



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 10:58 PM JST

PDB ID : 9XRL / pdb_00009xrl
EMDB ID : EMD-67147
Title : Structure of mouse cytoplasmic lattice (CPL) repeating unit
Authors : Chi, P.L.; Wang, X.; Li, J.L.; Deng, D.
Deposited on : 2025-11-19
Resolution : 3.74 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

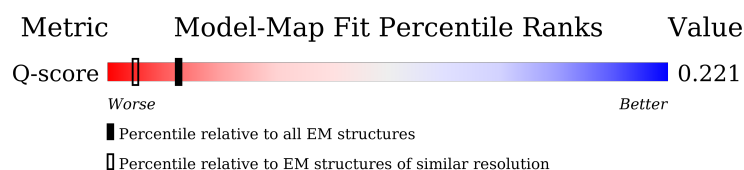
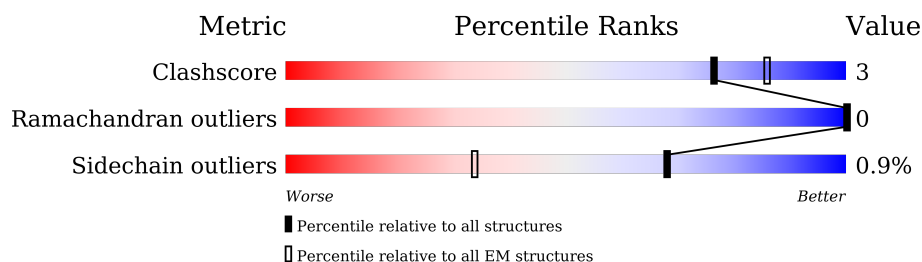
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 Å.

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



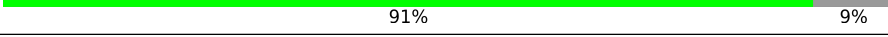
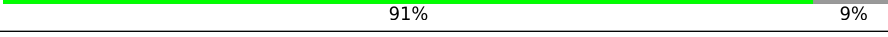
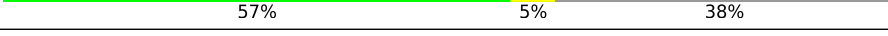
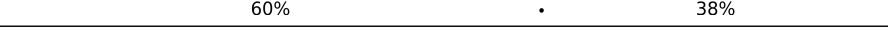
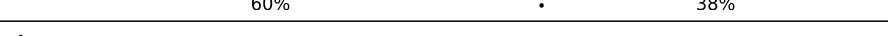
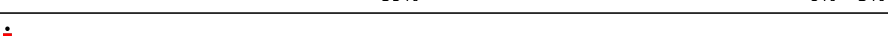
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10346 (3.24 - 4.24)

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	1	228	
1	3	228	
1	9	228	
2	4	440	

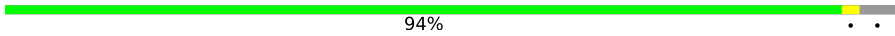
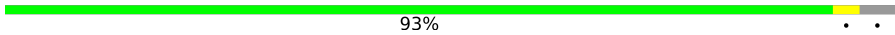
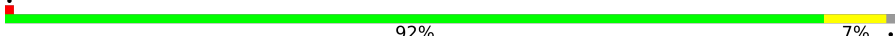
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Mol	Chain	Length	Quality of chain
2	6	440	
2	AA	440	
3	A	468	
4	D	163	
4	F	163	
4	O	163	
4	p	163	
4	q	163	
5	8	581	
5	AC	581	
5	E	581	
5	I	581	
5	P	581	
5	z	581	
6	H	937	
6	Q	937	
6	h	937	
6	i	937	
7	B	682	
7	K	682	
7	S	682	
7	T	682	
7	U	682	
7	V	682	
7	W	682	

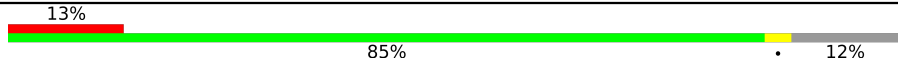
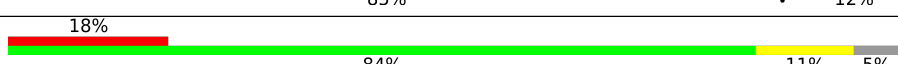
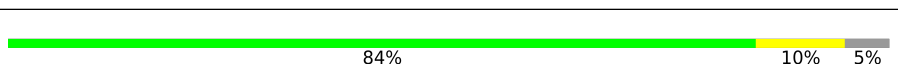
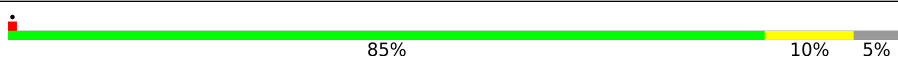
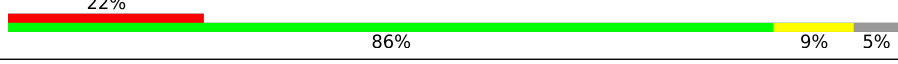
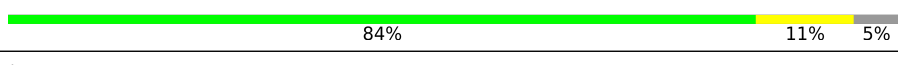
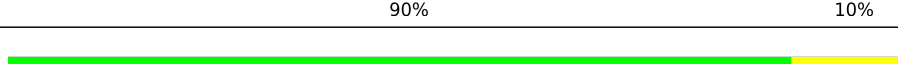
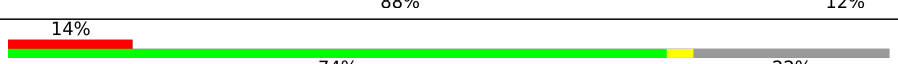
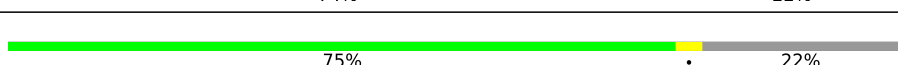
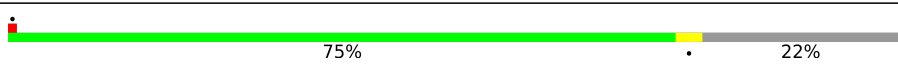
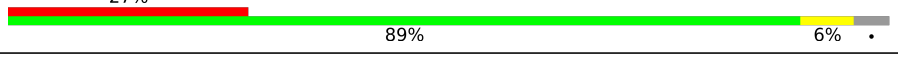
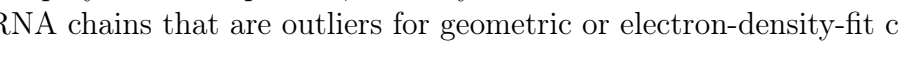
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Mol	Chain	Length	Quality of chain
7	X	682	
7	Y	682	
7	Z	682	
7	b	682	
7	c	682	
7	d	682	
7	f	682	
7	j	682	
7	m	682	
7	n	682	
7	o	682	
7	r	682	
7	s	682	
8	AH	164	
8	AI	164	
8	AJ	164	
8	AT	164	
8	e	164	
8	g	164	
9	k	469	
9	l	469	
10	AE	445	
10	AN	445	
10	t	445	
11	0	1059	

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Mol	Chain	Length	Quality of chain
11	2	1059	
11	5	1059	
11	7	1059	
11	AB	1059	
11	y	1059	
12	AF	451	
12	AO	451	
12	u	451	
13	AK	993	
13	AQ	993	
13	w	993	
14	AD	147	
14	AM	147	
14	AS	147	
15	AL	782	
15	AR	782	
15	x	782	
16	C	466	
16	L	466	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	GTP	AF	501	-	-	X	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 281032 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 Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	56	Total	C	N	O	S	0	0
			427	268	80	74	5		
1	3	56	Total	C	N	O	S	0	0
			453	288	84	75	6		
1	9	56	Total	C	N	O	S	0	0
			453	288	84	75	6		

- Molecule 2 is a protein called KH domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	124	Total	C	N	O	S	0	0
			977	633	167	171	6		
2	6	124	Total	C	N	O	S	0	0
			1028	667	178	175	8		
2	AA	124	Total	C	N	O	S	0	0
			1028	667	178	175	8		

- Molecule 3 is a protein called F-box and WD-40 domain protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	450	Total	C	N	O	S	0	0
			3650	2372	604	651	23		

- Molecule 4 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	148	Total	C	N	O	S	0	0
			1195	756	196	237	6		
4	p	148	Total	C	N	O	S	0	0
			1190	750	195	239	6		
4	O	148	Total	C	N	O	S	0	0
			1199	758	196	239	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	q	148	Total	C	N	O	S	0	0
			1190	750	195	239	6		
4	F	148	Total	C	N	O	S	0	0
			1199	758	196	239	6		

- Molecule 5 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	358	Total	C	N	O	S	0	0
			2799	1771	493	515	20		
5	I	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		
5	z	358	Total	C	N	O	S	0	0
			2813	1785	494	514	20		
5	P	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		
5	AC	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		
5	8	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		

- Molecule 6 is a protein called NLR family, pyrin domain containing 4F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	723	Total	C	N	O	S	0	0
			5803	3706	973	1070	54		
6	Q	636	Total	C	N	O	S	0	0
			5099	3248	850	948	53		
6	i	721	Total	C	N	O	S	0	0
			5738	3657	961	1064	56		
6	h	721	Total	C	N	O	S	0	0
			5781	3684	971	1071	55		

- Molecule 7 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	647	Total	C	N	O	S	0	0
			5102	3271	836	958	37		
7	T	654	Total	C	N	O	S	0	0
			5162	3310	849	965	38		
7	Y	658	Total	C	N	O	S	0	0
			5099	3279	836	949	35		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	656	Total	C	N	O	S	0	0
			5149	3304	845	962	38		
7	X	652	Total	C	N	O	S	0	0
			5161	3308	851	964	38		
7	Z	652	Total	C	N	O	S	0	0
			5133	3291	846	958	38		
7	V	652	Total	C	N	O	S	0	0
			5139	3297	845	959	38		
7	W	654	Total	C	N	O	S	0	0
			5151	3302	848	963	38		
7	n	658	Total	C	N	O	S	0	0
			5105	3282	839	949	35		
7	f	654	Total	C	N	O	S	0	0
			5168	3312	850	968	38		
7	s	656	Total	C	N	O	S	0	0
			5146	3303	845	960	38		
7	m	652	Total	C	N	O	S	0	0
			5161	3308	851	964	38		
7	o	652	Total	C	N	O	S	0	0
			5138	3294	845	961	38		
7	d	652	Total	C	N	O	S	0	0
			5130	3293	841	958	38		
7	j	654	Total	C	N	O	S	0	0
			5155	3305	849	963	38		
7	r	650	Total	C	N	O	S	0	0
			5144	3298	849	960	37		
7	B	651	Total	C	N	O	S	0	0
			5141	3293	849	962	37		
7	K	652	Total	C	N	O	S	0	0
			5145	3294	850	964	37		
7	U	655	Total	C	N	O	S	0	0
			5163	3304	853	968	38		
7	c	655	Total	C	N	O	S	0	0
			5167	3308	853	968	38		

- Molecule 8 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	128	Total	C	N	O	S	0	0
			928	590	164	169	5		
8	g	128	Total	C	N	O	S	0	0
			928	590	164	169	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	116	Total	C	N	O	S	0	0
			875	560	152	162	1		
8	AJ	116	Total	C	N	O	S	0	0
			938	600	162	171	5		
8	AI	116	Total	C	N	O	S	0	0
			935	597	162	171	5		
8	AT	128	Total	C	N	O	S	0	0
			928	590	164	169	5		

- Molecule 9 is a protein called Expressed sequence C85627.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	463	Total	C	N	O	S	0	0
			3729	2406	616	678	29		
9	l	463	Total	C	N	O	S	0	0
			3732	2409	616	678	29		

- Molecule 10 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	t	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
10	AE	430	Total	C	N	O	S	0	0
			3358	2110	572	650	26		
10	AN	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		

- Molecule 11 is a protein called NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	y	936	Total	C	N	O	S	0	0
			7262	4624	1230	1343	65		
11	AB	936	Total	C	N	O	S	0	0
			7322	4663	1239	1354	66		
11	0	935	Total	C	N	O	S	0	0
			7316	4658	1238	1354	66		
11	7	936	Total	C	N	O	S	0	0
			7319	4660	1239	1354	66		
11	5	935	Total	C	N	O	S	0	0
			7312	4655	1238	1353	66		
11	2	934	Total	C	N	O	S	0	0
			7221	4600	1222	1334	65		

- Molecule 12 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	u	430	Total	C	N	O	S	0	0
			3368	2136	573	637	22		
12	AF	430	Total	C	N	O	S	0	0
			3365	2135	573	635	22		
12	AO	430	Total	C	N	O	S	0	0
			3368	2136	573	637	22		

- Molecule 13 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	w	948	Total	C	N	O	S	0	0
			7473	4754	1292	1366	61		
13	AK	948	Total	C	N	O	S	0	0
			7417	4719	1284	1354	60		
13	AQ	948	Total	C	N	O	S	0	0
			7472	4754	1292	1365	61		

- Molecule 14 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AM	147	Total	C	N	O	S	0	0
			1167	748	197	215	7		
14	AS	147	Total	C	N	O	S	0	0
			1168	748	197	215	8		
14	AD	147	Total	C	N	O	S	0	0
			1168	748	197	215	8		

- Molecule 15 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	608	Total	C	N	O	S	0	0
			4872	3059	886	895	32		
15	AR	608	Total	C	N	O	S	0	0
			4872	3059	886	895	32		
15	x	608	Total	C	N	O	S	0	0
			4854	3050	881	891	32		

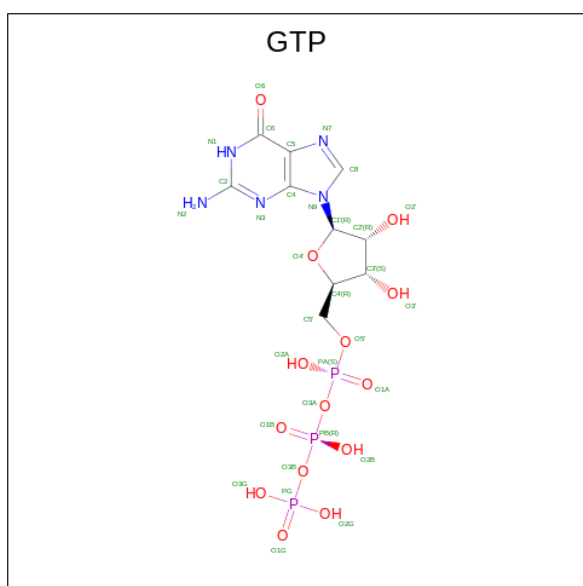
- Molecule 16 is a protein called F-box and WD-40 domain protein 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	449	Total	C	N	O	S	0	0
			3611	2322	617	643	29		
16	C	449	Total	C	N	O	S	0	0
			3601	2317	614	641	29		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	1	1	Total	Zn	0
			1	1	
17	3	1	Total	Zn	0
			1	1	
17	9	1	Total	Zn	0
			1	1	
17	AL	2	Total	Zn	0
			2	2	
17	AR	4	Total	Zn	0
			4	4	
17	x	4	Total	Zn	0
			4	4	

- Molecule 18 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
18	t	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	u	1	Total	C	N	O	P	0
			32	10	5	14	3	

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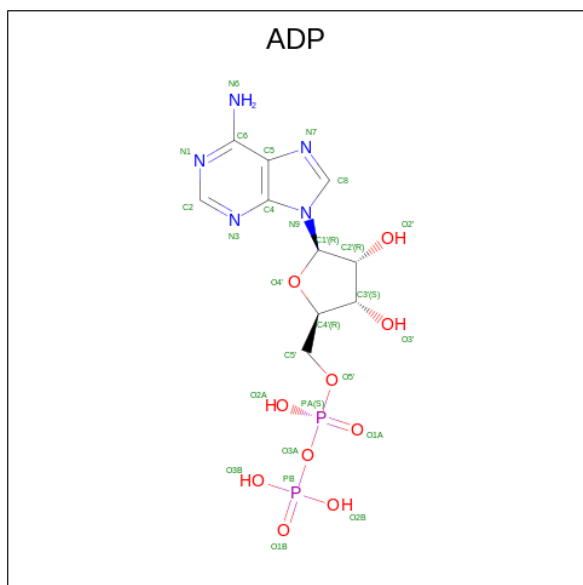
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Mol	Chain	Residues	Atoms					AltConf
18	AF	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	AO	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	AN	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	t	1	Total	Mg	0
			1	1	
19	u	1	Total	Mg	0
			1	1	
19	AO	1	Total	Mg	0
			1	1	
19	AN	1	Total	Mg	0
			1	1	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

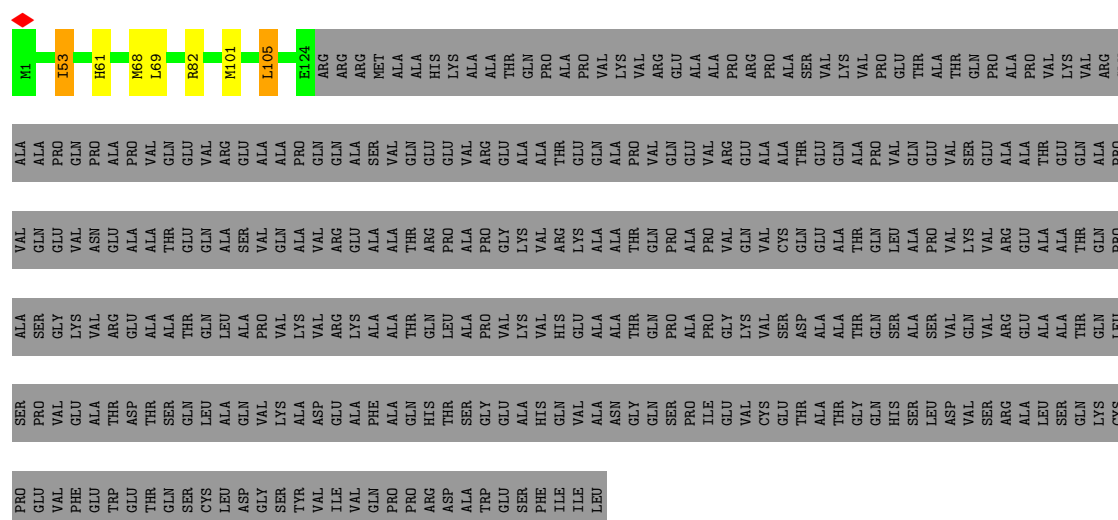


Mol	Chain	Residues	Atoms					AltConf
20	w	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

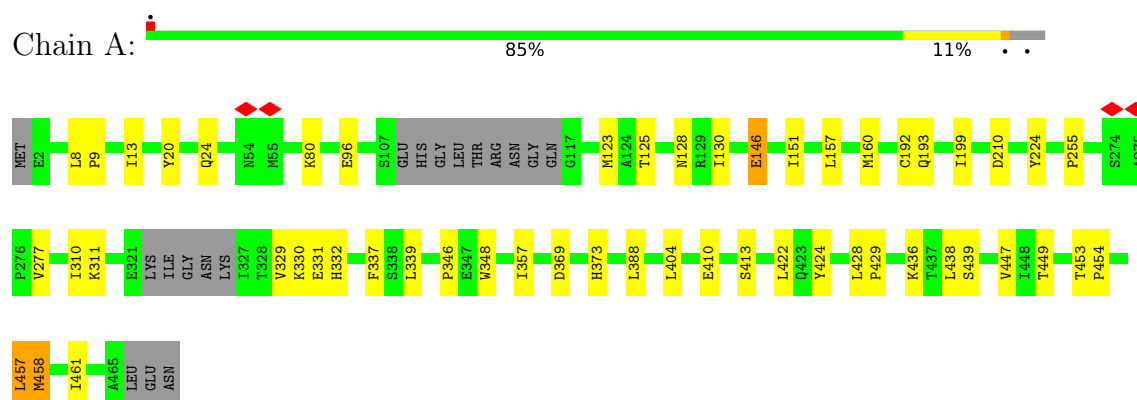
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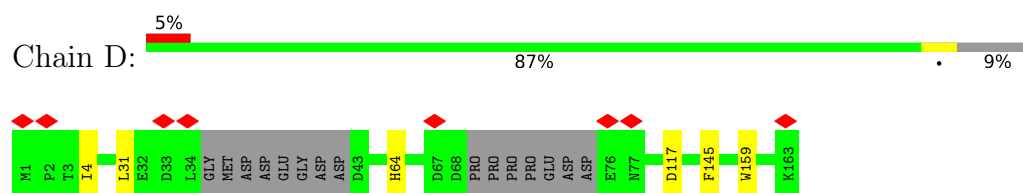
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	AQ	1	27	10	5	10	2	0



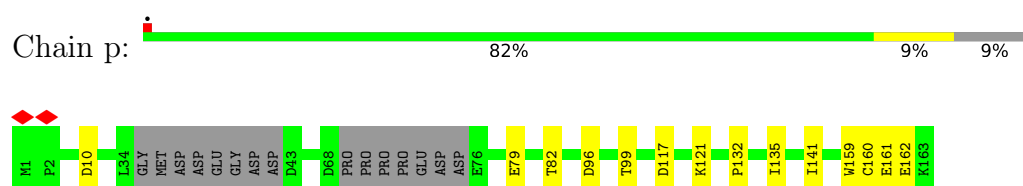
• Molecule 3: F-box and WD-40 domain protein 21



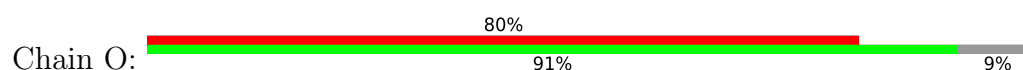
• Molecule 4: S-phase kinase-associated protein 1

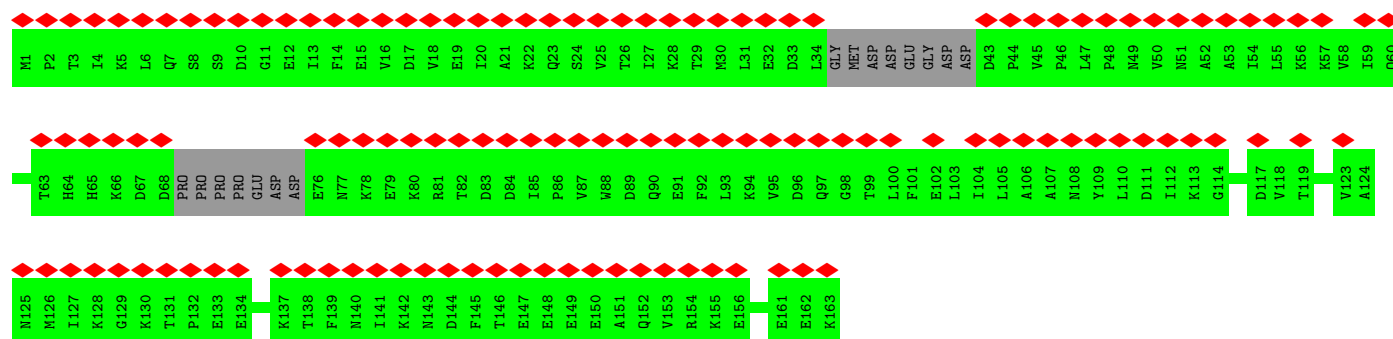


• Molecule 4: S-phase kinase-associated protein 1

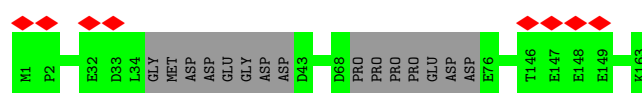
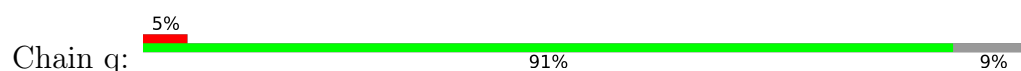


• Molecule 4: S-phase kinase-associated protein 1

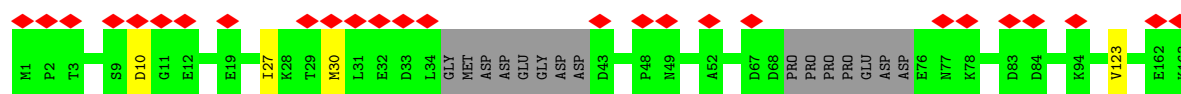
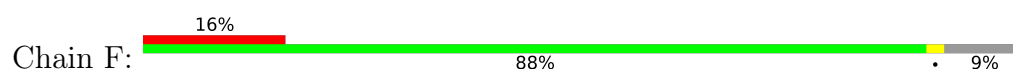




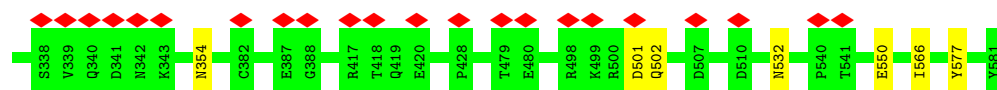
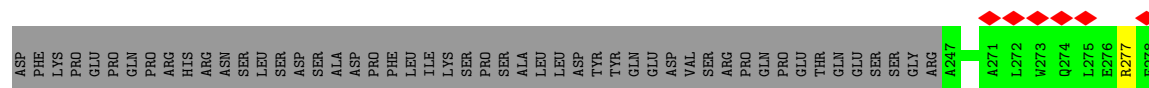
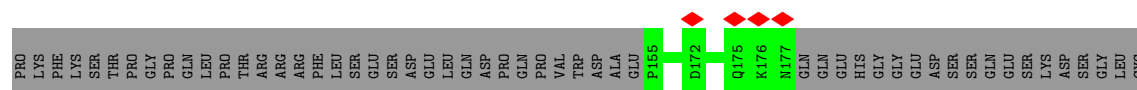
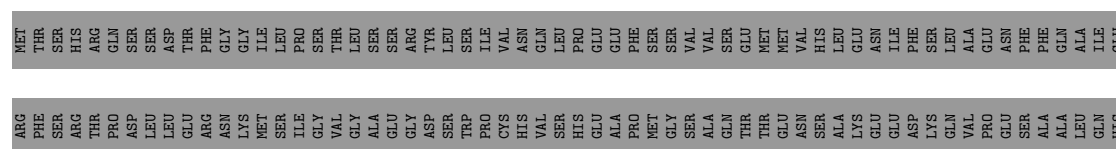
• Molecule 4: S-phase kinase-associated protein 1



• Molecule 4: S-phase kinase-associated protein 1



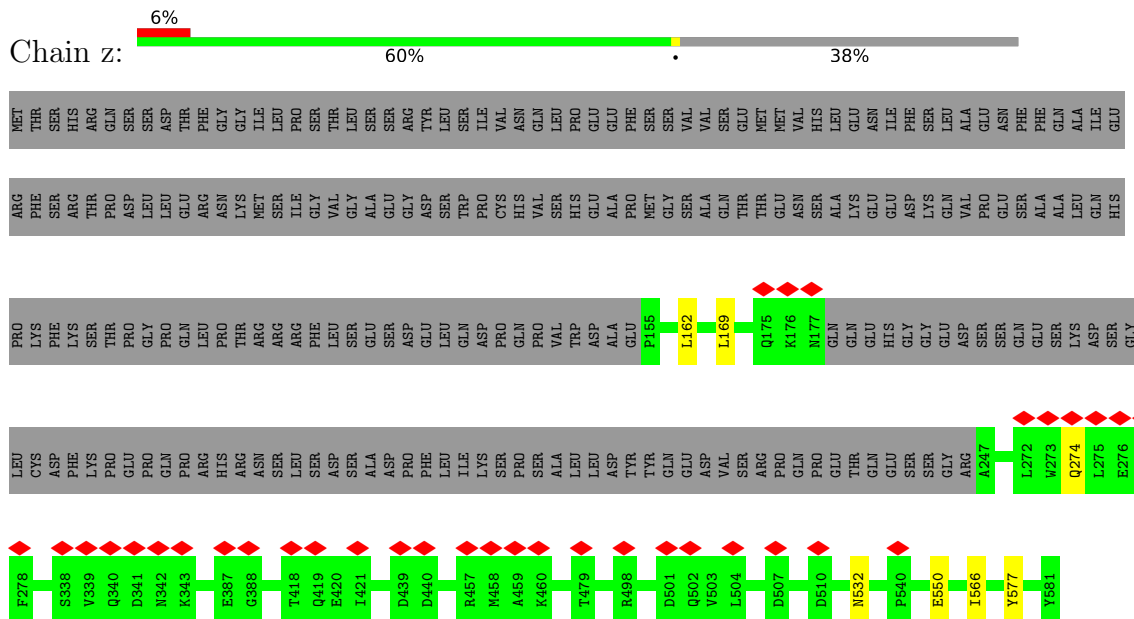
• Molecule 5: Transducin-like enhancer protein 6



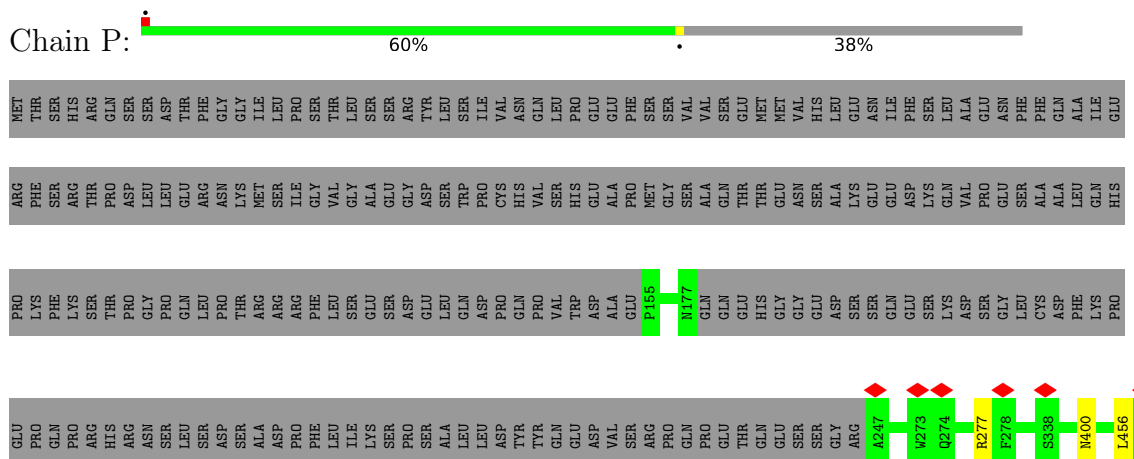
• Molecule 5: Transducin-like enhancer protein 6

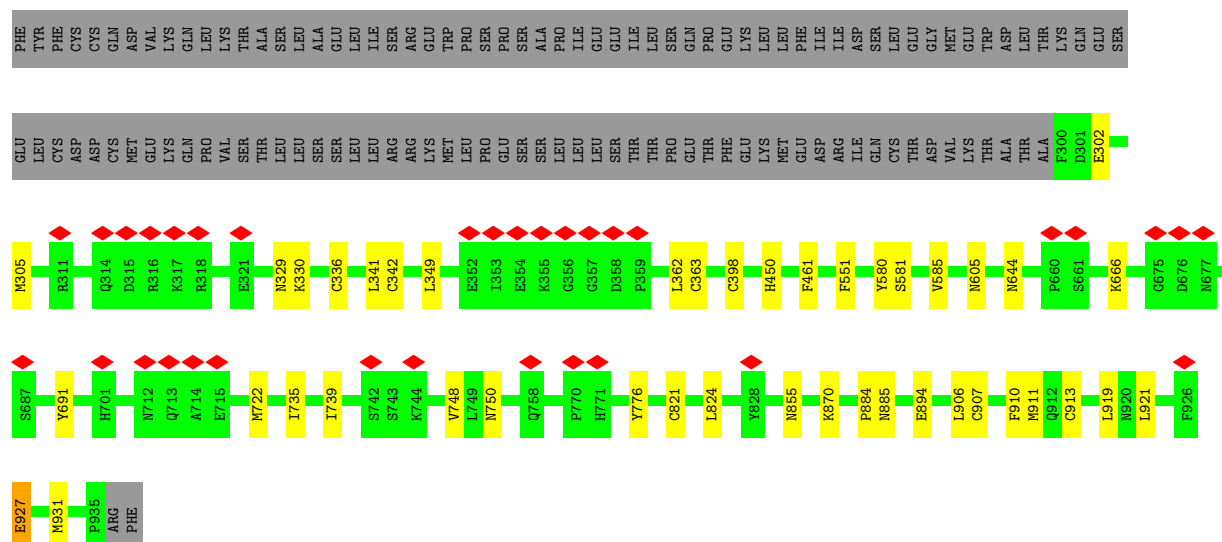


- Molecule 5: Transducin-like enhancer protein 6

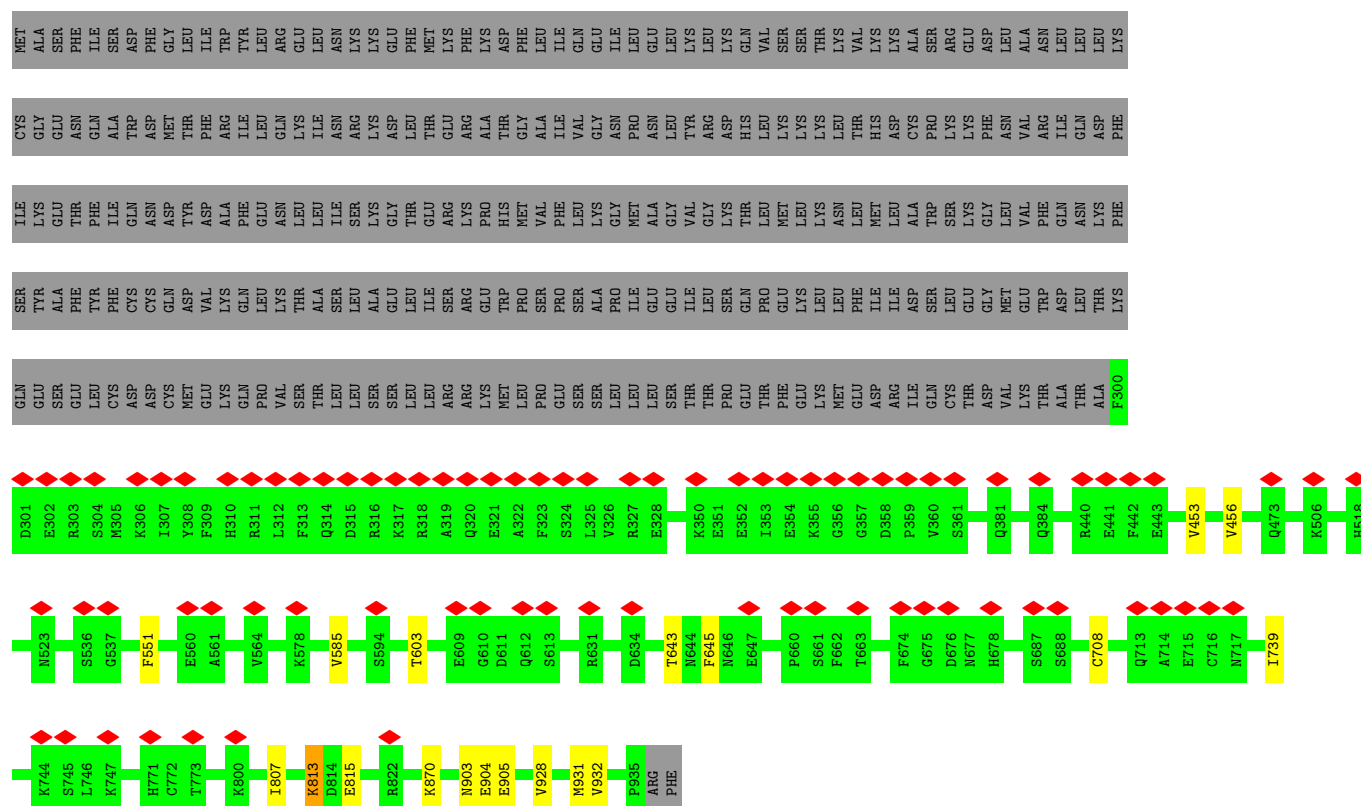


- Molecule 5: Transducin-like enhancer protein 6

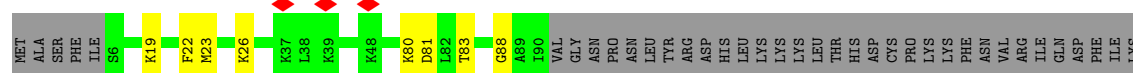


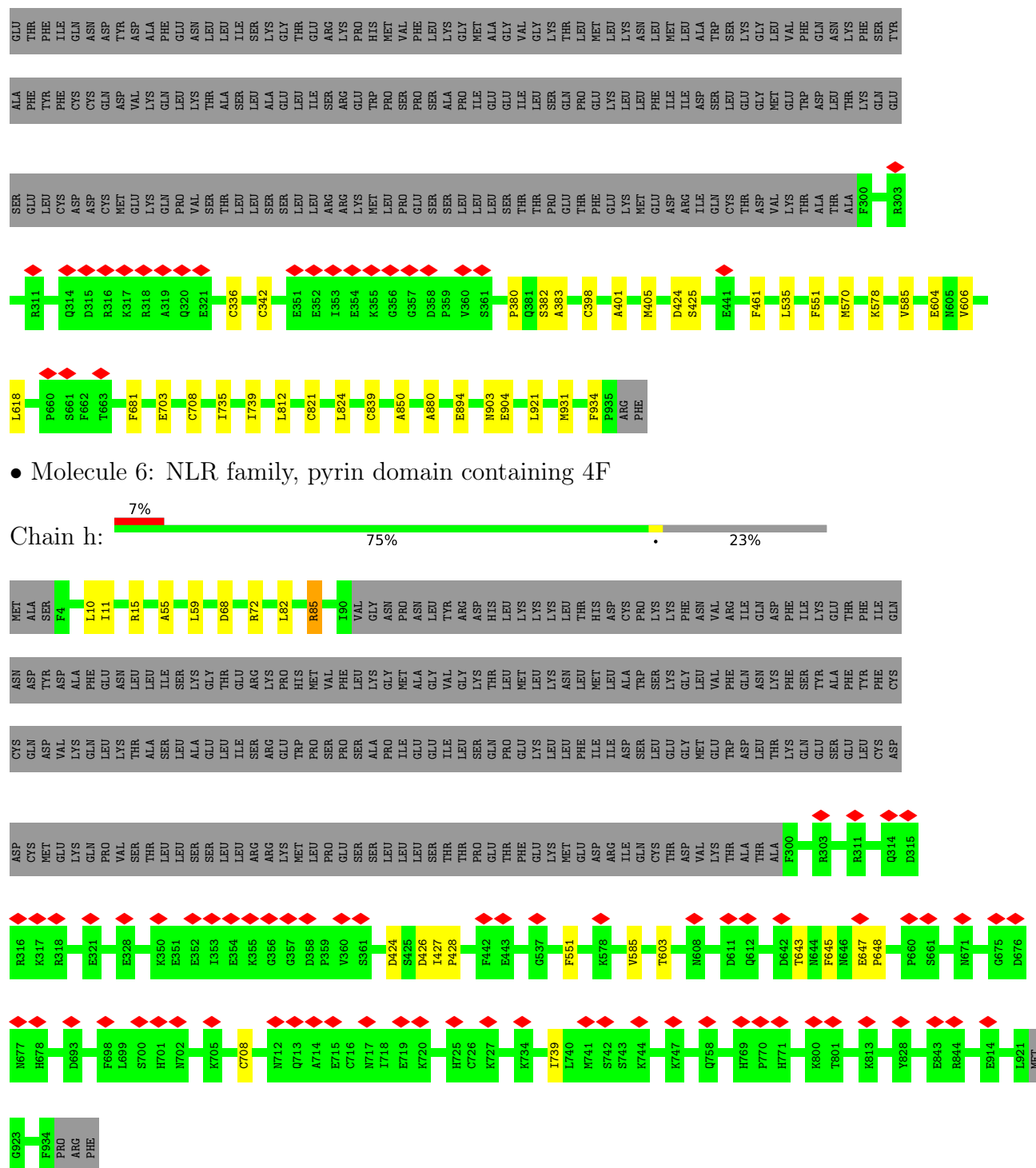


• Molecule 6: NLR family, pyrin domain containing 4F



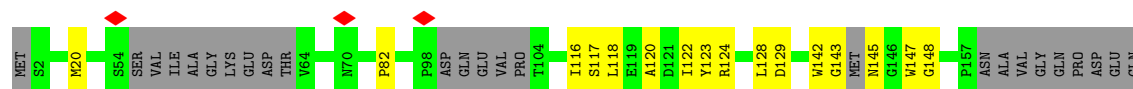
• Molecule 6: NLR family, pyrin domain containing 4F

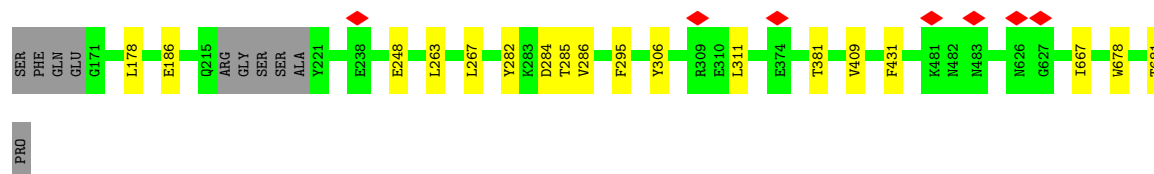




• Molecule 7: Inactive protein-arginine deiminase type-6

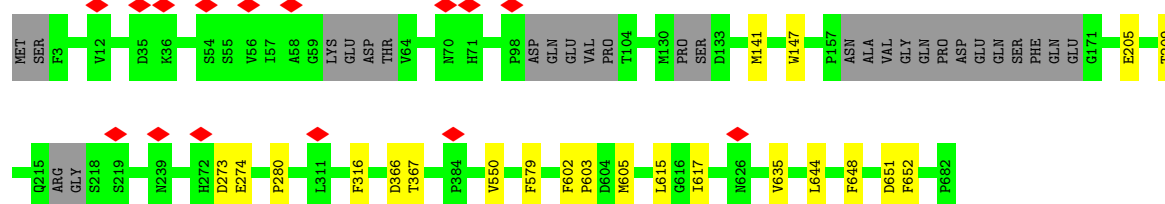
Chain S: 90% 5% 5%





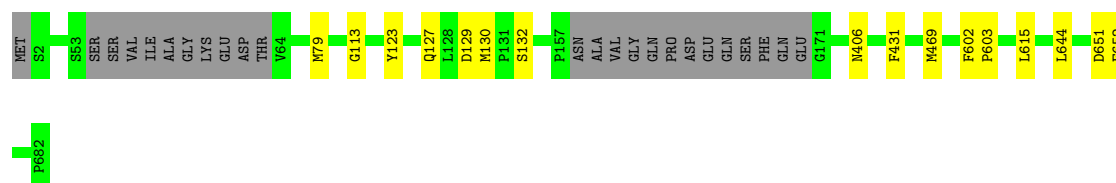
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain T: 93%



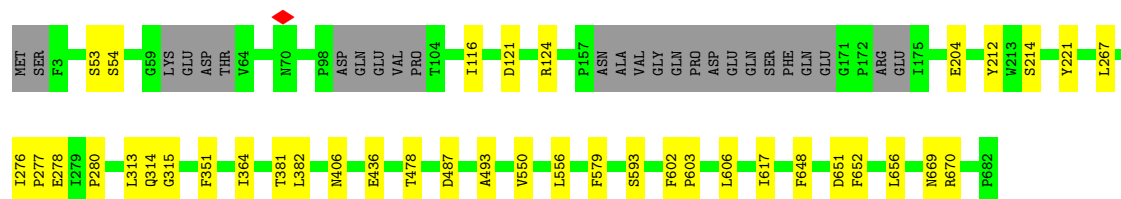
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain Y: 94%



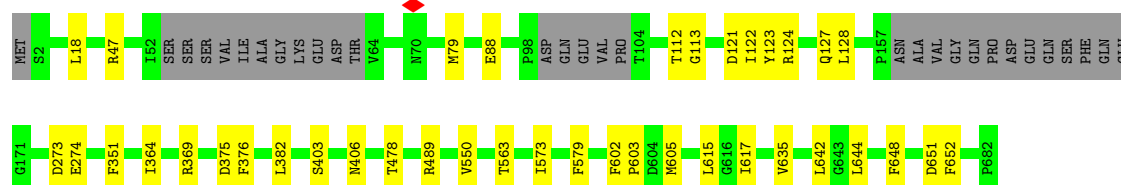
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain b: 90% 6%

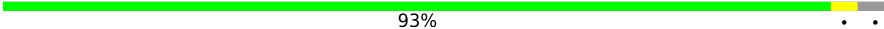


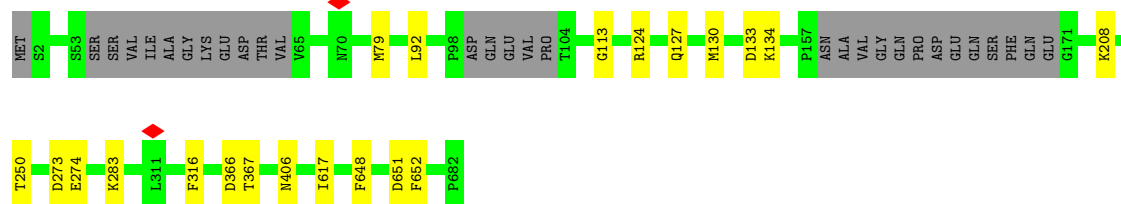
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain X: 90% 6%



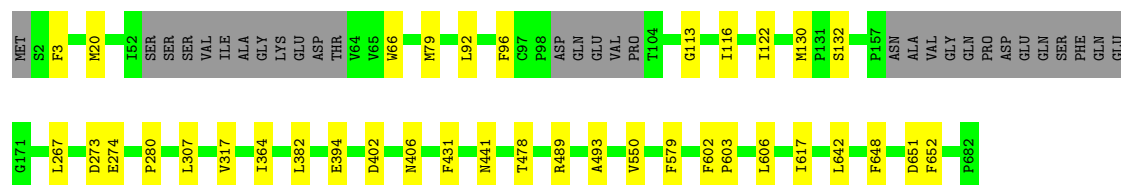
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain Z:  93%

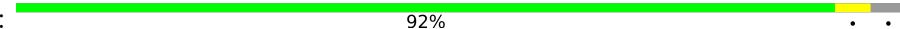


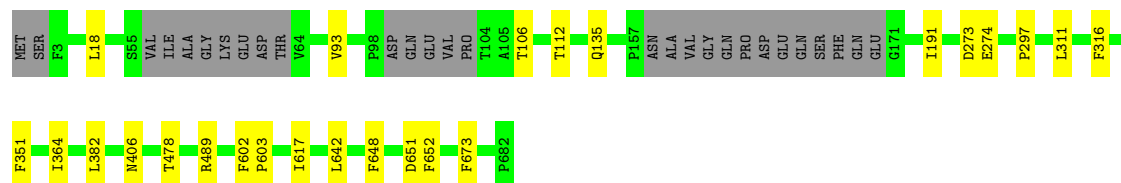
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain V:  90%



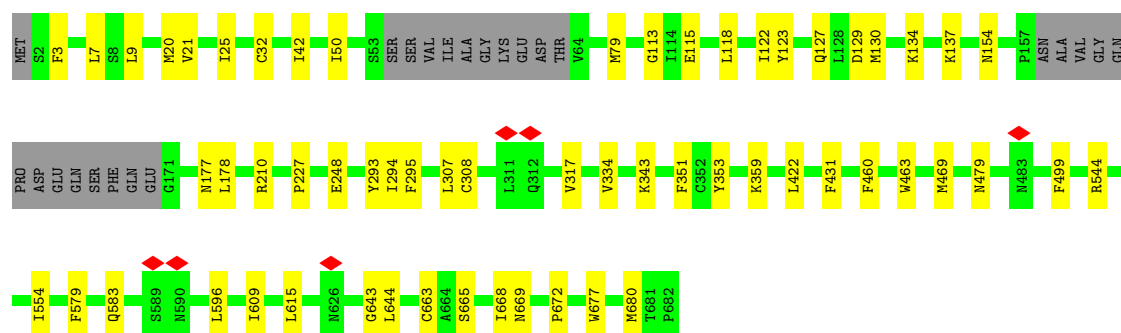
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain W:  92%



- Molecule 7: Inactive protein-arginine deiminase type-6

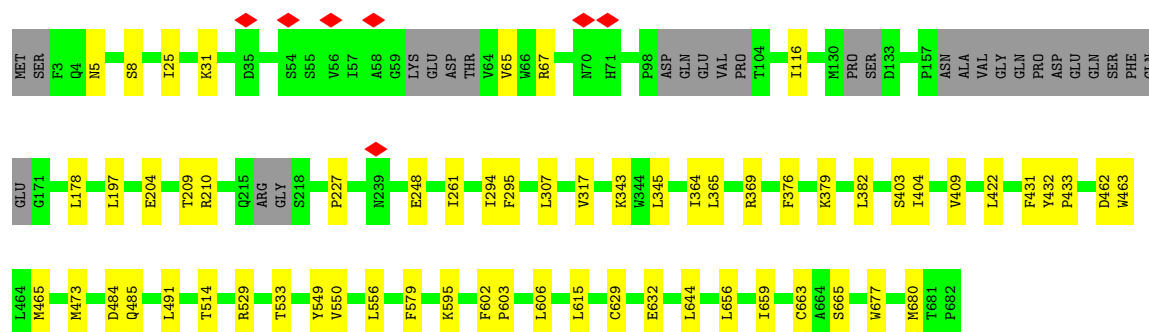
Chain n:  88%



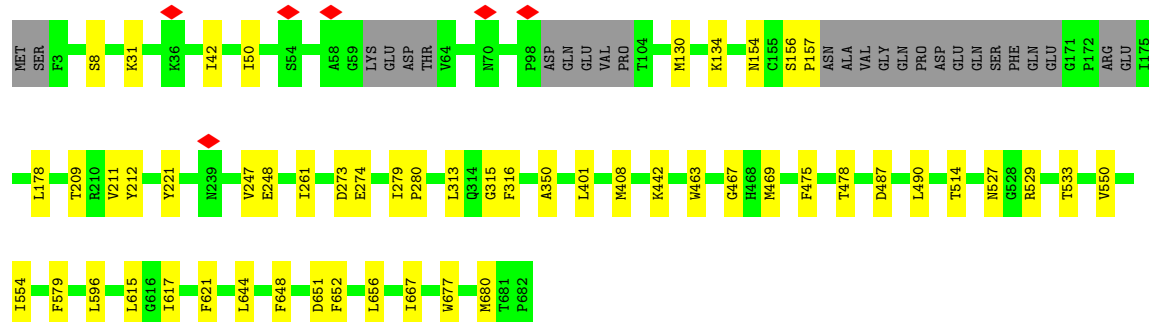
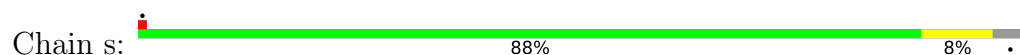
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain f:  87%

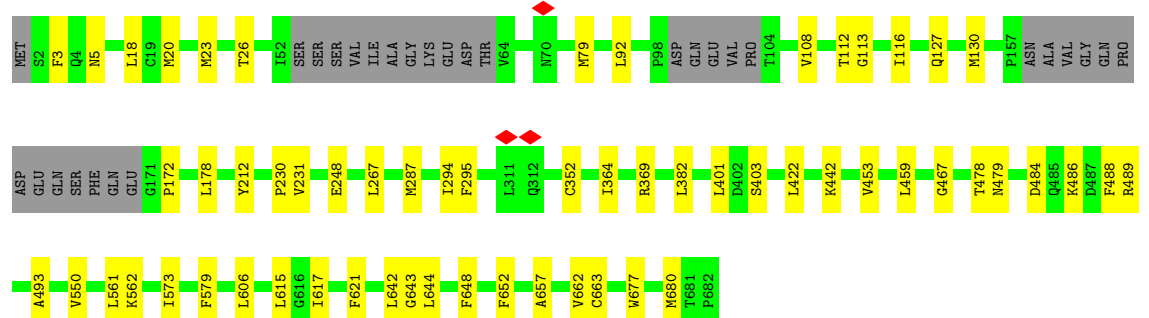
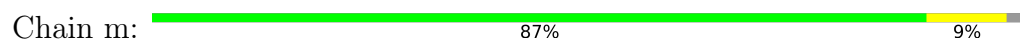




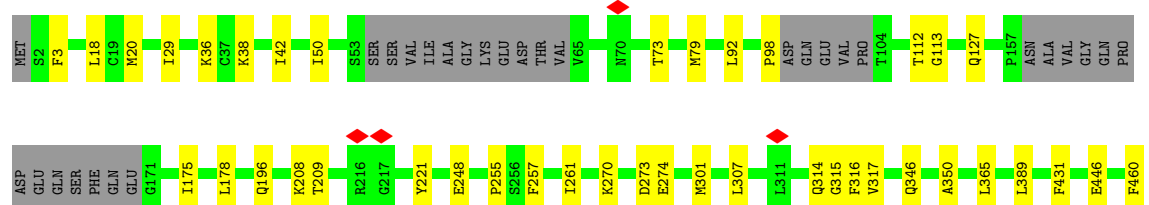
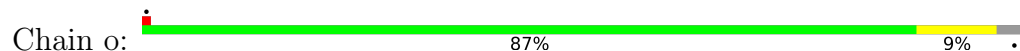
• Molecule 7: Inactive protein-arginine deiminase type-6



• Molecule 7: Inactive protein-arginine deiminase type-6



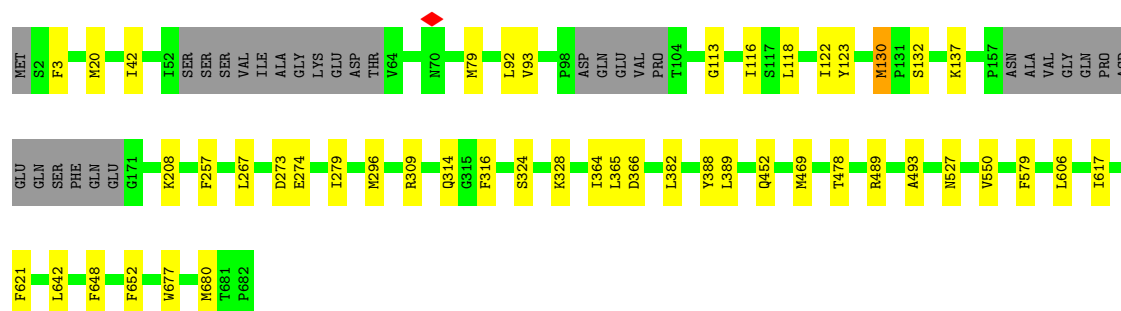
• Molecule 7: Inactive protein-arginine deiminase type-6





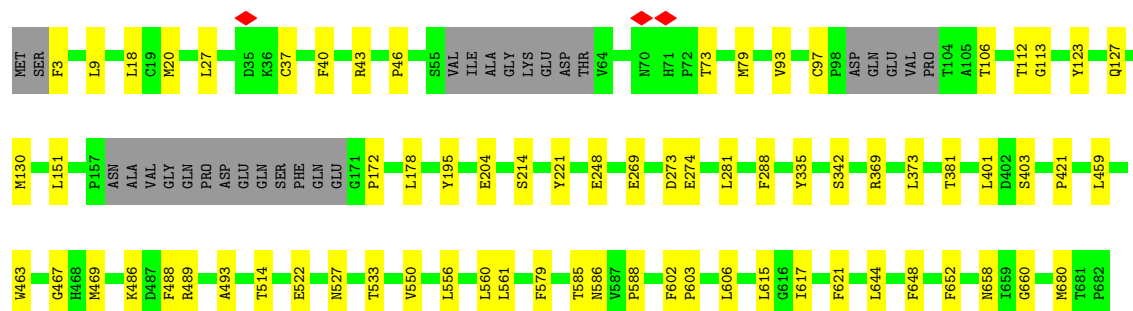
• Molecule 7: Inactive protein-arginine deiminase type-6

Chain d: 89% 7% .



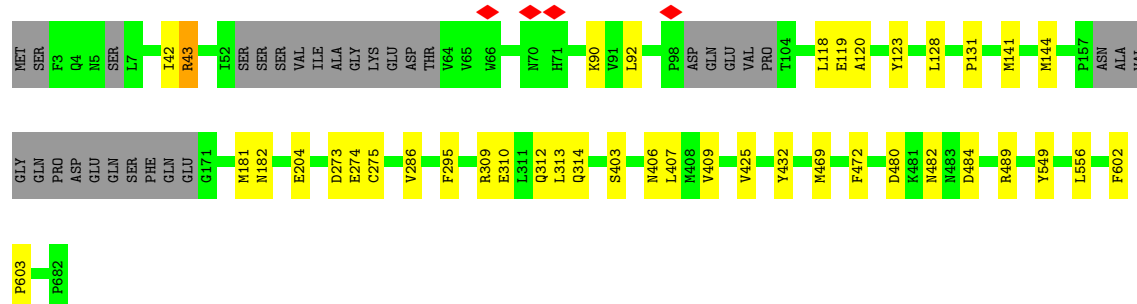
• Molecule 7: Inactive protein-arginine deiminase type-6

Chain j: 85% 11% .



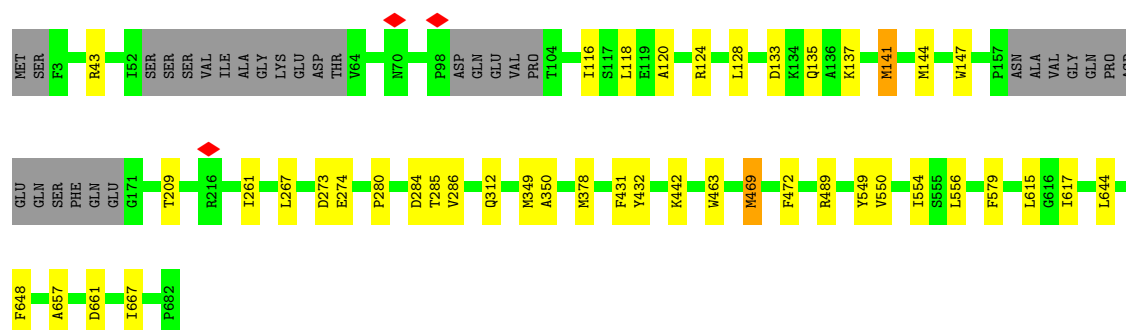
• Molecule 7: Inactive protein-arginine deiminase type-6

Chain r: 89% 6% 5%



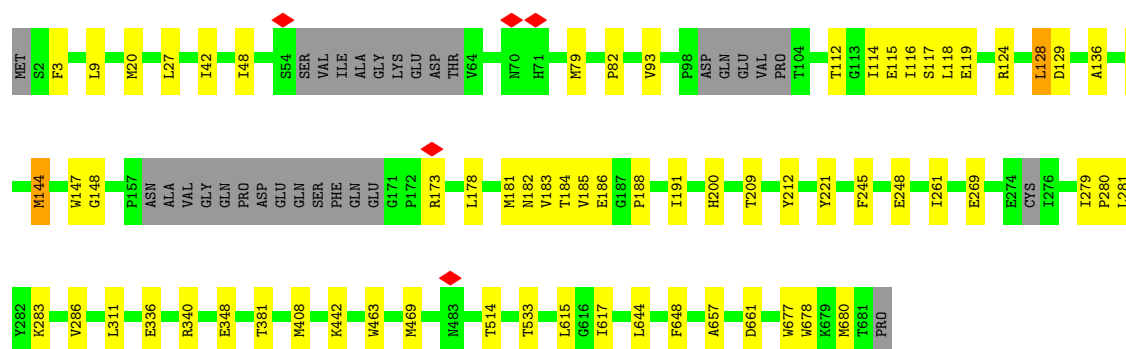
• Molecule 7: Inactive protein-arginine deiminase type-6

Chain B: 89% 6% 5%



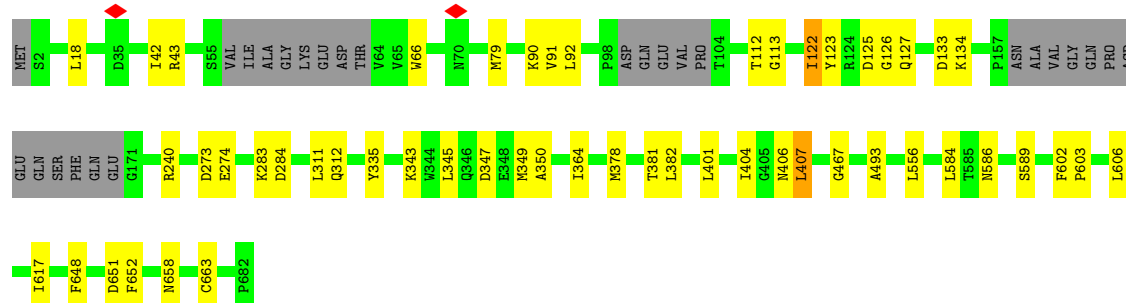
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain K: 86% 10% .



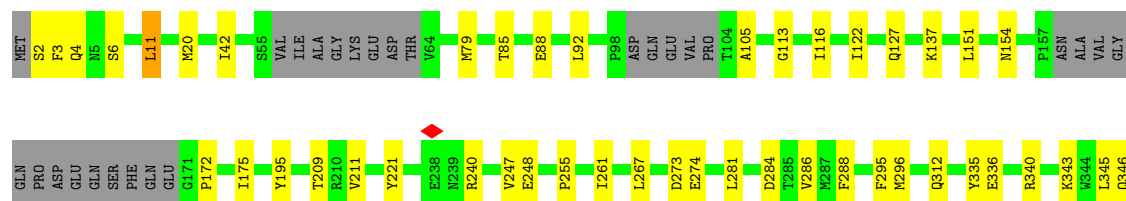
- Molecule 7: Inactive protein-arginine deiminase type-6

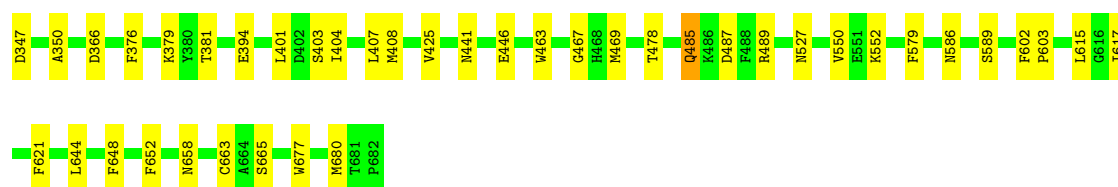
Chain U: 88% 7% .



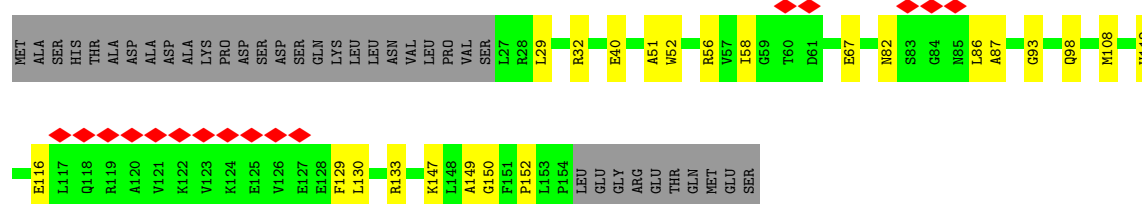
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain c: 83% 12% .

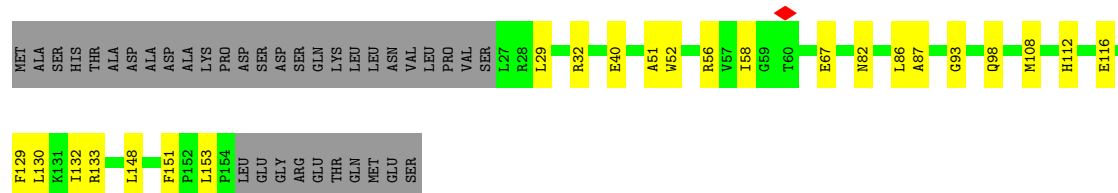




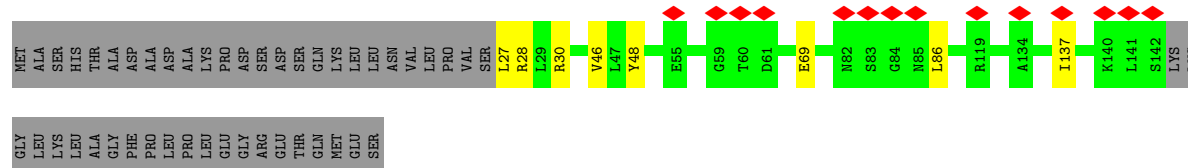
- Molecule 8: Oocyte-expressed protein homolog



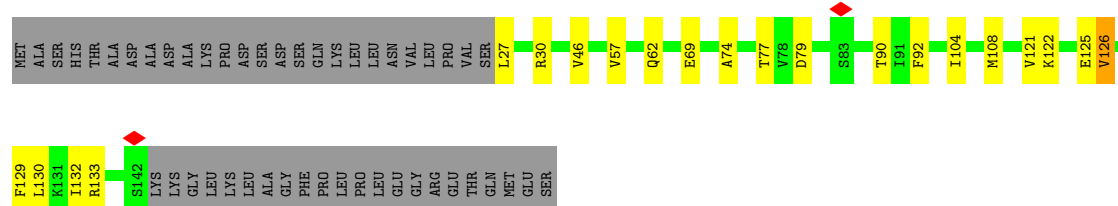
- Molecule 8: Oocyte-expressed protein homolog



- Molecule 8: Oocyte-expressed protein homolog

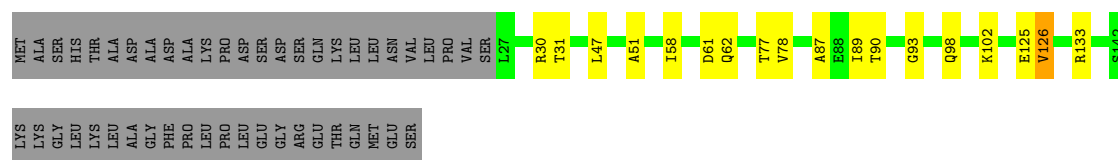


- Molecule 8: Oocyte-expressed protein homolog



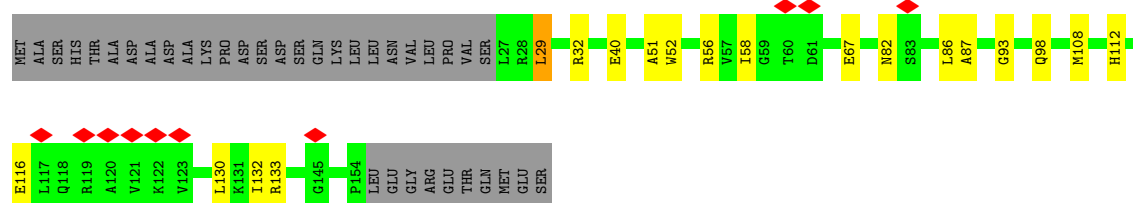
- Molecule 8: Oocyte-expressed protein homolog

Chain AI:  60% 10% 29%



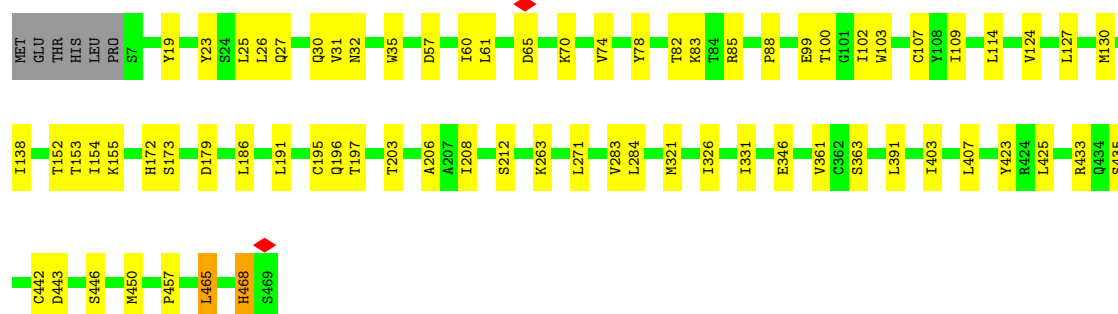
- Molecule 8: Oocyte-expressed protein homolog

Chain AT:  6% 66% 11% 22%

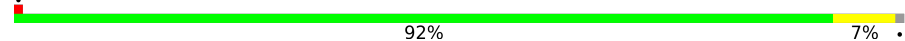


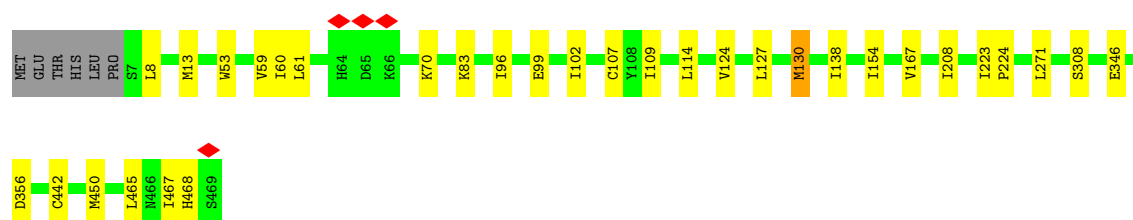
- Molecule 9: Expressed sequence C85627

Chain k:  84% 15%



- Molecule 9: Expressed sequence C85627

Chain l:  92% 7%

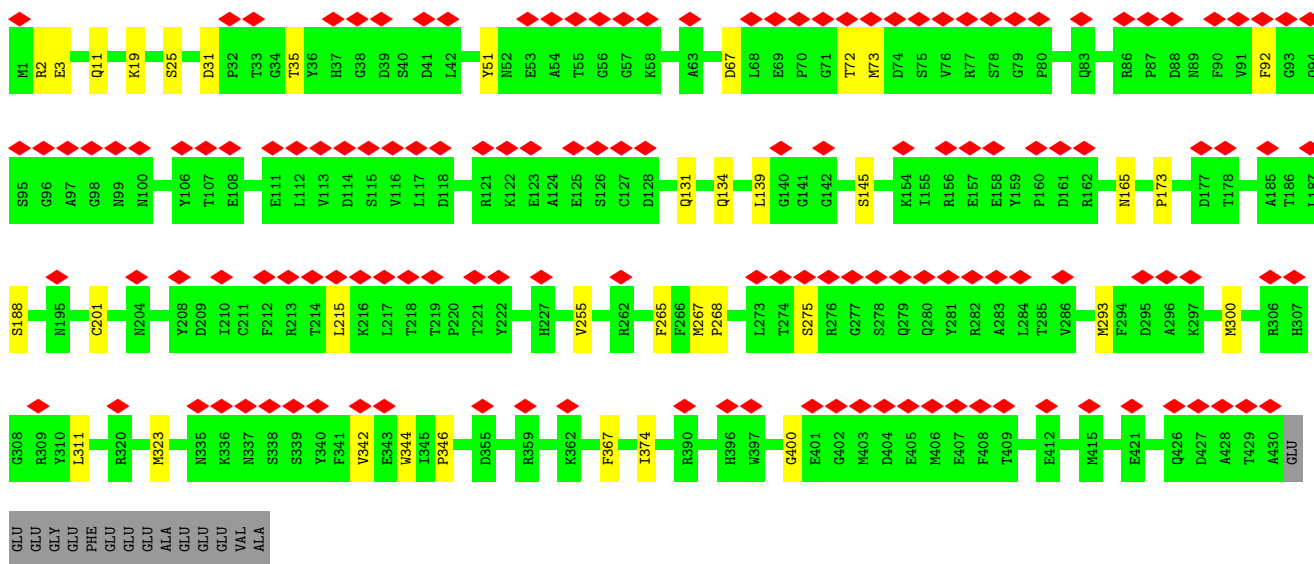


- Molecule 10: Tubulin beta-4B chain

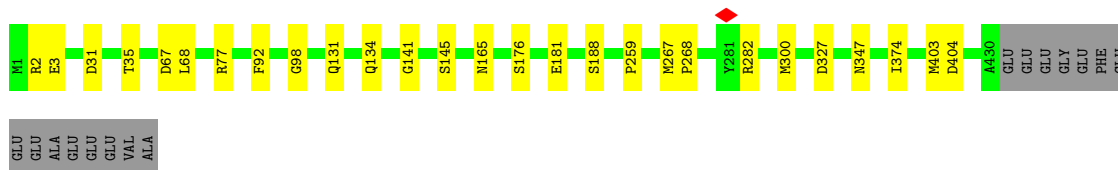
Chain t:  93%



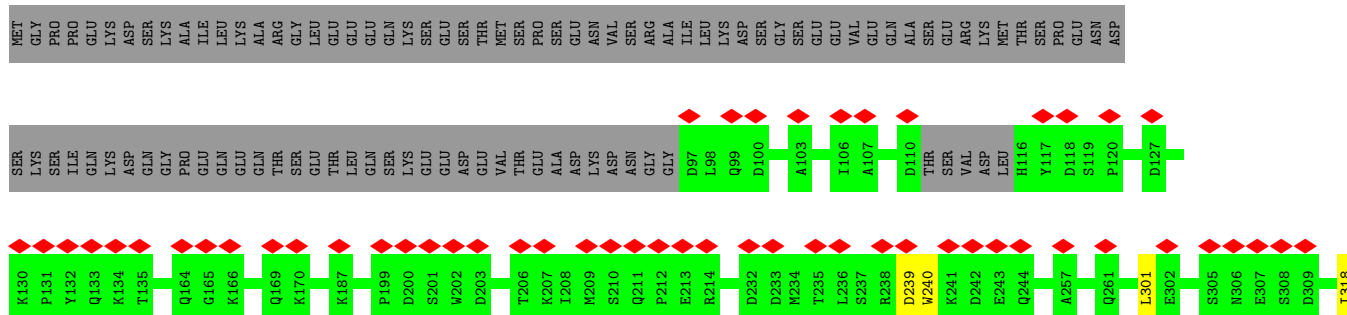
Chain AE:

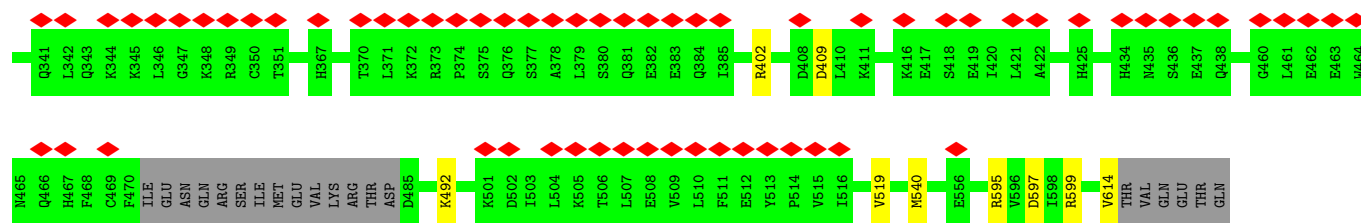


Chain AN: 91% 6%

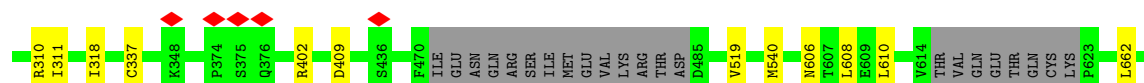
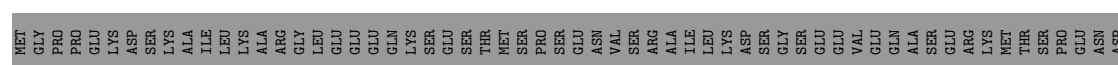


Chain y:

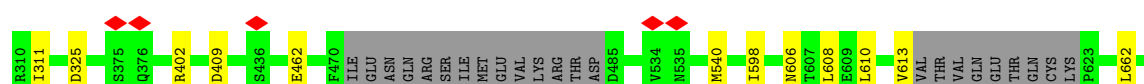
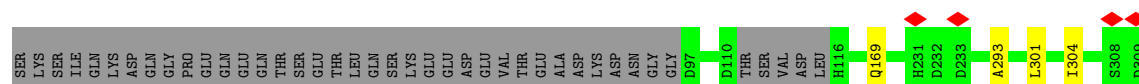
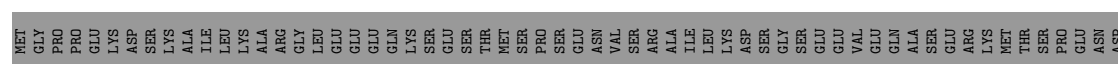
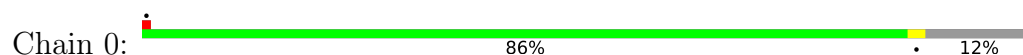




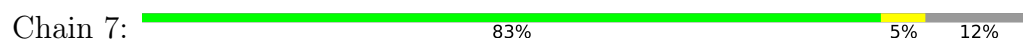
• Molecule 11: NACHT, LRR and PYD domains-containing protein 5

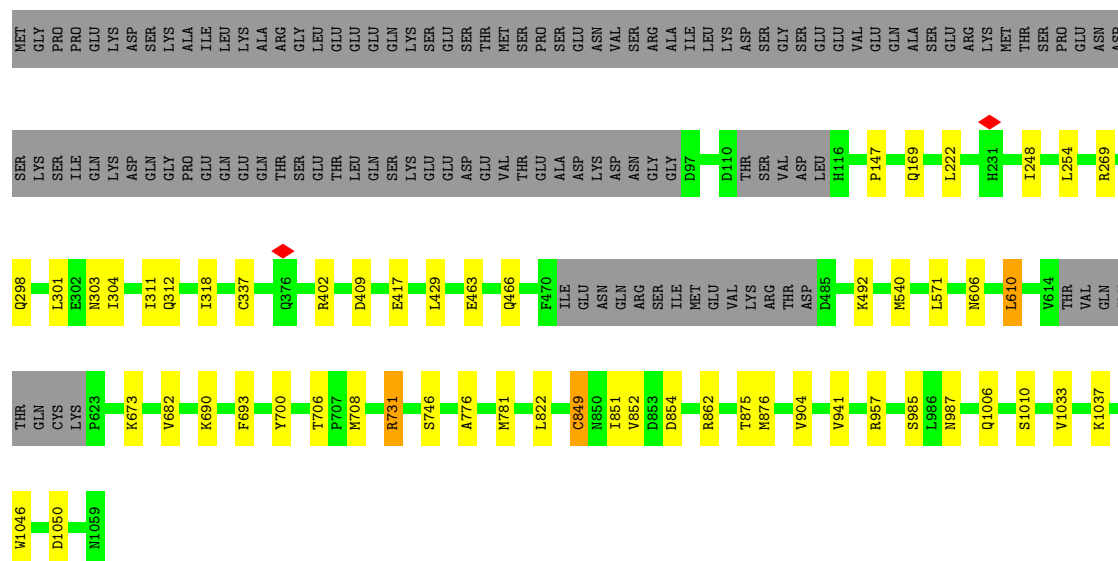


• Molecule 11: NACHT, LRR and PYD domains-containing protein 5



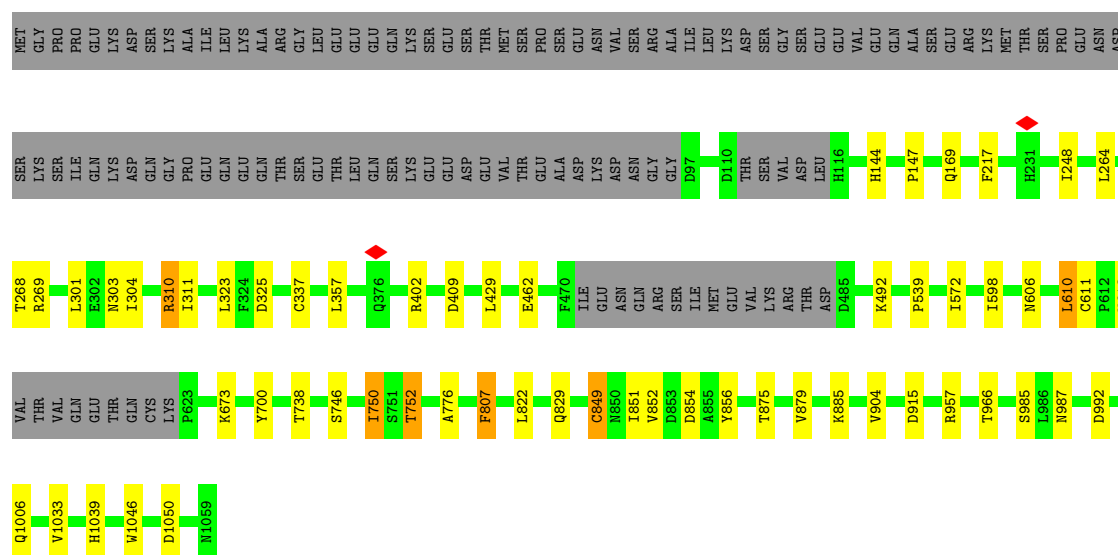
• Molecule 11: NACHT, LRR and PYD domains-containing protein 5





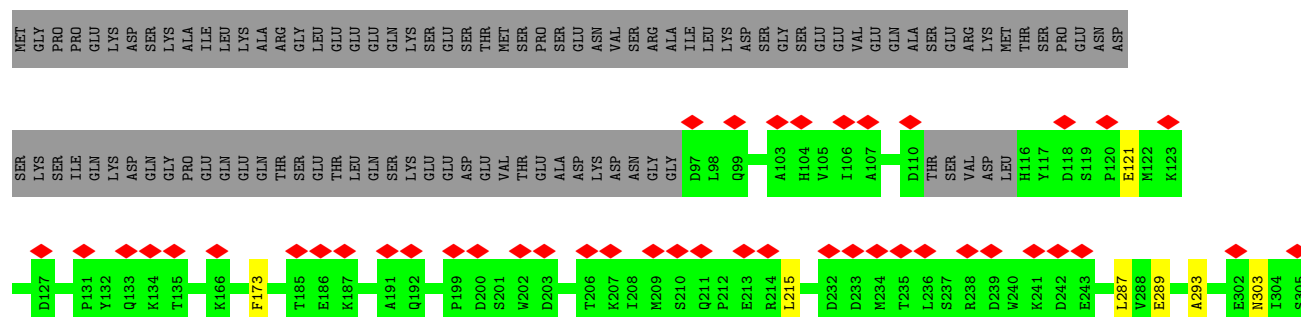
- Molecule 11: NACHT, LRR and PYD domains-containing protein 5

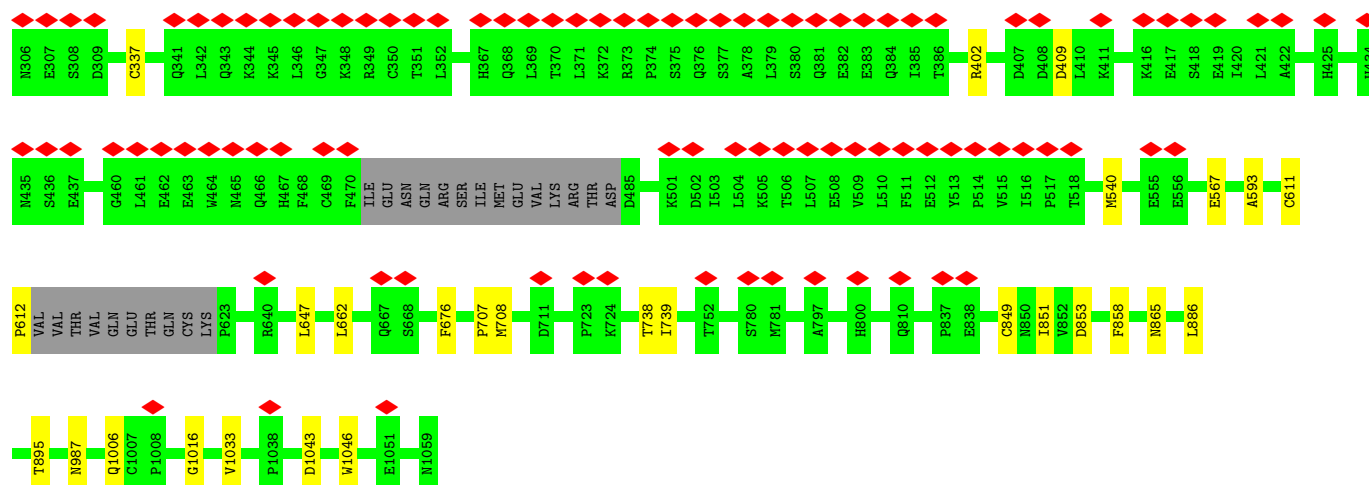
Chain 5: 83% 5% • 12%



- Molecule 11: NACHT, LRR and PYD domains-containing protein 5

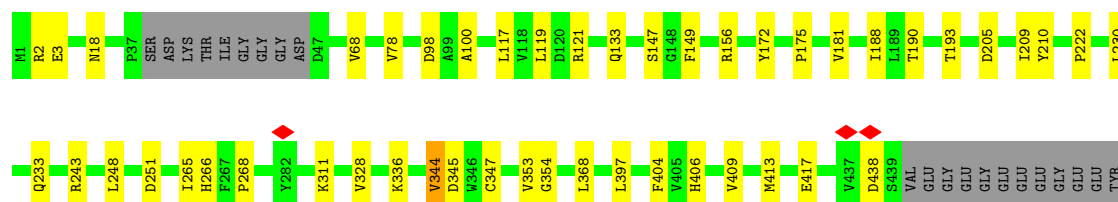
Chain 2: 13% 85% • 12%





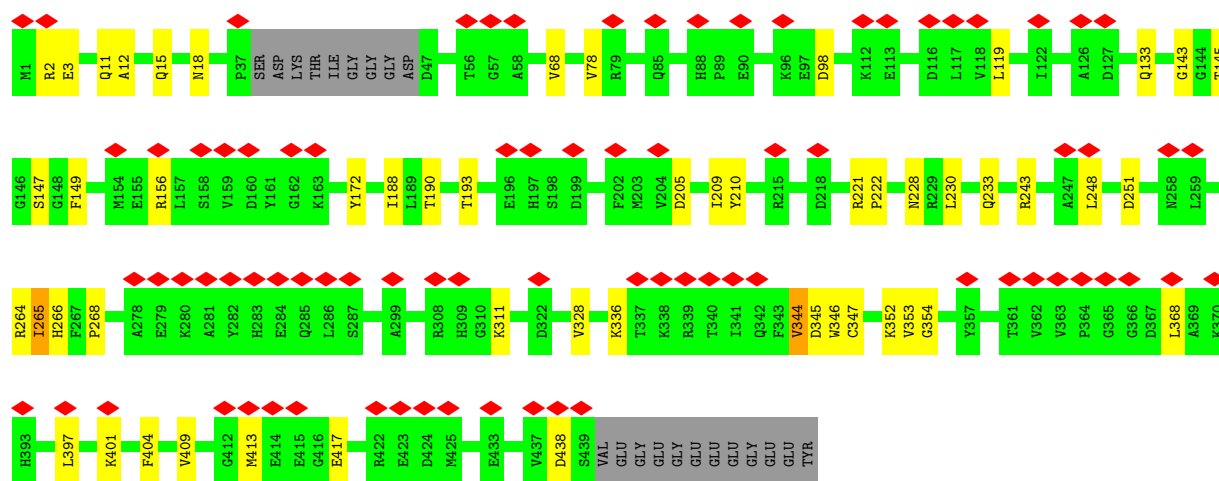
• Molecule 12: Tubulin alpha-1A chain

Chain u: 85% 10% 5%



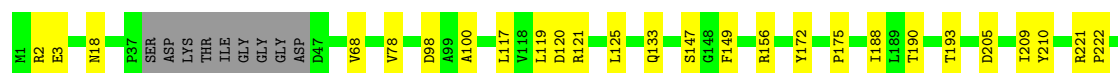
• Molecule 12: Tubulin alpha-1A chain

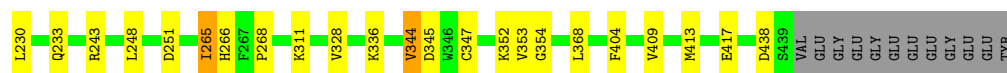
Chain AF: 18% 84% 11% 5%



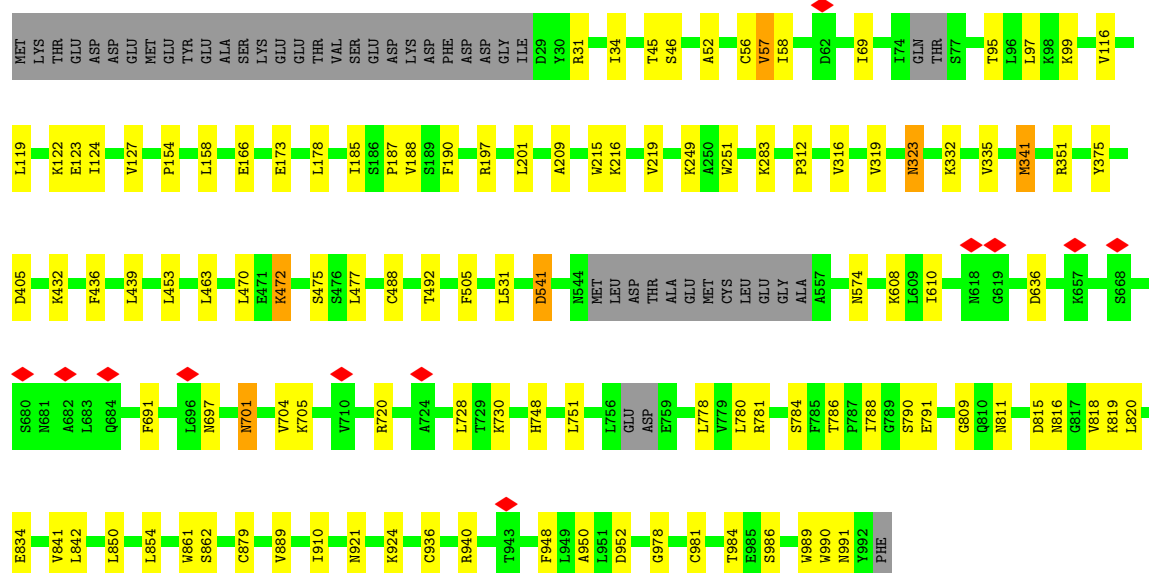
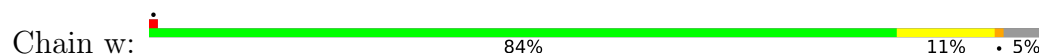
• Molecule 12: Tubulin alpha-1A chain

Chain AO: 84% 10% 5%

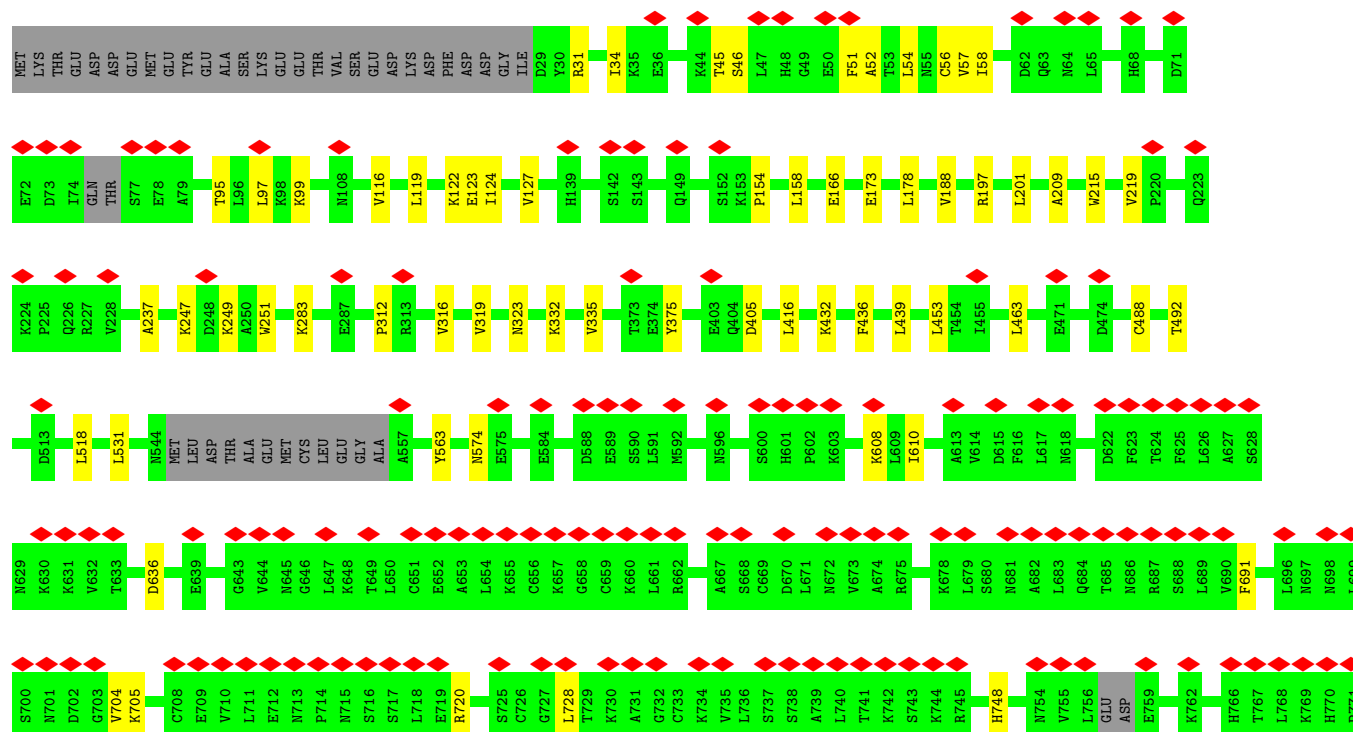
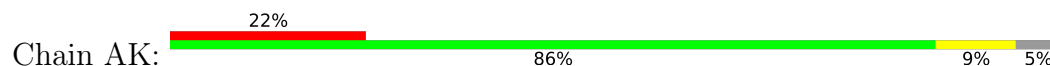




- Molecule 13: NACHT, LRR and PYD domains-containing protein 14

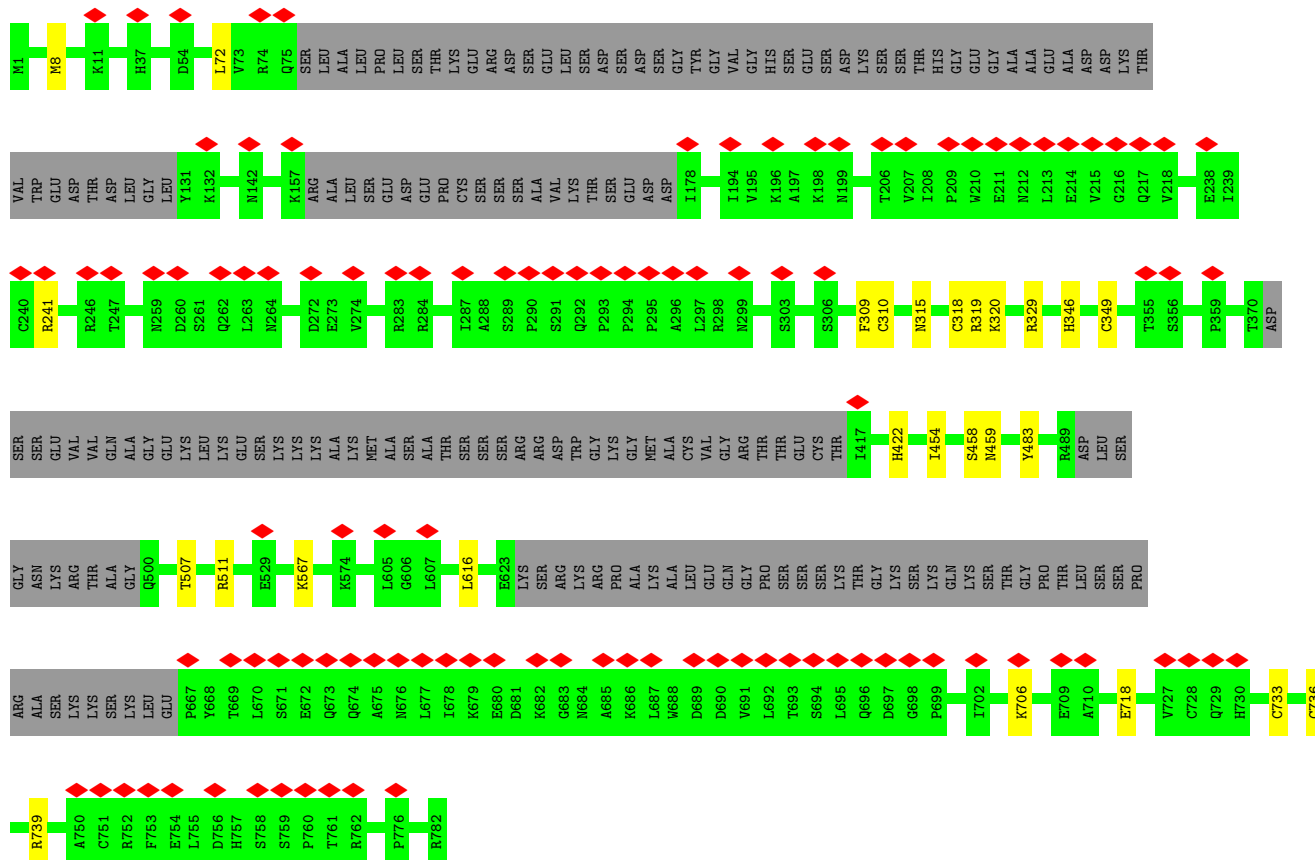
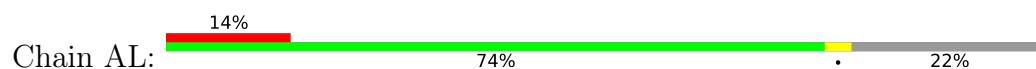


- Molecule 13: NACHT, LRR and PYD domains-containing protein 14

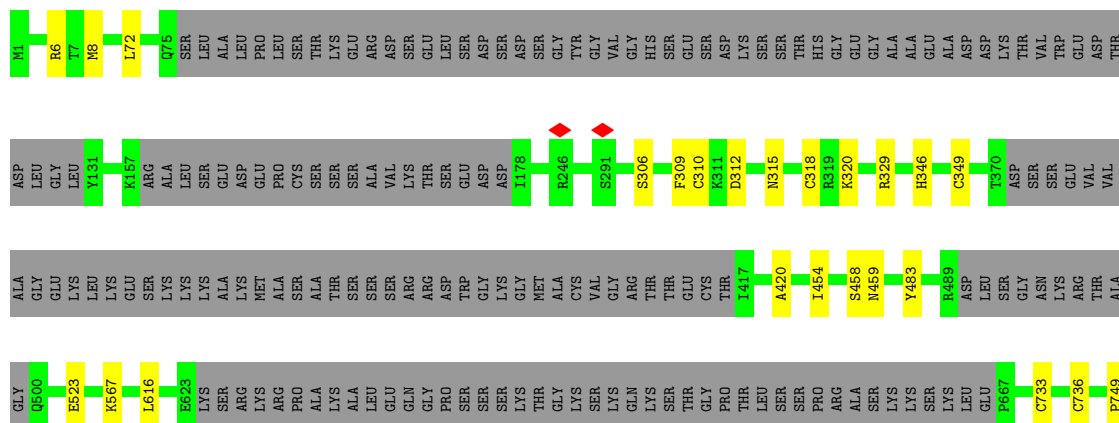
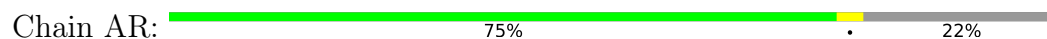




• Molecule 15: E3 ubiquitin-protein ligase UHRF1



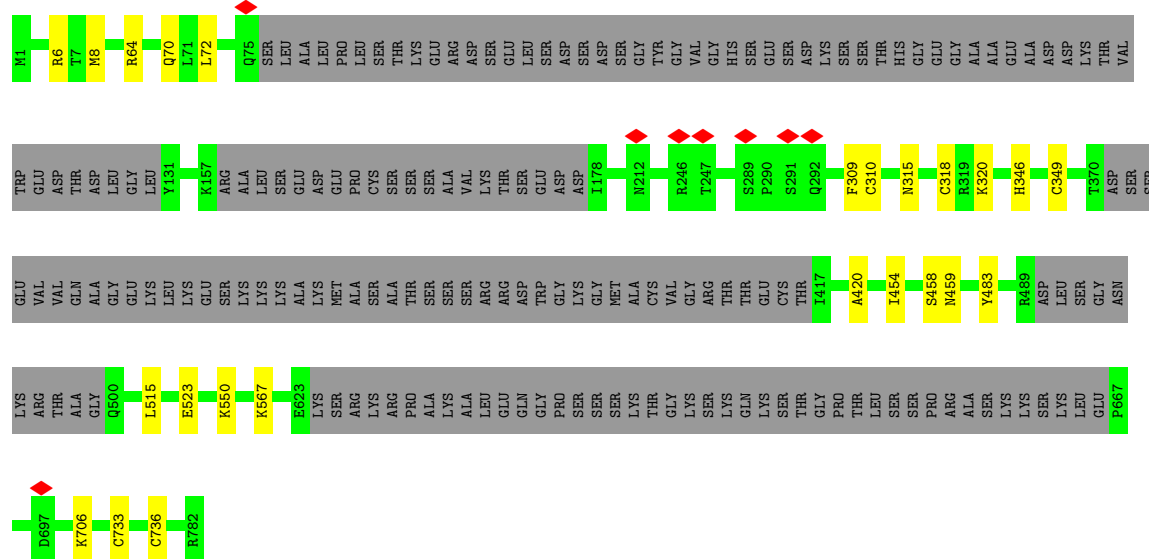
• Molecule 15: E3 ubiquitin-protein ligase UHRF1





- Molecule 15: E3 ubiquitin-protein ligase UHRF1

Chain x: 75% 22%



V164	T165	D166	M168	I172	R180	L188	T200	S203	G213	F218	V229	F232	G235	I236	D237	L249	I250	I251	Q254	R255	Y263	F283	A289	I299	S303	D309	I323	I329	L367	F368	D369	L373	Q376	E384
H394	L404	E410	S413	G426	TYR	LEU	PRO	LEU	SER	G432	K436	T437	L438	E441	L446	S450	SER	PRO	I453	M458	V464	CYS	SER											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	349408	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	611.328, 611.328, 611.328	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.194, 1.194, 1.194	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.16	0/440	0.34	0/598
1	3	0.13	0/469	0.32	0/637
1	9	0.18	0/469	0.35	0/637
2	4	0.18	0/1006	0.38	0/1367
2	6	0.14	0/1058	0.31	0/1431
2	AA	0.15	0/1058	0.34	0/1431
3	A	0.12	0/3749	0.29	0/5094
4	D	0.13	0/1212	0.29	0/1634
4	F	0.10	0/1216	0.25	0/1639
4	O	0.12	0/1216	0.25	0/1639
4	p	0.16	0/1205	0.32	0/1623
4	q	0.12	0/1205	0.28	0/1623
5	8	0.13	0/2879	0.28	0/3904
5	AC	0.17	0/2879	0.30	0/3904
5	E	0.16	0/2858	0.34	0/3875
5	I	0.12	0/2879	0.28	0/3904
5	P	0.15	0/2879	0.30	0/3904
5	z	0.17	0/2875	0.34	0/3899
6	H	0.11	0/5908	0.27	0/7956
6	Q	0.12	0/5195	0.30	0/7004
6	h	0.13	0/5883	0.34	2/7920 (0.0%)
6	i	0.11	0/5839	0.28	0/7868
7	B	0.15	0/5256	0.31	0/7126
7	K	0.13	0/5258	0.30	0/7126
7	S	0.33	0/5216	0.63	0/7073
7	T	0.14	0/5276	0.31	0/7150
7	U	0.30	0/5280	0.37	1/7157 (0.0%)
7	V	0.26	0/5255	0.33	0/7125
7	W	0.22	0/5268	0.33	0/7144
7	X	0.22	0/5278	0.33	0/7154
7	Y	0.19	0/5218	0.32	0/7091
7	Z	0.18	0/5250	0.32	0/7119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	b	0.24	0/5265	0.33	0/7139
7	c	0.27	0/5284	0.36	0/7162
7	d	0.23	0/5246	0.34	0/7114
7	f	0.15	0/5282	0.31	0/7158
7	j	0.22	0/5272	0.33	0/7148
7	m	0.21	0/5278	0.33	0/7154
7	n	0.17	0/5224	0.32	0/7098
7	o	0.16	0/5254	0.32	0/7124
7	r	0.32	0/5260	0.60	2/7131 (0.0%)
7	s	0.18	0/5262	0.31	0/7135
8	AH	0.19	0/892	0.38	0/1218
8	AI	0.11	0/953	0.27	0/1292
8	AJ	0.18	0/956	0.35	0/1296
8	AT	0.28	0/946	0.38	0/1294
8	e	0.28	0/946	0.38	0/1294
8	g	0.28	0/946	0.38	0/1294
9	k	0.14	0/3822	0.30	0/5197
9	l	0.17	0/3825	0.33	0/5201
10	AE	0.18	0/3433	0.31	0/4655
10	AN	0.11	0/3448	0.24	0/4673
10	t	0.13	0/3448	0.29	0/4673
11	0	0.16	0/7443	0.28	0/10068
11	2	0.16	0/7347	0.33	0/9945
11	5	0.12	0/7439	0.26	0/10063
11	7	0.13	0/7446	0.27	0/10073
11	AB	0.17	0/7449	0.30	0/10077
11	y	0.17	0/7389	0.32	0/10000
12	AF	0.18	0/3442	0.32	0/4673
12	AO	0.18	0/3445	0.32	0/4677
12	u	0.18	0/3445	0.32	0/4677
13	AK	0.16	0/7554	0.32	0/10222
13	AQ	0.16	0/7609	0.32	0/10291
13	w	0.16	0/7610	0.32	0/10292
14	AD	0.15	0/1203	0.31	0/1640
14	AM	0.15	0/1202	0.31	0/1639
14	AS	0.15	0/1203	0.31	0/1640
15	AL	0.16	0/4988	0.30	0/6753
15	AR	0.15	0/4988	0.30	0/6753
15	x	0.16	0/4970	0.30	0/6732
16	C	0.13	0/3687	0.31	0/5006
16	L	0.12	0/3697	0.32	0/5018
All	All	0.18	0/286730	0.33	5/388445 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	43	ARG	N-CA-C	6.83	120.03	108.90
7	U	311	LEU	CB-CA-C	-5.44	109.83	117.23
6	h	426	ASP	CA-C-N	5.33	123.60	120.24
6	h	426	ASP	C-N-CA	5.33	123.60	120.24
7	r	42	ILE	CB-CA-C	5.10	117.77	110.33

There are no chirality outliers.

There are no planarity outliers.

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	1	427	0	382	4	0
1	3	453	0	424	14	0
1	9	453	0	424	6	0
2	4	977	0	933	30	0
2	6	1028	0	1036	7	0
2	AA	1028	0	1036	13	0
3	A	3650	0	3613	23	0
4	D	1195	0	1198	8	0
4	F	1199	0	1202	3	0
4	O	1199	0	1202	0	0
4	p	1190	0	1194	25	0
4	q	1190	0	1194	0	0
5	8	2817	0	2801	15	0
5	AC	2817	0	2801	4	0
5	E	2799	0	2782	5	0
5	I	2817	0	2801	15	0
5	P	2817	0	2801	2	0
5	z	2813	0	2794	6	0
6	H	5803	0	5835	42	0
6	Q	5099	0	5098	12	0
6	h	5781	0	5793	14	0
6	i	5738	0	5726	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	5141	0	5149	42	0
7	K	5145	0	5157	54	0
7	S	5102	0	5087	44	0
7	T	5162	0	5174	13	0
7	U	5163	0	5151	50	0
7	V	5139	0	5151	32	0
7	W	5151	0	5153	22	0
7	X	5161	0	5179	29	0
7	Y	5099	0	5034	17	0
7	Z	5133	0	5130	12	0
7	b	5149	0	5151	34	0
7	c	5167	0	5162	72	0
7	d	5130	0	5136	49	0
7	f	5168	0	5180	45	0
7	j	5155	0	5164	78	0
7	m	5161	0	5179	50	0
7	n	5105	0	5045	43	0
7	o	5138	0	5142	35	0
7	r	5144	0	5151	33	0
7	s	5146	0	5149	36	0
8	AH	875	0	840	11	0
8	AI	935	0	947	13	0
8	AJ	938	0	956	18	0
8	AT	928	0	857	20	0
8	e	928	0	857	34	0
8	g	928	0	857	22	0
9	k	3729	0	3716	52	0
9	l	3732	0	3725	10	0
10	AE	3358	0	3226	28	0
10	AN	3373	0	3257	27	0
10	t	3373	0	3257	27	0
11	0	7316	0	7369	10	0
11	2	7221	0	7205	34	0
11	5	7312	0	7357	28	0
11	7	7319	0	7366	35	0
11	AB	7322	0	7375	17	0
11	y	7262	0	7254	44	0
12	AF	3365	0	3282	45	0
12	AO	3368	0	3284	35	0
12	u	3368	0	3284	38	0
13	AK	7417	0	7398	63	0
13	AQ	7472	0	7522	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	w	7473	0	7525	59	0
14	AD	1168	0	1150	10	0
14	AM	1167	0	1147	22	0
14	AS	1168	0	1150	9	0
15	AL	4872	0	4707	42	0
15	AR	4872	0	4701	26	0
15	x	4854	0	4666	26	0
16	C	3601	0	3620	40	0
16	L	3611	0	3635	13	0
17	1	1	0	0	0	0
17	3	1	0	0	0	0
17	9	1	0	0	0	0
17	AL	2	0	0	0	0
17	AR	4	0	0	0	0
17	x	4	0	0	0	0
18	AF	32	0	12	9	0
18	AN	32	0	12	7	0
18	AO	32	0	12	2	0
18	t	32	0	12	8	0
18	u	32	0	12	2	0
19	AN	1	0	0	0	0
19	AO	1	0	0	0	0
19	t	1	0	0	0	0
19	u	1	0	0	0	0
20	AK	27	0	12	0	0
20	AQ	27	0	12	0	0
20	w	27	0	12	0	0
All	All	281032	0	279482	1653	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 3.

All (1653) 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)
2:4:82:ARG:HA	6:i:424:ASP:CB	1.50	1.42
2:4:81:GLU:O	6:i:425:SER:N	1.63	1.30
6:H:913:CYS:O	8:e:147:LYS:NZ	1.67	1.27
7:j:586:ASN:HB2	15:AL:511:ARG:CD	1.70	1.21
15:AR:458:SER:HB2	7:U:586:ASN:OD1	1.37	1.21
7:n:127:GLN:CD	7:d:92:LEU:HD11	1.66	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:118:ALA:HB1	6:i:383:ALA:CB	1.73	1.18
15:AR:420:ALA:HB2	7:U:312:GLN:NE2	1.57	1.17
7:j:586:ASN:CB	15:AL:511:ARG:HD3	1.76	1.15
15:AR:458:SER:CB	7:U:586:ASN:OD1	1.96	1.13
7:n:127:GLN:HG3	7:d:92:LEU:CD1	1.80	1.12
7:d:364:ILE:HD12	7:d:382:LEU:HD11	1.24	1.11
7:j:586:ASN:CB	15:AL:511:ARG:CD	2.27	1.10
15:AR:420:ALA:CB	7:U:312:GLN:HE21	1.63	1.10
7:c:312:GLN:NE2	15:x:420:ALA:HB2	1.67	1.09
7:j:658:ASN:HD21	15:AL:459:ASN:ND2	1.50	1.08
15:AR:458:SER:OG	7:U:586:ASN:ND2	1.86	1.07
13:AQ:45:THR:HG22	13:AQ:51:PHE:O	1.51	1.07
1:3:54:MET:HE1	6:i:904:GLU:HG3	1.34	1.07
13:AK:45:THR:HG22	13:AK:51:PHE:O	1.51	1.07
7:n:127:GLN:HG3	7:d:92:LEU:HD12	1.31	1.06
2:4:118:ALA:CB	6:i:383:ALA:HB2	1.85	1.06
7:Y:127:GLN:HG3	7:V:92:LEU:CD1	1.84	1.06
15:AR:420:ALA:CB	7:U:312:GLN:NE2	2.17	1.06
7:W:489:ARG:HD2	7:W:642:LEU:HD13	1.36	1.05
9:k:26:LEU:HD12	4:p:160:CYS:SG	1.96	1.05
7:b:280:PRO:O	7:B:556:LEU:HD11	1.54	1.04
7:j:586:ASN:HB2	15:AL:511:ARG:HD3	1.29	1.04
2:4:118:ALA:HB1	6:i:383:ALA:HB2	1.40	1.04
8:AT:52:TRP:HZ2	8:AT:116:GLU:CB	1.70	1.04
13:AQ:842:LEU:HD11	13:AQ:846:ALA:HB3	1.37	1.03
8:e:52:TRP:HZ2	8:e:116:GLU:CB	1.70	1.02
7:c:312:GLN:HE21	15:x:420:ALA:CB	1.73	1.02
7:m:364:ILE:HD12	7:m:382:LEU:HD21	1.39	1.02
8:g:52:TRP:HZ2	8:g:116:GLU:CB	1.70	1.02
7:d:489:ARG:HD2	7:d:642:LEU:HD13	1.36	1.02
7:c:586:ASN:OD1	15:x:458:SER:HB2	1.59	1.01
13:AQ:842:LEU:HD11	13:AQ:846:ALA:CB	1.88	1.01
7:S:122:ILE:O	7:S:148:GLY:N	1.92	1.01
7:n:127:GLN:CD	7:d:92:LEU:CD1	2.34	1.00
9:k:85:ARG:NH2	4:p:161:GLU:O	1.96	0.99
7:S:118:LEU:N	7:S:284:ASP:OD2	1.93	0.99
7:d:489:ARG:HD2	7:d:642:LEU:CD1	1.92	0.99
7:j:588:PRO:HD3	15:AL:507:THR:HG21	1.45	0.98
6:H:910:PHE:O	8:e:147:LYS:HE2	1.63	0.98
7:n:127:GLN:CG	7:d:92:LEU:CD1	2.41	0.98
7:m:92:LEU:HD11	7:o:127:GLN:HG3	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:312:GLN:NE2	15:x:420:ALA:CB	2.25	0.98
8:e:133:ARG:HH11	11:y:318:ILE:HD11	1.27	0.98
7:B:141:MET:HE2	7:B:147:TRP:CH2	1.97	0.97
7:U:350:ALA:HB2	7:U:404:ILE:HG21	1.45	0.97
7:K:82:PRO:HG3	7:K:186:GLU:CB	1.95	0.97
7:c:586:ASN:OD1	15:x:458:SER:CB	2.11	0.97
12:AF:336:LYS:HE2	13:AK:57:VAL:HG22	1.46	0.97
11:y:858:PHE:CE1	11:2:886:LEU:HD23	1.99	0.96
7:c:350:ALA:HB2	7:c:404:ILE:HG21	1.45	0.96
7:d:364:ILE:HD11	7:d:382:LEU:HD21	1.47	0.96
10:AE:323:MET:HE3	12:AF:221:ARG:NH1	1.79	0.96
7:S:117:SER:HA	7:S:284:ASP:OD2	1.66	0.95
2:4:82:ARG:CA	6:i:424:ASP:CB	2.45	0.95
12:AF:228:ASN:OD1	18:AF:501:GTP:N1	1.99	0.94
7:W:489:ARG:HE	7:W:642:LEU:HD22	1.31	0.94
8:g:52:TRP:CZ2	8:g:116:GLU:CB	2.51	0.94
4:D:117:ASP:OD1	16:C:12:LYS:NZ	1.99	0.94
9:k:85:ARG:CZ	4:p:162:GLU:HA	1.97	0.94
7:r:118:LEU:HD23	7:r:286:VAL:HG12	1.49	0.94
8:e:52:TRP:CZ2	8:e:116:GLU:CB	2.51	0.94
8:AT:52:TRP:CZ2	8:AT:116:GLU:CB	2.51	0.94
7:f:364:ILE:CD1	7:f:382:LEU:HD21	1.97	0.93
9:l:127:LEU:HD21	9:l:130:MET:HA	1.46	0.93
6:H:910:PHE:O	8:e:147:LYS:CE	2.17	0.93
6:H:907:CYS:CB	8:e:149:ALA:HB3	2.00	0.92
7:W:489:ARG:NE	7:W:642:LEU:HD22	1.84	0.92
7:f:364:ILE:HD11	7:f:382:LEU:HD21	1.49	0.92
2:4:119:LEU:CD2	6:i:382:SER:O	2.19	0.91
7:m:364:ILE:HD12	7:m:382:LEU:CD2	1.99	0.91
7:m:92:LEU:CD1	7:o:127:GLN:HG3	1.99	0.91
15:AR:420:ALA:HB2	7:U:312:GLN:HE21	1.19	0.91
7:B:116:ILE:CD1	7:B:267:LEU:HD22	2.00	0.91
8:e:133:ARG:NH1	11:y:318:ILE:HD11	1.86	0.91
2:4:119:LEU:HD21	6:i:382:SER:O	1.71	0.90
6:h:10:LEU:CD2	6:h:59:LEU:HG	2.02	0.90
11:y:886:LEU:HD23	11:2:858:PHE:CE1	2.07	0.89
9:k:26:LEU:HD12	4:p:160:CYS:HB2	1.55	0.89
2:4:118:ALA:HB2	6:i:380:PRO:HG2	1.53	0.89
7:m:489:ARG:HE	7:m:642:LEU:HD22	1.38	0.89
7:K:128:LEU:HD22	7:K:182:ASN:ND2	1.87	0.89
7:j:586:ASN:HB3	15:AL:511:ARG:CZ	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AR:458:SER:OG	7:U:586:ASN:CG	2.16	0.88
9:k:26:LEU:HD12	4:p:160:CYS:CB	2.03	0.88
7:W:489:ARG:HD2	7:W:642:LEU:CD1	2.02	0.88
11:y:865:ASN:HD21	11:2:865:ASN:HD21	1.18	0.88
7:j:586:ASN:HB2	15:AL:511:ARG:HD2	1.56	0.88
6:H:911:MET:HA	8:e:147:LYS:HB2	1.56	0.88
7:d:364:ILE:CD1	7:d:382:LEU:HD21	2.03	0.88
10:AN:181:GLU:OE2	18:AN:501:GTP:H3'	1.73	0.88
1:3:54:MET:HE1	6:i:904:GLU:CG	2.02	0.88
7:j:586:ASN:HB3	15:AL:511:ARG:HD3	1.56	0.88
15:AR:459:ASN:ND2	7:U:658:ASN:HD21	1.73	0.87
11:y:886:LEU:HD23	11:2:858:PHE:CZ	2.10	0.87
7:S:118:LEU:HD21	7:S:263:LEU:O	1.73	0.87
9:k:127:LEU:HD21	9:k:130:MET:HA	1.54	0.86
9:k:26:LEU:CD1	4:p:160:CYS:SG	2.63	0.86
7:c:312:GLN:HE21	15:x:420:ALA:HB2	1.28	0.85
7:S:145:ASN:HA	7:U:66:TRP:CH2	2.11	0.84
8:g:82:ASN:HD21	8:g:130:LEU:HD22	1.43	0.84
7:S:118:LEU:HD23	7:S:285:THR:HA	1.57	0.84
7:j:586:ASN:HB3	15:AL:511:ARG:CD	2.08	0.84
8:AT:82:ASN:HD21	8:AT:130:LEU:HD22	1.43	0.84
12:AF:336:LYS:NZ	13:AK:56:CYS:O	2.09	0.83
14:AM:8:LYS:NZ	15:AL:718:GLU:OE2	2.12	0.83
7:d:364:ILE:CD1	7:d:382:LEU:HD11	2.08	0.83
8:g:52:TRP:CZ2	8:g:116:GLU:HA	2.14	0.82
7:Y:127:GLN:CD	7:V:92:LEU:HD11	2.04	0.82
6:h:10:LEU:HD22	6:h:59:LEU:HG	1.60	0.82
7:r:118:LEU:HD11	7:r:181:MET:SD	2.20	0.82
7:S:145:ASN:HA	7:U:66:TRP:CZ2	2.14	0.82
8:AT:52:TRP:CZ2	8:AT:116:GLU:HA	2.14	0.82
7:d:364:ILE:HD11	7:d:382:LEU:CD2	2.09	0.82
12:AF:12:ALA:N	18:AF:501:GTP:O2A	2.11	0.82
8:e:52:TRP:CZ2	8:e:116:GLU:HA	2.14	0.81
7:Y:127:GLN:CG	7:V:92:LEU:CD1	2.58	0.81
7:j:658:ASN:ND2	15:AL:459:ASN:ND2	2.27	0.81
7:X:489:ARG:HE	7:X:642:LEU:HD22	1.45	0.81
7:c:122:ILE:CD1	7:c:137:LYS:HG2	2.11	0.81
7:c:586:ASN:OD1	15:x:458:SER:OG	1.99	0.81
8:e:82:ASN:HD21	8:e:130:LEU:HD22	1.43	0.81
16:C:128:ASN:OD1	16:C:128:ASN:O	1.99	0.81
11:y:865:ASN:ND2	11:2:865:ASN:HD21	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:78:TYR:HE1	4:p:162:GLU:OE2	1.63	0.80
15:AR:458:SER:OG	7:U:586:ASN:OD1	1.98	0.80
7:Y:129:ASP:OD1	7:Y:130:MET:N	2.14	0.80
13:AQ:216:LYS:HB3	13:AQ:341:MET:HE1	1.63	0.80
7:j:586:ASN:ND2	15:AL:458:SER:HB2	1.97	0.80
16:C:125:THR:HG22	16:C:125:THR:O	1.82	0.80
11:AB:318:ILE:CD1	8:AT:133:ARG:HD2	2.11	0.80
1:3:54:MET:CE	6:i:904:GLU:HG3	2.11	0.79
7:m:489:ARG:NE	7:m:642:LEU:HD22	1.97	0.79
7:K:116:ILE:HA	7:K:184:THR:O	1.81	0.79
6:H:910:PHE:O	8:e:147:LYS:NZ	2.14	0.79
3:A:192:CYS:HA	3:A:210:ASP:HA	1.65	0.79
8:g:52:TRP:CZ2	8:g:116:GLU:CA	2.66	0.79
7:Y:127:GLN:HG3	7:V:92:LEU:HD12	1.64	0.79
16:C:127:THR:HG22	16:C:127:THR:O	1.83	0.79
13:AQ:819:LYS:HG2	13:AQ:849:ASP:OD2	1.83	0.79
7:S:120:ALA:CB	7:S:286:VAL:HG21	2.13	0.78
6:Q:807:ILE:O	6:Q:807:ILE:HG22	1.83	0.78
8:e:52:TRP:CZ2	8:e:116:GLU:CA	2.66	0.78
12:AF:11:GLN:HB3	18:AF:501:GTP:PA	2.23	0.78
8:AT:52:TRP:CZ2	8:AT:116:GLU:CA	2.66	0.77
7:c:2:SER:N	7:c:195:TYR:HH	1.81	0.77
7:s:596:LEU:CD1	7:r:275:CYS:O	2.33	0.77
10:AN:141:GLY:N	18:AN:501:GTP:H5'	1.99	0.77
15:AR:306:SER:OG	15:AR:312:ASP:OD2	2.00	0.77
11:y:858:PHE:CZ	11:2:886:LEU:HD23	2.20	0.77
7:B:116:ILE:HD12	7:B:267:LEU:HD22	1.67	0.77
7:j:586:ASN:CB	15:AL:511:ARG:NE	2.48	0.77
7:d:364:ILE:HD12	7:d:382:LEU:CD1	2.10	0.76
7:j:586:ASN:HB3	15:AL:511:ARG:NE	2.00	0.76
8:e:133:ARG:NH1	11:y:318:ILE:CD1	2.48	0.76
8:AH:46:VAL:HG11	11:2:293:ALA:HB3	1.67	0.76
7:n:615:LEU:HD11	7:n:644:LEU:HD13	1.66	0.76
7:V:489:ARG:HD2	7:V:642:LEU:HD13	1.68	0.76
14:AM:62:PHE:CZ	15:AL:739:ARG:HB3	2.21	0.76
7:m:615:LEU:HD11	7:m:644:LEU:HD13	1.69	0.75
7:U:349:MET:HE1	7:U:378:MET:HE3	1.68	0.75
2:4:81:GLU:O	6:i:424:ASP:C	2.29	0.75
14:AM:62:PHE:CE2	15:AL:739:ARG:HB3	2.21	0.75
7:b:204:GLU:OE2	7:B:442:LYS:NZ	2.20	0.75
7:j:585:THR:O	7:j:586:ASN:OD1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AF:228:ASN:CG	18:AF:501:GTP:HN1	1.95	0.75
11:AB:318:ILE:HD11	8:AT:133:ARG:HH11	1.50	0.75
7:B:141:MET:HE2	7:B:147:TRP:CZ3	2.21	0.74
7:K:115:GLU:O	7:K:185:VAL:HA	1.87	0.74
13:AK:45:THR:CG2	13:AK:51:PHE:O	2.33	0.74
6:Q:708:CYS:SG	6:Q:739:ILE:HD11	2.27	0.74
7:W:489:ARG:NE	7:W:642:LEU:CD2	2.50	0.74
7:m:489:ARG:HD2	7:m:642:LEU:HD13	1.69	0.74
7:r:295:PHE:HB2	7:r:409:VAL:HG21	1.68	0.74
7:S:120:ALA:HB2	7:S:286:VAL:HG21	1.68	0.74
7:B:141:MET:HE2	7:B:147:TRP:HH2	1.48	0.74
7:s:596:LEU:HD12	7:r:275:CYS:O	1.87	0.74
7:r:118:LEU:CD2	7:r:286:VAL:HG12	2.18	0.74
7:f:432:TYR:CD1	7:K:280:PRO:HB3	2.23	0.73
13:AQ:45:THR:CG2	13:AQ:51:PHE:O	2.33	0.73
7:S:118:LEU:HD23	7:S:285:THR:CA	2.18	0.73
7:W:478:THR:HG21	7:W:489:ARG:HG3	1.71	0.73
7:f:433:PRO:HD3	7:K:200:HIS:CE1	2.24	0.73
9:k:74:VAL:HG13	4:p:159:TRP:CB	2.19	0.73
12:AF:336:LYS:HE2	13:AK:57:VAL:CG2	2.19	0.73
6:H:907:CYS:HA	8:e:149:ALA:CB	2.18	0.73
7:j:127:GLN:OE1	7:r:92:LEU:CD1	2.37	0.73
7:m:364:ILE:CD1	7:m:382:LEU:CD2	2.67	0.73
15:AR:458:SER:CB	7:U:586:ASN:CG	2.61	0.73
7:b:276:ILE:HG23	7:B:549:TYR:CD1	2.24	0.73
7:c:615:LEU:HD11	7:c:644:LEU:HD13	1.71	0.73
2:4:118:ALA:HB3	6:i:383:ALA:HB2	1.70	0.72
7:S:118:LEU:CD2	7:S:263:LEU:O	2.37	0.72
11:y:886:LEU:CD2	11:2:858:PHE:CZ	2.71	0.72
7:S:116:ILE:CD1	7:S:267:LEU:HD22	2.18	0.72
6:H:911:MET:HA	8:e:147:LYS:CB	2.17	0.72
16:C:128:ASN:OD1	16:C:147:GLN:HB2	1.90	0.72
6:H:907:CYS:CA	8:e:149:ALA:HB3	2.20	0.72
16:C:404:LEU:HD21	16:C:446:LEU:HD21	1.70	0.72
5:E:354:ASN:HD22	6:i:88:GLY:HA2	1.55	0.72
10:t:345:ILE:CG2	12:u:181:VAL:HG11	2.20	0.72
7:j:369:ARG:NE	7:j:403:SER:OG	2.22	0.71
7:j:586:ASN:HB3	15:AL:511:ARG:NH1	2.05	0.71
7:f:433:PRO:CD	7:K:200:HIS:CE1	2.74	0.71
10:t:138:SER:OG	18:t:501:GTP:O1A	2.05	0.71
2:4:116:ILE:HD12	8:AH:137:ILE:CG2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:122:ILE:O	7:S:147:TRP:HB2	1.91	0.70
8:g:133:ARG:HH11	11:7:318:ILE:HD11	1.55	0.70
11:7:690:LYS:HG2	7:K:311:LEU:HD12	1.73	0.70
7:B:141:MET:HG3	7:B:147:TRP:CZ2	2.25	0.70
7:U:381:THR:HG22	7:U:381:THR:O	1.91	0.70
7:m:364:ILE:CD1	7:m:382:LEU:HD21	2.20	0.70
7:X:489:ARG:NE	7:X:642:LEU:HD22	2.07	0.70
7:S:129:ASP:OD2	7:U:90:LYS:HE2	1.91	0.70
9:k:78:TYR:CE1	4:p:162:GLU:OE2	2.44	0.70
7:j:335:TYR:OH	14:AM:80:SER:HA	1.91	0.70
14:AM:62:PHE:CZ	15:AL:739:ARG:CB	2.75	0.70
7:f:116:ILE:HD13	7:f:197:LEU:HD21	1.72	0.70
7:j:658:ASN:HD21	15:AL:459:ASN:HD21	1.40	0.70
7:o:38:LYS:HE3	7:o:98:PRO:HG3	1.73	0.69
7:j:586:ASN:O	15:AL:507:THR:HG22	1.93	0.69
7:c:343:LYS:HE3	7:c:346:GLN:OE1	1.92	0.69
13:AQ:69:ILE:HG21	13:AQ:110:TYR:OH	1.93	0.69
7:j:178:LEU:HD22	7:j:248:GLU:HB3	1.75	0.69
13:w:531:LEU:H	13:w:574:ASN:HD21	1.41	0.69
13:AQ:531:LEU:H	13:AQ:574:ASN:HD21	1.41	0.69
6:h:708:CYS:SG	6:h:739:ILE:HD11	2.33	0.69
1:3:66:GLN:OE1	6:i:904:GLU:OE1	2.11	0.69
7:S:117:SER:CA	7:S:284:ASP:OD2	2.39	0.68
7:V:478:THR:HG21	7:V:489:ARG:HG3	1.75	0.68
7:m:489:ARG:HD2	7:m:642:LEU:CD1	2.23	0.68
13:AK:531:LEU:H	13:AK:574:ASN:HD21	1.41	0.68
2:4:118:ALA:CB	6:i:380:PRO:HG2	2.24	0.68
10:AN:98:GLY:N	18:AN:501:GTP:O2G	2.26	0.68
9:l:53:TRP:HB3	9:l:59:VAL:HG21	1.76	0.68
7:n:127:GLN:OE1	7:d:92:LEU:HD11	1.91	0.68
7:o:178:LEU:HG	7:o:248:GLU:HB3	1.76	0.68
2:4:118:ALA:CB	6:i:383:ALA:CB	2.52	0.68
12:AF:11:GLN:HB3	18:AF:501:GTP:O1A	1.93	0.68
7:c:347:ASP:HB3	7:c:403:SER:HB3	1.76	0.68
7:n:129:ASP:OD1	7:n:130:MET:N	2.27	0.67
12:AF:336:LYS:CE	13:AK:57:VAL:HG22	2.23	0.67
7:s:529:ARG:HE	7:s:656:LEU:HD13	1.60	0.67
7:s:442:LYS:NZ	7:r:204:GLU:OE2	2.19	0.67
7:f:615:LEU:HD11	7:f:644:LEU:HD13	1.75	0.67
7:K:124:ARG:HD3	7:K:678:TRP:CD1	2.30	0.67
13:AQ:69:ILE:CG2	13:AQ:110:TYR:OH	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:105:LEU:HD23	8:AI:126:VAL:HG22	1.76	0.67
9:k:83:LYS:NZ	9:k:442:CYS:SG	2.68	0.67
13:AK:56:CYS:HB3	13:AK:99:LYS:HE2	1.77	0.67
2:4:81:GLU:O	6:i:424:ASP:CA	2.43	0.66
7:Y:127:GLN:CD	7:V:92:LEU:CD1	2.67	0.66
14:AM:88:ILE:CG2	14:AM:97:LEU:HD13	2.25	0.66
11:AB:311:ILE:HG23	8:AT:132:ILE:HD11	1.76	0.66
13:AQ:56:CYS:HB3	13:AQ:99:LYS:HE2	1.77	0.66
7:S:124:ARG:HD3	7:S:678:TRP:CD1	2.30	0.66
7:W:478:THR:CG2	7:W:489:ARG:HG3	2.25	0.66
10:t:141:GLY:N	18:t:501:GTP:H5'	2.10	0.66
7:c:122:ILE:HD12	7:c:137:LYS:HG2	1.76	0.66
13:w:56:CYS:HB3	13:w:99:LYS:HE2	1.78	0.66
14:AS:115:PRO:HB2	14:AS:128:LYS:HE3	1.77	0.66
11:0:775:ASN:HB3	16:L:168:MET:HE2	1.76	0.66
10:AN:141:GLY:CA	18:AN:501:GTP:H5'	2.26	0.66
14:AD:115:PRO:HB2	14:AD:128:LYS:HE3	1.77	0.66
7:c:586:ASN:CG	15:x:458:SER:OG	2.38	0.66
12:u:353:VAL:O	13:w:52:ALA:HB3	1.94	0.66
13:AQ:95:THR:HG22	13:AQ:99:LYS:HE3	1.78	0.66
2:6:53:ILE:HG22	8:AI:133:ARG:HG3	1.78	0.66
11:y:886:LEU:CD2	11:2:858:PHE:CE1	2.80	0.66
7:c:381:THR:HG22	7:c:381:THR:O	1.95	0.65
7:V:307:LEU:HD21	7:V:317:VAL:HG13	1.79	0.65
7:f:307:LEU:HD21	7:f:317:VAL:HG13	1.77	0.65
8:e:133:ARG:HH11	11:y:318:ILE:CD1	2.06	0.65
7:Y:127:GLN:HG3	7:V:92:LEU:HD13	1.73	0.65
2:6:101:MET:HG2	8:AI:126:VAL:HG21	1.79	0.65
13:w:95:THR:HG22	13:w:99:LYS:HE3	1.78	0.65
14:AM:115:PRO:HB2	14:AM:128:LYS:HE3	1.77	0.65
7:S:118:LEU:H	7:S:284:ASP:CG	2.00	0.65
7:B:141:MET:HG3	7:B:147:TRP:CH2	2.32	0.65
6:H:927:GLU:HA	8:e:152:PRO:HG3	1.77	0.65
7:s:212:TYR:HB3	7:s:221:TYR:HB3	1.79	0.65
7:c:122:ILE:HD13	7:c:137:LYS:HA	1.77	0.65
9:l:83:LYS:NZ	9:l:442:CYS:SG	2.70	0.64
13:AQ:842:LEU:CD1	13:AQ:846:ALA:CB	2.73	0.64
12:AO:353:VAL:O	13:AQ:52:ALA:HB3	1.97	0.64
7:r:118:LEU:HD23	7:r:286:VAL:CG1	2.24	0.64
7:B:116:ILE:HD13	7:B:267:LEU:HD22	1.80	0.64
7:c:345:LEU:HB3	7:c:665:SER:OG	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AK:95:THR:HG22	13:AK:99:LYS:HE3	1.78	0.64
10:t:345:ILE:HG23	12:u:181:VAL:HG11	1.79	0.64
6:H:907:CYS:HA	8:e:149:ALA:HB3	1.79	0.63
7:B:124:ARG:NH2	7:B:147:TRP:C	2.56	0.63
12:AO:336:LYS:HE2	13:AQ:57:VAL:HG22	1.80	0.63
15:AR:420:ALA:HB3	7:U:312:GLN:NE2	2.11	0.63
7:V:489:ARG:HD2	7:V:642:LEU:CD1	2.29	0.63
7:s:279:ILE:HG12	7:r:549:TYR:CE2	2.33	0.63
1:3:54:MET:CE	6:i:904:GLU:CG	2.74	0.63
10:AN:181:GLU:OE2	18:AN:501:GTP:C3'	2.45	0.63
9:k:130:MET:HG2	9:k:153:THR:HG23	1.81	0.63
7:f:364:ILE:HD12	7:f:382:LEU:HD21	1.77	0.63
7:d:478:THR:HG21	7:d:489:ARG:HG3	1.81	0.63
12:AO:336:LYS:NZ	13:AQ:56:CYS:O	2.22	0.63
6:H:907:CYS:CB	8:e:149:ALA:CB	2.77	0.62
10:t:252:LYS:HE3	12:u:98:ASP:OD2	2.00	0.62
7:S:129:ASP:OD2	7:U:90:LYS:CE	2.46	0.62
7:n:79:MET:HE2	7:n:113:GLY:HA3	1.81	0.62
15:AR:315:ASN:OD1	15:AR:567:LYS:NZ	2.23	0.62
11:5:572:ILE:HB	11:5:598:ILE:HG12	1.81	0.62
15:x:315:ASN:OD1	15:x:567:LYS:NZ	2.23	0.62
12:AF:2:ARG:HB3	12:AF:133:GLN:HG3	1.82	0.62
12:AO:18:ASN:HD21	12:AO:78:VAL:HG22	1.65	0.62
7:m:295:PHE:CE1	7:m:352:CYS:SG	2.93	0.62
7:f:364:ILE:HD12	7:f:382:LEU:HD11	1.82	0.62
1:1:73:PHE:CE1	8:e:108:MET:HE1	2.34	0.62
7:j:172:PRO:HG2	7:j:178:LEU:HD11	1.80	0.62
13:w:921:ASN:HA	13:w:950:ALA:HB3	1.82	0.62
12:AF:18:ASN:HD21	12:AF:78:VAL:HG22	1.65	0.62
1:9:54:MET:HE1	6:Q:904:GLU:HG3	1.82	0.62
12:u:2:ARG:HB3	12:u:133:GLN:HG3	1.82	0.62
7:K:269:GLU:HB3	7:K:279:ILE:CG2	2.30	0.62
6:h:10:LEU:HD21	6:h:55:ALA:O	2.00	0.62
7:c:586:ASN:ND2	15:x:458:SER:OG	2.33	0.61
2:4:118:ALA:HB1	6:i:383:ALA:HB3	1.80	0.61
9:k:197:THR:HG1	9:k:212:SER:HG	1.44	0.61
12:u:18:ASN:HD21	12:u:78:VAL:HG22	1.64	0.61
7:c:343:LYS:HD3	7:c:663:CYS:SG	2.39	0.61
13:AQ:921:ASN:HA	13:AQ:950:ALA:HB3	1.82	0.61
13:AQ:58:ILE:HD13	13:AQ:63:GLN:HG3	1.82	0.61
9:k:100:THR:HB	9:k:457:PRO:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:30:ARG:NH2	8:AH:69:GLU:OE2	2.33	0.61
12:AF:328:VAL:HG11	12:AF:353:VAL:HG11	1.83	0.61
15:AL:315:ASN:OD1	15:AL:567:LYS:NZ	2.23	0.61
7:c:312:GLN:NE2	15:x:420:ALA:HB3	2.14	0.61
10:t:141:GLY:HA3	18:t:501:GTP:O3A	2.00	0.61
7:j:9:LEU:HD21	7:j:27:LEU:HD21	1.83	0.61
11:y:858:PHE:CZ	11:2:886:LEU:CD2	2.83	0.61
12:AF:352:LYS:HG2	13:AK:54:LEU:HD23	1.83	0.61
2:4:116:ILE:HD12	8:AH:137:ILE:HG22	1.82	0.61
7:j:522:GLU:OE2	15:AL:422:HIS:HA	2.00	0.61
5:8:534:ILE:HD13	5:8:568:THR:HG21	1.83	0.61
1:1:73:PHE:HE1	8:e:108:MET:HE1	1.65	0.61
2:4:119:LEU:HD23	6:i:382:SER:O	2.01	0.61
10:t:181:GLU:OE2	18:t:501:GTP:H3'	2.01	0.61
8:AH:46:VAL:HG11	11:2:293:ALA:CB	2.30	0.61
12:AO:328:VAL:HG11	12:AO:353:VAL:HG11	1.83	0.61
7:d:116:ILE:HD13	7:d:267:LEU:HD13	1.82	0.61
7:j:615:LEU:HD11	7:j:644:LEU:HD13	1.83	0.61
11:7:402:ARG:NH2	11:7:409:ASP:OD2	2.33	0.61
4:D:64:HIS:HE1	10:AE:173:PRO:CB	2.13	0.60
7:f:431:PHE:CE2	7:K:283:LYS:HB2	2.35	0.60
7:j:335:TYR:CZ	14:AM:80:SER:HB3	2.36	0.60
7:K:136:ALA:O	7:K:147:TRP:NE1	2.33	0.60
13:AK:921:ASN:HA	13:AK:950:ALA:HB3	1.82	0.60
7:j:621:PHE:CE2	7:j:652:PHE:HB2	2.37	0.60
7:B:120:ALA:HB3	7:B:286:VAL:HG21	1.83	0.60
1:9:54:MET:CE	6:Q:904:GLU:HG3	2.32	0.60
8:AH:48:TYR:HB3	8:AH:86:LEU:HD11	1.84	0.60
7:S:120:ALA:HB3	7:S:286:VAL:HG21	1.84	0.60
6:Q:807:ILE:O	6:Q:807:ILE:CG2	2.48	0.60
7:c:4:GLN:HE21	7:c:6:SER:H	1.47	0.60
7:s:615:LEU:HD11	7:s:644:LEU:HD13	1.84	0.60
7:m:79:MET:HE2	7:m:113:GLY:HA3	1.84	0.60
12:AO:2:ARG:HB3	12:AO:133:GLN:HG3	1.82	0.60
16:C:213:GLY:HA2	16:C:235:GLY:HA2	1.83	0.60
16:C:237:ASP:N	16:C:251:ILE:O	2.35	0.60
10:t:347:ASN:OD1	12:u:175:PRO:HB3	2.01	0.60
7:b:280:PRO:O	7:B:556:LEU:CD1	2.39	0.60
10:AE:344:TRP:CE3	12:AF:401:LYS:HG3	2.36	0.60
13:AQ:781:ARG:HG3	13:AQ:809:GLY:HA3	1.83	0.60
8:g:129:PHE:CB	11:7:298:GLN:NE2	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t:347:ASN:CG	12:u:175:PRO:HB3	2.27	0.60
7:V:280:PRO:O	7:U:556:LEU:HD11	2.02	0.60
7:o:209:THR:HB	7:o:261:ILE:HD13	1.84	0.60
14:AM:88:ILE:HG23	14:AM:97:LEU:CD1	2.32	0.60
2:AA:105:LEU:O	2:AA:105:LEU:HD12	2.01	0.60
16:C:154:MET:HG3	16:C:165:THR:HG22	1.83	0.60
16:C:263:TYR:HB2	16:C:329:ILE:HD11	1.83	0.60
7:K:140:TRP:CD1	7:K:148:GLY:HA3	2.37	0.60
7:U:401:LEU:HD21	7:U:467:GLY:HA3	1.84	0.59
7:s:401:LEU:HD21	7:s:467:GLY:HA3	1.84	0.59
7:d:489:ARG:CD	7:d:642:LEU:HD13	2.23	0.59
7:b:276:ILE:CG2	7:B:549:TYR:CD1	2.85	0.59
10:AE:323:MET:HE3	12:AF:221:ARG:CZ	2.33	0.59
9:k:85:ARG:NH2	4:p:162:GLU:HA	2.16	0.59
7:c:347:ASP:O	7:c:404:ILE:N	2.34	0.59
8:g:133:ARG:NH1	11:7:318:ILE:HD11	2.17	0.59
7:d:79:MET:HE2	7:d:113:GLY:HA3	1.85	0.59
11:2:707:PRO:HG2	6:i:23:MET:HE2	1.85	0.59
7:m:401:LEU:HD21	7:m:467:GLY:HA3	1.84	0.59
12:u:328:VAL:HG11	12:u:353:VAL:HG11	1.83	0.59
10:t:347:ASN:HD21	12:u:175:PRO:HG3	1.68	0.59
7:b:277:PRO:HG2	7:B:549:TYR:OH	2.03	0.59
2:4:81:GLU:C	6:i:425:SER:H	1.99	0.59
8:e:133:ARG:HD2	11:y:318:ILE:CD1	2.33	0.59
7:b:364:ILE:HD12	7:b:382:LEU:HD21	1.83	0.59
7:X:364:ILE:HD12	7:X:382:LEU:HD21	1.85	0.59
7:K:615:LEU:HD11	7:K:644:LEU:HD13	1.85	0.59
7:X:489:ARG:HD2	7:X:642:LEU:HD13	1.85	0.58
7:c:343:LYS:CE	7:c:346:GLN:OE1	2.51	0.58
8:AJ:30:ARG:NH2	8:AJ:69:GLU:OE2	2.36	0.58
7:b:121:ASP:OD1	7:b:124:ARG:N	2.36	0.58
14:AM:88:ILE:HG23	14:AM:97:LEU:HD13	1.85	0.58
7:B:137:LYS:HG3	7:B:285:THR:O	2.03	0.58
9:k:19:TYR:HB3	4:p:82:THR:CG2	2.33	0.58
13:w:608:LYS:HE2	13:w:610:ILE:HD11	1.85	0.58
7:X:122:ILE:HD11	7:X:123:TYR:CE1	2.38	0.58
16:C:125:THR:O	16:C:125:THR:CG2	2.51	0.58
3:A:311:LYS:NZ	3:A:346:PRO:O	2.32	0.58
13:AK:57:VAL:HG12	13:AK:58:ILE:N	2.19	0.58
9:l:8:LEU:HD12	9:l:13:MET:HE3	1.84	0.58
7:s:316:PHE:HB2	7:s:651:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:489:ARG:NE	7:m:642:LEU:CD2	2.65	0.58
7:j:586:ASN:ND2	15:AL:458:SER:CB	2.64	0.58
7:K:20:MET:HE1	7:K:116:ILE:H	1.69	0.58
13:AK:608:LYS:HE2	13:AK:610:ILE:HD11	1.85	0.58
4:D:64:HIS:HE1	10:AE:173:PRO:HB2	1.68	0.58
7:c:404:ILE:HG23	7:c:407:LEU:HD23	1.86	0.58
13:AQ:57:VAL:HG12	13:AQ:58:ILE:N	2.19	0.58
8:AH:27:LEU:N	11:2:121:GLU:HG2	2.19	0.58
7:j:658:ASN:ND2	15:AL:459:ASN:CG	2.62	0.58
13:w:187:PRO:HD2	15:x:70:GLN:NE2	2.18	0.57
14:AM:86:LEU:HD13	14:AM:109:LEU:HD22	1.85	0.57
14:AS:86:LEU:HD13	14:AS:109:LEU:HD22	1.85	0.57
7:c:401:LEU:HD21	7:c:467:GLY:HA3	1.86	0.57
7:X:489:ARG:NE	7:X:642:LEU:CD2	2.67	0.57
11:7:301:LEU:HD12	11:7:304:ILE:HD11	1.85	0.57
7:V:116:ILE:CD1	7:V:267:LEU:HD22	2.34	0.57
7:d:550:VAL:HG11	7:d:579:PHE:CD1	2.39	0.57
7:f:484:ASP:OD1	7:f:485:GLN:N	2.37	0.57
11:AB:318:ILE:HD11	8:AT:133:ARG:NH1	2.19	0.57
11:7:147:PRO:HG3	11:7:269:ARG:HD3	1.85	0.57
13:AQ:608:LYS:HE2	13:AQ:610:ILE:HD11	1.85	0.57
3:A:449:THR:HA	3:A:454:PRO:HA	1.86	0.57
7:S:118:LEU:CD2	7:S:285:THR:HA	2.30	0.57
10:t:204:ASN:ND2	18:t:501:GTP:H1'	2.19	0.57
7:n:431:PHE:HB2	7:n:460:PHE:CD1	2.39	0.57
14:AD:86:LEU:HD13	14:AD:109:LEU:HD22	1.85	0.57
7:o:175:ILE:HG21	7:o:221:TYR:CZ	2.40	0.57
3:A:369:ASP:OD1	3:A:373:HIS:N	2.36	0.57
7:f:465:MET:HG2	7:f:659:ILE:HD11	1.87	0.57
7:j:369:ARG:HE	7:j:403:SER:HG	1.50	0.57
7:B:615:LEU:HD11	7:B:644:LEU:HD13	1.85	0.57
12:AF:11:GLN:HB3	18:AF:501:GTP:O2A	2.04	0.57
7:j:588:PRO:HD3	15:AL:507:THR:CG2	2.27	0.56
16:C:128:ASN:ND2	16:C:147:GLN:O	2.38	0.56
7:B:141:MET:CE	7:B:147:TRP:CH2	2.83	0.56
7:U:347:ASP:O	7:U:404:ILE:N	2.38	0.56
13:AQ:781:ARG:HG3	13:AQ:809:GLY:CA	2.35	0.56
2:4:81:GLU:O	6:i:424:ASP:N	2.38	0.56
13:w:178:LEU:HD11	13:w:197:ARG:HD2	1.87	0.56
13:AK:178:LEU:HD11	13:AK:197:ARG:HD2	1.87	0.56
10:t:141:GLY:H	18:t:501:GTP:H5'	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:56:ARG:HB3	8:g:112:HIS:CE1	2.41	0.56
11:y:886:LEU:HD21	11:2:858:PHE:CE2	2.40	0.56
7:d:3:PHE:CD1	7:d:20:MET:HG2	2.40	0.56
7:d:489:ARG:HD2	7:d:642:LEU:HD11	1.81	0.56
13:w:809:GLY:O	13:w:811:ASN:ND2	2.38	0.56
16:L:152:THR:CG2	16:L:168:MET:HE3	2.34	0.56
13:AK:809:GLY:O	13:AK:811:ASN:ND2	2.38	0.56
12:u:336:LYS:NZ	13:w:56:CYS:O	2.28	0.56
2:AA:53:ILE:HG22	8:AJ:133:ARG:HG3	1.85	0.56
7:K:269:GLU:HB3	7:K:279:ILE:HG22	1.87	0.56
7:V:116:ILE:HD12	7:V:267:LEU:HD22	1.87	0.56
11:AB:540:MET:HE2	11:AB:540:MET:HA	1.87	0.56
7:U:134:LYS:NZ	7:U:284:ASP:OD2	2.39	0.56
13:AK:127:VAL:HB	13:AK:188:VAL:HG21	1.87	0.56
13:AQ:127:VAL:HB	13:AQ:188:VAL:HG21	1.87	0.56
8:e:56:ARG:HB3	8:e:112:HIS:CE1	2.41	0.56
7:o:431:PHE:HB2	7:o:460:PHE:CD1	2.41	0.56
15:AR:616:LEU:HD22	13:AQ:316:VAL:HG11	1.88	0.56
8:g:132:ILE:HD11	11:7:311:ILE:CB	2.36	0.56
8:g:148:LEU:HB2	6:i:934:PHE:HB2	1.88	0.56
7:s:596:LEU:HD11	7:r:275:CYS:HA	1.87	0.56
11:5:147:PRO:HG3	11:5:269:ARG:HD3	1.88	0.56
6:H:855:ASN:OD1	11:y:738:THR:CG2	2.54	0.55
13:AQ:809:GLY:O	13:AQ:811:ASN:ND2	2.38	0.55
7:n:210:ARG:HG2	7:n:227:PRO:HD3	1.89	0.55
12:u:172:TYR:HB3	12:u:205:ASP:HA	1.88	0.55
11:5:301:LEU:HD12	11:5:304:ILE:HD11	1.87	0.55
8:AT:56:ARG:HB3	8:AT:112:HIS:CE1	2.41	0.55
8:e:86:LEU:HD23	8:e:130:LEU:HD11	1.88	0.55
13:w:127:VAL:HB	13:w:188:VAL:HG21	1.87	0.55
16:C:127:THR:HG22	16:C:146:VAL:HG22	1.86	0.55
6:Q:551:PHE:HB3	6:Q:585:VAL:HG12	1.89	0.55
9:k:203:THR:OG1	9:k:206:ALA:O	2.15	0.55
7:X:489:ARG:HD2	7:X:642:LEU:CD1	2.37	0.55
13:w:119:LEU:HB3	13:w:124:ILE:HD11	1.88	0.55
12:AO:172:TYR:HB3	12:AO:205:ASP:HA	1.88	0.55
10:t:261:PRO:HD3	12:u:406:HIS:CE1	2.41	0.55
12:AF:172:TYR:HB3	12:AF:205:ASP:HA	1.88	0.55
11:2:540:MET:HE2	11:2:540:MET:HA	1.87	0.55
3:A:410:GLU:OE1	3:A:413:SER:OG	2.24	0.55
7:S:143:GLY:HA2	7:S:681:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AB:318:ILE:HD12	8:AT:133:ARG:HD2	1.89	0.55
16:L:152:THR:HG22	16:L:168:MET:HE3	1.87	0.55
7:K:118:LEU:HD11	7:K:181:MET:SD	2.47	0.55
13:AQ:178:LEU:HD11	13:AQ:197:ARG:HD2	1.87	0.55
7:f:549:TYR:CD2	7:K:279:ILE:HD12	2.42	0.55
7:o:307:LEU:HD21	7:o:317:VAL:HG13	1.89	0.55
8:AT:86:LEU:HD23	8:AT:130:LEU:HD11	1.88	0.55
8:g:86:LEU:HD23	8:g:130:LEU:HD11	1.88	0.55
7:j:401:LEU:HD21	7:j:467:GLY:HA3	1.88	0.55
7:f:462:ASP:OD2	7:f:595:LYS:NZ	2.39	0.55
13:AK:119:LEU:HB3	13:AK:124:ILE:HD11	1.88	0.55
6:H:911:MET:CA	8:e:147:LYS:HB2	2.33	0.54
7:s:621:PHE:CE2	7:s:652:PHE:HB2	2.42	0.54
15:AL:241:ARG:HH12	13:AK:416:LEU:HD23	1.70	0.54
11:AB:287:LEU:O	8:AT:29:LEU:HA	2.07	0.54
7:K:82:PRO:CG	7:K:186:GLU:CB	2.78	0.54
6:Q:905:GLU:OE1	6:Q:905:GLU:N	2.40	0.54
10:t:259:PRO:HA	12:u:404:PHE:CD1	2.42	0.54
6:H:82:LEU:HA	6:H:85:ARG:HD2	1.90	0.54
7:S:20:MET:HE2	7:S:282:TYR:CZ	2.42	0.54
10:t:345:ILE:HG23	12:u:181:VAL:CG1	2.37	0.54
8:g:133:ARG:HD2	11:7:318:ILE:CD1	2.37	0.54
15:AL:733:CYS:HB2	15:AL:736:CYS:SG	2.47	0.54
11:7:849:CYS:O	11:7:851:ILE:HG12	2.06	0.54
14:AM:62:PHE:HZ	15:AL:739:ARG:HB2	1.72	0.54
12:AO:175:PRO:HG3	10:AN:347:ASN:HD21	1.72	0.54
15:AR:733:CYS:HB2	15:AR:736:CYS:SG	2.47	0.54
7:s:209:THR:HB	7:s:261:ILE:HD13	1.88	0.54
13:w:116:VAL:HG22	13:w:158:LEU:HB3	1.90	0.54
13:w:190:PHE:CE2	15:x:8:MET:HE1	2.43	0.54
7:c:172:PRO:HD2	7:c:175:ILE:HD11	1.89	0.54
7:j:46:PRO:HD3	7:r:131:PRO:HD3	1.89	0.54
5:I:536:VAL:HG12	5:I:545:LEU:HD12	1.90	0.54
9:k:363:SER:HB3	9:k:391:LEU:HD11	1.89	0.54
7:b:280:PRO:HB2	7:B:431:PHE:HD2	1.73	0.54
7:s:677:TRP:O	7:s:680:MET:HG2	2.08	0.54
15:x:733:CYS:HB2	15:x:736:CYS:SG	2.47	0.54
7:j:381:THR:HG22	7:j:381:THR:O	2.07	0.54
13:AK:116:VAL:HG22	13:AK:158:LEU:HB3	1.90	0.54
8:AT:93:GLY:O	8:AT:98:GLN:NE2	2.41	0.54
7:s:596:LEU:HD12	7:r:275:CYS:C	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:478:THR:HG21	7:m:489:ARG:HG3	1.90	0.53
7:o:79:MET:HE2	7:o:113:GLY:HA3	1.90	0.53
7:m:550:VAL:HG11	7:m:579:PHE:CD1	2.43	0.53
7:K:340:ARG:NH1	7:K:348:GLU:OE1	2.39	0.53
7:c:527:ASN:HD22	7:c:652:PHE:HE2	1.57	0.53
13:AQ:154:PRO:HB3	13:AQ:201:LEU:HD22	1.90	0.53
6:H:81:ASP:OD1	6:H:81:ASP:N	2.41	0.53
9:k:19:TYR:CE1	4:p:79:GLU:O	2.60	0.53
11:y:540:MET:HA	11:y:540:MET:HE2	1.89	0.53
7:X:273:ASP:OD1	7:X:274:GLU:N	2.41	0.53
7:j:3:PHE:CD1	7:j:281:LEU:HD13	2.44	0.53
12:AF:248:LEU:HD22	12:AF:354:GLY:HA3	1.90	0.53
13:AQ:119:LEU:HB3	13:AQ:124:ILE:HD11	1.88	0.53
1:l:72:ASN:OD1	1:l:73:PHE:N	2.42	0.53
7:r:118:LEU:CD2	7:r:286:VAL:CG1	2.86	0.53
7:S:145:ASN:OD1	7:U:66:TRP:CE3	2.62	0.53
7:s:514:THR:HG22	7:s:533:THR:HG22	1.90	0.53
12:u:266:HIS:O	12:u:268:PRO:HD3	2.09	0.53
12:AF:264:ARG:HG3	13:AK:247:LYS:HG3	1.90	0.53
1:3:67:VAL:HG12	8:g:151:PHE:CZ	2.44	0.53
7:S:118:LEU:HD23	7:S:285:THR:C	2.33	0.53
7:j:123:TYR:CD2	7:r:43:ARG:CZ	2.92	0.53
12:AF:98:ASP:HB2	18:AF:501:GTP:O3G	2.08	0.53
13:AQ:116:VAL:HG22	13:AQ:158:LEU:HB3	1.90	0.53
13:AQ:541:ASP:OD1	13:AQ:541:ASP:O	2.26	0.53
7:m:677:TRP:O	7:m:680:MET:HG2	2.09	0.53
7:j:43:ARG:NH2	7:r:123:TYR:HD2	2.07	0.53
7:j:335:TYR:OH	14:AM:80:SER:CA	2.57	0.53
7:m:295:PHE:CD1	7:m:352:CYS:SG	3.01	0.53
6:H:68:ASP:OD2	6:H:72:ARG:NH1	2.42	0.53
7:Z:79:MET:HE2	7:Z:113:GLY:HA3	1.90	0.53
7:f:343:LYS:NZ	7:f:663:CYS:SG	2.64	0.53
7:d:314:GLN:HG3	7:d:316:PHE:H	1.74	0.53
13:w:154:PRO:HB3	13:w:201:LEU:HD22	1.90	0.53
11:y:858:PHE:CE1	11:2:886:LEU:CD2	2.84	0.53
7:m:621:PHE:CE1	7:m:652:PHE:HB2	2.45	0.52
11:7:673:LYS:HG3	11:7:700:TYR:CD1	2.45	0.52
7:K:209:THR:HB	7:K:261:ILE:HD13	1.91	0.52
2:4:80:PRO:O	6:i:425:SER:CB	2.58	0.52
2:4:116:ILE:CD1	8:AH:137:ILE:HG22	2.40	0.52
7:S:145:ASN:CA	7:U:66:TRP:CZ2	2.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t:204:ASN:HD21	18:t:501:GTP:H1'	1.73	0.52
12:AO:266:HIS:O	12:AO:268:PRO:HD3	2.09	0.52
2:4:118:ALA:HB2	6:i:380:PRO:CG	2.34	0.52
10:AE:145:SER:HB2	10:AE:188:SER:OG	2.09	0.52
12:AO:409:VAL:HA	12:AO:413:MET:O	2.10	0.52
7:S:118:LEU:HD23	7:S:286:VAL:N	2.24	0.52
12:AF:266:HIS:O	12:AF:268:PRO:HD3	2.09	0.52
12:AF:346:TRP:CH2	13:AK:237:ALA:HB1	2.44	0.52
13:AK:936:CYS:O	13:AK:940:ARG:HG3	2.10	0.52
6:i:578:LYS:NZ	6:i:604:GLU:OE2	2.40	0.52
5:I:566:ILE:HG23	5:I:577:TYR:HB2	1.91	0.52
7:d:364:ILE:CD1	7:d:382:LEU:CD1	2.81	0.52
13:w:936:CYS:O	13:w:940:ARG:HG3	2.09	0.52
6:i:708:CYS:SG	6:i:739:ILE:HD11	2.49	0.52
7:Z:133:ASP:OD1	7:Z:134:LYS:N	2.43	0.52
7:m:18:LEU:HD12	7:m:112:THR:HB	1.90	0.52
7:d:20:MET:HE1	7:d:116:ILE:H	1.75	0.52
12:u:248:LEU:HD22	12:u:354:GLY:HA3	1.91	0.52
12:AF:409:VAL:HA	12:AF:413:MET:O	2.10	0.52
15:AL:616:LEU:HD22	13:AK:316:VAL:HG11	1.91	0.52
11:5:957:ARG:HG3	11:5:985:SER:HB3	1.92	0.52
13:AK:154:PRO:HB3	13:AK:201:LEU:HD22	1.90	0.52
13:AQ:58:ILE:CD1	13:AQ:63:GLN:HG3	2.40	0.52
6:H:329:ASN:ND2	6:H:363:CYS:O	2.40	0.52
7:j:127:GLN:OE1	7:r:92:LEU:HD11	2.10	0.52
11:5:849:CYS:O	11:5:851:ILE:HG12	2.10	0.52
15:x:454:ILE:HD11	15:x:483:TYR:HE2	1.75	0.52
13:AK:249:LYS:HE2	13:AK:283:LYS:HE3	1.92	0.52
16:C:289:ALA:HB1	16:C:299:ILE:HD11	1.92	0.52
7:K:118:LEU:HD23	7:K:286:VAL:HG12	1.91	0.52
10:AN:145:SER:HB2	10:AN:188:SER:OG	2.10	0.52
7:c:550:VAL:HG11	7:c:579:PHE:CD1	2.45	0.52
11:y:402:ARG:NH2	11:y:409:ASP:OD2	2.42	0.52
7:j:127:GLN:OE1	7:r:92:LEU:HD13	2.08	0.52
7:j:586:ASN:HA	15:AL:511:ARG:NE	2.25	0.52
13:AQ:249:LYS:HE2	13:AQ:283:LYS:HE3	1.92	0.52
6:H:551:PHE:HB3	6:H:585:VAL:HG12	1.92	0.52
7:X:615:LEU:HD11	7:X:644:LEU:HD13	1.92	0.52
7:m:662:VAL:O	7:m:663:CYS:SG	2.65	0.52
7:d:208:LYS:HD3	7:d:257:PHE:CD1	2.45	0.52
7:j:527:ASN:HD22	7:j:652:PHE:HE2	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:w:249:LYS:HE2	13:w:283:LYS:HE3	1.92	0.52
14:AM:62:PHE:HZ	15:AL:739:ARG:CB	2.21	0.52
13:AQ:936:CYS:O	13:AQ:940:ARG:HG3	2.10	0.52
7:S:178:LEU:HD22	7:S:248:GLU:HB3	1.90	0.51
7:m:92:LEU:HD22	7:m:108:VAL:HG22	1.91	0.51
7:m:369:ARG:NE	7:m:403:SER:OG	2.34	0.51
7:f:432:TYR:CE1	7:K:280:PRO:HB3	2.44	0.51
12:u:100:ALA:N	18:u:502:GTP:O2G	2.43	0.51
7:B:209:THR:HB	7:B:261:ILE:HD13	1.91	0.51
13:AK:46:SER:HA	13:AK:52:ALA:HA	1.93	0.51
7:S:117:SER:C	7:S:284:ASP:OD2	2.53	0.51
7:d:677:TRP:O	7:d:680:MET:HG2	2.10	0.51
7:j:335:TYR:CZ	14:AM:80:SER:CB	2.93	0.51
12:u:209:ILE:HG23	12:u:230:LEU:HD23	1.92	0.51
13:w:46:SER:HA	13:w:52:ALA:HA	1.92	0.51
12:AO:175:PRO:HG3	10:AN:347:ASN:ND2	2.26	0.51
12:AO:209:ILE:HG23	12:AO:230:LEU:HD23	1.93	0.51
15:AR:454:ILE:HD11	15:AR:483:TYR:HE2	1.75	0.51
16:C:127:THR:O	16:C:127:THR:CG2	2.53	0.51
7:c:589:SER:OG	15:x:523:GLU:OE1	2.12	0.51
9:k:88:PRO:HG3	9:k:423:TYR:HB2	1.92	0.51
9:l:127:LEU:HD11	9:l:154:ILE:HB	1.92	0.51
5:z:532:ASN:O	5:z:550:GLU:N	2.44	0.51
14:AM:62:PHE:CZ	15:AL:739:ARG:HB2	2.45	0.51
12:AO:248:LEU:HD22	12:AO:354:GLY:HA3	1.91	0.51
7:n:122:ILE:HG13	7:n:123:TYR:CD2	2.46	0.51
11:5:746:SER:OG	11:5:776:ALA:HB2	2.10	0.51
7:c:79:MET:HE2	7:c:113:GLY:HA3	1.93	0.51
7:W:617:ILE:O	7:W:648:PHE:HA	2.11	0.51
12:u:409:VAL:HA	12:u:413:MET:O	2.10	0.51
13:w:784:SER:N	13:w:811:ASN:OD1	2.44	0.51
2:AA:101:MET:HG2	8:AJ:126:VAL:HG21	1.93	0.51
7:r:310:GLU:N	7:r:310:GLU:OE1	2.44	0.51
7:U:79:MET:HE2	7:U:113:GLY:HA3	1.93	0.51
6:H:748:VAL:HG22	6:H:776:TYR:HB2	1.91	0.51
7:S:122:ILE:O	7:S:147:TRP:CA	2.59	0.51
7:V:550:VAL:HG11	7:V:579:PHE:CD1	2.46	0.51
11:5:1039:HIS:CE1	10:AN:282:ARG:HB3	2.46	0.51
8:AT:51:ALA:HA	8:AT:87:ALA:HB2	1.93	0.51
5:I:534:ILE:HD13	5:I:568:THR:HG21	1.92	0.51
8:g:93:GLY:O	8:g:98:GLN:NE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:489:ARG:CD	7:W:642:LEU:CD1	2.84	0.51
7:s:8:SER:HB3	7:s:31:LYS:HD3	1.92	0.51
7:m:127:GLN:CD	7:o:92:LEU:HD11	2.36	0.51
7:m:364:ILE:HD12	7:m:382:LEU:HD22	1.89	0.51
7:m:364:ILE:CD1	7:m:382:LEU:HD22	2.40	0.51
5:P:566:ILE:HG23	5:P:577:TYR:HB2	1.93	0.51
7:b:278:GLU:HB2	7:B:432:TYR:OH	2.11	0.51
7:b:280:PRO:HB3	7:B:432:TYR:CD1	2.46	0.51
7:X:128:LEU:N	7:X:128:LEU:HD12	2.26	0.51
7:s:280:PRO:O	7:r:556:LEU:HD11	2.11	0.51
7:d:489:ARG:CD	7:d:642:LEU:CD1	2.78	0.51
12:AF:413:MET:HE3	12:AF:417:GLU:HB2	1.93	0.51
15:AL:454:ILE:HD11	15:AL:483:TYR:HE2	1.75	0.51
13:AQ:784:SER:N	13:AQ:811:ASN:OD1	2.44	0.51
7:f:556:LEU:HD21	7:K:281:LEU:O	2.11	0.51
13:AQ:539:ARG:NH2	13:AQ:541:ASP:OD1	2.44	0.51
9:k:30:GLN:HB2	4:p:132:PRO:HB3	1.93	0.50
7:d:273:ASP:OD1	7:d:274:GLU:N	2.45	0.50
11:O:540:MET:HA	11:O:540:MET:HE2	1.91	0.50
13:AQ:472:LYS:HD2	13:AQ:505:PHE:CE2	2.46	0.50
13:AQ:791:GLU:HB2	13:AQ:820:LEU:HD13	1.94	0.50
1:3:75:MET:HE1	8:g:153:LEU:HD22	1.92	0.50
9:k:26:LEU:CD1	4:p:160:CYS:HB2	2.34	0.50
7:b:651:ASP:O	7:b:652:PHE:C	2.54	0.50
7:K:114:ILE:HA	7:K:186:GLU:O	2.11	0.50
1:3:73:PHE:CE1	8:g:108:MET:HE1	2.46	0.50
2:4:81:GLU:C	6:i:425:SER:N	2.59	0.50
4:D:4:ILE:HD12	4:D:31:LEU:HD21	1.94	0.50
10:t:259:PRO:HB3	12:u:404:PHE:CZ	2.47	0.50
10:t:345:ILE:CG2	12:u:181:VAL:CG1	2.87	0.50
7:o:615:LEU:HD11	7:o:644:LEU:HD13	1.93	0.50
8:e:93:GLY:O	8:e:98:GLN:NE2	2.41	0.50
7:f:550:VAL:HG11	7:f:579:PHE:CD1	2.46	0.50
7:m:178:LEU:HD22	7:m:248:GLU:HB3	1.94	0.50
7:o:365:LEU:HD13	7:o:389:LEU:HD23	1.93	0.50
12:u:311:LYS:NZ	12:u:438:ASP:OD1	2.45	0.50
14:AS:80:SER:HA	7:U:335:TYR:OH	2.12	0.50
2:AA:68:MET:O	8:AJ:121:VAL:HG12	2.11	0.50
16:C:200:THR:OG1	16:C:203:SER:O	2.29	0.50
13:AK:784:SER:N	13:AK:811:ASN:OD1	2.44	0.50
8:g:51:ALA:HA	8:g:87:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:j:37:CYS:HA	7:j:97:CYS:HA	1.92	0.50
13:w:531:LEU:N	13:w:574:ASN:HD21	2.09	0.50
12:AF:15:GLN:OE1	18:AF:501:GTP:O6	2.28	0.50
5:8:303:SER:HB2	5:8:560:THR:HB	1.94	0.50
5:8:566:ILE:HG23	5:8:577:TYR:HB2	1.94	0.50
7:K:112:THR:CG2	7:K:188:PRO:HG2	2.42	0.50
7:K:117:SER:O	7:K:183:VAL:HA	2.11	0.50
7:K:128:LEU:CD2	7:K:182:ASN:ND2	2.70	0.50
8:g:148:LEU:HB2	6:i:934:PHE:CB	2.41	0.50
8:AH:30:ARG:O	11:2:287:LEU:N	2.36	0.50
13:w:791:GLU:HB2	13:w:820:LEU:HD13	1.94	0.50
2:AA:105:LEU:HD21	8:AJ:129:PHE:CD1	2.46	0.50
11:0:746:SER:OG	11:0:776:ALA:HB2	2.11	0.50
11:5:875:THR:HG23	11:5:904:VAL:HB	1.93	0.50
6:H:821:CYS:HA	6:H:824:LEU:HB2	1.94	0.50
10:t:259:PRO:HA	12:u:404:PHE:CE1	2.46	0.50
7:b:214:SER:HB3	7:b:221:TYR:CD2	2.46	0.50
7:o:196:GLN:HE21	7:o:270:LYS:HG2	1.77	0.50
7:j:97:CYS:HB2	7:r:144:MET:HE1	1.93	0.50
13:w:948:PHE:CE1	13:w:981:CYS:HB2	2.47	0.50
12:AO:404:PHE:CD1	10:AN:259:PRO:HA	2.46	0.50
7:c:151:LEU:HG	7:c:288:PHE:HB3	1.94	0.50
5:I:455:ASP:HB3	5:I:458:MET:HB3	1.93	0.50
7:o:550:VAL:HG11	7:o:579:PHE:CD1	2.47	0.50
12:u:413:MET:HE3	12:u:417:GLU:HB2	1.93	0.50
11:7:693:PHE:HE2	7:K:311:LEU:HD11	1.76	0.50
7:B:463:TRP:CD1	7:B:463:TRP:H	2.28	0.50
7:S:122:ILE:O	7:S:147:TRP:CB	2.60	0.50
7:X:47:ARG:NH2	7:X:88:GLU:OE2	2.39	0.50
13:w:472:LYS:HD2	13:w:505:PHE:CE2	2.47	0.50
12:AF:209:ILE:HG23	12:AF:230:LEU:HD23	1.92	0.50
7:r:295:PHE:CB	7:r:409:VAL:HG21	2.37	0.50
5:E:566:ILE:HG23	5:E:577:TYR:HB2	1.93	0.49
6:H:894:GLU:HA	6:H:921:LEU:O	2.12	0.49
7:n:177:ASN:ND2	7:n:359:LYS:HD3	2.27	0.49
13:w:185:ILE:HG22	15:x:6:ARG:HH12	1.76	0.49
12:AF:233:GLN:HG3	12:AF:368:LEU:HD13	1.94	0.49
5:8:491:GLN:HG2	5:8:508:THR:HB	1.94	0.49
10:AN:67:ASP:OD1	10:AN:68:LEU:N	2.45	0.49
7:U:381:THR:O	7:U:381:THR:CG2	2.58	0.49
13:AK:791:GLU:HB2	13:AK:820:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:443:ASP:OD1	9:k:446:SER:OG	2.22	0.49
5:z:169:LEU:HD21	11:y:519:VAL:HG22	1.93	0.49
7:U:364:ILE:HD12	7:U:382:LEU:CD2	2.41	0.49
3:A:157:LEU:HD21	3:A:199:ILE:HG13	1.93	0.49
12:u:233:GLN:HG3	12:u:368:LEU:HD13	1.94	0.49
15:AR:459:ASN:ND2	7:U:658:ASN:ND2	2.52	0.49
11:2:849:CYS:O	11:2:851:ILE:HG12	2.12	0.49
13:AK:948:PHE:CE1	13:AK:981:CYS:HB2	2.47	0.49
6:h:82:LEU:HA	6:h:85:ARG:HD2	1.94	0.49
1:9:72:ASN:OD1	1:9:73:PHE:N	2.45	0.49
8:e:51:ALA:HA	8:e:87:ALA:HB2	1.93	0.49
12:AF:210:TYR:CE1	12:AF:222:PRO:HD2	2.48	0.49
12:AO:311:LYS:NZ	12:AO:438:ASP:OD1	2.45	0.49
12:AO:413:MET:HE3	12:AO:417:GLU:HB2	1.93	0.49
7:K:112:THR:HG21	7:K:188:PRO:HG2	1.94	0.49
13:AQ:46:SER:HA	13:AQ:52:ALA:HA	1.92	0.49
7:S:120:ALA:HB3	7:S:286:VAL:CG2	2.42	0.49
7:f:209:THR:HB	7:f:261:ILE:HD13	1.93	0.49
9:k:78:TYR:CD1	4:p:162:GLU:CD	2.90	0.49
9:k:127:LEU:HD11	9:k:154:ILE:HB	1.93	0.49
7:V:273:ASP:OD1	7:V:274:GLU:N	2.45	0.49
12:AO:233:GLN:HG3	12:AO:368:LEU:HD13	1.94	0.49
5:P:277:ARG:HA	5:P:277:ARG:NE	2.28	0.49
6:i:398:CYS:HB3	6:i:461:PHE:HB2	1.92	0.49
7:b:669:ASN:OD1	7:b:670:ARG:N	2.46	0.49
7:n:308:CYS:HA	7:n:334:VAL:HB	1.94	0.49
7:s:478:THR:OG1	7:s:487:ASP:O	2.27	0.49
7:o:582:GLU:OE1	7:o:599:ARG:NE	2.42	0.49
14:AM:33:TRP:HB2	14:AM:54:ILE:HB	1.95	0.49
16:L:213:GLY:HA2	16:L:235:GLY:HA2	1.94	0.49
13:AK:531:LEU:N	13:AK:574:ASN:HD21	2.09	0.49
7:Y:127:GLN:CG	7:V:92:LEU:HD13	2.36	0.49
13:w:704:VAL:HG21	13:w:728:LEU:HD21	1.95	0.49
13:AK:704:VAL:HG21	13:AK:728:LEU:HD21	1.95	0.49
7:j:130:MET:HE1	7:r:90:LYS:HE3	1.93	0.49
10:AE:2:ARG:HB3	10:AE:131:GLN:HG3	1.94	0.49
14:AS:33:TRP:HB2	14:AS:54:ILE:HB	1.95	0.49
7:c:295:PHE:CE1	7:c:407:LEU:HD21	2.48	0.49
13:AQ:948:PHE:CE1	13:AQ:981:CYS:HB2	2.47	0.49
7:f:431:PHE:CE2	7:K:283:LYS:CB	2.96	0.49
10:AE:3:GLU:OE1	10:AE:3:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AE:73:MET:HG3	10:AE:92:PHE:CD2	2.48	0.49
10:AN:176:SER:HB2	18:AN:501:GTP:O2'	2.13	0.49
7:c:407:LEU:HD12	7:c:425:VAL:HG13	1.95	0.49
6:h:10:LEU:HD22	6:h:59:LEU:CG	2.38	0.49
7:X:478:THR:HG21	7:X:489:ARG:HG3	1.95	0.48
7:Z:651:ASP:O	7:Z:652:PHE:C	2.56	0.48
7:V:651:ASP:O	7:V:652:PHE:C	2.55	0.48
7:W:18:LEU:HD12	7:W:112:THR:HB	1.94	0.48
12:AF:311:LYS:NZ	12:AF:438:ASP:OD1	2.45	0.48
8:AJ:46:VAL:HG11	11:O:293:ALA:HB3	1.94	0.48
7:r:409:VAL:HG22	7:r:425:VAL:HG22	1.94	0.48
16:C:142:TRP:CD1	16:C:180:ARG:HD3	2.48	0.48
9:k:179:ASP:HB3	9:k:186:LEU:HD11	1.94	0.48
7:X:121:ASP:OD1	7:X:124:ARG:N	2.46	0.48
7:V:364:ILE:HD12	7:V:382:LEU:HD21	1.95	0.48
12:AO:210:TYR:CE1	12:AO:222:PRO:HD2	2.48	0.48
16:C:446:LEU:HB2	16:C:458:MET:HB2	1.95	0.48
13:AQ:704:VAL:HG21	13:AQ:728:LEU:HD21	1.95	0.48
3:A:447:VAL:HG22	3:A:457:LEU:HD21	1.94	0.48
5:I:155:PRO:HB3	5:I:251:LEU:HD22	1.94	0.48
9:k:78:TYR:CD1	4:p:162:GLU:OE1	2.66	0.48
7:n:3:PHE:CD1	7:n:20:MET:HG2	2.47	0.48
7:d:617:ILE:O	7:d:648:PHE:HA	2.14	0.48
12:u:210:TYR:CE1	12:u:222:PRO:HD2	2.48	0.48
11:5:1006:GLN:HG3	11:5:1033:VAL:HG22	1.96	0.48
7:K:118:LEU:CD2	7:K:286:VAL:HG12	2.43	0.48
8:AI:30:ARG:NH1	8:AI:31:THR:O	2.45	0.48
5:E:532:ASN:O	5:E:550:GLU:N	2.46	0.48
7:o:208:LYS:HD3	7:o:257:PHE:CD1	2.49	0.48
7:d:364:ILE:CD1	7:d:382:LEU:CD2	2.77	0.48
2:4:81:GLU:O	6:i:424:ASP:CB	2.62	0.48
7:b:550:VAL:HG11	7:b:579:PHE:CD1	2.48	0.48
7:o:314:GLN:HG3	7:o:315:GLY:H	1.78	0.48
10:AE:215:LEU:HD13	10:AE:275:SER:HB3	1.95	0.48
7:B:273:ASP:OD1	7:B:274:GLU:N	2.47	0.48
9:k:26:LEU:HD11	4:p:160:CYS:SG	2.50	0.48
9:k:32:ASN:ND2	4:p:141:ILE:HG21	2.28	0.48
9:k:407:LEU:HD11	9:k:425:LEU:HD12	1.95	0.48
7:b:280:PRO:HD3	7:B:432:TYR:HE1	1.78	0.48
7:X:79:MET:HE2	7:X:113:GLY:HA3	1.96	0.48
7:o:316:PHE:HB2	7:o:651:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5:217:PHE:HB2	11:5:264:LEU:HD23	1.96	0.48
7:K:3:PHE:CD1	7:K:20:MET:HG2	2.49	0.48
5:I:286:LYS:HE3	5:I:575:SER:HB3	1.95	0.48
7:Y:79:MET:HE2	7:Y:113:GLY:HA3	1.96	0.48
7:W:651:ASP:O	7:W:652:PHE:C	2.57	0.48
14:AD:33:TRP:HB2	14:AD:54:ILE:HB	1.95	0.48
8:AT:52:TRP:CH2	8:AT:116:GLU:HA	2.49	0.48
9:k:284:LEU:HD21	9:k:321:MET:HE1	1.95	0.48
7:f:677:TRP:O	7:f:680:MET:HG2	2.14	0.48
16:C:410:GLU:OE1	16:C:413:SER:OG	2.31	0.48
5:8:302:SER:HB2	5:8:351:LEU:HD21	1.96	0.48
11:7:987:ASN:HB2	11:7:1046:TRP:CD2	2.48	0.48
13:AQ:788:ILE:H	13:AQ:788:ILE:HD12	1.78	0.48
3:A:436:LYS:HE2	3:A:438:LEU:HD21	1.96	0.48
7:S:142:TRP:HB3	7:S:681:THR:HA	1.96	0.48
13:w:788:ILE:H	13:w:788:ILE:HD12	1.78	0.48
11:5:673:LYS:HG3	11:5:700:TYR:CD1	2.49	0.48
7:K:408:MET:HG3	7:K:469:MET:HE3	1.96	0.48
7:c:658:ASN:HD21	15:x:459:ASN:ND2	2.12	0.48
7:S:123:TYR:HB2	7:U:43:ARG:NH2	2.28	0.48
5:AC:566:ILE:HG23	5:AC:577:TYR:HB2	1.96	0.48
11:AB:318:ILE:CD1	8:AT:133:ARG:NH1	2.77	0.48
11:AB:402:ARG:NH2	11:AB:409:ASP:OD2	2.47	0.48
7:r:273:ASP:OD1	7:r:274:GLU:N	2.47	0.48
3:A:13:ILE:HD13	4:F:123:VAL:HG11	1.96	0.47
10:t:67:ASP:OD1	10:t:68:LEU:N	2.47	0.47
7:Z:273:ASP:OD1	7:Z:274:GLU:N	2.47	0.47
7:f:294:ILE:HD13	7:f:422:LEU:HD13	1.96	0.47
8:AJ:30:ARG:HE	8:AJ:77:THR:HG23	1.78	0.47
13:AQ:217:ARG:HB2	13:AQ:341:MET:SD	2.53	0.47
6:i:606:VAL:HG12	6:i:618:LEU:HD21	1.95	0.47
6:i:850:ALA:HB1	6:i:880:ALA:HB2	1.95	0.47
7:b:277:PRO:HG2	7:B:549:TYR:CZ	2.49	0.47
7:m:459:LEU:HD11	7:m:561:LEU:HD21	1.97	0.47
7:o:486:LYS:HD3	7:o:488:PHE:CE2	2.49	0.47
7:o:621:PHE:CE2	7:o:652:PHE:HB2	2.49	0.47
7:X:550:VAL:HG11	7:X:579:PHE:CD1	2.50	0.47
16:L:100:ARG:O	16:L:101:ALA:HB3	2.12	0.47
14:AD:80:SER:HA	7:c:335:TYR:OH	2.13	0.47
11:2:987:ASN:HB2	11:2:1046:TRP:CD2	2.49	0.47
13:AK:788:ILE:HD12	13:AK:788:ILE:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:894:GLU:HA	6:i:921:LEU:O	2.13	0.47
6:H:885:ASN:HD21	11:y:710:ASP:CG	2.22	0.47
9:l:124:VAL:HG23	9:l:138:ILE:HD11	1.96	0.47
7:b:493:ALA:HB2	7:b:606:LEU:HD12	1.97	0.47
7:f:65:VAL:HG12	7:f:67:ARG:HG3	1.95	0.47
7:f:484:ASP:OD1	7:f:485:GLN:HG3	2.13	0.47
7:d:527:ASN:HD22	7:d:652:PHE:HE2	1.61	0.47
7:j:585:THR:O	7:j:586:ASN:CG	2.57	0.47
12:AF:264:ARG:HG3	13:AK:247:LYS:CG	2.45	0.47
16:C:249:LEU:HD13	16:C:299:ILE:HG12	1.96	0.47
7:B:118:LEU:N	7:B:284:ASP:OD2	2.29	0.47
13:AK:57:VAL:CG1	13:AK:58:ILE:N	2.78	0.47
13:AQ:834:GLU:HG2	13:AQ:862:SER:HB3	1.96	0.47
3:A:404:LEU:HD11	3:A:422:LEU:HD12	1.95	0.47
6:H:931:MET:HG2	8:e:150:GLY:O	2.14	0.47
9:k:35:TRP:HZ3	4:p:135:ILE:HG21	1.79	0.47
11:y:987:ASN:HB2	11:y:1046:TRP:CD2	2.49	0.47
7:b:212:TYR:HB3	7:b:221:TYR:HB3	1.96	0.47
7:s:154:ASN:ND2	7:s:248:GLU:OE1	2.44	0.47
7:U:602:PHE:O	7:U:603:PRO:C	2.57	0.47
8:g:52:TRP:CH2	8:g:116:GLU:HA	2.49	0.47
13:w:834:GLU:HG2	13:w:862:SER:HB3	1.96	0.47
7:U:349:MET:CE	7:U:378:MET:HE3	2.41	0.47
8:e:52:TRP:CH2	8:e:116:GLU:HA	2.49	0.47
7:T:316:PHE:HB2	7:T:651:ASP:OD2	2.15	0.47
11:y:849:CYS:O	11:y:851:ILE:HG12	2.13	0.47
7:b:602:PHE:O	7:b:603:PRO:C	2.57	0.47
7:m:617:ILE:O	7:m:648:PHE:HA	2.14	0.47
7:o:463:TRP:H	7:o:463:TRP:CD1	2.31	0.47
7:d:493:ALA:HB2	7:d:606:LEU:HD12	1.96	0.47
11:7:1006:GLN:HG3	11:7:1033:VAL:HG22	1.97	0.47
7:c:211:VAL:HG22	7:c:247:VAL:HG13	1.96	0.47
7:S:128:LEU:HG	7:S:128:LEU:O	2.14	0.47
7:j:606:LEU:HD23	7:j:606:LEU:HA	1.75	0.47
12:AO:221:ARG:HD2	10:AN:327:ASP:OD2	2.14	0.47
11:5:310:ARG:HB3	11:5:311:ILE:H	1.53	0.47
7:B:133:ASP:OD1	7:B:135:GLN:N	2.47	0.47
7:U:404:ILE:O	7:U:407:LEU:N	2.48	0.47
13:AQ:950:ALA:HA	13:AQ:978:GLY:O	2.15	0.47
6:H:855:ASN:OD1	11:y:738:THR:HG23	2.14	0.47
7:b:381:THR:O	7:b:381:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:w:950:ALA:HA	13:w:978:GLY:O	2.15	0.47
12:AO:100:ALA:N	18:AO:501:GTP:O2G	2.48	0.47
14:AS:95:PRO:HG2	15:AR:749:PRO:HB3	1.96	0.47
7:c:340:ARG:NH2	7:c:366:ASP:OD2	2.48	0.47
13:AQ:57:VAL:CG1	13:AQ:58:ILE:N	2.78	0.47
2:4:118:ALA:HB1	6:i:383:ALA:HB1	1.85	0.47
5:z:169:LEU:CD2	11:y:519:VAL:HG22	2.45	0.47
7:Z:127:GLN:NE2	7:Z:130:MET:SD	2.84	0.47
7:n:178:LEU:HD22	7:n:248:GLU:HB3	1.97	0.47
7:f:295:PHE:HB2	7:f:409:VAL:HG21	1.97	0.47
7:f:463:TRP:H	7:f:463:TRP:CD1	2.33	0.47
7:c:4:GLN:NE2	7:c:6:SER:H	2.12	0.47
7:s:178:LEU:HD22	7:s:248:GLU:HB3	1.96	0.46
7:s:617:ILE:O	7:s:648:PHE:HA	2.14	0.46
11:7:1050:ASP:OD1	11:7:1050:ASP:N	2.48	0.46
7:K:42:ILE:HG13	7:K:93:VAL:HG22	1.97	0.46
11:2:647:LEU:HD12	11:2:676:PHE:CE1	2.50	0.46
6:i:81:ASP:OD1	6:i:81:ASP:N	2.48	0.46
7:j:3:PHE:CE2	7:j:20:MET:HG2	2.51	0.46
7:j:586:ASN:CA	15:AL:511:ARG:NE	2.78	0.46
10:AE:134:GLN:HA	10:AE:165:ASN:O	2.16	0.46
2:AA:82:ARG:HA	6:h:424:ASP:HB2	1.97	0.46
11:0:849:CYS:O	11:0:851:ILE:HG12	2.16	0.46
7:B:550:VAL:O	7:B:554:ILE:HG13	2.15	0.46
7:U:273:ASP:OD1	7:U:274:GLU:N	2.48	0.46
13:AQ:69:ILE:HG22	13:AQ:110:TYR:OH	2.15	0.46
3:A:128:ASN:HB2	3:A:146:GLU:HG3	1.97	0.46
11:y:614:VAL:HG11	11:y:627:GLU:OE1	2.15	0.46
13:w:215:TRP:O	13:w:219:VAL:HG23	2.15	0.46
7:r:119:GLU:HB2	7:r:182:ASN:HB2	1.97	0.46
13:AK:950:ALA:HA	13:AK:978:GLY:O	2.15	0.46
3:A:255:PRO:HG3	10:AN:404:ASP:HA	1.97	0.46
7:f:204:GLU:OE2	7:K:442:LYS:NZ	2.44	0.46
7:d:478:THR:CG2	7:d:489:ARG:HG3	2.45	0.46
8:AJ:30:ARG:HE	8:AJ:77:THR:CG2	2.28	0.46
11:0:402:ARG:NH2	11:0:409:ASP:OD2	2.47	0.46
16:L:102:HIS:N	16:L:103:PRO:CD	2.79	0.46
5:8:397:THR:HG22	5:8:437:VAL:HG11	1.97	0.46
5:8:455:ASP:HB3	5:8:458:MET:HB3	1.98	0.46
13:AQ:215:TRP:O	13:AQ:219:VAL:HG23	2.16	0.46
7:S:82:PRO:HG3	7:S:186:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:651:ASP:O	7:Y:652:PHE:C	2.58	0.46
7:V:122:ILE:HD11	7:V:132:SER:HB2	1.98	0.46
7:o:3:PHE:CD1	7:o:20:MET:HG2	2.51	0.46
13:w:323:ASN:HD21	15:x:550:LYS:HA	1.80	0.46
12:AF:147:SER:HB2	12:AF:190:THR:HB	1.98	0.46
14:AS:140:GLU:O	14:AS:144:LYS:HB2	2.16	0.46
7:W:18:LEU:HD13	7:W:191:ILE:HD13	1.97	0.46
12:AF:3:GLU:N	12:AF:3:GLU:OE1	2.49	0.46
16:L:254:GLN:OE1	16:L:255:ARG:N	2.48	0.46
7:K:119:GLU:HB2	7:K:182:ASN:HB2	1.98	0.46
10:AN:2:ARG:HB3	10:AN:131:GLN:HG3	1.97	0.46
7:c:376:PHE:O	7:c:379:LYS:HG2	2.15	0.46
7:c:381:THR:O	7:c:381:THR:CG2	2.62	0.46
7:c:404:ILE:O	7:c:407:LEU:N	2.48	0.46
7:X:563:THR:HG21	7:W:135:GLN:HE21	1.81	0.46
7:V:394:GLU:OE1	7:V:441:ASN:ND2	2.49	0.46
7:V:493:ALA:HB2	7:V:606:LEU:HD12	1.97	0.46
7:W:93:VAL:O	7:W:106:THR:HA	2.15	0.46
13:w:701:ASN:N	13:w:701:ASN:HD22	2.13	0.46
7:c:85:THR:OG1	7:c:88:GLU:OE1	2.29	0.46
7:c:175:ILE:HD12	7:c:221:TYR:CD1	2.51	0.46
13:AK:834:GLU:HG2	13:AK:862:SER:HB3	1.96	0.46
4:p:10:ASP:OD1	4:p:10:ASP:N	2.39	0.46
7:s:550:VAL:O	7:s:554:ILE:HG13	2.16	0.46
10:AE:25:SER:OG	10:AE:51:TYR:OH	2.14	0.46
12:AO:3:GLU:N	12:AO:3:GLU:OE1	2.49	0.46
5:AC:277:ARG:HA	5:AC:277:ARG:NE	2.30	0.46
14:AD:140:GLU:O	14:AD:144:LYS:HB2	2.16	0.46
7:c:137:LYS:NZ	7:c:284:ASP:OD2	2.49	0.46
5:I:317:LYS:HD3	5:I:331:PRO:HG3	1.98	0.46
6:Q:643:THR:HG21	6:Q:645:PHE:CZ	2.51	0.46
9:k:31:VAL:HG12	9:k:32:ASN:HD22	1.80	0.46
9:k:173:SER:HB3	9:k:191:LEU:HB2	1.97	0.46
8:AH:28:ARG:H	11:2:121:GLU:HG2	1.81	0.46
7:b:313:LEU:HD12	7:b:315:GLY:H	1.80	0.46
7:j:469:MET:HE3	7:j:469:MET:HB2	1.83	0.46
11:5:303:ASN:ND2	11:5:337:CYS:HB3	2.31	0.46
7:U:493:ALA:HB2	7:U:606:LEU:HD12	1.98	0.46
7:U:651:ASP:O	7:U:652:PHE:C	2.57	0.46
6:h:551:PHE:HB3	6:h:585:VAL:HG12	1.98	0.46
10:t:145:SER:HB2	10:t:188:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:351:PHE:CZ	7:X:364:ILE:HD11	2.50	0.46
7:s:211:VAL:HG22	7:s:247:VAL:HG13	1.98	0.46
16:C:101:ALA:HA	16:C:436:LYS:HD2	1.98	0.46
11:7:682:VAL:HG22	11:7:706:THR:HG23	1.98	0.46
11:5:987:ASN:HB2	11:5:1046:TRP:CD2	2.51	0.46
13:AQ:531:LEU:N	13:AQ:574:ASN:HD21	2.09	0.46
1:3:76:TRP:O	1:3:80:LEU:HG	2.16	0.45
4:D:145:PHE:CE1	16:C:30:LYS:HG2	2.51	0.45
14:AM:140:GLU:O	14:AM:144:LYS:HB2	2.16	0.45
11:7:429:LEU:HD23	11:7:429:LEU:HA	1.86	0.45
11:5:1050:ASP:OD1	11:5:1050:ASP:N	2.48	0.45
10:AN:31:ASP:OD1	10:AN:35:THR:N	2.40	0.45
11:2:738:THR:HG22	11:2:739:ILE:N	2.31	0.45
10:t:261:PRO:HD3	12:u:406:HIS:ND1	2.31	0.45
7:Z:366:ASP:OD1	7:Z:367:THR:N	2.49	0.45
7:s:596:LEU:CD1	7:r:275:CYS:C	2.88	0.45
7:m:3:PHE:CD1	7:m:20:MET:HG2	2.51	0.45
12:u:3:GLU:N	12:u:3:GLU:OE1	2.49	0.45
4:F:10:ASP:OD1	4:F:10:ASP:N	2.36	0.45
5:8:162:LEU:HD23	11:7:492:LYS:HD2	1.98	0.45
11:7:222:LEU:HD21	11:7:254:LEU:HD11	1.98	0.45
11:2:611:CYS:SG	11:2:612:PRO:HD2	2.56	0.45
9:k:208:ILE:HD13	9:k:271:LEU:HD21	1.97	0.45
7:n:294:ILE:HD13	7:n:422:LEU:HD13	1.97	0.45
7:n:550:VAL:HG21	7:n:579:PHE:HB2	1.99	0.45
7:o:346:GLN:HB2	7:o:665:SER:HB3	1.98	0.45
10:AE:293:MET:HG2	10:AE:367:PHE:HB2	1.98	0.45
12:AO:147:SER:HB2	12:AO:190:THR:HB	1.97	0.45
11:5:402:ARG:NH2	11:5:409:ASP:OD2	2.49	0.45
5:z:566:ILE:HG23	5:z:577:TYR:HB2	1.97	0.45
7:n:154:ASN:HD21	7:n:210:ARG:NH2	2.14	0.45
12:AO:125:LEU:HD23	12:AO:125:LEU:HA	1.85	0.45
12:AO:175:PRO:HB3	10:AN:347:ASN:CG	2.41	0.45
16:C:213:GLY:HA3	16:C:232:PHE:O	2.17	0.45
1:3:66:GLN:OE1	6:i:904:GLU:CD	2.60	0.45
9:k:78:TYR:CE1	4:p:162:GLU:CD	2.95	0.45
11:y:862:ARG:HA	11:y:862:ARG:NE	2.32	0.45
7:n:42:ILE:HD13	7:n:50:ILE:HG21	1.99	0.45
7:j:93:VAL:O	7:j:106:THR:HA	2.15	0.45
10:AN:141:GLY:HA3	18:AN:501:GTP:O3A	2.16	0.45
13:AK:215:TRP:O	13:AK:219:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:735:ILE:O	6:i:739:ILE:HG13	2.17	0.45
3:A:224:TYR:HA	10:AE:400:GLY:O	2.17	0.45
7:T:605:MET:SD	7:T:635:VAL:HG21	2.57	0.45
7:X:617:ILE:O	7:X:648:PHE:HA	2.16	0.45
7:m:493:ALA:HB2	7:m:606:LEU:HD12	1.98	0.45
12:u:147:SER:HB2	12:u:190:THR:HB	1.98	0.45
12:AO:68:VAL:HG11	12:AO:149:PHE:CE2	2.52	0.45
11:AB:746:SER:OG	11:AB:776:ALA:HB2	2.16	0.45
8:AI:93:GLY:O	8:AI:98:GLN:NE2	2.49	0.45
6:H:398:CYS:HB3	6:H:461:PHE:HB2	1.99	0.45
5:I:162:LEU:HD23	11:5:492:LYS:HD2	1.99	0.45
9:k:19:TYR:OH	4:p:117:ASP:OD1	2.23	0.45
7:n:134:LYS:HA	7:n:134:LYS:HD2	1.71	0.45
13:w:436:PHE:O	13:w:492:THR:HG22	2.17	0.45
7:B:617:ILE:O	7:B:648:PHE:HA	2.16	0.45
7:c:255:PRO:HG3	7:c:446:GLU:HB3	1.99	0.45
13:AQ:781:ARG:HG3	13:AQ:809:GLY:C	2.41	0.45
10:t:261:PRO:HD3	12:u:406:HIS:CG	2.52	0.45
7:b:652:PHE:CZ	7:b:656:LEU:HD12	2.51	0.45
7:o:542:SER:O	7:o:546:GLN:HG3	2.17	0.45
7:K:617:ILE:O	7:K:648:PHE:HA	2.16	0.45
13:AK:748:HIS:HB3	13:AK:989:TRP:CZ2	2.52	0.45
13:AQ:436:PHE:O	13:AQ:492:THR:HG22	2.17	0.45
5:I:261:LEU:HD13	11:5:539:PRO:HG2	1.99	0.45
7:S:116:ILE:HD11	7:S:267:LEU:HD22	1.96	0.45
7:T:617:ILE:O	7:T:648:PHE:HA	2.17	0.45
7:n:351:PHE:CZ	7:n:669:ASN:HB2	2.52	0.45
7:f:210:ARG:HG2	7:f:227:PRO:HD3	1.99	0.45
7:f:365:LEU:HD23	7:f:404:ILE:HG12	1.98	0.45
7:d:324:SER:O	7:d:328:LYS:N	2.49	0.45
6:i:401:ALA:O	6:i:405:MET:HG2	2.17	0.45
9:k:465:LEU:HD12	9:k:465:LEU:HA	1.81	0.45
7:T:141:MET:HE2	7:T:147:TRP:CH2	2.52	0.45
7:o:18:LEU:HD12	7:o:112:THR:HB	1.99	0.45
10:AE:201:CYS:SG	10:AE:265:PHE:HB3	2.58	0.45
12:AO:344:VAL:HG22	12:AO:347:CYS:SG	2.57	0.45
7:K:140:TRP:HA	7:K:147:TRP:O	2.17	0.45
8:AI:47:LEU:HG	8:AI:89:ILE:HB	1.99	0.45
7:U:404:ILE:C	7:U:406:ASN:N	2.75	0.45
7:U:617:ILE:O	7:U:648:PHE:HA	2.17	0.45
7:c:469:MET:HE3	7:c:469:MET:HB2	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:356:ASP:OD1	9:l:356:ASP:N	2.50	0.44
7:b:406:ASN:CG	7:b:406:ASN:O	2.60	0.44
7:n:479:ASN:ND2	7:n:643:GLY:HA3	2.32	0.44
10:AE:31:ASP:OD1	10:AE:35:THR:N	2.47	0.44
16:L:219:ARG:O	16:L:223:LEU:N	2.49	0.44
5:8:532:ASN:O	5:8:550:GLU:N	2.47	0.44
8:AI:51:ALA:HA	8:AI:87:ALA:HB2	1.98	0.44
2:6:69:LEU:HD13	2:6:98:VAL:HG22	1.98	0.44
7:o:42:ILE:HD13	7:o:50:ILE:HG21	1.98	0.44
7:j:18:LEU:HD12	7:j:112:THR:HB	1.99	0.44
12:u:68:VAL:HG11	12:u:149:PHE:CE2	2.52	0.44
13:w:249:LYS:HG2	13:w:251:TRP:CZ2	2.53	0.44
13:w:850:LEU:O	13:w:854:LEU:HG	2.17	0.44
2:AA:105:LEU:HD21	8:AJ:129:PHE:HB3	1.99	0.44
10:AN:267:MET:HG2	10:AN:374:ILE:HD13	1.98	0.44
7:c:617:ILE:O	7:c:648:PHE:HA	2.17	0.44
13:AQ:380:MET:HE3	13:AQ:380:MET:HB2	1.91	0.44
3:A:20:TYR:O	3:A:24:GLN:HG2	2.17	0.44
5:E:277:ARG:NE	5:E:277:ARG:HA	2.33	0.44
7:Z:316:PHE:HB2	7:Z:651:ASP:OD2	2.18	0.44
13:w:332:LYS:HA	13:w:335:VAL:HG12	1.99	0.44
7:K:279:ILE:HG23	7:K:279:ILE:O	2.17	0.44
7:c:485:GLN:HE21	7:c:485:GLN:HA	1.82	0.44
13:AQ:850:LEU:O	13:AQ:854:LEU:HG	2.17	0.44
7:T:615:LEU:HD11	7:T:644:LEU:HD13	1.98	0.44
7:d:122:ILE:HG13	7:d:123:TYR:CD2	2.51	0.44
10:AE:267:MET:HG2	10:AE:374:ILE:HD13	2.00	0.44
12:AF:68:VAL:HG11	12:AF:149:PHE:CE2	2.52	0.44
15:AR:310:CYS:HB3	15:AR:318:CYS:HB3	1.99	0.44
15:AR:420:ALA:CB	7:U:312:GLN:HE22	2.22	0.44
2:AA:105:LEU:HD12	2:AA:105:LEU:C	2.42	0.44
10:AN:3:GLU:OE1	10:AN:3:GLU:N	2.51	0.44
10:AN:268:PRO:HG2	10:AN:300:MET:HB2	1.99	0.44
7:c:3:PHE:CE2	7:c:20:MET:HG2	2.53	0.44
7:c:343:LYS:CD	7:c:663:CYS:SG	3.05	0.44
7:c:677:TRP:O	7:c:680:MET:HG2	2.17	0.44
13:AK:436:PHE:O	13:AK:492:THR:HG22	2.17	0.44
1:3:72:ASN:OD1	1:3:73:PHE:N	2.50	0.44
6:H:907:CYS:CA	8:e:149:ALA:CB	2.85	0.44
7:b:53:SER:O	7:b:54:SER:OG	2.20	0.44
7:V:617:ILE:O	7:V:648:PHE:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:433:PRO:HD2	7:K:200:HIS:CE1	2.50	0.44
7:j:463:TRP:H	7:j:463:TRP:CD1	2.35	0.44
7:j:493:ALA:HB2	7:j:606:LEU:HD12	1.99	0.44
12:u:336:LYS:HE2	13:w:57:VAL:HG22	1.99	0.44
10:AE:268:PRO:HG2	10:AE:300:MET:HB2	2.00	0.44
12:AF:145:THR:HB	18:AF:501:GTP:O2B	2.17	0.44
16:C:369:ASP:OD1	16:C:373:LEU:N	2.43	0.44
5:8:463:LEU:HD13	5:8:500:ARG:HD3	1.99	0.44
11:5:885:LYS:HG2	11:5:915:ASP:OD2	2.17	0.44
13:AK:924:LYS:H	13:AK:952:ASP:CG	2.26	0.44
13:AQ:97:LEU:HD11	13:AQ:209:ALA:HB2	2.00	0.44
6:i:903:ASN:ND2	6:i:931:MET:SD	2.91	0.44
1:9:73:PHE:HE1	8:AT:108:MET:HE1	1.83	0.44
9:k:82:THR:HG21	9:k:468:HIS:NE2	2.31	0.44
4:p:96:ASP:OD1	4:p:99:THR:OG1	2.24	0.44
7:b:313:LEU:HD12	7:b:314:GLN:N	2.32	0.44
7:m:230:PRO:HG2	7:m:231:VAL:HG23	1.99	0.44
13:w:924:LYS:H	13:w:952:ASP:CG	2.26	0.44
15:AR:6:ARG:HH12	13:AQ:185:ILE:HG22	1.83	0.44
7:B:116:ILE:HD13	7:B:267:LEU:HD13	1.99	0.44
10:AN:134:GLN:HA	10:AN:165:ASN:O	2.18	0.44
13:AK:249:LYS:HG2	13:AK:251:TRP:CZ2	2.53	0.44
13:AQ:249:LYS:HG2	13:AQ:251:TRP:CZ2	2.53	0.44
1:3:44:LEU:HD23	1:3:44:LEU:HA	1.82	0.44
2:4:51:LEU:HD11	2:4:84:ALA:CB	2.47	0.44
4:D:159:TRP:HE3	16:C:23:LEU:HD12	1.83	0.44
7:T:205:GLU:O	7:T:209:THR:HG22	2.17	0.44
5:z:162:LEU:HD23	11:y:492:LYS:HD2	1.99	0.44
5:z:274:GLN:OE1	5:z:274:GLN:N	2.48	0.44
7:W:351:PHE:CZ	7:W:364:ILE:HD11	2.53	0.44
7:n:127:GLN:NE2	7:d:92:LEU:CD1	2.79	0.44
7:m:116:ILE:HD13	7:m:267:LEU:HD13	1.99	0.44
12:u:344:VAL:HG22	12:u:347:CYS:SG	2.57	0.44
13:w:97:LEU:HD11	13:w:209:ALA:HB2	2.00	0.44
13:w:432:LYS:HD2	13:w:488:CYS:SG	2.58	0.44
13:w:815:ASP:HA	13:w:818:VAL:HB	1.99	0.44
12:AF:344:VAL:HG22	12:AF:347:CYS:SG	2.57	0.44
14:AM:102:VAL:O	14:AM:106:ILE:HG13	2.18	0.44
7:U:18:LEU:HD12	7:U:112:THR:HB	2.00	0.44
7:c:336:GLU:H	7:c:336:GLU:CD	2.25	0.44
7:c:478:THR:HG21	7:c:489:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AK:58:ILE:O	13:AK:58:ILE:HG13	2.17	0.44
13:AQ:432:LYS:HD2	13:AQ:488:CYS:SG	2.58	0.44
13:AQ:815:ASP:HA	13:AQ:818:VAL:HB	1.99	0.44
2:4:115:GLU:HA	6:i:380:PRO:HB3	1.99	0.44
7:S:124:ARG:HD3	7:S:678:TRP:CG	2.53	0.44
9:l:127:LEU:CD2	9:l:130:MET:HA	2.33	0.44
7:X:364:ILE:HD12	7:X:382:LEU:CD2	2.47	0.44
7:V:602:PHE:O	7:V:603:PRO:C	2.60	0.44
7:d:621:PHE:CE2	7:d:652:PHE:HB2	2.53	0.44
7:j:459:LEU:HD11	7:j:561:LEU:HD21	2.00	0.44
13:w:705:LYS:HE2	13:w:705:LYS:HB3	1.80	0.44
10:AE:67:ASP:O	10:AE:92:PHE:HA	2.17	0.44
15:AL:310:CYS:HB3	15:AL:318:CYS:HB3	1.99	0.44
16:L:63:LEU:O	16:L:63:LEU:CD2	2.65	0.44
13:AK:432:LYS:HD2	13:AK:488:CYS:SG	2.58	0.44
13:AK:815:ASP:HA	13:AK:818:VAL:HB	1.99	0.44
13:AQ:748:HIS:HB3	13:AQ:989:TRP:CZ2	2.52	0.44
2:4:115:GLU:HA	6:i:380:PRO:CB	2.48	0.44
9:k:25:LEU:HD23	9:k:25:LEU:HA	1.86	0.44
9:k:403:ILE:HG23	9:k:433:ARG:HG3	2.00	0.44
7:Y:406:ASN:O	7:Y:469:MET:HE2	2.18	0.44
7:V:20:MET:HE1	7:V:116:ILE:H	1.83	0.44
7:f:369:ARG:HE	7:f:403:SER:HG	1.65	0.44
7:s:463:TRP:CD1	7:s:463:TRP:H	2.34	0.44
7:m:484:ASP:OD1	7:m:484:ASP:N	2.50	0.44
7:d:366:ASP:OD2	7:d:388:TYR:OH	2.23	0.44
7:K:514:THR:HG22	7:K:533:THR:HG22	2.00	0.44
7:K:657:ALA:HB1	7:K:661:ASP:HB2	1.99	0.44
15:x:310:CYS:HB3	15:x:318:CYS:HB3	1.99	0.44
13:AK:850:LEU:O	13:AK:854:LEU:HG	2.17	0.44
13:AQ:332:LYS:HA	13:AQ:335:VAL:HG12	1.99	0.44
6:i:80:LYS:O	6:i:83:THR:OG1	2.32	0.44
7:X:602:PHE:O	7:X:603:PRO:C	2.61	0.43
7:Z:617:ILE:O	7:Z:648:PHE:HA	2.18	0.43
7:n:343:LYS:HD3	7:n:663:CYS:SG	2.58	0.43
7:n:550:VAL:HG11	7:n:579:PHE:CD1	2.53	0.43
7:m:442:LYS:NZ	7:j:204:GLU:OE2	2.49	0.43
7:m:606:LEU:HD23	7:m:606:LEU:HA	1.77	0.43
13:w:748:HIS:HB3	13:w:989:TRP:CZ2	2.52	0.43
11:5:610:LEU:HD13	11:5:610:LEU:HA	1.81	0.43
11:2:738:THR:HG22	11:2:739:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:103:TRP:HB2	11:7:781:MET:HE3	2.00	0.43
7:T:550:VAL:HG11	7:T:579:PHE:CD1	2.53	0.43
7:T:651:ASP:O	7:T:652:PHE:C	2.61	0.43
7:f:8:SER:HB3	7:f:31:LYS:HD3	1.99	0.43
13:w:990:TRP:CG	13:w:991:ASN:N	2.86	0.43
15:AL:319:ARG:H	15:AL:319:ARG:HG2	1.64	0.43
11:AB:673:LYS:HG3	11:AB:700:TYR:CD1	2.53	0.43
16:C:42:TRP:CD1	16:C:67:LYS:HB2	2.53	0.43
7:c:154:ASN:ND2	7:c:248:GLU:OE1	2.38	0.43
7:c:487:ASP:OD1	7:c:487:ASP:N	2.46	0.43
13:AK:691:PHE:CD1	13:AK:720:ARG:HB2	2.53	0.43
1:3:73:PHE:HE1	8:g:108:MET:HE1	1.82	0.43
1:9:73:PHE:CE1	8:AT:108:MET:HE1	2.52	0.43
6:H:330:LYS:HB2	6:H:581:SER:HB2	2.01	0.43
7:m:294:ILE:HD13	7:m:422:LEU:HD13	2.00	0.43
7:d:365:LEU:HD13	7:d:389:LEU:HD23	2.00	0.43
7:j:560:LEU:HD12	7:j:560:LEU:HA	1.81	0.43
5:I:350:LEU:O	5:I:358:LEU:HD12	2.18	0.43
7:m:172:PRO:HD3	7:m:212:TYR:CZ	2.53	0.43
7:m:550:VAL:HG21	7:m:579:PHE:HB2	1.99	0.43
7:j:273:ASP:OD1	7:j:274:GLU:N	2.51	0.43
11:0:301:LEU:HD12	11:0:304:ILE:HD11	2.00	0.43
16:C:20:TYR:O	16:C:24:GLN:HG2	2.19	0.43
5:8:286:LYS:HE3	5:8:575:SER:HB3	2.00	0.43
7:B:550:VAL:HG11	7:B:579:PHE:CD1	2.53	0.43
14:AD:102:VAL:O	14:AD:106:ILE:HG13	2.18	0.43
7:c:394:GLU:OE1	7:c:441:ASN:ND2	2.48	0.43
13:AQ:705:LYS:HE2	13:AQ:705:LYS:HB3	1.80	0.43
6:i:812:LEU:HB3	6:i:839:CYS:HB3	2.00	0.43
7:S:311:LEU:HA	11:AB:715:LEU:HD22	1.99	0.43
7:s:273:ASP:OD1	7:s:274:GLU:N	2.52	0.43
7:s:408:MET:HG3	7:s:469:MET:HE3	1.99	0.43
7:d:606:LEU:HD23	7:d:606:LEU:HA	1.86	0.43
7:j:335:TYR:OH	14:AM:80:SER:CB	2.66	0.43
7:j:335:TYR:OH	14:AM:80:SER:HB3	2.18	0.43
7:j:550:VAL:HG11	7:j:579:PHE:CD1	2.53	0.43
10:AE:346:PRO:HG3	12:AF:397:LEU:HD12	2.01	0.43
11:7:731:ARG:HE	11:7:731:ARG:HB3	1.44	0.43
11:7:875:THR:HG23	11:7:904:VAL:HB	2.00	0.43
11:5:856:TYR:CE1	11:5:879:VAL:HG22	2.54	0.43
13:AK:610:ILE:HG23	13:AK:636:ASP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:t:165:ASN:OD1	10:t:166:THR:N	2.51	0.43
7:Y:127:GLN:OE1	7:V:92:LEU:HD11	2.18	0.43
7:n:677:TRP:O	7:n:680:MET:HG2	2.19	0.43
7:m:486:LYS:HD3	7:m:488:PHE:CE2	2.53	0.43
7:m:657:ALA:CB	7:m:663:CYS:SG	3.07	0.43
5:8:438:LYS:HD2	5:8:476:HIS:CE1	2.54	0.43
7:B:469:MET:HG3	7:B:472:PHE:HE2	1.84	0.43
13:AK:332:LYS:HA	13:AK:335:VAL:HG12	1.99	0.43
13:AQ:924:LYS:H	13:AQ:952:ASP:CG	2.26	0.43
9:k:57:ASP:OD1	9:k:57:ASP:N	2.49	0.43
10:t:12:CYS:HB2	18:t:501:GTP:C8	2.53	0.43
11:y:1006:GLN:HG3	11:y:1033:VAL:HG22	2.00	0.43
7:Y:127:GLN:CG	7:V:92:LEU:HD11	2.38	0.43
7:f:432:TYR:HE1	7:K:280:PRO:HD3	1.82	0.43
7:s:130:MET:HE2	7:s:134:LYS:HE2	2.01	0.43
10:AE:19:LYS:HA	10:AE:19:LYS:HD3	1.74	0.43
11:7:303:ASN:ND2	11:7:337:CYS:HB3	2.34	0.43
11:7:875:THR:HG22	11:7:876:MET:HG3	2.00	0.43
6:h:427:ILE:N	6:h:428:PRO:CD	2.82	0.43
3:A:428:LEU:HD12	3:A:429:PRO:HD2	2.00	0.43
6:H:302:GLU:HA	6:H:305:MET:HE3	2.01	0.43
7:S:122:ILE:C	7:S:147:TRP:HB2	2.44	0.43
7:S:381:THR:O	7:S:381:THR:HG22	2.18	0.43
7:b:351:PHE:CZ	7:b:364:ILE:HD11	2.53	0.43
7:s:313:LEU:HD12	7:s:315:GLY:H	1.83	0.43
7:o:255:PRO:HG3	7:o:446:GLU:HB3	2.01	0.43
13:w:439:LEU:HD11	13:w:463:LEU:HD12	2.01	0.43
13:w:691:PHE:CD1	13:w:720:ARG:HB2	2.53	0.43
15:AR:8:MET:HG3	15:AR:72:LEU:HD13	2.01	0.43
11:0:895:THR:HG22	11:0:895:THR:O	2.17	0.43
16:C:43:ARG:HA	16:C:66:TRP:CE3	2.54	0.43
13:AQ:670:ASP:O	13:AQ:675:ARG:NH1	2.52	0.43
2:4:92:PRO:N	2:4:93:PRO:CD	2.82	0.43
6:H:7:ASP:OD1	6:H:7:ASP:N	2.52	0.43
9:k:326:ILE:HD12	9:k:331:ILE:HD12	2.01	0.43
7:Y:615:LEU:HD11	7:Y:644:LEU:HD13	2.00	0.43
7:b:478:THR:OG1	7:b:487:ASP:O	2.29	0.43
7:n:307:LEU:HD21	7:n:317:VAL:HG13	2.01	0.43
7:f:178:LEU:HD22	7:f:248:GLU:HB3	1.99	0.43
7:s:350:ALA:HA	7:s:667:ILE:HD11	2.01	0.43
7:m:20:MET:HB2	7:m:23:MET:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:w:541:ASP:OD1	13:w:541:ASP:N	2.52	0.43
2:AA:61:HIS:CD2	8:AJ:132:ILE:HD13	2.53	0.43
11:7:708:MET:HE3	11:7:708:MET:HB3	1.87	0.43
10:AN:67:ASP:O	10:AN:92:PHE:HA	2.19	0.43
11:2:1016:GLY:HA2	11:2:1043:ASP:O	2.19	0.43
7:U:133:ASP:OD1	7:U:134:LYS:N	2.51	0.43
7:c:122:ILE:HD11	7:c:286:VAL:HG23	2.01	0.43
13:AQ:405:ASP:OD1	13:AQ:405:ASP:N	2.52	0.43
13:AQ:610:ILE:HG23	13:AQ:636:ASP:HB3	2.01	0.43
13:AQ:691:PHE:CD1	13:AQ:720:ARG:HB2	2.53	0.43
9:k:155:LYS:NZ	9:k:195:CYS:O	2.44	0.43
7:d:279:ILE:HD13	7:c:552:LYS:HD2	2.01	0.43
12:AO:98:ASP:HB2	18:AO:501:GTP:O3G	2.19	0.43
11:AB:895:THR:O	11:AB:895:THR:HG22	2.17	0.43
8:AJ:57:VAL:HG13	8:AJ:108:MET:HE2	2.01	0.43
16:C:46:CYS:SG	16:C:70:PHE:HB2	2.58	0.43
7:K:463:TRP:H	7:K:463:TRP:CD1	2.37	0.43
13:AQ:198:LYS:NZ	13:AQ:204:SER:O	2.52	0.43
6:i:22:PHE:CE2	6:i:26:LYS:HE3	2.54	0.43
2:6:50:LEU:HD22	8:AI:133:ARG:HH22	1.84	0.42
6:H:22:PHE:CE2	6:H:26:LYS:HE3	2.54	0.42
7:T:273:ASP:OD1	7:T:274:GLU:N	2.52	0.42
11:y:865:ASN:HD21	11:2:865:ASN:ND2	2.00	0.42
7:n:343:LYS:HA	7:n:665:SER:OG	2.19	0.42
7:n:343:LYS:HD2	7:n:665:SER:OG	2.19	0.42
7:m:489:ARG:HD3	7:m:573:ILE:HD11	2.01	0.42
13:w:405:ASP:OD1	13:w:405:ASP:N	2.52	0.42
10:AE:344:TRP:CD2	12:AF:401:LYS:HG3	2.54	0.42
12:AF:265:ILE:H	12:AF:265:ILE:HG12	1.66	0.42
12:AO:336:LYS:HE2	13:AQ:57:VAL:CG2	2.47	0.42
7:B:141:MET:CG	7:B:147:TRP:CH2	3.02	0.42
10:AN:403:MET:HE2	10:AN:403:MET:HB3	1.93	0.42
13:AK:97:LEU:HD11	13:AK:209:ALA:HB2	2.00	0.42
13:AK:990:TRP:CG	13:AK:991:ASN:N	2.86	0.42
6:i:551:PHE:HB3	6:i:585:VAL:HG12	2.00	0.42
6:Q:603:THR:OG1	6:Q:643:THR:HG23	2.19	0.42
7:W:311:LEU:HD22	7:W:311:LEU:H	1.84	0.42
7:s:280:PRO:HB3	7:r:432:TYR:CE1	2.54	0.42
7:j:130:MET:HB3	7:r:43:ARG:HH11	1.85	0.42
15:AR:523:GLU:OE1	7:U:589:SER:CB	2.67	0.42
11:AB:849:CYS:O	11:AB:851:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:0:751:SER:HA	16:L:98:GLU:HB2	2.00	0.42
15:x:309:PHE:CE2	15:x:320:LYS:HD2	2.55	0.42
7:S:431:PHE:CE2	7:T:280:PRO:HB2	2.53	0.42
7:V:79:MET:HE2	7:V:113:GLY:HA3	2.01	0.42
7:d:116:ILE:HD12	7:d:267:LEU:HD22	2.00	0.42
15:AL:309:PHE:CE2	15:AL:320:LYS:HD2	2.55	0.42
7:c:42:ILE:HA	7:c:92:LEU:O	2.19	0.42
6:i:19:LYS:O	6:i:23:MET:HG2	2.19	0.42
6:i:821:CYS:HA	6:i:824:LEU:HB2	2.01	0.42
5:I:491:GLN:HG2	5:I:508:THR:HB	2.01	0.42
7:T:602:PHE:O	7:T:603:PRO:C	2.61	0.42
7:b:436:GLU:OE1	7:b:593:SER:OG	2.36	0.42
7:V:406:ASN:O	7:V:406:ASN:CG	2.62	0.42
7:n:79:MET:HE3	7:n:79:MET:HB3	1.89	0.42
7:s:42:ILE:HD11	7:s:50:ILE:HD13	2.01	0.42
13:w:312:PRO:HD2	13:w:319:VAL:HG21	2.02	0.42
13:w:610:ILE:HG23	13:w:636:ASP:HB3	2.01	0.42
14:AS:102:VAL:O	14:AS:106:ILE:HG13	2.18	0.42
7:K:336:GLU:H	7:K:336:GLU:CD	2.27	0.42
11:2:567:GLU:HA	11:2:593:ALA:O	2.20	0.42
7:c:3:PHE:CD1	7:c:281:LEU:HD13	2.54	0.42
13:AQ:439:LEU:HD11	13:AQ:463:LEU:HD12	2.01	0.42
13:AQ:990:TRP:CG	13:AQ:991:ASN:N	2.86	0.42
6:i:681:PHE:HZ	6:i:703:GLU:HB3	1.84	0.42
4:D:159:TRP:CE3	16:C:23:LEU:HD12	2.54	0.42
6:Q:813:LYS:HD3	6:Q:813:LYS:HA	1.89	0.42
11:y:595:ARG:NH2	11:y:597:ASP:OD2	2.52	0.42
7:n:118:LEU:O	7:n:137:LYS:HE3	2.20	0.42
7:o:677:TRP:O	7:o:680:MET:HG2	2.19	0.42
7:c:407:LEU:CD1	7:c:425:VAL:HG13	2.49	0.42
13:AQ:312:PRO:HD2	13:AQ:319:VAL:HG21	2.02	0.42
2:6:54:MET:HA	8:AI:133:ARG:HD2	2.01	0.42
7:n:463:TRP:CD1	7:n:463:TRP:H	2.37	0.42
7:n:499:PHE:CZ	7:n:544:ARG:HG3	2.55	0.42
7:n:550:VAL:O	7:n:554:ILE:HG13	2.19	0.42
7:f:376:PHE:O	7:f:379:LYS:HG2	2.20	0.42
7:o:350:ALA:HA	7:o:667:ILE:HD11	2.00	0.42
7:j:617:ILE:O	7:j:648:PHE:HA	2.19	0.42
11:5:429:LEU:HD23	11:5:429:LEU:HA	1.85	0.42
7:K:212:TYR:HB3	7:K:221:TYR:HB3	2.02	0.42
3:A:424:TYR:CG	3:A:458:MET:HE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:906:LEU:HD22	6:H:919:LEU:HD21	2.02	0.42
7:X:651:ASP:O	7:X:652:PHE:C	2.63	0.42
7:V:66:TRP:CZ3	7:V:96:PHE:CE2	3.07	0.42
7:n:21:VAL:HG21	7:n:115:GLU:HB2	2.02	0.42
7:o:29:ILE:HD12	7:o:73:THR:HG22	2.01	0.42
7:j:514:THR:HG22	7:j:533:THR:HG22	2.01	0.42
15:AR:309:PHE:CE2	15:AR:320:LYS:HD2	2.55	0.42
2:AA:105:LEU:HD13	8:AJ:130:LEU:CD2	2.50	0.42
11:AB:303:ASN:ND2	11:AB:337:CYS:HB3	2.34	0.42
8:AJ:77:THR:OG1	8:AJ:90:THR:HB	2.20	0.42
7:U:122:ILE:HD13	7:U:123:TYR:CD2	2.55	0.42
6:h:647:GLU:HB3	6:h:648:PRO:HD3	2.01	0.42
11:y:239:ASP:OD1	11:y:240:TRP:N	2.53	0.42
7:Z:406:ASN:O	7:Z:406:ASN:CG	2.63	0.42
7:W:297:PRO:HD3	7:W:673:PHE:CZ	2.55	0.42
7:m:479:ASN:ND2	7:m:643:GLY:HA3	2.34	0.42
7:d:42:ILE:HG13	7:d:93:VAL:HG22	2.02	0.42
15:AR:346:HIS:HB2	15:AR:349:CYS:SG	2.60	0.42
7:r:120:ALA:CB	7:r:286:VAL:HG21	2.49	0.42
16:L:263:TYR:HB2	16:L:329:ILE:HD11	2.02	0.42
11:7:957:ARG:HG3	11:7:985:SER:HB3	2.02	0.42
11:7:1010:SER:O	11:7:1037:LYS:NZ	2.52	0.42
7:K:178:LEU:HD22	7:K:248:GLU:HB3	2.01	0.42
6:i:336:CYS:O	6:i:342:CYS:HB2	2.20	0.42
8:e:133:ARG:NH1	11:y:318:ILE:HD12	2.31	0.42
11:y:895:THR:O	11:y:895:THR:HG22	2.20	0.42
7:X:369:ARG:NE	7:X:403:SER:OG	2.43	0.42
7:f:345:LEU:HB3	7:f:665:SER:HB2	2.01	0.42
7:f:529:ARG:HE	7:f:656:LEU:HD13	1.84	0.42
7:o:301:MET:HE3	7:o:301:MET:HB2	1.90	0.42
7:d:452:GLN:H	7:d:452:GLN:HG3	1.65	0.42
10:AE:255:VAL:O	12:AF:404:PHE:CE1	2.73	0.42
15:AL:346:HIS:HB2	15:AL:349:CYS:SG	2.60	0.42
6:h:643:THR:HG21	6:h:645:PHE:CZ	2.55	0.42
5:E:501:ASP:OD1	5:E:502:GLN:N	2.52	0.42
6:H:605:ASN:OD1	6:H:644:ASN:ND2	2.51	0.42
11:y:1016:GLY:HA2	11:y:1043:ASP:O	2.20	0.42
11:y:1058:LYS:O	11:y:1059:ASN:C	2.63	0.42
13:w:730:LYS:H	13:w:730:LYS:HG2	1.68	0.42
10:AE:139:LEU:O	10:AE:145:SER:HB3	2.20	0.42
2:AA:69:LEU:CD2	8:AJ:122:LYS:HG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:131:SER:HB3	16:C:143:VAL:HG23	2.02	0.42
7:c:463:TRP:CD1	7:c:463:TRP:H	2.38	0.42
13:AK:705:LYS:HB3	13:AK:705:LYS:HE2	1.80	0.42
13:AQ:31:ARG:O	13:AQ:34:ILE:HG22	2.20	0.42
13:AQ:173:GLU:CD	13:AQ:173:GLU:H	2.28	0.42
3:A:80:LYS:NZ	3:A:439:SER:OG	2.53	0.41
4:D:64:HIS:CE1	10:AE:173:PRO:HB2	2.52	0.41
7:W:602:PHE:O	7:W:603:PRO:C	2.63	0.41
7:o:603:PRO:HD3	7:o:656:LEU:HD11	2.01	0.41
7:j:342:SER:OG	7:j:660:GLY:O	2.36	0.41
7:j:421:PRO:HD2	7:j:680:MET:HE3	2.01	0.41
15:AL:8:MET:HG3	15:AL:72:LEU:HD13	2.01	0.41
7:r:119:GLU:O	7:r:181:MET:HG3	2.20	0.41
5:8:274:GLN:OE1	5:8:274:GLN:N	2.52	0.41
7:K:188:PRO:HB2	7:K:191:ILE:HG22	2.01	0.41
14:AD:80:SER:HB3	7:c:335:TYR:CZ	2.55	0.41
7:U:364:ILE:HD12	7:U:382:LEU:HD21	2.01	0.41
15:x:346:HIS:HB2	15:x:349:CYS:SG	2.60	0.41
8:g:133:ARG:HD2	11:7:318:ILE:HD12	2.01	0.41
11:y:738:THR:HG22	11:y:739:ILE:N	2.35	0.41
7:V:402:ASP:OD1	7:V:441:ASN:N	2.34	0.41
7:n:7:LEU:HD12	7:n:25:ILE:HG21	2.02	0.41
7:j:79:MET:HE2	7:j:113:GLY:HA3	2.01	0.41
13:w:173:GLU:CD	13:w:173:GLU:H	2.28	0.41
12:AF:119:LEU:HD11	12:AF:156:ARG:HB3	2.02	0.41
5:AC:169:LEU:HD21	11:AB:519:VAL:HG22	2.02	0.41
8:AJ:74:ALA:HB1	8:AJ:92:PHE:O	2.20	0.41
16:C:106:ILE:HD13	16:C:106:ILE:HA	1.93	0.41
8:AI:47:LEU:HD22	8:AI:102:LYS:HG3	2.02	0.41
7:c:11:LEU:HD22	7:c:105:ALA:HB1	2.02	0.41
7:c:621:PHE:CE2	7:c:652:PHE:HB2	2.55	0.41
15:x:8:MET:HG3	15:x:72:LEU:HD13	2.01	0.41
13:AK:405:ASP:OD1	13:AK:405:ASP:N	2.52	0.41
13:AK:778:LEU:HG	13:AK:780:LEU:HG	2.03	0.41
3:A:310:ILE:HG23	3:A:339:LEU:O	2.19	0.41
9:k:19:TYR:CE1	4:p:121:LYS:HE2	2.55	0.41
7:f:629:CYS:SG	7:f:632:GLU:HG3	2.60	0.41
7:s:527:ASN:HD22	7:s:652:PHE:HE2	1.68	0.41
7:o:36:LYS:O	7:o:98:PRO:HD3	2.20	0.41
13:w:31:ARG:O	13:w:34:ILE:HG22	2.20	0.41
13:w:879:CYS:SG	13:w:910:ILE:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:7:303:ASN:CG	11:7:337:CYS:HB3	2.46	0.41
11:7:610:LEU:HD22	11:7:610:LEU:H	1.84	0.41
5:I:278:PHE:CE2	5:I:523:LYS:HE2	2.55	0.41
7:X:406:ASN:O	7:X:406:ASN:CG	2.62	0.41
7:W:406:ASN:CG	7:W:406:ASN:O	2.63	0.41
7:d:469:MET:HE3	7:d:469:MET:HB2	1.88	0.41
7:j:373:LEU:HD23	7:j:373:LEU:HA	1.85	0.41
12:AO:119:LEU:HD11	12:AO:156:ARG:HB3	2.02	0.41
16:C:188:LEU:HD11	16:C:218:PHE:CZ	2.56	0.41
14:AD:86:LEU:HD12	14:AD:86:LEU:HA	1.90	0.41
11:2:402:ARG:NH2	11:2:409:ASP:OD2	2.53	0.41
13:AK:439:LEU:HD11	13:AK:463:LEU:HD12	2.01	0.41
13:AK:879:CYS:SG	13:AK:910:ILE:HD11	2.60	0.41
3:A:8:LEU:HB3	3:A:9:PRO:HD3	2.03	0.41
6:H:884:PRO:HB2	11:y:709:LYS:HG3	2.02	0.41
9:k:263:LYS:HG2	9:k:283:VAL:HG22	2.02	0.41
10:t:430:ALA:HB1	12:u:397:LEU:CD2	2.50	0.41
7:Y:602:PHE:O	7:Y:603:PRO:C	2.62	0.41
7:X:18:LEU:HD12	7:X:112:THR:HB	2.03	0.41
7:X:127:GLN:CD	7:Z:92:LEU:HD11	2.46	0.41
7:f:514:THR:HG22	7:f:533:THR:HG22	2.02	0.41
5:AC:274:GLN:OE1	5:AC:274:GLN:N	2.48	0.41
7:r:602:PHE:O	7:r:603:PRO:C	2.64	0.41
7:B:124:ARG:NH2	7:B:147:TRP:O	2.53	0.41
8:AI:61:ASP:O	8:AI:62:GLN:HG2	2.20	0.41
11:2:303:ASN:ND2	11:2:337:CYS:HB3	2.35	0.41
7:U:343:LYS:HD3	7:U:663:CYS:SG	2.60	0.41
6:H:341:LEU:HD11	6:H:450:HIS:CE1	2.56	0.41
6:H:666:LYS:HE3	6:H:691:TYR:CE1	2.56	0.41
6:H:735:ILE:O	6:H:739:ILE:HG13	2.21	0.41
6:Q:903:ASN:ND2	6:Q:931:MET:SD	2.94	0.41
7:b:617:ILE:O	7:b:648:PHE:HA	2.21	0.41
7:W:316:PHE:N	7:W:651:ASP:OD2	2.41	0.41
7:d:130:MET:H	7:d:130:MET:HG2	1.61	0.41
12:AO:2:ARG:HB3	12:AO:133:GLN:CG	2.50	0.41
12:AO:352:LYS:HG2	13:AQ:54:LEU:HD23	2.02	0.41
12:AO:404:PHE:CE1	10:AN:259:PRO:HA	2.56	0.41
2:AA:105:LEU:HD23	8:AJ:126:VAL:HG22	2.03	0.41
16:C:367:LEU:HD22	16:C:376:GLN:OE1	2.20	0.41
4:F:27:ILE:HA	4:F:30:MET:HE3	2.02	0.41
11:7:540:MET:HE3	11:7:571:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5:750:ILE:H	11:5:750:ILE:HG12	1.74	0.41
11:2:895:THR:O	11:2:895:THR:HG22	2.20	0.41
1:1:70:LEU:N	1:1:70:LEU:HD22	2.36	0.41
3:A:130:ILE:HG23	3:A:151:ILE:HD13	2.03	0.41
10:t:3:GLU:OE1	10:t:3:GLU:N	2.53	0.41
7:T:316:PHE:CB	7:T:651:ASP:OD2	2.69	0.41
11:y:708:MET:HE3	11:y:708:MET:HB3	1.89	0.41
7:Z:208:LYS:HA	7:Z:250:THR:OG1	2.20	0.41
7:n:293:TYR:HE1	7:n:295:PHE:CZ	2.39	0.41
7:n:469:MET:HE3	7:n:469:MET:HB2	1.96	0.41
7:m:287:MET:HE2	7:m:287:MET:HB2	1.95	0.41
13:w:123:GLU:HB2	13:w:375:TYR:OH	2.20	0.41
15:AL:706:LYS:HD3	15:AL:706:LYS:HA	1.88	0.41
12:AO:265:ILE:H	12:AO:265:ILE:HG12	1.66	0.41
14:AS:17:PRO:HA	14:AS:18:PRO:HD3	1.95	0.41
7:K:144:MET:HE2	7:K:144:MET:HB3	1.63	0.41
13:AK:312:PRO:HD2	13:AK:319:VAL:HG21	2.02	0.41
13:AQ:122:LYS:HE3	13:AQ:166:GLU:CD	2.46	0.41
6:i:535:LEU:HD12	6:i:570:MET:HE1	2.03	0.41
1:3:54:MET:HE1	6:i:904:GLU:HG2	1.95	0.41
1:9:70:LEU:H	1:9:70:LEU:HD22	1.86	0.41
6:H:330:LYS:HE3	6:H:580:TYR:HD2	1.86	0.41
6:H:349:LEU:HD23	6:H:362:LEU:HD23	2.01	0.41
9:k:124:VAL:HG23	9:k:138:ILE:HD11	2.03	0.41
11:y:673:LYS:HG3	11:y:700:TYR:CD1	2.55	0.41
7:X:605:MET:SD	7:X:635:VAL:HG21	2.61	0.41
7:f:602:PHE:O	7:f:603:PRO:C	2.64	0.41
7:j:43:ARG:CZ	7:r:123:TYR:CD2	3.04	0.41
7:j:214:SER:HB2	7:j:221:TYR:CD2	2.56	0.41
13:w:351:ARG:HH12	15:x:64:ARG:HD3	1.86	0.41
13:w:778:LEU:HG	13:w:780:LEU:HG	2.03	0.41
12:AO:221:ARG:NH1	10:AN:327:ASP:OD2	2.53	0.41
11:0:775:ASN:ND2	16:L:168:MET:O	2.53	0.41
5:8:303:SER:HB3	5:8:561:GLU:CD	2.45	0.41
11:7:463:GLU:O	11:7:466:GLN:HG2	2.21	0.41
7:B:657:ALA:HB1	7:B:661:ASP:HB2	2.02	0.41
7:K:181:MET:O	7:K:245:PHE:N	2.43	0.41
13:AK:122:LYS:HE3	13:AK:166:GLU:CD	2.46	0.41
13:AK:123:GLU:HB2	13:AK:375:TYR:OH	2.20	0.41
13:AQ:879:CYS:SG	13:AQ:910:ILE:HD11	2.60	0.41
3:A:331:GLU:OE1	3:A:331:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:196:GLN:HG2	9:k:197:THR:HG23	2.02	0.41
11:y:599:ARG:HD2	11:y:599:ARG:N	2.36	0.41
7:Y:431:PHE:CE2	7:Z:283:LYS:HB2	2.55	0.41
7:b:364:ILE:HD12	7:b:382:LEU:CD2	2.48	0.41
7:X:369:ARG:HE	7:X:403:SER:HG	1.65	0.41
7:V:431:PHE:CE2	7:U:283:LYS:HB2	2.56	0.41
7:W:273:ASP:OD1	7:W:274:GLU:N	2.53	0.41
7:n:609:ILE:HG23	7:n:668:ILE:HD11	2.03	0.41
7:m:562:LYS:HE2	7:m:562:LYS:HB3	1.78	0.41
7:d:122:ILE:HD11	7:d:132:SER:HB2	2.02	0.41
7:d:296:MET:HE3	7:d:296:MET:HB2	1.97	0.41
7:j:602:PHE:O	7:j:603:PRO:C	2.64	0.41
12:AF:143:GLY:O	12:AF:147:SER:OG	2.28	0.41
11:AB:731:ARG:HE	11:AB:731:ARG:HB3	1.69	0.41
16:C:100:ARG:NH1	11:5:752:THR:HG23	2.36	0.41
16:C:283:PHE:CZ	16:C:303:SER:HB3	2.56	0.41
16:C:384:GLU:OE2	10:AN:77:ARG:NH1	2.53	0.41
11:7:746:SER:OG	11:7:776:ALA:HB2	2.20	0.41
11:5:144:HIS:HA	11:5:268:THR:O	2.21	0.41
11:5:323:LEU:HD12	11:5:357:LEU:HB2	2.03	0.41
7:K:677:TRP:O	7:K:680:MET:HG2	2.21	0.41
14:AD:17:PRO:HA	14:AD:18:PRO:HD3	1.95	0.41
11:2:1006:GLN:HG3	11:2:1033:VAL:HG22	2.02	0.41
13:AK:173:GLU:H	13:AK:173:GLU:CD	2.28	0.41
13:AK:518:LEU:HG	13:AK:563:TYR:HB3	2.03	0.41
13:AQ:778:LEU:HG	13:AQ:780:LEU:HG	2.03	0.41
6:H:336:CYS:O	6:H:342:CYS:HB2	2.21	0.41
7:S:295:PHE:HB3	7:S:409:VAL:HG21	2.03	0.41
9:l:223:ILE:HG23	9:l:224:PRO:HA	2.03	0.41
7:b:116:ILE:HD13	7:b:267:LEU:HD13	2.03	0.41
7:X:489:ARG:HD3	7:X:573:ILE:HD11	2.03	0.41
7:o:273:ASP:OD1	7:o:274:GLU:N	2.54	0.41
7:j:195:TYR:HD1	7:j:269:GLU:HA	1.86	0.41
13:w:122:LYS:HE3	13:w:166:GLU:CD	2.46	0.41
13:w:216:LYS:HB3	13:w:341:MET:HE1	2.03	0.41
10:AE:11:GLN:HA	10:AE:72:THR:HG21	2.03	0.41
7:B:116:ILE:CD1	7:B:267:LEU:CD2	2.86	0.41
7:B:350:ALA:HA	7:B:667:ILE:HD11	2.03	0.41
7:U:43:ARG:O	7:U:91:VAL:HG13	2.21	0.41
7:c:209:THR:HB	7:c:261:ILE:HD13	2.02	0.41
13:AQ:518:LEU:HG	13:AQ:563:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:603:THR:OG1	6:h:643:THR:HG23	2.21	0.41
8:AT:86:LEU:HD12	8:AT:86:LEU:HA	1.95	0.41
5:I:403:LEU:HG	5:I:413:ILE:HG12	2.03	0.40
7:S:306:TYR:HB2	7:S:667:ILE:HG23	2.03	0.40
8:e:129:PHE:HA	11:y:301:LEU:HD22	2.02	0.40
7:f:5:ASN:O	7:f:25:ILE:HG23	2.21	0.40
7:s:156:SER:HA	7:s:157:PRO:HD3	1.95	0.40
7:m:5:ASN:O	7:m:26:THR:N	2.42	0.40
7:j:18:LEU:HD12	7:j:18:LEU:HA	1.93	0.40
7:j:40:PHE:CZ	7:j:73:THR:HG21	2.55	0.40
7:j:151:LEU:HG	7:j:288:PHE:HB3	2.03	0.40
10:AE:311:LEU:HD23	10:AE:342:VAL:HG11	2.01	0.40
5:8:335:LEU:HD11	5:8:378:LEU:HD21	2.03	0.40
11:7:690:LYS:HA	11:7:693:PHE:CE2	2.56	0.40
11:7:862:ARG:HA	11:7:862:ARG:NE	2.36	0.40
7:B:349:MET:HE1	7:B:378:MET:HG2	2.03	0.40
14:AD:5:ARG:NH1	14:AD:61:PRO:HG3	2.36	0.40
7:U:42:ILE:HA	7:U:92:LEU:O	2.20	0.40
7:c:602:PHE:O	7:c:603:PRO:C	2.64	0.40
5:I:488:ALA:HA	5:I:512:THR:HG23	2.03	0.40
6:Q:453:VAL:O	6:Q:456:VAL:HG12	2.21	0.40
9:k:23:TYR:O	9:k:27:GLN:HG2	2.22	0.40
9:l:208:ILE:HD13	9:l:271:LEU:HD21	2.03	0.40
8:AH:28:ARG:NH2	11:2:289:GLU:HB3	2.36	0.40
7:b:280:PRO:HB2	7:B:431:PHE:CD2	2.55	0.40
7:b:556:LEU:HD11	7:B:280:PRO:HG2	2.03	0.40
7:X:375:ASP:OD1	7:X:376:PHE:N	2.51	0.40
7:n:583:GLN:HG3	7:n:596:LEU:HD23	2.04	0.40
7:f:656:LEU:HD23	7:f:656:LEU:HA	1.86	0.40
7:s:550:VAL:HG11	7:s:579:PHE:CD1	2.56	0.40
7:o:550:VAL:HG21	7:o:579:PHE:HB2	2.03	0.40
12:u:98:ASP:HB2	18:u:502:GTP:O3G	2.20	0.40
15:AL:241:ARG:HH12	13:AK:416:LEU:CD2	2.34	0.40
12:AO:117:LEU:O	12:AO:121:ARG:HG2	2.22	0.40
16:C:166:ILE:HG12	16:C:172:ILE:HG12	2.03	0.40
7:K:9:LEU:HD21	7:K:27:LEU:HD11	2.02	0.40
8:AI:58:ILE:HG21	8:AI:78:VAL:HG21	2.03	0.40
7:c:273:ASP:OD1	7:c:274:GLU:N	2.54	0.40
6:h:68:ASP:OD2	6:h:72:ARG:NH1	2.50	0.40
5:I:277:ARG:NE	5:I:277:ARG:HA	2.37	0.40
7:n:9:LEU:HB2	7:n:32:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:u:117:LEU:O	12:u:121:ARG:HG2	2.22	0.40
12:AF:397:LEU:HD23	12:AF:397:LEU:HA	1.95	0.40
14:AS:5:ARG:NH1	14:AS:61:PRO:HG3	2.36	0.40
8:AJ:104:ILE:HG23	6:h:11:ILE:HG21	2.02	0.40
16:L:142:TRP:CG	16:L:143:VAL:N	2.89	0.40
16:C:254:GLN:HG2	11:5:807:PHE:CE1	2.56	0.40
8:AI:77:THR:OG1	8:AI:90:THR:HB	2.21	0.40
11:2:708:MET:HE3	11:2:708:MET:HB3	1.96	0.40
7:c:296:MET:HE3	7:c:296:MET:HB2	1.92	0.40
13:AQ:123:GLU:HB2	13:AQ:375:TYR:OH	2.20	0.40
2:6:64:HIS:HD1	2:6:64:HIS:N	2.19	0.40
7:T:366:ASP:OD1	7:T:367:THR:N	2.55	0.40
11:y:647:LEU:HD12	11:y:676:PHE:CE1	2.56	0.40
7:Y:123:TYR:HE2	7:Y:132:SER:CB	2.34	0.40
7:W:364:ILE:HD12	7:W:382:LEU:CD2	2.52	0.40
7:f:473:MET:HA	7:f:491:LEU:O	2.22	0.40
7:f:606:LEU:HD23	7:f:606:LEU:HA	1.90	0.40
7:s:475:PHE:CE2	7:s:490:LEU:HD13	2.56	0.40
7:d:118:LEU:O	7:d:137:LYS:NZ	2.49	0.40
13:w:861:TRP:HA	13:w:889:VAL:HA	2.03	0.40
14:AM:86:LEU:HD12	14:AM:86:LEU:HA	1.90	0.40
11:5:966:THR:HA	11:5:992:ASP:O	2.21	0.40
7:c:116:ILE:HD12	7:c:267:LEU:HD22	2.03	0.40
15:x:706:LYS:HA	15:x:706:LYS:HD3	1.87	0.40
13:AK:31:ARG:O	13:AK:34:ILE:HG22	2.20	0.40
13:AK:861:TRP:HA	13:AK:889:VAL:HA	2.03	0.40
3:A:277:VAL:HG12	3:A:329:VAL:HG23	2.03	0.40
3:A:348:TRP:NE1	3:A:357:ILE:HG23	2.37	0.40
6:H:722:MET:HA	6:H:750:ASN:HB3	2.03	0.40
6:H:855:ASN:OD1	11:y:738:THR:HG22	2.20	0.40
7:S:122:ILE:HD12	7:S:147:TRP:CD1	2.57	0.40
9:k:27:GLN:OE1	4:p:132:PRO:HD3	2.21	0.40
9:k:152:THR:HG21	9:k:172:HIS:CD2	2.57	0.40
7:V:3:PHE:CD1	7:V:20:MET:HG2	2.56	0.40
7:n:353:TYR:CE2	7:n:672:PRO:HB3	2.57	0.40
7:m:79:MET:HE3	7:m:79:MET:HB3	1.88	0.40
7:m:422:LEU:HD12	7:m:453:VAL:HB	2.04	0.40
7:j:486:LYS:HD3	7:j:488:PHE:CE1	2.57	0.40
12:u:119:LEU:HD11	12:u:156:ARG:HB3	2.02	0.40
10:AE:323:MET:HB3	12:AF:221:ARG:HH11	1.86	0.40
12:AF:2:ARG:HB3	12:AF:133:GLN:CG	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:101:MET:HE3	8:AJ:126:VAL:HG23	2.04	0.40
16:C:81:THR:OG1	16:C:394:HIS:NE2	2.54	0.40
7:K:48:ILE:HG12	7:K:79:MET:SD	2.62	0.40
11:2:173:PHE:HB3	11:2:215:LEU:HD12	2.03	0.40
7:U:125:ASP:OD1	7:U:126:GLY:N	2.54	0.40
7:c:408:MET:HG3	7:c:469:MET:HE3	2.03	0.40
15:x:515:LEU:HD23	15:x:515:LEU:HA	1.90	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	1	54/228 (24%)	54 (100%)	0	0	100	100
1	3	54/228 (24%)	53 (98%)	1 (2%)	0	100	100
1	9	54/228 (24%)	52 (96%)	2 (4%)	0	100	100
2	4	122/440 (28%)	119 (98%)	3 (2%)	0	100	100
2	6	122/440 (28%)	121 (99%)	1 (1%)	0	100	100
2	AA	122/440 (28%)	120 (98%)	2 (2%)	0	100	100
3	A	444/468 (95%)	432 (97%)	12 (3%)	0	100	100
4	D	142/163 (87%)	142 (100%)	0	0	100	100
4	F	142/163 (87%)	142 (100%)	0	0	100	100
4	O	142/163 (87%)	142 (100%)	0	0	100	100
4	p	142/163 (87%)	142 (100%)	0	0	100	100
4	q	142/163 (87%)	142 (100%)	0	0	100	100
5	8	354/581 (61%)	345 (98%)	9 (2%)	0	100	100
5	AC	354/581 (61%)	344 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	354/581 (61%)	343 (97%)	11 (3%)	0	100	100
5	I	354/581 (61%)	342 (97%)	12 (3%)	0	100	100
5	P	354/581 (61%)	345 (98%)	9 (2%)	0	100	100
5	z	354/581 (61%)	343 (97%)	11 (3%)	0	100	100
6	H	719/937 (77%)	703 (98%)	16 (2%)	0	100	100
6	Q	634/937 (68%)	625 (99%)	9 (1%)	0	100	100
6	h	715/937 (76%)	708 (99%)	7 (1%)	0	100	100
6	i	717/937 (76%)	707 (99%)	10 (1%)	0	100	100
7	B	643/682 (94%)	639 (99%)	4 (1%)	0	100	100
7	K	642/682 (94%)	631 (98%)	11 (2%)	0	100	100
7	S	635/682 (93%)	626 (99%)	9 (1%)	0	100	100
7	T	642/682 (94%)	635 (99%)	7 (1%)	0	100	100
7	U	647/682 (95%)	628 (97%)	19 (3%)	0	100	100
7	V	644/682 (94%)	632 (98%)	12 (2%)	0	100	100
7	W	646/682 (95%)	638 (99%)	8 (1%)	0	100	100
7	X	644/682 (94%)	633 (98%)	11 (2%)	0	100	100
7	Y	652/682 (96%)	644 (99%)	8 (1%)	0	100	100
7	Z	644/682 (94%)	636 (99%)	8 (1%)	0	100	100
7	b	646/682 (95%)	635 (98%)	11 (2%)	0	100	100
7	c	647/682 (95%)	636 (98%)	11 (2%)	0	100	100
7	d	644/682 (94%)	638 (99%)	6 (1%)	0	100	100
7	f	642/682 (94%)	637 (99%)	5 (1%)	0	100	100
7	j	646/682 (95%)	639 (99%)	7 (1%)	0	100	100
7	m	644/682 (94%)	637 (99%)	7 (1%)	0	100	100
7	n	652/682 (96%)	644 (99%)	8 (1%)	0	100	100
7	o	644/682 (94%)	640 (99%)	4 (1%)	0	100	100
7	r	640/682 (94%)	632 (99%)	8 (1%)	0	100	100
7	s	646/682 (95%)	635 (98%)	11 (2%)	0	100	100
8	AH	114/164 (70%)	112 (98%)	2 (2%)	0	100	100
8	AI	114/164 (70%)	113 (99%)	1 (1%)	0	100	100
8	AJ	114/164 (70%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AT	126/164 (77%)	123 (98%)	3 (2%)	0	100	100
8	e	126/164 (77%)	123 (98%)	3 (2%)	0	100	100
8	g	126/164 (77%)	123 (98%)	3 (2%)	0	100	100
9	k	461/469 (98%)	456 (99%)	5 (1%)	0	100	100
9	l	461/469 (98%)	452 (98%)	9 (2%)	0	100	100
10	AE	428/445 (96%)	426 (100%)	2 (0%)	0	100	100
10	AN	428/445 (96%)	425 (99%)	3 (1%)	0	100	100
10	t	428/445 (96%)	422 (99%)	6 (1%)	0	100	100
11	0	927/1059 (88%)	910 (98%)	17 (2%)	0	100	100
11	2	926/1059 (87%)	910 (98%)	16 (2%)	0	100	100
11	5	927/1059 (88%)	910 (98%)	17 (2%)	0	100	100
11	7	928/1059 (88%)	915 (99%)	13 (1%)	0	100	100
11	AB	928/1059 (88%)	910 (98%)	18 (2%)	0	100	100
11	y	928/1059 (88%)	913 (98%)	15 (2%)	0	100	100
12	AF	426/451 (94%)	422 (99%)	4 (1%)	0	100	100
12	AO	426/451 (94%)	422 (99%)	4 (1%)	0	100	100
12	u	426/451 (94%)	422 (99%)	4 (1%)	0	100	100
13	AK	940/993 (95%)	933 (99%)	7 (1%)	0	100	100
13	AQ	940/993 (95%)	932 (99%)	8 (1%)	0	100	100
13	w	940/993 (95%)	932 (99%)	8 (1%)	0	100	100
14	AD	145/147 (99%)	145 (100%)	0	0	100	100
14	AM	145/147 (99%)	145 (100%)	0	0	100	100
14	AS	145/147 (99%)	145 (100%)	0	0	100	100
15	AL	596/782 (76%)	591 (99%)	5 (1%)	0	100	100
15	AR	596/782 (76%)	591 (99%)	5 (1%)	0	100	100
15	x	596/782 (76%)	592 (99%)	4 (1%)	0	100	100
16	C	441/466 (95%)	435 (99%)	6 (1%)	0	100	100
16	L	441/466 (95%)	432 (98%)	9 (2%)	0	100	100
All	All	35174/41823 (84%)	34675 (99%)	499 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	41/197 (21%)	41 (100%)	0	100	100
1	3	47/197 (24%)	46 (98%)	1 (2%)	47	64
1	9	47/197 (24%)	47 (100%)	0	100	100
2	4	99/357 (28%)	99 (100%)	0	100	100
2	6	112/357 (31%)	110 (98%)	2 (2%)	51	66
2	AA	112/357 (31%)	110 (98%)	2 (2%)	51	66
3	A	404/431 (94%)	390 (96%)	14 (4%)	32	54
4	D	136/150 (91%)	136 (100%)	0	100	100
4	F	137/150 (91%)	137 (100%)	0	100	100
4	O	137/150 (91%)	137 (100%)	0	100	100
4	p	136/150 (91%)	136 (100%)	0	100	100
4	q	136/150 (91%)	136 (100%)	0	100	100
5	8	313/516 (61%)	312 (100%)	1 (0%)	86	83
5	AC	313/516 (61%)	311 (99%)	2 (1%)	78	79
5	E	310/516 (60%)	310 (100%)	0	100	100
5	I	313/516 (61%)	311 (99%)	2 (1%)	78	79
5	P	313/516 (61%)	308 (98%)	5 (2%)	55	68
5	z	311/516 (60%)	311 (100%)	0	100	100
6	H	659/862 (76%)	653 (99%)	6 (1%)	70	74
6	Q	586/862 (68%)	581 (99%)	5 (1%)	70	74
6	h	656/862 (76%)	654 (100%)	2 (0%)	86	83
6	i	646/862 (75%)	646 (100%)	0	100	100
7	B	582/613 (95%)	575 (99%)	7 (1%)	63	71
7	K	584/613 (95%)	579 (99%)	5 (1%)	70	74
7	S	578/613 (94%)	578 (100%)	0	100	100
7	T	585/613 (95%)	585 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	583/613 (95%)	577 (99%)	6 (1%)	68	74
7	V	581/613 (95%)	580 (100%)	1 (0%)	87	86
7	W	583/613 (95%)	583 (100%)	0	100	100
7	X	586/613 (96%)	586 (100%)	0	100	100
7	Y	561/613 (92%)	561 (100%)	0	100	100
7	Z	579/613 (94%)	578 (100%)	1 (0%)	87	86
7	b	581/613 (95%)	581 (100%)	0	100	100
7	c	584/613 (95%)	580 (99%)	4 (1%)	76	77
7	d	579/613 (94%)	577 (100%)	2 (0%)	86	83
7	f	587/613 (96%)	587 (100%)	0	100	100
7	j	584/613 (95%)	582 (100%)	2 (0%)	86	83
7	m	586/613 (96%)	585 (100%)	1 (0%)	87	86
7	n	562/613 (92%)	562 (100%)	0	100	100
7	o	581/613 (95%)	581 (100%)	0	100	100
7	r	582/613 (95%)	567 (97%)	15 (3%)	40	60
7	s	580/613 (95%)	580 (100%)	0	100	100
8	AH	86/143 (60%)	86 (100%)	0	100	100
8	AI	102/143 (71%)	100 (98%)	2 (2%)	48	64
8	AJ	103/143 (72%)	98 (95%)	5 (5%)	22	48
8	AT	85/143 (59%)	80 (94%)	5 (6%)	18	44
8	e	85/143 (59%)	80 (94%)	5 (6%)	18	44
8	g	85/143 (59%)	80 (94%)	5 (6%)	18	44
9	k	423/435 (97%)	408 (96%)	15 (4%)	32	54
9	l	424/435 (98%)	407 (96%)	17 (4%)	28	52
10	AE	365/380 (96%)	365 (100%)	0	100	100
10	AN	368/380 (97%)	368 (100%)	0	100	100
10	t	368/380 (97%)	368 (100%)	0	100	100
11	0	823/960 (86%)	807 (98%)	16 (2%)	50	65
11	2	797/960 (83%)	795 (100%)	2 (0%)	86	83
11	5	821/960 (86%)	803 (98%)	18 (2%)	45	63
11	7	822/960 (86%)	810 (98%)	12 (2%)	57	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AB	823/960 (86%)	809 (98%)	14 (2%)	53	67
11	y	805/960 (84%)	805 (100%)	0	100	100
12	AF	361/378 (96%)	354 (98%)	7 (2%)	50	65
12	AO	362/378 (96%)	354 (98%)	8 (2%)	45	63
12	u	362/378 (96%)	355 (98%)	7 (2%)	50	65
13	AK	820/909 (90%)	818 (100%)	2 (0%)	87	86
13	AQ	839/909 (92%)	836 (100%)	3 (0%)	84	81
13	w	840/909 (92%)	815 (97%)	25 (3%)	36	57
14	AD	131/132 (99%)	129 (98%)	2 (2%)	57	68
14	AM	130/132 (98%)	130 (100%)	0	100	100
14	AS	131/132 (99%)	129 (98%)	2 (2%)	57	68
15	AL	524/682 (77%)	523 (100%)	1 (0%)	87	86
15	AR	524/682 (77%)	523 (100%)	1 (0%)	87	86
15	x	519/682 (76%)	519 (100%)	0	100	100
16	C	407/430 (95%)	395 (97%)	12 (3%)	37	57
16	L	409/430 (95%)	393 (96%)	16 (4%)	28	52
All	All	31316/37438 (84%)	31028 (99%)	288 (1%)	68	74

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	44	LEU
2	6	64	HIS
2	6	105	LEU
3	A	96	GLU
3	A	123	MET
3	A	125	THR
3	A	146	GLU
3	A	160	MET
3	A	193	GLN
3	A	330	LYS
3	A	332	HIS
3	A	337	PHE
3	A	388	LEU
3	A	453	THR
3	A	457	LEU

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Mol	Chain	Res	Type
3	A	458	MET
3	A	461	ILE
6	H	10	LEU
6	H	15	ARG
6	H	18	ASN
6	H	85	ARG
6	H	870	LYS
6	H	927	GLU
5	I	293	GLN
5	I	400	ASN
6	Q	813	LYS
6	Q	815	GLU
6	Q	870	LYS
6	Q	928	VAL
6	Q	932	VAL
8	e	29	LEU
8	e	32	ARG
8	e	40	GLU
8	e	58	ILE
8	e	67	GLU
9	k	60	ILE
9	k	61	LEU
9	k	65	ASP
9	k	70	LYS
9	k	99	GLU
9	k	102	ILE
9	k	107	CYS
9	k	109	ILE
9	k	114	LEU
9	k	346	GLU
9	k	361	VAL
9	k	435	SER
9	k	450	MET
9	k	465	LEU
9	k	468	HIS
9	l	60	ILE
9	l	61	LEU
9	l	70	LYS
9	l	96	ILE
9	l	99	GLU
9	l	102	ILE
9	l	107	CYS

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Mol	Chain	Res	Type
9	l	109	ILE
9	l	114	LEU
9	l	130	MET
9	l	167	VAL
9	l	308	SER
9	l	346	GLU
9	l	450	MET
9	l	465	LEU
9	l	467	ILE
9	l	468	HIS
8	g	29	LEU
8	g	32	ARG
8	g	40	GLU
8	g	58	ILE
8	g	67	GLU
7	Z	124	ARG
7	V	130	MET
7	m	130	MET
7	d	130	MET
7	d	309	ARG
7	j	489	ARG
7	j	556	LEU
12	u	188	ILE
12	u	193	THR
12	u	243	ARG
12	u	251	ASP
12	u	265	ILE
12	u	344	VAL
12	u	345	ASP
13	w	45	THR
13	w	57	VAL
13	w	58	ILE
13	w	69	ILE
13	w	316	VAL
13	w	323	ASN
13	w	341	MET
13	w	453	LEU
13	w	470	LEU
13	w	472	LYS
13	w	475	SER
13	w	477	LEU
13	w	541	ASP

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Mol	Chain	Res	Type
13	w	697	ASN
13	w	701	ASN
13	w	751	LEU
13	w	781	ARG
13	w	786	THR
13	w	790	SER
13	w	816	ASN
13	w	819	LYS
13	w	841	VAL
13	w	842	LEU
13	w	984	THR
13	w	986	SER
12	AF	188	ILE
12	AF	193	THR
12	AF	243	ARG
12	AF	251	ASP
12	AF	265	ILE
12	AF	344	VAL
12	AF	345	ASP
15	AL	329	ARG
12	AO	120	ASP
12	AO	188	ILE
12	AO	193	THR
12	AO	243	ARG
12	AO	251	ASP
12	AO	265	ILE
12	AO	344	VAL
12	AO	345	ASP
14	AS	21	CYS
14	AS	88	ILE
15	AR	329	ARG
5	P	400	ASN
5	P	456	LEU
5	P	567	ILE
5	P	571	ARG
5	P	573	CYS
2	AA	53	ILE
2	AA	105	LEU
5	AC	303	SER
5	AC	400	ASN
11	AB	169	GLN
11	AB	299	LEU

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Mol	Chain	Res	Type
11	AB	304	ILE
11	AB	310	ARG
11	AB	606	ASN
11	AB	608	LEU
11	AB	610	LEU
11	AB	662	LEU
11	AB	683	SER
11	AB	731	ARG
11	AB	733	ASP
11	AB	822	LEU
11	AB	849	CYS
11	AB	852	VAL
8	AJ	27	LEU
8	AJ	62	GLN
8	AJ	79	ASP
8	AJ	125	GLU
8	AJ	126	VAL
11	0	169	GLN
11	0	311	ILE
11	0	325	ASP
11	0	462	GLU
11	0	598	ILE
11	0	606	ASN
11	0	608	LEU
11	0	610	LEU
11	0	613	VAL
11	0	662	LEU
11	0	731	ARG
11	0	733	ASP
11	0	775	ASN
11	0	822	LEU
11	0	849	CYS
11	0	852	VAL
7	r	128	LEU
7	r	141	MET
7	r	309	ARG
7	r	312	GLN
7	r	313	LEU
7	r	314	GLN
7	r	403	SER
7	r	406	ASN
7	r	407	LEU

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Mol	Chain	Res	Type
7	r	469	MET
7	r	472	PHE
7	r	480	ASP
7	r	482	ASN
7	r	484	ASP
7	r	489	ARG
16	L	57	THR
16	L	60	LEU
16	L	63	LEU
16	L	97	PHE
16	L	98	GLU
16	L	106	ILE
16	L	108	ARG
16	L	109	HIS
16	L	125	THR
16	L	127	THR
16	L	128	ASN
16	L	164	VAL
16	L	229	VAL
16	L	323	ILE
16	L	438	LEU
16	L	441	GLU
16	C	57	THR
16	C	97	PHE
16	C	106	ILE
16	C	151	ILE
16	C	164	VAL
16	C	168	MET
16	C	229	VAL
16	C	255	ARG
16	C	309	ASP
16	C	323	ILE
16	C	438	LEU
16	C	441	GLU
5	8	400	ASN
11	7	169	GLN
11	7	248	ILE
11	7	312	GLN
11	7	417	GLU
11	7	606	ASN
11	7	610	LEU
11	7	731	ARG

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Mol	Chain	Res	Type
11	7	822	LEU
11	7	849	CYS
11	7	852	VAL
11	7	854	ASP
11	7	941	VAL
11	5	169	GLN
11	5	248	ILE
11	5	310	ARG
11	5	325	ASP
11	5	462	GLU
11	5	606	ASN
11	5	610	LEU
11	5	611	CYS
11	5	613	VAL
11	5	738	THR
11	5	750	ILE
11	5	752	THR
11	5	807	PHE
11	5	822	LEU
11	5	829	GLN
11	5	849	CYS
11	5	852	VAL
11	5	854	ASP
7	B	43	ARG
7	B	128	LEU
7	B	141	MET
7	B	144	MET
7	B	312	GLN
7	B	469	MET
7	B	489	ARG
7	K	128	LEU
7	K	129	ASP
7	K	144	MET
7	K	173	ARG
7	K	381	THR
8	AI	125	GLU
8	AI	126	VAL
14	AD	21	CYS
14	AD	88	ILE
11	2	662	LEU
11	2	853	ASP
7	U	122	ILE

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Mol	Chain	Res	Type
7	U	127	GLN
7	U	240	ARG
7	U	345	LEU
7	U	407	LEU
7	U	584	LEU
7	c	11	LEU
7	c	127	GLN
7	c	240	ARG
7	c	485	GLN
13	AK	323	ASN
13	AK	453	LEU
13	AQ	323	ASN
13	AQ	472	LYS
13	AQ	697	ASN
6	h	15	ARG
6	h	85	ARG
8	AT	29	LEU
8	AT	32	ARG
8	AT	40	GLU
8	AT	58	ILE
8	AT	67	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (280) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	43	HIS
1	3	43	HIS
3	A	214	ASN
3	A	415	GLN
4	D	64	HIS
4	D	97	GLN
5	E	267	GLN
5	E	441	ASN
6	H	678	HIS
5	I	267	GLN
7	S	71	HIS
7	S	135	GLN
7	S	314	GLN
7	S	341	GLN
7	S	355	GLN
7	S	471	GLN
6	Q	373	HIS

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Mol	Chain	Res	Type
6	Q	525	HIS
6	Q	526	HIS
6	Q	903	ASN
8	e	82	ASN
9	k	71	GLN
9	k	164	HIS
9	k	233	ASN
9	k	329	GLN
9	k	466	ASN
9	l	71	GLN
9	l	217	ASN
9	l	233	ASN
9	l	466	ASN
10	t	48	ASN
10	t	134	GLN
10	t	347	ASN
10	t	396	HIS
8	g	82	ASN
7	T	51	HIS
7	T	71	HIS
7	T	355	GLN
7	T	451	GLN
7	T	471	GLN
7	T	485	GLN
7	T	523	GLN
5	z	266	ASN
5	z	441	ASN
5	z	537	HIS
11	y	298	GLN
11	y	303	ASN
11	y	355	GLN
11	y	367	HIS
11	y	525	HIS
11	y	705	ASN
11	y	848	HIS
11	y	865	ASN
11	y	982	HIS
7	Y	135	GLN
7	Y	341	GLN
7	Y	355	GLN
7	Y	591	GLN
7	b	355	GLN

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Mol	Chain	Res	Type
7	b	396	HIS
7	b	471	GLN
7	b	614	ASN
7	X	355	GLN
7	X	592	GLN
7	X	614	ASN
7	Z	71	HIS
7	Z	341	GLN
7	Z	614	ASN
7	V	355	GLN
7	V	396	HIS
7	V	468	HIS
7	V	471	GLN
7	V	485	GLN
7	V	607	GLN
7	W	135	GLN
7	W	355	GLN
7	W	485	GLN
7	W	614	ASN
7	n	71	HIS
7	n	341	GLN
7	n	355	GLN
7	n	506	GLN
7	f	71	HIS
7	f	355	GLN
7	f	471	GLN
7	f	614	ASN
7	f	658	ASN
7	s	71	HIS
7	s	527	ASN
7	s	614	ASN
7	m	127	GLN
7	o	196	GLN
7	o	485	GLN
7	o	614	ASN
7	d	314	GLN
7	d	341	GLN
7	d	355	GLN
7	d	523	GLN
7	d	527	ASN
7	j	341	GLN
7	j	358	HIS

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Mol	Chain	Res	Type
7	j	527	ASN
7	j	614	ASN
12	u	15	GLN
12	u	18	ASN
12	u	266	HIS
12	u	301	GLN
12	u	406	HIS
13	w	270	HIS
13	w	273	HIS
13	w	323	ASN
13	w	353	HIS
13	w	383	HIS
13	w	479	GLN
13	w	574	ASN
13	w	634	HIS
13	w	697	ASN
13	w	754	ASN
10	AE	37	HIS
10	AE	48	ASN
12	AF	15	GLN
12	AF	18	ASN
12	AF	266	HIS
12	AF	301	GLN
15	AL	264	ASN
15	AL	459	ASN
15	AL	673	GLN
15	AL	744	GLN
12	AO	15	GLN
12	AO	18	ASN
12	AO	266	HIS
12	AO	301	GLN
15	AR	264	ASN
15	AR	744	GLN
15	AR	773	GLN
5	P	441	ASN
5	P	537	HIS
2	AA	61	HIS
2	AA	64	HIS
5	AC	400	ASN
5	AC	441	ASN
5	AC	537	HIS
11	AB	303	ASN

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Mol	Chain	Res	Type
11	AB	367	HIS
11	AB	431	GLN
11	AB	525	HIS
11	AB	606	ASN
11	AB	696	GLN
11	AB	848	HIS
11	AB	850	ASN
11	AB	865	ASN
11	AB	968	ASN
11	0	312	GLN
11	0	367	HIS
11	0	431	GLN
11	0	687	HIS
11	0	705	ASN
11	0	819	ASN
11	0	848	HIS
11	0	968	ASN
11	0	1011	ASN
7	r	135	GLN
7	r	312	GLN
7	r	355	GLN
7	r	591	GLN
7	r	614	ASN
16	L	59	GLN
16	L	128	ASN
16	L	214	ASN
16	L	230	ASN
16	C	4	HIS
16	C	59	GLN
16	C	136	HIS
16	C	230	ASN
16	C	256	HIS
16	C	332	HIS
5	8	465	HIS
11	7	298	GLN
11	7	303	ASN
11	7	355	GLN
11	7	367	HIS
11	7	431	GLN
11	7	466	GLN
11	7	467	HIS
11	7	525	HIS

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Mol	Chain	Res	Type
11	7	606	ASN
11	7	705	ASN
11	7	968	ASN
11	7	982	HIS
11	5	303	ASN
11	5	355	GLN
11	5	367	HIS
11	5	431	GLN
11	5	466	GLN
11	5	467	HIS
11	5	574	GLN
11	5	606	ASN
11	5	687	HIS
11	5	697	ASN
11	5	877	ASN
11	5	968	ASN
11	5	1006	GLN
11	5	1011	ASN
11	5	1039	HIS
7	B	127	GLN
7	B	135	GLN
7	B	312	GLN
7	B	341	GLN
7	B	355	GLN
7	B	471	GLN
7	B	607	GLN
7	B	614	ASN
7	B	658	ASN
7	K	71	HIS
7	K	135	GLN
7	K	341	GLN
7	K	346	GLN
7	K	482	ASN
7	K	506	GLN
10	AN	37	HIS
10	AN	48	ASN
10	AN	134	GLN
10	AN	227	HIS
10	AN	329	GLN
10	AN	347	ASN
11	2	270	ASN
11	2	303	ASN

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Mol	Chain	Res	Type
11	2	435	ASN
11	2	574	GLN
11	2	667	GLN
11	2	687	HIS
11	2	848	HIS
11	2	968	ASN
11	2	1011	ASN
7	U	71	HIS
7	U	312	GLN
7	U	355	GLN
7	U	614	ASN
7	U	658	ASN
7	c	4	GLN
7	c	71	HIS
7	c	127	GLN
7	c	177	ASN
7	c	312	GLN
7	c	482	ASN
7	c	485	GLN
7	c	658	ASN
15	x	264	ASN
15	x	450	HIS
15	x	673	GLN
15	x	744	GLN
13	AK	63	GLN
13	AK	270	HIS
13	AK	273	HIS
13	AK	323	ASN
13	AK	353	HIS
13	AK	383	HIS
13	AK	479	GLN
13	AK	574	ASN
13	AK	634	HIS
13	AK	754	ASN
13	AQ	270	HIS
13	AQ	273	HIS
13	AQ	323	ASN
13	AQ	353	HIS
13	AQ	383	HIS
13	AQ	479	GLN
13	AQ	574	ASN
13	AQ	634	HIS

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Mol	Chain	Res	Type
13	AQ	697	ASN
13	AQ	754	ASN
6	i	574	ASN
6	i	678	HIS
6	i	863	HIS
6	h	373	HIS
6	h	526	HIS
6	h	678	HIS
6	h	757	ASN
6	h	863	HIS
8	AT	82	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 17 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	$\# Z > 2$
18	GTP	u	502	19	30,34,34	2.17	7 (23%)	46,54,54	1.64	10 (21%)
18	GTP	AF	501	-	30,34,34	2.14	8 (26%)	46,54,54	1.57	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	ADP	AQ	1001	-	27,29,29	2.93	13 (48%)	42,45,45	1.87	12 (28%)
18	GTP	t	501	19	30,34,34	2.31	8 (26%)	46,54,54	1.63	12 (26%)
20	ADP	w	1001	-	27,29,29	2.93	13 (48%)	42,45,45	1.87	12 (28%)
18	GTP	AO	501	19	30,34,34	2.17	7 (23%)	46,54,54	1.64	10 (21%)
20	ADP	AK	1001	-	27,29,29	2.93	13 (48%)	42,45,45	1.87	12 (28%)
18	GTP	AN	501	19	30,34,34	2.31	8 (26%)	46,54,54	1.64	12 (26%)

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
18	GTP	u	502	19	-	9/22/38/38	0/3/3/3
18	GTP	AF	501	-	-	6/22/38/38	0/3/3/3
20	ADP	AQ	1001	-	-	8/16/32/32	0/3/3/3
18	GTP	t	501	19	-	4/22/38/38	0/3/3/3
20	ADP	w	1001	-	-	8/16/32/32	0/3/3/3
18	GTP	AO	501	19	-	9/22/38/38	0/3/3/3
20	ADP	AK	1001	-	-	8/16/32/32	0/3/3/3
18	GTP	AN	501	19	-	4/22/38/38	0/3/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AK	1001	ADP	PA-O5'	7.95	1.91	1.59
20	w	1001	ADP	PA-O5'	7.94	1.91	1.59
20	AQ	1001	ADP	PA-O5'	7.93	1.91	1.59
18	t	501	GTP	PA-O5'	7.78	1.90	1.59
18	AN	501	GTP	PA-O5'	7.78	1.90	1.59
18	AF	501	GTP	PA-O5'	7.02	1.87	1.59
18	u	502	GTP	PA-O5'	7.02	1.87	1.59
18	AO	501	GTP	PA-O5'	7.01	1.87	1.59
20	AQ	1001	ADP	C2-N1	4.58	1.42	1.33
20	AK	1001	ADP	C2-N1	4.57	1.42	1.33
20	w	1001	ADP	C2-N1	4.57	1.42	1.33
18	AN	501	GTP	C5'-C4'	4.48	1.65	1.51
18	t	501	GTP	C5'-C4'	4.48	1.65	1.51
20	AQ	1001	ADP	C5'-C4'	4.43	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AK	1001	ADP	C5'-C4'	4.43	1.65	1.51
20	w	1001	ADP	C5'-C4'	4.42	1.65	1.51
20	w	1001	ADP	C4-N9	4.32	1.47	1.37
20	AK	1001	ADP	C4-N9	4.30	1.47	1.37
20	AQ	1001	ADP	C4-N9	4.30	1.47	1.37
20	AK	1001	ADP	C1'-N9	4.26	1.58	1.46
20	w	1001	ADP	C1'-N9	4.26	1.58	1.46
20	AQ	1001	ADP	C1'-N9	4.25	1.58	1.46
18	AO	501	GTP	C5'-C4'	4.25	1.64	1.51
18	AF	501	GTP	C5'-C4'	4.24	1.64	1.51
18	u	502	GTP	C5'-C4'	4.24	1.64	1.51
20	w	1001	ADP	O5'-C5'	-3.94	1.29	1.44
20	AQ	1001	ADP	O5'-C5'	-3.94	1.29	1.44
20	AK	1001	ADP	O5'-C5'	-3.93	1.29	1.44
18	AO	501	GTP	O5'-C5'	-3.92	1.29	1.44
18	u	502	GTP	O5'-C5'	-3.90	1.29	1.44
18	AF	501	GTP	O5'-C5'	-3.88	1.29	1.44
18	t	501	GTP	O5'-C5'	-3.87	1.29	1.44
18	AN	501	GTP	O5'-C5'	-3.87	1.29	1.44
20	AQ	1001	ADP	C6-N6	3.84	1.43	1.34
20	w	1001	ADP	C6-N6	3.83	1.43	1.34
20	AK	1001	ADP	C6-N6	3.80	1.43	1.34
20	AK	1001	ADP	C4-N3	3.72	1.41	1.34
20	AQ	1001	ADP	C4-N3	3.71	1.41	1.34
20	w	1001	ADP	C4-N3	3.69	1.41	1.34
18	AN	501	GTP	C4-N3	3.49	1.42	1.34
18	t	501	GTP	C4-N3	3.48	1.42	1.34
18	AF	501	GTP	C4-N3	3.39	1.42	1.34
18	u	502	GTP	C4-N3	3.38	1.42	1.34
18	AO	501	GTP	C4-N3	3.38	1.42	1.34
18	u	502	GTP	C2-N2	2.93	1.41	1.34
18	AF	501	GTP	C2-N2	2.93	1.41	1.34
18	AO	501	GTP	C2-N2	2.93	1.41	1.34
18	AN	501	GTP	C2-N2	2.91	1.41	1.34
18	t	501	GTP	C2-N2	2.91	1.41	1.34
20	AK	1001	ADP	C5-C4	2.84	1.44	1.39
20	AQ	1001	ADP	C5-C4	2.84	1.44	1.39
20	w	1001	ADP	C5-C4	2.84	1.44	1.39
20	AQ	1001	ADP	C5-N7	2.75	1.44	1.39
20	w	1001	ADP	C5-N7	2.74	1.44	1.39
20	AK	1001	ADP	C5-N7	2.72	1.44	1.39
20	AK	1001	ADP	C8-N9	2.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	w	1001	ADP	C8-N9	2.63	1.42	1.37
20	AQ	1001	ADP	C8-N9	2.63	1.42	1.37
18	AN	501	GTP	C6-N1	2.52	1.43	1.38
18	t	501	GTP	C6-N1	2.51	1.43	1.38
18	t	501	GTP	C2-N3	2.30	1.38	1.33
18	AO	501	GTP	C2-N3	2.28	1.38	1.33
18	u	502	GTP	C2-N3	2.28	1.38	1.33
18	AN	501	GTP	C2-N3	2.27	1.38	1.33
18	AF	501	GTP	C2-N3	2.27	1.38	1.33
20	w	1001	ADP	C5-C6	2.25	1.47	1.41
20	AK	1001	ADP	C5-C6	2.24	1.47	1.41
20	AQ	1001	ADP	C5-C6	2.22	1.47	1.41
18	u	502	GTP	O3'-C3'	-2.19	1.37	1.43
18	AF	501	GTP	O3'-C3'	-2.19	1.37	1.43
18	AO	501	GTP	O3'-C3'	-2.18	1.37	1.43
18	AN	501	GTP	O3'-C3'	-2.06	1.38	1.43
18	t	501	GTP	O3'-C3'	-2.06	1.38	1.43
20	AK	1001	ADP	C8-N7	2.06	1.35	1.31
20	AQ	1001	ADP	C8-N7	2.05	1.35	1.31
20	w	1001	ADP	C8-N7	2.03	1.35	1.31
18	AF	501	GTP	C4-N9	2.01	1.43	1.38

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AN	501	GTP	O5'-PA-O1A	-4.54	91.32	109.07
18	t	501	GTP	O5'-PA-O1A	-4.54	91.33	109.07
20	w	1001	ADP	O5'-PA-O1A	-4.36	92.01	109.07
20	AQ	1001	ADP	O5'-PA-O1A	-4.36	92.04	109.07
18	u	502	GTP	O5'-PA-O1A	-4.31	92.23	109.07
18	AO	501	GTP	O5'-PA-O1A	-4.30	92.27	109.07
20	AQ	1001	ADP	C5-C4-N3	-3.92	121.63	126.75
18	AO	501	GTP	C5-C4-N3	-3.89	122.15	128.46
18	u	502	GTP	C5-C4-N3	-3.89	122.15	128.46
20	AQ	1001	ADP	O4'-C1'-N9	3.89	115.72	108.06
20	w	1001	ADP	O4'-C1'-N9	3.88	115.71	108.06
18	AF	501	GTP	C5-C4-N3	-3.88	122.17	128.46
20	AK	1001	ADP	O4'-C1'-N9	3.88	115.70	108.06
20	w	1001	ADP	C5-C4-N3	-3.88	121.69	126.75
20	AK	1001	ADP	C5-C4-N3	-3.86	121.71	126.75
18	AN	501	GTP	C5-C4-N3	-3.69	122.48	128.46
18	t	501	GTP	C5-C4-N3	-3.67	122.50	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AQ	1001	ADP	N3-C4-N9	3.57	132.97	127.08
20	w	1001	ADP	N3-C4-N9	3.56	132.95	127.08
20	AK	1001	ADP	N3-C4-N9	3.54	132.92	127.08
20	AK	1001	ADP	O5'-PA-O1A	-3.41	95.73	109.07
20	AK	1001	ADP	O2A-PA-O5'	-3.39	92.01	107.75
18	AF	501	GTP	O2A-PA-O5'	-3.34	92.22	107.75
18	u	502	GTP	N9-C4-N3	3.15	132.26	125.94
18	AF	501	GTP	N9-C4-N3	3.14	132.25	125.94
18	AO	501	GTP	N9-C4-N3	3.14	132.25	125.94
18	AF	501	GTP	O5'-PA-O1A	-3.07	97.06	109.07
20	AQ	1001	ADP	C5-N7-C8	3.00	107.77	103.51
20	AK	1001	ADP	C5-N7-C8	2.99	107.76	103.51
20	w	1001	ADP	C5-N7-C8	2.99	107.76	103.51
18	AN	501	GTP	N9-C4-N3	2.88	131.72	125.94
18	t	501	GTP	N9-C4-N3	2.88	131.72	125.94
20	AK	1001	ADP	C1'-N9-C8	-2.73	120.97	127.14
20	w	1001	ADP	C1'-N9-C8	-2.72	121.00	127.14
20	AQ	1001	ADP	C1'-N9-C8	-2.71	121.02	127.14
18	AF	501	GTP	C1'-N9-C4	2.60	134.23	126.50
18	AO	501	GTP	C1'-N9-C4	2.60	134.22	126.50
18	u	502	GTP	C1'-N9-C4	2.60	134.22	126.50
20	w	1001	ADP	O2A-PA-O5'	-2.59	95.71	107.75
18	AN	501	GTP	O6-C6-N1	-2.59	115.16	120.12
20	AQ	1001	ADP	O2A-PA-O5'	-2.58	95.75	107.75
18	t	501	GTP	O6-C6-N1	-2.56	115.21	120.12
18	AO	501	GTP	O6-C6-N1	-2.52	115.29	120.12
18	u	502	GTP	O6-C6-N1	-2.52	115.29	120.12
18	AF	501	GTP	O6-C6-N1	-2.51	115.30	120.12
18	u	502	GTP	O2G-PG-O3B	2.50	113.02	104.64
18	AO	501	GTP	O2G-PG-O3B	2.50	113.00	104.64
20	AK	1001	ADP	C4-N9-C1'	2.47	132.49	126.59
20	w	1001	ADP	C4-N9-C1'	2.46	132.45	126.59
20	AQ	1001	ADP	C4-N9-C1'	2.45	132.43	126.59
18	AF	501	GTP	C2-N3-C4	2.41	116.59	112.30
18	AO	501	GTP	C2-N3-C4	2.41	116.59	112.30
18	u	502	GTP	C2-N3-C4	2.41	116.59	112.30
18	AN	501	GTP	O2G-PG-O3B	2.39	112.65	104.64
18	AN	501	GTP	O2A-PA-O5'	-2.39	96.66	107.75
18	t	501	GTP	O2A-PA-O5'	-2.38	96.69	107.75
18	t	501	GTP	O2G-PG-O3B	2.38	112.61	104.64
18	AN	501	GTP	C2-N3-C4	2.37	116.52	112.30
18	t	501	GTP	C2-N3-C4	2.37	116.51	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AN	501	GTP	C2-N1-C6	-2.30	120.90	125.10
18	AO	501	GTP	O2A-PA-O5'	-2.30	97.07	107.75
18	u	502	GTP	O2A-PA-O5'	-2.30	97.08	107.75
18	t	501	GTP	C2-N1-C6	-2.27	120.96	125.10
18	u	502	GTP	C2-N1-C6	-2.25	121.00	125.10
18	AF	501	GTP	C2-N1-C6	-2.24	121.02	125.10
18	AO	501	GTP	C2-N1-C6	-2.23	121.03	125.10
20	AQ	1001	ADP	C2-N3-C4	2.23	117.02	111.75
18	AO	501	GTP	C4'-O4'-C1'	2.22	114.37	109.47
20	w	1001	ADP	C2-N3-C4	2.22	116.99	111.75
20	AK	1001	ADP	C2-N3-C4	2.21	116.97	111.75
18	AF	501	GTP	C4'-O4'-C1'	2.21	114.34	109.47
18	u	502	GTP	C4'-O4'-C1'	2.20	114.33	109.47
20	AQ	1001	ADP	C2'-C1'-N9	-2.19	107.77	113.30
20	w	1001	ADP	C2'-C1'-N9	-2.18	107.78	113.30
20	AK	1001	ADP	C2'-C1'-N9	-2.17	107.79	113.30
20	AQ	1001	ADP	N3-C2-N1	-2.16	125.23	128.60
20	w	1001	ADP	N3-C2-N1	-2.15	125.24	128.60
20	AK	1001	ADP	N3-C2-N1	-2.15	125.24	128.60
20	w	1001	ADP	O3B-PB-O2B	2.14	115.80	107.64
20	AQ	1001	ADP	O3B-PB-O2B	2.14	115.80	107.64
18	AN	501	GTP	C2'-C3'-C4'	-2.12	98.53	102.64
18	t	501	GTP	C2'-C3'-C4'	-2.11	98.55	102.64
18	AN	501	GTP	O4'-C4'-C5'	2.10	116.29	109.37
18	t	501	GTP	O4'-C4'-C5'	2.10	116.28	109.37
20	AK	1001	ADP	O3A-PB-O1B	-2.10	99.54	111.19
18	t	501	GTP	C1'-N9-C4	2.09	132.72	126.50
18	AN	501	GTP	C1'-N9-C4	2.09	132.71	126.50
18	AN	501	GTP	O4'-C1'-N9	2.03	113.01	108.36
18	t	501	GTP	O4'-C1'-N9	2.03	113.00	108.36

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	t	501	GTP	C5'-O5'-PA-O3A
18	t	501	GTP	C5'-O5'-PA-O1A
18	u	502	GTP	C5'-O5'-PA-O3A
18	u	502	GTP	C5'-O5'-PA-O2A
18	u	502	GTP	O4'-C4'-C5'-O5'
18	u	502	GTP	C3'-C4'-C5'-O5'
18	AF	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
18	AF	501	GTP	O4'-C4'-C5'-O5'
18	AF	501	GTP	C3'-C4'-C5'-O5'
18	AO	501	GTP	C5'-O5'-PA-O3A
18	AO	501	GTP	C5'-O5'-PA-O2A
18	AO	501	GTP	O4'-C4'-C5'-O5'
18	AO	501	GTP	C3'-C4'-C5'-O5'
18	AN	501	GTP	C5'-O5'-PA-O3A
18	AN	501	GTP	C5'-O5'-PA-O1A
20	w	1001	ADP	PA-O3A-PB-O3B
20	w	1001	ADP	O4'-C4'-C5'-O5'
20	AK	1001	ADP	PA-O3A-PB-O2B
20	AK	1001	ADP	PA-O3A-PB-O3B
20	AK	1001	ADP	O4'-C4'-C5'-O5'
20	AQ	1001	ADP	PA-O3A-PB-O3B
20	AQ	1001	ADP	O4'-C4'-C5'-O5'
18	t	501	GTP	O4'-C4'-C5'-O5'
18	AN	501	GTP	O4'-C4'-C5'-O5'
20	w	1001	ADP	C3'-C4'-C5'-O5'
20	AK	1001	ADP	C3'-C4'-C5'-O5'
20	AQ	1001	ADP	C3'-C4'-C5'-O5'
18	t	501	GTP	C3'-C4'-C5'-O5'
18	AN	501	GTP	C3'-C4'-C5'-O5'
18	u	502	GTP	PG-O3B-PB-O1B
18	AO	501	GTP	PG-O3B-PB-O1B
20	w	1001	ADP	C2'-C1'-N9-C8
20	AK	1001	ADP	C2'-C1'-N9-C8
20	AQ	1001	ADP	C2'-C1'-N9-C8
18	u	502	GTP	C5'-O5'-PA-O1A
18	AF	501	GTP	C5'-O5'-PA-O1A
18	AF	501	GTP	C5'-O5'-PA-O2A
18	AO	501	GTP	C5'-O5'-PA-O1A
18	u	502	GTP	PG-O3B-PB-O2B
18	AO	501	GTP	PG-O3B-PB-O2B
20	w	1001	ADP	C2'-C1'-N9-C4
20	AK	1001	ADP	C2'-C1'-N9-C4
20	AQ	1001	ADP	C2'-C1'-N9-C4
20	w	1001	ADP	PA-O3A-PB-O1B
20	AQ	1001	ADP	PA-O3A-PB-O1B
20	w	1001	ADP	O4'-C1'-N9-C8
20	AK	1001	ADP	O4'-C1'-N9-C8
20	AQ	1001	ADP	O4'-C1'-N9-C8
18	u	502	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
18	u	502	GTP	PA-O3A-PB-O2B
18	AF	501	GTP	PG-O3B-PB-O1B
18	AO	501	GTP	PA-O3A-PB-O1B
18	AO	501	GTP	PA-O3A-PB-O2B
20	w	1001	ADP	C5'-O5'-PA-O1A
20	AQ	1001	ADP	C5'-O5'-PA-O1A
20	AK	1001	ADP	PA-O3A-PB-O1B

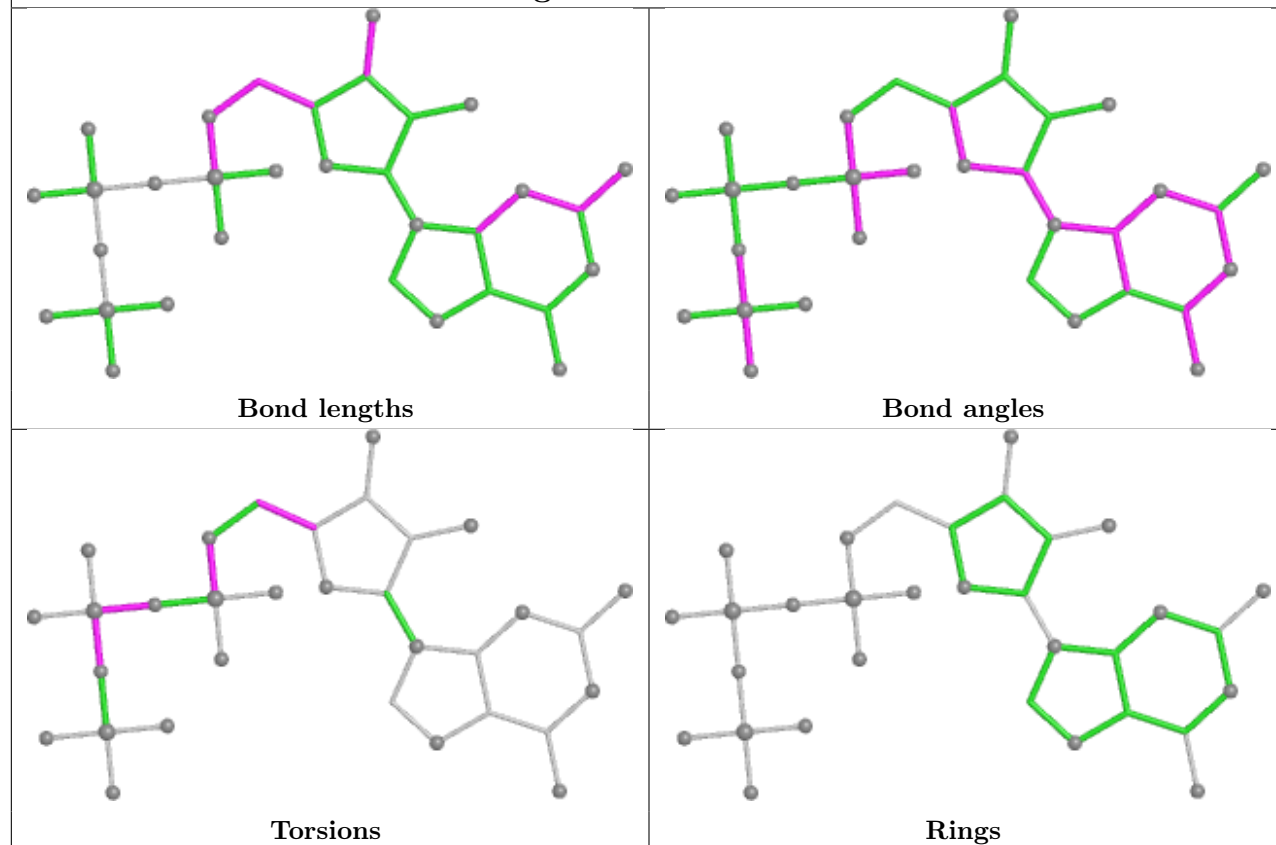
There are no ring outliers.

5 monomers are involved in 28 short contacts:

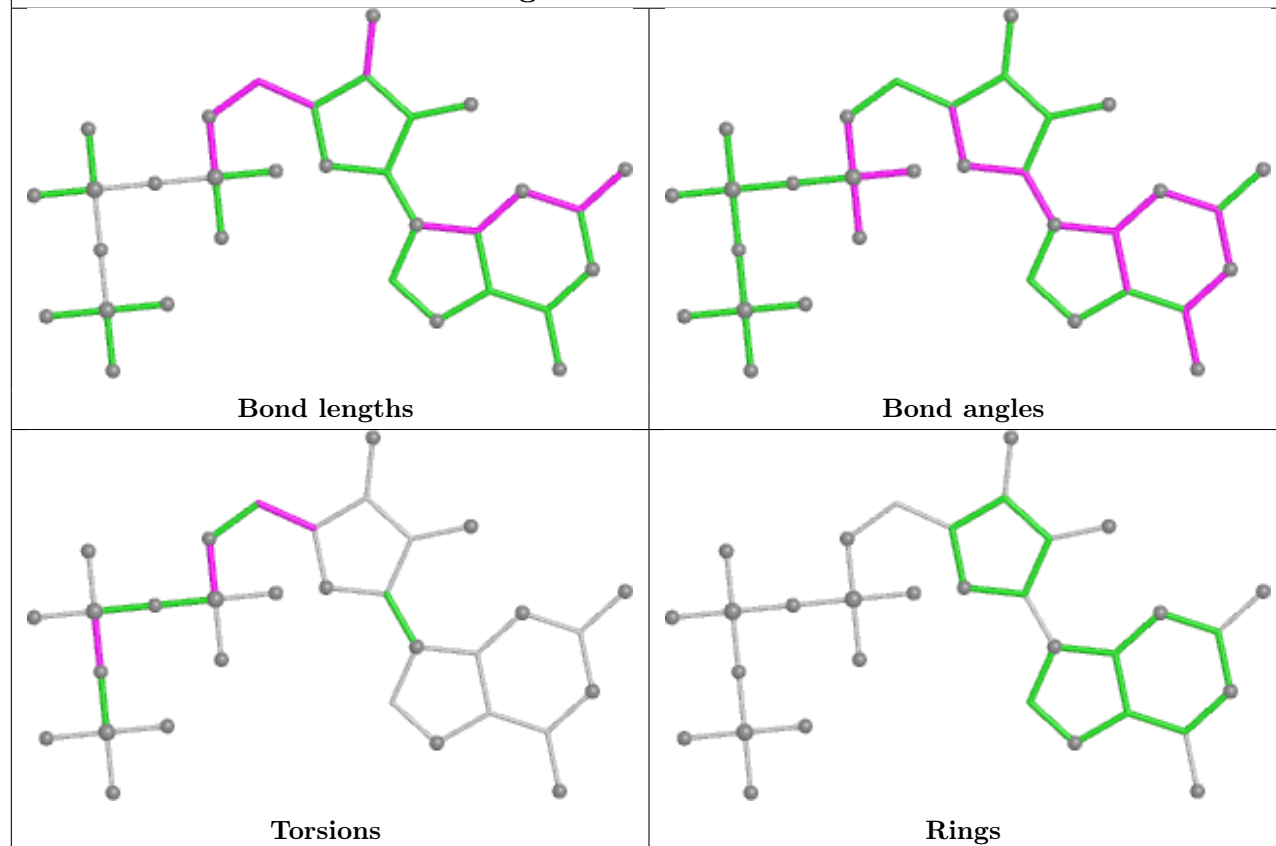
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	u	502	GTP	2	0
18	AF	501	GTP	9	0
18	t	501	GTP	8	0
18	AO	501	GTP	2	0
18	AN	501	GTP	7	0

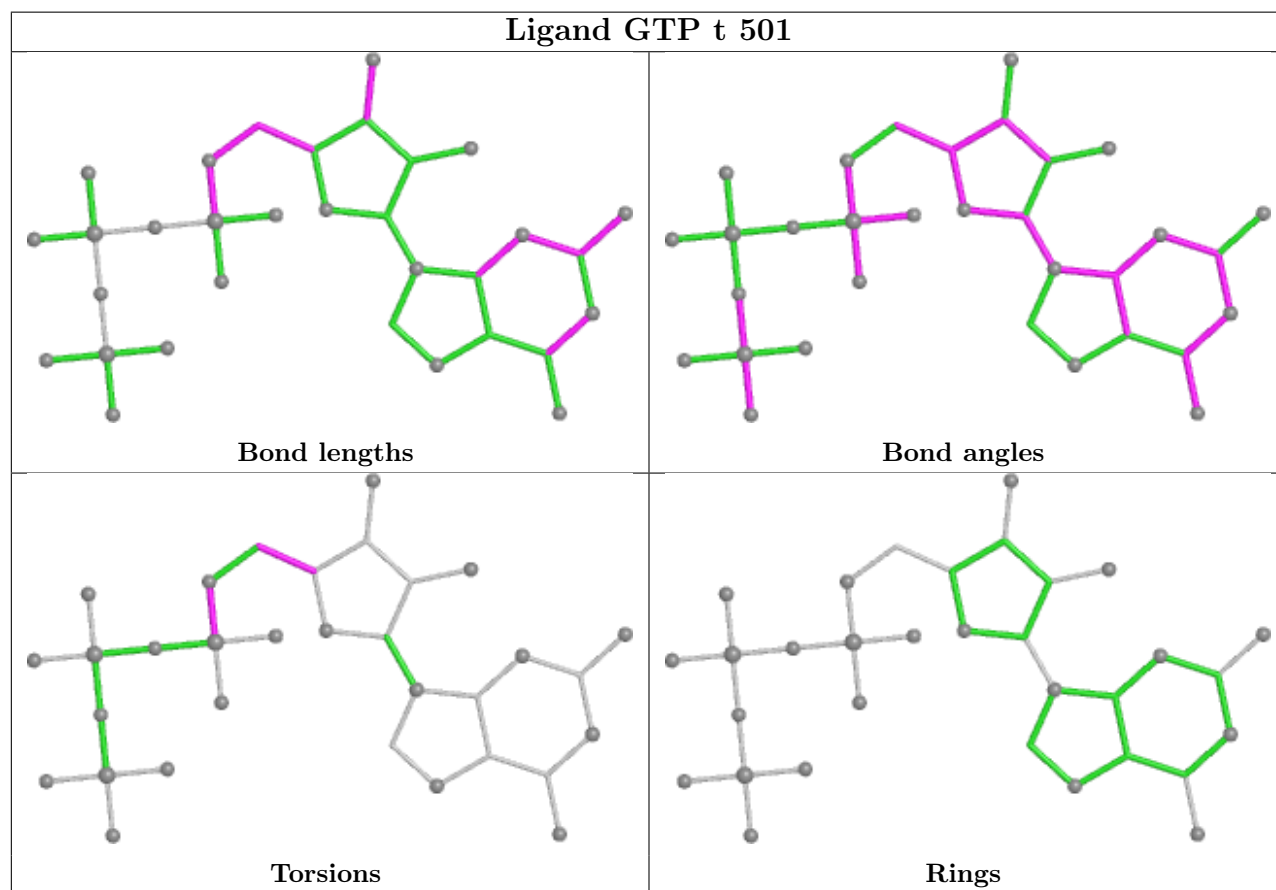
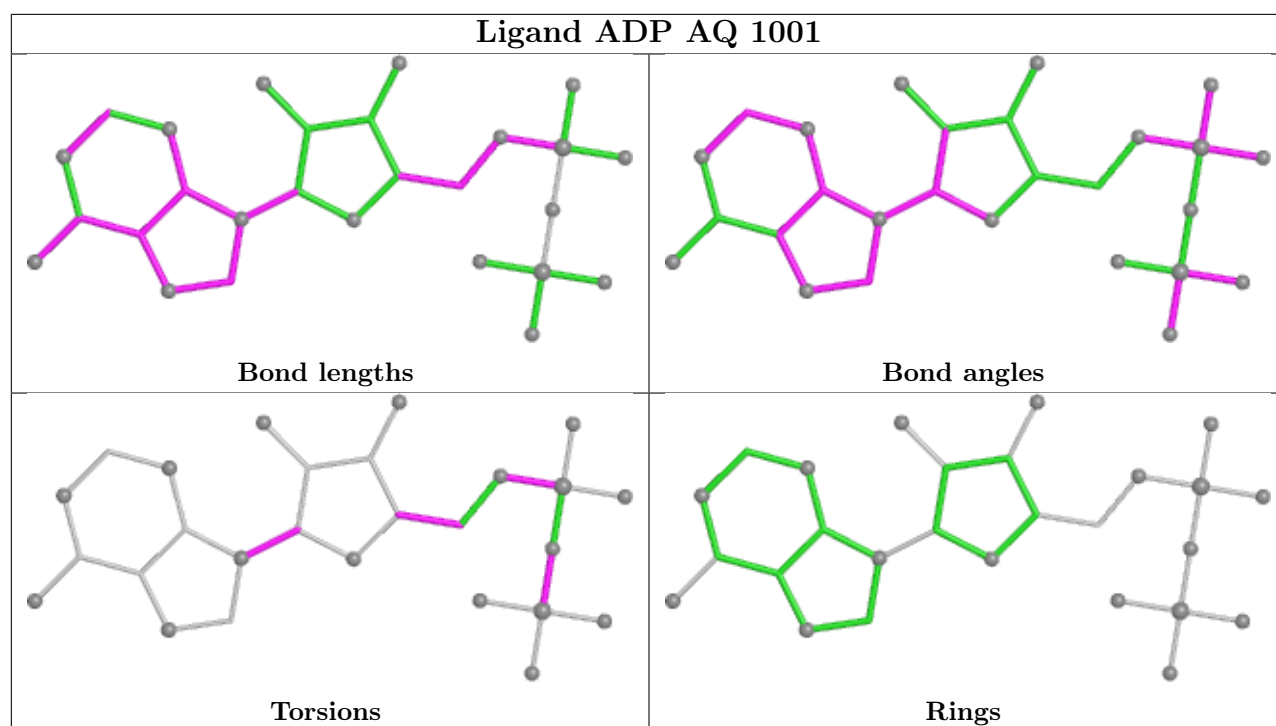
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

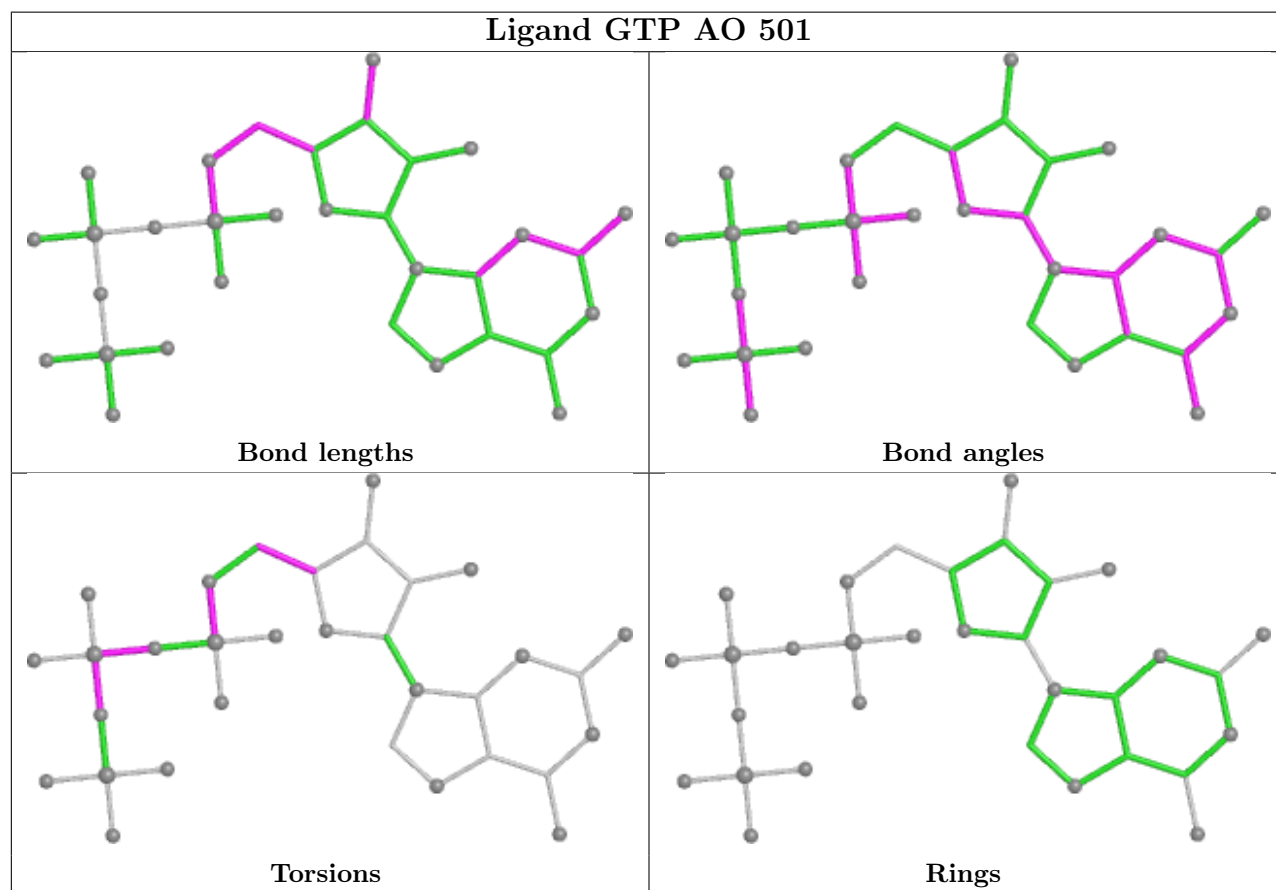
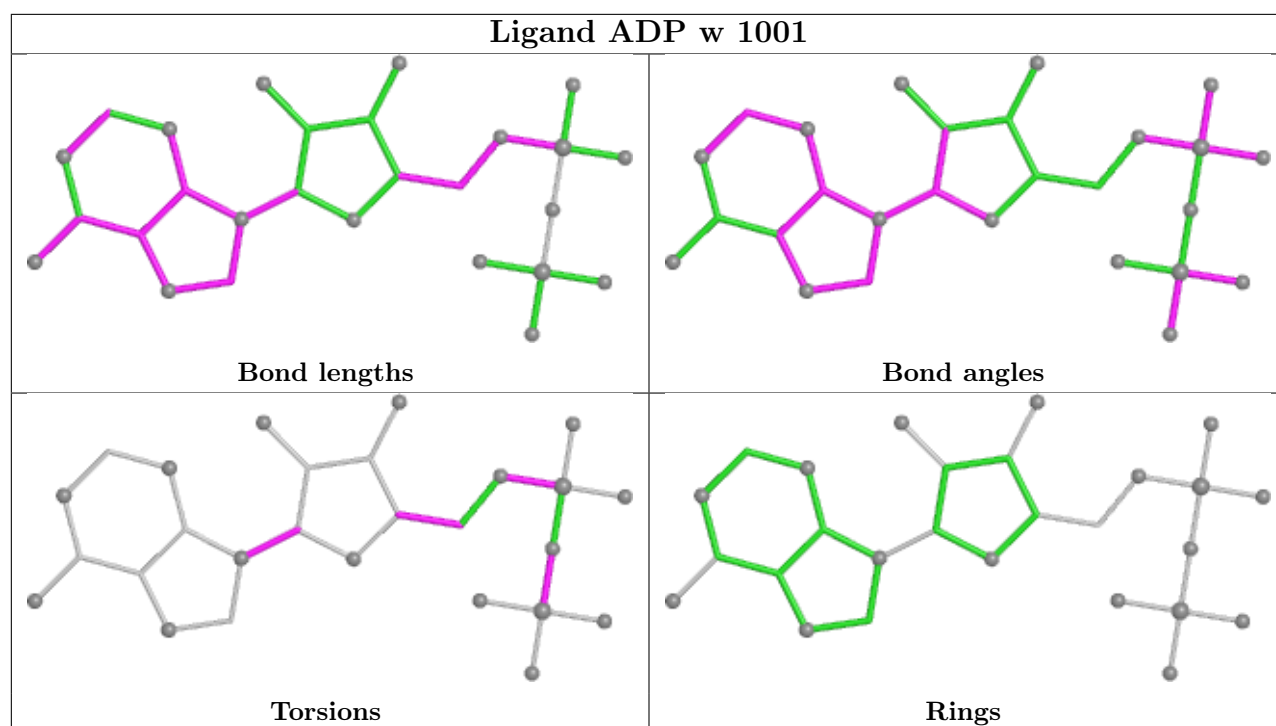
Ligand GTP u 502

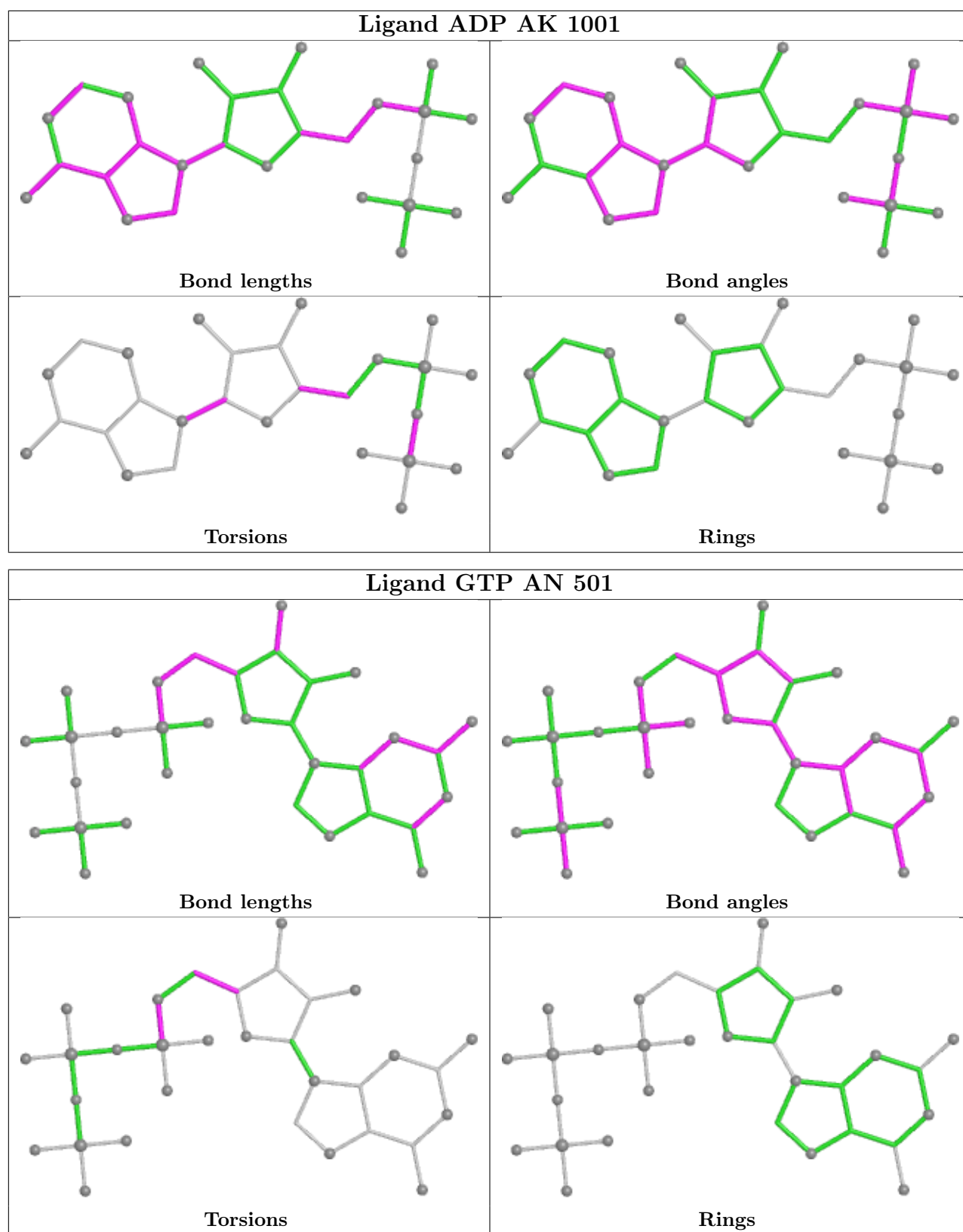


Ligand GTP AF 501









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

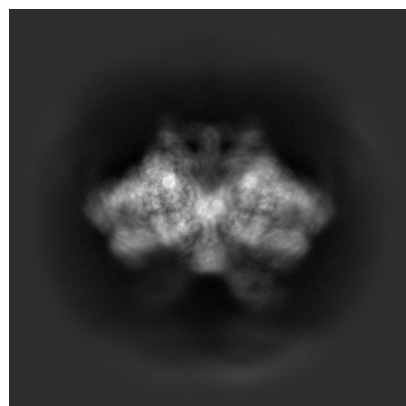
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67147. These allow visual inspection of the internal detail of the map and identification of artifacts.

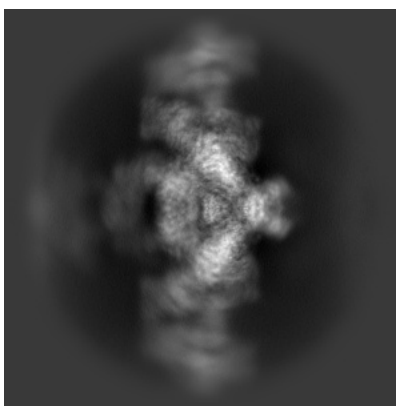
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

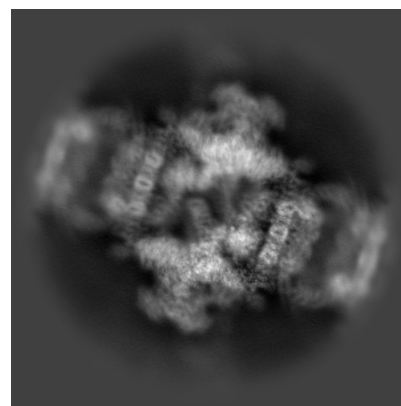
6.1.1 Primary map



X

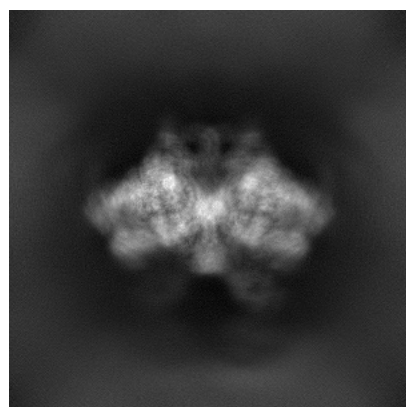


Y

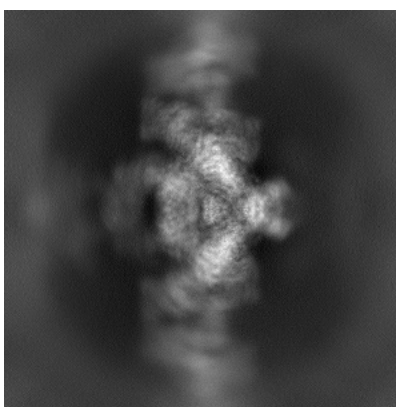


Z

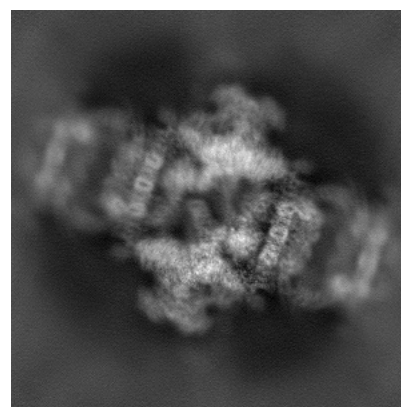
6.1.2 Raw map



X



Y

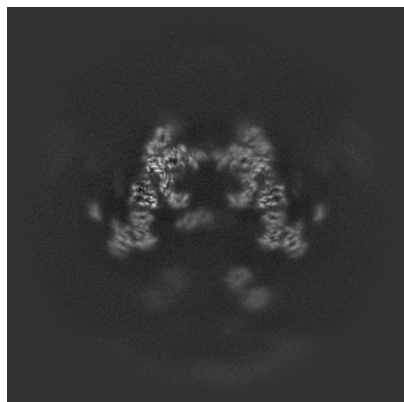


Z

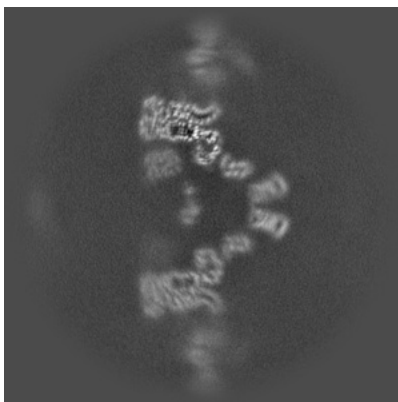
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

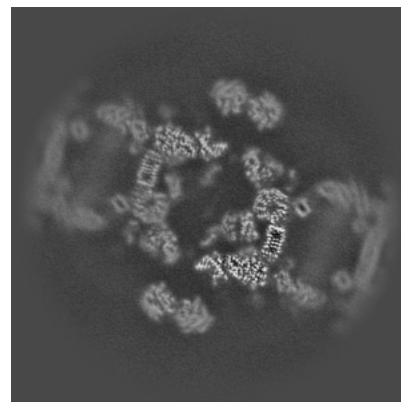
6.2.1 Primary map



X Index: 256

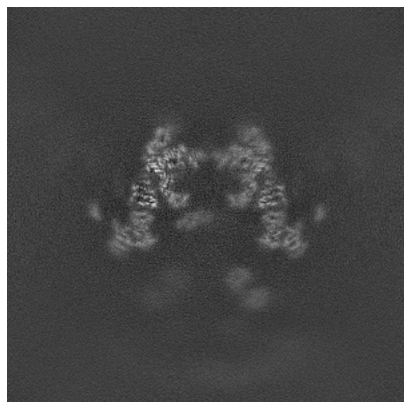


Y Index: 256

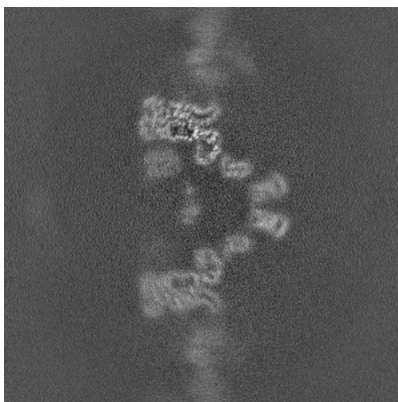


Z Index: 256

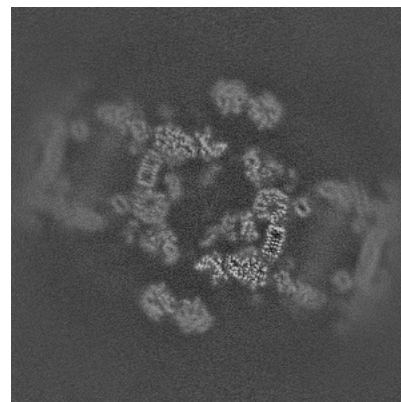
6.2.2 Raw map



X Index: 256



Y Index: 256

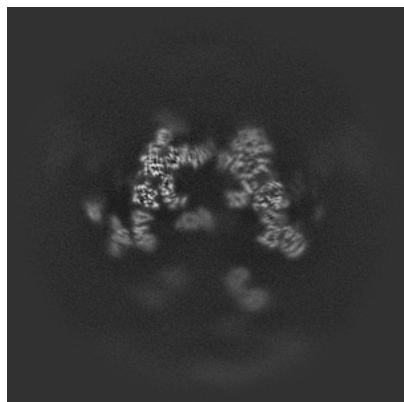


Z Index: 256

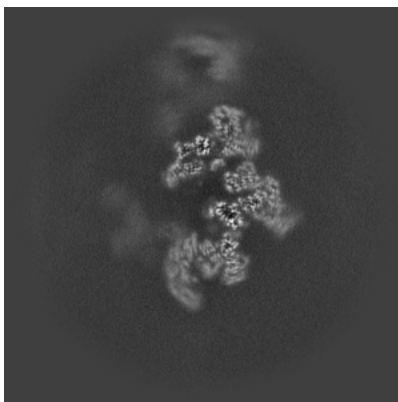
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

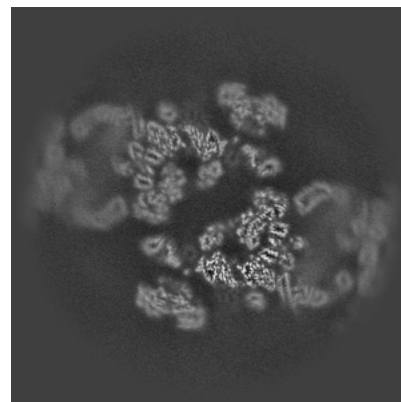
6.3.1 Primary map



X Index: 252

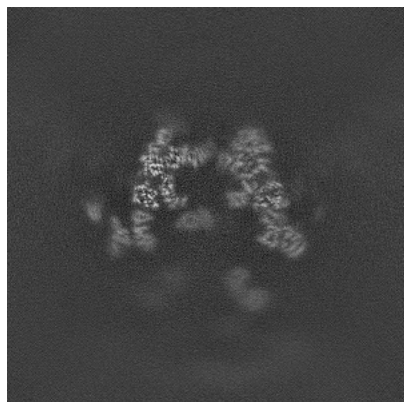


Y Index: 205

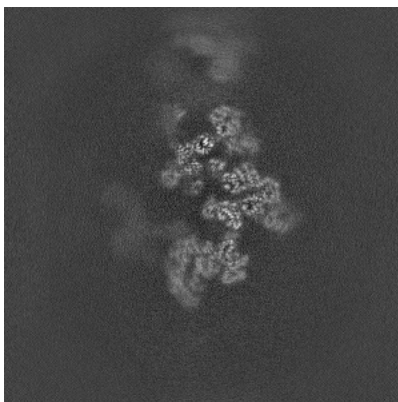


Z Index: 267

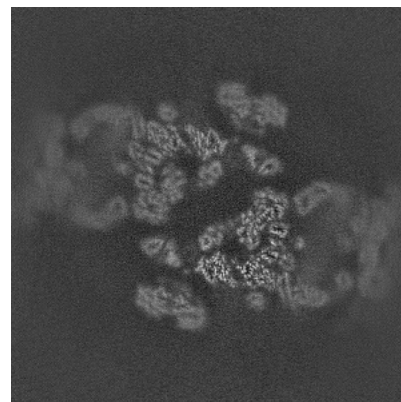
6.3.2 Raw map



X Index: 252



Y Index: 209

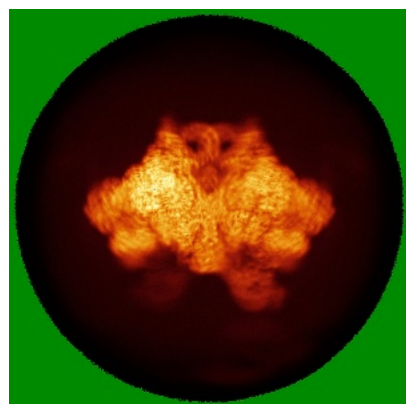


Z Index: 266

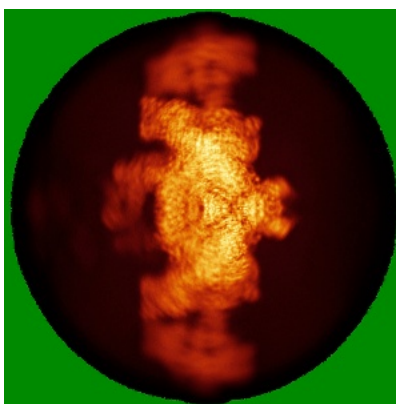
The images above show the largest variance slices of the map in three orthogonal directions.

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

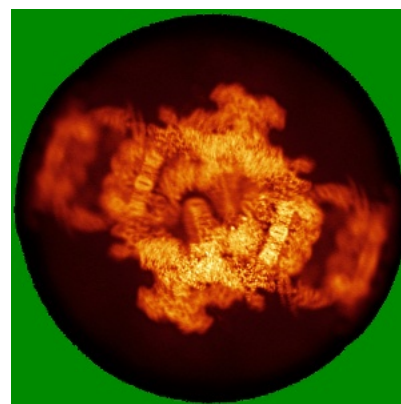
6.4.1 Primary map



X

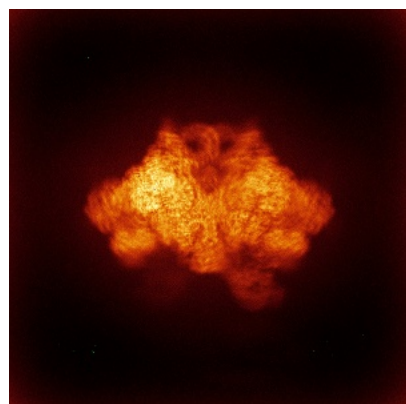


Y

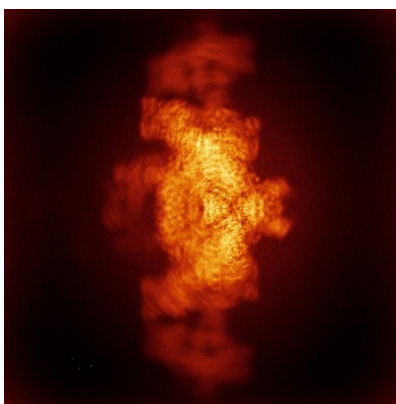


Z

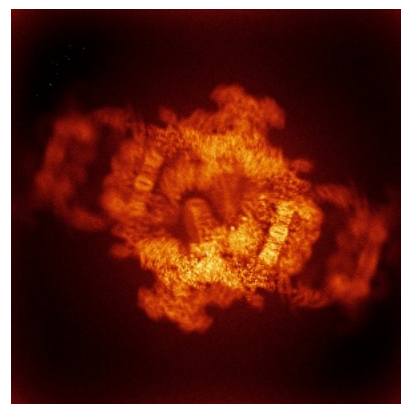
6.4.2 Raw map



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.

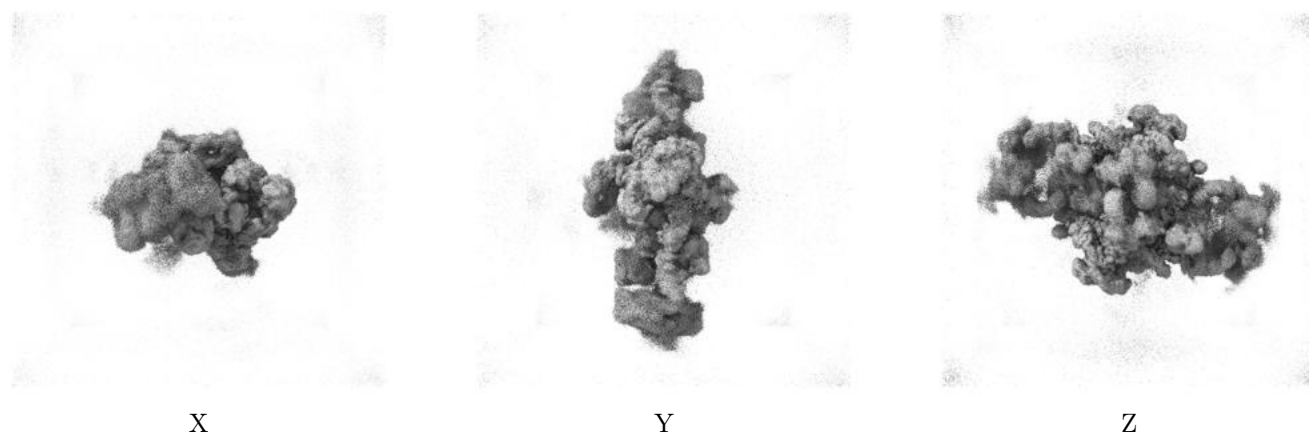
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

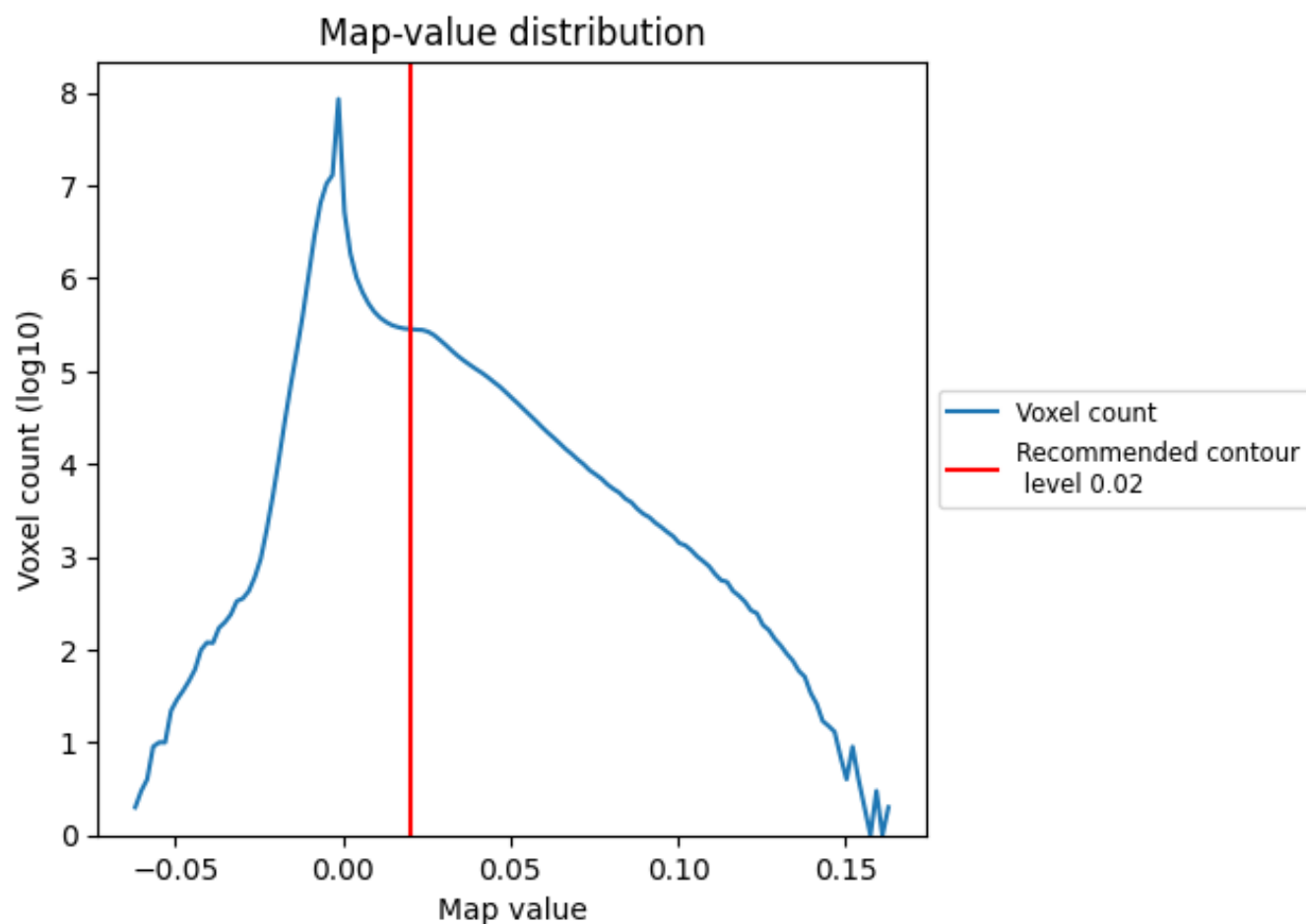
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

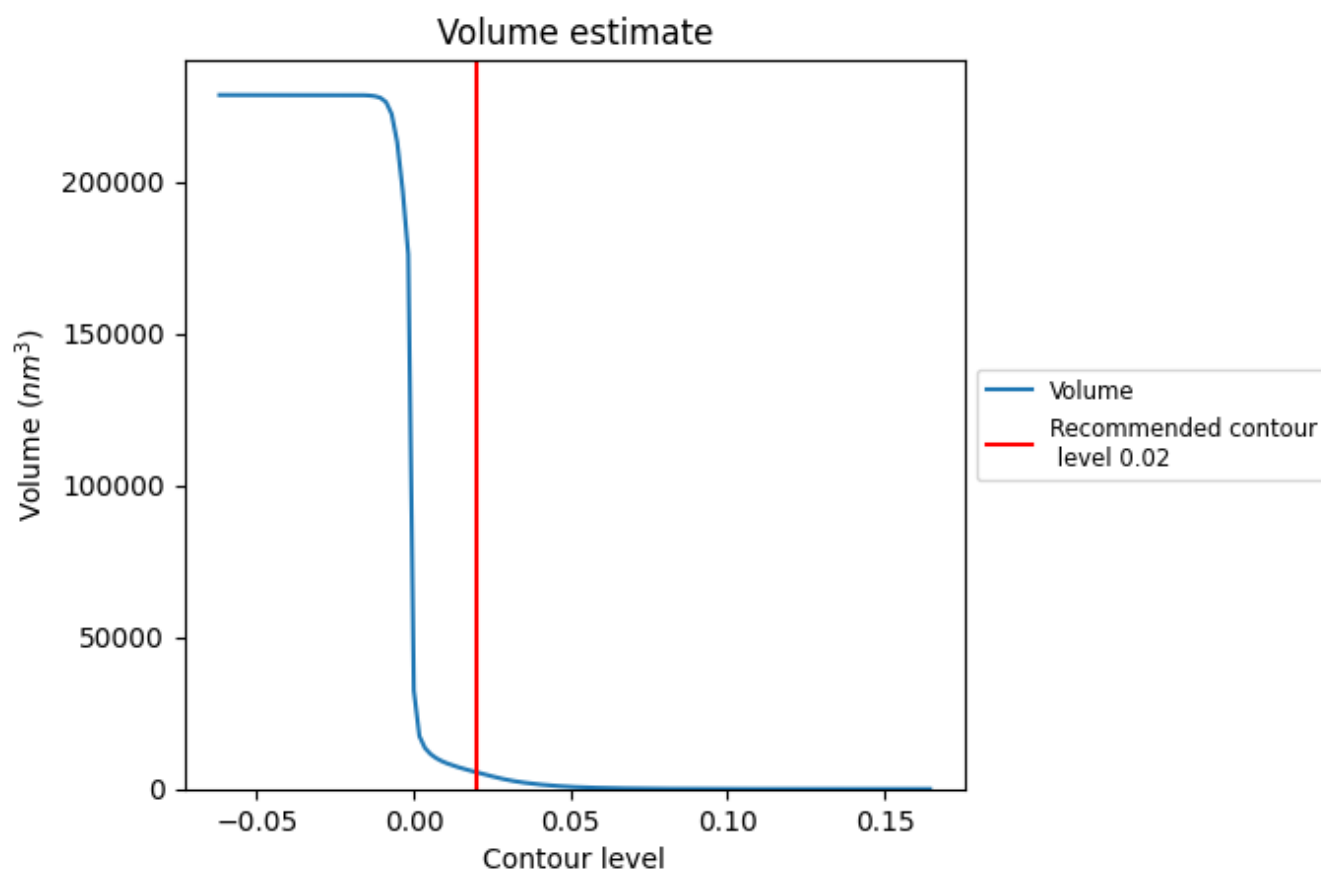
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

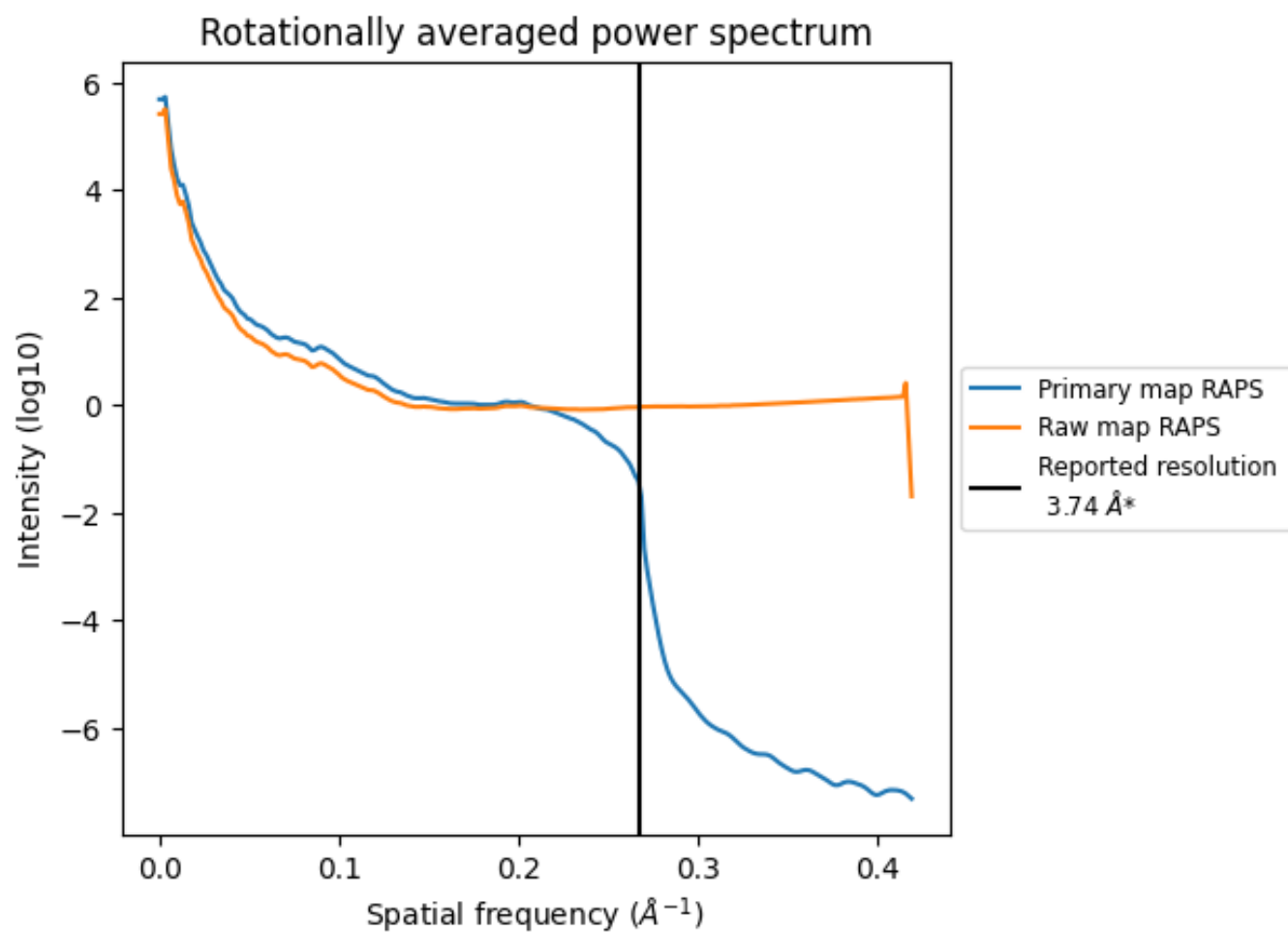
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5490 nm^3 ; this corresponds to an approximate mass of 4959 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

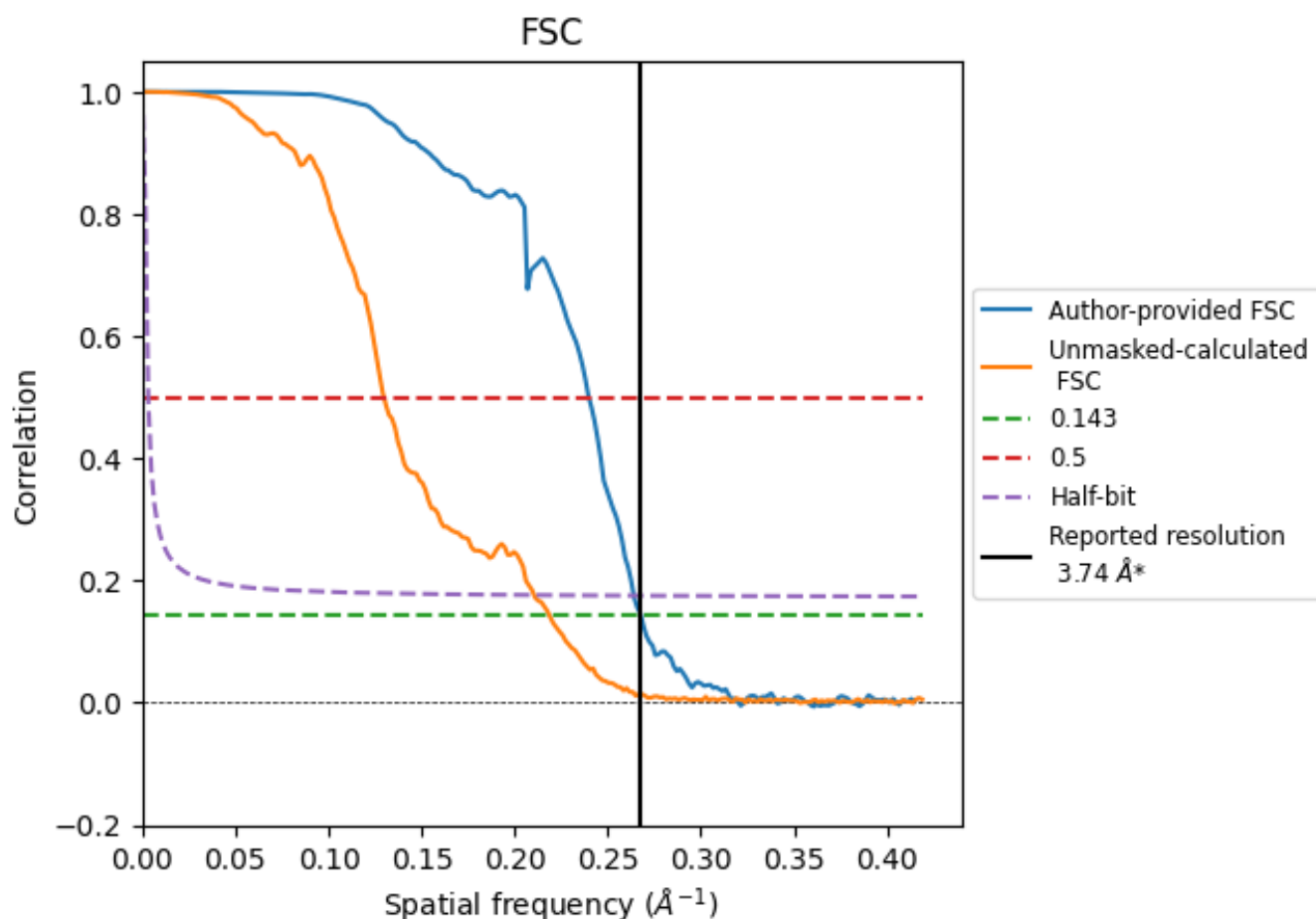


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.267 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

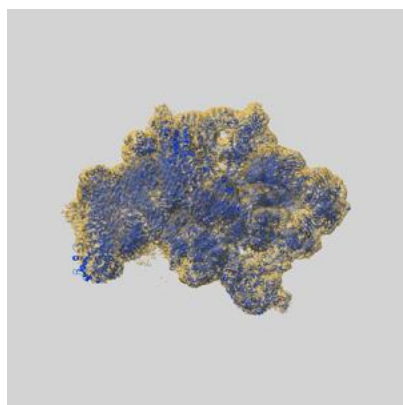
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	3.74	4.17	3.79
Unmasked-calculated*	4.57	7.70	4.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.74 by more than 10 %

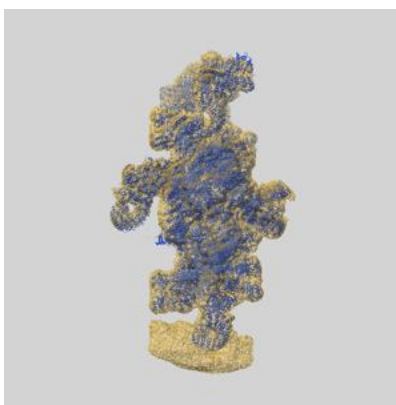
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67147 and PDB model 9XRL. Per-residue inclusion information can be found in section 3 on page 14.

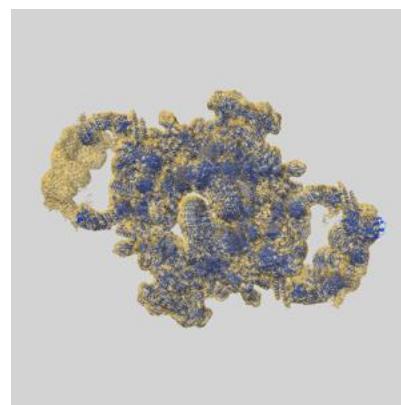
9.1 Map-model overlay [i](#)



X



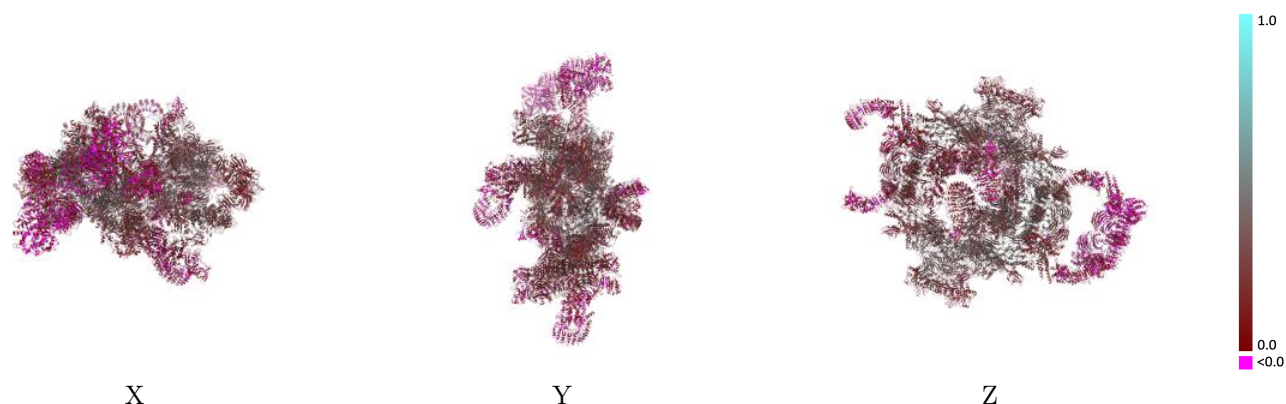
Y



Z

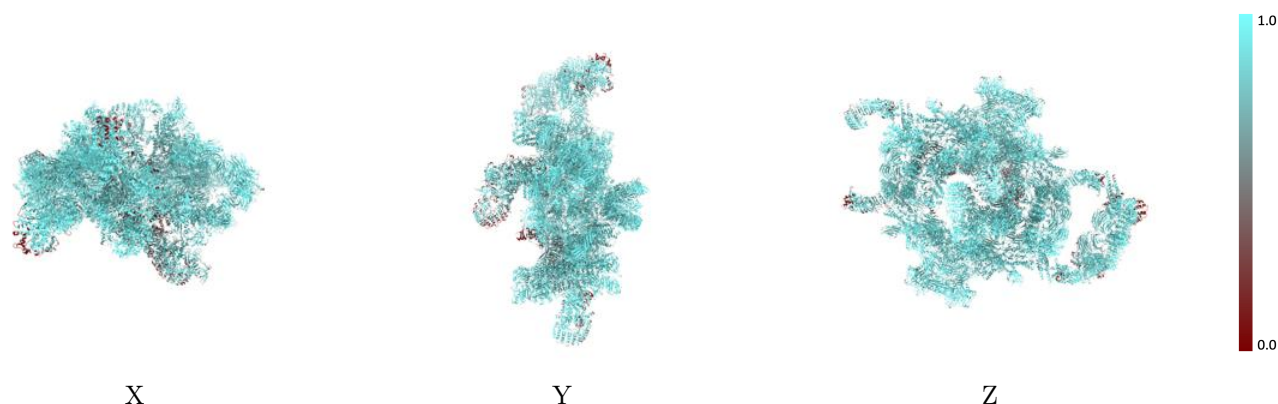
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



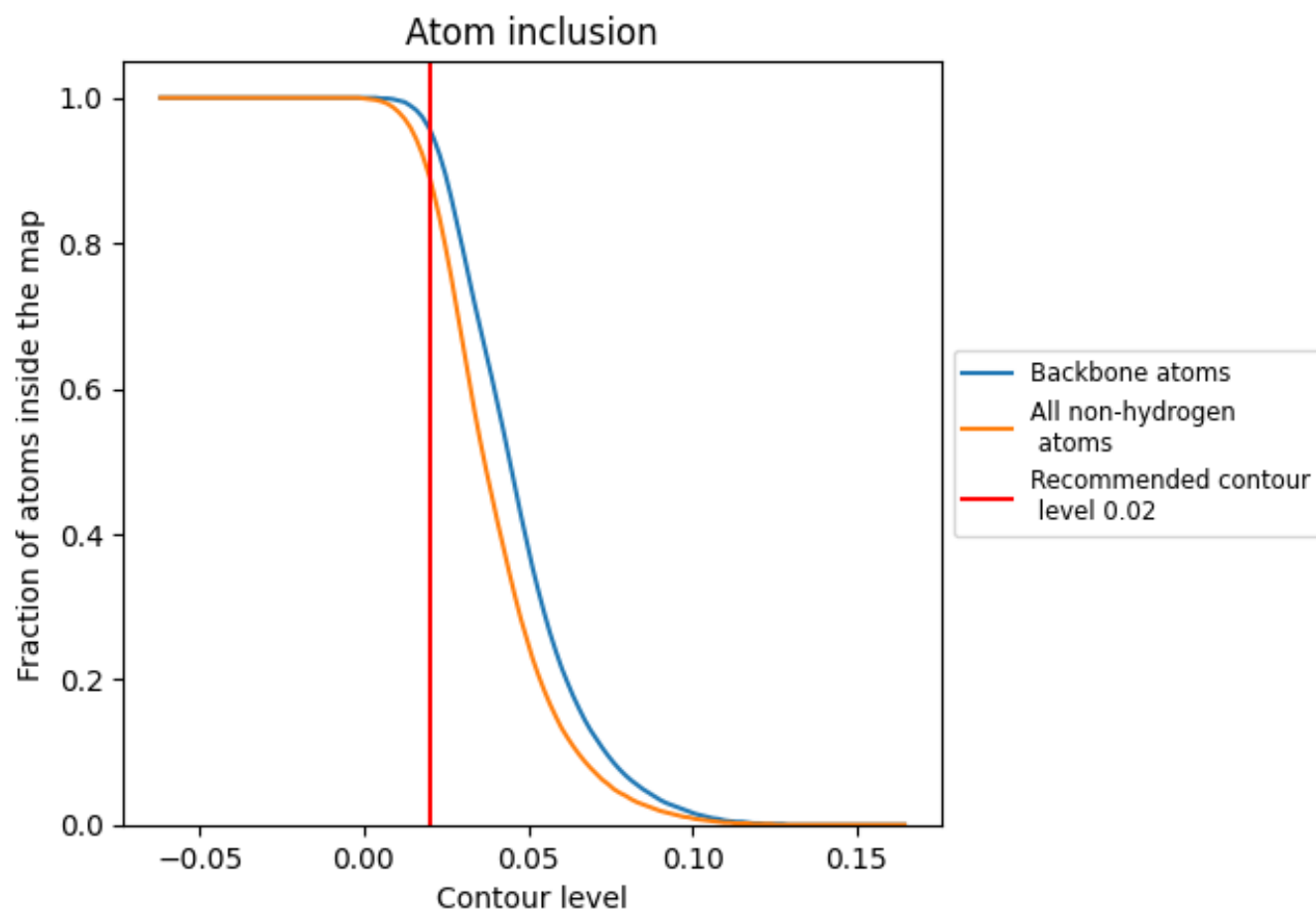
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.2210
0	 0.9230	 0.1970
1	 0.9500	 0.0520
2	 0.8070	 0.0420
3	 0.9770	 0.3130
4	 0.7940	 0.0550
5	 0.9350	 0.3000
6	 0.8910	 0.2380
7	 0.9360	 0.2900
8	 0.9500	 0.3220
9	 0.9750	 0.2030
A	 0.8610	 0.3070
AA	 0.8810	 0.1810
AB	 0.9250	 0.1700
AC	 0.9380	 0.1690
AD	 0.9340	 0.3040
AE	 0.5320	 0.1740
AF	 0.6800	 0.1420
AH	 0.8430	 0.0440
AI	 0.9180	 0.2630
AJ	 0.9170	 0.1740
AK	 0.6820	 0.1000
AL	 0.7360	 0.1370
AM	 0.8510	 0.2130
AN	 0.9240	 0.3320
AO	 0.9440	 0.3190
AQ	 0.9510	 0.2420
AR	 0.9550	 0.2810
AS	 0.9500	 0.3830
AT	 0.9150	 0.1490
B	 0.9260	 0.3630
C	 0.9340	 0.3720
D	 0.8730	 0.2040
E	 0.8630	 0.0410
F	 0.6860	 0.1460



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Chain	Atom inclusion	Q-score
H	 0.8650	 0.1240
I	 0.9440	 0.3000
K	 0.9180	 0.3270
L	 0.5670	 0.1310
O	 0.1290	 0.0530
P	 0.9370	 0.1550
Q	 0.7620	 0.0900
S	 0.9200	 0.2420
T	 0.9210	 0.1710
U	 0.9430	 0.3870
V	 0.9590	 0.3570
W	 0.9510	 0.2410
X	 0.9560	 0.2240
Y	 0.9650	 0.2340
Z	 0.9580	 0.2110
b	 0.9460	 0.3760
c	 0.9360	 0.3450
d	 0.9510	 0.3090
e	 0.8650	 0.0460
f	 0.9330	 0.2860
g	 0.9500	 0.2860
h	 0.8300	 0.0970
i	 0.8730	 0.1480
j	 0.9390	 0.2940
k	 0.9430	 0.3340
l	 0.9330	 0.1990
m	 0.9470	 0.2570
n	 0.9600	 0.2210
o	 0.9520	 0.2020
p	 0.8820	 0.1770
q	 0.8210	 0.1170
r	 0.9250	 0.3170
s	 0.9370	 0.3240
t	 0.9220	 0.1800
u	 0.9340	 0.1900
w	 0.9210	 0.1480
x	 0.9290	 0.2020
y	 0.8270	 0.0440
z	 0.8600	 0.0320