



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:08 AM UTC

PDB ID : 5FTL / pdb_00005ftl
EMDB ID : EMD-3297
Title : Cryo-EM structure of human p97 bound to ATPgS (Conformation I)
Authors : Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Huryn, D.; Arkin, M.; Subramaniam, S.
Deposited on : 2016-01-14
Resolution : 3.30 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:

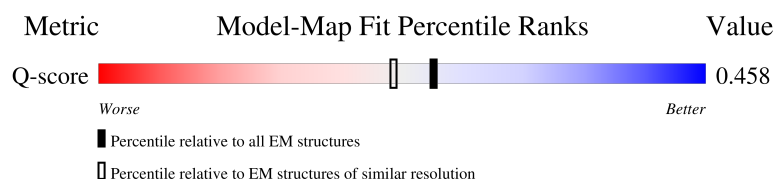
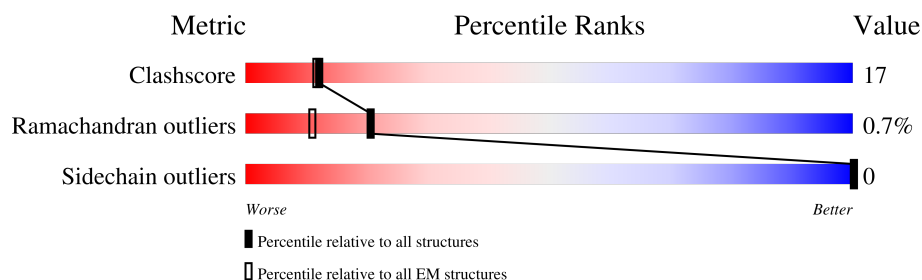
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

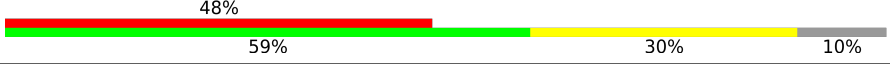
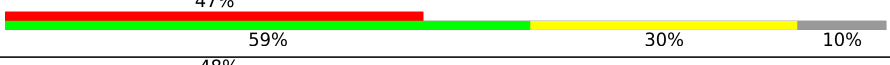
The reported resolution of this entry is 3.30 Å.

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	15087 (2.80 - 3.80)

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	806	
1	B	806	
1	C	806	
1	D	806	

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Mol	Chain	Length	Quality of chain
1	E	806	47% 59% 30% 10%
1	F	806	48% 58% 31% 10%

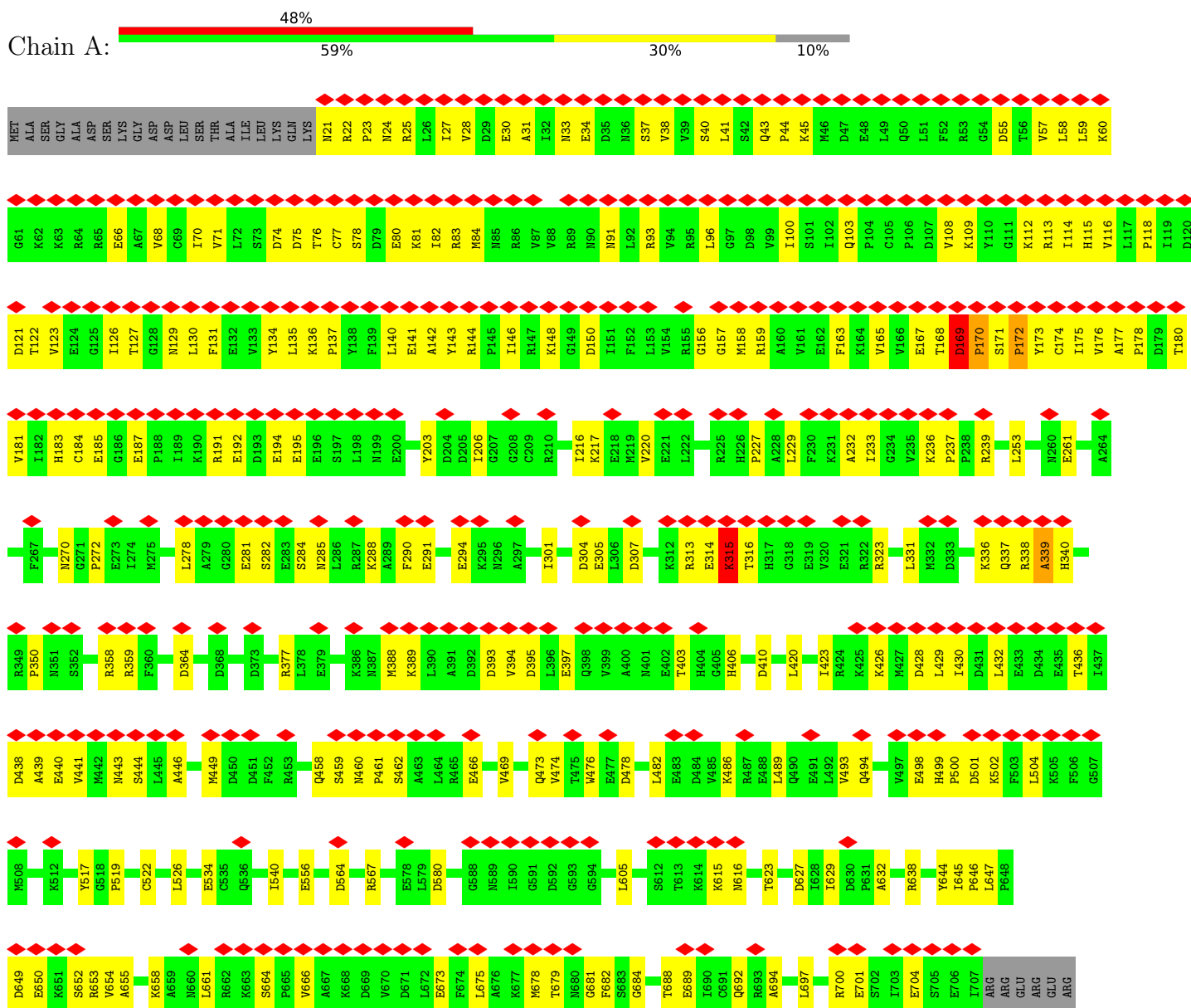
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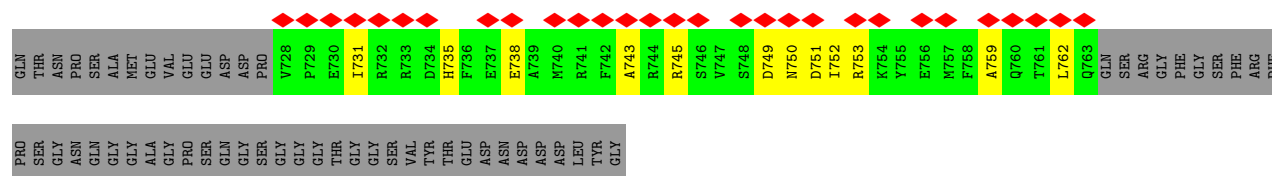
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10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

3 Residue-property plots

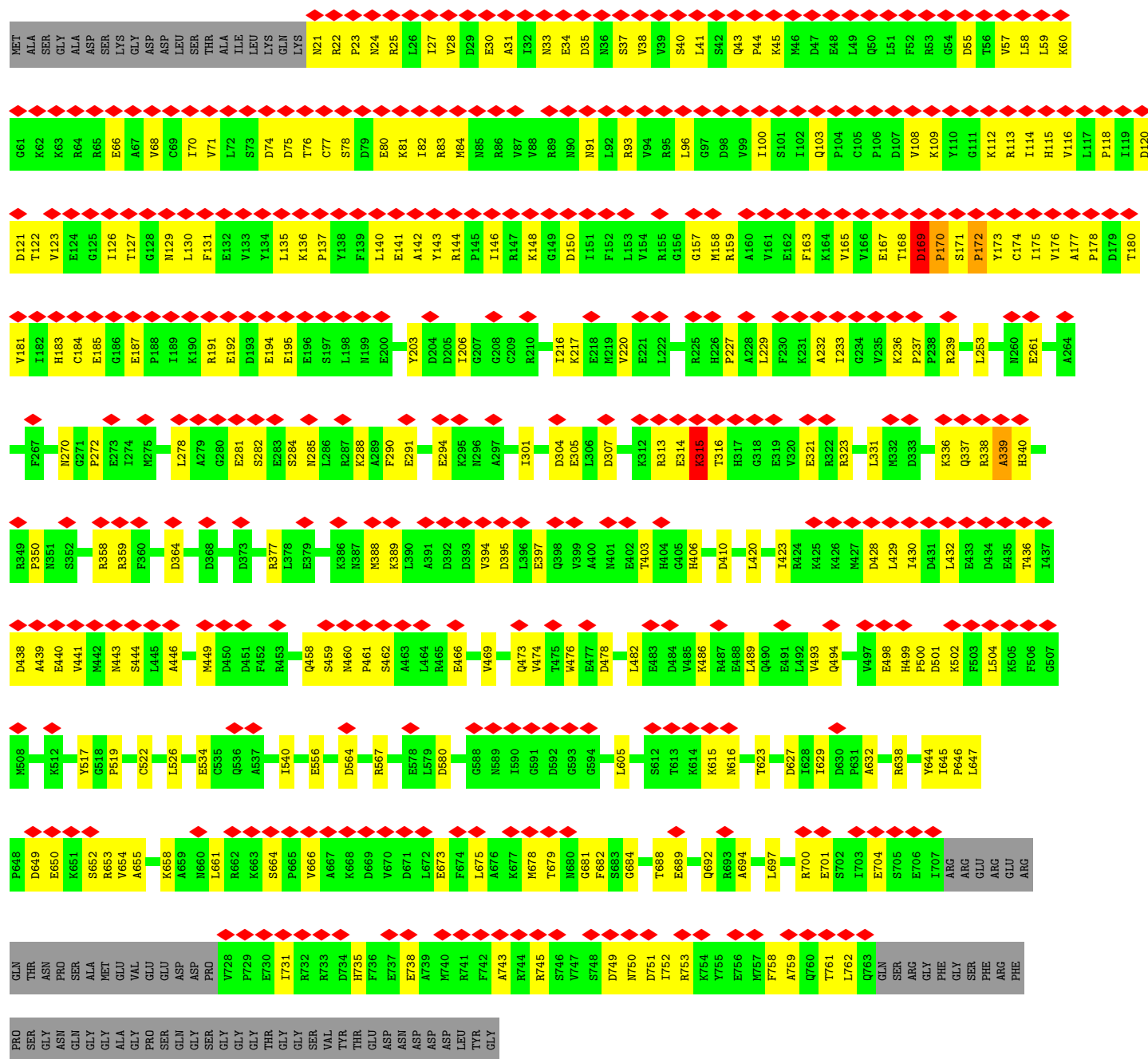
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

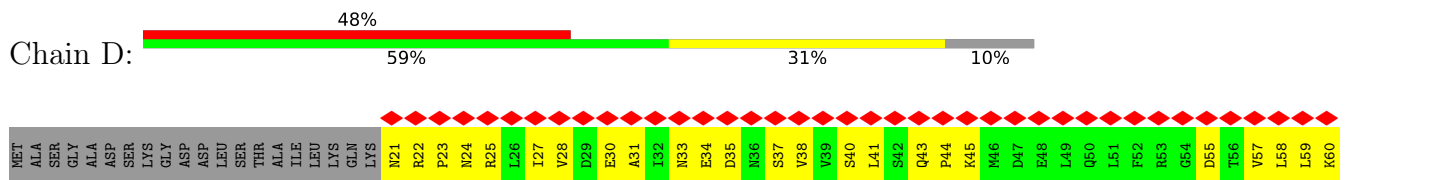


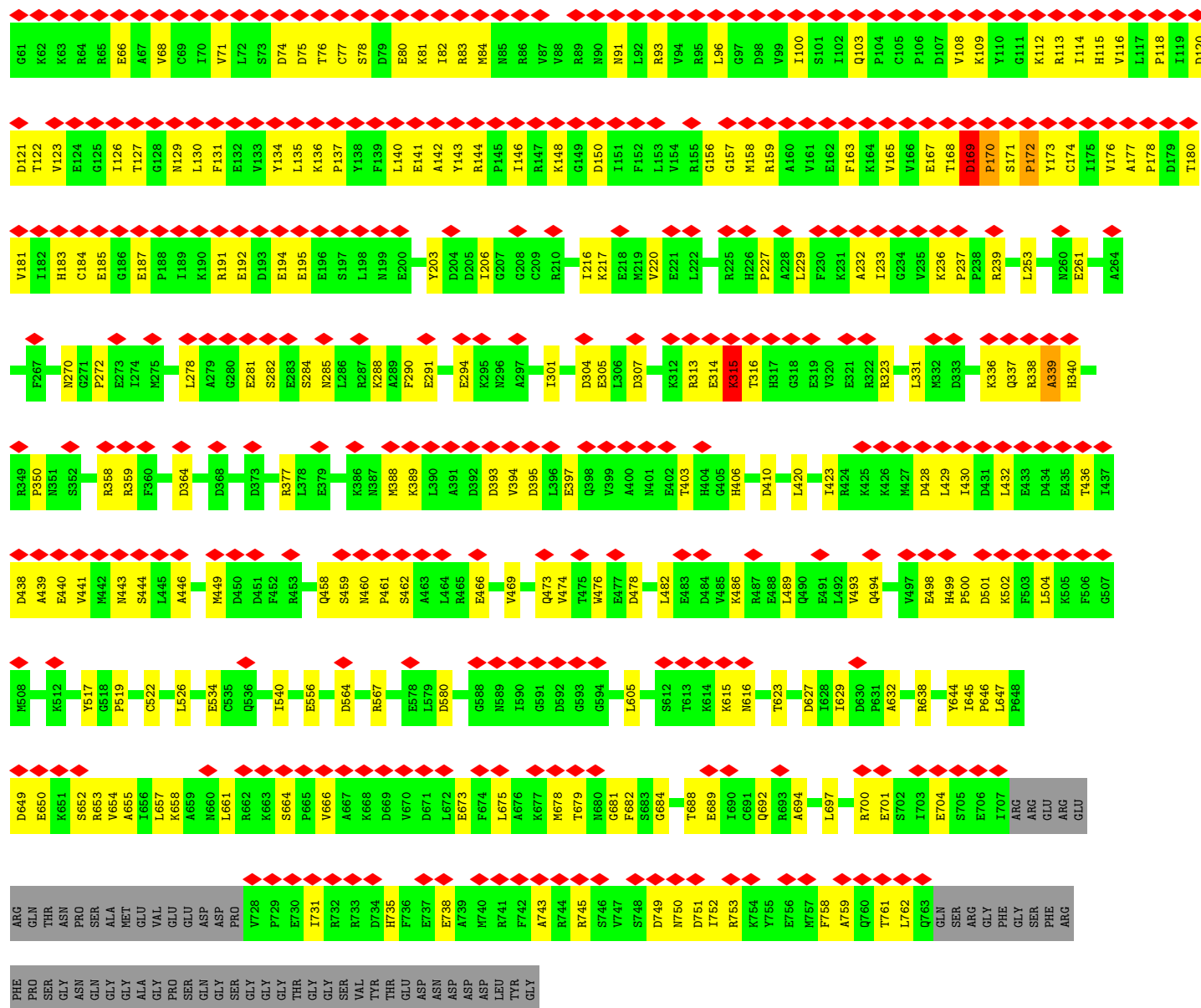


• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



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PHE	ARG		F503	L432	K336
	ARG	Y644	L504	E439	Q337
	GLU	I645	K505	D434	R338
	ARG	L647	F506	E435	A339
	PHE	P648	G507	T436	H340
	PRO	D649	M508	I437	
	THR	E650		D438	R349
	ASN	K651	K512	A439	P350
	GLN	S652		E440	N351
	GLY	R653	Y517	V441	S352
GLY	V654	G518	M442		
ALA	A655	P519	N443	R358	
VAL	K658	C522	S444	R359	
GLU	A659	L526	L445	F360	
PRO	N660		A446		
GLN	L661	E534	M449	D364	
SER	R662	C535	D450	D369	
GLY	K663	Q536	D451		
GLY	S664	A537	F452	D373	
THR	E730		R453		
THR	I731	I540	Q458	R377	
GLY	V666	E556	S459	L378	
GLY	A667	D564	M460	E379	
SER	R732	R567	P461	K386	
VAL	R733	E578	S462	N387	
THR	D734	D580	A463	K388	
THR	F736	L579	R465	K389	
GLU	E737		E466		
ASP	E738	G588	V469		
ASP	A739	N589	Q473	L396	
ASP	M740	I590	V474	E397	
LEU	R741	G591	T475	Q398	
THR	F742	G593	N476	V399	
GLY	A743	G594	E477	A400	
GLY	R744	L605	D478	N401	
PRO	R745		E483	E402	
PRO	F746	S612	D484	T403	
GLN	T747	T613	V485	H404	
GLN	S748	K614	K486	G405	
SER	D749	K615	R487	H406	
GLY	N750	N616	E488		
D751	D751	T623	L489	D410	
L752	L752	D627	Q490	L420	
R753	R753	I628	E491	T423	
R754	R754	I629	V493	R424	
L755	L755	D630	Q494	K425	
L756	L756	P631	V497	K426	
L757	L757	A632	E498	M427	
F758	F758	R638	H499	D428	
A759	A759		P500	L429	
Q760	Q760		D501	L430	
T761	T761		K502	D431	
L762	L762				
L763	L763				
GLN	GLN				
SER	SER				
ARG	ARG				
GLY	GLY				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	33882	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	950	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	36980	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0179	Depositor
Map size ($\text{\AA}$)	186.576, 186.576, 186.576	wwPDB
Map dimensions	276, 276, 276	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.676, 0.676, 0.676	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/5751	0.64	0/7767
1	B	0.44	0/5751	0.64	0/7767
1	C	0.44	0/5751	0.64	0/7767
1	D	0.44	0/5751	0.64	0/7767
1	E	0.44	0/5751	0.64	0/7767
1	F	0.44	0/5751	0.64	2/7767 (0.0%)
All	All	0.44	0/34506	0.64	2/46602 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
All	All	0	24

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	664	SER	CA-C-N	-5.02	113.56	119.84
1	F	664	SER	C-N-CA	-5.02	113.56	119.84

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ASP	Peptide
1	A	172	PRO	Peptide
1	A	23	PRO	Peptide
1	A	315	LYS	Peptide
1	B	169	ASP	Peptide
1	B	172	PRO	Peptide
1	B	23	PRO	Peptide
1	B	315	LYS	Peptide
1	C	169	ASP	Peptide
1	C	172	PRO	Peptide
1	C	23	PRO	Peptide
1	C	315	LYS	Peptide
1	D	169	ASP	Peptide
1	D	172	PRO	Peptide
1	D	23	PRO	Peptide
1	D	315	LYS	Peptide
1	E	169	ASP	Peptide
1	E	172	PRO	Peptide
1	E	23	PRO	Peptide
1	E	315	LYS	Peptide
1	F	169	ASP	Peptide
1	F	172	PRO	Peptide
1	F	23	PRO	Peptide
1	F	315	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5659	0	5731	202	0
1	B	5659	0	5731	203	0
1	C	5659	0	5731	200	0
1	D	5659	0	5731	204	0
1	E	5659	0	5731	201	0
1	F	5659	0	5731	204	0
2	A	54	0	24	3	0
2	B	54	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	54	0	24	3	0
2	D	54	0	24	3	0
2	E	54	0	24	3	0
2	F	54	0	24	3	0
All	All	34278	0	34530	1184	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 17.

All (1184) 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:294:GLU:OE2	1:C:338:ARG:HG3	1.53	1.08
1:A:294:GLU:OE2	1:A:338:ARG:HG3	1.53	1.07
1:E:294:GLU:OE2	1:E:338:ARG:HG3	1.53	1.07
1:D:294:GLU:OE2	1:D:338:ARG:HG3	1.53	1.06
1:F:294:GLU:OE2	1:F:338:ARG:HG3	1.53	1.06
1:B:294:GLU:OE2	1:B:338:ARG:HG3	1.53	1.06
1:B:294:GLU:CD	1:B:338:ARG:HG3	1.81	1.06
1:E:294:GLU:CD	1:E:338:ARG:HG3	1.81	1.05
1:F:294:GLU:CD	1:F:338:ARG:HG3	1.81	1.05
1:A:294:GLU:CD	1:A:338:ARG:HG3	1.81	1.05
1:C:294:GLU:CD	1:C:338:ARG:HG3	1.81	1.05
1:D:294:GLU:CD	1:D:338:ARG:HG3	1.81	1.05
1:F:127:THR:HB	1:F:438:ASP:HA	1.56	0.88
1:E:127:THR:HB	1:E:438:ASP:HA	1.56	0.87
1:A:127:THR:HB	1:A:438:ASP:HA	1.56	0.87
1:B:127:THR:HB	1:B:438:ASP:HA	1.56	0.87
1:C:127:THR:HB	1:C:438:ASP:HA	1.56	0.87
1:D:127:THR:HB	1:D:438:ASP:HA	1.56	0.86
1:F:701:GLU:HA	1:F:704:GLU:HB3	1.68	0.76
1:A:701:GLU:HA	1:A:704:GLU:HB3	1.68	0.76
1:A:294:GLU:CD	1:A:338:ARG:CG	2.59	0.75
1:B:701:GLU:HA	1:B:704:GLU:HB3	1.68	0.75
1:E:701:GLU:HA	1:E:704:GLU:HB3	1.68	0.75
1:C:701:GLU:HA	1:C:704:GLU:HB3	1.68	0.75
1:D:294:GLU:CD	1:D:338:ARG:CG	2.59	0.75
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.69	0.74
1:A:294:GLU:CD	1:A:338:ARG:HE	1.95	0.74
1:B:294:GLU:CD	1:B:338:ARG:HE	1.95	0.74
1:D:701:GLU:HA	1:D:704:GLU:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.69	0.74
1:C:294:GLU:CD	1:C:338:ARG:HE	1.95	0.74
1:E:294:GLU:CD	1:E:338:ARG:CG	2.59	0.74
1:F:294:GLU:CD	1:F:338:ARG:CG	2.59	0.74
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.69	0.74
1:D:294:GLU:CD	1:D:338:ARG:HE	1.95	0.74
1:E:294:GLU:CD	1:E:338:ARG:HE	1.94	0.74
1:C:294:GLU:CD	1:C:338:ARG:CG	2.59	0.73
1:F:294:GLU:CD	1:F:338:ARG:HE	1.95	0.73
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.69	0.73
1:E:294:GLU:OE1	1:E:338:ARG:NE	2.21	0.73
1:F:294:GLU:OE1	1:F:338:ARG:NE	2.21	0.73
1:E:157:GLY:HA2	1:E:443:ASN:HA	1.71	0.73
1:E:519:PRO:HG3	1:E:647:LEU:HD12	1.71	0.73
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.69	0.73
1:D:519:PRO:HG3	1:D:647:LEU:HD12	1.71	0.73
1:B:157:GLY:HA2	1:B:443:ASN:HA	1.71	0.73
1:B:519:PRO:HG3	1:B:647:LEU:HD12	1.71	0.73
1:F:519:PRO:HG3	1:F:647:LEU:HD12	1.71	0.73
1:F:439:ALA:O	1:F:443:ASN:ND2	2.22	0.72
1:A:294:GLU:OE1	1:A:338:ARG:NE	2.21	0.72
1:D:294:GLU:OE1	1:D:338:ARG:NE	2.21	0.72
1:E:439:ALA:O	1:E:443:ASN:ND2	2.22	0.72
1:C:294:GLU:OE1	1:C:338:ARG:NE	2.21	0.72
1:B:294:GLU:CD	1:B:338:ARG:CG	2.59	0.72
1:C:439:ALA:O	1:C:443:ASN:ND2	2.22	0.72
1:A:439:ALA:O	1:A:443:ASN:ND2	2.22	0.72
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.69	0.72
1:F:157:GLY:HA2	1:F:443:ASN:HA	1.71	0.72
1:A:157:GLY:HA2	1:A:443:ASN:HA	1.71	0.72
1:B:439:ALA:O	1:B:443:ASN:ND2	2.22	0.72
1:D:157:GLY:HA2	1:D:443:ASN:HA	1.71	0.72
1:C:519:PRO:HG3	1:C:647:LEU:HD12	1.71	0.72
1:D:439:ALA:O	1:D:443:ASN:ND2	2.22	0.72
1:B:294:GLU:OE1	1:B:338:ARG:NE	2.21	0.71
1:E:337:GLN:HA	1:E:337:GLN:NE2	2.05	0.71
1:C:157:GLY:HA2	1:C:443:ASN:HA	1.71	0.71
1:A:519:PRO:HG3	1:A:647:LEU:HD12	1.71	0.71
1:D:337:GLN:NE2	1:D:337:GLN:HA	2.05	0.71
1:B:337:GLN:HA	1:B:337:GLN:NE2	2.05	0.71
1:A:337:GLN:HA	1:A:337:GLN:NE2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:GLN:HA	1:C:337:GLN:NE2	2.05	0.70
1:D:142:ALA:HB1	1:D:144:ARG:HG3	1.74	0.70
1:B:142:ALA:HB1	1:B:144:ARG:HG3	1.74	0.69
1:D:77:CYS:SG	1:D:78:SER:N	2.66	0.69
1:F:337:GLN:HA	1:F:337:GLN:NE2	2.05	0.69
1:E:142:ALA:HB1	1:E:144:ARG:HG3	1.74	0.69
1:C:142:ALA:HB1	1:C:144:ARG:HG3	1.74	0.69
1:E:77:CYS:SG	1:E:78:SER:N	2.66	0.69
1:B:443:ASN:OD1	1:B:444:SER:N	2.26	0.69
1:D:443:ASN:OD1	1:D:444:SER:N	2.26	0.69
1:C:443:ASN:OD1	1:C:444:SER:N	2.26	0.68
1:F:77:CYS:SG	1:F:78:SER:N	2.66	0.68
1:E:443:ASN:OD1	1:E:444:SER:N	2.26	0.68
1:A:77:CYS:SG	1:A:78:SER:N	2.66	0.68
1:A:142:ALA:HB1	1:A:144:ARG:HG3	1.74	0.68
1:F:443:ASN:OD1	1:F:444:SER:N	2.26	0.68
1:A:443:ASN:OD1	1:A:444:SER:N	2.26	0.68
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.26	0.68
1:D:281:GLU:O	1:D:285:ASN:ND2	2.28	0.67
1:C:281:GLU:O	1:C:285:ASN:ND2	2.28	0.67
1:B:59:LEU:HB3	1:B:100:ILE:HD11	1.76	0.67
1:B:281:GLU:O	1:B:285:ASN:ND2	2.28	0.67
1:F:281:GLU:O	1:F:285:ASN:ND2	2.28	0.67
1:A:281:GLU:O	1:A:285:ASN:ND2	2.28	0.67
1:C:59:LEU:HB3	1:C:100:ILE:HD11	1.76	0.67
1:F:142:ALA:HB1	1:F:144:ARG:HG3	1.74	0.67
1:E:59:LEU:HB3	1:E:100:ILE:HD11	1.76	0.67
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.26	0.67
1:A:476:TRP:NE1	1:A:534:GLU:OE1	2.26	0.66
1:E:694:ALA:HB1	1:E:731:ILE:HD11	1.78	0.66
1:F:59:LEU:HB3	1:F:100:ILE:HD11	1.76	0.66
1:E:281:GLU:O	1:E:285:ASN:ND2	2.28	0.66
1:A:91:ASN:ND2	1:A:150:ASP:OD1	2.29	0.66
1:C:430:ILE:HG22	1:C:432:LEU:HG	1.78	0.66
1:E:316:THR:HG21	1:F:315:LYS:HE2	1.78	0.66
1:E:430:ILE:HG22	1:E:432:LEU:HG	1.78	0.66
1:A:694:ALA:HB1	1:A:731:ILE:HD11	1.77	0.66
1:B:430:ILE:HG22	1:B:432:LEU:HG	1.78	0.66
1:A:59:LEU:HB3	1:A:100:ILE:HD11	1.76	0.66
1:D:91:ASN:ND2	1:D:150:ASP:OD1	2.29	0.66
1:E:91:ASN:ND2	1:E:150:ASP:OD1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:HG21	1:B:315:LYS:HE2	1.78	0.66
1:B:694:ALA:HB1	1:B:731:ILE:HD11	1.77	0.66
1:C:694:ALA:HB1	1:C:731:ILE:HD11	1.78	0.66
1:F:649:ASP:OD1	1:F:650:GLU:N	2.29	0.66
1:A:430:ILE:HG22	1:A:432:LEU:HG	1.78	0.66
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.26	0.66
1:C:77:CYS:SG	1:C:78:SER:N	2.66	0.66
1:D:430:ILE:HG22	1:D:432:LEU:HG	1.78	0.66
1:B:91:ASN:ND2	1:B:150:ASP:OD1	2.29	0.65
1:D:476:TRP:NE1	1:D:534:GLU:OE1	2.26	0.65
1:B:316:THR:HG21	1:C:315:LYS:HE2	1.78	0.65
1:F:430:ILE:HG22	1:F:432:LEU:HG	1.78	0.65
1:D:694:ALA:HB1	1:D:731:ILE:HD11	1.77	0.65
1:F:313:ARG:HG3	1:F:314:GLU:H	1.61	0.65
1:A:313:ARG:HG3	1:A:314:GLU:H	1.62	0.65
1:D:59:LEU:HB3	1:D:100:ILE:HD11	1.76	0.65
1:A:232:ALA:O	1:B:159:ARG:NH2	2.30	0.65
1:A:315:LYS:HE2	1:F:316:THR:HG21	1.79	0.65
1:B:232:ALA:O	1:C:159:ARG:NH2	2.30	0.65
1:A:143:TYR:HE1	1:A:178:PRO:HD3	1.62	0.65
1:B:313:ARG:HG3	1:B:314:GLU:H	1.61	0.65
1:E:313:ARG:HG3	1:E:314:GLU:H	1.61	0.65
1:C:313:ARG:HG3	1:C:314:GLU:H	1.61	0.65
1:D:313:ARG:HG3	1:D:314:GLU:H	1.62	0.65
1:F:143:TYR:HE1	1:F:178:PRO:HD3	1.62	0.65
1:A:159:ARG:NH2	1:F:232:ALA:O	2.30	0.65
1:D:316:THR:HG21	1:E:315:LYS:HE2	1.79	0.65
1:F:91:ASN:ND2	1:F:150:ASP:OD1	2.29	0.65
1:F:694:ALA:HB1	1:F:731:ILE:HD11	1.77	0.65
1:A:649:ASP:OD1	1:A:650:GLU:N	2.29	0.64
1:A:21:ASN:O	1:A:25:ARG:NH2	2.31	0.64
1:B:21:ASN:O	1:B:25:ARG:NH2	2.31	0.64
1:D:338:ARG:HG2	1:D:338:ARG:O	1.98	0.64
1:C:91:ASN:ND2	1:C:150:ASP:OD1	2.29	0.64
1:C:21:ASN:O	1:C:25:ARG:NH2	2.31	0.64
1:C:316:THR:HG21	1:D:315:LYS:HE2	1.79	0.64
1:E:232:ALA:O	1:F:159:ARG:NH2	2.30	0.64
1:A:338:ARG:O	1:A:338:ARG:HG2	1.97	0.64
1:B:143:TYR:HE1	1:B:178:PRO:HD3	1.62	0.64
1:D:232:ALA:O	1:E:159:ARG:NH2	2.30	0.64
1:F:21:ASN:O	1:F:25:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:ARG:O	1:F:338:ARG:HG2	1.97	0.64
1:E:338:ARG:O	1:E:338:ARG:HG2	1.97	0.64
1:C:338:ARG:O	1:C:338:ARG:HG2	1.97	0.64
1:E:143:TYR:HE1	1:E:178:PRO:HD3	1.62	0.64
1:A:440:GLU:HA	1:A:443:ASN:HD21	1.63	0.63
1:E:476:TRP:NE1	1:E:534:GLU:OE1	2.26	0.63
1:B:440:GLU:HA	1:B:443:ASN:HD21	1.64	0.63
1:C:143:TYR:HE1	1:C:178:PRO:HD3	1.61	0.63
1:A:749:ASP:OD1	1:A:750:ASN:N	2.32	0.63
1:B:338:ARG:O	1:B:338:ARG:HG2	1.97	0.63
1:D:21:ASN:O	1:D:25:ARG:NH2	2.31	0.63
1:D:749:ASP:OD1	1:D:750:ASN:N	2.32	0.63
1:F:440:GLU:HA	1:F:443:ASN:HD21	1.64	0.63
1:D:143:TYR:HE1	1:D:178:PRO:HD3	1.62	0.63
1:E:350:PRO:O	1:E:358:ARG:NH2	2.32	0.63
1:E:440:GLU:HA	1:E:443:ASN:HD21	1.63	0.63
1:E:647:LEU:HD13	1:E:752:ILE:HD13	1.80	0.63
1:F:116:VAL:HG12	1:F:165:VAL:HA	1.81	0.63
1:C:440:GLU:HA	1:C:443:ASN:HD21	1.63	0.63
1:E:649:ASP:OD1	1:E:650:GLU:N	2.29	0.63
1:D:440:GLU:HA	1:D:443:ASN:HD21	1.63	0.63
1:F:45:LYS:NZ	1:F:77:CYS:SG	2.72	0.63
1:B:749:ASP:OD1	1:B:750:ASN:N	2.32	0.62
1:C:45:LYS:NZ	1:C:77:CYS:SG	2.72	0.62
1:C:647:LEU:HD13	1:C:752:ILE:HD13	1.81	0.62
1:F:350:PRO:O	1:F:358:ARG:NH2	2.32	0.62
1:A:116:VAL:HG12	1:A:165:VAL:HA	1.81	0.62
1:B:45:LYS:NZ	1:B:77:CYS:SG	2.72	0.62
1:B:77:CYS:SG	1:B:78:SER:N	2.66	0.62
1:B:116:VAL:HG12	1:B:165:VAL:HA	1.81	0.62
1:B:350:PRO:O	1:B:358:ARG:NH2	2.32	0.62
1:E:116:VAL:HG12	1:E:165:VAL:HA	1.81	0.62
1:A:45:LYS:NZ	1:A:77:CYS:SG	2.72	0.62
1:A:337:GLN:O	1:A:338:ARG:HB3	1.99	0.62
1:C:232:ALA:O	1:D:159:ARG:NH2	2.31	0.62
1:D:45:LYS:NZ	1:D:77:CYS:SG	2.72	0.62
1:D:350:PRO:O	1:D:358:ARG:NH2	2.32	0.62
1:E:749:ASP:OD1	1:E:750:ASN:N	2.32	0.62
1:F:647:LEU:HD13	1:F:752:ILE:HD13	1.80	0.62
1:F:749:ASP:OD1	1:F:750:ASN:N	2.32	0.62
1:A:476:TRP:HE1	1:A:534:GLU:CD	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:ASP:OD1	1:C:750:ASN:N	2.32	0.62
1:E:21:ASN:O	1:E:25:ARG:NH2	2.31	0.62
1:F:476:TRP:HE1	1:F:534:GLU:CD	2.07	0.62
1:C:350:PRO:O	1:C:358:ARG:NH2	2.32	0.62
1:C:649:ASP:OD1	1:C:650:GLU:N	2.29	0.62
1:A:350:PRO:O	1:A:358:ARG:NH2	2.32	0.62
1:D:116:VAL:HG12	1:D:165:VAL:HA	1.81	0.62
1:A:406:HIS:CE1	1:A:461:PRO:HA	2.35	0.62
1:B:647:LEU:HD13	1:B:752:ILE:HD13	1.81	0.62
1:C:476:TRP:HE1	1:C:534:GLU:CD	2.07	0.62
1:C:116:VAL:HG12	1:C:165:VAL:HA	1.81	0.62
1:D:337:GLN:O	1:D:338:ARG:HB3	1.99	0.62
1:D:647:LEU:HD13	1:D:752:ILE:HD13	1.80	0.62
1:E:337:GLN:HA	1:E:337:GLN:HE21	1.65	0.62
1:E:476:TRP:HE1	1:E:534:GLU:CD	2.07	0.62
1:B:406:HIS:CE1	1:B:461:PRO:HA	2.35	0.62
1:E:45:LYS:NZ	1:E:77:CYS:SG	2.72	0.61
1:F:337:GLN:HA	1:F:337:GLN:HE21	1.65	0.61
1:E:337:GLN:O	1:E:338:ARG:HB3	1.99	0.61
1:D:476:TRP:HE1	1:D:534:GLU:CD	2.07	0.61
1:B:476:TRP:HE1	1:B:534:GLU:CD	2.07	0.61
1:D:649:ASP:OD1	1:D:650:GLU:N	2.29	0.61
1:F:406:HIS:CE1	1:F:461:PRO:HA	2.35	0.61
1:B:337:GLN:O	1:B:338:ARG:HB3	1.99	0.61
1:B:649:ASP:OD1	1:B:650:GLU:N	2.29	0.61
1:C:337:GLN:O	1:C:338:ARG:HB3	1.99	0.61
1:D:337:GLN:HA	1:D:337:GLN:HE21	1.65	0.61
1:A:337:GLN:HA	1:A:337:GLN:HE21	1.65	0.61
1:A:647:LEU:HD13	1:A:752:ILE:HD13	1.81	0.61
1:F:337:GLN:O	1:F:338:ARG:HB3	1.99	0.60
1:C:406:HIS:CE1	1:C:461:PRO:HA	2.35	0.60
1:E:501:ASP:OD1	1:E:502:LYS:N	2.35	0.60
1:C:337:GLN:HA	1:C:337:GLN:HE21	1.65	0.60
1:A:112:LYS:N	1:A:169:ASP:OD2	2.31	0.60
1:A:501:ASP:OD1	1:A:502:LYS:N	2.35	0.60
1:E:673:GLU:OE1	1:E:673:GLU:N	2.34	0.60
1:B:337:GLN:HA	1:B:337:GLN:HE21	1.65	0.60
1:E:406:HIS:CE1	1:E:461:PRO:HA	2.35	0.60
1:D:406:HIS:CE1	1:D:461:PRO:HA	2.35	0.60
1:E:359:ARG:HH12	1:F:305:GLU:CD	2.10	0.59
1:F:673:GLU:OE1	1:F:673:GLU:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:501:ASP:OD1	1:F:502:LYS:N	2.35	0.59
1:C:501:ASP:OD1	1:C:502:LYS:N	2.35	0.59
1:A:130:LEU:HD21	1:A:163:PHE:CE1	2.38	0.59
1:B:130:LEU:HD21	1:B:163:PHE:CE1	2.38	0.59
1:A:305:GLU:CD	1:F:359:ARG:HH12	2.10	0.59
1:D:112:LYS:N	1:D:169:ASP:OD2	2.31	0.59
1:D:130:LEU:HD21	1:D:163:PHE:CE1	2.38	0.59
1:E:130:LEU:HD21	1:E:163:PHE:CE1	2.38	0.59
1:A:359:ARG:HH12	1:B:305:GLU:CD	2.11	0.59
1:C:130:LEU:HD21	1:C:163:PHE:CE1	2.38	0.59
1:F:130:LEU:HD21	1:F:163:PHE:CE1	2.38	0.59
1:B:458:GLN:O	1:B:461:PRO:HD2	2.03	0.59
1:F:458:GLN:O	1:F:461:PRO:HD2	2.03	0.59
1:C:359:ARG:HH12	1:D:305:GLU:CD	2.11	0.58
1:F:294:GLU:CD	1:F:338:ARG:NE	2.61	0.58
1:B:359:ARG:HH12	1:C:305:GLU:CD	2.10	0.58
1:D:458:GLN:O	1:D:461:PRO:HD2	2.03	0.58
1:D:501:ASP:OD1	1:D:502:LYS:N	2.35	0.58
1:A:294:GLU:CD	1:A:338:ARG:NE	2.61	0.58
1:C:458:GLN:O	1:C:461:PRO:HD2	2.03	0.58
1:E:458:GLN:O	1:E:461:PRO:HD2	2.03	0.58
1:B:501:ASP:OD1	1:B:502:LYS:N	2.35	0.58
1:F:112:LYS:N	1:F:169:ASP:OD2	2.31	0.58
1:A:108:VAL:HG22	1:A:109:LYS:H	1.69	0.58
1:A:750:ASN:OD1	1:A:751:ASP:N	2.37	0.58
1:B:108:VAL:HG22	1:B:109:LYS:H	1.69	0.58
1:D:359:ARG:HH12	1:E:305:GLU:CD	2.11	0.58
1:F:750:ASN:OD1	1:F:751:ASP:N	2.37	0.58
1:B:750:ASN:OD1	1:B:751:ASP:N	2.37	0.57
1:C:294:GLU:CD	1:C:338:ARG:NE	2.61	0.57
1:E:112:LYS:N	1:E:169:ASP:OD2	2.31	0.57
1:A:458:GLN:O	1:A:461:PRO:HD2	2.03	0.57
1:C:750:ASN:OD1	1:C:751:ASP:N	2.37	0.57
1:E:294:GLU:CD	1:E:338:ARG:NE	2.61	0.57
1:A:673:GLU:OE1	1:A:673:GLU:N	2.34	0.57
1:B:294:GLU:CD	1:B:338:ARG:NE	2.61	0.57
1:A:143:TYR:HA	1:A:176:VAL:O	2.05	0.57
1:C:108:VAL:HG22	1:C:109:LYS:H	1.69	0.57
1:C:564:ASP:OD1	1:C:567:ARG:NH1	2.37	0.57
1:E:394:VAL:HA	1:E:449:MET:HE2	1.87	0.57
1:F:108:VAL:HG22	1:F:109:LYS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:TYR:HA	1:B:176:VAL:O	2.05	0.57
1:D:143:TYR:HA	1:D:176:VAL:O	2.05	0.57
1:E:750:ASN:OD1	1:E:751:ASP:N	2.37	0.57
1:B:203:TYR:CZ	1:B:261:GLU:HG2	2.40	0.57
1:C:143:TYR:HA	1:C:176:VAL:O	2.05	0.57
1:D:750:ASN:OD1	1:D:751:ASP:N	2.37	0.57
1:A:294:GLU:HG3	1:A:338:ARG:HG2	1.87	0.57
1:A:564:ASP:OD1	1:A:567:ARG:NH1	2.37	0.57
1:F:394:VAL:HA	1:F:449:MET:HE2	1.87	0.57
1:F:615:LYS:HG2	1:F:616:ASN:H	1.70	0.57
1:D:394:VAL:HA	1:D:449:MET:HE2	1.87	0.57
1:F:294:GLU:HG3	1:F:338:ARG:HG2	1.87	0.57
1:B:615:LYS:HG2	1:B:616:ASN:H	1.70	0.56
1:E:294:GLU:HG3	1:E:338:ARG:HG2	1.87	0.56
1:C:203:TYR:CZ	1:C:261:GLU:HG2	2.40	0.56
1:D:108:VAL:HG22	1:D:109:LYS:H	1.69	0.56
1:D:294:GLU:CD	1:D:338:ARG:NE	2.61	0.56
1:D:615:LYS:HG2	1:D:616:ASN:H	1.70	0.56
1:A:146:ILE:HG23	1:A:165:VAL:HG21	1.88	0.56
1:A:203:TYR:CZ	1:A:261:GLU:HG2	2.40	0.56
1:B:112:LYS:N	1:B:169:ASP:OD2	2.31	0.56
1:B:146:ILE:HG23	1:B:165:VAL:HG21	1.88	0.56
1:B:556:GLU:N	1:B:556:GLU:OE1	2.38	0.56
1:C:146:ILE:HG23	1:C:165:VAL:HG21	1.87	0.56
1:C:364:ASP:OD1	1:C:364:ASP:N	2.35	0.56
1:E:108:VAL:HG22	1:E:109:LYS:H	1.69	0.56
1:F:143:TYR:HA	1:F:176:VAL:O	2.05	0.56
1:F:564:ASP:OD1	1:F:567:ARG:NH1	2.37	0.56
1:B:75:ASP:OD1	1:B:76:THR:N	2.37	0.56
1:C:294:GLU:HG3	1:C:338:ARG:HG2	1.87	0.56
1:D:203:TYR:CZ	1:D:261:GLU:HG2	2.40	0.56
1:E:564:ASP:OD1	1:E:567:ARG:NH1	2.37	0.56
1:F:146:ILE:HG23	1:F:165:VAL:HG21	1.88	0.56
1:C:615:LYS:HG2	1:C:616:ASN:H	1.70	0.56
1:E:203:TYR:CZ	1:E:261:GLU:HG2	2.40	0.56
1:B:129:ASN:OD1	1:B:131:PHE:N	2.39	0.56
1:F:129:ASN:OD1	1:F:131:PHE:N	2.39	0.56
1:A:170:PRO:O	1:A:173:TYR:HB3	2.06	0.56
1:C:394:VAL:HA	1:C:449:MET:HE2	1.87	0.56
1:C:556:GLU:N	1:C:556:GLU:OE1	2.38	0.56
1:E:129:ASN:OD1	1:E:131:PHE:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:TYR:HA	1:E:176:VAL:O	2.05	0.56
1:A:129:ASN:OD1	1:A:131:PHE:N	2.39	0.56
1:A:650:GLU:HG3	1:A:653:ARG:NH2	2.21	0.56
1:D:294:GLU:HG3	1:D:338:ARG:HG2	1.87	0.56
1:E:146:ILE:HG23	1:E:165:VAL:HG21	1.88	0.56
1:A:394:VAL:HA	1:A:449:MET:HE2	1.87	0.55
1:B:170:PRO:O	1:B:173:TYR:HB3	2.06	0.55
1:B:564:ASP:OD1	1:B:567:ARG:NH1	2.37	0.55
1:D:239:ARG:NH2	1:D:337:GLN:H	2.04	0.55
1:E:170:PRO:O	1:E:173:TYR:HB3	2.06	0.55
1:F:650:GLU:HG3	1:F:653:ARG:NH2	2.21	0.55
1:F:170:PRO:O	1:F:173:TYR:HB3	2.06	0.55
1:F:203:TYR:CZ	1:F:261:GLU:HG2	2.40	0.55
1:B:394:VAL:HA	1:B:449:MET:HE2	1.87	0.55
1:B:650:GLU:HG3	1:B:653:ARG:NH2	2.21	0.55
1:D:129:ASN:OD1	1:D:131:PHE:N	2.39	0.55
1:D:146:ILE:HG23	1:D:165:VAL:HG21	1.88	0.55
1:D:290:PHE:CD1	1:D:301:ILE:HD13	2.42	0.55
1:E:290:PHE:CD1	1:E:301:ILE:HD13	2.42	0.55
1:B:294:GLU:HG3	1:B:338:ARG:HG2	1.87	0.55
1:B:673:GLU:OE1	1:B:673:GLU:N	2.34	0.55
1:C:650:GLU:HG3	1:C:653:ARG:NH2	2.21	0.55
1:E:615:LYS:HG2	1:E:616:ASN:H	1.70	0.55
1:A:239:ARG:NH2	1:A:337:GLN:H	2.04	0.55
1:A:615:LYS:HG2	1:A:616:ASN:H	1.70	0.55
1:C:129:ASN:OD1	1:C:131:PHE:N	2.39	0.55
1:D:170:PRO:O	1:D:173:TYR:HB3	2.06	0.55
1:E:650:GLU:HG3	1:E:653:ARG:NH2	2.21	0.55
1:A:290:PHE:CD1	1:A:301:ILE:HD13	2.42	0.55
1:B:239:ARG:NH2	1:B:337:GLN:H	2.04	0.55
1:B:364:ASP:OD1	1:B:364:ASP:N	2.35	0.55
1:C:239:ARG:NH2	1:C:337:GLN:H	2.04	0.55
1:C:290:PHE:CD1	1:C:301:ILE:HD13	2.42	0.55
1:D:75:ASP:OD1	1:D:76:THR:N	2.37	0.55
1:A:632:ALA:O	1:A:638:ARG:NH1	2.40	0.54
1:B:290:PHE:CD1	1:B:301:ILE:HD13	2.42	0.54
1:C:76:THR:OG1	1:C:83:ARG:NH1	2.39	0.54
1:C:170:PRO:O	1:C:173:TYR:HB3	2.06	0.54
1:D:556:GLU:OE1	1:D:556:GLU:N	2.38	0.54
1:F:239:ARG:NH2	1:F:337:GLN:H	2.04	0.54
1:D:31:ALA:HB2	1:D:84:MET:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:GLU:HG3	1:D:653:ARG:NH2	2.21	0.54
1:E:498:GLU:OE1	1:E:499:HIS:NE2	2.41	0.54
1:E:632:ALA:O	1:E:638:ARG:NH1	2.40	0.54
1:F:31:ALA:HB2	1:F:84:MET:C	2.33	0.54
1:A:31:ALA:HB2	1:A:84:MET:C	2.33	0.54
1:D:498:GLU:OE1	1:D:499:HIS:NE2	2.41	0.54
1:E:112:LYS:HG2	1:E:113:ARG:HG3	1.90	0.54
1:F:290:PHE:CD1	1:F:301:ILE:HD13	2.42	0.54
1:E:31:ALA:HB2	1:E:84:MET:C	2.33	0.54
1:E:127:THR:OG1	1:E:436:THR:O	2.26	0.54
1:E:654:VAL:O	1:E:658:LYS:HG2	2.08	0.54
1:A:338:ARG:O	1:A:339:ALA:HB3	2.08	0.54
1:B:498:GLU:OE1	1:B:499:HIS:NE2	2.41	0.54
1:E:428:ASP:OD1	1:E:429:LEU:N	2.41	0.54
1:F:498:GLU:OE1	1:F:499:HIS:NE2	2.41	0.54
1:F:632:ALA:O	1:F:638:ARG:NH1	2.40	0.54
1:C:31:ALA:HB2	1:C:84:MET:C	2.33	0.54
1:A:498:GLU:OE1	1:A:499:HIS:NE2	2.41	0.54
1:D:76:THR:OG1	1:D:83:ARG:NH1	2.39	0.54
1:D:564:ASP:OD1	1:D:567:ARG:NH1	2.37	0.54
1:E:76:THR:OG1	1:E:83:ARG:NH1	2.39	0.54
1:E:239:ARG:NH2	1:E:337:GLN:H	2.04	0.54
1:F:428:ASP:OD1	1:F:429:LEU:N	2.41	0.54
1:C:112:LYS:N	1:C:169:ASP:OD2	2.31	0.54
1:F:112:LYS:HG2	1:F:113:ARG:HG3	1.90	0.54
1:F:654:VAL:O	1:F:658:LYS:HG2	2.08	0.54
1:B:654:VAL:O	1:B:658:LYS:HG2	2.08	0.53
1:A:654:VAL:O	1:A:658:LYS:HG2	2.08	0.53
1:B:109:LYS:HD3	1:B:173:TYR:CE1	2.44	0.53
1:B:112:LYS:HG2	1:B:113:ARG:HG3	1.90	0.53
1:D:428:ASP:OD1	1:D:429:LEU:N	2.41	0.53
1:E:78:SER:OG	1:E:81:LYS:HG2	2.09	0.53
1:F:109:LYS:HD3	1:F:173:TYR:CE1	2.44	0.53
1:A:109:LYS:HD3	1:A:173:TYR:CE1	2.44	0.53
1:B:31:ALA:HB2	1:B:84:MET:C	2.33	0.53
1:C:338:ARG:O	1:C:339:ALA:HB3	2.08	0.53
1:D:338:ARG:O	1:D:339:ALA:HB3	2.08	0.53
1:A:428:ASP:OD1	1:A:429:LEU:N	2.41	0.53
1:B:76:THR:OG1	1:B:83:ARG:NH1	2.39	0.53
1:B:282:SER:O	1:B:285:ASN:N	2.40	0.53
1:F:127:THR:OG1	1:F:436:THR:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:SER:O	1:A:285:ASN:N	2.40	0.53
1:B:428:ASP:OD1	1:B:429:LEU:N	2.41	0.53
1:C:112:LYS:HG2	1:C:113:ARG:HG3	1.90	0.53
1:D:78:SER:OG	1:D:81:LYS:HG2	2.09	0.53
1:D:112:LYS:HG2	1:D:113:ARG:HG3	1.90	0.53
1:D:127:THR:OG1	1:D:436:THR:O	2.26	0.53
1:E:282:SER:O	1:E:285:ASN:N	2.40	0.53
1:A:75:ASP:OD1	1:A:76:THR:N	2.37	0.53
1:C:127:THR:OG1	1:C:436:THR:O	2.26	0.53
1:C:498:GLU:OE1	1:C:499:HIS:NE2	2.41	0.53
1:E:233:ILE:HD11	1:F:158:MET:HB2	1.91	0.53
1:F:78:SER:OG	1:F:81:LYS:HG2	2.09	0.53
1:B:338:ARG:O	1:B:339:ALA:HB3	2.08	0.53
1:D:177:ALA:O	1:D:180:THR:HG22	2.09	0.53
1:D:526:LEU:HD11	2:D:900:ADP:H2'	1.91	0.53
1:D:673:GLU:OE1	1:D:673:GLU:N	2.34	0.53
1:F:177:ALA:O	1:F:180:THR:HG22	2.09	0.53
1:C:109:LYS:HD3	1:C:173:TYR:CE1	2.44	0.53
1:C:526:LEU:HD11	2:C:900:ADP:H2'	1.91	0.53
1:F:338:ARG:O	1:F:339:ALA:HB3	2.08	0.53
1:A:177:ALA:O	1:A:180:THR:HG22	2.09	0.53
1:A:233:ILE:HD11	1:B:158:MET:HB2	1.91	0.53
1:B:233:ILE:HD11	1:C:158:MET:HB2	1.91	0.53
1:C:203:TYR:CE2	1:C:217:LYS:HE2	2.44	0.53
1:C:428:ASP:OD1	1:C:429:LEU:N	2.41	0.53
1:C:654:VAL:O	1:C:658:LYS:HG2	2.08	0.53
1:D:203:TYR:CE2	1:D:217:LYS:HE2	2.44	0.53
1:E:556:GLU:OE1	1:E:556:GLU:N	2.38	0.53
1:A:78:SER:OG	1:A:81:LYS:HG2	2.09	0.53
1:B:127:THR:OG1	1:B:436:THR:O	2.26	0.53
1:C:282:SER:O	1:C:285:ASN:N	2.40	0.53
1:E:177:ALA:O	1:E:180:THR:HG22	2.09	0.53
1:E:203:TYR:CE2	1:E:217:LYS:HE2	2.44	0.53
1:E:526:LEU:HD11	2:E:900:ADP:H2'	1.91	0.53
1:B:203:TYR:CE2	1:B:217:LYS:HE2	2.44	0.52
1:D:282:SER:O	1:D:285:ASN:N	2.40	0.52
1:D:654:VAL:O	1:D:658:LYS:HG2	2.08	0.52
1:E:336:LYS:O	1:E:337:GLN:C	2.51	0.52
1:F:701:GLU:OE2	1:F:735:HIS:NE2	2.42	0.52
1:E:338:ARG:O	1:E:339:ALA:HB3	2.08	0.52
1:E:701:GLU:OE2	1:E:735:HIS:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:526:LEU:HD11	2:F:900:ADP:H2'	1.91	0.52
1:A:336:LYS:O	1:A:337:GLN:C	2.51	0.52
1:B:78:SER:OG	1:B:81:LYS:HG2	2.09	0.52
1:C:78:SER:OG	1:C:81:LYS:HG2	2.09	0.52
1:C:403:THR:HB	1:C:406:HIS:ND1	2.25	0.52
1:D:336:LYS:O	1:D:337:GLN:C	2.51	0.52
1:F:403:THR:HB	1:F:406:HIS:ND1	2.24	0.52
1:F:605:LEU:HD22	1:F:638:ARG:HD3	1.92	0.52
1:A:526:LEU:HD11	2:A:900:ADP:H2'	1.91	0.52
1:B:93:ARG:HH21	1:B:194:GLU:HG3	1.75	0.52
1:B:526:LEU:HD11	2:B:900:ADP:H2'	1.91	0.52
1:C:177:ALA:O	1:C:180:THR:HG22	2.09	0.52
1:D:109:LYS:HD3	1:D:173:TYR:CE1	2.44	0.52
1:A:112:LYS:HG2	1:A:113:ARG:HG3	1.90	0.52
1:A:556:GLU:OE1	1:A:556:GLU:N	2.38	0.52
1:A:605:LEU:HD22	1:A:638:ARG:HD3	1.92	0.52
1:D:239:ARG:HH22	1:D:337:GLN:H	1.58	0.52
1:E:239:ARG:HH22	1:E:337:GLN:H	1.58	0.52
1:F:203:TYR:CE2	1:F:217:LYS:HE2	2.44	0.52
1:F:556:GLU:OE1	1:F:556:GLU:N	2.38	0.52
1:A:158:MET:HB2	1:F:233:ILE:HD11	1.92	0.52
1:A:701:GLU:OE2	1:A:735:HIS:NE2	2.42	0.52
1:B:177:ALA:O	1:B:180:THR:HG22	2.09	0.52
1:B:403:THR:HB	1:B:406:HIS:ND1	2.24	0.52
1:C:673:GLU:OE1	1:C:673:GLU:N	2.34	0.52
1:D:233:ILE:HD11	1:E:158:MET:HB2	1.91	0.52
1:E:109:LYS:HD3	1:E:173:TYR:CE1	2.44	0.52
1:C:605:LEU:HD22	1:C:638:ARG:HD3	1.92	0.52
1:C:632:ALA:O	1:C:638:ARG:NH1	2.40	0.52
1:D:93:ARG:HH21	1:D:194:GLU:HG3	1.75	0.52
1:F:76:THR:OG1	1:F:83:ARG:NH1	2.39	0.52
1:A:127:THR:OG1	1:A:436:THR:O	2.26	0.52
1:A:403:THR:HB	1:A:406:HIS:ND1	2.25	0.52
1:B:460:ASN:OD1	1:B:460:ASN:N	2.43	0.52
1:B:473:GLN:OE1	1:B:473:GLN:N	2.32	0.52
1:B:605:LEU:HD22	1:B:638:ARG:HD3	1.92	0.52
1:C:236:LYS:HD2	1:C:237:PRO:HD2	1.92	0.52
1:C:239:ARG:HH22	1:C:337:GLN:H	1.58	0.52
1:D:158:MET:HG2	1:D:388:MET:HB3	1.92	0.52
1:A:364:ASP:OD1	1:A:364:ASP:N	2.35	0.52
1:C:158:MET:HG2	1:C:388:MET:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ARG:HH22	1:F:337:GLN:H	1.58	0.52
1:F:697:LEU:HD11	1:F:738:GLU:OE1	2.10	0.52
1:C:233:ILE:HD11	1:D:158:MET:HB2	1.92	0.52
1:D:701:GLU:OE2	1:D:735:HIS:NE2	2.42	0.52
1:E:75:ASP:OD1	1:E:76:THR:N	2.37	0.52
1:A:203:TYR:CE2	1:A:217:LYS:HE2	2.44	0.51
1:B:33:ASN:OD1	1:B:34:GLU:N	2.44	0.51
1:E:460:ASN:OD1	1:E:460:ASN:N	2.43	0.51
1:A:76:THR:OG1	1:A:83:ARG:NH1	2.39	0.51
1:A:697:LEU:HD11	1:A:738:GLU:OE1	2.10	0.51
1:B:236:LYS:HD2	1:B:237:PRO:HD2	1.92	0.51
1:B:697:LEU:HD11	1:B:738:GLU:OE1	2.10	0.51
1:C:697:LEU:HD11	1:C:738:GLU:OE1	2.10	0.51
1:E:403:THR:HB	1:E:406:HIS:ND1	2.24	0.51
1:E:605:LEU:HD22	1:E:638:ARG:HD3	1.92	0.51
1:F:389:LYS:HZ2	1:F:446:ALA:HB2	1.75	0.51
1:A:33:ASN:OD1	1:A:34:GLU:N	2.43	0.51
1:D:389:LYS:NZ	1:D:446:ALA:HB2	2.25	0.51
1:D:605:LEU:HD22	1:D:638:ARG:HD3	1.92	0.51
1:E:93:ARG:HH21	1:E:194:GLU:HG3	1.75	0.51
1:F:389:LYS:NZ	1:F:446:ALA:HB2	2.25	0.51
1:B:337:GLN:NE2	1:B:337:GLN:CA	2.73	0.51
1:C:75:ASP:OD1	1:C:76:THR:N	2.37	0.51
1:C:644:TYR:CZ	1:C:646:PRO:HB3	2.46	0.51
1:A:460:ASN:OD1	1:A:460:ASN:N	2.43	0.51
1:B:389:LYS:HZ2	1:B:446:ALA:HB2	1.75	0.51
1:B:644:TYR:CZ	1:B:646:PRO:HB3	2.46	0.51
1:A:131:PHE:HA	1:A:135:LEU:HD13	1.93	0.51
1:D:236:LYS:HD2	1:D:237:PRO:HD2	1.92	0.51
1:E:131:PHE:HA	1:E:135:LEU:HD13	1.93	0.51
1:E:700:ARG:O	1:E:704:GLU:N	2.32	0.51
1:F:93:ARG:HH21	1:F:194:GLU:HG3	1.75	0.51
1:C:33:ASN:OD1	1:C:34:GLU:N	2.43	0.51
1:D:403:THR:HB	1:D:406:HIS:ND1	2.25	0.51
1:D:460:ASN:N	1:D:460:ASN:OD1	2.43	0.51
1:D:644:TYR:CZ	1:D:646:PRO:HB3	2.46	0.51
1:F:131:PHE:HA	1:F:135:LEU:HD13	1.93	0.51
1:F:282:SER:O	1:F:285:ASN:N	2.40	0.51
1:A:236:LYS:HD2	1:A:237:PRO:HD2	1.92	0.51
1:D:30:GLU:HB3	1:D:96:LEU:HD21	1.93	0.51
1:E:697:LEU:HD11	1:E:738:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ARG:HH22	1:B:337:GLN:H	1.58	0.51
1:D:473:GLN:OE1	1:D:473:GLN:N	2.32	0.51
1:E:389:LYS:NZ	1:E:446:ALA:HB2	2.26	0.51
1:A:30:GLU:HB3	1:A:96:LEU:HD21	1.93	0.51
1:A:239:ARG:HH22	1:A:337:GLN:H	1.58	0.51
1:B:30:GLU:HB3	1:B:96:LEU:HD21	1.93	0.51
1:C:93:ARG:HH21	1:C:194:GLU:HG3	1.75	0.51
1:C:336:LYS:O	1:C:337:GLN:C	2.51	0.51
1:C:460:ASN:OD1	1:C:460:ASN:N	2.43	0.51
1:D:253:LEU:HD13	2:D:807:ADP:H2'	1.93	0.51
1:C:701:GLU:OE2	1:C:735:HIS:NE2	2.42	0.50
1:D:33:ASN:OD1	1:D:34:GLU:N	2.44	0.50
1:D:697:LEU:HD11	1:D:738:GLU:OE1	2.10	0.50
1:A:337:GLN:NE2	1:A:337:GLN:CA	2.73	0.50
1:B:389:LYS:NZ	1:B:446:ALA:HB2	2.26	0.50
1:C:253:LEU:HD13	2:C:807:ADP:H2'	1.93	0.50
1:E:33:ASN:OD1	1:E:34:GLU:N	2.44	0.50
1:E:134:TYR:OH	1:E:156:GLY:O	2.25	0.50
1:F:441:VAL:O	1:F:444:SER:OG	2.28	0.50
1:A:93:ARG:HH21	1:A:194:GLU:HG3	1.75	0.50
1:E:158:MET:HG2	1:E:388:MET:HB3	1.92	0.50
1:E:253:LEU:HD13	2:E:807:ADP:H2'	1.93	0.50
1:A:644:TYR:CZ	1:A:646:PRO:HB3	2.46	0.50
1:B:701:GLU:OE2	1:B:735:HIS:NE2	2.42	0.50
1:D:131:PHE:HA	1:D:135:LEU:HD13	1.93	0.50
1:F:131:PHE:HZ	1:F:184:CYS:H	1.59	0.50
1:A:158:MET:HG2	1:A:388:MET:HB3	1.92	0.50
1:A:389:LYS:NZ	1:A:446:ALA:HB2	2.26	0.50
1:B:227:PRO:HB3	1:B:340:HIS:CD2	2.47	0.50
1:B:517:TYR:CZ	1:B:644:TYR:HB2	2.47	0.50
1:C:30:GLU:HB3	1:C:96:LEU:HD21	1.93	0.50
1:C:420:LEU:HD23	1:C:423:ILE:HD12	1.93	0.50
1:D:420:LEU:HD23	1:D:423:ILE:HD12	1.93	0.50
1:F:406:HIS:HD2	1:F:410:ASP:HB3	1.77	0.50
1:F:460:ASN:N	1:F:460:ASN:OD1	2.43	0.50
1:A:227:PRO:HB3	1:A:340:HIS:CD2	2.47	0.50
1:A:420:LEU:HD23	1:A:423:ILE:HD12	1.93	0.50
1:E:236:LYS:HD2	1:E:237:PRO:HD2	1.92	0.50
1:E:406:HIS:HD2	1:E:410:ASP:HB3	1.77	0.50
1:E:517:TYR:CZ	1:E:644:TYR:HB2	2.46	0.50
1:E:644:TYR:CZ	1:E:646:PRO:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:MET:HG2	1:F:388:MET:HB3	1.92	0.50
1:B:420:LEU:HD23	1:B:423:ILE:HD12	1.93	0.50
1:B:666:VAL:HA	1:B:731:ILE:HG22	1.94	0.50
1:B:700:ARG:O	1:B:704:GLU:N	2.32	0.50
1:C:517:TYR:CZ	1:C:644:TYR:HB2	2.47	0.50
1:C:700:ARG:O	1:C:704:GLU:N	2.32	0.50
1:E:74:ASP:OD2	1:E:77:CYS:HB3	2.12	0.50
1:E:131:PHE:HZ	1:E:184:CYS:H	1.59	0.50
1:F:75:ASP:OD1	1:F:76:THR:N	2.37	0.50
1:F:420:LEU:HD23	1:F:423:ILE:HD12	1.93	0.50
1:A:666:VAL:HA	1:A:731:ILE:HG22	1.94	0.50
1:B:131:PHE:HA	1:B:135:LEU:HD13	1.93	0.50
1:B:158:MET:HG2	1:B:388:MET:HB3	1.92	0.50
1:B:253:LEU:HD13	2:B:807:ADP:H2'	1.93	0.50
1:C:127:THR:CB	1:C:438:ASP:HA	2.37	0.50
1:E:57:VAL:O	1:E:68:VAL:HG13	2.12	0.50
1:E:121:ASP:OD1	1:E:122:THR:N	2.45	0.50
1:E:420:LEU:HD23	1:E:423:ILE:HD12	1.93	0.50
1:F:30:GLU:HB3	1:F:96:LEU:HD21	1.93	0.50
1:F:33:ASN:OD1	1:F:34:GLU:N	2.43	0.50
1:F:74:ASP:OD2	1:F:77:CYS:HB3	2.12	0.50
1:F:236:LYS:HD2	1:F:237:PRO:HD2	1.92	0.50
1:F:666:VAL:HA	1:F:731:ILE:HG22	1.94	0.50
1:A:517:TYR:CZ	1:A:644:TYR:HB2	2.47	0.50
1:C:227:PRO:HB3	1:C:340:HIS:CD2	2.47	0.50
1:C:389:LYS:NZ	1:C:446:ALA:HB2	2.26	0.50
1:D:57:VAL:O	1:D:68:VAL:HG13	2.12	0.50
1:A:121:ASP:OD1	1:A:122:THR:N	2.45	0.49
1:B:121:ASP:OD1	1:B:122:THR:N	2.45	0.49
1:C:406:HIS:HD2	1:C:410:ASP:HB3	1.77	0.49
1:A:700:ARG:O	1:A:704:GLU:N	2.32	0.49
1:C:57:VAL:O	1:C:68:VAL:HG13	2.12	0.49
1:A:131:PHE:HZ	1:A:184:CYS:H	1.60	0.49
1:A:406:HIS:HD2	1:A:410:ASP:HB3	1.77	0.49
1:D:406:HIS:HD2	1:D:410:ASP:HB3	1.77	0.49
1:F:336:LYS:O	1:F:337:GLN:C	2.51	0.49
1:F:517:TYR:CZ	1:F:644:TYR:HB2	2.47	0.49
1:F:644:TYR:CZ	1:F:646:PRO:HB3	2.46	0.49
1:B:632:ALA:O	1:B:638:ARG:NH1	2.40	0.49
1:E:337:GLN:NE2	1:E:337:GLN:CA	2.73	0.49
1:F:227:PRO:HB3	1:F:340:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD13	2:A:807:ADP:H2'	1.93	0.49
1:C:666:VAL:HA	1:C:731:ILE:HG22	1.94	0.49
1:D:632:ALA:O	1:D:638:ARG:NH1	2.40	0.49
1:E:30:GLU:HB3	1:E:96:LEU:HD21	1.93	0.49
1:E:666:VAL:HA	1:E:731:ILE:HG22	1.94	0.49
1:F:57:VAL:O	1:F:68:VAL:HG13	2.12	0.49
1:F:239:ARG:HH22	1:F:336:LYS:HA	1.78	0.49
1:A:57:VAL:O	1:A:68:VAL:HG13	2.12	0.49
1:A:389:LYS:HZ1	1:A:446:ALA:HB2	1.78	0.49
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.53	0.49
1:C:758:PHE:O	1:C:761:THR:OG1	2.29	0.49
1:D:74:ASP:OD2	1:D:77:CYS:HB3	2.12	0.49
1:D:169:ASP:O	1:D:171:SER:N	2.46	0.49
1:D:517:TYR:CZ	1:D:644:TYR:HB2	2.47	0.49
1:A:169:ASP:O	1:A:171:SER:N	2.46	0.49
1:A:759:ALA:HA	1:A:762:LEU:HD12	1.95	0.49
1:C:121:ASP:OD1	1:C:122:THR:N	2.45	0.49
1:D:239:ARG:HH22	1:D:336:LYS:HA	1.78	0.49
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.53	0.49
1:A:74:ASP:OD2	1:A:77:CYS:HB3	2.12	0.49
1:B:406:HIS:HD2	1:B:410:ASP:HB3	1.77	0.49
1:C:74:ASP:OD2	1:C:77:CYS:HB3	2.12	0.49
1:C:131:PHE:HA	1:C:135:LEU:HD13	1.93	0.49
1:D:227:PRO:HB3	1:D:340:HIS:CD2	2.47	0.49
1:E:169:ASP:O	1:E:171:SER:N	2.46	0.49
1:F:121:ASP:OD1	1:F:122:THR:N	2.45	0.49
1:F:253:LEU:HD13	2:F:807:ADP:H2'	1.93	0.49
1:B:239:ARG:HH22	1:B:336:LYS:HA	1.78	0.49
1:B:759:ALA:HA	1:B:762:LEU:HD12	1.95	0.49
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.53	0.49
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.53	0.49
1:B:57:VAL:O	1:B:68:VAL:HG13	2.12	0.49
1:B:169:ASP:O	1:B:171:SER:N	2.46	0.49
1:B:675:LEU:HA	1:B:678:MET:SD	2.53	0.49
1:C:169:ASP:O	1:C:171:SER:N	2.46	0.49
1:E:127:THR:CB	1:E:438:ASP:HA	2.37	0.49
1:E:675:LEU:HA	1:E:678:MET:SD	2.53	0.49
1:B:74:ASP:OD2	1:B:77:CYS:HB3	2.12	0.48
1:D:131:PHE:HZ	1:D:184:CYS:H	1.60	0.48
1:E:227:PRO:HB3	1:E:340:HIS:CD2	2.47	0.48
1:E:759:ALA:HA	1:E:762:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:759:ALA:HA	1:F:762:LEU:HD12	1.95	0.48
1:C:675:LEU:HA	1:C:678:MET:SD	2.53	0.48
1:C:681:GLY:HA3	1:C:745:ARG:HH21	1.78	0.48
1:C:759:ALA:HA	1:C:762:LEU:HD12	1.95	0.48
1:D:666:VAL:HA	1:D:731:ILE:HG22	1.94	0.48
1:D:681:GLY:HA3	1:D:745:ARG:HH21	1.78	0.48
1:F:675:LEU:HA	1:F:678:MET:SD	2.53	0.48
1:B:131:PHE:HZ	1:B:184:CYS:H	1.59	0.48
1:B:336:LYS:O	1:B:337:GLN:C	2.51	0.48
1:C:60:LYS:HA	1:C:66:GLU:HG2	1.96	0.48
1:D:121:ASP:OD1	1:D:122:THR:N	2.45	0.48
1:F:364:ASP:OD1	1:F:364:ASP:N	2.35	0.48
1:B:60:LYS:HA	1:B:66:GLU:HG2	1.96	0.48
1:C:114:ILE:HD13	1:C:168:THR:HG23	1.96	0.48
1:D:191:ARG:HH21	1:D:195:GLU:HG2	1.79	0.48
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.53	0.48
1:D:675:LEU:HA	1:D:678:MET:SD	2.53	0.48
1:E:123:VAL:O	1:E:126:ILE:HG12	2.14	0.48
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.53	0.48
1:D:681:GLY:CA	1:D:745:ARG:HE	2.27	0.48
1:D:759:ALA:HA	1:D:762:LEU:HD12	1.95	0.48
1:F:169:ASP:O	1:F:171:SER:N	2.46	0.48
1:F:681:GLY:CA	1:F:745:ARG:HE	2.27	0.48
1:A:675:LEU:HA	1:A:678:MET:SD	2.53	0.48
1:B:123:VAL:O	1:B:126:ILE:HG12	2.14	0.48
1:B:284:SER:O	1:B:288:LYS:HG2	2.14	0.48
1:C:627:ASP:OD1	1:C:627:ASP:N	2.46	0.48
1:C:681:GLY:CA	1:C:745:ARG:HE	2.27	0.48
1:D:123:VAL:O	1:D:126:ILE:HG12	2.14	0.48
1:A:284:SER:O	1:A:288:LYS:HG2	2.14	0.48
1:B:681:GLY:HA3	1:B:745:ARG:HH21	1.78	0.48
1:C:239:ARG:HH22	1:C:336:LYS:HA	1.78	0.48
1:C:284:SER:O	1:C:288:LYS:HG2	2.14	0.48
1:D:60:LYS:HA	1:D:66:GLU:HG2	1.96	0.48
1:D:127:THR:CB	1:D:438:ASP:HA	2.37	0.48
1:E:681:GLY:CA	1:E:745:ARG:HE	2.27	0.48
1:F:123:VAL:O	1:F:126:ILE:HG12	2.14	0.48
1:A:60:LYS:HA	1:A:66:GLU:HG2	1.96	0.48
1:A:681:GLY:CA	1:A:745:ARG:HE	2.27	0.48
1:C:131:PHE:HZ	1:C:184:CYS:H	1.59	0.48
1:E:466:GLU:N	1:E:466:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:TYR:OH	1:A:156:GLY:O	2.25	0.48
1:D:284:SER:O	1:D:288:LYS:HG2	2.14	0.48
1:E:114:ILE:HD13	1:E:168:THR:HG23	1.96	0.48
1:A:123:VAL:O	1:A:126:ILE:HG12	2.14	0.48
1:E:28:VAL:HG23	1:E:96:LEU:HA	1.96	0.48
1:E:681:GLY:HA3	1:E:745:ARG:HH21	1.79	0.48
1:F:700:ARG:O	1:F:704:GLU:N	2.32	0.48
1:A:239:ARG:HH22	1:A:336:LYS:HA	1.78	0.47
1:B:114:ILE:HD13	1:B:168:THR:HG23	1.96	0.47
1:D:114:ILE:HD13	1:D:168:THR:HG23	1.96	0.47
1:D:337:GLN:NE2	1:D:337:GLN:CA	2.73	0.47
1:F:466:GLU:OE1	1:F:466:GLU:N	2.47	0.47
1:A:681:GLY:HA3	1:A:745:ARG:HH21	1.78	0.47
1:C:191:ARG:HH21	1:C:195:GLU:HG2	1.79	0.47
1:E:239:ARG:HH22	1:E:336:LYS:HA	1.78	0.47
1:F:681:GLY:HA3	1:F:745:ARG:HH21	1.78	0.47
1:A:191:ARG:HH21	1:A:195:GLU:HG2	1.79	0.47
1:B:627:ASP:N	1:B:627:ASP:OD1	2.46	0.47
1:C:123:VAL:O	1:C:126:ILE:HG12	2.14	0.47
1:D:28:VAL:HG23	1:D:96:LEU:HA	1.96	0.47
1:E:191:ARG:HH21	1:E:195:GLU:HG2	1.79	0.47
1:A:466:GLU:OE1	1:A:466:GLU:N	2.47	0.47
1:C:37:SER:O	1:C:38:VAL:HG23	2.14	0.47
1:C:109:LYS:HD3	1:C:173:TYR:CD1	2.50	0.47
1:D:37:SER:O	1:D:38:VAL:HG23	2.14	0.47
1:E:33:ASN:OD1	1:E:35:ASP:N	2.31	0.47
1:E:60:LYS:HA	1:E:66:GLU:HG2	1.96	0.47
1:F:284:SER:O	1:F:288:LYS:HG2	2.14	0.47
1:B:681:GLY:CA	1:B:745:ARG:HE	2.27	0.47
1:C:337:GLN:NE2	1:C:337:GLN:CA	2.73	0.47
1:D:679:THR:HB	1:D:682:PHE:HB2	1.97	0.47
1:F:28:VAL:HG23	1:F:96:LEU:HA	1.96	0.47
1:F:60:LYS:HA	1:F:66:GLU:HG2	1.96	0.47
1:F:191:ARG:HH21	1:F:195:GLU:HG2	1.79	0.47
1:A:37:SER:O	1:A:38:VAL:HG23	2.14	0.47
1:C:28:VAL:HG23	1:C:96:LEU:HA	1.96	0.47
1:C:466:GLU:N	1:C:466:GLU:OE1	2.47	0.47
1:A:109:LYS:HD3	1:A:173:TYR:CD1	2.50	0.47
1:A:473:GLN:OE1	1:A:473:GLN:N	2.32	0.47
1:C:679:THR:HB	1:C:682:PHE:HB2	1.97	0.47
1:D:134:TYR:OH	1:D:156:GLY:O	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLU:N	1:D:466:GLU:OE1	2.47	0.47
1:E:109:LYS:HD3	1:E:173:TYR:CD1	2.50	0.47
1:E:284:SER:O	1:E:288:LYS:HG2	2.14	0.47
1:F:37:SER:O	1:F:38:VAL:HG23	2.14	0.47
1:F:109:LYS:HD3	1:F:173:TYR:CD1	2.50	0.47
1:F:134:TYR:OH	1:F:156:GLY:O	2.25	0.47
1:A:679:THR:HB	1:A:682:PHE:HB2	1.97	0.47
1:F:114:ILE:HD13	1:F:168:THR:HG23	1.96	0.47
1:F:229:LEU:O	1:F:233:ILE:HG22	2.15	0.47
1:F:288:LYS:HA	1:F:291:GLU:OE2	2.15	0.47
1:F:337:GLN:NE2	1:F:337:GLN:CA	2.73	0.47
1:A:58:LEU:HD22	1:A:103:GLN:NE2	2.30	0.47
1:B:58:LEU:HD22	1:B:103:GLN:NE2	2.30	0.47
1:B:679:THR:HB	1:B:682:PHE:HB2	1.97	0.47
1:E:644:TYR:CE2	1:E:646:PRO:HB3	2.50	0.47
1:F:679:THR:HB	1:F:682:PHE:HB2	1.97	0.47
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.50	0.47
1:B:466:GLU:N	1:B:466:GLU:OE1	2.47	0.47
1:E:136:LYS:HB2	1:E:137:PRO:HD3	1.97	0.47
1:F:627:ASP:OD1	1:F:627:ASP:N	2.46	0.47
1:A:28:VAL:HG23	1:A:96:LEU:HA	1.96	0.46
1:A:229:LEU:O	1:A:233:ILE:HG22	2.15	0.46
1:B:191:ARG:HH21	1:B:195:GLU:HG2	1.79	0.46
1:B:288:LYS:HA	1:B:291:GLU:OE2	2.15	0.46
1:C:58:LEU:HD22	1:C:103:GLN:NE2	2.30	0.46
1:D:109:LYS:HD3	1:D:173:TYR:CD1	2.50	0.46
1:D:700:ARG:O	1:D:704:GLU:N	2.32	0.46
1:E:22:ARG:NH1	1:E:24:ASN:OD1	2.49	0.46
1:E:679:THR:HB	1:E:682:PHE:HB2	1.97	0.46
1:F:58:LEU:HD22	1:F:103:GLN:NE2	2.30	0.46
1:F:136:LYS:HB2	1:F:137:PRO:HD3	1.97	0.46
1:A:114:ILE:HD13	1:A:168:THR:HG23	1.96	0.46
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.96	0.46
1:B:109:LYS:HD3	1:B:173:TYR:CD1	2.50	0.46
1:C:270:ASN:OD1	1:C:272:PRO:HD2	2.16	0.46
1:D:22:ARG:NH1	1:D:24:ASN:OD1	2.49	0.46
1:F:290:PHE:CE2	1:F:331:LEU:HB3	2.51	0.46
1:F:644:TYR:CE2	1:F:646:PRO:HB3	2.50	0.46
1:A:389:LYS:HE3	1:A:443:ASN:O	2.16	0.46
1:B:37:SER:O	1:B:38:VAL:HG23	2.14	0.46
1:C:136:LYS:HB2	1:C:137:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PHE:HZ	1:D:184:CYS:N	2.14	0.46
1:D:644:TYR:CE2	1:D:646:PRO:HB3	2.50	0.46
1:E:37:SER:O	1:E:38:VAL:HG23	2.14	0.46
1:E:288:LYS:HA	1:E:291:GLU:OE2	2.15	0.46
1:B:136:LYS:HB2	1:B:137:PRO:HD3	1.97	0.46
1:C:473:GLN:OE1	1:C:473:GLN:N	2.32	0.46
1:D:58:LEU:HD22	1:D:103:GLN:NE2	2.30	0.46
1:D:288:LYS:HA	1:D:291:GLU:OE2	2.15	0.46
1:E:131:PHE:HZ	1:E:184:CYS:N	2.14	0.46
1:F:22:ARG:NH1	1:F:24:ASN:OD1	2.49	0.46
1:F:689:GLU:HA	1:F:692:GLN:HB2	1.97	0.46
1:A:270:ASN:OD1	1:A:272:PRO:HD2	2.16	0.46
1:A:689:GLU:HA	1:A:692:GLN:HB2	1.97	0.46
1:B:229:LEU:O	1:B:233:ILE:HG22	2.15	0.46
1:B:389:LYS:HE3	1:B:443:ASN:O	2.16	0.46
1:B:644:TYR:CE2	1:B:646:PRO:HB3	2.50	0.46
1:E:229:LEU:O	1:E:233:ILE:HG22	2.15	0.46
1:F:270:ASN:OD1	1:F:272:PRO:HD2	2.15	0.46
1:A:290:PHE:CE2	1:A:331:LEU:HB3	2.51	0.46
1:B:270:ASN:OD1	1:B:272:PRO:HD2	2.16	0.46
1:C:22:ARG:NH1	1:C:24:ASN:OD1	2.49	0.46
1:C:33:ASN:OD1	1:C:35:ASP:N	2.31	0.46
1:C:229:LEU:O	1:C:233:ILE:HG22	2.15	0.46
1:C:288:LYS:HA	1:C:291:GLU:OE2	2.15	0.46
1:C:290:PHE:CE2	1:C:331:LEU:HB3	2.51	0.46
1:D:270:ASN:OD1	1:D:272:PRO:HD2	2.16	0.46
1:E:58:LEU:HD22	1:E:103:GLN:NE2	2.30	0.46
1:F:389:LYS:HE3	1:F:443:ASN:O	2.16	0.46
1:B:131:PHE:HZ	1:B:184:CYS:N	2.14	0.46
1:D:229:LEU:O	1:D:233:ILE:HG22	2.15	0.46
1:D:489:LEU:O	1:D:493:VAL:HG22	2.16	0.46
1:A:22:ARG:NH1	1:A:24:ASN:OD1	2.49	0.46
1:A:294:GLU:HG3	1:A:338:ARG:CG	2.46	0.46
1:A:493:VAL:HG23	1:A:494:GLN:N	2.31	0.46
1:B:689:GLU:HA	1:B:692:GLN:HB2	1.97	0.46
1:E:290:PHE:CE2	1:E:331:LEU:HB3	2.51	0.46
1:E:364:ASP:OD1	1:E:364:ASP:N	2.35	0.46
1:F:294:GLU:HG3	1:F:338:ARG:CG	2.46	0.46
1:A:131:PHE:HZ	1:A:184:CYS:N	2.14	0.46
1:A:288:LYS:HA	1:A:291:GLU:OE2	2.15	0.46
1:A:627:ASP:OD1	1:A:627:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:NH1	1:B:24:ASN:OD1	2.49	0.46
1:C:441:VAL:O	1:C:444:SER:OG	2.28	0.46
1:C:689:GLU:HA	1:C:692:GLN:HB2	1.97	0.46
1:D:290:PHE:CE2	1:D:331:LEU:HB3	2.51	0.46
1:E:294:GLU:HG3	1:E:338:ARG:CG	2.46	0.46
1:E:627:ASP:OD1	1:E:627:ASP:N	2.46	0.46
1:F:131:PHE:HZ	1:F:184:CYS:N	2.14	0.46
1:C:389:LYS:HE3	1:C:443:ASN:O	2.16	0.46
1:C:644:TYR:CE2	1:C:646:PRO:HB3	2.50	0.46
1:E:270:ASN:OD1	1:E:272:PRO:HD2	2.16	0.46
1:F:493:VAL:HG23	1:F:494:GLN:N	2.31	0.46
1:A:136:LYS:HB2	1:A:137:PRO:HD3	1.97	0.45
1:C:148:LYS:HE3	1:C:167:GLU:HA	1.98	0.45
1:C:489:LEU:O	1:C:493:VAL:HG22	2.16	0.45
1:D:136:LYS:HB2	1:D:137:PRO:HD3	1.97	0.45
1:E:43:GLN:HB3	1:E:44:PRO:HD3	1.99	0.45
1:E:389:LYS:HE3	1:E:443:ASN:O	2.16	0.45
1:A:176:VAL:HG13	1:A:180:THR:HG21	1.99	0.45
1:C:131:PHE:HZ	1:C:184:CYS:N	2.14	0.45
1:D:689:GLU:HA	1:D:692:GLN:HB2	1.97	0.45
1:E:176:VAL:HG13	1:E:180:THR:HG21	1.99	0.45
1:E:489:LEU:O	1:E:493:VAL:HG22	2.16	0.45
1:E:661:LEU:O	1:E:664:SER:O	2.35	0.45
1:F:43:GLN:HB3	1:F:44:PRO:HD3	1.99	0.45
1:D:148:LYS:HE3	1:D:167:GLU:HA	1.98	0.45
1:D:389:LYS:HE3	1:D:443:ASN:O	2.16	0.45
1:F:176:VAL:HG13	1:F:180:THR:HG21	1.99	0.45
1:B:290:PHE:CE2	1:B:331:LEU:HB3	2.51	0.45
1:E:689:GLU:HA	1:E:692:GLN:HB2	1.97	0.45
1:F:661:LEU:O	1:F:664:SER:O	2.35	0.45
1:A:112:LYS:O	1:A:181:VAL:HG12	2.17	0.45
1:B:148:LYS:HE3	1:B:167:GLU:HA	1.99	0.45
1:B:323:ARG:NH1	1:C:278:LEU:HD23	2.32	0.45
1:D:323:ARG:NH1	1:E:278:LEU:HD23	2.32	0.45
1:F:118:PRO:HG3	1:F:130:LEU:HD22	1.99	0.45
1:B:294:GLU:HG3	1:B:338:ARG:CG	2.46	0.45
1:B:459:SER:O	1:B:462:SER:HB2	2.17	0.45
1:B:493:VAL:HG23	1:B:494:GLN:N	2.31	0.45
1:D:176:VAL:HG13	1:D:180:THR:HG21	1.99	0.45
1:D:294:GLU:HG3	1:D:338:ARG:CG	2.46	0.45
1:E:474:VAL:HG23	1:E:478:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD23	1:F:323:ARG:NH1	2.31	0.45
1:B:140:LEU:HB3	1:B:141:GLU:OE1	2.17	0.45
1:D:118:PRO:HG3	1:D:130:LEU:HD22	1.99	0.45
1:D:140:LEU:HB3	1:D:141:GLU:OE1	2.17	0.45
1:E:118:PRO:HG3	1:E:130:LEU:HD22	1.99	0.45
1:E:140:LEU:HB3	1:E:141:GLU:OE1	2.17	0.45
1:E:148:LYS:HE3	1:E:167:GLU:HA	1.98	0.45
1:F:474:VAL:HG23	1:F:478:ASP:HB2	1.99	0.45
1:B:43:GLN:HB3	1:B:44:PRO:HD3	1.99	0.45
1:B:176:VAL:HG13	1:B:180:THR:HG21	1.99	0.45
1:B:661:LEU:O	1:B:664:SER:O	2.35	0.45
1:C:176:VAL:HG13	1:C:180:THR:HG21	1.99	0.45
1:C:459:SER:O	1:C:462:SER:HB2	2.17	0.45
1:D:112:LYS:O	1:D:181:VAL:HG12	2.17	0.45
1:D:474:VAL:HG23	1:D:478:ASP:HB2	1.99	0.45
1:D:627:ASP:OD1	1:D:627:ASP:N	2.46	0.45
1:A:118:PRO:HG3	1:A:130:LEU:HD22	1.99	0.45
1:B:489:LEU:O	1:B:493:VAL:HG22	2.16	0.45
1:C:140:LEU:HB3	1:C:141:GLU:OE1	2.17	0.45
1:D:364:ASP:OD1	1:D:364:ASP:N	2.35	0.45
1:D:441:VAL:O	1:D:444:SER:OG	2.28	0.45
1:E:493:VAL:HG23	1:E:494:GLN:N	2.31	0.45
1:F:140:LEU:HB3	1:F:141:GLU:OE1	2.17	0.45
1:A:661:LEU:O	1:A:664:SER:O	2.35	0.45
1:C:493:VAL:HG23	1:C:494:GLN:N	2.31	0.45
1:C:43:GLN:HB3	1:C:44:PRO:HD3	1.99	0.44
1:C:112:LYS:O	1:C:181:VAL:HG12	2.17	0.44
1:D:493:VAL:HG23	1:D:494:GLN:N	2.31	0.44
1:C:130:LEU:HD11	1:C:163:PHE:HZ	1.83	0.44
1:C:469:VAL:HG22	1:C:540:ILE:HG12	2.00	0.44
1:D:33:ASN:OD1	1:D:35:ASP:N	2.31	0.44
1:E:45:LYS:HG2	1:E:80:GLU:OE2	2.18	0.44
1:F:489:LEU:O	1:F:493:VAL:HG22	2.16	0.44
1:A:45:LYS:HG2	1:A:80:GLU:OE2	2.18	0.44
1:A:474:VAL:HG23	1:A:478:ASP:HB2	1.99	0.44
1:C:96:LEU:HD13	1:C:261:GLU:OE2	2.18	0.44
1:D:136:LYS:O	1:D:140:LEU:HD13	2.18	0.44
1:D:459:SER:O	1:D:462:SER:HB2	2.17	0.44
1:F:112:LYS:O	1:F:181:VAL:HG12	2.17	0.44
1:A:489:LEU:O	1:A:493:VAL:HG22	2.16	0.44
1:B:33:ASN:OD1	1:B:35:ASP:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PRO:HG3	1:B:130:LEU:HD22	1.99	0.44
1:B:469:VAL:HG22	1:B:540:ILE:HG12	2.00	0.44
1:C:118:PRO:HG3	1:C:130:LEU:HD22	1.99	0.44
1:C:474:VAL:HG23	1:C:478:ASP:HB2	1.99	0.44
1:D:45:LYS:HG2	1:D:80:GLU:OE2	2.18	0.44
1:D:469:VAL:HG22	1:D:540:ILE:HG12	2.00	0.44
1:A:43:GLN:HB3	1:A:44:PRO:HD3	1.99	0.44
1:C:45:LYS:HG2	1:C:80:GLU:OE2	2.18	0.44
1:E:96:LEU:HD13	1:E:261:GLU:OE2	2.18	0.44
1:C:136:LYS:O	1:C:140:LEU:HD13	2.18	0.44
1:D:43:GLN:HB3	1:D:44:PRO:HD3	1.98	0.44
1:F:96:LEU:HD13	1:F:261:GLU:OE2	2.18	0.44
1:A:96:LEU:HD13	1:A:261:GLU:OE2	2.18	0.44
1:A:323:ARG:NH1	1:B:278:LEU:HD23	2.33	0.44
1:B:45:LYS:HG2	1:B:80:GLU:OE2	2.18	0.44
1:B:59:LEU:O	1:B:66:GLU:HA	2.18	0.44
1:C:294:GLU:HG3	1:C:338:ARG:CG	2.46	0.44
1:C:661:LEU:O	1:C:664:SER:O	2.35	0.44
1:D:130:LEU:HD11	1:D:163:PHE:HZ	1.83	0.44
1:F:45:LYS:HG2	1:F:80:GLU:OE2	2.18	0.44
1:F:148:LYS:HE3	1:F:167:GLU:HA	1.98	0.44
1:B:109:LYS:HD2	1:B:173:TYR:C	2.43	0.44
1:D:96:LEU:HD13	1:D:261:GLU:OE2	2.18	0.44
1:A:109:LYS:HD2	1:A:173:TYR:C	2.43	0.44
1:A:148:LYS:HE3	1:A:167:GLU:HA	1.99	0.44
1:A:459:SER:O	1:A:462:SER:HB2	2.17	0.44
1:D:661:LEU:O	1:D:664:SER:O	2.35	0.44
1:E:323:ARG:NH1	1:F:278:LEU:HD23	2.32	0.44
1:E:469:VAL:HG22	1:E:540:ILE:HG12	2.00	0.44
1:F:109:LYS:HD2	1:F:173:TYR:C	2.43	0.44
1:F:136:LYS:O	1:F:140:LEU:HD13	2.18	0.44
1:A:469:VAL:HG22	1:A:540:ILE:HG12	2.00	0.43
1:B:112:LYS:O	1:B:181:VAL:HG12	2.17	0.43
1:B:130:LEU:HD11	1:B:163:PHE:HZ	1.83	0.43
1:C:59:LEU:O	1:C:66:GLU:HA	2.18	0.43
1:C:109:LYS:HD2	1:C:173:TYR:C	2.43	0.43
1:D:109:LYS:HD2	1:D:173:TYR:C	2.43	0.43
1:E:112:LYS:O	1:E:181:VAL:HG12	2.17	0.43
1:E:473:GLN:OE1	1:E:473:GLN:N	2.32	0.43
1:A:136:LYS:O	1:A:140:LEU:HD13	2.18	0.43
1:A:140:LEU:HB3	1:A:141:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:O	1:B:82:ILE:HG22	2.19	0.43
1:B:136:LYS:O	1:B:140:LEU:HD13	2.18	0.43
1:C:206:ILE:HG12	1:C:253:LEU:HD23	2.01	0.43
1:C:323:ARG:NH1	1:D:278:LEU:HD23	2.33	0.43
1:D:59:LEU:O	1:D:66:GLU:HA	2.18	0.43
1:F:59:LEU:O	1:F:66:GLU:HA	2.18	0.43
1:F:459:SER:O	1:F:462:SER:HB2	2.17	0.43
1:B:307:ASP:N	1:B:307:ASP:OD1	2.51	0.43
1:C:192:GLU:OE1	1:C:192:GLU:N	2.52	0.43
1:C:389:LYS:HZ2	1:C:446:ALA:HB2	1.83	0.43
1:E:59:LEU:O	1:E:66:GLU:HA	2.18	0.43
1:E:115:HIS:NE2	1:E:185:GLU:HG2	2.34	0.43
1:B:96:LEU:HD13	1:B:261:GLU:OE2	2.18	0.43
1:B:115:HIS:NE2	1:B:185:GLU:HG2	2.34	0.43
1:B:474:VAL:HG23	1:B:478:ASP:HB2	1.99	0.43
1:E:130:LEU:HD11	1:E:163:PHE:HZ	1.83	0.43
1:E:441:VAL:O	1:E:444:SER:OG	2.28	0.43
1:F:206:ILE:HG12	1:F:253:LEU:HD23	2.00	0.43
1:F:469:VAL:HG22	1:F:540:ILE:HG12	2.00	0.43
1:B:143:TYR:CE1	1:B:178:PRO:HD3	2.49	0.43
1:B:206:ILE:HG12	1:B:253:LEU:HD23	2.01	0.43
1:C:143:TYR:CE1	1:C:178:PRO:HD3	2.48	0.43
1:D:27:ILE:O	1:D:82:ILE:HG22	2.19	0.43
1:E:206:ILE:HG12	1:E:253:LEU:HD23	2.00	0.43
1:E:459:SER:O	1:E:462:SER:HB2	2.17	0.43
1:E:500:PRO:O	1:E:504:LEU:HD13	2.19	0.43
1:F:307:ASP:OD1	1:F:307:ASP:N	2.51	0.43
1:F:473:GLN:OE1	1:F:473:GLN:N	2.32	0.43
1:A:130:LEU:HD11	1:A:163:PHE:HZ	1.83	0.43
1:B:41:LEU:C	1:B:74:ASP:HB3	2.44	0.43
1:B:82:ILE:HG12	1:B:84:MET:HG3	2.00	0.43
1:E:109:LYS:HD2	1:E:173:TYR:C	2.43	0.43
1:E:136:LYS:O	1:E:140:LEU:HD13	2.18	0.43
1:F:315:LYS:NZ	1:F:321:GLU:OE2	2.43	0.43
1:F:684:GLY:HA3	2:F:900:ADP:C8	2.54	0.43
1:A:41:LEU:C	1:A:74:ASP:HB3	2.44	0.43
1:A:206:ILE:HG12	1:A:253:LEU:HD23	2.01	0.43
1:A:429:LEU:HD12	1:A:430:ILE:N	2.34	0.43
1:A:441:VAL:O	1:A:444:SER:OG	2.28	0.43
1:A:684:GLY:HA3	2:A:900:ADP:C8	2.54	0.43
1:B:130:LEU:HD11	1:B:163:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HA	1:B:304:ASP:HB3	2.00	0.43
1:D:270:ASN:HA	1:D:304:ASP:HB3	2.00	0.43
1:D:294:GLU:CG	1:D:338:ARG:CG	2.97	0.43
1:D:500:PRO:O	1:D:504:LEU:HD13	2.19	0.43
1:D:758:PHE:O	1:D:761:THR:OG1	2.29	0.43
1:F:130:LEU:HD11	1:F:163:PHE:HZ	1.83	0.43
1:F:192:GLU:N	1:F:192:GLU:OE1	2.52	0.43
1:A:59:LEU:O	1:A:66:GLU:HA	2.18	0.43
1:A:115:HIS:NE2	1:A:185:GLU:HG2	2.34	0.43
1:A:216:ILE:O	1:A:220:VAL:HG22	2.19	0.43
1:B:684:GLY:HA3	2:B:900:ADP:C8	2.54	0.43
1:C:429:LEU:HD12	1:C:430:ILE:N	2.34	0.43
1:D:115:HIS:NE2	1:D:185:GLU:HG2	2.34	0.43
1:D:684:GLY:HA3	2:D:900:ADP:C8	2.54	0.43
1:E:143:TYR:CE1	1:E:178:PRO:HD3	2.48	0.43
1:E:270:ASN:HA	1:E:304:ASP:HB3	2.00	0.43
1:F:216:ILE:O	1:F:220:VAL:HG22	2.19	0.43
1:F:500:PRO:O	1:F:504:LEU:HD13	2.19	0.43
1:A:192:GLU:N	1:A:192:GLU:OE1	2.52	0.43
1:B:192:GLU:N	1:B:192:GLU:OE1	2.52	0.43
1:C:294:GLU:CG	1:C:338:ARG:CG	2.97	0.43
1:D:41:LEU:C	1:D:74:ASP:HB3	2.44	0.43
1:D:206:ILE:HG12	1:D:253:LEU:HD23	2.01	0.43
1:A:130:LEU:HD11	1:A:163:PHE:CZ	2.54	0.43
1:B:429:LEU:HD12	1:B:430:ILE:N	2.34	0.43
1:E:684:GLY:HA3	2:E:900:ADP:C8	2.54	0.43
1:F:82:ILE:HG12	1:F:84:MET:HG3	2.01	0.43
1:F:115:HIS:NE2	1:F:185:GLU:HG2	2.34	0.43
1:F:130:LEU:HD11	1:F:163:PHE:CZ	2.54	0.43
1:F:393:ASP:OD1	1:F:393:ASP:N	2.52	0.43
1:B:294:GLU:CG	1:B:338:ARG:CG	2.97	0.42
1:C:41:LEU:C	1:C:74:ASP:HB3	2.44	0.42
1:D:130:LEU:HD11	1:D:163:PHE:CZ	2.54	0.42
1:D:389:LYS:HZ2	1:D:446:ALA:HB2	1.83	0.42
1:E:41:LEU:C	1:E:74:ASP:HB3	2.44	0.42
1:E:429:LEU:HD12	1:E:430:ILE:N	2.34	0.42
1:F:429:LEU:HD12	1:F:430:ILE:N	2.34	0.42
1:A:127:THR:CB	1:A:438:ASP:HA	2.37	0.42
1:A:270:ASN:HA	1:A:304:ASP:HB3	2.00	0.42
1:C:27:ILE:O	1:C:82:ILE:HG22	2.19	0.42
1:D:109:LYS:HE2	1:D:174:CYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PRO:HB2	1:D:173:TYR:HD2	1.84	0.42
1:E:130:LEU:HD11	1:E:163:PHE:CZ	2.54	0.42
1:A:27:ILE:O	1:A:82:ILE:HG22	2.19	0.42
1:A:307:ASP:OD1	1:A:307:ASP:N	2.51	0.42
1:C:130:LEU:HD11	1:C:163:PHE:CZ	2.54	0.42
1:D:113:ARG:NH2	1:D:183:HIS:CD2	2.88	0.42
1:D:192:GLU:N	1:D:192:GLU:OE1	2.52	0.42
1:E:113:ARG:NH2	1:E:183:HIS:CD2	2.88	0.42
1:E:170:PRO:HB2	1:E:173:TYR:HD2	1.84	0.42
1:F:27:ILE:O	1:F:82:ILE:HG22	2.19	0.42
1:F:113:ARG:NH2	1:F:183:HIS:CD2	2.88	0.42
1:A:82:ILE:HG12	1:A:84:MET:HG3	2.00	0.42
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.54	0.42
1:A:500:PRO:O	1:A:504:LEU:HD13	2.19	0.42
1:B:216:ILE:O	1:B:220:VAL:HG22	2.19	0.42
1:C:307:ASP:OD1	1:C:307:ASP:N	2.51	0.42
1:C:500:PRO:O	1:C:504:LEU:HD13	2.19	0.42
1:D:82:ILE:HG12	1:D:84:MET:HG3	2.00	0.42
1:D:429:LEU:HD12	1:D:430:ILE:N	2.34	0.42
1:E:82:ILE:HG12	1:E:84:MET:HG3	2.00	0.42
1:E:109:LYS:HE2	1:E:174:CYS:O	2.19	0.42
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.54	0.42
1:E:216:ILE:O	1:E:220:VAL:HG22	2.19	0.42
1:E:682:PHE:CZ	1:E:743:ALA:HB1	2.55	0.42
1:E:750:ASN:HA	1:E:753:ARG:HG2	2.02	0.42
1:F:120:ASP:OD1	1:F:120:ASP:N	2.52	0.42
1:F:187:GLU:O	1:F:187:GLU:HG2	2.19	0.42
1:B:109:LYS:HE2	1:B:174:CYS:O	2.19	0.42
1:C:115:HIS:NE2	1:C:185:GLU:HG2	2.34	0.42
1:D:203:TYR:CE2	1:D:261:GLU:HG2	2.54	0.42
1:E:307:ASP:N	1:E:307:ASP:OD1	2.51	0.42
1:F:109:LYS:HE2	1:F:174:CYS:O	2.19	0.42
1:F:682:PHE:CZ	1:F:743:ALA:HB1	2.55	0.42
1:A:187:GLU:O	1:A:187:GLU:HG2	2.19	0.42
1:A:294:GLU:CG	1:A:338:ARG:CG	2.97	0.42
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.54	0.42
1:B:652:SER:O	1:B:655:ALA:N	2.53	0.42
1:B:758:PHE:O	1:B:761:THR:OG1	2.29	0.42
1:C:114:ILE:HG22	1:C:116:VAL:HG13	2.02	0.42
1:C:652:SER:O	1:C:655:ALA:N	2.53	0.42
1:D:393:ASP:OD1	1:D:393:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:682:PHE:CZ	1:D:743:ALA:HB1	2.55	0.42
1:E:27:ILE:O	1:E:82:ILE:HG22	2.19	0.42
1:E:192:GLU:N	1:E:192:GLU:OE1	2.52	0.42
1:F:41:LEU:C	1:F:74:ASP:HB3	2.44	0.42
1:F:294:GLU:CG	1:F:338:ARG:CG	2.97	0.42
1:A:109:LYS:HE2	1:A:174:CYS:O	2.19	0.42
1:A:652:SER:O	1:A:655:ALA:N	2.53	0.42
1:B:500:PRO:O	1:B:504:LEU:HD13	2.19	0.42
1:C:113:ARG:NH2	1:C:183:HIS:CD2	2.88	0.42
1:C:393:ASP:OD1	1:C:393:ASP:N	2.52	0.42
1:C:750:ASN:HA	1:C:753:ARG:HG2	2.02	0.42
1:D:750:ASN:HA	1:D:753:ARG:HG2	2.02	0.42
1:E:294:GLU:CG	1:E:338:ARG:CG	2.97	0.42
1:E:393:ASP:OD1	1:E:393:ASP:N	2.52	0.42
1:F:750:ASN:HA	1:F:753:ARG:HG2	2.02	0.42
1:A:114:ILE:HG22	1:A:116:VAL:HG13	2.02	0.42
1:A:143:TYR:CE1	1:A:178:PRO:HD3	2.49	0.42
1:B:114:ILE:HG22	1:B:116:VAL:HG13	2.02	0.42
1:B:120:ASP:N	1:B:120:ASP:OD1	2.52	0.42
1:C:82:ILE:HG12	1:C:84:MET:HG3	2.00	0.42
1:C:109:LYS:HE2	1:C:174:CYS:O	2.19	0.42
1:C:170:PRO:HB2	1:C:173:TYR:HD2	1.84	0.42
1:C:216:ILE:O	1:C:220:VAL:HG22	2.19	0.42
1:C:684:GLY:HA3	2:C:900:ADP:C8	2.54	0.42
1:D:652:SER:O	1:D:655:ALA:N	2.53	0.42
1:F:114:ILE:HG22	1:F:116:VAL:HG13	2.02	0.42
1:F:652:SER:O	1:F:655:ALA:N	2.53	0.42
1:B:170:PRO:HB2	1:B:173:TYR:HD2	1.84	0.42
1:B:187:GLU:HG2	1:B:187:GLU:O	2.19	0.42
1:B:750:ASN:HA	1:B:753:ARG:HG2	2.02	0.42
1:C:270:ASN:HA	1:C:304:ASP:HB3	2.00	0.42
1:D:187:GLU:O	1:D:187:GLU:HG2	2.19	0.42
1:D:216:ILE:O	1:D:220:VAL:HG22	2.19	0.42
1:E:120:ASP:OD1	1:E:120:ASP:N	2.52	0.42
1:F:270:ASN:HA	1:F:304:ASP:HB3	2.00	0.42
1:A:113:ARG:NH2	1:A:183:HIS:CD2	2.88	0.41
1:A:170:PRO:HB2	1:A:173:TYR:HD2	1.84	0.41
1:A:393:ASP:OD1	1:A:393:ASP:N	2.52	0.41
1:D:114:ILE:HG22	1:D:116:VAL:HG13	2.02	0.41
1:E:42:SER:HB2	1:E:45:LYS:HZ3	1.85	0.41
1:C:682:PHE:CZ	1:C:743:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:GLU:O	1:F:401:ASN:N	2.39	0.41
1:F:476:TRP:CZ3	1:F:486:LYS:HG2	2.55	0.41
1:A:682:PHE:CZ	1:A:743:ALA:HB1	2.55	0.41
1:B:517:TYR:HA	1:B:623:THR:O	2.20	0.41
1:E:652:SER:O	1:E:655:ALA:N	2.53	0.41
1:F:203:TYR:CE2	1:F:261:GLU:HG2	2.54	0.41
1:A:519:PRO:HD2	1:A:645:ILE:O	2.21	0.41
1:A:750:ASN:HA	1:A:753:ARG:HG2	2.02	0.41
1:B:113:ARG:NH2	1:B:183:HIS:CD2	2.88	0.41
1:D:395:ASP:HB2	1:D:397:GLU:OE1	2.21	0.41
1:D:580:ASP:HB3	1:D:629:ILE:HD11	2.02	0.41
1:F:170:PRO:HB2	1:F:173:TYR:HD2	1.84	0.41
1:B:682:PHE:CZ	1:B:743:ALA:HB1	2.55	0.41
1:C:580:ASP:HB3	1:C:629:ILE:HD11	2.02	0.41
1:D:120:ASP:OD1	1:D:120:ASP:N	2.52	0.41
1:E:114:ILE:HG22	1:E:116:VAL:HG13	2.02	0.41
1:B:395:ASP:HB2	1:B:397:GLU:OE1	2.21	0.41
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.54	0.41
1:C:395:ASP:HB2	1:C:397:GLU:OE1	2.21	0.41
1:D:55:ASP:OD1	1:D:71:VAL:HG22	2.21	0.41
1:D:517:TYR:HA	1:D:623:THR:O	2.20	0.41
1:E:187:GLU:O	1:E:187:GLU:HG2	2.19	0.41
1:E:476:TRP:CZ3	1:E:486:LYS:HG2	2.55	0.41
1:E:517:TYR:HA	1:E:623:THR:O	2.20	0.41
1:C:55:ASP:OD1	1:C:71:VAL:HG22	2.21	0.41
1:C:517:TYR:HA	1:C:623:THR:O	2.20	0.41
1:D:397:GLU:H	1:D:397:GLU:CD	2.28	0.41
1:F:38:VAL:HA	1:F:70:ILE:O	2.21	0.41
1:A:38:VAL:HA	1:A:70:ILE:O	2.21	0.41
1:A:476:TRP:CZ3	1:A:486:LYS:HG2	2.55	0.41
1:B:38:VAL:HA	1:B:70:ILE:O	2.21	0.41
1:C:187:GLU:O	1:C:187:GLU:HG2	2.19	0.41
1:D:657:LEU:HD23	1:D:657:LEU:HA	1.92	0.41
1:E:519:PRO:HD2	1:E:645:ILE:O	2.21	0.41
1:F:127:THR:CB	1:F:438:ASP:HA	2.37	0.41
1:F:517:TYR:HA	1:F:623:THR:O	2.20	0.41
1:A:290:PHE:CD2	1:A:331:LEU:HB3	2.56	0.41
1:A:395:ASP:HB2	1:A:397:GLU:OE1	2.21	0.41
1:A:517:TYR:HA	1:A:623:THR:O	2.20	0.41
1:B:55:ASP:OD1	1:B:71:VAL:HG22	2.21	0.41
1:B:482:LEU:O	1:B:486:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:TYR:CE1	1:D:178:PRO:HD3	2.49	0.41
1:D:377:ARG:NE	1:D:403:THR:O	2.54	0.41
1:D:476:TRP:CZ3	1:D:486:LYS:HG2	2.55	0.41
1:E:55:ASP:OD1	1:E:71:VAL:HG22	2.21	0.41
1:F:519:PRO:HD2	1:F:645:ILE:O	2.21	0.41
1:A:109:LYS:O	1:A:175:ILE:HB	2.21	0.41
1:A:688:THR:O	1:A:692:GLN:HG3	2.21	0.41
1:B:127:THR:CB	1:B:438:ASP:HA	2.37	0.41
1:B:290:PHE:CD2	1:B:331:LEU:HB3	2.56	0.41
1:B:441:VAL:O	1:B:444:SER:OG	2.28	0.41
1:C:120:ASP:OD1	1:C:120:ASP:N	2.52	0.41
1:D:688:THR:O	1:D:692:GLN:HG3	2.21	0.41
1:B:377:ARG:NE	1:B:403:THR:O	2.54	0.40
1:B:580:ASP:HB3	1:B:629:ILE:HD11	2.02	0.40
1:C:397:GLU:H	1:C:397:GLU:CD	2.28	0.40
1:C:476:TRP:CZ3	1:C:486:LYS:HG2	2.55	0.40
1:C:519:PRO:HD2	1:C:645:ILE:O	2.21	0.40
1:D:482:LEU:O	1:D:486:LYS:HG3	2.21	0.40
1:E:377:ARG:NE	1:E:403:THR:O	2.54	0.40
1:E:395:ASP:HB2	1:E:397:GLU:OE1	2.21	0.40
1:F:310:ALA:HA	1:F:325:VAL:HG22	2.03	0.40
1:F:669:ASP:N	1:F:669:ASP:OD1	2.54	0.40
1:A:580:ASP:HB3	1:A:629:ILE:HD11	2.02	0.40
1:B:519:PRO:HD2	1:B:645:ILE:O	2.21	0.40
1:C:290:PHE:CD2	1:C:331:LEU:HB3	2.56	0.40
1:C:426:LYS:HD2	1:C:426:LYS:HA	1.88	0.40
1:E:580:ASP:HB3	1:E:629:ILE:HD11	2.02	0.40
1:F:438:ASP:HB2	1:F:440:GLU:CD	2.47	0.40
1:F:688:THR:O	1:F:692:GLN:HG3	2.21	0.40
1:A:482:LEU:O	1:A:486:LYS:HG3	2.21	0.40
1:B:109:LYS:O	1:B:175:ILE:HB	2.22	0.40
1:B:476:TRP:CZ3	1:B:486:LYS:HG2	2.55	0.40
1:B:688:THR:O	1:B:692:GLN:HG3	2.21	0.40
1:E:349:ARG:HA	1:E:350:PRO:HD3	1.97	0.40
1:E:438:ASP:HB2	1:E:440:GLU:CD	2.47	0.40
1:F:55:ASP:OD1	1:F:71:VAL:HG22	2.21	0.40
1:F:580:ASP:HB3	1:F:629:ILE:HD11	2.02	0.40
1:A:377:ARG:NE	1:A:403:THR:O	2.54	0.40
1:A:426:LYS:HD2	1:A:426:LYS:HA	1.88	0.40
1:D:307:ASP:OD1	1:D:307:ASP:N	2.51	0.40
1:D:438:ASP:HB2	1:D:440:GLU:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:PRO:HD2	1:D:645:ILE:O	2.21	0.40
1:A:55:ASP:OD1	1:A:71:VAL:HG22	2.21	0.40
1:B:315:LYS:NZ	1:B:321:GLU:OE2	2.42	0.40
1:E:482:LEU:O	1:E:486:LYS:HG3	2.21	0.40
1:F:143:TYR:CE1	1:F:178:PRO:HD3	2.48	0.40
1:F:377:ARG:NE	1:F:403:THR:O	2.54	0.40
1:F:395:ASP:HB2	1:F:397:GLU:OE1	2.21	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	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	18	49
1	B	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	18	49
1	C	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	18	49
1	D	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	18	49
1	E	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	18	49
1	F	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	18	49
All	All	4314/4836 (89%)	4020 (93%)	264 (6%)	30 (1%)	20	49

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ASP
1	B	169	ASP
1	C	169	ASP
1	D	169	ASP
1	E	169	ASP

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Mol	Chain	Res	Type
1	F	169	ASP
1	A	339	ALA
1	B	339	ALA
1	C	339	ALA
1	D	339	ALA
1	E	339	ALA
1	F	339	ALA
1	A	170	PRO
1	B	170	PRO
1	C	170	PRO
1	D	170	PRO
1	E	170	PRO
1	F	170	PRO
1	A	315	LYS
1	B	315	LYS
1	C	315	LYS
1	D	315	LYS
1	E	315	LYS
1	F	315	LYS
1	A	172	PRO
1	B	172	PRO
1	C	172	PRO
1	D	172	PRO
1	E	172	PRO
1	F	172	PRO

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	615/678 (91%)	615 (100%)	0	100	100
1	B	615/678 (91%)	615 (100%)	0	100	100
1	C	615/678 (91%)	615 (100%)	0	100	100
1	D	615/678 (91%)	615 (100%)	0	100	100
1	E	615/678 (91%)	615 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	615/678 (91%)	615 (100%)	0	100	100
All	All	3690/4068 (91%)	3690 (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 (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	115	HIS
1	A	183	HIS
1	A	285	ASN
1	A	337	GLN
1	A	340	HIS
1	A	384	HIS
1	A	533	ASN
1	B	36	ASN
1	B	115	HIS
1	B	183	HIS
1	B	285	ASN
1	B	337	GLN
1	B	340	HIS
1	B	384	HIS
1	B	533	ASN
1	C	36	ASN
1	C	115	HIS
1	C	183	HIS
1	C	285	ASN
1	C	337	GLN
1	C	340	HIS
1	C	384	HIS
1	C	499	HIS
1	C	533	ASN
1	D	36	ASN
1	D	115	HIS
1	D	183	HIS
1	D	285	ASN
1	D	337	GLN
1	D	340	HIS
1	D	384	HIS
1	D	533	ASN

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Mol	Chain	Res	Type
1	E	36	ASN
1	E	115	HIS
1	E	183	HIS
1	E	285	ASN
1	E	337	GLN
1	E	340	HIS
1	E	384	HIS
1	E	533	ASN
1	F	36	ASN
1	F	115	HIS
1	F	183	HIS
1	F	285	ASN
1	F	337	GLN
1	F	340	HIS
1	F	384	HIS
1	F	533	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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	ADP	E	807	-	28,29,29	1.41	5 (17%)	43,45,45	1.97	11 (25%)
2	ADP	F	807	-	28,29,29	1.40	5 (17%)	43,45,45	1.97	11 (25%)
2	ADP	C	900	-	28,29,29	1.35	5 (17%)	43,45,45	1.84	9 (20%)
2	ADP	E	900	-	28,29,29	1.34	5 (17%)	43,45,45	1.83	9 (20%)
2	ADP	F	900	-	28,29,29	1.34	5 (17%)	43,45,45	1.84	9 (20%)
2	ADP	C	807	-	28,29,29	1.40	5 (17%)	43,45,45	1.97	11 (25%)
2	ADP	D	807	-	28,29,29	1.40	5 (17%)	43,45,45	1.97	11 (25%)
2	ADP	D	900	-	28,29,29	1.35	5 (17%)	43,45,45	1.84	9 (20%)
2	ADP	A	807	-	28,29,29	1.41	5 (17%)	43,45,45	1.97	11 (25%)
2	ADP	A	900	-	28,29,29	1.35	5 (17%)	43,45,45	1.84	9 (20%)
2	ADP	B	900	-	28,29,29	1.35	5 (17%)	43,45,45	1.84	9 (20%)
2	ADP	B	807	-	28,29,29	1.41	5 (17%)	43,45,45	1.97	11 (25%)

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	ADP	E	807	-	-	2/16/32/32	0/3/3/3
2	ADP	F	807	-	-	2/16/32/32	0/3/3/3
2	ADP	C	900	-	-	3/16/32/32	0/3/3/3
2	ADP	E	900	-	-	3/16/32/32	0/3/3/3
2	ADP	F	900	-	-	3/16/32/32	0/3/3/3
2	ADP	C	807	-	-	2/16/32/32	0/3/3/3
2	ADP	D	807	-	-	2/16/32/32	0/3/3/3
2	ADP	D	900	-	-	3/16/32/32	0/3/3/3
2	ADP	A	807	-	-	2/16/32/32	0/3/3/3
2	ADP	A	900	-	-	3/16/32/32	0/3/3/3
2	ADP	B	900	-	-	3/16/32/32	0/3/3/3
2	ADP	B	807	-	-	2/16/32/32	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	ADP	C5-C4	3.89	1.46	1.39
2	F	900	ADP	C5-C4	3.89	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ADP	C5-C4	3.89	1.46	1.39
2	D	900	ADP	C5-C4	3.89	1.46	1.39
2	B	900	ADP	C5-C4	3.88	1.46	1.39
2	E	900	ADP	C5-C4	3.88	1.46	1.39
2	B	807	ADP	C5-C4	3.69	1.45	1.39
2	E	807	ADP	C5-C4	3.67	1.45	1.39
2	A	807	ADP	C5-C4	3.66	1.45	1.39
2	D	807	ADP	C5-C4	3.66	1.45	1.39
2	C	807	ADP	C5-C4	3.66	1.45	1.39
2	F	807	ADP	C5-C4	3.66	1.45	1.39
2	B	807	ADP	C5-N7	-3.24	1.33	1.39
2	E	807	ADP	C5-N7	-3.24	1.33	1.39
2	A	807	ADP	C5-N7	-3.21	1.33	1.39
2	D	807	ADP	C5-N7	-3.21	1.33	1.39
2	C	807	ADP	C5-N7	-3.18	1.33	1.39
2	F	807	ADP	C5-N7	-3.18	1.33	1.39
2	C	900	ADP	C5-N7	-2.94	1.33	1.39
2	B	900	ADP	C5-N7	-2.92	1.33	1.39
2	A	900	ADP	C5-N7	-2.92	1.33	1.39
2	D	900	ADP	C5-N7	-2.92	1.33	1.39
2	F	900	ADP	C5-N7	-2.92	1.33	1.39
2	E	900	ADP	C5-N7	-2.87	1.33	1.39
2	B	807	ADP	C8-N9	-2.75	1.32	1.37
2	E	807	ADP	C8-N9	-2.75	1.32	1.37
2	A	807	ADP	C8-N9	-2.75	1.32	1.37
2	D	807	ADP	C8-N9	-2.75	1.32	1.37
2	C	807	ADP	C8-N9	-2.73	1.32	1.37
2	F	807	ADP	C8-N9	-2.73	1.32	1.37
2	E	807	ADP	C4-N9	-2.56	1.32	1.37
2	C	807	ADP	C4-N9	-2.53	1.32	1.37
2	B	807	ADP	C4-N9	-2.52	1.32	1.37
2	F	807	ADP	C4-N9	-2.51	1.32	1.37
2	A	807	ADP	C4-N9	-2.51	1.32	1.37
2	D	807	ADP	C4-N9	-2.51	1.32	1.37
2	C	900	ADP	C4-N9	-2.49	1.32	1.37
2	B	900	ADP	C4-N9	-2.49	1.32	1.37
2	A	900	ADP	C4-N9	-2.48	1.32	1.37
2	D	900	ADP	C4-N9	-2.48	1.32	1.37
2	F	900	ADP	C4-N9	-2.44	1.32	1.37
2	E	900	ADP	C4-N9	-2.43	1.32	1.37
2	D	900	ADP	C8-N9	-2.21	1.33	1.37
2	E	900	ADP	C8-N9	-2.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ADP	C8-N9	-2.17	1.33	1.37
2	B	900	ADP	C8-N9	-2.16	1.33	1.37
2	B	807	ADP	C5-C6	2.16	1.47	1.41
2	E	807	ADP	C5-C6	2.16	1.47	1.41
2	C	807	ADP	C5-C6	2.15	1.47	1.41
2	F	807	ADP	C5-C6	2.15	1.47	1.41
2	A	807	ADP	C5-C6	2.15	1.47	1.41
2	C	900	ADP	C8-N9	-2.14	1.33	1.37
2	F	900	ADP	C8-N9	-2.14	1.33	1.37
2	C	900	ADP	C5-C6	2.12	1.46	1.41
2	D	807	ADP	C5-C6	2.12	1.46	1.41
2	A	900	ADP	C5-C6	2.10	1.46	1.41
2	D	900	ADP	C5-C6	2.10	1.46	1.41
2	B	900	ADP	C5-C6	2.10	1.46	1.41
2	F	900	ADP	C5-C6	2.08	1.46	1.41
2	E	900	ADP	C5-C6	2.07	1.46	1.41

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	807	ADP	C5-C4-N3	-6.30	118.04	126.72
2	D	807	ADP	C5-C4-N3	-6.29	118.05	126.72
2	C	807	ADP	C5-C4-N3	-6.28	118.07	126.72
2	F	807	ADP	C5-C4-N3	-6.28	118.07	126.72
2	A	807	ADP	C5-C4-N3	-6.27	118.08	126.72
2	B	807	ADP	C5-C4-N3	-6.27	118.08	126.72
2	D	900	ADP	C5-C4-N3	-5.80	118.74	126.72
2	A	900	ADP	C5-C4-N3	-5.77	118.78	126.72
2	B	900	ADP	C5-C4-N3	-5.76	118.78	126.72
2	C	900	ADP	C5-C4-N3	-5.76	118.79	126.72
2	F	900	ADP	C5-C4-N3	-5.76	118.79	126.72
2	E	900	ADP	C5-C4-N3	-5.75	118.80	126.72
2	B	807	ADP	N3-C4-N9	5.03	135.73	127.17
2	D	807	ADP	N3-C4-N9	5.02	135.71	127.17
2	E	807	ADP	N3-C4-N9	5.02	135.70	127.17
2	A	807	ADP	N3-C4-N9	5.01	135.69	127.17
2	C	807	ADP	N3-C4-N9	5.00	135.68	127.17
2	F	807	ADP	N3-C4-N9	4.99	135.65	127.17
2	D	900	ADP	N3-C4-N9	4.74	135.23	127.17
2	B	900	ADP	N3-C4-N9	4.72	135.19	127.17
2	A	900	ADP	N3-C4-N9	4.72	135.19	127.17
2	F	900	ADP	N3-C4-N9	4.71	135.18	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	900	ADP	N3-C4-N9	4.70	135.16	127.17
2	C	900	ADP	N3-C4-N9	4.69	135.15	127.17
2	D	900	ADP	C2-N3-C4	3.68	120.81	111.83
2	D	807	ADP	C2-N3-C4	3.67	120.78	111.83
2	B	900	ADP	C2-N3-C4	3.66	120.78	111.83
2	E	807	ADP	C2-N3-C4	3.66	120.78	111.83
2	A	900	ADP	C2-N3-C4	3.66	120.77	111.83
2	C	900	ADP	C2-N3-C4	3.66	120.77	111.83
2	F	900	ADP	C2-N3-C4	3.66	120.77	111.83
2	F	807	ADP	C2-N3-C4	3.66	120.77	111.83
2	E	900	ADP	C2-N3-C4	3.66	120.76	111.83
2	B	807	ADP	C2-N3-C4	3.66	120.76	111.83
2	A	807	ADP	C2-N3-C4	3.65	120.75	111.83
2	C	807	ADP	C2-N3-C4	3.65	120.75	111.83
2	F	807	ADP	C4-C5-N7	-3.60	106.46	110.58
2	A	807	ADP	C4-C5-N7	-3.58	106.49	110.58
2	D	807	ADP	C4-C5-N7	-3.58	106.49	110.58
2	C	807	ADP	C4-C5-N7	-3.58	106.49	110.58
2	E	807	ADP	C4-C5-N7	-3.57	106.50	110.58
2	B	807	ADP	C4-C5-N7	-3.54	106.54	110.58
2	B	900	ADP	N3-C2-N1	-3.30	123.58	128.58
2	F	900	ADP	N3-C2-N1	-3.30	123.59	128.58
2	D	900	ADP	N3-C2-N1	-3.30	123.59	128.58
2	A	900	ADP	N3-C2-N1	-3.28	123.62	128.58
2	C	900	ADP	N3-C2-N1	-3.27	123.63	128.58
2	E	900	ADP	N3-C2-N1	-3.27	123.64	128.58
2	C	900	ADP	C4-C5-N7	-2.90	107.27	110.58
2	E	900	ADP	C4-C5-N7	-2.89	107.28	110.58
2	A	900	ADP	C4-C5-N7	-2.89	107.28	110.58
2	D	900	ADP	C4-C5-N7	-2.89	107.28	110.58
2	F	900	ADP	C4-C5-N7	-2.88	107.29	110.58
2	B	900	ADP	C4-C5-N7	-2.88	107.29	110.58
2	F	807	ADP	N3-C2-N1	-2.86	124.25	128.58
2	C	807	ADP	N3-C2-N1	-2.85	124.27	128.58
2	A	807	ADP	N3-C2-N1	-2.85	124.27	128.58
2	D	807	ADP	N3-C2-N1	-2.85	124.27	128.58
2	E	807	ADP	N3-C2-N1	-2.83	124.30	128.58
2	B	807	ADP	N3-C2-N1	-2.82	124.31	128.58
2	B	807	ADP	C4-N9-C8	2.79	108.67	105.74
2	C	807	ADP	C4-N9-C8	2.77	108.65	105.74
2	E	807	ADP	C4-N9-C8	2.77	108.64	105.74
2	A	807	ADP	C4-N9-C8	2.76	108.64	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	807	ADP	C4-N9-C8	2.76	108.64	105.74
2	F	807	ADP	C4-N9-C8	2.75	108.63	105.74
2	B	900	ADP	C4-N9-C8	2.72	108.60	105.74
2	D	900	ADP	C4-N9-C8	2.68	108.56	105.74
2	A	900	ADP	C4-N9-C8	2.68	108.55	105.74
2	F	900	ADP	C4-N9-C8	2.65	108.53	105.74
2	E	900	ADP	C4-N9-C8	2.65	108.52	105.74
2	F	807	ADP	C5-N7-C8	2.63	107.59	103.45
2	A	807	ADP	C5-N7-C8	2.63	107.59	103.45
2	D	807	ADP	C5-N7-C8	2.63	107.59	103.45
2	C	900	ADP	C4-N9-C8	2.63	108.50	105.74
2	C	807	ADP	C5-N7-C8	2.62	107.56	103.45
2	B	807	ADP	C5-N7-C8	2.61	107.55	103.45
2	E	807	ADP	C5-N7-C8	2.61	107.55	103.45
2	A	807	ADP	C2'-C1'-N9	-2.48	107.13	113.30
2	E	807	ADP	C2'-C1'-N9	-2.48	107.13	113.30
2	B	807	ADP	C2'-C1'-N9	-2.48	107.14	113.30
2	D	807	ADP	C2'-C1'-N9	-2.48	107.15	113.30
2	F	807	ADP	C2'-C1'-N9	-2.48	107.15	113.30
2	C	807	ADP	C2'-C1'-N9	-2.47	107.17	113.30
2	F	807	ADP	C3'-C2'-C1'	2.45	106.09	101.46
2	C	807	ADP	C3'-C2'-C1'	2.44	106.08	101.46
2	A	807	ADP	C3'-C2'-C1'	2.44	106.07	101.46
2	B	807	ADP	C3'-C2'-C1'	2.43	106.07	101.46
2	E	807	ADP	C3'-C2'-C1'	2.43	106.06	101.46
2	D	807	ADP	C3'-C2'-C1'	2.42	106.05	101.46
2	E	900	ADP	C3'-C2'-C1'	2.38	105.97	101.46
2	A	900	ADP	C3'-C2'-C1'	2.38	105.96	101.46
2	D	900	ADP	C3'-C2'-C1'	2.38	105.96	101.46
2	F	900	ADP	C3'-C2'-C1'	2.38	105.96	101.46
2	C	900	ADP	C3'-C2'-C1'	2.37	105.95	101.46
2	B	900	ADP	C3'-C2'-C1'	2.36	105.92	101.46
2	F	900	ADP	C5-N7-C8	2.09	106.73	103.45
2	C	900	ADP	C5-N7-C8	2.08	106.72	103.45
2	B	900	ADP	C5-N7-C8	2.08	106.72	103.45
2	F	900	ADP	O2A-PA-O1A	2.07	122.07	112.44
2	E	900	ADP	O2A-PA-O1A	2.07	122.07	112.44
2	A	900	ADP	C5-N7-C8	2.07	106.70	103.45
2	A	900	ADP	O2A-PA-O1A	2.07	122.06	112.44
2	C	900	ADP	O2A-PA-O1A	2.07	122.06	112.44
2	E	900	ADP	C5-N7-C8	2.06	106.69	103.45
2	B	900	ADP	O2A-PA-O1A	2.06	122.03	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	ADP	O2A-PA-O1A	2.06	122.03	112.44
2	D	900	ADP	C5-N7-C8	2.05	106.68	103.45
2	C	807	ADP	N9-C8-N7	-2.04	111.05	113.94
2	F	807	ADP	N9-C8-N7	-2.04	111.05	113.94
2	A	807	ADP	N9-C8-N7	-2.04	111.05	113.94
2	D	807	ADP	N9-C8-N7	-2.04	111.05	113.94
2	B	807	ADP	N9-C8-N7	-2.04	111.05	113.94
2	E	807	ADP	N9-C8-N7	-2.04	111.05	113.94
2	D	807	ADP	O3A-PB-O1B	-2.01	100.44	111.04
2	C	807	ADP	O3A-PB-O1B	-2.01	100.45	111.04
2	F	807	ADP	O3A-PB-O1B	-2.01	100.45	111.04
2	B	807	ADP	O3A-PB-O1B	-2.01	100.46	111.04
2	E	807	ADP	O3A-PB-O1B	-2.01	100.46	111.04
2	A	807	ADP	O3A-PB-O1B	-2.01	100.48	111.04

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	ADP	C5'-O5'-PA-O3A
2	A	900	ADP	C5'-O5'-PA-O1A
2	A	900	ADP	C5'-O5'-PA-O2A
2	A	900	ADP	C5'-O5'-PA-O3A
2	B	807	ADP	C5'-O5'-PA-O3A
2	B	900	ADP	C5'-O5'-PA-O1A
2	B	900	ADP	C5'-O5'-PA-O2A
2	B	900	ADP	C5'-O5'-PA-O3A
2	C	807	ADP	C5'-O5'-PA-O3A
2	C	900	ADP	C5'-O5'-PA-O1A
2	C	900	ADP	C5'-O5'-PA-O2A
2	C	900	ADP	C5'-O5'-PA-O3A
2	D	807	ADP	C5'-O5'-PA-O3A
2	D	900	ADP	C5'-O5'-PA-O1A
2	D	900	ADP	C5'-O5'-PA-O2A
2	D	900	ADP	C5'-O5'-PA-O3A
2	E	807	ADP	C5'-O5'-PA-O3A
2	E	900	ADP	C5'-O5'-PA-O1A
2	E	900	ADP	C5'-O5'-PA-O2A
2	E	900	ADP	C5'-O5'-PA-O3A
2	F	807	ADP	C5'-O5'-PA-O3A
2	F	900	ADP	C5'-O5'-PA-O1A
2	F	900	ADP	C5'-O5'-PA-O2A

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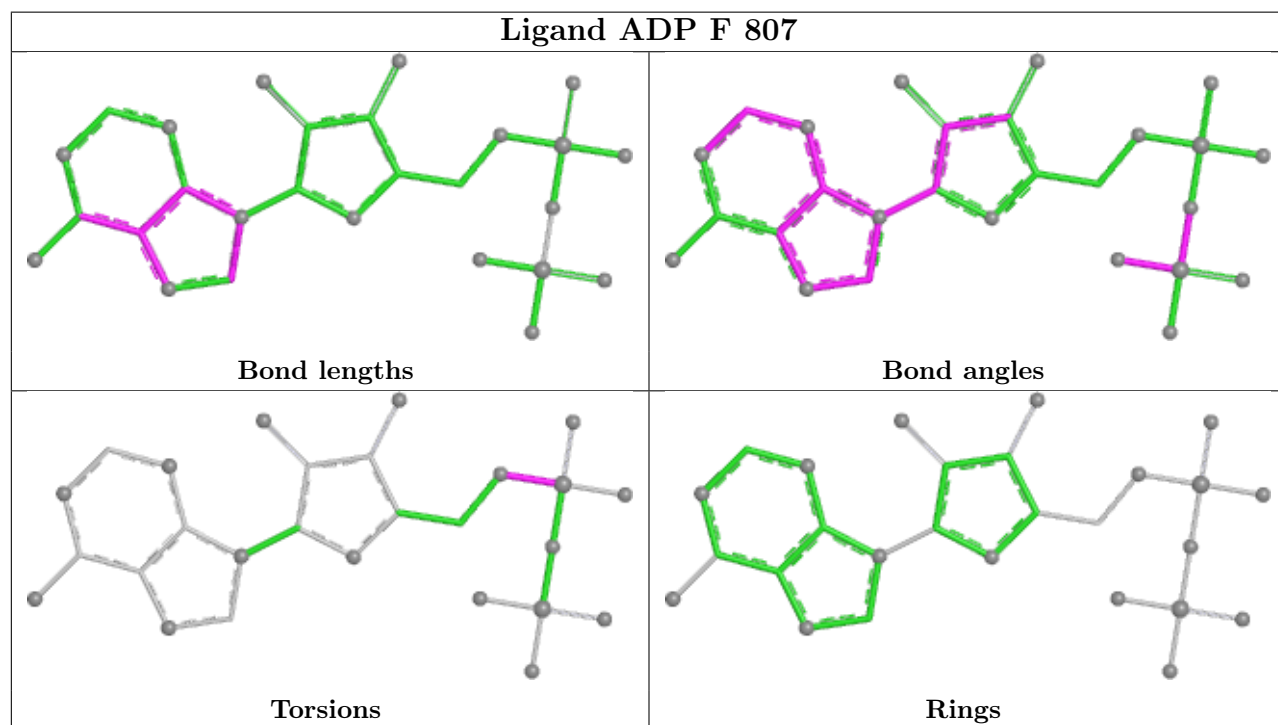
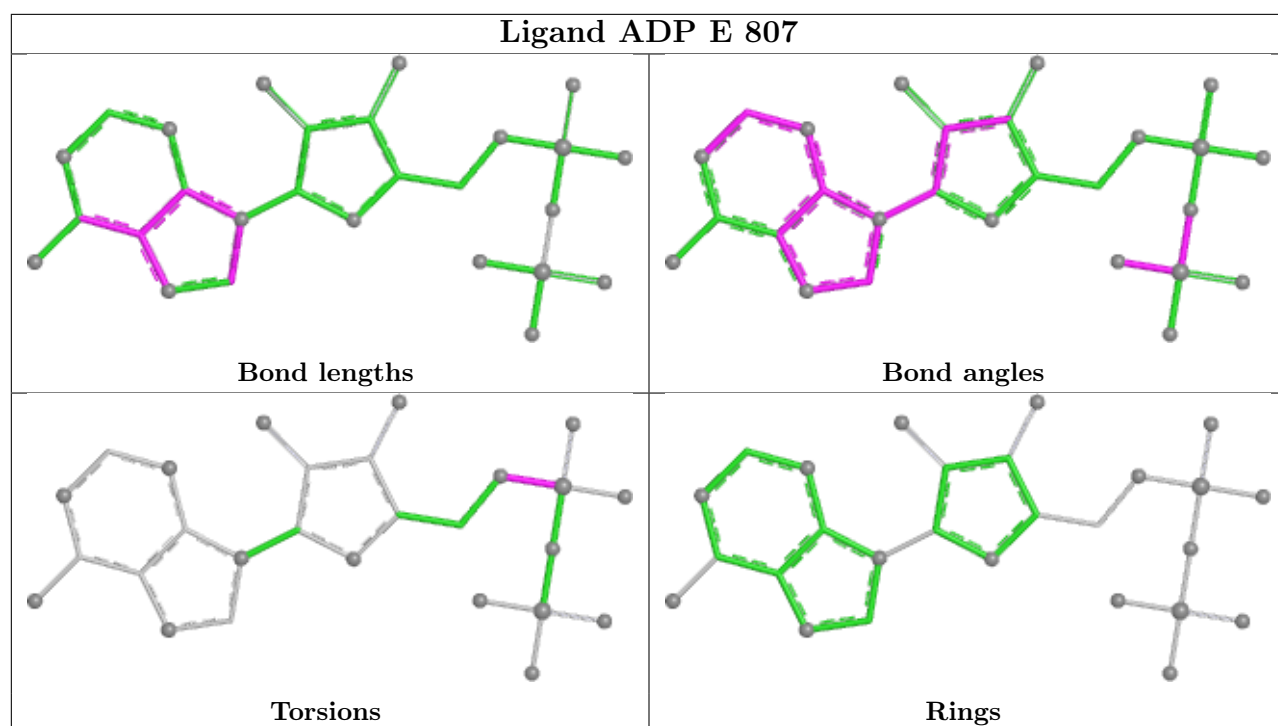
Mol	Chain	Res	Type	Atoms
2	F	900	ADP	C5'-O5'-PA-O3A
2	A	807	ADP	C5'-O5'-PA-O1A
2	B	807	ADP	C5'-O5'-PA-O1A
2	C	807	ADP	C5'-O5'-PA-O1A
2	D	807	ADP	C5'-O5'-PA-O1A
2	E	807	ADP	C5'-O5'-PA-O1A
2	F	807	ADP	C5'-O5'-PA-O1A

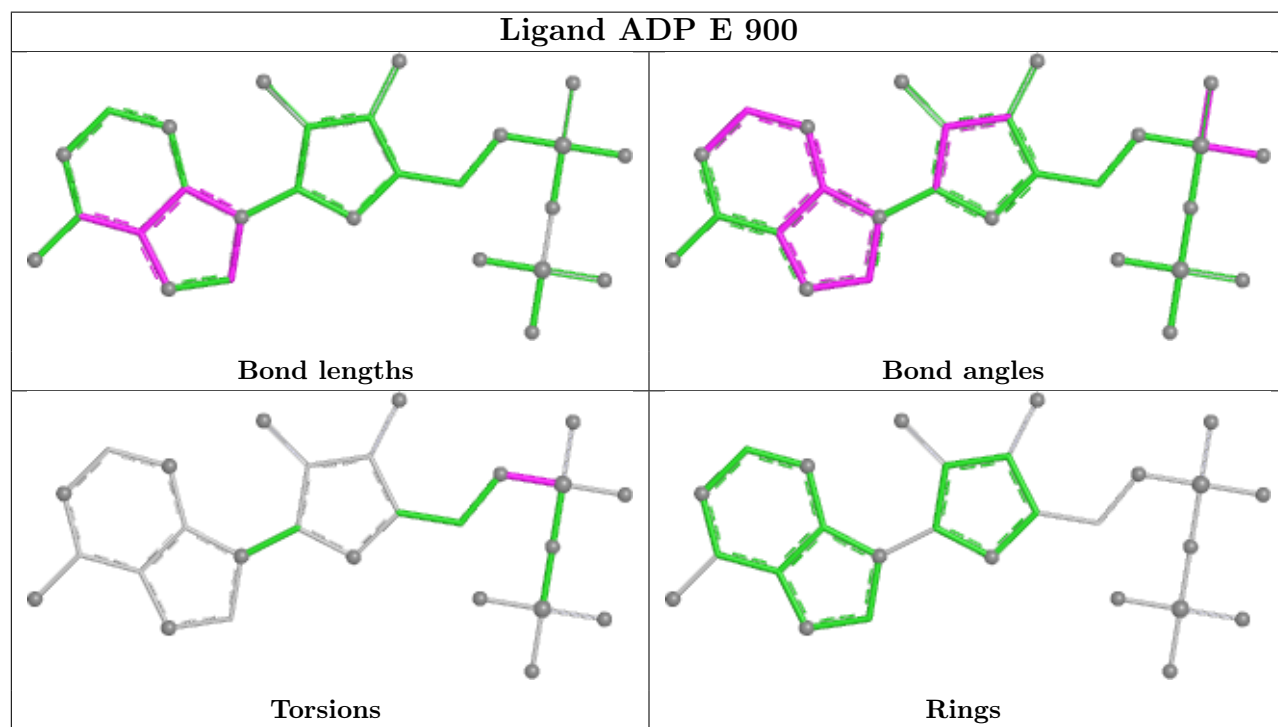
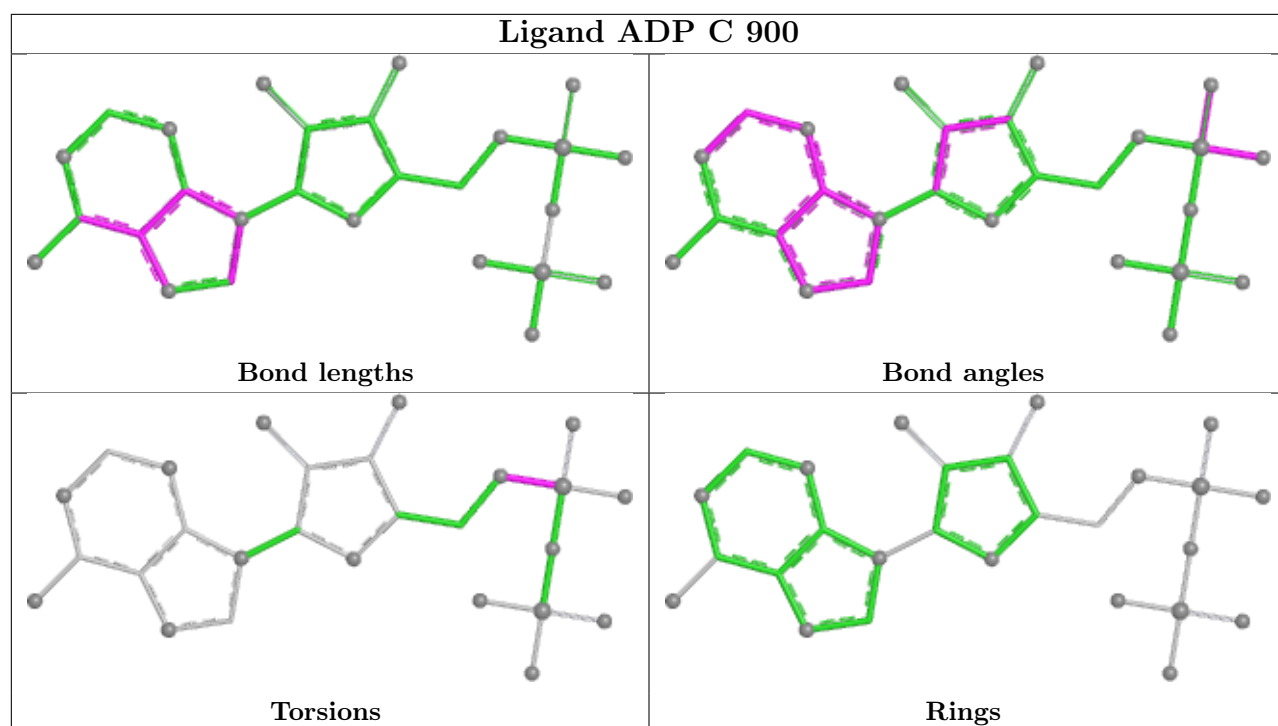
There are no ring outliers.

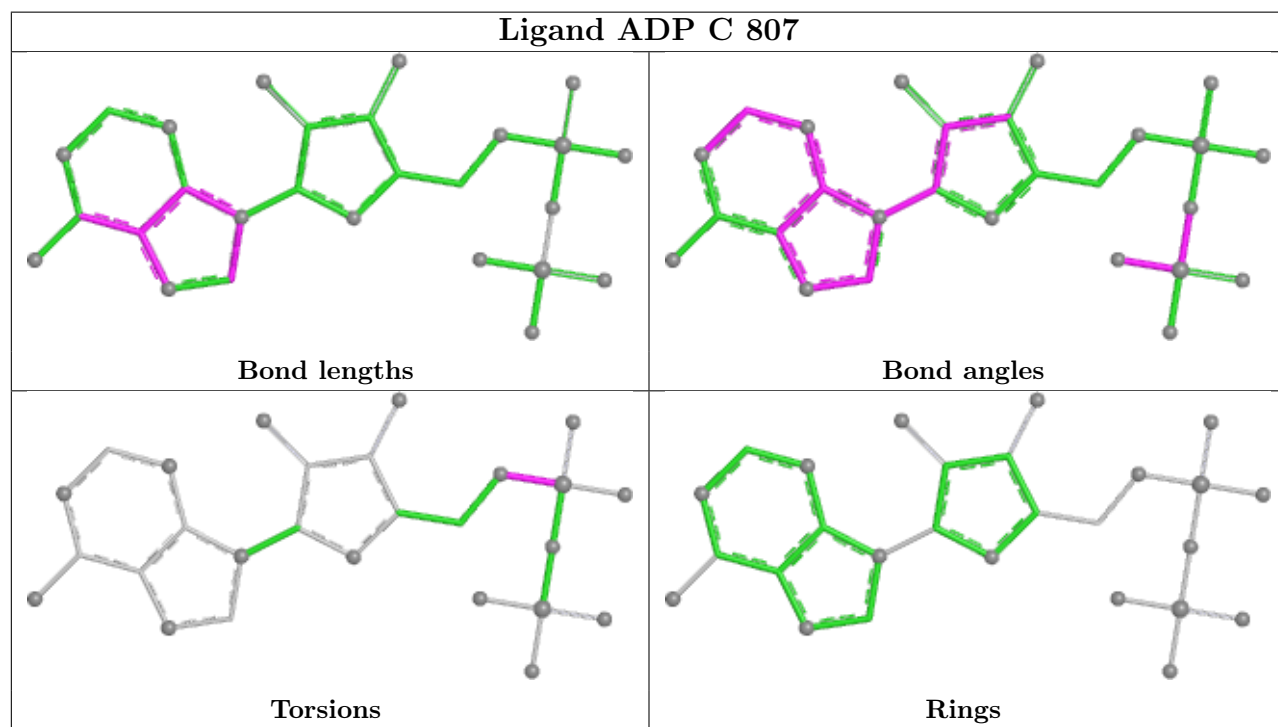
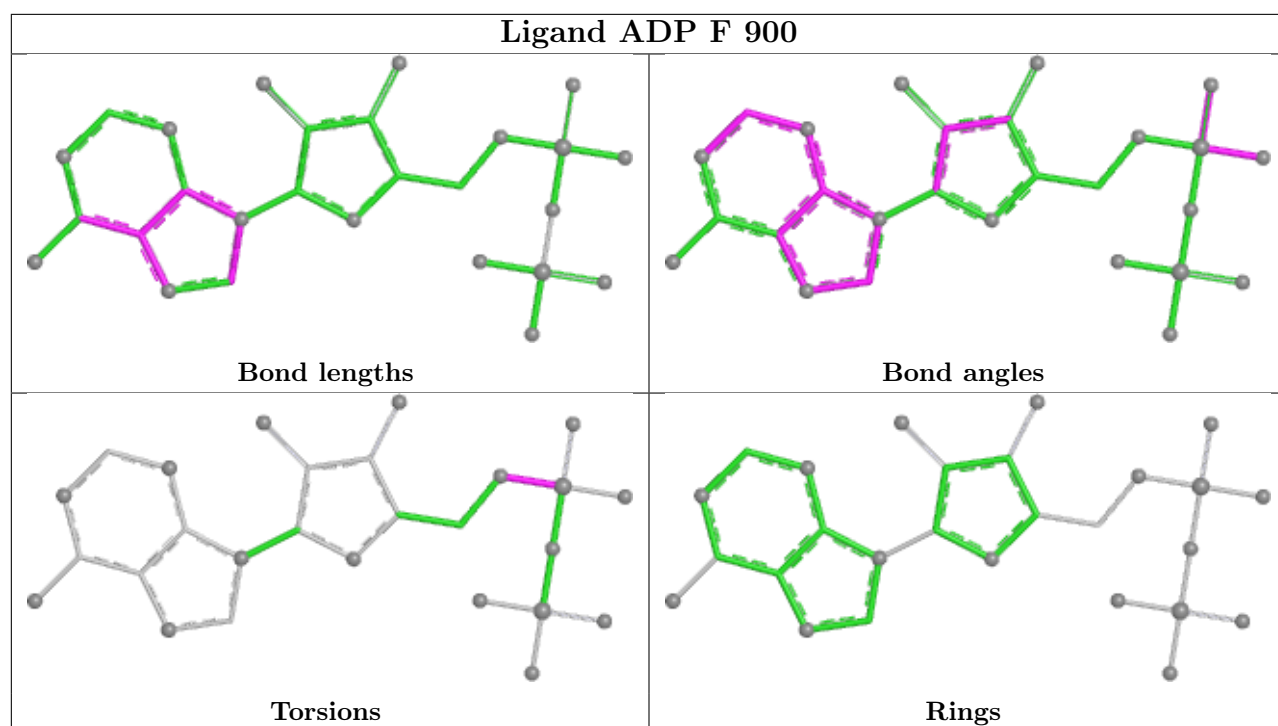
12 monomers are involved in 18 short contacts:

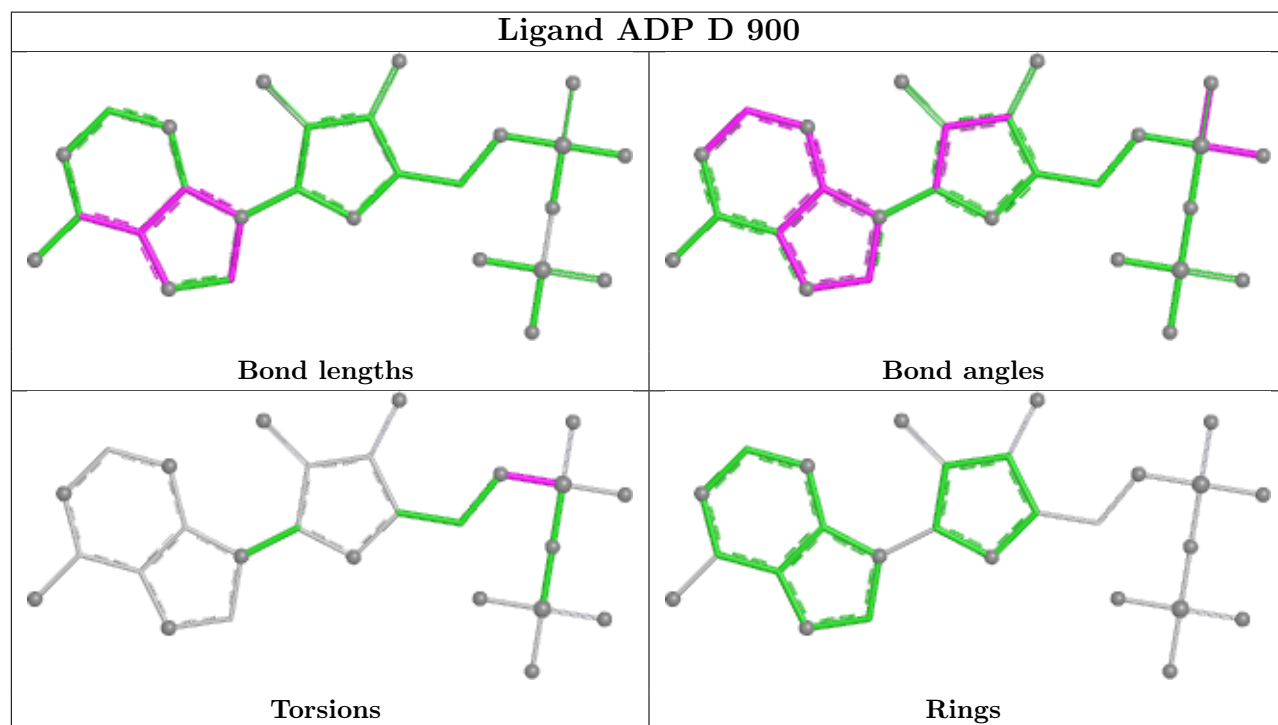
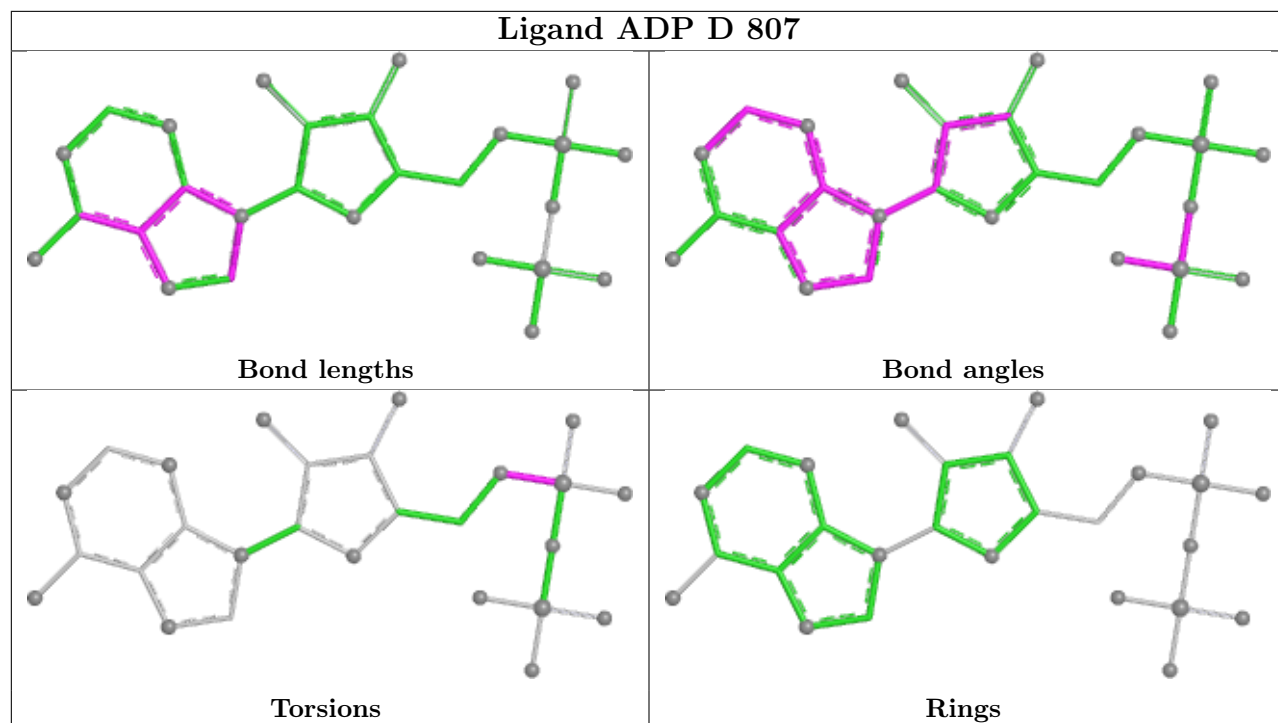
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	807	ADP	1	0
2	F	807	ADP	1	0
2	C	900	ADP	2	0
2	E	900	ADP	2	0
2	F	900	ADP	2	0
2	C	807	ADP	1	0
2	D	807	ADP	1	0
2	D	900	ADP	2	0
2	A	807	ADP	1	0
2	A	900	ADP	2	0
2	B	900	ADP	2	0
2	B	807	ADP	1	0

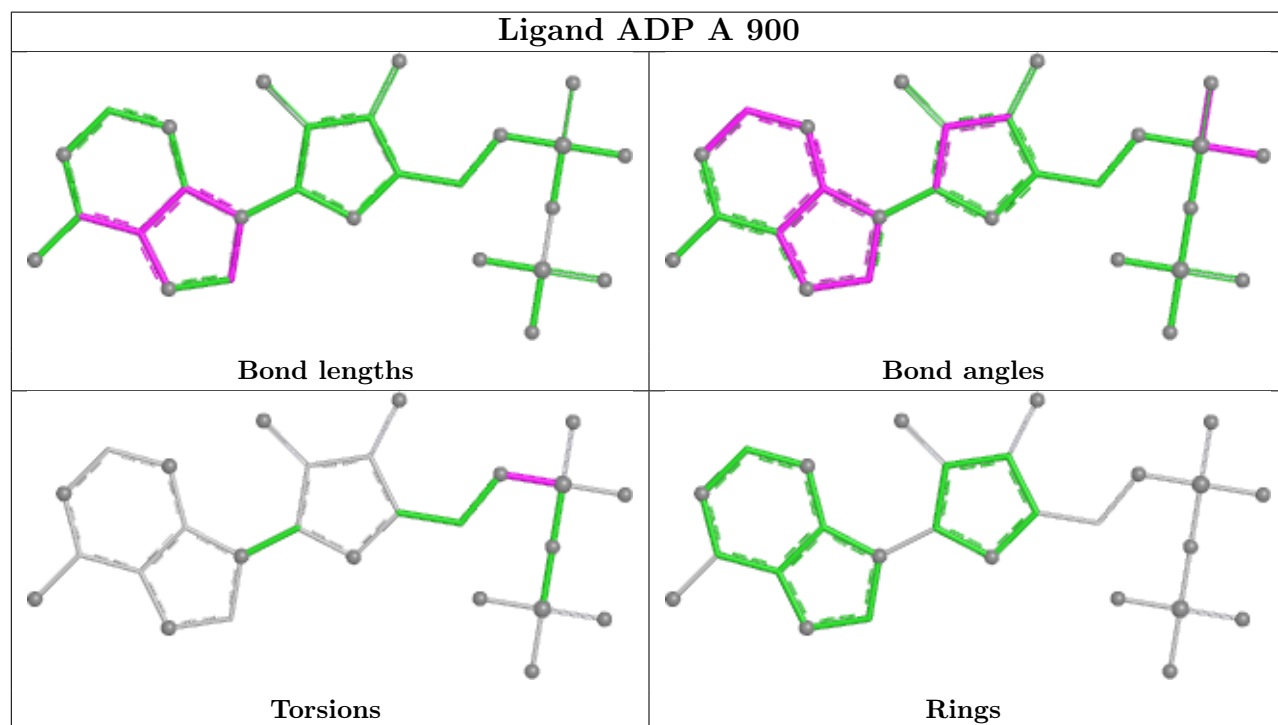
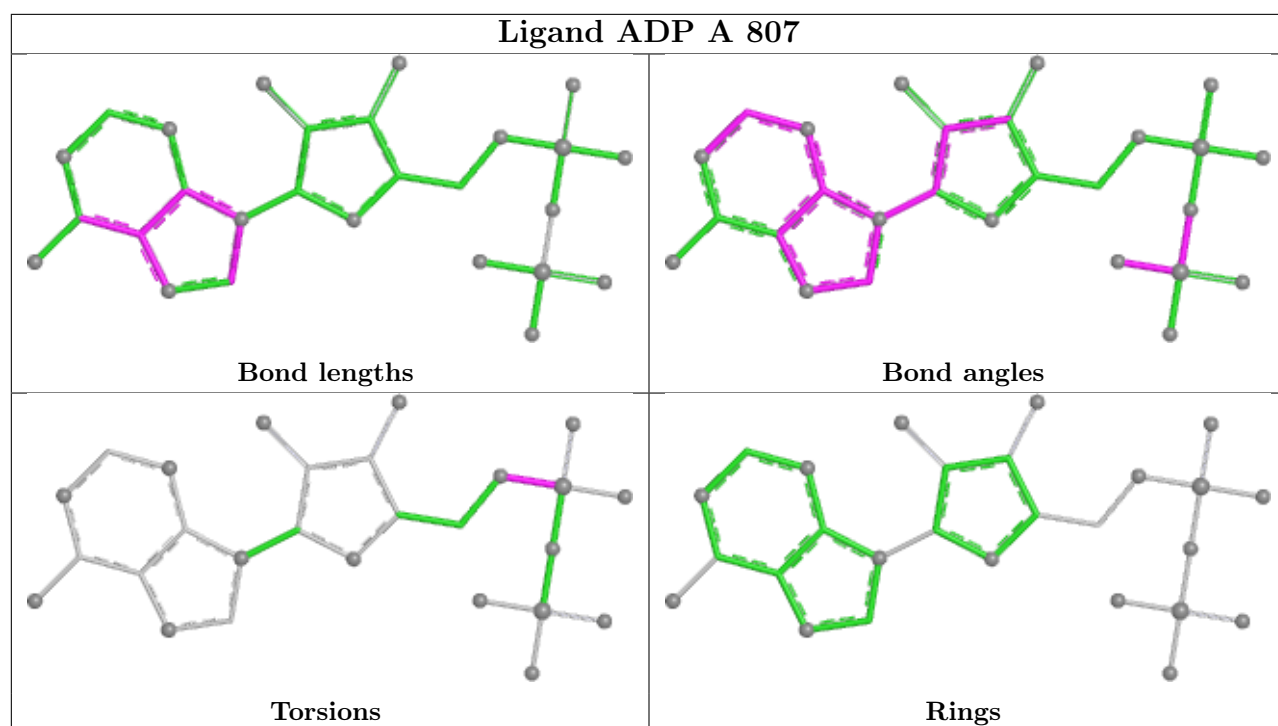
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

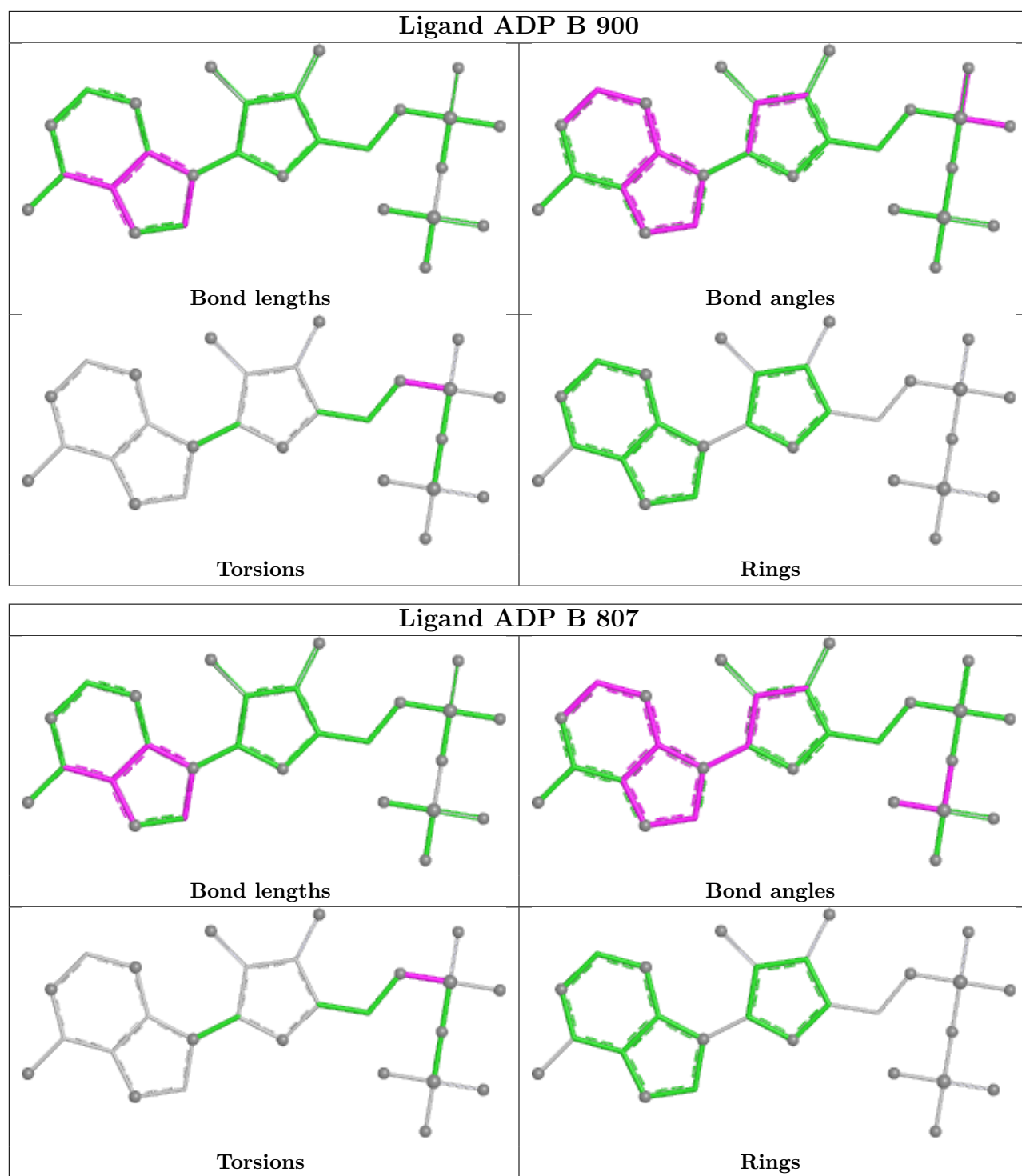












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

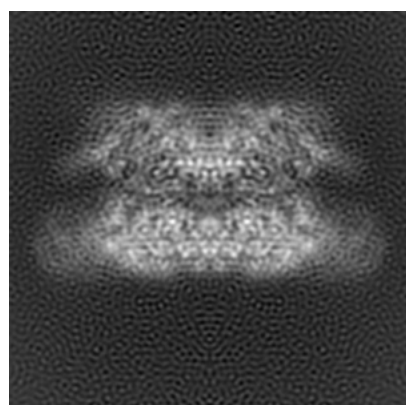
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3297. These allow visual inspection of the internal detail of the map and identification of artifacts.

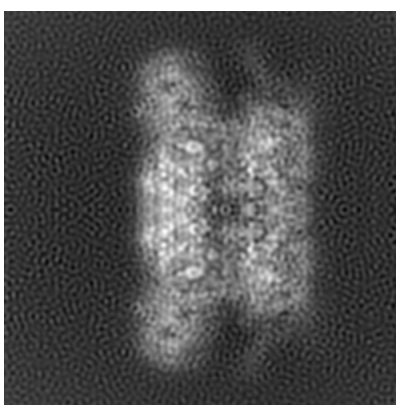
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

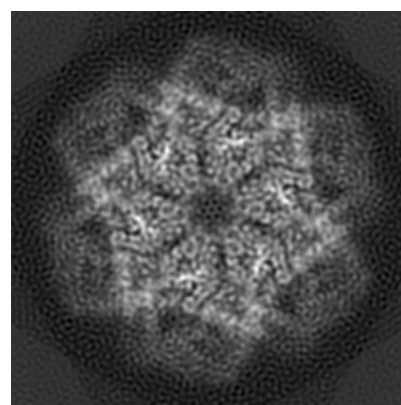
6.1.1 Primary map



X



Y

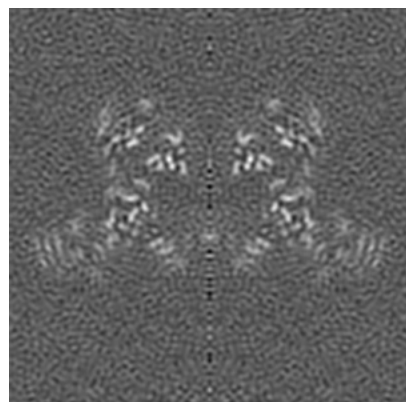


Z

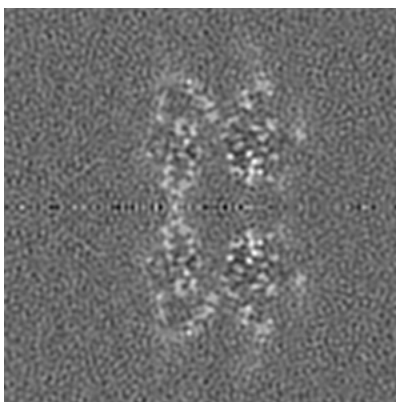
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

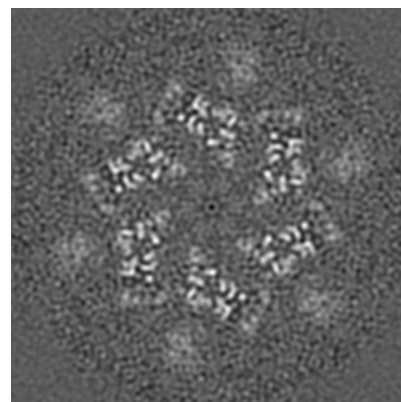
6.2.1 Primary map



X Index: 138



Y Index: 138

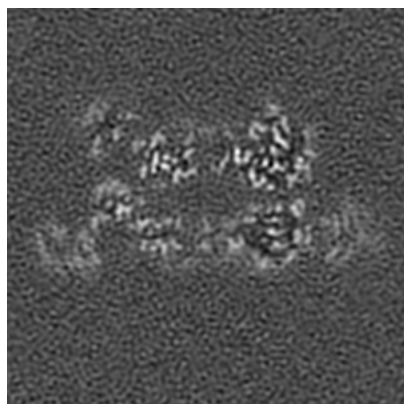


Z Index: 138

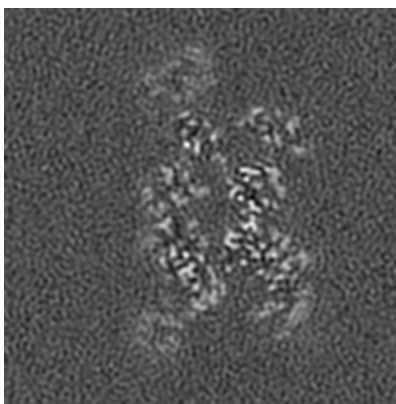
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

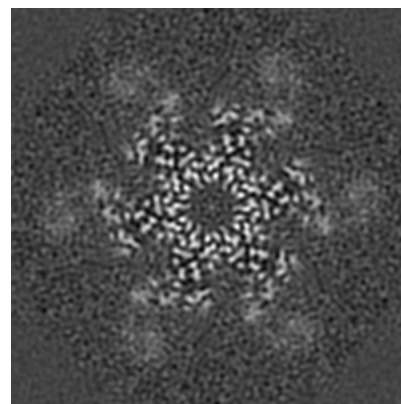
6.3.1 Primary map



X Index: 152



Y Index: 167

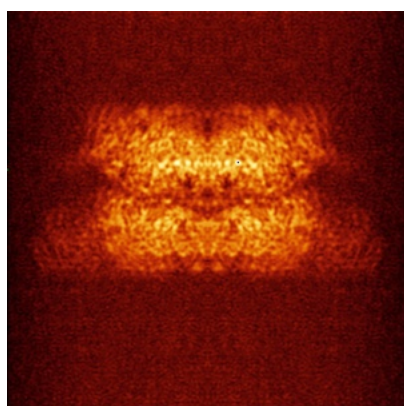


Z Index: 170

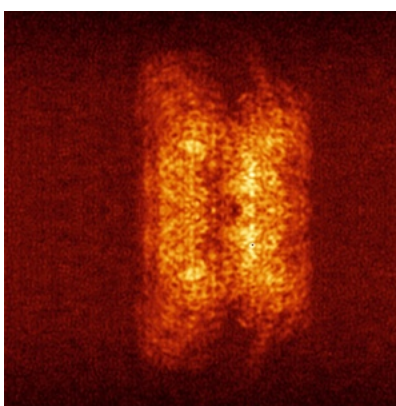
The images above show the largest variance slices of the map in three orthogonal directions.

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

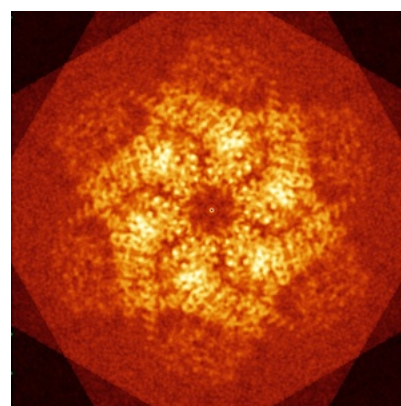
6.4.1 Primary map



X



Y

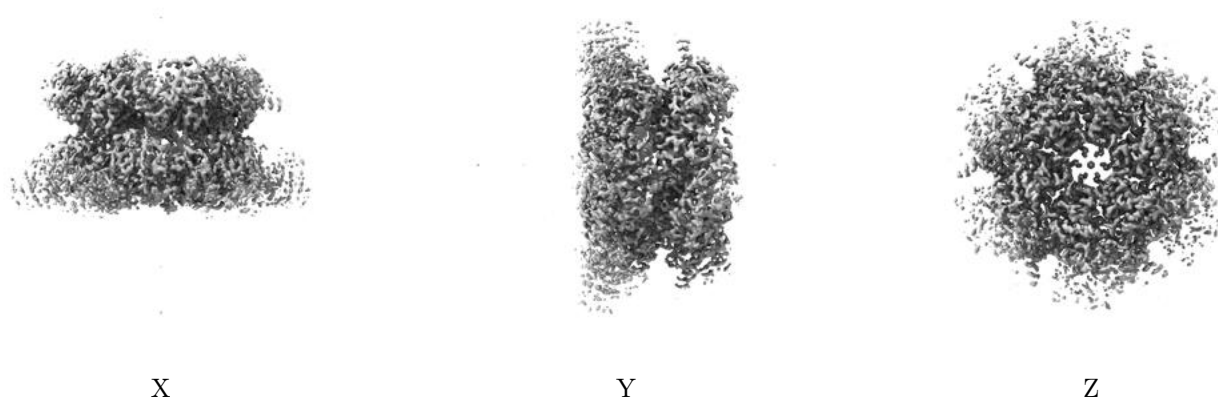


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0179. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

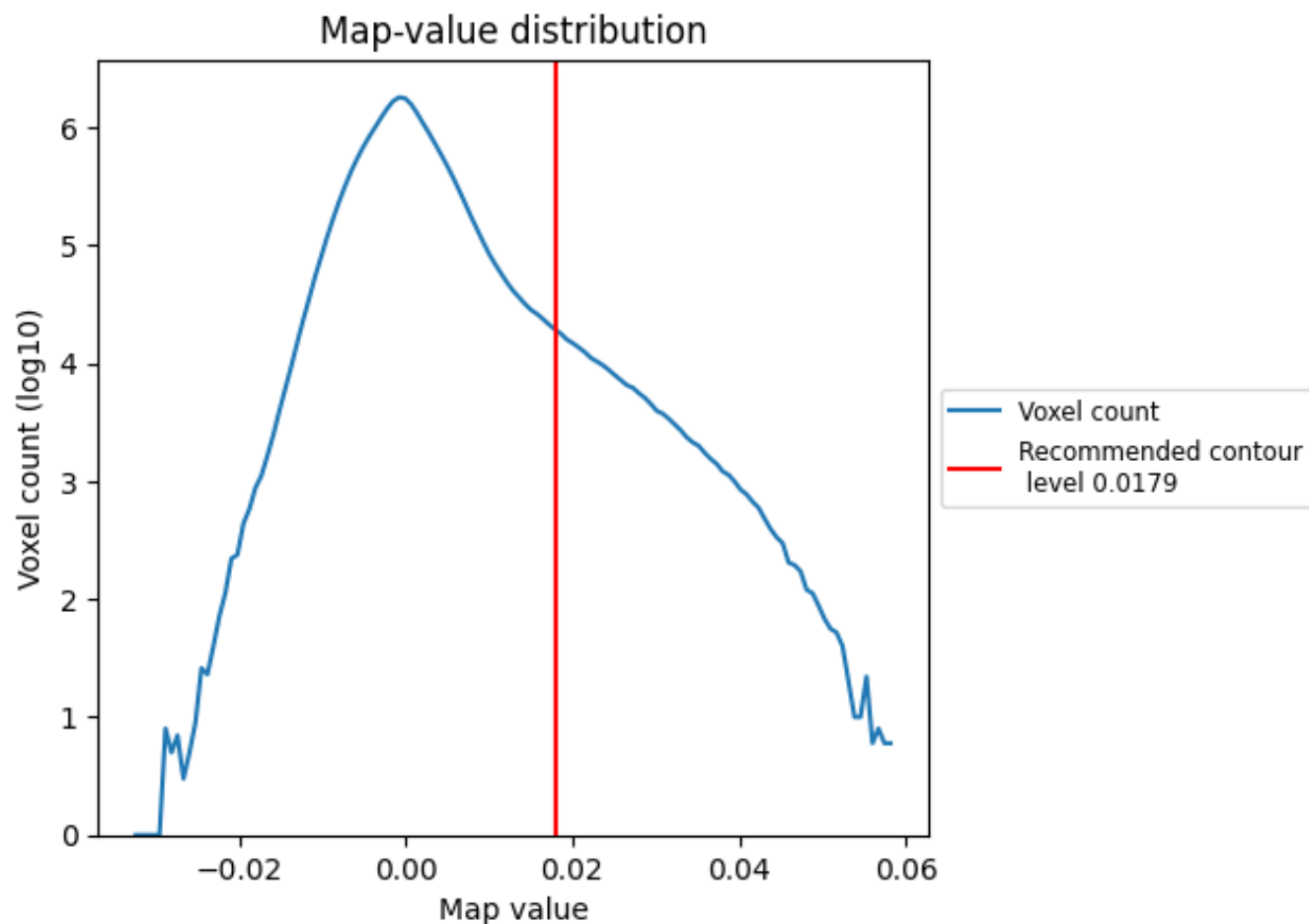
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

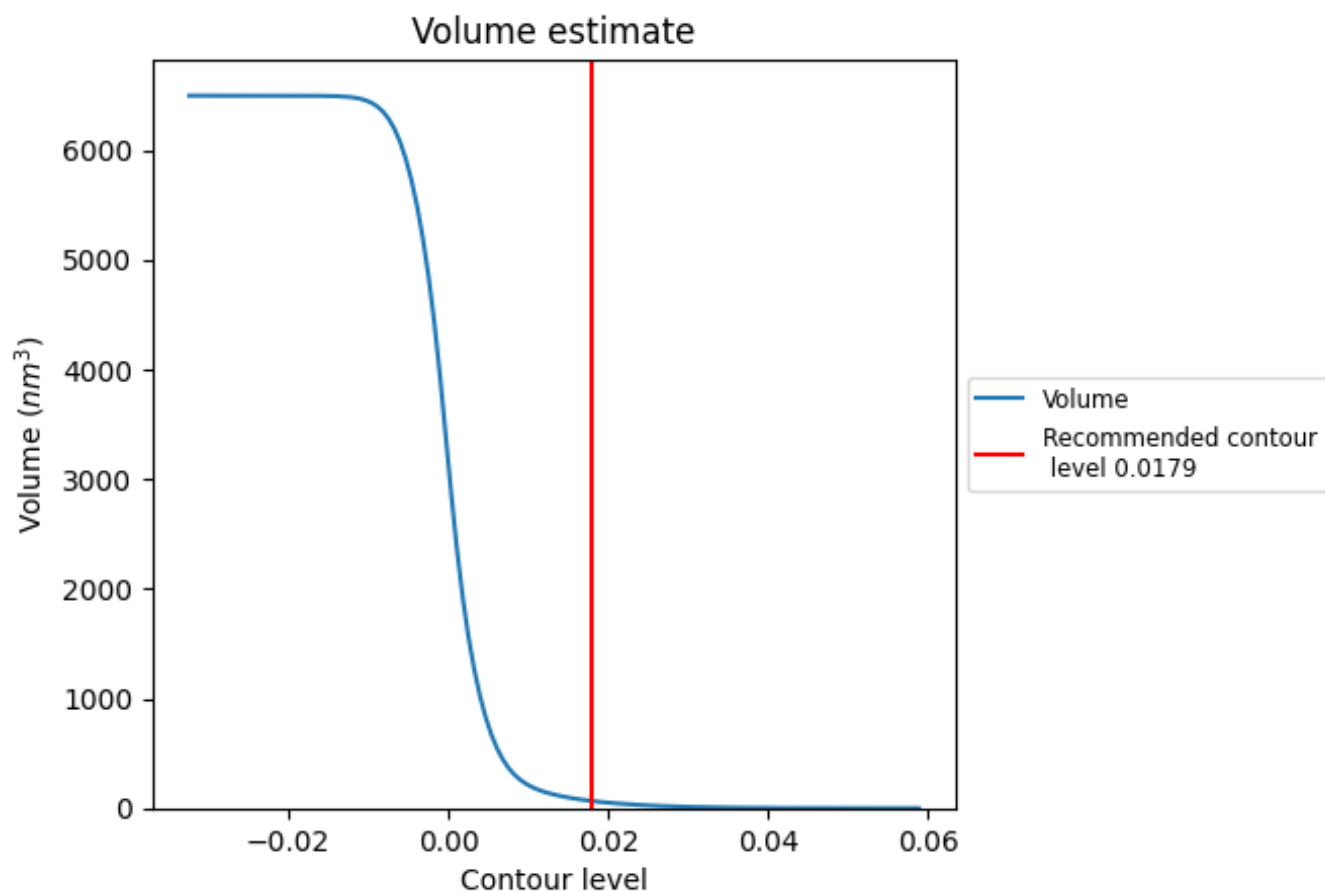
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

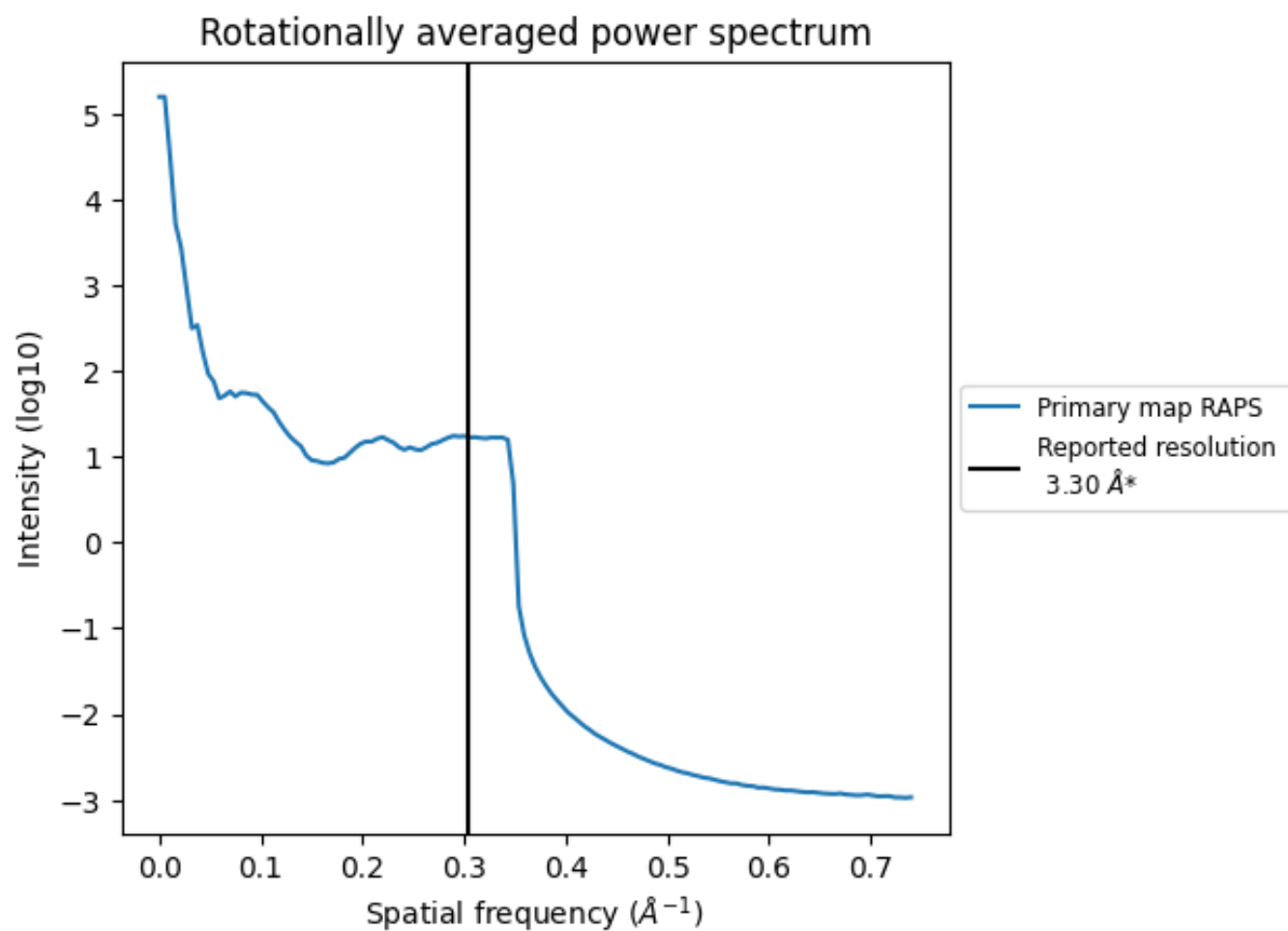
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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 0.303 Å⁻¹

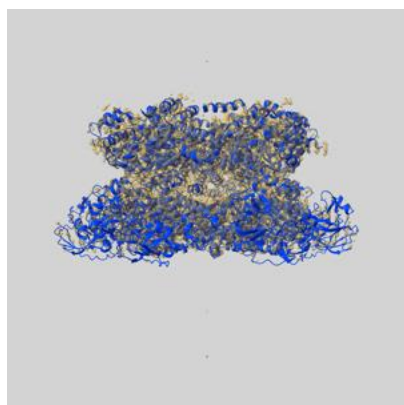
8 Fourier-Shell correlation

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

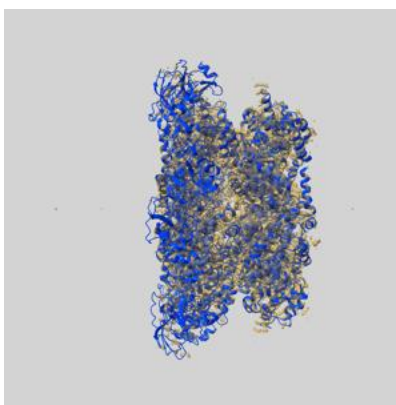
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3297 and PDB model 5FTL. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

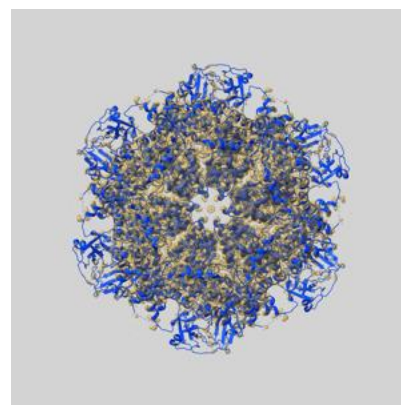
9.1 Map-model overlay [i](#)



X



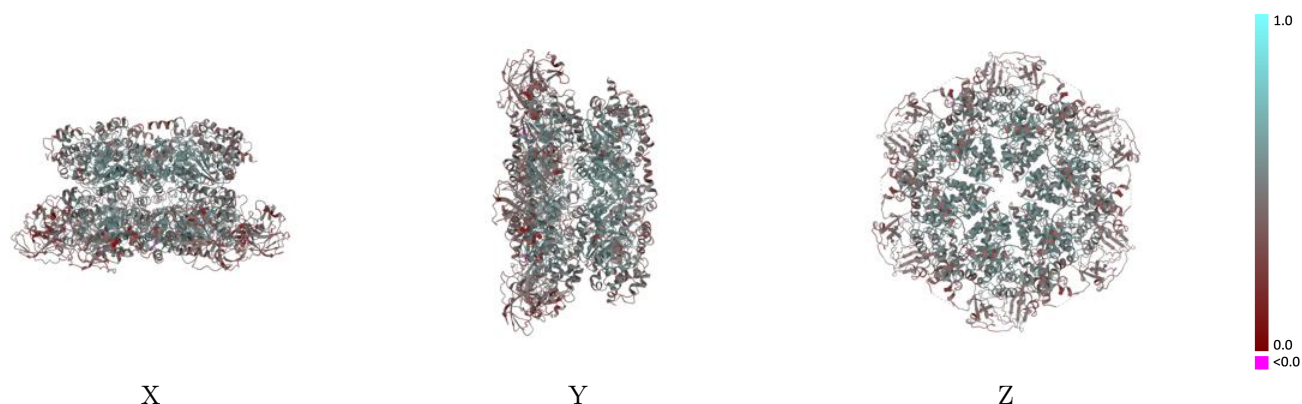
Y



Z

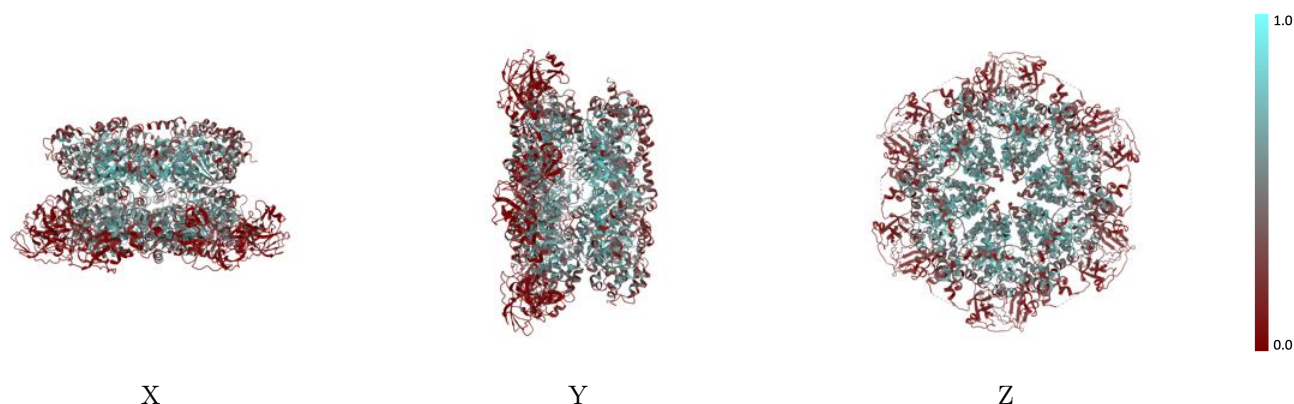
The images above show the 3D surface view of the map at the recommended contour level 0.0179 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



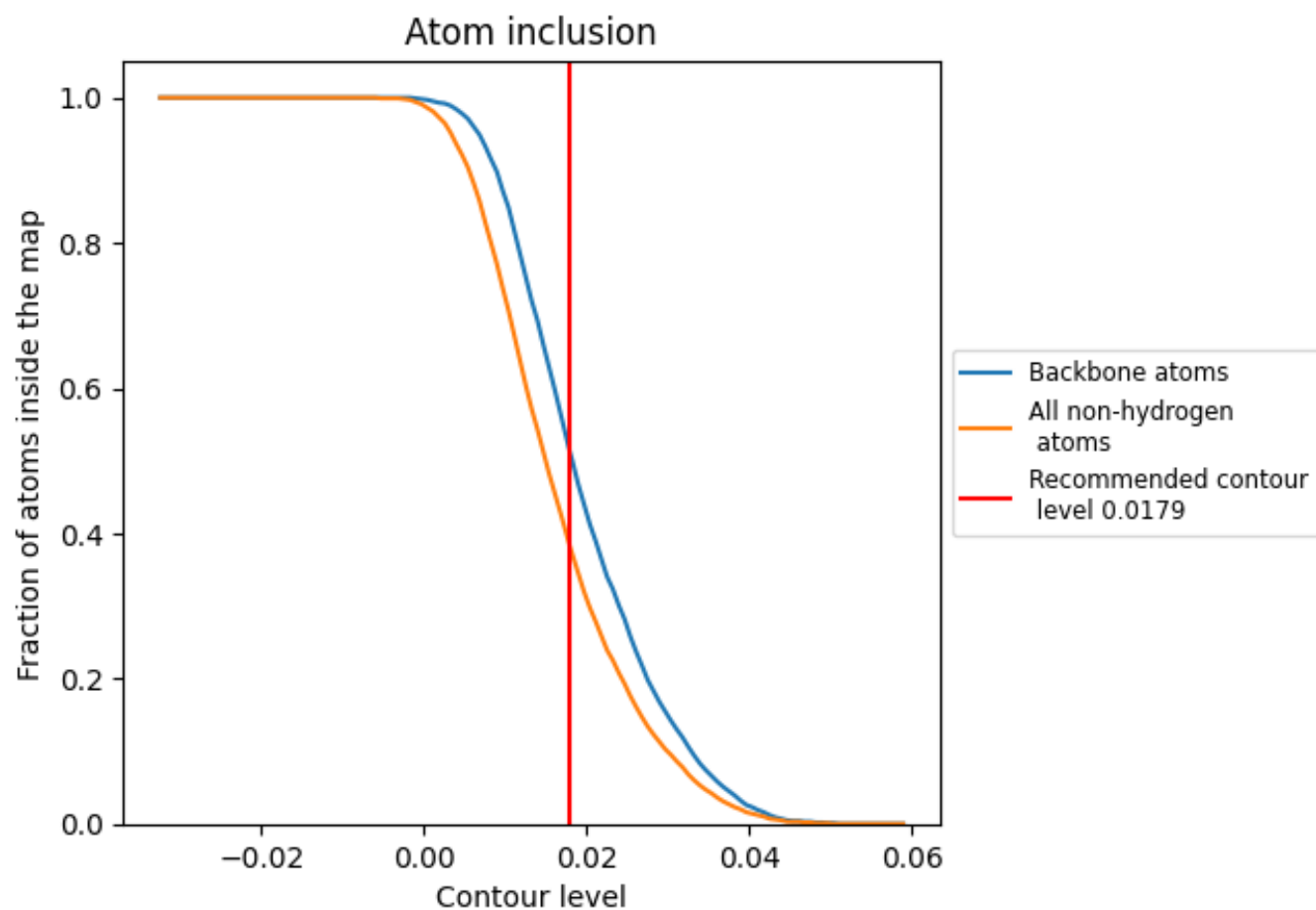
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0179).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 38% 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 (0.0179) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3830	0.4580
A	0.3830	0.4590
B	0.3820	0.4580
C	0.3830	0.4580
D	0.3830	0.4580
E	0.3830	0.4580
F	0.3830	0.4580

1.0

0.0

<0.0