



Full wwPDB EM Validation Report ⓘ

Sep 5, 2026 – 01:50 PM EDT

PDB ID : 10WP / pdb_000010wp
EMDB ID : EMD-75504
Title : MPXV replisome bound to forked DNA
Authors : Yu, Z.; Abraham, J.
Deposited on : 2026-02-11
Resolution : 6.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

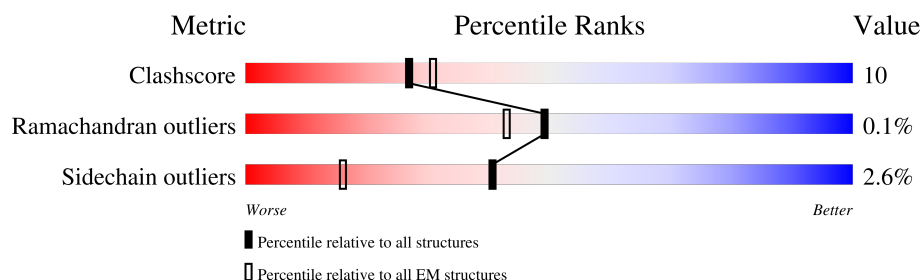
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	D	785	19% 64% 22% 14%
1	E	785	29% 54% 17% 28%
1	F	785	18% 32% 12% 55%
1	G	785	10% 34% 10% 55%
1	H	785	13% 31% 10% 59%
1	I	785	12% 35% 9% 55%
2	T	27	63% 74% 26%
3	A	1006	45% 70% 25%

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Mol	Chain	Length	Quality of chain
4	C	426	54% 70% 20% 10%
5	B	218	39% 90% 10%
6	S	22	91% 82% 18%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35220 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Uncoating factor OPG117.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	674	Total	C	N	O	S	0	0
			5469	3479	932	1027	31		
1	E	566	Total	C	N	O	S	0	0
			4599	2923	779	869	28		
1	I	351	Total	C	N	O	S	0	0
			2857	1831	482	529	15		
1	F	351	Total	C	N	O	S	0	0
			2855	1832	482	526	15		
1	H	324	Total	C	N	O	S	0	0
			2635	1684	452	485	14		
1	G	351	Total	C	N	O	S	0	0
			2856	1831	483	528	14		

- Molecule 2 is a DNA chain called lagging strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	27	Total	C	N	O	P	0	0
			548	268	83	170	27		

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	981	Total	C	N	O	S	0	0
			8036	5136	1340	1507	53		

- Molecule 4 is a protein called DNA polymerase processivity factor component OPG148.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	385	Total	C	N	O	S	0	0
			3141	2028	513	590	10		

- Molecule 5 is a protein called Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	218	Total	C	N	O	S	0	0
			1773	1149	292	326	6		

- Molecule 6 is a DNA chain called leading strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	22	Total	C	N	O	P	0	0
			450	219	72	137	22		

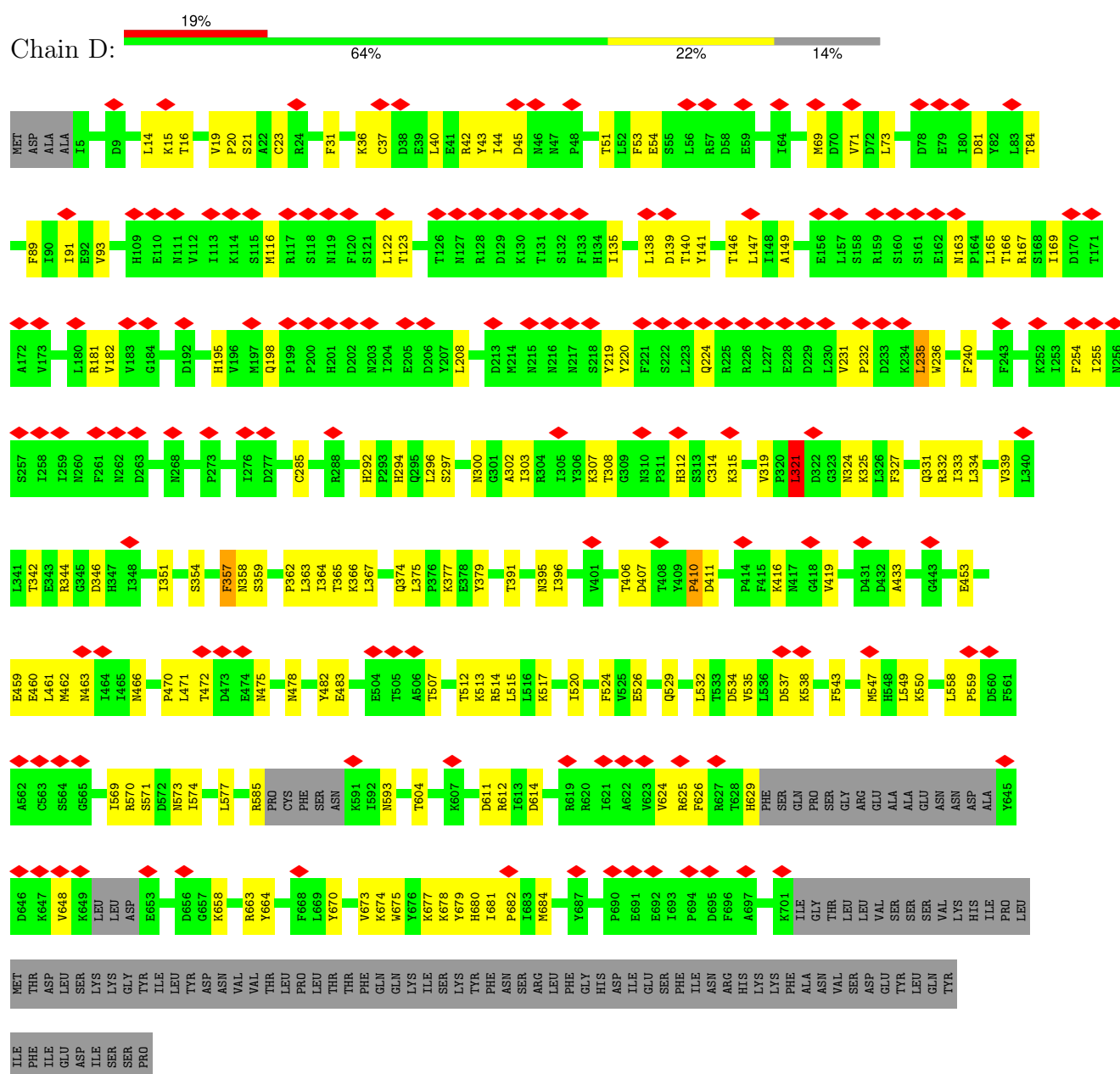
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	Zn	0
			1	1	

3 Residue-property plots

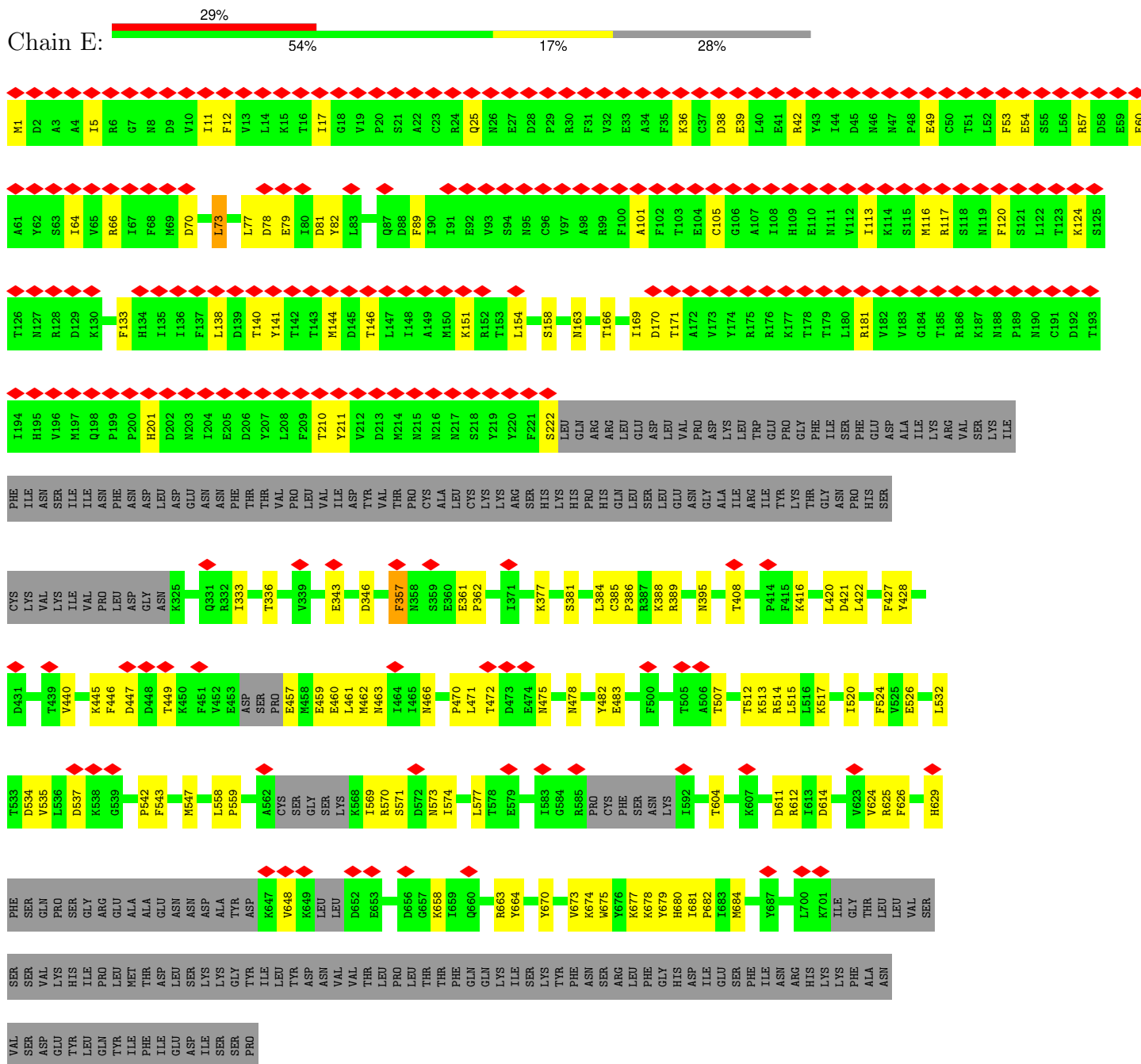
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Uncoating factor OPG117



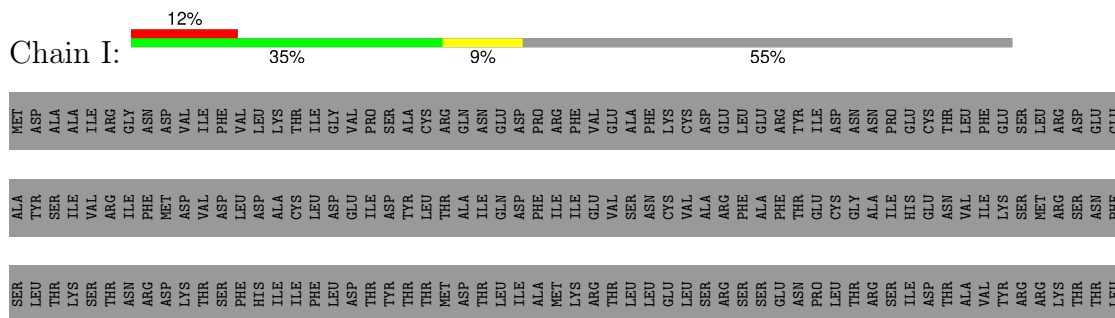
● Molecule 1: Uncoating factor OPG117

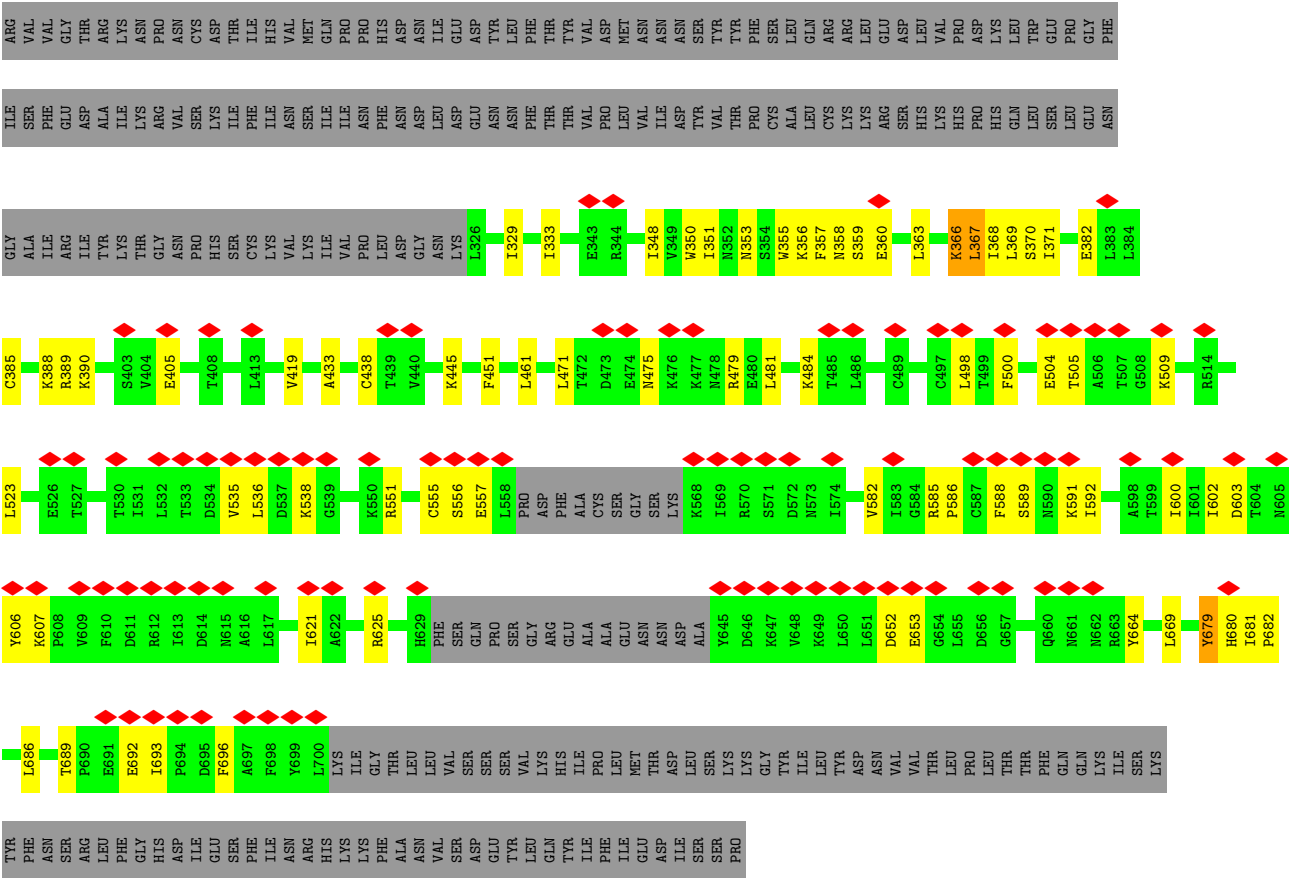
Chain E:



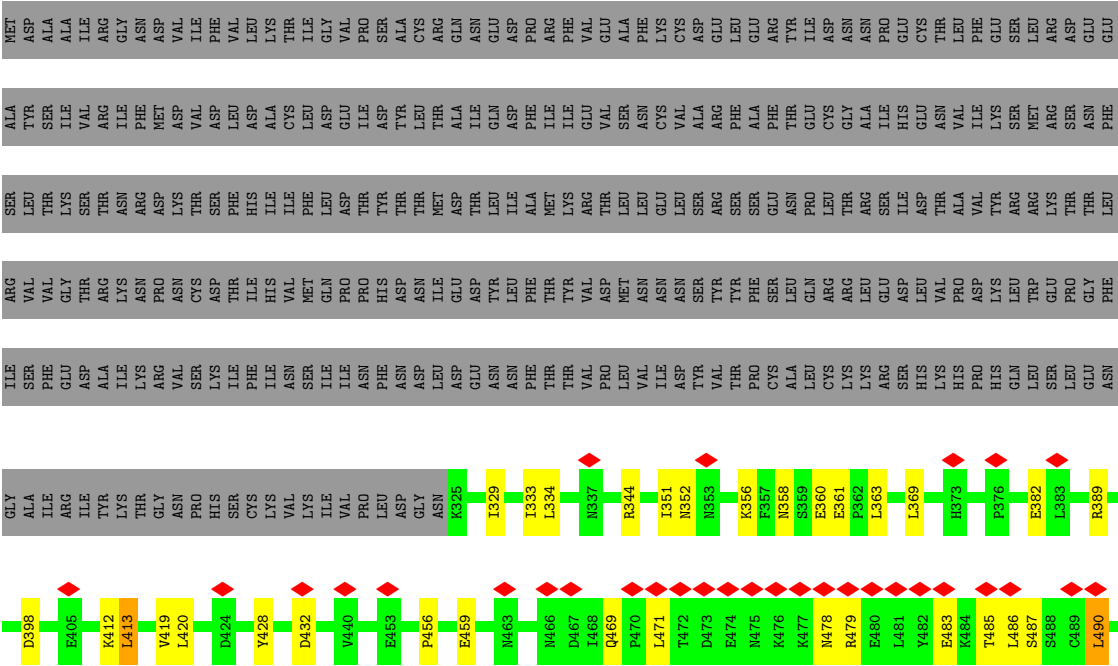
● Molecule 1: Uncoating factor OPG117

Chain I:



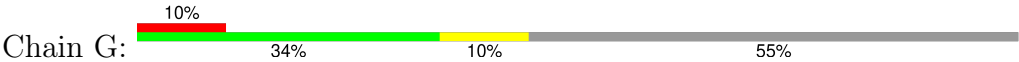


● Molecule 1: Uncoating factor OPG117



ILE	GLY	THR	LEU	LEU	VAL	SER	SER	SER	VAL	VAL	ASP	ASP	GLU	TYR	LEU	GLN	THR	ILE	PRO	LEU	LEU	THR	THR	ASP	LEU	SER	LEU	LEU	LYS	LYS	GLY	GLY	TYR	TYR	PRO
ARG	HIS	LYS	LYS	PHE	ALA	ASN	VAL	SER	SER	ASP	ASP	GLU	GLY	TYR	LEU	GLN	THR	ILE	PRO	LEU	LEU	THR	THR	ASP	LEU	SER	LEU	LEU	LYS	LYS	GLY	GLY	TYR	TYR	PRO

● Molecule 1: Uncoating factor OPG117



MET	ASP	ALA	ILE	ARG	GLY	ASN	VAL	ASP	ASP	VAL	ILE	CYS	THR	ILE	ASP	VAL	PRO	SER	ASP	GLY	VAL	PRO	THR	ASP	GLY	LEU	LEU	LYS	LYS	GLY	GLY	ASP	ASP	GLU
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ALA	TYR	SER	ILE	VAL	ARG	ILE	PHE	ASP	ASP	VAL	ASP	ASP	VAL	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	PHE
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ARG	VAL	VAL	GLY	THR	THR	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	PHE
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ILE	SER	PHE	GLY	ASP	ALA	ILE	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
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GLY	ALA	ILE	ARG	ILE	TYR	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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R397	D398	N399	L400	V401	D402	E405	T408	Y409	P410	D411	K412	G418	V419	L420	D421	L422	V423	D424	G425	N426	F427	C438	T439	V440	S441	T442	F446	D447	E453	P456	E459	M462	N463	I464	I465	N466	P470	L471	T472	D473	E474	N475	K476	K477	N478	Y482	E483
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T494	K495	F500	E504	T505	A506	T507	S510	T511	T512	K513	R514	L515	L516	K517	S518	A519	I520	F524	T527	L532	T533	D534	V535	L536	D537	K538	G539	P540	N541	P542	F543	M547	L558	PRO	ASP	PHE	ALA	CYS	GLY	GLY	ASN	ASN	ASP	LYS	LYS	I569	R570	S571	D572	N573	I574	K575	K576
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L577	T578	E579	F580	I583	G584	R585	PRO	CYS	PHE	SER	ASN	K591	I592	A598	T604	K607	P608	V609	F610	D611	R612	I613	D614	N615	M618	V623	R624	R625	F626	R627	T628	H629	F630	SER	GLN	PRO	SER	GLY	ARG	ALA	ALA	GLU	ASN	ASN	ASP	A644	Y645	D646	K647	V648	K649	L650
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L651	D652	E653	D656	I659	Q660	N661	N662	F668	L669	V673	K674	Y675	K677	K678	Y679	H680	I681	P682	I683	K684	L686	Y687	P690	E691	F694	D695	F696	A697	L700	K701	ILE	GLY	THR	LEU	VAL	SER	SER	GLN	TYR	VAL	VAL	LYS	HIS	ILE	PRO	LEU	MET	THR	ASP	LEU	SER
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LYS	LYS	GLY	TYR	ILE	LEU	TYR	ASP	ASN	VAL	VAL	THR	LEU	PRO	LEU	THR	THR	PHE	GLN	GLN	LYS	ILE	SER	SER	TYR	PHE	ASN	ASN	ARG	HIS	LYS	LYS	PHE	ILE	ALA	ASN	VAL	SER	ASP	GLY	TYR	LEU	SER	GLN	TYR	VAL	ILE	PHE	ILE	GLY	ASP
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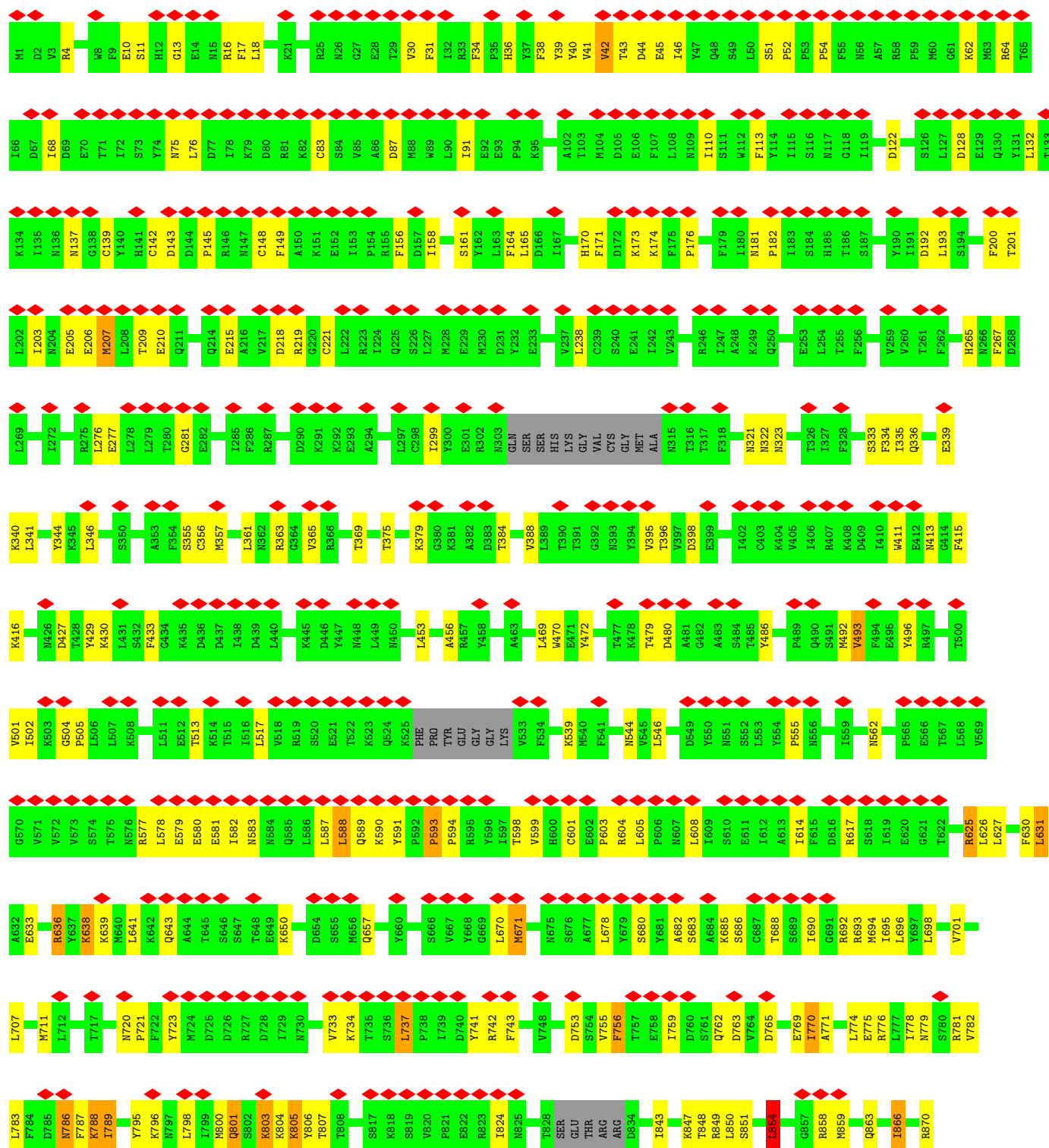
ILE	SER	SER	PRO
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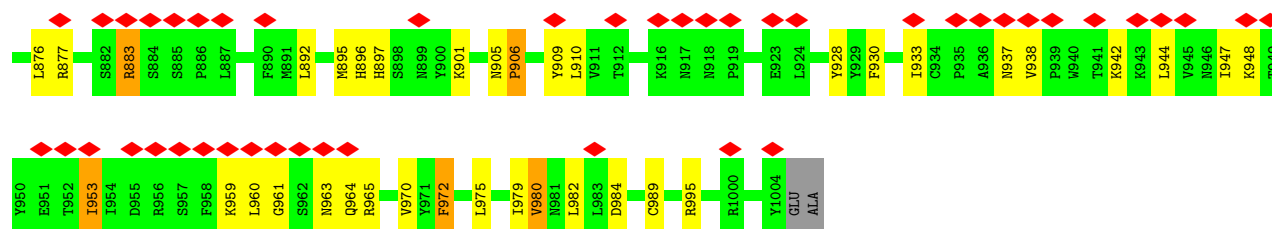
● Molecule 2: lagging strand



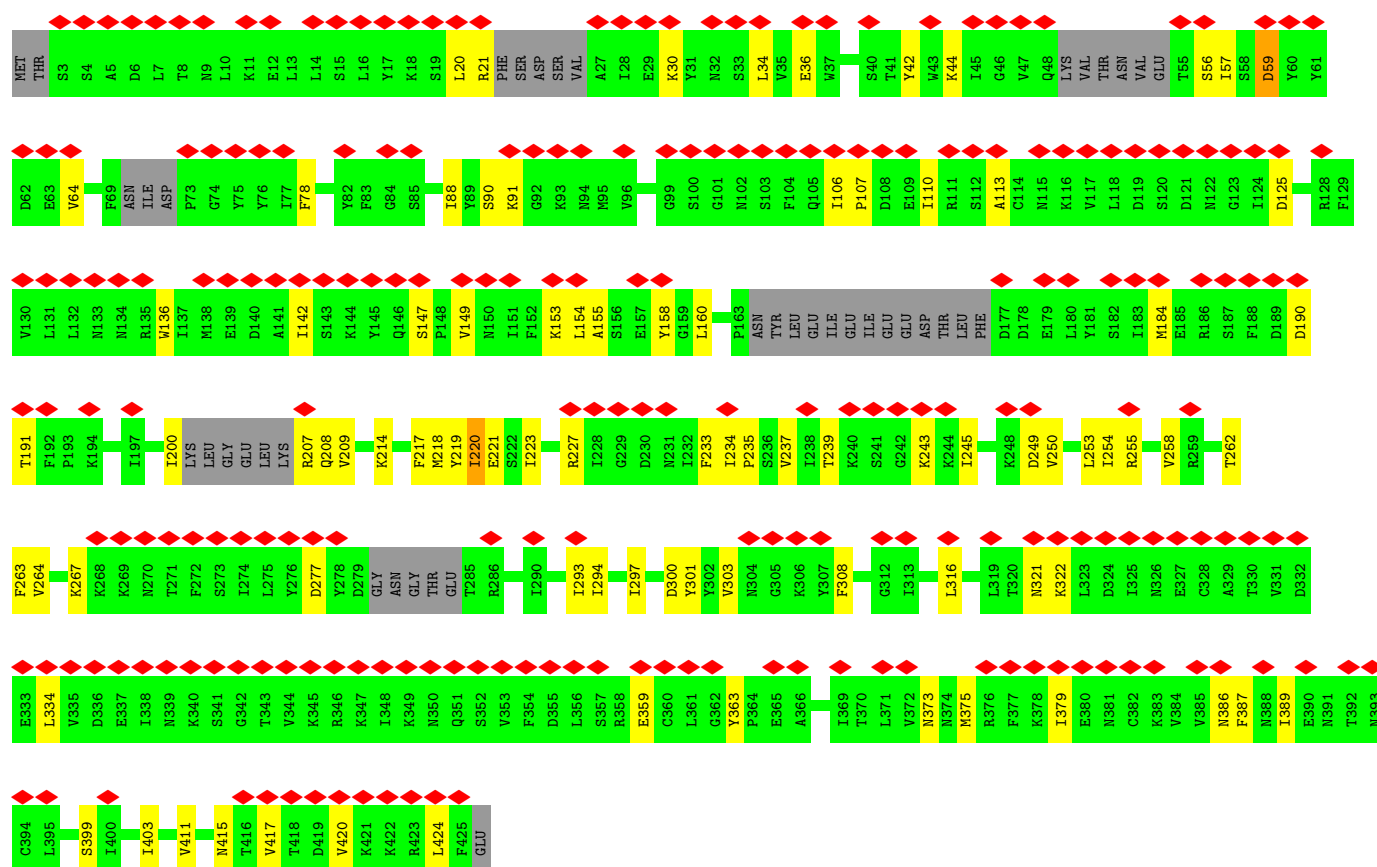


• Molecule 3: DNA polymerase

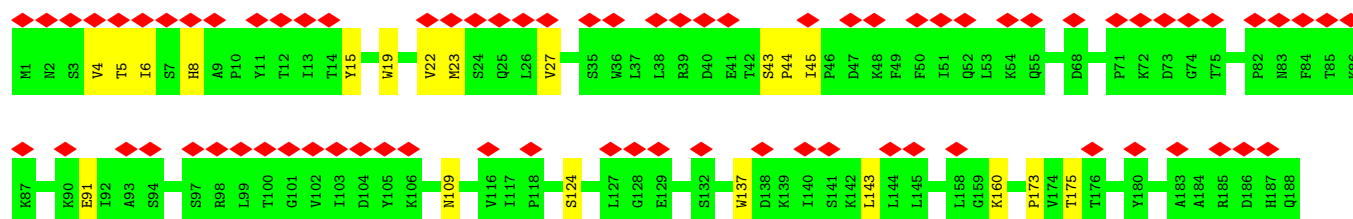
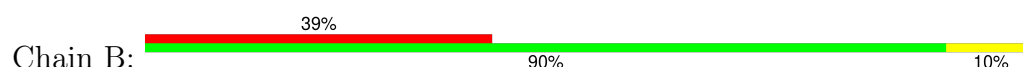


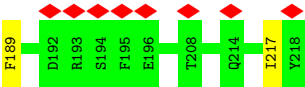


• Molecule 4: DNA polymerase processivity factor component OPG148

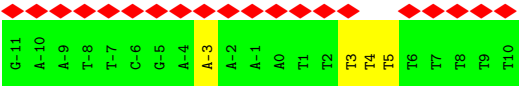
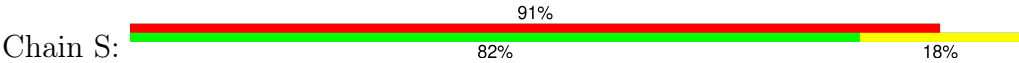


• Molecule 5: Uracil-DNA glycosylase





• Molecule 6: leading strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.268	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	378.88, 378.88, 378.88	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

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

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	D	0.73	1/5579 (0.0%)	0.97	14/7542 (0.2%)
1	E	0.48	0/4684	0.70	3/6324 (0.0%)
1	F	0.60	0/2914	0.78	5/3934 (0.1%)
1	G	0.47	0/2912	0.66	1/3927 (0.0%)
1	H	0.44	0/2684	0.63	1/3614 (0.0%)
1	I	0.54	1/2915 (0.0%)	0.76	5/3935 (0.1%)
2	T	0.39	0/609	0.74	0/935
3	A	1.01	2/8206 (0.0%)	1.35	44/11081 (0.4%)
4	C	0.53	0/3199	0.73	2/4306 (0.0%)
5	B	0.42	0/1823	0.55	0/2479
6	S	0.43	0/502	0.74	0/773
All	All	0.69	4/36027 (0.0%)	0.93	75/48850 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	333	ILE	C-O	-6.06	1.16	1.24
3	A	41	VAL	N-CA	5.14	1.52	1.46
1	I	367	LEU	C-O	-5.12	1.18	1.24
3	A	161	SER	CA-CB	-5.09	1.45	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	593	PRO	N-CA-C	9.71	122.54	110.70
3	A	980	VAL	N-CA-C	-9.29	103.64	111.91
3	A	171	PHE	CA-CB-CG	9.22	123.02	113.80
3	A	580	GLU	N-CA-C	-8.56	103.42	114.04
1	E	381	SER	N-CA-C	-8.56	104.86	114.62
3	A	972	PHE	N-CA-C	-8.10	103.18	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	369	LEU	CA-C-N	-7.60	110.10	120.28
1	I	369	LEU	C-N-CA	-7.60	110.10	120.28
3	A	200	PHE	CA-CB-CG	7.52	121.32	113.80
3	A	756	PHE	CA-CB-CG	6.90	120.70	113.80
1	D	321	LEU	N-CA-C	6.84	120.40	109.24
1	H	513	LYS	N-CA-C	-6.83	103.84	111.28
3	A	930	PHE	CA-CB-CG	6.66	120.46	113.80
1	I	582	VAL	CA-C-N	-6.66	115.27	122.59
1	I	582	VAL	C-N-CA	-6.66	115.27	122.59
3	A	469	LEU	N-CA-C	-6.53	105.13	113.23
3	A	156	PHE	CA-CB-CG	6.48	120.28	113.80
3	A	267	PHE	CB-CA-C	-6.48	102.39	112.31
1	F	522	ASP	O-C-N	6.37	129.67	122.22
3	A	42	VAL	N-CA-C	6.33	116.61	107.88
3	A	164	PHE	CA-C-O	-6.15	114.22	121.16
1	D	333	ILE	CA-C-N	-5.95	111.27	120.31
1	D	333	ILE	C-N-CA	-5.95	111.27	120.31
3	A	31	PHE	CA-CB-CG	5.91	119.71	113.80
3	A	960	LEU	N-CA-C	-5.88	104.22	111.75
1	D	315	LYS	CA-C-N	-5.85	115.29	123.13
1	D	315	LYS	C-N-CA	-5.85	115.29	123.13
3	A	40	TYR	CA-C-O	-5.85	115.01	121.33
3	A	804	LYS	N-CA-C	-5.76	105.56	112.59
1	G	439	THR	O-C-N	5.75	130.06	122.30
3	A	38	PHE	CA-CB-CG	5.72	119.53	113.80
3	A	589	GLN	N-CA-C	-5.69	106.69	113.97
3	A	866	ILE	N-CA-C	-5.69	107.72	113.47
3	A	901	LYS	N-CA-C	-5.66	106.76	113.38
3	A	470	TRP	N-CA-C	-5.65	105.88	112.89
3	A	76	LEU	N-CA-C	5.61	117.62	109.71
3	A	948	LYS	N-CA-C	-5.61	108.22	114.62
3	A	883	ARG	N-CA-C	-5.58	103.70	111.52
3	A	44	ASP	N-CA-C	-5.58	105.29	111.71
1	D	410	PRO	CB-CA-C	-5.54	102.42	111.56
1	D	333	ILE	N-CA-C	-5.53	104.03	111.44
1	F	546	ASN	N-CA-C	-5.51	105.17	111.07
1	D	359	SER	N-CA-C	-5.48	106.36	113.16
3	A	854	LEU	N-CA-C	-5.41	106.53	113.23
4	C	220	ILE	CA-C-N	-5.36	111.30	121.54
4	C	220	ILE	C-N-CA	-5.36	111.30	121.54
3	A	34	PHE	CA-CB-CG	5.36	119.16	113.80
3	A	415	PHE	CA-CB-CG	5.33	119.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	906	PRO	N-CA-CB	-5.31	97.67	103.25
1	F	582	VAL	CA-C-N	-5.31	115.74	122.43
1	F	582	VAL	C-N-CA	-5.31	115.74	122.43
3	A	206	GLU	N-CA-C	-5.30	107.00	112.93
1	D	232	PRO	CB-CA-C	-5.26	102.88	111.56
3	A	493	VAL	N-CA-C	-5.24	107.29	113.42
3	A	877	ARG	N-CA-C	-5.24	107.44	113.88
3	A	207	MET	N-CA-C	-5.24	106.84	114.12
1	I	366	LYS	CA-C-O	-5.21	115.33	120.70
1	F	689	THR	CB-CA-C	5.21	115.13	110.44
3	A	801	GLN	N-CA-C	-5.21	107.58	114.04
3	A	778	ILE	N-CA-C	-5.19	107.10	111.56
1	E	408	THR	N-CA-C	5.18	119.23	113.01
3	A	39	TYR	CA-C-O	-5.17	115.18	121.28
1	D	146	THR	CB-CA-C	5.17	118.64	109.65
3	A	480	ASP	N-CA-C	-5.15	107.66	114.04
3	A	323	ASN	N-CA-C	-5.13	105.77	111.36
3	A	562	ASN	CB-CA-C	5.12	118.72	111.86
3	A	276	LEU	N-CA-C	-5.09	107.02	113.18
1	E	357	PHE	CA-CB-CG	5.08	118.88	113.80
3	A	472	TYR	N-CA-C	-5.06	107.66	113.88
3	A	149	PHE	N-CA-C	-5.05	106.96	112.72
1	D	357	PHE	CA-CB-CG	5.04	118.84	113.80
1	D	331	GLN	CA-C-N	-5.04	112.64	120.31
1	D	331	GLN	C-N-CA	-5.04	112.64	120.31
3	A	803	LYS	N-CA-C	-5.01	106.33	112.90
1	D	149	ALA	N-CA-C	-5.01	104.97	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5469	0	5473	115	0
1	E	4599	0	4592	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2855	0	2892	81	0
1	G	2856	0	2892	58	0
1	H	2635	0	2674	60	0
1	I	2857	0	2889	52	0
2	T	548	0	315	7	0
3	A	8036	0	7991	177	0
4	C	3141	0	3151	63	0
5	B	1773	0	1764	17	0
6	S	450	0	255	3	0
7	D	1	0	0	0	0
All	All	35220	0	34888	692	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 10.

All (692) 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)
3:A:513:THR:CG2	3:A:625:ARG:HH22	1.33	1.40
3:A:513:THR:CG2	3:A:625:ARG:NH2	1.86	1.37
3:A:513:THR:HG23	3:A:625:ARG:NH2	1.38	1.33
3:A:513:THR:HG21	3:A:625:ARG:CZ	1.70	1.22
3:A:858:ARG:O	3:A:859:MET:HE2	1.49	1.12
1:F:681:ILE:HG23	1:F:682:PRO:HD3	1.38	1.06
1:F:681:ILE:CG2	1:F:682:PRO:HD3	1.85	1.05
3:A:340:LYS:O	3:A:341:LEU:HG	1.61	1.01
3:A:961:GLY:HA2	3:A:964:GLN:HB3	1.45	0.99
3:A:513:THR:HG21	3:A:625:ARG:NH1	1.80	0.97
3:A:513:THR:CG2	3:A:625:ARG:CZ	2.37	0.96
5:B:4:VAL:HG11	5:B:27:VAL:HG21	1.48	0.95
3:A:513:THR:HG21	3:A:625:ARG:NH2	1.68	0.93
1:F:540:PRO:HB2	1:F:587:CYS:HA	1.51	0.91
3:A:587:LEU:CD1	3:A:588:LEU:HD22	2.01	0.90
3:A:192:ASP:OD1	3:A:193:LEU:N	2.09	0.86
3:A:756:PHE:HE2	3:A:800:MET:HE3	1.42	0.84
1:F:681:ILE:HG23	1:F:682:PRO:CD	2.07	0.83
1:I:681:ILE:HG23	1:I:682:PRO:HD3	1.60	0.82
1:D:163:ASN:HB3	1:D:166:THR:HG22	1.61	0.81
3:A:513:THR:CG2	3:A:625:ARG:NH1	2.40	0.80
3:A:798:LEU:HD11	3:A:800:MET:HE2	1.61	0.80
3:A:486:TYR:CD1	3:A:501:VAL:CG1	2.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:486:TYR:CG	3:A:501:VAL:HG13	2.17	0.80
3:A:340:LYS:O	3:A:341:LEU:CG	2.30	0.79
3:A:980:VAL:HG13	3:A:989:CYS:HB3	1.66	0.78
3:A:192:ASP:CG	3:A:193:LEU:H	1.91	0.77
1:F:681:ILE:HG22	1:F:682:PRO:HD3	1.66	0.77
3:A:427:ASP:HB3	3:A:429:TYR:CE2	2.19	0.76
1:D:15:LYS:HG3	1:D:51:THR:O	1.85	0.76
1:G:535:VAL:CG1	1:G:538:LYS:HG2	2.15	0.76
1:I:484:LYS:HG3	1:I:680:HIS:NE2	1.99	0.76
1:D:391:THR:HG21	2:T:19:DA:H2"	1.68	0.76
4:C:200:ILE:HG22	4:C:207:ARG:HG2	1.68	0.75
3:A:579:GLU:HA	3:A:582:ILE:HG12	1.68	0.75
1:E:346:ASP:HB2	1:E:357:PHE:HE1	1.50	0.75
1:F:568:LYS:O	1:F:570:ARG:NH2	2.20	0.75
1:I:586:PRO:HB2	1:I:589:SER:HB2	1.69	0.74
3:A:743:PHE:HB3	3:A:759:ILE:HD11	1.69	0.74
1:H:544:ILE:HG21	1:H:584:GLY:HA3	1.68	0.74
3:A:42:VAL:CG1	3:A:46:ILE:HB	2.18	0.74
3:A:587:LEU:HD12	3:A:588:LEU:HD22	1.69	0.73
3:A:513:THR:CG2	3:A:625:ARG:HH12	2.01	0.73
3:A:851:SER:HA	3:A:854:LEU:HD22	1.70	0.73
3:A:577:ARG:HD2	4:C:373:ASN:HA	1.70	0.72
3:A:587:LEU:HD11	3:A:588:LEU:HD22	1.70	0.72
3:A:501:VAL:HG12	3:A:501:VAL:O	1.89	0.72
3:A:883:ARG:HH12	3:A:965:ARG:HG3	1.54	0.72
3:A:843:ILE:HG12	3:A:847:LYS:HE3	1.71	0.72
1:H:512:THR:HG22	1:H:515:LEU:HD12	1.73	0.71
3:A:375:THR:HG22	3:A:379:LYS:HE2	1.71	0.71
1:F:382:GLU:N	1:F:382:GLU:OE2	2.24	0.70
1:E:346:ASP:HB2	1:E:357:PHE:CE1	2.26	0.70
3:A:513:THR:HG23	3:A:625:ARG:HH22	0.56	0.70
4:C:142:ILE:HG22	4:C:207:ARG:NH1	2.06	0.70
3:A:42:VAL:HG13	3:A:46:ILE:HB	1.73	0.69
3:A:411:TRP:HE1	3:A:416:LYS:HD2	1.57	0.69
4:C:249:ASP:OD1	4:C:250:VAL:N	2.25	0.69
1:F:523:LEU:HD22	1:F:551:ARG:HG3	1.74	0.69
3:A:340:LYS:C	3:A:341:LEU:HG	2.17	0.69
1:D:236:TRP:HD1	3:A:995:ARG:HD3	1.58	0.68
1:H:512:THR:HA	1:H:515:LEU:HB2	1.74	0.68
1:D:36:LYS:HG2	1:D:37:CYS:N	2.09	0.68
3:A:555:PRO:HA	3:A:627:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:720:ASN:OD1	3:A:721:PRO:HD2	1.93	0.67
1:F:351:ILE:O	1:F:356:LYS:NZ	2.27	0.67
3:A:209:THR:HG22	3:A:210:GLU:N	2.09	0.67
3:A:176:PRO:HA	3:A:181:ASN:HD22	1.59	0.67
1:D:585:ARG:HH12	1:E:542:PRO:HB3	1.59	0.66
3:A:627:LEU:HA	3:A:630:PHE:HB2	1.78	0.66
1:D:363:LEU:HD13	1:D:366:LYS:HD2	1.78	0.66
1:F:578:THR:HG21	1:F:620:ARG:HD3	1.77	0.66
1:G:681:ILE:HG23	1:G:682:PRO:HD3	1.78	0.66
1:E:681:ILE:HG23	1:E:682:PRO:HD3	1.78	0.65
1:H:681:ILE:HG23	1:H:682:PRO:HD3	1.78	0.65
1:D:681:ILE:HG23	1:D:682:PRO:HD3	1.78	0.65
1:F:490:LEU:HD11	1:F:669:LEU:HD13	1.79	0.65
1:F:578:THR:HG21	1:F:620:ARG:HH11	1.62	0.65
1:D:391:THR:HG23	1:E:386:PRO:HG2	1.79	0.64
1:F:344:ARG:HH12	1:F:593:ASN:HB3	1.62	0.64
1:G:418:GLY:HA3	1:G:427:PHE:CZ	2.32	0.64
3:A:603:PRO:HB3	3:A:608:LEU:HB3	1.78	0.63
3:A:395:VAL:HG22	3:A:433:PHE:CE1	2.34	0.63
1:I:498:LEU:HD22	1:I:600:ILE:HB	1.80	0.63
1:I:681:ILE:CG2	1:I:682:PRO:HD3	2.28	0.63
3:A:395:VAL:HG12	3:A:396:THR:N	2.14	0.63
1:F:578:THR:HG21	1:F:620:ARG:NH1	2.13	0.63
1:H:428:TYR:HB2	1:H:433:ALA:HB2	1.81	0.63
1:D:296:LEU:HD22	1:D:303:ILE:HG22	1.81	0.63
3:A:43:THR:HG22	3:A:45:GLU:H	1.62	0.62
3:A:756:PHE:CE2	3:A:800:MET:HE3	2.29	0.62
1:G:358:ASN:ND2	1:G:360:GLU:OE2	2.32	0.62
1:D:296:LEU:HD22	1:D:303:ILE:CG2	2.30	0.62
1:D:362:PRO:O	1:D:366:LYS:HG3	2.00	0.62
1:F:510:SER:OG	1:F:514:ARG:NH2	2.33	0.62
4:C:113:ALA:HB1	4:C:160:LEU:HD23	1.81	0.62
1:D:20:PRO:HG2	1:D:23:CYS:HB2	1.82	0.62
1:F:622:ALA:HB1	1:F:689:THR:H	1.65	0.62
3:A:598:THR:HG22	3:A:614:ILE:HG12	1.82	0.61
5:B:22:VAL:HG13	5:B:23:MET:HE2	1.80	0.61
1:G:535:VAL:HG11	1:G:538:LYS:HG2	1.82	0.61
1:F:578:THR:CG2	1:F:620:ARG:NH1	2.64	0.61
1:F:618:MET:HG2	1:F:696:PHE:CG	2.36	0.61
3:A:486:TYR:CG	3:A:501:VAL:CG1	2.81	0.61
1:H:507:THR:HG21	1:H:626:PHE:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:892:LEU:N	3:A:892:LEU:HD12	2.16	0.61
4:C:142:ILE:HG22	4:C:207:ARG:CZ	2.31	0.61
1:E:520:ILE:HD11	1:E:524:PHE:HB2	1.83	0.60
3:A:707:LEU:HG	3:A:741:TYR:O	2.01	0.60
1:D:303:ILE:HD12	1:D:321:LEU:HG	1.82	0.60
1:E:1:MET:HE1	1:E:5:ILE:HB	1.83	0.60
1:F:546:ASN:O	1:F:550:LYS:HE2	2.00	0.60
1:G:520:ILE:HD11	1:G:524:PHE:HB2	1.83	0.60
4:C:411:VAL:O	4:C:415:ASN:ND2	2.35	0.60
1:E:395:ASN:OD1	1:G:389:ARG:NH2	2.34	0.60
1:D:520:ILE:HD11	1:D:524:PHE:HB2	1.84	0.60
1:F:456:PRO:HA	1:F:459:GLU:HG2	1.84	0.60
1:F:413:LEU:HD21	1:F:490:LEU:HD22	1.83	0.60
3:A:858:ARG:C	3:A:859:MET:HE2	2.25	0.60
5:B:43:SER:HB2	5:B:44:PRO:HD3	1.82	0.60
1:D:507:THR:HG21	1:D:626:PHE:HB3	1.83	0.60
3:A:75:ASN:OD1	3:A:75:ASN:C	2.45	0.59
3:A:581:GLU:HB2	4:C:379:ILE:HD12	1.83	0.59
1:E:36:LYS:HD3	1:E:38:ASP:H	1.67	0.59
1:F:500:PHE:HB2	1:F:623:VAL:HG22	1.84	0.59
1:E:124:LYS:HA	1:E:133:PHE:HB3	1.83	0.59
1:F:568:LYS:N	1:F:570:ARG:HH22	2.00	0.59
5:B:109:ASN:HB2	5:B:217:ILE:HD11	1.84	0.59
1:G:535:VAL:HG13	1:G:538:LYS:HG2	1.83	0.59
1:H:514:ARG:O	1:H:517:LYS:HB2	2.02	0.59
1:D:14:LEU:HD12	1:D:31:PHE:O	2.03	0.59
1:E:39:GLU:O	1:E:42:ARG:NH1	2.35	0.59
1:E:507:THR:HG21	1:E:626:PHE:HB3	1.83	0.59
3:A:501:VAL:CG1	3:A:501:VAL:O	2.50	0.59
5:B:6:ILE:HG22	5:B:8:HIS:H	1.67	0.59
1:D:462:MET:HA	1:D:462:MET:HE2	1.84	0.58
1:F:329:ILE:O	1:F:333:ILE:HG12	2.02	0.58
3:A:947:ILE:HG21	3:A:970:VAL:HG11	1.85	0.58
1:E:462:MET:HE2	1:E:462:MET:HA	1.84	0.58
1:E:483:GLU:HB3	1:E:679:TYR:HE2	1.68	0.58
4:C:57:ILE:HG13	4:C:88:ILE:HG21	1.84	0.58
3:A:277:GLU:HA	3:A:281:GLY:HA2	1.84	0.58
1:H:389:ARG:NH2	1:G:395:ASN:OD1	2.37	0.58
1:H:483:GLU:HB3	1:H:679:TYR:HE2	1.68	0.58
3:A:707:LEU:HD21	3:A:741:TYR:HB3	1.85	0.58
1:D:303:ILE:HG22	1:D:303:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:GLU:HB3	1:D:679:TYR:HE2	1.68	0.58
1:D:513:LYS:NZ	1:D:526:GLU:OE1	2.30	0.58
1:G:507:THR:HG21	1:G:626:PHE:HB3	1.83	0.58
3:A:341:LEU:HD12	3:A:344:TYR:HE1	1.69	0.58
1:G:483:GLU:HB3	1:G:679:TYR:HE2	1.68	0.58
4:C:64:VAL:HG12	4:C:209:VAL:HG23	1.85	0.58
1:D:419:VAL:HG12	1:D:433:ALA:HB1	1.86	0.57
1:D:324:ASN:HB2	1:E:384:LEU:HD13	1.84	0.57
1:D:36:LYS:HG2	1:D:37:CYS:H	1.69	0.57
4:C:56:SER:HA	4:C:59:ASP:HB3	1.86	0.57
1:G:421:ASP:HB3	1:G:425:GLY:HA3	1.85	0.57
1:F:660:GLN:N	1:F:660:GLN:OE1	2.38	0.57
1:G:471:LEU:H	1:G:471:LEU:HD23	1.70	0.57
3:A:980:VAL:CG1	3:A:989:CYS:HB3	2.32	0.57
4:C:253:LEU:HD22	4:C:258:VAL:HG11	1.86	0.57
1:G:462:MET:HA	1:G:462:MET:HE2	1.84	0.57
1:E:471:LEU:H	1:E:471:LEU:HD23	1.70	0.57
1:I:556:SER:HA	1:I:603:ASP:HB3	1.87	0.57
5:B:4:VAL:HG23	5:B:15:TYR:CE1	2.39	0.57
1:D:20:PRO:HB3	2:T:7:DT:H1'	1.85	0.56
1:G:482:TYR:HD1	1:G:624:VAL:HG11	1.70	0.56
1:H:482:TYR:HD1	1:H:624:VAL:HG11	1.70	0.56
1:E:482:TYR:HD1	1:E:624:VAL:HG11	1.70	0.56
1:E:513:LYS:NZ	1:E:526:GLU:OE1	2.30	0.56
1:D:471:LEU:HD23	1:D:471:LEU:H	1.70	0.56
1:H:421:ASP:OD1	1:H:422:LEU:N	2.37	0.56
1:D:116:MET:HB3	1:D:140:THR:HG21	1.87	0.56
1:F:478:ASN:ND2	1:F:625:ARG:O	2.36	0.56
1:F:652:ASP:OD1	1:F:653:GLU:N	2.38	0.56
1:H:389:ARG:NH1	1:G:398:ASP:OD2	2.39	0.56
1:I:405:GLU:OE1	1:I:405:GLU:N	2.37	0.56
3:A:62:LYS:HD3	3:A:87:ASP:HA	1.88	0.56
3:A:341:LEU:HD12	3:A:344:TYR:CE1	2.41	0.56
3:A:395:VAL:CG1	3:A:396:THR:H	2.19	0.56
1:E:66:ARG:HE	1:E:138:LEU:HA	1.71	0.56
4:C:30:LYS:O	4:C:34:LEU:HG	2.05	0.56
4:C:250:VAL:O	4:C:254:ILE:HG12	2.05	0.56
1:H:518:SER:HB3	1:H:664:TYR:CZ	2.41	0.56
4:C:375:MET:HG2	4:C:389:ILE:HD13	1.88	0.56
1:I:693:ILE:HG22	1:I:696:PHE:H	1.70	0.55
1:F:558:LEU:HD23	1:F:604:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:614:ASP:OD1	1:F:614:ASP:N	2.37	0.55
4:C:234:ILE:HD12	4:C:235:PRO:HD2	1.88	0.55
1:D:312:HIS:ND1	1:D:312:HIS:O	2.40	0.55
1:I:360:GLU:OE2	1:I:360:GLU:N	2.28	0.55
1:D:482:TYR:HD1	1:D:624:VAL:HG11	1.70	0.55
1:I:555:CYS:HB3	1:I:602:ILE:HD12	1.89	0.55
3:A:192:ASP:CG	3:A:193:LEU:N	2.58	0.55
4:C:42:TYR:HB3	5:B:175:THR:HG23	1.89	0.55
1:H:585:ARG:HH11	1:H:586:PRO:HD2	1.71	0.55
1:D:377:LYS:HE3	1:D:377:LYS:HA	1.88	0.55
4:C:399:SER:O	4:C:403:ILE:HG12	2.07	0.55
5:B:4:VAL:CG1	5:B:27:VAL:HG21	2.29	0.55
3:A:905:ASN:OD1	3:A:906:PRO:HD2	2.07	0.55
1:H:423:VAL:HG23	1:H:424:ASP:OD1	2.07	0.54
1:E:158:SER:HB3	1:E:169:ILE:HG22	1.88	0.54
1:I:419:VAL:HG12	1:I:433:ALA:HB1	1.89	0.54
1:D:138:LEU:C	1:D:140:THR:H	2.14	0.54
3:A:395:VAL:CG1	3:A:396:THR:N	2.71	0.54
1:D:670:TYR:O	1:D:674:LYS:HG2	2.08	0.54
1:E:670:TYR:O	1:E:674:LYS:HG2	2.08	0.54
1:F:351:ILE:HD12	1:F:352:ASN:H	1.72	0.54
3:A:340:LYS:O	3:A:341:LEU:CD2	2.56	0.54
3:A:843:ILE:CG1	3:A:847:LYS:HE3	2.36	0.54
3:A:356:CYS:SG	3:A:357:MET:N	2.80	0.54
3:A:944:LEU:HB3	3:A:947:ILE:HD11	1.89	0.54
1:I:679:TYR:O	1:I:680:HIS:HD2	1.91	0.54
1:H:382:GLU:OE2	1:H:382:GLU:N	2.41	0.54
1:G:418:GLY:CA	1:G:427:PHE:CZ	2.91	0.54
4:C:220:ILE:N	4:C:262:THR:O	2.41	0.54
3:A:937:ASN:OD1	3:A:937:ASN:O	2.26	0.53
1:E:673:VAL:O	1:E:677:LYS:HG2	2.08	0.53
1:H:658:LYS:HB2	1:H:663:ARG:HG3	1.89	0.53
3:A:339:GLU:CD	3:A:341:LEU:HD11	2.34	0.53
1:I:481:LEU:HD11	1:I:689:THR:HG21	1.90	0.53
1:D:54:GLU:OE1	1:D:208:LEU:HD23	2.09	0.53
4:C:190:ASP:OD1	4:C:191:THR:N	2.41	0.53
1:D:675:TRP:CD1	1:D:678:LYS:HZ3	2.27	0.53
1:H:664:TYR:HB2	1:H:667:ALA:HB3	1.90	0.53
3:A:892:LEU:N	3:A:892:LEU:CD1	2.71	0.53
4:C:107:PRO:HG3	4:C:136:TRP:CD1	2.43	0.53
1:G:329:ILE:O	1:G:333:ILE:HG12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:673:VAL:O	1:G:677:LYS:HG2	2.08	0.53
1:F:498:LEU:HB2	1:F:620:ARG:O	2.09	0.53
1:F:569:ILE:HB	1:F:610:PHE:CD1	2.43	0.53
1:D:673:VAL:O	1:D:677:LYS:HG2	2.08	0.53
1:E:113:ILE:HD12	1:E:117:ARG:HH21	1.74	0.53
1:E:427:PHE:CZ	1:E:446:PHE:HB2	2.44	0.53
1:D:324:ASN:HB3	1:D:327:PHE:HB2	1.91	0.52
3:A:502:ILE:HD13	3:A:678:LEU:HD22	1.91	0.52
1:E:120:PHE:O	1:E:201:HIS:CE1	2.63	0.52
3:A:176:PRO:HA	3:A:181:ASN:ND2	2.24	0.52
3:A:783:LEU:HD13	3:A:788:LYS:HA	1.91	0.52
1:D:462:MET:SD	1:D:466:ASN:ND2	2.83	0.52
1:E:462:MET:SD	1:E:466:ASN:ND2	2.83	0.52
4:C:363:TYR:CD1	4:C:403:ILE:HD12	2.44	0.52
1:G:462:MET:SD	1:G:466:ASN:ND2	2.83	0.52
1:D:139:ASP:O	1:D:219:TYR:HB3	2.09	0.52
1:I:475:ASN:HB3	1:I:479:ARG:HB2	1.90	0.52
3:A:265:HIS:O	3:A:299:ILE:HG21	2.09	0.52
3:A:587:LEU:HD12	3:A:588:LEU:N	2.24	0.52
1:E:416:LYS:HZ2	1:E:445:LYS:HG2	1.75	0.52
3:A:209:THR:CG2	3:A:210:GLU:N	2.72	0.52
4:C:155:ALA:HB1	4:C:160:LEU:HD11	1.91	0.52
1:I:351:ILE:H	1:I:356:LYS:HZ1	1.58	0.52
3:A:961:GLY:C	3:A:963:ASN:H	2.18	0.52
1:E:60:GLU:N	1:E:60:GLU:OE1	2.43	0.52
1:E:421:ASP:HB2	1:E:428:TYR:HE2	1.75	0.52
3:A:170:HIS:HB3	3:A:182:PRO:HD2	1.91	0.52
3:A:883:ARG:NH1	3:A:965:ARG:HG3	2.24	0.52
1:D:54:GLU:OE1	1:D:208:LEU:CD2	2.58	0.52
1:H:518:SER:HB3	1:H:664:TYR:CE1	2.45	0.52
3:A:633:GLU:HA	3:A:636:ARG:HD2	1.92	0.52
4:C:221:GLU:N	4:C:221:GLU:OE1	2.43	0.52
1:D:54:GLU:HB2	1:D:182:VAL:CG2	2.41	0.51
1:F:556:SER:HA	1:F:603:ASP:HB3	1.91	0.51
3:A:173:LYS:O	3:A:174:LYS:HG3	2.11	0.51
3:A:395:VAL:HG12	3:A:396:THR:H	1.74	0.51
3:A:737:LEU:HD21	3:A:770:ILE:HA	1.91	0.51
5:B:4:VAL:HG23	5:B:15:TYR:HE1	1.75	0.51
1:E:514:ARG:HA	1:E:517:LYS:HG2	1.92	0.51
1:E:54:GLU:OE2	1:E:210:THR:OG1	2.25	0.51
1:I:389:ARG:NH1	1:F:398:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:VAL:HG21	1:F:550:LYS:HG3	1.93	0.51
3:A:582:ILE:HG22	4:C:379:ILE:HG21	1.91	0.51
4:C:218:MET:O	4:C:263:PHE:HA	2.10	0.51
4:C:223:ILE:HG13	4:C:237:VAL:HG12	1.93	0.51
1:G:573:ASN:O	1:G:577:LEU:HG	2.11	0.51
1:I:382:GLU:OE1	1:I:388:LYS:HD3	2.09	0.51
1:I:451:PHE:HE1	1:I:669:LEU:HB3	1.75	0.51
5:B:45:ILE:HD12	5:B:45:ILE:H	1.75	0.51
1:E:573:ASN:O	1:E:577:LEU:HG	2.11	0.51
3:A:68:ILE:HD13	3:A:517:LEU:HB3	1.92	0.51
3:A:427:ASP:HB3	3:A:429:TYR:CZ	2.45	0.51
3:A:590:LYS:HD3	3:A:591:TYR:CE1	2.45	0.51
1:E:163:ASN:HB2	1:E:166:THR:HG22	1.93	0.51
1:I:585:ARG:HH12	1:I:588:PHE:H	1.59	0.51
1:G:680:HIS:HB3	1:G:684:MET:HG3	1.93	0.51
1:G:684:MET:O	1:G:685:LYS:HD3	2.11	0.51
1:E:680:HIS:HB3	1:E:684:MET:HG3	1.93	0.51
1:F:681:ILE:CG2	1:F:682:PRO:CD	2.71	0.51
1:D:169:ILE:HG13	1:D:169:ILE:O	2.10	0.51
1:E:532:LEU:HD12	1:E:569:ILE:HG23	1.93	0.51
3:A:599:VAL:HG11	3:A:686:SER:HB3	1.93	0.51
1:E:151:LYS:HG3	1:E:171:THR:OG1	2.11	0.51
1:E:385:CYS:HB2	1:E:388:LYS:HD2	1.92	0.51
1:H:532:LEU:HD12	1:H:569:ILE:HG23	1.93	0.51
1:D:236:TRP:CD1	3:A:995:ARG:HD3	2.42	0.50
1:D:514:ARG:HA	1:D:517:LYS:HG2	1.92	0.50
1:D:680:HIS:HB3	1:D:684:MET:HG3	1.93	0.50
1:F:622:ALA:HB2	1:F:688:PRO:HA	1.93	0.50
1:G:514:ARG:HA	1:G:517:LYS:HG2	1.92	0.50
1:D:54:GLU:CD	1:D:208:LEU:HD22	2.37	0.50
1:D:573:ASN:O	1:D:577:LEU:HG	2.11	0.50
1:I:505:THR:HG21	1:F:615:ASN:HB3	1.92	0.50
3:A:128:ASP:OD1	3:A:148:CYS:HA	2.11	0.50
1:F:662:ASN:HB3	1:F:665:ARG:HB2	1.93	0.50
3:A:4:ARG:HH11	3:A:158:ILE:HG12	1.76	0.50
3:A:132:LEU:HD23	3:A:142:CYS:HB2	1.93	0.50
3:A:604:ARG:HH21	3:A:682:ALA:HB2	1.76	0.50
1:G:629:HIS:HB3	1:G:648:VAL:HG13	1.94	0.50
1:G:675:TRP:CD1	1:G:678:LYS:HZ3	2.30	0.50
1:E:101:ALA:HA	1:E:105:CYS:HB2	1.94	0.50
1:I:329:ILE:O	1:I:333:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:573:ASN:O	1:H:577:LEU:HG	2.11	0.50
3:A:587:LEU:HD11	3:A:588:LEU:CD2	2.39	0.50
3:A:707:LEU:CD2	3:A:741:TYR:HB3	2.41	0.50
1:E:470:PRO:HB2	1:E:472:THR:HG23	1.94	0.50
1:F:622:ALA:CB	1:F:689:THR:H	2.24	0.50
1:I:586:PRO:HB2	1:I:589:SER:CB	2.39	0.50
1:G:470:PRO:HB2	1:G:472:THR:HG23	1.94	0.50
1:E:116:MET:HB3	1:E:140:THR:HG21	1.93	0.50
1:E:361:GLU:N	1:E:362:PRO:HD2	2.27	0.50
1:E:629:HIS:HB3	1:E:648:VAL:HG13	1.94	0.50
1:I:367:LEU:O	1:I:371:ILE:N	2.31	0.50
3:A:62:LYS:HE2	3:A:87:ASP:HB2	1.92	0.50
3:A:363:ARG:O	3:A:363:ARG:HG3	2.12	0.50
3:A:593:PRO:HB3	3:A:723:TYR:CE1	2.47	0.50
1:F:568:LYS:HB2	1:F:570:ARG:NH2	2.27	0.50
1:H:465:ILE:HG22	1:H:479:ARG:HH21	1.77	0.50
4:C:147:SER:O	4:C:149:VAL:N	2.44	0.50
4:C:219:TYR:HA	4:C:262:THR:O	2.12	0.49
1:E:11:ILE:HD11	1:E:211:TYR:HD1	1.77	0.49
4:C:237:VAL:HG23	4:C:245:ILE:HB	1.94	0.49
1:D:532:LEU:HD12	1:D:569:ILE:HG23	1.93	0.49
1:E:64:ILE:HD11	1:E:141:TYR:HB3	1.94	0.49
1:F:471:LEU:HD23	1:F:471:LEU:H	1.77	0.49
3:A:13:GLY:O	3:A:16:ARG:HD3	2.12	0.49
4:C:149:VAL:HG12	4:C:153:LYS:NZ	2.26	0.49
1:E:420:LEU:HD22	1:E:446:PHE:CZ	2.47	0.49
1:H:680:HIS:HB3	1:H:684:MET:HG3	1.93	0.49
1:F:618:MET:HG2	1:F:696:PHE:HB3	1.95	0.49
3:A:807:THR:HA	3:A:824:ILE:O	2.13	0.49
1:D:470:PRO:HB2	1:D:472:THR:HG23	1.94	0.49
1:H:393:GLU:OE1	1:H:397:ARG:HD2	2.12	0.49
3:A:209:THR:HG22	3:A:210:GLU:H	1.78	0.49
4:C:21:ARG:NH1	4:C:57:ILE:HD11	2.28	0.49
1:E:675:TRP:CD1	1:E:678:LYS:HZ3	2.30	0.49
1:G:382:GLU:N	1:G:382:GLU:OE2	2.41	0.49
1:H:468:ILE:HG21	1:H:512:THR:CG2	2.43	0.49
4:C:78:PHE:CE2	4:C:184:MET:HE3	2.48	0.49
1:H:414:PRO:HA	1:H:419:VAL:HG22	1.94	0.49
3:A:375:THR:HG22	3:A:379:LYS:CE	2.41	0.49
3:A:671:MET:HE2	3:A:671:MET:HB2	1.75	0.49
4:C:221:GLU:OE1	4:C:239:THR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:VAL:HG22	1:D:21:SER:H	1.78	0.48
1:I:367:LEU:O	1:I:368:ILE:C	2.54	0.48
3:A:539:LYS:HD2	3:A:982:LEU:O	2.13	0.48
4:C:227:ARG:HG2	4:C:233:PHE:CE1	2.48	0.48
3:A:779:ASN:HB3	3:A:788:LYS:HG2	1.95	0.48
3:A:591:TYR:CD1	3:A:614:ILE:HD13	2.48	0.48
1:D:406:THR:OG1	1:D:407:ASP:OD1	2.23	0.48
1:F:412:LYS:HB3	1:F:419:VAL:HG21	1.95	0.48
1:F:536:LEU:HD13	1:F:544:ILE:HG21	1.95	0.48
4:C:125:ASP:HB3	4:C:142:ILE:HG13	1.96	0.48
3:A:883:ARG:HH12	3:A:965:ARG:CG	2.25	0.48
3:A:933:ILE:HG21	3:A:964:GLN:HE21	1.78	0.48
1:E:25:GLN:OE1	1:E:25:GLN:N	2.45	0.48
1:E:343:GLU:HG2	1:E:343:GLU:O	2.14	0.48
3:A:854:LEU:N	3:A:854:LEU:HD13	2.29	0.48
3:A:895:MET:C	3:A:896:HIS:ND1	2.71	0.48
1:D:300:ASN:HD21	2:T:14:DA:H1'	1.79	0.47
1:D:342:THR:HG22	1:D:346:ASP:O	2.14	0.47
1:D:512:THR:HA	1:D:515:LEU:HD12	1.96	0.47
1:D:407:ASP:OD2	1:D:549:LEU:HD13	2.14	0.47
1:D:614:ASP:OD1	1:D:614:ASP:N	2.47	0.47
1:I:585:ARG:HG3	1:I:591:LYS:O	2.13	0.47
1:D:629:HIS:HB3	1:D:648:VAL:HG13	1.94	0.47
1:E:614:ASP:N	1:E:614:ASP:OD1	2.48	0.47
3:A:876:LEU:HG	3:A:972:PHE:CD2	2.49	0.47
5:B:19:TRP:HB3	5:B:23:MET:HE3	1.96	0.47
1:E:89:PHE:HD1	1:E:166:THR:HB	1.79	0.47
1:H:353:ASN:HD21	1:H:430:GLY:H	1.60	0.47
3:A:959:LYS:C	3:A:961:GLY:N	2.67	0.47
1:I:475:ASN:HD22	1:I:479:ARG:HD3	1.79	0.47
1:H:614:ASP:OD1	1:H:614:ASP:N	2.48	0.47
3:A:137:ASN:C	3:A:139:CYS:H	2.23	0.47
1:D:351:ILE:HD11	1:D:363:LEU:CD1	2.44	0.47
1:I:350:TRP:CZ2	1:I:353:ASN:HA	2.50	0.47
1:I:625:ARG:NH1	1:I:692:GLU:OE2	2.47	0.47
4:C:322:LYS:HE3	4:C:359:GLU:HB3	1.95	0.47
5:B:124:SER:HB3	5:B:137:TRP:HE1	1.79	0.47
1:G:512:THR:HA	1:G:515:LEU:HD12	1.96	0.47
1:D:36:LYS:CG	1:D:37:CYS:N	2.76	0.47
1:D:339:VAL:HG23	1:D:367:LEU:CD2	2.45	0.47
3:A:51:SER:HB3	3:A:52:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:20:LEU:O	4:C:21:ARG:C	2.58	0.47
1:I:504:GLU:O	1:I:509:LYS:NZ	2.47	0.47
2:T:25:DT:H2''	2:T:26:DT:H71	1.96	0.47
3:A:782:VAL:HG12	3:A:782:VAL:O	2.14	0.47
1:D:71:VAL:CG1	1:D:73:LEU:CD1	2.93	0.47
1:D:357:PHE:O	1:D:358:ASN:C	2.57	0.47
1:D:543:PHE:HB2	1:D:547:MET:HE2	1.97	0.47
1:E:144:MET:HE3	1:E:144:MET:HA	1.96	0.47
1:E:512:THR:HA	1:E:515:LEU:HD12	1.96	0.47
1:F:568:LYS:C	1:F:570:ARG:NH2	2.73	0.47
1:F:622:ALA:HB2	1:F:688:PRO:CA	2.45	0.47
3:A:11:SER:HB3	3:A:17:PHE:H	1.79	0.47
3:A:486:TYR:CD1	3:A:501:VAL:HG13	2.40	0.47
4:C:214:LYS:O	4:C:267:LYS:HG3	2.15	0.47
3:A:720:ASN:OD1	3:A:721:PRO:CD	2.62	0.46
3:A:800:MET:SD	3:A:806:TYR:HB3	2.55	0.46
1:G:614:ASP:N	1:G:614:ASP:OD1	2.47	0.46
1:D:374:GLN:C	1:D:375:LEU:HD12	2.40	0.46
1:F:358:ASN:ND2	1:F:360:GLU:OE2	2.45	0.46
1:H:402:ASP:OD1	1:H:402:ASP:N	2.38	0.46
6:S:4:DT:H2''	6:S:5:DT:O5'	2.15	0.46
1:H:478:ASN:HD21	1:H:625:ARG:H	1.64	0.46
1:E:478:ASN:HD21	1:E:625:ARG:H	1.64	0.46
1:H:471:LEU:HD23	1:H:471:LEU:H	1.80	0.46
3:A:333:SER:HA	3:A:336:GLN:HE21	1.79	0.46
1:G:393:GLU:OE2	1:G:397:ARG:NH1	2.37	0.46
1:G:411:ASP:O	1:G:412:LYS:HD3	2.15	0.46
1:G:456:PRO:HA	1:G:459:GLU:OE1	2.15	0.46
1:D:81:ASP:HA	1:D:84:THR:HG22	1.98	0.46
1:H:407:ASP:HB2	1:H:595:ARG:NH1	2.31	0.46
1:D:585:ARG:NH1	1:E:542:PRO:HB3	2.27	0.46
1:I:358:ASN:OD1	1:I:359:SER:N	2.48	0.46
1:D:461:LEU:HD13	1:D:664:TYR:HB3	1.98	0.46
1:H:339:VAL:O	1:H:340:LEU:HD23	2.15	0.46
3:A:411:TRP:HE1	3:A:416:LYS:CD	2.27	0.46
3:A:492:MET:HE3	3:A:496:TYR:CE2	2.50	0.46
5:B:4:VAL:HG12	5:B:5:THR:N	2.31	0.46
1:G:439:THR:HG22	1:G:440:VAL:HG13	1.97	0.46
1:F:547:MET:C	1:F:550:LYS:HG2	2.41	0.46
1:H:512:THR:CA	1:H:515:LEU:HB2	2.44	0.46
4:C:239:THR:OG1	4:C:243:LYS:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ASP:HB3	1:E:170:ASP:OD1	2.16	0.45
1:E:571:SER:H	1:E:612:ARG:NH1	2.15	0.45
4:C:154:LEU:HD11	4:C:158:TYR:CZ	2.51	0.45
1:D:571:SER:H	1:D:612:ARG:NH1	2.14	0.45
1:I:348:ILE:HG22	1:I:357:PHE:HB3	1.96	0.45
1:G:571:SER:H	1:G:612:ARG:NH1	2.14	0.45
1:D:147:LEU:HD23	1:D:147:LEU:HA	1.86	0.45
1:D:334:LEU:HD13	1:D:396:ILE:HD11	1.98	0.45
1:D:478:ASN:HD21	1:D:625:ARG:H	1.63	0.45
1:F:352:ASN:HB2	1:F:356:LYS:HZ1	1.82	0.45
3:A:583:ASN:O	3:A:587:LEU:HD23	2.17	0.45
3:A:801:GLN:HB3	3:A:805:LYS:HB3	1.99	0.45
1:E:570:ARG:HB2	1:E:573:ASN:ND2	2.32	0.45
1:F:504:GLU:O	1:F:509:LYS:NZ	2.46	0.45
1:H:342:THR:HG22	1:H:346:ASP:H	1.80	0.45
4:C:417:VAL:HA	4:C:420:VAL:HG12	1.98	0.45
1:G:478:ASN:HD21	1:G:625:ARG:H	1.64	0.45
1:G:627:ARG:HH21	1:G:644:ALA:C	2.25	0.45
1:D:54:GLU:HB2	1:D:182:VAL:HG22	1.98	0.45
1:D:570:ARG:HB2	1:D:573:ASN:ND2	2.32	0.45
1:F:483:GLU:HB3	1:F:679:TYR:HE1	1.82	0.45
1:H:571:SER:H	1:H:612:ARG:NH1	2.14	0.45
2:T:-2:DT:OP2	5:B:160:LYS:HB2	2.17	0.45
3:A:513:THR:HG22	3:A:625:ARG:HH12	1.77	0.45
5:B:22:VAL:HG23	5:B:143:LEU:HG	1.98	0.45
3:A:590:LYS:HD3	3:A:591:TYR:CZ	2.51	0.45
3:A:733:VAL:HG11	3:A:781:ARG:HG3	1.98	0.45
4:C:107:PRO:HG2	4:C:110:ILE:HB	1.98	0.45
1:D:460:GLU:CD	1:D:663:ARG:HH21	2.25	0.45
1:D:585:ARG:HH12	1:E:542:PRO:CB	2.27	0.45
1:F:428:TYR:HB3	1:F:432:ASP:HB2	1.99	0.45
3:A:909:TYR:O	3:A:910:LEU:C	2.59	0.45
1:E:461:LEU:HD13	1:E:664:TYR:HB3	1.98	0.45
4:C:78:PHE:HE2	4:C:184:MET:HE3	1.81	0.45
4:C:300:ASP:OD1	4:C:300:ASP:N	2.47	0.45
1:G:570:ARG:HB2	1:G:573:ASN:ND2	2.32	0.45
3:A:427:ASP:O	3:A:429:TYR:CD2	2.70	0.45
4:C:255:ARG:HH12	4:C:277:ASP:HB2	1.82	0.45
1:G:333:ILE:O	1:G:336:THR:HG22	2.17	0.45
1:E:534:ASP:OD1	1:E:535:VAL:N	2.50	0.44
1:F:553:VAL:HG23	1:F:600:ILE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:569:ILE:HB	1:F:610:PHE:HD1	1.82	0.44
1:H:468:ILE:HG21	1:H:512:THR:HG21	1.99	0.44
1:I:355:TRP:HB2	1:I:438:CYS:O	2.16	0.44
1:I:679:TYR:O	1:I:680:HIS:CD2	2.69	0.44
1:F:358:ASN:HB3	1:F:361:GLU:O	2.18	0.44
1:F:469:GLN:HB3	1:F:479:ARG:HD3	1.99	0.44
1:H:387:ARG:NH2	6:S:-3:DA:OP2	2.50	0.44
3:A:215:GLU:O	3:A:218:ASP:HB2	2.18	0.44
1:G:543:PHE:HB2	1:G:547:MET:HE2	1.98	0.44
1:D:459:GLU:O	1:D:463:ASN:OD1	2.35	0.44
1:D:571:SER:O	1:D:574:ILE:HG13	2.17	0.44
3:A:10:GLU:HB3	3:A:18:LEU:HD12	1.98	0.44
1:H:570:ARG:HB2	1:H:573:ASN:ND2	2.32	0.44
1:D:285:CYS:SG	1:D:314:CYS:SG	3.14	0.44
1:E:422:LEU:HD22	1:E:673:VAL:HG22	1.99	0.44
1:E:447:ASP:C	1:E:449:THR:N	2.75	0.44
1:E:460:GLU:CD	1:E:663:ARG:HH21	2.25	0.44
1:E:543:PHE:HB2	1:E:547:MET:HE2	1.98	0.44
3:A:398:ASP:OD1	3:A:398:ASP:O	2.35	0.44
1:D:294:HIS:CE1	1:D:307:LYS:HB2	2.53	0.44
1:D:534:ASP:OD1	1:D:535:VAL:N	2.50	0.44
1:H:353:ASN:ND2	1:H:430:GLY:H	2.14	0.44
4:C:303:VAL:HG22	4:C:308:PHE:HE1	1.82	0.44
6:S:3:DT:H2''	6:S:4:DT:O4'	2.18	0.44
1:D:138:LEU:C	1:D:140:THR:N	2.76	0.44
1:H:571:SER:O	1:H:574:ILE:HG13	2.17	0.44
1:G:459:GLU:O	1:G:463:ASN:OD1	2.35	0.44
1:E:12:PHE:CG	1:E:57:ARG:HD3	2.53	0.44
1:E:77:LEU:HB3	1:E:81:ASP:HB3	1.99	0.44
1:E:459:GLU:O	1:E:463:ASN:OD1	2.35	0.44
1:E:460:GLU:HB2	1:E:664:TYR:HE2	1.83	0.44
1:F:369:LEU:HD22	1:H:398:ASP:HB3	2.00	0.44
1:F:412:LYS:HB3	1:F:419:VAL:CG2	2.47	0.44
1:F:547:MET:O	1:F:548:HIS:C	2.61	0.44
1:G:324:ASN:OD1	1:G:325:LYS:N	2.48	0.44
1:G:571:SER:O	1:G:574:ILE:HG13	2.17	0.44
1:F:486:LEU:HD12	1:F:486:LEU:HA	1.83	0.44
1:H:428:TYR:HB3	1:H:432:ASP:OD2	2.18	0.44
3:A:502:ILE:HG12	3:A:502:ILE:O	2.17	0.44
3:A:504:GLY:N	3:A:505:PRO:HD2	2.33	0.43
1:G:378:GLU:OE2	1:G:378:GLU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:LYS:HG3	1:D:379:TYR:CE1	2.53	0.43
1:I:366:LYS:O	1:I:370:SER:N	2.33	0.43
1:I:385:CYS:HB3	1:I:388:LYS:HD2	2.00	0.43
1:F:611:ASP:OD1	1:F:612:ARG:N	2.49	0.43
4:C:277:ASP:OD1	4:C:277:ASP:N	2.39	0.43
1:E:571:SER:O	1:E:574:ILE:HG13	2.17	0.43
1:F:607:LYS:HD3	1:F:608:PRO:HD2	2.00	0.43
3:A:753:ASP:OD2	3:A:803:LYS:HE2	2.19	0.43
3:A:774:LEU:HD23	3:A:774:LEU:HA	1.87	0.43
1:E:629:HIS:CD2	1:E:648:VAL:HG13	2.54	0.43
1:F:389:ARG:NH2	1:H:395:ASN:OD1	2.50	0.43
3:A:54:PRO:HB3	3:A:91:ILE:HB	2.00	0.43
1:H:407:ASP:HB2	1:H:595:ARG:HH12	1.82	0.43
1:H:490:LEU:HD11	1:H:672:LEU:HD13	1.99	0.43
3:A:64:ARG:HE	3:A:83:CYS:HB3	1.83	0.43
3:A:143:ASP:O	3:A:145:PRO:HD3	2.19	0.43
3:A:590:LYS:CE	3:A:591:TYR:OH	2.67	0.43
3:A:863:GLN:HA	3:A:866:ILE:HG12	2.00	0.43
4:C:107:PRO:HG3	4:C:136:TRP:NE1	2.34	0.43
1:D:460:GLU:HB2	1:D:664:TYR:HE2	1.83	0.43
1:H:333:ILE:O	1:H:336:THR:HG22	2.18	0.43
1:H:396:ILE:HD13	1:H:396:ILE:HA	1.87	0.43
3:A:209:THR:CG2	3:A:210:GLU:H	2.31	0.43
3:A:578:LEU:HD23	3:A:578:LEU:O	2.19	0.43
4:C:255:ARG:NH1	4:C:277:ASP:HB2	2.33	0.43
1:E:154:LEU:HD12	1:E:154:LEU:HA	1.82	0.43
1:E:333:ILE:O	1:E:336:THR:HG22	2.19	0.43
1:I:606:TYR:OH	1:F:614:ASP:OD2	2.32	0.43
3:A:219:ARG:H	3:A:219:ARG:HG3	1.57	0.43
4:C:30:LYS:HA	4:C:30:LYS:HD3	1.69	0.43
1:D:123:THR:HB	1:D:195:HIS:HB3	1.99	0.43
1:D:344:ARG:HB3	1:D:593:ASN:HD21	1.84	0.43
1:I:390:LYS:HB2	1:I:390:LYS:HE2	1.79	0.43
1:I:607:LYS:HD3	1:I:607:LYS:HA	1.88	0.43
1:H:655:LEU:HA	1:H:658:LYS:HE2	2.01	0.43
3:A:62:LYS:CE	3:A:87:ASP:HB2	2.49	0.43
3:A:546:LEU:HD13	3:A:771:ALA:HB2	2.00	0.43
3:A:928:TYR:HB2	3:A:953:ILE:HD11	2.00	0.43
1:G:629:HIS:CD2	1:G:648:VAL:HG13	2.54	0.43
1:D:354:SER:HB3	1:D:416:LYS:O	2.18	0.43
1:E:78:ASP:O	1:E:79:GLU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:607:LYS:NZ	1:F:693:ILE:HA	2.34	0.43
1:D:550:LYS:HE2	1:D:550:LYS:HB2	1.92	0.43
1:E:678:LYS:HB2	1:E:678:LYS:HE2	1.76	0.43
4:C:90:SER:OG	4:C:91:LYS:N	2.52	0.43
1:G:402:ASP:OD1	1:G:402:ASP:N	2.46	0.43
1:D:558:LEU:HD23	1:D:559:PRO:O	2.19	0.42
1:I:484:LYS:HG3	1:I:680:HIS:CE1	2.53	0.42
4:C:218:MET:HE2	4:C:218:MET:HB3	1.81	0.42
1:D:69:MET:HE2	1:D:89:PHE:HZ	1.84	0.42
1:D:235:LEU:HD23	3:A:870:ARG:HE	1.84	0.42
3:A:486:TYR:CE1	3:A:501:VAL:CG1	3.03	0.42
3:A:631:LEU:HD22	3:A:631:LEU:HA	1.62	0.42
1:D:292:HIS:HB3	1:D:308:THR:O	2.19	0.42
1:E:17:ILE:HG22	1:E:53:PHE:CE2	2.54	0.42
1:F:515:LEU:HD23	1:F:515:LEU:HA	1.86	0.42
1:H:512:THR:O	1:H:515:LEU:HB2	2.18	0.42
4:C:208:GLN:N	4:C:208:GLN:OE1	2.52	0.42
1:D:141:TYR:O	1:D:220:TYR:HA	2.20	0.42
1:E:558:LEU:HD23	1:E:559:PRO:O	2.19	0.42
1:E:658:LYS:HD2	1:E:663:ARG:HD3	2.01	0.42
2:T:24:DA:H2'	2:T:25:DT:H72	2.00	0.42
3:A:486:TYR:CD1	3:A:501:VAL:HG12	2.52	0.42
3:A:789:ILE:HD13	3:A:789:ILE:HA	1.63	0.42
1:D:658:LYS:HD2	1:D:663:ARG:HD3	2.01	0.42
1:I:652:ASP:OD1	1:I:653:GLU:N	2.52	0.42
1:F:557:GLU:OE2	1:H:612:ARG:NE	2.53	0.42
1:F:568:LYS:CA	1:F:570:ARG:HH22	2.32	0.42
3:A:961:GLY:C	3:A:963:ASN:N	2.77	0.42
1:D:89:PHE:CE1	1:D:93:VAL:HG21	2.55	0.42
1:H:558:LEU:HD23	1:H:559:PRO:O	2.19	0.42
4:C:217:PHE:HA	4:C:264:VAL:O	2.19	0.42
4:C:233:PHE:HE2	4:C:301:TYR:HE1	1.68	0.42
1:I:523:LEU:HD22	1:I:551:ARG:HG3	2.01	0.42
1:F:586:PRO:HB2	1:F:589:SER:HB3	2.01	0.42
1:F:618:MET:SD	1:F:696:PHE:HB3	2.60	0.42
1:E:73:LEU:HA	1:E:73:LEU:HD23	1.74	0.42
1:E:146:THR:HG21	1:E:222:SER:HA	2.01	0.42
3:A:453:LEU:HA	3:A:456:ALA:HB3	2.02	0.42
4:C:316:LEU:HD11	4:C:334:LEU:HD11	2.02	0.42
1:D:513:LYS:HG2	1:D:517:LYS:NZ	2.35	0.42
1:F:617:LEU:HG	1:F:621:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:420:VAL:HG22	4:C:424:LEU:HD12	2.00	0.42
5:B:91:GLU:HG2	5:B:189:PHE:HD2	1.85	0.42
1:G:520:ILE:HD11	1:G:524:PHE:HD2	1.85	0.42
1:E:475:ASN:HD21	1:E:478:ASN:HD22	1.68	0.42
1:E:513:LYS:HG2	1:E:517:LYS:NZ	2.35	0.42
1:I:535:VAL:HB	1:I:538:LYS:HE3	2.02	0.42
1:F:547:MET:O	1:F:550:LYS:HG2	2.20	0.42
3:A:203:ILE:HB	3:A:238:LEU:HG	2.02	0.42
1:D:69:MET:SD	1:D:93:VAL:HG11	2.60	0.41
1:D:520:ILE:HD11	1:D:524:PHE:HD2	1.85	0.41
3:A:848:THR:OG1	3:A:849:ARG:N	2.52	0.41
3:A:938:VAL:O	3:A:965:ARG:NH2	2.53	0.41
4:C:386:ASN:OD1	4:C:387:PHE:N	2.52	0.41
1:G:483:GLU:HG2	1:G:675:TRP:CD2	2.55	0.41
1:H:420:LEU:HD22	1:H:446:PHE:CE1	2.55	0.41
1:H:550:LYS:HE2	1:H:550:LYS:HB2	1.92	0.41
1:D:42:ARG:O	1:D:43:TYR:C	2.63	0.41
1:D:395:ASN:OD1	1:E:389:ARG:NH2	2.53	0.41
1:D:475:ASN:HD21	1:D:478:ASN:HD22	1.68	0.41
1:E:49:GLU:OE2	1:E:49:GLU:N	2.48	0.41
1:E:53:PHE:CE1	1:E:181:ARG:HB2	2.55	0.41
1:I:389:ARG:NH2	1:F:395:ASN:OD1	2.54	0.41
1:D:42:ARG:O	1:D:45:ASP:N	2.52	0.41
1:D:483:GLU:HG2	1:D:675:TRP:CD2	2.55	0.41
1:I:505:THR:HB	1:F:616:ALA:HB2	2.02	0.41
3:A:638:LYS:HB2	3:A:638:LYS:HE2	1.66	0.41
1:E:535:VAL:HG22	1:E:537:ASP:H	1.86	0.41
1:I:556:SER:C	1:I:557:GLU:HG3	2.46	0.41
1:F:586:PRO:HD3	1:F:592:ILE:HA	2.02	0.41
3:A:207:MET:HB3	3:A:207:MET:HE2	1.87	0.41
3:A:850:LEU:HD12	3:A:850:LEU:HA	1.91	0.41
4:C:293:ILE:O	4:C:297:ILE:HG12	2.20	0.41
1:G:465:ILE:HD13	1:G:465:ILE:HA	1.92	0.41
1:G:532:LEU:HA	1:G:573:ASN:HD22	1.85	0.41
1:I:500:PHE:HE2	1:I:621:ILE:HD12	1.85	0.41
1:I:585:ARG:NH1	1:I:588:PHE:H	2.18	0.41
1:F:334:LEU:HD12	1:F:334:LEU:HA	1.88	0.41
1:D:558:LEU:HD22	1:D:604:THR:OG1	2.21	0.41
1:I:367:LEU:HA	1:I:370:SER:HB3	2.03	0.41
1:G:513:LYS:HG2	1:G:517:LYS:NZ	2.35	0.41
1:H:364:ILE:O	1:H:368:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:7:DT:H6	2:T:7:DT:H2'	1.71	0.41
3:A:384:THR:O	3:A:388:VAL:HG23	2.21	0.41
3:A:737:LEU:HD12	3:A:737:LEU:HA	1.85	0.41
1:D:254:PHE:O	1:D:255:ILE:HB	2.21	0.41
1:D:611:ASP:OD2	1:D:612:ARG:NH1	2.54	0.41
1:E:483:GLU:HG2	1:E:675:TRP:CD2	2.55	0.41
1:E:520:ILE:HD11	1:E:524:PHE:HD2	1.85	0.41
1:I:382:GLU:OE1	1:I:382:GLU:O	2.39	0.41
1:I:461:LEU:HD13	1:I:664:TYR:HB3	2.03	0.41
1:I:471:LEU:O	1:I:471:LEU:HD12	2.21	0.41
1:F:486:LEU:HD21	1:F:668:PHE:HZ	1.85	0.41
3:A:355:SER:HB2	3:A:430:LYS:HE3	2.03	0.41
3:A:479:THR:O	3:A:479:THR:HG22	2.21	0.41
3:A:783:LEU:HB3	3:A:787:PHE:O	2.21	0.41
3:A:896:HIS:CD2	3:A:897:HIS:H	2.38	0.41
1:G:475:ASN:HD21	1:G:478:ASN:HD22	1.68	0.41
1:D:302:ALA:HA	1:D:321:LEU:HB2	2.03	0.41
1:D:535:VAL:HG22	1:D:537:ASP:H	1.86	0.41
1:F:661:ASN:OD1	1:F:661:ASN:N	2.42	0.41
1:H:475:ASN:HD21	1:H:478:ASN:HD22	1.68	0.41
3:A:346:LEU:HD12	3:A:346:LEU:HA	1.69	0.41
3:A:395:VAL:CG2	3:A:433:PHE:CE1	3.02	0.41
4:C:44:LYS:HG3	5:B:173:PRO:HB2	2.01	0.41
1:G:334:LEU:HD12	1:G:334:LEU:HA	1.86	0.41
1:G:418:GLY:C	1:G:427:PHE:CE1	2.99	0.41
1:D:16:THR:HG21	1:D:31:PHE:HD2	1.86	0.40
1:D:240:PHE:HZ	1:D:332:ARG:HG3	1.86	0.40
1:I:445:LYS:HE2	1:I:445:LYS:HB3	1.81	0.40
3:A:795:TYR:HB3	3:A:798:LEU:HB2	2.02	0.40
1:D:53:PHE:CE1	1:D:181:ARG:HG2	2.56	0.40
1:D:538:LYS:O	1:D:538:LYS:HG3	2.21	0.40
1:H:611:ASP:OD2	1:H:612:ARG:NH1	2.54	0.40
3:A:110:ILE:O	3:A:113:PHE:HB3	2.21	0.40
1:D:364:ILE:O	1:D:365:THR:C	2.64	0.40
1:D:529:GLN:H	1:D:529:GLN:CD	2.27	0.40
1:E:611:ASP:OD2	1:E:612:ARG:NH1	2.54	0.40
1:F:360:GLU:H	1:F:360:GLU:HG3	1.71	0.40
1:H:421:ASP:OD2	1:H:428:TYR:OH	2.34	0.40
1:H:558:LEU:HD22	1:H:604:THR:OG1	2.21	0.40
3:A:340:LYS:O	3:A:341:LEU:HD23	2.21	0.40
1:G:419:VAL:N	1:G:427:PHE:CE1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:558:LEU:HD22	1:G:604:THR:OG1	2.21	0.40
1:G:611:ASP:OD2	1:G:612:ARG:NH1	2.54	0.40
1:D:40:LEU:O	1:D:44:ILE:HG12	2.22	0.40
1:D:71:VAL:CG1	1:D:73:LEU:HD12	2.52	0.40
1:E:558:LEU:HD22	1:E:604:THR:OG1	2.21	0.40
1:H:678:LYS:HE2	1:H:678:LYS:HB2	1.76	0.40
3:A:711:MET:HE2	3:A:711:MET:HB2	1.98	0.40
4:C:293:ILE:HG13	4:C:294:ILE:N	2.37	0.40
4:C:321:ASN:OD1	4:C:322:LYS:N	2.54	0.40
1:G:355:TRP:HB2	1:G:438:CYS:O	2.20	0.40
1:D:165:LEU:C	1:D:167:ARG:H	2.29	0.40
1:F:487:SER:HB3	1:F:675:TRP:HB3	2.04	0.40
3:A:544:ASN:O	3:A:759:ILE:HG22	2.21	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	D	666/785 (85%)	609 (91%)	56 (8%)	1 (0%)	43	78
1	E	552/785 (70%)	531 (96%)	21 (4%)	0	100	100
1	F	345/785 (44%)	324 (94%)	20 (6%)	1 (0%)	36	72
1	G	343/785 (44%)	324 (94%)	18 (5%)	1 (0%)	36	72
1	H	314/785 (40%)	305 (97%)	9 (3%)	0	100	100
1	I	345/785 (44%)	326 (94%)	19 (6%)	0	100	100
3	A	973/1006 (97%)	889 (91%)	82 (8%)	2 (0%)	43	78
4	C	371/426 (87%)	357 (96%)	14 (4%)	0	100	100
5	B	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
All	All	4125/6360 (65%)	3871 (94%)	249 (6%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	786	ASN
1	G	410	PRO
1	F	682	PRO
1	D	410	PRO
3	A	594	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	D	624/725 (86%)	612 (98%)	12 (2%)	50	67
1	E	522/725 (72%)	517 (99%)	5 (1%)	68	78
1	F	324/725 (45%)	315 (97%)	9 (3%)	38	60
1	G	322/725 (44%)	320 (99%)	2 (1%)	78	83
1	H	298/725 (41%)	298 (100%)	0	100	100
1	I	324/725 (45%)	319 (98%)	5 (2%)	57	72
3	A	910/929 (98%)	844 (93%)	66 (7%)	13	34
4	C	358/396 (90%)	355 (99%)	3 (1%)	73	80
5	B	200/200 (100%)	200 (100%)	0	100	100
All	All	3882/5875 (66%)	3780 (97%)	102 (3%)	41	62

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	91	ILE
1	D	122	LEU
1	D	135	ILE
1	D	198	GLN
1	D	224	GLN
1	D	231	VAL
1	D	235	LEU
1	D	297	SER

Continued on next page...

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Mol	Chain	Res	Type
1	D	319	VAL
1	D	321	LEU
1	D	411	ASP
1	D	453	GLU
1	E	73	LEU
1	E	82	TYR
1	E	377	LYS
1	E	440	VAL
1	E	457	GLU
1	I	363	LEU
1	I	536	LEU
1	I	592	ILE
1	I	679	TYR
1	I	686	LEU
1	F	363	LEU
1	F	413	LEU
1	F	420	LEU
1	F	485	THR
1	F	490	LEU
1	F	536	LEU
1	F	585	ARG
1	F	677	LYS
1	F	686	LEU
3	A	30	VAL
3	A	36	HIS
3	A	122	ASP
3	A	165	LEU
3	A	201	THR
3	A	205	GLU
3	A	221	CYS
3	A	321	ASN
3	A	322	ASN
3	A	334	PHE
3	A	335	ILE
3	A	361	LEU
3	A	365	VAL
3	A	369	THR
3	A	413	ASN
3	A	493	VAL
3	A	588	LEU
3	A	601	CYS
3	A	605	LEU

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Mol	Chain	Res	Type
3	A	617	ARG
3	A	625	ARG
3	A	626	LEU
3	A	631	LEU
3	A	636	ARG
3	A	638	LYS
3	A	639	LYS
3	A	641	LEU
3	A	643	GLN
3	A	650	LYS
3	A	657	GLN
3	A	670	LEU
3	A	671	MET
3	A	680	SER
3	A	683	SER
3	A	685	LYS
3	A	688	THR
3	A	690	ILE
3	A	692	ARG
3	A	693	ARG
3	A	694	MET
3	A	695	ILE
3	A	696	LEU
3	A	698	LEU
3	A	701	VAL
3	A	734	LYS
3	A	737	LEU
3	A	742	ARG
3	A	755	VAL
3	A	762	GLN
3	A	763	ASP
3	A	765	ASP
3	A	769	GLU
3	A	770	ILE
3	A	775	GLU
3	A	776	ARG
3	A	786	ASN
3	A	788	LYS
3	A	789	ILE
3	A	796	LYS
3	A	805	LYS
3	A	854	LEU

Continued on next page...

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Mol	Chain	Res	Type
3	A	942	LYS
3	A	953	ILE
3	A	975	LEU
3	A	979	ILE
3	A	984	ASP
4	C	36	GLU
4	C	59	ASP
4	C	106	ILE
1	G	423	VAL
1	G	442	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	8	ASN
1	D	46	ASN
1	D	95	ASN
1	D	134	HIS
1	D	163	ASN
1	D	198	GLN
1	D	201	HIS
1	D	224	GLN
1	D	300	ASN
1	D	324	ASN
1	D	478	ASN
1	D	546	ASN
1	E	8	ASN
1	E	134	HIS
1	E	163	ASN
1	E	201	HIS
1	E	328	ASN
1	E	373	HIS
1	E	478	ASN
1	E	548	HIS
1	E	594	ASN
1	E	629	HIS
1	I	478	ASN
1	I	548	HIS
1	I	661	ASN
1	I	662	ASN
1	I	680	HIS
1	F	541	ASN

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Mol	Chain	Res	Type
1	F	573	ASN
1	H	469	GLN
1	H	478	ASN
3	A	48	GLN
3	A	170	HIS
3	A	181	ASN
3	A	185	HIS
3	A	204	ASN
3	A	225	GLN
3	A	303	ASN
3	A	323	ASN
3	A	336	GLN
3	A	352	ASN
3	A	413	ASN
3	A	538	GLN
3	A	543	ASN
3	A	583	ASN
3	A	584	ASN
3	A	589	GLN
3	A	607	ASN
3	A	657	GLN
3	A	703	ASN
3	A	709	ASN
3	A	762	GLN
3	A	801	GLN
3	A	841	ASN
3	A	897	HIS
3	A	899	ASN
3	A	937	ASN
3	A	964	GLN
3	A	994	GLN
4	C	48	GLN
4	C	115	ASN
4	C	318	GLN
1	G	478	ASN
1	G	529	GLN
1	G	573	ASN
1	G	629	HIS
1	G	661	ASN
1	G	662	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	1:DT	O3'	6:DT	P	27.58

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75504. These allow visual inspection of the internal detail of the map and identification of artifacts.

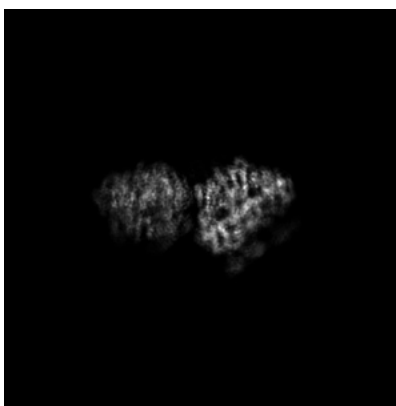
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

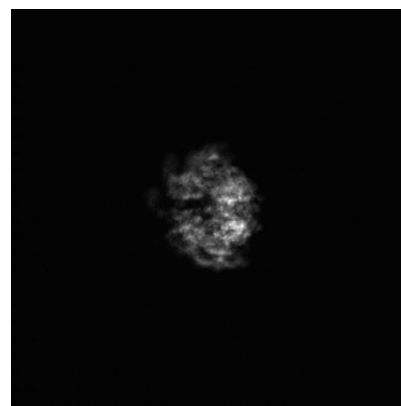
6.1.1 Primary map



X

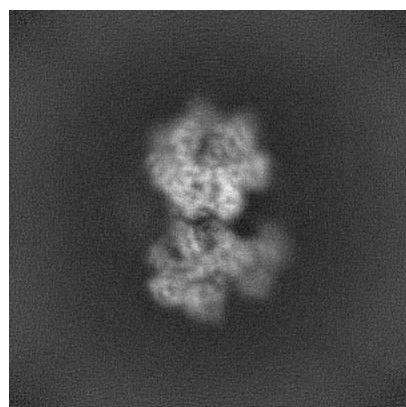


Y

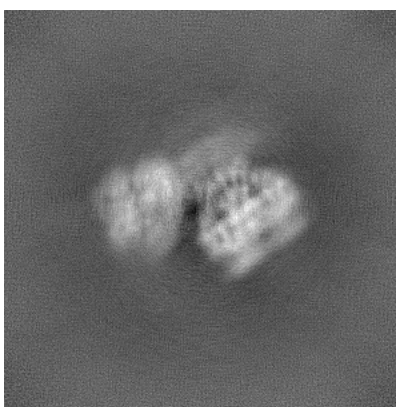


Z

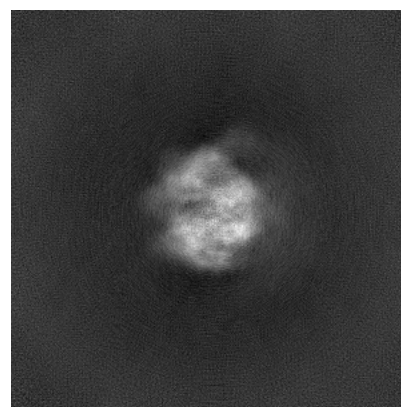
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

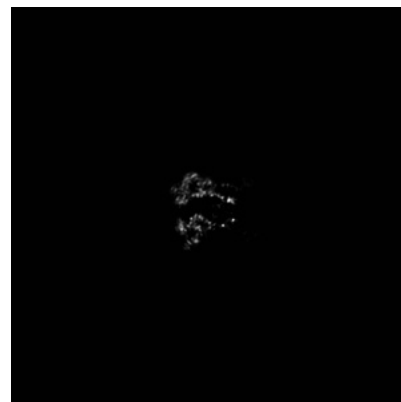
6.2.1 Primary map



X Index: 256

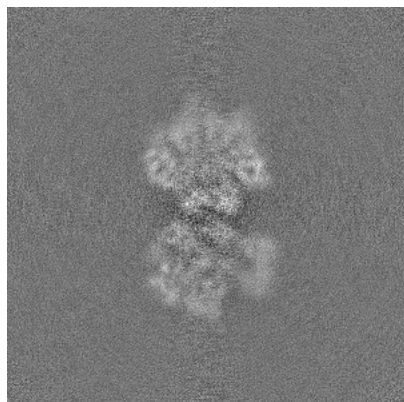


Y Index: 256

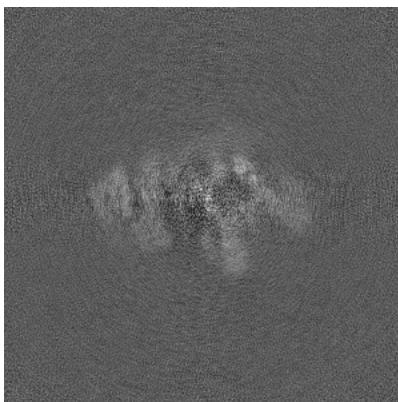


Z Index: 256

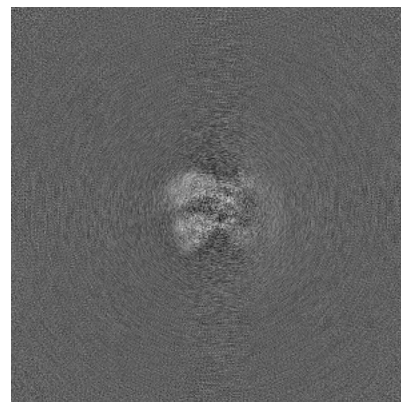
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

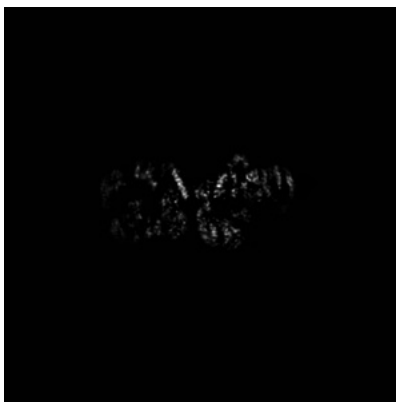
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

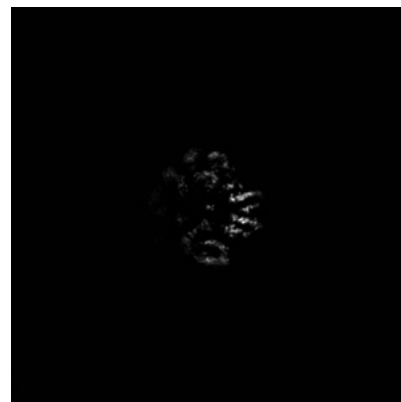
6.3.1 Primary map



X Index: 275

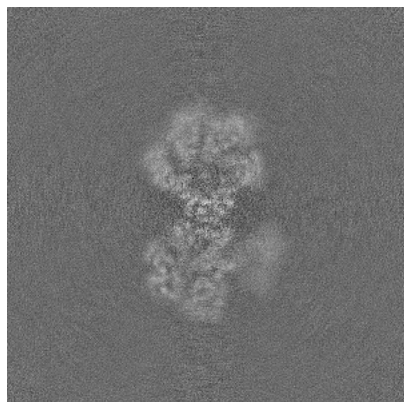


Y Index: 232

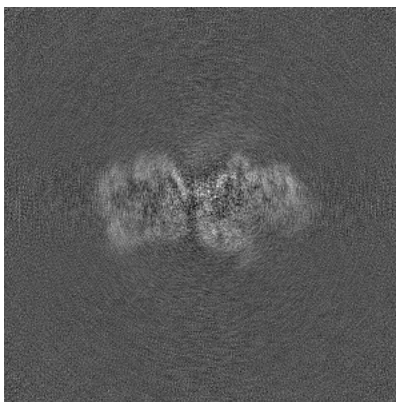


Z Index: 307

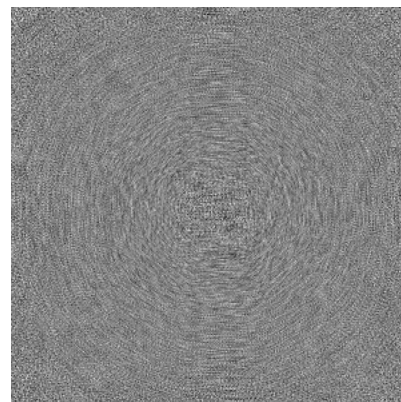
6.3.2 Raw map



X Index: 269



Y Index: 233

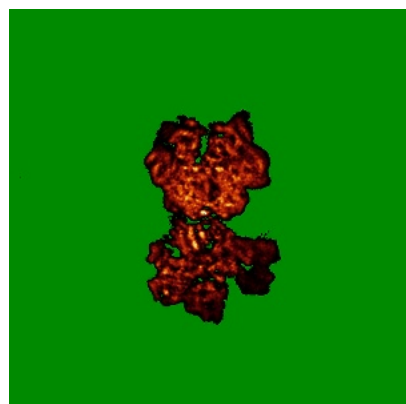


Z Index: 0

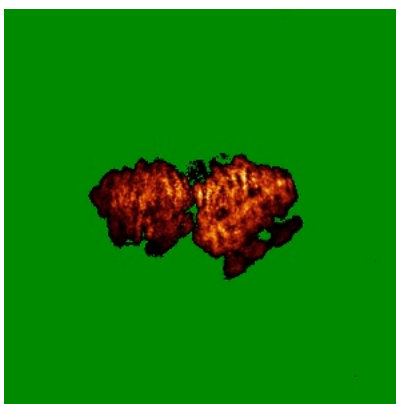
The images above show the largest variance slices of the map in three orthogonal directions.

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

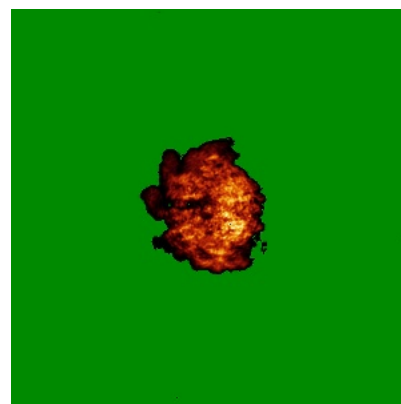
6.4.1 Primary map



X

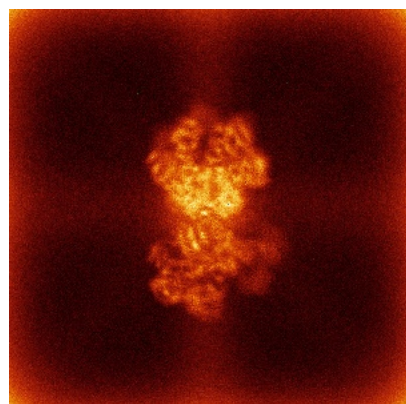


Y

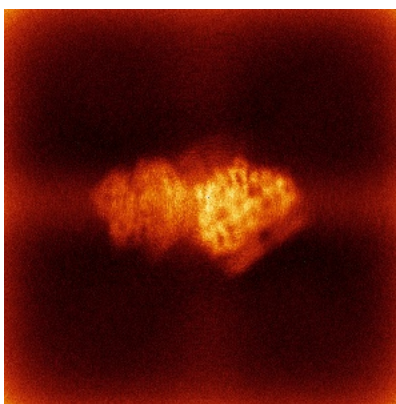


Z

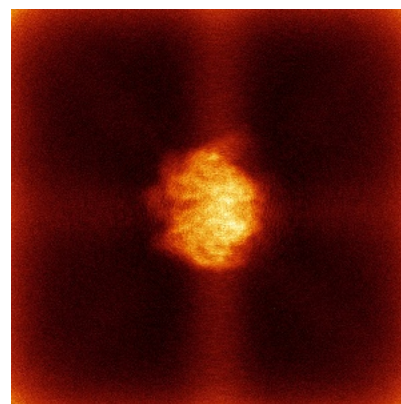
6.4.2 Raw map



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](#)

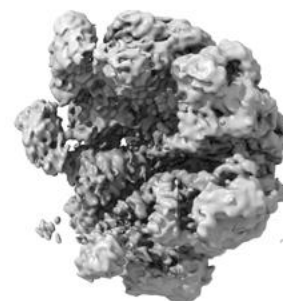
6.5.1 Primary map



X



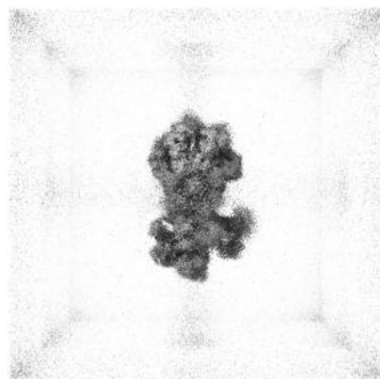
Y



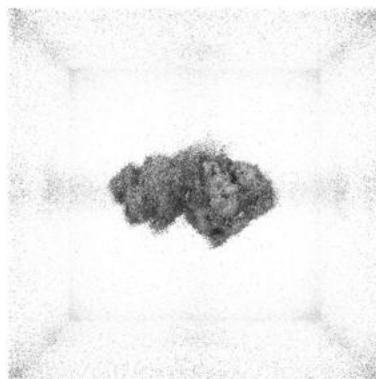
Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

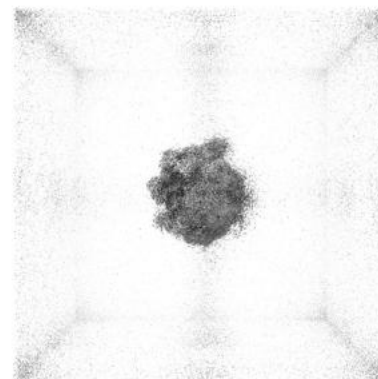
6.5.2 Raw map



X



Y



Z

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.

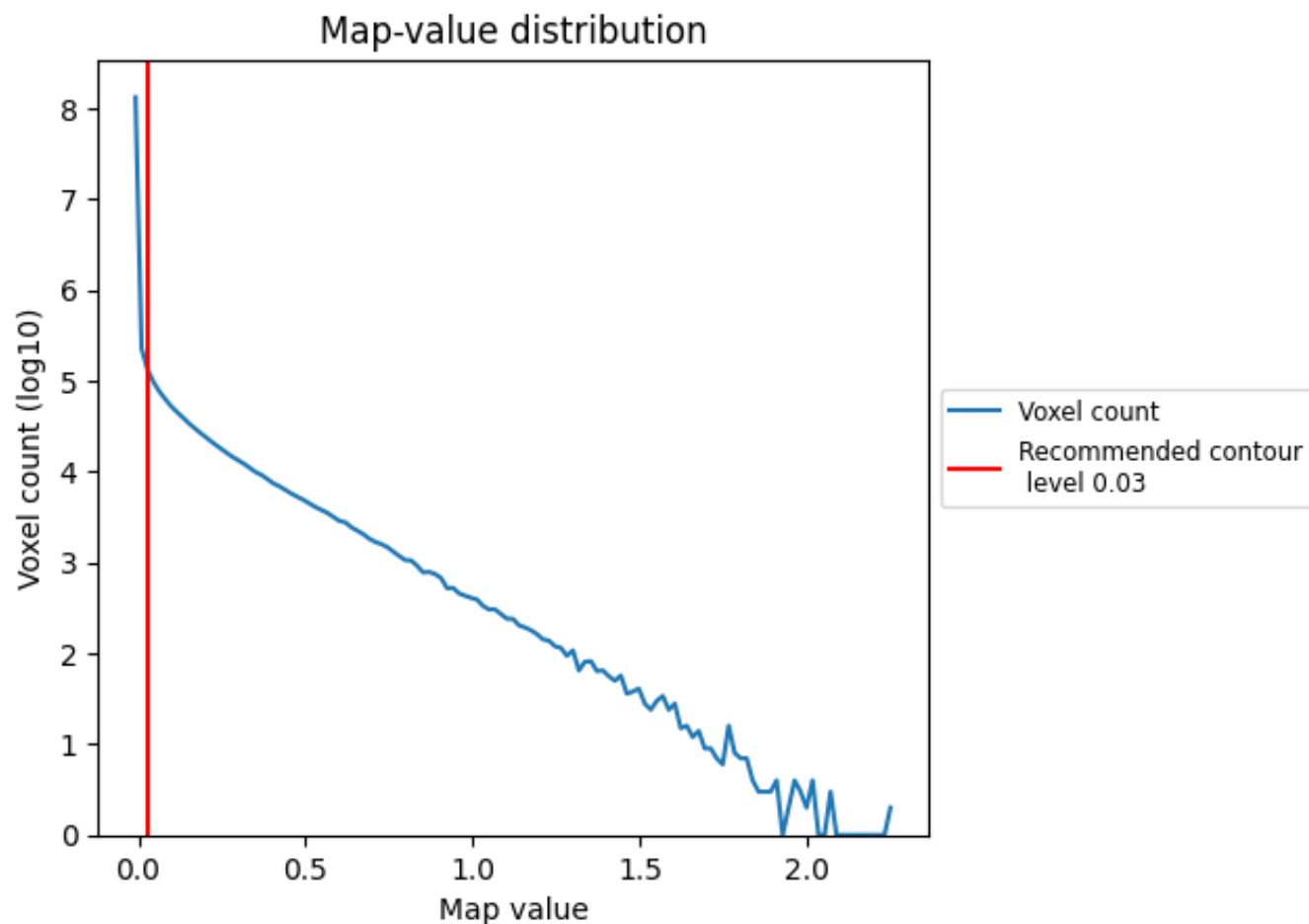
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

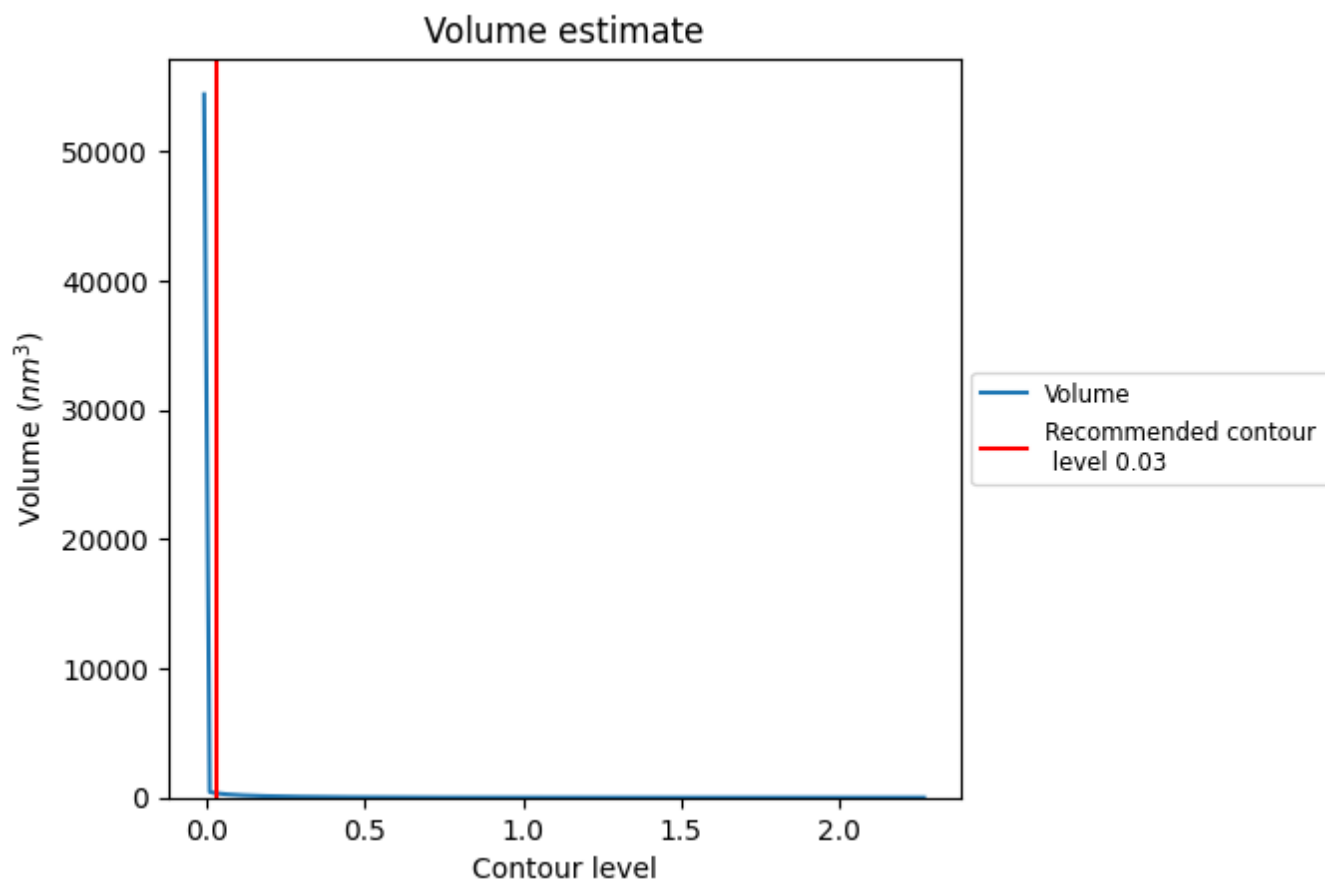
This section contains the results of statistical analysis of the map.

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.

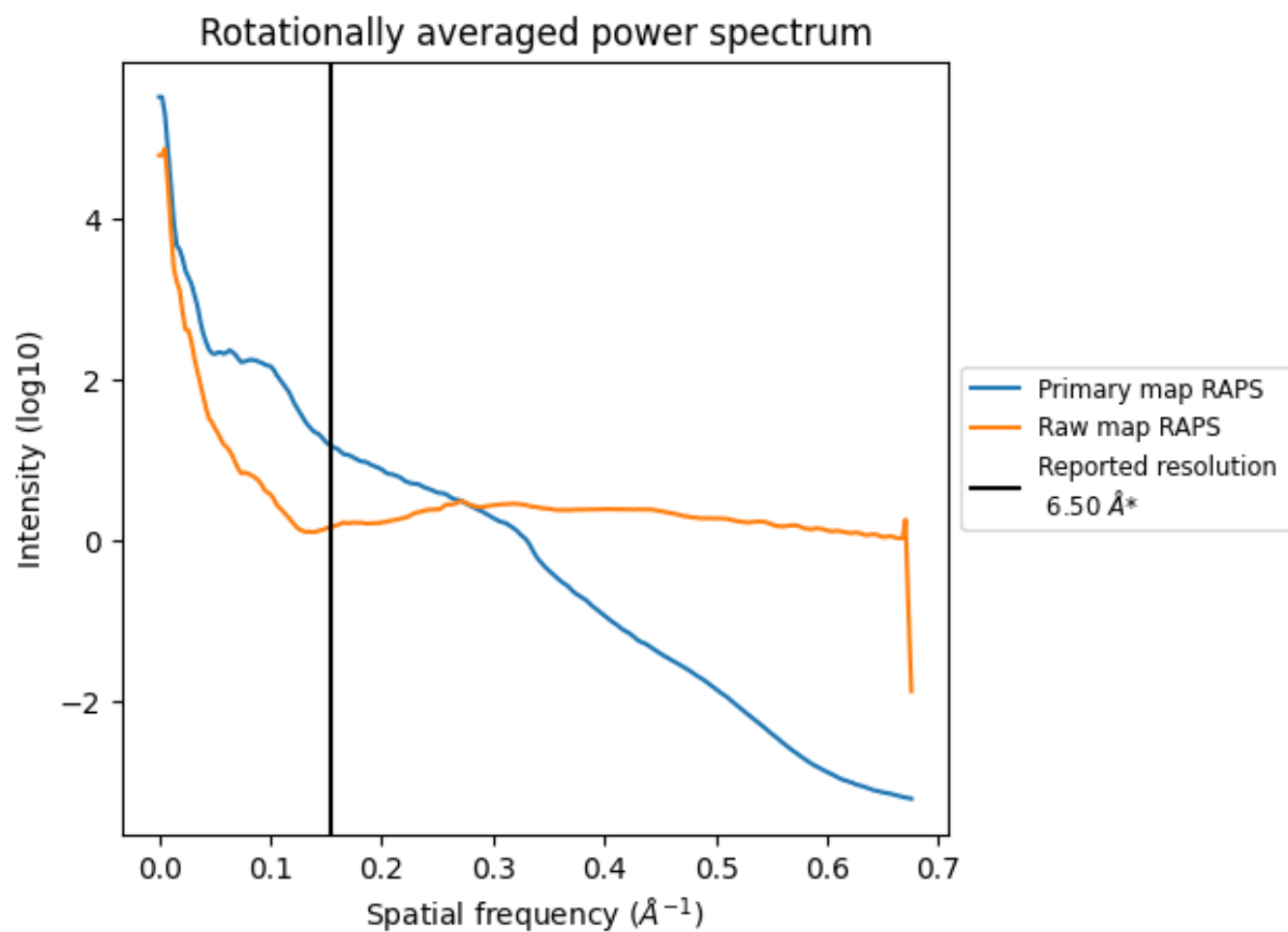
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 335 nm³; this corresponds to an approximate mass of 303 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 ⓘ

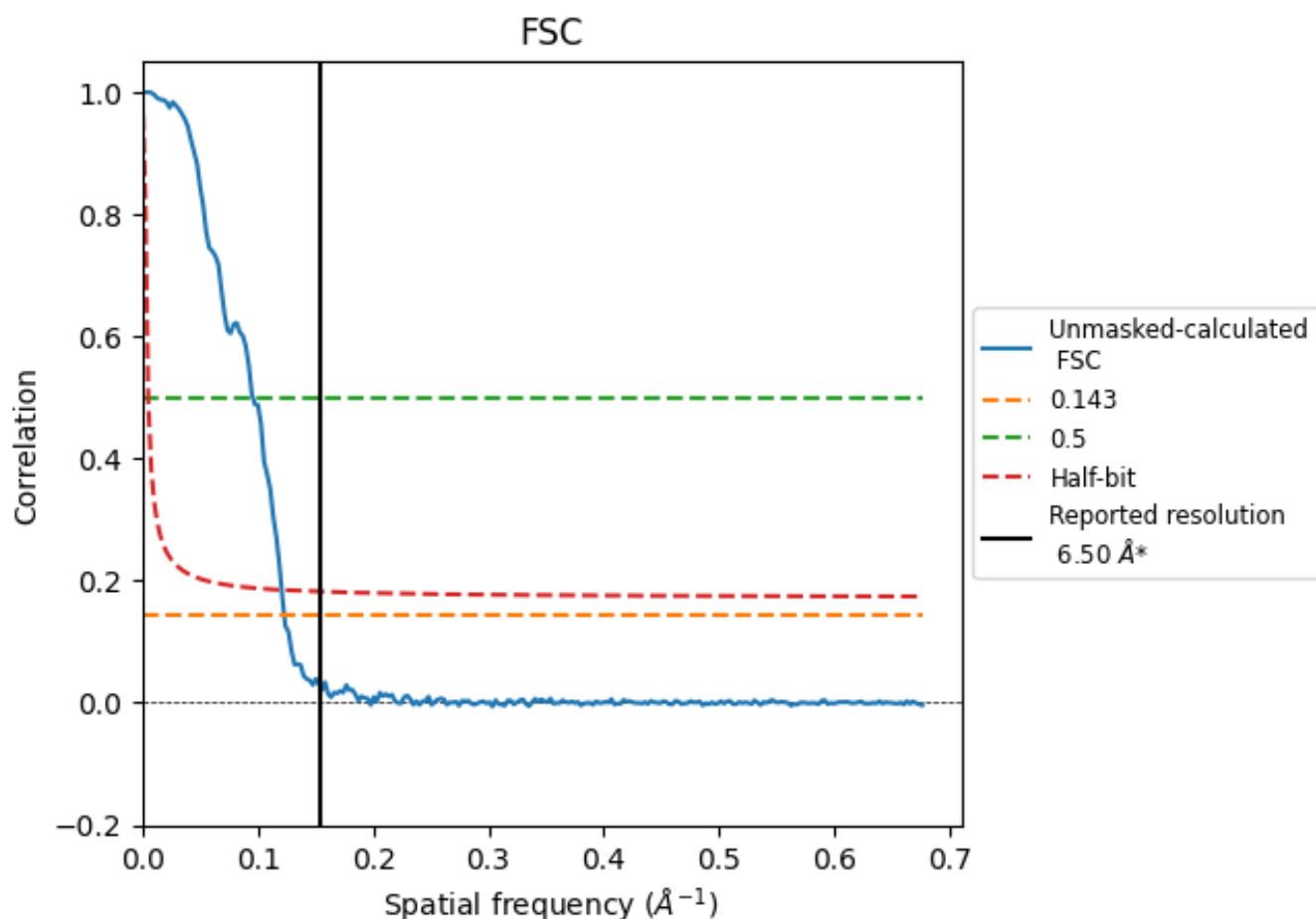


*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

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 0.154 Å⁻¹

8.2 Resolution estimates [i](#)

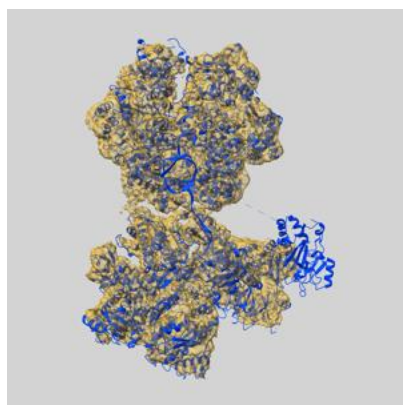
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.12	10.45	8.28

*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 8.12 differs from the reported value 6.5 by more than 10 %

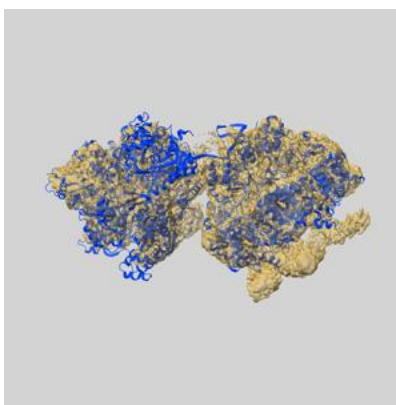
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75504 and PDB model 10WP. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

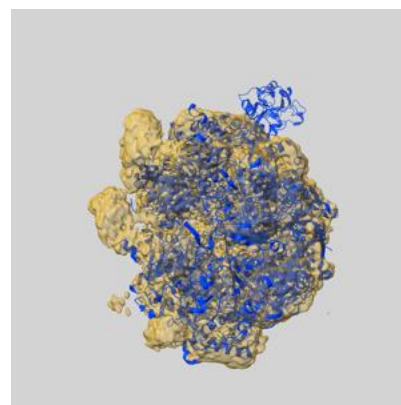
9.1 Map-model overlay [i](#)



X



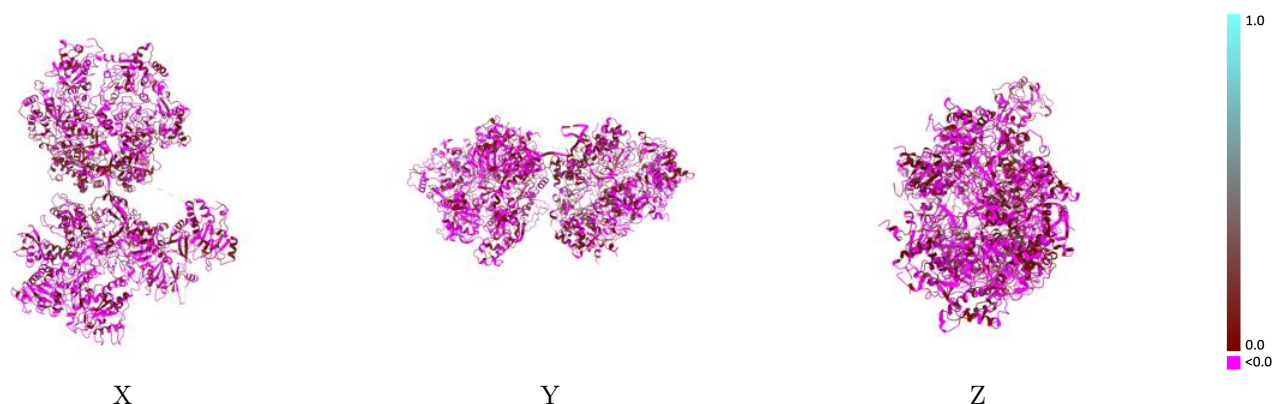
Y



Z

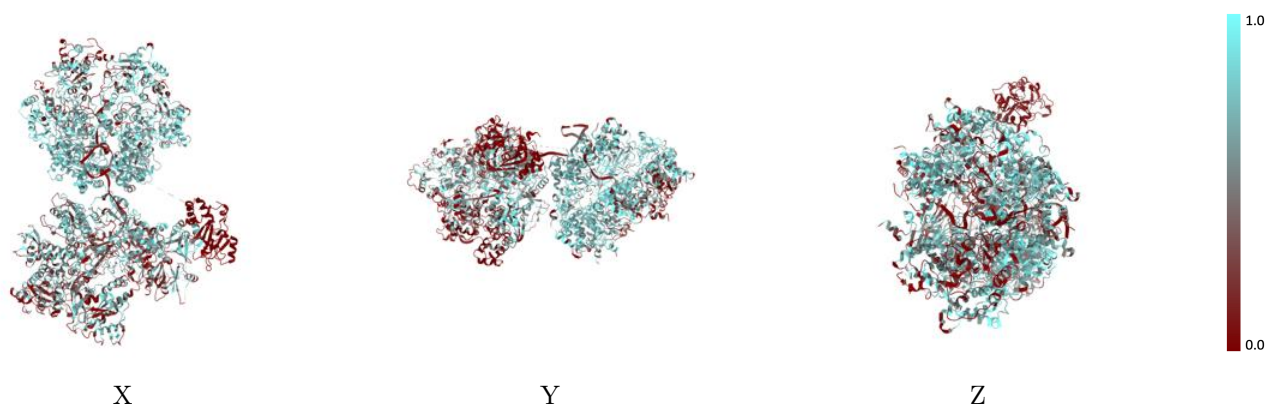
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



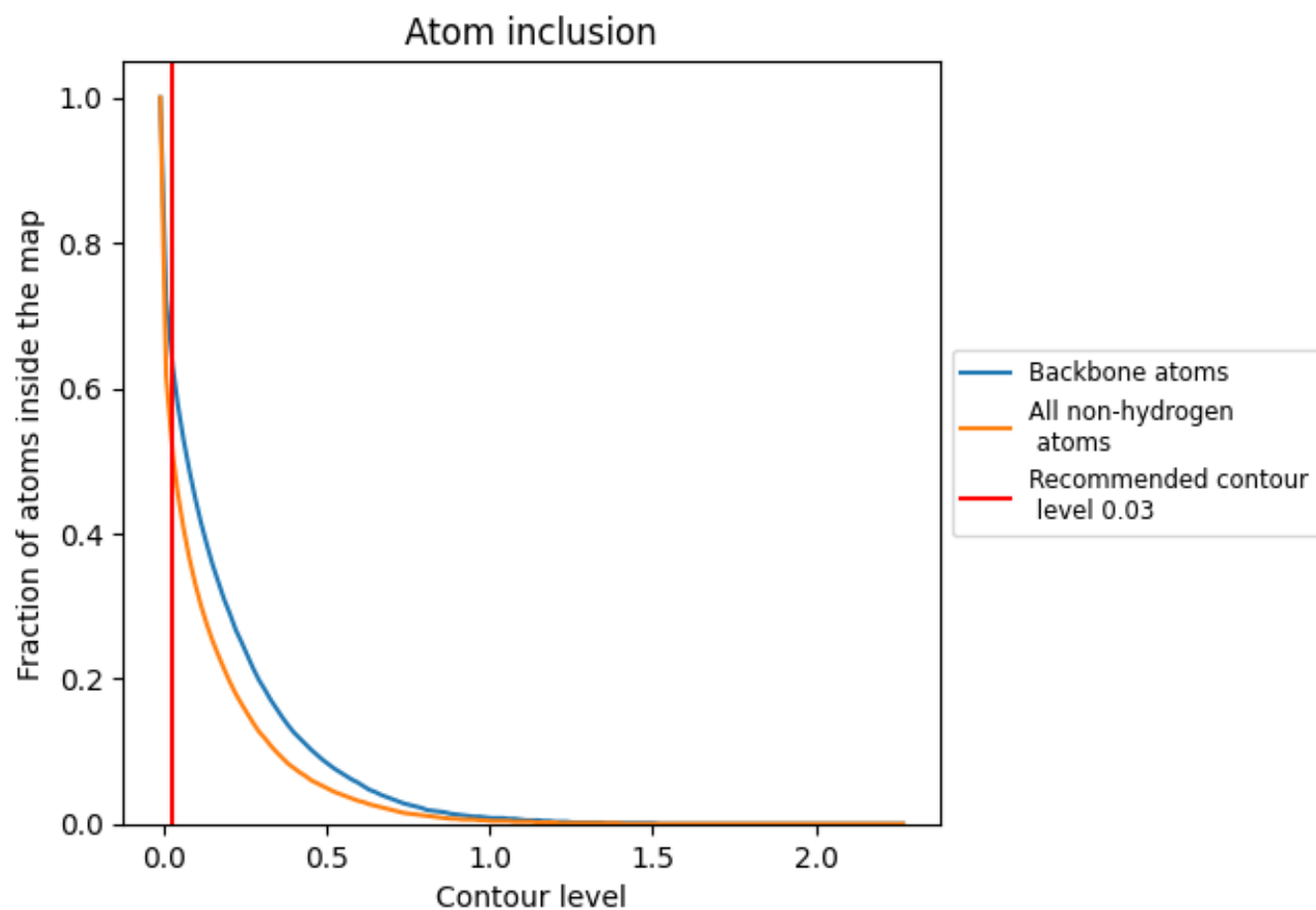
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 51% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5090	-0.0090
A	0.4350	-0.0450
B	0.5230	-0.0460
C	0.3720	-0.0280
D	0.6260	0.0270
E	0.4840	0.0200
F	0.4920	-0.0060
G	0.6350	-0.0060
H	0.5750	-0.0080
I	0.5980	0.0140
S	0.1420	-0.0450
T	0.3190	-0.0110

1.0

0.0

<0.0