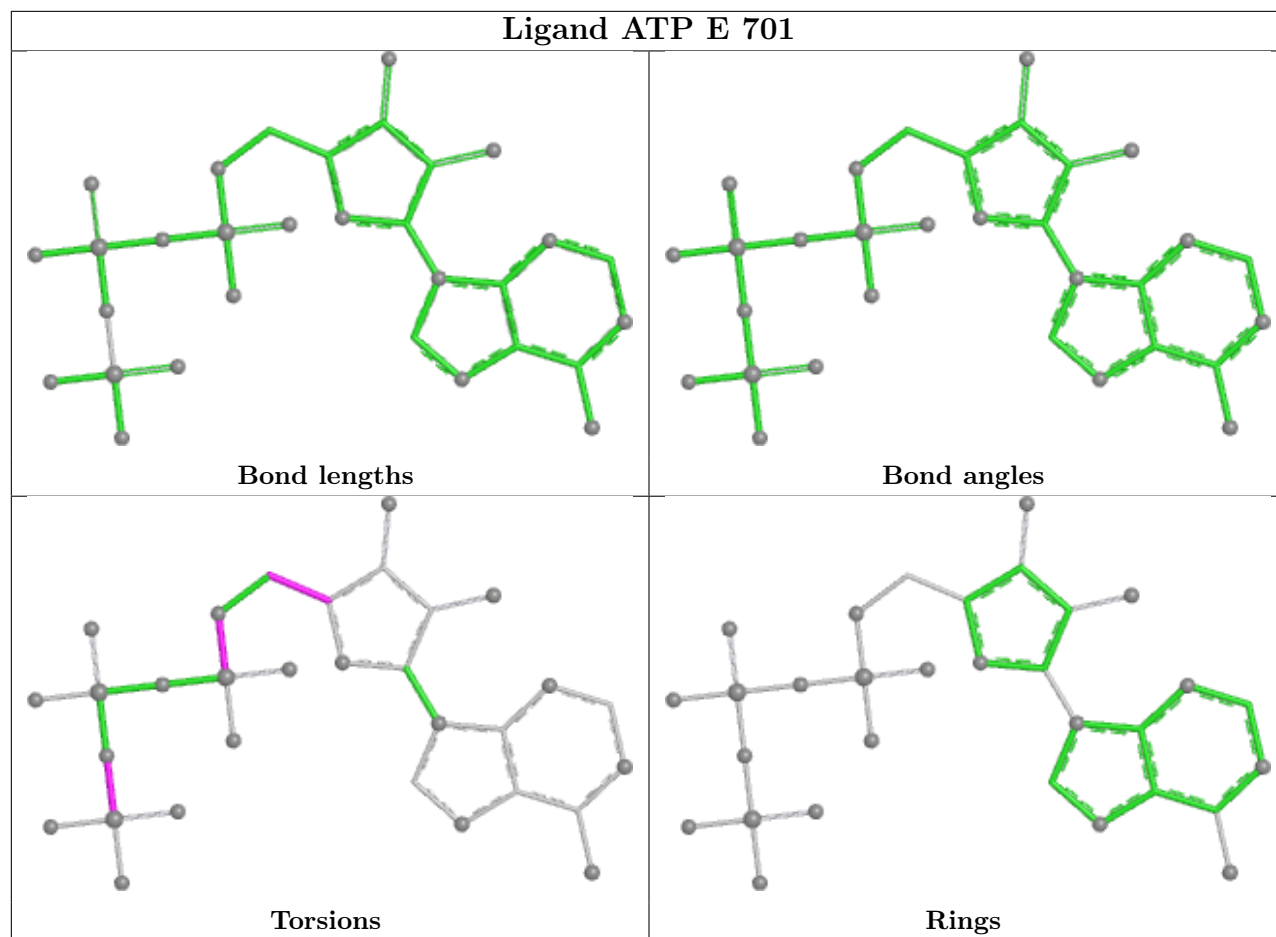
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	ATP	1	0
3	C	701	ATP	1	0
3	E	701	ATP	2	0
3	B	701	ATP	1	0

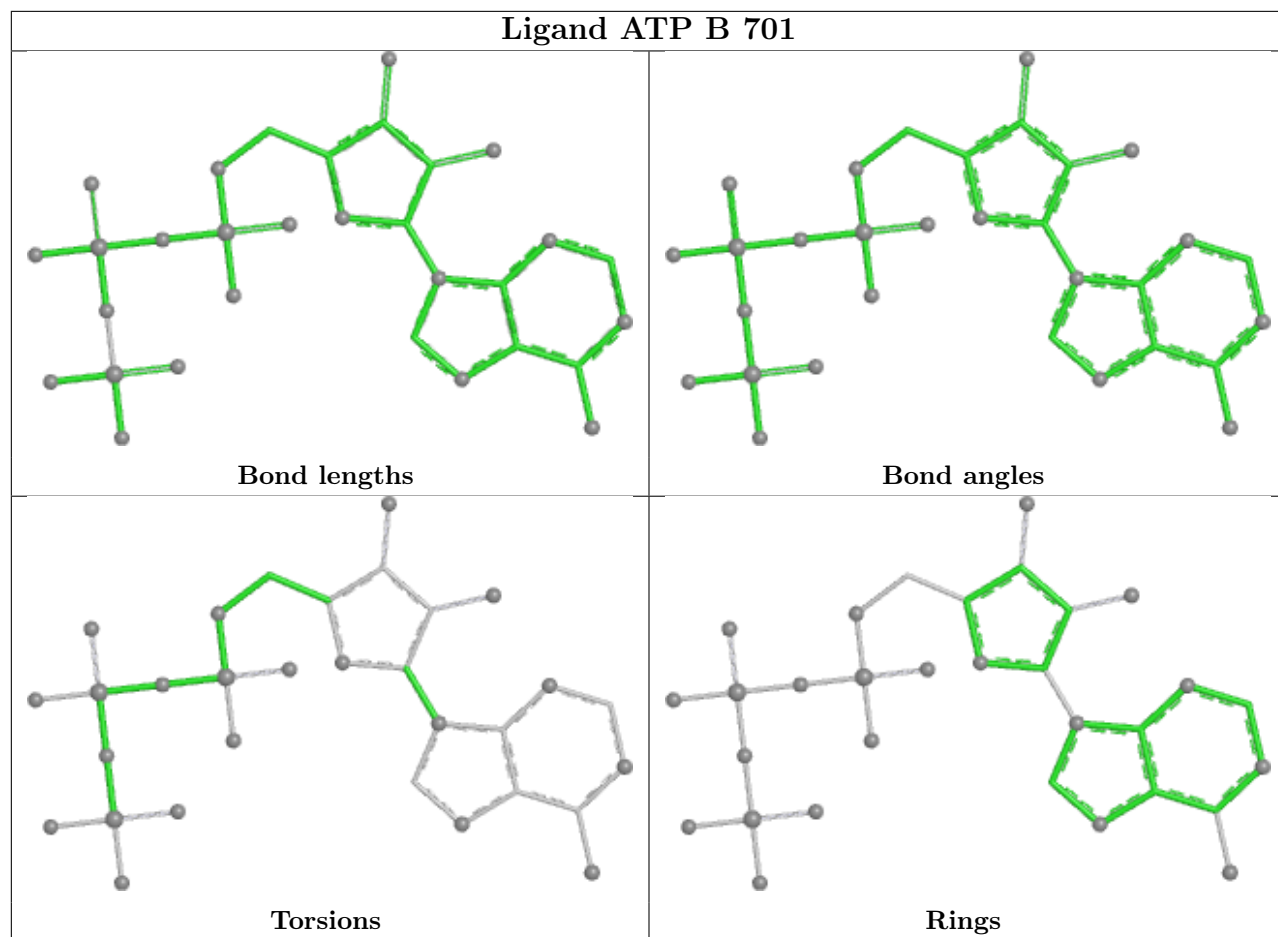
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

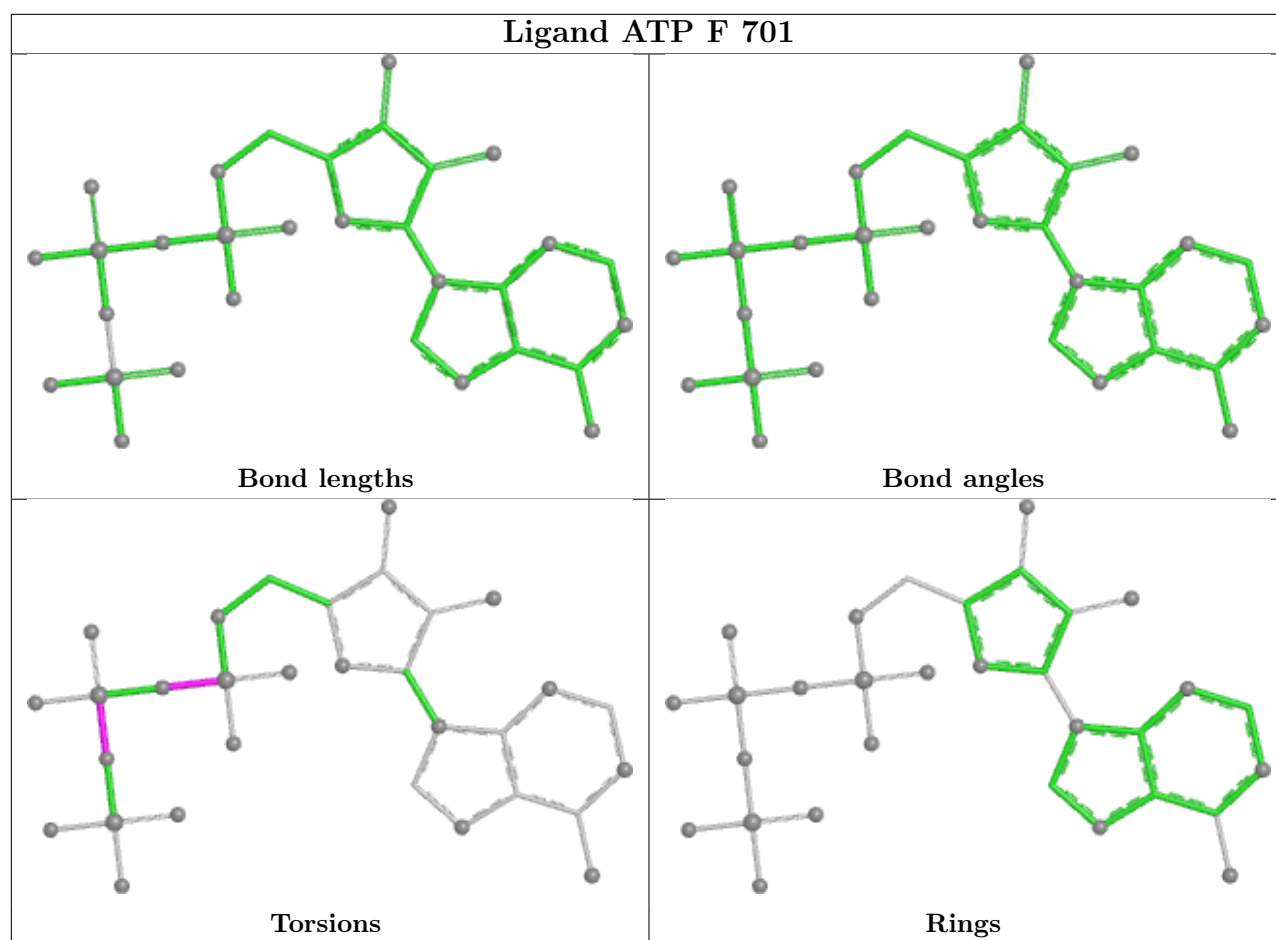












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

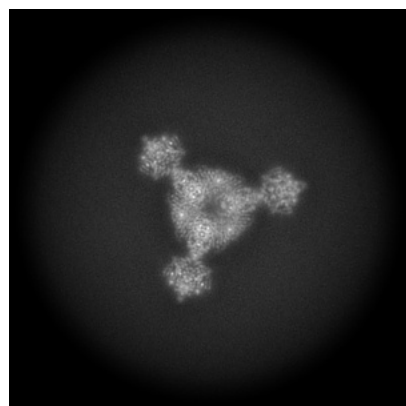
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39750. These allow visual inspection of the internal detail of the map and identification of artifacts.

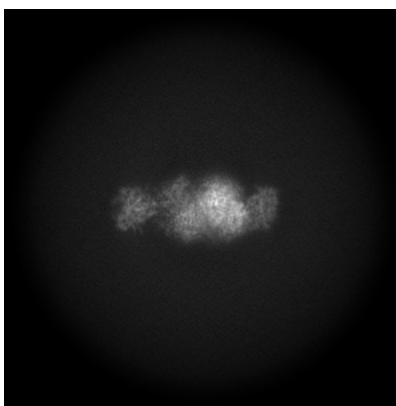
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

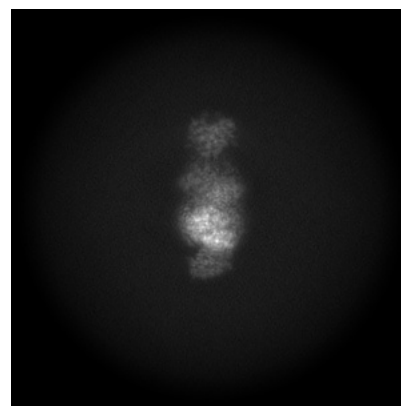
6.1.1 Primary map



X

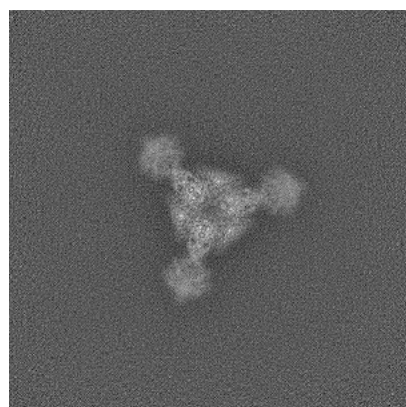


Y

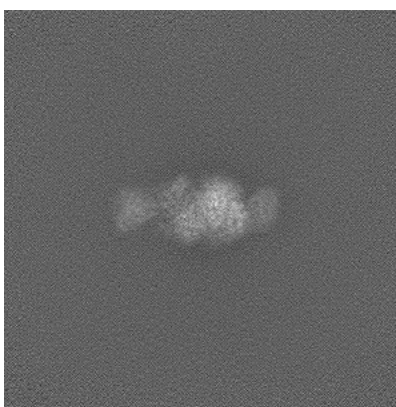


Z

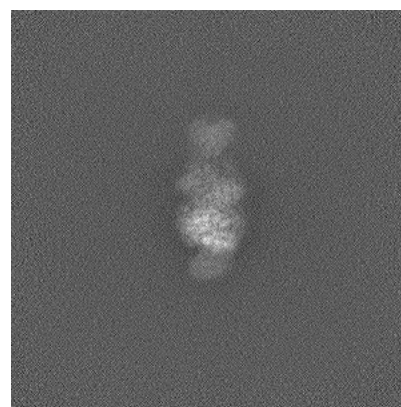
6.1.2 Raw map



X



Y

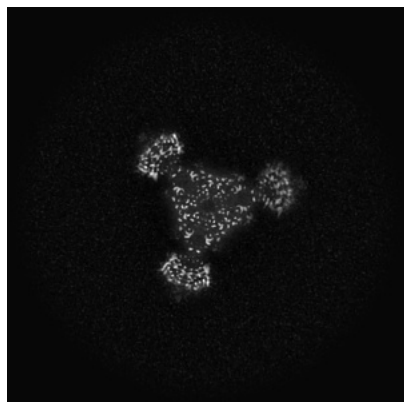


Z

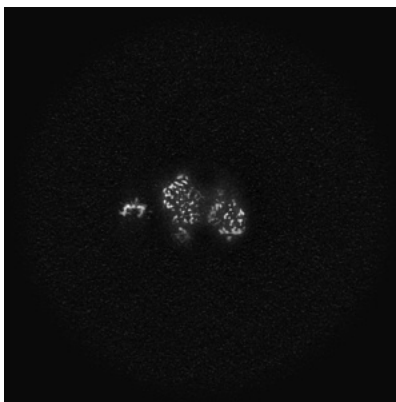
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

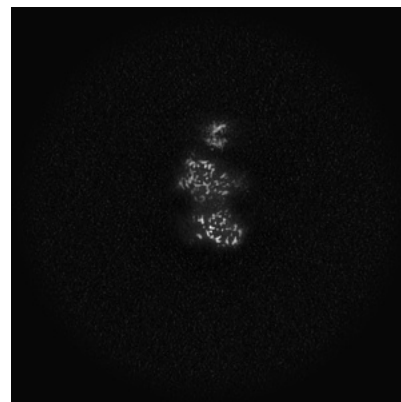
6.2.1 Primary map



X Index: 256

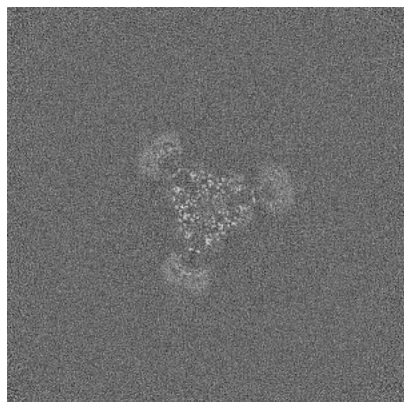


Y Index: 256

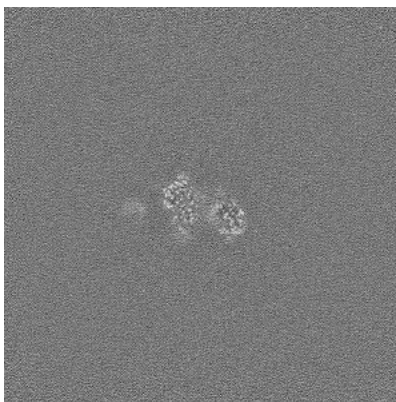


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

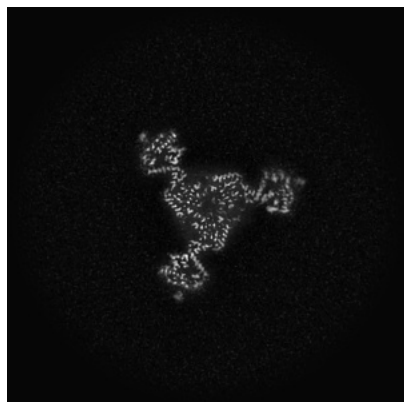


Z Index: 256

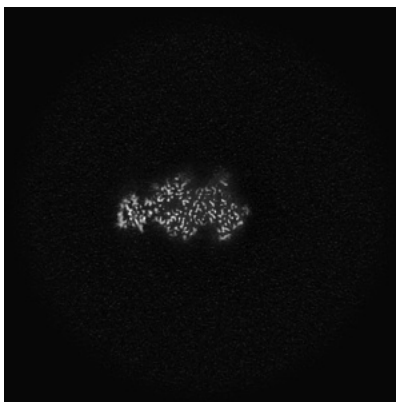
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

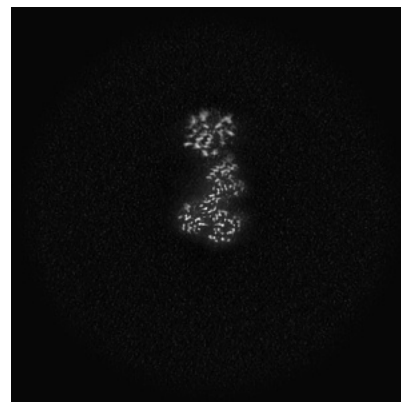
6.3.1 Primary map



X Index: 263

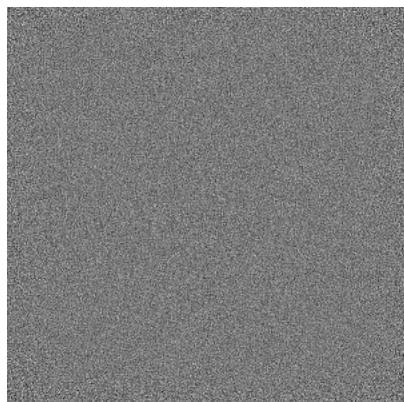


Y Index: 242

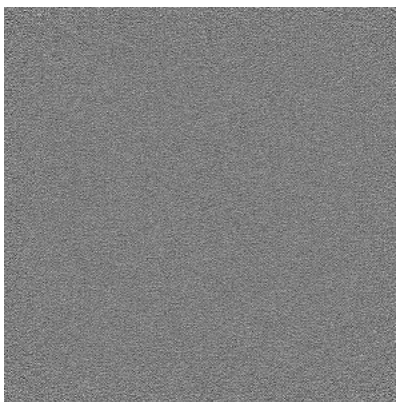


Z Index: 281

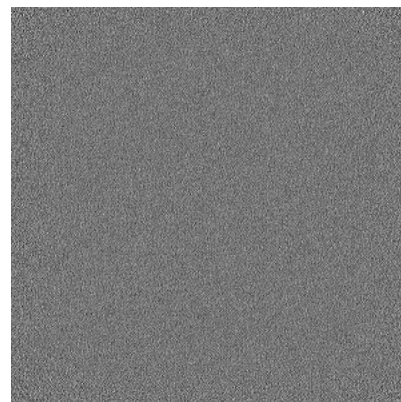
6.3.2 Raw map



X Index: 0



Y Index: 0

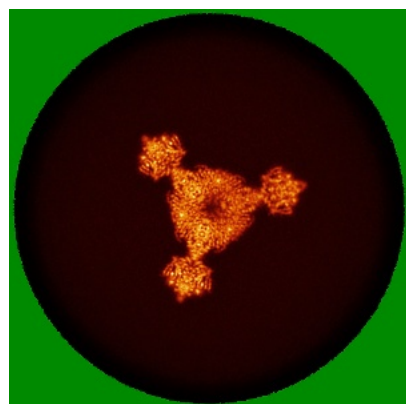


Z Index: 0

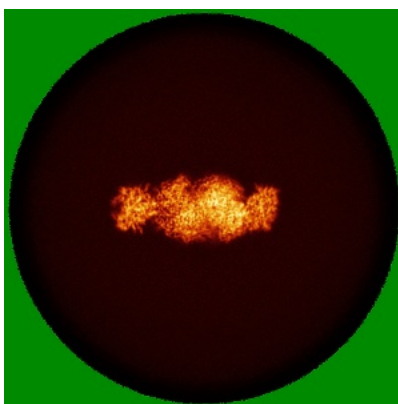
The images above show the largest variance slices of the map in three orthogonal directions.

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

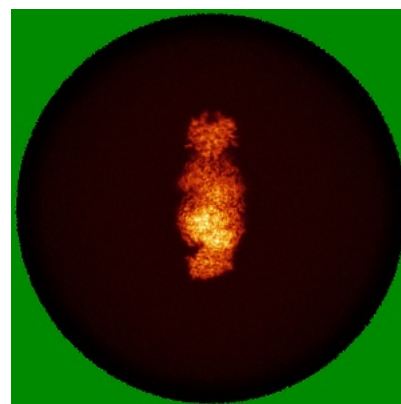
6.4.1 Primary map



X

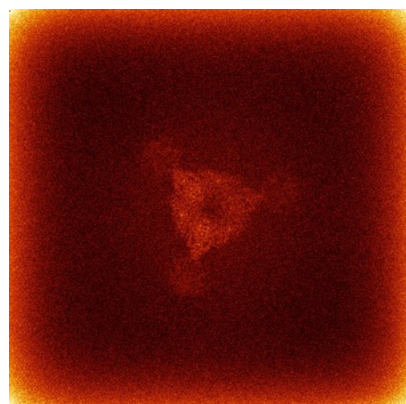


Y

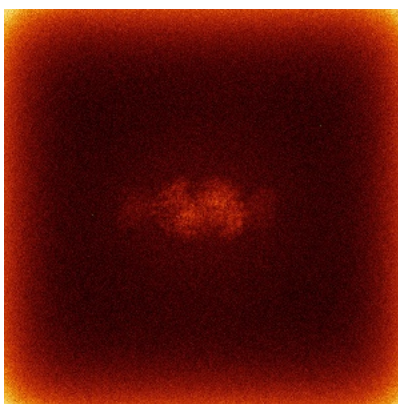


Z

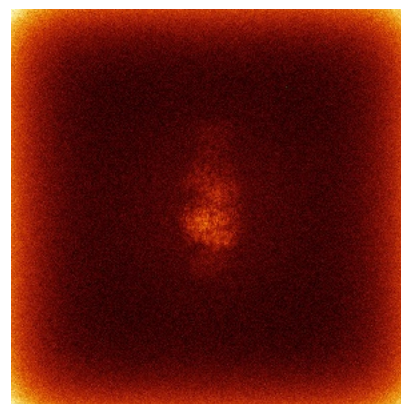
6.4.2 Raw map



X



Y

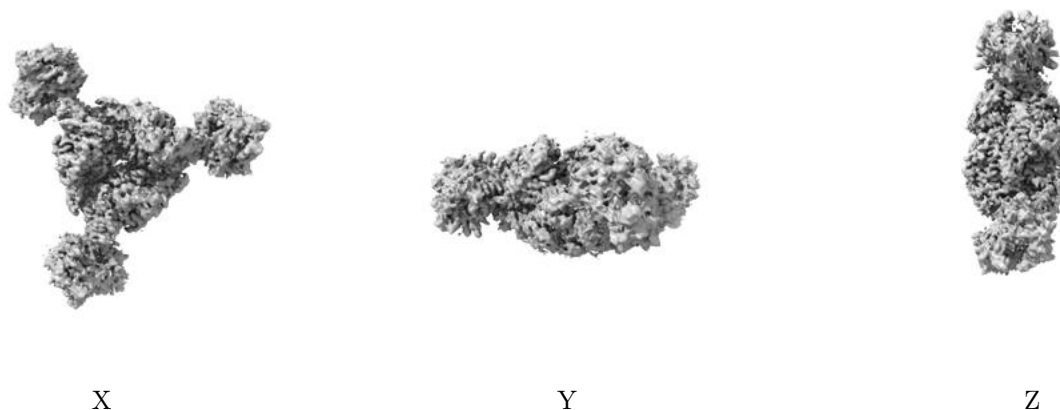


Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

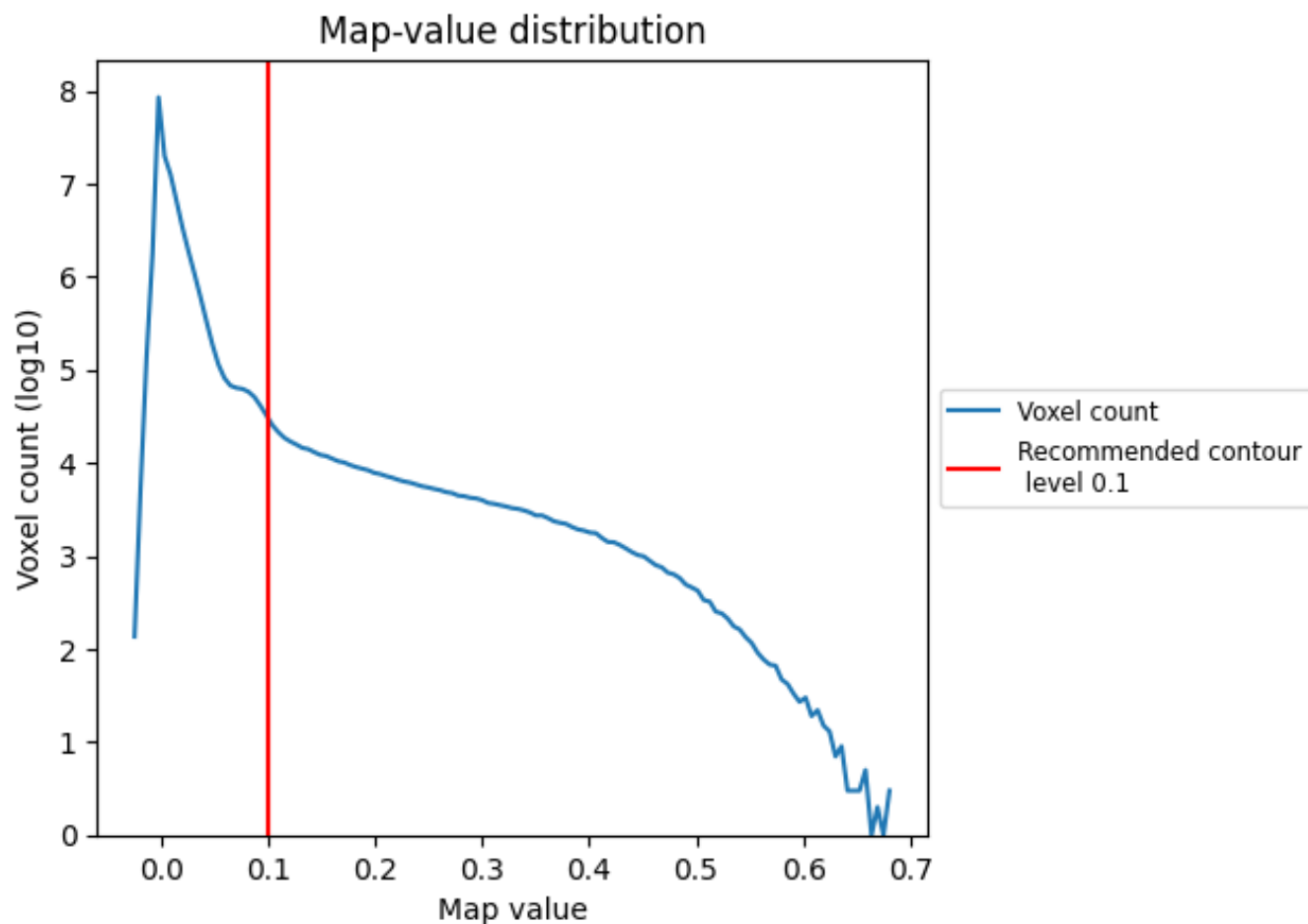
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

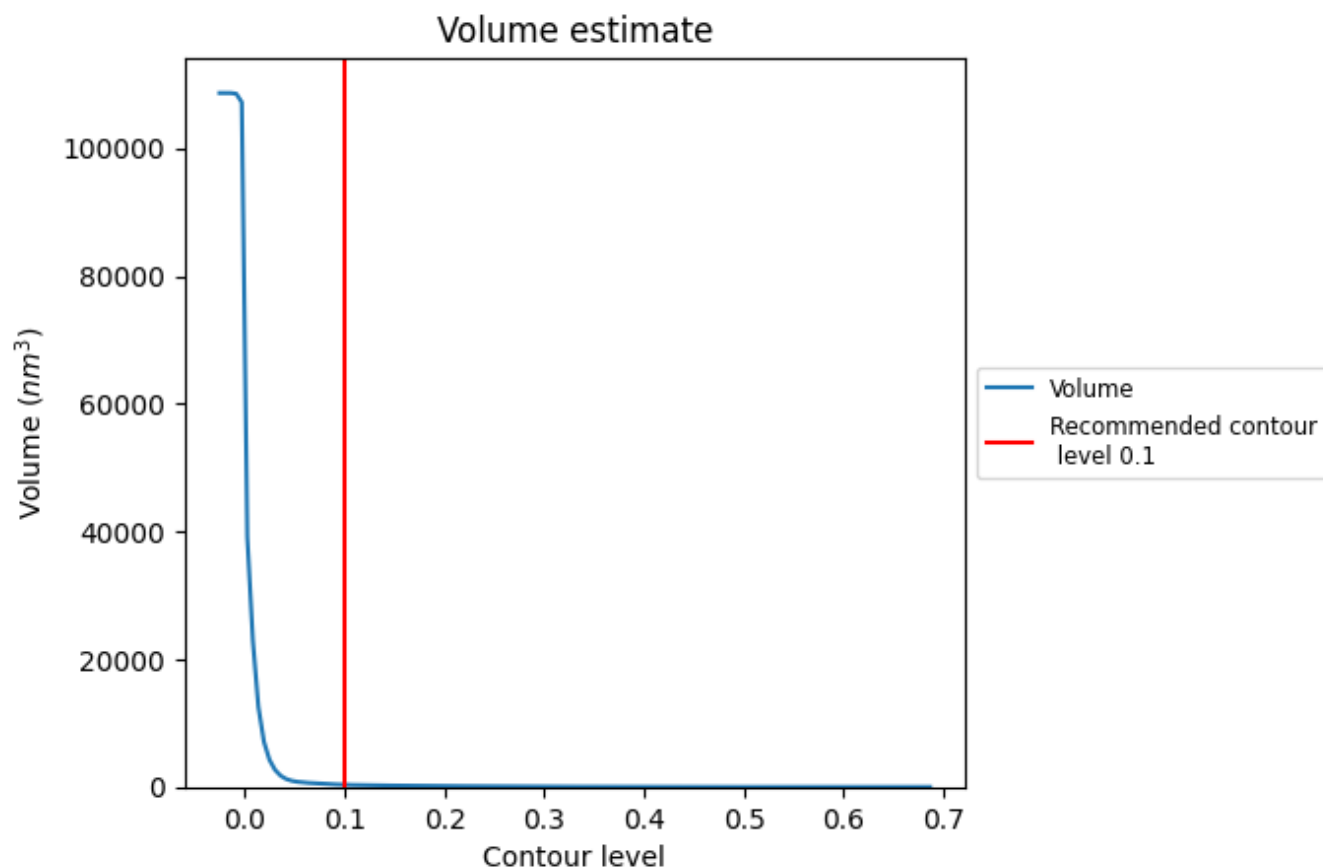
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

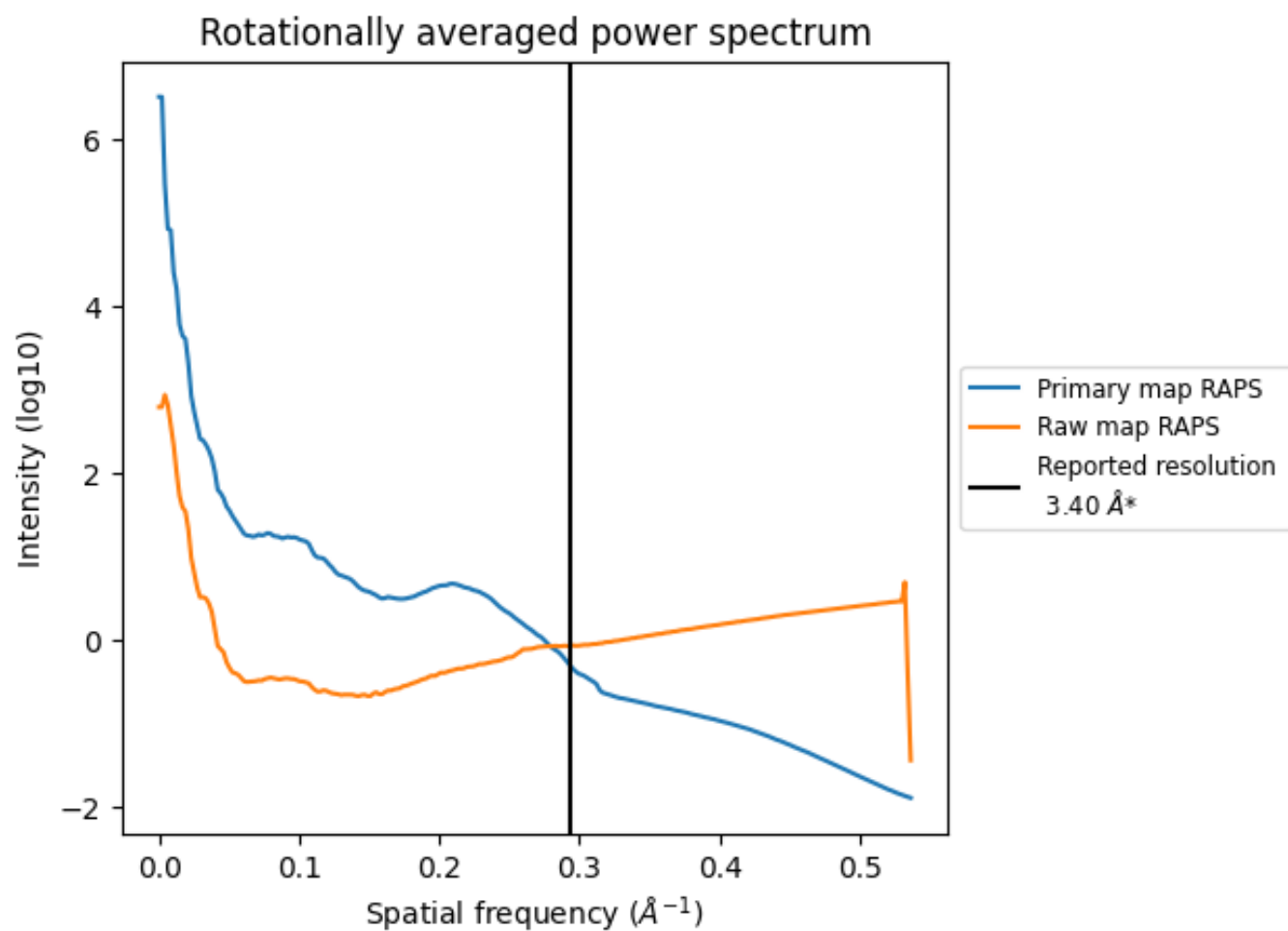
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 348 nm^3 ; this corresponds to an approximate mass of 314 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 [i](#)

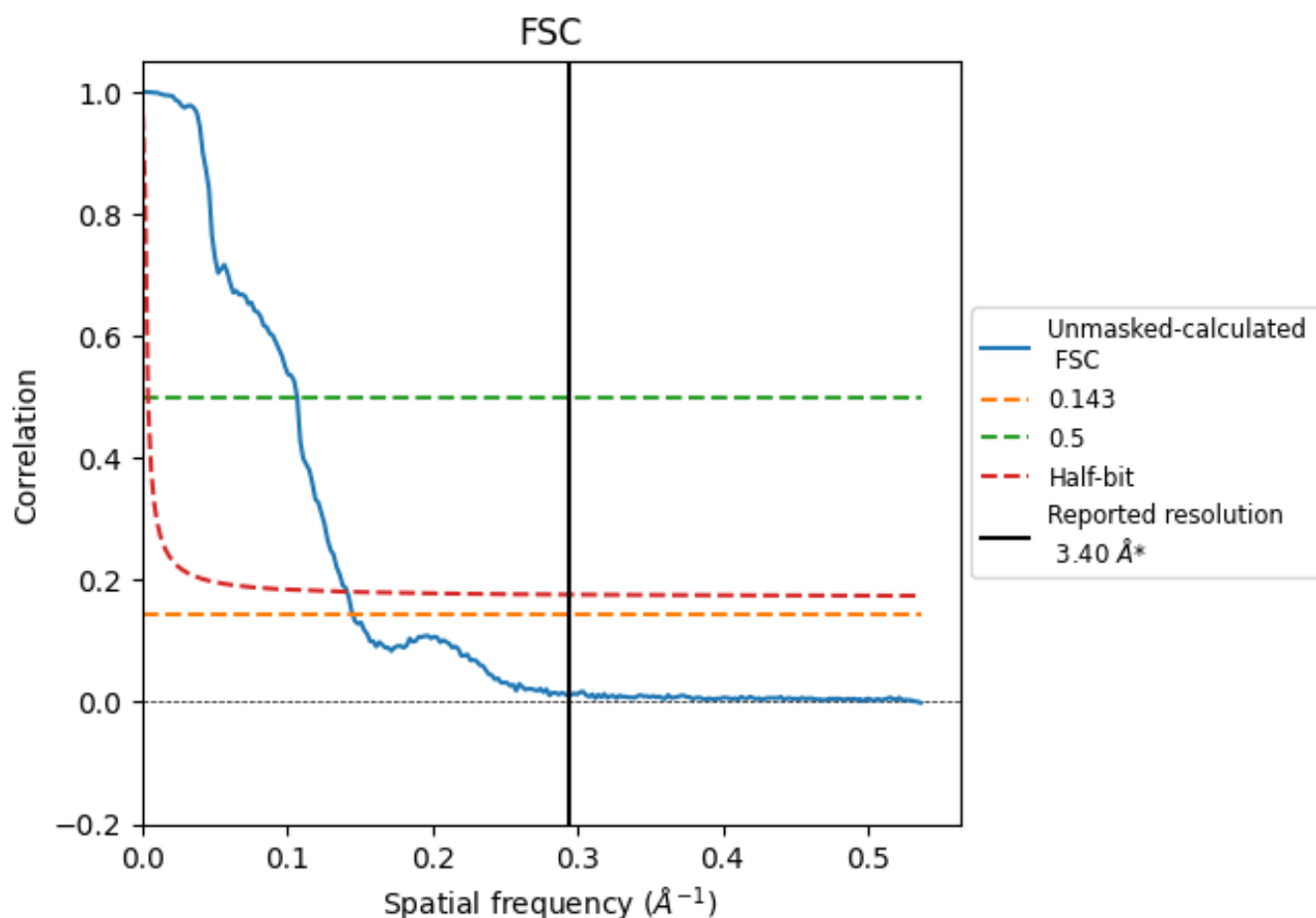


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

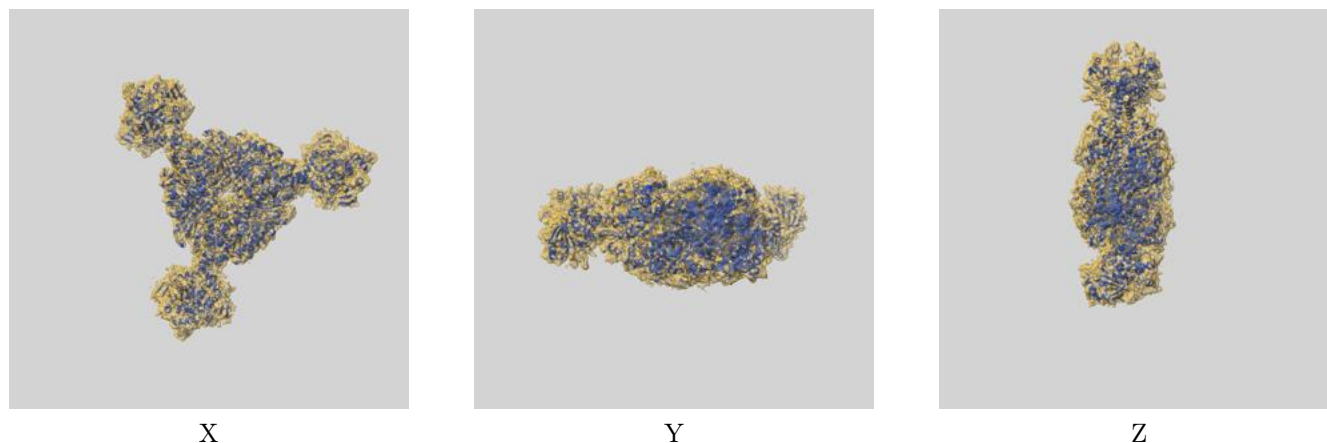
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.89	9.36	7.08

*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 6.89 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

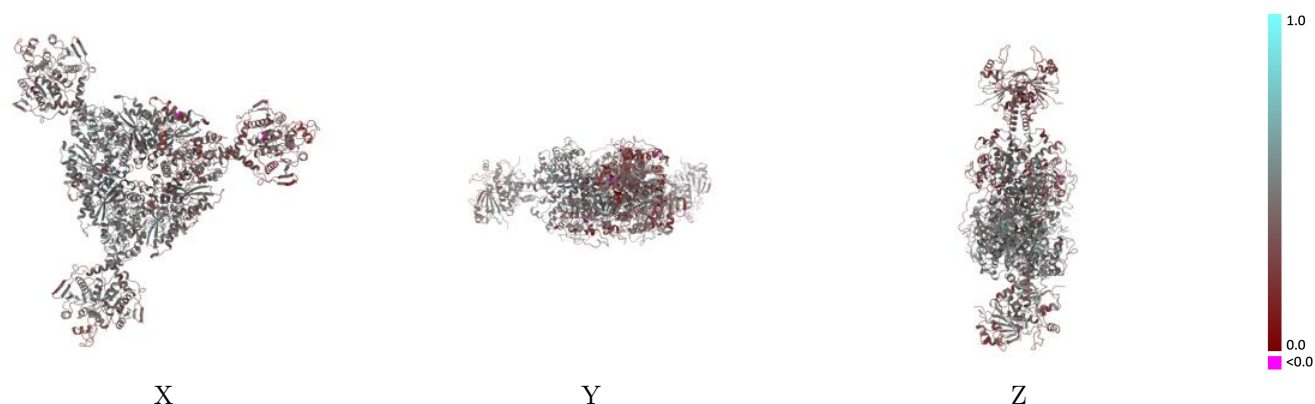
This section contains information regarding the fit between EMDB map EMD-39750 and PDB model 8Z3P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

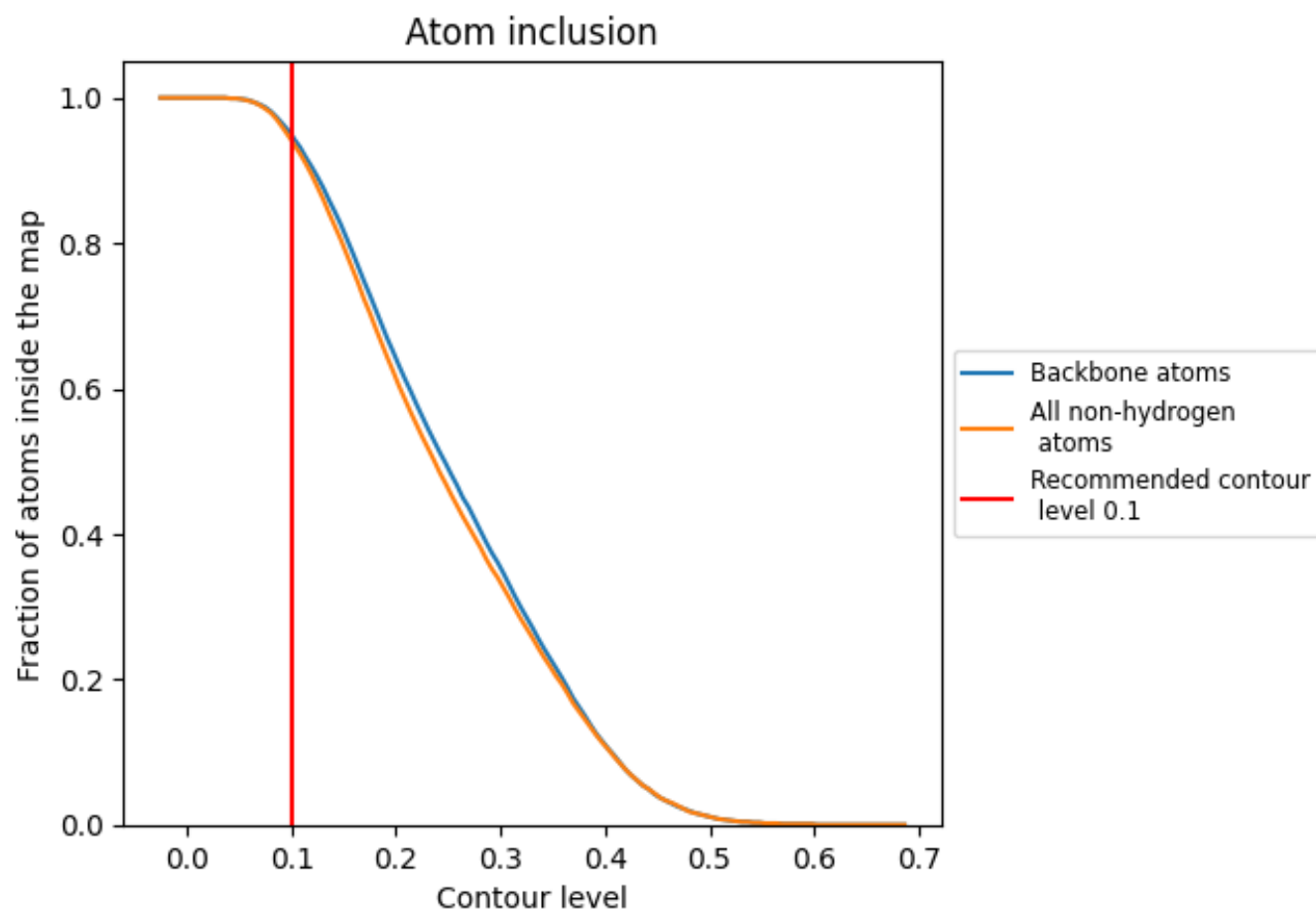


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.4200
A	0.9140	0.3600
B	0.9540	0.4400
C	0.9640	0.4550
D	0.9610	0.4430
E	0.9530	0.4480
F	0.9160	0.3710
X	1.0000	0.4740
Y	1.0000	0.4680
Z	1.0000	0.4150

1.0

0.0

<0.0