



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:40 AM UTC

PDB ID : 8BMO / pdb_00008bmo
EMDB ID : EMD-16119
Title : Structure of GroEL:GroES complex exhibiting ADP-conformation in trans ring obtained under the continuous turnover conditions
Authors : Dhurandhar, M.; Torino, S.; Efremov, R.
Deposited on : 2022-11-10
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

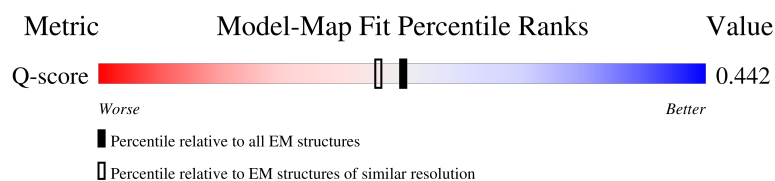
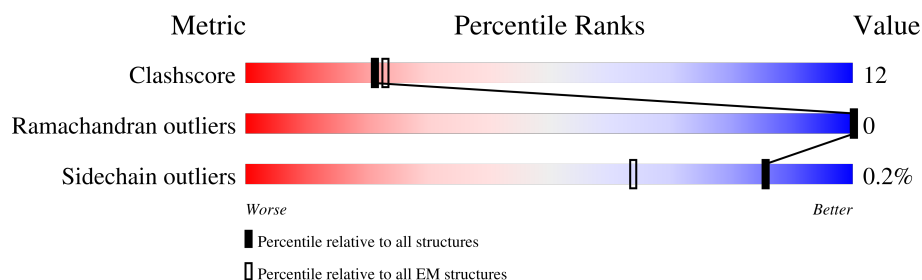
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



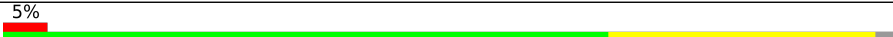
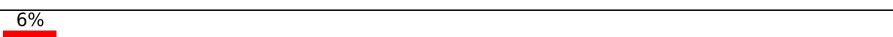
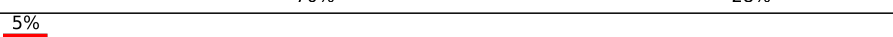
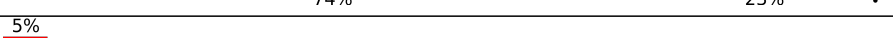
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	E	548	

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Mol	Chain	Length	Quality of chain
1	F	548	
1	H	548	
1	I	548	
1	J	548	
1	L	548	
1	M	548	
1	O	548	
1	P	548	
1	R	548	
1	S	548	
2	D	98	
2	G	98	
2	K	98	
2	N	98	
2	Q	98	
2	T	98	
2	W	98	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 59346 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 Chaperonin GroEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	524	Total	C	N	O	S	0	0
			3849	2394	662	773	20		
1	I	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	A	524	Total	C	N	O	S	0	0
			3849	2394	662	773	20		
1	B	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	E	524	Total	C	N	O	S	0	0
			3849	2394	662	773	20		
1	F	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	H	524	Total	C	N	O	S	0	0
			3849	2394	662	773	20		
1	J	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	L	524	Total	C	N	O	S	0	0
			3849	2394	662	773	20		
1	M	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	O	524	Total	C	N	O	S	0	0
			3849	2394	662	773	20		
1	P	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	R	524	Total	C	N	O	S	0	0
			3849	2394	662	773	20		
1	S	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		

- Molecule 2 is a protein called Co-chaperonin GroES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	96	Total	C	N	O	S	0	0
			714	444	125	144	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	96	Total	C	N	O	S	0	0
			714	444	125	144	1		
2	G	96	Total	C	N	O	S	0	0
			714	444	125	144	1		
2	K	96	Total	C	N	O	S	0	0
			714	444	125	144	1		
2	N	96	Total	C	N	O	S	0	0
			714	444	125	144	1		
2	Q	96	Total	C	N	O	S	0	0
			714	444	125	144	1		
2	T	96	Total	C	N	O	S	0	0
			714	444	125	144	1		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	0	MET	-	initiating methionine	UNP P0A6F9
W	1	ALA	-	expression tag	UNP P0A6F9
D	0	MET	-	initiating methionine	UNP P0A6F9
D	1	ALA	-	expression tag	UNP P0A6F9
G	0	MET	-	initiating methionine	UNP P0A6F9
G	1	ALA	-	expression tag	UNP P0A6F9
K	0	MET	-	initiating methionine	UNP P0A6F9
K	1	ALA	-	expression tag	UNP P0A6F9
N	0	MET	-	initiating methionine	UNP P0A6F9
N	1	ALA	-	expression tag	UNP P0A6F9
Q	0	MET	-	initiating methionine	UNP P0A6F9
Q	1	ALA	-	expression tag	UNP P0A6F9
T	0	MET	-	initiating methionine	UNP P0A6F9
T	1	ALA	-	expression tag	UNP P0A6F9

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

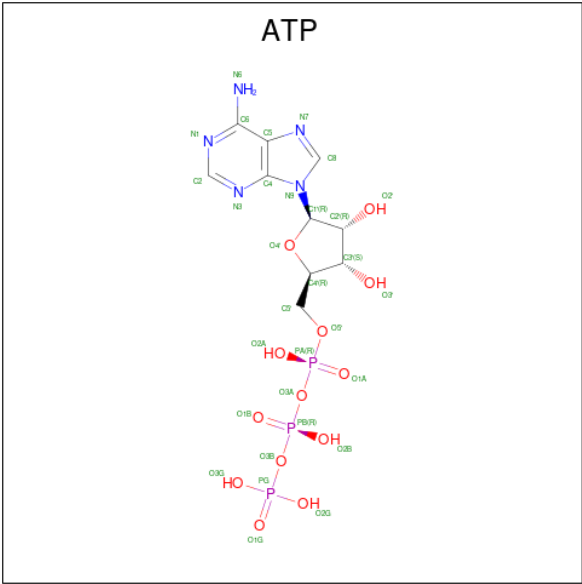
Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Mg	0
			1	1	
3	I	1	Total	Mg	0
			1	1	
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	
3	H	1	Total	Mg	0
			1	1	
3	J	1	Total	Mg	0
			1	1	
3	L	1	Total	Mg	0
			1	1	
3	M	1	Total	Mg	0
			1	1	
3	O	1	Total	Mg	0
			1	1	
3	P	1	Total	Mg	0
			1	1	
3	R	1	Total	Mg	0
			1	1	
3	S	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



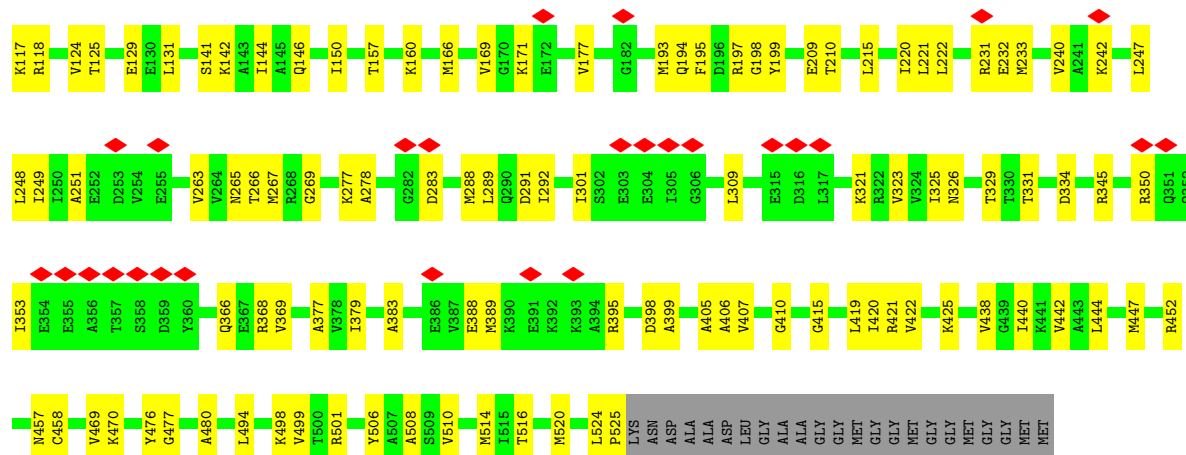
Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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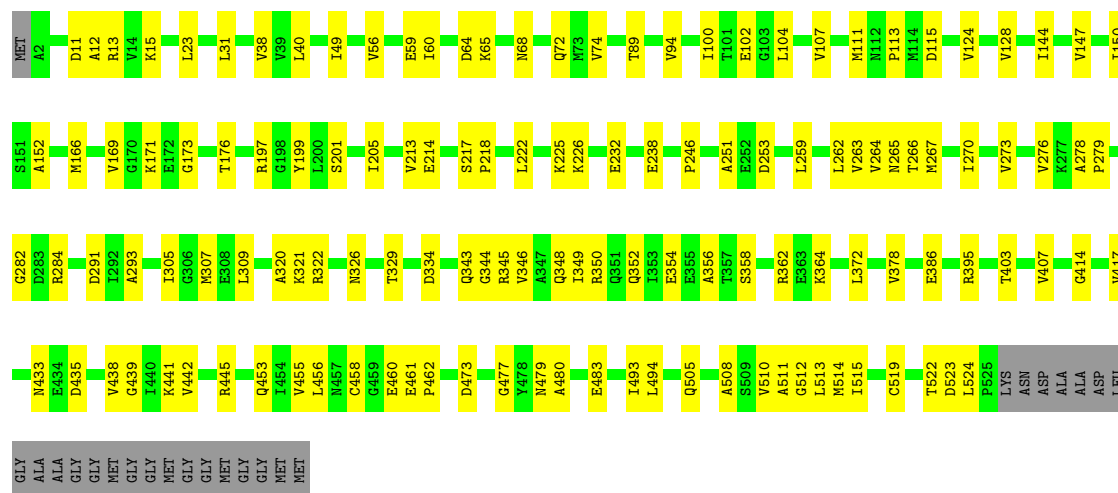
Mol	Chain	Residues	Atoms					AltConf
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	O	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	P	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	R	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	S	1	Total	C	N	O	P	0
			31	10	5	13	3	





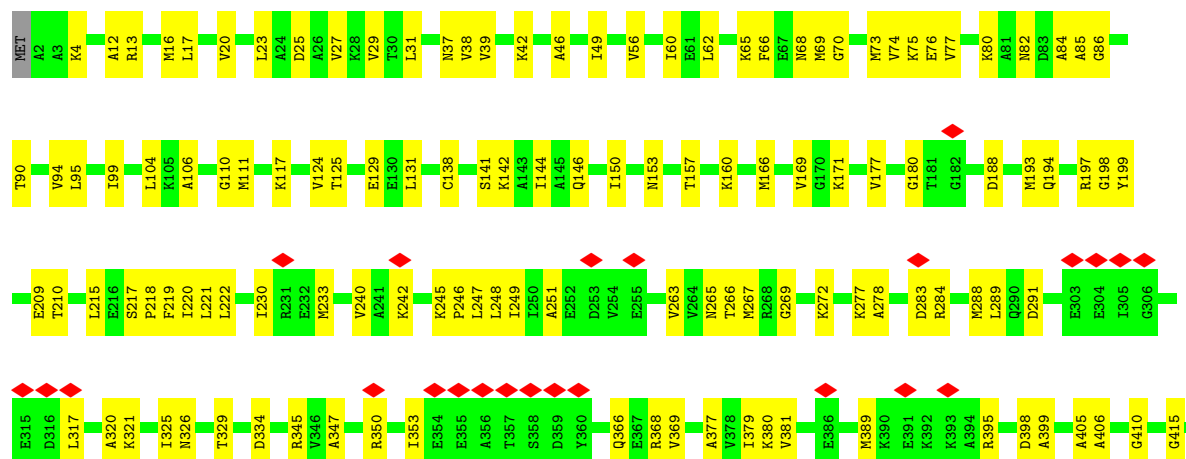
• Molecule 1: Chaperonin GroEL

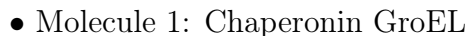
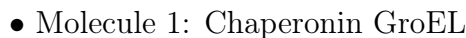
Chain F: 72% 24%



• Molecule 1: Chaperonin GroEL

Chain H: 68% 28%





MET	M447	V324	G173	MET
MET	E448	I325	I176	A2
		N326	V177	A12
	Q453	T329	R197	A13
	I454	T330		V14
	V455	T331		K15
	L456	I332	I205	
	N457	I333		L23
	G458	D334	V213	
	G459	G335		L31
	E460		S217	
	E461	R345		K34
	E462	V346	D224	
	D473	A347		V38
		Q348	N229	V39
	G477	I349	T230	L40
		R350	R231	
	A480	Q351		V56
	E483	I353	E238	
		E354	A239	E59
	I493	F355	K245	I60
		A356		
	L504	I357	L248	D64
	Q505	S358		N68
			L262	M69
	A508	R362		
			N265	
	A511	L372		Q72
	G512		I270	M73
	L513	V378	V271	V74
	M514		K272	K75
	I515	E366	V273	E76
		V367	A274	
		E368		T89
	C519	M389	P279	
	M520	K390	G280	V94
	P525	L400	R285	E102
LYS	ASN			G103
ASP	ALA	T403	M288	L104
ALA	ALA	V407		K105
ASP	LEU	V417	D291	
GLY	GLY		I301	V124
ALA	ALA	I420	S302	A127
GLY	GLY			V128
GLY	GLY	A423	I305	I144
GLY	GLY		G306	
MET	MET	V438	M307	I150
GLY	GLY	G439	E308	
GLY	GLY	I440	L309	I162
MET	MET	K441		M166
GLY	GLY	V442	L314	
GLY	GLY			
MET	MET	A443	A320	V169
GLY	GLY	L444	K321	G170
GLY	GLY	R445	R322	K171
GLY	GLY	I446	E323	E172

Chain 0: 68% 28%

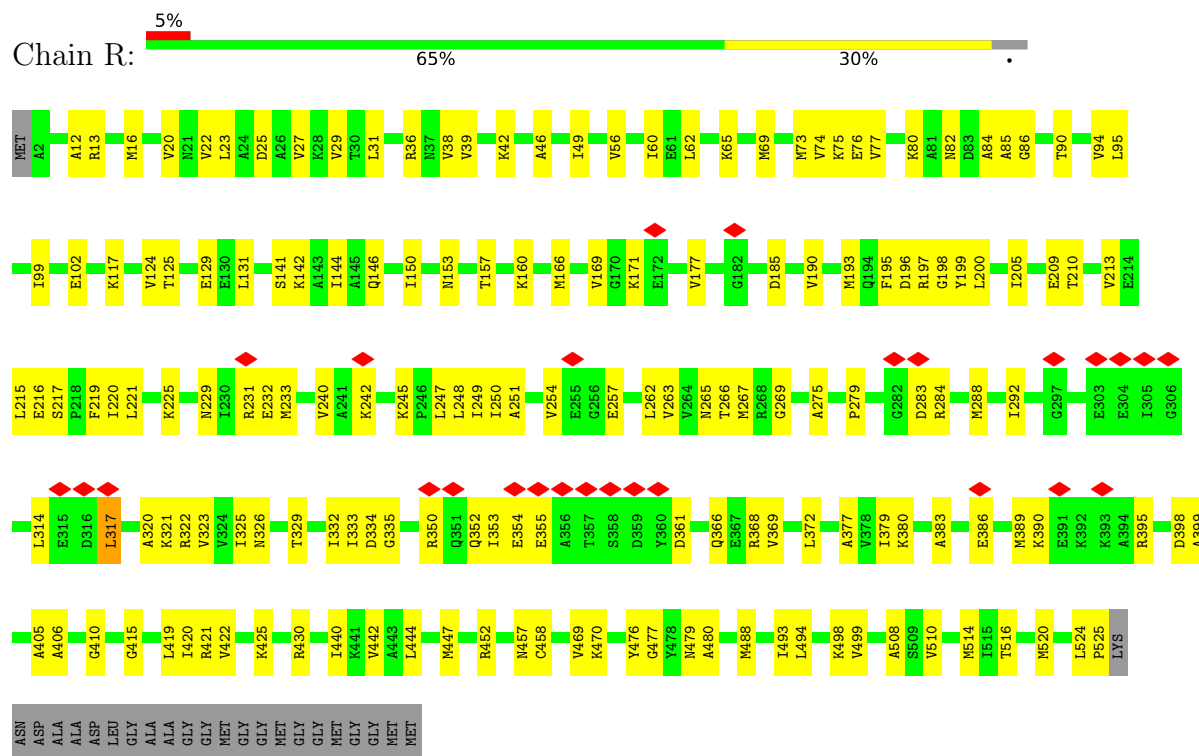
MET	R452	R350	R231	M110	MET
MET	N457	Q351	E232	G111	A2
	C458	Q352	N233	M111	A12
	V469	I353	V240	M114	M16
	K470	E354	A241	K117	V20
	Y476	E355	K242	A123	L23
	Q477	A356	P246	V124	A24
	A480	T357	L247	T125	D25
		S358	L248	E129	A26
		D359	D253	E130	V27
	E483	Y360	V254	L131	K28
	N487	D361	E255	S141	T29
	M488	Q366	E256	K142	V30
	T489	E367	G257	A143	L31
	Q490	R368	V263	I144	N37
	N491	V369	T266	A145	V38
			M267	Q146	V39
	L494	L372	K272	I150	K42
	K498	V376	D283	T157	A46
	V499	I379	R284	V158	L49
	Y506	K380	K286	G159	V56
	A507	A383	N287	M166	
	S509	E386	A288	K171	L60
	V510		L289	V174	K65
	M514	R389	Q290	V177	M69
	I515	E391	D291	D185	M73
	T516	K392	T292	V190	V74
	M520	K393	E303	K306	K75
	P625	V396	I305	G306	E76
LYS	ASN	R404			V77
ASP	ASP	A405			
ALA	ALA	A406			
ASP	ASP	V407	E315	M193	X80
LEU	LEU	E408	D316	F195	A81
GLY	GLY	E409	L317	D196	N82
ALA	ALA	G410	K321	R197	A85
GLY	GLY	G415	R322	G198	G86
GLY	GLY	T420	V323	Y199	
MET	MET	R421	V324	E209	T89
GLY	GLY	V422	N326	T210	T90
MET	MET	K425	T329	L215	Y94
GLY	GLY	V438	T333	F219	L95
GLY	GLY	P439	D334	L220	
GLY	GLY	L440	R345	L222	Y99
		L444	V346	L221	I100
			A247		L107

Chain P: 71% 24% .

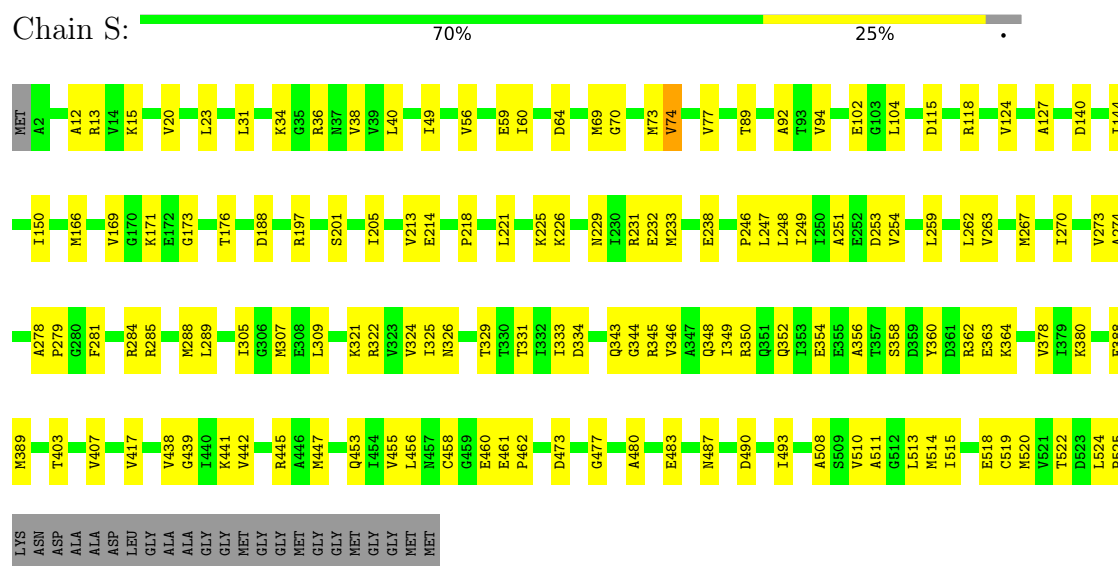
M166	M167	M168	M169	G170	K171	E172	G173	G174	M175	M176	M177	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	A251	E252	A253	D254	D255	A256	L257	L258	A259	A260	T261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	V294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	M311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	E365	D366	L367	E368	L369	L370	L371	L372	L373	L374	L375	E376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L72
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• Molecule 1: Chaperonin GroEL



• Molecule 1: Chaperonin GroEL



- Molecule 2: Co-chaperonin GroES

Chain W:  67% 31%



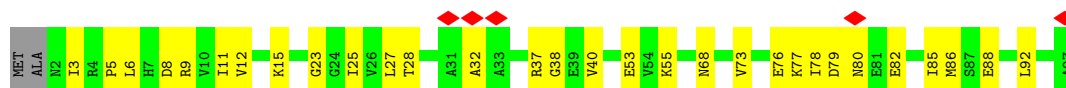
- Molecule 2: Co-chaperonin GroES

Chain D:  5% 68% 30%



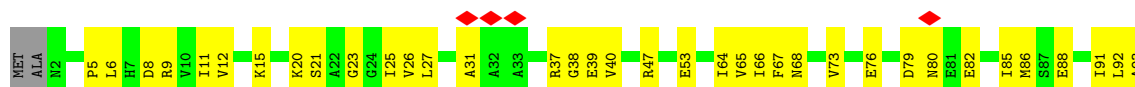
- Molecule 2: Co-chaperonin GroES

Chain G:  5% 67% 31%



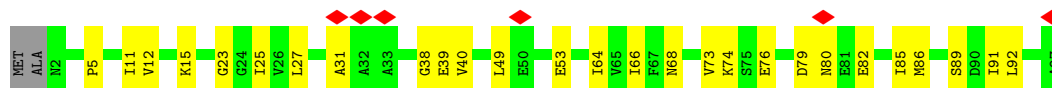
- Molecule 2: Co-chaperonin GroES

Chain K:  5% 60% 38%



- Molecule 2: Co-chaperonin GroES

Chain N:  6% 70% 28%

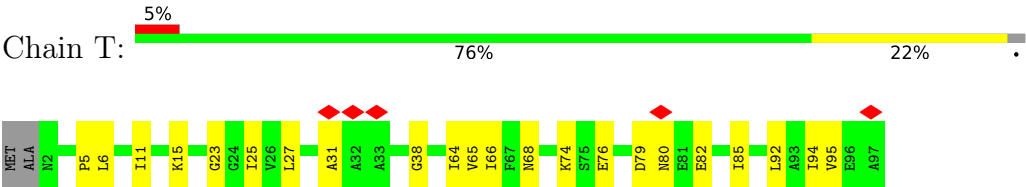


- Molecule 2: Co-chaperonin GroES

Chain Q:  5% 74% 23%



- Molecule 2: Co-chaperonin GroES



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	4612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	376.31998, 376.31998, 376.31998	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9599999, 0.9599999, 0.9599999	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/3877	0.30	0/5236
1	B	0.19	0/3879	0.30	0/5238
1	C	0.15	0/3877	0.33	0/5236
1	E	0.15	0/3877	0.33	0/5236
1	F	0.18	0/3879	0.30	0/5238
1	H	0.15	0/3877	0.32	0/5236
1	I	0.18	0/3879	0.30	0/5238
1	J	0.19	0/3879	0.31	0/5238
1	L	0.15	0/3877	0.32	0/5236
1	M	0.19	0/3879	0.32	0/5238
1	O	0.15	0/3877	0.30	0/5236
1	P	0.19	0/3879	0.31	0/5238
1	R	0.15	0/3877	0.32	0/5236
1	S	0.18	0/3879	0.31	0/5238
2	D	0.12	0/718	0.32	0/966
2	G	0.12	0/718	0.29	0/966
2	K	0.12	0/718	0.31	0/966
2	N	0.11	0/718	0.30	0/966
2	Q	0.11	0/718	0.29	0/966
2	T	0.11	0/718	0.31	0/966
2	W	0.12	0/718	0.31	0/966
All	All	0.16	0/59318	0.31	0/80080

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3849	0	3965	92	0
1	B	3851	0	3972	92	0
1	C	3849	0	3965	109	0
1	E	3849	0	3965	98	0
1	F	3851	0	3972	86	0
1	H	3849	0	3965	101	0
1	I	3851	0	3972	75	0
1	J	3851	0	3972	103	0
1	L	3849	0	3965	106	0
1	M	3851	0	3972	88	0
1	O	3849	0	3965	104	0
1	P	3851	0	3972	91	0
1	R	3849	0	3965	124	0
1	S	3851	0	3972	91	0
2	D	714	0	732	22	0
2	G	714	0	732	24	0
2	K	714	0	732	30	0
2	N	714	0	732	18	0
2	Q	714	0	732	17	0
2	T	714	0	732	19	0
2	W	714	0	732	23	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	31	0	12	1	0
4	E	31	0	12	2	0
4	F	31	0	12	1	0
4	H	31	0	12	2	0
4	I	31	0	12	1	0
4	J	31	0	12	2	0
4	L	31	0	12	1	0
4	M	31	0	12	2	0
4	O	31	0	12	1	0
4	P	31	0	12	2	0
4	R	31	0	12	1	0
4	S	31	0	12	1	0
All	All	59346	0	60851	1421	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 12.

All (1421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.63	0.80
1:O:77:VAL:HG21	1:O:510:VAL:HB	1.63	0.80
1:M:291:ASP:HB3	1:M:372:LEU:HD21	1.66	0.78
1:O:220:ILE:HG13	1:O:248:LEU:HD21	1.67	0.77
1:M:262:LEU:HD22	1:M:273:VAL:HG11	1.66	0.77
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.66	0.76
1:J:262:LEU:HD22	1:J:273:VAL:HG11	1.67	0.76
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.68	0.76
1:R:220:ILE:HG13	1:R:248:LEU:HD21	1.66	0.75
1:P:262:LEU:HD22	1:P:273:VAL:HG11	1.69	0.74
1:L:524:LEU:HD12	1:L:525:PRO:HD2	1.70	0.74
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.67	0.74
1:F:291:ASP:HB3	1:F:372:LEU:HD11	1.70	0.73
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.70	0.73
1:I:20:VAL:HG21	1:I:514:MET:HE1	1.71	0.73
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.70	0.72
1:O:263:VAL:O	1:O:266:THR:OG1	2.05	0.72
2:W:5:PRO:HG3	2:W:11:ILE:HG12	1.70	0.72
1:O:124:VAL:HG21	1:O:508:ALA:HB2	1.70	0.72
1:R:77:VAL:HG21	1:R:510:VAL:HB	1.69	0.72
1:R:124:VAL:HG21	1:R:508:ALA:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:O	1:B:265:ASN:ND2	2.23	0.72
1:H:220:ILE:HG13	1:H:248:LEU:HD21	1.70	0.72
1:B:262:LEU:HD22	1:B:273:VAL:HG11	1.72	0.72
1:L:124:VAL:HG21	1:L:508:ALA:HB2	1.71	0.72
1:H:452:ARG:NH2	1:M:461:GLU:OE2	2.24	0.71
1:O:386:GLU:HA	1:O:389:MET:HG2	1.70	0.71
1:I:461:GLU:OE2	1:R:452:ARG:NH2	2.23	0.71
1:R:177:VAL:HG12	1:R:379:ILE:HB	1.73	0.71
1:F:262:LEU:HD22	1:F:273:VAL:HG21	1.71	0.71
1:C:452:ARG:NH2	1:B:461:GLU:OE2	2.24	0.71
1:S:262:LEU:HD22	1:S:273:VAL:HG11	1.72	0.71
1:C:220:ILE:HG13	1:C:248:LEU:HD21	1.73	0.70
1:E:177:VAL:HG12	1:E:379:ILE:HB	1.72	0.70
1:H:124:VAL:HG21	1:H:508:ALA:HB2	1.71	0.70
1:C:124:VAL:HG21	1:C:508:ALA:HB2	1.71	0.70
1:E:124:VAL:HG21	1:E:508:ALA:HB2	1.72	0.70
1:O:197:ARG:H	1:O:329:THR:HA	1.57	0.70
2:Q:5:PRO:HG3	2:Q:11:ILE:HG12	1.72	0.70
1:H:177:VAL:HG12	1:H:379:ILE:HB	1.73	0.70
1:C:177:VAL:HG12	1:C:379:ILE:HB	1.72	0.69
1:A:85:ALA:HB1	1:A:499:VAL:HG22	1.72	0.69
1:F:197:ARG:HE	1:F:279:PRO:HA	1.56	0.69
1:L:16:MET:HE3	1:L:520:MET:HE3	1.74	0.69
1:A:177:VAL:HG12	1:A:379:ILE:HB	1.72	0.69
2:N:15:LYS:HG3	2:N:38:GLY:HA2	1.74	0.69
1:C:85:ALA:HB1	1:C:499:VAL:HG22	1.75	0.69
1:L:177:VAL:HG12	1:L:379:ILE:HB	1.73	0.69
1:E:220:ILE:HG13	1:E:248:LEU:HD21	1.73	0.69
1:H:406:ALA:O	1:H:410:GLY:N	2.24	0.69
2:G:15:LYS:HG3	2:G:38:GLY:HA2	1.75	0.69
1:O:215:LEU:HB2	1:O:323:VAL:HG12	1.75	0.69
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.74	0.68
1:O:177:VAL:HG12	1:O:379:ILE:HB	1.75	0.68
1:A:270:ILE:HG13	1:A:271:VAL:HG13	1.73	0.68
1:E:215:LEU:HB2	1:E:323:VAL:HG12	1.74	0.68
1:A:215:LEU:HB2	1:A:323:VAL:HG12	1.74	0.68
1:I:197:ARG:HE	1:I:279:PRO:HA	1.58	0.68
1:E:263:VAL:HG12	1:E:267:MET:HE1	1.76	0.68
1:L:230:ILE:HA	1:L:233:MET:HE1	1.76	0.68
1:R:197:ARG:H	1:R:329:THR:HA	1.58	0.68
2:T:5:PRO:HG3	2:T:11:ILE:HG12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:ALA:HB1	1:H:499:VAL:HG22	1.75	0.67
1:L:76:GLU:HG3	1:O:46:ALA:HB2	1.76	0.67
1:M:23:LEU:HD22	1:M:74:VAL:HG13	1.75	0.67
1:A:111:MET:HE1	1:A:438:VAL:HG21	1.76	0.67
1:L:111:MET:HE1	1:L:438:VAL:HG21	1.77	0.67
1:R:84:ALA:O	1:R:498:LYS:NZ	2.28	0.67
2:K:9:ARG:NH2	2:N:89:SER:O	2.27	0.67
1:L:84:ALA:O	1:L:498:LYS:NZ	2.28	0.67
1:M:321:LYS:HB3	1:M:334:ASP:HB2	1.77	0.67
1:J:321:LYS:HB3	1:J:334:ASP:HB2	1.76	0.67
2:K:37:ARG:HG2	2:K:66:ILE:HG12	1.77	0.67
1:S:321:LYS:HB3	1:S:334:ASP:HB2	1.76	0.67
1:E:389:MET:HE3	1:E:389:MET:HA	1.77	0.67
1:S:34:LYS:NZ	1:S:483:GLU:OE2	2.28	0.66
1:H:84:ALA:O	1:H:498:LYS:NZ	2.28	0.66
1:L:197:ARG:H	1:L:329:THR:HA	1.61	0.66
1:R:73:MET:HE2	1:R:514:MET:HG2	1.78	0.66
1:C:84:ALA:O	1:C:498:LYS:NZ	2.28	0.66
1:C:46:ALA:HB2	1:R:76:GLU:HG3	1.77	0.66
1:E:76:GLU:HG3	1:H:46:ALA:HB2	1.78	0.66
1:L:85:ALA:HB1	1:L:499:VAL:HG22	1.78	0.66
1:E:452:ARG:NH2	1:J:461:GLU:OE2	2.25	0.66
1:H:76:GLU:HG3	1:L:46:ALA:HB2	1.78	0.66
1:H:111:MET:HE1	1:H:438:VAL:HG21	1.78	0.65
1:P:251:ALA:O	1:P:278:ALA:N	2.27	0.65
1:R:13:ARG:HA	1:R:16:MET:HG3	1.78	0.65
1:A:301:ILE:HG13	1:A:307:MET:HG3	1.78	0.65
1:A:69:MET:O	1:A:73:MET:HG2	1.96	0.65
1:C:406:ALA:O	1:C:410:GLY:N	2.29	0.65
1:E:111:MET:HE1	1:E:438:VAL:HG21	1.78	0.65
1:H:389:MET:HE3	1:H:389:MET:HA	1.79	0.65
1:A:220:ILE:HG13	1:A:248:LEU:HD21	1.78	0.65
1:O:452:ARG:NH2	1:S:461:GLU:OE2	2.23	0.65
2:W:47:ARG:NH2	2:W:88:GLU:OE1	2.29	0.65
1:R:406:ALA:O	1:R:410:GLY:N	2.29	0.65
1:C:39:VAL:HG22	1:C:49:ILE:HG12	1.78	0.65
1:C:76:GLU:HG3	1:A:46:ALA:HB2	1.79	0.64
1:A:84:ALA:O	1:A:498:LYS:NZ	2.28	0.64
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.79	0.64
1:I:144:ILE:HG21	1:I:166:MET:HE2	1.79	0.64
1:A:452:ARG:NH2	1:F:461:GLU:OE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:MET:HE1	1:E:73:MET:HE2	1.80	0.64
1:O:23:LEU:HD23	1:O:74:VAL:HG13	1.79	0.64
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.80	0.64
1:S:251:ALA:O	1:S:278:ALA:N	2.27	0.64
2:W:68:ASN:HB2	2:W:92:LEU:HD21	1.77	0.64
1:B:34:LYS:NZ	1:B:483:GLU:OE2	2.31	0.64
1:B:321:LYS:HB3	1:B:334:ASP:HB2	1.80	0.64
1:J:225:LYS:HD3	1:J:309:LEU:HD11	1.81	0.63
2:W:15:LYS:HG3	2:W:38:GLY:HA2	1.79	0.63
1:S:127:ALA:HB2	1:S:447:MET:HE1	1.80	0.63
1:I:34:LYS:NZ	1:I:483:GLU:OE2	2.30	0.63
1:I:225:LYS:HD3	1:I:309:LEU:HD11	1.80	0.63
1:M:171:LYS:O	1:M:171:LYS:NZ	2.27	0.63
1:O:76:GLU:HG3	1:R:46:ALA:HB2	1.80	0.63
1:R:240:VAL:HG11	1:R:247:LEU:HB2	1.81	0.63
1:O:39:VAL:HG22	1:O:49:ILE:HG12	1.80	0.63
1:A:406:ALA:O	1:A:410:GLY:N	2.31	0.63
1:R:76:GLU:OE1	1:R:80:LYS:NZ	2.31	0.63
1:R:85:ALA:HB1	1:R:499:VAL:HG22	1.80	0.63
1:C:197:ARG:H	1:C:329:THR:HA	1.64	0.63
1:H:233:MET:H	1:H:233:MET:HE3	1.63	0.63
1:C:265:ASN:O	1:C:269:GLY:N	2.31	0.63
1:E:197:ARG:H	1:E:329:THR:HA	1.63	0.63
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.81	0.63
1:R:27:VAL:HG12	1:R:90:THR:HG23	1.81	0.62
1:A:197:ARG:H	1:A:329:THR:HA	1.64	0.62
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.80	0.62
1:E:85:ALA:HB1	1:E:499:VAL:HG22	1.81	0.62
1:L:301:ILE:HG23	1:L:307:MET:HG3	1.81	0.62
1:O:76:GLU:OE1	1:O:80:LYS:NZ	2.31	0.62
1:P:261:THR:O	1:P:265:ASN:ND2	2.26	0.62
1:S:124:VAL:HG21	1:S:508:ALA:HB2	1.82	0.62
1:S:197:ARG:HE	1:S:279:PRO:HA	1.64	0.62
1:I:124:VAL:HG21	1:I:508:ALA:HB2	1.81	0.62
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.82	0.62
1:M:34:LYS:NZ	1:M:483:GLU:OE2	2.32	0.62
1:B:38:VAL:HG22	1:F:519:CYS:HB3	1.81	0.62
2:D:11:ILE:HG22	2:D:41:LEU:HB2	1.80	0.62
1:F:214:GLU:OE2	1:F:322:ARG:NH1	2.32	0.62
1:H:153:ASN:OD1	1:H:395:ARG:NH1	2.32	0.62
2:W:92:LEU:HB3	2:T:85:ILE:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:O	1:B:514:MET:HG3	2.00	0.62
2:D:15:LYS:HG3	2:D:38:GLY:HA2	1.82	0.62
1:E:76:GLU:OE1	1:E:80:LYS:NZ	2.32	0.62
2:N:11:ILE:HD12	2:N:85:ILE:HG12	1.82	0.62
2:D:27:LEU:HB3	2:D:32:ALA:HB2	1.82	0.62
2:G:68:ASN:HB2	2:G:92:LEU:HD21	1.80	0.62
1:J:324:VAL:HG22	1:J:331:THR:HB	1.82	0.62
2:K:5:PRO:HG3	2:K:11:ILE:HG12	1.81	0.62
1:F:225:LYS:HD3	1:F:309:LEU:HD11	1.81	0.62
1:L:76:GLU:OE1	1:L:80:LYS:NZ	2.32	0.62
1:O:240:VAL:HG11	1:O:247:LEU:HB2	1.82	0.62
1:E:39:VAL:HG22	1:E:49:ILE:HG12	1.81	0.61
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.82	0.61
1:R:221:LEU:HD22	1:R:317:LEU:HD22	1.82	0.61
1:C:221:LEU:HD22	1:C:317:LEU:HD22	1.80	0.61
1:C:404:ARG:O	1:C:408:GLU:HG2	2.00	0.61
1:J:214:GLU:OE2	1:J:322:ARG:NH1	2.33	0.61
1:O:185:ASP:HA	1:O:380:LYS:O	2.00	0.61
1:I:262:LEU:HD22	1:I:273:VAL:HG11	1.83	0.61
1:A:76:GLU:HG3	1:E:46:ALA:HB2	1.81	0.61
1:O:406:ALA:O	1:O:410:GLY:N	2.30	0.61
1:H:197:ARG:H	1:H:329:THR:HA	1.64	0.61
2:Q:74:LYS:NZ	2:Q:76:GLU:OE1	2.33	0.61
1:I:214:GLU:OE2	1:I:322:ARG:NH1	2.33	0.61
1:R:12:ALA:HB1	1:R:520:MET:HG3	1.81	0.61
1:B:225:LYS:HD3	1:B:309:LEU:HD11	1.81	0.61
1:F:23:LEU:HD22	1:F:74:VAL:HG13	1.82	0.61
1:P:201:SER:HB2	1:P:259:LEU:HD21	1.82	0.61
1:C:153:ASN:OD1	1:C:395:ARG:NH1	2.34	0.61
1:P:38:VAL:HG22	1:S:519:CYS:HB3	1.82	0.61
2:T:11:ILE:HD12	2:T:85:ILE:HG12	1.81	0.61
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.82	0.60
1:H:23:LEU:HD23	1:H:74:VAL:HG13	1.83	0.60
1:J:23:LEU:HD22	1:J:74:VAL:HG13	1.82	0.60
1:L:421:ARG:NH1	1:L:469:VAL:O	2.31	0.60
1:P:197:ARG:HE	1:P:279:PRO:HA	1.66	0.60
1:R:265:ASN:O	1:R:269:GLY:N	2.32	0.60
1:R:389:MET:HA	1:R:389:MET:HE3	1.83	0.60
1:F:201:SER:HB2	1:F:259:LEU:HD21	1.82	0.60
1:B:124:VAL:HG21	1:B:508:ALA:HB2	1.83	0.60
1:J:38:VAL:HG22	1:M:519:CYS:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:5:PRO:HG3	2:N:11:ILE:HG12	1.83	0.60
1:B:169:VAL:HB	1:B:173:GLY:HA3	1.84	0.60
1:B:231:ARG:HA	1:B:234:LEU:HG	1.83	0.60
1:M:265:ASN:HD22	1:M:270:ILE:HD11	1.66	0.60
1:A:166:MET:SD	1:A:171:LYS:HA	2.41	0.60
1:H:240:VAL:HG11	1:H:247:LEU:HB2	1.84	0.60
1:R:185:ASP:HA	1:R:380:LYS:O	2.02	0.60
1:B:171:LYS:O	1:B:171:LYS:NZ	2.29	0.60
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.84	0.60
1:A:23:LEU:HD23	1:A:74:VAL:HG13	1.83	0.60
1:S:171:LYS:O	1:S:171:LYS:NZ	2.29	0.60
1:B:356:ALA:O	1:B:362:ARG:NH2	2.35	0.60
1:F:321:LYS:HB3	1:F:334:ASP:HB2	1.83	0.60
1:L:389:MET:HE3	1:L:389:MET:HA	1.82	0.60
2:N:73:VAL:HG23	2:N:86:MET:HB3	1.82	0.60
1:F:171:LYS:O	1:F:171:LYS:NZ	2.29	0.59
1:O:166:MET:SD	1:O:171:LYS:HA	2.41	0.59
1:R:421:ARG:O	1:R:425:LYS:HG2	2.01	0.59
1:E:193:MET:HE1	1:E:195:PHE:HB3	1.83	0.59
1:C:76:GLU:OE1	1:C:80:LYS:NZ	2.35	0.59
1:J:124:VAL:HG21	1:J:508:ALA:HB2	1.84	0.59
1:R:233:MET:SD	1:R:233:MET:N	2.75	0.59
1:I:321:LYS:HB3	1:I:334:ASP:HB2	1.84	0.59
1:F:199:TYR:HA	1:F:276:VAL:HG12	1.83	0.59
1:O:321:LYS:HB2	1:O:334:ASP:HB3	1.84	0.59
1:P:229:ASN:OD1	1:P:231:ARG:NE	2.36	0.59
1:S:322:ARG:HB2	1:S:333:ILE:HB	1.84	0.59
1:O:383:ALA:H	1:O:389:MET:HE1	1.67	0.59
1:P:225:LYS:HD3	1:P:309:LEU:HD11	1.85	0.59
2:T:68:ASN:HB2	2:T:92:LEU:HD21	1.83	0.59
1:E:406:ALA:O	1:E:410:GLY:N	2.34	0.59
1:M:301:ILE:HG21	1:M:309:LEU:HD23	1.85	0.59
1:A:386:GLU:HA	1:A:389:MET:HG2	1.83	0.59
1:B:15:LYS:NZ	1:B:64:ASP:OD2	2.33	0.59
2:D:47:ARG:NH2	2:D:88:GLU:OE1	2.35	0.59
1:I:171:LYS:O	1:I:171:LYS:NZ	2.29	0.59
1:P:356:ALA:O	1:P:362:ARG:NH2	2.35	0.59
1:R:166:MET:SD	1:R:171:LYS:HA	2.43	0.59
1:R:421:ARG:NH1	1:R:469:VAL:O	2.34	0.59
1:C:69:MET:O	1:C:73:MET:HG2	2.02	0.59
2:W:9:ARG:NH2	2:D:89:SER:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HD22	1:B:74:VAL:HG13	1.85	0.59
1:I:519:CYS:HB3	1:S:38:VAL:HG22	1.83	0.58
1:P:124:VAL:HG21	1:P:508:ALA:HB2	1.85	0.58
1:A:421:ARG:NH1	1:A:469:VAL:O	2.34	0.58
1:F:124:VAL:HG21	1:F:508:ALA:HB2	1.85	0.58
1:J:169:VAL:HB	1:J:173:GLY:HA3	1.84	0.58
1:S:238:GLU:HG2	2:T:23:GLY:HA3	1.85	0.58
1:M:38:VAL:HG22	1:P:519:CYS:HB3	1.85	0.58
1:R:39:VAL:HG22	1:R:49:ILE:HG12	1.85	0.58
1:R:240:VAL:HG21	1:R:247:LEU:HD13	1.85	0.58
1:L:166:MET:SD	1:L:171:LYS:HA	2.43	0.58
1:P:23:LEU:HD22	1:P:74:VAL:HG13	1.85	0.58
1:R:23:LEU:HD23	1:R:74:VAL:HG13	1.85	0.58
1:C:12:ALA:HB1	1:C:520:MET:HG3	1.85	0.58
1:B:458:CYS:SG	1:B:480:ALA:HB1	2.43	0.58
1:F:169:VAL:HB	1:F:173:GLY:HA3	1.85	0.58
1:L:215:LEU:HB2	1:L:323:VAL:HG12	1.84	0.58
2:G:73:VAL:HG23	2:G:86:MET:HB3	1.84	0.58
1:I:38:VAL:HG22	1:B:519:CYS:HB3	1.84	0.58
1:A:193:MET:HE1	1:A:195:PHE:HB3	1.84	0.58
1:J:302:SER:HB3	1:J:305:ILE:HG22	1.86	0.58
1:I:199:TYR:HA	1:I:276:VAL:HG12	1.86	0.58
1:B:230:ILE:HG12	1:B:261:THR:HG21	1.84	0.58
1:B:238:GLU:O	1:B:242:LYS:HD3	2.04	0.58
2:K:47:ARG:NH2	2:K:88:GLU:OE1	2.36	0.58
1:M:291:ASP:OD1	1:M:345:ARG:NE	2.37	0.58
1:P:344:GLY:O	1:P:348:GLN:HG3	2.03	0.58
2:K:21:SER:HB3	2:K:25:ILE:HG23	1.85	0.58
2:T:74:LYS:NZ	2:T:76:GLU:OE1	2.36	0.58
1:C:193:MET:HE1	1:C:195:PHE:HB3	1.84	0.58
1:I:23:LEU:HD22	1:I:74:VAL:HG13	1.86	0.58
1:J:356:ALA:O	1:J:362:ARG:NH2	2.37	0.58
2:K:68:ASN:HB2	2:K:92:LEU:HD21	1.86	0.58
1:O:69:MET:O	1:O:73:MET:HG3	2.04	0.58
1:C:166:MET:SD	1:C:171:LYS:HA	2.44	0.57
2:W:65:VAL:HG12	2:W:94:ILE:HG22	1.86	0.57
1:O:284:ARG:HH22	1:O:361:ASP:HA	1.68	0.57
1:P:458:CYS:SG	1:P:480:ALA:HB1	2.44	0.57
1:S:356:ALA:O	1:S:362:ARG:NH2	2.36	0.57
1:S:458:CYS:SG	1:S:480:ALA:HB1	2.44	0.57
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.86	0.57
1:S:225:LYS:HD3	1:S:309:LEU:HD11	1.86	0.57
1:E:405:ALA:HB1	1:E:498:LYS:HB3	1.87	0.57
1:F:31:LEU:HD22	1:F:94:VAL:HG21	1.85	0.57
1:L:23:LEU:HD23	1:L:74:VAL:HG13	1.86	0.57
1:M:356:ALA:O	1:M:362:ARG:NH2	2.37	0.57
1:S:144:ILE:HG21	1:S:166:MET:HE2	1.85	0.57
1:C:386:GLU:HA	1:C:389:MET:HG2	1.86	0.57
1:C:389:MET:HE3	1:C:389:MET:HA	1.86	0.57
1:I:356:ALA:O	1:I:362:ARG:NH2	2.37	0.57
2:W:9:ARG:NH1	2:D:91:ILE:O	2.36	0.57
1:J:171:LYS:O	1:J:171:LYS:NZ	2.27	0.57
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.86	0.57
1:R:193:MET:HE1	1:R:195:PHE:HB3	1.86	0.57
1:I:169:VAL:HB	1:I:173:GLY:HA3	1.86	0.57
1:M:31:LEU:HD22	1:M:94:VAL:HG21	1.86	0.57
1:P:230:ILE:HG13	1:P:258:ALA:HA	1.86	0.57
1:S:226:LYS:HE3	1:S:253:ASP:HB3	1.87	0.57
1:C:281:PHE:H	1:C:284:ARG:HB2	1.69	0.57
1:F:473:ASP:N	1:F:473:ASP:OD1	2.38	0.57
1:M:169:VAL:HB	1:M:173:GLY:HA3	1.86	0.57
1:B:31:LEU:HD22	1:B:94:VAL:HG21	1.85	0.57
1:A:321:LYS:HB2	1:A:334:ASP:HB3	1.87	0.57
1:B:322:ARG:HB3	1:B:333:ILE:HB	1.86	0.57
1:H:39:VAL:HG22	1:H:49:ILE:HG12	1.86	0.57
1:J:205:ILE:HA	1:J:213:VAL:HG22	1.86	0.57
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.45	0.57
1:M:124:VAL:HG21	1:M:508:ALA:HB2	1.86	0.57
1:O:27:VAL:HG12	1:O:90:THR:HG23	1.86	0.57
1:C:60:ILE:O	1:C:75:LYS:NZ	2.35	0.57
1:L:141:SER:HA	1:L:144:ILE:HD12	1.86	0.57
1:M:197:ARG:HE	1:M:279:PRO:HA	1.69	0.57
1:O:347:ALA:O	1:O:351:GLN:NE2	2.38	0.57
1:A:76:GLU:OE1	1:A:80:LYS:NZ	2.38	0.56
1:P:169:VAL:HB	1:P:173:GLY:HA3	1.87	0.56
1:P:510:VAL:HG12	1:P:514:MET:HE2	1.87	0.56
1:F:356:ALA:O	1:F:362:ARG:NH2	2.38	0.56
1:J:102:GLU:OE1	1:J:445:ARG:NH1	2.38	0.56
2:K:73:VAL:HG23	2:K:86:MET:HB3	1.87	0.56
2:Q:65:VAL:HG12	2:Q:94:ILE:HG22	1.87	0.56
1:R:249:ILE:HG22	1:R:251:ALA:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:169:VAL:HB	1:S:173:GLY:HA3	1.86	0.56
1:E:60:ILE:O	1:E:75:LYS:NZ	2.37	0.56
1:E:421:ARG:NH2	1:E:476:TYR:O	2.38	0.56
1:L:39:VAL:HG22	1:L:49:ILE:HG12	1.87	0.56
1:L:406:ALA:O	1:L:410:GLY:N	2.34	0.56
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.86	0.56
1:S:15:LYS:NZ	1:S:64:ASP:OD2	2.32	0.56
2:W:76:GLU:HG2	2:D:66:ILE:HD13	1.87	0.56
1:A:39:VAL:HG22	1:A:49:ILE:HG12	1.88	0.56
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.45	0.56
1:J:203:TYR:HB3	1:J:267:MET:HE3	1.87	0.56
2:Q:79:ASP:O	2:Q:80:ASN:ND2	2.38	0.56
1:E:265:ASN:O	1:E:269:GLY:N	2.38	0.56
1:H:230:ILE:HA	1:H:233:MET:HE1	1.86	0.56
1:R:405:ALA:HB1	1:R:498:LYS:HB3	1.87	0.56
1:I:102:GLU:OE1	1:I:445:ARG:NH1	2.39	0.56
1:M:326:ASN:OD1	1:M:329:THR:N	2.29	0.56
1:R:215:LEU:HB2	1:R:323:VAL:HG12	1.88	0.56
1:I:344:GLY:O	1:I:348:GLN:HG3	2.06	0.56
1:B:12:ALA:HB1	1:B:520:MET:HG3	1.88	0.56
1:F:38:VAL:HG22	1:J:519:CYS:HB3	1.88	0.56
1:L:197:ARG:HA	1:L:277:LYS:HE3	1.87	0.56
1:L:215:LEU:HD13	1:L:246:PRO:HB2	1.87	0.56
1:P:200:LEU:HD23	1:P:276:VAL:HA	1.88	0.56
2:D:7:HIS:NE2	2:G:88:GLU:OE2	2.39	0.56
2:D:73:VAL:HG23	2:D:86:MET:HB3	1.88	0.56
1:M:348:GLN:O	1:M:352:GLN:HG3	2.05	0.56
2:D:68:ASN:HB2	2:D:92:LEU:HD21	1.87	0.56
1:F:523:ASP:OD1	1:F:524:LEU:N	2.39	0.56
1:S:201:SER:HB2	1:S:259:LEU:HD21	1.86	0.56
1:C:405:ALA:HB1	1:C:498:LYS:HB3	1.88	0.55
1:S:20:VAL:HG21	1:S:514:MET:HE1	1.88	0.55
1:B:324:VAL:HG22	1:B:331:THR:HB	1.87	0.55
1:J:281:PHE:HB2	1:J:284:ARG:HH12	1.71	0.55
2:K:79:ASP:O	2:K:80:ASN:ND2	2.40	0.55
1:E:23:LEU:HD23	1:E:74:VAL:HG13	1.89	0.55
1:E:166:MET:SD	1:E:171:LYS:HA	2.47	0.55
1:E:321:LYS:HB2	1:E:334:ASP:HB3	1.88	0.55
1:B:473:ASP:OD1	1:B:473:ASP:N	2.39	0.55
1:H:405:ALA:HB1	1:H:498:LYS:HB3	1.89	0.55
1:P:221:LEU:HD23	1:P:249:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:386:GLU:O	1:R:390:LYS:HG3	2.06	0.55
1:S:326:ASN:OD1	1:S:329:THR:N	2.32	0.55
1:R:200:LEU:HD13	1:R:254:VAL:H	1.71	0.55
1:L:265:ASN:O	1:L:269:GLY:N	2.39	0.55
1:M:12:ALA:HB1	1:M:520:MET:HG3	1.87	0.55
1:B:151:SER:HB2	1:B:399:ALA:HA	1.87	0.55
1:F:144:ILE:HG21	1:F:166:MET:HE2	1.89	0.55
1:H:421:ARG:NH2	1:H:476:TYR:O	2.39	0.55
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.46	0.55
1:R:209:GLU:HG2	1:R:210:THR:HG23	1.89	0.55
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.88	0.55
2:G:79:ASP:O	2:G:80:ASN:ND2	2.40	0.55
1:M:473:ASP:N	1:M:473:ASP:OD1	2.39	0.55
1:O:31:LEU:O	1:O:457:ASN:ND2	2.37	0.55
1:R:153:ASN:OD1	1:R:395:ARG:NH1	2.40	0.55
1:A:31:LEU:O	1:A:457:ASN:ND2	2.37	0.55
1:F:15:LYS:NZ	1:F:64:ASP:OD2	2.31	0.55
1:R:284:ARG:HH22	1:R:361:ASP:HA	1.70	0.55
1:E:69:MET:HE2	1:E:520:MET:HE2	1.87	0.54
1:H:265:ASN:O	1:H:269:GLY:N	2.39	0.54
1:P:31:LEU:HD22	1:P:94:VAL:HG21	1.89	0.54
1:P:226:LYS:HE3	1:P:253:ASP:HB3	1.89	0.54
2:D:11:ILE:HB	2:D:42:ALA:HB3	1.89	0.54
2:Q:15:LYS:HG3	2:Q:38:GLY:HA2	1.88	0.54
1:H:20:VAL:HG21	1:H:514:MET:HE1	1.89	0.54
1:P:473:ASP:OD1	1:P:473:ASP:N	2.40	0.54
1:S:23:LEU:HD22	1:S:74:VAL:HG13	1.89	0.54
1:C:31:LEU:HD22	1:C:94:VAL:HG21	1.90	0.54
1:F:49:ILE:HD12	1:J:513:LEU:HD13	1.88	0.54
1:M:89:THR:OG1	4:M:602:ATP:O2G	2.23	0.54
1:M:144:ILE:HG21	1:M:166:MET:HE2	1.89	0.54
1:M:238:GLU:HG2	2:N:23:GLY:HA3	1.89	0.54
1:O:85:ALA:HB1	1:O:499:VAL:HG22	1.88	0.54
2:D:37:ARG:HG2	2:D:66:ILE:HG12	1.89	0.54
1:C:281:PHE:HB3	1:A:181:THR:HB	1.88	0.54
1:C:295:LEU:HD21	1:C:372:LEU:HD22	1.88	0.54
1:E:73:MET:HE1	1:H:49:ILE:HD11	1.89	0.54
1:O:196:ASP:OD1	1:O:196:ASP:N	2.40	0.54
1:P:69:MET:HE2	1:P:522:THR:HB	1.89	0.54
1:P:214:GLU:OE2	1:P:322:ARG:NH2	2.40	0.54
1:I:217:SER:O	1:I:245:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:326:ASN:OD1	1:I:329:THR:N	2.27	0.54
1:I:473:ASP:OD1	1:I:473:ASP:N	2.40	0.54
1:E:209:GLU:HG2	1:E:210:THR:HG23	1.90	0.54
1:M:229:ASN:OD1	1:M:231:ARG:NE	2.41	0.54
1:P:321:LYS:HB2	1:P:334:ASP:HB2	1.89	0.54
1:S:89:THR:OG1	4:S:602:ATP:O2G	2.24	0.54
1:C:421:ARG:NH1	1:C:469:VAL:O	2.33	0.54
1:C:421:ARG:NH2	1:C:476:TYR:O	2.41	0.54
1:J:447:MET:HE2	1:J:504:LEU:HD21	1.90	0.54
1:M:73:MET:HE3	1:M:514:MET:HG2	1.90	0.54
1:C:194:GLN:NE2	1:C:331:THR:OG1	2.41	0.53
1:E:350:ARG:HA	1:E:353:ILE:HD12	1.89	0.53
1:F:102:GLU:OE1	1:F:445:ARG:NH1	2.41	0.53
1:F:263:VAL:HG12	1:F:267:MET:HE1	1.89	0.53
1:P:171:LYS:O	1:P:171:LYS:NZ	2.28	0.53
1:P:284:ARG:O	1:P:288:MET:HG3	2.08	0.53
1:R:60:ILE:O	1:R:75:LYS:NZ	2.37	0.53
1:R:263:VAL:O	1:R:266:THR:HG22	2.08	0.53
1:S:221:LEU:HD23	1:S:249:ILE:HG12	1.89	0.53
1:A:117:LYS:HD2	1:A:516:THR:HG21	1.90	0.53
1:E:31:LEU:HD22	1:E:94:VAL:HG21	1.89	0.53
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.91	0.53
1:M:15:LYS:NZ	1:M:64:ASP:OD2	2.34	0.53
1:O:487:ASN:O	1:O:491:MET:HG3	2.07	0.53
1:R:150:ILE:HG21	1:R:494:LEU:O	2.09	0.53
1:C:415:GLY:HA2	4:C:602:ATP:H1'	1.91	0.53
1:E:415:GLY:HA2	4:E:602:ATP:H1'	1.91	0.53
1:P:291:ASP:OD1	1:P:345:ARG:NE	2.41	0.53
1:I:12:ALA:HB1	1:I:520:MET:HG3	1.91	0.53
1:B:89:THR:OG1	4:B:602:ATP:O2G	2.25	0.53
1:I:291:ASP:OD1	1:I:345:ARG:NE	2.41	0.53
1:E:31:LEU:O	1:E:457:ASN:ND2	2.36	0.53
1:H:291:ASP:OD2	1:H:368:ARG:NH1	2.41	0.53
1:J:15:LYS:NZ	1:J:64:ASP:OD2	2.36	0.53
1:L:381:VAL:HG13	1:L:389:MET:HE1	1.89	0.53
1:L:421:ARG:NH2	1:L:476:TYR:O	2.41	0.53
1:C:209:GLU:HG2	1:C:210:THR:HG23	1.91	0.53
1:I:89:THR:OG1	4:I:602:ATP:O2G	2.26	0.53
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.49	0.53
1:P:89:THR:OG1	4:P:602:ATP:O2G	2.23	0.53
2:Q:11:ILE:HD12	2:Q:85:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:102:GLU:OE1	1:S:445:ARG:NH1	2.42	0.53
1:O:233:MET:SD	1:O:233:MET:N	2.81	0.53
1:P:205:ILE:HA	1:P:213:VAL:HG22	1.90	0.53
1:P:447:MET:HE2	1:P:504:LEU:HD21	1.91	0.53
1:E:498:LYS:HG3	1:E:501:ARG:HH21	1.73	0.53
1:O:284:ARG:O	1:O:288:MET:HE3	2.08	0.53
1:O:421:ARG:NH1	1:O:469:VAL:O	2.36	0.53
1:S:270:ILE:HD12	2:T:25:ILE:HA	1.90	0.53
2:G:5:PRO:HG3	2:G:11:ILE:HG12	1.91	0.53
2:G:6:LEU:HD11	2:K:94:ILE:HG23	1.90	0.53
1:P:102:GLU:OE1	1:P:445:ARG:NH1	2.41	0.53
1:I:280:GLY:O	1:I:285:ARG:NH2	2.41	0.53
2:W:64:ILE:HB	2:W:95:VAL:HB	1.91	0.53
1:H:209:GLU:HG2	1:H:210:THR:HG23	1.91	0.53
1:R:458:CYS:SG	1:R:480:ALA:HB1	2.49	0.53
1:A:262:LEU:O	1:A:266:THR:OG1	2.25	0.52
1:B:281:PHE:O	1:B:285:ARG:N	2.34	0.52
1:J:264:VAL:O	1:J:268:ARG:HG2	2.09	0.52
2:K:65:VAL:HG12	2:K:94:ILE:HG22	1.91	0.52
1:L:263:VAL:O	1:L:266:THR:HG22	2.09	0.52
1:O:458:CYS:SG	1:O:480:ALA:HB1	2.49	0.52
1:R:350:ARG:HA	1:R:353:ILE:HD12	1.90	0.52
1:S:473:ASP:OD1	1:S:473:ASP:N	2.42	0.52
1:M:224:ASP:HB2	1:M:302:SER:HB2	1.92	0.52
1:L:142:LYS:HG3	1:L:146:GLN:HE21	1.75	0.52
1:M:229:ASN:CG	1:M:230:ILE:N	2.66	0.52
1:P:238:GLU:HG2	2:Q:23:GLY:HA3	1.90	0.52
1:R:250:ILE:HG13	1:R:250:ILE:O	2.09	0.52
1:R:284:ARG:O	1:R:288:MET:HE3	2.09	0.52
1:A:209:GLU:HG2	1:A:210:THR:HG23	1.92	0.52
1:M:217:SER:O	1:M:245:LYS:NZ	2.42	0.52
1:O:389:MET:HE3	1:O:389:MET:HA	1.91	0.52
1:P:326:ASN:OD1	1:P:329:THR:N	2.35	0.52
2:Q:82:GLU:OE1	2:Q:82:GLU:N	2.42	0.52
1:R:196:ASP:OD1	1:R:196:ASP:N	2.41	0.52
1:S:31:LEU:HD22	1:S:94:VAL:HG21	1.92	0.52
1:A:31:LEU:HD22	1:A:94:VAL:HG21	1.90	0.52
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.92	0.52
1:F:348:GLN:O	1:F:352:GLN:HG3	2.09	0.52
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.49	0.52
1:J:111:MET:HE3	1:J:438:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:350:ARG:HA	1:O:353:ILE:HD12	1.92	0.52
1:R:421:ARG:NH2	1:R:476:TYR:O	2.43	0.52
1:R:477:GLY:HA3	1:R:488:MET:HE2	1.90	0.52
1:J:197:ARG:HE	1:J:279:PRO:HA	1.74	0.52
1:J:473:ASP:N	1:J:473:ASP:OD1	2.40	0.52
1:L:405:ALA:HB1	1:L:498:LYS:HB3	1.92	0.52
1:M:150:ILE:HG13	1:M:493:ILE:HA	1.92	0.52
1:O:477:GLY:HA3	1:O:488:MET:HE2	1.91	0.52
1:R:31:LEU:O	1:R:457:ASN:ND2	2.36	0.52
1:L:150:ILE:HG21	1:L:494:LEU:O	2.10	0.52
1:P:348:GLN:O	1:P:352:GLN:HG3	2.10	0.52
1:C:142:LYS:HG3	1:C:146:GLN:NE2	2.25	0.52
1:C:458:CYS:SG	1:C:480:ALA:HB1	2.49	0.52
1:C:117:LYS:HD2	1:C:516:THR:HG21	1.92	0.52
1:C:421:ARG:O	1:C:425:LYS:HG2	2.10	0.52
1:A:405:ALA:HB1	1:A:498:LYS:HB3	1.92	0.52
1:H:60:ILE:O	1:H:75:LYS:NZ	2.34	0.52
1:H:117:LYS:HD2	1:H:516:THR:HG21	1.91	0.52
1:O:209:GLU:HG2	1:O:210:THR:HG23	1.91	0.52
1:P:322:ARG:HB2	1:P:333:ILE:HB	1.92	0.52
1:P:479:ASN:HB2	1:P:491:MET:HE1	1.91	0.52
1:I:348:GLN:O	1:I:352:GLN:HG3	2.10	0.52
1:E:458:CYS:SG	1:E:480:ALA:HB1	2.50	0.52
1:H:197:ARG:HA	1:H:277:LYS:HE3	1.91	0.52
1:H:421:ARG:O	1:H:425:LYS:HG2	2.10	0.52
1:J:13:ARG:HD2	1:J:104:LEU:HD22	1.92	0.52
1:J:150:ILE:HG13	1:J:493:ILE:HA	1.92	0.52
1:L:142:LYS:HG3	1:L:146:GLN:NE2	2.25	0.52
1:C:23:LEU:HD23	1:C:74:VAL:HG13	1.92	0.51
1:I:456:LEU:HB2	1:I:462:PRO:HG3	1.92	0.51
1:E:469:VAL:HG22	1:E:477:GLY:HA2	1.92	0.51
1:O:60:ILE:O	1:O:75:LYS:NZ	2.36	0.51
1:O:368:ARG:O	1:O:372:LEU:HG	2.10	0.51
1:S:205:ILE:HA	1:S:213:VAL:HG22	1.91	0.51
2:T:79:ASP:O	2:T:80:ASN:ND2	2.43	0.51
1:L:209:GLU:HG2	1:L:210:THR:HG23	1.92	0.51
2:N:82:GLU:N	2:N:82:GLU:OE2	2.43	0.51
1:C:150:ILE:HG21	1:C:494:LEU:O	2.10	0.51
1:B:348:GLN:O	1:B:352:GLN:HG3	2.10	0.51
1:H:415:GLY:HA2	4:H:602:ATP:H1'	1.92	0.51
1:M:324:VAL:HG22	1:M:331:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:20:VAL:HG21	1:R:514:MET:HE1	1.93	0.51
1:R:190:VAL:HG21	1:R:333:ILE:HG23	1.93	0.51
1:C:111:MET:HE1	1:C:438:VAL:HG21	1.93	0.51
2:D:11:ILE:CD1	2:D:85:ILE:HG12	2.41	0.51
1:F:291:ASP:OD1	1:F:345:ARG:NE	2.41	0.51
1:L:31:LEU:HD22	1:L:94:VAL:HG21	1.92	0.51
1:O:404:ARG:O	1:O:408:GLU:HG2	2.10	0.51
1:S:281:PHE:HB2	1:S:284:ARG:HH12	1.75	0.51
2:T:15:LYS:HG3	2:T:38:GLY:HA2	1.92	0.51
1:E:291:ASP:OD2	1:E:368:ARG:NH1	2.43	0.51
1:F:218:PRO:HB3	1:F:246:PRO:HB2	1.93	0.51
1:L:194:GLN:O	1:L:371:LYS:NZ	2.38	0.51
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.50	0.51
1:A:291:ASP:OD2	1:A:368:ARG:NH1	2.44	0.51
1:E:420:ILE:HG23	1:E:470:LYS:HG2	1.93	0.51
1:E:421:ARG:NH1	1:E:469:VAL:O	2.33	0.51
1:O:150:ILE:HG21	1:O:494:LEU:O	2.11	0.51
1:R:200:LEU:HD12	1:R:275:ALA:HB1	1.92	0.51
2:K:9:ARG:NH1	2:N:91:ILE:O	2.43	0.51
1:M:102:GLU:OE1	1:M:445:ARG:NH1	2.43	0.51
1:B:201:SER:HB2	1:B:259:LEU:HD21	1.93	0.51
1:H:142:LYS:HG3	1:H:146:GLN:NE2	2.25	0.51
1:H:421:ARG:NH1	1:H:469:VAL:O	2.33	0.51
1:J:291:ASP:OD1	1:J:345:ARG:NE	2.44	0.51
1:M:358:SER:O	1:M:362:ARG:HG2	2.11	0.51
1:M:438:VAL:O	1:M:442:VAL:HG13	2.11	0.51
1:P:305:ILE:HG23	1:P:307:MET:HG2	1.93	0.51
1:R:190:VAL:HB	1:R:334:ASP:HB2	1.93	0.51
2:W:27:LEU:HD22	2:W:31:ALA:HB1	1.91	0.51
1:E:222:LEU:HB3	1:E:289:LEU:HD12	1.92	0.51
1:P:358:SER:O	1:P:362:ARG:HG2	2.10	0.51
1:R:142:LYS:HG3	1:R:146:GLN:NE2	2.26	0.51
1:S:305:ILE:HG23	1:S:307:MET:HG2	1.92	0.51
1:A:197:ARG:HA	1:A:277:LYS:HE3	1.94	0.51
1:B:199:TYR:HA	1:B:276:VAL:HG12	1.93	0.51
1:E:142:LYS:HG3	1:E:146:GLN:NE2	2.25	0.51
1:P:350:ARG:O	1:P:354:GLU:HG2	2.11	0.51
1:R:95:LEU:O	1:R:99:ILE:HG13	2.11	0.51
1:S:150:ILE:HG13	1:S:493:ILE:HA	1.92	0.51
1:S:344:GLY:O	1:S:348:GLN:HG3	2.11	0.51
1:I:350:ARG:O	1:I:354:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:HG3	1:A:146:GLN:NE2	2.26	0.50
1:E:16:MET:HE3	1:E:520:MET:HE3	1.91	0.50
1:E:65:LYS:O	1:E:69:MET:HG3	2.11	0.50
1:H:150:ILE:HG21	1:H:494:LEU:O	2.11	0.50
1:J:124:VAL:HG21	1:J:508:ALA:CB	2.40	0.50
1:R:31:LEU:HD22	1:R:94:VAL:HG21	1.94	0.50
2:T:82:GLU:N	2:T:82:GLU:OE1	2.44	0.50
1:A:142:LYS:HG3	1:A:146:GLN:HE21	1.76	0.50
1:A:415:GLY:HA2	4:A:602:ATP:H1'	1.93	0.50
1:E:82:ASN:O	1:E:86:GLY:N	2.44	0.50
1:E:194:GLN:NE2	1:E:331:THR:OG1	2.44	0.50
1:F:305:ILE:HG23	1:F:307:MET:HG2	1.92	0.50
1:O:142:LYS:HG3	1:O:146:GLN:NE2	2.25	0.50
1:B:350:ARG:O	1:B:354:GLU:HG2	2.11	0.50
1:S:124:VAL:HG21	1:S:508:ALA:CB	2.41	0.50
1:A:233:MET:SD	1:A:233:MET:N	2.81	0.50
1:J:479:ASN:HB2	1:J:491:MET:HE1	1.94	0.50
1:L:291:ASP:OD2	1:L:368:ARG:NH1	2.42	0.50
1:C:350:ARG:HA	1:C:353:ILE:HD12	1.93	0.50
1:B:278:ALA:HB1	1:B:289:LEU:HD21	1.92	0.50
2:D:74:LYS:NZ	2:D:76:GLU:OE1	2.43	0.50
1:H:420:ILE:HG23	1:H:470:LYS:HG2	1.94	0.50
1:J:350:ARG:O	1:J:354:GLU:HG2	2.12	0.50
2:K:27:LEU:HD22	2:K:31:ALA:HB1	1.92	0.50
1:L:219:PHE:HB3	1:L:317:LEU:HD13	1.93	0.50
1:O:111:MET:HE1	1:O:438:VAL:HG21	1.94	0.50
1:O:421:ARG:NH2	1:O:476:TYR:O	2.45	0.50
1:P:200:LEU:HB3	1:P:259:LEU:HD11	1.92	0.50
1:B:358:SER:O	1:B:362:ARG:HG2	2.11	0.50
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.93	0.50
1:F:150:ILE:HG13	1:F:493:ILE:HA	1.93	0.50
1:M:350:ARG:O	1:M:354:GLU:HG2	2.12	0.50
1:S:278:ALA:HB1	1:S:289:LEU:HD21	1.93	0.50
1:C:49:ILE:HD11	1:R:73:MET:HE1	1.94	0.50
1:C:197:ARG:HA	1:C:277:LYS:HE3	1.94	0.50
1:I:358:SER:O	1:I:362:ARG:HG2	2.10	0.50
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.41	0.50
1:F:350:ARG:O	1:F:354:GLU:HG2	2.11	0.50
1:J:280:GLY:O	1:J:285:ARG:NH2	2.44	0.50
1:J:346:VAL:HG23	1:J:369:VAL:HG22	1.94	0.50
1:J:438:VAL:O	1:J:442:VAL:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:124:VAL:HG21	1:P:508:ALA:CB	2.41	0.50
1:R:415:GLY:HA2	4:R:602:ATP:H1'	1.94	0.50
1:S:213:VAL:HB	1:S:325:ILE:HB	1.93	0.50
1:C:219:PHE:CE2	1:C:245:LYS:HB2	2.46	0.50
1:J:238:GLU:HG2	2:K:23:GLY:HA3	1.94	0.50
1:L:415:GLY:HA2	4:L:602:ATP:H1'	1.94	0.50
1:M:456:LEU:HB2	1:M:462:PRO:HG3	1.94	0.50
1:S:247:LEU:HB3	1:S:273:VAL:HG22	1.93	0.50
1:C:82:ASN:O	1:C:86:GLY:N	2.41	0.50
1:E:197:ARG:HA	1:E:277:LYS:HE3	1.94	0.49
1:F:49:ILE:HD13	1:J:513:LEU:HB3	1.93	0.49
1:F:238:GLU:HG2	2:G:23:GLY:HA3	1.92	0.49
1:O:415:GLY:HA2	4:O:602:ATP:H1'	1.94	0.49
1:I:238:GLU:HG2	2:W:23:GLY:HA3	1.94	0.49
2:W:66:ILE:HD13	2:T:76:GLU:HG2	1.93	0.49
1:A:150:ILE:HG21	1:A:494:LEU:O	2.12	0.49
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.40	0.49
1:A:95:LEU:O	1:A:99:ILE:HG13	2.12	0.49
1:H:284:ARG:O	1:H:288:MET:HE3	2.11	0.49
1:F:115:ASP:OD2	1:F:433:ASN:ND2	2.39	0.49
1:H:166:MET:SD	1:H:171:LYS:HA	2.52	0.49
1:J:326:ASN:OD1	1:J:329:THR:N	2.33	0.49
1:J:456:LEU:HB2	1:J:462:PRO:HG3	1.94	0.49
2:N:53:GLU:OE1	2:N:53:GLU:N	2.45	0.49
1:C:199:TYR:HD2	1:C:325:ILE:HG22	1.77	0.49
1:C:291:ASP:OD2	1:C:368:ARG:NH1	2.44	0.49
1:E:117:LYS:HD2	1:E:516:THR:HG21	1.93	0.49
1:F:510:VAL:HG12	1:F:514:MET:HE2	1.93	0.49
1:H:350:ARG:HA	1:H:353:ILE:HD12	1.94	0.49
1:J:348:GLN:O	1:J:352:GLN:HG3	2.11	0.49
1:L:222:LEU:HB3	1:L:289:LEU:HD12	1.94	0.49
1:J:31:LEU:HD22	1:J:94:VAL:HG21	1.94	0.49
1:P:455:VAL:HG13	1:P:460:GLU:HB2	1.94	0.49
2:G:9:ARG:HD3	2:K:92:LEU:HD12	1.94	0.49
1:H:469:VAL:HG22	1:H:477:GLY:HA2	1.95	0.49
1:L:487:ASN:O	1:L:491:MET:HG3	2.13	0.49
1:A:194:GLN:NE2	1:A:331:THR:OG1	2.45	0.49
1:A:199:TYR:HD2	1:A:325:ILE:HG22	1.77	0.49
1:H:222:LEU:HB3	1:H:289:LEU:HD12	1.94	0.49
1:L:31:LEU:O	1:L:457:ASN:ND2	2.37	0.49
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:68:ASN:HB2	2:Q:92:LEU:HD21	1.95	0.49
1:S:12:ALA:HB1	1:S:520:MET:HG3	1.94	0.49
1:S:350:ARG:O	1:S:354:GLU:HG2	2.13	0.49
1:I:347:ALA:O	1:I:351:GLN:HG2	2.13	0.49
1:F:166:MET:HE1	1:F:407:VAL:HG11	1.95	0.49
1:F:456:LEU:HB2	1:F:462:PRO:HG3	1.95	0.49
1:H:31:LEU:HD22	1:H:94:VAL:HG21	1.95	0.49
1:J:188:ASP:OD2	1:J:380:LYS:NZ	2.43	0.49
1:I:417:VAL:HG21	1:I:477:GLY:HA3	1.95	0.49
1:I:438:VAL:O	1:I:442:VAL:HG13	2.13	0.49
1:B:238:GLU:HG2	2:D:23:GLY:HA3	1.95	0.49
1:B:291:ASP:OD1	1:B:345:ARG:NE	2.45	0.49
1:J:358:SER:O	1:J:362:ARG:HG2	2.13	0.49
2:N:74:LYS:NZ	2:N:76:GLU:OE1	2.46	0.48
2:Q:37:ARG:HD3	2:Q:95:VAL:HG21	1.93	0.48
1:R:254:VAL:HG11	1:R:262:LEU:HD12	1.94	0.48
1:B:242:LYS:NZ	2:D:23:GLY:O	2.46	0.48
1:E:95:LEU:O	1:E:99:ILE:HG13	2.13	0.48
1:E:142:LYS:HG3	1:E:146:GLN:HE21	1.78	0.48
1:E:150:ILE:HG21	1:E:494:LEU:O	2.13	0.48
2:G:3:ILE:HG12	2:G:78:ILE:HD12	1.95	0.48
1:S:284:ARG:O	1:S:288:MET:HG3	2.12	0.48
1:C:263:VAL:HA	1:C:266:THR:HG22	1.95	0.48
1:I:271:VAL:HG22	1:I:273:VAL:HG23	1.95	0.48
1:A:283:ASP:OD1	1:A:283:ASP:N	2.44	0.48
1:E:283:ASP:N	1:E:283:ASP:OD1	2.44	0.48
1:M:417:VAL:HG21	1:M:477:GLY:HA3	1.95	0.48
1:O:242:LYS:HB3	1:O:242:LYS:HE3	1.60	0.48
1:R:219:PHE:CE2	1:R:245:LYS:HB2	2.48	0.48
1:L:242:LYS:HB3	1:L:242:LYS:HE3	1.61	0.48
1:O:31:LEU:HD22	1:O:94:VAL:HG21	1.96	0.48
1:O:158:VAL:HG13	1:O:396:VAL:HG22	1.96	0.48
1:O:267:MET:SD	1:O:267:MET:N	2.87	0.48
1:R:386:GLU:O	1:R:389:MET:HB2	2.14	0.48
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.42	0.48
1:A:76:GLU:O	1:A:80:LYS:HG2	2.14	0.48
1:A:420:ILE:HG23	1:A:470:LYS:HG2	1.95	0.48
1:E:199:TYR:HD2	1:E:325:ILE:HG22	1.77	0.48
1:F:455:VAL:HG13	1:F:460:GLU:HB2	1.96	0.48
1:L:193:MET:SD	1:L:194:GLN:N	2.86	0.48
1:O:69:MET:CE	1:O:520:MET:HE2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:117:LYS:HD2	1:O:516:THR:HG21	1.96	0.48
1:I:510:VAL:O	1:I:514:MET:HG3	2.13	0.48
1:B:217:SER:O	1:B:245:LYS:NZ	2.42	0.48
1:B:248:LEU:HD13	1:B:325:ILE:HD11	1.94	0.48
1:H:95:LEU:O	1:H:99:ILE:HG13	2.14	0.48
1:L:421:ARG:O	1:L:425:LYS:HG2	2.14	0.48
1:P:144:ILE:HG21	1:P:166:MET:HE2	1.96	0.48
2:T:64:ILE:HB	2:T:95:VAL:HB	1.95	0.48
1:C:76:GLU:O	1:C:80:LYS:HG2	2.14	0.48
1:I:231:ARG:HA	1:I:234:LEU:HD23	1.95	0.48
1:A:60:ILE:O	1:A:75:LYS:NZ	2.34	0.48
1:B:271:VAL:HG22	1:B:273:VAL:HG23	1.96	0.48
1:J:221:LEU:HD23	1:J:249:ILE:HG12	1.95	0.48
1:O:246:PRO:HB3	1:O:272:LYS:HB2	1.95	0.48
2:Q:85:ILE:HG21	2:T:92:LEU:HB3	1.94	0.48
1:S:438:VAL:O	1:S:442:VAL:HG13	2.14	0.48
1:A:141:SER:HA	1:A:144:ILE:HD12	1.95	0.48
1:J:144:ILE:HG21	1:J:166:MET:HE2	1.96	0.48
1:J:322:ARG:HB3	1:J:333:ILE:HB	1.95	0.48
1:L:498:LYS:HG3	1:L:501:ARG:HH21	1.79	0.48
1:P:100:ILE:HD11	1:P:514:MET:HE3	1.95	0.48
1:R:69:MET:O	1:R:73:MET:HG2	2.14	0.48
1:R:288:MET:O	1:R:292:ILE:HG12	2.14	0.48
1:B:102:GLU:OE1	1:B:445:ARG:NH1	2.46	0.48
1:B:326:ASN:OD1	1:B:329:THR:N	2.33	0.48
1:E:157:THR:HA	1:E:160:LYS:HG2	1.96	0.48
1:H:283:ASP:OD1	1:H:283:ASP:N	2.46	0.48
1:J:89:THR:OG1	4:J:602:ATP:O2G	2.30	0.48
1:L:221:LEU:HD22	1:L:249:ILE:HG23	1.95	0.48
1:O:20:VAL:HG21	1:O:514:MET:HE1	1.95	0.48
1:O:421:ARG:O	1:O:425:LYS:HG2	2.14	0.48
1:C:95:LEU:O	1:C:99:ILE:HG13	2.14	0.48
1:C:284:ARG:O	1:C:288:MET:HE3	2.14	0.48
1:I:284:ARG:O	1:I:288:MET:HG3	2.13	0.48
1:B:150:ILE:HG13	1:B:493:ILE:HA	1.96	0.48
1:B:166:MET:HG2	1:B:175:ILE:CD1	2.44	0.48
1:O:82:ASN:HB2	1:O:89:THR:HG22	1.96	0.48
1:O:95:LEU:O	1:O:99:ILE:HG13	2.14	0.48
1:P:479:ASN:HB2	1:P:491:MET:CE	2.44	0.48
1:S:307:MET:HE2	1:S:307:MET:HB3	1.85	0.48
1:I:150:ILE:HG13	1:I:493:ILE:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:LYS:HG3	1:H:146:GLN:HE21	1.78	0.47
1:L:82:ASN:O	1:L:86:GLY:N	2.44	0.47
1:L:95:LEU:O	1:L:99:ILE:HG13	2.14	0.47
1:O:100:ILE:HG12	1:O:514:MET:HE2	1.95	0.47
2:Q:76:GLU:HG2	2:T:66:ILE:HD13	1.94	0.47
1:S:232:GLU:HG2	1:S:233:MET:HG3	1.95	0.47
1:I:239:ALA:HB1	1:I:314:LEU:HD21	1.96	0.47
1:A:100:ILE:HD13	1:A:514:MET:HE2	1.96	0.47
1:H:82:ASN:O	1:H:86:GLY:N	2.46	0.47
1:H:219:PHE:CE2	1:H:245:LYS:HB2	2.50	0.47
1:P:271:VAL:HG22	1:P:273:VAL:HG23	1.97	0.47
2:D:8:ASP:OD1	2:D:8:ASP:N	2.47	0.47
1:E:421:ARG:O	1:E:425:LYS:HG2	2.15	0.47
1:J:488:MET:HE2	1:J:488:MET:HA	1.95	0.47
1:L:125:THR:O	1:L:129:GLU:HG2	2.14	0.47
1:M:40:LEU:HD13	1:M:59:GLU:HG3	1.96	0.47
1:O:209:GLU:HG3	1:O:390:LYS:HB2	1.96	0.47
1:P:345:ARG:O	1:P:349:ILE:HG13	2.14	0.47
1:A:421:ARG:O	1:A:425:LYS:HG2	2.14	0.47
1:B:282:GLY:C	1:B:284:ARG:H	2.21	0.47
1:F:152:ALA:O	1:F:395:ARG:NH1	2.46	0.47
1:J:271:VAL:HG22	1:J:273:VAL:HG23	1.96	0.47
1:M:68:ASN:O	1:M:72:GLN:HG2	2.15	0.47
1:O:125:THR:O	1:O:129:GLU:HG2	2.14	0.47
1:R:383:ALA:HB3	1:R:389:MET:SD	2.55	0.47
1:C:142:LYS:HG3	1:C:146:GLN:HE21	1.79	0.47
1:C:157:THR:HA	1:C:160:LYS:HG2	1.96	0.47
1:H:199:TYR:HD2	1:H:325:ILE:HG22	1.78	0.47
2:N:79:ASP:O	2:N:80:ASN:ND2	2.47	0.47
1:O:440:ILE:O	1:O:444:LEU:HG	2.15	0.47
1:P:177:VAL:HG23	1:P:400:LEU:HD22	1.96	0.47
2:Q:39:GLU:HA	2:Q:64:ILE:HA	1.96	0.47
1:S:487:ASN:HB3	1:S:490:ASP:HB2	1.96	0.47
1:B:239:ALA:HB1	1:B:314:LEU:HD21	1.96	0.47
1:J:69:MET:HE2	1:J:522:THR:HB	1.96	0.47
1:J:386:GLU:HB3	1:M:76:GLU:OE2	2.14	0.47
1:L:12:ALA:O	1:L:16:MET:HG3	2.15	0.47
1:L:60:ILE:O	1:L:75:LYS:NZ	2.36	0.47
1:O:199:TYR:HD2	1:O:325:ILE:HG22	1.79	0.47
1:P:66:PHE:HA	1:P:69:MET:HE3	1.96	0.47
1:R:142:LYS:HG3	1:R:146:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:321:LYS:HB2	1:R:334:ASP:HB3	1.96	0.47
1:C:420:ILE:HG23	1:C:470:LYS:HG2	1.95	0.47
1:I:291:ASP:HB3	1:I:372:LEU:HD11	1.96	0.47
1:A:157:THR:HA	1:A:160:LYS:HG2	1.97	0.47
1:A:222:LEU:HB3	1:A:289:LEU:HD12	1.95	0.47
1:H:66:PHE:O	1:H:69:MET:HG2	2.15	0.47
2:N:39:GLU:HA	2:N:64:ILE:HA	1.96	0.47
1:O:76:GLU:O	1:O:80:LYS:HG2	2.15	0.47
1:P:150:ILE:HG13	1:P:493:ILE:HA	1.97	0.47
1:P:242:LYS:HD3	1:P:242:LYS:N	2.30	0.47
1:S:456:LEU:HB2	1:S:462:PRO:HG3	1.96	0.47
1:L:157:THR:HA	1:L:160:LYS:HG2	1.96	0.47
1:L:283:ASP:O	1:L:286:LYS:HG3	2.15	0.47
1:P:417:VAL:HG21	1:P:477:GLY:HA3	1.95	0.47
1:R:125:THR:O	1:R:129:GLU:HG2	2.15	0.47
1:R:205:ILE:HA	1:R:213:VAL:HG22	1.97	0.47
1:C:125:THR:O	1:C:129:GLU:HG2	2.15	0.47
1:F:11:ASP:OD1	1:F:12:ALA:N	2.48	0.47
1:H:157:THR:HA	1:H:160:LYS:HG2	1.97	0.47
1:J:232:GLU:OE1	1:J:232:GLU:N	2.48	0.47
1:L:420:ILE:HG23	1:L:470:LYS:HG2	1.96	0.47
1:I:339:GLU:O	1:I:343:GLN:HG2	2.15	0.47
1:F:128:VAL:HG21	1:F:505:GLN:HE21	1.80	0.47
2:G:8:ASP:OD1	2:G:8:ASP:N	2.48	0.47
1:O:420:ILE:HG23	1:O:470:LYS:HG2	1.97	0.47
1:A:421:ARG:NH2	1:A:476:TYR:O	2.49	0.46
2:G:15:LYS:HD3	2:G:37:ARG:HG3	1.98	0.46
1:J:239:ALA:HB1	1:J:314:LEU:HD21	1.96	0.46
1:L:350:ARG:HA	1:L:353:ILE:HD12	1.97	0.46
1:M:320:ALA:HA	1:M:335:GLY:HA2	1.97	0.46
1:R:117:LYS:HD2	1:R:516:THR:HG21	1.97	0.46
1:R:199:TYR:HD2	1:R:325:ILE:HG22	1.80	0.46
1:R:322:ARG:HB3	1:R:333:ILE:HD12	1.97	0.46
1:C:31:LEU:O	1:C:457:ASN:ND2	2.37	0.46
1:E:242:LYS:HE3	1:E:242:LYS:HB3	1.62	0.46
1:F:438:VAL:O	1:F:442:VAL:HG13	2.15	0.46
1:H:141:SER:HA	1:H:144:ILE:HD12	1.97	0.46
1:L:219:PHE:CE2	1:L:245:LYS:HB2	2.50	0.46
1:O:131:LEU:HG	1:O:422:VAL:HG21	1.96	0.46
1:O:350:ARG:O	1:O:354:GLU:HG2	2.15	0.46
1:P:438:VAL:O	1:P:442:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:345:ARG:O	1:I:349:ILE:HG13	2.16	0.46
2:W:3:ILE:HG13	2:W:78:ILE:HG21	1.97	0.46
1:A:383:ALA:N	1:A:389:MET:HE1	2.30	0.46
1:E:141:SER:HA	1:E:144:ILE:HD12	1.97	0.46
1:H:131:LEU:HG	1:H:422:VAL:HG21	1.97	0.46
1:O:283:ASP:OD1	1:O:283:ASP:N	2.48	0.46
1:O:346:VAL:HG12	1:O:372:LEU:HD12	1.98	0.46
1:R:157:THR:HA	1:R:160:LYS:HG2	1.97	0.46
1:A:69:MET:HE2	1:A:520:MET:HE2	1.96	0.46
2:D:82:GLU:N	2:D:82:GLU:OE1	2.49	0.46
1:F:89:THR:OG1	4:F:602:ATP:O2G	2.31	0.46
1:H:12:ALA:O	1:H:16:MET:HG3	2.15	0.46
1:J:417:VAL:HG21	1:J:477:GLY:HA3	1.97	0.46
1:O:157:THR:HA	1:O:160:LYS:HG2	1.96	0.46
1:O:405:ALA:HB1	1:O:498:LYS:HB3	1.97	0.46
1:P:364:LYS:HA	1:P:364:LYS:HD2	1.77	0.46
1:R:229:ASN:HD21	1:R:231:ARG:HB3	1.81	0.46
2:T:11:ILE:CD1	2:T:85:ILE:HG12	2.46	0.46
1:A:77:VAL:HG13	1:A:506:TYR:HB3	1.98	0.46
1:F:441:LYS:HA	1:F:441:LYS:HD3	1.69	0.46
2:G:6:LEU:HD12	2:K:93:ALA:HA	1.96	0.46
1:J:265:ASN:ND2	2:K:25:ILE:HD12	2.30	0.46
2:K:11:ILE:HD12	2:K:85:ILE:HG12	1.98	0.46
1:P:56:VAL:O	1:P:60:ILE:HG12	2.16	0.46
1:C:12:ALA:HB1	1:C:520:MET:SD	2.56	0.46
1:I:105:LYS:HE3	1:O:110:GLY:HA3	1.97	0.46
1:F:40:LEU:HD13	1:F:59:GLU:HG3	1.98	0.46
1:F:262:LEU:O	1:F:266:THR:OG1	2.27	0.46
1:F:265:ASN:HD22	1:F:270:ILE:HD11	1.80	0.46
2:G:53:GLU:OE1	2:G:53:GLU:N	2.49	0.46
1:J:224:ASP:HB2	1:J:302:SER:HB2	1.98	0.46
1:O:190:VAL:HG21	1:O:333:ILE:HG23	1.98	0.46
1:B:441:LYS:HA	1:B:441:LYS:HD3	1.70	0.46
1:E:69:MET:O	1:E:73:MET:HG2	2.15	0.46
1:E:125:THR:O	1:E:129:GLU:HG2	2.15	0.46
1:E:263:VAL:HA	1:E:266:THR:HG22	1.96	0.46
1:F:345:ARG:O	1:F:349:ILE:HG13	2.16	0.46
1:H:42:LYS:HA	1:H:42:LYS:HD3	1.78	0.46
1:O:283:ASP:O	1:O:286:LYS:HG3	2.16	0.46
1:P:40:LEU:HD13	1:P:59:GLU:HG3	1.97	0.46
1:R:82:ASN:O	1:R:86:GLY:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:350:ARG:O	1:R:354:GLU:HG2	2.15	0.46
1:S:455:VAL:HG13	1:S:460:GLU:HB2	1.97	0.46
1:C:440:ILE:O	1:C:444:LEU:HG	2.16	0.46
1:A:440:ILE:O	1:A:444:LEU:HG	2.15	0.46
1:B:16:MET:HE2	1:B:16:MET:HB3	1.85	0.46
1:E:76:GLU:O	1:E:80:LYS:HG2	2.15	0.46
1:E:198:GLY:HA2	1:E:326:ASN:O	2.16	0.46
1:F:326:ASN:OD1	1:F:329:THR:N	2.32	0.46
1:F:364:LYS:HA	1:F:364:LYS:HD2	1.79	0.46
1:H:76:GLU:O	1:H:80:LYS:HG2	2.16	0.46
2:K:82:GLU:N	2:K:82:GLU:OE1	2.48	0.46
1:L:246:PRO:HB3	1:L:272:LYS:HB2	1.97	0.46
1:R:131:LEU:HG	1:R:422:VAL:HG21	1.96	0.46
1:C:301:ILE:HD11	1:C:309:LEU:HA	1.97	0.46
1:A:350:ARG:HA	1:A:353:ILE:HD12	1.98	0.46
1:E:131:LEU:HG	1:E:422:VAL:HG21	1.97	0.46
1:O:142:LYS:HG3	1:O:146:GLN:HE21	1.81	0.46
1:R:420:ILE:HG23	1:R:470:LYS:HG2	1.97	0.46
1:I:403:THR:O	1:I:407:VAL:HG13	2.16	0.46
1:A:204:PHE:HD1	1:A:266:THR:HG21	1.80	0.46
1:J:56:VAL:O	1:J:60:ILE:HG12	2.16	0.46
1:J:403:THR:O	1:J:407:VAL:HG13	2.16	0.46
1:M:56:VAL:O	1:M:60:ILE:HG12	2.16	0.46
1:M:302:SER:HB3	1:M:305:ILE:HG22	1.98	0.46
1:S:56:VAL:O	1:S:60:ILE:HG12	2.16	0.46
1:I:40:LEU:HD13	1:I:59:GLU:HG3	1.98	0.45
2:W:82:GLU:N	2:W:82:GLU:OE1	2.49	0.45
1:B:69:MET:HE1	1:B:520:MET:HB3	1.98	0.45
1:E:110:GLY:HA3	1:M:105:LYS:HE3	1.98	0.45
1:H:125:THR:O	1:H:129:GLU:HG2	2.15	0.45
1:J:152:ALA:O	1:J:395:ARG:NH1	2.49	0.45
1:J:268:ARG:HB2	1:J:270:ILE:HG12	1.97	0.45
1:J:479:ASN:HB2	1:J:491:MET:CE	2.46	0.45
1:L:440:ILE:O	1:L:444:LEU:HG	2.16	0.45
1:S:345:ARG:O	1:S:349:ILE:HG13	2.16	0.45
1:C:69:MET:HE2	1:C:520:MET:HE2	1.97	0.45
1:C:240:VAL:HG21	1:C:247:LEU:HD13	1.98	0.45
2:W:64:ILE:HD12	2:W:64:ILE:H	1.81	0.45
1:B:174:VAL:HG22	1:B:366:GLN:HG3	1.97	0.45
1:B:403:THR:O	1:B:407:VAL:HG13	2.17	0.45
1:E:171:LYS:HE3	1:E:407:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:ALA:O	1:F:278:ALA:N	2.45	0.45
1:L:16:MET:HE1	1:L:73:MET:CE	2.46	0.45
1:M:345:ARG:O	1:M:349:ILE:HG13	2.16	0.45
1:M:347:ALA:O	1:M:351:GLN:HG2	2.17	0.45
1:O:77:VAL:HG13	1:O:506:TYR:HB3	1.98	0.45
1:R:76:GLU:O	1:R:80:LYS:HG2	2.16	0.45
1:S:69:MET:HE2	1:S:522:THR:HB	1.98	0.45
1:S:214:GLU:OE2	1:S:322:ARG:NH2	2.48	0.45
1:C:232:GLU:HG2	1:C:233:MET:CE	2.47	0.45
1:C:346:VAL:HG23	1:C:350:ARG:HH21	1.82	0.45
1:I:56:VAL:O	1:I:60:ILE:HG12	2.16	0.45
1:F:270:ILE:HD12	2:G:25:ILE:HA	1.98	0.45
1:J:231:ARG:HA	1:J:234:LEU:HD23	1.98	0.45
1:L:118:ARG:NH2	1:O:483:GLU:OE2	2.50	0.45
1:C:288:MET:O	1:C:292:ILE:HG12	2.17	0.45
1:C:383:ALA:HB3	1:C:389:MET:SD	2.56	0.45
1:I:69:MET:HE1	1:I:520:MET:HB3	1.97	0.45
1:E:440:ILE:O	1:E:444:LEU:HG	2.15	0.45
1:H:106:ALA:O	1:H:111:MET:HG3	2.16	0.45
1:H:291:ASP:OD1	1:H:345:ARG:NE	2.50	0.45
1:M:280:GLY:O	1:M:285:ARG:NH2	2.49	0.45
1:S:321:LYS:HG3	1:S:322:ARG:HG2	1.99	0.45
1:I:514:MET:HE3	1:I:514:MET:HB3	1.83	0.45
2:G:77:LYS:O	2:K:37:ARG:NH2	2.50	0.45
1:H:70:GLY:O	1:H:73:MET:HG2	2.16	0.45
1:J:345:ARG:O	1:J:349:ILE:HG13	2.16	0.45
1:J:487:ASN:O	1:J:491:MET:HG3	2.17	0.45
1:L:117:LYS:HD2	1:L:516:THR:HG21	1.98	0.45
1:L:199:TYR:HD2	1:L:325:ILE:HG22	1.81	0.45
1:O:141:SER:HA	1:O:144:ILE:HD12	1.98	0.45
1:B:40:LEU:HD13	1:B:59:GLU:HG3	1.98	0.45
1:B:56:VAL:O	1:B:60:ILE:HG12	2.15	0.45
1:B:284:ARG:O	1:B:288:MET:HE3	2.17	0.45
1:B:479:ASN:HB2	1:B:491:MET:CE	2.47	0.45
2:G:27:LEU:HB3	2:G:32:ALA:HB2	1.98	0.45
2:G:55:LYS:HB3	2:G:55:LYS:HE3	1.82	0.45
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.99	0.45
1:P:31:LEU:HD23	1:P:453:GLN:HB3	1.99	0.45
1:R:419:LEU:HD22	1:R:447:MET:HG3	1.99	0.45
1:C:38:VAL:HG11	1:C:56:VAL:HG13	1.99	0.45
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.99	0.45
1:A:198:GLY:HA2	1:A:326:ASN:O	2.16	0.45
1:B:254:VAL:O	1:B:259:LEU:HD12	2.16	0.45
1:B:456:LEU:HB2	1:B:462:PRO:HG3	1.98	0.45
1:J:234:LEU:HD12	2:K:25:ILE:HG21	1.98	0.45
1:L:76:GLU:O	1:L:80:LYS:HG2	2.17	0.45
1:M:271:VAL:HG22	1:M:273:VAL:HG23	1.99	0.45
1:O:25:ASP:O	1:O:29:VAL:HG13	2.17	0.45
1:S:20:VAL:CG2	1:S:514:MET:HE1	2.46	0.45
1:S:403:THR:O	1:S:407:VAL:HG13	2.16	0.45
1:I:233:MET:HE3	1:I:233:MET:HB2	1.85	0.45
1:A:150:ILE:HD11	4:A:602:ATP:N7	2.32	0.45
1:E:25:ASP:O	1:E:29:VAL:HG13	2.16	0.45
1:F:56:VAL:O	1:F:60:ILE:HG12	2.17	0.45
1:F:68:ASN:O	1:F:72:GLN:HG2	2.16	0.45
1:H:110:GLY:HA3	1:P:105:LYS:HE3	1.99	0.45
1:L:13:ARG:HA	1:L:16:MET:HG3	1.98	0.45
1:M:177:VAL:HG23	1:M:400:LEU:HD22	1.97	0.45
1:P:15:LYS:NZ	1:P:64:ASP:OD2	2.35	0.45
1:R:22:VAL:HG11	1:R:62:LEU:HD11	1.98	0.45
2:W:94:ILE:HG23	2:T:6:LEU:HD11	1.99	0.45
1:A:125:THR:O	1:A:129:GLU:HG2	2.16	0.45
1:B:438:VAL:O	1:B:442:VAL:HG13	2.16	0.45
1:B:511:ALA:O	1:B:515:ILE:HG23	2.17	0.45
1:B:513:LEU:HD23	1:B:513:LEU:HA	1.83	0.45
1:E:38:VAL:HG11	1:E:56:VAL:HG13	1.99	0.45
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.99	0.45
1:O:82:ASN:O	1:O:86:GLY:N	2.47	0.45
1:I:386:GLU:HB3	1:B:76:GLU:OE2	2.17	0.45
1:A:110:GLY:HA3	1:J:105:LYS:HE3	1.98	0.45
1:B:31:LEU:HD23	1:B:453:GLN:HB3	1.97	0.45
1:H:263:VAL:HG12	1:H:267:MET:HE1	1.99	0.45
1:L:477:GLY:HA3	1:L:488:MET:HE2	1.99	0.45
1:M:403:THR:O	1:M:407:VAL:HG13	2.17	0.45
1:O:73:MET:HE3	1:R:49:ILE:HD11	1.99	0.45
1:R:198:GLY:HA2	1:R:326:ASN:O	2.16	0.45
1:S:513:LEU:HD23	1:S:513:LEU:HA	1.85	0.45
1:C:314:LEU:HD12	1:C:317:LEU:HD12	2.00	0.44
1:A:69:MET:CE	1:A:520:MET:HE2	2.47	0.44
1:L:131:LEU:HG	1:L:422:VAL:HG21	1.99	0.44
1:M:307:MET:H	1:M:307:MET:HG2	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:11:ASP:OD1	1:P:12:ALA:N	2.50	0.44
1:C:131:LEU:HG	1:C:422:VAL:HG21	1.97	0.44
2:W:8:ASP:HB3	2:W:47:ARG:HB2	2.00	0.44
1:E:73:MET:CE	1:H:49:ILE:HD11	2.46	0.44
1:E:232:GLU:HG2	1:E:233:MET:CE	2.47	0.44
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.98	0.44
1:M:128:VAL:HG21	1:M:505:GLN:HE21	1.82	0.44
1:O:222:LEU:HB3	1:O:289:LEU:HD12	1.99	0.44
1:R:232:GLU:HG2	1:R:233:MET:CE	2.47	0.44
1:A:25:ASP:O	1:A:29:VAL:HG13	2.18	0.44
1:B:115:ASP:OD1	1:B:118:ARG:NH1	2.49	0.44
1:J:226:LYS:HE3	1:J:253:ASP:HB3	1.99	0.44
1:L:65:LYS:O	1:L:69:MET:HG3	2.16	0.44
1:M:307:MET:HE2	1:M:307:MET:HB3	1.91	0.44
2:N:12:VAL:HG22	2:N:40:VAL:HG22	1.99	0.44
1:E:150:ILE:HD11	4:E:602:ATP:N7	2.33	0.44
1:F:100:ILE:HD11	1:F:514:MET:HE3	1.98	0.44
1:F:217:SER:HA	1:F:320:ALA:O	2.18	0.44
1:H:198:GLY:HA2	1:H:326:ASN:O	2.18	0.44
1:H:215:LEU:HB3	1:H:218:PRO:HB3	1.99	0.44
1:J:217:SER:O	1:J:245:LYS:NZ	2.40	0.44
1:J:291:ASP:HB3	1:J:372:LEU:HD11	2.00	0.44
1:M:13:ARG:HD2	1:M:104:LEU:HD22	1.98	0.44
1:O:174:VAL:HG12	1:O:376:VAL:HG13	2.00	0.44
1:P:279:PRO:HG2	1:P:288:MET:HE3	1.99	0.44
1:A:82:ASN:O	1:A:86:GLY:N	2.50	0.44
1:H:25:ASP:O	1:H:29:VAL:HG13	2.18	0.44
1:H:76:GLU:OE1	1:H:80:LYS:NZ	2.50	0.44
1:J:265:ASN:ND2	2:K:26:VAL:H	2.16	0.44
1:J:441:LYS:HA	1:J:441:LYS:HD3	1.70	0.44
2:N:68:ASN:HB2	2:N:92:LEU:HD21	1.98	0.44
1:O:198:GLY:HA2	1:O:326:ASN:O	2.17	0.44
1:O:232:GLU:HG2	1:O:233:MET:CE	2.48	0.44
1:O:291:ASP:OD1	1:O:345:ARG:NE	2.51	0.44
1:R:38:VAL:HG11	1:R:56:VAL:HG13	2.00	0.44
1:B:68:ASN:O	1:B:72:GLN:HG2	2.17	0.44
1:B:347:ALA:O	1:B:351:GLN:HG2	2.18	0.44
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.98	0.44
1:H:221:LEU:HD22	1:H:249:ILE:HG23	1.99	0.44
1:H:251:ALA:O	1:H:278:ALA:N	2.51	0.44
1:J:40:LEU:HD13	1:J:59:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:383:ALA:HB2	1:L:392:LYS:HD3	1.99	0.44
1:M:31:LEU:HD23	1:M:453:GLN:HB3	2.00	0.44
1:P:441:LYS:HA	1:P:441:LYS:HD3	1.71	0.44
1:R:185:ASP:OD1	1:R:185:ASP:N	2.50	0.44
1:C:242:LYS:HE3	1:C:242:LYS:HB3	1.62	0.44
1:A:404:ARG:O	1:A:408:GLU:HG2	2.18	0.44
1:B:345:ARG:O	1:B:349:ILE:HG13	2.17	0.44
1:B:346:VAL:HG23	1:B:369:VAL:HG22	2.00	0.44
1:E:169:VAL:HG11	1:E:377:ALA:HB2	2.00	0.44
1:F:358:SER:O	1:F:362:ARG:HG2	2.18	0.44
1:H:215:LEU:HD23	1:H:246:PRO:HB2	2.00	0.44
1:L:386:GLU:HA	1:L:389:MET:HB2	1.99	0.44
1:M:69:MET:HE1	1:M:520:MET:HB3	2.00	0.44
1:M:386:GLU:HB3	1:P:76:GLU:OE2	2.17	0.44
1:B:195:PHE:HB2	1:B:279:PRO:HB3	1.99	0.44
1:B:417:VAL:HG21	1:B:477:GLY:HA3	2.00	0.44
1:F:226:LYS:HE3	1:F:253:ASP:HB3	2.00	0.44
1:F:344:GLY:O	1:F:348:GLN:HG3	2.17	0.44
1:L:25:ASP:O	1:L:29:VAL:HG13	2.18	0.44
1:L:193:MET:HG3	1:L:332:ILE:HG22	2.00	0.44
1:L:321:LYS:HB2	1:L:334:ASP:HB3	2.00	0.44
1:R:321:LYS:HD3	1:R:321:LYS:HA	1.66	0.44
1:C:141:SER:HA	1:C:144:ILE:HD12	1.99	0.44
1:C:263:VAL:O	1:C:267:MET:SD	2.76	0.44
1:I:513:LEU:HD11	1:S:388:GLU:HA	2.00	0.44
1:E:37:ASN:HB3	1:E:49:ILE:HG23	1.99	0.44
2:G:78:ILE:HG12	2:G:79:ASP:OD2	2.18	0.44
1:H:440:ILE:O	1:H:444:LEU:HG	2.16	0.44
1:J:229:ASN:OD1	1:J:231:ARG:NH2	2.47	0.44
1:M:389:MET:HE2	1:M:389:MET:HB2	1.78	0.44
1:O:123:ALA:HB2	1:O:440:ILE:HG12	1.99	0.44
1:P:13:ARG:HD2	1:P:104:LEU:HD22	2.00	0.44
1:P:144:ILE:HD13	1:P:144:ILE:HA	1.85	0.44
1:R:366:GLN:HA	1:R:369:VAL:HG22	2.00	0.44
1:C:47:PRO:HG3	1:R:69:MET:HG2	2.00	0.43
1:I:511:ALA:O	1:I:515:ILE:HG23	2.17	0.43
1:A:131:LEU:HG	1:A:422:VAL:HG21	1.99	0.43
1:J:222:LEU:HB3	1:J:289:LEU:HD12	2.00	0.43
1:M:441:LYS:HA	1:M:441:LYS:HD3	1.69	0.43
1:O:366:GLN:HA	1:O:369:VAL:HG22	2.00	0.43
1:O:469:VAL:HG22	1:O:477:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:302:SER:HB3	1:P:305:ILE:HG22	1.99	0.43
1:R:225:LYS:HB3	1:R:225:LYS:HE3	1.61	0.43
1:S:358:SER:O	1:S:362:ARG:HG2	2.18	0.43
1:A:76:GLU:HG3	1:E:46:ALA:CB	2.48	0.43
1:A:524:LEU:HG	1:A:525:PRO:HD2	1.99	0.43
1:E:524:LEU:HG	1:E:525:PRO:HD2	2.00	0.43
1:H:321:LYS:HB2	1:H:334:ASP:HB3	2.01	0.43
1:J:228:SER:HB2	1:J:255:GLU:OE2	2.18	0.43
1:R:16:MET:HE3	1:R:520:MET:HE2	2.00	0.43
1:S:510:VAL:O	1:S:514:MET:HG3	2.18	0.43
1:A:251:ALA:O	1:A:278:ALA:N	2.51	0.43
1:A:469:VAL:HG22	1:A:477:GLY:HA2	1.99	0.43
1:B:479:ASN:HB2	1:B:491:MET:HE1	1.99	0.43
2:G:11:ILE:CD1	2:G:85:ILE:HG12	2.48	0.43
1:M:390:LYS:HE2	1:M:390:LYS:HB3	1.89	0.43
1:M:439:GLY:O	1:M:442:VAL:HG22	2.18	0.43
1:R:196:ASP:HA	1:R:329:THR:HA	2.00	0.43
1:H:524:LEU:HG	1:H:525:PRO:HD2	2.01	0.43
1:M:265:ASN:ND2	2:N:25:ILE:HG13	2.34	0.43
1:M:387:VAL:HG13	1:P:76:GLU:OE1	2.18	0.43
1:M:513:LEU:HD23	1:M:513:LEU:HA	1.81	0.43
1:O:12:ALA:O	1:O:16:MET:HG3	2.19	0.43
1:P:456:LEU:HB2	1:P:462:PRO:HG3	1.99	0.43
1:R:25:ASP:O	1:R:29:VAL:HG13	2.19	0.43
1:S:13:ARG:HD2	1:S:104:LEU:HD22	2.00	0.43
1:C:383:ALA:HB1	1:C:388:GLU:CD	2.42	0.43
2:W:20:LYS:HG2	2:W:26:VAL:HG22	1.99	0.43
1:A:70:GLY:O	1:A:73:MET:HG3	2.17	0.43
1:J:16:MET:HE2	1:J:16:MET:HB3	1.85	0.43
1:J:177:VAL:HG23	1:J:400:LEU:HD22	1.99	0.43
1:L:16:MET:HE2	1:L:514:MET:HE2	2.01	0.43
1:L:180:GLY:HA2	1:L:380:LYS:HB3	2.00	0.43
1:M:322:ARG:HB3	1:M:333:ILE:HB	2.00	0.43
1:P:439:GLY:O	1:P:442:VAL:HG22	2.18	0.43
1:R:283:ASP:OD1	1:R:283:ASP:N	2.51	0.43
1:R:352:GLN:HA	1:R:355:GLU:HG2	2.00	0.43
2:T:65:VAL:HA	2:T:94:ILE:HA	2.01	0.43
1:C:25:ASP:O	1:C:29:VAL:HG13	2.18	0.43
1:C:198:GLY:HA2	1:C:326:ASN:O	2.18	0.43
1:C:233:MET:SD	1:C:233:MET:N	2.90	0.43
1:C:498:LYS:HG3	1:C:501:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:439:GLY:O	1:I:442:VAL:HG22	2.18	0.43
1:B:305:ILE:HG23	1:B:307:MET:HE3	2.01	0.43
1:E:251:ALA:O	1:E:278:ALA:N	2.51	0.43
1:F:65:LYS:HB2	1:F:522:THR:HG21	2.01	0.43
1:J:439:GLY:O	1:J:442:VAL:HG22	2.18	0.43
1:L:77:VAL:HG13	1:L:506:TYR:HB3	2.01	0.43
1:L:263:VAL:HG12	1:L:267:MET:HE1	2.00	0.43
1:M:127:ALA:HB2	1:M:447:MET:HE1	1.99	0.43
2:Q:47:ARG:NH2	2:Q:88:GLU:OE1	2.52	0.43
1:R:232:GLU:HG2	1:R:233:MET:HE1	1.99	0.43
1:R:263:VAL:O	1:R:267:MET:SD	2.77	0.43
1:C:42:LYS:HA	1:C:42:LYS:HD3	1.78	0.43
1:C:321:LYS:HA	1:C:321:LYS:HD3	1.69	0.43
1:I:77:VAL:HG12	1:I:92:ALA:HB1	2.00	0.43
1:F:107:VAL:HG22	1:F:113:PRO:HG3	2.00	0.43
1:H:138:CYS:O	1:H:171:LYS:NZ	2.50	0.43
1:H:188:ASP:OD2	1:H:380:LYS:NZ	2.37	0.43
1:O:114:MET:HE2	1:R:36:ARG:HD3	2.01	0.43
1:R:250:ILE:HD11	1:R:279:PRO:HD2	2.01	0.43
1:R:314:LEU:HD12	1:R:317:LEU:HD12	2.01	0.43
1:C:269:GLY:HA3	1:R:257:GLU:CD	2.43	0.43
1:I:31:LEU:HD22	1:I:94:VAL:HG21	2.01	0.43
1:B:177:VAL:HG23	1:B:400:LEU:HD22	2.01	0.43
1:B:215:LEU:HD23	1:B:246:PRO:HB2	1.99	0.43
1:F:111:MET:HG3	1:F:435:ASP:OD2	2.18	0.43
1:F:222:LEU:HD22	1:F:293:ALA:HB2	2.01	0.43
1:H:219:PHE:HB3	1:H:317:LEU:HD22	2.00	0.43
1:P:140:ASP:OD1	1:P:140:ASP:N	2.50	0.43
1:P:511:ALA:O	1:P:515:ILE:HG23	2.18	0.43
1:S:514:MET:HB3	1:S:514:MET:HE2	1.73	0.43
1:B:200:LEU:HD23	1:B:276:VAL:HA	2.01	0.43
1:E:221:LEU:HD22	1:E:249:ILE:HG23	1.99	0.43
1:H:263:VAL:HA	1:H:266:THR:HG22	1.99	0.43
1:H:366:GLN:HA	1:H:369:VAL:HG22	2.01	0.43
1:L:76:GLU:HG3	1:O:46:ALA:CB	2.48	0.43
1:M:74:VAL:HB	1:M:514:MET:HE1	2.00	0.43
1:C:291:ASP:O	1:C:295:LEU:HG	2.19	0.43
1:C:524:LEU:HG	1:C:525:PRO:HD2	1.99	0.43
1:B:247:LEU:HD23	1:B:273:VAL:HG22	2.00	0.43
1:F:264:VAL:HG21	2:G:28:THR:HG21	2.01	0.43
1:F:403:THR:O	1:F:407:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:11:ASP:OD1	1:J:12:ALA:N	2.52	0.43
1:L:283:ASP:OD1	1:L:283:ASP:N	2.51	0.43
1:L:479:ASN:HB2	1:L:491:MET:SD	2.59	0.43
1:S:439:GLY:O	1:S:442:VAL:HG22	2.19	0.43
1:C:49:ILE:HD11	1:R:73:MET:CE	2.49	0.42
1:C:215:LEU:HD12	1:C:248:LEU:HB3	2.00	0.42
1:B:147:VAL:HG23	1:B:494:LEU:HD12	2.01	0.42
1:B:217:SER:HA	1:B:320:ALA:O	2.19	0.42
1:F:343:GLN:O	1:F:346:VAL:HG12	2.19	0.42
1:J:54:VAL:HB	1:J:89:THR:HG21	2.01	0.42
2:K:76:GLU:HG2	2:N:66:ILE:HD13	2.01	0.42
1:P:199:TYR:HA	1:P:276:VAL:HG12	2.01	0.42
1:R:284:ARG:NH2	1:R:361:ASP:HA	2.33	0.42
1:S:176:THR:HG23	1:S:378:VAL:HG22	2.01	0.42
1:I:217:SER:HA	1:I:320:ALA:O	2.19	0.42
1:E:419:LEU:HD22	1:E:447:MET:HG3	2.00	0.42
1:F:439:GLY:O	1:F:442:VAL:HG22	2.19	0.42
1:H:38:VAL:HG11	1:H:56:VAL:HG13	2.00	0.42
1:J:325:ILE:HG23	1:J:330:THR:OG1	2.19	0.42
2:K:67:PHE:HB3	2:K:91:ILE:HD13	2.01	0.42
1:L:217:SER:HA	1:L:320:ALA:O	2.19	0.42
1:R:469:VAL:HG22	1:R:477:GLY:HA2	2.00	0.42
1:S:40:LEU:HD13	1:S:59:GLU:HG3	2.00	0.42
1:I:305:ILE:HG23	1:I:307:MET:HE3	2.01	0.42
1:I:322:ARG:HB3	1:I:333:ILE:HB	2.01	0.42
1:B:128:VAL:HG21	1:B:505:GLN:HE21	1.84	0.42
1:B:166:MET:HA	1:B:169:VAL:HG22	2.00	0.42
1:E:13:ARG:HA	1:E:16:MET:HG3	2.01	0.42
1:F:511:ALA:O	1:F:515:ILE:HG23	2.19	0.42
1:H:169:VAL:HG11	1:H:377:ALA:HB2	2.02	0.42
1:J:387:VAL:HG13	1:M:76:GLU:OE1	2.19	0.42
1:P:513:LEU:HD23	1:P:513:LEU:HA	1.82	0.42
1:B:82:ASN:HB2	1:B:89:THR:HG21	2.02	0.42
1:E:76:GLU:HG3	1:H:46:ALA:CB	2.48	0.42
1:H:180:GLY:N	1:H:381:VAL:O	2.46	0.42
1:J:389:MET:HE2	1:J:389:MET:HB2	1.93	0.42
2:K:53:GLU:N	2:K:53:GLU:OE1	2.53	0.42
1:L:42:LYS:HA	1:L:42:LYS:HD3	1.78	0.42
1:L:65:LYS:HB3	1:L:65:LYS:HE3	1.88	0.42
1:I:320:ALA:HA	1:I:335:GLY:HA2	2.02	0.42
1:F:479:ASN:O	1:F:483:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:321:LYS:HD3	1:L:321:LYS:HA	1.66	0.42
1:M:31:LEU:HD12	4:M:602:ATP:H5'1	2.02	0.42
1:O:37:ASN:HB3	1:O:49:ILE:HG23	2.00	0.42
1:O:219:PHE:CD1	1:O:317:LEU:HG	2.55	0.42
1:S:263:VAL:O	1:S:267:MET:SD	2.78	0.42
1:S:417:VAL:HG21	1:S:477:GLY:HA3	2.00	0.42
1:C:69:MET:SD	1:A:41:ASP:HB2	2.59	0.42
1:I:518:GLU:HB2	1:S:36:ARG:HG3	2.02	0.42
1:A:62:LEU:HB2	1:A:68:ASN:HA	2.02	0.42
1:B:439:GLY:O	1:B:442:VAL:HG22	2.20	0.42
2:K:20:LYS:HG2	2:K:26:VAL:HG22	2.01	0.42
2:K:39:GLU:HA	2:K:64:ILE:HA	2.02	0.42
1:M:324:VAL:CG2	1:M:331:THR:HB	2.50	0.42
1:P:31:LEU:HD12	4:P:602:ATP:H5'1	2.01	0.42
1:R:440:ILE:O	1:R:444:LEU:HG	2.20	0.42
1:S:324:VAL:HG22	1:S:331:THR:HB	2.01	0.42
2:T:65:VAL:HG12	2:T:94:ILE:HG22	2.00	0.42
1:C:366:GLN:HA	1:C:369:VAL:HG22	2.02	0.42
1:I:15:LYS:NZ	1:I:64:ASP:OD2	2.33	0.42
2:W:57:LEU:HD13	2:W:88:GLU:HB2	2.01	0.42
1:A:477:GLY:HA3	1:A:488:MET:HE2	2.00	0.42
1:E:69:MET:CE	1:E:520:MET:HE2	2.50	0.42
1:E:77:VAL:HG13	1:E:506:TYR:HB3	2.02	0.42
1:F:31:LEU:HD23	1:F:453:GLN:HB3	2.01	0.42
1:J:217:SER:HA	1:J:320:ALA:O	2.18	0.42
2:K:12:VAL:HG22	2:K:40:VAL:HG22	2.02	0.42
2:K:15:LYS:HG3	2:K:38:GLY:HA2	2.02	0.42
1:L:106:ALA:O	1:L:111:MET:HG3	2.19	0.42
1:L:479:ASN:CG	1:L:493:ILE:HD11	2.45	0.42
2:Q:11:ILE:CD1	2:Q:85:ILE:HG12	2.50	0.42
1:E:383:ALA:HB1	1:E:388:GLU:CD	2.44	0.42
2:G:12:VAL:HG22	2:G:40:VAL:HG22	2.02	0.42
1:H:13:ARG:NH1	1:H:517:THR:O	2.53	0.42
1:M:248:LEU:HA	1:M:274:ALA:O	2.20	0.42
1:R:320:ALA:HA	1:R:335:GLY:HA2	2.02	0.42
1:S:188:ASP:OD2	1:S:380:LYS:NZ	2.45	0.42
1:C:246:PRO:HB3	1:C:272:LYS:HB2	2.02	0.42
1:I:15:LYS:HD3	1:I:66:PHE:HB2	2.02	0.42
1:I:177:VAL:HG23	1:I:400:LEU:HD22	2.02	0.42
1:A:42:LYS:HA	1:A:42:LYS:HD3	1.75	0.42
1:A:231:ARG:NH2	1:A:232:GLU:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:HG2	1:A:233:MET:CE	2.50	0.42
1:B:196:ASP:OD1	1:B:196:ASP:N	2.53	0.42
1:E:232:GLU:HG2	1:E:233:MET:HE3	2.01	0.42
1:E:366:GLN:HA	1:E:369:VAL:HG22	2.02	0.42
1:J:479:ASN:O	1:J:483:GLU:N	2.53	0.42
1:P:217:SER:HA	1:P:320:ALA:O	2.20	0.42
1:S:389:MET:HE2	1:S:389:MET:HB2	1.97	0.42
1:C:13:ARG:NH1	1:C:517:THR:O	2.53	0.42
1:C:69:MET:HG2	1:A:47:PRO:HG3	2.02	0.42
1:C:169:VAL:HG11	1:C:377:ALA:HB2	2.02	0.42
1:I:222:LEU:HD22	1:I:293:ALA:HB2	2.02	0.42
1:B:49:ILE:HD12	1:F:513:LEU:HB3	2.02	0.42
2:D:8:ASP:HA	2:D:57:LEU:HD21	2.02	0.42
1:E:291:ASP:OD1	1:E:345:ARG:NE	2.53	0.42
1:F:147:VAL:HG23	1:F:494:LEU:HD12	2.02	0.42
1:F:386:GLU:HB3	1:J:76:GLU:OE2	2.20	0.42
1:H:65:LYS:HB3	1:H:65:LYS:HE3	1.90	0.42
1:J:115:ASP:OD2	1:J:433:ASN:ND2	2.44	0.42
1:J:414:GLY:HA3	1:J:493:ILE:HG22	2.01	0.42
1:L:198:GLY:HA2	1:L:326:ASN:O	2.20	0.42
1:R:217:SER:HA	1:R:320:ALA:O	2.19	0.42
1:S:77:VAL:HG12	1:S:92:ALA:HB1	2.02	0.42
1:S:115:ASP:OD1	1:S:118:ARG:NH1	2.51	0.42
1:A:366:GLN:HA	1:A:369:VAL:HG22	2.02	0.41
1:E:16:MET:HE1	1:E:73:MET:CE	2.49	0.41
1:E:118:ARG:NH2	1:H:483:GLU:OE2	2.53	0.41
1:H:193:MET:SD	1:H:194:GLN:N	2.93	0.41
1:J:73:MET:HE2	1:J:514:MET:CG	2.50	0.41
1:J:327:LYS:O	1:J:327:LYS:NZ	2.35	0.41
1:M:176:THR:HG23	1:M:378:VAL:HG22	2.02	0.41
1:M:423:ALA:HA	1:M:444:LEU:HD22	2.01	0.41
1:O:390:LYS:HB3	1:O:390:LYS:HE2	1.89	0.41
1:P:324:VAL:HG22	1:P:331:THR:HB	2.02	0.41
1:R:524:LEU:HG	1:R:525:PRO:HD2	2.01	0.41
1:C:489:ILE:HG12	1:C:494:LEU:HD21	2.02	0.41
2:D:53:GLU:OE1	2:D:53:GLU:N	2.53	0.41
1:H:17:LEU:HB2	1:H:104:LEU:HD12	2.00	0.41
1:L:180:GLY:N	1:L:381:VAL:O	2.48	0.41
1:P:152:ALA:O	1:P:395:ARG:NH1	2.53	0.41
2:Q:50:GLU:H	2:Q:50:GLU:HG3	1.61	0.41
1:S:248:LEU:HD13	1:S:325:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:441:LYS:HA	1:S:441:LYS:HD3	1.72	0.41
1:C:215:LEU:HD22	1:C:246:PRO:CB	2.51	0.41
1:B:194:GLN:HG2	1:B:331:THR:OG1	2.21	0.41
1:F:414:GLY:HA3	1:F:493:ILE:HG22	2.02	0.41
2:G:76:GLU:HG2	2:K:66:ILE:HD13	2.02	0.41
1:J:31:LEU:HD12	4:J:602:ATP:H5'1	2.02	0.41
1:J:232:GLU:HG2	1:J:233:MET:HG3	2.03	0.41
1:L:169:VAL:HG11	1:L:377:ALA:HB2	2.02	0.41
1:P:111:MET:HE3	1:P:438:VAL:HG21	2.02	0.41
1:P:176:THR:HG23	1:P:378:VAL:HG22	2.03	0.41
1:P:263:VAL:O	1:P:267:MET:SD	2.79	0.41
1:S:140:ASP:OD1	1:S:140:ASP:N	2.53	0.41
1:S:229:ASN:OD1	1:S:231:ARG:NH1	2.52	0.41
1:S:285:ARG:O	1:S:289:LEU:HD23	2.20	0.41
1:C:20:VAL:HG22	1:C:74:VAL:HG11	2.02	0.41
1:C:398:ASP:OD1	1:C:399:ALA:N	2.54	0.41
1:A:301:ILE:HD11	1:A:309:LEU:HA	2.02	0.41
1:H:233:MET:HE3	1:H:233:MET:N	2.31	0.41
1:M:60:ILE:HD13	1:M:60:ILE:HA	1.91	0.41
2:N:27:LEU:HD12	2:N:31:ALA:HB1	2.03	0.41
1:O:42:LYS:HA	1:O:42:LYS:HD3	1.76	0.41
1:O:284:ARG:NH2	1:O:361:ASP:HA	2.34	0.41
1:P:196:ASP:OD1	1:P:196:ASP:N	2.53	0.41
1:P:226:LYS:HE3	1:P:226:LYS:HB2	1.81	0.41
1:P:247:LEU:HB3	1:P:273:VAL:HG22	2.02	0.41
1:S:70:GLY:HA2	1:S:73:MET:HE3	2.03	0.41
1:C:62:LEU:HB2	1:C:68:ASN:HA	2.03	0.41
1:B:20:VAL:HG21	1:B:514:MET:HE1	2.03	0.41
1:E:288:MET:O	1:E:292:ILE:HG12	2.21	0.41
1:E:301:ILE:HD11	1:E:309:LEU:HA	2.02	0.41
1:L:248:LEU:HD12	1:L:325:ILE:HD11	2.03	0.41
1:L:366:GLN:HA	1:L:369:VAL:HG22	2.02	0.41
1:P:233:MET:HE3	1:P:233:MET:HB2	1.85	0.41
1:R:16:MET:HG2	1:R:520:MET:CE	2.51	0.41
1:R:42:LYS:HD3	1:R:42:LYS:HA	1.80	0.41
1:S:364:LYS:HA	1:S:364:LYS:HD2	1.75	0.41
1:C:17:LEU:HB2	1:C:104:LEU:HD12	2.01	0.41
1:C:321:LYS:HB2	1:C:334:ASP:HB3	2.03	0.41
1:F:60:ILE:HD13	1:F:60:ILE:HA	1.91	0.41
1:H:4:LYS:HD2	1:L:59:GLU:O	2.20	0.41
1:H:395:ARG:HA	1:H:398:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:489:ILE:HG12	1:L:494:LEU:HD21	2.01	0.41
1:P:262:LEU:O	1:P:266:THR:OG1	2.32	0.41
1:I:385:THR:HG21	1:B:510:VAL:HG23	2.02	0.41
2:W:6:LEU:HB3	2:W:7:HIS:HD2	1.86	0.41
1:A:69:MET:HE3	1:E:39:VAL:HG12	2.03	0.41
1:A:346:VAL:O	1:A:350:ARG:HG3	2.20	0.41
2:D:12:VAL:HB	2:D:86:MET:HE1	2.02	0.41
2:G:82:GLU:OE1	2:G:82:GLU:N	2.54	0.41
1:H:398:ASP:OD1	1:H:399:ALA:N	2.54	0.41
1:J:66:PHE:HD1	1:J:520:MET:HE3	1.86	0.41
1:J:68:ASN:O	1:J:72:GLN:HG2	2.20	0.41
1:L:144:ILE:HD13	1:L:166:MET:HG3	2.02	0.41
1:L:383:ALA:N	1:L:389:MET:SD	2.94	0.41
1:L:395:ARG:HA	1:L:398:ASP:OD2	2.21	0.41
1:M:217:SER:HA	1:M:320:ALA:O	2.20	0.41
1:O:12:ALA:HB1	1:O:520:MET:HG3	2.02	0.41
1:P:68:ASN:O	1:P:72:GLN:HG2	2.20	0.41
1:R:229:ASN:ND2	1:R:231:ARG:HB3	2.36	0.41
1:R:398:ASP:OD1	1:R:399:ALA:N	2.54	0.41
1:S:248:LEU:HA	1:S:274:ALA:O	2.21	0.41
1:S:343:GLN:O	1:S:346:VAL:HG12	2.20	0.41
1:C:65:LYS:HB3	1:C:65:LYS:HE3	1.88	0.41
1:C:232:GLU:HG2	1:C:233:MET:HE1	2.02	0.41
1:A:264:VAL:O	1:A:268:ARG:HG2	2.21	0.41
1:A:389:MET:HA	1:A:389:MET:HE3	2.03	0.41
1:B:512:GLY:HA2	1:B:515:ILE:HG12	2.03	0.41
2:D:39:GLU:HA	2:D:64:ILE:HA	2.03	0.41
1:E:73:MET:CE	1:E:514:MET:HG2	2.51	0.41
1:F:512:GLY:HA2	1:F:515:ILE:HG12	2.02	0.41
1:H:16:MET:HE2	1:H:514:MET:SD	2.61	0.41
1:L:291:ASP:OD1	1:L:345:ARG:NE	2.54	0.41
1:M:288:MET:HA	1:M:291:ASP:OD2	2.21	0.41
2:N:49:LEU:HD12	2:N:53:GLU:O	2.21	0.41
1:O:65:LYS:HE3	1:O:65:LYS:HB3	1.87	0.41
1:O:73:MET:CE	1:R:49:ILE:HD11	2.50	0.41
1:O:257:GLU:CD	1:O:257:GLU:H	2.29	0.41
1:P:346:VAL:HG23	1:P:369:VAL:HG22	2.03	0.41
1:P:479:ASN:O	1:P:483:GLU:N	2.53	0.41
1:R:193:MET:H	1:R:332:ILE:HG22	1.85	0.41
1:R:368:ARG:O	1:R:372:LEU:HG	2.20	0.41
1:C:294:THR:HG23	1:C:295:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:11:ILE:CD1	2:W:85:ILE:HG12	2.51	0.41
2:W:13:LYS:HB2	2:W:41:LEU:HD11	2.03	0.41
1:A:513:LEU:HB3	1:E:49:ILE:CD1	2.51	0.41
1:F:270:ILE:H	1:F:270:ILE:HG12	1.67	0.41
1:H:37:ASN:HB3	1:H:49:ILE:HG23	2.03	0.41
1:J:176:THR:HG23	1:J:378:VAL:HG22	2.02	0.41
1:J:413:ALA:HB1	1:J:488:MET:HG3	2.03	0.41
1:M:162:ILE:O	1:M:166:MET:HG3	2.21	0.41
1:M:229:ASN:ND2	1:M:230:ILE:H	2.19	0.41
1:M:239:ALA:HB1	1:M:314:LEU:HD21	2.01	0.41
1:M:511:ALA:O	1:M:515:ILE:HG23	2.20	0.41
1:O:38:VAL:HG11	1:O:56:VAL:HG13	2.03	0.41
1:O:232:GLU:HG2	1:O:233:MET:HE1	2.02	0.41
1:O:489:ILE:HG12	1:O:494:LEU:HD21	2.03	0.41
2:Q:55:LYS:HB3	2:Q:55:LYS:HE3	1.94	0.41
1:R:65:LYS:HB3	1:R:65:LYS:HE3	1.88	0.41
1:R:102:GLU:HB2	1:R:442:VAL:HG13	2.02	0.41
1:R:141:SER:HA	1:R:144:ILE:HD12	2.02	0.41
1:R:231:ARG:NH2	1:R:232:GLU:HB3	2.36	0.41
1:R:395:ARG:HA	1:R:398:ASP:OD2	2.20	0.41
1:R:430:ARG:HD3	1:R:430:ARG:HA	1.87	0.41
1:R:479:ASN:CG	1:R:493:ILE:HD11	2.46	0.41
1:S:31:LEU:HD23	1:S:453:GLN:HB3	2.03	0.41
1:S:226:LYS:HE3	1:S:226:LYS:HB2	1.81	0.41
1:S:511:ALA:O	1:S:515:ILE:HG23	2.20	0.41
1:F:265:ASN:HB3	1:F:270:ILE:HG13	2.03	0.41
1:H:217:SER:HA	1:H:320:ALA:O	2.21	0.41
1:H:513:LEU:HB3	1:L:49:ILE:CD1	2.51	0.41
1:J:115:ASP:OD1	1:J:118:ARG:NH1	2.52	0.41
1:M:420:ILE:HD13	1:M:448:GLU:HG2	2.03	0.41
1:M:447:MET:HE2	1:M:504:LEU:HD21	2.03	0.41
1:S:254:VAL:O	1:S:259:LEU:HD12	2.21	0.41
1:I:73:MET:SD	1:S:49:ILE:HD11	2.61	0.40
1:H:31:LEU:O	1:H:457:ASN:ND2	2.39	0.40
1:H:347:ALA:HA	1:H:350:ARG:HE	1.86	0.40
1:O:107:VAL:HG21	1:O:515:ILE:HG23	2.03	0.40
1:S:218:PRO:HB3	1:S:246:PRO:HB2	2.03	0.40
1:I:258:ALA:O	1:I:262:LEU:HG	2.21	0.40
1:A:242:LYS:HB3	1:A:242:LYS:HE3	1.62	0.40
1:A:288:MET:O	1:A:292:ILE:HG12	2.21	0.40
1:A:479:ASN:CG	1:A:493:ILE:HD11	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASP:OD2	1:B:433:ASN:ND2	2.46	0.40
1:E:102:GLU:HB2	1:E:442:VAL:HG13	2.03	0.40
1:E:231:ARG:NH2	1:E:232:GLU:HB3	2.35	0.40
1:F:232:GLU:OE1	1:F:232:GLU:N	2.54	0.40
1:H:62:LEU:HB2	1:H:68:ASN:HA	2.02	0.40
1:L:37:ASN:HB3	1:L:49:ILE:HG23	2.02	0.40
1:L:38:VAL:HG11	1:L:56:VAL:HG13	2.03	0.40
1:L:346:VAL:O	1:L:350:ARG:HG3	2.20	0.40
1:R:216:GLU:HA	1:R:322:ARG:HG3	2.03	0.40
1:S:349:ILE:HA	1:S:352:GLN:HG3	2.02	0.40
2:T:27:LEU:HD12	2:T:31:ALA:HB1	2.03	0.40
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.92	0.40
1:I:176:THR:HG23	1:I:378:VAL:HG22	2.04	0.40
1:I:389:MET:HE2	1:I:389:MET:HB2	1.89	0.40
1:A:395:ARG:HA	1:A:398:ASP:OD2	2.21	0.40
1:B:262:LEU:O	1:B:266:THR:OG1	2.35	0.40
1:E:398:ASP:OD1	1:E:399:ALA:N	2.54	0.40
1:F:176:THR:HG23	1:F:378:VAL:HG22	2.02	0.40
1:F:282:GLY:C	1:F:284:ARG:H	2.30	0.40
1:H:150:ILE:HD11	4:H:602:ATP:N7	2.37	0.40
2:K:8:ASP:N	2:K:8:ASP:OD1	2.48	0.40
1:L:69:MET:CE	1:L:520:MET:HE2	2.52	0.40
1:L:188:ASP:OD2	1:L:380:LYS:NZ	2.44	0.40
1:O:193:MET:SD	1:O:194:GLN:N	2.95	0.40
1:R:242:LYS:HE3	1:R:242:LYS:HB3	1.61	0.40
1:C:291:ASP:OD1	1:C:345:ARG:NE	2.55	0.40
1:C:395:ARG:HA	1:C:398:ASP:OD2	2.21	0.40
1:E:395:ARG:HA	1:E:398:ASP:OD2	2.21	0.40
1:F:65:LYS:NZ	1:F:523:ASP:HB3	2.36	0.40
1:H:242:LYS:HE3	1:H:242:LYS:HB3	1.60	0.40
1:J:282:GLY:C	1:J:284:ARG:H	2.29	0.40
1:J:420:ILE:HG23	1:J:470:LYS:HG2	2.02	0.40
1:J:512:GLY:HA2	1:J:515:ILE:HG12	2.02	0.40
1:M:229:ASN:CG	1:M:230:ILE:H	2.29	0.40
1:O:288:MET:O	1:O:292:ILE:HG12	2.22	0.40
1:P:36:ARG:HG3	1:S:518:GLU:HB2	2.04	0.40
1:P:288:MET:HA	1:P:291:ASP:OD2	2.22	0.40
1:R:169:VAL:HG11	1:R:377:ALA:HB2	2.02	0.40
1:S:360:TYR:O	1:S:363:GLU:HG2	2.21	0.40
1:C:46:ALA:CB	1:R:76:GLU:HG3	2.50	0.40
1:C:479:ASN:HB2	1:C:491:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:LEU:O	1:C:517:THR:OG1	2.30	0.40
1:B:54:VAL:HB	1:B:89:THR:HG21	2.02	0.40
1:E:40:LEU:HD13	1:E:59:GLU:HG3	2.04	0.40
1:J:74:VAL:HB	1:J:514:MET:HE1	2.03	0.40
1:L:172:GLU:OE1	1:L:172:GLU:N	2.54	0.40
1:S:524:LEU:HD23	1:S:525:PRO:HD2	2.04	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	B	300/548 (55%)	294 (98%)	6 (2%)	0	100	100
1	E	522/548 (95%)	515 (99%)	7 (1%)	0	100	100
1	F	522/548 (95%)	513 (98%)	9 (2%)	0	100	100
1	H	522/548 (95%)	512 (98%)	10 (2%)	0	100	100
1	J	522/548 (95%)	511 (98%)	11 (2%)	0	100	100
1	L	522/548 (95%)	512 (98%)	10 (2%)	0	100	100
1	M	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	O	522/548 (95%)	507 (97%)	15 (3%)	0	100	100
1	P	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	R	522/548 (95%)	512 (98%)	10 (2%)	0	100	100
1	S	522/548 (95%)	515 (99%)	7 (1%)	0	100	100
2	D	94/98 (96%)	90 (96%)	4 (4%)	0	100	100
2	G	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
2	K	94/98 (96%)	90 (96%)	4 (4%)	0	100	100
2	N	94/98 (96%)	91 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	94/98 (96%)	90 (96%)	4 (4%)	0	100	100
2	T	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
All	All	6084/6616 (92%)	5964 (98%)	120 (2%)	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	A	403/415 (97%)	403 (100%)	0	100	100
1	B	403/415 (97%)	401 (100%)	2 (0%)	81	81
1	C	403/415 (97%)	402 (100%)	1 (0%)	87	85
1	E	76/415 (18%)	76 (100%)	0	100	100
1	H	69/415 (17%)	69 (100%)	0	100	100
1	I	403/415 (97%)	402 (100%)	1 (0%)	87	85
1	J	403/415 (97%)	403 (100%)	0	100	100
1	L	403/415 (97%)	403 (100%)	0	100	100
1	M	403/415 (97%)	402 (100%)	1 (0%)	87	85
1	O	403/415 (97%)	403 (100%)	0	100	100
1	P	403/415 (97%)	403 (100%)	0	100	100
1	R	403/415 (97%)	402 (100%)	1 (0%)	87	85
1	S	403/415 (97%)	402 (100%)	1 (0%)	87	85
2	D	49/80 (61%)	49 (100%)	0	100	100
2	K	77/80 (96%)	76 (99%)	1 (1%)	61	71
2	N	77/80 (96%)	77 (100%)	0	100	100
2	Q	77/80 (96%)	77 (100%)	0	100	100
2	T	77/80 (96%)	77 (100%)	0	100	100
2	W	77/80 (96%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5012/5875 (85%)	5004 (100%)	8 (0%)	85	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	317	LEU
1	I	289	LEU
1	B	151	SER
1	B	288	MET
2	K	6	LEU
1	M	270	ILE
1	R	317	LEU
1	S	74	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	319	GLN
1	I	343	GLN
1	I	479	ASN
1	A	290	GLN
1	B	68	ASN
1	B	72	GLN
1	B	82	ASN
1	B	112	ASN
1	B	479	ASN
1	J	432	GLN
2	K	80	ASN
1	L	290	GLN
1	M	432	GLN
2	N	80	ASN
1	O	290	GLN
1	O	319	GLN
1	O	348	GLN
1	O	475	ASN
1	P	290	GLN
1	P	479	ASN
2	Q	80	ASN
1	R	290	GLN
1	R	348	GLN
2	T	80	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	$\# Z > 2$
4	ATP	H	602	3	32,33,33	0.37	0	48,52,52	0.27	0
4	ATP	S	602	3	32,33,33	0.45	0	48,52,52	0.45	0
4	ATP	E	602	3	32,33,33	0.39	0	48,52,52	0.28	0
4	ATP	R	602	3	32,33,33	0.34	0	48,52,52	0.27	0
4	ATP	M	602	3	32,33,33	0.52	0	48,52,52	0.47	0
4	ATP	I	602	3	32,33,33	0.50	0	48,52,52	0.45	0
4	ATP	O	602	3	32,33,33	0.38	0	48,52,52	0.27	0
4	ATP	F	602	3	32,33,33	0.50	0	48,52,52	0.45	0
4	ATP	L	602	3	32,33,33	0.36	0	48,52,52	0.27	0
4	ATP	B	602	3	32,33,33	0.48	0	48,52,52	0.45	0
4	ATP	A	602	3	32,33,33	0.37	0	48,52,52	0.27	0
4	ATP	P	602	3	32,33,33	0.51	0	48,52,52	0.46	0
4	ATP	J	602	3	32,33,33	0.51	0	48,52,52	0.46	0
4	ATP	C	602	3	32,33,33	0.36	0	48,52,52	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	H	602	3	-	5/22/38/38	0/3/3/3
4	ATP	S	602	3	-	7/22/38/38	0/3/3/3
4	ATP	E	602	3	-	5/22/38/38	0/3/3/3
4	ATP	R	602	3	-	6/22/38/38	0/3/3/3
4	ATP	M	602	3	-	7/22/38/38	0/3/3/3
4	ATP	I	602	3	-	6/22/38/38	0/3/3/3
4	ATP	O	602	3	-	5/22/38/38	0/3/3/3
4	ATP	F	602	3	-	7/22/38/38	0/3/3/3
4	ATP	L	602	3	-	4/22/38/38	0/3/3/3
4	ATP	B	602	3	-	7/22/38/38	0/3/3/3
4	ATP	A	602	3	-	5/22/38/38	0/3/3/3
4	ATP	P	602	3	-	8/22/38/38	0/3/3/3
4	ATP	J	602	3	-	6/22/38/38	0/3/3/3
4	ATP	C	602	3	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	602	ATP	C5'-O5'-PA-O1A
4	I	602	ATP	C5'-O5'-PA-O2A
4	I	602	ATP	C5'-O5'-PA-O3A
4	I	602	ATP	O4'-C4'-C5'-O5'
4	B	602	ATP	C5'-O5'-PA-O1A
4	B	602	ATP	C5'-O5'-PA-O2A
4	B	602	ATP	C5'-O5'-PA-O3A
4	B	602	ATP	O4'-C4'-C5'-O5'
4	F	602	ATP	PB-O3B-PG-O2G
4	F	602	ATP	C5'-O5'-PA-O1A
4	F	602	ATP	C5'-O5'-PA-O2A
4	F	602	ATP	C5'-O5'-PA-O3A
4	F	602	ATP	O4'-C4'-C5'-O5'
4	J	602	ATP	PB-O3B-PG-O2G
4	J	602	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	J	602	ATP	C5'-O5'-PA-O2A
4	J	602	ATP	C5'-O5'-PA-O3A
4	J	602	ATP	O4'-C4'-C5'-O5'
4	M	602	ATP	PB-O3B-PG-O2G
4	M	602	ATP	C5'-O5'-PA-O1A
4	M	602	ATP	C5'-O5'-PA-O2A
4	M	602	ATP	C5'-O5'-PA-O3A
4	M	602	ATP	O4'-C4'-C5'-O5'
4	P	602	ATP	PB-O3B-PG-O2G
4	P	602	ATP	C5'-O5'-PA-O1A
4	P	602	ATP	C5'-O5'-PA-O2A
4	P	602	ATP	C5'-O5'-PA-O3A
4	P	602	ATP	O4'-C4'-C5'-O5'
4	S	602	ATP	C5'-O5'-PA-O1A
4	S	602	ATP	C5'-O5'-PA-O2A
4	S	602	ATP	C5'-O5'-PA-O3A
4	S	602	ATP	O4'-C4'-C5'-O5'
4	R	602	ATP	C3'-C4'-C5'-O5'
4	C	602	ATP	C3'-C4'-C5'-O5'
4	A	602	ATP	C3'-C4'-C5'-O5'
4	H	602	ATP	C3'-C4'-C5'-O5'
4	L	602	ATP	C3'-C4'-C5'-O5'
4	O	602	ATP	C3'-C4'-C5'-O5'
4	I	602	ATP	C3'-C4'-C5'-O5'
4	F	602	ATP	C3'-C4'-C5'-O5'
4	J	602	ATP	C3'-C4'-C5'-O5'
4	M	602	ATP	C3'-C4'-C5'-O5'
4	P	602	ATP	C3'-C4'-C5'-O5'
4	S	602	ATP	C3'-C4'-C5'-O5'
4	B	602	ATP	C3'-C4'-C5'-O5'
4	E	602	ATP	C3'-C4'-C5'-O5'
4	R	602	ATP	O4'-C4'-C5'-O5'
4	L	602	ATP	O4'-C4'-C5'-O5'
4	O	602	ATP	O4'-C4'-C5'-O5'
4	C	602	ATP	O4'-C4'-C5'-O5'
4	A	602	ATP	O4'-C4'-C5'-O5'
4	H	602	ATP	O4'-C4'-C5'-O5'
4	C	602	ATP	PA-O3A-PB-O1B
4	A	602	ATP	PA-O3A-PB-O1B
4	E	602	ATP	O4'-C4'-C5'-O5'
4	O	602	ATP	PA-O3A-PB-O1B
4	E	602	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	H	602	ATP	PA-O3A-PB-O1B
4	R	602	ATP	PG-O3B-PB-O3A
4	B	602	ATP	PB-O3B-PG-O2G
4	S	602	ATP	PB-O3B-PG-O2G
4	A	602	ATP	PG-O3B-PB-O2B
4	A	602	ATP	PA-O3A-PB-O2B
4	H	602	ATP	PA-O3A-PB-O2B
4	O	602	ATP	PG-O3B-PB-O2B
4	O	602	ATP	PA-O3A-PB-O2B
4	R	602	ATP	PG-O3B-PB-O1B
4	C	602	ATP	PG-O3B-PB-O2B
4	C	602	ATP	PA-O3A-PB-O2B
4	I	602	ATP	PA-O3A-PB-O2B
4	B	602	ATP	PA-O3A-PB-O2B
4	E	602	ATP	PG-O3B-PB-O2B
4	E	602	ATP	PA-O3A-PB-O2B
4	F	602	ATP	PA-O3A-PB-O2B
4	H	602	ATP	PG-O3B-PB-O2B
4	L	602	ATP	PA-O3A-PB-O2B
4	M	602	ATP	PB-O3A-PA-O2A
4	P	602	ATP	PA-O3A-PB-O2B
4	P	602	ATP	PB-O3A-PA-O2A
4	R	602	ATP	PG-O3B-PB-O2B
4	R	602	ATP	PA-O3A-PB-O2B
4	S	602	ATP	PA-O3A-PB-O2B
4	L	602	ATP	PG-O3B-PB-O3A

There are no ring outliers.

14 monomers are involved in 20 short contacts:

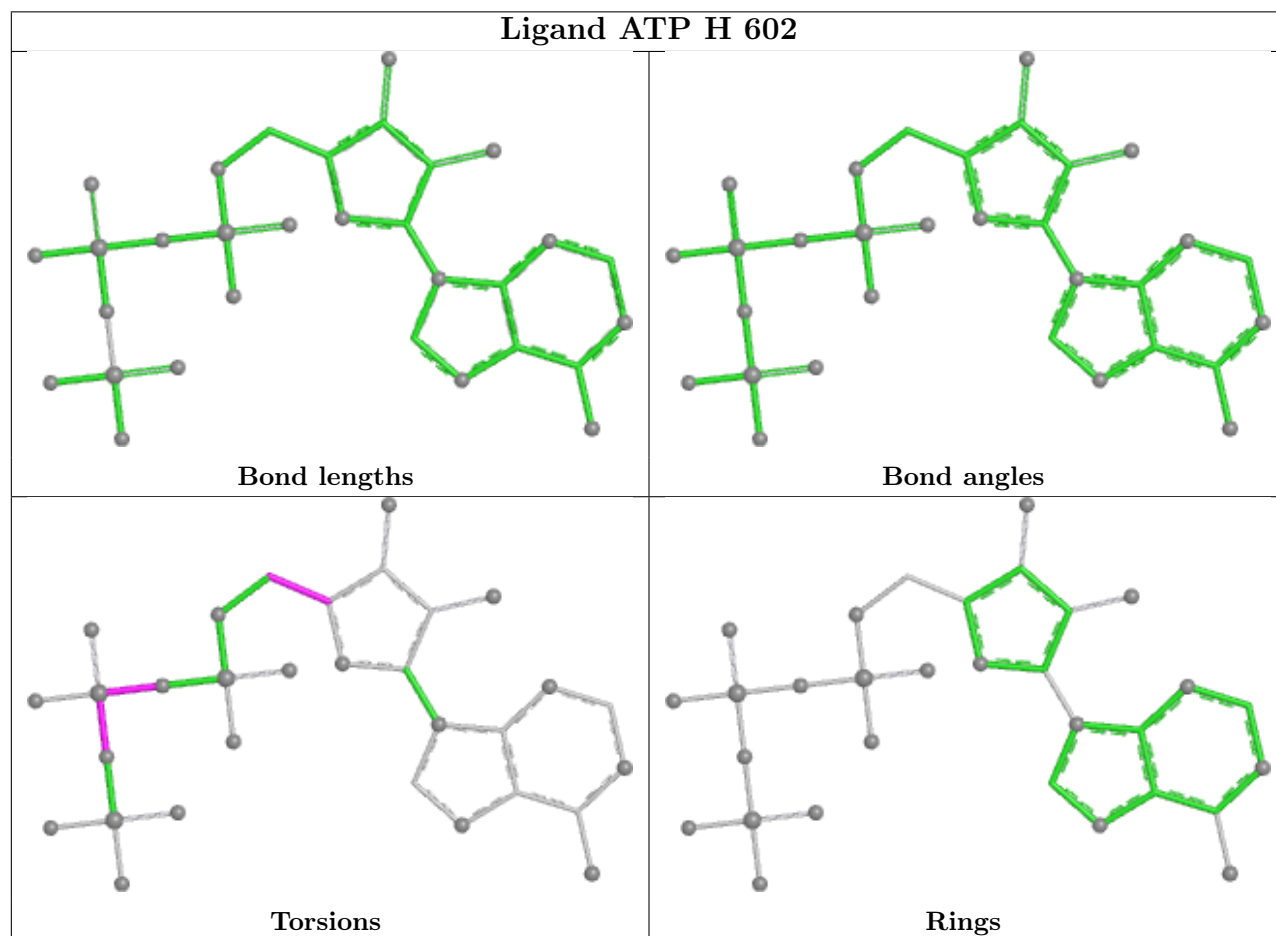
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	602	ATP	2	0
4	S	602	ATP	1	0
4	E	602	ATP	2	0
4	R	602	ATP	1	0
4	M	602	ATP	2	0
4	I	602	ATP	1	0
4	O	602	ATP	1	0
4	F	602	ATP	1	0
4	L	602	ATP	1	0
4	B	602	ATP	1	0
4	A	602	ATP	2	0

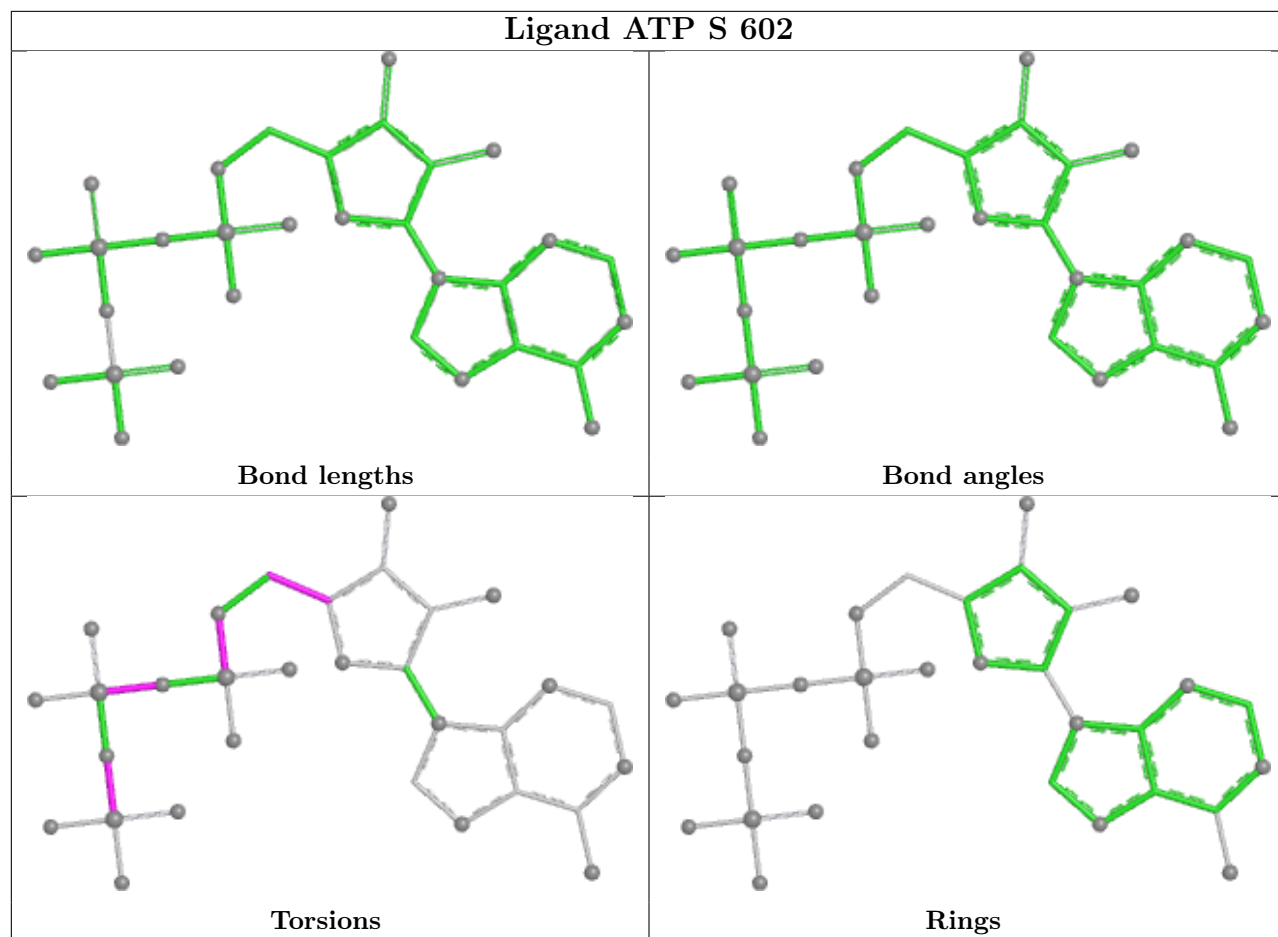
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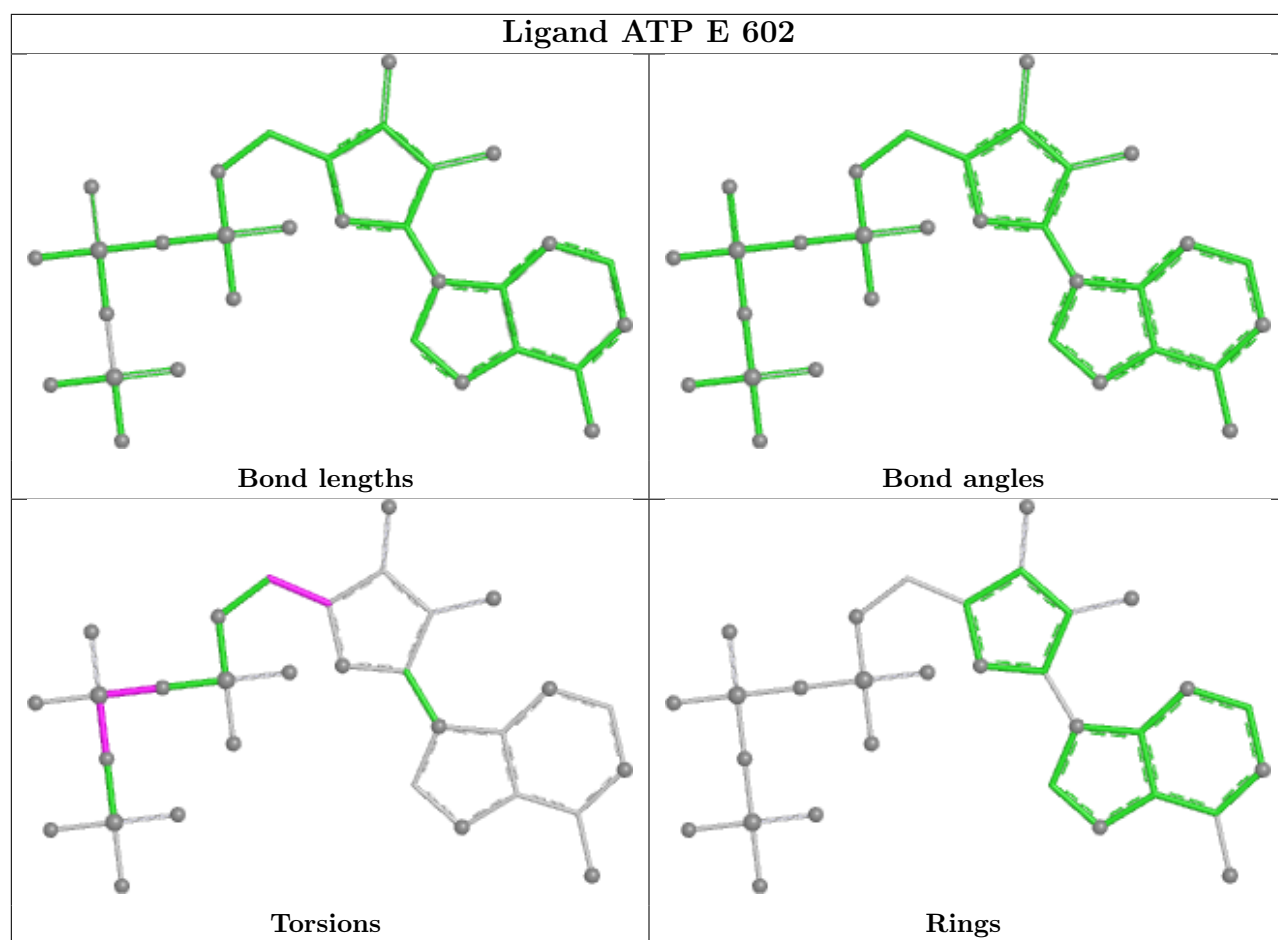
Continued from previous page...

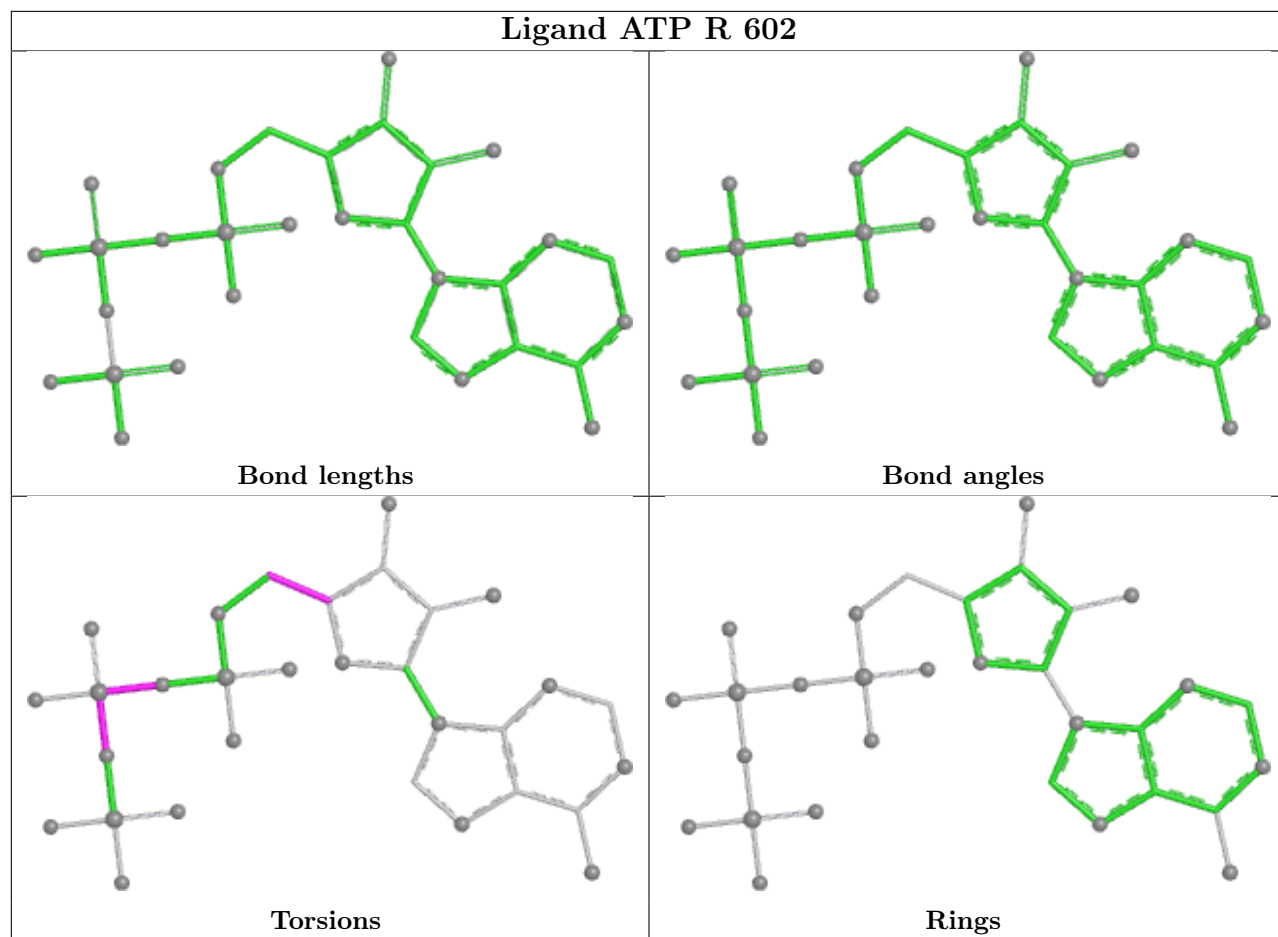
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	602	ATP	2	0
4	J	602	ATP	2	0
4	C	602	ATP	1	0

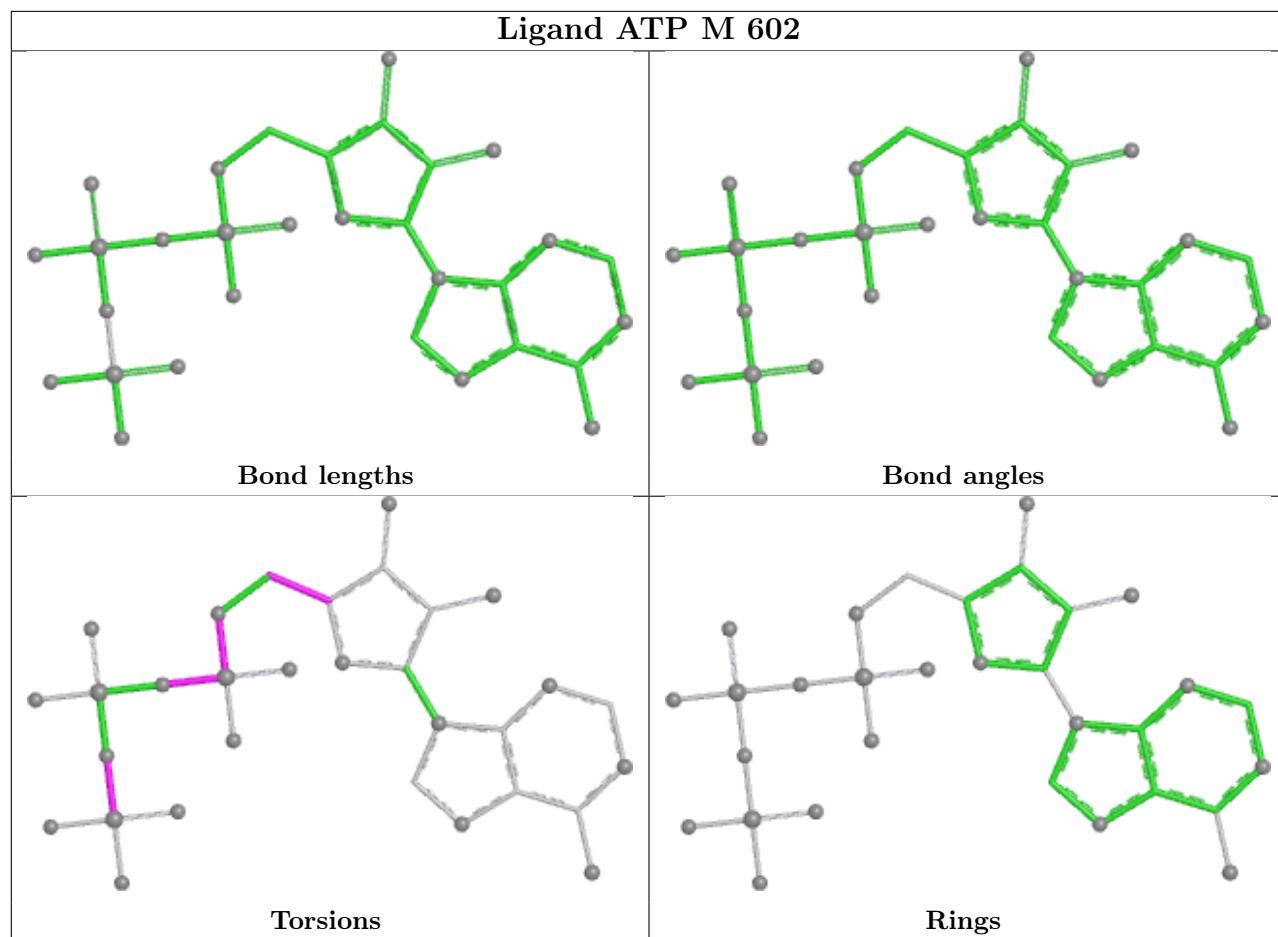
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

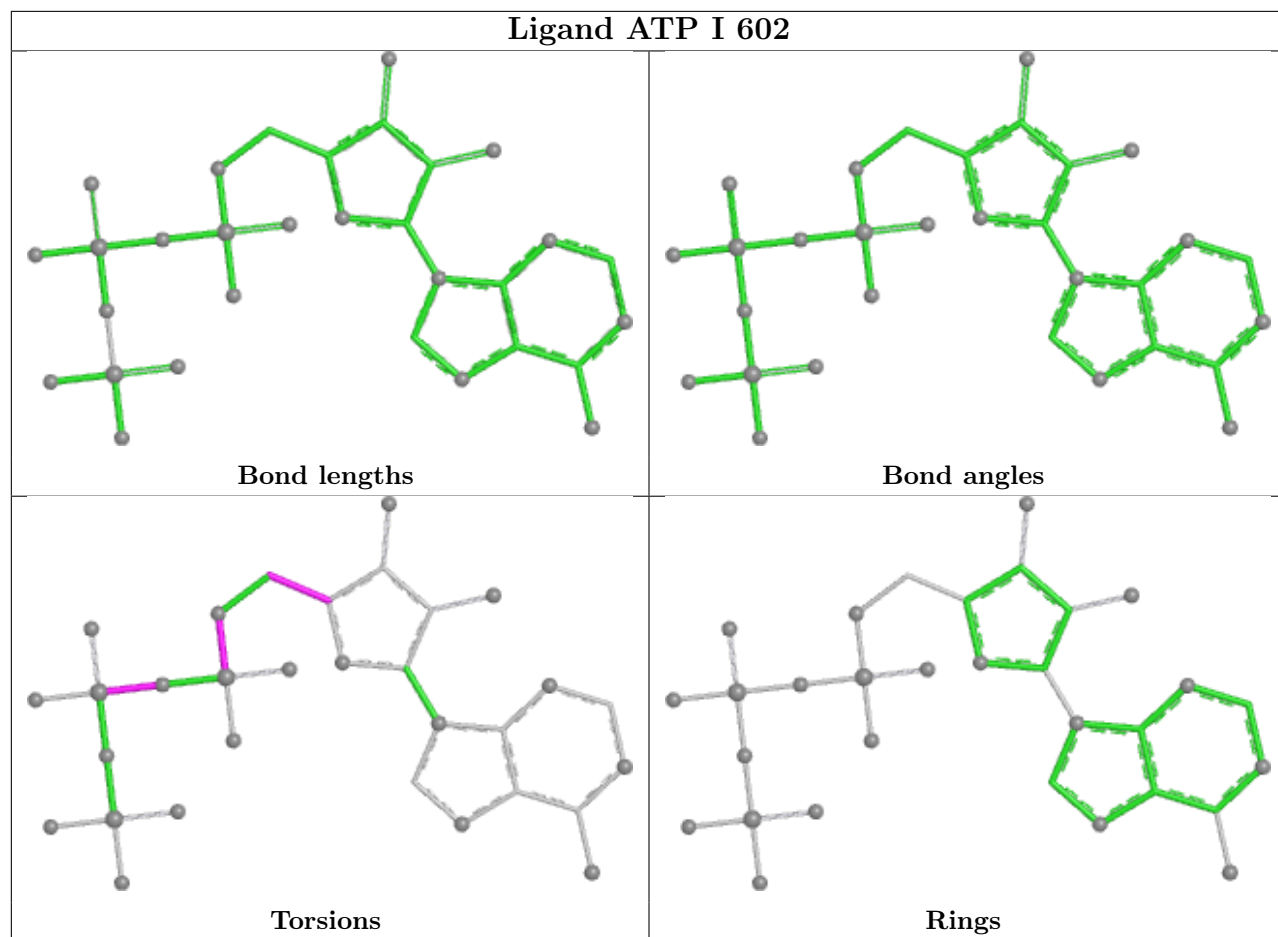


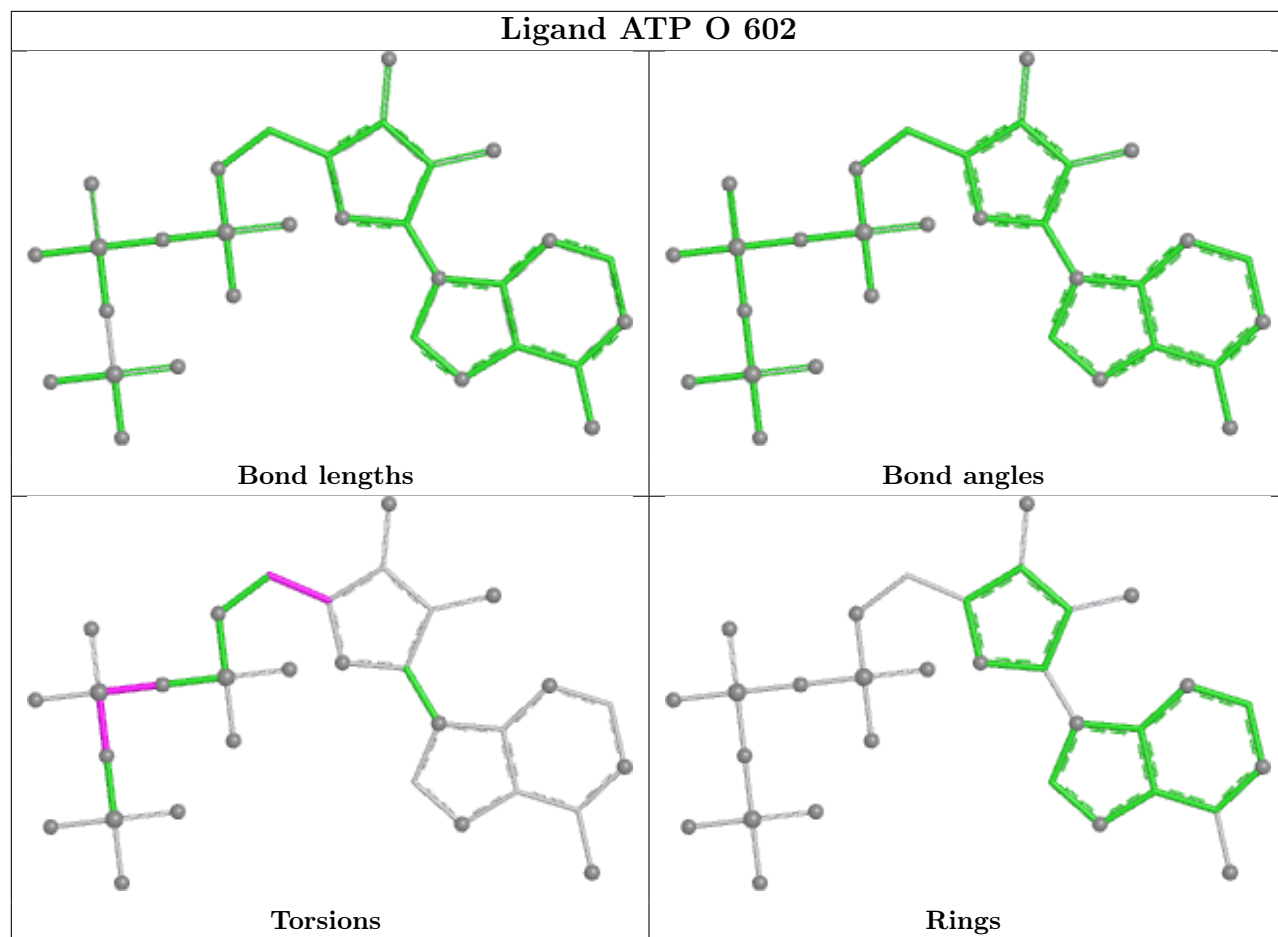


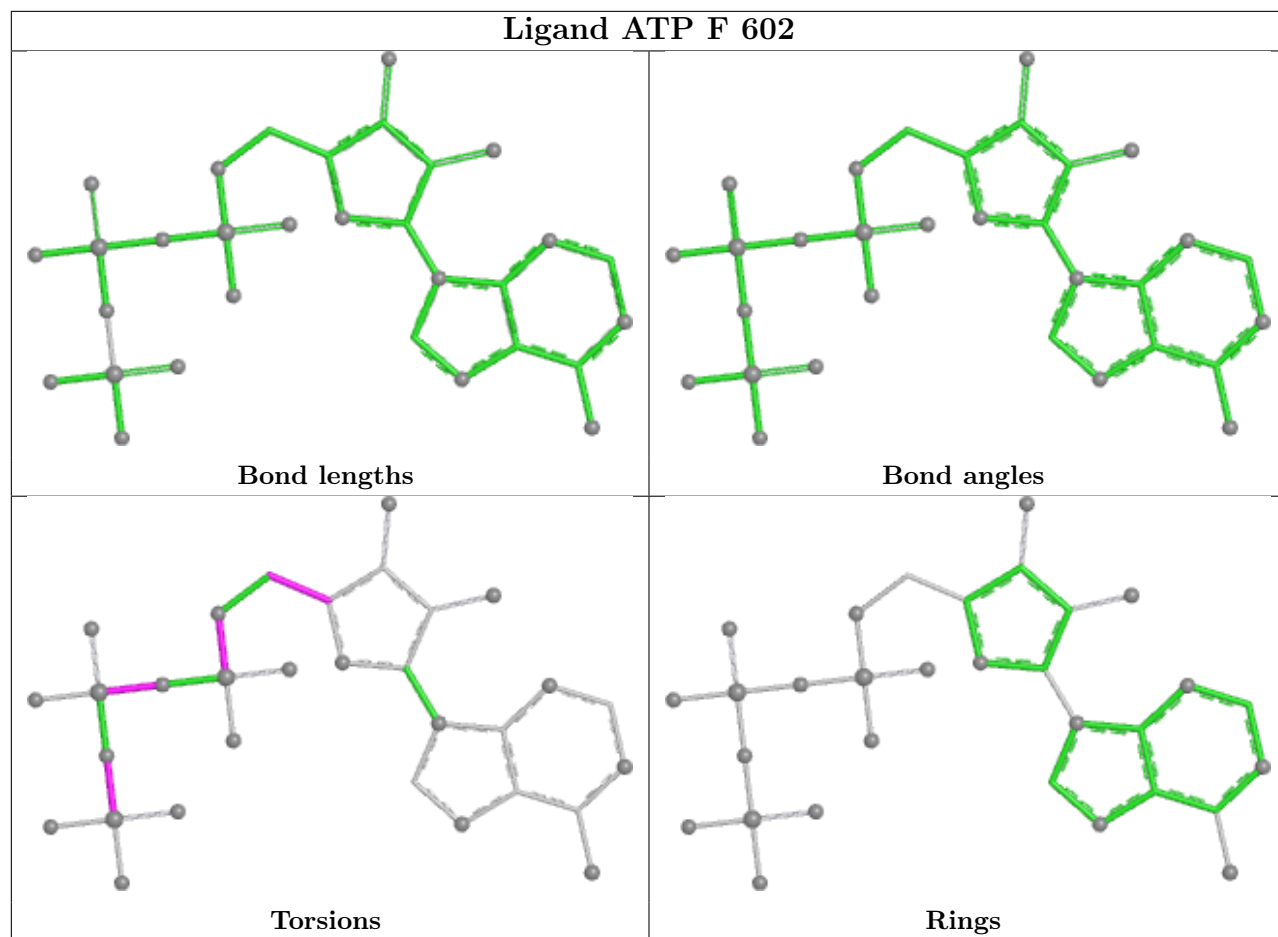


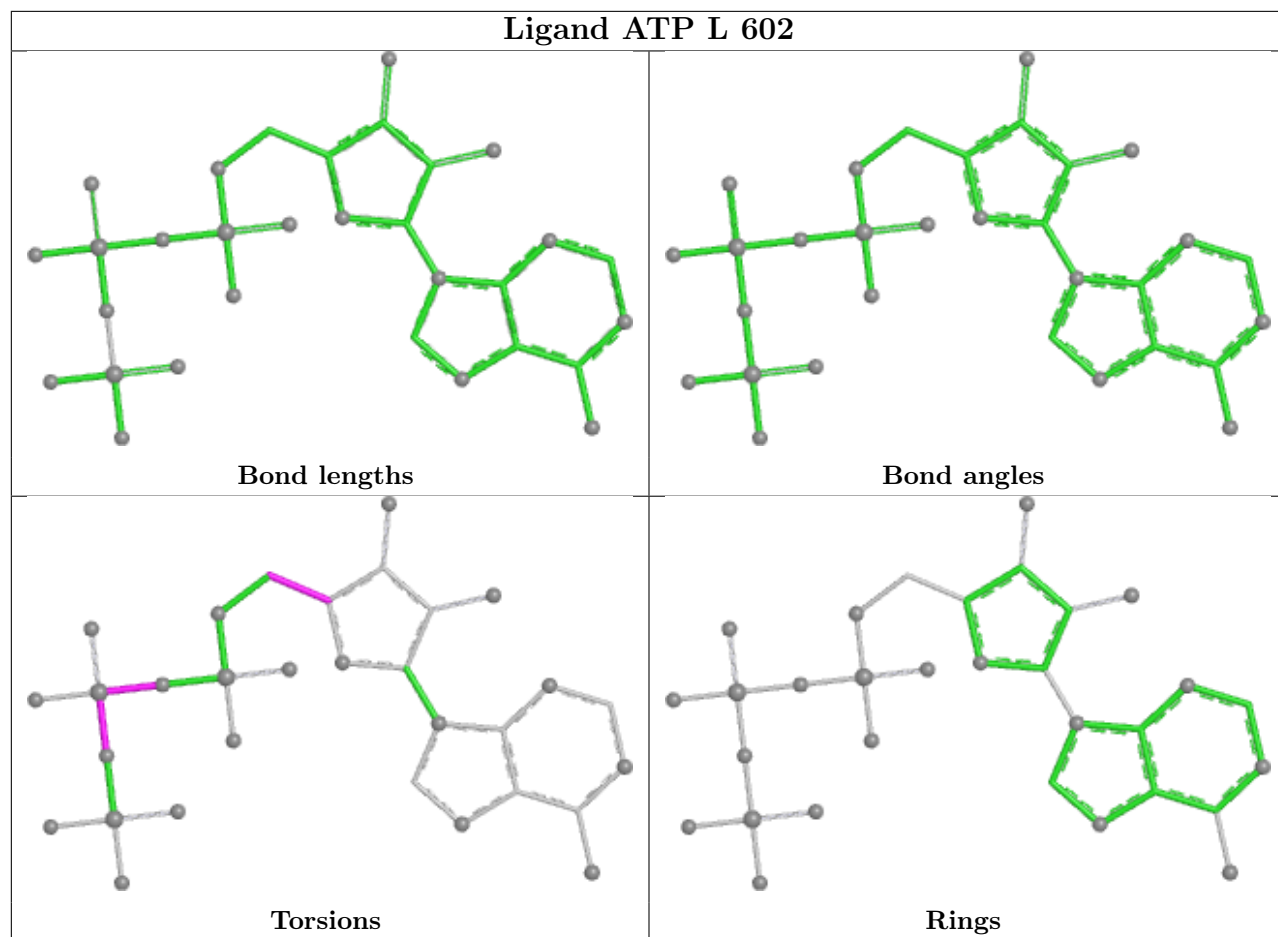


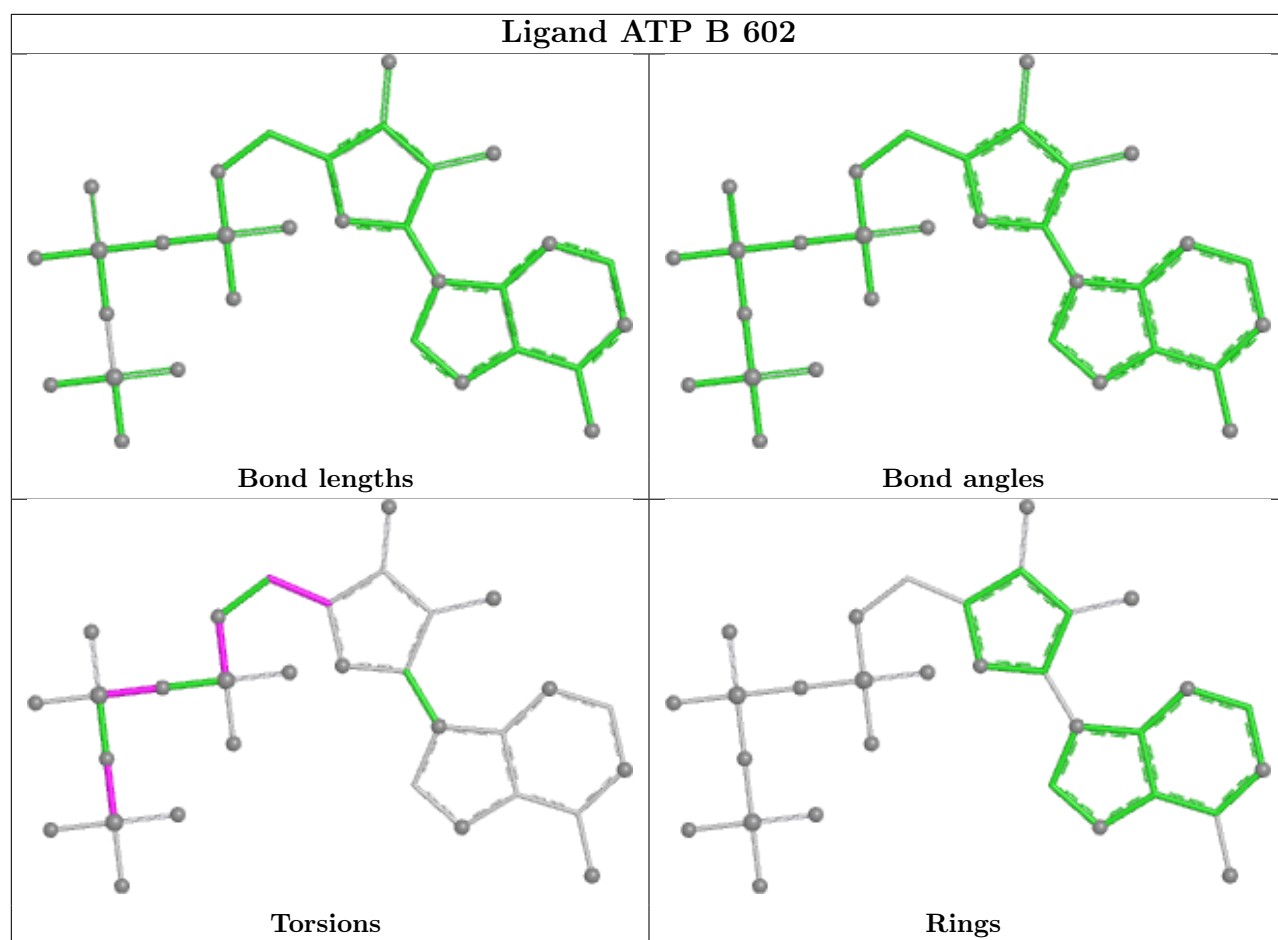


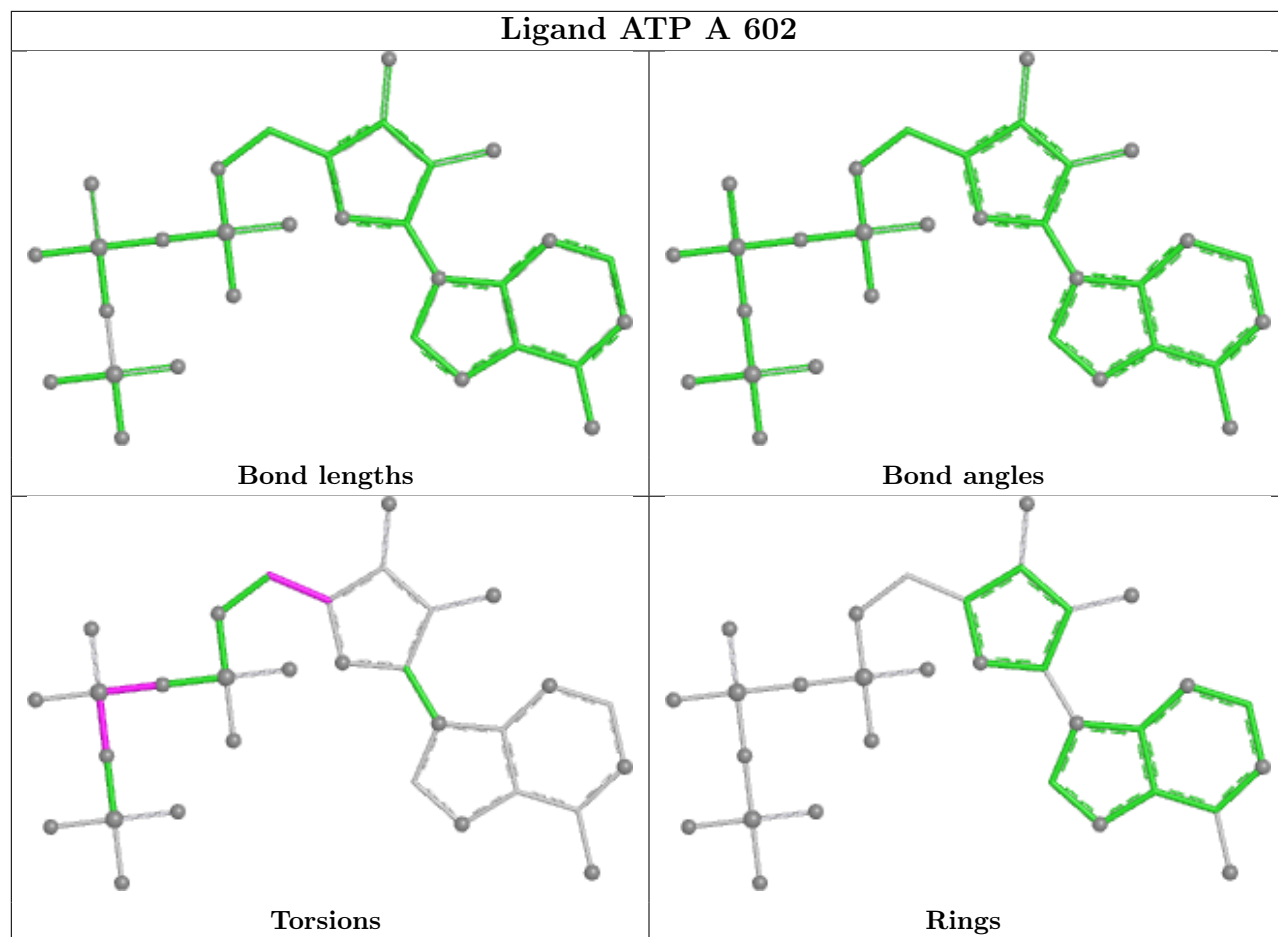


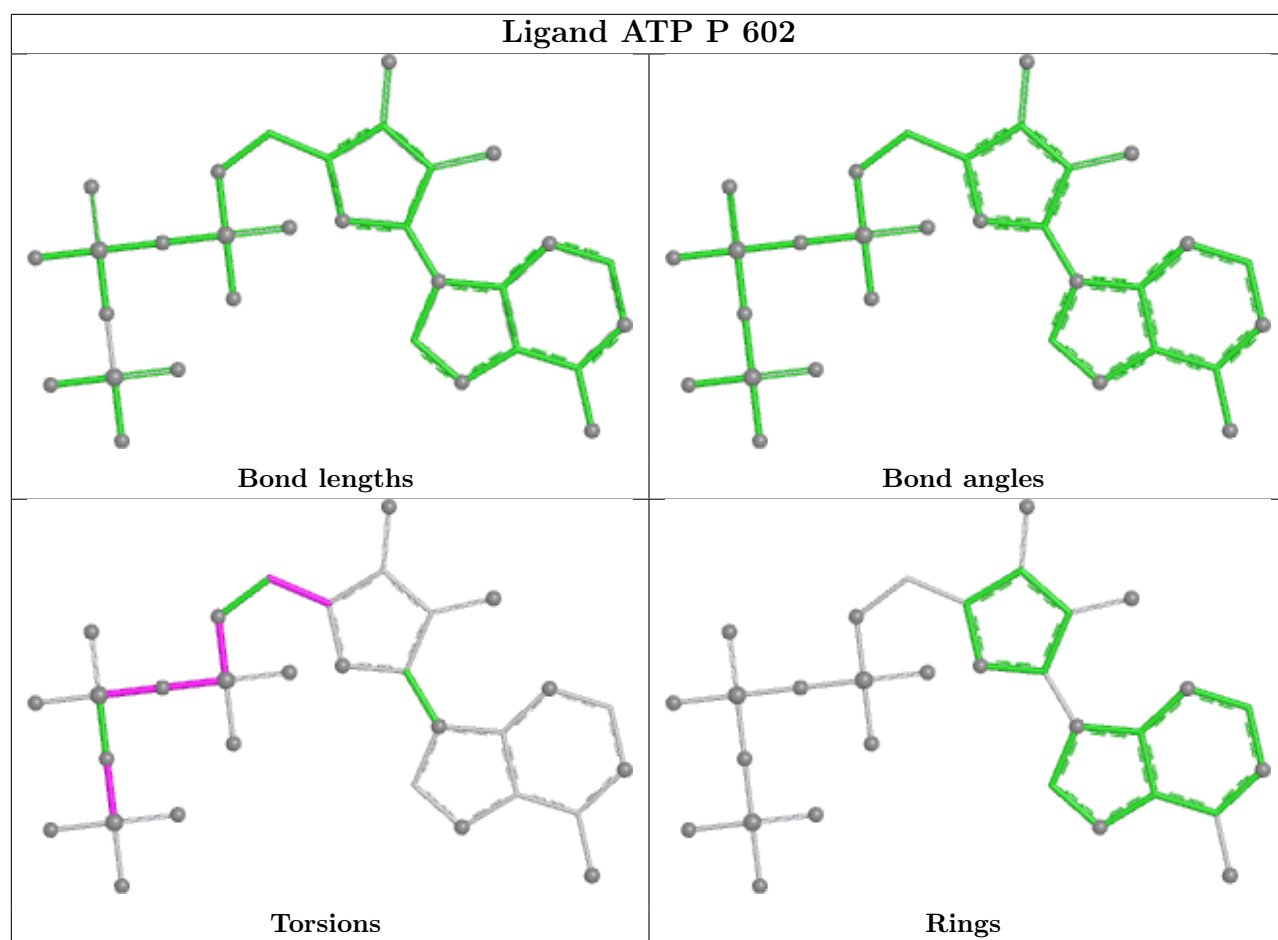


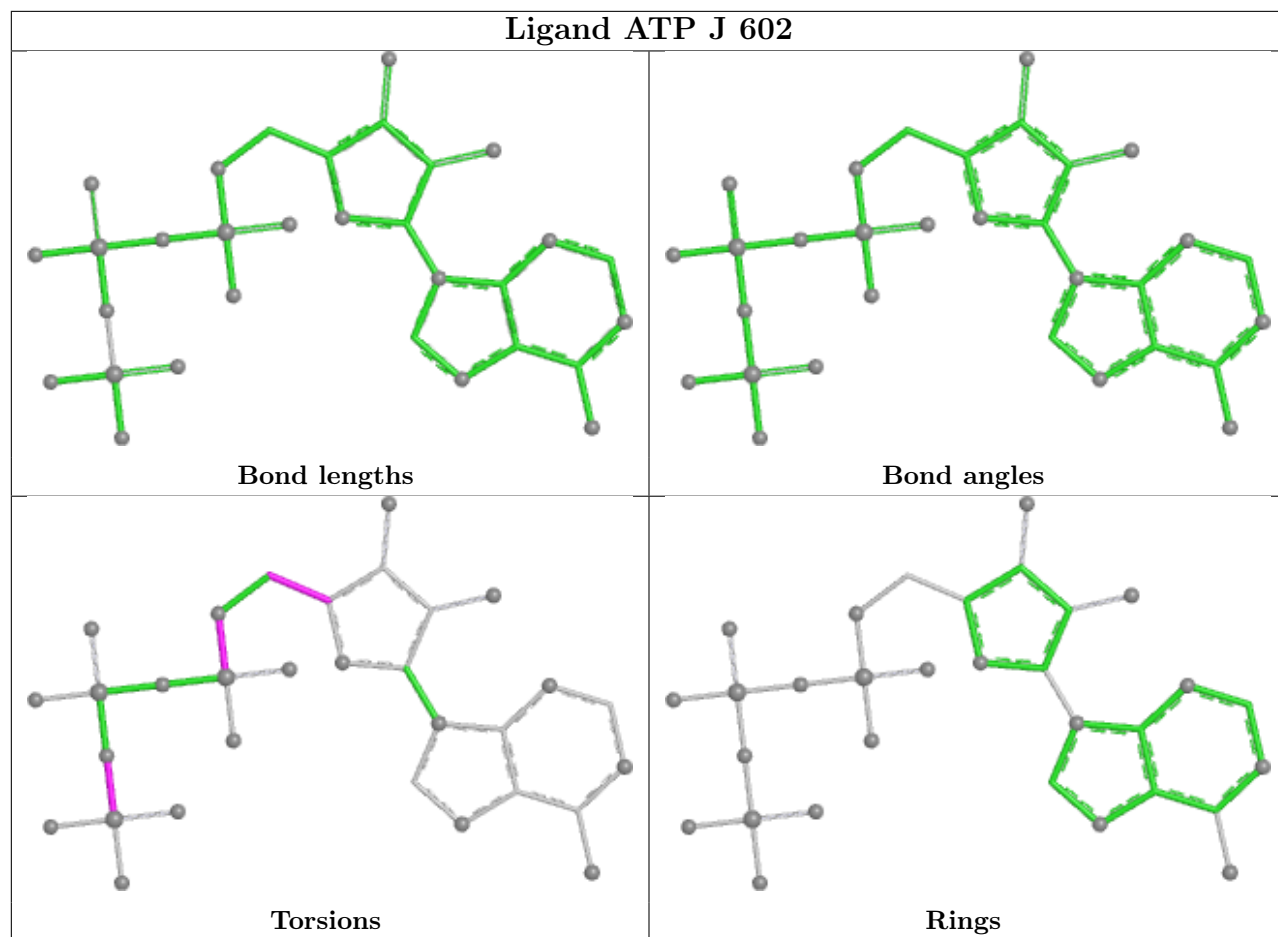


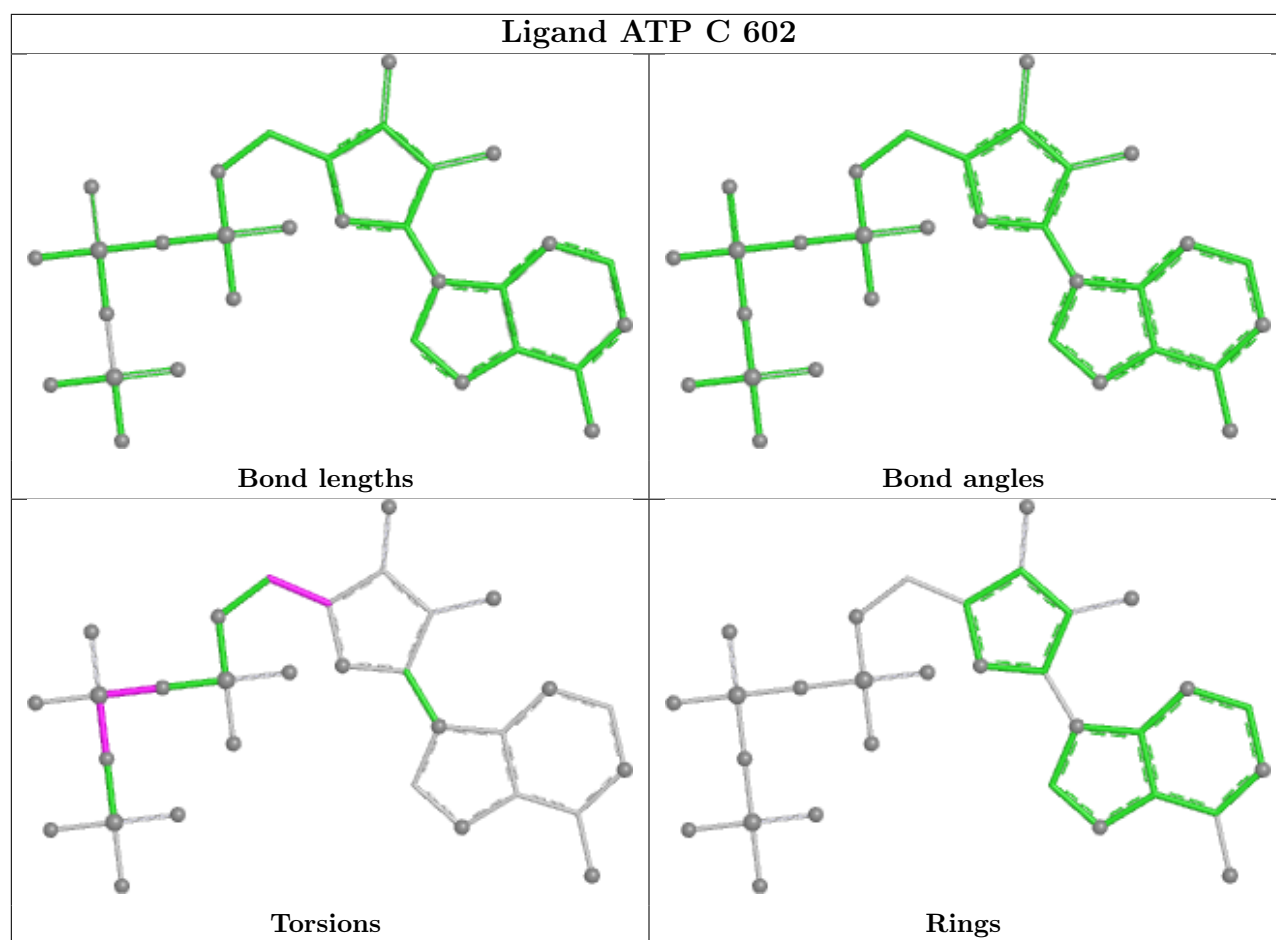












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

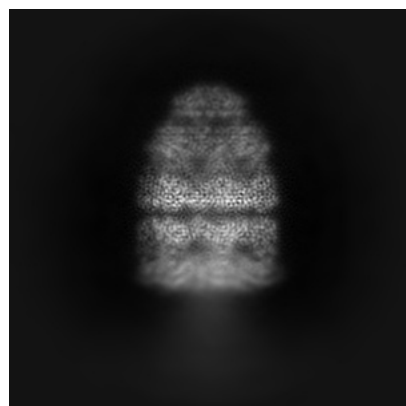
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16119. These allow visual inspection of the internal detail of the map and identification of artifacts.

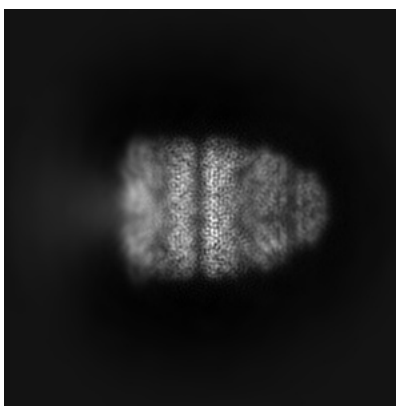
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

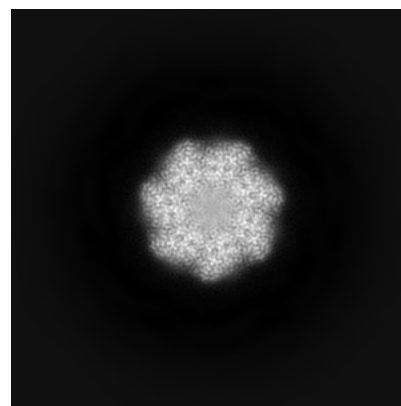
6.1.1 Primary map



X

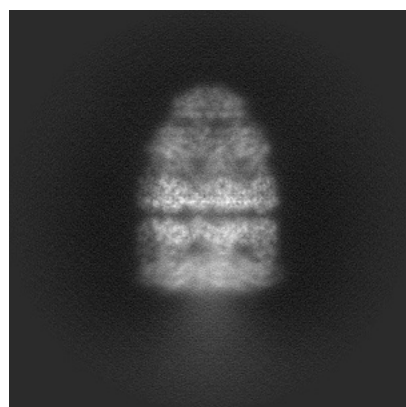


Y

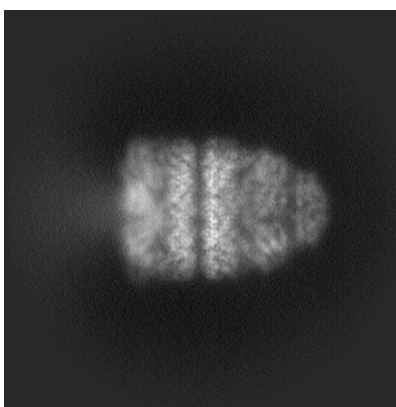


Z

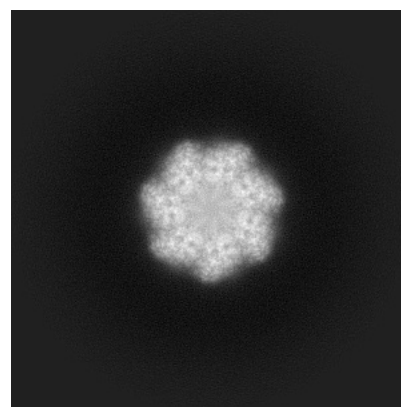
6.1.2 Raw map



X



Y

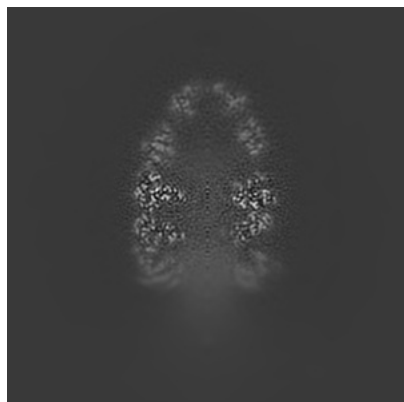


Z

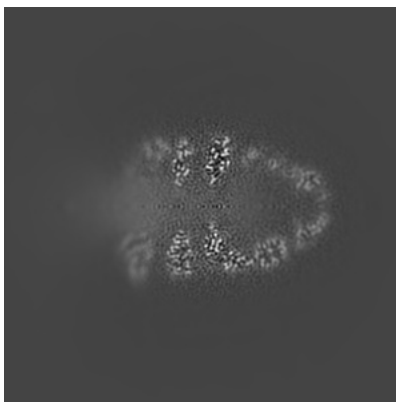
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

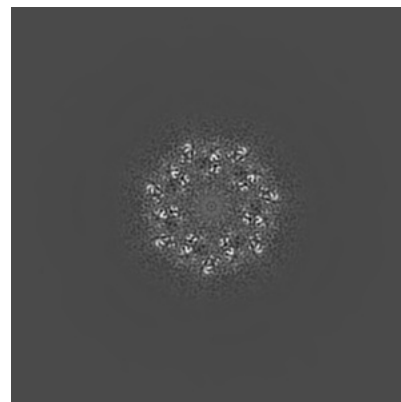
6.2.1 Primary map



X Index: 196

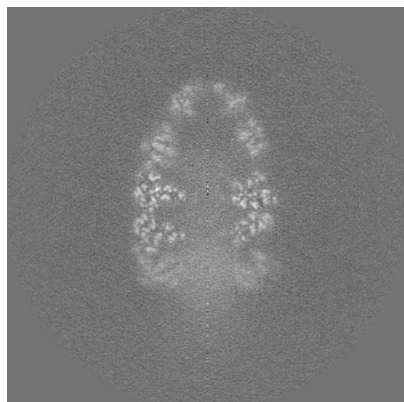


Y Index: 196

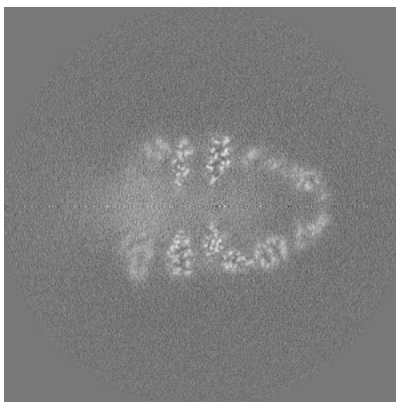


Z Index: 196

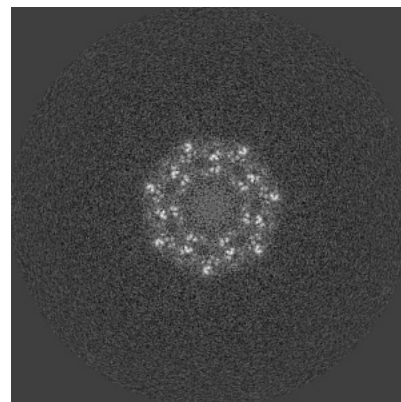
6.2.2 Raw map



X Index: 196



Y Index: 196

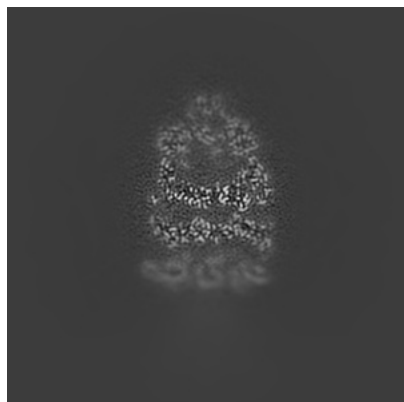


Z Index: 196

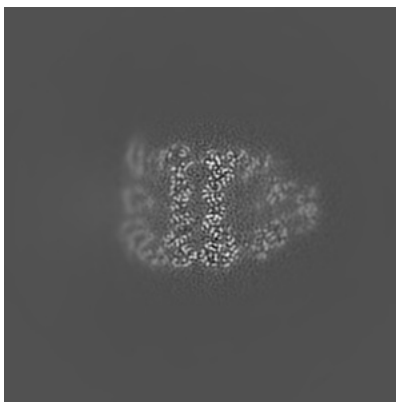
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

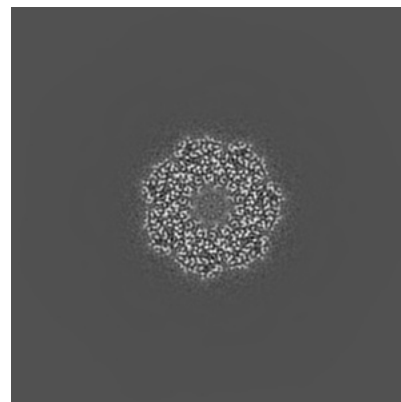
6.3.1 Primary map



X Index: 162

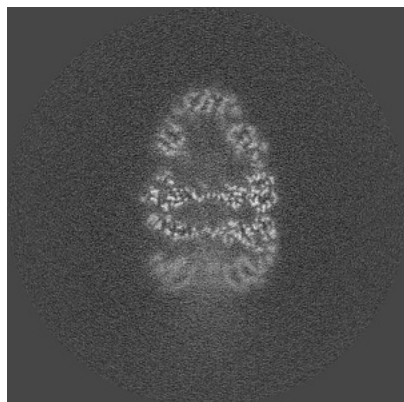


Y Index: 163

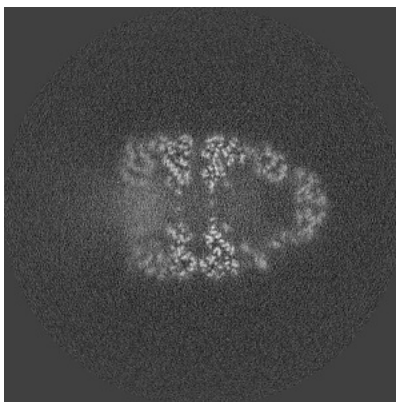


Z Index: 204

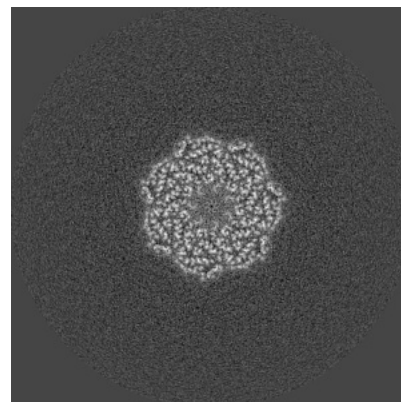
6.3.2 Raw map



X Index: 172



Y Index: 213

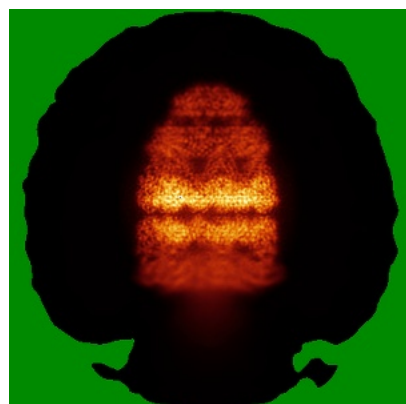


Z Index: 204

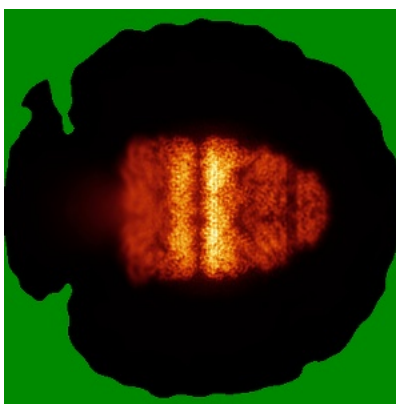
The images above show the largest variance slices of the map in three orthogonal directions.

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

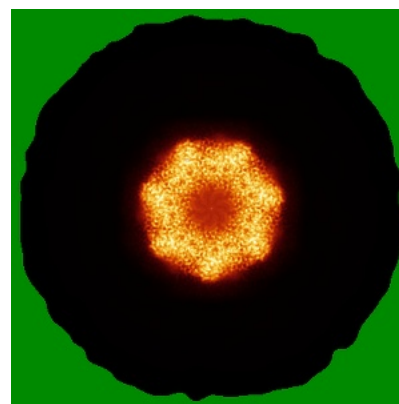
6.4.1 Primary map



X

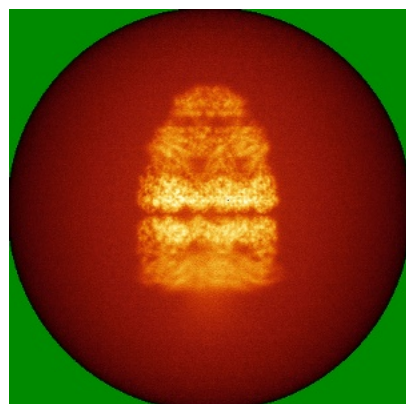


Y

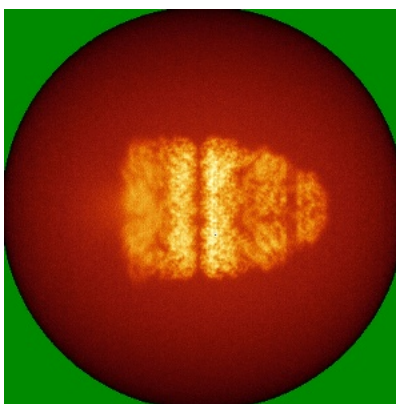


Z

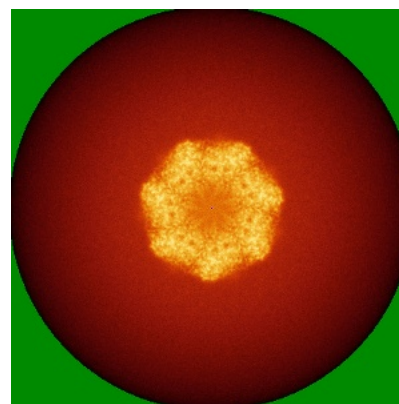
6.4.2 Raw map



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](#)

This section was not generated.

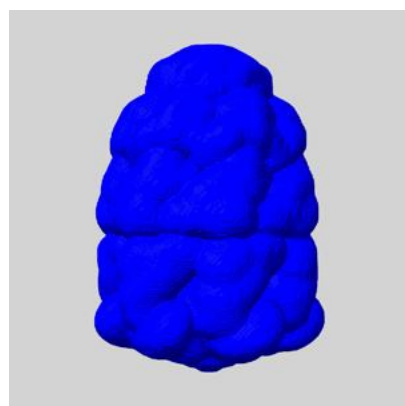
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

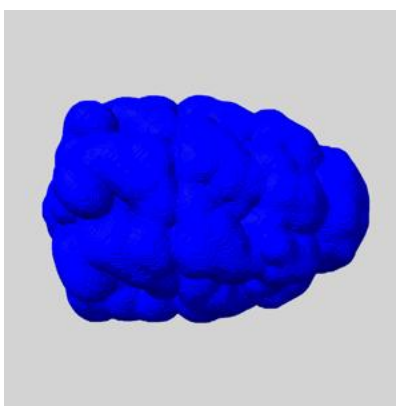
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

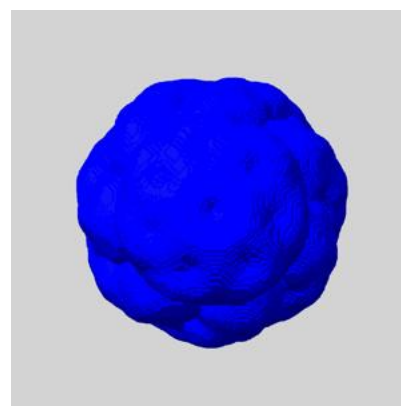
6.6.1 emd_16119_msk_1.map [i](#)



X



Y

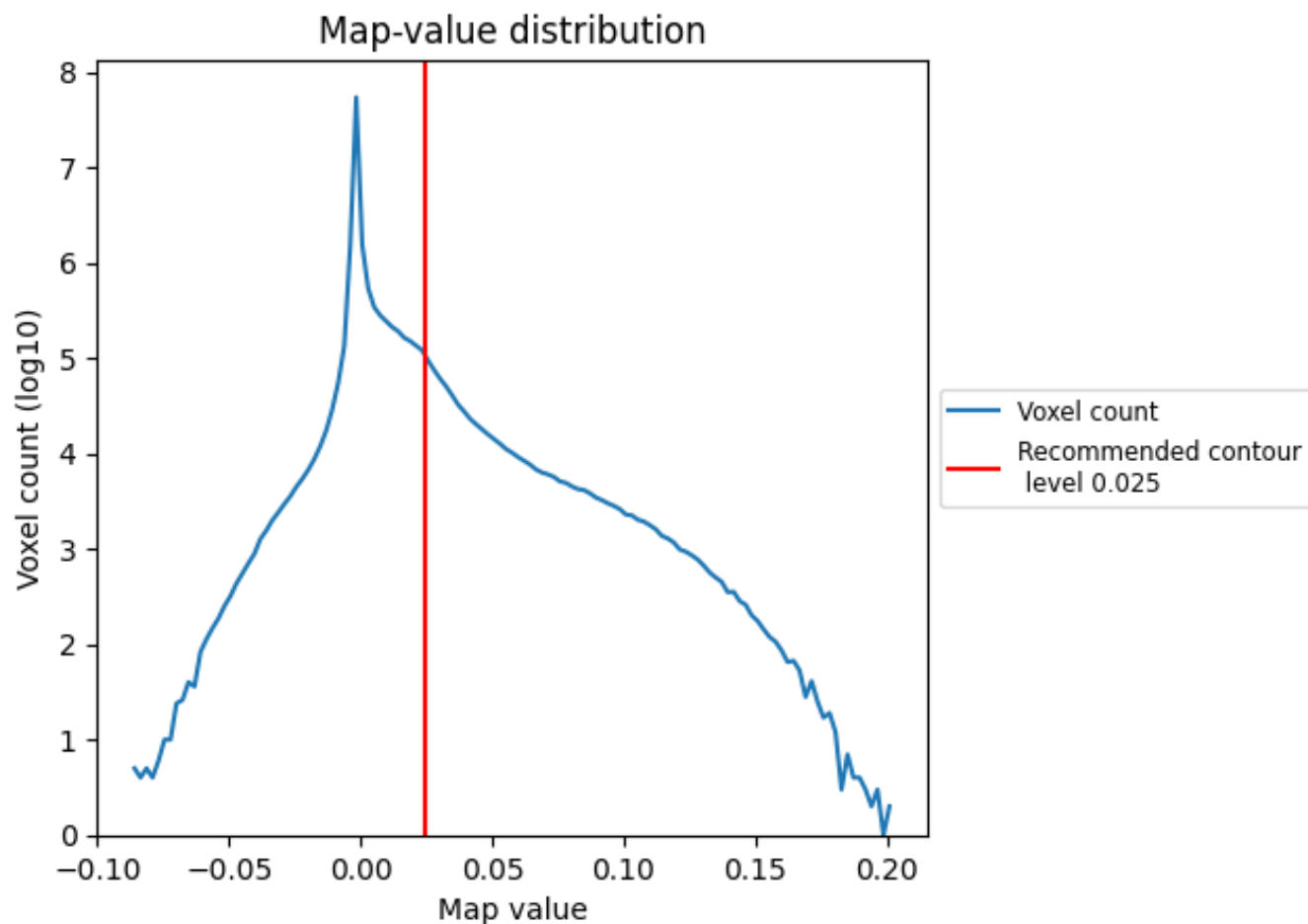


Z

7 Map analysis [i](#)

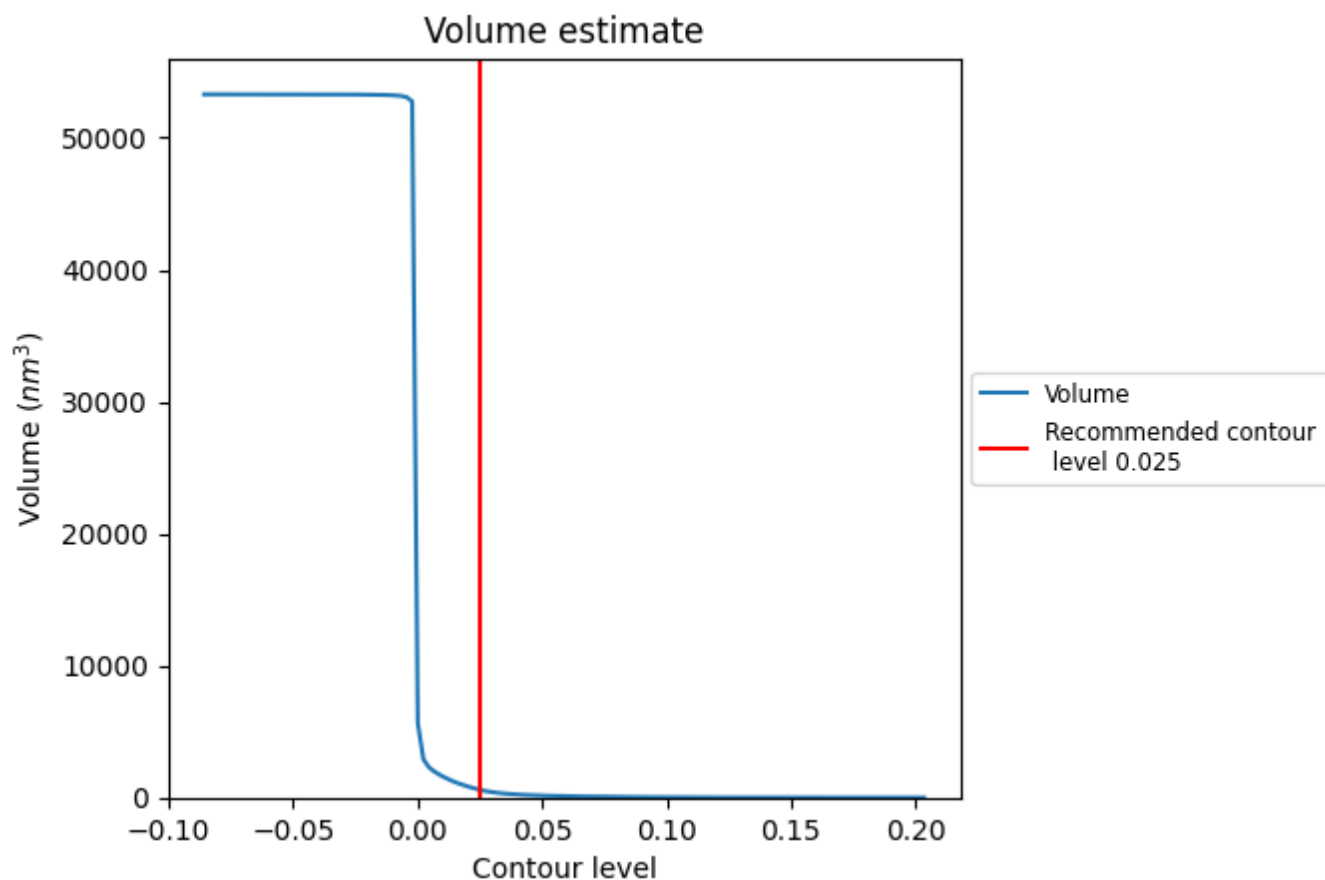
This section contains the results of statistical analysis of the map.

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.

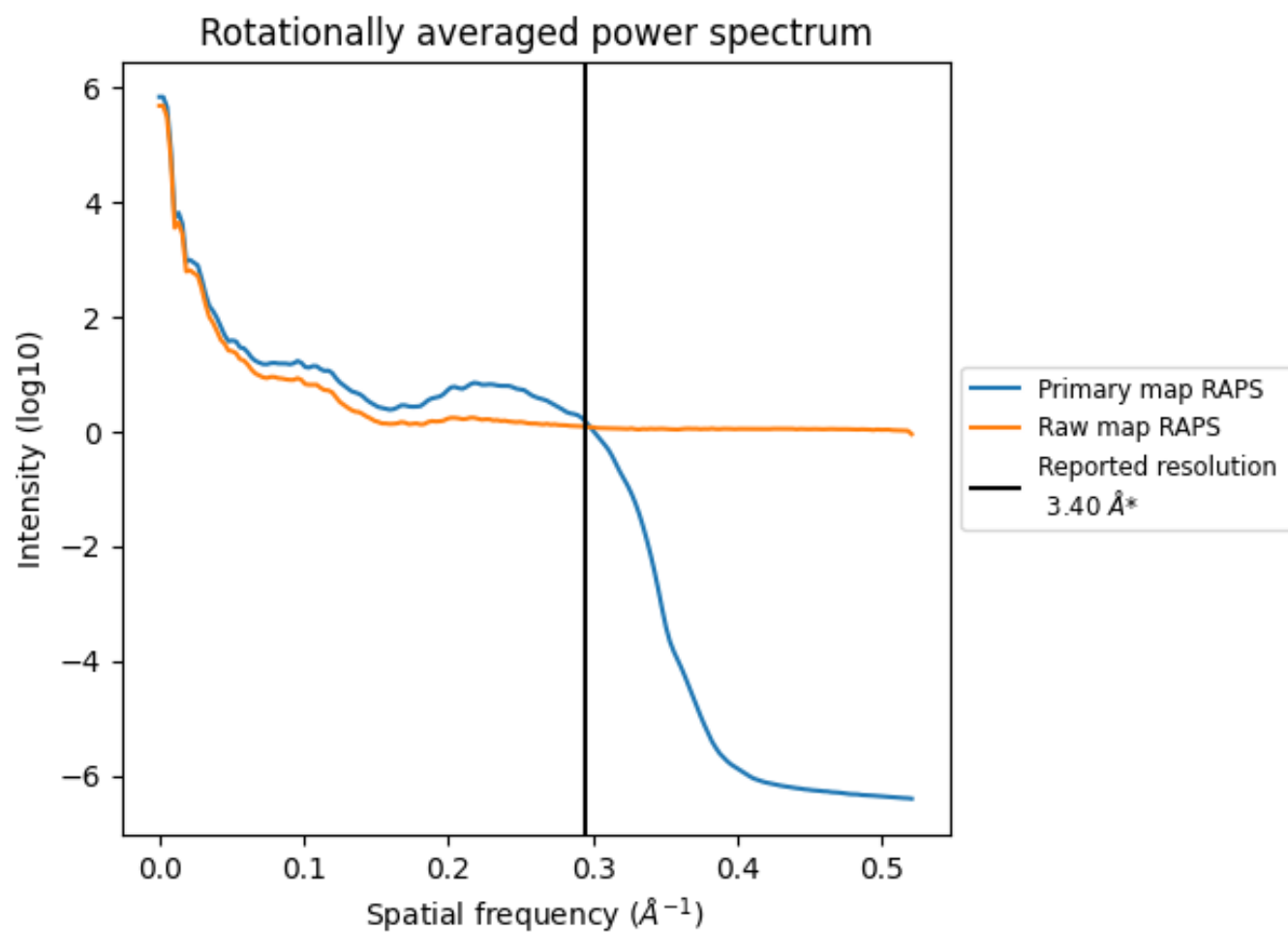
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 583 nm³; this corresponds to an approximate mass of 527 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 ⓘ

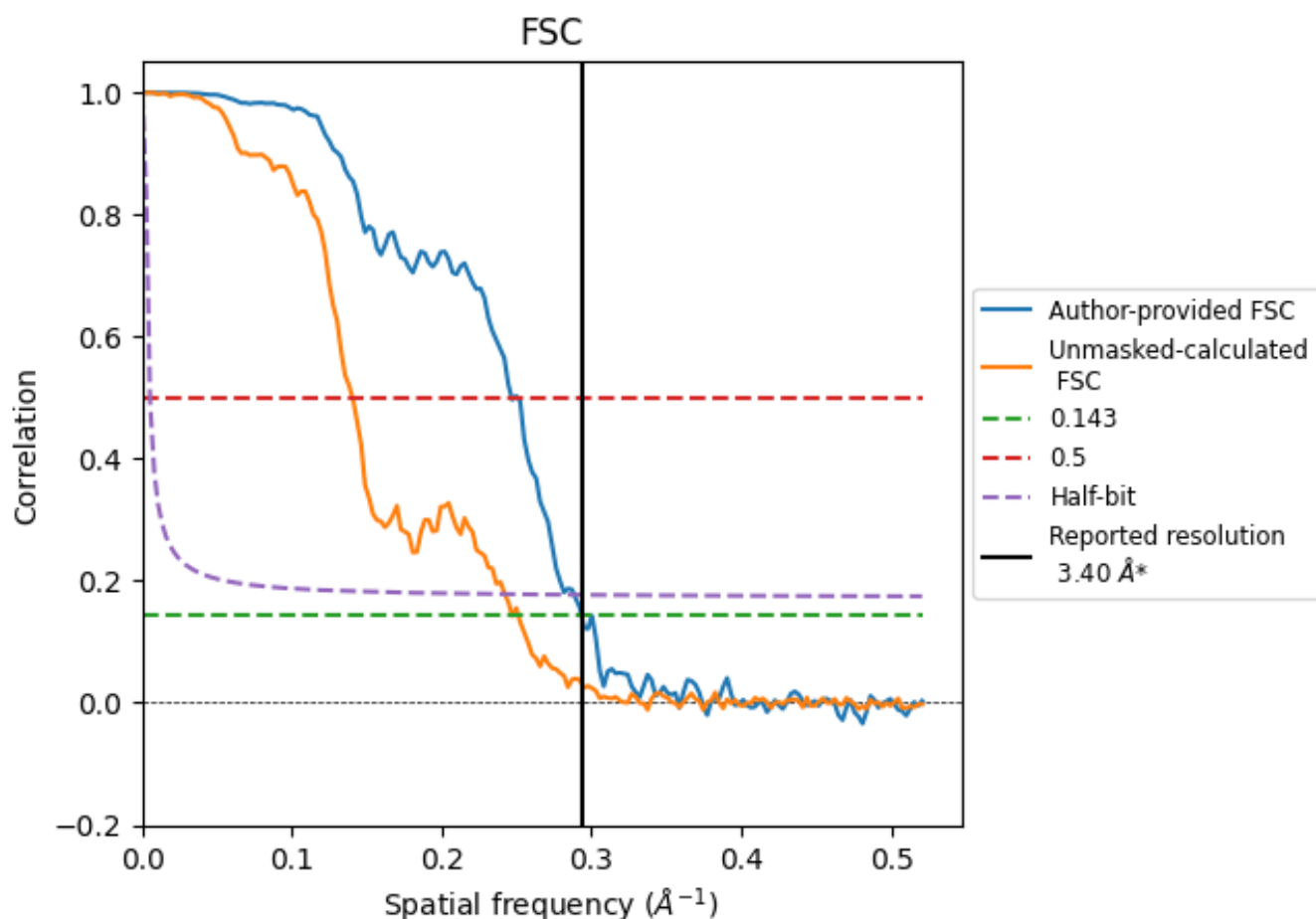


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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

8.2 Resolution estimates [i](#)

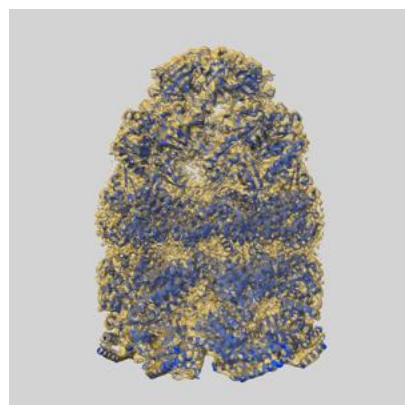
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	4.05	3.47
Unmasked-calculated*	4.05	7.12	4.13

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

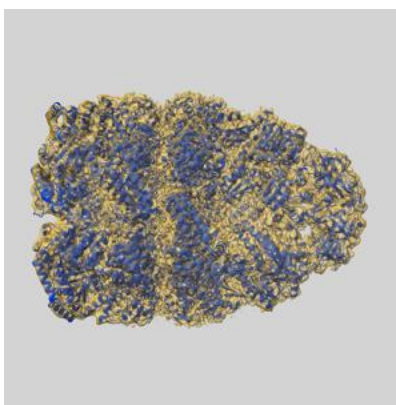
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16119 and PDB model 8BMO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

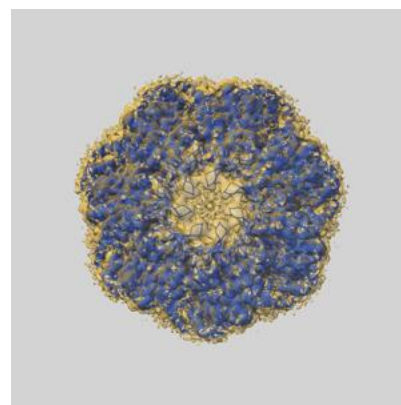
9.1 Map-model overlay [i](#)



X



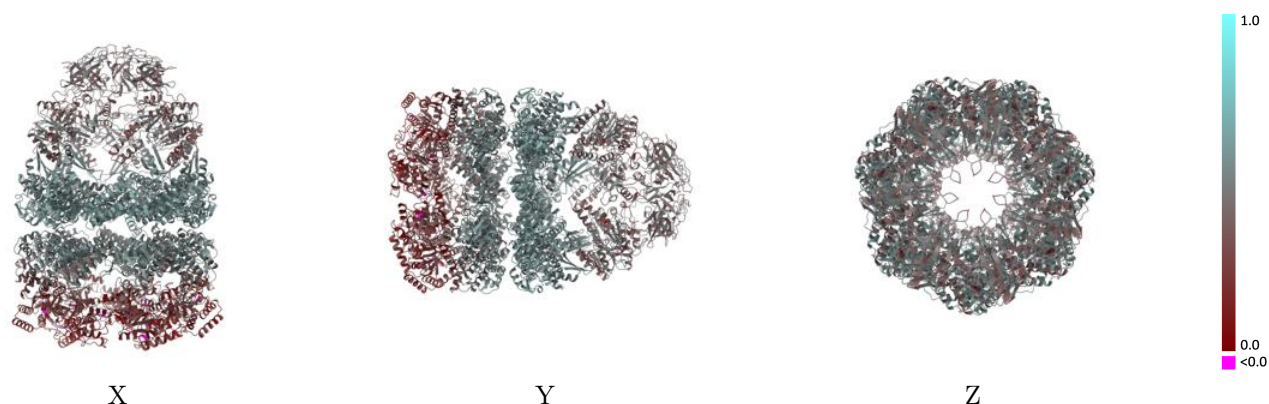
Y



Z

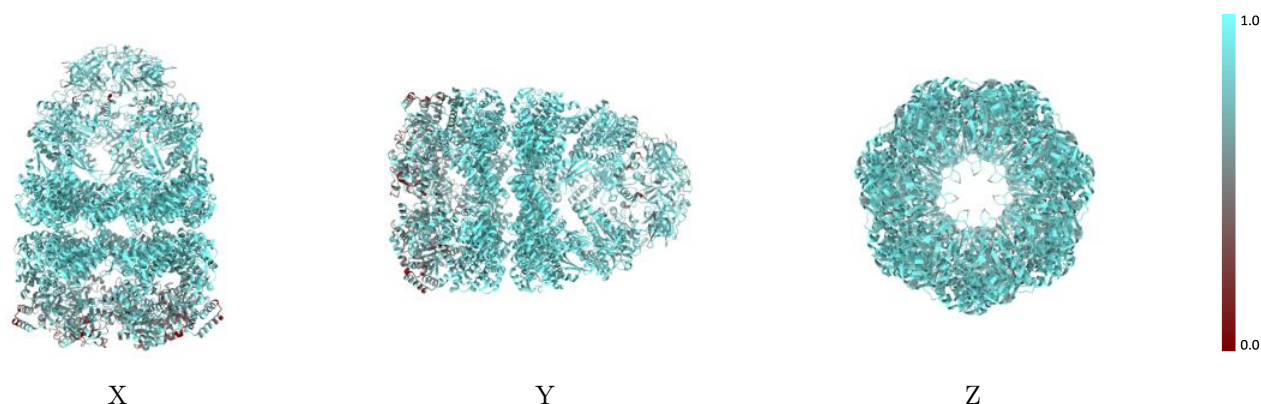
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



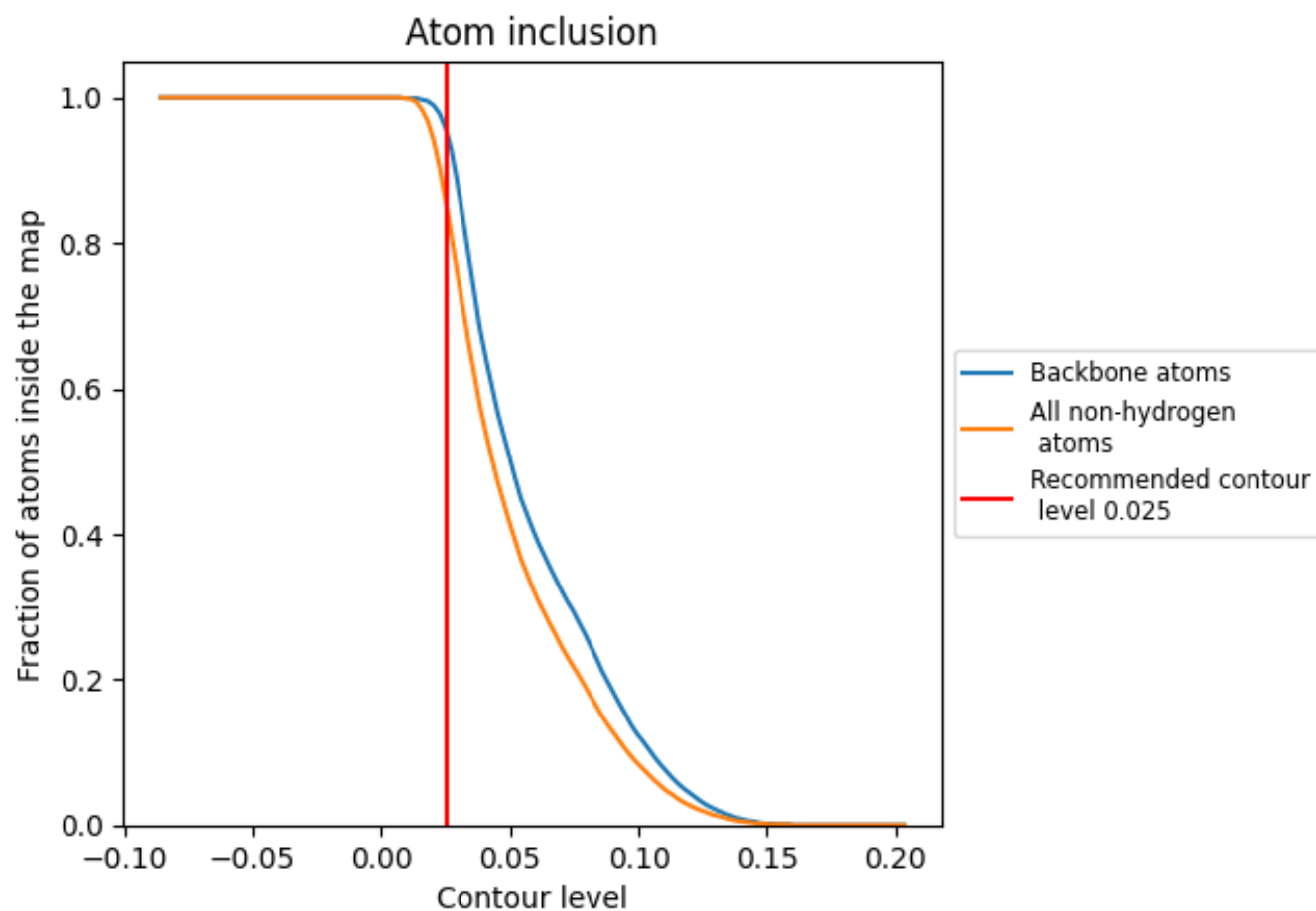
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 86% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.4420
A	 0.8070	 0.3730
B	 0.9240	 0.5170
C	 0.8090	 0.3730
D	 0.7780	 0.4180
E	 0.8100	 0.3730
F	 0.9230	 0.5140
G	 0.7790	 0.4240
H	 0.8100	 0.3730
I	 0.9220	 0.5140
J	 0.9220	 0.5140
K	 0.7700	 0.4180
L	 0.8060	 0.3690
M	 0.9220	 0.5150
N	 0.7740	 0.4180
O	 0.8110	 0.3770
P	 0.9240	 0.5140
Q	 0.7680	 0.4180
R	 0.8120	 0.3760
S	 0.9210	 0.5130
T	 0.7740	 0.4250
W	 0.7750	 0.4230

