



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:32 AM UTC

PDB ID : 7RL7 / pdb_00007rl7
EMDB ID : EMD-24519
Title : Cryo-EM structure of human p97-R155H mutant bound to ATPgS.
Authors : Caffrey, B.; Zhu, X.; Berezuk, A.; Tuttle, K.; Chittori, S.; Subramaniam, S.
Deposited on : 2021-07-23
Resolution : 3.00 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

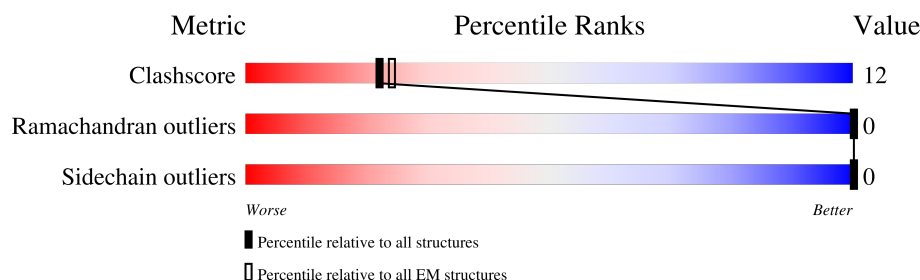
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	821	67% 23% 10%
1	B	821	69% 21% 10%
1	C	821	67% 23% 10%
1	D	821	68% 22% 10%
1	E	821	68% 22% 10%
1	F	821	66% 24% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34950 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	737	Total	C	N	O	S	0	0
			5761	3627	1013	1091	30		
1	B	737	Total	C	N	O	S	0	0
			5761	3627	1013	1091	30		
1	C	737	Total	C	N	O	S	0	0
			5761	3627	1013	1091	30		
1	D	737	Total	C	N	O	S	0	0
			5761	3627	1013	1091	30		
1	E	737	Total	C	N	O	S	0	0
			5761	3627	1013	1091	30		
1	F	737	Total	C	N	O	S	0	0
			5761	3627	1013	1091	30		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P55072
A	-13	HIS	-	expression tag	UNP P55072
A	-12	HIS	-	expression tag	UNP P55072
A	-11	HIS	-	expression tag	UNP P55072
A	-10	HIS	-	expression tag	UNP P55072
A	-9	HIS	-	expression tag	UNP P55072
A	-8	GLY	-	expression tag	UNP P55072
A	-7	THR	-	expression tag	UNP P55072
A	-6	SER	-	expression tag	UNP P55072
A	-5	GLU	-	expression tag	UNP P55072
A	-4	ASN	-	expression tag	UNP P55072
A	-3	LEU	-	expression tag	UNP P55072
A	-2	TYR	-	expression tag	UNP P55072
A	-1	PHE	-	expression tag	UNP P55072
A	0	GLN	-	expression tag	UNP P55072
A	1	GLY	-	expression tag	UNP P55072
A	155	HIS	ARG	engineered mutation	UNP P55072
B	-14	HIS	-	expression tag	UNP P55072

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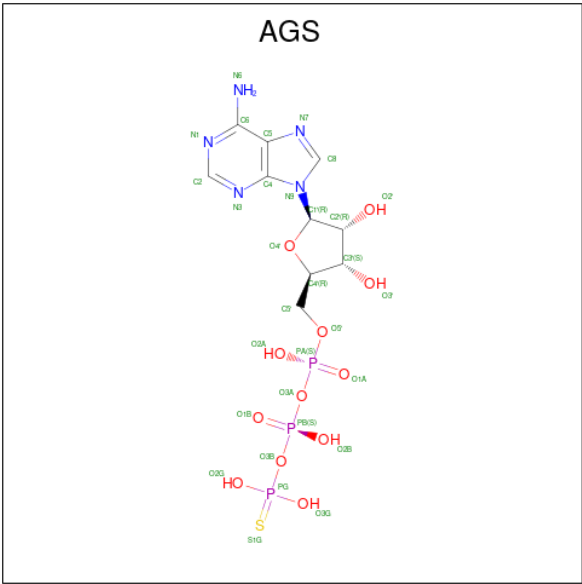
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P55072
B	-12	HIS	-	expression tag	UNP P55072
B	-11	HIS	-	expression tag	UNP P55072
B	-10	HIS	-	expression tag	UNP P55072
B	-9	HIS	-	expression tag	UNP P55072
B	-8	GLY	-	expression tag	UNP P55072
B	-7	THR	-	expression tag	UNP P55072
B	-6	SER	-	expression tag	UNP P55072
B	-5	GLU	-	expression tag	UNP P55072
B	-4	ASN	-	expression tag	UNP P55072
B	-3	LEU	-	expression tag	UNP P55072
B	-2	TYR	-	expression tag	UNP P55072
B	-1	PHE	-	expression tag	UNP P55072
B	0	GLN	-	expression tag	UNP P55072
B	1	GLY	-	expression tag	UNP P55072
B	155	HIS	ARG	engineered mutation	UNP P55072
C	-14	HIS	-	expression tag	UNP P55072
C	-13	HIS	-	expression tag	UNP P55072
C	-12	HIS	-	expression tag	UNP P55072
C	-11	HIS	-	expression tag	UNP P55072
C	-10	HIS	-	expression tag	UNP P55072
C	-9	HIS	-	expression tag	UNP P55072
C	-8	GLY	-	expression tag	UNP P55072
C	-7	THR	-	expression tag	UNP P55072
C	-6	SER	-	expression tag	UNP P55072
C	-5	GLU	-	expression tag	UNP P55072
C	-4	ASN	-	expression tag	UNP P55072
C	-3	LEU	-	expression tag	UNP P55072
C	-2	TYR	-	expression tag	UNP P55072
C	-1	PHE	-	expression tag	UNP P55072
C	0	GLN	-	expression tag	UNP P55072
C	1	GLY	-	expression tag	UNP P55072
C	155	HIS	ARG	engineered mutation	UNP P55072
D	-14	HIS	-	expression tag	UNP P55072
D	-13	HIS	-	expression tag	UNP P55072
D	-12	HIS	-	expression tag	UNP P55072
D	-11	HIS	-	expression tag	UNP P55072
D	-10	HIS	-	expression tag	UNP P55072
D	-9	HIS	-	expression tag	UNP P55072
D	-8	GLY	-	expression tag	UNP P55072
D	-7	THR	-	expression tag	UNP P55072
D	-6	SER	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLU	-	expression tag	UNP P55072
D	-4	ASN	-	expression tag	UNP P55072
D	-3	LEU	-	expression tag	UNP P55072
D	-2	TYR	-	expression tag	UNP P55072
D	-1	PHE	-	expression tag	UNP P55072
D	0	GLN	-	expression tag	UNP P55072
D	1	GLY	-	expression tag	UNP P55072
D	155	HIS	ARG	engineered mutation	UNP P55072
E	-14	HIS	-	expression tag	UNP P55072
E	-13	HIS	-	expression tag	UNP P55072
E	-12	HIS	-	expression tag	UNP P55072
E	-11	HIS	-	expression tag	UNP P55072
E	-10	HIS	-	expression tag	UNP P55072
E	-9	HIS	-	expression tag	UNP P55072
E	-8	GLY	-	expression tag	UNP P55072
E	-7	THR	-	expression tag	UNP P55072
E	-6	SER	-	expression tag	UNP P55072
E	-5	GLU	-	expression tag	UNP P55072
E	-4	ASN	-	expression tag	UNP P55072
E	-3	LEU	-	expression tag	UNP P55072
E	-2	TYR	-	expression tag	UNP P55072
E	-1	PHE	-	expression tag	UNP P55072
E	0	GLN	-	expression tag	UNP P55072
E	1	GLY	-	expression tag	UNP P55072
E	155	HIS	ARG	engineered mutation	UNP P55072
F	-14	HIS	-	expression tag	UNP P55072
F	-13	HIS	-	expression tag	UNP P55072
F	-12	HIS	-	expression tag	UNP P55072
F	-11	HIS	-	expression tag	UNP P55072
F	-10	HIS	-	expression tag	UNP P55072
F	-9	HIS	-	expression tag	UNP P55072
F	-8	GLY	-	expression tag	UNP P55072
F	-7	THR	-	expression tag	UNP P55072
F	-6	SER	-	expression tag	UNP P55072
F	-5	GLU	-	expression tag	UNP P55072
F	-4	ASN	-	expression tag	UNP P55072
F	-3	LEU	-	expression tag	UNP P55072
F	-2	TYR	-	expression tag	UNP P55072
F	-1	PHE	-	expression tag	UNP P55072
F	0	GLN	-	expression tag	UNP P55072
F	1	GLY	-	expression tag	UNP P55072
F	155	HIS	ARG	engineered mutation	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

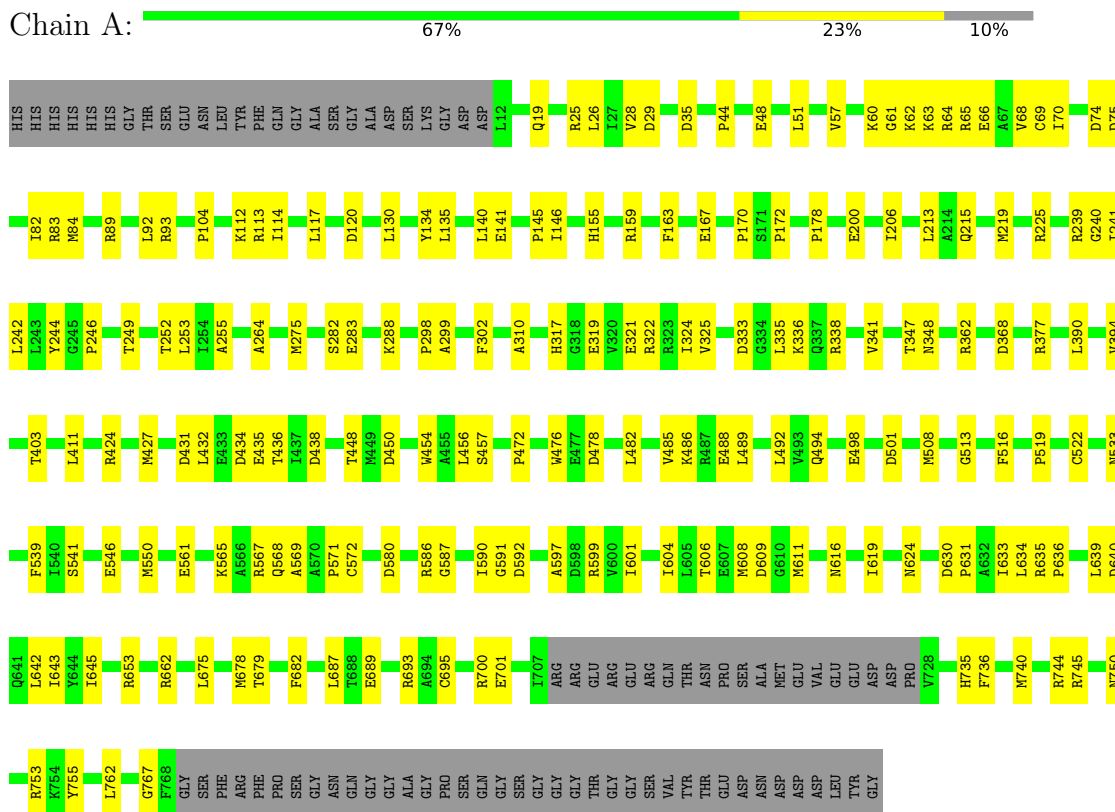
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Mg 2	0
3	B	2	Total 2	Mg 2	0
3	C	2	Total 2	Mg 2	0
3	D	2	Total 2	Mg 2	0
3	E	2	Total 2	Mg 2	0
3	F	2	Total 2	Mg 2	0

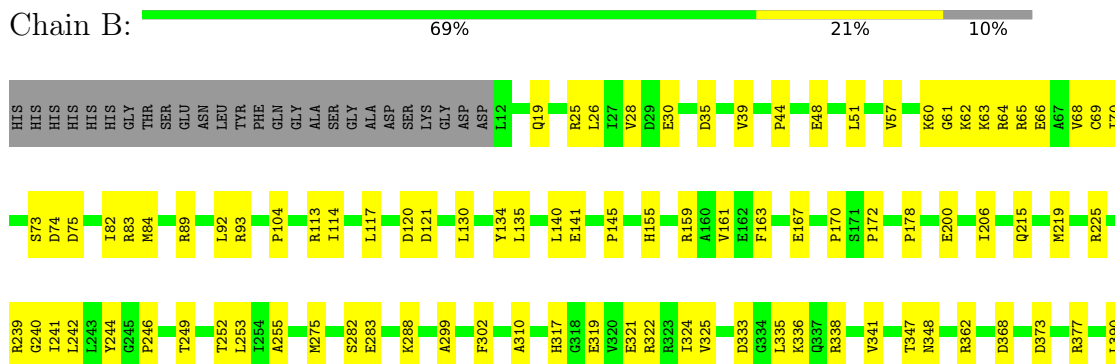
3 Residue-property plots

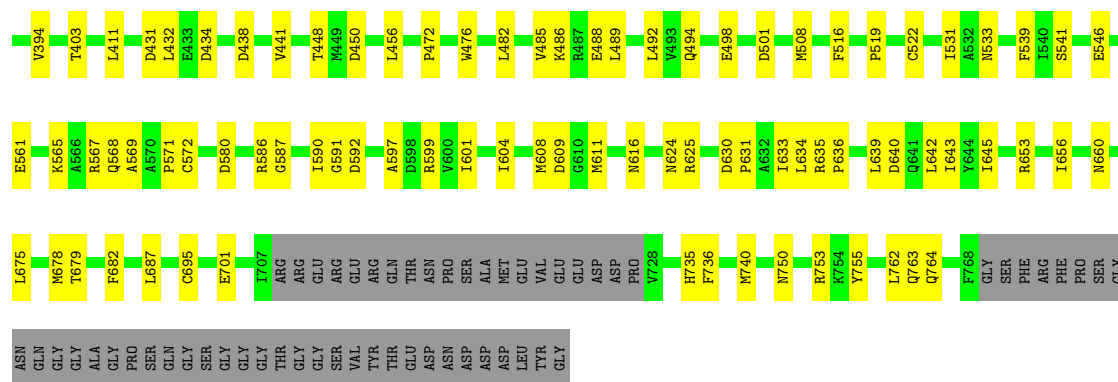
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Transitional endoplasmic reticulum ATPase

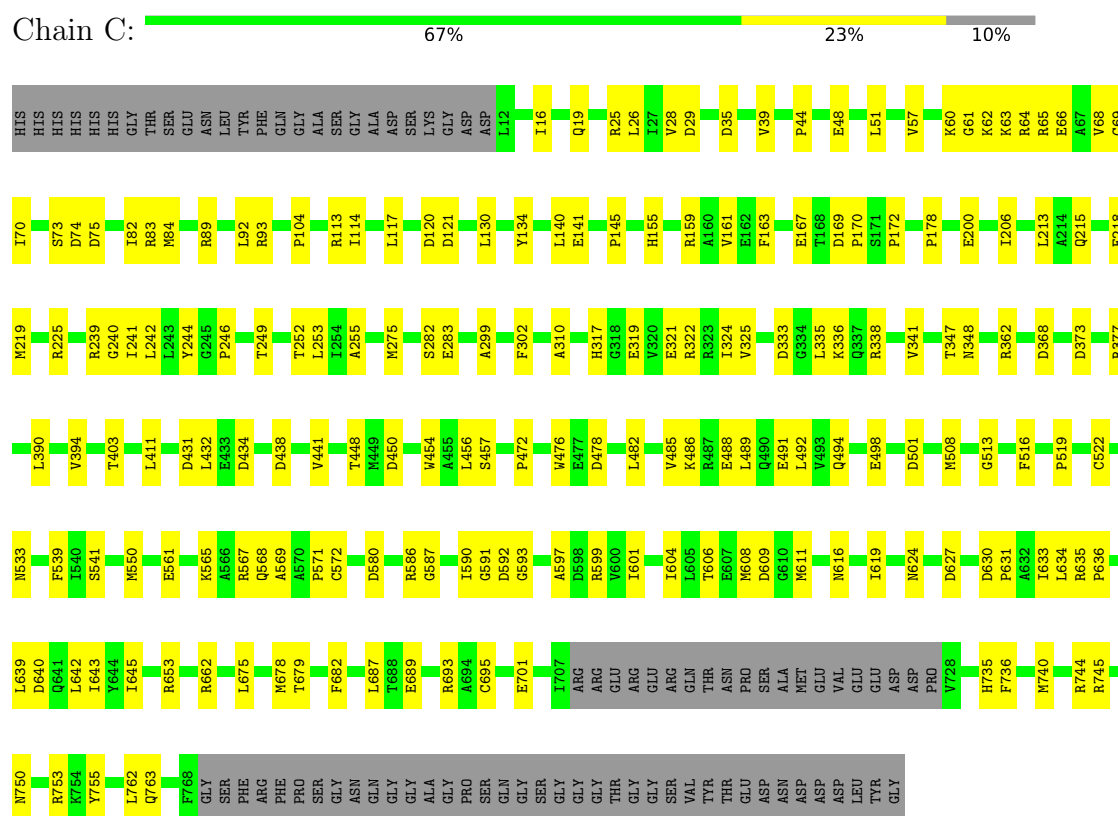


- Molecule 1: Transitional endoplasmic reticulum ATPase

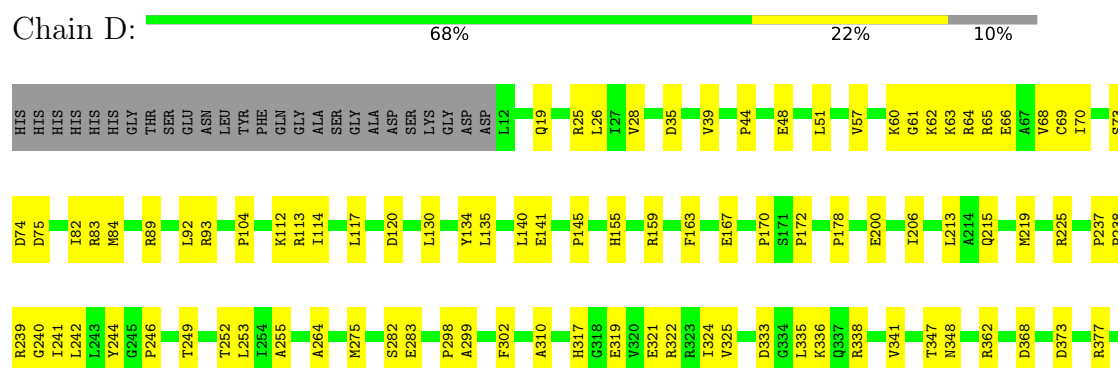


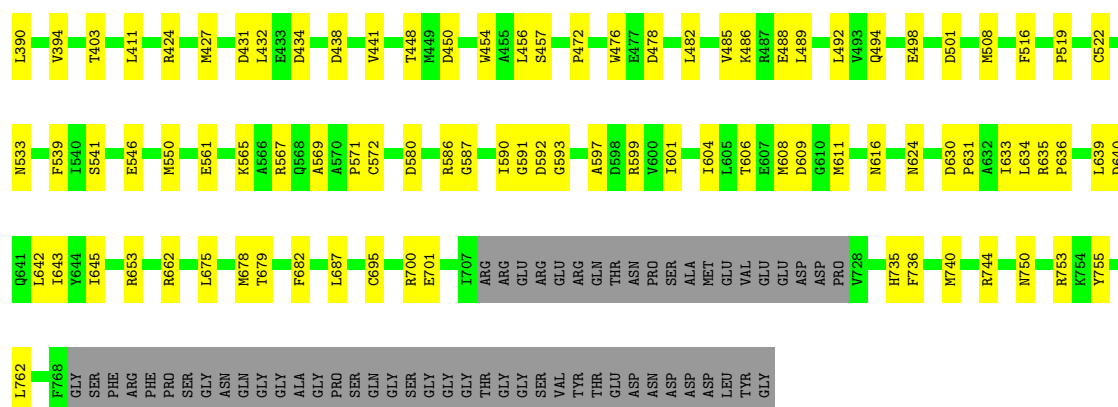


- Molecule 1: Transitional endoplasmic reticulum ATPase



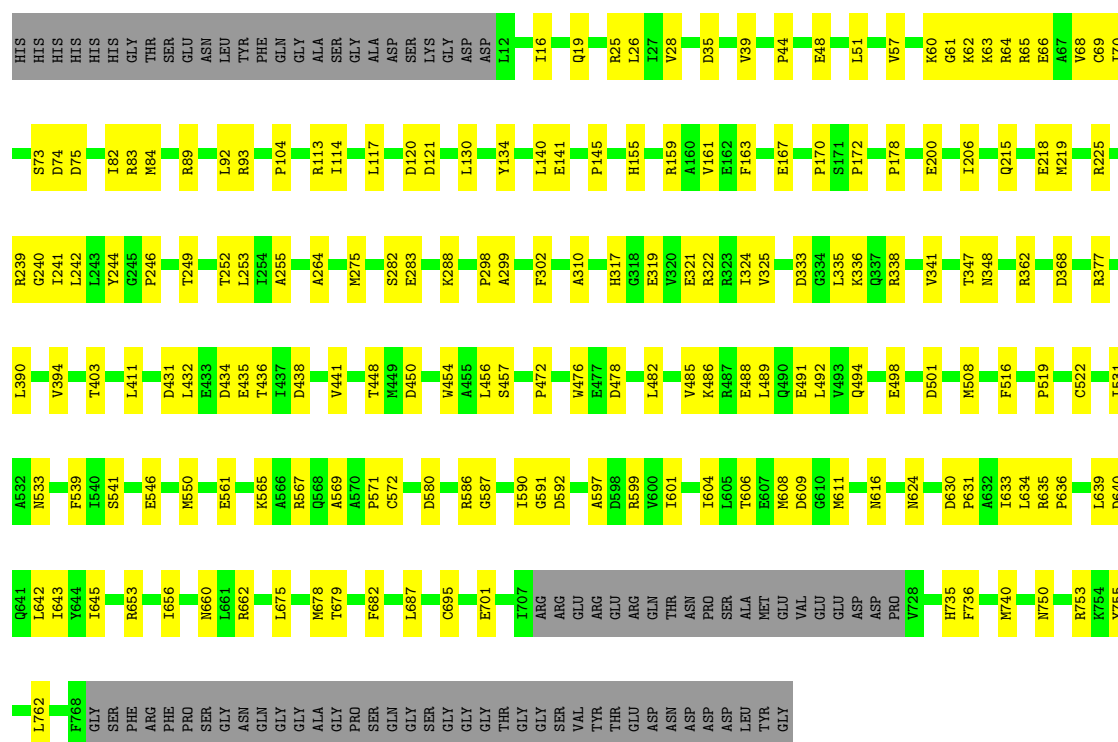
- Molecule 1: Transitional endoplasmic reticulum ATPase





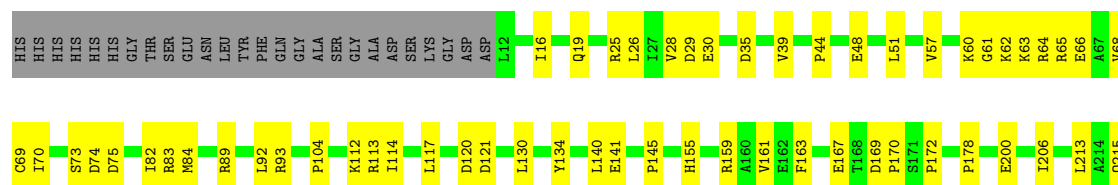
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E: 68% 22% 10%



- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F: 66% 24% 10%



LEU	TYR	GLY	GLU	I619	M508	D373	E218
			VAL	N624	G513	M219	
PHE	ARG	GLY	ASP	D627	F516	R377	R225
			ASP				
PRO	THR	GLY	ASP	D630	F519	L380	P237
			PRO	P631	P520	P238	
H735	F736	GLY	ASP	A632	G521	V394	R239
			ASP	A633	G522	G240	
H740	N750	GLY	ASP	L634	G521	T403	G249
			ASP	L635	G522	T241	
N750	R753	GLY	ASP	R636	T531	L411	L242
			ASP	R637	T532	L243	
R754	Y755	GLY	ASP	L639	N533	R424	Y244
			ASP	D640	N534	G245	
L762	Q764	GLY	ASP	P641	F539	M427	P246
			ASP	L642	F540	D431	
Q764	F768	GLY	ASP	L643	S541	L432	T249
			ASP	L644	S542	L433	
F768	SER	GLY	ASP	L645	E546	D434	T252
			ASP	L646	E547	D435	
F768	SER	GLY	ASP	L647	N550	T436	L254
			ASP	L648	N551	A255	
F768	SER	GLY	ASP	L649	E561	L437	A255
			ASP	L650	E562	L438	
F768	SER	GLY	ASP	L651	K565	D438	M275
			ASP	L652	K566	T448	
F768	SER	GLY	ASP	L653	S567	M449	S282
			ASP	L654	S568	E283	
F768	SER	GLY	ASP	L655	A569	D450	E283
			ASP	L656	A570	A299	
F768	SER	GLY	ASP	L657	P571	W454	A299
			ASP	L658	P572	F302	
F768	SER	GLY	ASP	L659	C572	L456	F302
			ASP	L660	C573	S457	
F768	SER	GLN	ASP	L661	D580	L464	A310
			ASP	L662	D581	L465	
F768	SER	GLY	ASP	L663	E586	P472	H317
			ASP	L664	E587	G318	
F768	SER	ALA	ASP	E689	A589	E319	G318
			ASP			V320	
F768	SER	GLY	ASP	L665	T590	W476	E321
			ASP	L666	T591	E477	R322
F768	SER	GLN	ASP	A694	G591	D478	R322
			ASP	C695	D592	R323	
F768	SER	GLY	ASP	R700	A597	L482	I324
			ASP	E701	D598	V325	
F768	SER	GLY	ASP	L707	B598	V485	D333
			ASP			K486	G334
F768	THR	GLY	ASP	ARG	T601	E487	L335
			ASP			E488	L336
F768	THR	GLY	ASP	ARG	L604	L489	Q337
			ASP			Q490	R338
F768	THR	VAL	ASP	ARG	L605	Q490	R338
			ASP			E491	V341
F768	THR	GLN	ASP	ARG	E607	L492	V341
			ASP			W493	T347
F768	THR	GLU	ASP	THR	H608	Q494	N348
			ASP			D609	R362
F768	THR	ASP	ASP	ASN	G610	E498	T347
			ASP			N611	N348
F768	THR	ASP	ASP	ASP	N611	E498	R362
			ASP			D501	T369
F768	THR	ASP	ASP	ALA	N616	D501	T369
			ASP			W571	T369

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	284092	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 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	0.15	0/5855	0.39	0/7906
1	B	0.15	0/5855	0.39	0/7906
1	C	0.15	0/5855	0.39	0/7906
1	D	0.14	0/5855	0.39	0/7906
1	E	0.15	0/5855	0.39	0/7906
1	F	0.14	0/5855	0.39	0/7906
All	All	0.15	0/35130	0.39	0/47436

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5761	0	5833	144	0
1	B	5761	0	5833	135	0
1	C	5761	0	5833	145	0
1	D	5761	0	5833	140	0
1	E	5761	0	5833	137	0
1	F	5761	0	5833	151	0
2	A	62	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	62	0	24	2	0
2	C	62	0	24	3	0
2	D	62	0	24	4	0
2	E	62	0	24	3	0
2	F	62	0	24	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	34950	0	35142	807	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 (807) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:HB3	1:C:92:LEU:CD2	1.58	1.33
1:D:65:ARG:HB3	1:D:92:LEU:CD2	1.57	1.33
1:A:65:ARG:HB3	1:A:92:LEU:CD2	1.58	1.32
1:B:65:ARG:HB3	1:B:92:LEU:CD2	1.58	1.32
1:F:65:ARG:HB3	1:F:92:LEU:CD2	1.58	1.31
1:E:65:ARG:HB3	1:E:92:LEU:CD2	1.57	1.29
1:E:65:ARG:CB	1:E:92:LEU:HD21	1.72	1.20
1:F:65:ARG:CB	1:F:92:LEU:HD21	1.72	1.19
1:B:65:ARG:CB	1:B:92:LEU:HD21	1.72	1.18
1:C:65:ARG:CB	1:C:92:LEU:HD21	1.72	1.18
1:D:65:ARG:CB	1:D:92:LEU:HD21	1.72	1.18
1:A:65:ARG:CB	1:A:92:LEU:HD21	1.72	1.18
1:B:51:LEU:HD22	1:B:104:PRO:HG3	1.32	1.10
1:E:51:LEU:HD22	1:E:104:PRO:HG3	1.33	1.07
1:D:51:LEU:HD22	1:D:104:PRO:HG3	1.33	1.07
1:A:51:LEU:HD22	1:A:104:PRO:HG3	1.32	1.07
1:C:51:LEU:HD22	1:C:104:PRO:HG3	1.32	1.07
1:F:51:LEU:HD22	1:F:104:PRO:HG3	1.33	1.04
1:A:65:ARG:HB3	1:A:92:LEU:HD21	1.03	1.03
1:D:65:ARG:HB3	1:D:92:LEU:HD21	1.03	1.03
1:F:65:ARG:HB3	1:F:92:LEU:HD21	1.03	1.03
1:C:65:ARG:HB3	1:C:92:LEU:HD21	1.03	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:O	1:A:92:LEU:HD11	1.59	1.02
1:E:65:ARG:HB3	1:E:92:LEU:HD21	1.03	1.02
1:F:65:ARG:O	1:F:92:LEU:HD11	1.59	1.02
1:B:65:ARG:O	1:B:92:LEU:HD11	1.59	1.01
1:B:65:ARG:HB3	1:B:92:LEU:HD21	1.03	1.01
1:C:65:ARG:O	1:C:92:LEU:HD11	1.60	1.00
1:E:65:ARG:O	1:E:92:LEU:HD11	1.60	1.00
1:D:65:ARG:O	1:D:92:LEU:HD11	1.59	1.00
1:D:65:ARG:C	1:D:92:LEU:HD11	1.95	0.91
1:C:65:ARG:C	1:C:92:LEU:HD11	1.95	0.91
1:B:65:ARG:C	1:B:92:LEU:HD11	1.95	0.91
1:E:65:ARG:C	1:E:92:LEU:HD11	1.95	0.91
1:A:51:LEU:CD2	1:A:104:PRO:HG3	2.02	0.90
1:F:65:ARG:O	1:F:92:LEU:CD1	2.19	0.90
1:A:65:ARG:C	1:A:92:LEU:HD11	1.95	0.90
1:E:51:LEU:CD2	1:E:104:PRO:HG3	2.02	0.90
1:A:322:ARG:HH12	1:B:317:HIS:HB3	1.36	0.90
1:B:65:ARG:O	1:B:92:LEU:CD1	2.19	0.90
1:D:51:LEU:CD2	1:D:104:PRO:HG3	2.02	0.90
1:F:65:ARG:C	1:F:92:LEU:HD11	1.95	0.89
1:B:51:LEU:CD2	1:B:104:PRO:HG3	2.02	0.89
1:C:65:ARG:O	1:C:92:LEU:CD1	2.19	0.89
1:A:65:ARG:O	1:A:92:LEU:CD1	2.19	0.89
1:C:51:LEU:CD2	1:C:104:PRO:HG3	2.02	0.89
1:D:65:ARG:O	1:D:92:LEU:CD1	2.19	0.89
1:F:51:LEU:CD2	1:F:104:PRO:HG3	2.02	0.89
1:E:65:ARG:O	1:E:92:LEU:CD1	2.19	0.89
1:E:65:ARG:HB3	1:E:92:LEU:HD23	1.57	0.86
1:F:65:ARG:HB3	1:F:92:LEU:HD23	1.57	0.86
1:E:322:ARG:HH12	1:F:317:HIS:HB3	1.41	0.85
1:C:65:ARG:CA	1:C:92:LEU:HD21	2.08	0.83
1:A:65:ARG:CA	1:A:92:LEU:HD21	2.08	0.83
1:F:65:ARG:CA	1:F:92:LEU:HD21	2.08	0.83
1:B:65:ARG:CA	1:B:92:LEU:HD21	2.08	0.83
1:D:65:ARG:CA	1:D:92:LEU:HD21	2.08	0.83
1:E:65:ARG:CA	1:E:92:LEU:HD21	2.08	0.82
1:A:65:ARG:HB3	1:A:92:LEU:HD23	1.57	0.81
1:C:65:ARG:HB3	1:C:92:LEU:HD23	1.57	0.81
1:B:65:ARG:HB3	1:B:92:LEU:HD23	1.57	0.81
1:D:65:ARG:HB3	1:D:92:LEU:HD23	1.57	0.79
1:B:225:ARG:NH1	1:C:432:LEU:O	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ARG:HH12	1:D:317:HIS:HB3	1.51	0.76
1:E:338:ARG:H	1:E:338:ARG:HD3	1.53	0.74
1:F:338:ARG:H	1:F:338:ARG:HD3	1.53	0.74
1:A:636:PRO:HA	1:A:640:ASP:HB3	1.70	0.74
1:A:51:LEU:CD2	1:A:104:PRO:CG	2.66	0.74
1:B:51:LEU:CD2	1:B:104:PRO:CG	2.66	0.73
1:C:51:LEU:CD2	1:C:104:PRO:CG	2.66	0.73
1:F:51:LEU:CD2	1:F:104:PRO:CG	2.66	0.73
1:E:636:PRO:HA	1:E:640:ASP:HB3	1.70	0.73
1:F:62:LYS:O	1:F:92:LEU:CD2	2.37	0.73
1:B:338:ARG:H	1:B:338:ARG:HD3	1.53	0.73
1:C:338:ARG:H	1:C:338:ARG:HD3	1.53	0.73
1:D:338:ARG:H	1:D:338:ARG:HD3	1.53	0.73
1:A:62:LYS:O	1:A:92:LEU:CD2	2.37	0.73
1:B:62:LYS:O	1:B:92:LEU:CD2	2.37	0.73
1:D:322:ARG:HH12	1:E:317:HIS:HB3	1.52	0.73
1:B:636:PRO:HA	1:B:640:ASP:HB3	1.70	0.73
1:E:62:LYS:O	1:E:92:LEU:CD2	2.37	0.73
1:D:62:LYS:O	1:D:92:LEU:CD2	2.37	0.72
1:E:51:LEU:CD2	1:E:104:PRO:CG	2.66	0.72
1:A:338:ARG:H	1:A:338:ARG:HD3	1.53	0.72
1:C:62:LYS:O	1:C:92:LEU:CD2	2.37	0.72
1:D:51:LEU:CD2	1:D:104:PRO:CG	2.66	0.72
1:D:636:PRO:HA	1:D:640:ASP:HB3	1.70	0.72
1:F:636:PRO:HA	1:F:640:ASP:HB3	1.70	0.72
1:B:322:ARG:HH12	1:C:317:HIS:HB3	1.53	0.72
1:C:636:PRO:HA	1:C:640:ASP:HB3	1.70	0.72
1:B:62:LYS:O	1:B:92:LEU:HD22	1.90	0.72
1:F:65:ARG:C	1:F:92:LEU:HD21	2.15	0.72
1:E:65:ARG:C	1:E:92:LEU:HD21	2.15	0.71
1:C:62:LYS:O	1:C:92:LEU:HD22	1.90	0.71
1:E:62:LYS:O	1:E:92:LEU:HD22	1.90	0.71
1:C:65:ARG:C	1:C:92:LEU:HD21	2.15	0.71
1:A:65:ARG:C	1:A:92:LEU:HD21	2.16	0.71
1:D:62:LYS:O	1:D:92:LEU:HD22	1.90	0.71
1:A:317:HIS:HB3	1:F:322:ARG:HH12	1.55	0.71
1:D:65:ARG:C	1:D:92:LEU:HD21	2.16	0.71
1:B:65:ARG:C	1:B:92:LEU:HD21	2.16	0.70
1:F:62:LYS:O	1:F:92:LEU:HD22	1.90	0.70
1:A:62:LYS:O	1:A:92:LEU:HD22	1.90	0.70
1:E:239:ARG:NH1	1:E:335:LEU:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ARG:NH1	1:D:335:LEU:O	2.25	0.70
1:A:348:ASN:ND2	2:A:901:AGS:S1G	2.65	0.70
1:F:239:ARG:NH1	1:F:335:LEU:O	2.25	0.70
1:E:678:MET:HE3	1:E:678:MET:HA	1.74	0.70
1:C:239:ARG:NH1	1:C:335:LEU:O	2.25	0.69
1:F:348:ASN:ND2	2:F:901:AGS:S1G	2.65	0.69
1:B:348:ASN:ND2	2:B:901:AGS:S1G	2.65	0.69
1:E:348:ASN:ND2	2:E:901:AGS:S1G	2.65	0.69
1:C:348:ASN:ND2	2:C:901:AGS:S1G	2.65	0.69
1:B:239:ARG:NH1	1:B:335:LEU:O	2.25	0.69
1:D:678:MET:HE3	1:D:678:MET:HA	1.74	0.69
1:F:678:MET:HA	1:F:678:MET:HE3	1.74	0.69
1:A:239:ARG:NH1	1:A:335:LEU:O	2.25	0.69
1:D:348:ASN:ND2	2:D:901:AGS:S1G	2.65	0.69
1:A:432:LEU:O	1:F:225:ARG:NH1	2.26	0.68
1:A:678:MET:HA	1:A:678:MET:HE3	1.74	0.68
1:C:678:MET:HE3	1:C:678:MET:HA	1.74	0.68
1:D:225:ARG:NH1	1:E:432:LEU:O	2.27	0.68
1:B:678:MET:HE3	1:B:678:MET:HA	1.74	0.68
1:E:82:ILE:HG12	1:E:84:MET:HE1	1.78	0.66
1:D:82:ILE:HG12	1:D:84:MET:HE1	1.78	0.66
1:F:633:ILE:HG12	1:F:639:LEU:HD12	1.78	0.66
1:F:82:ILE:HG12	1:F:84:MET:HE1	1.78	0.66
1:A:633:ILE:HG12	1:A:639:LEU:HD12	1.78	0.65
1:C:225:ARG:NH1	1:D:432:LEU:O	2.29	0.65
1:E:633:ILE:HG12	1:E:639:LEU:HD12	1.78	0.65
1:B:82:ILE:HG12	1:B:84:MET:HE1	1.77	0.65
1:A:82:ILE:HG12	1:A:84:MET:HE1	1.78	0.65
1:C:82:ILE:HG12	1:C:84:MET:HE1	1.78	0.65
1:B:633:ILE:HG12	1:B:639:LEU:HD12	1.78	0.64
1:D:633:ILE:HG12	1:D:639:LEU:HD12	1.78	0.64
1:C:633:ILE:HG12	1:C:639:LEU:HD12	1.78	0.64
1:E:66:GLU:HA	1:E:92:LEU:HD11	1.80	0.64
1:F:66:GLU:HA	1:F:92:LEU:HD11	1.80	0.64
1:A:66:GLU:HA	1:A:92:LEU:HD11	1.80	0.63
1:C:66:GLU:HA	1:C:92:LEU:HD11	1.80	0.63
1:D:66:GLU:HA	1:D:92:LEU:HD11	1.80	0.63
1:E:215:GLN:O	1:E:219:MET:HG2	1.99	0.63
1:A:448:THR:OG1	1:A:450:ASP:OD1	2.17	0.63
1:B:215:GLN:O	1:B:219:MET:HG2	1.99	0.63
1:A:215:GLN:O	1:A:219:MET:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:GLN:O	1:F:219:MET:HG2	1.99	0.63
1:F:63:LYS:NZ	1:F:200:GLU:O	2.28	0.63
1:B:448:THR:OG1	1:B:450:ASP:OD1	2.17	0.63
1:D:215:GLN:O	1:D:219:MET:HG2	1.99	0.63
1:B:66:GLU:HA	1:B:92:LEU:HD11	1.80	0.62
1:C:448:THR:OG1	1:C:450:ASP:OD1	2.17	0.62
1:E:377:ARG:HB2	1:E:411:LEU:HD11	1.81	0.62
1:F:597:ALA:HA	1:F:601:ILE:HD11	1.81	0.62
1:B:377:ARG:HB2	1:B:411:LEU:HD11	1.81	0.62
1:E:225:ARG:NH1	1:F:432:LEU:O	2.32	0.62
1:E:604:ILE:O	1:E:608:MET:HG3	1.99	0.62
1:F:377:ARG:HB2	1:F:411:LEU:HD11	1.80	0.62
1:F:604:ILE:O	1:F:608:MET:HG3	1.99	0.62
1:C:215:GLN:O	1:C:219:MET:HG2	1.99	0.62
1:C:377:ARG:HB2	1:C:411:LEU:HD11	1.81	0.62
1:A:597:ALA:HA	1:A:601:ILE:HD11	1.81	0.62
1:B:642:LEU:HD13	1:B:762:LEU:HD23	1.82	0.62
1:C:604:ILE:O	1:C:608:MET:HG3	1.99	0.62
1:A:377:ARG:HB2	1:A:411:LEU:HD11	1.80	0.62
1:A:642:LEU:HD13	1:A:762:LEU:HD23	1.82	0.62
1:C:642:LEU:HD13	1:C:762:LEU:HD23	1.82	0.62
1:D:377:ARG:HB2	1:D:411:LEU:HD11	1.80	0.61
1:D:597:ALA:HA	1:D:601:ILE:HD11	1.81	0.61
1:B:604:ILE:O	1:B:608:MET:HG3	1.99	0.61
1:D:604:ILE:O	1:D:608:MET:HG3	1.99	0.61
1:F:642:LEU:HD13	1:F:762:LEU:HD23	1.82	0.61
1:E:597:ALA:HA	1:E:601:ILE:HD11	1.81	0.61
1:C:597:ALA:HA	1:C:601:ILE:HD11	1.81	0.61
1:A:604:ILE:O	1:A:608:MET:HG3	1.99	0.61
1:F:448:THR:OG1	1:F:450:ASP:OD1	2.17	0.60
1:B:597:ALA:HA	1:B:601:ILE:HD11	1.81	0.60
1:D:642:LEU:HD13	1:D:762:LEU:HD23	1.82	0.60
1:E:642:LEU:HD13	1:E:762:LEU:HD23	1.82	0.60
1:E:448:THR:OG1	1:E:450:ASP:OD1	2.17	0.60
1:B:508:MET:HG3	1:C:695:CYS:SG	2.42	0.60
1:A:63:LYS:NZ	1:A:200:GLU:O	2.28	0.59
1:B:66:GLU:CA	1:B:92:LEU:HD11	2.33	0.59
1:A:225:ARG:NH1	1:B:432:LEU:O	2.36	0.59
1:A:65:ARG:CB	1:A:92:LEU:CD2	2.48	0.59
1:A:66:GLU:CA	1:A:92:LEU:HD11	2.33	0.59
1:E:61:GLY:H	1:E:92:LEU:HD13	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLU:CA	1:C:92:LEU:HD11	2.33	0.59
1:D:66:GLU:CA	1:D:92:LEU:HD11	2.33	0.58
1:B:275:MET:HE1	1:B:321:GLU:HG3	1.85	0.58
1:C:65:ARG:O	1:C:92:LEU:HD21	2.03	0.58
1:E:66:GLU:CA	1:E:92:LEU:HD11	2.33	0.58
1:A:275:MET:HE1	1:A:321:GLU:HG3	1.85	0.58
1:A:590:ILE:HD11	1:B:591:GLY:HA2	1.86	0.58
1:D:448:THR:OG1	1:D:450:ASP:OD1	2.17	0.58
1:E:65:ARG:CB	1:E:92:LEU:CD2	2.48	0.58
1:F:66:GLU:CA	1:F:92:LEU:HD11	2.33	0.58
1:D:65:ARG:O	1:D:92:LEU:HD21	2.04	0.58
1:F:472:PRO:O	1:F:533:ASN:ND2	2.34	0.58
1:D:275:MET:HE1	1:D:321:GLU:HG3	1.85	0.58
1:D:590:ILE:HD11	1:E:591:GLY:HA2	1.84	0.58
1:E:275:MET:HE1	1:E:321:GLU:HG3	1.85	0.58
1:E:390:LEU:HB3	1:E:394:VAL:HG21	1.86	0.58
1:F:390:LEU:HB3	1:F:394:VAL:HG21	1.86	0.58
1:F:624:ASN:O	1:F:755:TYR:OH	2.20	0.58
1:D:61:GLY:H	1:D:92:LEU:HD13	1.68	0.58
1:E:65:ARG:O	1:E:92:LEU:HD21	2.04	0.58
1:B:65:ARG:O	1:B:92:LEU:HD21	2.04	0.58
1:D:390:LEU:HB3	1:D:394:VAL:HG21	1.86	0.58
1:A:65:ARG:O	1:A:92:LEU:HD21	2.04	0.57
1:A:322:ARG:NH1	1:B:317:HIS:HB3	2.13	0.57
1:F:61:GLY:H	1:F:92:LEU:HD13	1.68	0.57
1:A:390:LEU:HB3	1:A:394:VAL:HG21	1.86	0.57
1:D:63:LYS:NZ	1:D:200:GLU:O	2.28	0.57
1:A:114:ILE:HD11	1:A:167:GLU:O	2.04	0.57
1:B:35:ASP:N	1:B:35:ASP:OD1	2.37	0.57
1:B:61:GLY:H	1:B:92:LEU:HD13	1.68	0.57
1:C:61:GLY:H	1:C:92:LEU:HD13	1.68	0.57
1:C:390:LEU:HB3	1:C:394:VAL:HG21	1.86	0.57
1:E:377:ARG:NH1	1:E:403:THR:O	2.38	0.57
1:F:275:MET:HE1	1:F:321:GLU:HG3	1.86	0.57
1:B:60:LYS:HD3	1:B:66:GLU:HB3	1.87	0.57
1:D:377:ARG:NH1	1:D:403:THR:O	2.38	0.57
1:F:65:ARG:O	1:F:92:LEU:HD21	2.03	0.57
1:F:377:ARG:NH1	1:F:403:THR:O	2.38	0.57
1:B:390:LEU:HB3	1:B:394:VAL:HG21	1.86	0.57
1:F:35:ASP:OD1	1:F:35:ASP:N	2.37	0.57
1:B:206:ILE:HD13	1:B:253:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LYS:HD3	1:F:66:GLU:HB3	1.87	0.57
1:A:61:GLY:H	1:A:92:LEU:HD13	1.68	0.56
1:C:206:ILE:HD13	1:C:253:LEU:HD23	1.87	0.56
1:B:63:LYS:NZ	1:B:200:GLU:O	2.28	0.56
1:B:561:GLU:OE1	1:B:561:GLU:N	2.31	0.56
1:C:60:LYS:HD3	1:C:66:GLU:HB3	1.87	0.56
1:C:275:MET:HE1	1:C:321:GLU:HG3	1.85	0.56
1:E:35:ASP:OD1	1:E:35:ASP:N	2.37	0.56
1:A:206:ILE:HD13	1:A:253:LEU:HD23	1.87	0.56
1:D:35:ASP:N	1:D:35:ASP:OD1	2.37	0.56
1:E:60:LYS:HD3	1:E:66:GLU:HB3	1.87	0.56
1:B:252:THR:OG1	2:B:901:AGS:O1B	2.24	0.56
1:B:472:PRO:O	1:B:533:ASN:ND2	2.34	0.56
1:C:65:ARG:O	1:C:92:LEU:CD2	2.54	0.56
1:C:377:ARG:NH1	1:C:403:THR:O	2.38	0.56
1:A:65:ARG:O	1:A:92:LEU:CD2	2.54	0.56
1:A:113:ARG:HD2	1:A:178:PRO:HA	1.88	0.56
1:C:113:ARG:HD2	1:C:178:PRO:HA	1.88	0.56
1:B:624:ASN:O	1:B:755:TYR:OH	2.20	0.56
1:F:65:ARG:O	1:F:92:LEU:CD2	2.54	0.56
1:A:35:ASP:OD1	1:A:35:ASP:N	2.37	0.56
1:A:60:LYS:HD3	1:A:66:GLU:HB3	1.87	0.56
1:B:113:ARG:HD2	1:B:178:PRO:HA	1.88	0.56
1:D:113:ARG:HD2	1:D:178:PRO:HA	1.88	0.56
1:F:206:ILE:HD13	1:F:253:LEU:HD23	1.87	0.56
1:A:377:ARG:NH1	1:A:403:THR:O	2.38	0.56
1:A:591:GLY:HA2	1:F:590:ILE:HD11	1.88	0.56
1:C:252:THR:OG1	2:C:901:AGS:O1B	2.24	0.56
1:F:117:LEU:HB2	1:F:163:PHE:CE1	2.42	0.56
1:E:113:ARG:HD2	1:E:178:PRO:HA	1.88	0.55
1:F:113:ARG:HD2	1:F:178:PRO:HA	1.88	0.55
1:D:65:ARG:O	1:D:92:LEU:CD2	2.54	0.55
1:D:246:PRO:HD2	1:D:249:THR:HG21	1.88	0.55
1:E:65:ARG:O	1:E:92:LEU:CD2	2.54	0.55
1:E:130:LEU:O	1:E:134:TYR:OH	2.21	0.55
1:C:590:ILE:HD11	1:D:591:GLY:HA2	1.86	0.55
1:D:206:ILE:HD13	1:D:253:LEU:HD23	1.87	0.55
1:A:117:LEU:HB2	1:A:163:PHE:CE1	2.42	0.55
1:A:252:THR:OG1	2:A:901:AGS:O1B	2.24	0.55
1:B:65:ARG:O	1:B:92:LEU:CD2	2.54	0.55
1:C:63:LYS:NZ	1:C:200:GLU:O	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:HB2	1:E:163:PHE:CE1	2.42	0.55
1:B:377:ARG:NH1	1:B:403:THR:O	2.38	0.55
1:C:35:ASP:OD1	1:C:35:ASP:N	2.37	0.55
1:C:472:PRO:O	1:C:533:ASN:ND2	2.34	0.55
1:E:561:GLU:OE1	1:E:561:GLU:N	2.32	0.55
1:E:624:ASN:O	1:E:755:TYR:OH	2.20	0.55
1:A:114:ILE:HG12	1:A:167:GLU:HB2	1.88	0.55
1:E:206:ILE:HD13	1:E:253:LEU:HD23	1.87	0.55
1:C:117:LEU:HB2	1:C:163:PHE:CE1	2.42	0.55
1:B:65:ARG:CB	1:B:92:LEU:CD2	2.48	0.55
1:B:586:ARG:HH11	1:B:592:ASP:HB3	1.72	0.55
1:D:252:THR:OG1	2:D:901:AGS:O1B	2.24	0.55
1:F:252:THR:OG1	2:F:901:AGS:O1B	2.24	0.55
1:C:624:ASN:O	1:C:755:TYR:OH	2.20	0.55
1:F:155:HIS:O	1:F:159:ARG:NH1	2.40	0.55
1:D:60:LYS:HD3	1:D:66:GLU:HB3	1.87	0.54
1:D:155:HIS:O	1:D:159:ARG:NH1	2.40	0.54
1:E:155:HIS:O	1:E:159:ARG:NH1	2.40	0.54
1:E:246:PRO:HD2	1:E:249:THR:HG21	1.88	0.54
1:A:472:PRO:O	1:A:533:ASN:ND2	2.34	0.54
1:D:117:LEU:HB2	1:D:163:PHE:CE1	2.42	0.54
1:D:586:ARG:HH11	1:D:592:ASP:HB3	1.72	0.54
1:B:155:HIS:O	1:B:159:ARG:NH1	2.40	0.54
1:C:586:ARG:HH11	1:C:592:ASP:HB3	1.72	0.54
1:E:252:THR:OG1	2:E:901:AGS:O1B	2.24	0.54
1:F:246:PRO:HD2	1:F:249:THR:HG21	1.88	0.54
1:A:695:CYS:SG	1:F:508:MET:HG3	2.47	0.54
1:B:246:PRO:HD2	1:B:249:THR:HG21	1.88	0.54
1:C:155:HIS:O	1:C:159:ARG:NH1	2.40	0.54
1:E:586:ARG:HH11	1:E:592:ASP:HB3	1.73	0.54
1:A:246:PRO:HD2	1:A:249:THR:HG21	1.88	0.54
1:B:117:LEU:HB2	1:B:163:PHE:CE1	2.42	0.54
1:C:454:TRP:O	1:C:457:SER:OG	2.22	0.54
1:D:130:LEU:O	1:D:134:TYR:OH	2.21	0.54
1:D:624:ASN:O	1:D:755:TYR:OH	2.20	0.54
1:F:586:ARG:HH11	1:F:592:ASP:HB3	1.73	0.54
1:A:624:ASN:O	1:A:755:TYR:OH	2.20	0.54
1:A:586:ARG:HH11	1:A:592:ASP:HB3	1.72	0.54
1:A:155:HIS:O	1:A:159:ARG:NH1	2.40	0.54
1:C:336:LYS:HB2	1:C:338:ARG:CZ	2.38	0.54
1:C:246:PRO:HD2	1:C:249:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:LEU:O	1:F:134:TYR:OH	2.21	0.54
1:B:336:LYS:HB2	1:B:338:ARG:CZ	2.38	0.53
1:D:454:TRP:O	1:D:457:SER:OG	2.22	0.53
1:D:494:GLN:HG2	1:D:498:GLU:OE2	2.09	0.53
1:E:336:LYS:HB2	1:E:338:ARG:CZ	2.38	0.53
1:F:336:LYS:HB2	1:F:338:ARG:CZ	2.38	0.53
1:E:494:GLN:HG2	1:E:498:GLU:OE2	2.09	0.53
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.91	0.53
1:A:336:LYS:HB2	1:A:338:ARG:CZ	2.38	0.53
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.91	0.53
1:C:494:GLN:HG2	1:C:498:GLU:OE2	2.09	0.53
1:D:336:LYS:HB2	1:D:338:ARG:CZ	2.38	0.53
1:C:65:ARG:CB	1:C:92:LEU:CD2	2.48	0.53
1:E:63:LYS:NZ	1:E:200:GLU:O	2.28	0.53
1:E:472:PRO:O	1:E:533:ASN:ND2	2.34	0.53
1:A:494:GLN:HG2	1:A:498:GLU:OE2	2.09	0.52
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.91	0.52
1:F:494:GLN:HG2	1:F:498:GLU:OE2	2.09	0.52
1:A:454:TRP:O	1:A:457:SER:OG	2.22	0.52
1:C:508:MET:HG3	1:D:695:CYS:SG	2.50	0.52
1:B:494:GLN:HG2	1:B:498:GLU:OE2	2.09	0.52
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.91	0.52
1:B:438:ASP:OD1	1:B:438:ASP:N	2.42	0.52
1:E:68:VAL:HG11	1:E:145:PRO:HG2	1.92	0.52
1:F:68:VAL:HG11	1:F:145:PRO:HG2	1.92	0.52
1:A:561:GLU:OE1	1:A:561:GLU:N	2.31	0.52
1:D:472:PRO:O	1:D:533:ASN:ND2	2.34	0.52
1:E:438:ASP:N	1:E:438:ASP:OD1	2.42	0.52
1:A:640:ASP:N	1:A:640:ASP:OD1	2.43	0.52
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.91	0.51
1:C:482:LEU:HD21	1:C:645:ILE:HG23	1.92	0.51
1:D:640:ASP:OD1	1:D:640:ASP:N	2.43	0.51
1:B:482:LEU:HD21	1:B:645:ILE:HG23	1.93	0.51
1:C:640:ASP:OD1	1:C:640:ASP:N	2.43	0.51
1:F:310:ALA:HA	1:F:325:VAL:HG22	1.91	0.51
1:A:489:LEU:HD11	1:A:516:PHE:HZ	1.76	0.51
1:A:606:THR:HG23	1:B:546:GLU:HG2	1.92	0.51
1:B:489:LEU:HD11	1:B:516:PHE:HZ	1.76	0.51
1:A:701:GLU:OE1	1:A:735:HIS:NE2	2.37	0.51
1:D:561:GLU:OE1	1:D:561:GLU:N	2.32	0.51
1:A:68:VAL:HG11	1:A:145:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:VAL:HG11	1:D:145:PRO:HG2	1.92	0.51
1:D:482:LEU:HD21	1:D:645:ILE:HG23	1.93	0.51
1:F:438:ASP:OD1	1:F:438:ASP:N	2.42	0.51
1:A:438:ASP:OD1	1:A:438:ASP:N	2.42	0.51
1:E:242:LEU:HD11	1:E:347:THR:HG22	1.93	0.51
1:E:640:ASP:OD1	1:E:640:ASP:N	2.43	0.51
1:F:489:LEU:HD11	1:F:516:PHE:HZ	1.76	0.51
1:D:508:MET:HG3	1:E:695:CYS:SG	2.51	0.51
1:E:454:TRP:O	1:E:457:SER:OG	2.22	0.51
1:E:482:LEU:HD21	1:E:645:ILE:HG23	1.93	0.51
1:F:640:ASP:N	1:F:640:ASP:OD1	2.43	0.51
1:E:590:ILE:HD11	1:F:591:GLY:HA2	1.92	0.50
1:A:57:VAL:HG23	1:A:104:PRO:HA	1.94	0.50
1:C:606:THR:HG23	1:D:546:GLU:HG2	1.92	0.50
1:B:57:VAL:HG23	1:B:104:PRO:HA	1.94	0.50
1:E:489:LEU:HD11	1:E:516:PHE:HZ	1.76	0.50
1:A:482:LEU:HD21	1:A:645:ILE:HG23	1.93	0.50
1:C:489:LEU:HD11	1:C:516:PHE:HZ	1.76	0.50
1:D:66:GLU:N	1:D:92:LEU:HD11	2.26	0.50
1:A:69:CYS:SG	1:A:70:ILE:N	2.84	0.50
1:B:68:VAL:HG11	1:B:145:PRO:HG2	1.92	0.50
1:F:242:LEU:HD11	1:F:347:THR:HG22	1.93	0.50
1:F:454:TRP:O	1:F:457:SER:OG	2.22	0.50
1:F:482:LEU:HD21	1:F:645:ILE:HG23	1.92	0.50
1:C:68:VAL:HG11	1:C:145:PRO:HG2	1.92	0.50
1:C:57:VAL:HG23	1:C:104:PRO:HA	1.94	0.50
1:E:322:ARG:NH1	1:F:317:HIS:HB3	2.20	0.50
1:F:57:VAL:HG23	1:F:104:PRO:HA	1.94	0.50
1:E:69:CYS:SG	1:E:70:ILE:N	2.84	0.50
1:D:242:LEU:HD11	1:D:347:THR:HG22	1.93	0.49
1:C:69:CYS:SG	1:C:70:ILE:N	2.84	0.49
1:D:140:LEU:O	1:D:141:GLU:HG3	2.13	0.49
1:E:140:LEU:O	1:E:141:GLU:HG3	2.12	0.49
1:A:114:ILE:HD12	1:A:146:ILE:CD1	2.42	0.49
1:C:66:GLU:N	1:C:92:LEU:HD11	2.26	0.49
1:C:140:LEU:O	1:C:141:GLU:HG3	2.12	0.49
1:E:57:VAL:HG23	1:E:104:PRO:HA	1.94	0.49
1:E:508:MET:HG3	1:F:695:CYS:SG	2.51	0.49
1:F:140:LEU:O	1:F:141:GLU:HG3	2.13	0.49
1:B:242:LEU:HD11	1:B:347:THR:HG22	1.93	0.49
1:D:57:VAL:HG23	1:D:104:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:GLU:HG3	1:E:324:ILE:HD13	1.95	0.49
1:D:69:CYS:SG	1:D:70:ILE:N	2.84	0.49
1:E:606:THR:HG23	1:F:546:GLU:HG2	1.93	0.49
1:A:242:LEU:HD11	1:A:347:THR:HG22	1.93	0.49
1:B:640:ASP:OD1	1:B:640:ASP:N	2.43	0.49
1:C:242:LEU:HD11	1:C:347:THR:HG22	1.93	0.49
1:F:69:CYS:SG	1:F:70:ILE:N	2.84	0.49
1:F:283:GLU:HG3	1:F:324:ILE:HD13	1.95	0.49
1:A:140:LEU:O	1:A:141:GLU:HG3	2.12	0.49
1:C:438:ASP:N	1:C:438:ASP:OD1	2.42	0.49
1:C:701:GLU:OE1	1:C:735:HIS:NE2	2.37	0.49
1:D:489:LEU:HD11	1:D:516:PHE:HZ	1.76	0.49
1:E:66:GLU:N	1:E:92:LEU:HD11	2.26	0.49
1:B:66:GLU:N	1:B:92:LEU:HD11	2.26	0.49
1:C:39:VAL:H	1:C:73:SER:HG	1.58	0.49
1:D:283:GLU:HG3	1:D:324:ILE:HD13	1.95	0.49
1:D:571:PRO:HB3	1:D:616:ASN:HB3	1.95	0.49
1:F:539:PHE:CE2	1:F:541:SER:HB2	2.48	0.49
1:F:701:GLU:OE1	1:F:735:HIS:NE2	2.37	0.49
1:C:571:PRO:HB3	1:C:616:ASN:HB3	1.95	0.49
1:E:571:PRO:HB3	1:E:616:ASN:HB3	1.95	0.49
1:E:539:PHE:CE2	1:E:541:SER:HB2	2.48	0.48
1:A:587:GLY:HA3	1:A:591:GLY:HA3	1.96	0.48
1:B:140:LEU:O	1:B:141:GLU:HG3	2.12	0.48
1:F:561:GLU:OE1	1:F:561:GLU:N	2.31	0.48
1:B:571:PRO:HB3	1:B:616:ASN:HB3	1.95	0.48
1:B:587:GLY:HA3	1:B:591:GLY:HA3	1.96	0.48
1:F:571:PRO:HB3	1:F:616:ASN:HB3	1.95	0.48
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.54	0.48
1:A:539:PHE:CE2	1:A:541:SER:HB2	2.48	0.48
1:B:69:CYS:SG	1:B:70:ILE:N	2.84	0.48
1:B:763:GLN:NE2	1:C:744:ARG:HB3	2.29	0.48
1:D:587:GLY:HA3	1:D:591:GLY:HA3	1.96	0.48
1:E:587:GLY:HA3	1:E:591:GLY:HA3	1.96	0.48
1:A:283:GLU:HG3	1:A:324:ILE:HD13	1.95	0.48
1:A:571:PRO:HB3	1:A:616:ASN:HB3	1.95	0.48
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.54	0.48
1:C:283:GLU:HG3	1:C:324:ILE:HD13	1.95	0.48
1:F:587:GLY:HA3	1:F:591:GLY:HA3	1.96	0.48
1:B:283:GLU:HG3	1:B:324:ILE:HD13	1.95	0.48
1:D:539:PHE:CE2	1:D:541:SER:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:HG2	1:F:606:THR:HG23	1.95	0.47
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.54	0.47
1:C:587:GLY:HA3	1:C:591:GLY:HA3	1.96	0.47
1:F:66:GLU:N	1:F:92:LEU:HD11	2.26	0.47
1:A:66:GLU:N	1:A:92:LEU:HD11	2.26	0.47
1:D:606:THR:HG23	1:E:546:GLU:HG2	1.96	0.47
1:D:630:ASP:OD1	1:D:630:ASP:N	2.48	0.47
1:B:586:ARG:HH21	1:B:599:ARG:HH22	1.62	0.47
1:D:438:ASP:OD1	1:D:438:ASP:N	2.42	0.47
1:D:701:GLU:OE1	1:D:735:HIS:NE2	2.37	0.47
1:E:586:ARG:HH21	1:E:599:ARG:HH22	1.62	0.47
1:F:586:ARG:HH21	1:F:599:ARG:HH22	1.63	0.47
1:B:539:PHE:CE2	1:B:541:SER:HB2	2.49	0.47
1:D:65:ARG:CB	1:D:92:LEU:CD2	2.48	0.47
1:A:586:ARG:HH21	1:A:599:ARG:HH22	1.63	0.47
1:C:130:LEU:O	1:C:134:TYR:OH	2.21	0.47
1:C:586:ARG:HH21	1:C:599:ARG:HH22	1.63	0.47
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.54	0.47
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.54	0.47
1:F:501:ASP:OD1	1:F:501:ASP:N	2.47	0.47
1:A:700:ARG:NE	1:F:491:GLU:OE2	2.48	0.47
1:C:19:GLN:HB2	1:C:25:ARG:NH2	2.30	0.47
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.54	0.47
1:C:539:PHE:CE2	1:C:541:SER:HB2	2.48	0.47
1:A:744:ARG:HB3	1:F:763:GLN:NE2	2.30	0.47
1:D:586:ARG:HH21	1:D:599:ARG:HH22	1.62	0.47
1:E:701:GLU:OE1	1:E:735:HIS:NE2	2.37	0.46
1:E:740:MET:HE3	1:E:740:MET:O	2.15	0.46
1:B:701:GLU:OE1	1:B:735:HIS:NE2	2.38	0.46
1:C:561:GLU:OE1	1:C:561:GLU:N	2.31	0.46
1:D:501:ASP:OD1	1:D:501:ASP:N	2.47	0.46
1:B:319:GLU:OE2	1:B:322:ARG:NH1	2.43	0.46
1:B:501:ASP:N	1:B:501:ASP:OD1	2.47	0.46
1:B:590:ILE:HD11	1:C:591:GLY:HA2	1.98	0.46
1:C:319:GLU:OE2	1:C:322:ARG:NH1	2.43	0.46
1:D:19:GLN:HB2	1:D:25:ARG:NH2	2.30	0.46
1:F:740:MET:HE3	1:F:740:MET:O	2.15	0.46
1:C:675:LEU:HD21	1:C:736:PHE:HB3	1.98	0.46
1:A:427:MET:HE1	1:F:16:ILE:HD12	1.97	0.46
1:A:675:LEU:HD21	1:A:736:PHE:HB3	1.98	0.46
1:C:631:PRO:HA	1:C:634:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:PRO:HA	1:D:634:LEU:HD23	1.98	0.46
1:B:19:GLN:HB2	1:B:25:ARG:NH2	2.30	0.46
1:D:740:MET:HE3	1:D:740:MET:O	2.15	0.46
1:E:488:GLU:O	1:E:492:LEU:HG	2.16	0.46
1:F:19:GLN:HB2	1:F:25:ARG:NH2	2.30	0.46
1:F:488:GLU:O	1:F:492:LEU:HG	2.16	0.46
1:A:567:ARG:HH21	1:A:611:MET:HG2	1.81	0.46
1:B:44:PRO:O	1:B:48:GLU:HG2	2.16	0.46
1:B:488:GLU:O	1:B:492:LEU:HG	2.16	0.46
1:B:675:LEU:HD21	1:B:736:PHE:HB3	1.98	0.46
1:F:44:PRO:O	1:F:48:GLU:HG2	2.16	0.46
1:F:65:ARG:CB	1:F:92:LEU:CD2	2.48	0.46
1:F:675:LEU:HD21	1:F:736:PHE:HB3	1.98	0.46
1:A:114:ILE:HD12	1:A:146:ILE:HD12	1.98	0.46
1:A:333:ASP:OD2	1:A:362:ARG:NH2	2.48	0.46
1:B:255:ALA:HB2	1:B:302:PHE:CZ	2.51	0.46
1:C:488:GLU:O	1:C:492:LEU:HG	2.16	0.46
1:A:653:ARG:HG2	1:A:687:LEU:HD11	1.98	0.46
1:E:19:GLN:HB2	1:E:25:ARG:NH2	2.30	0.46
1:A:19:GLN:HB2	1:A:25:ARG:NH2	2.30	0.45
1:A:631:PRO:HA	1:A:634:LEU:HD23	1.98	0.45
1:B:631:PRO:HA	1:B:634:LEU:HD23	1.98	0.45
1:B:653:ARG:HG2	1:B:687:LEU:HD11	1.98	0.45
1:C:255:ALA:HB2	1:C:302:PHE:CZ	2.51	0.45
1:D:255:ALA:HB2	1:D:302:PHE:CZ	2.51	0.45
1:D:488:GLU:O	1:D:492:LEU:HG	2.16	0.45
1:D:675:LEU:HD21	1:D:736:PHE:HB3	1.98	0.45
1:E:44:PRO:O	1:E:48:GLU:HG2	2.16	0.45
1:E:403:THR:HG23	1:E:456:LEU:HD21	1.98	0.45
1:E:631:PRO:HA	1:E:634:LEU:HD23	1.98	0.45
1:B:567:ARG:HH21	1:B:611:MET:HG2	1.81	0.45
1:F:567:ARG:HH21	1:F:611:MET:HG2	1.81	0.45
1:A:255:ALA:HB2	1:A:302:PHE:CZ	2.51	0.45
1:E:675:LEU:HD21	1:E:736:PHE:HB3	1.98	0.45
1:F:403:THR:HG23	1:F:456:LEU:HD21	1.98	0.45
1:F:631:PRO:HA	1:F:634:LEU:HD23	1.98	0.45
1:A:488:GLU:O	1:A:492:LEU:HG	2.16	0.45
1:A:740:MET:HE3	1:A:740:MET:O	2.15	0.45
1:C:501:ASP:OD1	1:C:501:ASP:N	2.47	0.45
1:C:653:ARG:HG2	1:C:687:LEU:HD11	1.98	0.45
1:C:740:MET:HE3	1:C:740:MET:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:HD2	1:D:64:ARG:N	2.32	0.45
1:A:61:GLY:N	1:A:92:LEU:HD13	2.32	0.45
1:A:64:ARG:N	1:A:64:ARG:HD2	2.32	0.45
1:B:740:MET:O	1:B:740:MET:HE3	2.15	0.45
1:C:403:THR:HG23	1:C:456:LEU:HD21	1.98	0.45
1:C:485:VAL:HG13	1:C:643:ILE:HG21	1.98	0.45
1:D:44:PRO:O	1:D:48:GLU:HG2	2.16	0.45
1:E:501:ASP:N	1:E:501:ASP:OD1	2.47	0.45
1:E:653:ARG:HG2	1:E:687:LEU:HD11	1.99	0.45
1:F:485:VAL:HG13	1:F:643:ILE:HG21	1.98	0.45
1:B:61:GLY:N	1:B:92:LEU:HD13	2.32	0.45
1:B:64:ARG:HD2	1:B:64:ARG:N	2.31	0.45
1:C:44:PRO:O	1:C:48:GLU:HG2	2.16	0.45
1:C:64:ARG:N	1:C:64:ARG:HD2	2.32	0.45
1:C:630:ASP:N	1:C:630:ASP:OD1	2.48	0.45
1:F:255:ALA:HB2	1:F:302:PHE:CZ	2.51	0.45
1:A:485:VAL:HG13	1:A:643:ILE:HG21	1.98	0.45
1:C:16:ILE:HD12	1:D:427:MET:HE1	1.99	0.45
1:C:218:GLU:CD	1:D:424:ARG:HH21	2.24	0.45
1:E:255:ALA:HB2	1:E:302:PHE:CZ	2.51	0.45
1:E:561:GLU:O	1:E:565:LYS:HB2	2.17	0.45
1:F:64:ARG:HD2	1:F:64:ARG:N	2.31	0.45
1:F:630:ASP:N	1:F:630:ASP:OD1	2.48	0.45
1:D:485:VAL:HG13	1:D:643:ILE:HG21	1.98	0.45
1:D:653:ARG:HG2	1:D:687:LEU:HD11	1.98	0.45
1:E:567:ARG:HH21	1:E:611:MET:HG2	1.81	0.45
1:B:630:ASP:OD1	1:B:630:ASP:N	2.48	0.45
1:C:567:ARG:HH21	1:C:611:MET:HG2	1.81	0.45
1:F:561:GLU:O	1:F:565:LYS:HB2	2.17	0.45
1:B:39:VAL:H	1:B:73:SER:HG	1.61	0.45
1:C:679:THR:HB	1:C:682:PHE:CG	2.52	0.45
1:B:403:THR:HG23	1:B:456:LEU:HD21	1.98	0.44
1:C:491:GLU:OE2	1:D:700:ARG:NE	2.48	0.44
1:D:403:THR:HG23	1:D:456:LEU:HD21	1.98	0.44
1:D:561:GLU:O	1:D:565:LYS:HB2	2.17	0.44
1:D:567:ARG:HH21	1:D:611:MET:HG2	1.81	0.44
1:E:491:GLU:OE2	1:F:700:ARG:NE	2.51	0.44
1:F:61:GLY:N	1:F:92:LEU:HD13	2.32	0.44
1:F:653:ARG:HG2	1:F:687:LEU:HD11	1.98	0.44
1:A:44:PRO:O	1:A:48:GLU:HG2	2.16	0.44
1:A:561:GLU:O	1:A:565:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ASP:N	1:A:630:ASP:OD1	2.48	0.44
1:C:61:GLY:N	1:C:92:LEU:HD13	2.32	0.44
1:D:679:THR:HB	1:D:682:PHE:CG	2.52	0.44
1:E:64:ARG:HD2	1:E:64:ARG:N	2.32	0.44
1:E:333:ASP:OD2	1:E:362:ARG:NH2	2.48	0.44
1:F:319:GLU:OE2	1:F:322:ARG:NH1	2.43	0.44
1:C:609:ASP:OD1	1:C:635:ARG:NH2	2.50	0.44
1:B:333:ASP:OD2	1:B:362:ARG:NH2	2.48	0.44
1:C:29:ASP:OD1	1:C:29:ASP:N	2.51	0.44
1:C:561:GLU:O	1:C:565:LYS:HB2	2.17	0.44
1:D:26:LEU:HD11	1:D:82:ILE:H	1.83	0.44
1:F:609:ASP:OD1	1:F:635:ARG:NH2	2.50	0.44
1:A:112:LYS:NZ	1:A:113:ARG:O	2.40	0.44
1:B:485:VAL:HG13	1:B:643:ILE:HG21	1.98	0.44
1:B:531:ILE:HD12	1:B:531:ILE:HA	1.86	0.44
1:B:609:ASP:OD1	1:B:635:ARG:NH2	2.50	0.44
1:D:593:GLY:HA3	1:E:592:ASP:HB2	1.99	0.44
1:D:609:ASP:OD1	1:D:635:ARG:NH2	2.50	0.44
1:E:485:VAL:HG13	1:E:643:ILE:HG21	1.98	0.44
1:C:120:ASP:OD1	1:C:120:ASP:N	2.51	0.44
1:E:218:GLU:CD	1:F:424:ARG:HH21	2.25	0.44
1:B:26:LEU:HD11	1:B:82:ILE:H	1.83	0.44
1:B:299:ALA:HB3	1:B:341:VAL:HG22	2.00	0.44
1:E:39:VAL:H	1:E:73:SER:HG	1.59	0.44
1:E:630:ASP:OD1	1:E:630:ASP:N	2.48	0.44
1:A:299:ALA:HB3	1:A:341:VAL:HG22	2.00	0.43
1:A:319:GLU:OE2	1:A:322:ARG:NH1	2.43	0.43
1:A:424:ARG:HH21	1:F:218:GLU:CD	2.26	0.43
1:B:120:ASP:N	1:B:120:ASP:OD1	2.51	0.43
1:B:373:ASP:OD1	1:B:373:ASP:N	2.51	0.43
1:B:561:GLU:O	1:B:565:LYS:HB2	2.17	0.43
1:F:299:ALA:HB3	1:F:341:VAL:HG22	2.00	0.43
1:A:501:ASP:OD1	1:A:501:ASP:N	2.47	0.43
1:B:336:LYS:HB2	1:B:338:ARG:NH1	2.33	0.43
1:E:679:THR:HB	1:E:682:PHE:CG	2.52	0.43
1:A:679:THR:HB	1:A:682:PHE:CG	2.52	0.43
1:B:679:THR:HB	1:B:682:PHE:CG	2.52	0.43
1:D:170:PRO:HB2	1:D:172:PRO:HD2	2.00	0.43
1:D:319:GLU:OE2	1:D:322:ARG:NH1	2.43	0.43
1:E:609:ASP:OD1	1:E:635:ARG:NH2	2.51	0.43
1:F:333:ASP:OD2	1:F:362:ARG:NH2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:679:THR:HB	1:F:682:PHE:CG	2.52	0.43
1:A:609:ASP:OD1	1:A:635:ARG:NH2	2.50	0.43
1:B:170:PRO:HB2	1:B:172:PRO:HD2	2.01	0.43
1:C:170:PRO:HB2	1:C:172:PRO:HD2	2.01	0.43
1:D:28:VAL:HG23	1:D:83:ARG:HA	2.00	0.43
1:F:244:TYR:CZ	1:F:368:ASP:HB2	2.54	0.43
1:A:170:PRO:HB2	1:A:172:PRO:HD2	2.01	0.43
1:A:336:LYS:HB2	1:A:338:ARG:NH1	2.34	0.43
1:C:28:VAL:HG23	1:C:83:ARG:HA	2.00	0.43
1:C:74:ASP:O	1:C:75:ASP:HB2	2.19	0.43
1:D:39:VAL:H	1:D:73:SER:HG	1.62	0.43
1:D:120:ASP:N	1:D:120:ASP:OD1	2.51	0.43
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.87	0.43
1:A:508:MET:HG3	1:B:695:CYS:SG	2.58	0.43
1:B:244:TYR:CZ	1:B:368:ASP:HB2	2.54	0.43
1:C:336:LYS:HB2	1:C:338:ARG:NH1	2.33	0.43
1:D:333:ASP:OD2	1:D:362:ARG:NH2	2.48	0.43
1:D:476:TRP:CZ3	1:D:486:LYS:HG2	2.54	0.43
1:E:61:GLY:N	1:E:92:LEU:HD13	2.32	0.43
1:E:74:ASP:O	1:E:75:ASP:HB2	2.19	0.43
1:E:170:PRO:HB2	1:E:172:PRO:HD2	2.01	0.43
1:E:299:ALA:HB3	1:E:341:VAL:HG22	2.00	0.43
1:A:26:LEU:HD11	1:A:82:ILE:H	1.83	0.43
1:A:403:THR:HG23	1:A:456:LEU:HD21	1.98	0.43
1:C:373:ASP:OD1	1:C:373:ASP:N	2.51	0.43
1:F:29:ASP:OD1	1:F:29:ASP:N	2.50	0.43
1:F:170:PRO:HB2	1:F:172:PRO:HD2	2.01	0.43
1:C:244:TYR:CZ	1:C:368:ASP:HB2	2.54	0.43
1:D:336:LYS:HB2	1:D:338:ARG:NH1	2.33	0.43
1:E:336:LYS:HB2	1:E:338:ARG:NH1	2.33	0.43
1:E:531:ILE:HD12	1:E:531:ILE:HA	1.86	0.43
1:A:244:TYR:CZ	1:A:368:ASP:HB2	2.54	0.43
1:B:28:VAL:HG23	1:B:83:ARG:HA	2.00	0.43
1:B:569:ALA:O	1:B:572:CYS:HB2	2.19	0.43
1:C:114:ILE:HD13	1:C:167:GLU:HB2	2.01	0.43
1:D:431:ASP:HB2	1:D:434:ASP:HB2	2.01	0.43
1:D:750:ASN:O	1:D:753:ARG:HG2	2.19	0.43
1:E:476:TRP:CZ3	1:E:486:LYS:HG2	2.54	0.43
1:F:74:ASP:O	1:F:75:ASP:HB2	2.18	0.43
1:A:120:ASP:OD1	1:A:120:ASP:N	2.51	0.43
1:A:745:ARG:O	1:F:764:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASP:OD1	1:B:580:ASP:N	2.52	0.43
1:C:333:ASP:OD2	1:C:362:ARG:NH2	2.48	0.43
1:C:431:ASP:HB2	1:C:434:ASP:HB2	2.01	0.43
1:C:750:ASN:O	1:C:753:ARG:HG2	2.19	0.43
1:D:114:ILE:HD13	1:D:167:GLU:HB2	2.01	0.43
1:E:244:TYR:CZ	1:E:368:ASP:HB2	2.54	0.43
1:E:569:ALA:O	1:E:572:CYS:HB2	2.19	0.43
1:F:120:ASP:OD1	1:F:120:ASP:N	2.51	0.43
1:F:237:PRO:HA	1:F:238:PRO:HD3	1.92	0.43
1:F:336:LYS:HB2	1:F:338:ARG:NH1	2.34	0.43
1:C:299:ALA:HB3	1:C:341:VAL:HG22	2.00	0.42
1:C:476:TRP:CZ3	1:C:486:LYS:HG2	2.54	0.42
1:C:550:MET:O	1:C:550:MET:HG2	2.19	0.42
1:E:114:ILE:HD13	1:E:167:GLU:HB2	2.01	0.42
1:F:26:LEU:HD11	1:F:82:ILE:H	1.83	0.42
1:F:569:ALA:O	1:F:572:CYS:HB2	2.19	0.42
1:A:28:VAL:HG23	1:A:83:ARG:HA	2.00	0.42
1:A:569:ALA:O	1:A:572:CYS:HB2	2.19	0.42
1:C:26:LEU:HD11	1:C:82:ILE:H	1.83	0.42
1:C:569:ALA:O	1:C:572:CYS:HB2	2.19	0.42
1:D:61:GLY:N	1:D:92:LEU:HD13	2.32	0.42
1:F:66:GLU:HA	1:F:92:LEU:CD1	2.49	0.42
1:F:112:LYS:HE2	1:F:112:LYS:HB2	1.87	0.42
1:F:114:ILE:HD13	1:F:167:GLU:HB2	2.01	0.42
1:A:74:ASP:O	1:A:75:ASP:HB2	2.19	0.42
1:A:240:GLY:C	1:A:241:ILE:HD12	2.44	0.42
1:F:750:ASN:O	1:F:753:ARG:HG2	2.19	0.42
1:B:240:GLY:C	1:B:241:ILE:HD12	2.45	0.42
1:B:764:GLN:NE2	1:C:745:ARG:O	2.52	0.42
1:D:299:ALA:HB3	1:D:341:VAL:HG22	2.00	0.42
1:E:26:LEU:HD11	1:E:82:ILE:H	1.83	0.42
1:E:120:ASP:OD1	1:E:120:ASP:N	2.51	0.42
1:E:431:ASP:HB2	1:E:434:ASP:HB2	2.01	0.42
1:F:476:TRP:CZ3	1:F:486:LYS:HG2	2.54	0.42
1:B:74:ASP:O	1:B:75:ASP:HB2	2.19	0.42
1:B:240:GLY:HA3	1:B:362:ARG:O	2.20	0.42
1:B:431:ASP:HB2	1:B:434:ASP:HB2	2.01	0.42
1:E:319:GLU:OE2	1:E:322:ARG:NH1	2.43	0.42
1:F:30:GLU:H	1:F:30:GLU:HG3	1.69	0.42
1:F:240:GLY:C	1:F:241:ILE:HD12	2.44	0.42
1:A:550:MET:HG2	1:A:550:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLN:H	1:A:568:GLN:HG2	1.69	0.42
1:C:240:GLY:C	1:C:241:ILE:HD12	2.44	0.42
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.87	0.42
1:D:240:GLY:HA3	1:D:362:ARG:O	2.20	0.42
1:D:244:TYR:CZ	1:D:368:ASP:HB2	2.54	0.42
1:E:66:GLU:HA	1:E:92:LEU:CD1	2.49	0.42
1:E:288:LYS:HA	1:E:288:LYS:HD3	1.87	0.42
1:F:28:VAL:HG23	1:F:83:ARG:HA	2.00	0.42
1:F:627:ASP:OD1	1:F:627:ASP:N	2.53	0.42
1:A:66:GLU:HA	1:A:92:LEU:CD1	2.49	0.42
1:A:240:GLY:HA3	1:A:362:ARG:O	2.20	0.42
1:B:288:LYS:HA	1:B:288:LYS:HD3	1.87	0.42
1:B:476:TRP:CZ3	1:B:486:LYS:HG2	2.54	0.42
1:C:478:ASP:OD1	1:C:662:ARG:NH1	2.53	0.42
1:D:240:GLY:C	1:D:241:ILE:HD12	2.44	0.42
1:E:89:ARG:HD3	1:E:93:ARG:NE	2.34	0.42
1:A:84:MET:N	1:A:84:MET:HE2	2.35	0.42
1:A:282:SER:OG	1:A:324:ILE:HD11	2.20	0.42
1:A:476:TRP:CZ3	1:A:486:LYS:HG2	2.54	0.42
1:A:580:ASP:OD1	1:A:580:ASP:N	2.52	0.42
1:B:30:GLU:H	1:B:30:GLU:HG3	1.69	0.42
1:B:114:ILE:HD13	1:B:167:GLU:HB2	2.01	0.42
1:B:750:ASN:O	1:B:753:ARG:HG2	2.19	0.42
1:E:478:ASP:OD1	1:E:662:ARG:NH1	2.53	0.42
1:E:750:ASN:O	1:E:753:ARG:HG2	2.19	0.42
1:B:89:ARG:HD3	1:B:93:ARG:NE	2.34	0.42
1:C:580:ASP:N	1:C:580:ASP:OD1	2.52	0.42
1:C:627:ASP:OD1	1:C:627:ASP:N	2.53	0.42
1:D:74:ASP:O	1:D:75:ASP:HB2	2.19	0.42
1:D:112:LYS:NZ	1:D:113:ARG:O	2.41	0.42
1:E:28:VAL:HG23	1:E:83:ARG:HA	2.00	0.42
1:F:213:LEU:HD23	1:F:213:LEU:HA	1.87	0.42
1:F:282:SER:OG	1:F:324:ILE:HD11	2.20	0.42
1:F:431:ASP:HB2	1:F:434:ASP:HB2	2.01	0.42
1:F:464:LEU:HD23	1:F:464:LEU:HA	1.95	0.42
1:C:240:GLY:HA3	1:C:362:ARG:O	2.20	0.41
1:D:84:MET:N	1:D:84:MET:HE2	2.35	0.41
1:D:282:SER:OG	1:D:324:ILE:HD11	2.20	0.41
1:E:550:MET:O	1:E:550:MET:HG2	2.19	0.41
1:F:649:ASP:OD1	1:F:649:ASP:N	2.48	0.41
1:A:130:LEU:O	1:A:134:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ASP:HB2	1:A:434:ASP:HB2	2.01	0.41
1:A:750:ASN:O	1:A:753:ARG:HG2	2.19	0.41
1:B:282:SER:OG	1:B:324:ILE:HD11	2.20	0.41
1:C:593:GLY:HA3	1:D:592:ASP:HB2	2.02	0.41
1:D:550:MET:O	1:D:550:MET:HG2	2.19	0.41
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.93	0.41
1:C:89:ARG:HD3	1:C:93:ARG:NE	2.34	0.41
1:D:89:ARG:HD3	1:D:93:ARG:NE	2.35	0.41
1:D:569:ALA:O	1:D:572:CYS:HB2	2.19	0.41
1:E:240:GLY:C	1:E:241:ILE:HD12	2.45	0.41
1:E:240:GLY:HA3	1:E:362:ARG:O	2.20	0.41
1:F:240:GLY:HA3	1:F:362:ARG:O	2.20	0.41
1:A:29:ASP:OD1	1:A:29:ASP:N	2.50	0.41
1:B:586:ARG:HH21	1:B:599:ARG:NH2	2.19	0.41
1:C:565:LYS:HB2	1:C:565:LYS:HE3	1.90	0.41
1:D:478:ASP:OD1	1:D:662:ARG:NH1	2.53	0.41
1:D:586:ARG:HH21	1:D:599:ARG:NH2	2.19	0.41
1:E:656:ILE:O	1:E:660:ASN:ND2	2.48	0.41
1:F:89:ARG:HD3	1:F:93:ARG:NE	2.34	0.41
1:B:656:ILE:O	1:B:660:ASN:ND2	2.48	0.41
1:C:84:MET:N	1:C:84:MET:HE2	2.35	0.41
1:C:763:GLN:NE2	1:D:744:ARG:HB3	2.34	0.41
1:D:580:ASP:OD1	1:D:580:ASP:N	2.52	0.41
1:F:478:ASP:OD1	1:F:662:ARG:NH1	2.53	0.41
1:F:519:PRO:HA	1:F:520:PRO:HD3	1.95	0.41
1:E:84:MET:HE2	1:E:84:MET:N	2.35	0.41
1:F:39:VAL:H	1:F:73:SER:HG	1.61	0.41
1:F:550:MET:HG2	1:F:550:MET:O	2.19	0.41
1:F:580:ASP:N	1:F:580:ASP:OD1	2.52	0.41
1:A:288:LYS:HA	1:A:288:LYS:HD3	1.87	0.41
1:B:66:GLU:HA	1:B:92:LEU:CD1	2.49	0.41
1:D:66:GLU:HA	1:D:92:LEU:CD1	2.49	0.41
1:E:282:SER:OG	1:E:324:ILE:HD11	2.20	0.41
1:F:586:ARG:HH21	1:F:599:ARG:NH2	2.19	0.41
1:F:689:GLU:OE2	1:F:693:ARG:NH2	2.53	0.41
1:C:636:PRO:HD2	2:D:902:AGS:S1G	2.61	0.41
1:F:84:MET:N	1:F:84:MET:HE2	2.35	0.41
1:F:275:MET:CE	1:F:321:GLU:HG3	2.50	0.41
1:F:435:GLU:HG2	1:F:436:THR:HG22	2.03	0.41
1:A:513:GLY:HA2	1:A:619:ILE:O	2.21	0.41
1:A:586:ARG:HH21	1:A:599:ARG:NH2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:O	1:B:134:TYR:OH	2.21	0.41
1:C:213:LEU:HD23	1:C:213:LEU:HA	1.87	0.41
1:C:282:SER:OG	1:C:324:ILE:HD11	2.20	0.41
1:C:513:GLY:HA2	1:C:619:ILE:O	2.21	0.41
1:C:568:GLN:H	1:C:568:GLN:HG2	1.69	0.41
1:E:580:ASP:N	1:E:580:ASP:OD1	2.52	0.41
1:E:586:ARG:HH21	1:E:599:ARG:NH2	2.19	0.41
1:F:531:ILE:HD12	1:F:531:ILE:HA	1.86	0.41
1:A:89:ARG:HD3	1:A:93:ARG:NE	2.35	0.41
1:C:66:GLU:HA	1:C:92:LEU:CD1	2.49	0.41
1:C:438:ASP:O	1:C:441:VAL:HG22	2.21	0.41
1:F:169:ASP:HB2	1:F:170:PRO:HD3	2.03	0.41
1:C:121:ASP:OD1	1:C:161:VAL:HG11	2.21	0.40
1:C:586:ARG:HH21	1:C:599:ARG:NH2	2.19	0.40
1:C:689:GLU:OE2	1:C:693:ARG:NH2	2.53	0.40
1:D:264:ALA:HA	1:D:298:PRO:HB2	2.03	0.40
1:D:438:ASP:O	1:D:441:VAL:HG22	2.22	0.40
1:D:565:LYS:HB2	1:D:565:LYS:HE3	1.90	0.40
1:E:435:GLU:HG2	1:E:436:THR:HG22	2.03	0.40
1:A:478:ASP:OD1	1:A:662:ARG:NH1	2.53	0.40
1:A:689:GLU:OE2	1:A:693:ARG:NH2	2.53	0.40
2:C:901:AGS:O2A	2:C:901:AGS:O2B	2.39	0.40
1:D:275:MET:CE	1:D:321:GLU:HG3	2.50	0.40
2:D:901:AGS:O2A	2:D:901:AGS:O2B	2.39	0.40
1:E:438:ASP:O	1:E:441:VAL:HG22	2.22	0.40
1:F:373:ASP:OD1	1:F:373:ASP:N	2.51	0.40
1:A:435:GLU:HG2	1:A:436:THR:HG22	2.03	0.40
1:A:767:GLY:O	1:B:625:ARG:HD2	2.21	0.40
1:B:590:ILE:HG23	1:B:591:GLY:N	2.37	0.40
1:C:590:ILE:HG23	1:C:591:GLY:N	2.37	0.40
1:E:264:ALA:HA	1:E:298:PRO:HB2	2.03	0.40
2:E:901:AGS:O2B	2:E:901:AGS:O2A	2.39	0.40
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.93	0.40
1:C:169:ASP:HB2	1:C:170:PRO:HD3	2.03	0.40
1:D:237:PRO:HA	1:D:238:PRO:HD3	1.92	0.40
1:D:373:ASP:OD1	1:D:373:ASP:N	2.51	0.40
1:E:16:ILE:HD12	1:F:427:MET:HE1	2.03	0.40
1:F:513:GLY:HA2	1:F:619:ILE:O	2.21	0.40
1:A:264:ALA:HA	1:A:298:PRO:HB2	2.03	0.40
1:B:84:MET:N	1:B:84:MET:HE2	2.35	0.40
1:B:121:ASP:OD1	1:B:161:VAL:HG11	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ASP:O	1:B:441:VAL:HG22	2.22	0.40
1:B:568:GLN:H	1:B:568:GLN:HG2	1.69	0.40
1:C:89:ARG:HD3	1:C:93:ARG:HE	1.87	0.40
1:D:135:LEU:HD23	1:D:135:LEU:HA	1.93	0.40
1:E:121:ASP:OD1	1:E:161:VAL:HG11	2.22	0.40
1:F:121:ASP:OD1	1:F:161:VAL:HG11	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/821 (89%)	686 (94%)	47 (6%)	0	100	100
1	B	733/821 (89%)	689 (94%)	44 (6%)	0	100	100
1	C	733/821 (89%)	688 (94%)	45 (6%)	0	100	100
1	D	733/821 (89%)	688 (94%)	45 (6%)	0	100	100
1	E	733/821 (89%)	688 (94%)	45 (6%)	0	100	100
1	F	733/821 (89%)	688 (94%)	45 (6%)	0	100	100
All	All	4398/4926 (89%)	4127 (94%)	271 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	626/691 (91%)	626 (100%)	0	100	100
1	B	626/691 (91%)	626 (100%)	0	100	100
1	C	626/691 (91%)	626 (100%)	0	100	100
1	D	626/691 (91%)	626 (100%)	0	100	100
1	E	626/691 (91%)	626 (100%)	0	100	100
1	F	626/691 (91%)	626 (100%)	0	100	100
All	All	3756/4146 (91%)	3756 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	A	398	GLN
1	A	443	ASN
1	A	499	HIS
1	A	602	ASN
1	B	260	ASN
1	B	285	ASN
1	B	398	GLN
1	B	443	ASN
1	B	499	HIS
1	C	260	ASN
1	C	285	ASN
1	C	398	GLN
1	C	443	ASN
1	C	499	HIS
1	C	602	ASN
1	D	260	ASN
1	D	285	ASN
1	D	398	GLN
1	D	499	HIS
1	D	602	ASN
1	E	285	ASN
1	E	398	GLN
1	E	499	HIS
1	E	602	ASN
1	F	260	ASN
1	F	285	ASN
1	F	398	GLN

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Mol	Chain	Res	Type
1	F	443	ASN
1	F	499	HIS

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 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
2	AGS	A	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	F	902	3	32,33,33	0.49	1 (3%)	45,52,52	0.68	1 (2%)
2	AGS	C	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	F	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	B	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	C	902	3	32,33,33	0.50	1 (3%)	45,52,52	0.68	1 (2%)
2	AGS	D	902	3	32,33,33	0.49	1 (3%)	45,52,52	0.68	1 (2%)
2	AGS	B	902	3	32,33,33	0.50	1 (3%)	45,52,52	0.68	1 (2%)
2	AGS	E	902	3	32,33,33	0.50	1 (3%)	45,52,52	0.68	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	D	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	E	901	3	32,33,33	0.51	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	A	902	3	32,33,33	0.50	1 (3%)	45,52,52	0.68	1 (2%)

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
2	AGS	A	901	3	-	7/21/38/38	0/3/3/3
2	AGS	F	902	3	-	3/21/38/38	0/3/3/3
2	AGS	C	901	3	-	7/21/38/38	0/3/3/3
2	AGS	F	901	3	-	7/21/38/38	0/3/3/3
2	AGS	B	901	3	-	7/21/38/38	0/3/3/3
2	AGS	C	902	3	-	3/21/38/38	0/3/3/3
2	AGS	D	902	3	-	3/21/38/38	0/3/3/3
2	AGS	B	902	3	-	3/21/38/38	0/3/3/3
2	AGS	E	902	3	-	3/21/38/38	0/3/3/3
2	AGS	D	901	3	-	7/21/38/38	0/3/3/3
2	AGS	E	901	3	-	7/21/38/38	0/3/3/3
2	AGS	A	902	3	-	3/21/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	AGS	PG-S1G	2.09	1.95	1.90
2	B	902	AGS	PG-S1G	2.09	1.95	1.90
2	A	902	AGS	PG-S1G	2.07	1.95	1.90
2	D	901	AGS	PG-S1G	2.07	1.95	1.90
2	A	901	AGS	PG-S1G	2.06	1.95	1.90
2	C	902	AGS	PG-S1G	2.06	1.95	1.90
2	D	902	AGS	PG-S1G	2.06	1.95	1.90
2	E	902	AGS	PG-S1G	2.06	1.95	1.90
2	B	901	AGS	PG-S1G	2.05	1.95	1.90
2	F	902	AGS	PG-S1G	2.05	1.95	1.90
2	C	901	AGS	PG-S1G	2.05	1.95	1.90
2	F	901	AGS	PG-S1G	2.03	1.95	1.90

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	AGS	PB-O3B-PG	-3.82	119.17	133.17
2	C	901	AGS	PB-O3B-PG	-3.82	119.18	133.17
2	A	901	AGS	PB-O3B-PG	-3.82	119.19	133.17
2	E	901	AGS	PB-O3B-PG	-3.81	119.22	133.17
2	F	901	AGS	PB-O3B-PG	-3.81	119.22	133.17
2	B	901	AGS	PB-O3B-PG	-3.80	119.25	133.17
2	E	902	AGS	PB-O3B-PG	-3.76	119.40	133.17
2	A	902	AGS	PB-O3B-PG	-3.76	119.41	133.17
2	D	902	AGS	PB-O3B-PG	-3.76	119.42	133.17
2	B	902	AGS	PB-O3B-PG	-3.76	119.43	133.17
2	F	902	AGS	PB-O3B-PG	-3.75	119.44	133.17
2	C	902	AGS	PB-O3B-PG	-3.74	119.47	133.17

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	AGS	C5'-O5'-PA-O1A
2	A	901	AGS	C5'-O5'-PA-O2A
2	A	901	AGS	C5'-O5'-PA-O3A
2	B	901	AGS	C5'-O5'-PA-O1A
2	B	901	AGS	C5'-O5'-PA-O2A
2	B	901	AGS	C5'-O5'-PA-O3A
2	C	901	AGS	C5'-O5'-PA-O1A
2	C	901	AGS	C5'-O5'-PA-O2A
2	C	901	AGS	C5'-O5'-PA-O3A
2	D	901	AGS	C5'-O5'-PA-O1A
2	D	901	AGS	C5'-O5'-PA-O2A
2	D	901	AGS	C5'-O5'-PA-O3A
2	E	901	AGS	C5'-O5'-PA-O1A
2	E	901	AGS	C5'-O5'-PA-O2A
2	E	901	AGS	C5'-O5'-PA-O3A
2	F	901	AGS	C5'-O5'-PA-O1A
2	F	901	AGS	C5'-O5'-PA-O2A
2	F	901	AGS	C5'-O5'-PA-O3A
2	A	901	AGS	O4'-C4'-C5'-O5'
2	B	901	AGS	O4'-C4'-C5'-O5'
2	C	901	AGS	O4'-C4'-C5'-O5'
2	D	901	AGS	O4'-C4'-C5'-O5'
2	E	901	AGS	O4'-C4'-C5'-O5'
2	F	901	AGS	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	901	AGS	PA-O3A-PB-O2B
2	A	902	AGS	PA-O3A-PB-O1B
2	B	901	AGS	PA-O3A-PB-O2B
2	B	902	AGS	PA-O3A-PB-O1B
2	C	901	AGS	PA-O3A-PB-O2B
2	C	902	AGS	PA-O3A-PB-O1B
2	D	901	AGS	PA-O3A-PB-O2B
2	D	902	AGS	PA-O3A-PB-O1B
2	E	901	AGS	PA-O3A-PB-O2B
2	E	902	AGS	PA-O3A-PB-O1B
2	F	901	AGS	PA-O3A-PB-O2B
2	F	902	AGS	PA-O3A-PB-O1B
2	A	901	AGS	C3'-C4'-C5'-O5'
2	B	901	AGS	C3'-C4'-C5'-O5'
2	C	901	AGS	C3'-C4'-C5'-O5'
2	D	901	AGS	C3'-C4'-C5'-O5'
2	E	901	AGS	C3'-C4'-C5'-O5'
2	F	901	AGS	C3'-C4'-C5'-O5'
2	A	902	AGS	PB-O3B-PG-O3G
2	B	902	AGS	PB-O3B-PG-O3G
2	C	902	AGS	PB-O3B-PG-O3G
2	D	902	AGS	PB-O3B-PG-O3G
2	E	902	AGS	PB-O3B-PG-O3G
2	F	902	AGS	PB-O3B-PG-O3G
2	A	901	AGS	PA-O3A-PB-O1B
2	B	901	AGS	PA-O3A-PB-O1B
2	C	901	AGS	PA-O3A-PB-O1B
2	D	901	AGS	PA-O3A-PB-O1B
2	E	901	AGS	PA-O3A-PB-O1B
2	F	901	AGS	PA-O3A-PB-O1B
2	A	902	AGS	PA-O3A-PB-O2B
2	B	902	AGS	PA-O3A-PB-O2B
2	C	902	AGS	PA-O3A-PB-O2B
2	D	902	AGS	PA-O3A-PB-O2B
2	E	902	AGS	PA-O3A-PB-O2B
2	F	902	AGS	PA-O3A-PB-O2B

There are no ring outliers.

7 monomers are involved in 16 short contacts:

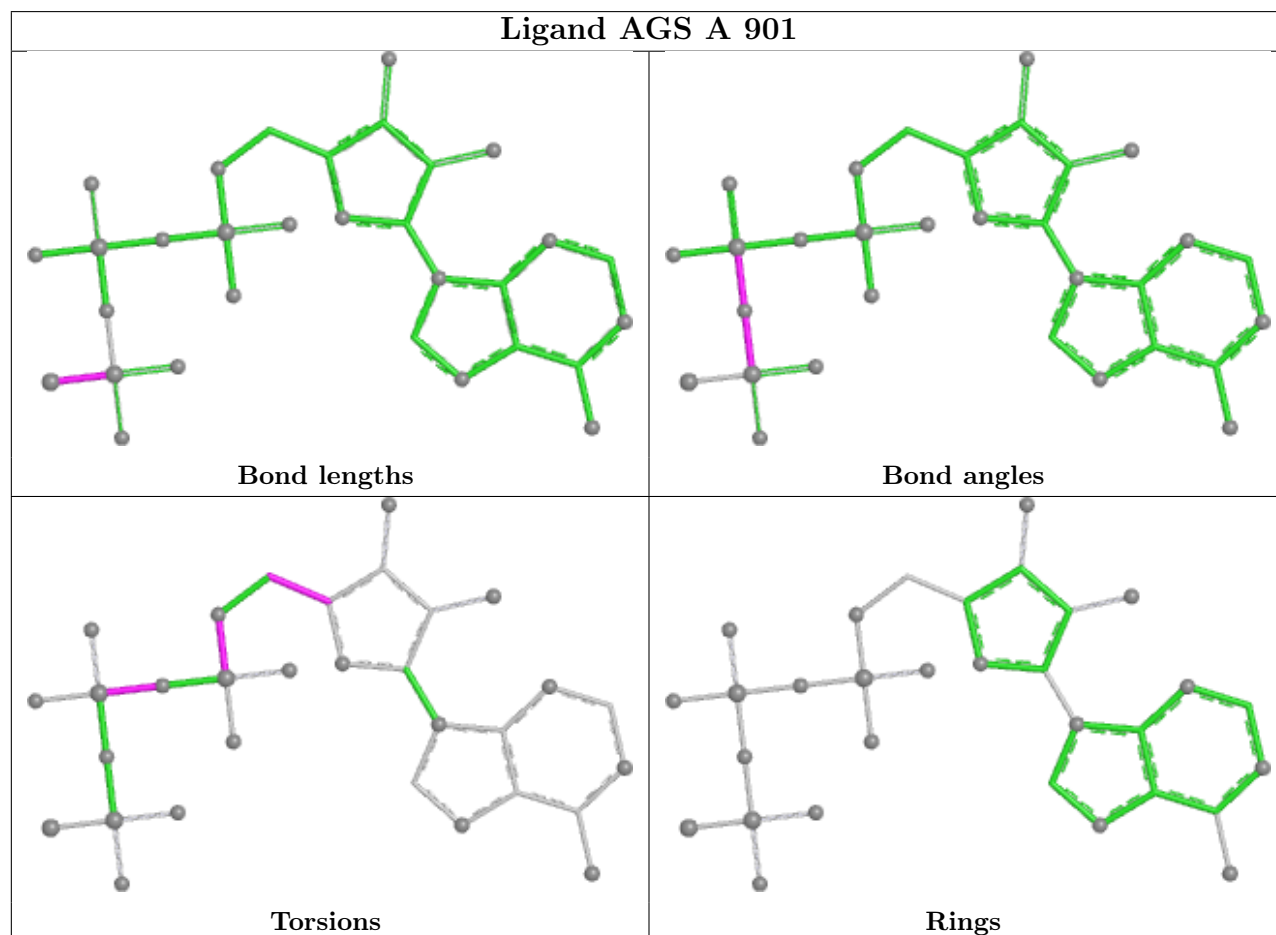
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	2	0

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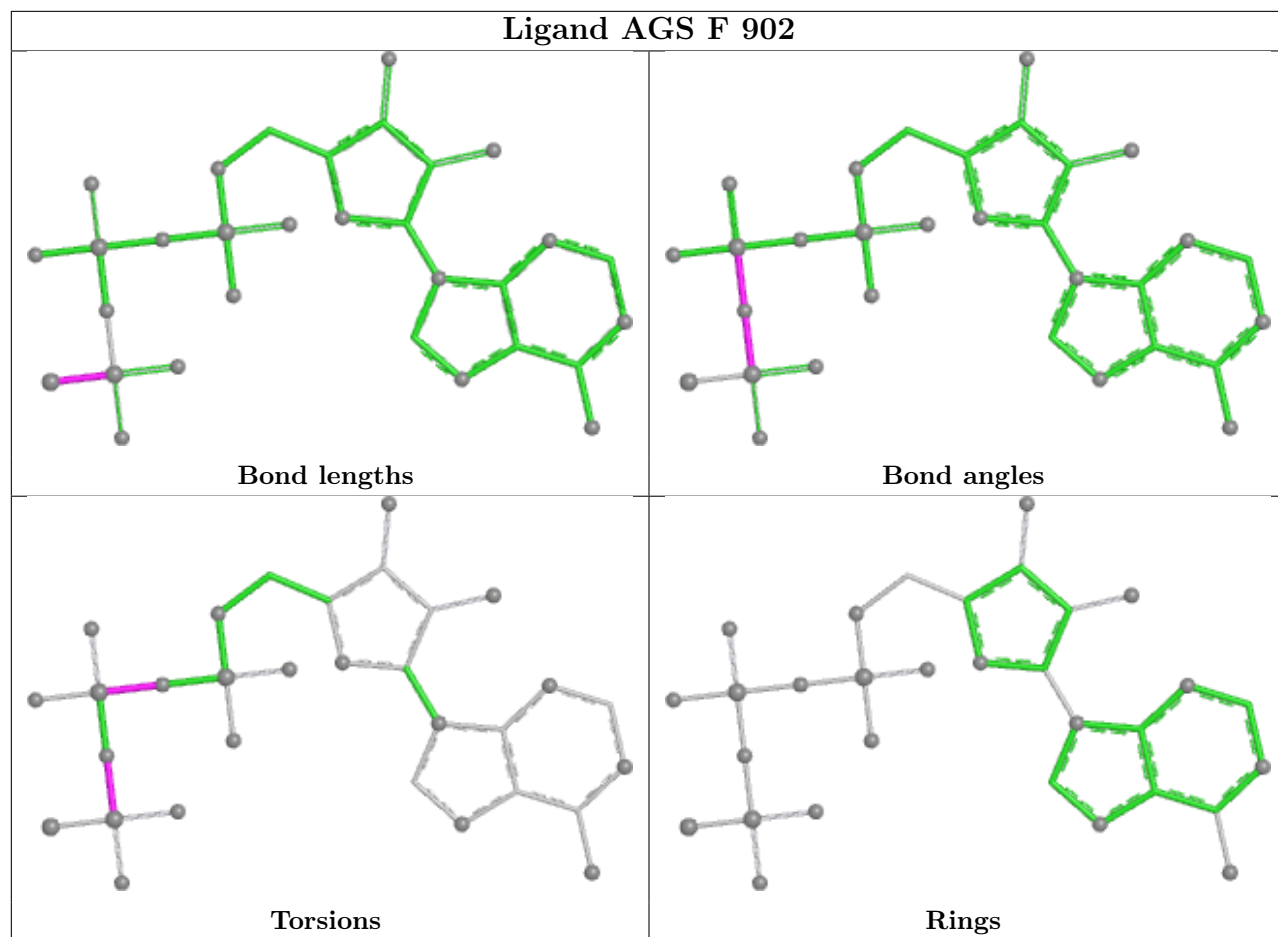
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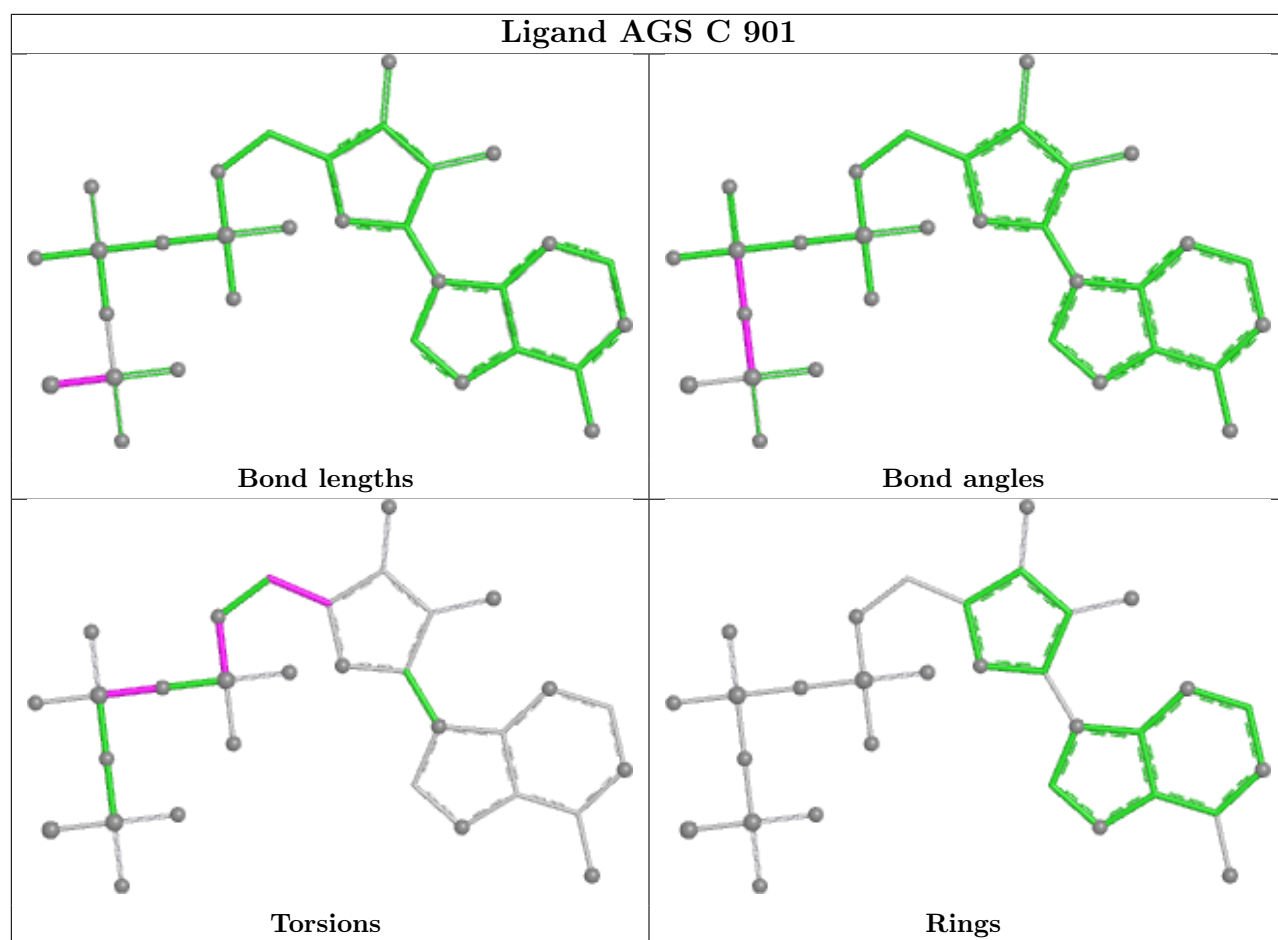
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	AGS	3	0
2	F	901	AGS	2	0
2	B	901	AGS	2	0
2	D	902	AGS	1	0
2	D	901	AGS	3	0
2	E	901	AGS	3	0

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

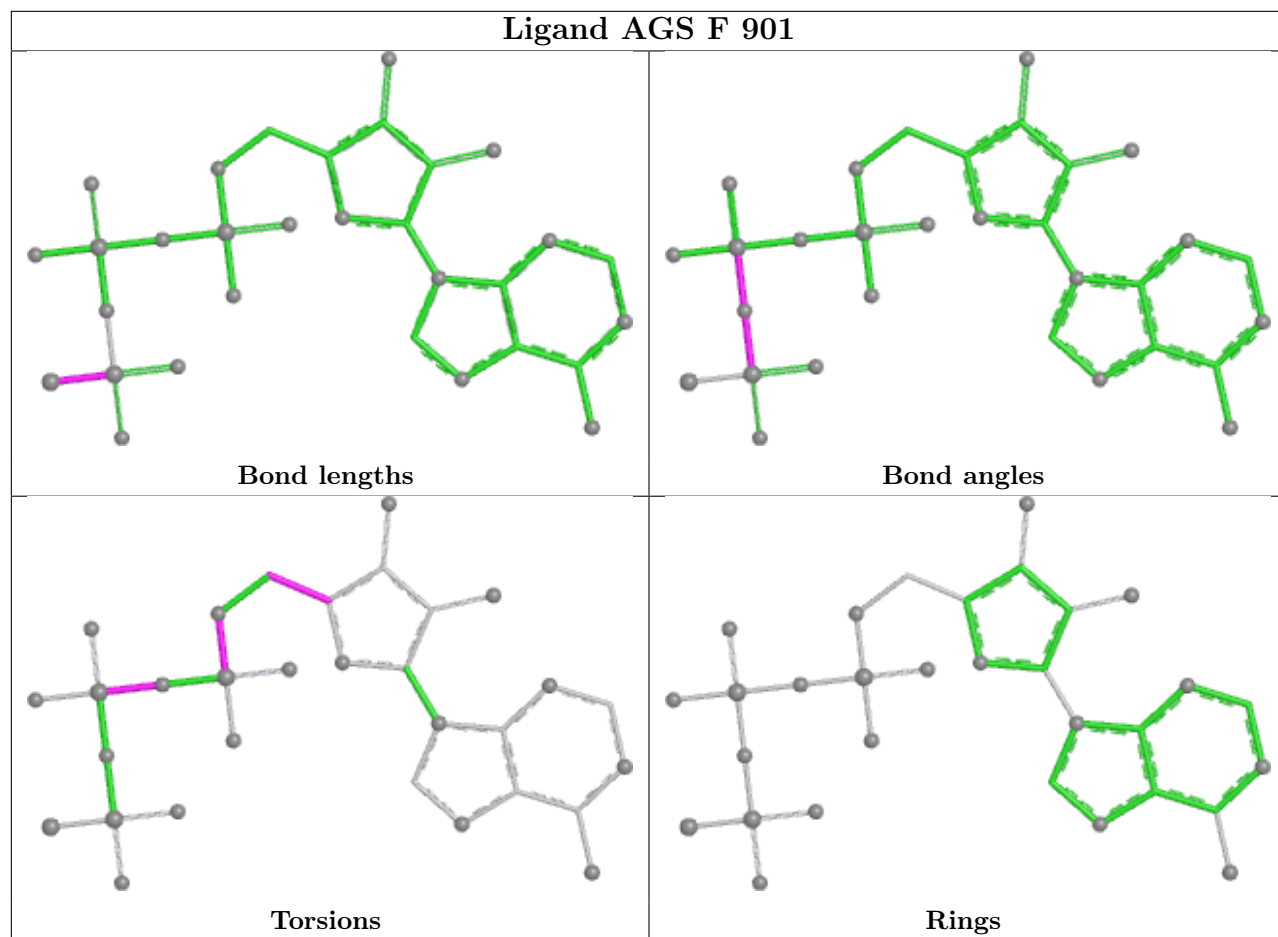


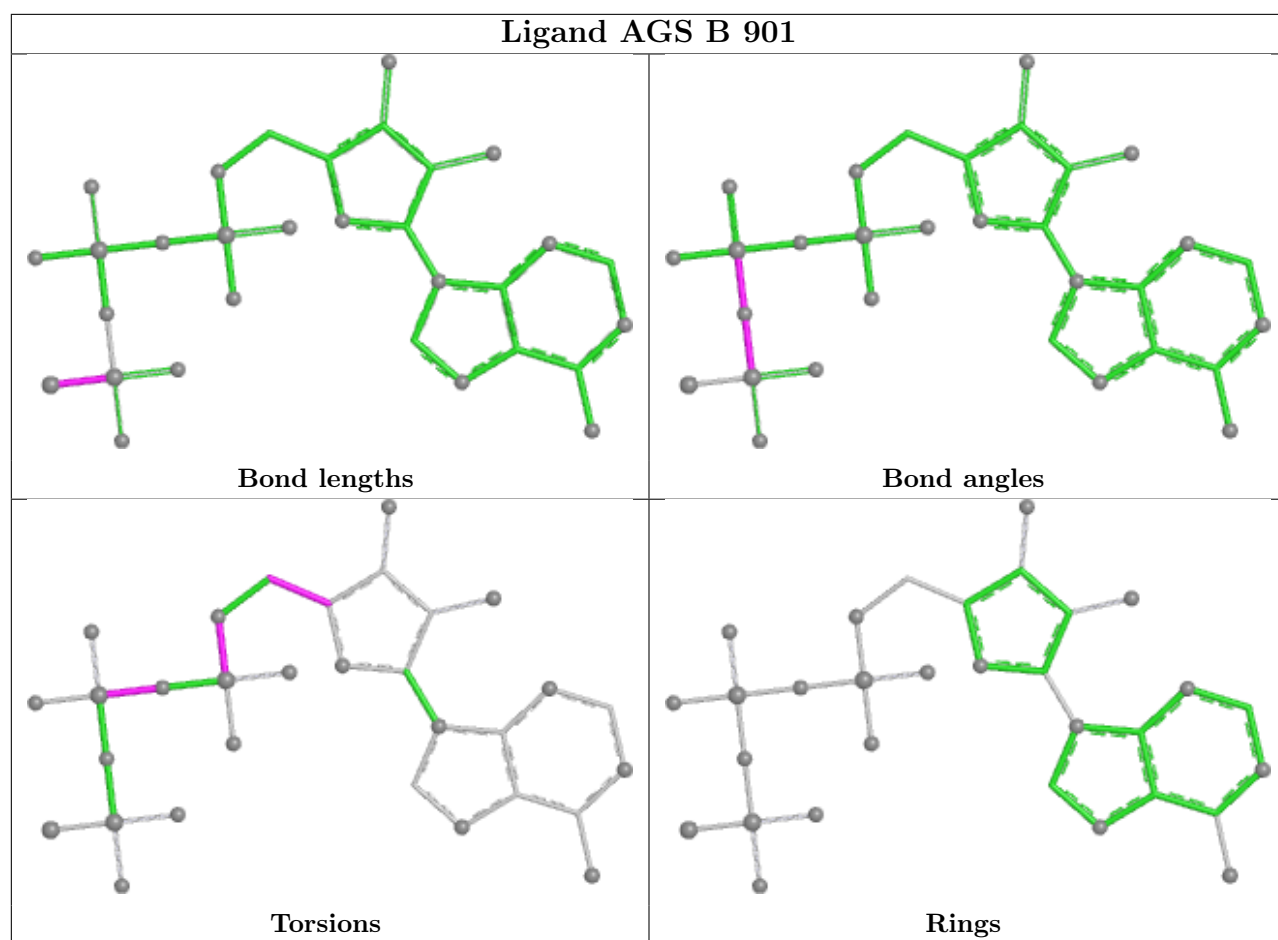
Ligand AGS F 902

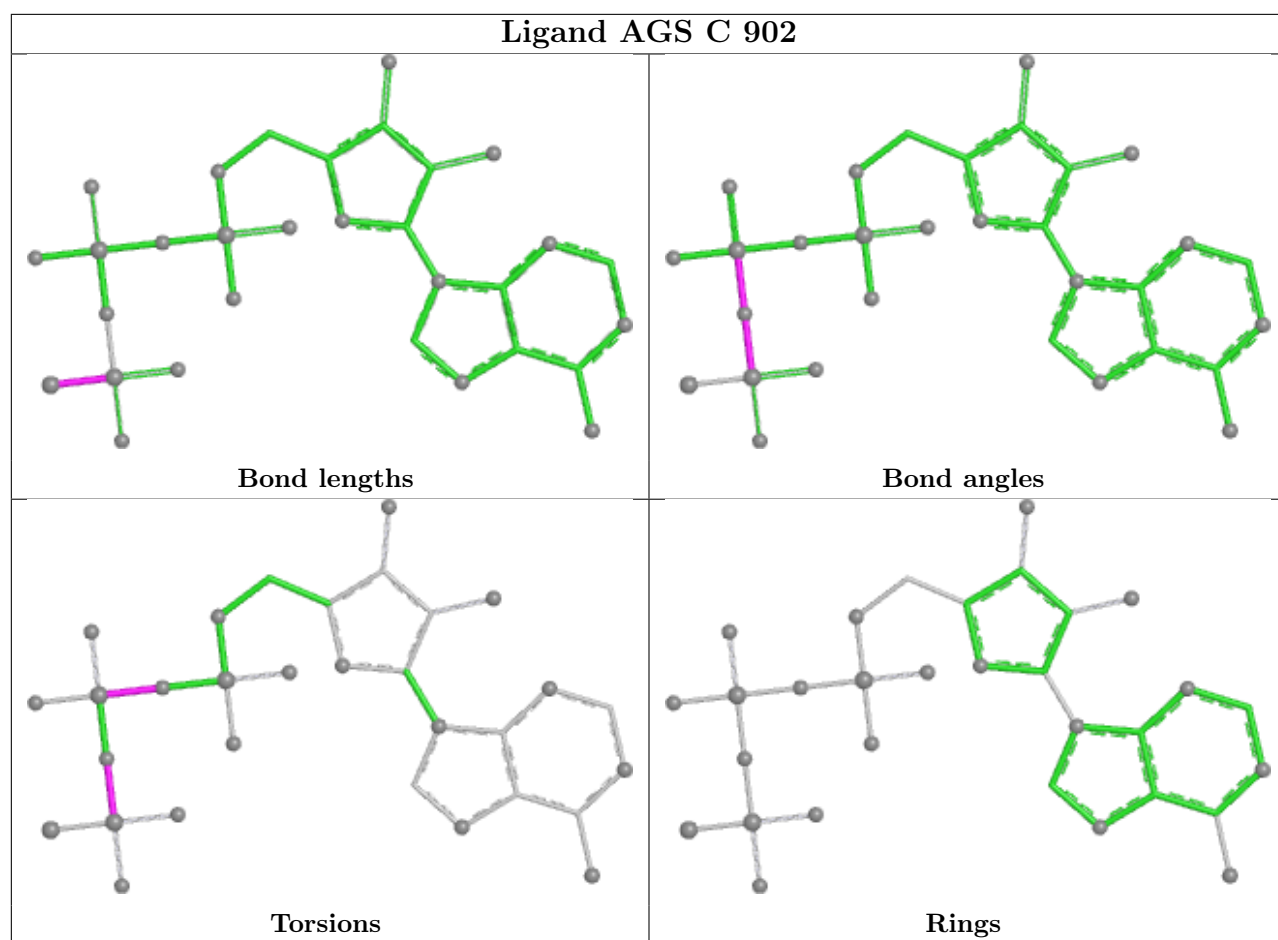


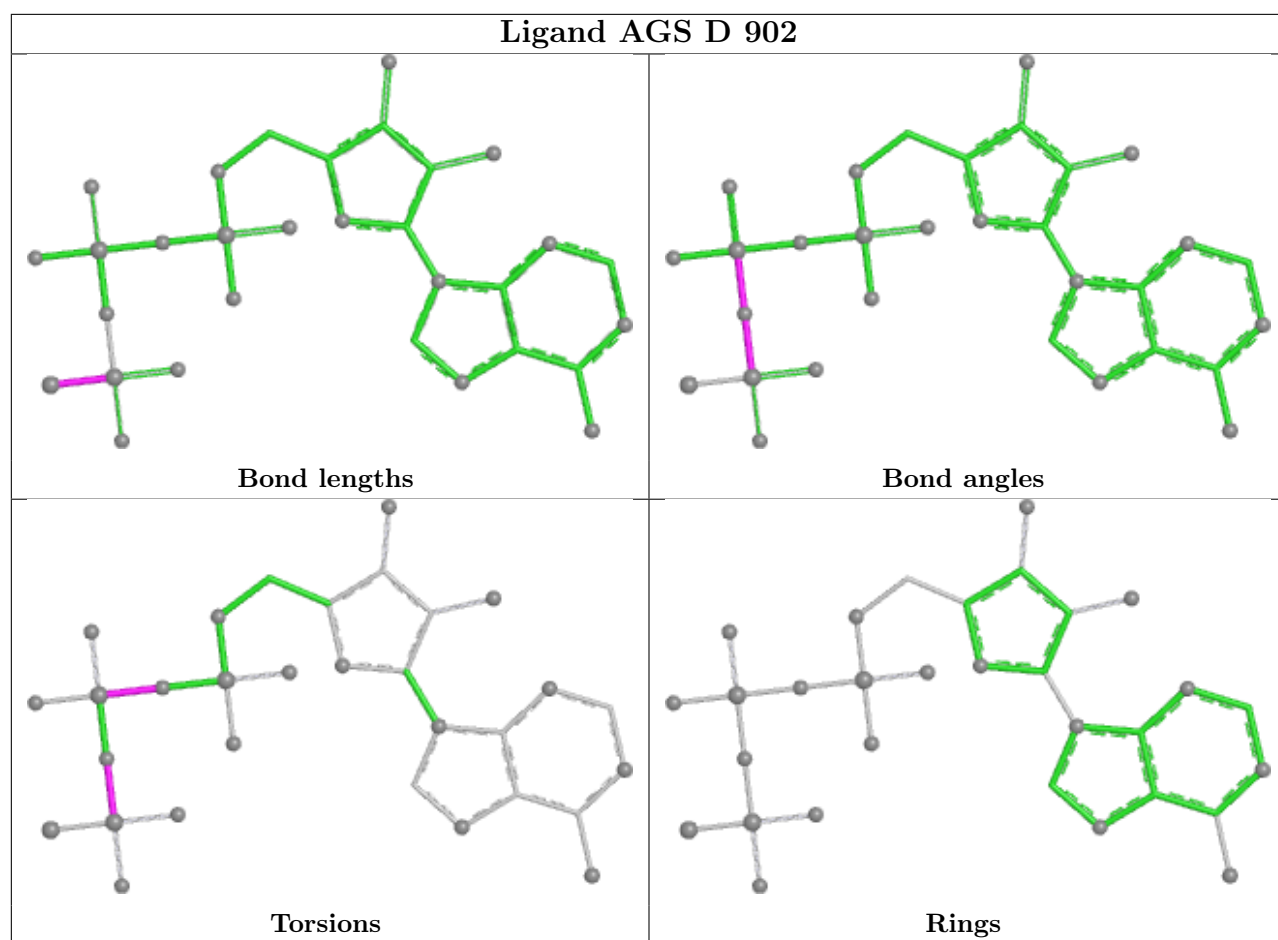


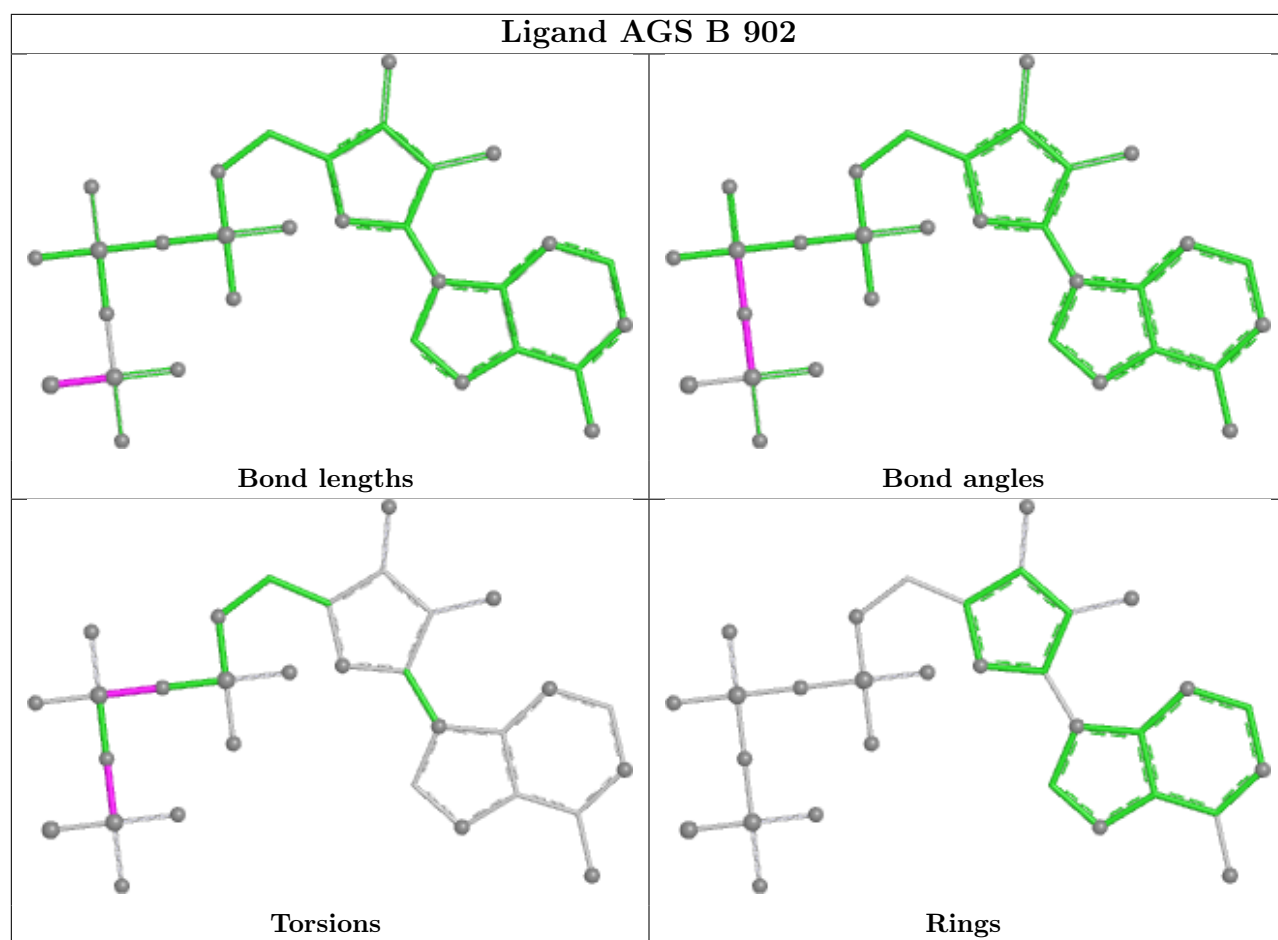
Ligand AGS F 901

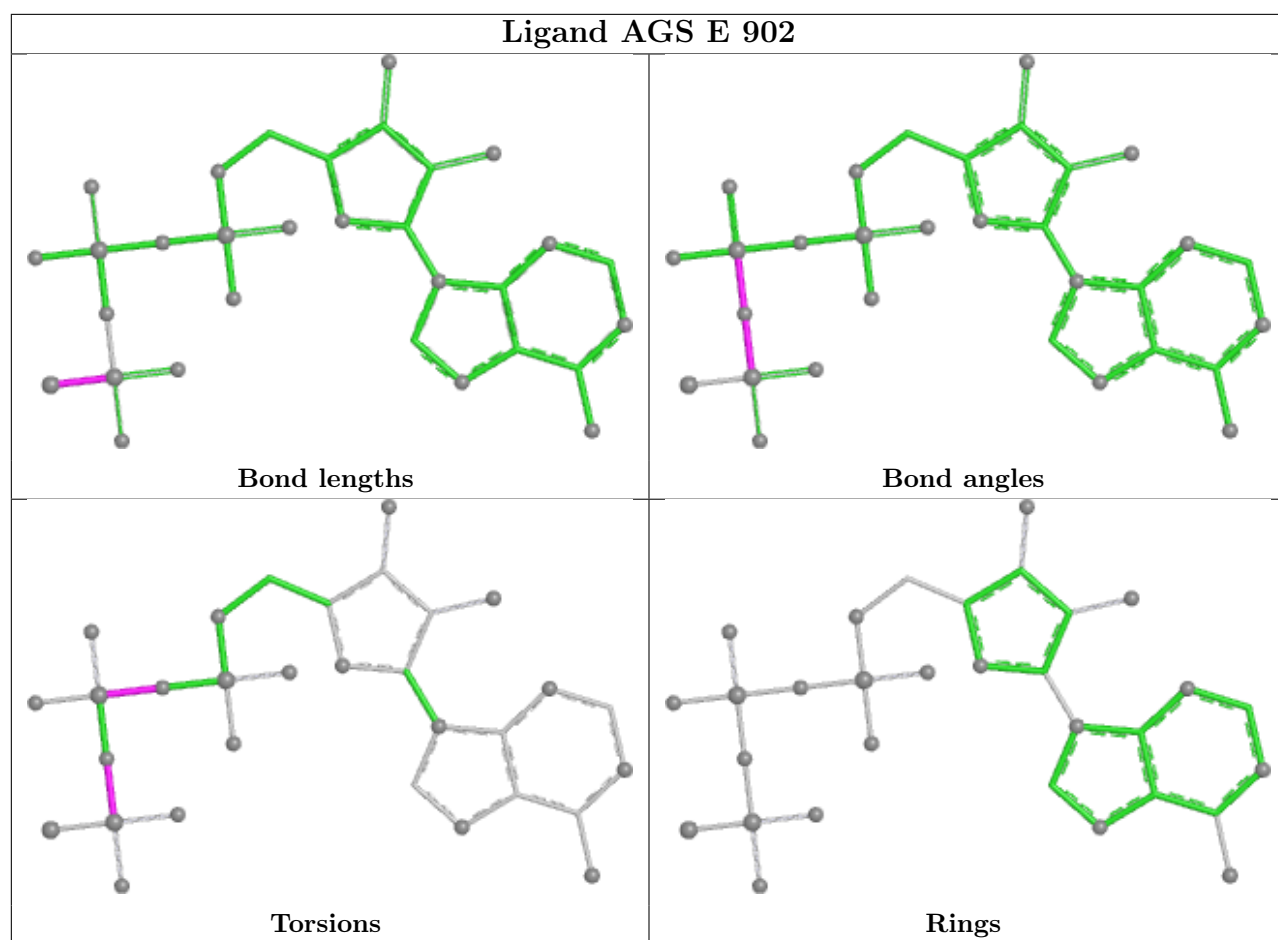


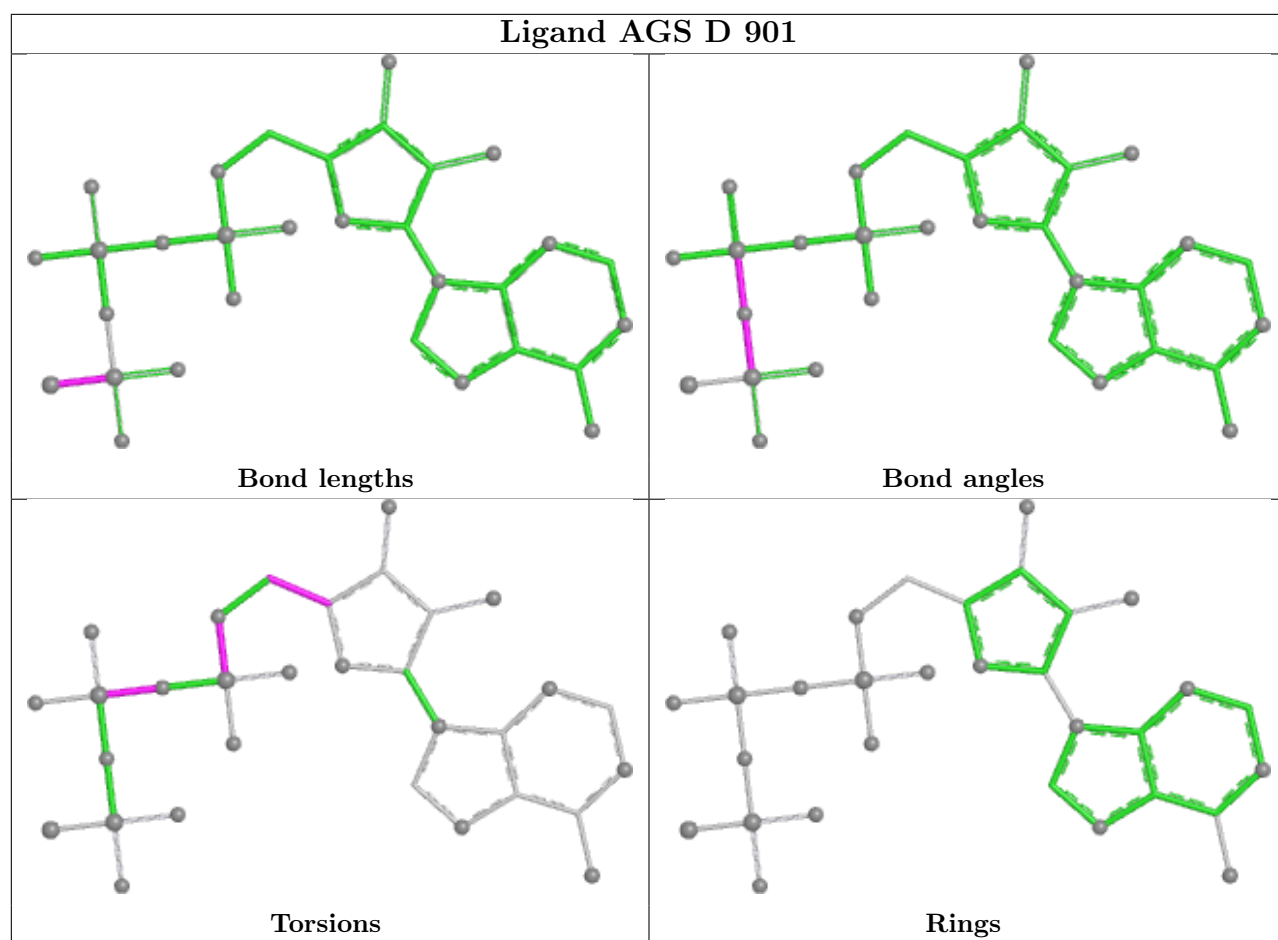


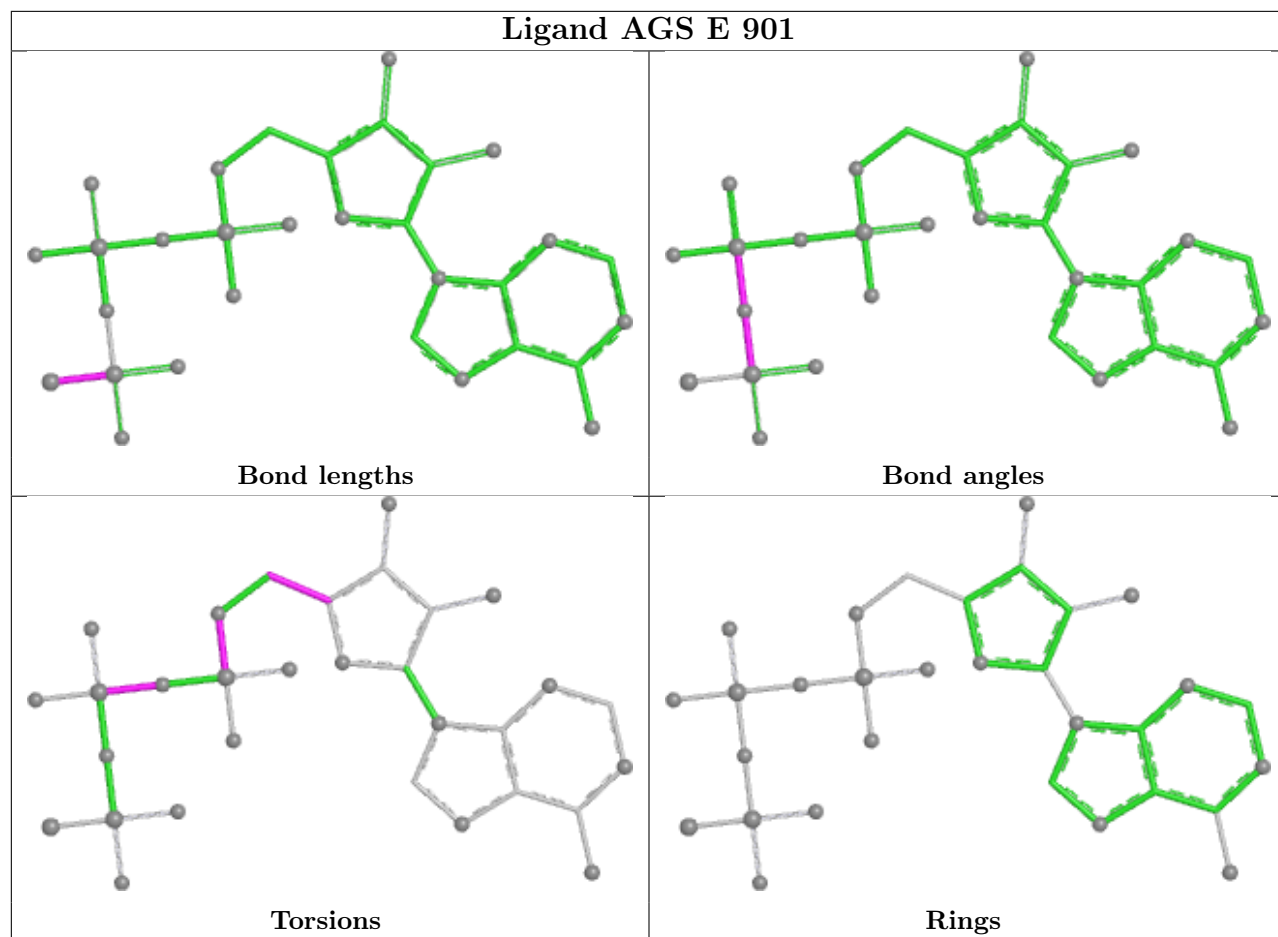


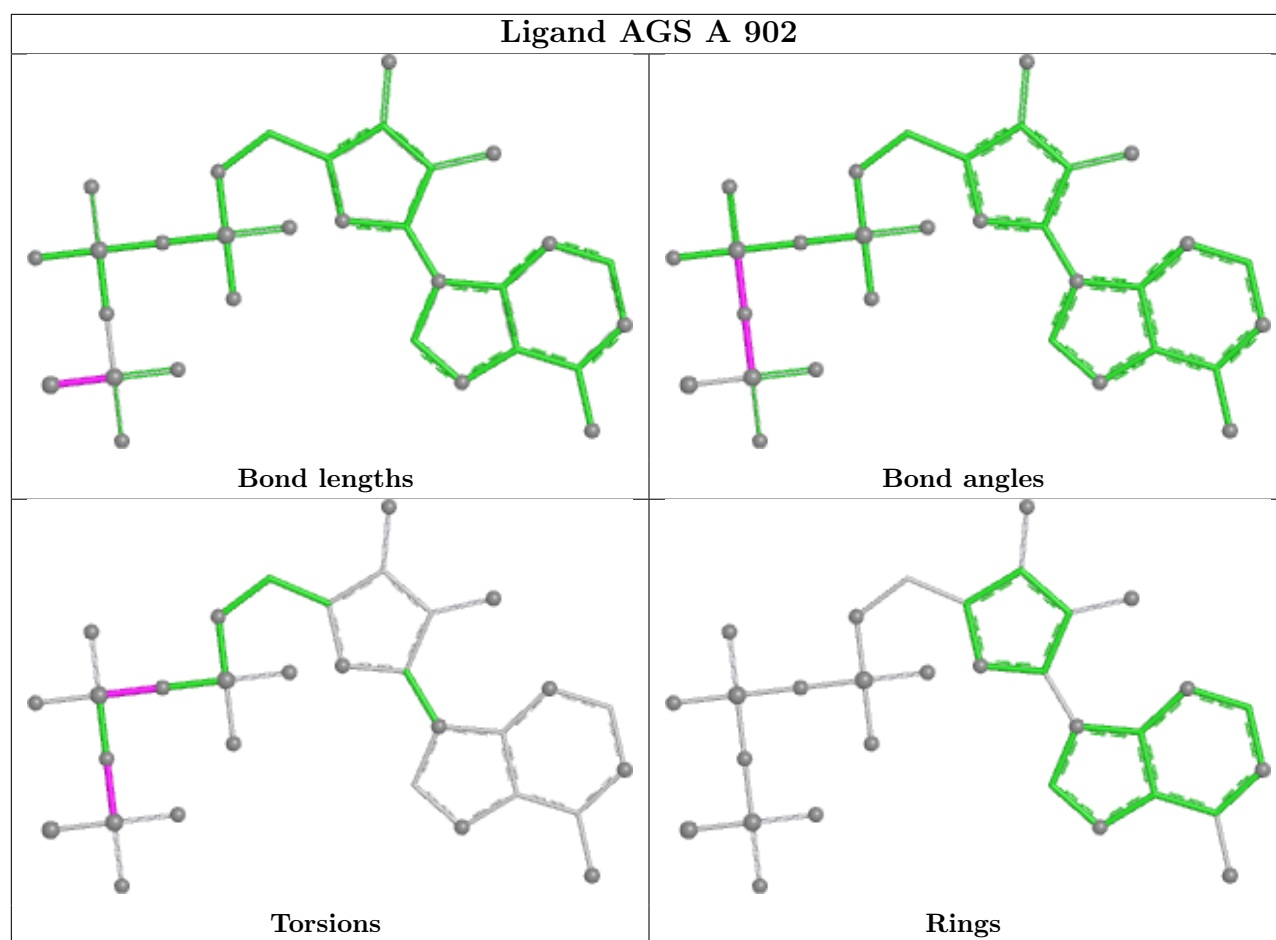












5.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-24519. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.