



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 09:24 AM EDT

PDB ID : 5UIE
EMDB ID : EMD-8549
Title : Vps4-Vta1 complex
Authors : Monroe, N.; Shen, P.; Han, H.; Sundquist, W.I.; Hill, C.P.
Deposited on : 2017-01-13
Resolution : 5.70 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

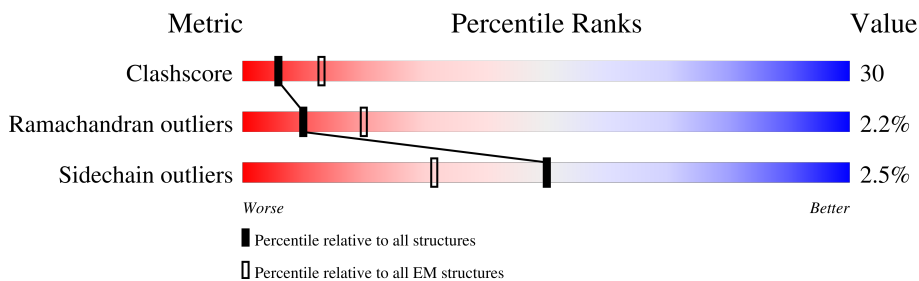
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	437	
1	B	437	
1	C	437	
1	D	437	
1	E	437	
1	F	437	
2	G	9	
3	H	330	

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Mol	Chain	Length	Quality of chain
3	I	330	 15% 10% 5% 85%
3	J	330	 13% 8% 87%
3	K	330	 14% 9% 5% 86%
3	L	330	 13% 5% 8% 87%
3	M	330	 14% 9% 5% 86%
3	N	330	 13% 5% 8% 87%
3	O	330	 13% 5% 8% 87%
3	P	330	 13% 5% 8% 87%
3	Q	330	 13% 5% 7% 87%
3	R	330	 13% 5% 7% 87%
3	S	330	 13% 5% 8% 87%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18682 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Vacuolar protein sorting-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	312	Total 2412	C 1522	N 409	O 472	S 9	0	0
1	B	311	Total 2407	C 1519	N 408	O 471	S 9	0	0
1	C	311	Total 2407	C 1519	N 408	O 471	S 9	0	0
1	D	311	Total 2407	C 1519	N 408	O 471	S 9	0	0
1	E	308	Total 2387	C 1507	N 405	O 466	S 9	0	0
1	F	302	Total 2344	C 1484	N 396	O 455	S 9	0	0

- Molecule 2 is a protein called DOA4-independent degradation protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	9	Total 43	C 26	N 8	O 9	0	0

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein VTA1.

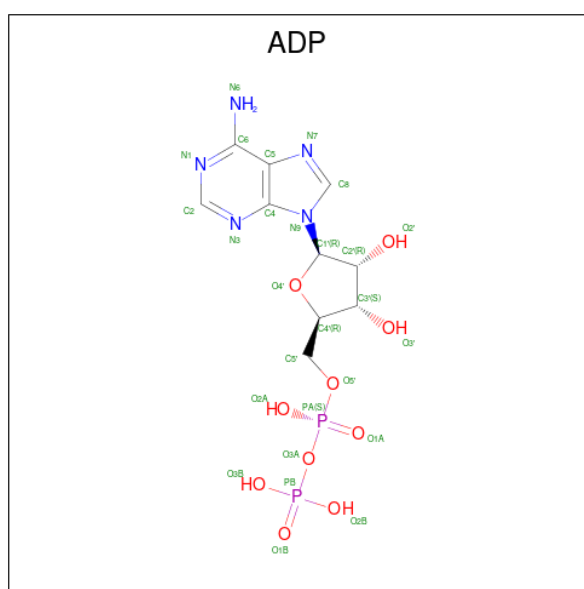
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	42	Total 331	C 209	N 54	O 68		0	0
3	I	51	Total 404	C 255	N 65	O 83	S 1	0	0
3	J	42	Total 331	C 209	N 54	O 68		0	0
3	K	47	Total 371	C 236	N 60	O 74	S 1	0	0
3	L	42	Total 331	C 209	N 54	O 68		0	0
3	M	47	Total 371	C 236	N 60	O 74	S 1	0	0

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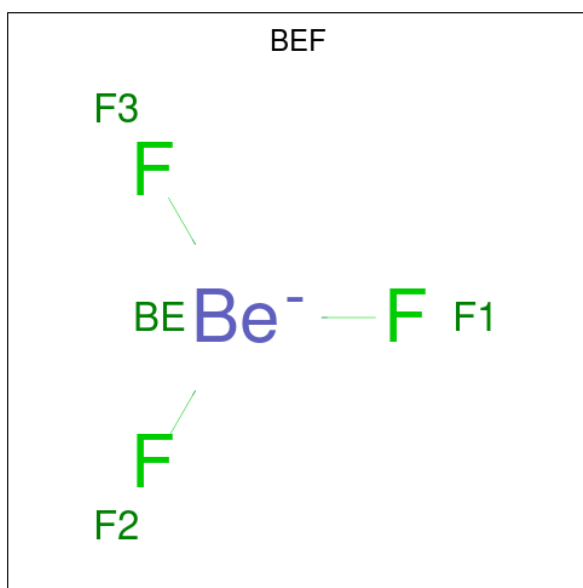
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	N	42	Total 331	C 209	N 54	O 68	0	0
3	O	42	Total 331	C 209	N 54	O 68	0	0
3	P	42	Total 331	C 209	N 54	O 68	0	0
3	Q	42	Total 331	C 209	N 54	O 68	0	0
3	R	42	Total 331	C 209	N 54	O 68	0	0
3	S	42	Total 331	C 209	N 54	O 68	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
5	A	1	4	1	3	0
5	C	1	8	2	6	0
5	C	1	8	2	6	0

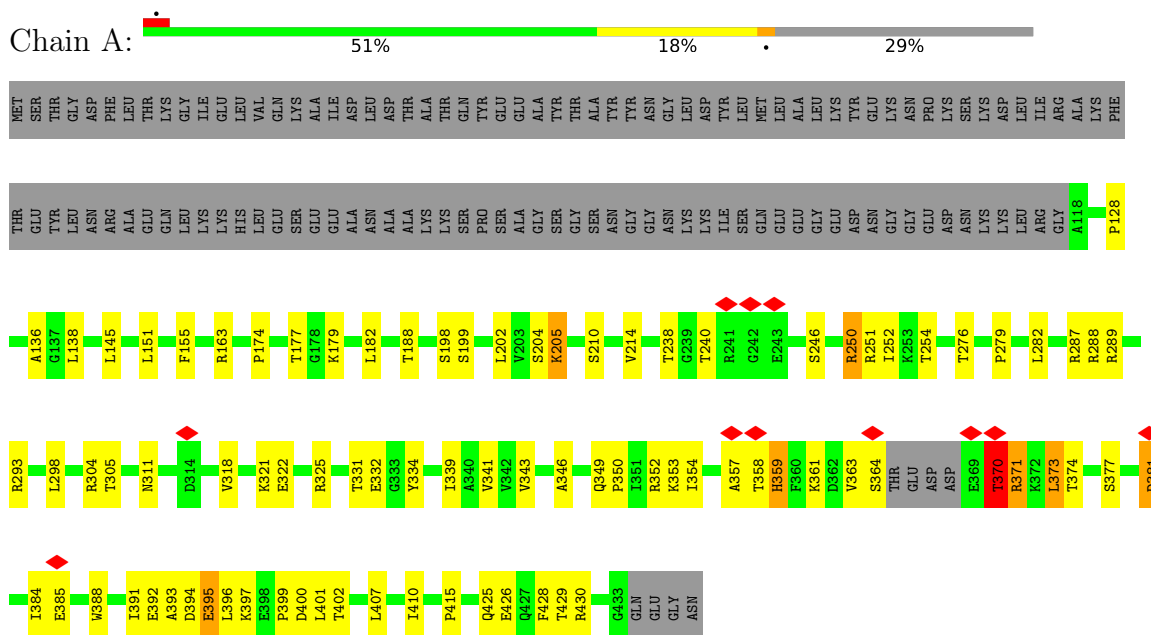
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0
6	B	1	1	1	0
6	C	1	1	1	0

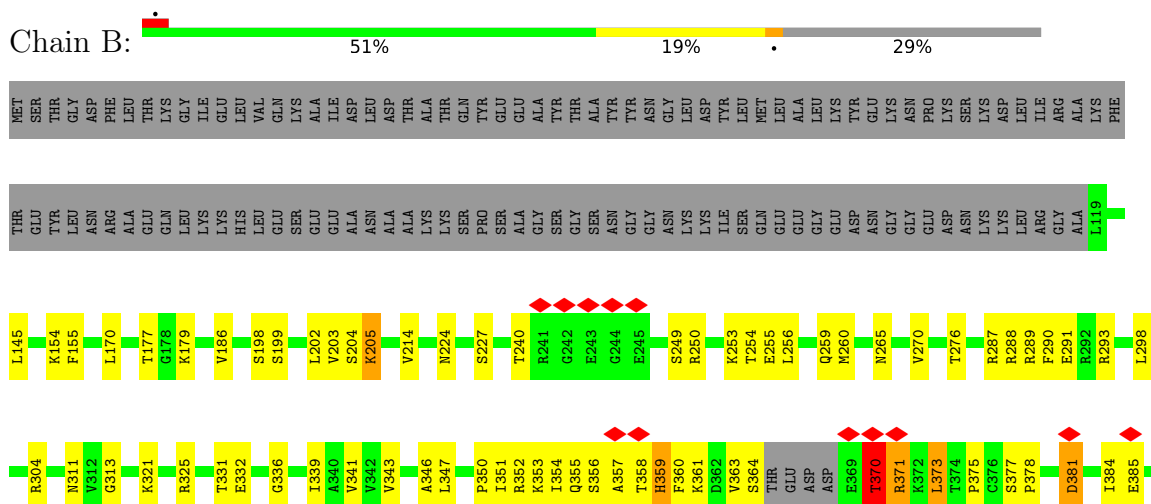
3 Residue-property plots

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

- Molecule 1: Vacuolar protein sorting-associated protein 4

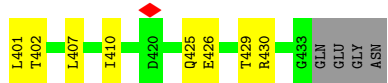
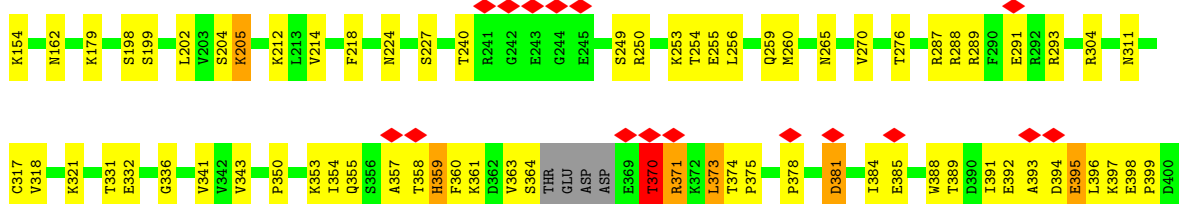
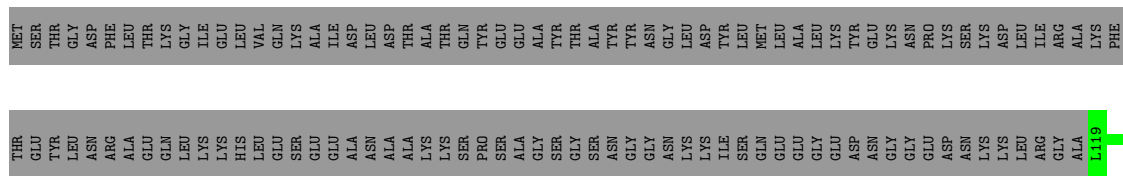


- Molecule 1: Vacuolar protein sorting-associated protein 4

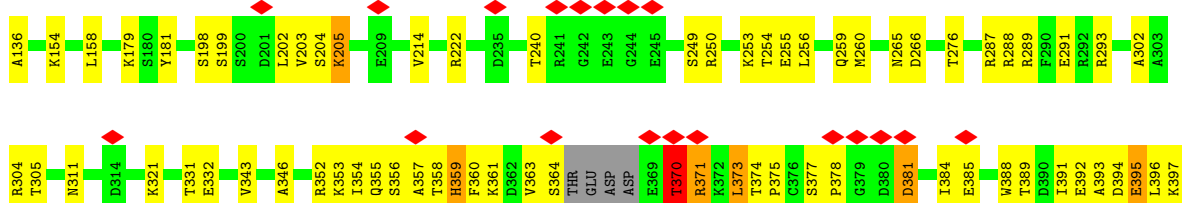
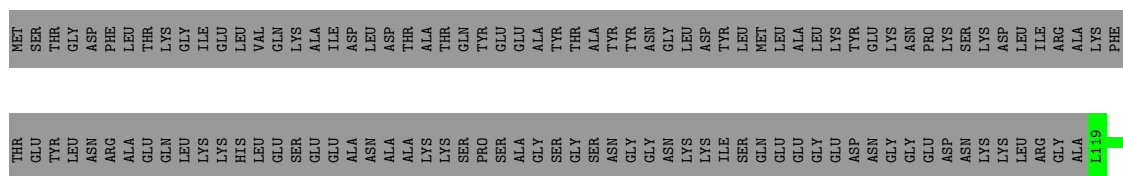




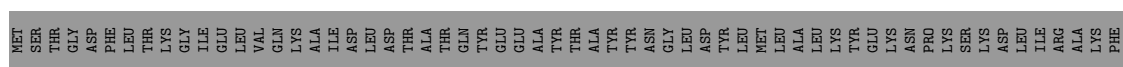
• Molecule 1: Vacuolar protein sorting-associated protein 4

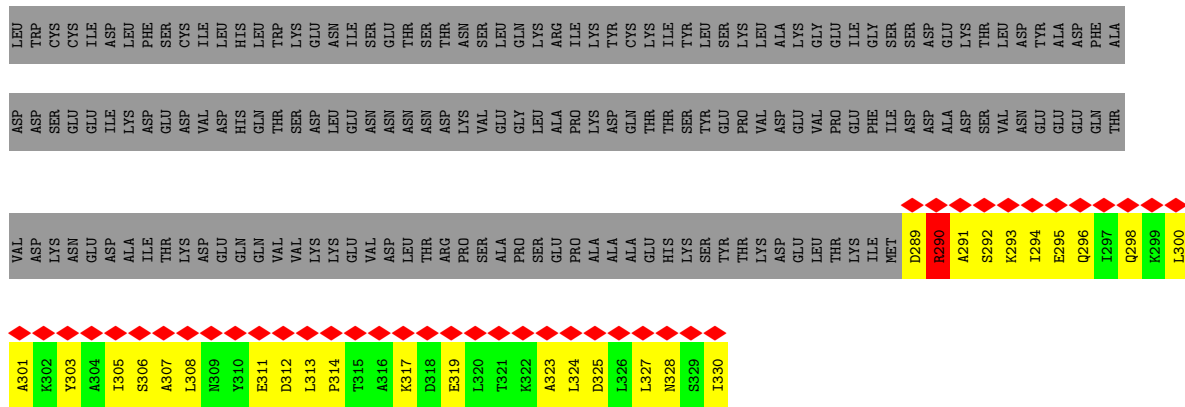


• Molecule 1: Vacuolar protein sorting-associated protein 4

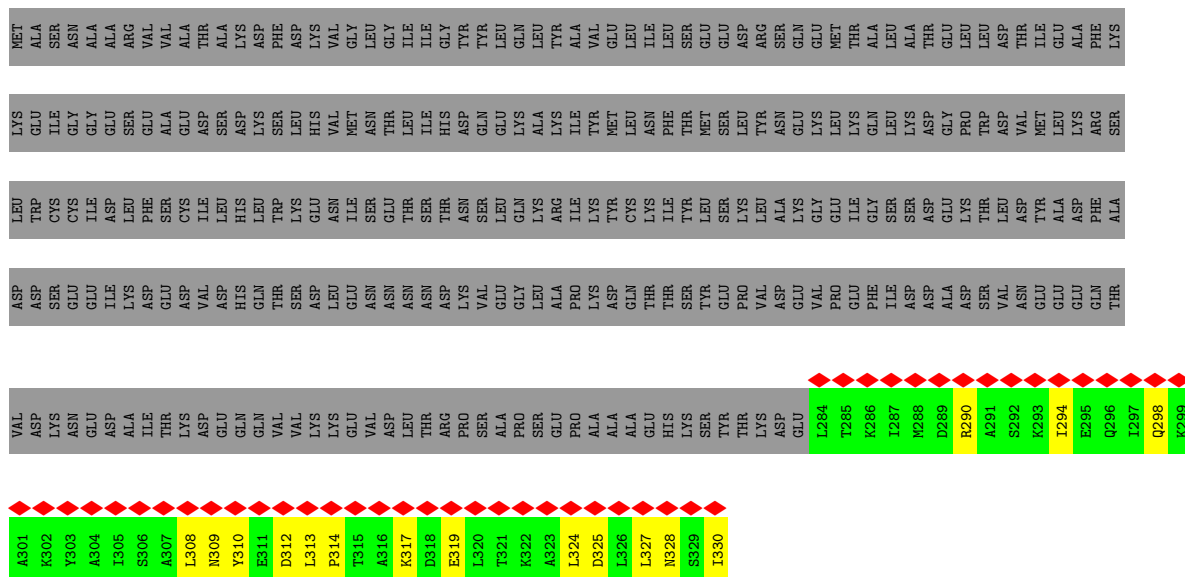


• Molecule 1: Vacuolar protein sorting-associated protein 4

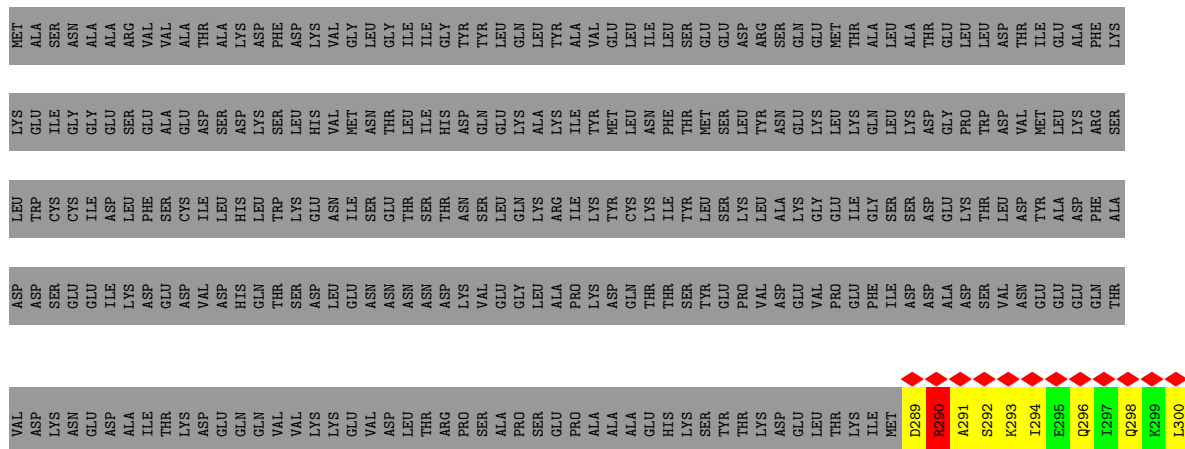




● Molecule 3: Vacuolar protein sorting-associated protein VTA1

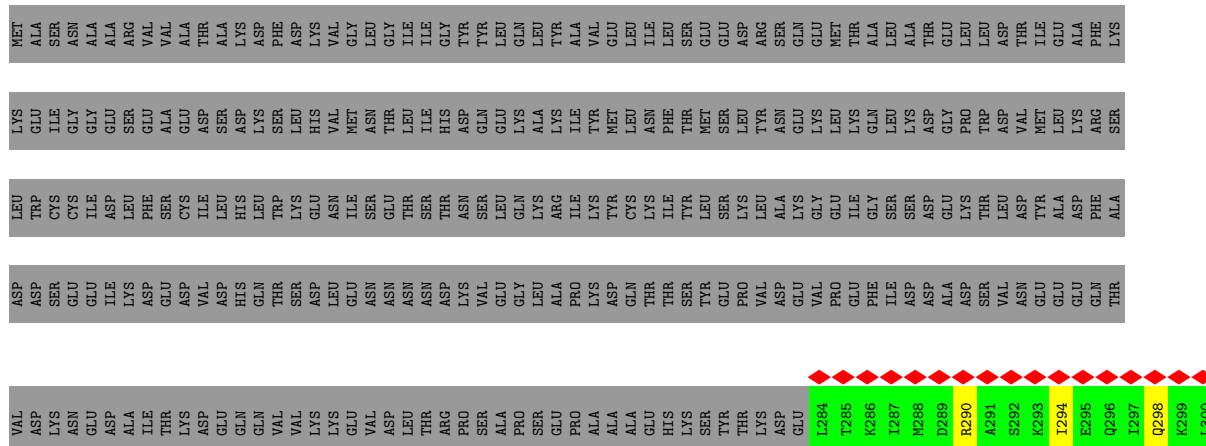


● Molecule 3: Vacuolar protein sorting-associated protein VTA1





● Molecule 3: Vacuolar protein sorting-associated protein VTA1

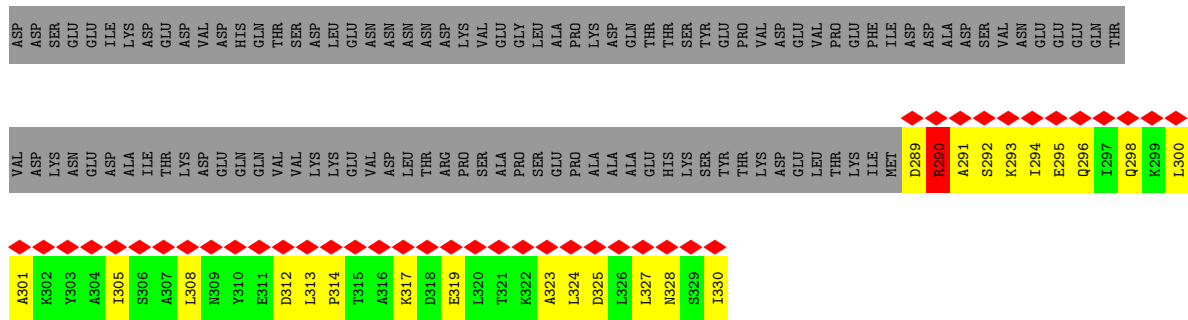


● Molecule 3: Vacuolar protein sorting-associated protein VTA1

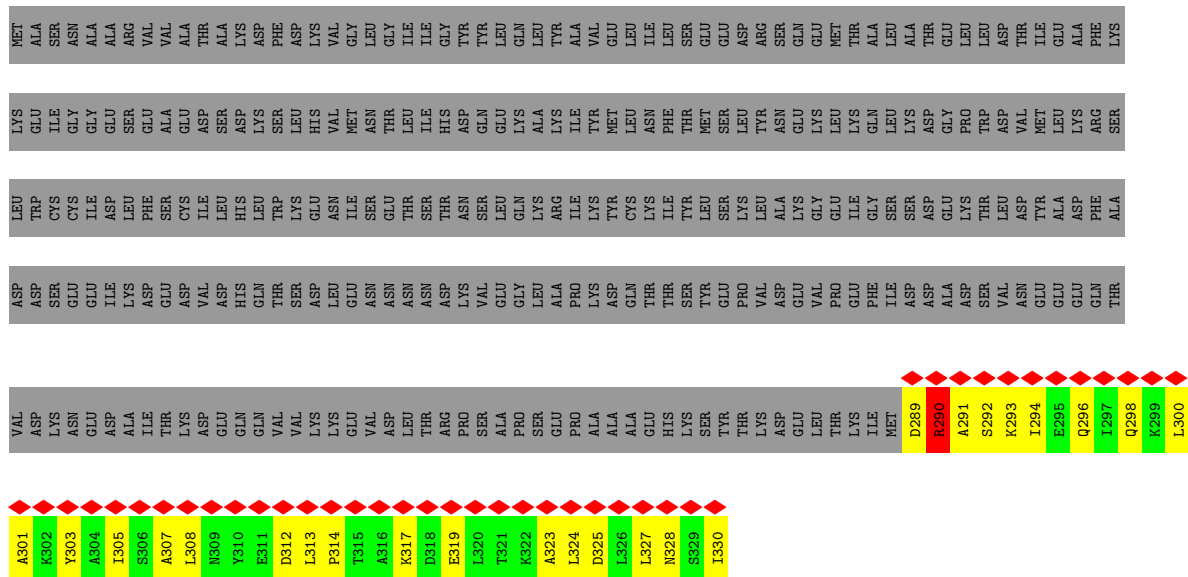


● Molecule 3: Vacuolar protein sorting-associated protein VTA1

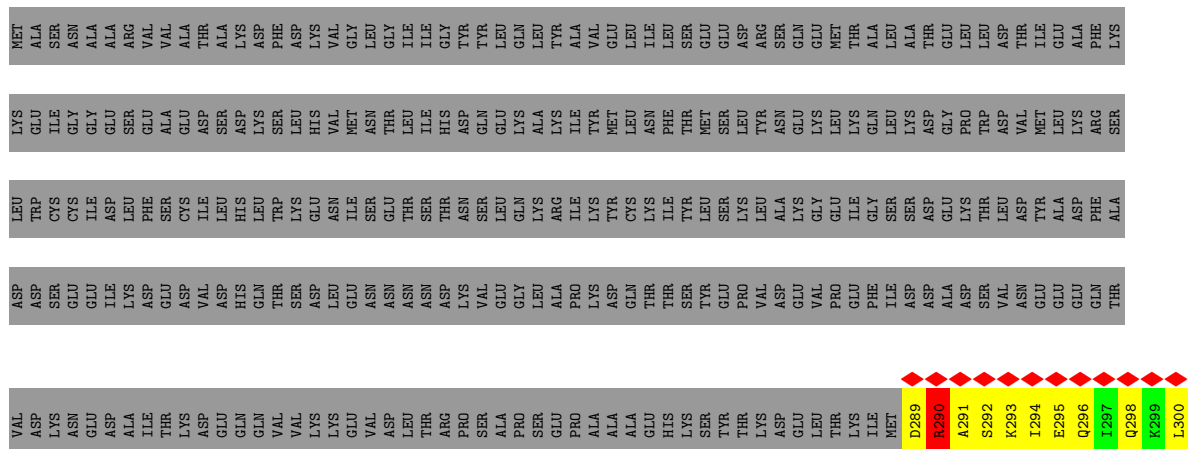




• Molecule 3: Vacuolar protein sorting-associated protein VTA1



• Molecule 3: Vacuolar protein sorting-associated protein VTA1



A301	K302	Y303	A304	I305	S306	A307	L308	N309	Y310	E311	D312	L313	P314	T315	A316	K317	D318	E319	L320	T321	K322	A323	L324	D325	L326	L327	N328	S329	I330
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.017	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0222	Depositor
Map size (Å)	194.442, 194.442, 194.442	wwPDB
Map dimensions	138, 138, 138	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.409, 1.409, 1.409	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ACE, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/2453	0.55	0/3315
1	B	0.36	0/2448	0.55	0/3308
1	C	0.36	0/2448	0.55	0/3308
1	D	0.36	0/2448	0.56	0/3308
1	E	0.35	0/2428	0.57	0/3281
1	F	0.60	0/2384	0.69	2/3222 (0.1%)
3	H	0.52	0/333	0.75	0/447
3	I	0.54	0/406	0.66	0/544
3	J	0.52	0/333	0.75	0/447
3	K	0.52	0/373	0.68	0/500
3	L	0.52	0/333	0.75	0/447
3	M	0.52	0/373	0.68	0/500
3	N	0.52	0/333	0.75	0/447
3	O	0.52	0/333	0.75	0/447
3	P	0.52	0/333	0.75	0/447
3	Q	0.52	0/333	0.75	0/447
3	R	0.53	0/333	0.75	0/447
3	S	0.53	0/333	0.75	0/447
All	All	0.43	0/18758	0.61	2/25309 (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
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	269	GLY	N-CA-C	5.16	126.00	113.10
1	F	287	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	LYS	Peptide
1	A	250	ARG	Sidechain
1	B	205	LYS	Peptide
1	B	270	VAL	Mainchain
1	B	414	ARG	Peptide
1	C	205	LYS	Peptide
1	C	270	VAL	Mainchain
1	D	205	LYS	Peptide
1	E	356	SER	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2412	0	2435	178	0
1	B	2407	0	2430	179	0
1	C	2407	0	2430	124	0
1	D	2407	0	2430	147	0
1	E	2387	0	2407	154	0
1	F	2344	0	2371	208	0
2	G	43	0	12	0	0
3	H	331	0	344	36	0
3	I	404	0	425	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	331	0	344	37	0
3	K	371	0	395	24	0
3	L	331	0	344	39	0
3	M	371	0	395	34	0
3	N	331	0	344	36	0
3	O	331	0	344	38	0
3	P	331	0	344	39	0
3	Q	331	0	344	29	0
3	R	331	0	344	27	0
3	S	331	0	344	59	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	2	0
4	E	27	0	12	1	0
5	A	4	0	0	0	0
5	C	8	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	18682	0	18886	1118	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 30.

All (1118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ILE:HD13	1:C:375:PRO:CG	1.31	1.61
1:F:354:ILE:CG2	1:F:396:LEU:HD21	1.20	1.59
1:B:354:ILE:HA	1:B:375:PRO:CG	1.14	1.59
1:C:354:ILE:HD13	1:C:375:PRO:CD	1.31	1.55
1:A:254:THR:CB	1:F:205:LYS:HD3	1.12	1.54
1:D:389:THR:CG2	1:E:154:LYS:HZ1	1.16	1.54
1:C:354:ILE:CD1	1:C:375:PRO:HD3	1.39	1.50
1:A:325:ARG:HH12	3:S:312:ASP:CB	1.24	1.49
1:F:323:ASP:CB	1:F:403:ILE:HD12	1.46	1.46
1:A:254:THR:CB	1:F:205:LYS:CD	1.95	1.45
1:A:305:THR:HG21	3:S:310:TYR:CE1	1.48	1.44
1:B:354:ILE:O	1:B:360:PHE:CZ	1.72	1.42
1:C:354:ILE:CD1	1:C:375:PRO:CD	1.90	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:CD	3:S:309:ASN:O	1.65	1.41
1:E:318:VAL:CG1	1:E:402:THR:HA	1.51	1.40
1:D:389:THR:CG2	1:E:154:LYS:NZ	1.87	1.36
1:B:321:LYS:HG2	3:I:310:TYR:CD1	1.59	1.36
1:A:325:ARG:NH1	3:S:312:ASP:HB2	1.36	1.36
1:B:321:LYS:CG	3:I:310:TYR:HD1	1.38	1.35
1:E:301:LEU:HD13	3:O:310:TYR:CD1	1.62	1.35
1:E:318:VAL:HB	1:E:401:LEU:O	1.26	1.34
1:B:354:ILE:CA	1:B:375:PRO:CG	2.02	1.33
1:A:325:ARG:NH1	3:S:312:ASP:CB	1.89	1.32
1:F:317:CYS:CB	1:F:401:LEU:HD23	1.60	1.31
1:B:321:LYS:CG	3:I:310:TYR:CD1	2.14	1.30
1:E:318:VAL:HG11	1:E:402:THR:CA	1.61	1.30
1:E:201:ASP:CG	1:F:250:ARG:NH2	1.83	1.29
1:E:404:LYS:HE2	3:P:311:GLU:CG	1.45	1.29
1:C:354:ILE:HA	1:C:375:PRO:CG	1.64	1.28
1:A:254:THR:HB	1:F:205:LYS:CD	1.61	1.27
1:A:254:THR:OG1	1:F:205:LYS:HD3	1.24	1.27
1:B:321:LYS:HD3	3:I:310:TYR:CD1	1.69	1.26
1:B:321:LYS:CD	3:I:310:TYR:CD1	2.19	1.26
1:F:354:ILE:CG2	1:F:396:LEU:CD2	2.14	1.25
1:A:250:ARG:NH1	1:F:204:SER:HB3	1.49	1.25
1:B:354:ILE:CA	1:B:375:PRO:HG2	1.64	1.25
1:F:360:PHE:CG	1:F:391:ILE:HD11	1.72	1.25
1:D:321:LYS:CD	3:M:310:TYR:HA	1.67	1.24
1:C:358:THR:O	1:C:359:HIS:CD2	1.90	1.24
1:A:388:TRP:CZ3	1:B:155:PHE:CZ	2.25	1.23
1:E:201:ASP:OD1	1:F:250:ARG:NH2	1.72	1.22
1:B:354:ILE:CA	1:B:375:PRO:HG3	1.65	1.22
1:B:355:GLN:NE2	1:B:388:TRP:CD2	2.08	1.22
1:B:355:GLN:CG	1:B:388:TRP:CD1	2.23	1.21
1:A:388:TRP:HZ3	1:B:155:PHE:CZ	1.60	1.19
1:B:354:ILE:HG13	1:B:375:PRO:CD	1.72	1.19
1:D:389:THR:HG22	1:E:154:LYS:NZ	1.51	1.19
1:F:354:ILE:HG21	1:F:396:LEU:CD2	1.69	1.19
1:A:322:GLU:CG	3:S:310:TYR:O	1.90	1.19
1:F:317:CYS:HB3	1:F:401:LEU:CD2	1.73	1.19
1:A:388:TRP:CZ3	1:B:155:PHE:CE2	2.31	1.18
1:A:254:THR:HG21	1:F:205:LYS:CG	1.74	1.18
1:E:404:LYS:CE	3:P:311:GLU:HG3	1.74	1.17
1:E:201:ASP:OD2	1:F:250:ARG:NH2	1.71	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:O	1:B:359:HIS:CD2	1.96	1.16
1:E:201:ASP:OD1	1:F:250:ARG:CZ	1.93	1.16
1:B:355:GLN:CD	1:B:388:TRP:CD1	2.18	1.16
1:B:355:GLN:HG2	1:B:388:TRP:CG	1.80	1.16
1:A:254:THR:HB	1:F:205:LYS:CE	1.74	1.16
1:B:355:GLN:HG2	1:B:388:TRP:CB	1.76	1.16
1:E:404:LYS:CE	3:P:311:GLU:CG	2.23	1.16
1:F:323:ASP:HB3	1:F:403:ILE:HD12	1.16	1.15
1:E:301:LEU:HD13	3:O:310:TYR:CE1	1.82	1.15
1:A:305:THR:HG21	3:S:310:TYR:CZ	1.83	1.12
1:F:319:LEU:HD21	1:F:403:ILE:HA	1.30	1.12
1:E:393:ALA:HB1	1:F:157:HIS:CE1	1.81	1.12
1:C:354:ILE:HA	1:C:375:PRO:HG3	1.14	1.11
1:A:251:ARG:O	1:F:205:LYS:NZ	1.82	1.11
1:F:253:LYS:HE3	1:F:283:ASP:OD2	1.47	1.11
1:A:240:THR:HG21	1:A:250:ARG:HH21	1.07	1.11
1:B:354:ILE:HA	1:B:375:PRO:HG2	1.12	1.11
1:D:321:LYS:CG	3:M:310:TYR:HA	1.79	1.11
1:A:254:THR:CG2	1:F:205:LYS:CD	2.29	1.10
1:C:354:ILE:HD13	1:C:375:PRO:HG2	1.31	1.10
1:D:389:THR:HG23	1:E:154:LYS:NZ	1.67	1.10
1:B:358:THR:OG1	1:B:385:GLU:HG3	1.52	1.10
1:A:254:THR:HG21	1:F:205:LYS:HG2	1.19	1.09
1:B:355:GLN:CD	1:B:388:TRP:CG	2.26	1.09
1:C:354:ILE:HD12	1:C:375:PRO:HD3	1.26	1.09
1:A:250:ARG:NH1	1:F:204:SER:CB	2.16	1.08
1:D:321:LYS:HD3	3:M:310:TYR:HA	1.36	1.08
1:D:302:ALA:O	3:M:310:TYR:OH	1.72	1.08
1:B:355:GLN:HG2	1:B:388:TRP:HB3	1.24	1.07
1:F:319:LEU:CD2	1:F:403:ILE:HB	1.84	1.07
1:B:354:ILE:HG13	1:B:375:PRO:HD3	1.12	1.06
1:D:373:LEU:HD12	1:D:391:ILE:HD13	1.38	1.05
1:F:373:LEU:HD12	1:F:391:ILE:HD13	1.38	1.05
1:A:373:LEU:HD12	1:A:391:ILE:HD13	1.38	1.05
1:C:358:THR:O	1:C:359:HIS:CG	2.09	1.05
1:A:325:ARG:HH12	3:S:312:ASP:CG	1.57	1.04
1:B:355:GLN:CG	1:B:388:TRP:CG	2.38	1.04
1:D:389:THR:HG22	1:E:154:LYS:HZ1	0.99	1.04
1:A:353:LYS:HD2	1:A:399:PRO:HG2	1.36	1.03
1:D:321:LYS:HD3	3:M:310:TYR:CA	1.88	1.03
1:A:163:ARG:HD3	1:F:351:ILE:HG12	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:CG2	3:S:310:TYR:CE1	2.41	1.03
1:A:321:LYS:HD3	3:S:309:ASN:O	0.87	1.03
1:C:354:ILE:CD1	1:C:375:PRO:CG	2.24	1.03
1:C:373:LEU:HD12	1:C:391:ILE:HD13	1.38	1.03
1:E:301:LEU:CD1	3:O:310:TYR:CD1	2.40	1.03
1:E:373:LEU:HD12	1:E:391:ILE:CD1	1.89	1.03
1:B:325:ARG:NH1	3:I:312:ASP:OD2	1.91	1.02
1:C:373:LEU:HD12	1:C:391:ILE:CD1	1.89	1.02
1:A:373:LEU:HD12	1:A:391:ILE:CD1	1.89	1.02
1:D:354:ILE:HA	1:D:375:PRO:CG	1.89	1.02
1:A:254:THR:HG21	1:F:205:LYS:CD	1.88	1.02
1:B:355:GLN:NE2	1:B:388:TRP:CG	2.26	1.02
1:B:373:LEU:HD12	1:B:391:ILE:HD13	1.38	1.02
1:D:321:LYS:HG2	3:M:310:TYR:HA	1.39	1.02
1:F:373:LEU:HD12	1:F:391:ILE:CD1	1.89	1.02
1:B:321:LYS:HG2	3:I:310:TYR:HD1	0.85	1.02
1:B:373:LEU:HD12	1:B:391:ILE:CD1	1.89	1.02
1:B:354:ILE:CG1	1:B:375:PRO:HD3	1.90	1.02
1:D:352:ARG:O	1:D:356:SER:HB3	1.59	1.01
1:E:201:ASP:CG	1:F:250:ARG:HH22	1.52	1.01
1:F:360:PHE:CG	1:F:391:ILE:CD1	2.41	1.01
1:F:354:ILE:HG23	1:F:396:LEU:HD11	1.39	1.01
1:A:250:ARG:HH11	1:F:204:SER:CB	1.71	1.01
1:A:322:GLU:HG2	3:S:310:TYR:O	1.54	1.01
1:D:373:LEU:HD12	1:D:391:ILE:CD1	1.89	1.01
1:F:323:ASP:CA	1:F:403:ILE:HD12	1.91	1.01
1:D:361:LYS:HD2	1:D:381:ASP:O	1.61	1.00
1:E:318:VAL:CB	1:E:401:LEU:O	2.07	1.00
1:E:361:LYS:HD2	1:E:381:ASP:O	1.61	1.00
1:D:358:THR:HG21	3:N:303:TYR:CE1	1.97	1.00
1:A:254:THR:CG2	1:F:205:LYS:HD3	1.90	1.00
1:F:361:LYS:HD2	1:F:381:ASP:O	1.61	1.00
1:C:354:ILE:HG23	1:C:360:PHE:HE2	1.27	0.99
1:C:361:LYS:HD2	1:C:381:ASP:O	1.61	0.99
1:E:325:ARG:NH2	3:O:310:TYR:O	1.94	0.99
1:B:361:LYS:HD2	1:B:381:ASP:O	1.61	0.99
1:F:357:ALA:HB1	1:F:375:PRO:HG3	1.45	0.99
1:E:373:LEU:HD12	1:E:391:ILE:HD13	1.38	0.99
1:B:358:THR:O	1:B:359:HIS:CG	2.15	0.99
1:A:251:ARG:CZ	1:F:205:LYS:O	2.10	0.98
1:A:361:LYS:HD2	1:A:381:ASP:O	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ILE:HA	1:D:375:PRO:HG3	1.41	0.98
1:D:377:SER:OG	3:N:307:ALA:HA	1.62	0.98
1:F:323:ASP:CB	1:F:403:ILE:CD1	2.41	0.98
1:C:358:THR:OG1	1:C:385:GLU:HG3	1.62	0.98
1:D:358:THR:OG1	1:D:385:GLU:HG3	1.62	0.98
1:A:322:GLU:OE2	3:S:310:TYR:O	1.81	0.98
1:A:254:THR:CG2	1:F:205:LYS:HE2	1.94	0.97
1:F:360:PHE:HD1	1:F:386:MET:HG3	1.30	0.97
1:A:377:SER:OG	3:H:307:ALA:HA	1.64	0.97
1:B:354:ILE:HG12	1:B:360:PHE:HE2	1.28	0.97
1:F:354:ILE:HG23	1:F:396:LEU:HD21	1.46	0.97
1:B:354:ILE:CD1	1:B:396:LEU:CD1	2.43	0.96
1:B:354:ILE:HD11	1:B:396:LEU:HD12	1.47	0.96
1:D:389:THR:CB	1:E:154:LYS:HZ1	1.77	0.96
1:A:254:THR:HB	1:F:205:LYS:NZ	1.80	0.96
1:D:321:LYS:CD	3:M:310:TYR:CA	2.41	0.96
1:F:319:LEU:HD23	1:F:403:ILE:HB	1.47	0.96
1:D:321:LYS:HD3	3:M:309:ASN:O	1.65	0.96
1:D:354:ILE:HD11	1:D:398:GLU:HA	1.45	0.96
1:C:357:ALA:HB2	3:L:306:SER:HB2	1.48	0.95
1:D:388:TRP:CE3	1:E:155:PHE:HE2	1.82	0.95
1:A:254:THR:HB	1:F:205:LYS:HD3	1.15	0.95
1:B:354:ILE:HD13	1:B:396:LEU:HD11	1.45	0.95
1:A:321:LYS:HG2	3:S:310:TYR:CD1	2.01	0.95
1:F:323:ASP:HB3	1:F:403:ILE:CD1	1.98	0.94
1:A:388:TRP:CZ3	1:B:155:PHE:HZ	1.73	0.94
1:A:254:THR:CG2	1:F:205:LYS:CE	2.46	0.94
1:A:388:TRP:HZ3	1:B:155:PHE:HZ	1.03	0.94
1:B:346:ALA:O	1:B:401:LEU:CD2	2.15	0.94
1:E:357:ALA:HB1	3:P:306:SER:HB2	1.50	0.93
1:F:360:PHE:CD1	1:F:391:ILE:HD11	2.04	0.93
1:A:240:THR:CG2	1:A:250:ARG:HH21	1.81	0.93
1:D:321:LYS:HD3	3:M:309:ASN:C	1.89	0.93
1:B:355:GLN:HG2	1:B:388:TRP:CD1	1.97	0.92
1:B:354:ILE:HG13	1:B:375:PRO:CG	1.97	0.92
1:E:388:TRP:HZ2	1:F:147:GLU:OE1	1.50	0.92
1:C:354:ILE:HA	1:C:375:PRO:HG2	1.52	0.92
1:D:358:THR:O	1:D:359:HIS:CD2	2.22	0.92
1:A:305:THR:HG21	3:S:310:TYR:HE1	1.16	0.92
1:A:388:TRP:CZ3	1:B:155:PHE:HE2	1.87	0.91
1:E:393:ALA:HB1	1:F:157:HIS:HE1	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ILE:CD1	1:B:396:LEU:HD11	2.01	0.91
1:F:354:ILE:HG22	1:F:396:LEU:HD21	1.48	0.91
1:A:325:ARG:HH11	3:S:312:ASP:HB2	1.21	0.91
1:A:254:THR:CB	1:F:205:LYS:CE	2.42	0.90
1:A:325:ARG:NH1	3:S:312:ASP:OD2	2.04	0.90
1:C:318:VAL:HG11	1:C:402:THR:HA	1.52	0.90
1:D:305:THR:HB	3:M:310:TYR:OH	1.68	0.89
1:A:358:THR:O	1:A:359:HIS:CD2	2.26	0.89
1:B:355:GLN:HB3	1:B:388:TRP:CD1	2.08	0.89
1:A:353:LYS:CD	1:A:399:PRO:HG2	2.02	0.89
1:B:358:THR:OG1	1:B:385:GLU:CG	2.21	0.89
1:E:388:TRP:CZ2	1:F:147:GLU:OE1	2.26	0.89
1:B:354:ILE:HA	1:B:375:PRO:HG3	0.89	0.89
1:C:355:GLN:HG2	1:C:388:TRP:CD2	2.08	0.89
1:A:163:ARG:CD	1:F:351:ILE:HG12	2.03	0.89
1:A:322:GLU:CD	3:S:310:TYR:O	2.11	0.89
1:F:319:LEU:CD2	1:F:403:ILE:HA	2.03	0.88
1:F:360:PHE:CD2	1:F:391:ILE:CD1	2.56	0.88
1:A:240:THR:HG21	1:A:250:ARG:NH2	1.87	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CB	2.51	0.88
1:D:354:ILE:CG2	1:D:396:LEU:HD11	2.02	0.88
1:B:321:LYS:CD	3:I:310:TYR:HD1	1.71	0.88
1:B:354:ILE:O	1:B:360:PHE:HZ	1.26	0.88
1:E:301:LEU:CD1	3:O:310:TYR:CG	2.56	0.88
1:F:319:LEU:HD21	1:F:403:ILE:CA	2.04	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CA	2.51	0.88
1:B:355:GLN:CB	1:B:388:TRP:CD1	2.57	0.87
1:C:354:ILE:HG23	1:C:360:PHE:CE2	2.09	0.87
1:A:354:ILE:HD13	1:A:396:LEU:HD21	1.57	0.87
1:A:325:ARG:HH12	3:S:312:ASP:HB3	1.37	0.86
1:F:323:ASP:CG	1:F:403:ILE:HD12	1.96	0.86
1:A:388:TRP:CH2	1:B:155:PHE:HE2	1.92	0.86
1:F:354:ILE:HG23	1:F:396:LEU:CD1	2.06	0.85
1:A:163:ARG:HG3	1:F:348:MET:SD	2.16	0.85
1:A:254:THR:HB	1:F:205:LYS:HZ3	1.39	0.85
1:D:354:ILE:HD11	1:D:398:GLU:CA	2.06	0.85
1:D:388:TRP:HE3	1:E:155:PHE:HE2	1.20	0.85
1:A:250:ARG:HD2	1:F:204:SER:HB2	1.59	0.85
1:D:388:TRP:CD2	1:E:154:LYS:NZ	2.36	0.85
1:B:321:LYS:HD2	3:I:310:TYR:HA	1.59	0.84
1:B:354:ILE:CB	1:B:375:PRO:CG	2.54	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:OG	3:J:307:ALA:HA	1.75	0.84
1:E:385:GLU:OE2	3:P:303:TYR:OH	1.95	0.84
1:E:357:ALA:CB	3:P:306:SER:HB2	2.08	0.84
1:F:355:GLN:O	1:F:388:TRP:CD1	2.31	0.83
1:A:325:ARG:CZ	3:S:312:ASP:OD2	2.26	0.83
1:F:354:ILE:HG21	1:F:396:LEU:HD21	0.85	0.83
1:E:318:VAL:HG11	1:E:402:THR:HA	0.84	0.83
1:A:254:THR:OG1	1:F:205:LYS:CD	2.12	0.83
1:E:301:LEU:HD13	3:O:310:TYR:CG	2.13	0.83
1:C:358:THR:OG1	1:C:385:GLU:CG	2.27	0.83
1:B:321:LYS:NZ	3:I:309:ASN:O	2.11	0.82
1:E:408:LYS:CE	3:Q:295:GLU:HB2	2.09	0.82
1:B:321:LYS:CG	3:I:310:TYR:CE1	2.61	0.82
1:A:251:ARG:NH1	1:F:205:LYS:O	2.11	0.82
1:D:389:THR:CA	1:E:154:LYS:HZ1	1.92	0.82
1:E:302:ALA:HB2	3:O:309:ASN:O	1.79	0.82
1:A:305:THR:HB	3:S:310:TYR:OH	1.80	0.82
1:D:385:GLU:OE2	3:N:303:TYR:OH	1.97	0.82
1:C:358:THR:HG23	1:C:359:HIS:CD2	2.14	0.81
1:C:354:ILE:CA	1:C:375:PRO:CG	2.53	0.81
1:D:354:ILE:HD11	1:D:398:GLU:HB3	1.61	0.81
1:F:350:PRO:HB3	1:F:399:PRO:O	1.80	0.81
1:B:354:ILE:HA	1:B:375:PRO:CB	2.11	0.81
1:D:389:THR:CA	1:E:154:LYS:NZ	2.44	0.81
1:B:354:ILE:O	1:B:360:PHE:CE2	2.33	0.81
3:J:311:GLU:CD	3:K:290:ARG:HH12	1.84	0.81
3:H:311:GLU:CD	3:I:290:ARG:HH12	1.84	0.80
3:L:311:GLU:CD	3:M:290:ARG:HH12	1.85	0.80
1:C:357:ALA:HB2	3:L:306:SER:CB	2.11	0.80
1:D:354:ILE:HG21	1:D:396:LEU:HD11	1.62	0.80
1:B:354:ILE:HD13	1:B:396:LEU:CD1	2.10	0.80
1:B:355:GLN:HB3	1:B:388:TRP:HD1	1.42	0.80
1:E:186:VAL:O	1:E:190:ALA:HB2	1.82	0.80
1:A:321:LYS:HG2	3:S:310:TYR:HD1	1.42	0.80
1:B:321:LYS:HD3	3:I:310:TYR:CE1	2.17	0.80
1:F:317:CYS:HB3	1:F:401:LEU:HD23	0.83	0.80
1:D:352:ARG:O	1:D:356:SER:CB	2.30	0.80
1:D:388:TRP:CE3	1:E:155:PHE:CE2	2.70	0.80
1:F:385:GLU:OE2	3:R:303:TYR:OH	1.99	0.80
1:E:249:SER:O	1:E:253:LYS:HB3	1.82	0.79
1:A:358:THR:OG1	1:A:385:GLU:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:ALA:HB1	3:P:306:SER:CB	2.12	0.79
1:C:249:SER:O	1:C:253:LYS:HB3	1.82	0.79
1:B:321:LYS:CD	3:I:309:ASN:O	2.31	0.79
1:A:305:THR:CG2	3:S:310:TYR:HE1	1.86	0.79
1:A:254:THR:HG22	1:F:205:LYS:HE2	1.64	0.79
1:A:358:THR:HG23	1:A:359:HIS:CD2	2.18	0.79
1:B:249:SER:O	1:B:253:LYS:HB3	1.82	0.79
1:D:249:SER:O	1:D:253:LYS:HB3	1.82	0.79
1:E:408:LYS:HE3	3:Q:295:GLU:HB2	1.65	0.79
1:C:354:ILE:CD1	1:C:375:PRO:HD2	2.12	0.79
1:C:354:ILE:HD11	1:C:375:PRO:HD3	1.61	0.79
1:C:358:THR:O	1:C:359:HIS:CB	2.30	0.78
1:D:354:ILE:O	1:D:360:PHE:HZ	1.65	0.78
1:F:317:CYS:CB	1:F:401:LEU:CD2	2.45	0.78
1:A:321:LYS:HD2	3:S:309:ASN:O	1.81	0.78
1:D:321:LYS:HD3	3:M:310:TYR:N	1.97	0.78
1:E:146:LYS:O	1:E:150:ILE:HB	1.82	0.78
1:E:301:LEU:HD12	3:O:310:TYR:CG	2.18	0.78
1:E:201:ASP:OD1	1:F:250:ARG:NH1	2.14	0.78
1:B:354:ILE:CG1	1:B:375:PRO:CG	2.62	0.78
1:D:354:ILE:HA	1:D:375:PRO:HG2	1.65	0.78
1:E:358:THR:HG21	3:P:303:TYR:CE1	2.19	0.78
1:F:204:SER:O	1:F:207:MET:SD	2.41	0.78
1:B:321:LYS:HD3	3:I:309:ASN:O	1.82	0.78
1:C:396:LEU:HD23	1:D:158:LEU:HD21	1.65	0.78
3:P:289:ASP:O	3:P:290:ARG:HB3	1.84	0.78
3:S:289:ASP:O	3:S:290:ARG:HB3	1.84	0.78
1:A:246:SER:HA	1:A:250:ARG:HG2	1.64	0.78
1:C:354:ILE:CA	1:C:375:PRO:HG2	2.14	0.78
3:N:291:ALA:HA	3:N:294:ILE:HD11	1.66	0.77
1:B:354:ILE:HG12	1:B:360:PHE:CE2	2.18	0.77
1:D:354:ILE:CD1	1:D:398:GLU:HB3	2.14	0.77
3:O:291:ALA:HA	3:O:294:ILE:HD11	1.66	0.77
3:Q:291:ALA:HA	3:Q:294:ILE:HD11	1.66	0.77
3:J:291:ALA:HA	3:J:294:ILE:HD11	1.66	0.77
1:D:358:THR:O	1:D:359:HIS:CG	2.37	0.77
3:J:289:ASP:O	3:J:290:ARG:HB3	1.84	0.77
3:S:291:ALA:HA	3:S:294:ILE:HD11	1.66	0.77
1:B:358:THR:HG23	1:B:359:HIS:CD2	2.20	0.77
3:H:291:ALA:HA	3:H:294:ILE:HD11	1.66	0.77
3:L:291:ALA:HA	3:L:294:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:291:ALA:HA	3:P:294:ILE:HD11	1.66	0.77
1:C:361:LYS:CD	1:C:381:ASP:O	2.33	0.77
1:F:319:LEU:HD22	1:F:403:ILE:HB	1.65	0.77
3:L:289:ASP:O	3:L:290:ARG:HB3	1.84	0.77
3:Q:289:ASP:O	3:Q:290:ARG:HB3	1.84	0.77
1:B:358:THR:O	1:B:359:HIS:CB	2.32	0.76
1:E:361:LYS:CD	1:E:381:ASP:O	2.33	0.76
1:D:354:ILE:O	1:D:360:PHE:CZ	2.39	0.76
3:H:308:LEU:HD12	3:I:298:GLN:HG3	1.67	0.76
3:J:308:LEU:HD12	3:K:298:GLN:HG3	1.67	0.76
1:C:358:THR:O	1:C:359:HIS:HD2	1.67	0.76
3:O:289:ASP:O	3:O:290:ARG:HB3	1.84	0.76
1:B:361:LYS:CD	1:B:381:ASP:O	2.33	0.76
1:D:361:LYS:CD	1:D:381:ASP:O	2.33	0.76
3:H:289:ASP:O	3:H:290:ARG:HB3	1.84	0.75
3:N:289:ASP:O	3:N:290:ARG:HB3	1.84	0.75
1:D:354:ILE:HD11	1:D:398:GLU:CB	2.16	0.75
3:L:308:LEU:HD12	3:M:298:GLN:HG3	1.67	0.75
3:R:289:ASP:O	3:R:290:ARG:HB3	1.84	0.75
3:R:291:ALA:HA	3:R:294:ILE:HD11	1.66	0.75
1:D:346:ALA:O	1:D:401:LEU:HD13	1.86	0.75
1:D:389:THR:CG2	1:E:154:LYS:HZ2	1.94	0.75
1:F:323:ASP:CG	1:F:403:ILE:CD1	2.55	0.75
1:B:355:GLN:CD	1:B:388:TRP:CD2	2.57	0.75
1:A:358:THR:O	1:A:359:HIS:CB	2.34	0.75
1:C:354:ILE:HD11	1:C:375:PRO:CD	2.09	0.75
1:A:353:LYS:HD2	1:A:399:PRO:CG	2.16	0.75
1:A:358:THR:O	1:A:359:HIS:CG	2.39	0.75
1:A:361:LYS:CD	1:A:381:ASP:O	2.33	0.75
1:B:346:ALA:O	1:B:401:LEU:HD21	1.85	0.74
1:E:404:LYS:HE2	3:P:311:GLU:HG3	0.78	0.74
1:E:375:PRO:HB2	3:P:310:TYR:OH	1.86	0.74
1:F:361:LYS:CD	1:F:381:ASP:O	2.33	0.74
1:D:346:ALA:O	1:D:401:LEU:CD1	2.36	0.74
1:E:318:VAL:HG11	1:E:402:THR:CB	2.17	0.74
1:F:319:LEU:HD23	1:F:403:ILE:CB	2.14	0.74
1:D:389:THR:HG22	1:E:154:LYS:CE	2.16	0.74
1:B:354:ILE:CB	1:B:375:PRO:HG2	2.16	0.73
1:A:305:THR:CG2	3:S:310:TYR:CZ	2.68	0.73
1:B:354:ILE:CG1	1:B:375:PRO:CD	2.58	0.73
1:A:325:ARG:NH1	3:S:312:ASP:CG	2.25	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:GLU:O	1:E:151:LEU:HB3	1.88	0.73
1:A:250:ARG:HH11	1:F:204:SER:HB2	1.53	0.72
1:C:321:LYS:HG2	3:K:310:TYR:HD1	1.53	0.72
1:D:358:THR:O	1:D:359:HIS:CB	2.37	0.72
1:B:355:GLN:CB	1:B:388:TRP:HD1	2.00	0.72
1:F:323:ASP:OD1	1:F:403:ILE:HD13	1.89	0.72
1:C:318:VAL:HB	1:C:401:LEU:O	1.90	0.72
1:D:394:ASP:O	1:D:396:LEU:N	2.24	0.71
1:C:394:ASP:O	1:C:396:LEU:N	2.24	0.71
1:D:389:THR:HA	1:E:154:LYS:NZ	2.05	0.71
1:E:408:LYS:NZ	3:Q:295:GLU:HB2	2.06	0.71
1:F:394:ASP:O	1:F:396:LEU:N	2.24	0.71
1:C:321:LYS:HD3	3:K:309:ASN:O	1.90	0.71
1:E:394:ASP:O	1:E:396:LEU:N	2.24	0.71
1:F:360:PHE:CD1	1:F:391:ILE:CD1	2.71	0.71
1:D:358:THR:HG23	1:D:359:HIS:CD2	2.25	0.71
1:A:305:THR:CB	3:S:310:TYR:OH	2.39	0.71
1:B:355:GLN:OE1	1:B:388:TRP:NE1	2.24	0.71
1:B:354:ILE:HD11	1:B:396:LEU:CD1	2.12	0.70
1:D:358:THR:OG1	1:D:385:GLU:CG	2.37	0.70
1:E:318:VAL:CG1	1:E:401:LEU:O	2.39	0.70
1:F:355:GLN:O	1:F:388:TRP:NE1	2.24	0.70
1:F:373:LEU:CD1	1:F:391:ILE:CD1	2.69	0.70
1:B:398:GLU:OE1	1:B:398:GLU:N	2.21	0.70
1:D:402:THR:O	1:D:405:ASP:HB2	1.90	0.70
1:E:403:ILE:O	1:E:406:PHE:N	2.24	0.70
1:F:360:PHE:CE2	1:F:391:ILE:HD12	2.26	0.70
1:A:388:TRP:CH2	1:B:154:LYS:NZ	2.59	0.70
1:D:354:ILE:HG23	1:D:396:LEU:HD11	1.72	0.70
1:F:346:ALA:CB	1:F:406:PHE:CD2	2.74	0.70
1:F:349:GLN:OE1	1:F:352:ARG:HD2	1.92	0.70
1:B:354:ILE:HG13	1:B:375:PRO:HG3	1.69	0.70
1:C:318:VAL:CG1	1:C:402:THR:HA	2.22	0.70
1:A:250:ARG:HH12	1:F:204:SER:HB3	1.55	0.70
1:A:251:ARG:HH12	1:F:206:TRP:HA	1.57	0.70
1:A:305:THR:CG2	3:S:310:TYR:OH	2.39	0.69
1:B:354:ILE:CG1	1:B:375:PRO:HG3	2.19	0.69
1:F:346:ALA:HB3	1:F:406:PHE:CE2	2.27	0.69
1:B:352:ARG:O	1:B:356:SER:HB2	1.92	0.69
1:F:317:CYS:HA	1:F:401:LEU:HB3	1.72	0.69
1:A:325:ARG:NH2	3:S:312:ASP:OD2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:LEU:CD1	1:E:391:ILE:HD13	2.20	0.69
1:A:373:LEU:CD1	1:A:391:ILE:HD13	2.20	0.69
1:A:373:LEU:CD1	1:A:391:ILE:CD1	2.69	0.69
1:A:394:ASP:O	1:A:396:LEU:N	2.24	0.69
1:B:354:ILE:N	1:B:375:PRO:HG2	2.07	0.69
1:B:373:LEU:CD1	1:B:391:ILE:CD1	2.69	0.69
1:E:373:LEU:CD1	1:E:391:ILE:CD1	2.69	0.69
1:B:355:GLN:CG	1:B:388:TRP:HB3	2.15	0.68
1:B:398:GLU:HB2	1:B:399:PRO:HD2	1.74	0.68
1:A:254:THR:CG2	1:F:205:LYS:CG	2.59	0.68
1:B:346:ALA:O	1:B:401:LEU:HD22	1.93	0.68
1:C:350:PRO:HB3	1:C:399:PRO:HD2	1.74	0.68
1:D:373:LEU:CD1	1:D:391:ILE:CD1	2.69	0.68
1:F:323:ASP:HA	1:F:403:ILE:HD12	1.74	0.68
1:D:373:LEU:CD1	1:D:391:ILE:HD13	2.20	0.68
1:F:263:VAL:HG12	1:F:267:SER:CB	2.23	0.68
1:B:394:ASP:O	1:B:396:LEU:N	2.24	0.68
1:F:373:LEU:CD1	1:F:391:ILE:HD13	2.20	0.68
1:B:354:ILE:CD1	1:B:396:LEU:HD12	2.11	0.68
3:R:290:ARG:H	3:R:293:LYS:HG2	1.58	0.68
1:A:155:PHE:HE2	1:F:388:TRP:CZ3	2.12	0.67
1:B:358:THR:O	1:B:359:HIS:HD2	1.70	0.67
1:A:250:ARG:CD	1:F:204:SER:HB2	2.22	0.67
1:A:251:ARG:NH1	1:F:206:TRP:HA	2.09	0.67
1:A:322:GLU:OE2	3:S:311:GLU:HB2	1.94	0.67
3:J:308:LEU:HD12	3:K:298:GLN:CG	2.25	0.67
1:E:318:VAL:HG12	1:E:402:THR:HA	1.66	0.67
1:B:373:LEU:CD1	1:B:391:ILE:HD13	2.20	0.67
1:F:263:VAL:HG12	1:F:267:SER:HB2	1.77	0.67
1:C:374:THR:HB	1:C:397:LYS:HB3	1.76	0.67
1:F:253:LYS:CE	1:F:283:ASP:OD2	2.34	0.67
3:J:308:LEU:HD13	3:K:294:ILE:HG23	1.77	0.66
1:D:389:THR:HG23	1:E:154:LYS:HZ2	1.52	0.66
1:B:355:GLN:NE2	1:B:388:TRP:CE3	2.62	0.66
1:F:360:PHE:CD2	1:F:391:ILE:HD12	2.30	0.66
3:N:291:ALA:HA	3:N:294:ILE:CD1	2.26	0.66
3:R:291:ALA:HA	3:R:294:ILE:CD1	2.26	0.66
3:S:291:ALA:HA	3:S:294:ILE:CD1	2.26	0.66
1:A:358:THR:O	1:A:359:HIS:HB2	1.95	0.66
3:H:291:ALA:HA	3:H:294:ILE:CD1	2.26	0.66
3:H:308:LEU:HD13	3:I:294:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LEU:CD1	1:C:391:ILE:CD1	2.69	0.66
3:Q:291:ALA:HA	3:Q:294:ILE:CD1	2.26	0.66
1:D:389:THR:N	1:E:154:LYS:HZ3	1.94	0.66
1:E:393:ALA:CB	1:F:157:HIS:CE1	2.69	0.66
1:F:323:ASP:OD1	1:F:403:ILE:CD1	2.44	0.66
3:H:308:LEU:HD12	3:I:298:GLN:CG	2.25	0.66
1:B:355:GLN:CG	1:B:388:TRP:CB	2.64	0.65
3:L:308:LEU:HD13	3:M:294:ILE:HG23	1.77	0.65
3:O:291:ALA:HA	3:O:294:ILE:CD1	2.26	0.65
3:P:291:ALA:HA	3:P:294:ILE:CD1	2.26	0.65
1:B:203:VAL:O	1:C:212:LYS:NZ	2.30	0.65
1:F:405:ASP:O	1:F:408:LYS:HB3	1.97	0.65
3:L:291:ALA:HA	3:L:294:ILE:CD1	2.26	0.65
3:L:308:LEU:HD12	3:M:298:GLN:CG	2.25	0.65
1:E:359:HIS:CE1	1:E:385:GLU:HB2	2.31	0.65
3:J:291:ALA:HA	3:J:294:ILE:CD1	2.26	0.65
1:F:317:CYS:CB	1:F:401:LEU:HB3	2.25	0.65
1:B:388:TRP:HH2	1:C:154:LYS:HD3	1.60	0.65
1:D:359:HIS:CE1	1:D:385:GLU:HB2	2.31	0.65
1:B:359:HIS:CE1	1:B:385:GLU:HB2	2.31	0.65
1:A:359:HIS:CE1	1:A:385:GLU:HB2	2.31	0.65
1:C:354:ILE:O	1:C:360:PHE:CZ	2.50	0.65
1:C:359:HIS:CE1	1:C:385:GLU:HB2	2.31	0.65
1:F:253:LYS:HE3	1:F:283:ASP:CG	2.16	0.65
1:C:373:LEU:CD1	1:C:391:ILE:HD13	2.20	0.64
1:E:179:LYS:NZ	1:E:276:THR:O	2.29	0.64
1:A:346:ALA:O	1:A:401:LEU:CD2	2.45	0.64
1:B:355:GLN:CD	1:B:388:TRP:NE1	2.50	0.64
1:A:358:THR:HG21	3:H:303:TYR:CE1	2.32	0.64
1:B:357:ALA:HB2	3:J:306:SER:HB2	1.79	0.64
1:D:377:SER:OG	3:N:307:ALA:CA	2.41	0.64
1:F:323:ASP:HA	1:F:403:ILE:CD1	2.28	0.64
1:A:346:ALA:O	1:A:401:LEU:HD21	1.98	0.64
1:C:354:ILE:CA	1:C:375:PRO:HG3	2.08	0.63
1:B:355:GLN:CD	1:B:388:TRP:CE2	2.72	0.63
1:B:347:LEU:CD2	1:B:401:LEU:HD11	2.29	0.63
1:D:321:LYS:CD	3:M:309:ASN:O	2.46	0.63
1:B:355:GLN:OE1	1:B:388:TRP:CD1	2.51	0.62
1:F:354:ILE:HG23	1:F:396:LEU:CD2	2.13	0.62
1:E:388:TRP:HZ3	1:F:151:LEU:HD13	1.64	0.62
1:F:167:SER:OG	1:F:263:VAL:HG21	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:ILE:HB	1:F:273:LEU:HD23	1.80	0.62
1:A:318:VAL:HG11	1:A:402:THR:HA	1.81	0.62
1:B:354:ILE:CG1	1:B:360:PHE:HE2	2.07	0.62
1:F:353:LYS:O	1:F:357:ALA:HB2	2.00	0.62
1:A:388:TRP:CE3	1:B:155:PHE:CZ	2.85	0.62
1:C:389:THR:HG22	1:D:154:LYS:NZ	2.14	0.62
1:A:251:ARG:HA	1:F:205:LYS:HD2	1.80	0.62
1:C:378:PRO:HG2	3:L:303:TYR:HB3	1.82	0.62
1:D:321:LYS:HG2	3:M:310:TYR:CA	2.23	0.62
1:D:358:THR:O	1:D:359:HIS:HB2	2.00	0.61
1:F:357:ALA:CB	1:F:375:PRO:HG3	2.26	0.61
1:B:259:GLN:O	1:B:265:ASN:ND2	2.33	0.61
1:D:259:GLN:O	1:D:265:ASN:ND2	2.33	0.61
1:E:304:ARG:HH12	1:E:332:GLU:HA	1.65	0.61
1:E:318:VAL:CG1	1:E:402:THR:CA	2.44	0.61
1:A:426:GLU:O	1:A:430:ARG:HB2	2.01	0.61
1:D:403:ILE:O	1:D:406:PHE:N	2.32	0.61
1:E:256:LEU:O	1:E:260:MET:HB2	2.00	0.61
1:A:305:THR:HG21	3:S:310:TYR:OH	2.00	0.61
1:B:256:LEU:O	1:B:260:MET:HB2	2.00	0.61
1:F:323:ASP:CA	1:F:403:ILE:CD1	2.74	0.61
1:A:350:PRO:HB3	1:A:399:PRO:HD2	1.81	0.61
1:C:426:GLU:O	1:C:430:ARG:HB2	2.01	0.61
1:C:304:ARG:HH12	1:C:332:GLU:HA	1.66	0.60
1:D:304:ARG:HH12	1:D:332:GLU:HA	1.65	0.60
1:D:357:ALA:HB1	3:N:306:SER:HB2	1.83	0.60
1:E:318:VAL:HG11	1:E:402:THR:CG2	2.30	0.60
1:D:256:LEU:O	1:D:260:MET:HB2	2.00	0.60
1:E:259:GLN:O	1:E:265:ASN:ND2	2.33	0.60
1:F:319:LEU:HD23	1:F:403:ILE:CA	2.30	0.60
1:A:357:ALA:HB2	3:H:306:SER:HB2	1.83	0.60
1:A:377:SER:OG	3:H:307:ALA:CA	2.46	0.60
1:C:259:GLN:O	1:C:265:ASN:ND2	2.33	0.60
3:J:290:ARG:O	3:J:294:ILE:HG12	2.02	0.60
1:A:136:ALA:H	4:A:501:ADP:HN62	1.49	0.60
1:A:304:ARG:HH12	1:A:332:GLU:HA	1.65	0.60
1:C:256:LEU:O	1:C:260:MET:HB2	2.00	0.60
1:F:317:CYS:HB2	1:F:401:LEU:CG	2.30	0.60
1:E:378:PRO:HG2	3:P:303:TYR:HB3	1.82	0.60
1:D:398:GLU:OE1	1:E:163:ARG:NH1	2.28	0.60
1:D:426:GLU:O	1:D:430:ARG:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:290:ARG:O	3:H:294:ILE:HG12	2.02	0.60
3:R:290:ARG:O	3:R:294:ILE:HG12	2.02	0.60
1:E:358:THR:OG1	1:E:385:GLU:HG3	2.01	0.60
3:S:290:ARG:O	3:S:294:ILE:HG12	2.02	0.60
1:A:246:SER:OG	1:A:250:ARG:CZ	2.49	0.60
3:L:290:ARG:O	3:L:294:ILE:HG12	2.02	0.60
3:Q:290:ARG:O	3:Q:294:ILE:HG12	2.02	0.59
1:B:304:ARG:HH12	1:B:332:GLU:HA	1.65	0.59
1:B:426:GLU:O	1:B:430:ARG:HB2	2.01	0.59
1:E:426:GLU:O	1:E:430:ARG:HB2	2.01	0.59
1:F:317:CYS:CA	1:F:401:LEU:HB3	2.32	0.59
1:D:346:ALA:HB1	1:D:401:LEU:HD11	1.83	0.59
3:N:290:ARG:O	3:N:294:ILE:HG12	2.02	0.59
3:P:290:ARG:O	3:P:294:ILE:HG12	2.02	0.59
1:B:347:LEU:HD23	1:B:401:LEU:HD11	1.85	0.59
1:F:418:ASN:OD1	1:F:419:GLU:N	2.35	0.59
3:O:290:ARG:O	3:O:294:ILE:HG12	2.02	0.59
1:A:246:SER:HA	1:A:250:ARG:CG	2.30	0.59
1:E:358:THR:O	1:E:359:HIS:HB2	2.02	0.59
1:F:360:PHE:CZ	1:F:388:TRP:HA	2.38	0.59
1:C:354:ILE:HD13	1:C:375:PRO:HG3	1.66	0.58
1:F:346:ALA:HB3	1:F:406:PHE:CD2	2.37	0.58
1:F:360:PHE:CB	1:F:391:ILE:HD11	2.29	0.58
1:F:404:LYS:HA	1:F:407:LEU:HD12	1.85	0.58
1:C:355:GLN:HG2	1:C:388:TRP:CE3	2.38	0.58
1:F:360:PHE:CZ	1:F:391:ILE:HD12	2.39	0.58
1:C:321:LYS:HG2	3:K:310:TYR:CD1	2.36	0.58
1:A:155:PHE:CE2	1:F:388:TRP:CZ3	2.91	0.58
1:C:394:ASP:C	1:C:396:LEU:H	2.07	0.58
1:D:388:TRP:HE3	1:E:155:PHE:CE2	2.12	0.58
1:E:388:TRP:CZ2	1:F:147:GLU:HB3	2.39	0.58
1:C:358:THR:HG21	3:L:303:TYR:CZ	2.37	0.58
1:E:350:PRO:CG	1:E:401:LEU:HD13	2.32	0.58
3:H:298:GLN:HG3	3:I:308:LEU:HD12	1.86	0.58
3:N:298:GLN:HG3	3:O:308:LEU:HD12	1.86	0.58
1:D:136:ALA:H	4:D:501:ADP:HN62	1.50	0.57
1:E:408:LYS:HZ2	3:Q:295:GLU:HB2	1.67	0.57
1:B:350:PRO:HB2	1:B:398:GLU:CG	2.34	0.57
1:F:308:PHE:O	1:F:312:VAL:HG13	2.04	0.57
3:H:300:LEU:HD12	3:H:323:ALA:CA	2.34	0.57
3:J:298:GLN:HG3	3:K:308:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:300:LEU:HD12	3:L:323:ALA:CA	2.34	0.57
1:B:357:ALA:CB	3:J:306:SER:HB2	2.35	0.57
1:D:255:GLU:O	1:D:259:GLN:HB3	2.04	0.57
1:D:358:THR:CG2	3:N:303:TYR:CE1	2.81	0.57
1:E:224:ASN:O	1:E:227:SER:OG	2.23	0.57
3:N:300:LEU:HD12	3:N:323:ALA:CA	2.34	0.57
1:E:255:GLU:O	1:E:259:GLN:HB3	2.04	0.57
1:E:394:ASP:C	1:E:396:LEU:H	2.07	0.57
3:P:300:LEU:HD12	3:P:323:ALA:CA	2.35	0.57
1:B:354:ILE:CB	1:B:375:PRO:HG3	2.26	0.57
1:C:255:GLU:O	1:C:259:GLN:HB3	2.04	0.57
3:Q:300:LEU:HD12	3:Q:323:ALA:CA	2.34	0.57
3:R:298:GLN:HG3	3:S:308:LEU:HD12	1.86	0.57
1:A:128:PRO:O	1:A:188:THR:OG1	2.23	0.57
1:F:204:SER:O	1:F:207:MET:HG3	2.03	0.57
1:D:389:THR:HA	1:E:154:LYS:CE	2.34	0.57
1:E:122:ALA:O	1:F:250:ARG:NH2	2.37	0.57
3:R:300:LEU:HD12	3:R:323:ALA:CA	2.35	0.57
3:S:300:LEU:HD12	3:S:323:ALA:CA	2.34	0.57
1:D:373:LEU:HD11	1:D:391:ILE:HG12	1.87	0.57
1:E:318:VAL:HG11	1:E:402:THR:HG23	1.87	0.57
1:F:373:LEU:HD11	1:F:391:ILE:HG12	1.87	0.57
3:P:308:LEU:HD12	3:Q:298:GLN:HG3	1.86	0.57
1:A:254:THR:HG21	1:F:205:LYS:CE	2.22	0.57
1:B:355:GLN:NE2	1:B:388:TRP:CE2	2.69	0.57
3:J:300:LEU:HD12	3:J:323:ALA:CA	2.34	0.57
3:P:298:GLN:HG3	3:Q:308:LEU:HD12	1.86	0.57
1:D:354:ILE:CA	1:D:375:PRO:HG2	2.33	0.57
1:E:373:LEU:HD12	1:E:391:ILE:HD11	1.84	0.57
1:B:255:GLU:O	1:B:259:GLN:HB3	2.04	0.56
1:F:394:ASP:C	1:F:396:LEU:H	2.07	0.56
1:A:357:ALA:CB	3:H:306:SER:HB2	2.35	0.56
1:A:373:LEU:HD12	1:A:391:ILE:HD11	1.84	0.56
1:E:373:LEU:HD11	1:E:391:ILE:HG12	1.87	0.56
3:O:300:LEU:HD12	3:O:323:ALA:CA	2.34	0.56
1:E:358:THR:HG23	1:E:359:HIS:CD2	2.40	0.56
3:N:308:LEU:HD12	3:O:298:GLN:HG3	1.86	0.56
1:F:317:CYS:CB	1:F:401:LEU:CG	2.82	0.56
3:L:298:GLN:HG3	3:M:308:LEU:HD12	1.86	0.56
1:B:398:GLU:H	1:B:398:GLU:CD	2.08	0.56
1:E:408:LYS:HE3	3:Q:295:GLU:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:PHE:CD1	1:F:386:MET:HG3	2.23	0.56
1:B:358:THR:O	1:B:359:HIS:HB2	2.06	0.56
1:D:304:ARG:NH1	1:D:331:THR:O	2.39	0.56
1:F:204:SER:O	1:F:207:MET:CG	2.53	0.56
3:R:308:LEU:HD12	3:S:298:GLN:HG3	1.86	0.56
1:A:341:VAL:HG11	1:B:291:GLU:HB2	1.88	0.56
1:A:394:ASP:C	1:A:396:LEU:H	2.07	0.56
1:C:304:ARG:NH1	1:C:331:THR:O	2.39	0.56
1:C:321:LYS:HD3	3:K:310:TYR:CD1	2.40	0.56
1:B:353:LYS:O	1:B:375:PRO:HB3	2.06	0.56
1:A:304:ARG:NH1	1:A:331:THR:O	2.39	0.55
1:B:373:LEU:HD11	1:B:391:ILE:HG12	1.87	0.55
1:B:304:ARG:NH1	1:B:331:THR:O	2.39	0.55
1:A:250:ARG:NH1	1:F:204:SER:HB2	2.11	0.55
1:B:354:ILE:CD1	1:B:375:PRO:HD3	2.35	0.55
1:C:373:LEU:HD12	1:C:391:ILE:HD11	1.84	0.55
1:C:373:LEU:HD11	1:C:391:ILE:HG12	1.87	0.55
1:F:349:GLN:OE1	1:F:352:ARG:NH1	2.39	0.55
1:A:373:LEU:HD11	1:A:391:ILE:HG12	1.87	0.55
1:E:304:ARG:NH1	1:E:331:THR:O	2.39	0.55
3:J:290:ARG:HG3	3:J:291:ALA:N	2.22	0.55
1:D:373:LEU:HD12	1:D:391:ILE:HD11	1.84	0.55
1:E:319:LEU:HD11	1:E:403:ILE:HB	1.88	0.55
3:S:290:ARG:HG3	3:S:291:ALA:N	2.22	0.55
1:A:358:THR:OG1	1:A:385:GLU:CG	2.55	0.55
3:N:290:ARG:HG3	3:N:291:ALA:N	2.22	0.55
1:D:287:ARG:O	1:D:293:ARG:NH2	2.38	0.54
1:C:358:THR:C	1:C:359:HIS:CG	2.80	0.54
1:B:287:ARG:O	1:B:293:ARG:NH2	2.38	0.54
1:D:357:ALA:CB	3:N:306:SER:HB2	2.37	0.54
1:F:304:ARG:NH1	1:F:328:GLY:O	2.40	0.54
3:L:290:ARG:HG3	3:L:291:ALA:N	2.22	0.54
1:D:353:LYS:O	1:D:375:PRO:CB	2.55	0.54
1:D:353:LYS:O	1:D:375:PRO:CG	2.56	0.54
1:F:360:PHE:HB3	1:F:373:LEU:HB2	1.90	0.54
1:F:354:ILE:HG23	1:F:396:LEU:CG	2.37	0.54
1:A:210:SER:HB2	1:A:252:ILE:HD11	1.89	0.54
1:D:249:SER:O	1:D:253:LYS:CB	2.55	0.54
1:D:394:ASP:C	1:D:396:LEU:H	2.07	0.54
3:H:290:ARG:HG3	3:H:291:ALA:N	2.22	0.54
1:A:322:GLU:HG3	3:S:310:TYR:O	1.97	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:LYS:NZ	1:F:283:ASP:OD1	2.33	0.54
1:A:174:PRO:HG3	1:A:425:GLN:HG3	1.90	0.53
3:R:290:ARG:HG3	3:R:291:ALA:N	2.22	0.53
1:A:240:THR:CB	1:A:250:ARG:HH21	2.21	0.53
1:F:323:ASP:HB3	1:F:403:ILE:CG1	2.39	0.53
3:O:290:ARG:HG3	3:O:291:ALA:N	2.22	0.53
1:E:388:TRP:CH2	1:F:147:GLU:HB3	2.43	0.53
1:F:342:VAL:HG12	1:F:413:THR:HB	1.91	0.53
3:Q:290:ARG:HG3	3:Q:291:ALA:N	2.22	0.53
1:B:354:ILE:CG1	1:B:360:PHE:CE2	2.87	0.53
1:E:336:GLY:HA3	4:E:501:ADP:C8	2.43	0.53
1:E:393:ALA:HB1	1:F:157:HIS:NE2	2.18	0.53
1:B:394:ASP:C	1:B:396:LEU:H	2.09	0.53
1:D:222:ARG:HD2	1:D:266:ASP:HB2	1.91	0.53
3:P:290:ARG:HG3	3:P:291:ALA:N	2.22	0.53
1:A:254:THR:CG2	1:F:205:LYS:HG2	2.13	0.53
1:B:321:LYS:HG3	3:I:310:TYR:CE1	2.44	0.53
3:O:310:TYR:O	3:O:310:TYR:CD2	2.62	0.53
1:D:393:ALA:O	1:D:394:ASP:OD1	2.27	0.53
1:B:393:ALA:O	1:B:394:ASP:OD1	2.27	0.53
1:C:318:VAL:CG1	1:C:401:LEU:O	2.56	0.53
1:D:353:LYS:C	1:D:375:PRO:HG2	2.30	0.53
1:F:317:CYS:HB2	1:F:401:LEU:HG	1.91	0.53
1:C:249:SER:O	1:C:253:LYS:CB	2.55	0.53
1:E:207:MET:O	1:E:207:MET:HG2	2.09	0.53
1:B:426:GLU:O	1:B:430:ARG:CB	2.57	0.52
1:F:357:ALA:HB1	1:F:375:PRO:CG	2.30	0.52
3:P:330:ILE:HG22	3:P:330:ILE:OXT	2.10	0.52
1:D:426:GLU:O	1:D:430:ARG:CB	2.57	0.52
1:A:426:GLU:O	1:A:430:ARG:CB	2.57	0.52
1:C:426:GLU:O	1:C:430:ARG:CB	2.57	0.52
1:E:249:SER:O	1:E:253:LYS:CB	2.55	0.52
1:E:426:GLU:O	1:E:430:ARG:CB	2.57	0.52
1:D:388:TRP:CZ3	1:E:155:PHE:CE2	2.97	0.52
3:M:330:ILE:HG22	3:M:330:ILE:OXT	2.10	0.52
3:S:330:ILE:HG22	3:S:330:ILE:OXT	2.10	0.52
1:A:287:ARG:O	1:A:293:ARG:NH2	2.38	0.52
1:E:393:ALA:O	1:E:394:ASP:OD1	2.27	0.52
3:H:330:ILE:HG22	3:H:330:ILE:OXT	2.09	0.52
1:A:251:ARG:NE	1:F:205:LYS:O	2.42	0.52
1:A:349:GLN:OE1	1:A:352:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:THR:N	1:E:154:LYS:NZ	2.54	0.52
3:I:330:ILE:HG22	3:I:330:ILE:OXT	2.10	0.52
3:K:325:ASP:HA	3:K:328:ASN:HD22	1.75	0.52
3:L:325:ASP:HA	3:L:328:ASN:HD22	1.75	0.52
3:P:325:ASP:HA	3:P:328:ASN:HD22	1.75	0.52
1:C:354:ILE:N	1:C:375:PRO:HG2	2.25	0.52
1:C:358:THR:O	1:C:359:HIS:HB2	2.08	0.52
1:D:403:ILE:HG23	1:D:404:LYS:N	2.25	0.52
1:F:339:ILE:HA	1:F:342:VAL:HG22	1.91	0.52
3:L:330:ILE:OXT	3:L:330:ILE:HG22	2.10	0.52
1:B:358:THR:C	1:B:359:HIS:CG	2.82	0.52
1:C:355:GLN:HG2	1:C:388:TRP:CE2	2.45	0.52
1:F:354:ILE:CG2	1:F:396:LEU:CG	2.86	0.52
1:A:246:SER:CA	1:A:250:ARG:HG2	2.37	0.51
1:C:393:ALA:O	1:C:394:ASP:OD1	2.27	0.51
1:D:181:TYR:HB2	4:D:501:ADP:H5'2	1.92	0.51
3:M:325:ASP:HA	3:M:328:ASN:HD22	1.75	0.51
3:O:330:ILE:HG22	3:O:330:ILE:OXT	2.10	0.51
1:B:249:SER:O	1:B:253:LYS:CB	2.55	0.51
1:C:354:ILE:O	1:C:360:PHE:HZ	1.93	0.51
3:K:330:ILE:HG22	3:K:330:ILE:OXT	2.10	0.51
3:J:330:ILE:HG22	3:J:330:ILE:OXT	2.10	0.51
1:A:179:LYS:NZ	1:A:276:THR:O	2.39	0.51
1:A:393:ALA:O	1:A:394:ASP:OD1	2.27	0.51
1:C:288:ARG:NH2	5:C:501:BEF:F3	2.33	0.51
1:F:377:SER:OG	3:R:307:ALA:HA	2.10	0.51
3:R:330:ILE:HG22	3:R:330:ILE:OXT	2.10	0.51
3:O:325:ASP:HA	3:O:328:ASN:HD22	1.75	0.51
3:Q:325:ASP:HA	3:Q:328:ASN:HD22	1.75	0.51
1:E:238:THR:HG21	1:E:282:LEU:HA	1.91	0.51
1:F:378:PRO:HD2	3:R:307:ALA:HB2	1.92	0.51
3:J:325:ASP:HA	3:J:328:ASN:HD22	1.75	0.51
1:C:354:ILE:HG21	1:C:396:LEU:HD11	1.92	0.51
1:F:393:ALA:O	1:F:394:ASP:OD1	2.27	0.51
3:H:325:ASP:HA	3:H:328:ASN:HD22	1.75	0.51
3:N:330:ILE:HG22	3:N:330:ILE:OXT	2.10	0.51
3:R:325:ASP:HA	3:R:328:ASN:HD22	1.75	0.51
3:S:325:ASP:HA	3:S:328:ASN:HD22	1.75	0.51
1:E:318:VAL:CG1	1:E:402:THR:HG23	2.41	0.51
3:I:325:ASP:HA	3:I:328:ASN:HD22	1.75	0.51
1:E:350:PRO:HG2	1:E:401:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:LEU:HD12	1:F:391:ILE:HD11	1.84	0.50
3:H:289:ASP:HA	3:H:292:SER:OG	2.12	0.50
3:N:289:ASP:HA	3:N:292:SER:OG	2.12	0.50
3:O:293:LYS:HZ2	3:O:330:ILE:HD13	1.76	0.50
1:D:378:PRO:HG2	3:N:303:TYR:O	2.11	0.50
1:E:403:ILE:O	1:E:404:LYS:C	2.48	0.50
3:J:289:ASP:HA	3:J:292:SER:OG	2.12	0.50
3:P:293:LYS:HZ2	3:P:330:ILE:HD13	1.76	0.50
1:A:155:PHE:CE2	1:F:388:TRP:HZ3	2.30	0.50
3:O:289:ASP:HA	3:O:292:SER:OG	2.12	0.50
3:S:289:ASP:HA	3:S:292:SER:OG	2.12	0.50
1:C:311:ASN:HB3	1:C:343:VAL:HG11	1.94	0.50
1:E:301:LEU:HD13	3:O:310:TYR:CZ	2.41	0.50
3:P:289:ASP:HA	3:P:292:SER:OG	2.12	0.50
3:Q:289:ASP:HA	3:Q:292:SER:OG	2.12	0.50
3:H:293:LYS:HZ2	3:H:330:ILE:HD13	1.77	0.50
1:A:311:ASN:HB3	1:A:343:VAL:HG11	1.94	0.50
1:E:357:ALA:HB1	3:P:306:SER:OG	2.12	0.50
1:F:350:PRO:O	1:F:354:ILE:HG13	2.11	0.50
3:Q:330:ILE:OXT	3:Q:330:ILE:HG22	2.10	0.50
3:R:289:ASP:HA	3:R:292:SER:OG	2.12	0.50
1:C:393:ALA:O	1:C:394:ASP:CG	2.50	0.50
1:E:147:GLU:O	1:E:151:LEU:CB	2.58	0.50
1:E:311:ASN:HB3	1:E:343:VAL:HG11	1.94	0.50
1:F:393:ALA:O	1:F:394:ASP:CG	2.50	0.50
3:N:325:ASP:HA	3:N:328:ASN:HD22	1.75	0.50
1:D:392:GLU:HB2	1:D:395:GLU:CD	2.33	0.49
1:F:404:LYS:O	1:F:407:LEU:HB2	2.12	0.49
1:A:392:GLU:HB2	1:A:395:GLU:CD	2.33	0.49
1:B:311:ASN:HB3	1:B:343:VAL:HG11	1.94	0.49
1:E:375:PRO:CB	3:P:310:TYR:OH	2.58	0.49
1:A:388:TRP:CH2	1:B:155:PHE:CE2	2.76	0.49
1:C:392:GLU:HB2	1:C:395:GLU:CD	2.33	0.49
1:D:302:ALA:HA	3:M:310:TYR:CE2	2.48	0.49
1:E:393:ALA:O	1:E:394:ASP:CG	2.50	0.49
3:L:289:ASP:HA	3:L:292:SER:OG	2.11	0.49
1:A:155:PHE:HE2	1:F:388:TRP:HZ3	1.60	0.49
1:B:355:GLN:OE1	1:B:388:TRP:CE2	2.66	0.49
1:A:393:ALA:O	1:A:394:ASP:CG	2.50	0.49
1:B:377:SER:OG	3:J:307:ALA:CA	2.55	0.49
1:C:218:PHE:HD2	1:C:259:GLN:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLU:HB2	1:E:395:GLU:CD	2.33	0.49
1:F:392:GLU:HB2	1:F:395:GLU:CD	2.33	0.49
3:J:313:LEU:N	3:J:314:PRO:CD	2.76	0.49
1:C:354:ILE:CD1	1:C:375:PRO:HG3	2.33	0.49
1:B:321:LYS:CD	3:I:310:TYR:HA	2.39	0.49
1:B:373:LEU:HD12	1:B:391:ILE:HD11	1.84	0.49
1:D:250:ARG:O	1:D:254:THR:OG1	2.28	0.49
1:F:360:PHE:HE1	1:F:387:SER:C	2.16	0.49
3:O:327:LEU:HD12	3:O:327:LEU:O	2.13	0.49
3:P:327:LEU:HD12	3:P:327:LEU:O	2.13	0.49
3:R:313:LEU:N	3:R:314:PRO:CD	2.76	0.49
3:S:327:LEU:O	3:S:327:LEU:HD12	2.13	0.49
1:C:318:VAL:CB	1:C:401:LEU:O	2.60	0.49
1:E:357:ALA:CB	3:P:306:SER:CB	2.80	0.49
3:L:313:LEU:N	3:L:314:PRO:CD	2.76	0.49
3:M:313:LEU:N	3:M:314:PRO:CD	2.76	0.49
3:M:327:LEU:HD12	3:M:327:LEU:O	2.13	0.49
1:A:254:THR:HG21	1:F:205:LYS:HE2	1.81	0.48
1:D:393:ALA:O	1:D:394:ASP:CG	2.50	0.48
1:F:203:VAL:HG21	1:F:236:ALA:O	2.13	0.48
1:A:246:SER:CA	1:A:250:ARG:CG	2.92	0.48
1:A:246:SER:HB3	1:A:250:ARG:HG3	1.93	0.48
1:A:318:VAL:CG1	1:A:401:LEU:O	2.61	0.48
1:D:311:ASN:HB3	1:D:343:VAL:HG11	1.94	0.48
1:E:287:ARG:O	1:E:293:ARG:NH2	2.38	0.48
3:H:327:LEU:HD12	3:H:327:LEU:O	2.13	0.48
3:I:313:LEU:N	3:I:314:PRO:CD	2.76	0.48
3:O:313:LEU:N	3:O:314:PRO:CD	2.76	0.48
1:A:388:TRP:CE3	1:B:155:PHE:HZ	2.26	0.48
1:B:392:GLU:HB2	1:B:395:GLU:CD	2.33	0.48
1:D:250:ARG:O	1:D:254:THR:CB	2.62	0.48
3:J:327:LEU:HD12	3:J:327:LEU:O	2.13	0.48
3:N:327:LEU:O	3:N:327:LEU:HD12	2.13	0.48
3:Q:293:LYS:HZ2	3:Q:330:ILE:HD13	1.78	0.48
1:B:393:ALA:O	1:B:394:ASP:CG	2.50	0.48
1:C:202:LEU:HD22	1:C:214:VAL:HG22	1.95	0.48
1:E:250:ARG:O	1:E:254:THR:CB	2.62	0.48
3:L:327:LEU:HD12	3:L:327:LEU:O	2.13	0.48
1:C:287:ARG:O	1:C:293:ARG:NH2	2.38	0.48
1:A:202:LEU:HD22	1:A:214:VAL:HG22	1.95	0.48
1:C:250:ARG:O	1:C:254:THR:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:ALA:HB2	3:P:306:SER:HB2	1.94	0.48
1:F:257:LEU:HD23	1:F:289:ARG:HG3	1.95	0.48
3:H:313:LEU:N	3:H:314:PRO:CD	2.76	0.48
3:Q:313:LEU:N	3:Q:314:PRO:CD	2.76	0.48
1:F:253:LYS:HZ1	1:F:283:ASP:CG	2.16	0.48
1:D:179:LYS:NZ	1:D:276:THR:O	2.44	0.48
3:I:327:LEU:O	3:I:327:LEU:HD12	2.13	0.48
3:K:327:LEU:HD12	3:K:327:LEU:O	2.13	0.48
3:N:296:GLN:HE21	3:N:300:LEU:HG	1.79	0.48
3:N:313:LEU:N	3:N:314:PRO:CD	2.76	0.48
1:A:395:GLU:O	1:A:395:GLU:HG3	2.14	0.48
1:B:202:LEU:HD22	1:B:214:VAL:HG22	1.95	0.48
3:O:296:GLN:HE21	3:O:300:LEU:HG	1.79	0.48
3:P:313:LEU:N	3:P:314:PRO:CD	2.76	0.48
3:R:296:GLN:HE21	3:R:300:LEU:HG	1.79	0.48
1:B:250:ARG:O	1:B:254:THR:CB	2.62	0.48
1:C:354:ILE:HD13	1:C:375:PRO:HD2	1.64	0.48
1:C:357:ALA:CB	3:L:306:SER:CB	2.88	0.48
1:C:395:GLU:O	1:C:395:GLU:HG3	2.14	0.48
1:F:166:THR:HG23	1:F:291:GLU:CD	2.34	0.48
1:F:351:ILE:O	1:F:355:GLN:HG3	2.14	0.48
3:L:296:GLN:HE21	3:L:300:LEU:HG	1.79	0.48
3:P:296:GLN:HE21	3:P:300:LEU:HG	1.79	0.48
1:D:255:GLU:O	1:D:259:GLN:CB	2.63	0.47
3:J:296:GLN:HE21	3:J:300:LEU:HG	1.79	0.47
3:R:327:LEU:HD12	3:R:327:LEU:O	2.13	0.47
1:C:336:GLY:HA3	4:C:502:ADP:C8	2.49	0.47
1:F:166:THR:HG23	1:F:291:GLU:OE1	2.13	0.47
3:S:313:LEU:N	3:S:314:PRO:CD	2.76	0.47
1:C:179:LYS:NZ	1:C:276:THR:O	2.46	0.47
1:C:321:LYS:CG	3:K:310:TYR:HD1	2.26	0.47
1:D:354:ILE:HG23	1:D:396:LEU:CD1	2.44	0.47
1:D:395:GLU:O	1:D:395:GLU:HG3	2.14	0.47
1:F:206:TRP:O	1:F:209:GLU:HG2	2.14	0.47
1:B:341:VAL:HG11	1:C:291:GLU:HB2	1.96	0.47
1:B:395:GLU:O	1:B:395:GLU:HG3	2.14	0.47
1:C:396:LEU:CD2	1:D:158:LEU:HD21	2.38	0.47
3:K:313:LEU:N	3:K:314:PRO:CD	2.76	0.47
3:L:293:LYS:HZ2	3:L:330:ILE:HD13	1.78	0.47
3:Q:296:GLN:HE21	3:Q:300:LEU:HG	1.79	0.47
3:Q:327:LEU:HD12	3:Q:327:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:296:GLN:HE21	3:S:300:LEU:HG	1.79	0.47
1:A:254:THR:OG1	1:F:205:LYS:HB2	2.15	0.47
1:C:341:VAL:HG11	1:D:291:GLU:HB2	1.95	0.47
1:E:403:ILE:HG13	1:E:406:PHE:HB2	1.95	0.47
1:E:403:ILE:HG12	1:E:407:LEU:HG	1.97	0.47
1:C:394:ASP:OD1	1:C:395:GLU:N	2.48	0.47
1:D:202:LEU:HD22	1:D:214:VAL:HG22	1.95	0.47
1:E:255:GLU:O	1:E:259:GLN:CB	2.62	0.47
1:E:395:GLU:HG3	1:E:395:GLU:O	2.14	0.47
1:F:311:ASN:HB3	1:F:343:VAL:HG11	1.97	0.47
1:C:389:THR:HG22	1:D:154:LYS:HZ1	1.76	0.47
1:D:321:LYS:HD2	3:M:310:TYR:CA	2.41	0.47
1:B:358:THR:HG21	3:J:303:TYR:CZ	2.50	0.47
1:C:255:GLU:O	1:C:259:GLN:CB	2.62	0.47
1:C:358:THR:O	1:C:358:THR:HG23	2.13	0.47
1:F:395:GLU:O	1:F:395:GLU:HG3	2.14	0.47
1:F:394:ASP:OD1	1:F:395:GLU:N	2.48	0.47
3:P:328:ASN:OD1	3:Q:317:LYS:HE3	2.15	0.47
1:D:394:ASP:OD1	1:D:395:GLU:N	2.48	0.46
1:E:358:THR:O	1:E:359:HIS:CB	2.63	0.46
1:E:394:ASP:OD1	1:E:395:GLU:N	2.48	0.46
3:H:328:ASN:OD1	3:I:317:LYS:HE3	2.16	0.46
3:L:317:LYS:HE3	3:M:328:ASN:OD1	2.16	0.46
1:B:336:GLY:HA3	4:B:501:ADP:C8	2.50	0.46
3:H:324:LEU:O	3:H:328:ASN:ND2	2.49	0.46
3:L:324:LEU:O	3:L:328:ASN:ND2	2.49	0.46
3:L:328:ASN:OD1	3:M:317:LYS:HE3	2.16	0.46
3:P:324:LEU:O	3:P:328:ASN:ND2	2.49	0.46
3:R:324:LEU:O	3:R:328:ASN:ND2	2.49	0.46
1:B:255:GLU:O	1:B:259:GLN:CB	2.62	0.46
3:I:324:LEU:O	3:I:328:ASN:ND2	2.49	0.46
3:J:328:ASN:OD1	3:K:317:LYS:HE3	2.15	0.46
3:N:317:LYS:HE3	3:O:328:ASN:OD1	2.16	0.46
3:N:324:LEU:O	3:N:328:ASN:ND2	2.49	0.46
3:N:328:ASN:OD1	3:O:317:LYS:HE3	2.16	0.46
3:Q:324:LEU:O	3:Q:328:ASN:ND2	2.49	0.46
1:A:394:ASP:OD1	1:A:395:GLU:N	2.48	0.46
1:B:224:ASN:O	1:B:227:SER:OG	2.33	0.46
1:B:394:ASP:OD1	1:B:395:GLU:N	2.48	0.46
1:E:393:ALA:CB	1:F:157:HIS:NE2	2.78	0.46
3:H:296:GLN:HE21	3:H:300:LEU:HG	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:311:GLU:OE1	3:I:290:ARG:NH1	2.49	0.46
3:O:301:ALA:O	3:O:305:ILE:HG13	2.16	0.46
1:D:403:ILE:HG23	1:D:404:LYS:H	1.81	0.46
3:J:301:ALA:O	3:J:305:ILE:HG13	2.16	0.46
3:M:324:LEU:O	3:M:328:ASN:ND2	2.49	0.46
3:O:324:LEU:O	3:O:328:ASN:ND2	2.49	0.46
3:R:328:ASN:OD1	3:S:317:LYS:HE3	2.16	0.46
3:H:301:ALA:O	3:H:305:ILE:HG13	2.16	0.46
3:J:293:LYS:HZ2	3:J:330:ILE:HD13	1.80	0.46
3:L:311:GLU:OE1	3:M:290:ARG:NH1	2.49	0.46
1:A:177:THR:HG22	1:A:298:LEU:HD23	1.97	0.46
1:E:132:TRP:CD1	1:E:189:GLU:HG3	2.51	0.46
1:F:225:LYS:HD3	1:F:269:GLY:HA3	1.98	0.46
1:C:198:SER:OG	1:C:199:SER:N	2.49	0.46
1:D:377:SER:HG	3:N:307:ALA:HA	1.73	0.46
1:F:212:LYS:HE3	1:F:216:GLN:HE21	1.81	0.46
3:H:317:LYS:HE3	3:I:328:ASN:OD1	2.16	0.46
3:R:317:LYS:HE3	3:S:328:ASN:OD1	2.16	0.46
1:A:322:GLU:OE2	3:S:311:GLU:CB	2.61	0.45
1:D:353:LYS:O	1:D:375:PRO:HB3	2.15	0.45
1:B:378:PRO:HG2	3:J:303:TYR:HB3	1.98	0.45
1:C:407:LEU:HD23	1:C:410:ILE:HD12	1.99	0.45
1:D:204:SER:HA	1:E:212:LYS:HZ3	1.80	0.45
1:F:317:CYS:CB	1:F:401:LEU:CB	2.93	0.45
3:N:293:LYS:HZ2	3:N:330:ILE:HD13	1.81	0.45
3:N:301:ALA:O	3:N:305:ILE:HG13	2.16	0.45
3:P:317:LYS:HE3	3:Q:328:ASN:OD1	2.16	0.45
1:A:325:ARG:NH1	3:S:312:ASP:HB3	2.06	0.45
1:A:407:LEU:HD23	1:A:410:ILE:HD12	1.98	0.45
1:F:139:GLU:H	1:F:139:GLU:HG2	1.45	0.45
1:F:315:THR:HG21	1:F:347:LEU:HD22	1.98	0.45
3:K:324:LEU:O	3:K:328:ASN:ND2	2.49	0.45
1:C:358:THR:CG2	3:L:303:TYR:CZ	3.00	0.45
1:F:354:ILE:HG12	1:F:398:GLU:HA	1.76	0.45
3:S:324:LEU:O	3:S:328:ASN:ND2	2.49	0.45
1:A:388:TRP:HH2	1:B:154:LYS:NZ	2.10	0.45
1:B:170:LEU:HB2	1:B:290:PHE:HB3	1.98	0.45
1:B:288:ARG:NH2	1:B:289:ARG:HH12	2.15	0.45
1:B:347:LEU:HA	1:B:401:LEU:HD21	1.99	0.45
3:J:317:LYS:HE3	3:K:328:ASN:OD1	2.16	0.45
3:J:324:LEU:O	3:J:328:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:301:ALA:O	3:L:305:ILE:HG13	2.16	0.45
3:R:301:ALA:O	3:R:305:ILE:HG13	2.16	0.45
1:A:198:SER:OG	1:A:199:SER:N	2.49	0.45
1:B:407:LEU:HD23	1:B:410:ILE:HD12	1.99	0.45
1:C:317:CYS:HA	1:C:401:LEU:HB2	1.98	0.45
1:D:204:SER:HA	1:E:212:LYS:NZ	2.32	0.45
1:D:378:PRO:HD2	3:N:307:ALA:HB2	1.98	0.45
1:F:323:ASP:CG	1:F:403:ILE:HG21	2.36	0.45
1:A:279:PRO:HB2	1:A:428:PHE:CE2	2.52	0.45
1:B:321:LYS:CE	3:I:309:ASN:O	2.65	0.45
3:P:301:ALA:O	3:P:305:ILE:HG13	2.16	0.45
3:S:301:ALA:O	3:S:305:ILE:HG13	2.16	0.45
1:B:370:THR:O	1:B:371:ARG:O	2.35	0.45
1:E:288:ARG:NH2	1:E:289:ARG:HH12	2.15	0.45
1:E:407:LEU:HD23	1:E:410:ILE:HD12	1.99	0.45
3:N:300:LEU:HD12	3:N:323:ALA:HA	1.99	0.45
3:P:300:LEU:HD12	3:P:323:ALA:HA	1.99	0.45
1:D:288:ARG:NH2	1:D:289:ARG:HH12	2.15	0.45
1:D:355:GLN:HE22	1:E:147:GLU:HG3	1.81	0.45
3:J:311:GLU:OE1	3:K:290:ARG:NH1	2.49	0.45
3:L:311:GLU:CD	3:M:290:ARG:NH1	2.64	0.45
1:B:250:ARG:O	1:B:254:THR:OG1	2.28	0.45
1:C:250:ARG:O	1:C:254:THR:OG1	2.28	0.45
1:D:370:THR:O	1:D:371:ARG:O	2.35	0.45
3:Q:301:ALA:O	3:Q:305:ILE:HG13	2.16	0.45
1:A:358:THR:O	1:A:359:HIS:HD2	1.91	0.44
1:D:198:SER:OG	1:D:199:SER:N	2.49	0.44
1:D:355:GLN:HA	1:D:388:TRP:CD1	2.52	0.44
1:F:370:THR:O	1:F:371:ARG:O	2.35	0.44
3:J:311:GLU:CD	3:K:290:ARG:NH1	2.64	0.44
3:R:300:LEU:HD12	3:R:323:ALA:HA	1.99	0.44
1:E:256:LEU:O	1:E:260:MET:CB	2.65	0.44
1:A:370:THR:O	1:A:371:ARG:O	2.35	0.44
1:B:321:LYS:CD	3:I:310:TYR:CE1	2.77	0.44
1:B:352:ARG:O	1:B:356:SER:CB	2.63	0.44
1:C:355:GLN:HA	1:C:388:TRP:CE3	2.52	0.44
1:D:204:SER:OG	1:D:205:LYS:N	2.50	0.44
1:D:353:LYS:O	1:D:375:PRO:HG2	2.18	0.44
3:L:300:LEU:HD12	3:L:323:ALA:HA	1.99	0.44
1:C:354:ILE:HD11	1:C:375:PRO:HD2	1.91	0.44
1:C:370:THR:O	1:C:371:ARG:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:THR:O	1:E:371:ARG:O	2.35	0.44
3:O:300:LEU:HD12	3:O:323:ALA:HA	1.99	0.44
1:A:288:ARG:NH2	1:A:289:ARG:HH12	2.15	0.44
1:A:363:VAL:O	1:A:364:SER:HB3	2.18	0.44
1:B:353:LYS:O	1:B:375:PRO:CB	2.65	0.44
1:E:330:MET:HG3	1:E:410:ILE:HG21	1.99	0.44
1:B:204:SER:OG	1:B:205:LYS:N	2.50	0.44
1:D:407:LEU:HD23	1:D:410:ILE:HD12	1.99	0.44
1:A:204:SER:OG	1:A:205:LYS:N	2.50	0.44
1:A:374:THR:HB	1:A:397:LYS:HB3	2.00	0.44
1:B:198:SER:OG	1:B:199:SER:N	2.49	0.44
1:C:218:PHE:CD2	1:C:259:GLN:HG3	2.52	0.44
1:C:363:VAL:O	1:C:364:SER:HB3	2.18	0.44
1:E:250:ARG:O	1:E:254:THR:OG1	2.28	0.44
1:A:388:TRP:CH2	1:B:154:LYS:CE	3.01	0.44
3:O:310:TYR:O	3:O:310:TYR:CG	2.71	0.44
1:C:256:LEU:O	1:C:260:MET:CB	2.65	0.43
1:B:179:LYS:NZ	1:B:276:THR:O	2.50	0.43
1:C:204:SER:OG	1:C:205:LYS:N	2.50	0.43
1:D:363:VAL:O	1:D:364:SER:HB3	2.18	0.43
1:F:346:ALA:CB	1:F:406:PHE:CE2	2.96	0.43
1:F:360:PHE:HD1	1:F:386:MET:CG	2.14	0.43
3:J:300:LEU:HD12	3:J:323:ALA:HA	1.99	0.43
3:S:300:LEU:HD12	3:S:323:ALA:HA	1.99	0.43
1:B:363:VAL:O	1:B:364:SER:HB3	2.18	0.43
1:C:288:ARG:NH2	1:C:289:ARG:HH12	2.15	0.43
1:F:132:TRP:CE2	1:F:189:GLU:HG3	2.53	0.43
1:F:363:VAL:O	1:F:364:SER:HB3	2.18	0.43
1:D:374:THR:HB	1:D:397:LYS:HB3	2.01	0.43
3:Q:300:LEU:HD12	3:Q:323:ALA:HA	1.99	0.43
1:B:177:THR:HG22	1:B:298:LEU:HD23	2.00	0.43
1:F:317:CYS:HB2	1:F:401:LEU:HB3	2.01	0.43
1:A:322:GLU:HG2	3:S:310:TYR:HB3	2.00	0.43
1:D:373:LEU:CD1	1:D:391:ILE:HG12	2.49	0.43
1:E:363:VAL:O	1:E:364:SER:HB3	2.18	0.43
1:E:374:THR:HB	1:E:397:LYS:HB3	2.01	0.43
1:F:290:PHE:O	1:F:291:GLU:C	2.55	0.43
1:A:350:PRO:HB3	1:A:399:PRO:CD	2.45	0.43
1:C:373:LEU:CD1	1:C:391:ILE:HG12	2.49	0.43
1:E:373:LEU:CD1	1:E:391:ILE:HG12	2.49	0.43
1:B:256:LEU:O	1:B:260:MET:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HA	1:B:354:ILE:HG22	2.00	0.43
3:L:308:LEU:CD1	3:M:298:GLN:HG3	2.44	0.43
1:B:358:THR:O	1:B:358:THR:HG23	2.19	0.43
3:H:300:LEU:HD12	3:H:323:ALA:HA	1.99	0.43
1:A:373:LEU:CD1	1:A:391:ILE:HG12	2.49	0.43
1:A:425:GLN:O	1:A:429:THR:CB	2.67	0.43
1:B:373:LEU:CD1	1:B:391:ILE:HG12	2.49	0.43
1:D:358:THR:O	1:D:359:HIS:HD2	1.88	0.43
1:E:301:LEU:CD1	3:O:310:TYR:CD2	3.02	0.43
3:H:311:GLU:CD	3:I:290:ARG:NH1	2.64	0.43
1:F:360:PHE:CE1	1:F:391:ILE:HD12	2.54	0.42
1:F:373:LEU:CD1	1:F:391:ILE:HG12	2.49	0.42
3:L:317:LYS:N	3:M:327:LEU:HD21	2.35	0.42
1:A:318:VAL:HG12	1:A:401:LEU:O	2.19	0.42
1:D:425:GLN:O	1:D:429:THR:CB	2.67	0.42
1:F:174:PRO:HB3	1:F:421:ASP:OD2	2.19	0.42
3:H:327:LEU:HD21	3:I:317:LYS:N	2.35	0.42
3:N:327:LEU:HD21	3:O:317:LYS:N	2.35	0.42
1:C:353:LYS:O	1:C:375:PRO:HB3	2.19	0.42
1:F:155:PHE:HB3	1:F:158:LEU:HD23	2.01	0.42
3:O:300:LEU:HD12	3:O:323:ALA:N	2.35	0.42
3:P:327:LEU:HD21	3:Q:317:LYS:N	2.35	0.42
1:C:358:THR:HG21	3:L:303:TYR:OH	2.20	0.42
1:D:358:THR:C	1:D:359:HIS:CG	2.92	0.42
1:E:403:ILE:CG1	1:E:407:LEU:HG	2.50	0.42
1:F:355:GLN:O	1:F:388:TRP:CE2	2.73	0.42
3:J:317:LYS:N	3:K:327:LEU:HD21	2.35	0.42
3:R:317:LYS:N	3:S:327:LEU:HD21	2.35	0.42
1:A:138:LEU:HD13	1:A:182:LEU:HD13	2.02	0.42
1:C:240:THR:HB	1:C:253:LYS:HE2	2.02	0.42
1:D:354:ILE:CG2	1:D:396:LEU:CD1	2.86	0.42
1:F:374:THR:HB	1:F:397:LYS:HB3	2.01	0.42
3:J:300:LEU:HD12	3:J:323:ALA:N	2.35	0.42
3:P:300:LEU:HD12	3:P:323:ALA:N	2.35	0.42
3:P:317:LYS:N	3:Q:327:LEU:HD21	2.35	0.42
1:E:425:GLN:O	1:E:429:THR:CB	2.67	0.42
3:H:300:LEU:HD12	3:H:323:ALA:N	2.35	0.42
1:C:357:ALA:CB	3:L:306:SER:OG	2.68	0.42
1:D:250:ARG:O	1:D:254:THR:HB	2.20	0.42
1:D:256:LEU:O	1:D:260:MET:CB	2.65	0.42
3:J:327:LEU:HD21	3:K:317:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:327:LEU:HD21	3:S:317:LYS:N	2.35	0.42
1:A:358:THR:C	1:A:359:HIS:CG	2.93	0.42
1:B:359:HIS:HA	1:B:384:ILE:O	2.20	0.42
3:H:317:LYS:N	3:I:327:LEU:HD21	2.35	0.42
1:C:353:LYS:O	1:C:375:PRO:CB	2.68	0.41
1:E:359:HIS:HA	1:E:384:ILE:O	2.20	0.41
1:F:422:LEU:O	1:F:426:GLU:HG3	2.19	0.41
3:J:308:LEU:CD1	3:K:298:GLN:HG3	2.44	0.41
3:L:327:LEU:HD21	3:M:317:LYS:N	2.35	0.41
3:R:300:LEU:HD12	3:R:323:ALA:N	2.35	0.41
1:A:238:THR:HG21	1:A:282:LEU:HD12	2.02	0.41
1:E:253:LYS:HB3	1:E:253:LYS:HE3	1.88	0.41
1:F:263:VAL:HA	1:F:267:SER:HA	1.85	0.41
3:L:300:LEU:HD12	3:L:323:ALA:N	2.35	0.41
3:N:317:LYS:N	3:O:327:LEU:HD21	2.35	0.41
3:Q:300:LEU:HD12	3:Q:323:ALA:N	2.35	0.41
3:R:330:ILE:OXT	3:R:330:ILE:CG2	2.68	0.41
1:C:425:GLN:O	1:C:429:THR:CB	2.67	0.41
1:D:203:VAL:O	1:E:212:LYS:NZ	2.45	0.41
1:D:240:THR:HB	1:D:253:LYS:HE2	2.02	0.41
1:D:377:SER:OG	3:N:307:ALA:CB	2.69	0.41
1:B:250:ARG:O	1:B:254:THR:HB	2.20	0.41
1:E:250:ARG:O	1:E:254:THR:HB	2.20	0.41
1:F:237:LEU:CD1	1:F:256:LEU:HD22	2.50	0.41
3:N:300:LEU:HD12	3:N:323:ALA:N	2.35	0.41
3:O:330:ILE:OXT	3:O:330:ILE:CG2	2.68	0.41
3:S:293:LYS:HZ2	3:S:330:ILE:HD13	1.84	0.41
1:A:151:LEU:CD1	1:F:355:GLN:HG2	2.51	0.41
1:A:334:TYR:CD1	1:A:415:PRO:HG3	2.54	0.41
1:B:313:GLY:HA3	1:C:162:ASN:ND2	2.36	0.41
1:B:425:GLN:O	1:B:429:THR:CB	2.67	0.41
1:C:354:ILE:CD1	1:C:375:PRO:HG2	2.17	0.41
1:F:265:ASN:N	1:F:265:ASN:HD22	2.17	0.41
3:P:330:ILE:OXT	3:P:330:ILE:CG2	2.68	0.41
3:Q:330:ILE:OXT	3:Q:330:ILE:CG2	2.68	0.41
1:D:358:THR:O	1:D:358:THR:HG23	2.21	0.41
1:D:359:HIS:HA	1:D:384:ILE:O	2.20	0.41
3:H:305:ILE:HD13	3:I:302:LYS:HG3	2.03	0.41
3:S:300:LEU:HD12	3:S:323:ALA:N	2.35	0.41
1:C:250:ARG:O	1:C:254:THR:HB	2.20	0.41
1:E:240:THR:HB	1:E:253:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:305:ILE:HD13	3:M:302:LYS:HG3	2.03	0.41
3:S:295:GLU:O	3:S:295:GLU:HG2	2.21	0.41
1:F:263:VAL:CG1	1:F:267:SER:HB2	2.46	0.41
3:S:330:ILE:OXT	3:S:330:ILE:CG2	2.68	0.41
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.92	0.41
1:A:353:LYS:HD2	1:A:399:PRO:CB	2.51	0.41
1:B:240:THR:HB	1:B:253:LYS:HE2	2.02	0.41
1:C:260:MET:SD	1:C:289:ARG:HB3	2.61	0.41
1:F:209:GLU:HG2	1:F:209:GLU:H	1.45	0.41
3:I:330:ILE:OXT	3:I:330:ILE:CG2	2.68	0.41
1:A:358:THR:O	1:A:358:THR:HG23	2.21	0.41
1:B:358:THR:OG1	1:B:385:GLU:HG2	2.17	0.41
1:C:321:LYS:CD	3:K:310:TYR:CD1	3.03	0.41
1:D:358:THR:HG21	3:N:303:TYR:CZ	2.49	0.41
1:E:301:LEU:HB3	3:O:310:TYR:CD1	2.56	0.41
1:F:225:LYS:NZ	1:F:268:GLN:O	2.43	0.41
3:J:295:GLU:O	3:J:295:GLU:HG2	2.21	0.41
1:B:145:LEU:HD13	1:B:186:VAL:HG21	2.03	0.40
1:B:350:PRO:HB2	1:B:398:GLU:HG3	2.04	0.40
1:C:224:ASN:O	1:C:227:SER:OG	2.40	0.40
3:J:330:ILE:OXT	3:J:330:ILE:CG2	2.68	0.40
3:K:330:ILE:OXT	3:K:330:ILE:CG2	2.68	0.40
3:L:330:ILE:OXT	3:L:330:ILE:CG2	2.68	0.40
3:M:330:ILE:OXT	3:M:330:ILE:CG2	2.68	0.40
3:O:295:GLU:O	3:O:295:GLU:HG2	2.21	0.40
1:B:347:LEU:HD21	1:B:401:LEU:HD11	2.03	0.40
1:E:304:ARG:HG2	1:E:339:ILE:HD11	2.03	0.40
1:F:200:SER:HB3	1:F:233:GLU:OE1	2.21	0.40
1:A:357:ALA:CB	3:H:306:SER:CB	3.00	0.40
1:A:359:HIS:HA	1:A:384:ILE:O	2.20	0.40
1:C:359:HIS:HA	1:C:384:ILE:O	2.20	0.40
1:E:197:VAL:HG22	1:E:198:SER:O	2.22	0.40
1:E:233:GLU:HA	1:E:276:THR:HA	2.02	0.40
1:F:330:MET:HE2	1:F:330:MET:HB2	1.76	0.40
1:B:304:ARG:HG2	1:B:339:ILE:HD11	2.03	0.40
1:B:350:PRO:HB3	1:B:399:PRO:HD2	2.03	0.40
3:N:330:ILE:OXT	3:N:330:ILE:CG2	2.68	0.40
1:A:304:ARG:HG2	1:A:339:ILE:HD11	2.03	0.40
3:H:330:ILE:OXT	3:H:330:ILE:CG2	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/437 (70%)	280 (91%)	23 (8%)	5 (2%)	9	43
1	B	307/437 (70%)	271 (88%)	31 (10%)	5 (2%)	9	43
1	C	307/437 (70%)	275 (90%)	27 (9%)	5 (2%)	9	43
1	D	307/437 (70%)	272 (89%)	30 (10%)	5 (2%)	9	43
1	E	304/437 (70%)	268 (88%)	31 (10%)	5 (2%)	9	43
1	F	296/437 (68%)	275 (93%)	15 (5%)	6 (2%)	7	37
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	I	49/330 (15%)	43 (88%)	5 (10%)	1 (2%)	7	37
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	K	45/330 (14%)	39 (87%)	5 (11%)	1 (2%)	6	35
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	M	45/330 (14%)	39 (87%)	5 (11%)	1 (2%)	6	35
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	O	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	Q	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
3	S	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	2	20
All	All	2328/6582 (35%)	2041 (88%)	235 (10%)	52 (2%)	10	35

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	371	ARG
1	A	395	GLU
1	B	359	HIS

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Mol	Chain	Res	Type
1	B	371	ARG
1	B	395	GLU
1	C	359	HIS
1	C	371	ARG
1	C	395	GLU
1	D	359	HIS
1	D	371	ARG
1	D	395	GLU
1	E	371	ARG
1	E	395	GLU
1	F	371	ARG
1	F	395	GLU
1	F	207	MET
3	H	312	ASP
3	I	312	ASP
3	J	312	ASP
3	K	312	ASP
3	L	312	ASP
3	M	312	ASP
3	N	312	ASP
3	O	312	ASP
3	P	312	ASP
3	Q	312	ASP
3	R	312	ASP
3	S	312	ASP
1	A	381	ASP
1	B	381	ASP
1	C	381	ASP
1	D	381	ASP
1	E	381	ASP
1	F	359	HIS
1	F	381	ASP
1	E	359	HIS
3	H	290	ARG
3	J	290	ARG
3	L	290	ARG
3	N	290	ARG
3	O	290	ARG
3	P	290	ARG
3	Q	290	ARG
3	R	290	ARG
3	S	290	ARG

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Mol	Chain	Res	Type
1	A	370	THR
1	B	370	THR
1	C	370	THR
1	D	370	THR
1	E	370	THR
1	F	370	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	265/367 (72%)	262 (99%)	3 (1%)	73 84
1	B	265/367 (72%)	259 (98%)	6 (2%)	50 70
1	C	265/367 (72%)	262 (99%)	3 (1%)	73 84
1	D	265/367 (72%)	261 (98%)	4 (2%)	65 80
1	E	262/367 (71%)	259 (99%)	3 (1%)	73 84
1	F	258/367 (70%)	247 (96%)	11 (4%)	29 53
3	H	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	I	45/294 (15%)	44 (98%)	1 (2%)	52 71
3	J	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	K	41/294 (14%)	40 (98%)	1 (2%)	49 69
3	L	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	M	41/294 (14%)	40 (98%)	1 (2%)	49 69
3	N	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	O	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	P	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	Q	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	R	36/294 (12%)	34 (94%)	2 (6%)	21 46
3	S	36/294 (12%)	34 (94%)	2 (6%)	21 46
All	All	2031/5730 (35%)	1980 (98%)	51 (2%)	50 68

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	THR
1	A	373	LEU
1	A	400	ASP
1	B	370	THR
1	B	373	LEU
1	B	396	LEU
1	B	397	LYS
1	B	398	GLU
1	B	402	THR
1	C	370	THR
1	C	373	LEU
1	C	398	GLU
1	D	370	THR
1	D	373	LEU
1	D	398	GLU
1	D	402	THR
1	E	370	THR
1	E	373	LEU
1	E	402	THR
1	F	127	LYS
1	F	139	GLU
1	F	200	SER
1	F	209	GLU
1	F	240	THR
1	F	278	ILE
1	F	291	GLU
1	F	370	THR
1	F	373	LEU
1	F	412	SER
1	F	417	VAL
3	H	290	ARG
3	H	319	GLU
3	I	319	GLU
3	J	290	ARG
3	J	319	GLU
3	K	319	GLU
3	L	290	ARG
3	L	319	GLU
3	M	319	GLU
3	N	290	ARG
3	N	319	GLU
3	O	290	ARG

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Mol	Chain	Res	Type
3	O	319	GLU
3	P	290	ARG
3	P	319	GLU
3	Q	290	ARG
3	Q	319	GLU
3	R	290	ARG
3	R	319	GLU
3	S	290	ARG
3	S	319	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	B	359	HIS
1	C	359	HIS
1	D	355	GLN
1	D	359	HIS
1	E	359	HIS
1	E	425	GLN
1	F	216	GLN
1	F	265	ASN
3	H	296	GLN
3	I	298	GLN
3	J	296	GLN
3	K	298	GLN
3	L	296	GLN
3	M	298	GLN
3	N	296	GLN
3	O	296	GLN
3	P	296	GLN
3	Q	296	GLN
3	R	296	GLN
3	S	296	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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
5	BEF	C	503	4	0,3,3	-	-	-		
4	ADP	A	501	5	24,29,29	0.94	2 (8%)	29,45,45	1.22	3 (10%)
5	BEF	A	502	4	0,3,3	-	-	-		
4	ADP	E	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.47	4 (13%)
4	ADP	C	502	5	24,29,29	0.81	1 (4%)	29,45,45	1.23	4 (13%)
4	ADP	D	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
5	BEF	C	501	4	0,3,3	-	-	-		
4	ADP	B	501	5	24,29,29	0.95	1 (4%)	29,45,45	1.29	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	501	5	-	4/12/32/32	0/3/3/3
4	ADP	E	501	-	-	4/12/32/32	0/3/3/3
4	ADP	C	502	5	-	2/12/32/32	0/3/3/3
4	ADP	D	501	-	-	1/12/32/32	0/3/3/3
4	ADP	B	501	5	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501	ADP	C5-C4	2.52	1.47	1.40
4	D	501	ADP	C5-C4	2.44	1.47	1.40
4	A	501	ADP	PB-O1B	2.28	1.57	1.50
4	C	502	ADP	C8-N7	-2.10	1.31	1.34
4	B	501	ADP	C8-N7	-2.08	1.31	1.34
4	A	501	ADP	C8-N7	-2.07	1.31	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	ADP	PA-O3A-PB	-4.01	119.06	132.83
4	E	501	ADP	C3'-C2'-C1'	3.72	106.57	100.98
4	E	501	ADP	PA-O3A-PB	-3.34	121.37	132.83
4	B	501	ADP	PA-O3A-PB	-3.12	122.13	132.83
4	E	501	ADP	N3-C2-N1	-3.05	123.91	128.68
4	C	502	ADP	C3'-C2'-C1'	2.92	105.38	100.98
4	D	501	ADP	N3-C2-N1	-2.92	124.11	128.68
4	D	501	ADP	C3'-C2'-C1'	2.89	105.33	100.98
4	D	501	ADP	C4-C5-N7	-2.71	106.57	109.40
4	C	502	ADP	O2A-PA-O5'	2.68	120.19	107.75
4	E	501	ADP	C4-C5-N7	-2.59	106.70	109.40
4	B	501	ADP	C3'-C2'-C1'	2.49	104.72	100.98
4	A	501	ADP	O5'-PA-O1A	2.46	118.67	109.07
4	B	501	ADP	O2A-PA-O5'	2.45	119.14	107.75
4	A	501	ADP	O3B-PB-O3A	2.39	112.65	104.64
4	B	501	ADP	O3B-PB-O3A	2.20	112.03	104.64
4	C	502	ADP	PA-O3A-PB	-2.17	125.39	132.83
4	C	502	ADP	O2B-PB-O3A	2.07	111.56	104.64
4	A	501	ADP	C5-C6-N6	2.05	123.47	120.35
4	B	501	ADP	C5-C6-N6	2.02	123.43	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	501	ADP	PA-O3A-PB-O2B
4	E	501	ADP	C5'-O5'-PA-O3A
4	C	502	ADP	O4'-C4'-C5'-O5'
4	A	501	ADP	C5'-O5'-PA-O3A
4	E	501	ADP	C5'-O5'-PA-O1A
4	C	502	ADP	C3'-C4'-C5'-O5'

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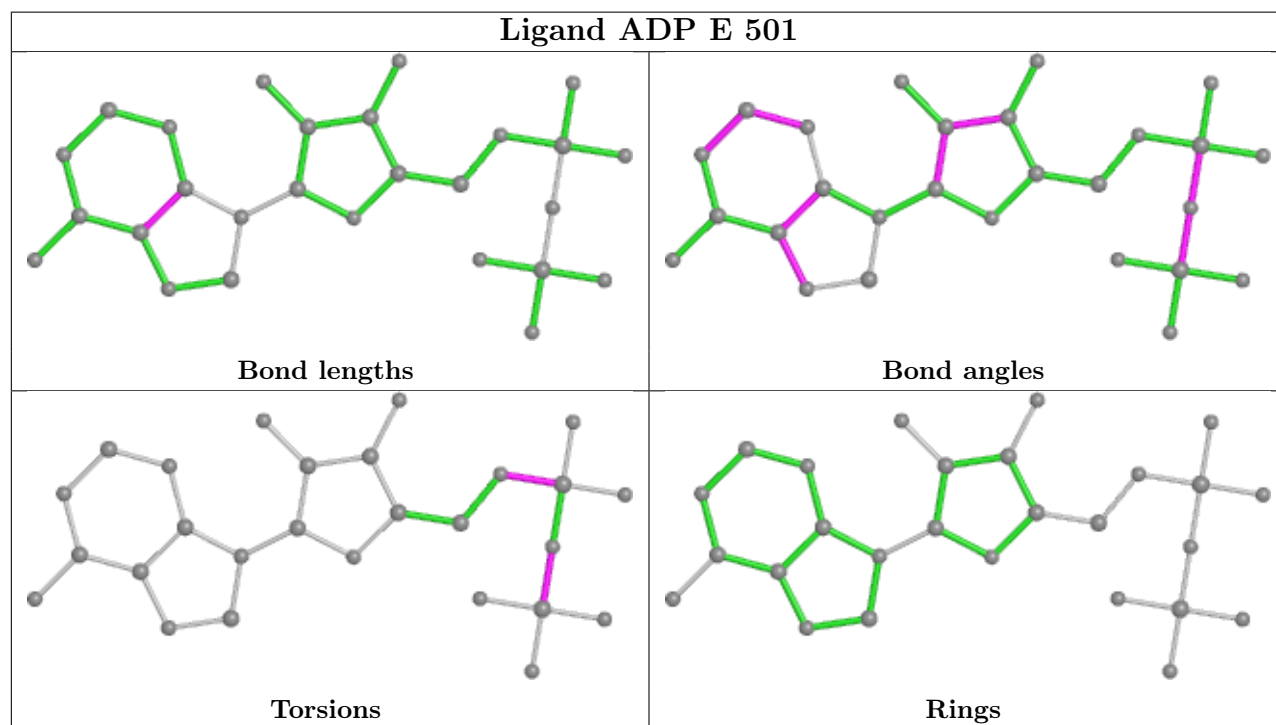
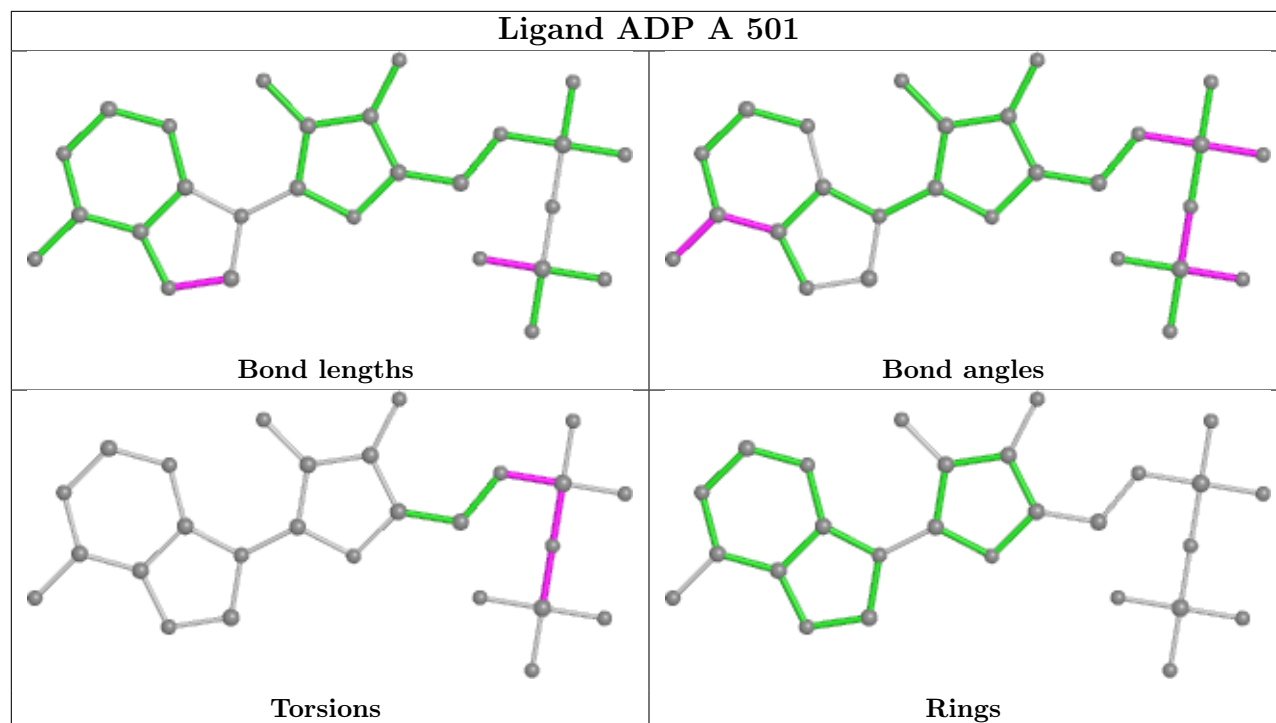
Mol	Chain	Res	Type	Atoms
4	A	501	ADP	PA-O3A-PB-O1B
4	E	501	ADP	PA-O3A-PB-O3B
4	D	501	ADP	C5'-O5'-PA-O3A
4	A	501	ADP	PB-O3A-PA-O2A
4	A	501	ADP	C5'-O5'-PA-O1A

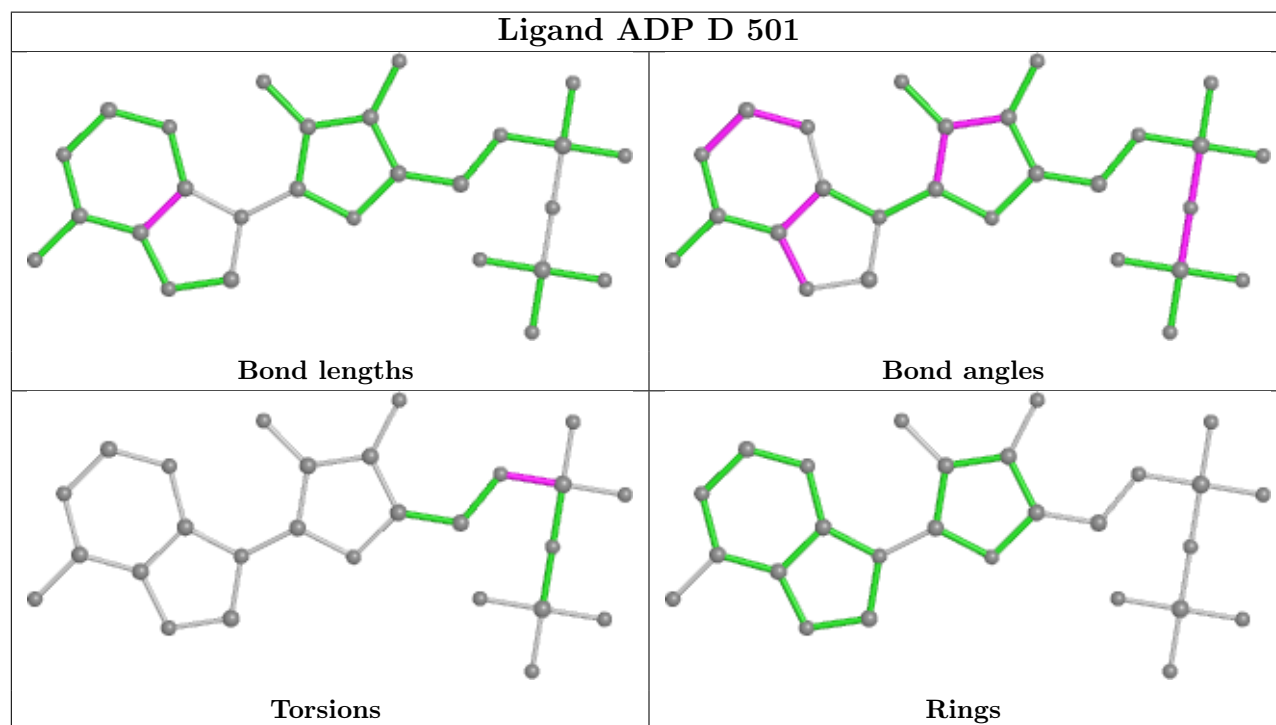
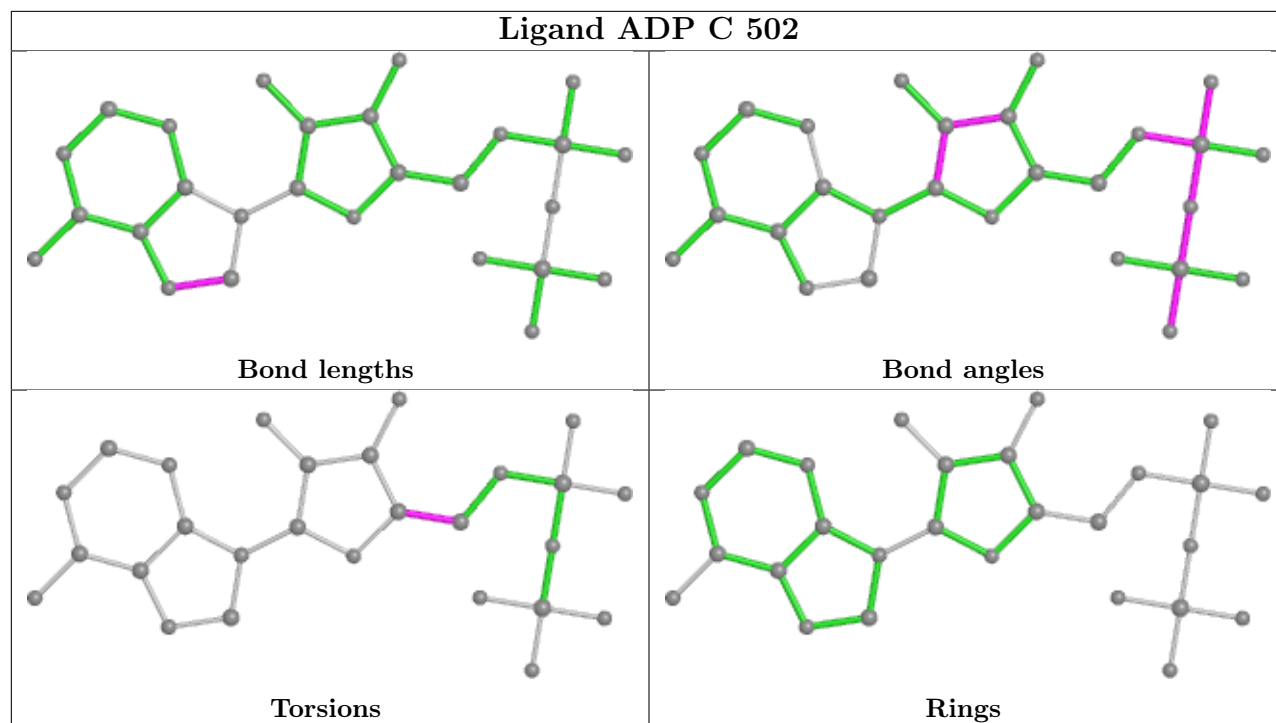
There are no ring outliers.

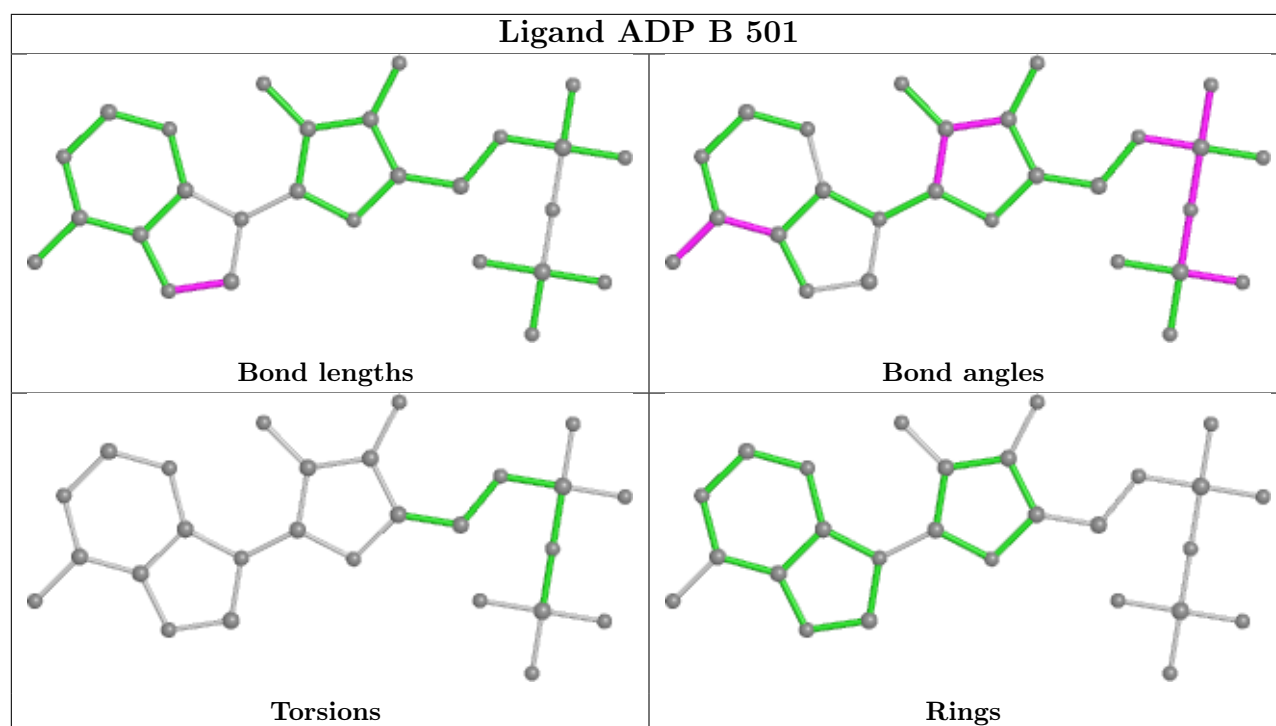
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	ADP	1	0
4	E	501	ADP	1	0
4	C	502	ADP	1	0
4	D	501	ADP	2	0
5	C	501	BEF	1	0
4	B	501	ADP	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.

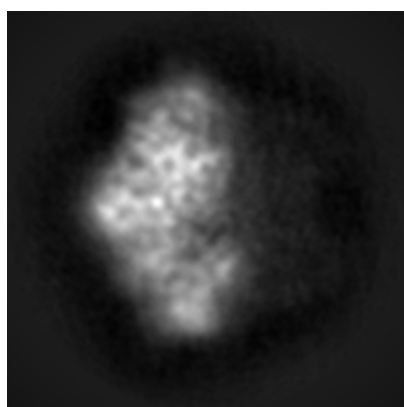
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8549. These allow visual inspection of the internal detail of the map and identification of artifacts.

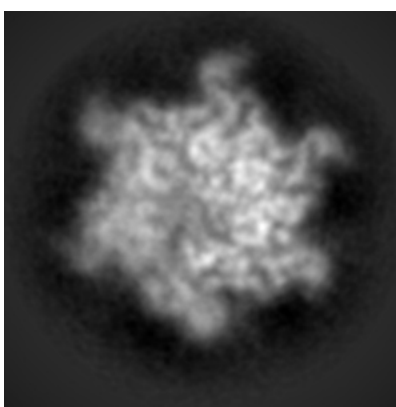
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

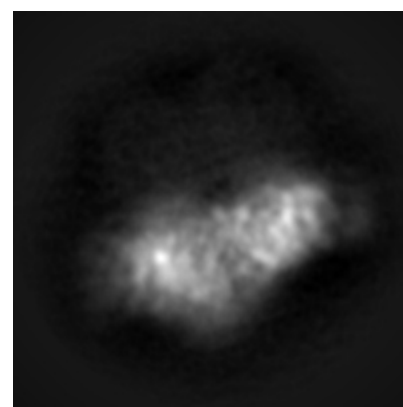
6.1.1 Primary map



X



Y

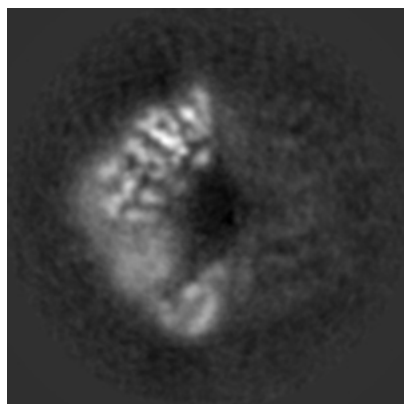


Z

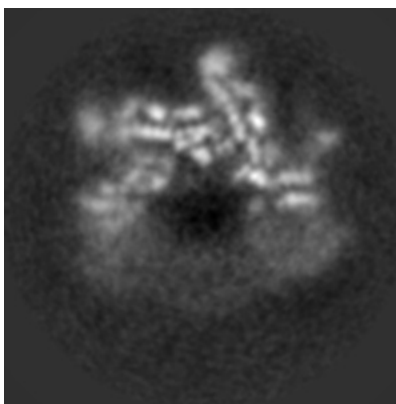
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

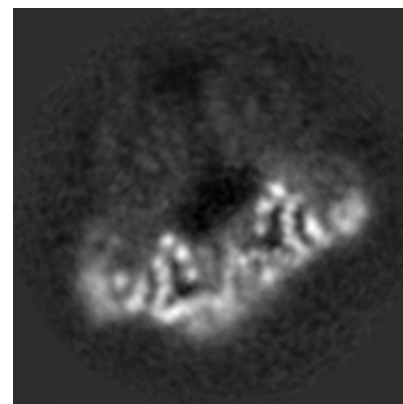
6.2.1 Primary map



X Index: 69



Y Index: 69

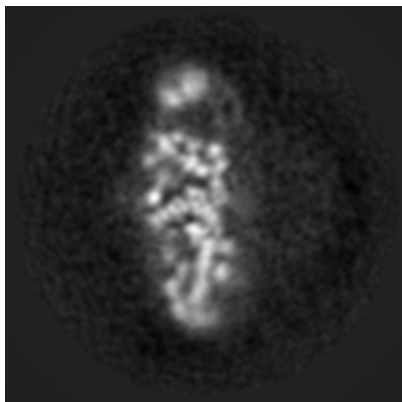


Z Index: 69

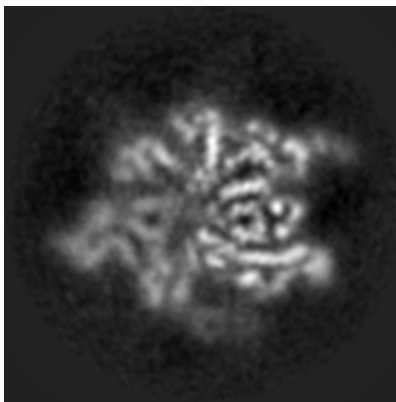
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

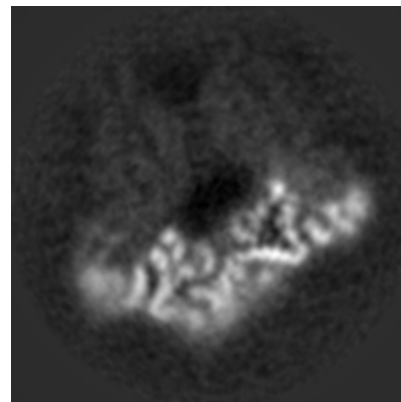
6.3.1 Primary map



X Index: 94



Y Index: 52



Z Index: 71

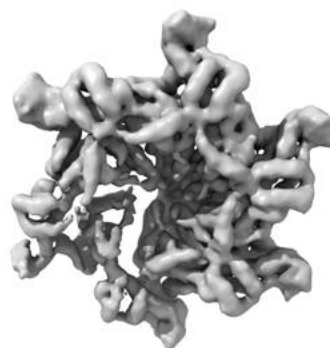
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0222. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

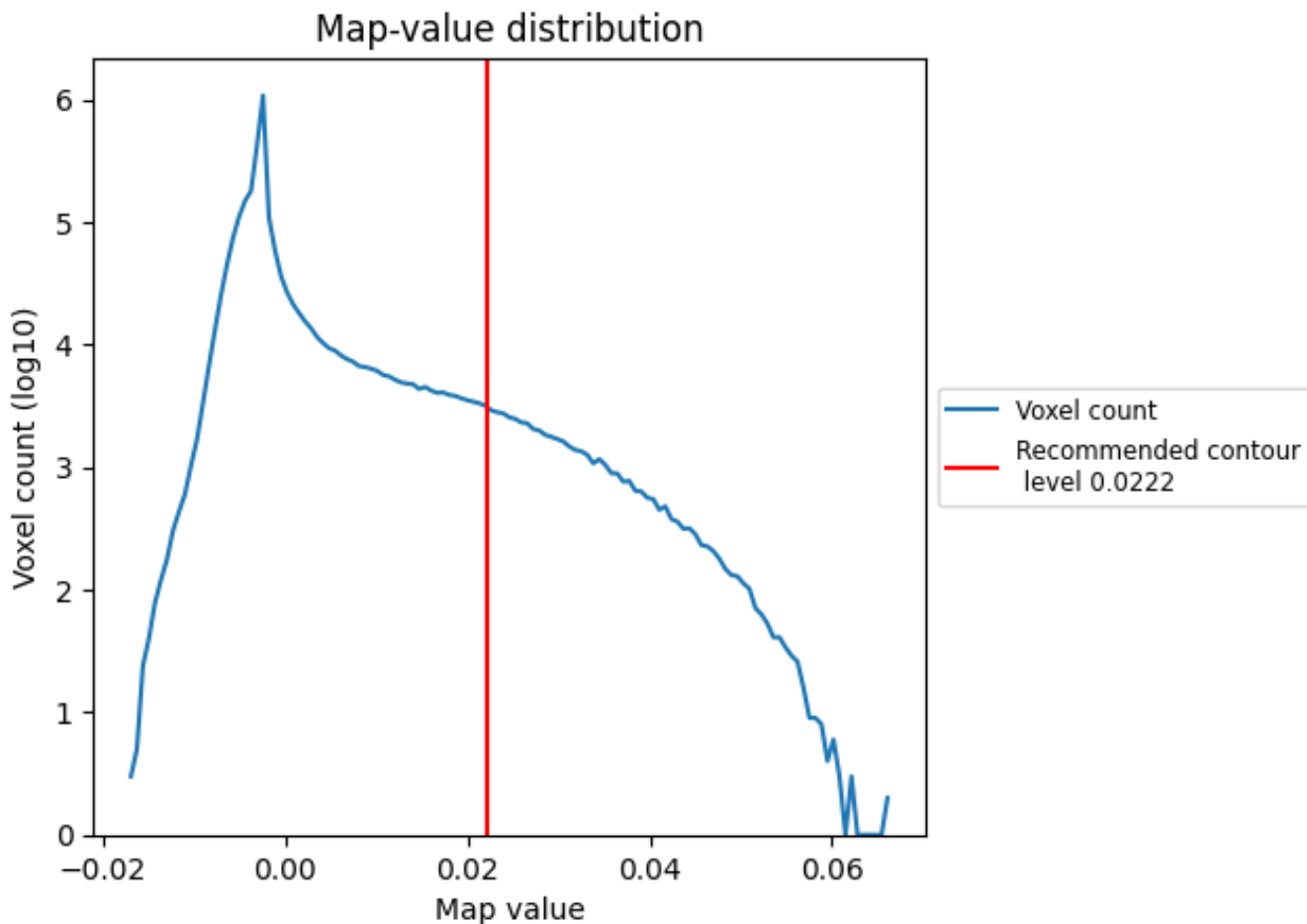
6.5 Mask visualisation

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

7 Map analysis [i](#)

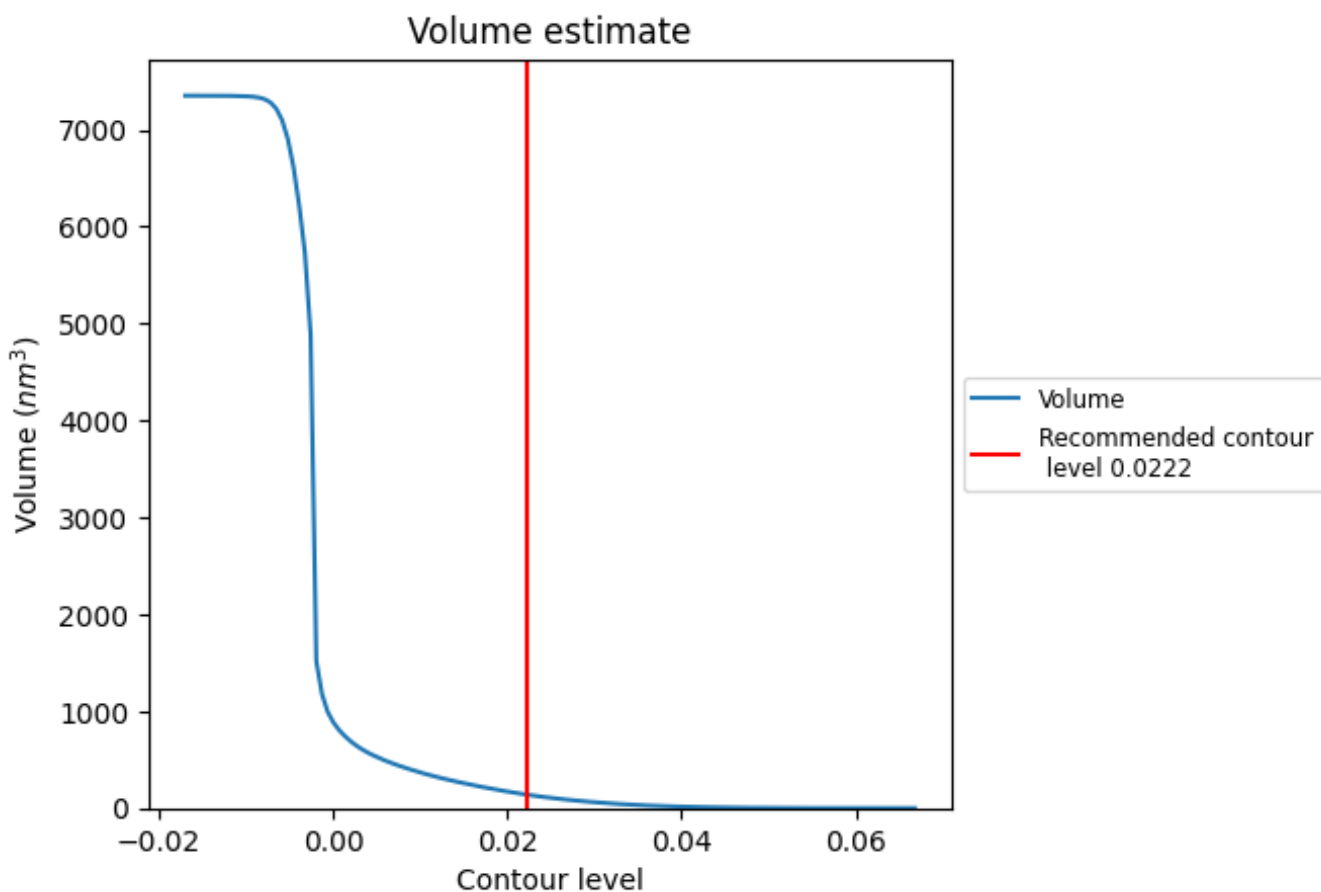
This section contains the results of statistical analysis of the map.

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.

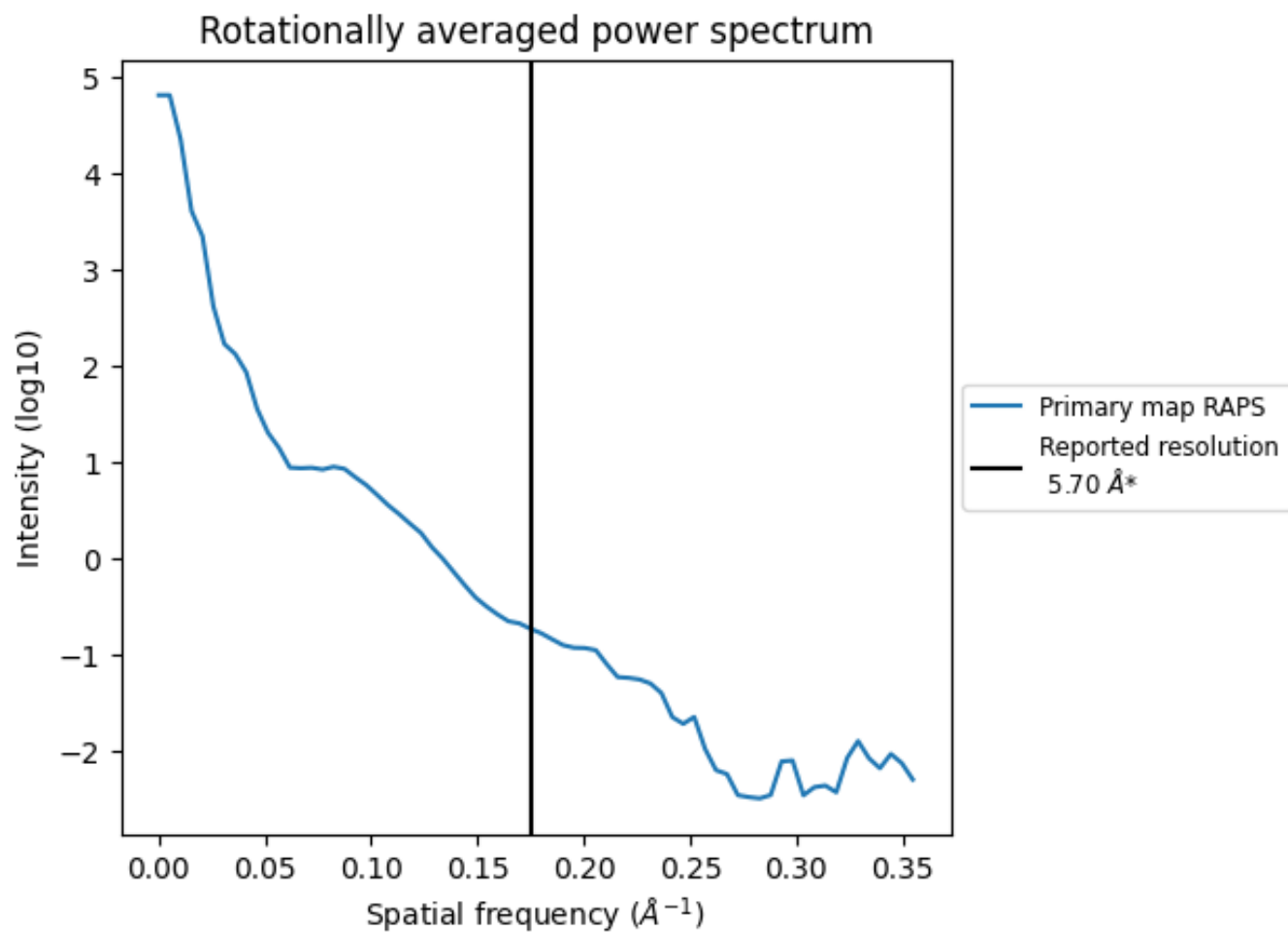
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm^3 ; this corresponds to an approximate mass of 126 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 0.175 Å⁻¹

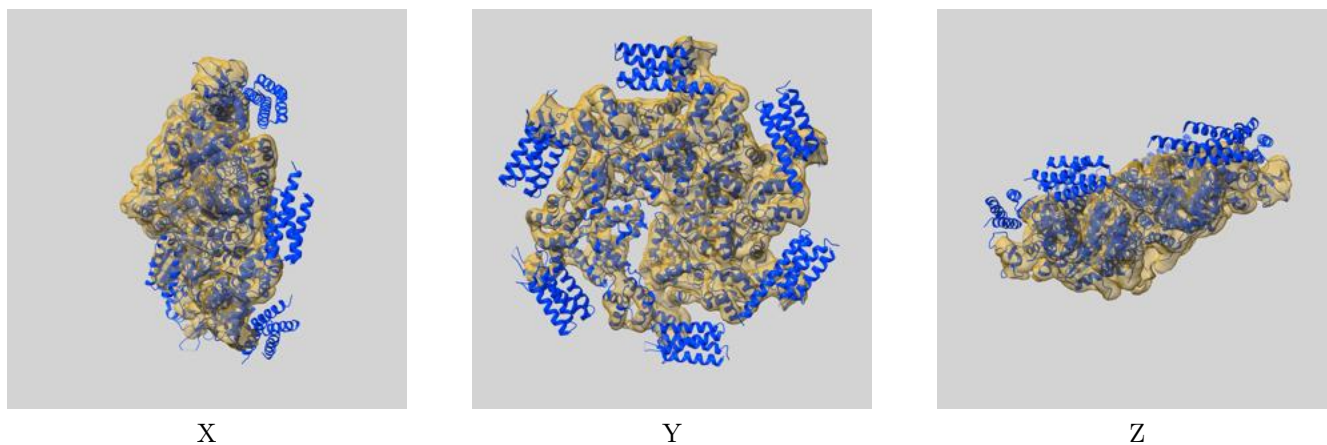
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

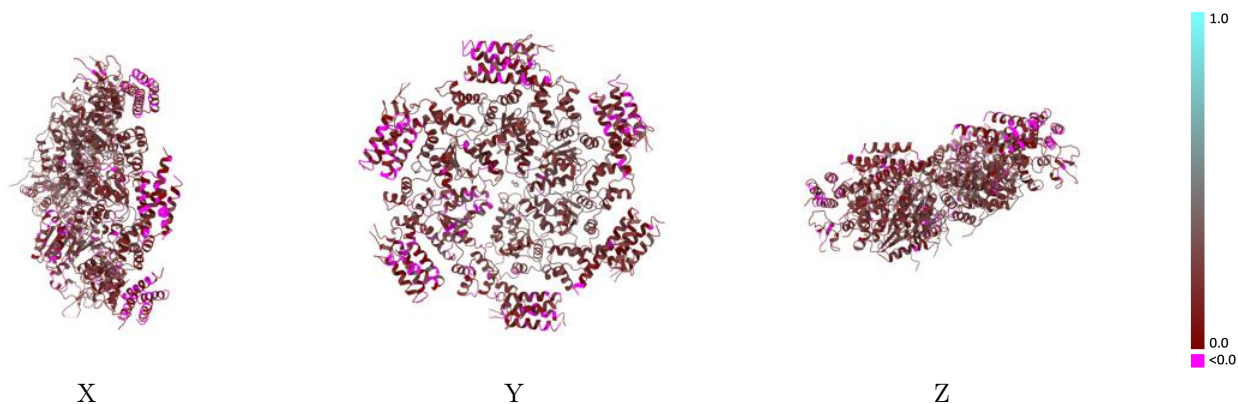
This section contains information regarding the fit between EMDB map EMD-8549 and PDB model 5UIE. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



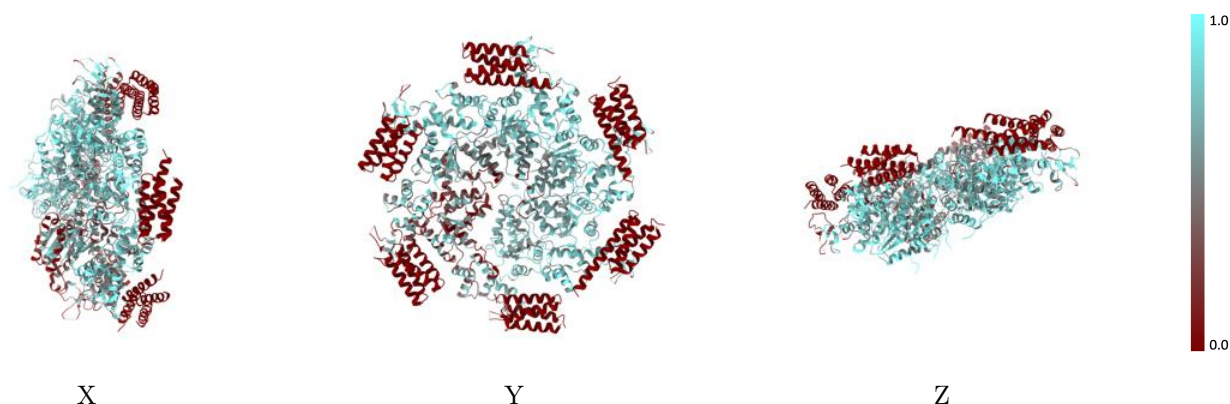
The images above show the 3D surface view of the map at the recommended contour level 0.0222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



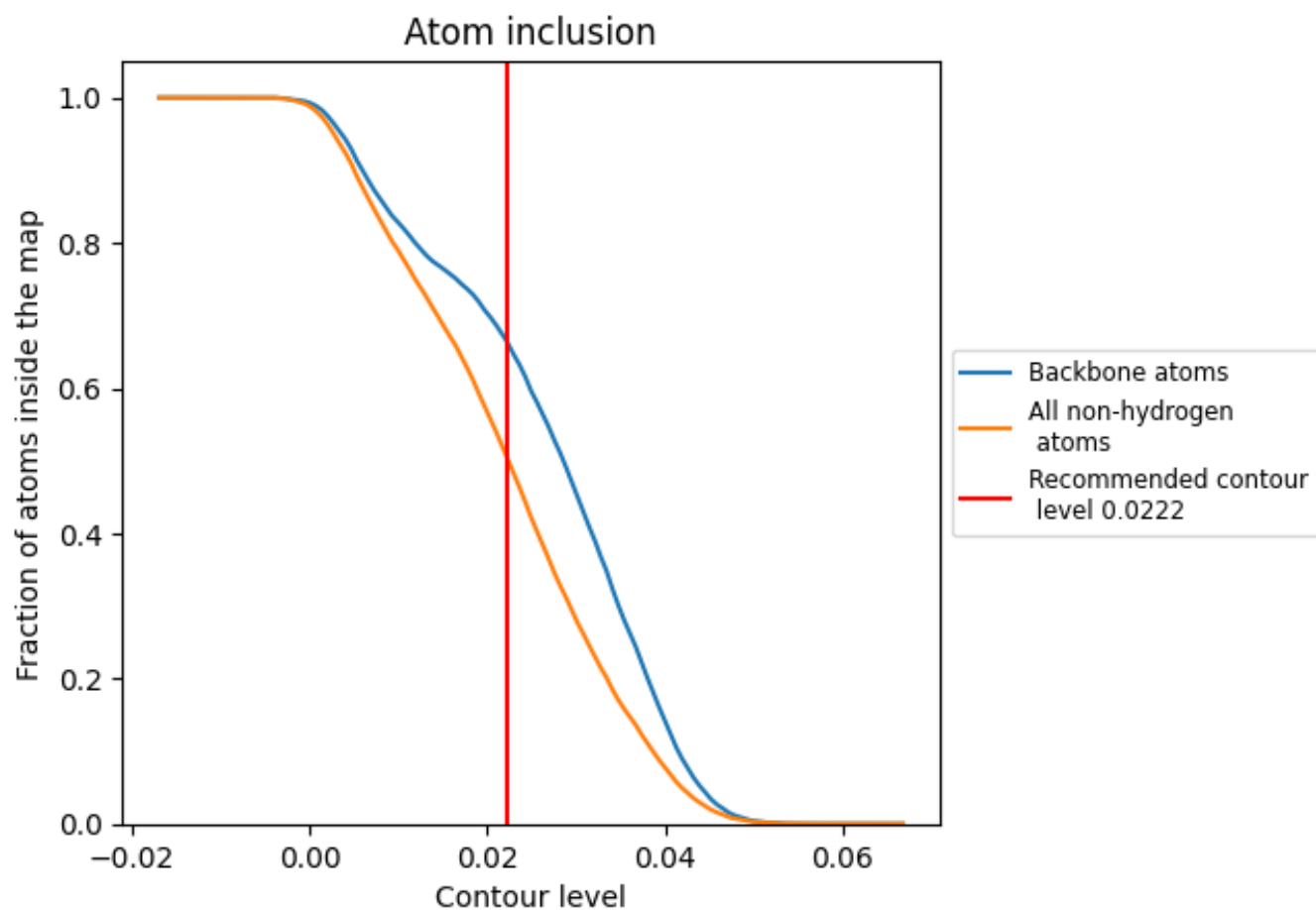
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0222).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 50% 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 (0.0222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5038	 0.1850
A	 0.7499	 0.2250
B	 0.7473	 0.2420
C	 0.7448	 0.2460
D	 0.7158	 0.2350
E	 0.5365	 0.2040
F	 0.3731	 0.1220
G	 0.9286	 0.3320
H	 0.0000	 0.1690
I	 0.0000	 0.1240
J	 0.0000	 0.0870
K	 0.0000	 0.1000
L	 0.0000	 0.0450
M	 0.0000	 0.0700
N	 0.0000	 0.0160
O	 0.0000	 0.0410
P	 0.0000	 0.0900
Q	 0.0000	 0.0910
R	 0.0000	 0.0920
S	 0.0000	 0.1070

