



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:11 AM UTC

PDB ID : 8OM7 / pdb_00008om7
EMDB ID : EMD-16970
Title : Human Mitochondrial Lon Y186E Mutant ADP Bound
Authors : Kereiche, S.; Bauer, J.A.; Matyas, P.; Novacek, J.; Kutejova, E.
Deposited on : 2023-03-31
Resolution : 3.74 Å (reported)
Based on initial model : 7NFY

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:

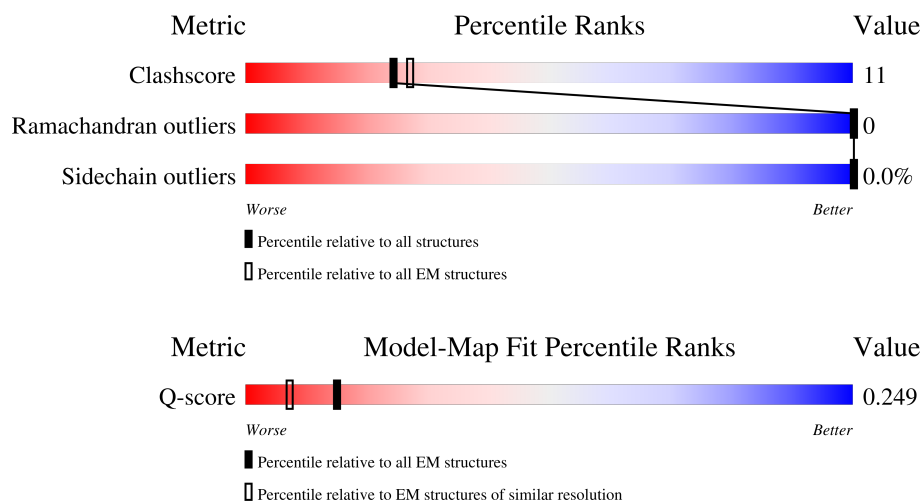
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	869	29% 68% 22% 11%
1	B	869	29% 67% 22% 11%
1	C	869	30% 69% 20% 11%
1	D	869	31% 69% 21% 11%

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Mol	Chain	Length	Quality of chain
1	E	869	39% 69% 20% 11%
1	F	869	36% 71% 19% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 74748 atoms, of which 37758 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 Lon protease homolog, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	776	Total	C	H	N	O	S	0	0
			12419	3893	6281	1066	1152	27		
1	B	776	Total	C	H	N	O	S	0	0
			12419	3893	6281	1066	1152	27		
1	C	776	Total	C	H	N	O	S	0	0
			12419	3893	6281	1066	1152	27		
1	D	776	Total	C	H	N	O	S	0	0
			12419	3893	6281	1066	1152	27		
1	E	776	Total	C	H	N	O	S	0	0
			12419	3893	6281	1066	1152	27		
1	F	776	Total	C	H	N	O	S	0	0
			12419	3893	6281	1066	1152	27		

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MET	-	initiating methionine	UNP P36776
A	92	GLY	-	expression tag	UNP P36776
A	93	HIS	-	expression tag	UNP P36776
A	94	HIS	-	expression tag	UNP P36776
A	95	HIS	-	expression tag	UNP P36776
A	96	HIS	-	expression tag	UNP P36776
A	97	HIS	-	expression tag	UNP P36776
A	98	HIS	-	expression tag	UNP P36776
A	99	ASP	-	expression tag	UNP P36776
A	100	TYR	-	expression tag	UNP P36776
A	101	ASP	-	expression tag	UNP P36776
A	102	ILE	-	expression tag	UNP P36776
A	103	PRO	-	expression tag	UNP P36776
A	104	THR	-	expression tag	UNP P36776
A	105	THR	-	expression tag	UNP P36776
A	106	GLU	-	expression tag	UNP P36776
A	107	ASN	-	expression tag	UNP P36776
A	108	LEU	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
A	109	TYR	-	expression tag	UNP P36776
A	110	PHE	-	expression tag	UNP P36776
A	111	GLN	-	expression tag	UNP P36776
A	112	GLY	-	expression tag	UNP P36776
A	113	ALA	-	expression tag	UNP P36776
A	114	HIS	-	expression tag	UNP P36776
A	186	GLU	TYR	engineered mutation	UNP P36776
B	91	MET	-	initiating methionine	UNP P36776
B	92	GLY	-	expression tag	UNP P36776
B	93	HIS	-	expression tag	UNP P36776
B	94	HIS	-	expression tag	UNP P36776
B	95	HIS	-	expression tag	UNP P36776
B	96	HIS	-	expression tag	UNP P36776
B	97	HIS	-	expression tag	UNP P36776
B	98	HIS	-	expression tag	UNP P36776
B	99	ASP	-	expression tag	UNP P36776
B	100	TYR	-	expression tag	UNP P36776
B	101	ASP	-	expression tag	UNP P36776
B	102	ILE	-	expression tag	UNP P36776
B	103	PRO	-	expression tag	UNP P36776
B	104	THR	-	expression tag	UNP P36776
B	105	THR	-	expression tag	UNP P36776
B	106	GLU	-	expression tag	UNP P36776
B	107	ASN	-	expression tag	UNP P36776
B	108	LEU	-	expression tag	UNP P36776
B	109	TYR	-	expression tag	UNP P36776
B	110	PHE	-	expression tag	UNP P36776
B	111	GLN	-	expression tag	UNP P36776
B	112	GLY	-	expression tag	UNP P36776
B	113	ALA	-	expression tag	UNP P36776
B	114	HIS	-	expression tag	UNP P36776
B	186	GLU	TYR	engineered mutation	UNP P36776
C	91	MET	-	initiating methionine	UNP P36776
C	92	GLY	-	expression tag	UNP P36776
C	93	HIS	-	expression tag	UNP P36776
C	94	HIS	-	expression tag	UNP P36776
C	95	HIS	-	expression tag	UNP P36776
C	96	HIS	-	expression tag	UNP P36776
C	97	HIS	-	expression tag	UNP P36776
C	98	HIS	-	expression tag	UNP P36776
C	99	ASP	-	expression tag	UNP P36776
C	100	TYR	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
C	101	ASP	-	expression tag	UNP P36776
C	102	ILE	-	expression tag	UNP P36776
C	103	PRO	-	expression tag	UNP P36776
C	104	THR	-	expression tag	UNP P36776
C	105	THR	-	expression tag	UNP P36776
C	106	GLU	-	expression tag	UNP P36776
C	107	ASN	-	expression tag	UNP P36776
C	108	LEU	-	expression tag	UNP P36776
C	109	TYR	-	expression tag	UNP P36776
C	110	PHE	-	expression tag	UNP P36776
C	111	GLN	-	expression tag	UNP P36776
C	112	GLY	-	expression tag	UNP P36776
C	113	ALA	-	expression tag	UNP P36776
C	114	HIS	-	expression tag	UNP P36776
C	186	GLU	TYR	engineered mutation	UNP P36776
D	91	MET	-	initiating methionine	UNP P36776
D	92	GLY	-	expression tag	UNP P36776
D	93	HIS	-	expression tag	UNP P36776
D	94	HIS	-	expression tag	UNP P36776
D	95	HIS	-	expression tag	UNP P36776
D	96	HIS	-	expression tag	UNP P36776
D	97	HIS	-	expression tag	UNP P36776
D	98	HIS	-	expression tag	UNP P36776
D	99	ASP	-	expression tag	UNP P36776
D	100	TYR	-	expression tag	UNP P36776
D	101	ASP	-	expression tag	UNP P36776
D	102	ILE	-	expression tag	UNP P36776
D	103	PRO	-	expression tag	UNP P36776
D	104	THR	-	expression tag	UNP P36776
D	105	THR	-	expression tag	UNP P36776
D	106	GLU	-	expression tag	UNP P36776
D	107	ASN	-	expression tag	UNP P36776
D	108	LEU	-	expression tag	UNP P36776
D	109	TYR	-	expression tag	UNP P36776
D	110	PHE	-	expression tag	UNP P36776
D	111	GLN	-	expression tag	UNP P36776
D	112	GLY	-	expression tag	UNP P36776
D	113	ALA	-	expression tag	UNP P36776
D	114	HIS	-	expression tag	UNP P36776
D	186	GLU	TYR	engineered mutation	UNP P36776
E	91	MET	-	initiating methionine	UNP P36776
E	92	GLY	-	expression tag	UNP P36776

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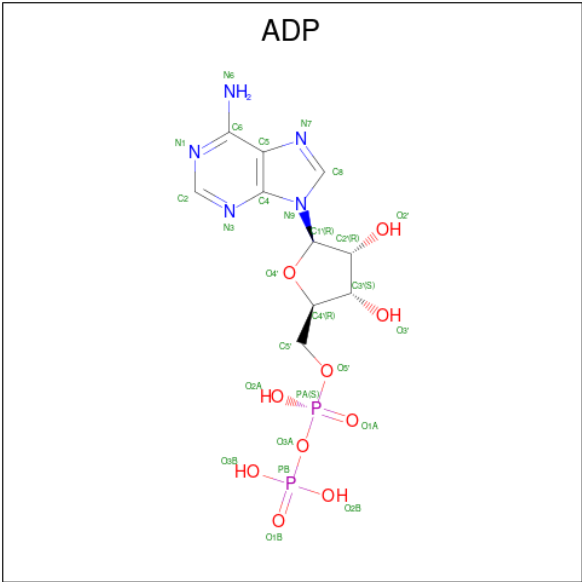
Chain	Residue	Modelled	Actual	Comment	Reference
E	93	HIS	-	expression tag	UNP P36776
E	94	HIS	-	expression tag	UNP P36776
E	95	HIS	-	expression tag	UNP P36776
E	96	HIS	-	expression tag	UNP P36776
E	97	HIS	-	expression tag	UNP P36776
E	98	HIS	-	expression tag	UNP P36776
E	99	ASP	-	expression tag	UNP P36776
E	100	TYR	-	expression tag	UNP P36776
E	101	ASP	-	expression tag	UNP P36776
E	102	ILE	-	expression tag	UNP P36776
E	103	PRO	-	expression tag	UNP P36776
E	104	THR	-	expression tag	UNP P36776
E	105	THR	-	expression tag	UNP P36776
E	106	GLU	-	expression tag	UNP P36776
E	107	ASN	-	expression tag	UNP P36776
E	108	LEU	-	expression tag	UNP P36776
E	109	TYR	-	expression tag	UNP P36776
E	110	PHE	-	expression tag	UNP P36776
E	111	GLN	-	expression tag	UNP P36776
E	112	GLY	-	expression tag	UNP P36776
E	113	ALA	-	expression tag	UNP P36776
E	114	HIS	-	expression tag	UNP P36776
E	186	GLU	TYR	engineered mutation	UNP P36776
F	91	MET	-	initiating methionine	UNP P36776
F	92	GLY	-	expression tag	UNP P36776
F	93	HIS	-	expression tag	UNP P36776
F	94	HIS	-	expression tag	UNP P36776
F	95	HIS	-	expression tag	UNP P36776
F	96	HIS	-	expression tag	UNP P36776
F	97	HIS	-	expression tag	UNP P36776
F	98	HIS	-	expression tag	UNP P36776
F	99	ASP	-	expression tag	UNP P36776
F	100	TYR	-	expression tag	UNP P36776
F	101	ASP	-	expression tag	UNP P36776
F	102	ILE	-	expression tag	UNP P36776
F	103	PRO	-	expression tag	UNP P36776
F	104	THR	-	expression tag	UNP P36776
F	105	THR	-	expression tag	UNP P36776
F	106	GLU	-	expression tag	UNP P36776
F	107	ASN	-	expression tag	UNP P36776
F	108	LEU	-	expression tag	UNP P36776
F	109	TYR	-	expression tag	UNP P36776

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Chain	Residue	Modelled	Actual	Comment	Reference
F	110	PHE	-	expression tag	UNP P36776
F	111	GLN	-	expression tag	UNP P36776
F	112	GLY	-	expression tag	UNP P36776
F	113	ALA	-	expression tag	UNP P36776
F	114	HIS	-	expression tag	UNP P36776
F	186	GLU	TYR	engineered mutation	UNP P36776

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

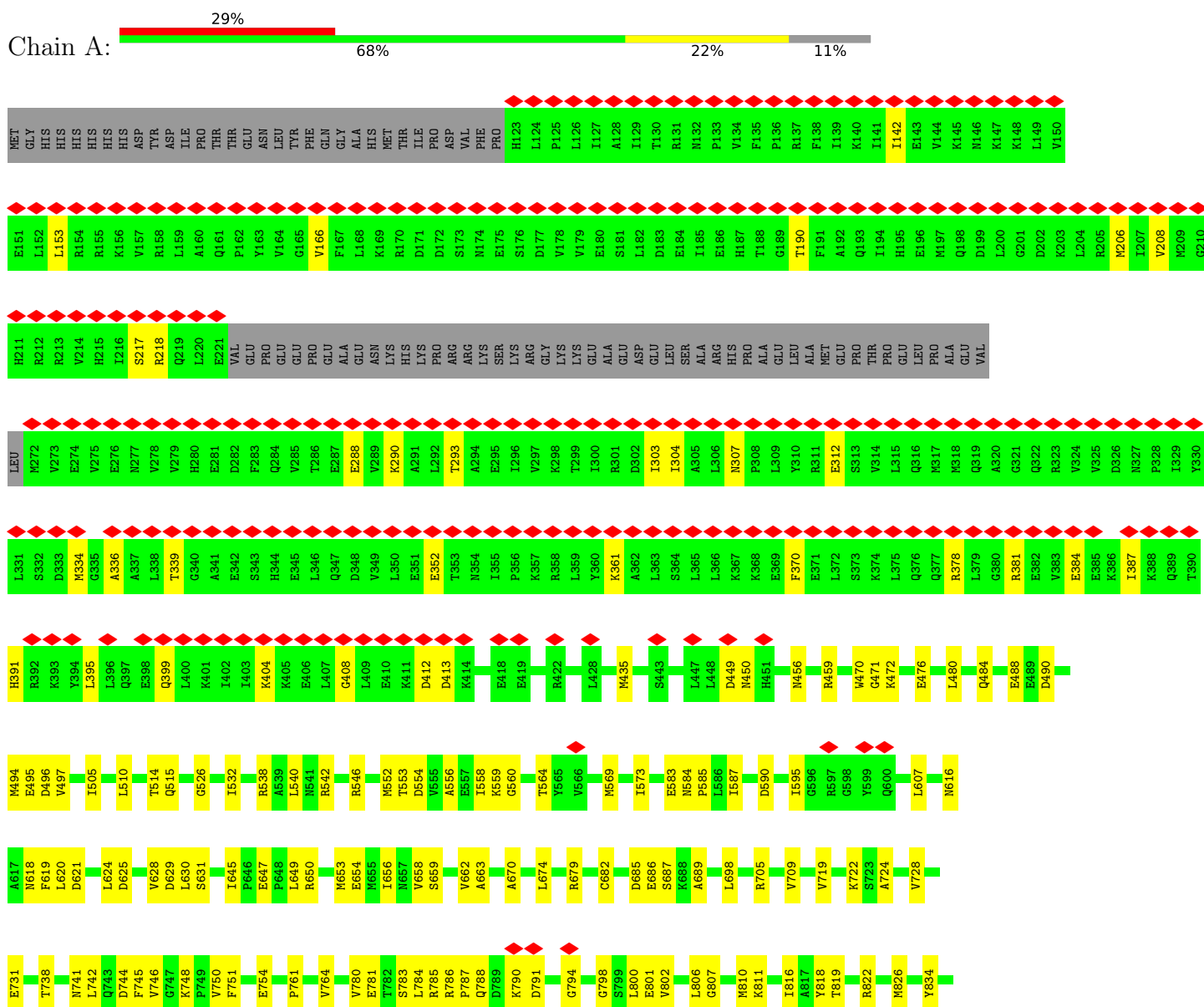


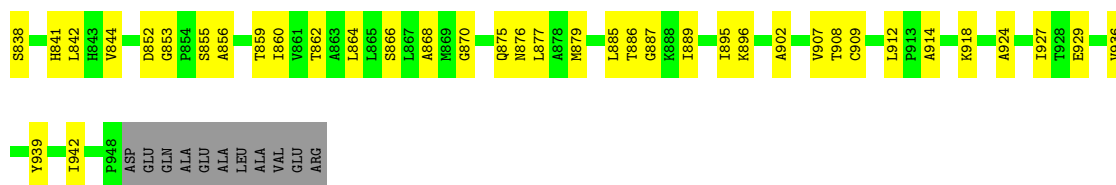
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	C	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

3 Residue-property plots

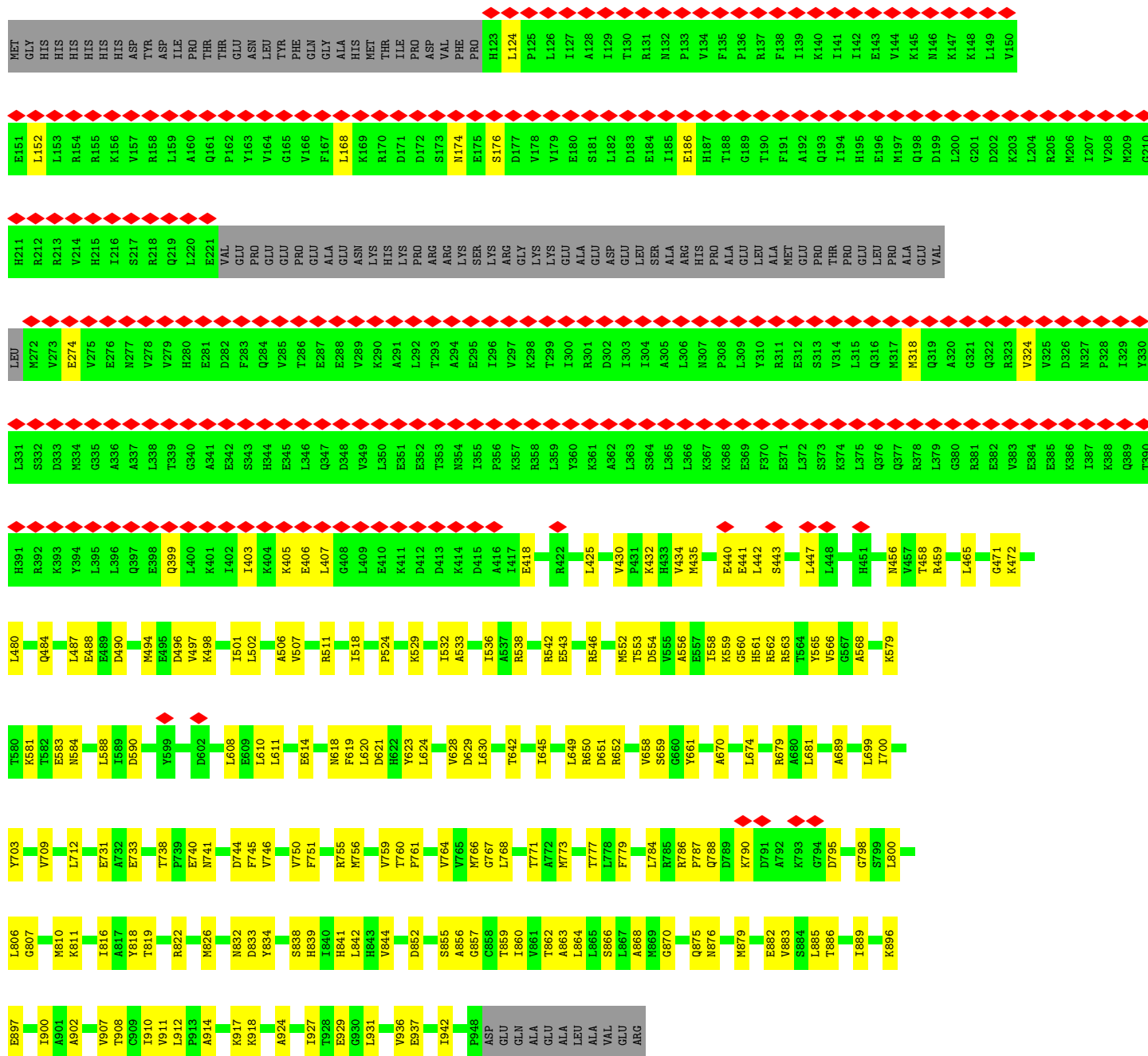
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Lon protease homolog, mitochondrial

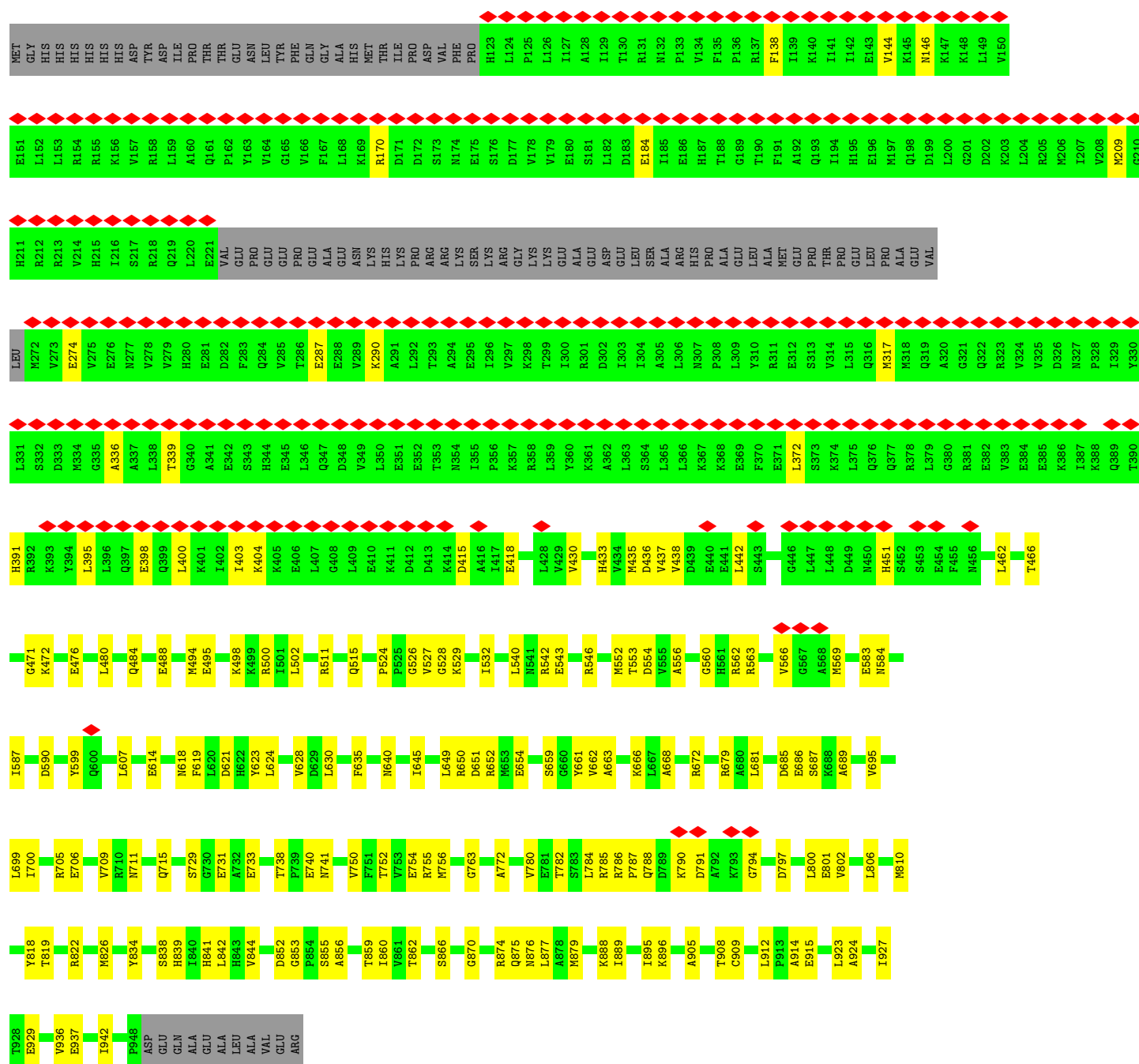




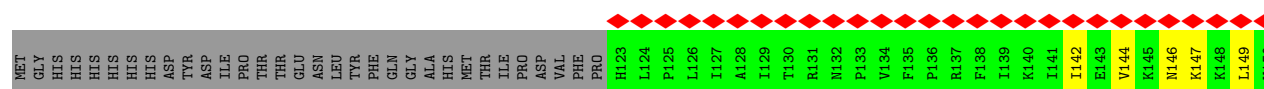
- Molecule 1: Lon protease homolog, mitochondrial



- Molecule 1: Lon protease homolog, mitochondrial



- Molecule 1: Lon protease homolog, mitochondrial



K996	F779	E647	G551	S452	H591	L331
T899	T782	P648	M552	S453	R392	S332
I900	L649	L649	T553	E454	K393	D333
T908	S783	R650	D554	F455	Y394	M334
L912	L784	V658	V555	M456	L395	G335
P913	R785	S659	A556	V457	L396	A336
A914	R786	G660	K559	T458	Q397	A337
L923	P787	V662	G560	R459	L338	L338
A924	Q788	A663	H561	L462	T339	G340
T927	D789	K666	R562	T466	L400	A341
T928	K791	I669	H563	L470	K401	G342
E929	A792	A670	T564	G471	I402	E343
G530	K793	L674	Y565	K472	K404	H344
L931	L800	L674	G567	Y473	K405	E345
V936	L806	R679	E583	S474	E406	L346
E937	G807	A689	N584	N475	L407	Q347
H938	R808	L689	L588	E476	G408	D348
Y939	M810	E706	I589	N477	L409	V349
T942	K811	L712	D590	L478	E410	L350
P948	Y818	L712	G596	D490	K411	E351
ASP	R822	V716	R597	H491	D412	E352
GLU	M826	V719	G598	D496	D413	T353
GLN	L835	V719	Y599	V497	K414	N354
ALA	L841	K722	Q600	K498	D415	I355
GLU	H841	V728	G601	L502	A416	P356
ALA	L842	E731	D602	I505	I417	K357
VAL	T849	L611	P603	A506	E418	R358
GLU	D852	T738	L611	V507	E419	L359
ARG	S855	N741	E914	S508	R422	Y360
	A856	D744	N618	Q509	E423	K361
	T859	F745	F619	L510	R424	A362
	I860	V753	L620	R511	L425	L363
	A863	E754	D621	G512	K426	S364
	S866	R755	H622	S513	E427	L365
	G870	M756	Y623	T514	L428	L366
	Q875	D758	L624	Q515	K367	K367
	N876	V759	D625	G516	V429	K368
	G887	T760	V626	K517	V430	E369
	K888	G763	P627	I518	P431	F370
	I895	M766	V628	L519	K432	E371
			D629	V527	H433	L372
			L630	I532	V434	S373
			S631	R538	M435	K374
			K632	R542	D436	L375
			T638	E543	V437	Q376
				R546	V438	Q377
				F547	D439	R378
					E440	L379
					E441	G380
					L442	R381
					S443	E382
					K444	V383
					L445	E384
					G446	E385
					L447	K386
					L448	I387
					D449	K388
					N450	Q389
					H451	T390

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39948	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.140	Depositor
Minimum map value	-0.442	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	469.8, 469.8, 469.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.566, 1.566, 1.566	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: 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	0.12	0/6239	0.29	0/8422
1	B	0.12	0/6239	0.30	0/8422
1	C	0.11	0/6239	0.28	0/8422
1	D	0.11	0/6239	0.30	0/8422
1	E	0.11	0/6239	0.29	0/8422
1	F	0.10	0/6239	0.27	0/8422
All	All	0.11	0/37434	0.29	0/50532

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	6138	6281	6283	153	0
1	B	6138	6281	6283	155	0
1	C	6138	6281	6283	145	0
1	D	6138	6281	6283	144	0
1	E	6138	6281	6283	132	0
1	F	6138	6281	6283	120	0
2	A	27	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	12	12	0	0
2	C	27	12	12	3	0
2	D	27	12	12	3	0
2	E	27	12	12	1	0
2	F	27	12	12	1	0
All	All	36990	37758	37770	797	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 11.

All (797) 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:E:834:TYR:O	1:E:838:SER:OG	1.92	0.88
1:D:810:MET:HE3	1:D:810:MET:HA	1.56	0.88
1:F:756:MET:HE2	1:F:756:MET:H	1.35	0.88
1:B:787:PRO:O	1:B:790:LYS:NZ	2.07	0.86
1:E:679:ARG:NH2	1:E:689:ALA:O	2.08	0.86
1:F:856:ALA:O	1:F:859:THR:OG1	1.94	0.85
1:D:834:TYR:O	1:D:838:SER:OG	1.93	0.85
1:C:738:THR:OG1	1:C:741:ASN:OD1	1.93	0.84
1:B:834:TYR:O	1:B:838:SER:OG	1.96	0.84
1:A:918:LYS:NZ	1:D:749:PRO:O	2.12	0.83
1:E:738:THR:OG1	1:E:741:ASN:OD1	1.95	0.83
1:F:852:ASP:O	1:F:855:SER:OG	1.96	0.82
1:D:679:ARG:NH2	1:D:689:ALA:O	2.12	0.82
1:C:834:TYR:O	1:C:838:SER:OG	1.97	0.81
1:C:435:MET:HE3	1:C:435:MET:HA	1.62	0.81
1:D:738:THR:OG1	1:D:741:ASN:OD1	1.97	0.81
1:B:885:LEU:HD23	1:B:885:LEU:O	1.81	0.81
1:A:738:THR:OG1	1:A:741:ASN:OD1	1.99	0.81
1:E:206:MET:HA	1:E:206:MET:HE2	1.64	0.80
1:A:764:VAL:HG23	1:A:781:GLU:HB2	1.62	0.79
1:A:552:MET:SD	1:A:553:THR:N	2.55	0.79
1:F:476:GLU:OE1	1:F:542:ARG:NH2	2.14	0.79
1:B:524:PRO:O	1:B:529:LYS:NZ	2.16	0.79
1:D:788:GLN:N	1:D:788:GLN:OE1	2.16	0.79
1:C:705:ARG:NH1	1:C:752:THR:O	2.15	0.79
1:B:786:ARG:NH1	1:C:797:ASP:OD1	2.15	0.78
1:D:710:ARG:NH2	2:D:1001:ADP:O3A	2.16	0.78
1:A:834:TYR:O	1:A:838:SER:OG	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:ASP:OD1	1:D:687:SER:OG	2.01	0.78
1:C:788:GLN:N	1:C:788:GLN:OE1	2.17	0.78
1:C:471:GLY:N	1:C:583:GLU:OE1	2.17	0.77
1:A:558:ILE:HG23	1:A:573:ILE:HD11	1.66	0.77
1:D:645:ILE:O	1:D:650:ARG:NH2	2.18	0.77
1:A:515:GLN:NE2	1:A:631:SER:O	2.18	0.77
1:D:764:VAL:HG23	1:D:781:GLU:HB2	1.67	0.77
1:B:738:THR:OG1	1:B:741:ASN:OD1	2.00	0.77
1:D:529:LYS:NZ	2:D:1001:ADP:O3B	2.17	0.77
1:E:476:GLU:OE1	1:E:514:THR:OG1	2.03	0.76
1:C:528:GLY:N	2:C:1001:ADP:O2B	2.19	0.76
1:E:206:MET:SD	1:E:207:ILE:N	2.58	0.76
1:C:640:ASN:ND2	1:C:772:ALA:O	2.18	0.76
1:C:685:ASP:OD2	1:C:687:SER:OG	2.02	0.76
1:A:556:ALA:O	1:A:560:GLY:N	2.18	0.76
1:C:787:PRO:O	1:C:790:LYS:NZ	2.13	0.76
1:C:442:LEU:HD23	1:C:462:LEU:HD21	1.67	0.75
1:A:788:GLN:N	1:A:788:GLN:OE1	2.19	0.75
1:C:852:ASP:O	1:C:855:SER:OG	2.03	0.75
1:F:788:GLN:N	1:F:788:GLN:OE1	2.20	0.75
1:F:738:THR:OG1	1:F:741:ASN:OD1	2.03	0.75
1:C:563:ARG:O	1:C:563:ARG:NE	2.19	0.75
1:A:497:VAL:HG21	1:A:658:VAL:HG12	1.69	0.74
1:A:290:LYS:O	1:A:293:THR:OG1	2.04	0.74
1:C:556:ALA:O	1:C:560:GLY:N	2.20	0.74
1:B:174:ASN:OD1	1:B:176:SER:OG	2.03	0.74
1:F:808:GLU:N	1:F:808:GLU:OE1	2.21	0.74
1:B:494:MET:SD	1:B:532:ILE:HD12	2.28	0.74
1:B:788:GLN:OE1	1:B:788:GLN:N	2.20	0.74
1:C:543:GLU:N	1:C:543:GLU:OE1	2.20	0.73
1:E:686:GLU:N	1:E:686:GLU:OE1	2.20	0.73
1:B:566:VAL:O	1:C:562:ARG:NH1	2.21	0.73
1:A:552:MET:SD	1:A:554:ASP:N	2.62	0.73
1:E:186:GLU:OE1	1:E:347:GLN:NE2	2.22	0.73
1:E:647:GLU:OE1	1:E:650:ARG:NH1	2.22	0.73
1:A:744:ASP:OD1	1:A:745:PHE:N	2.22	0.72
1:D:500:ARG:NH2	1:D:654:GLU:OE2	2.22	0.72
1:A:559:LYS:NZ	1:A:620:LEU:O	2.22	0.72
1:B:700:ILE:HG12	1:B:712:LEU:HD11	1.70	0.72
1:F:559:LYS:NZ	1:F:620:LEU:O	2.21	0.72
1:A:490:ASP:OD2	1:A:538:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:808:GLU:N	1:D:808:GLU:OE1	2.21	0.72
1:B:937:GLU:N	1:B:937:GLU:OE1	2.22	0.72
1:E:788:GLN:OE1	1:E:788:GLN:N	2.22	0.72
1:B:471:GLY:N	1:B:583:GLU:OE1	2.23	0.72
1:C:929:GLU:N	1:C:929:GLU:OE1	2.23	0.72
1:E:274:GLU:OE1	1:E:274:GLU:N	2.23	0.72
1:B:929:GLU:N	1:B:929:GLU:OE1	2.22	0.71
1:F:527:VAL:O	1:F:661:TYR:OH	2.06	0.71
1:A:621:ASP:OD1	1:A:624:LEU:N	2.22	0.71
1:A:705:ARG:NH2	1:A:754:GLU:O	2.23	0.71
1:B:432:LYS:O	1:B:435:MET:HE3	1.90	0.71
1:F:645:ILE:O	1:F:650:ARG:NH2	2.23	0.71
1:B:563:ARG:HA	1:B:568:ALA:HB3	1.72	0.70
1:E:941:GLU:N	1:E:941:GLU:OE1	2.23	0.70
1:A:856:ALA:O	1:A:859:THR:OG1	2.08	0.70
1:D:793:LYS:O	1:D:793:LYS:NZ	2.16	0.70
1:B:579:LYS:O	1:B:581:LYS:NZ	2.24	0.70
1:A:456:ASN:OD1	1:A:459:ARG:NH1	2.25	0.70
1:A:875:GLN:N	1:A:875:GLN:OE1	2.25	0.70
1:B:318:MET:HA	1:B:318:MET:HE2	1.74	0.70
1:D:543:GLU:OE1	1:D:544:TYR:N	2.24	0.70
1:D:405:LYS:O	1:D:407:LEU:HD22	1.91	0.69
1:D:856:ALA:O	1:D:859:THR:OG1	2.09	0.69
1:C:614:GLU:N	1:C:614:GLU:OE1	2.25	0.69
1:E:856:ALA:O	1:E:859:THR:OG1	2.08	0.69
1:B:856:ALA:O	1:B:859:THR:OG1	2.09	0.69
1:C:495:GLU:N	1:C:495:GLU:OE1	2.25	0.69
1:D:929:GLU:N	1:D:929:GLU:OE1	2.25	0.69
1:B:561:HIS:HB2	1:B:568:ALA:HB1	1.73	0.69
1:E:590:ASP:OD1	1:E:638:THR:OG1	2.10	0.69
1:C:569:MET:HE3	1:C:569:MET:N	2.07	0.69
1:C:740:GLU:N	1:C:740:GLU:OE1	2.24	0.69
1:C:542:ARG:NH1	1:C:584:ASN:O	2.24	0.69
1:F:863:ALA:O	1:F:866:SER:OG	2.10	0.69
1:A:495:GLU:OE1	1:A:495:GLU:N	2.26	0.69
1:C:937:GLU:N	1:C:937:GLU:OE1	2.26	0.68
1:E:711:ASN:OD1	1:E:715:GLN:NE2	2.26	0.68
1:E:478:LEU:O	1:E:509:GLN:NE2	2.26	0.68
2:E:1001:ADP:H5'2	2:E:1001:ADP:O2B	1.93	0.68
1:A:387:ILE:HD11	1:C:398:GLU:OE1	1.94	0.68
1:E:403:ILE:HG23	1:E:404:LYS:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:556:ALA:O	1:F:560:GLY:N	2.27	0.68
1:A:679:ARG:NH2	1:A:689:ALA:O	2.27	0.68
1:D:659:SER:O	1:D:896:LYS:NZ	2.26	0.68
1:D:574:ILE:H	1:D:574:ILE:HD12	1.58	0.67
1:E:411:LYS:NZ	1:E:413:ASP:OD1	2.24	0.67
1:F:543:GLU:OE1	1:F:543:GLU:N	2.27	0.67
1:B:914:ALA:N	1:B:936:VAL:O	2.28	0.67
1:E:798:GLY:O	1:E:818:TYR:OH	2.09	0.67
1:E:929:GLU:N	1:E:929:GLU:OE1	2.26	0.67
1:A:484:GLN:NE2	1:A:488:GLU:OE2	2.28	0.67
1:C:862:THR:HG21	1:C:879:MET:CE	2.24	0.67
1:C:875:GLN:OE1	1:C:875:GLN:N	2.26	0.67
1:F:452:SER:OG	1:F:454:GLU:OE1	2.12	0.67
1:B:681:LEU:O	1:C:511:ARG:NE	2.28	0.67
1:C:552:MET:SD	1:C:553:THR:N	2.68	0.67
1:D:733:GLU:N	1:D:733:GLU:OE1	2.27	0.67
1:E:151:GLU:OE1	1:E:154:ARG:NH2	2.28	0.67
1:E:442:LEU:HD23	1:E:462:LEU:HD21	1.76	0.66
1:D:924:ALA:O	1:D:927:ILE:HG22	1.95	0.66
1:B:543:GLU:N	1:B:543:GLU:OE1	2.28	0.66
1:F:758:ASP:O	1:F:875:GLN:NE2	2.29	0.66
1:A:546:ARG:NH2	1:A:590:ASP:OD2	2.29	0.66
1:D:552:MET:SD	1:D:553:THR:N	2.69	0.66
1:A:476:GLU:OE1	1:A:514:THR:OG1	2.13	0.66
1:F:274:GLU:N	1:F:274:GLU:OE1	2.29	0.66
1:F:456:ASN:OD1	1:F:459:ARG:NH1	2.28	0.66
1:A:542:ARG:NH1	1:A:584:ASN:O	2.30	0.65
1:E:142:ILE:HD12	1:E:208:VAL:HG11	1.77	0.65
1:D:542:ARG:NH1	1:D:584:ASN:O	2.28	0.65
1:C:524:PRO:O	1:C:529:LYS:NZ	2.30	0.65
1:D:471:GLY:N	1:D:583:GLU:OE2	2.28	0.65
1:C:607:LEU:HD23	1:C:649:LEU:HD11	1.78	0.65
1:F:491:HIS:CD2	1:F:532:ILE:HG22	2.32	0.65
1:F:806:LEU:HD13	1:F:811:LYS:HB2	1.79	0.65
1:E:418:GLU:OE1	1:E:442:LEU:HD22	1.96	0.65
1:A:914:ALA:N	1:A:936:VAL:O	2.29	0.65
1:C:856:ALA:O	1:C:859:THR:OG1	2.12	0.65
1:D:731:GLU:N	1:D:731:GLU:OE1	2.29	0.64
1:B:800:LEU:HD11	1:B:842:LEU:HD23	1.79	0.64
1:F:670:ALA:HB2	1:F:712:LEU:HD21	1.80	0.64
1:D:810:MET:HE1	1:D:854:PRO:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:914:ALA:N	1:F:936:VAL:O	2.30	0.63
1:C:526:GLY:N	2:C:1001:ADP:O3B	2.31	0.63
1:C:874:ARG:NH2	1:C:877:LEU:HD13	2.14	0.63
1:D:895:ILE:HD11	1:D:912:LEU:HD12	1.80	0.63
1:F:712:LEU:HD12	1:F:712:LEU:O	1.98	0.63
1:E:490:ASP:O	1:E:491:HIS:ND1	2.31	0.63
1:C:914:ALA:N	1:C:936:VAL:O	2.30	0.63
1:E:914:ALA:N	1:E:936:VAL:O	2.31	0.63
1:A:783:SER:OG	1:B:885:LEU:HD21	1.97	0.63
1:A:647:GLU:OE1	1:A:650:ARG:NH1	2.31	0.63
1:B:784:LEU:HD11	1:B:786:ARG:O	1.98	0.63
1:D:744:ASP:OD1	1:D:745:PHE:N	2.31	0.63
1:D:472:LYS:N	1:D:583:GLU:OE1	2.31	0.63
1:D:475:ASN:O	1:D:541:ASN:ND2	2.32	0.63
1:E:441:GLU:OE1	1:E:444:LYS:NZ	2.28	0.63
1:B:862:THR:HG21	1:B:879:MET:CE	2.29	0.62
1:B:875:GLN:N	1:B:875:GLN:OE1	2.32	0.62
1:E:653:MET:O	1:E:655:MET:HE1	1.99	0.62
1:B:771:THR:HG23	1:B:773:MET:O	1.99	0.62
1:D:889:ILE:N	1:D:937:GLU:O	2.32	0.62
1:F:744:ASP:OD1	1:F:745:PHE:N	2.32	0.62
1:B:897:GLU:N	1:B:897:GLU:OE1	2.32	0.62
1:D:875:GLN:N	1:D:875:GLN:OE1	2.33	0.62
1:A:731:GLU:OE1	1:A:731:GLU:N	2.31	0.62
1:B:441:GLU:OE2	1:B:458:THR:HG22	1.99	0.62
1:B:750:VAL:HG13	1:B:751:PHE:CD1	2.34	0.62
1:C:587:ILE:HD12	1:C:587:ILE:H	1.63	0.62
1:D:785:ARG:NE	1:D:801:GLU:OE1	2.33	0.62
1:A:654:GLU:N	1:A:654:GLU:OE1	2.33	0.62
1:A:336:ALA:O	1:A:339:THR:OG1	2.10	0.62
1:E:401:LYS:HA	1:E:407:LEU:HD22	1.81	0.62
1:E:787:PRO:O	1:E:790:LYS:NZ	2.32	0.62
1:A:472:LYS:N	1:A:583:GLU:OE1	2.32	0.61
1:C:451:HIS:ND1	1:E:448:LEU:HD13	2.14	0.61
1:C:651:ASP:OD1	1:C:652:ARG:N	2.34	0.61
1:B:621:ASP:OD1	1:B:624:LEU:N	2.33	0.61
1:D:785:ARG:NH2	1:D:801:GLU:OE2	2.33	0.61
1:F:190:THR:OG1	1:F:213:ARG:NH1	2.33	0.61
1:C:681:LEU:O	1:E:511:ARG:NH1	2.34	0.61
1:F:476:GLU:OE2	1:F:514:THR:HG21	2.00	0.61
1:A:785:ARG:NE	1:A:801:GLU:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:ILE:HG23	1:A:885:LEU:HB2	1.81	0.61
1:B:324:VAL:O	1:D:147:LYS:NZ	2.33	0.61
1:F:643:ASP:OD2	1:F:849:THR:OG1	2.19	0.61
1:C:418:GLU:OE1	1:C:442:LEU:HD22	2.00	0.61
1:F:929:GLU:OE1	1:F:929:GLU:N	2.34	0.61
1:F:787:PRO:O	1:F:790:LYS:NZ	2.34	0.61
1:C:274:GLU:OE1	1:C:274:GLU:N	2.34	0.61
1:A:685:ASP:OD1	1:A:686:GLU:N	2.33	0.60
1:C:645:ILE:O	1:C:650:ARG:NH2	2.33	0.60
1:E:726:LYS:HE3	1:E:735:VAL:HG22	1.83	0.60
1:D:552:MET:HE1	1:D:554:ASP:O	2.01	0.60
1:D:614:GLU:OE1	1:D:614:GLU:N	2.34	0.60
1:E:887:GLY:O	1:E:939:TYR:N	2.35	0.60
1:F:590:ASP:OD1	1:F:638:THR:OG1	2.18	0.60
1:C:430:VAL:HG11	1:C:435:MET:SD	2.41	0.60
1:A:387:ILE:HD11	1:C:398:GLU:CD	2.26	0.60
1:D:430:VAL:HG13	1:D:435:MET:HE2	1.83	0.60
1:B:852:ASP:O	1:B:855:SER:OG	2.17	0.60
1:E:903:LYS:NZ	1:E:927:ILE:O	2.35	0.60
1:C:731:GLU:N	1:C:731:GLU:OE1	2.35	0.60
1:D:559:LYS:NZ	1:D:620:LEU:O	2.35	0.60
1:D:889:ILE:HD11	1:D:942:ILE:HD12	1.84	0.60
1:D:911:VAL:C	1:D:912:LEU:HD23	2.27	0.60
1:E:876:ASN:OD1	1:E:908:THR:HG22	2.02	0.59
1:D:852:ASP:O	1:D:855:SER:OG	2.18	0.59
1:A:885:LEU:HD23	1:D:781:GLU:OE1	2.02	0.59
1:D:418:GLU:HG2	1:D:442:LEU:HD22	1.85	0.59
1:D:629:ASP:OD2	1:D:632:LYS:NZ	2.34	0.59
1:F:866:SER:O	1:F:870:GLY:N	2.35	0.59
1:E:556:ALA:O	1:E:560:GLY:N	2.35	0.59
1:E:866:SER:O	1:E:870:GLY:N	2.35	0.59
1:B:518:ILE:HG21	1:B:611:LEU:HD23	1.84	0.59
1:D:456:ASN:OD1	1:D:459:ARG:NH1	2.35	0.59
1:A:682:CYS:SG	1:B:511:ARG:NH2	2.76	0.59
1:A:645:ILE:O	1:A:650:ARG:NH2	2.36	0.59
1:A:859:THR:O	1:A:862:THR:HG22	2.03	0.59
1:C:818:TYR:OH	1:C:822:ARG:NH2	2.36	0.58
1:E:430:VAL:HG11	1:E:435:MET:SD	2.43	0.58
1:E:559:LYS:NZ	1:E:620:LEU:O	2.34	0.58
1:F:508:SER:HB2	1:F:514:THR:HG23	1.84	0.58
1:B:484:GLN:NE2	1:B:488:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:SER:OG	1:E:480:LEU:HD13	2.02	0.58
1:C:756:MET:HE3	1:E:890:LEU:HD22	1.85	0.58
1:C:621:ASP:OD1	1:C:624:LEU:N	2.36	0.58
1:A:569:MET:SD	1:A:569:MET:N	2.77	0.58
1:A:929:GLU:OE1	1:A:929:GLU:N	2.35	0.58
1:C:784:LEU:HD11	1:C:786:ARG:O	2.03	0.58
1:D:352:GLU:O	1:D:358:ARG:NH2	2.34	0.58
1:E:645:ILE:O	1:E:650:ARG:NH2	2.36	0.58
1:B:733:GLU:OE1	1:B:733:GLU:N	2.35	0.58
1:B:501:ILE:HG21	1:B:536:ILE:HD13	1.85	0.58
1:E:456:ASN:OD1	1:E:459:ARG:NH1	2.36	0.58
1:E:614:GLU:N	1:E:614:GLU:OE1	2.37	0.58
1:A:748:LYS:HE2	1:B:918:LYS:HD2	1.85	0.58
1:B:124:LEU:HD22	1:B:152:LEU:HD11	1.86	0.58
1:D:498:LYS:O	1:D:502:LEU:HD23	2.03	0.58
1:E:621:ASP:OD1	1:E:624:LEU:N	2.34	0.58
1:F:430:VAL:HG11	1:F:435:MET:SD	2.44	0.58
1:F:662:VAL:HA	1:F:900:ILE:HD11	1.86	0.58
1:A:810:MET:HE1	1:A:853:GLY:C	2.29	0.58
1:B:546:ARG:NH2	1:B:590:ASP:OD2	2.36	0.58
1:B:645:ILE:O	1:B:650:ARG:NH2	2.37	0.58
1:B:659:SER:O	1:B:896:LYS:NZ	2.37	0.58
1:B:844:VAL:HG23	1:B:844:VAL:O	2.04	0.58
1:A:810:MET:HA	1:A:810:MET:HE2	1.84	0.57
1:C:498:LYS:O	1:C:502:LEU:HD23	2.04	0.57
1:F:306:LEU:O	1:F:377:GLN:NE2	2.37	0.57
1:F:810:MET:HE3	1:F:810:MET:HA	1.86	0.57
1:A:497:VAL:CG2	1:A:658:VAL:HG12	2.35	0.57
1:C:791:ASP:OD2	1:C:794:GLY:N	2.38	0.57
1:D:494:MET:CE	1:D:532:ILE:HD13	2.34	0.57
1:A:787:PRO:CA	1:B:826:MET:HE1	2.35	0.57
1:A:895:ILE:HD11	1:A:912:LEU:HD13	1.87	0.57
1:C:889:ILE:HD11	1:C:942:ILE:HD12	1.85	0.57
1:A:217:SER:O	1:A:218:ARG:NE	2.38	0.57
1:D:495:GLU:OE1	1:D:495:GLU:N	2.38	0.57
1:A:526:GLY:N	2:A:1001:ADP:O3B	2.38	0.57
1:E:552:MET:CE	1:E:558:ILE:HD11	2.35	0.57
1:F:547:PHE:O	1:F:590:ASP:N	2.37	0.57
1:A:800:LEU:HD11	1:A:842:LEU:HD23	1.87	0.56
1:C:403:ILE:HD12	1:E:403:ILE:HD13	1.87	0.56
1:C:785:ARG:NE	1:C:801:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:LEU:HD23	1:D:540:LEU:O	2.05	0.56
1:E:860:ILE:O	1:E:864:LEU:HD22	2.05	0.56
1:B:559:LYS:NZ	1:B:620:LEU:O	2.38	0.56
1:C:484:GLN:NE2	1:C:488:GLU:OE2	2.38	0.56
1:D:798:GLY:O	1:D:818:TYR:OH	2.17	0.56
1:A:682:CYS:O	1:B:511:ARG:NH1	2.37	0.56
1:B:496:ASP:OD1	1:B:497:VAL:N	2.38	0.56
1:C:862:THR:HG21	1:C:879:MET:HE1	1.86	0.56
1:E:552:MET:HE1	1:E:558:ILE:HD11	1.88	0.56
1:F:474:SER:OG	1:F:584:ASN:OD1	2.16	0.56
1:A:619:PHE:O	1:A:628:VAL:HG22	2.06	0.56
1:F:496:ASP:N	1:F:496:ASP:OD1	2.38	0.56
1:F:462:LEU:O	1:F:466:THR:HG23	2.05	0.56
1:D:621:ASP:OD1	1:D:624:LEU:N	2.35	0.56
1:C:546:ARG:NH2	1:C:590:ASP:OD2	2.39	0.56
1:A:844:VAL:HG23	1:A:844:VAL:O	2.05	0.56
1:A:877:LEU:HD12	1:A:909:CYS:O	2.05	0.56
1:F:889:ILE:HD11	1:F:942:ILE:HD12	1.88	0.56
1:C:494:MET:SD	1:C:532:ILE:HD12	2.46	0.56
1:C:500:ARG:NH2	1:C:654:GLU:OE2	2.37	0.56
1:F:889:ILE:N	1:F:937:GLU:O	2.38	0.56
1:F:895:ILE:HD11	1:F:912:LEU:HD13	1.86	0.56
1:B:552:MET:SD	1:B:554:ASP:N	2.79	0.55
1:B:608:LEU:HD22	1:B:649:LEU:CD2	2.36	0.55
1:F:334:MET:SD	1:F:335:GLY:N	2.80	0.55
1:A:685:ASP:OD2	1:A:687:SER:OG	2.23	0.55
1:C:862:THR:HG21	1:C:879:MET:HE3	1.88	0.55
1:F:669:ILE:HG23	2:F:1001:ADP:C2	2.41	0.55
1:F:887:GLY:O	1:F:939:TYR:N	2.36	0.55
1:C:750:VAL:HG23	1:C:750:VAL:O	2.06	0.55
1:B:841:HIS:HD1	1:C:819:THR:HG21	1.72	0.55
1:D:784:LEU:HD11	1:D:786:ARG:O	2.06	0.55
1:B:882:GLU:OE1	1:B:883:VAL:N	2.40	0.55
1:E:727:ILE:HD11	1:E:735:VAL:HG23	1.89	0.55
1:C:540:LEU:HD23	1:C:540:LEU:O	2.06	0.55
1:D:842:LEU:C	1:D:842:LEU:HD12	2.32	0.55
1:E:726:LYS:O	1:E:730:GLY:N	2.40	0.55
1:A:784:LEU:HD11	1:A:786:ARG:O	2.07	0.55
1:B:405:LYS:NZ	1:B:406:GLU:OE2	2.40	0.55
1:C:621:ASP:OD1	1:C:623:TYR:N	2.40	0.55
1:C:685:ASP:OD1	1:C:686:GLU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:LEU:O	1:D:409:LEU:HD12	2.06	0.55
1:E:773:MET:O	1:E:773:MET:SD	2.64	0.55
1:D:556:ALA:O	1:D:560:GLY:N	2.33	0.55
1:E:771:THR:HG23	1:E:773:MET:O	2.07	0.55
1:F:895:ILE:O	1:F:899:THR:OG1	2.21	0.55
1:C:566:VAL:O	1:C:566:VAL:HG13	2.07	0.55
1:F:272:MET:SD	1:F:272:MET:N	2.80	0.55
1:A:142:ILE:HD12	1:A:208:VAL:HG11	1.87	0.54
1:A:862:THR:HG21	1:A:879:MET:CE	2.37	0.54
1:B:552:MET:SD	1:B:553:THR:N	2.80	0.54
1:C:511:ARG:NH1	1:C:515:GLN:OE1	2.40	0.54
1:D:153:LEU:HD21	1:D:206:MET:HE1	1.88	0.54
1:E:757:TYR:O	1:E:760:THR:OG1	2.24	0.54
1:B:798:GLY:O	1:B:818:TYR:OH	2.22	0.54
1:C:896:LYS:HG3	1:C:923:LEU:HD22	1.89	0.54
1:B:876:ASN:OD1	1:B:908:THR:HG22	2.07	0.54
1:A:807:GLY:O	1:A:811:LYS:N	2.34	0.54
1:C:679:ARG:NH2	1:C:689:ALA:O	2.41	0.54
1:C:895:ILE:HD11	1:C:912:LEU:HD22	1.89	0.54
1:D:761:PRO:O	1:D:764:VAL:HG12	2.07	0.54
1:A:304:ILE:HD12	1:A:312:GLU:OE1	2.08	0.54
1:D:491:HIS:HD2	1:D:532:ILE:HD12	1.73	0.54
1:F:156:LYS:NZ	1:F:163:TYR:O	2.38	0.54
1:A:819:THR:HG21	1:D:841:HIS:HD1	1.72	0.54
1:C:336:ALA:O	1:C:339:THR:OG1	2.21	0.54
1:C:430:VAL:HG21	1:C:435:MET:SD	2.48	0.54
1:D:863:ALA:O	1:D:866:SER:OG	2.19	0.54
1:A:659:SER:O	1:A:896:LYS:NZ	2.41	0.53
1:E:465:LEU:HD13	1:E:624:LEU:HD11	1.89	0.53
1:E:496:ASP:OD1	1:E:497:VAL:N	2.41	0.53
1:A:399:GLN:HG2	1:F:383:VAL:HG11	1.90	0.53
1:F:642:THR:O	1:F:645:ILE:HG22	2.08	0.53
1:F:731:GLU:OE1	1:F:731:GLU:N	2.34	0.53
1:E:294:ALA:O	1:E:297:VAL:HG22	2.08	0.53
1:A:352:GLU:OE2	1:A:361:LYS:NZ	2.40	0.53
1:F:679:ARG:NH2	1:F:689:ALA:O	2.41	0.53
1:F:385:GLU:OE2	1:F:385:GLU:HA	2.09	0.53
1:B:784:LEU:HD12	1:B:839:HIS:O	2.08	0.53
1:B:889:ILE:HD11	1:B:942:ILE:HD12	1.90	0.53
1:C:476:GLU:OE1	1:C:476:GLU:N	2.39	0.53
1:D:787:PRO:O	1:D:790:LYS:NZ	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:800:LEU:HD11	1:D:842:LEU:HD23	1.89	0.53
1:C:552:MET:SD	1:C:554:ASP:N	2.82	0.53
1:C:844:VAL:HG23	1:C:844:VAL:O	2.09	0.53
1:C:436:ASP:OD1	1:C:437:VAL:N	2.42	0.53
1:C:733:GLU:N	1:C:733:GLU:OE1	2.41	0.53
1:A:886:THR:HG22	1:A:886:THR:O	2.09	0.53
1:A:384:GLU:HA	1:A:387:ILE:HD12	1.89	0.52
1:A:780:VAL:HG23	1:A:844:VAL:HG12	1.91	0.52
1:E:666:LYS:HD3	1:E:709:VAL:HG22	1.92	0.52
1:F:547:PHE:N	1:F:588:LEU:O	2.40	0.52
1:A:682:CYS:HA	1:B:511:ARG:CZ	2.39	0.52
1:C:472:LYS:N	1:C:583:GLU:OE2	2.41	0.52
1:D:597:ARG:NH2	1:D:602:ASP:OD1	2.42	0.52
1:A:510:LEU:HD12	1:D:728:VAL:HG22	1.90	0.52
1:B:833:ASP:OD1	1:B:833:ASP:C	2.51	0.52
1:D:484:GLN:NE2	1:D:488:GLU:OE2	2.42	0.52
1:E:784:LEU:HD11	1:E:786:ARG:O	2.08	0.52
1:F:442:LEU:HD23	1:F:462:LEU:HD21	1.92	0.52
1:F:756:MET:HE2	1:F:756:MET:N	2.13	0.52
1:A:787:PRO:O	1:A:790:LYS:NZ	2.35	0.52
1:C:915:GLU:OE1	1:C:915:GLU:N	2.43	0.52
1:D:820:PHE:CD2	1:D:883:VAL:HG11	2.44	0.52
1:C:442:LEU:CD2	1:C:462:LEU:HD21	2.38	0.52
1:E:597:ARG:CG	1:E:597:ARG:O	2.58	0.52
1:F:806:LEU:HD12	1:F:806:LEU:C	2.34	0.52
1:E:498:LYS:O	1:E:502:LEU:HD23	2.10	0.52
1:F:619:PHE:O	1:F:628:VAL:HG22	2.10	0.52
1:C:619:PHE:O	1:C:628:VAL:HG22	2.10	0.52
1:E:764:VAL:HG23	1:E:781:GLU:HA	1.91	0.52
1:A:862:THR:HG21	1:A:879:MET:HE1	1.91	0.51
1:B:731:GLU:OE1	1:B:731:GLU:N	2.38	0.51
1:A:412:ASP:HB3	1:B:447:LEU:HD21	1.91	0.51
1:A:471:GLY:N	1:A:583:GLU:OE2	2.39	0.51
1:B:610:LEU:HD21	1:B:619:PHE:CZ	2.46	0.51
1:B:619:PHE:O	1:B:628:VAL:HG22	2.10	0.51
1:D:911:VAL:O	1:D:912:LEU:HD23	2.10	0.51
1:B:810:MET:HE2	1:B:810:MET:HA	1.93	0.51
1:E:144:VAL:HB	1:E:204:LEU:HD23	1.92	0.51
1:A:786:ARG:NH2	1:B:795:ASP:O	2.39	0.51
1:C:810:MET:HE1	1:C:853:GLY:C	2.36	0.51
1:E:442:LEU:CD2	1:E:462:LEU:HD21	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:LYS:N	1:E:583:GLU:OE1	2.43	0.51
1:B:773:MET:O	1:B:773:MET:SD	2.69	0.51
1:C:784:LEU:HD12	1:C:839:HIS:O	2.10	0.51
1:A:826:MET:HE1	1:D:787:PRO:N	2.26	0.51
1:B:621:ASP:OD1	1:B:623:TYR:N	2.44	0.51
1:B:740:GLU:OE1	1:B:740:GLU:N	2.34	0.51
1:C:786:ARG:HG2	1:C:787:PRO:HD2	1.93	0.51
1:D:914:ALA:N	1:D:936:VAL:O	2.39	0.51
1:E:681:LEU:HD23	1:E:681:LEU:C	2.35	0.51
1:A:658:VAL:HG23	1:A:658:VAL:O	2.11	0.51
1:A:786:ARG:HG3	1:A:787:PRO:HD2	1.92	0.51
1:B:318:MET:HE1	1:D:203:LYS:CE	2.41	0.51
1:C:755:ARG:NH1	1:C:905:ALA:O	2.44	0.51
1:D:503:GLU:OE2	1:F:722:LYS:N	2.44	0.51
1:E:750:VAL:HG22	1:E:750:VAL:O	2.10	0.51
1:F:659:SER:OG	1:F:896:LYS:NZ	2.40	0.51
1:B:614:GLU:OE1	1:B:614:GLU:N	2.43	0.50
1:D:911:VAL:HG11	1:D:942:ILE:HG12	1.94	0.50
1:A:288:GLU:OE2	1:E:342:GLU:N	2.44	0.50
1:A:573:ILE:HD12	1:A:573:ILE:H	1.76	0.50
1:D:501:ILE:HG21	1:D:536:ILE:HD12	1.92	0.50
1:A:494:MET:SD	1:A:532:ILE:HD12	2.50	0.50
1:C:866:SER:O	1:C:870:GLY:N	2.43	0.50
1:D:287:GLU:O	1:D:290:LYS:NZ	2.41	0.50
1:E:705:ARG:NH2	1:E:750:VAL:O	2.45	0.50
1:D:658:VAL:HG13	1:D:658:VAL:O	2.11	0.50
1:E:863:ALA:O	1:E:866:SER:OG	2.28	0.50
1:D:438:VAL:HG12	1:D:442:LEU:HD11	1.93	0.50
1:D:597:ARG:HG3	1:D:597:ARG:O	2.12	0.50
1:D:619:PHE:O	1:D:628:VAL:HG12	2.12	0.50
1:D:653:MET:SD	1:D:653:MET:N	2.85	0.50
1:B:889:ILE:N	1:B:937:GLU:O	2.40	0.50
1:C:662:VAL:HG22	1:C:663:ALA:H	1.77	0.50
1:A:866:SER:O	1:A:870:GLY:N	2.44	0.50
1:C:527:VAL:O	1:C:661:TYR:OH	2.30	0.50
1:C:859:THR:O	1:C:862:THR:HG22	2.11	0.50
1:B:924:ALA:O	1:B:927:ILE:HG22	2.12	0.50
1:E:628:VAL:HG23	1:E:630:LEU:CD1	2.42	0.50
1:B:556:ALA:O	1:B:560:GLY:N	2.36	0.49
1:B:914:ALA:O	1:B:917:LYS:HB3	2.12	0.49
1:C:709:VAL:HG12	1:C:709:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:866:SER:O	1:D:870:GLY:N	2.43	0.49
1:D:876:ASN:OD1	1:D:908:THR:HG22	2.11	0.49
1:F:755:ARG:HE	1:F:766:MET:HE1	1.77	0.49
1:C:527:VAL:N	2:C:1001:ADP:O2B	2.44	0.49
1:C:802:VAL:HG23	1:C:842:LEU:HD11	1.95	0.49
1:E:546:ARG:NH2	1:E:590:ASP:OD2	2.46	0.49
1:F:773:MET:O	1:F:773:MET:SD	2.70	0.49
1:F:800:LEU:HD11	1:F:842:LEU:HD23	1.95	0.49
1:A:818:TYR:OH	1:A:822:ARG:NH2	2.46	0.49
1:C:924:ALA:O	1:C:927:ILE:HG22	2.11	0.49
1:B:816:ILE:HG23	1:B:885:LEU:HB2	1.95	0.49
1:C:415:ASP:O	1:C:418:GLU:HB3	2.13	0.49
1:A:497:VAL:HG22	1:A:656:ILE:HG21	1.94	0.49
1:D:153:LEU:HD21	1:D:206:MET:CE	2.42	0.49
1:F:784:LEU:HD11	1:F:786:ARG:O	2.13	0.49
1:F:928:THR:HA	1:F:931:LEU:HD21	1.95	0.49
1:A:887:GLY:O	1:A:939:TYR:N	2.40	0.49
1:B:766:MET:SD	1:B:777:THR:OG1	2.70	0.49
1:C:372:LEU:HD13	1:D:402:ILE:HD11	1.95	0.49
1:E:501:ILE:O	1:E:505:ILE:HG12	2.13	0.49
1:B:418:GLU:CG	1:B:442:LEU:HD22	2.43	0.48
1:D:647:GLU:OE1	1:D:650:ARG:NH1	2.43	0.48
1:E:698:LEU:HD22	1:E:742:LEU:CD2	2.43	0.48
1:D:518:ILE:HG21	1:D:611:LEU:HD23	1.95	0.48
1:E:688:LYS:NZ	1:E:733:GLU:OE1	2.43	0.48
1:A:435:MET:HE2	1:A:435:MET:HA	1.94	0.48
1:A:842:LEU:C	1:A:842:LEU:HD12	2.38	0.48
1:C:404:LYS:HB2	1:E:403:ILE:HG21	1.95	0.48
1:C:780:VAL:HG23	1:C:844:VAL:HG12	1.95	0.48
1:C:787:PRO:HA	1:E:826:MET:CE	2.44	0.48
1:D:418:GLU:OE2	1:D:442:LEU:HD13	2.14	0.48
1:F:647:GLU:OE1	1:F:650:ARG:NH1	2.46	0.48
1:A:798:GLY:O	1:A:818:TYR:OH	2.25	0.48
1:B:507:VAL:HG22	1:B:511:ARG:CZ	2.44	0.48
1:C:842:LEU:C	1:C:842:LEU:HD12	2.38	0.48
1:C:287:GLU:O	1:C:290:LYS:NZ	2.44	0.48
1:A:618:ASN:N	1:A:618:ASN:OD1	2.45	0.48
1:B:418:GLU:HG3	1:B:442:LEU:HD22	1.94	0.48
1:A:629:ASP:C	1:A:630:LEU:HD12	2.39	0.48
1:A:724:ALA:O	1:A:728:VAL:HG23	2.14	0.48
1:A:889:ILE:HD11	1:A:942:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:MET:O	1:A:494:MET:HG3	2.14	0.48
1:A:742:LEU:CD1	1:A:746:VAL:HG12	2.44	0.48
1:B:318:MET:HE1	1:D:203:LYS:HE3	1.96	0.48
1:B:759:VAL:O	1:B:760:THR:OG1	2.25	0.48
1:E:334:MET:HE3	1:E:334:MET:O	2.13	0.48
1:F:835:LEU:C	1:F:835:LEU:HD23	2.39	0.48
1:A:653:MET:SD	1:A:653:MET:N	2.87	0.48
1:A:852:ASP:O	1:A:855:SER:OG	2.28	0.48
1:C:876:ASN:OD1	1:C:908:THR:HG22	2.14	0.48
1:F:472:LYS:N	1:F:583:GLU:OE1	2.47	0.48
1:A:924:ALA:O	1:A:927:ILE:HG22	2.13	0.47
1:F:842:LEU:C	1:F:842:LEU:HD12	2.38	0.47
1:B:274:GLU:N	1:B:274:GLU:OE1	2.46	0.47
1:B:886:THR:O	1:B:886:THR:HG22	2.14	0.47
1:C:418:GLU:CD	1:C:442:LEU:HD22	2.39	0.47
1:C:618:ASN:N	1:C:618:ASN:OD1	2.47	0.47
1:F:490:ASP:OD1	1:F:538:ARG:NH2	2.47	0.47
1:F:666:LYS:NZ	1:F:706:GLU:O	2.40	0.47
1:F:699:LEU:HD22	1:F:712:LEU:HD13	1.96	0.47
1:C:317:MET:N	1:C:317:MET:HE2	2.29	0.47
1:B:490:ASP:OD2	1:B:538:ARG:NH2	2.48	0.47
1:B:700:ILE:CG1	1:B:712:LEU:HD11	2.44	0.47
1:B:795:ASP:OD1	1:B:795:ASP:N	2.47	0.47
1:F:175:GLU:OE1	1:F:175:GLU:N	2.46	0.47
1:A:722:LYS:HD2	1:A:745:PHE:O	2.15	0.47
1:B:679:ARG:NH2	1:B:689:ALA:O	2.47	0.47
1:D:565:TYR:HB2	1:D:568:ALA:HB2	1.95	0.47
1:F:822:ARG:O	1:F:826:MET:HG3	2.15	0.47
1:F:896:LYS:HG3	1:F:923:LEU:HD22	1.97	0.47
1:A:819:THR:HG21	1:D:841:HIS:ND1	2.29	0.47
1:D:557:GLU:O	1:D:572:LYS:N	2.45	0.47
1:D:802:VAL:HG23	1:D:842:LEU:HD11	1.95	0.47
1:D:887:GLY:O	1:D:939:TYR:N	2.44	0.47
1:A:496:ASP:OD1	1:A:497:VAL:N	2.48	0.47
1:B:542:ARG:NH1	1:B:584:ASN:O	2.39	0.47
1:C:802:VAL:HG13	1:C:806:LEU:HD13	1.95	0.47
1:E:698:LEU:HD23	1:E:698:LEU:C	2.39	0.47
1:F:490:ASP:O	1:F:491:HIS:ND1	2.48	0.47
1:F:924:ALA:O	1:F:927:ILE:HG22	2.15	0.47
1:A:864:LEU:O	1:A:868:ALA:N	2.46	0.47
1:D:480:LEU:HD22	1:D:502:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:LEU:O	1:E:186:GLU:HB2	2.15	0.47
1:B:806:LEU:HD12	1:B:811:LYS:HG2	1.97	0.46
1:B:911:VAL:C	1:B:912:LEU:HD22	2.40	0.46
1:E:784:LEU:HD12	1:E:839:HIS:O	2.15	0.46
1:A:558:ILE:CG2	1:A:573:ILE:HD11	2.42	0.46
1:E:726:LYS:CE	1:E:735:VAL:HG22	2.46	0.46
1:D:274:GLU:N	1:D:274:GLU:OE1	2.49	0.46
1:F:621:ASP:OD1	1:F:624:LEU:N	2.40	0.46
1:B:859:THR:O	1:B:862:THR:HG22	2.15	0.46
1:E:611:LEU:HD22	1:E:649:LEU:HD13	1.98	0.46
1:C:810:MET:HE2	1:C:810:MET:HA	1.98	0.46
1:E:788:GLN:HA	1:E:790:LYS:HZ3	1.81	0.46
1:B:440:GLU:O	1:B:443:SER:OG	2.31	0.46
1:B:642:THR:O	1:B:645:ILE:HG22	2.16	0.46
1:C:841:HIS:HD1	1:E:819:THR:HG21	1.81	0.46
1:A:802:VAL:HG13	1:A:806:LEU:HD13	1.97	0.46
1:B:746:VAL:O	1:B:746:VAL:HG22	2.16	0.46
1:F:349:VAL:HG22	1:F:361:LYS:CD	2.46	0.46
1:A:698:LEU:HD23	1:A:698:LEU:O	2.16	0.46
1:C:170:ARG:NE	1:C:184:GLU:OE1	2.48	0.46
1:D:142:ILE:HB	1:D:206:MET:HB2	1.98	0.46
1:E:619:PHE:O	1:E:628:VAL:HG22	2.15	0.46
1:E:864:LEU:O	1:E:868:ALA:N	2.48	0.46
1:F:818:TYR:OH	1:F:822:ARG:NH2	2.49	0.46
1:A:616:ASN:ND2	1:A:630:LEU:O	2.49	0.45
1:C:144:VAL:HG12	1:C:146:ASN:H	1.81	0.45
1:C:800:LEU:HD11	1:C:842:LEU:HD23	1.98	0.45
1:D:496:ASP:OD1	1:D:497:VAL:N	2.45	0.45
1:B:832:ASN:OD1	1:B:833:ASP:N	2.49	0.45
1:E:698:LEU:HD23	1:E:698:LEU:O	2.16	0.45
1:F:345:GLU:O	1:F:349:VAL:HG23	2.16	0.45
1:F:876:ASN:OD1	1:F:908:THR:HG22	2.17	0.45
1:A:413:ASP:O	1:A:450:ASN:ND2	2.47	0.45
1:A:761:PRO:O	1:A:764:VAL:HG12	2.16	0.45
1:A:876:ASN:OD1	1:A:908:THR:HG22	2.16	0.45
1:C:403:ILE:CD1	1:E:403:ILE:HD13	2.47	0.45
1:C:438:VAL:HG12	1:C:442:LEU:HD11	1.99	0.45
1:D:810:MET:HA	1:D:810:MET:CE	2.36	0.45
1:F:546:ARG:NH2	1:F:590:ASP:OD2	2.50	0.45
1:A:748:LYS:HE2	1:B:918:LYS:CD	2.47	0.45
1:B:629:ASP:C	1:B:630:LEU:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:ARG:NH1	1:C:754:GLU:OE1	2.49	0.45
1:D:895:ILE:O	1:D:899:THR:OG1	2.29	0.45
1:E:744:ASP:OD1	1:E:745:PHE:N	2.49	0.45
1:F:384:GLU:O	1:F:388:LYS:HG2	2.17	0.45
1:A:470:TRP:HH2	1:A:628:VAL:HG12	1.81	0.45
1:B:658:VAL:HG13	1:B:658:VAL:O	2.16	0.45
1:D:819:THR:HG21	1:F:841:HIS:ND1	2.32	0.45
1:E:727:ILE:CD1	1:E:735:VAL:HG23	2.47	0.45
1:E:859:THR:O	1:E:860:ILE:C	2.60	0.45
1:A:480:LEU:C	1:A:480:LEU:HD23	2.42	0.45
1:A:679:ARG:NH1	1:A:686:GLU:OE1	2.40	0.45
1:C:711:ASN:OD1	1:C:715:GLN:NE2	2.45	0.45
1:F:859:THR:O	1:F:860:ILE:C	2.60	0.45
1:A:334:MET:SD	1:A:334:MET:C	3.00	0.45
1:A:787:PRO:HA	1:B:826:MET:HE1	1.99	0.45
1:B:498:LYS:O	1:B:502:LEU:HD23	2.17	0.45
1:B:744:ASP:OD1	1:B:745:PHE:N	2.50	0.45
1:B:859:THR:O	1:B:860:ILE:C	2.59	0.45
1:C:462:LEU:O	1:C:466:THR:HG23	2.17	0.45
1:E:317:MET:C	1:E:317:MET:SD	2.99	0.45
1:E:698:LEU:HD22	1:E:742:LEU:HD23	1.96	0.45
1:A:670:ALA:HA	1:A:674:LEU:HB2	1.99	0.45
1:B:403:ILE:O	1:B:407:LEU:HD23	2.17	0.45
1:C:138:PHE:N	1:C:209:MET:SD	2.90	0.45
1:C:628:VAL:HG23	1:C:630:LEU:CD1	2.46	0.44
1:D:662:VAL:HG12	1:D:663:ALA:N	2.32	0.44
1:E:761:PRO:O	1:E:764:VAL:HG12	2.16	0.44
1:B:533:ALA:CB	1:B:588:LEU:HD22	2.47	0.44
1:B:618:ASN:OD1	1:B:618:ASN:N	2.50	0.44
1:D:414:LYS:O	1:D:419:GLU:N	2.42	0.44
1:D:607:LEU:HD21	1:D:649:LEU:HD11	1.99	0.44
1:D:773:MET:HG3	1:D:773:MET:O	2.18	0.44
1:C:852:ASP:OD1	1:C:852:ASP:C	2.61	0.44
1:F:716:VAL:HA	1:F:719:VAL:HG12	1.99	0.44
1:A:303:ILE:O	1:A:307:ASN:N	2.45	0.44
1:A:902:ALA:O	1:A:907:VAL:HG12	2.16	0.44
1:B:651:ASP:OD1	1:B:652:ARG:N	2.50	0.44
1:A:750:VAL:HG23	1:A:751:PHE:N	2.32	0.44
1:B:472:LYS:N	1:B:583:GLU:OE1	2.51	0.44
1:D:438:VAL:O	1:D:442:LEU:HG	2.18	0.44
1:D:709:VAL:HG12	1:D:709:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ALA:O	1:D:610:LEU:HG	2.17	0.44
1:F:628:VAL:HG23	1:F:630:LEU:CD1	2.47	0.44
1:A:585:PRO:HG2	1:A:587:ILE:HD11	2.00	0.44
1:B:879:MET:HB3	1:B:911:VAL:HB	1.99	0.44
1:D:494:MET:HE1	1:D:532:ILE:HD13	1.99	0.44
1:E:562:ARG:O	1:E:563:ARG:HB3	2.18	0.44
1:B:628:VAL:HG23	1:B:630:LEU:CD1	2.48	0.44
1:C:787:PRO:HD3	1:E:826:MET:HE3	1.99	0.44
1:D:420:LYS:O	1:D:420:LYS:NZ	2.37	0.44
1:C:666:LYS:HB3	1:C:700:ILE:HD12	2.00	0.44
1:E:475:ASN:O	1:E:541:ASN:ND2	2.51	0.44
1:F:331:LEU:O	1:F:334:MET:SD	2.76	0.44
1:B:608:LEU:HD22	1:B:649:LEU:HD21	1.98	0.43
1:B:761:PRO:O	1:B:764:VAL:HG12	2.17	0.43
1:E:770:TRP:NE1	1:E:897:GLU:OE1	2.51	0.43
1:F:415:ASP:O	1:F:419:GLU:N	2.49	0.43
1:F:620:LEU:HD23	1:F:620:LEU:H	1.83	0.43
1:A:505:ILE:HD11	1:A:540:LEU:HD13	2.00	0.43
1:A:658:VAL:O	1:A:658:VAL:CG2	2.65	0.43
1:D:584:ASN:OD1	1:D:584:ASN:N	2.51	0.43
1:D:607:LEU:HD12	1:D:611:LEU:CD1	2.49	0.43
1:D:895:ILE:HD12	1:D:916:ASN:HB3	2.00	0.43
1:C:859:THR:O	1:C:860:ILE:C	2.61	0.43
1:D:510:LEU:HD12	1:F:728:VAL:HG22	2.00	0.43
1:E:751:PHE:HD1	1:E:752:THR:N	2.16	0.43
1:B:670:ALA:HA	1:B:674:LEU:HB2	2.00	0.43
1:B:787:PRO:HA	1:C:826:MET:HE1	2.01	0.43
1:B:709:VAL:HG12	1:B:709:VAL:O	2.19	0.43
1:B:918:LYS:HE3	1:B:918:LYS:HB3	1.88	0.43
1:D:549:VAL:HG22	1:D:549:VAL:O	2.17	0.43
1:D:688:LYS:O	1:D:735:VAL:N	2.45	0.43
1:E:440:GLU:O	1:E:444:LYS:HG3	2.19	0.43
1:E:662:VAL:HG22	1:E:663:ALA:N	2.34	0.43
1:F:434:VAL:CG1	1:F:626:VAL:HG11	2.48	0.43
1:F:807:GLY:O	1:F:811:LYS:N	2.45	0.43
1:A:153:LEU:HD13	1:A:206:MET:HE2	2.01	0.43
1:A:476:GLU:CD	1:A:514:THR:HG1	2.21	0.43
1:B:863:ALA:O	1:B:866:SER:OG	2.24	0.43
1:C:587:ILE:HD12	1:C:587:ILE:N	2.33	0.43
1:C:662:VAL:HG22	1:C:663:ALA:N	2.34	0.43
1:C:763:GLY:O	1:C:782:THR:OG1	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:VAL:O	1:E:430:VAL:HG13	2.18	0.43
1:E:695:VAL:O	1:E:699:LEU:HD23	2.19	0.43
1:F:662:VAL:HG22	1:F:663:ALA:H	1.83	0.43
1:B:487:LEU:O	1:B:498:LYS:NZ	2.52	0.43
1:B:561:HIS:CB	1:B:568:ALA:HB1	2.46	0.43
1:C:527:VAL:O	1:C:527:VAL:HG12	2.19	0.43
1:D:149:LEU:O	1:D:153:LEU:HG	2.18	0.43
1:D:608:LEU:O	1:D:612:ASP:N	2.52	0.43
1:C:435:MET:HA	1:C:435:MET:CE	2.43	0.43
1:D:565:TYR:CD1	1:F:566:VAL:HG12	2.54	0.43
1:E:529:LYS:HA	1:E:532:ILE:HG22	2.01	0.43
1:F:128:ALA:HB3	1:F:149:LEU:HD11	2.01	0.43
1:A:404:LYS:O	1:A:408:GLY:N	2.35	0.43
1:A:709:VAL:O	1:A:709:VAL:HG12	2.18	0.43
1:A:781:GLU:OE2	1:B:885:LEU:HB3	2.19	0.43
1:E:616:ASN:OD1	1:E:617:ALA:N	2.52	0.43
1:E:842:LEU:HD12	1:E:842:LEU:C	2.44	0.43
1:B:168:LEU:O	1:B:186:GLU:HG2	2.18	0.43
1:B:565:TYR:HB2	1:B:568:ALA:HB2	2.00	0.43
1:B:756:MET:SD	1:C:888:LYS:NZ	2.81	0.43
1:B:857:GLY:HA2	1:B:860:ILE:HD12	2.00	0.43
1:C:540:LEU:HD23	1:C:540:LEU:C	2.44	0.43
1:F:611:LEU:HD22	1:F:649:LEU:CD1	2.49	0.43
1:B:844:VAL:O	1:B:844:VAL:CG2	2.66	0.42
1:C:695:VAL:O	1:C:699:LEU:HD23	2.18	0.42
1:E:142:ILE:CD1	1:E:208:VAL:HG11	2.49	0.42
1:A:470:TRP:CH2	1:A:628:VAL:HG12	2.54	0.42
1:A:497:VAL:HG21	1:A:658:VAL:CG1	2.46	0.42
1:A:584:ASN:N	1:A:585:PRO:CD	2.82	0.42
1:B:931:LEU:HD12	1:B:931:LEU:O	2.19	0.42
1:D:540:LEU:O	1:D:541:ASN:HB3	2.19	0.42
1:E:810:MET:HE1	1:E:853:GLY:C	2.43	0.42
1:A:628:VAL:HG23	1:A:630:LEU:CD1	2.50	0.42
1:B:434:VAL:HG23	1:B:465:LEU:HD11	2.01	0.42
1:B:496:ASP:OD1	1:B:497:VAL:HG23	2.19	0.42
1:D:477:ASN:OD1	1:D:478:LEU:N	2.52	0.42
1:D:859:THR:O	1:D:860:ILE:C	2.61	0.42
1:E:547:PHE:N	1:E:588:LEU:O	2.51	0.42
1:B:661:TYR:C	1:B:900:ILE:HD11	2.45	0.42
1:B:818:TYR:OH	1:B:822:ARG:NH2	2.52	0.42
1:E:298:LYS:O	1:E:302:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:ALA:O	1:B:907:VAL:HG12	2.19	0.42
1:F:434:VAL:HG13	1:F:626:VAL:HG11	2.00	0.42
1:B:766:MET:HG3	1:B:779:PHE:CE1	2.54	0.42
1:D:549:VAL:O	1:D:552:MET:HB3	2.20	0.42
1:E:924:ALA:O	1:E:927:ILE:HG22	2.18	0.42
1:F:418:GLU:OE1	1:F:442:LEU:HD22	2.20	0.42
1:F:527:VAL:HG11	1:F:658:VAL:HG12	2.01	0.42
1:F:662:VAL:HG22	1:F:663:ALA:N	2.34	0.42
1:A:552:MET:SD	1:A:552:MET:C	3.02	0.42
1:A:625:ASP:OD1	1:A:625:ASP:N	2.52	0.42
1:A:719:VAL:HG23	1:A:745:PHE:HB3	2.01	0.42
1:A:885:LEU:HG	1:D:781:GLU:OE2	2.20	0.42
1:C:480:LEU:HD22	1:C:502:LEU:CD1	2.50	0.42
1:C:877:LEU:HD12	1:C:909:CYS:O	2.20	0.42
1:D:167:PHE:O	1:D:168:LEU:HD22	2.20	0.42
1:D:895:ILE:HD11	1:D:912:LEU:CD1	2.49	0.42
1:E:480:LEU:HD21	1:E:505:ILE:HB	2.02	0.42
1:E:604:SER:O	1:E:608:LEU:HD23	2.20	0.42
1:E:803:THR:CB	1:E:841:HIS:HE2	2.29	0.42
1:F:477:ASN:OD1	1:F:478:LEU:N	2.52	0.42
1:F:527:VAL:O	1:F:527:VAL:HG12	2.18	0.42
1:F:699:LEU:C	1:F:699:LEU:HD23	2.45	0.42
1:A:378:ARG:HA	1:A:381:ARG:HG2	2.01	0.42
1:A:802:VAL:HG23	1:A:842:LEU:HD11	2.02	0.42
1:B:755:ARG:O	1:B:756:MET:C	2.62	0.42
1:C:666:LYS:NZ	1:C:706:GLU:O	2.41	0.42
1:D:621:ASP:OD1	1:D:623:TYR:N	2.53	0.42
1:E:800:LEU:HD11	1:E:842:LEU:HD23	2.01	0.42
1:A:303:ILE:HD11	1:A:370:PHE:HB2	2.01	0.42
1:A:859:THR:O	1:A:860:ILE:C	2.61	0.42
1:D:844:VAL:HG13	1:D:844:VAL:O	2.19	0.42
1:F:430:VAL:O	1:F:430:VAL:HG13	2.18	0.42
1:A:449:ASP:OD1	1:A:449:ASP:N	2.53	0.42
1:A:742:LEU:HD11	1:A:746:VAL:CG1	2.50	0.42
1:B:699:LEU:HD12	1:B:703:TYR:HB2	2.02	0.42
1:C:433:HIS:HA	1:C:436:ASP:OD2	2.19	0.42
1:D:649:LEU:HD23	1:D:653:MET:HE1	2.01	0.42
1:D:725:TYR:CD1	1:D:725:TYR:C	2.98	0.42
1:F:143:GLU:N	1:F:143:GLU:OE1	2.53	0.42
1:F:498:LYS:O	1:F:502:LEU:HD23	2.20	0.42
1:F:763:GLY:O	1:F:782:THR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ILE:HD11	1:A:607:LEU:HD11	2.01	0.41
1:F:670:ALA:HA	1:F:674:LEU:HB2	2.02	0.41
1:B:562:ARG:O	1:B:563:ARG:HB3	2.20	0.41
1:C:587:ILE:HD13	1:C:635:PHE:CE1	2.56	0.41
1:F:842:LEU:HD12	1:F:842:LEU:O	2.20	0.41
1:A:791:ASP:OD2	1:A:794:GLY:N	2.53	0.41
1:A:841:HIS:ND1	1:B:819:THR:HG21	2.36	0.41
1:B:561:HIS:O	1:B:623:TYR:HA	2.21	0.41
1:D:144:VAL:HG12	1:D:146:ASN:H	1.84	0.41
1:D:816:ILE:HD13	1:F:841:HIS:CE1	2.55	0.41
1:E:496:ASP:OD1	1:E:497:VAL:HG23	2.19	0.41
1:F:759:VAL:O	1:F:760:THR:OG1	2.27	0.41
1:B:620:LEU:H	1:B:620:LEU:HD23	1.85	0.41
1:B:768:LEU:CD1	1:B:910:ILE:HD11	2.50	0.41
1:C:668:ALA:O	1:C:672:ARG:HG2	2.20	0.41
1:E:705:ARG:NE	1:E:751:PHE:O	2.53	0.41
1:D:600:GLN:OE1	1:D:600:GLN:O	2.39	0.41
1:D:859:THR:O	1:D:862:THR:HG22	2.20	0.41
1:F:476:GLU:CD	1:F:514:THR:HG21	2.45	0.41
1:E:837:THR:O	1:E:837:THR:OG1	2.33	0.41
1:A:391:HIS:O	1:A:395:LEU:HG	2.21	0.41
1:B:399:GLN:O	1:B:403:ILE:HG12	2.20	0.41
1:B:864:LEU:O	1:B:868:ALA:N	2.54	0.41
1:D:685:ASP:OD1	1:D:687:SER:N	2.54	0.41
1:C:552:MET:SD	1:C:552:MET:C	3.04	0.41
1:C:659:SER:CB	1:C:896:LYS:HZ2	2.26	0.41
1:C:787:PRO:CD	1:E:826:MET:HE3	2.51	0.41
1:D:415:ASP:OD1	1:D:416:ALA:N	2.53	0.41
1:B:456:ASN:OD1	1:B:459:ARG:NH1	2.54	0.41
1:B:756:MET:HE2	1:B:756:MET:HA	2.01	0.41
1:B:807:GLY:O	1:B:811:LYS:HG3	2.21	0.41
1:B:876:ASN:C	1:B:907:VAL:HG23	2.45	0.41
1:C:391:HIS:O	1:C:395:LEU:HG	2.20	0.41
1:E:649:LEU:O	1:E:649:LEU:HD12	2.21	0.41
1:A:166:VAL:O	1:A:190:THR:N	2.49	0.41
1:A:781:GLU:CD	1:B:886:THR:OG1	2.64	0.41
1:E:637:CYS:SG	1:E:638:THR:N	2.93	0.41
1:E:710:ARG:O	1:E:714:LYS:HG2	2.21	0.41
1:F:618:ASN:OD1	1:F:618:ASN:N	2.53	0.41
1:A:826:MET:HE1	1:D:787:PRO:CA	2.51	0.40
1:E:852:ASP:O	1:E:855:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:766:MET:HE3	1:F:779:PHE:CZ	2.56	0.40
1:A:662:VAL:HG22	1:A:663:ALA:H	1.85	0.40
1:B:866:SER:O	1:B:870:GLY:N	2.54	0.40
1:C:400:LEU:HA	1:E:403:ILE:HD11	2.03	0.40
1:C:562:ARG:O	1:C:563:ARG:HB3	2.21	0.40
1:C:599:TYR:CD1	1:C:599:TYR:C	3.00	0.40
1:D:584:ASN:N	1:D:585:PRO:CD	2.84	0.40
1:E:859:THR:O	1:E:862:THR:HG22	2.21	0.40
1:F:602:ASP:N	1:F:603:PRO:CD	2.84	0.40
1:B:480:LEU:HD11	1:B:506:ALA:HB2	2.04	0.40
1:B:558:ILE:HG22	1:B:558:ILE:O	2.22	0.40
1:C:569:MET:HE3	1:C:569:MET:H	1.84	0.40
1:D:528:GLY:N	2:D:1001:ADP:O2A	2.42	0.40
1:E:533:ALA:CB	1:E:588:LEU:HD22	2.52	0.40
1:E:755:ARG:HA	1:E:755:ARG:HE	1.87	0.40
1:F:508:SER:CB	1:F:514:THR:HG23	2.51	0.40
1:F:646:PRO:O	1:F:650:ARG:N	2.50	0.40
1:A:649:LEU:HD23	1:A:649:LEU:O	2.22	0.40
1:B:430:VAL:O	1:B:430:VAL:HG13	2.21	0.40
1:B:842:LEU:HD12	1:B:842:LEU:C	2.46	0.40
1:D:620:LEU:HD12	1:D:625:ASP:O	2.22	0.40
1:D:903:LYS:NZ	1:D:927:ILE:O	2.54	0.40
1:E:702:GLN:HA	1:E:751:PHE:HB3	2.04	0.40
1:F:611:LEU:HD22	1:F:649:LEU:HD11	2.03	0.40
1:A:564:THR:HG21	1:D:567:GLY:HA2	2.04	0.40
1:A:587:ILE:H	1:A:587:ILE:HD12	1.86	0.40
1:B:425:LEU:HD23	1:B:425:LEU:C	2.47	0.40
1:B:766:MET:HG2	1:B:767:GLY:N	2.37	0.40
1:D:853:GLY:N	1:D:854:PRO:CD	2.85	0.40
1:E:306:LEU:HD12	1:E:370:PHE:HE1	1.86	0.40
1:E:763:GLY:O	1:E:782:THR:OG1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	772/869 (89%)	740 (96%)	32 (4%)	0	100	100
1	B	772/869 (89%)	734 (95%)	38 (5%)	0	100	100
1	C	772/869 (89%)	745 (96%)	27 (4%)	0	100	100
1	D	772/869 (89%)	746 (97%)	26 (3%)	0	100	100
1	E	772/869 (89%)	744 (96%)	28 (4%)	0	100	100
1	F	772/869 (89%)	750 (97%)	22 (3%)	0	100	100
All	All	4632/5214 (89%)	4459 (96%)	173 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	675/755 (89%)	675 (100%)	0	100	100
1	B	675/755 (89%)	675 (100%)	0	100	100
1	C	675/755 (89%)	675 (100%)	0	100	100
1	D	675/755 (89%)	675 (100%)	0	100	100
1	E	675/755 (89%)	674 (100%)	1 (0%)	88	88
1	F	675/755 (89%)	675 (100%)	0	100	100
All	All	4050/4530 (89%)	4049 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	751	PHE

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

Mol	Chain	Res	Type
1	A	377	GLN
1	A	515	GLN
1	A	600	GLN
1	A	615	GLN
1	B	187	HIS
1	B	219	GLN
1	B	344	HIS
1	B	615	GLN
1	C	174	ASN
1	C	187	HIS
1	C	193	GLN
1	C	451	HIS
1	C	622	HIS
1	C	640	ASN
1	C	805	GLN
1	C	828	HIS
1	D	211	HIS
1	D	307	ASN
1	E	307	ASN
1	E	347	GLN
1	E	664	GLN
1	F	307	ASN
1	F	715	GLN
1	F	875	GLN

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](#)

6 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	F	1001	-	28,29,29	1.39	4 (14%)	43,45,45	1.86	10 (23%)
2	ADP	D	1001	-	28,29,29	1.40	4 (14%)	43,45,45	1.85	10 (23%)
2	ADP	C	1001	-	28,29,29	1.39	4 (14%)	43,45,45	1.88	10 (23%)
2	ADP	A	1001	-	28,29,29	1.39	4 (14%)	43,45,45	1.86	11 (25%)
2	ADP	B	1001	-	28,29,29	1.39	4 (14%)	43,45,45	1.89	11 (25%)
2	ADP	E	1001	-	28,29,29	1.44	5 (17%)	43,45,45	2.19	12 (27%)

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	F	1001	-	-	3/16/32/32	0/3/3/3
2	ADP	D	1001	-	-	6/16/32/32	0/3/3/3
2	ADP	C	1001	-	-	7/16/32/32	0/3/3/3
2	ADP	A	1001	-	-	5/16/32/32	0/3/3/3
2	ADP	B	1001	-	-	8/16/32/32	0/3/3/3
2	ADP	E	1001	-	-	9/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	ADP	C5-C4	4.64	1.47	1.39
2	F	1001	ADP	C5-C4	4.56	1.47	1.39
2	B	1001	ADP	C5-C4	4.54	1.47	1.39
2	D	1001	ADP	C5-C4	4.53	1.47	1.39
2	C	1001	ADP	C5-C4	4.51	1.47	1.39
2	A	1001	ADP	C5-C4	4.48	1.47	1.39
2	E	1001	ADP	C5-C6	2.75	1.48	1.41
2	D	1001	ADP	C5-C6	2.71	1.48	1.41
2	C	1001	ADP	C5-C6	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ADP	C5-C6	2.68	1.48	1.41
2	A	1001	ADP	C5-C6	2.67	1.48	1.41
2	F	1001	ADP	C5-C6	2.63	1.48	1.41
2	C	1001	ADP	C8-N7	2.45	1.36	1.31
2	E	1001	ADP	C8-N7	2.43	1.36	1.31
2	A	1001	ADP	C8-N7	2.42	1.36	1.31
2	D	1001	ADP	C8-N7	2.42	1.36	1.31
2	B	1001	ADP	C8-N7	2.41	1.36	1.31
2	D	1001	ADP	C5-N7	-2.38	1.34	1.39
2	A	1001	ADP	C5-N7	-2.37	1.34	1.39
2	F	1001	ADP	C5-N7	-2.36	1.34	1.39
2	F	1001	ADP	C8-N7	2.34	1.36	1.31
2	E	1001	ADP	PA-O3A	2.31	1.62	1.59
2	B	1001	ADP	C5-N7	-2.28	1.34	1.39
2	E	1001	ADP	C5-N7	-2.28	1.34	1.39
2	C	1001	ADP	C5-N7	-2.25	1.35	1.39

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1001	ADP	O5'-C5'-C4'	7.29	133.83	108.99
2	E	1001	ADP	C5-C4-N3	-5.85	118.66	126.72
2	D	1001	ADP	C5-C4-N3	-5.81	118.72	126.72
2	B	1001	ADP	C5-C4-N3	-5.74	118.82	126.72
2	F	1001	ADP	C5-C4-N3	-5.74	118.82	126.72
2	A	1001	ADP	C5-C4-N3	-5.72	118.84	126.72
2	C	1001	ADP	C5-C4-N3	-5.67	118.92	126.72
2	E	1001	ADP	N3-C4-N9	4.57	134.94	127.17
2	B	1001	ADP	N3-C4-N9	4.53	134.87	127.17
2	F	1001	ADP	N3-C4-N9	4.52	134.85	127.17
2	C	1001	ADP	N3-C4-N9	4.36	134.58	127.17
2	D	1001	ADP	N3-C4-N9	4.25	134.39	127.17
2	A	1001	ADP	N3-C4-N9	4.24	134.39	127.17
2	E	1001	ADP	C2-N3-C4	3.89	121.33	111.83
2	A	1001	ADP	C2-N3-C4	3.87	121.29	111.83
2	C	1001	ADP	C2-N3-C4	3.86	121.26	111.83
2	B	1001	ADP	C2-N3-C4	3.86	121.26	111.83
2	D	1001	ADP	C2-N3-C4	3.85	121.24	111.83
2	F	1001	ADP	C2-N3-C4	3.80	121.11	111.83
2	D	1001	ADP	C4-C5-N7	-3.74	106.30	110.58
2	A	1001	ADP	N3-C2-N1	-3.73	122.93	128.58
2	E	1001	ADP	N3-C2-N1	-3.71	122.97	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ADP	N3-C2-N1	-3.69	123.00	128.58
2	A	1001	ADP	C4-C5-N7	-3.68	106.37	110.58
2	C	1001	ADP	C4-C5-N7	-3.68	106.38	110.58
2	C	1001	ADP	N3-C2-N1	-3.66	123.04	128.58
2	E	1001	ADP	C4-C5-N7	-3.64	106.42	110.58
2	D	1001	ADP	N3-C2-N1	-3.62	123.10	128.58
2	B	1001	ADP	C4-C5-N7	-3.58	106.49	110.58
2	F	1001	ADP	N3-C2-N1	-3.57	123.18	128.58
2	F	1001	ADP	C4-C5-N7	-3.44	106.64	110.58
2	B	1001	ADP	C4-N9-C8	2.97	108.86	105.74
2	C	1001	ADP	C4-N9-C8	2.87	108.75	105.74
2	A	1001	ADP	C5-N7-C8	2.79	107.83	103.45
2	E	1001	ADP	C5-N7-C8	2.79	107.83	103.45
2	D	1001	ADP	C5-N7-C8	2.78	107.82	103.45
2	B	1001	ADP	C5-N7-C8	2.77	107.80	103.45
2	E	1001	ADP	C4-N9-C8	2.76	108.64	105.74
2	F	1001	ADP	C4-N9-C8	2.76	108.63	105.74
2	C	1001	ADP	C5-N7-C8	2.74	107.76	103.45
2	F	1001	ADP	C5-N7-C8	2.64	107.60	103.45
2	A	1001	ADP	C4-N9-C8	2.47	108.33	105.74
2	B	1001	ADP	N9-C8-N7	-2.39	110.55	113.94
2	C	1001	ADP	C6-C5-N7	2.36	136.64	132.09
2	C	1001	ADP	N9-C8-N7	-2.34	110.61	113.94
2	A	1001	ADP	C6-C5-N7	2.33	136.58	132.09
2	E	1001	ADP	C3'-C2'-C1'	2.30	105.82	101.46
2	F	1001	ADP	C3'-C2'-C1'	2.29	105.80	101.46
2	D	1001	ADP	C6-C5-N7	2.29	136.50	132.09
2	B	1001	ADP	C3'-C2'-C1'	2.28	105.78	101.46
2	A	1001	ADP	N9-C8-N7	-2.28	110.70	113.94
2	E	1001	ADP	N9-C8-N7	-2.28	110.71	113.94
2	D	1001	ADP	C4-N9-C8	2.28	108.13	105.74
2	B	1001	ADP	C6-C5-N7	2.24	136.42	132.09
2	E	1001	ADP	C6-C5-N7	2.24	136.40	132.09
2	F	1001	ADP	N9-C8-N7	-2.21	110.79	113.94
2	D	1001	ADP	N9-C8-N7	-2.16	110.87	113.94
2	E	1001	ADP	C2-N1-C6	2.11	122.20	118.73
2	F	1001	ADP	C6-C5-N7	2.10	136.14	132.09
2	A	1001	ADP	C2-N1-C6	2.07	122.13	118.73
2	B	1001	ADP	C2-N1-C6	2.06	122.11	118.73
2	A	1001	ADP	C3'-C2'-C1'	2.06	105.35	101.46
2	D	1001	ADP	C2-N1-C6	2.04	122.08	118.73
2	C	1001	ADP	C2-N1-C6	2.01	122.04	118.73

There are no chirality outliers.

All (38) torsion outliers are listed below:

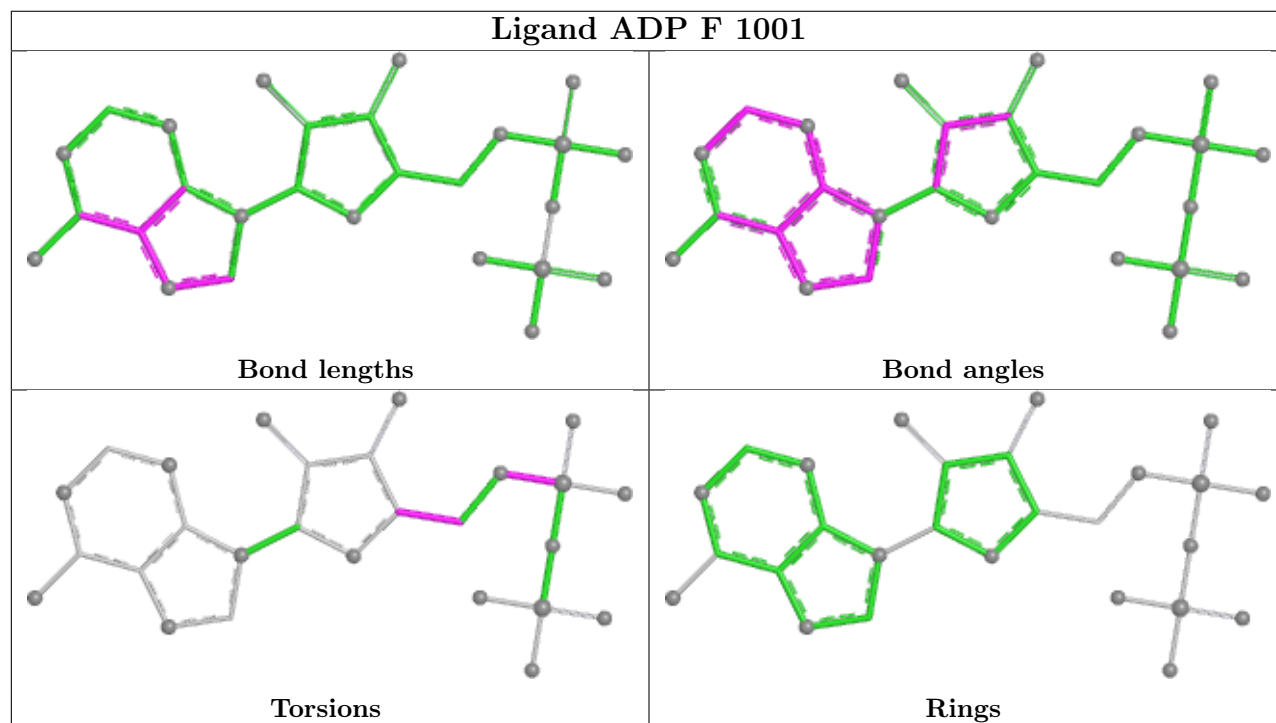
Mol	Chain	Res	Type	Atoms
2	B	1001	ADP	PA-O3A-PB-O2B
2	B	1001	ADP	C5'-O5'-PA-O2A
2	B	1001	ADP	C5'-O5'-PA-O3A
2	B	1001	ADP	O4'-C1'-N9-C8
2	B	1001	ADP	O4'-C1'-N9-C4
2	C	1001	ADP	C5'-O5'-PA-O2A
2	C	1001	ADP	C5'-O5'-PA-O3A
2	C	1001	ADP	O4'-C4'-C5'-O5'
2	D	1001	ADP	C5'-O5'-PA-O1A
2	D	1001	ADP	C5'-O5'-PA-O2A
2	D	1001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	PA-O3A-PB-O2B
2	E	1001	ADP	C5'-O5'-PA-O2A
2	E	1001	ADP	C5'-O5'-PA-O3A
2	F	1001	ADP	C5'-O5'-PA-O3A
2	C	1001	ADP	C3'-C4'-C5'-O5'
2	E	1001	ADP	O4'-C4'-C5'-O5'
2	A	1001	ADP	C2'-C1'-N9-C8
2	E	1001	ADP	C3'-C4'-C5'-O5'
2	A	1001	ADP	C2'-C1'-N9-C4
2	D	1001	ADP	C3'-C4'-C5'-O5'
2	E	1001	ADP	PB-O3A-PA-O5'
2	A	1001	ADP	PB-O3A-PA-O2A
2	C	1001	ADP	PB-O3A-PA-O2A
2	D	1001	ADP	C2'-C1'-N9-C8
2	E	1001	ADP	C5'-O5'-PA-O1A
2	F	1001	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	PB-O3A-PA-O1A
2	B	1001	ADP	O4'-C4'-C5'-O5'
2	D	1001	ADP	O4'-C1'-N9-C8
2	B	1001	ADP	PA-O3A-PB-O3B
2	E	1001	ADP	PA-O3A-PB-O3B
2	C	1001	ADP	C2'-C1'-N9-C8
2	B	1001	ADP	PA-O3A-PB-O1B
2	E	1001	ADP	PA-O3A-PB-O1B
2	A	1001	ADP	O4'-C1'-N9-C8
2	A	1001	ADP	PB-O3A-PA-O1A
2	F	1001	ADP	O4'-C4'-C5'-O5'

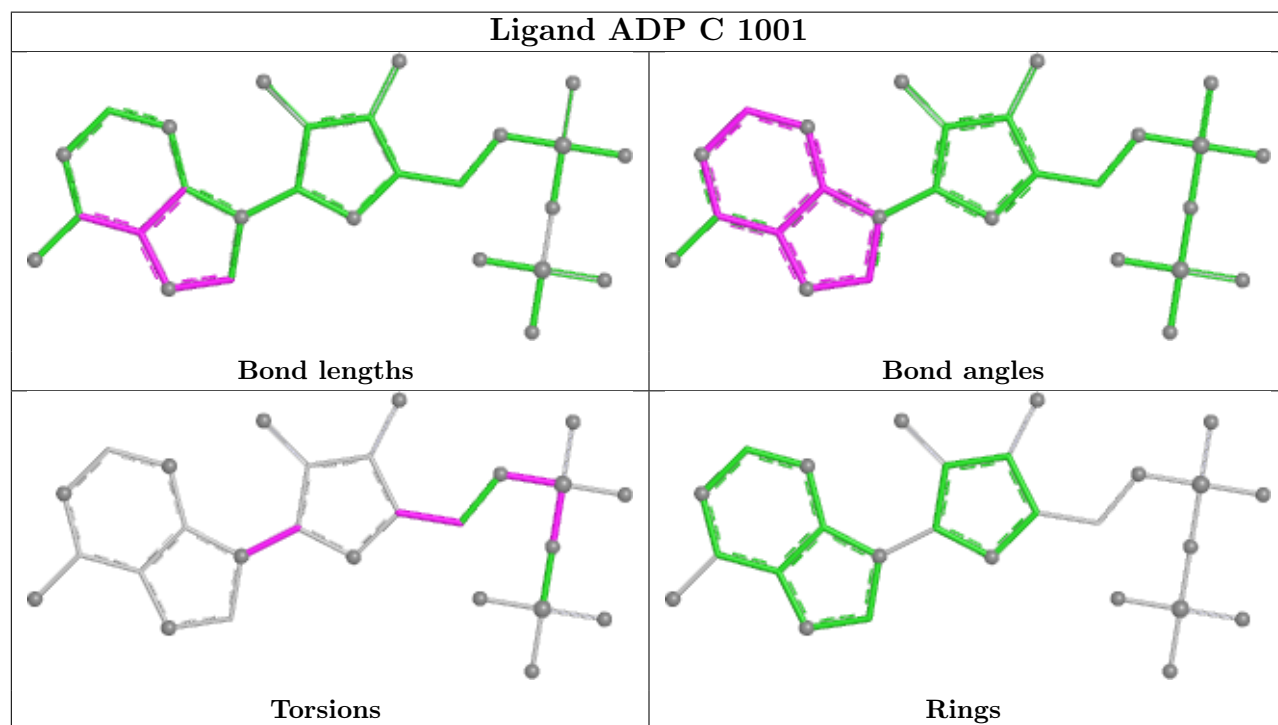
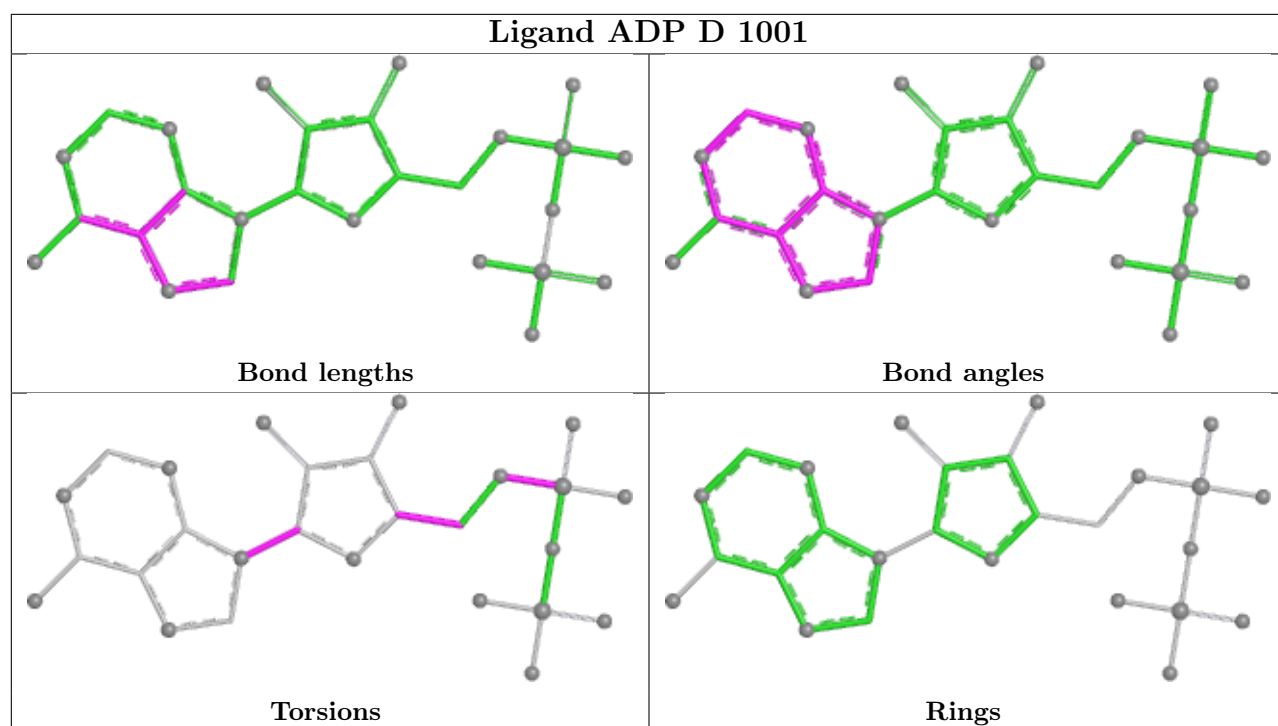
There are no ring outliers.

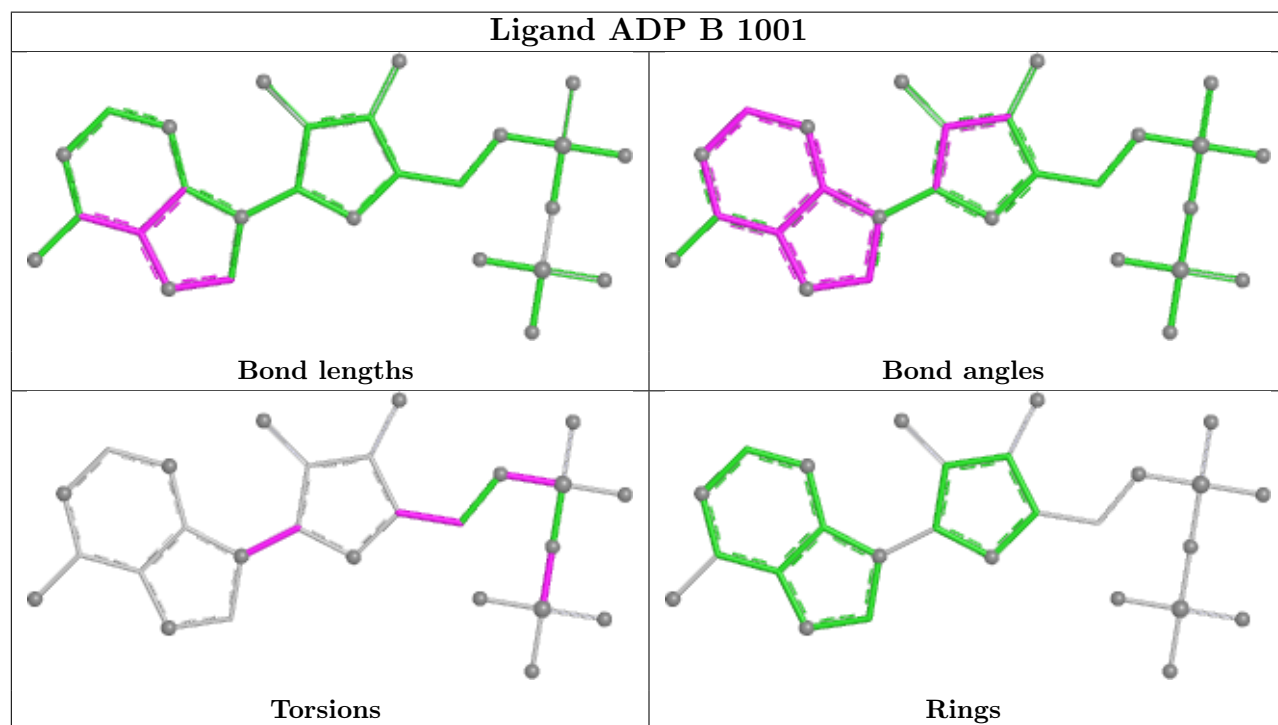
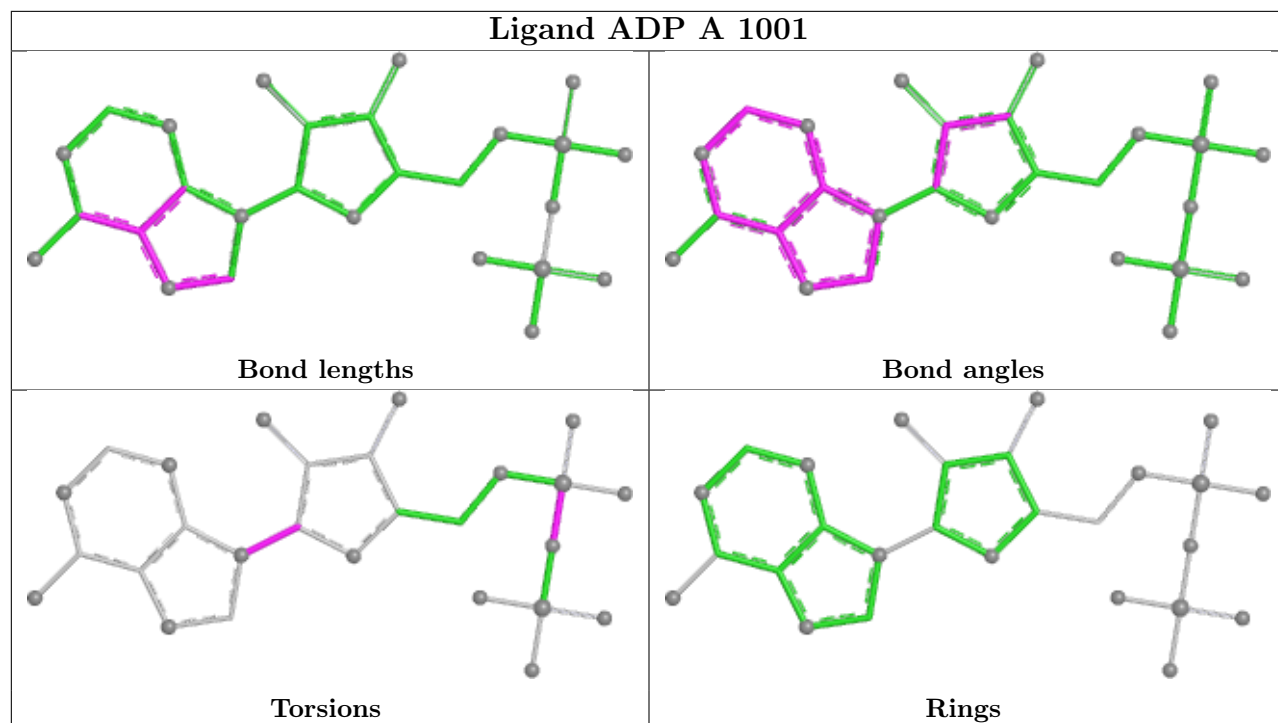
5 monomers are involved in 9 short contacts:

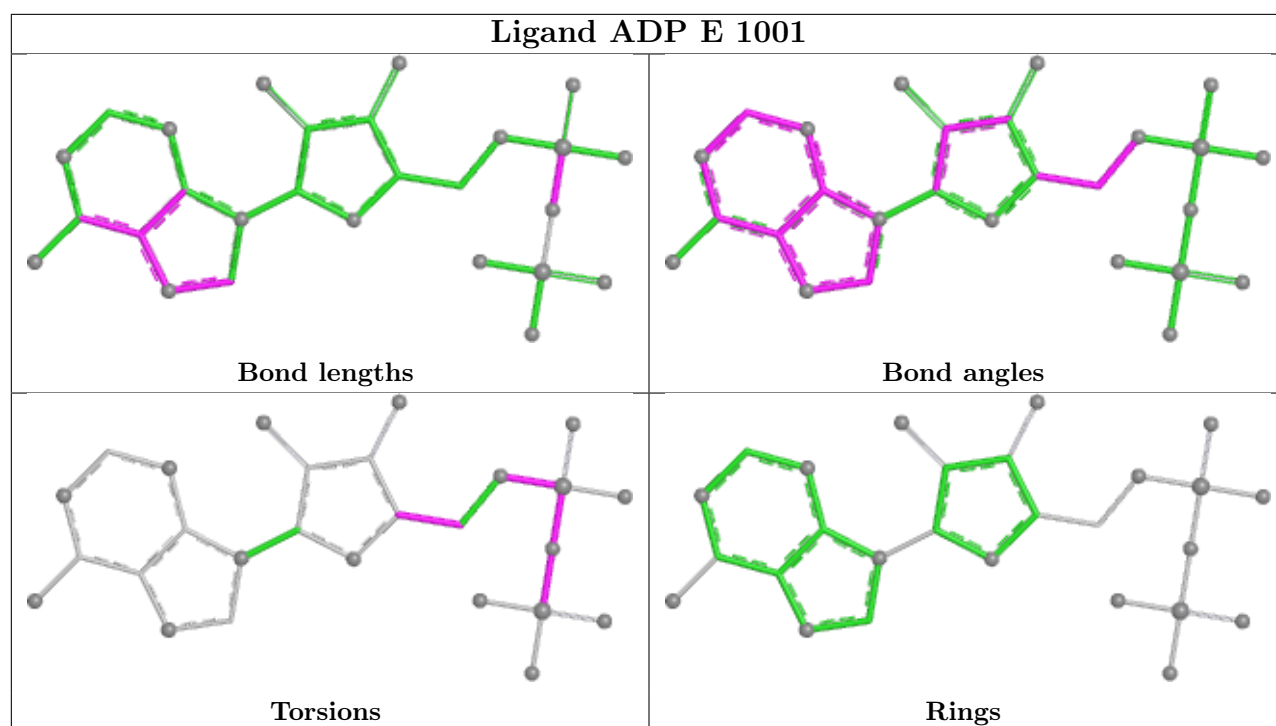
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1001	ADP	1	0
2	D	1001	ADP	3	0
2	C	1001	ADP	3	0
2	A	1001	ADP	1	0
2	E	1001	ADP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

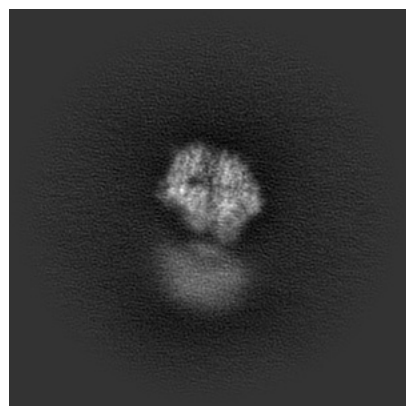
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16970. These allow visual inspection of the internal detail of the map and identification of artifacts.

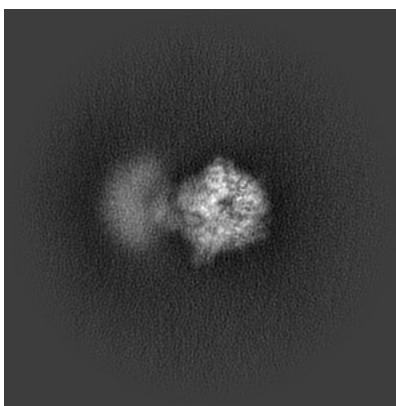
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

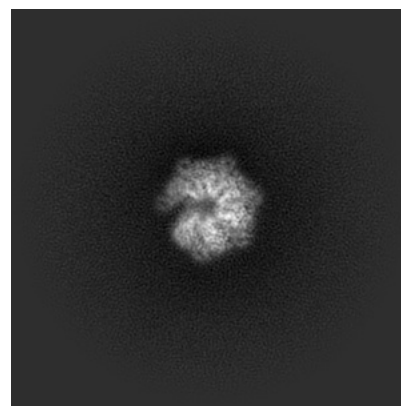
6.1.1 Primary map



X

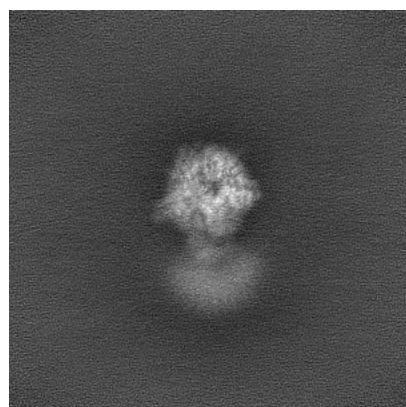


Y

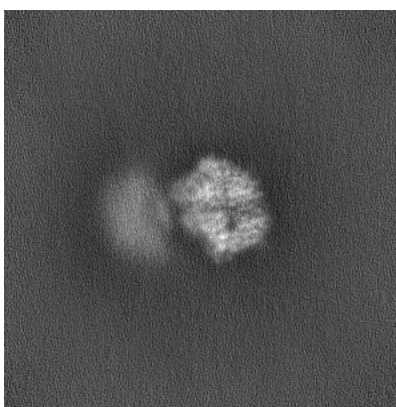


Z

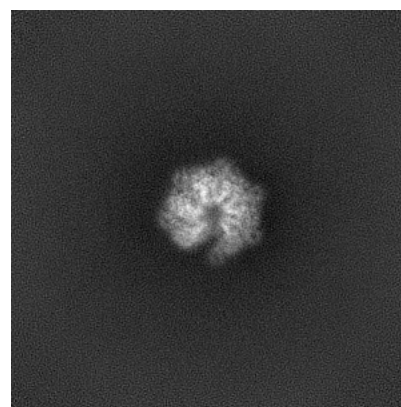
6.1.2 Raw map



X



Y

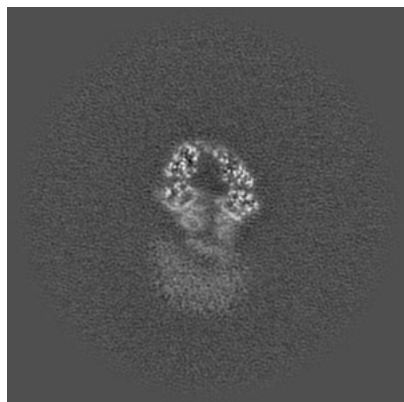


Z

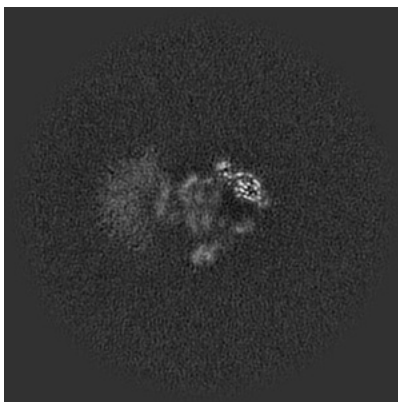
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

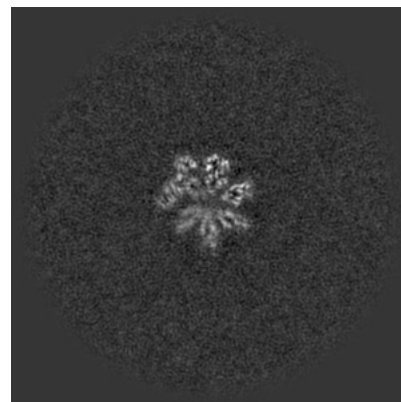
6.2.1 Primary map



X Index: 150



Y Index: 150

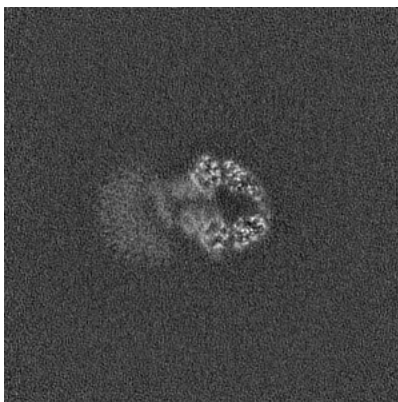


Z Index: 150

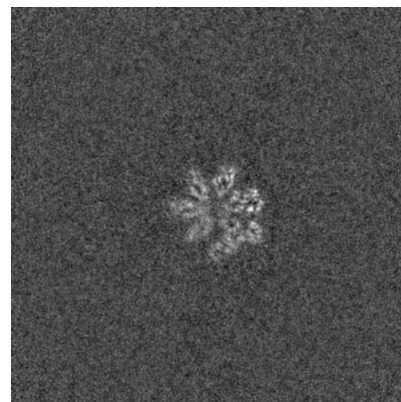
6.2.2 Raw map



X Index: 150



Y Index: 150

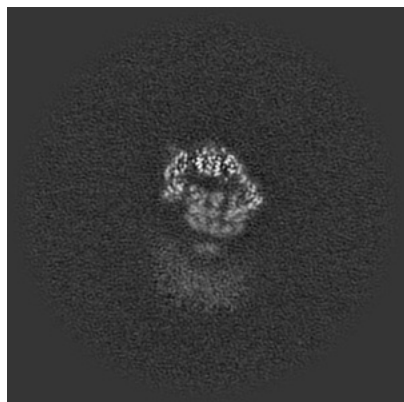


Z Index: 150

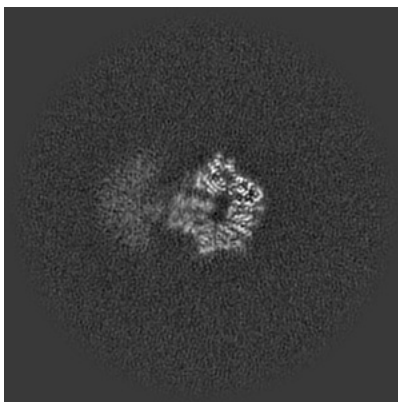
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

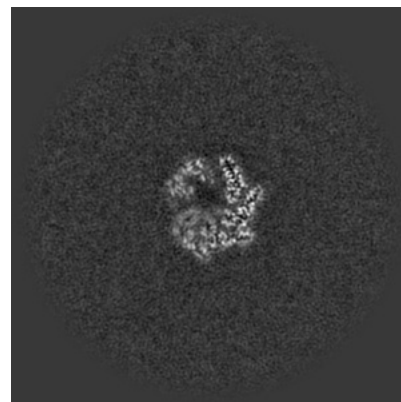
6.3.1 Primary map



X Index: 158

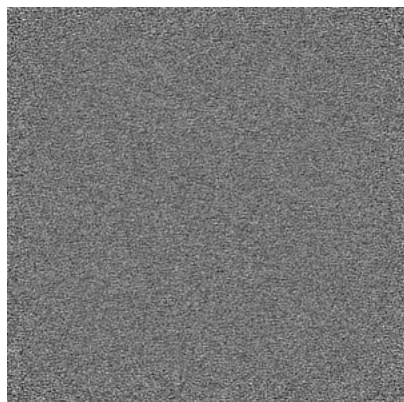


Y Index: 162

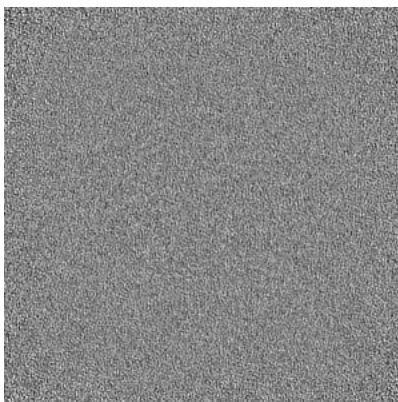


Z Index: 162

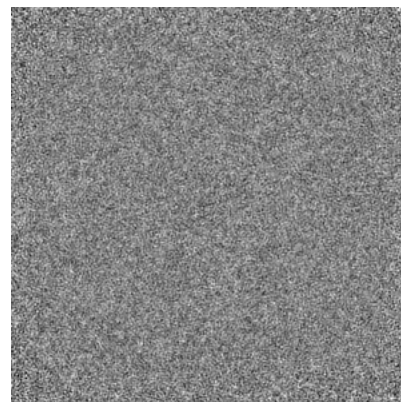
6.3.2 Raw map



X Index: 0



Y Index: 0

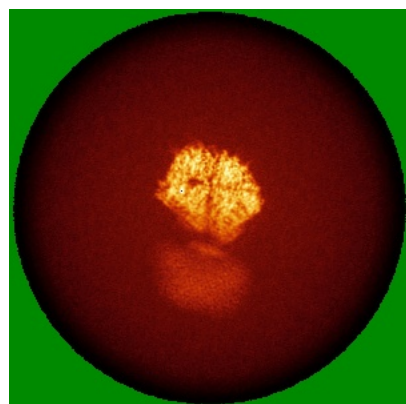


Z Index: 0

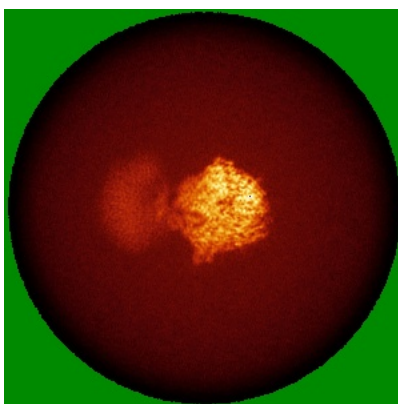
The images above show the largest variance slices of the map in three orthogonal directions.

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

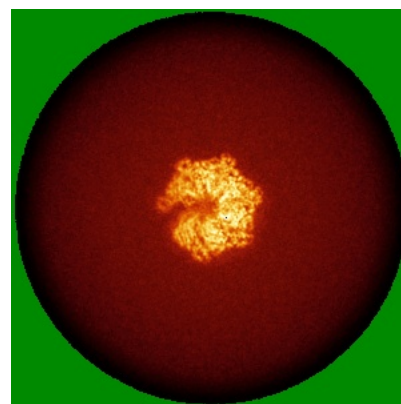
6.4.1 Primary map



X

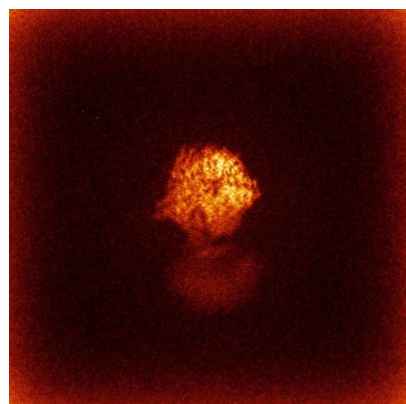


Y

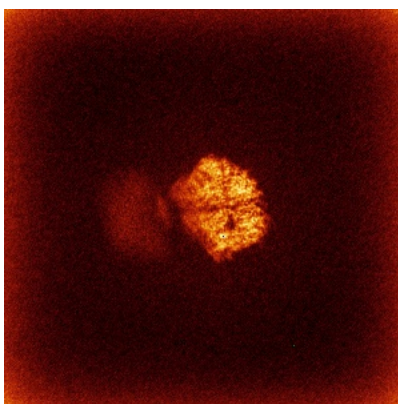


Z

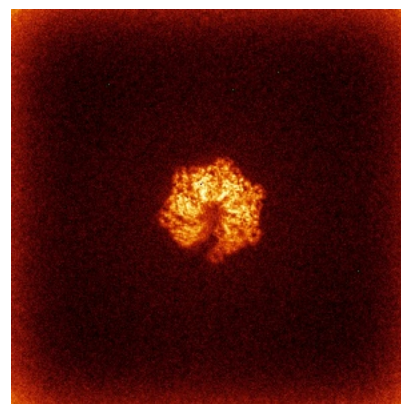
6.4.2 Raw map



X



Y

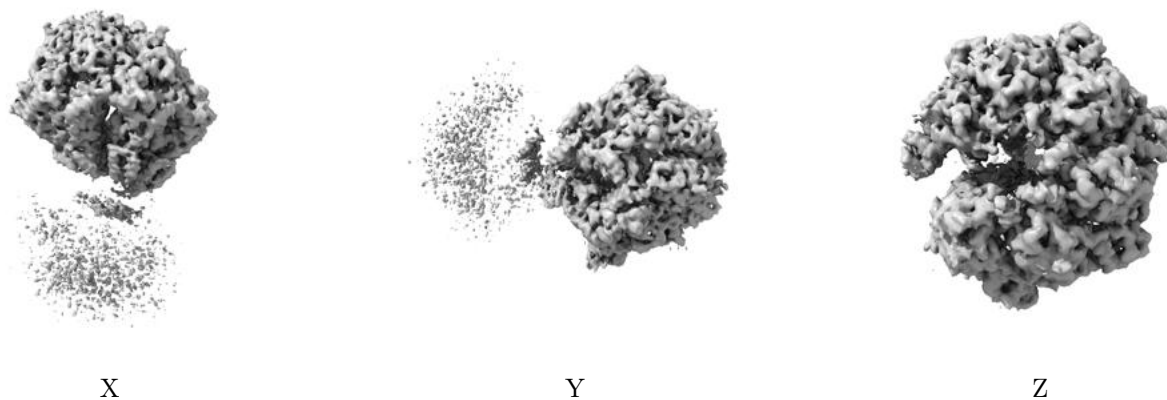


Z

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

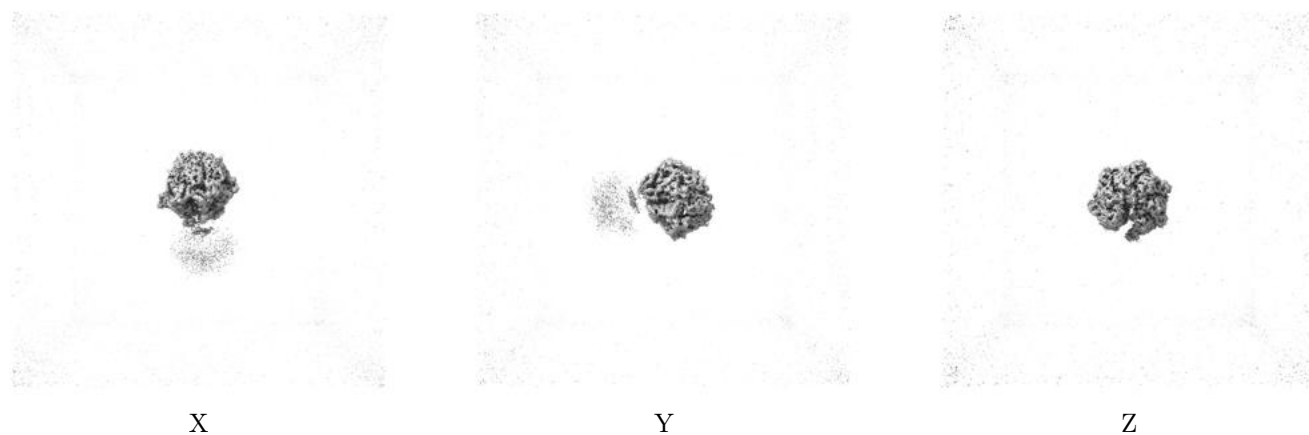
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

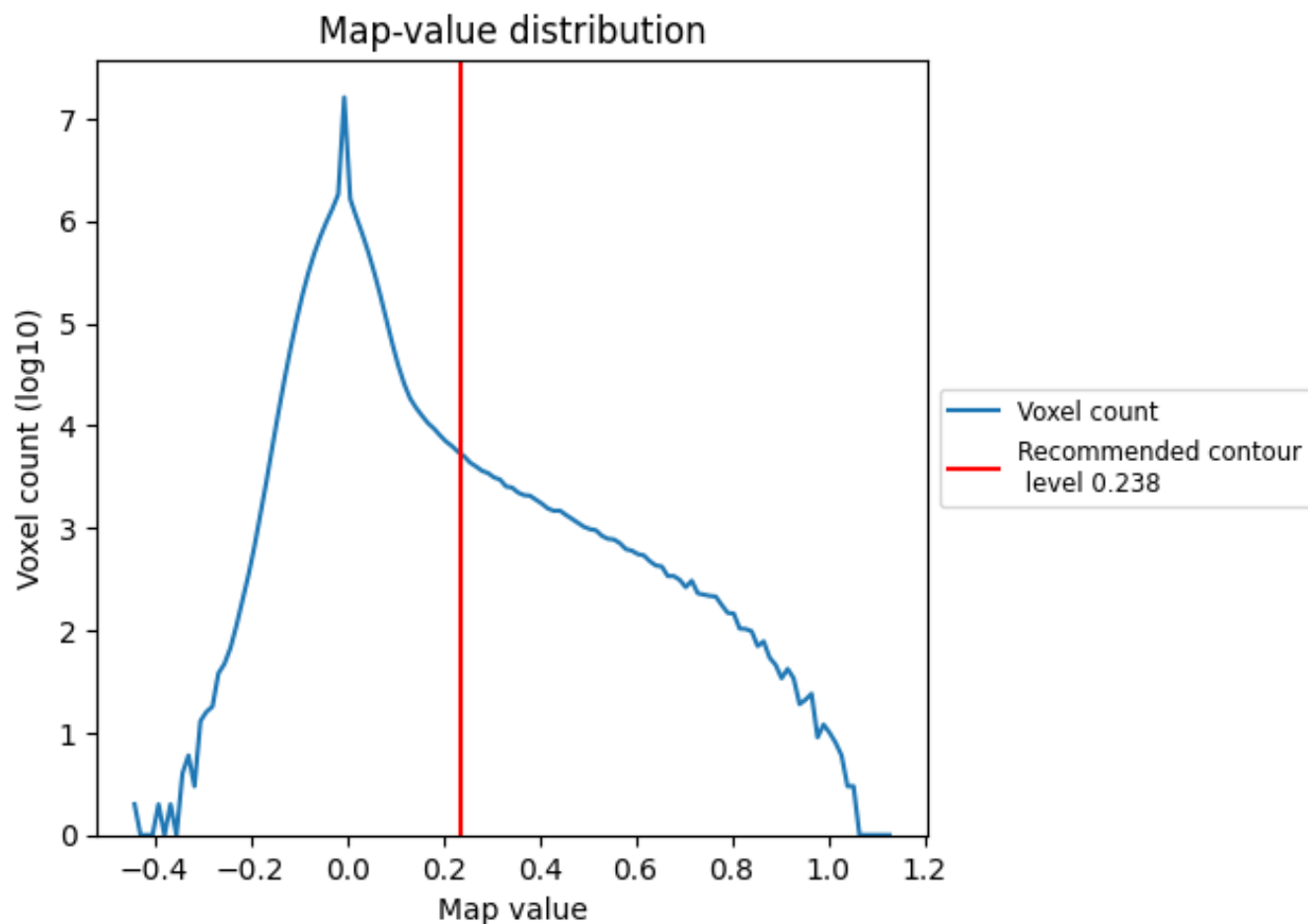
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

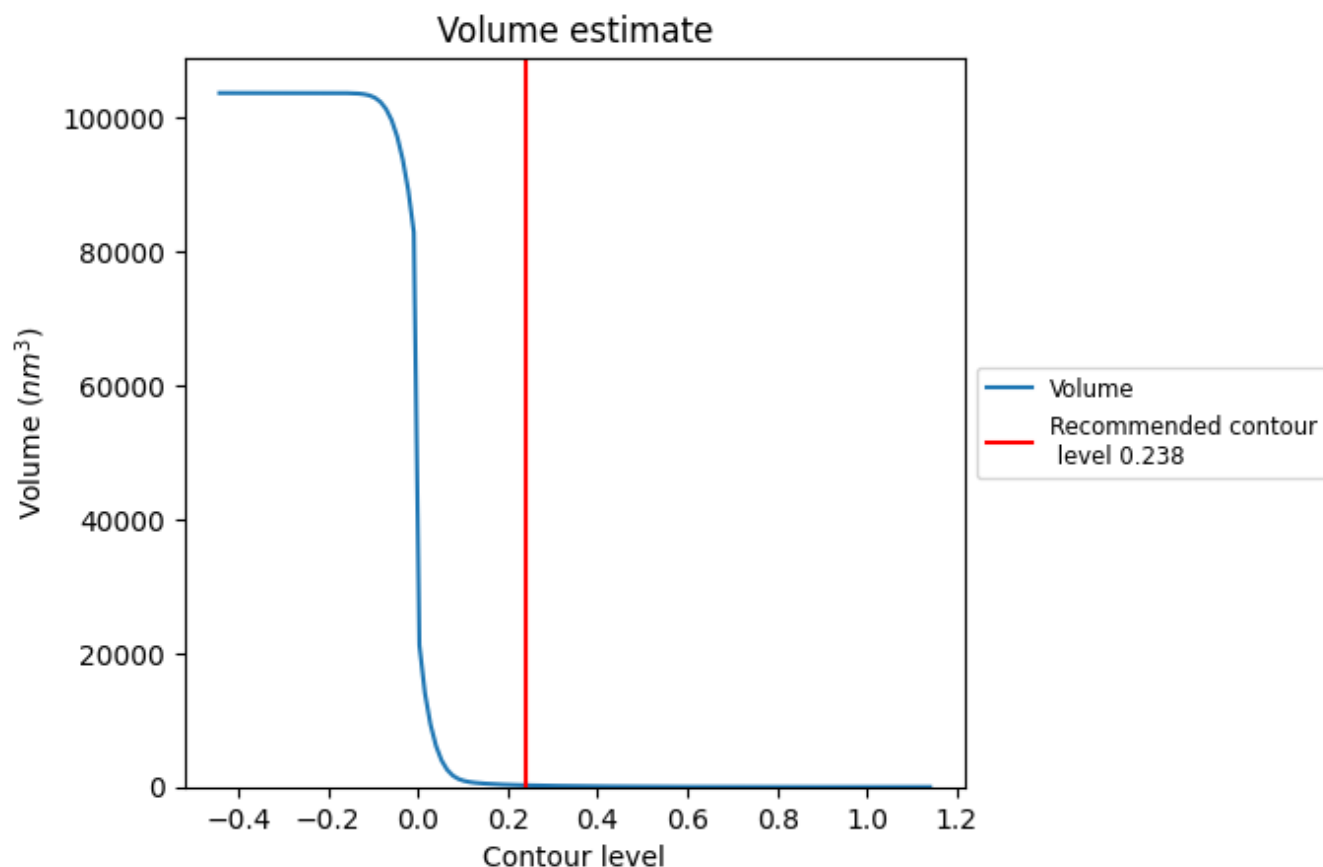
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

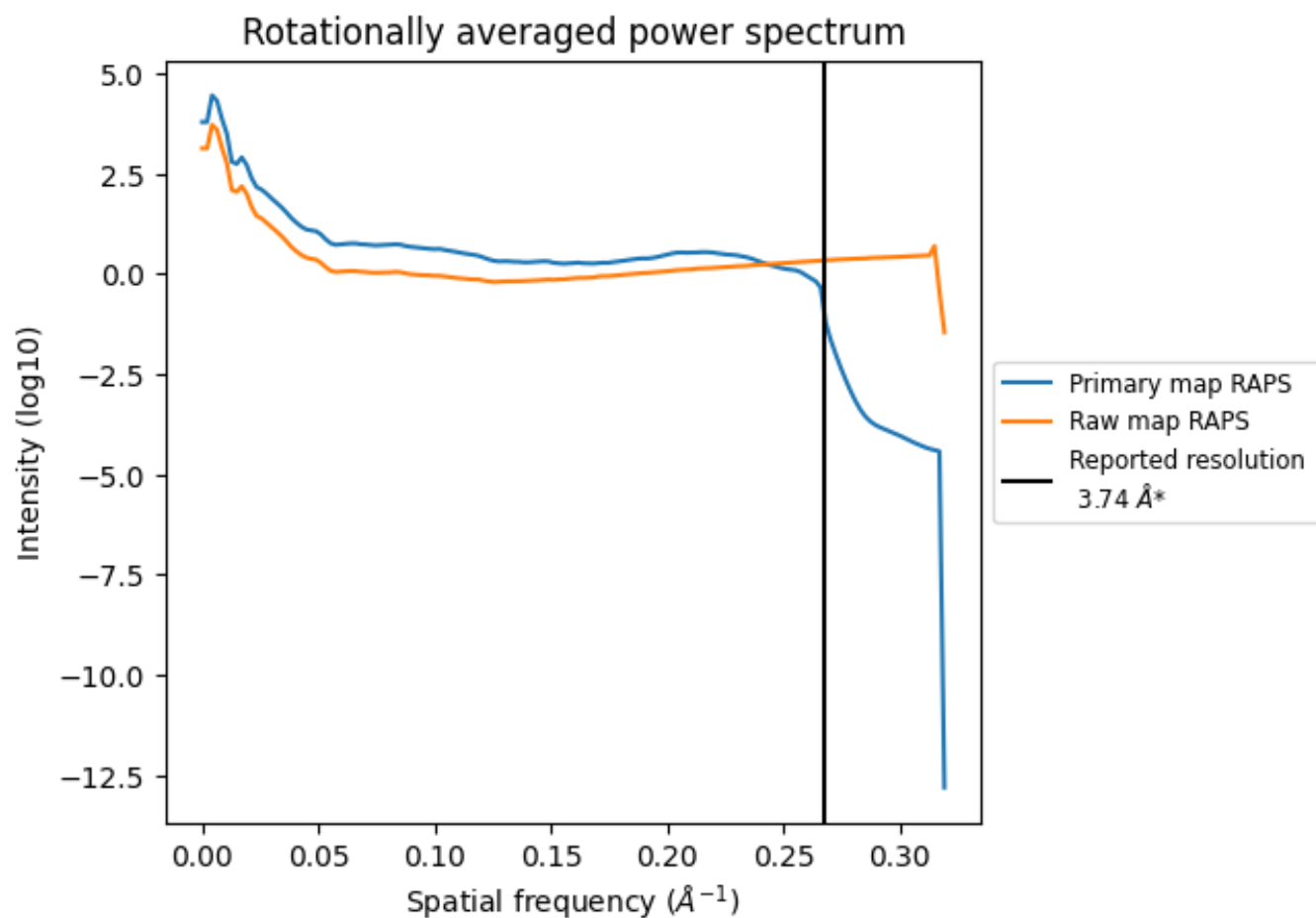
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm^3 ; this corresponds to an approximate mass of 227 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

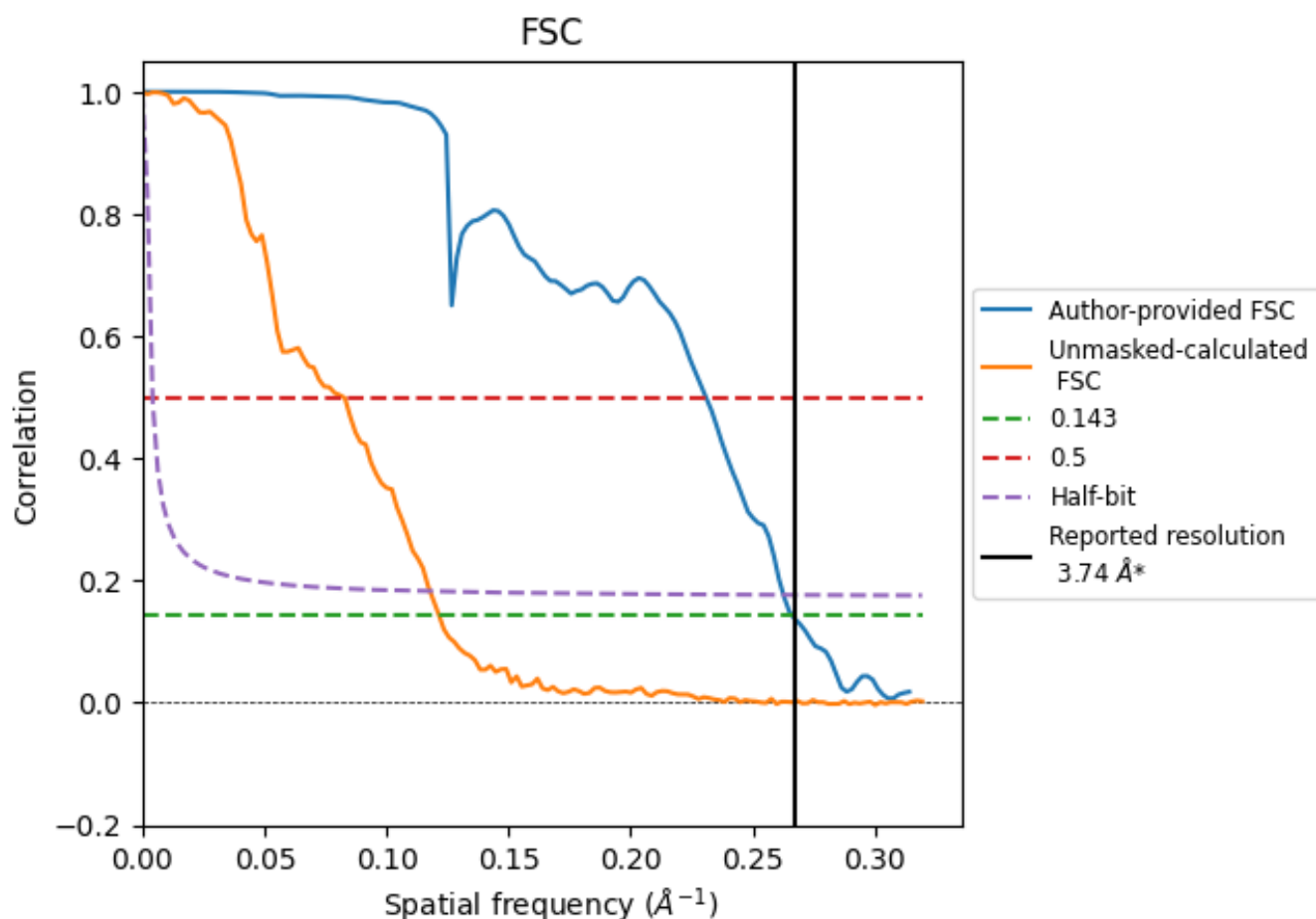


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

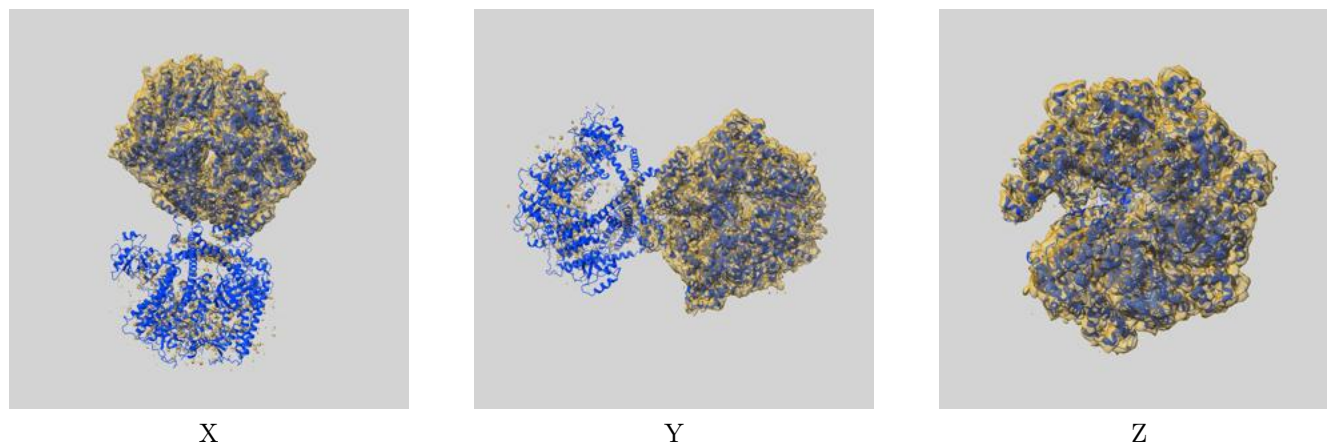
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	3.76	4.33	3.81
Unmasked-calculated*	8.23	12.15	8.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.23 differs from the reported value 3.74 by more than 10 %

9 Map-model fit [i](#)

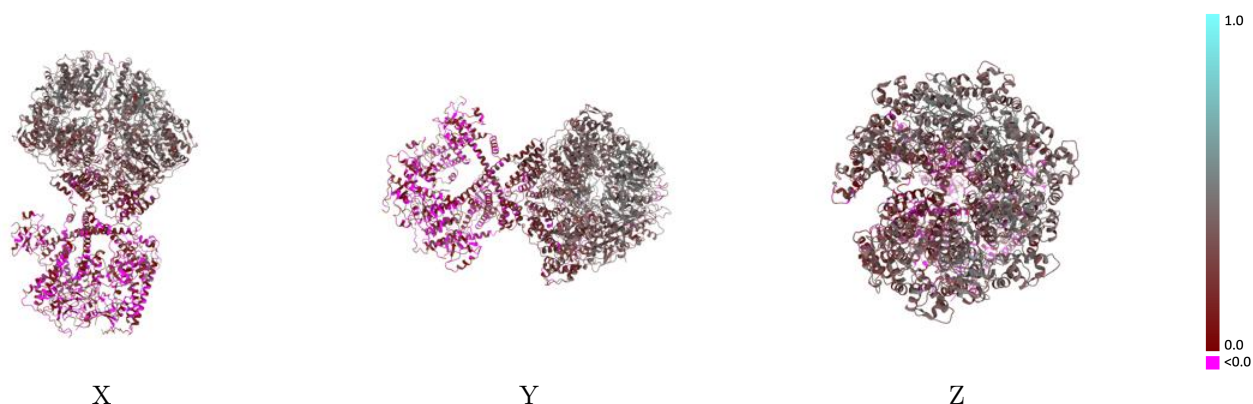
This section contains information regarding the fit between EMDB map EMD-16970 and PDB model 8OM7. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



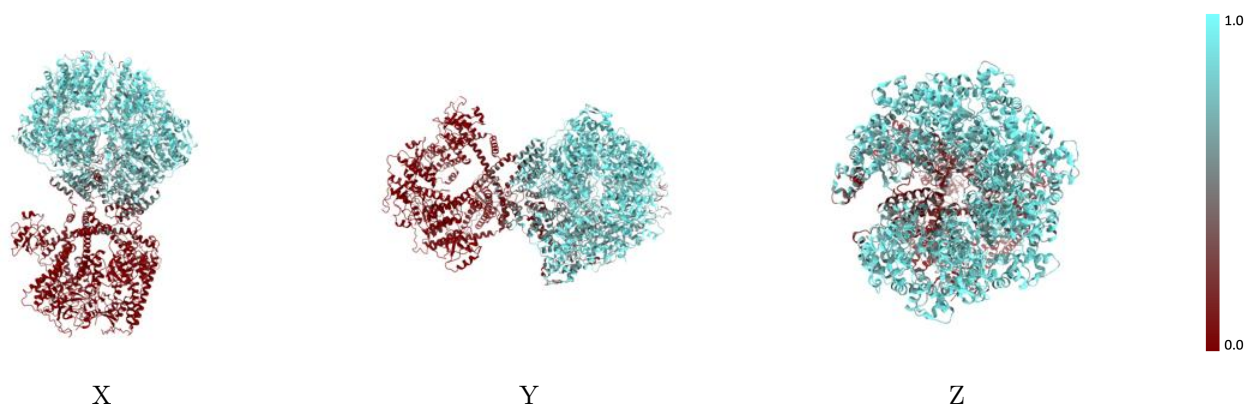
The images above show the 3D surface view of the map at the recommended contour level 0.238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



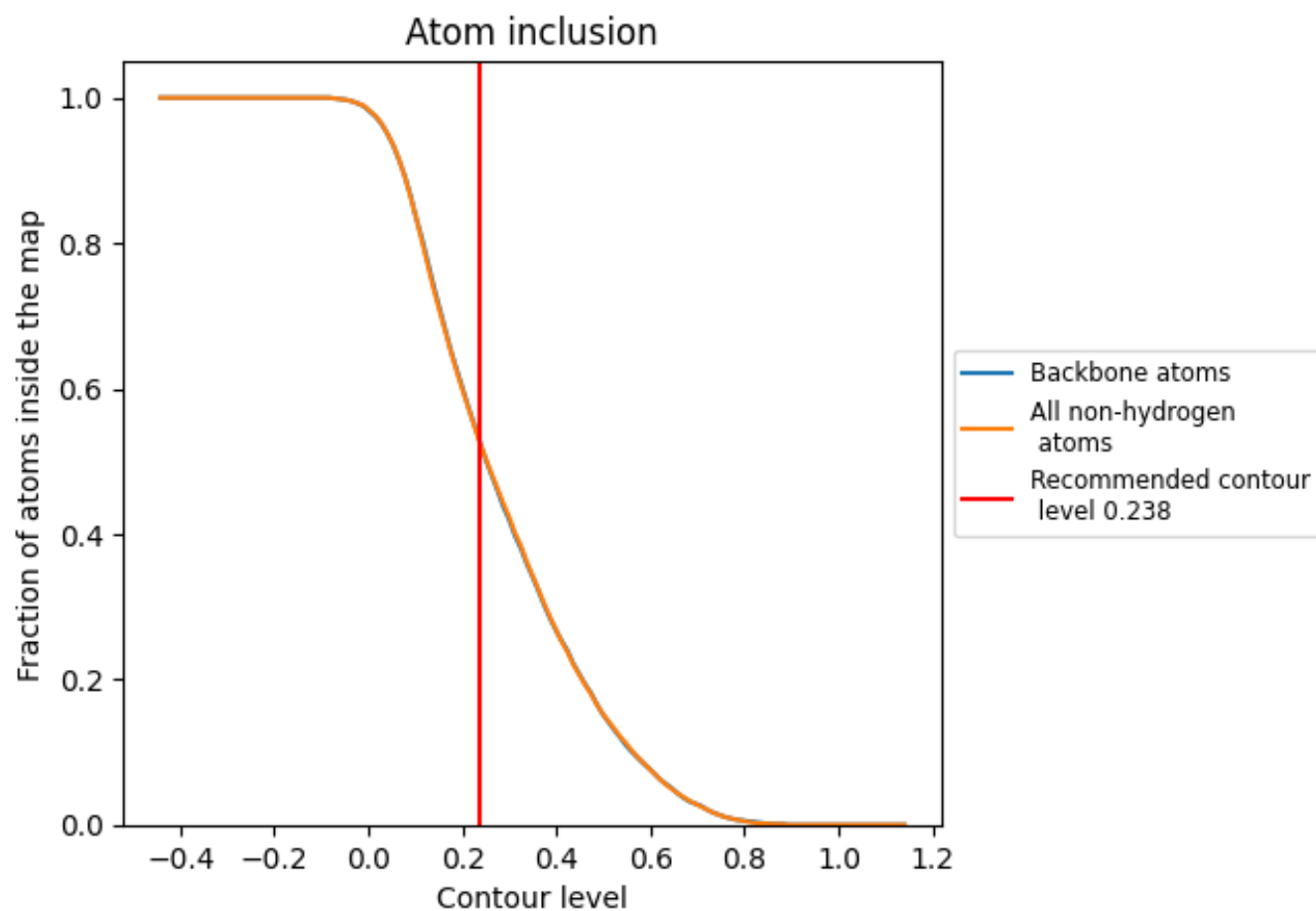
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.238).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5240	0.2490
A	0.5750	0.2750
B	0.5730	0.2740
C	0.5590	0.2680
D	0.5530	0.2590
E	0.4460	0.2100
F	0.4780	0.2100

1.0

0.0

<0.0