WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 01:49 am GMT

PDB ID	:	6TNZ
EMDB ID	:	EMD-10540
Title	:	Human polymerase delta-FEN1-PCNA toolbelt
Authors	:	Lancey, C.; Hamdan, S.M.; De Biasio, A.
Deposited on	:	2019-12-10
Resolution	:	4.05 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:

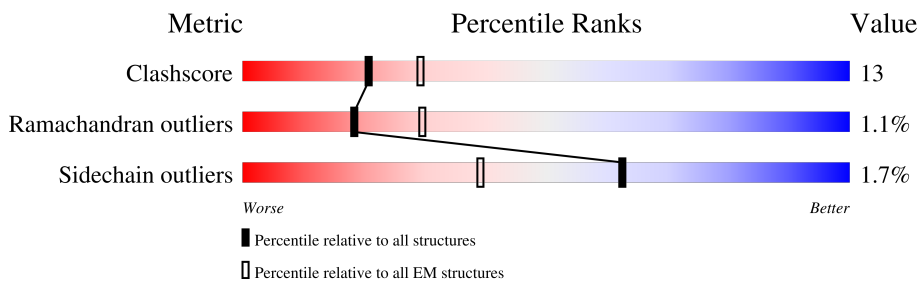|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.05 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	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		1.1%
Sidechain outliers		1.7%

Worse   *Better*

■ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1107	6% · 79% · 12% · 9%
2	B	469	· 79% · 13% · 8%
3	C	474	· 27% · 70%
4	D	137	· 36% · 11% ·· 52%
5	E	264	21% · 67% · 28% · 5%
5	F	264	· 80% · 15% · 6%
5	G	264	6% · 75% · 20% · 6%
6	H	380	68% · 32% · 41% · 8% · 19%

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Mol	Chain	Length	Quality of chain
7	P	25	88% • 8%
8	T	38	68% • 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SF4	A	1202	-	-	X	-

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 22008 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 DNA polymerase delta catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1010	Total 7926	C 5028	N 1405	O 1447	S 46	1	0

- Molecule 2 is a protein called DNA polymerase delta subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	431	Total 3304	C 2103	N 553	O 630	S 18	0	0

- Molecule 3 is a protein called DNA polymerase delta subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	143	Total 1130	C 715	N 196	O 214	S 5	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	initiating methionine	UNP Q15054
C	-6	TRP	-	expression tag	UNP Q15054
C	-5	SER	-	expression tag	UNP Q15054
C	-4	HIS	-	expression tag	UNP Q15054
C	-3	PRO	-	expression tag	UNP Q15054
C	-2	GLN	-	expression tag	UNP Q15054
C	-1	PHE	-	expression tag	UNP Q15054
C	0	GLU	-	expression tag	UNP Q15054
C	1	LYS	-	expression tag	UNP Q15054

- Molecule 4 is a protein called DNA polymerase delta subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	66	Total 554	C 359	N 97	O 94	S 4	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-29	MET	-	initiating methionine	UNP Q9HCU8
D	-28	HIS	-	expression tag	UNP Q9HCU8
D	-27	HIS	-	expression tag	UNP Q9HCU8
D	-26	HIS	-	expression tag	UNP Q9HCU8
D	-25	HIS	-	expression tag	UNP Q9HCU8
D	-24	HIS	-	expression tag	UNP Q9HCU8
D	-23	HIS	-	expression tag	UNP Q9HCU8
D	-22	SER	-	expression tag	UNP Q9HCU8
D	-21	ARG	-	expression tag	UNP Q9HCU8
D	-20	ALA	-	expression tag	UNP Q9HCU8
D	-19	TRP	-	expression tag	UNP Q9HCU8
D	-18	ARG	-	expression tag	UNP Q9HCU8
D	-17	HIS	-	expression tag	UNP Q9HCU8
D	-16	PRO	-	expression tag	UNP Q9HCU8
D	-15	GLN	-	expression tag	UNP Q9HCU8
D	-14	PHE	-	expression tag	UNP Q9HCU8
D	-13	GLY	-	expression tag	UNP Q9HCU8
D	-12	GLY	-	expression tag	UNP Q9HCU8
D	-11	HIS	-	expression tag	UNP Q9HCU8
D	-10	HIS	-	expression tag	UNP Q9HCU8
D	-9	HIS	-	expression tag	UNP Q9HCU8
D	-8	HIS	-	expression tag	UNP Q9HCU8
D	-7	HIS	-	expression tag	UNP Q9HCU8
D	-6	HIS	-	expression tag	UNP Q9HCU8
D	-5	GLU	-	expression tag	UNP Q9HCU8
D	-4	ASN	-	expression tag	UNP Q9HCU8
D	-3	LEU	-	expression tag	UNP Q9HCU8
D	-2	TYR	-	expression tag	UNP Q9HCU8
D	-1	PHE	-	expression tag	UNP Q9HCU8
D	0	GLN	-	expression tag	UNP Q9HCU8
D	1	SER	-	expression tag	UNP Q9HCU8

- Molecule 5 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	251	Total	C	N	O	S	0	0
			1924	1211	314	383	16		
5	F	249	Total	C	N	O	S	0	0
			1913	1205	312	380	16		
5	G	249	Total	C	N	O	S	0	0
			1913	1204	314	379	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P12004
E	-1	PRO	-	expression tag	UNP P12004
E	0	HIS	-	expression tag	UNP P12004
F	-2	GLY	-	expression tag	UNP P12004
F	-1	PRO	-	expression tag	UNP P12004
F	0	HIS	-	expression tag	UNP P12004
G	-2	GLY	-	expression tag	UNP P12004
G	-1	PRO	-	expression tag	UNP P12004
G	0	HIS	-	expression tag	UNP P12004

- Molecule 6 is a protein called Flap endonuclease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	306	2282	1436	396	437	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	181	ALA	ASP	conflict	UNP P39748

- Molecule 7 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	P	23	469	225	84	137	23	0	0

- Molecule 8 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	T	27	555	266	100	162	27	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	A	1	1	1	0

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

SF4
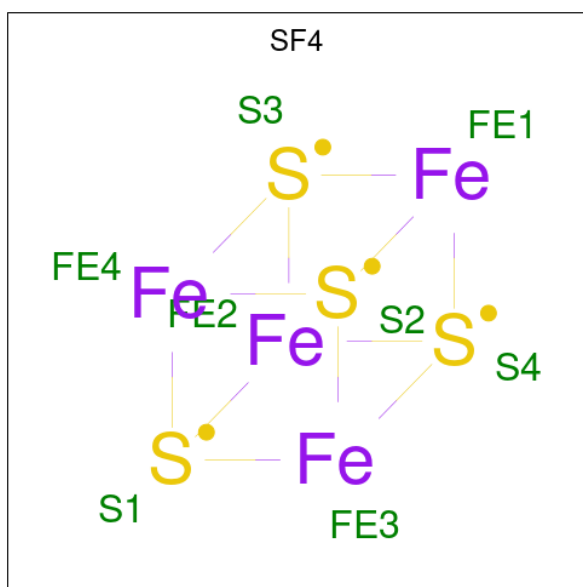
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
10	A	1	8	4	4	0

- Molecule 11 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

TTP
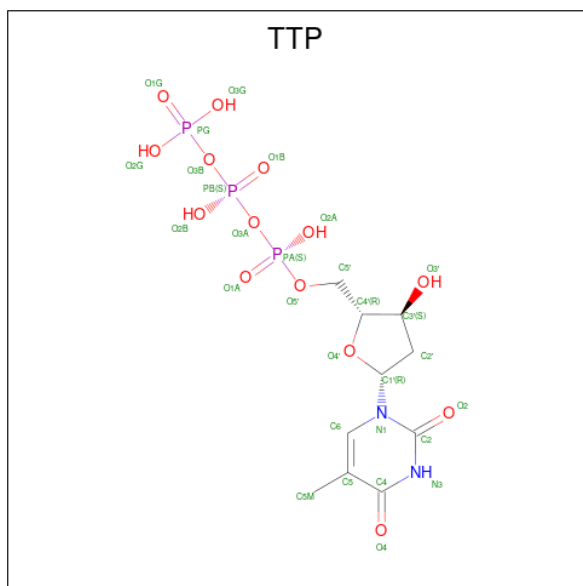
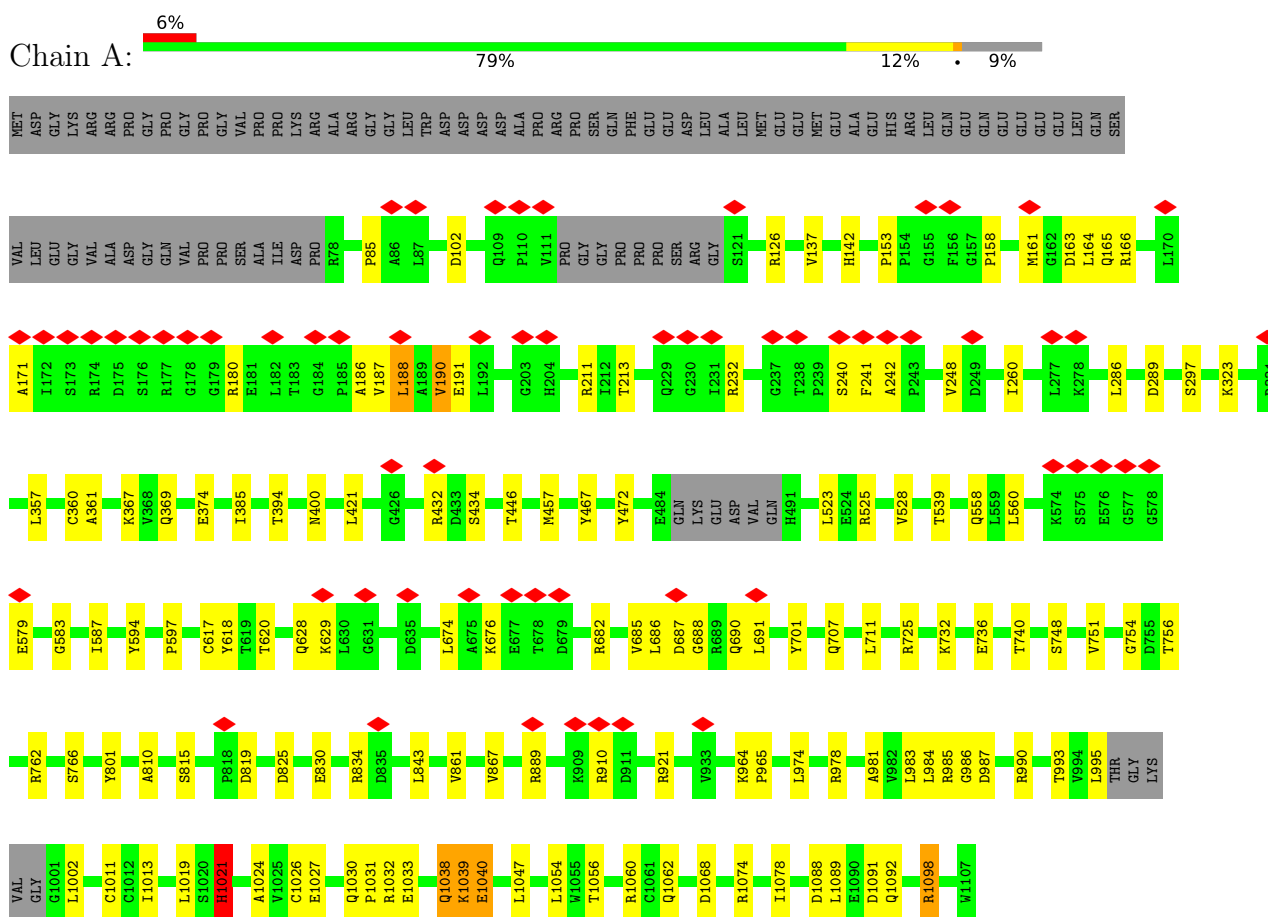| Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	A	1	29	10	2	14	3	0

3 Residue-property plots ⓘ

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

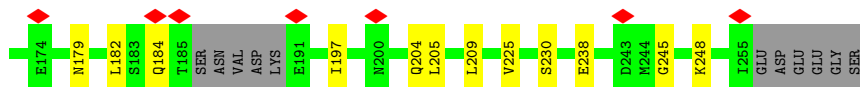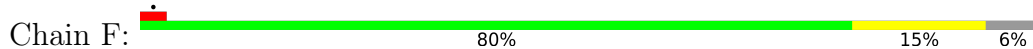• Molecule 1: DNA polymerase delta catalytic subunit

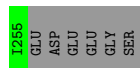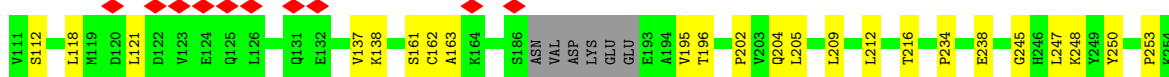• Molecule 2: DNA polymerase delta subunit 2

D167 D168 G169 D175 Y176 D180 Q184 D193 G207 G208 D220 R240 N246 S251 T252 Q253 S254 ARG SER ILE ASN LYS ALA LYS TYR LEU THR LYS LYS THR GLN ALA A271 S272 V273 V276 D293 V294 M295 P296 G297 E298 P307 Q308 Q309 M315

V328 T329 N330 P331 Y332 Q333 D337 Q347 S356 S357 E366 A378 P379 C398 C404 G405 N406 T407 I415 T427 L439 V440 N441 I450 E458 D459 D460 D461 L462 GLY LEU GLY LEU PRO

• Molecule 3: DNA polymerase delta subunit 3

Chain C:

27%　　　　　　　　　　70%

MET TRP SER HIS PRO GLN PHE GLU LYS A2 D3 Q4 L5 Y6 N35 K38 D43 R49 S53 G54 V59 L62 N70 G71 V79 E86 I103 Q104 K105 A106 M107 L108 K109 D110 N128 A139 R143 A144 PRO ALA GLU SER SER SER SER

LYS LYS PHE GLU GLN SER HIS LEU HIS MET SER SER GLU THR GLN ALA ASN GLU LEU THR THR ASN GLY HIS GLY PRO PRO ALA SER LYS GLN VAL SER GLN GLN PRO LYS GLY ILE MET GLY MET PHE ALA SER LYS ALA ALA LYS THR GLN GLU THR ASN LYS GLU THR LYS

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

PRO LYS LEU ALA THR PRO ALA GLY LEU LYS LYS SER SER LYS LYS ALA GLU PRO VAL LYS VAL LEU GLN LYS GLU GLY LYS LYS ARG GLY LYS ARG VAL ALA MET LEU LEU SER ASP GLU GLU THR LYS GLU THR GLU GLN ALA VAL LYS GLU GLU LYS ILE GLU VAL GLN PRO THR VAL SER VAL THR GLU ASN MET ARG LYS LYS ARG ARG ILE LYS LEU PRO GLU GLU SER ASP SER SER

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

LEU ASP GLY GLY CYS ILE VAL THR GLU LYS VAL TYR GLU SER GLU SER CYS THR ASP SER GLU GLU LEU ASN MET LYS THR SER SER VAL HIS ARG PRO PRO ALA MET THR VAL LYS SER GLU SER GLY GLU ASN ARG LYS ARG ARG LYS ARG VAL LEU LYS SER LYS GLY THR ALA LEU GLY LYS

ALA ASN ARG GLN VAL SER ILE THR GLY PHE PHE GLN ARG LYS

• Molecule 4: DNA polymerase delta subunit 4

Chain D:

36%　　11%　　52%

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

GLU LEU GLY GLU GLU PRO GLN PRO ARG ASP GLU E42 E43 A44 E45 L46 E47 R50 D53 C61 T62 R66 R69 R72 E79 L88 K89 R96 F97 L101 Y105 P106 L107
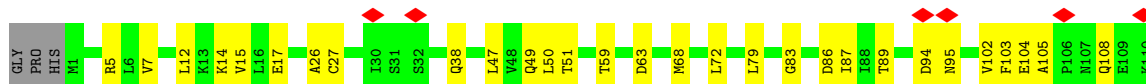
• Molecule 5: Proliferating cell nuclear antigen

Chain E:

21%

67%　　　　　　　　28%　　5%

GLY PRO HIS M1 F2 E3 A4 L12 L16 L19 E25 A26 C27 W28 D29 S32 Q38 S39 M40 D41 S42 S43 H44 L47 E55 G56 T59 Y60 R61 C62 D63 R64 M68 G69 I87 I88 T89 A92 E93 D94 N95 A96 D97 A100 L101 V102 F103

E104 S112 D113 Y114 E115 M116 K117 L118 M119 D120 L121 D122 V123 E124 Q125 L126 G127 I128 P129 E130 Q131 E132 Y133 S134 V137 K138 M139 P140 L151 I154 V159 I160 S161 C162 A163 K164 D165 G166 V167 K168 F169 S170 N179 Q184 T185 S186 ASN VAL ASP LYS E191 E192 E193

• Molecule 5: Proliferating cell nuclear antigen

Chain F:

| 80% | 15% | 6% |

• Molecule 5: Proliferating cell nuclear antigen

Chain G:

6%

| 75% | 20% | 6% |

• Molecule 6: Flap endonuclease 1

Chain H:

68%

| 32% | 41% | 8% | 19% |

E303 E304 E305 L306 I307 K308 F309 M310 C311 G312 E313 K314 Q315 F316 S317 E318 E319 R320 I321 R322 S323 G324 V325 K326 R327 L328 S329 K330 S331 R332 Q333 G334 S335 T336 Q337 G338 R339 L340 F343 F344 K345 V346 T347 G348 S349 L350 S351 S352 A353 LYS ARG GLU PRO GLU PRO LYS GLY SER

THR LYS LYS ALA LYS THR GLY ALA ALA GLY LYS PHE LYS ARG GLY LYS

• Molecule 7: DNA primer

Chain P:

88% 8%

DA DG C3 C25

• Molecule 8: DNA template

Chain T:

68% 29%

DC DT DG DC DA DC DG DA DA T-3 T21 A22 G23 DC DT

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	44	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	57471	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0073	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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, TTP, SF4, DOC

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	0.39	0/8094	0.64	0/10971
2	B	0.41	0/3380	0.61	0/4604
3	C	0.36	0/1149	0.58	0/1553
4	D	0.42	0/574	0.69	0/783
5	E	0.31	0/1949	0.61	0/2632
5	F	0.35	0/1937	0.62	0/2614
5	G	0.31	0/1938	0.59	0/2617
6	H	0.35	1/2322 (0.0%)	0.58	0/3141
7	P	0.83	0/505	1.05	0/777
8	T	0.86	0/622	1.11	1/958 (0.1%)
All	All	0.41	1/22470 (0.0%)	0.65	1/30650 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	338	GLY	N-CA	-5.47	1.37	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	21	DT	O4'-C1'-N1	5.39	111.78	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts   ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7926	0	7967	128	0
2	B	3304	0	3255	32	0
3	C	1130	0	1138	8	0
4	D	554	0	537	11	0
5	E	1924	0	1929	145	0
5	F	1913	0	1922	24	0
5	G	1913	0	1928	31	0
6	H	2282	0	2178	308	0
7	P	469	0	261	0	0
8	T	555	0	307	0	0
9	A	1	0	0	0	0
10	A	8	0	0	2	0
11	A	29	0	10	0	0
All	All	22008	0	21432	584	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 13.

All (584) 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)
5:E:234:PRO:HG2	6:H:344:PHE:CZ	1.31	1.58
1:A:861:VAL:CG1	1:A:985:ARG:HD3	1.40	1.48
5:E:27:CYS:SG	6:H:350:LEU:CG	2.02	1.47
1:A:688:GLY:HA2	1:A:691:LEU:CD2	1.43	1.46
1:A:861:VAL:HG11	1:A:985:ARG:NE	1.28	1.42
5:E:27:CYS:SG	6:H:350:LEU:HD12	1.60	1.41
1:A:861:VAL:CG1	1:A:985:ARG:CD	1.98	1.41
5:E:27:CYS:SG	6:H:350:LEU:CD1	2.10	1.40
5:E:129:PRO:CD	6:H:344:PHE:CD1	2.06	1.38
1:A:861:VAL:HG13	1:A:985:ARG:CD	1.52	1.34
5:E:40:MET:CE	5:E:126:LEU:HD21	1.58	1.33
5:E:252:ALA:HB2	6:H:340:LEU:CD2	1.62	1.27
5:E:27:CYS:SG	6:H:350:LEU:HG	1.66	1.23
5:E:234:PRO:HG2	6:H:344:PHE:CE2	1.72	1.22
5:E:234:PRO:CG	6:H:344:PHE:CZ	2.22	1.22
5:E:232:ASP:O	6:H:343:PHE:CE1	1.92	1.20
5:E:69:GLY:HA3	5:E:121:LEU:CD1	1.72	1.18
5:E:129:PRO:HD3	6:H:344:PHE:CD1	1.70	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:ALA:HB1	1:A:985:ARG:NH1	1.61	1.16
5:E:126:LEU:HA	6:H:347:THR:N	1.60	1.14
1:A:861:VAL:CG1	1:A:985:ARG:NE	2.09	1.14
6:H:28:GLY:HA2	6:H:335:SER:N	1.59	1.14
5:E:129:PRO:HD2	6:H:344:PHE:CD1	1.80	1.11
5:E:252:ALA:CB	6:H:340:LEU:HD23	1.83	1.09
1:A:688:GLY:O	1:A:691:LEU:HG	1.53	1.08
5:E:27:CYS:SG	6:H:350:LEU:CB	2.42	1.07
1:A:688:GLY:HA2	1:A:691:LEU:HD23	1.37	1.05
5:E:125:GLN:O	6:H:348:GLY:N	1.87	1.04
1:A:981:ALA:CB	1:A:985:ARG:HH12	1.70	1.04
5:E:129:PRO:HD2	6:H:344:PHE:CE1	1.91	1.04
5:E:126:LEU:CA	6:H:347:THR:H	1.70	1.03
5:E:69:GLY:HA3	5:E:121:LEU:HD11	1.37	1.03
5:E:129:PRO:CD	6:H:344:PHE:HD1	1.52	1.02
1:A:688:GLY:HA2	1:A:691:LEU:HD21	1.06	1.01
1:A:688:GLY:CA	1:A:691:LEU:CD2	2.38	1.00
6:H:28:GLY:HA2	6:H:334:GLY:C	1.81	1.00
5:E:126:LEU:CB	6:H:346:VAL:HA	1.92	1.00
5:E:40:MET:HE3	5:E:126:LEU:HD21	1.42	1.00
5:E:27:CYS:SG	6:H:350:LEU:HB3	2.01	1.00
1:A:981:ALA:HB1	1:A:985:ARG:HH12	0.83	0.99
5:E:252:ALA:HB2	6:H:340:LEU:HD23	0.99	0.98
6:H:27:PHE:CD2	6:H:77:ASN:O	2.16	0.97
6:H:330:LYS:HE2	6:H:330:LYS:HA	1.44	0.97
1:A:688:GLY:CA	1:A:691:LEU:HD21	1.96	0.96
5:E:126:LEU:HB3	6:H:346:VAL:HA	1.46	0.95
5:E:40:MET:CE	5:E:126:LEU:CD2	2.45	0.95
1:A:861:VAL:HG11	1:A:985:ARG:CD	1.81	0.95
1:A:1026:CYS:O	1:A:1030:GLN:HG3	1.67	0.95
6:H:29:ARG:HD3	6:H:173:TYR:CD2	2.01	0.94
1:A:861:VAL:HG13	1:A:985:ARG:HD3	0.95	0.94
5:E:69:GLY:CA	5:E:121:LEU:CD1	2.45	0.93
5:E:69:GLY:CA	5:E:121:LEU:HD11	1.98	0.93
5:E:234:PRO:HG2	6:H:344:PHE:HZ	1.15	0.92
6:H:238:ILE:HG23	6:H:241:ILE:HD11	1.51	0.92
6:H:26:TYR:CE1	6:H:29:ARG:NH1	2.38	0.91
5:E:44:HIS:CD2	6:H:339:ARG:HD3	2.07	0.90
5:E:123:VAL:O	6:H:349:SER:HA	1.72	0.90
5:E:40:MET:HE2	5:E:126:LEU:HD21	1.53	0.90
5:E:232:ASP:O	6:H:343:PHE:CZ	2.24	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:28:GLY:HA3	6:H:335:SER:HA	1.54	0.89
5:E:123:VAL:O	6:H:349:SER:CA	2.21	0.89
6:H:184:THR:HG22	6:H:227:CYS:SG	2.11	0.89
5:E:69:GLY:HA3	5:E:121:LEU:HD12	1.54	0.89
5:E:121:LEU:N	6:H:352:SER:OG	2.06	0.88
6:H:71:THR:HG21	6:H:150:ILE:HD13	1.53	0.87
5:E:121:LEU:HB2	6:H:352:SER:H	1.39	0.85
5:E:252:ALA:CB	6:H:340:LEU:CD2	2.50	0.85
5:E:121:LEU:O	6:H:351:SER:HB3	1.75	0.85
1:A:164:LEU:HB3	1:A:190:VAL:HG11	1.59	0.85
6:H:27:PHE:CD1	6:H:78:GLY:HA3	2.12	0.84
5:E:123:VAL:O	6:H:349:SER:CB	2.25	0.84
5:E:234:PRO:CG	6:H:344:PHE:HZ	1.75	0.83
5:E:121:LEU:O	6:H:351:SER:CB	2.27	0.83
5:E:129:PRO:CG	6:H:344:PHE:HD1	1.92	0.83
6:H:254:LYS:H	6:H:254:LYS:HD2	1.41	0.82
5:E:120:ASP:HA	6:H:352:SER:OG	1.79	0.82
6:H:28:GLY:CA	6:H:335:SER:N	2.42	0.82
5:E:125:GLN:N	6:H:348:GLY:O	2.12	0.82
5:E:126:LEU:HA	6:H:347:THR:H	0.75	0.81
6:H:28:GLY:CA	6:H:334:GLY:C	2.48	0.81
6:H:28:GLY:CA	6:H:335:SER:HA	2.11	0.81
5:E:121:LEU:O	6:H:351:SER:HA	1.82	0.80
5:E:121:LEU:O	6:H:351:SER:CA	2.29	0.79
1:A:1038:GLN:HE22	2:B:273:VAL:HA	1.48	0.79
6:H:152:TYR:O	6:H:153:LEU:HD12	1.82	0.79
5:E:252:ALA:HB2	6:H:340:LEU:CG	2.13	0.79
1:A:188:LEU:HA	1:A:213:THR:O	1.82	0.77
1:A:861:VAL:HG11	1:A:985:ARG:HE	0.96	0.77
6:H:27:PHE:CE1	6:H:334:GLY:HA2	2.19	0.77
5:E:69:GLY:CA	5:E:121:LEU:HD12	2.13	0.77
5:E:125:GLN:O	6:H:347:THR:N	2.19	0.76
6:H:26:TYR:CD1	6:H:29:ARG:NH1	2.53	0.76
5:E:123:VAL:O	6:H:349:SER:HB3	1.85	0.76
6:H:30:LYS:O	6:H:172:VAL:HG22	1.87	0.75
1:A:1078:ILE:HG13	10:A:1202:SF4:S1	2.26	0.75
5:E:125:GLN:OE1	6:H:350:LEU:HB2	1.86	0.75
6:H:67:MET:HE1	6:H:83:TYR:CD2	2.21	0.75
1:A:861:VAL:HG12	1:A:985:ARG:HD3	1.63	0.74
6:H:254:LYS:HD2	6:H:254:LYS:N	2.01	0.74
5:E:232:ASP:OD1	6:H:343:PHE:HZ	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:26:TYR:CE2	6:H:204:ILE:HG12	2.23	0.74
6:H:152:TYR:C	6:H:153:LEU:HD12	2.08	0.74
5:E:234:PRO:CG	6:H:344:PHE:CE2	2.62	0.73
1:A:861:VAL:HG13	1:A:985:ARG:HD2	1.66	0.73
6:H:284:LEU:O	6:H:286:PRO:HD3	1.87	0.73
6:H:177:THR:HG22	6:H:178:GLU:H	1.52	0.73
5:E:40:MET:HE2	5:E:126:LEU:CD2	2.13	0.73
1:A:1011:CYS:O	1:A:1098:ARG:NH1	2.22	0.72
5:E:125:GLN:O	6:H:347:THR:CA	2.37	0.72
1:A:164:LEU:HB3	1:A:190:VAL:HG21	1.72	0.72
1:A:188:LEU:N	1:A:188:LEU:HD23	2.04	0.71
6:H:221:GLU:HG2	6:H:284:LEU:HD11	1.71	0.71
5:E:128:ILE:HD11	6:H:344:PHE:CZ	2.25	0.71
5:F:166:GLY:HA3	5:F:182:LEU:O	1.90	0.71
6:H:272:GLU:HG3	6:H:273:ASN:H	1.56	0.71
5:E:120:ASP:HA	6:H:352:SER:HG	1.56	0.70
6:H:28:GLY:CA	6:H:335:SER:CA	2.69	0.69
1:A:688:GLY:CA	1:A:691:LEU:HD23	2.13	0.69
5:E:103:PHE:HB2	5:E:112:SER:HB2	1.75	0.69
6:H:321:ILE:O	6:H:325:VAL:HG22	1.93	0.69
5:E:234:PRO:HA	5:E:251:LEU:O	1.94	0.68
6:H:242:GLY:H	6:H:245:ARG:HB3	1.58	0.68
6:H:282:LEU:O	6:H:286:PRO:HG3	1.94	0.68
6:H:134:THR:HG22	6:H:135:LYS:H	1.58	0.68
5:E:126:LEU:HD13	6:H:344:PHE:HB2	1.76	0.68
6:H:264:ASP:N	6:H:265:PRO:HD2	2.09	0.68
6:H:27:PHE:CG	6:H:78:GLY:HA3	2.29	0.67
6:H:219:ASN:H	6:H:222:GLN:NE2	1.92	0.67
5:E:127:GLY:O	6:H:344:PHE:HB3	1.93	0.67
6:H:11:ALA:O	6:H:15:PRO:HG3	1.93	0.67
5:E:29:ASP:OD1	6:H:350:LEU:HD21	1.94	0.67
1:A:1091:ASP:OD1	1:A:1092:GLN:N	2.28	0.67
6:H:63:HIS:O	6:H:64:LEU:HD23	1.94	0.67
6:H:3:ILE:HG22	6:H:6:LEU:HB2	1.77	0.66
6:H:336:THR:HG22	6:H:337:GLN:H	1.61	0.66
6:H:78:GLY:O	6:H:334:GLY:HA3	1.96	0.66
1:A:1024:ALA:HB2	1:A:1098:ARG:HB3	1.76	0.66
5:G:27:CYS:HB3	5:G:121:LEU:HD21	1.78	0.66
6:H:264:ASP:H	6:H:265:PRO:CD	2.09	0.66
6:H:260:VAL:HG23	6:H:261:ARG:H	1.59	0.65
1:A:1026:CYS:O	1:A:1030:GLN:CG	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:GLY:HA2	5:F:197:ILE:HD13	1.77	0.65
1:A:525:ARG:O	1:A:682:ARG:NH2	2.29	0.65
5:E:120:ASP:CA	6:H:352:SER:OG	2.43	0.65
6:H:27:PHE:CD2	6:H:77:ASN:C	2.70	0.65
6:H:289:LEU:HD12	6:H:289:LEU:O	1.97	0.65
5:E:252:ALA:N	6:H:340:LEU:HD21	2.12	0.65
6:H:264:ASP:H	6:H:265:PRO:HD2	1.62	0.65
5:E:120:ASP:C	6:H:352:SER:OG	2.36	0.64
6:H:137:HIS:H	6:H:137:HIS:CD2	2.13	0.64
6:H:200:LYS:HB3	6:H:202:LEU:HD13	1.79	0.64
6:H:340:LEU:HD22	6:H:344:PHE:HE2	1.62	0.64
5:E:40:MET:HE3	5:E:126:LEU:CD2	2.18	0.64
5:E:238:GLU:HG3	5:E:248:LYS:HG2	1.80	0.64
1:A:1002:LEU:HD21	5:F:47:LEU:HB2	1.79	0.64
5:G:47:LEU:HB3	5:G:250:TYR:HB2	1.80	0.64
6:H:340:LEU:HD22	6:H:344:PHE:CE2	2.34	0.63
6:H:263:LEU:HD12	6:H:263:LEU:O	1.98	0.63
6:H:27:PHE:CD1	6:H:334:GLY:HA2	2.33	0.62
6:H:28:GLY:HA2	6:H:335:SER:CA	2.28	0.62
6:H:64:LEU:HD11	6:H:140:GLU:HG2	1.80	0.62
5:E:128:ILE:CD1	6:H:344:PHE:CZ	2.82	0.62
5:E:129:PRO:HD3	6:H:344:PHE:CG	2.30	0.62
1:A:995:LEU:HB2	5:F:123:VAL:HA	1.80	0.62
5:E:40:MET:HE1	5:E:126:LEU:HD21	1.71	0.62
6:H:26:TYR:OH	6:H:206:GLU:HG3	1.98	0.62
5:E:125:GLN:C	6:H:347:THR:HB	2.20	0.62
1:A:188:LEU:HD23	1:A:188:LEU:H	1.65	0.62
2:B:73:TRP:NE1	2:B:175:ASP:OD2	2.33	0.62
1:A:674:LEU:HD13	1:A:686:LEU:HB2	1.82	0.61
5:E:128:ILE:CD1	6:H:344:PHE:CE2	2.84	0.61
6:H:162:SER:O	6:H:165:ALA:HB3	2.00	0.61
6:H:304:GLU:HA	6:H:307:ILE:HG22	1.81	0.61
6:H:141:CYS:C	6:H:143:HIS:H	2.02	0.61
6:H:159:ALA:O	6:H:162:SER:N	2.33	0.61
6:H:9:LEU:O	6:H:13:VAL:HG13	2.00	0.61
1:A:432:ARG:HH21	1:A:434:SER:HB2	1.66	0.61
4:D:42:GLU:OE2	4:D:96:ARG:NH2	2.34	0.60
4:D:53:ASP:OD2	4:D:66:ARG:NH2	2.31	0.60
5:E:87:ILE:HB	5:E:104:GLU:HB2	1.82	0.60
1:A:583:GLY:O	1:A:725:ARG:NH1	2.34	0.60
5:E:226:THR:HB	5:E:238:GLU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:311:CYS:SG	6:H:318:GLU:HA	2.42	0.60
1:A:1013:ILE:HD12	1:A:1024:ALA:HB1	1.84	0.60
1:A:525:ARG:HG2	1:A:682:ARG:HH22	1.67	0.60
5:F:5:ARG:HB3	5:F:59:THR:HB	1.84	0.60
1:A:995:LEU:HD22	5:F:124:GLU:H	1.67	0.60
6:H:218:LEU:HB2	6:H:222:GLN:HB2	1.83	0.60
4:D:61:CYS:SG	4:D:72:ARG:NH2	2.75	0.59
6:H:28:GLY:HA3	6:H:335:SER:CA	2.28	0.59
6:H:134:THR:HG22	6:H:135:LYS:N	2.17	0.59
1:A:1027:GLU:HA	1:A:1030:GLN:CD	2.23	0.59
1:A:186:ALA:HB3	1:A:188:LEU:CD2	2.33	0.59
1:A:187:VAL:HG22	1:A:187:VAL:O	2.02	0.59
1:A:1088:ASP:HA	1:A:1091:ASP:OD2	2.02	0.59
1:A:986:GLY:O	1:A:990:ARG:N	2.36	0.59
5:E:234:PRO:CB	6:H:344:PHE:HZ	2.15	0.59
6:H:137:HIS:H	6:H:137:HIS:HD2	1.51	0.59
6:H:14:ALA:N	6:H:15:PRO:HD3	2.18	0.59
6:H:27:PHE:CE1	6:H:78:GLY:HA3	2.38	0.59
6:H:241:ILE:HG21	6:H:249:LEU:HD22	1.85	0.58
6:H:270:VAL:HG13	6:H:271:PRO:HD2	1.84	0.58
5:G:238:GLU:HG3	5:G:248:LYS:HG2	1.85	0.58
5:E:133:TYR:HA	5:E:230:SER:HB2	1.85	0.58
1:A:1062:GLN:NE2	1:A:1068:ASP:O	2.37	0.58
2:B:184:GLN:HB2	2:B:398:CYS:HB3	1.85	0.58
1:A:186:ALA:HB3	1:A:188:LEU:HD21	1.86	0.58
5:E:125:GLN:O	6:H:347:THR:HB	2.03	0.58
5:F:7:VAL:HA	5:F:87:ILE:HG23	1.86	0.58
5:G:104:GLU:HB3	5:G:108:GLN:HE22	1.69	0.58
5:F:152:SER:HA	5:F:209:LEU:HD13	1.86	0.57
6:H:264:ASP:N	6:H:265:PRO:CD	2.66	0.57
1:A:539:THR:HA	1:A:558:GLN:HE21	1.69	0.57
5:E:121:LEU:HB2	6:H:352:SER:N	2.16	0.57
6:H:194:LEU:HG	6:H:194:LEU:O	2.04	0.57
1:A:357:LEU:HD11	1:A:374:GLU:HG2	1.85	0.57
1:A:688:GLY:O	1:A:691:LEU:CG	2.41	0.57
1:A:1056:THR:HG23	1:A:1060:ARG:HH21	1.70	0.57
6:H:308:LYS:NZ	6:H:308:LYS:HB3	2.19	0.57
1:A:161:MET:O	1:A:165:GLN:NE2	2.37	0.57
1:A:628:GLN:HB3	1:A:629:LYS:HD3	1.86	0.57
1:A:1039:LYS:O	1:A:1040:GLU:HG2	2.04	0.57
5:E:254:LYS:HA	6:H:337:GLN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:LEU:O	1:A:990:ARG:NH1	2.38	0.57
2:B:1:MET:HG2	2:B:441:ASN:HD22	1.69	0.57
6:H:135:LYS:HD2	6:H:135:LYS:C	2.25	0.57
5:E:126:LEU:HB2	6:H:345:LYS:O	2.04	0.56
5:E:126:LEU:HB2	6:H:346:VAL:HA	1.82	0.56
1:A:981:ALA:O	1:A:985:ARG:HG3	2.05	0.56
6:H:29:ARG:HD3	6:H:173:TYR:CE2	2.41	0.56
5:F:5:ARG:NH2	5:F:104:GLU:OE1	2.38	0.56
6:H:37:MET:SD	6:H:177:THR:HG22	2.46	0.56
6:H:268:TYR:N	6:H:269:PRO:HD3	2.20	0.56
6:H:275:LEU:HD22	6:H:275:LEU:N	2.21	0.56
5:E:125:GLN:O	6:H:347:THR:C	2.44	0.56
5:E:237:VAL:HG22	5:E:249:TYR:HB2	1.86	0.56
5:G:234:PRO:HA	5:G:253:PRO:HD3	1.87	0.56
6:H:300:GLU:CD	6:H:301:PRO:HD2	2.25	0.56
5:E:29:ASP:OD1	6:H:350:LEU:CD2	2.53	0.56
5:G:89:THR:HB	5:G:102:VAL:HB	1.87	0.56
6:H:199:ALA:O	6:H:201:LYS:N	2.38	0.56
6:H:260:VAL:HG23	6:H:261:ARG:N	2.20	0.56
6:H:218:LEU:HB2	6:H:222:GLN:CB	2.36	0.56
6:H:265:PRO:C	6:H:267:LYS:H	2.07	0.56
6:H:307:ILE:HD11	6:H:311:CYS:SG	2.46	0.56
1:A:587:ILE:HD13	1:A:732:LYS:HD3	1.88	0.56
2:B:134:VAL:HG11	2:B:141:ARG:HH11	1.70	0.56
6:H:6:LEU:HD22	6:H:10:ILE:HD11	1.87	0.56
1:A:142:HIS:NE2	1:A:289:ASP:OD1	2.38	0.56
6:H:26:TYR:OH	6:H:204:ILE:HD11	2.05	0.56
6:H:225:ASP:O	6:H:229:LEU:HG	2.06	0.56
1:A:1030:GLN:H	1:A:1031:PRO:CD	2.19	0.55
2:B:307:PRO:O	2:B:309:GLN:NE2	2.37	0.55
5:E:129:PRO:HD3	6:H:344:PHE:HD1	1.27	0.55
1:A:1030:GLN:N	1:A:1031:PRO:CD	2.69	0.55
6:H:322:ARG:O	6:H:325:VAL:HG23	2.06	0.55
6:H:27:PHE:CG	6:H:77:ASN:O	2.60	0.55
6:H:71:THR:O	6:H:75:MET:HG2	2.06	0.55
5:E:47:LEU:HB3	5:E:250:TYR:HD2	1.72	0.55
1:A:981:ALA:CB	1:A:985:ARG:NH1	2.44	0.55
3:C:35:ASN:HA	3:C:38:LYS:HD2	1.88	0.55
6:H:14:ALA:HB1	6:H:215:GLU:HG3	1.89	0.54
1:A:153:PRO:HD2	1:A:158:PRO:HG2	1.88	0.54
6:H:258:GLU:OE1	6:H:262:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:GLY:C	1:A:691:LEU:HG	2.24	0.54
6:H:74:MET:O	6:H:79:ILE:HB	2.08	0.54
5:E:89:THR:HB	5:E:102:VAL:HB	1.90	0.54
5:E:232:ASP:OD1	6:H:343:PHE:CZ	2.56	0.54
2:B:295:MET:HG3	2:B:328:VAL:HG23	1.89	0.54
5:G:51:THR:O	5:G:245:GLY:HA3	2.08	0.54
6:H:33:ILE:HG22	6:H:34:ASP:N	2.22	0.54
2:B:32:TYR:HH	2:B:332:TYR:HH	1.52	0.54
4:D:66:ARG:NH1	4:D:97:PHE:O	2.41	0.54
6:H:330:LYS:HE2	6:H:330:LYS:CA	2.27	0.54
5:E:161:SER:HB3	5:E:168:LYS:HB2	1.90	0.54
6:H:332:ARG:O	6:H:333:GLN:CB	2.56	0.54
2:B:298:GLU:HG3	2:B:347:GLN:HE21	1.73	0.53
4:D:47:GLU:OE1	4:D:50:ARG:NH1	2.41	0.53
6:H:69:TYR:O	6:H:72:ILE:HB	2.08	0.53
6:H:27:PHE:HD1	6:H:334:GLY:O	1.91	0.53
2:B:356:SER:OG	2:B:357:SER:N	2.40	0.53
5:E:252:ALA:HB2	6:H:340:LEU:HA	1.90	0.53
5:E:44:HIS:NE2	6:H:339:ARG:HD3	2.23	0.53
1:A:687:ASP:O	1:A:691:LEU:HD23	2.09	0.53
5:G:162:CYS:O	5:G:202:PRO:HA	2.08	0.53
6:H:65:MET:O	6:H:68:PHE:HB3	2.09	0.53
5:G:137:VAL:HA	5:G:196:THR:O	2.08	0.53
2:B:404:CYS:SG	2:B:405:GLY:N	2.79	0.53
5:E:234:PRO:CD	6:H:344:PHE:CZ	2.91	0.53
2:B:330:ASN:HB3	2:B:331:PRO:HD3	1.90	0.53
5:E:113:ASP:OD1	5:E:113:ASP:N	2.40	0.53
1:A:164:LEU:CB	1:A:190:VAL:HG21	2.38	0.53
5:F:91:ARG:HB3	5:F:100:ALA:HB3	1.90	0.53
1:A:617:CYS:HB3	1:A:620:THR:HG22	1.91	0.52
5:E:2:PHE:HB3	5:E:92:ALA:HB3	1.91	0.52
6:H:134:THR:C	6:H:136:GLN:H	2.11	0.52
3:C:110:ASP:OD1	3:C:110:ASP:N	2.42	0.52
5:E:44:HIS:HD2	6:H:339:ARG:HD3	1.68	0.52
5:G:103:PHE:HB2	5:G:112:SER:HB2	1.92	0.52
6:H:141:CYS:C	6:H:143:HIS:N	2.63	0.52
6:H:220:GLN:O	6:H:223:PHE:HB3	2.09	0.52
5:F:113:ASP:OD1	5:F:113:ASP:N	2.40	0.52
6:H:26:TYR:HH	6:H:206:GLU:HG3	1.73	0.52
6:H:273:ASN:O	6:H:275:LEU:HD22	2.09	0.52
3:C:59:VAL:HG12	3:C:103:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:7:VAL:HA	5:G:87:ILE:HG23	1.92	0.52
6:H:27:PHE:CE2	6:H:77:ASN:C	2.83	0.52
2:B:308:GLN:OE1	2:B:330:ASN:ND2	2.42	0.52
1:A:171:ALA:H	1:A:180:ARG:HG3	1.75	0.52
1:A:232:ARG:HH12	1:A:242:ALA:HB3	1.75	0.52
1:A:1027:GLU:HA	1:A:1030:GLN:NE2	2.25	0.52
6:H:302:ASN:HD22	6:H:302:ASN:C	2.14	0.52
5:E:124:GLU:HA	6:H:348:GLY:O	2.10	0.51
6:H:181:ALA:O	6:H:184:THR:N	2.42	0.51
6:H:321:ILE:O	6:H:321:ILE:HG22	2.11	0.51
1:A:394:THR:HG22	1:A:457:MET:HB2	1.91	0.51
6:H:88:LYS:HG3	6:H:88:LYS:O	2.10	0.51
6:H:303:GLU:O	6:H:307:ILE:HG22	2.11	0.51
1:A:164:LEU:HB3	1:A:190:VAL:CG1	2.37	0.51
5:E:125:GLN:O	6:H:347:THR:CB	2.58	0.51
1:A:102:ASP:HB3	1:A:126:ARG:HB2	1.93	0.51
5:F:184:GLN:NE2	5:F:197:ILE:O	2.43	0.51
6:H:209:LEU:HD21	6:H:220:GLN:OE1	2.11	0.50
1:A:688:GLY:HA2	1:A:691:LEU:CG	2.34	0.50
6:H:3:ILE:HD12	6:H:3:ILE:N	2.25	0.50
6:H:61:THR:HG22	6:H:61:THR:O	2.12	0.50
1:A:191:GLU:HB3	1:A:211:ARG:HB3	1.93	0.50
5:E:128:ILE:HD12	6:H:344:PHE:CD2	2.46	0.50
6:H:275:LEU:HD22	6:H:275:LEU:H	1.76	0.50
6:H:275:LEU:C	6:H:277:LYS:H	2.14	0.50
6:H:336:THR:HG22	6:H:337:GLN:N	2.24	0.50
5:E:44:HIS:CD2	6:H:339:ARG:CD	2.87	0.50
5:E:128:ILE:HD12	6:H:344:PHE:CG	2.46	0.50
5:F:16:LEU:HD22	5:F:79:LEU:HD12	1.93	0.50
1:A:984:LEU:HA	1:A:987:ASP:HB2	1.94	0.50
5:G:38:GLN:HG2	5:G:49:GLN:HG2	1.92	0.50
2:B:99:LYS:H	2:B:155:THR:HB	1.77	0.49
5:E:184:GLN:HG3	5:E:197:ILE:HD12	1.93	0.49
5:E:206:THR:HG23	5:E:254:LYS:HB2	1.92	0.49
1:A:974:LEU:HD22	1:A:978:ARG:HD3	1.95	0.49
5:G:161:SER:HB3	5:G:204:GLN:HE21	1.78	0.49
6:H:177:THR:HG22	6:H:178:GLU:N	2.23	0.49
6:H:275:LEU:C	6:H:277:LYS:N	2.66	0.49
5:E:16:LEU:HA	5:E:19:LEU:HB2	1.94	0.49
6:H:71:THR:HG21	6:H:150:ILE:CD1	2.36	0.49
1:A:587:ILE:HD12	1:A:754:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:105:ALA:O	5:G:108:GLN:NE2	2.45	0.49
5:G:138:LYS:O	5:G:195:VAL:HA	2.12	0.49
6:H:26:TYR:HD1	6:H:29:ARG:HD2	1.77	0.49
6:H:263:LEU:HD12	6:H:263:LEU:C	2.33	0.49
6:H:316:PHE:HD1	6:H:317:SER:H	1.61	0.49
1:A:1021:HIS:C	1:A:1021:HIS:CD2	2.86	0.49
1:A:248:VAL:HG11	1:A:560:LEU:HD11	1.95	0.49
2:B:18:SER:OG	2:B:19:ALA:N	2.45	0.49
1:A:421:LEU:H	1:A:421:LEU:HD22	1.78	0.48
2:B:276:VAL:HG11	2:B:315:MET:HB3	1.95	0.48
6:H:245:ARG:HG2	6:H:245:ARG:HH11	1.78	0.48
5:E:122:ASP:HA	6:H:351:SER:OG	2.13	0.48
6:H:221:GLU:HA	6:H:224:VAL:HG23	1.95	0.48
6:H:238:ILE:HG23	6:H:241:ILE:CD1	2.35	0.48
1:A:188:LEU:H	1:A:188:LEU:CD2	2.24	0.48
6:H:26:TYR:CZ	6:H:204:ILE:HG12	2.48	0.48
6:H:330:LYS:HA	6:H:330:LYS:CE	2.31	0.48
1:A:736:GLU:HG3	1:A:751:VAL:HG23	1.94	0.48
5:F:160:ILE:O	5:F:204:GLN:HA	2.13	0.48
1:A:1047:LEU:HB3	1:A:1089:LEU:HD13	1.96	0.48
2:B:49:GLN:NE2	4:D:62:THR:OG1	2.46	0.48
5:E:162:CYS:O	5:E:202:PRO:HA	2.14	0.48
5:F:169:PHE:O	5:F:179:ASN:HA	2.14	0.48
6:H:80:LYS:HB3	6:H:298:TRP:CE2	2.49	0.48
5:E:44:HIS:HD2	6:H:339:ARG:CD	2.25	0.48
6:H:167:VAL:HG12	6:H:188:PRO:CG	2.43	0.48
1:A:1039:LYS:O	1:A:1040:GLU:CG	2.61	0.47
6:H:175:ALA:O	6:H:190:LEU:HD12	2.14	0.47
1:A:964:LYS:HG3	1:A:965:PRO:HD3	1.95	0.47
5:E:69:GLY:HA2	5:E:121:LEU:CD1	2.38	0.47
6:H:10:ILE:HG22	6:H:18:ILE:HD11	1.95	0.47
6:H:336:THR:O	6:H:337:GLN:O	2.32	0.47
5:E:128:ILE:HD12	6:H:344:PHE:CD1	2.49	0.47
6:H:67:MET:CE	6:H:145:LEU:HD21	2.44	0.47
5:G:68:MET:HB3	5:G:118:LEU:HD11	1.94	0.47
6:H:24:LYS:HA	6:H:77:ASN:HD22	1.79	0.47
1:A:467:TYR:O	1:A:472:TYR:OH	2.32	0.47
5:E:129:PRO:CG	6:H:344:PHE:CD1	2.78	0.47
5:E:69:GLY:HA2	5:E:121:LEU:HD11	1.93	0.47
5:G:205:LEU:HD13	5:G:253:PRO:HG3	1.95	0.47
3:C:6:TYR:OH	3:C:43:ASP:OD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:GLU:OE1	4:D:79:GLU:HA	2.13	0.47
5:E:218:ALA:HA	5:E:221:LEU:HD23	1.96	0.47
6:H:30:LYS:HA	6:H:80:LYS:O	2.14	0.47
6:H:202:LEU:N	6:H:202:LEU:HD12	2.29	0.47
5:E:12:LEU:HD23	5:E:88:ILE:HG21	1.96	0.47
5:E:138:LYS:O	5:E:195:VAL:HA	2.15	0.47
5:F:13:LYS:NZ	5:F:82:ALA:O	2.43	0.47
6:H:251:GLN:O	6:H:254:LYS:NZ	2.43	0.47
1:A:240:SER:HA	1:A:241:PHE:HA	1.62	0.47
1:A:810:ALA:HA	1:A:825:ASP:O	2.15	0.47
1:A:1054:LEU:HD23	2:B:107:ILE:HD13	1.96	0.47
1:A:1039:LYS:O	1:A:1040:GLU:CB	2.62	0.46
6:H:27:PHE:CE1	6:H:78:GLY:CA	2.97	0.46
6:H:167:VAL:HG12	6:H:188:PRO:HG2	1.96	0.46
5:E:240:LYS:HD3	5:E:246:HIS:HB3	1.96	0.46
6:H:63:HIS:CD2	6:H:137:HIS:HB2	2.50	0.46
5:E:252:ALA:CA	6:H:340:LEU:CD2	2.93	0.46
1:A:1088:ASP:O	1:A:1091:ASP:OD1	2.32	0.46
1:A:360:CYS:SG	1:A:361:ALA:N	2.84	0.46
5:E:252:ALA:CA	6:H:340:LEU:HD23	2.43	0.46
5:G:50:LEU:HD13	5:G:247:LEU:HD13	1.97	0.46
6:H:135:LYS:HA	6:H:138:ASN:HB3	1.97	0.46
2:B:240:ARG:NH2	2:B:293:ASP:OD2	2.37	0.46
6:H:3:ILE:N	6:H:3:ILE:CD1	2.79	0.46
1:A:163:ASP:HA	1:A:166:ARG:HB2	1.98	0.46
5:F:51:THR:O	5:F:245:GLY:HA3	2.16	0.46
4:D:50:ARG:HG3	4:D:101:LEU:HD21	1.96	0.46
5:E:137:VAL:HA	5:E:196:THR:O	2.16	0.46
6:H:64:LEU:HA	6:H:67:MET:HB2	1.97	0.46
6:H:199:ALA:O	6:H:200:LYS:C	2.54	0.46
6:H:239:ARG:HG3	6:H:239:ARG:HH11	1.80	0.46
2:B:83:CYS:HB3	2:B:140:GLN:HE22	1.80	0.46
5:E:134:SER:HA	5:E:200:ASN:HD21	1.81	0.46
5:F:159:VAL:HA	5:F:205:LEU:O	2.16	0.46
1:A:1098:ARG:HG2	1:A:1098:ARG:NH2	2.31	0.46
2:B:439:LEU:HG	2:B:450:ILE:HD11	1.98	0.45
3:C:104:GLN:NE2	3:C:106:ALA:O	2.49	0.45
6:H:67:MET:HE1	6:H:145:LEU:HD11	1.97	0.45
6:H:37:MET:HE1	6:H:178:GLU:HB2	1.98	0.45
5:G:5:ARG:HB3	5:G:59:THR:HB	1.99	0.45
6:H:167:VAL:HG12	6:H:188:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:140:PRO:HG3	5:E:193:GLU:HA	1.98	0.45
6:H:3:ILE:HG12	6:H:227:CYS:HB3	1.98	0.45
6:H:6:LEU:HD22	6:H:10:ILE:CD1	2.47	0.45
6:H:219:ASN:CB	6:H:222:GLN:HE21	2.29	0.45
2:B:246:ASN:H	2:B:297:GLY:HA3	1.82	0.45
5:E:128:ILE:HD12	6:H:344:PHE:CE2	2.51	0.45
6:H:215:GLU:C	6:H:217:GLY:H	2.19	0.45
2:B:366:GLU:HG3	2:B:415:ILE:HD13	1.99	0.45
1:A:843:LEU:HD22	1:A:867:VAL:HG11	1.99	0.45
2:B:70:GLN:HG2	2:B:77:VAL:HG11	1.99	0.45
6:H:35:ALA:HB3	6:H:84:VAL:O	2.17	0.45
6:H:204:ILE:HD11	6:H:206:GLU:HG3	1.99	0.45
6:H:238:ILE:O	6:H:240:GLY:N	2.50	0.45
1:A:834:ARG:HH21	1:A:921:ARG:HH11	1.65	0.45
1:A:1030:GLN:H	1:A:1031:PRO:HD2	1.82	0.45
6:H:298:TRP:HE3	6:H:298:TRP:H	1.64	0.45
6:H:202:LEU:HA	6:H:203:PRO:HD3	1.84	0.45
6:H:135:LYS:HD2	6:H:135:LYS:O	2.17	0.44
1:A:736:GLU:OE2	1:A:751:VAL:N	2.39	0.44
5:G:26:ALA:HB3	5:G:72:LEU:HD21	1.99	0.44
5:G:94:ASP:OD1	5:G:94:ASP:N	2.50	0.44
6:H:134:THR:C	6:H:136:GLN:N	2.70	0.44
6:H:134:THR:O	6:H:137:HIS:CD2	2.71	0.44
6:H:244:LYS:HE3	6:H:244:LYS:HB2	1.86	0.44
5:E:126:LEU:HD12	5:E:126:LEU:C	2.38	0.44
5:F:151:LEU:HD22	5:F:171:ALA:HB3	1.99	0.44
1:A:164:LEU:CB	1:A:190:VAL:HG11	2.41	0.44
1:A:187:VAL:O	1:A:187:VAL:HG13	2.18	0.44
2:B:161:VAL:HG23	2:B:176:TYR:HB3	2.00	0.44
5:G:212:LEU:O	5:G:216:THR:OG1	2.29	0.44
5:E:252:ALA:HB2	6:H:340:LEU:HG	1.99	0.44
5:G:79:LEU:HA	5:G:103:PHE:HZ	1.82	0.44
6:H:166:LEU:O	6:H:169:ALA:N	2.50	0.44
6:H:91:GLN:HA	6:H:91:GLN:OE1	2.17	0.44
2:B:193:ASP:N	2:B:193:ASP:OD1	2.49	0.44
5:E:128:ILE:HD11	6:H:344:PHE:CE2	2.52	0.44
6:H:10:ILE:HD13	6:H:212:ILE:HD11	1.99	0.44
6:H:200:LYS:CB	6:H:202:LEU:HD13	2.47	0.44
5:E:56:GLY:HA3	5:E:244:MET:HA	1.99	0.44
6:H:220:GLN:O	6:H:224:VAL:HG23	2.18	0.44
1:A:1078:ILE:CG1	10:A:1202:SF4:S1	2.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:236:GLU:HG3	6:H:271:PRO:HB3	2.00	0.43
1:A:594:TYR:HB2	1:A:801:TYR:HB3	2.00	0.43
1:A:815:SER:OG	1:A:819:ASP:OD2	2.35	0.43
3:C:128:ASN:N	3:C:128:ASN:OD1	2.51	0.43
4:D:66:ARG:HG2	4:D:88:LEU:HD11	2.01	0.43
5:F:238:GLU:HG3	5:F:248:LYS:HG2	2.00	0.43
1:A:682:ARG:HA	1:A:685:VAL:HG22	2.00	0.43
5:F:133:TYR:HA	5:F:230:SER:HB2	1.99	0.43
5:G:12:LEU:HA	5:G:15:VAL:HB	2.00	0.43
6:H:30:LYS:C	6:H:172:VAL:HG22	2.38	0.43
6:H:204:ILE:HD12	6:H:205:GLN:N	2.33	0.43
5:E:25:GLU:OE2	5:E:121:LEU:HD22	2.19	0.43
5:E:124:GLU:HA	6:H:349:SER:OG	2.19	0.43
5:E:128:ILE:HD12	6:H:344:PHE:CE1	2.54	0.43
5:E:254:LYS:HA	6:H:338:GLY:H	1.83	0.43
6:H:254:LYS:O	6:H:255:SER:HB3	2.18	0.43
1:A:687:ASP:OD1	1:A:690:GLN:NE2	2.50	0.43
5:E:162:CYS:HB3	5:E:199:MET:HE1	2.00	0.43
5:F:141:SER:HB3	5:F:225:VAL:HG13	2.01	0.43
6:H:63:HIS:C	6:H:64:LEU:HD23	2.38	0.43
6:H:218:LEU:HD12	6:H:218:LEU:O	2.19	0.43
6:H:239:ARG:HG3	6:H:239:ARG:NH1	2.33	0.43
1:A:1030:GLN:N	1:A:1031:PRO:HD2	2.34	0.43
1:A:617:CYS:SG	1:A:618:TYR:N	2.92	0.43
5:E:254:LYS:HD2	6:H:337:GLN:CB	2.49	0.43
5:G:83:GLY:N	5:G:86:ASP:OD2	2.52	0.43
1:A:1098:ARG:CG	1:A:1098:ARG:HH21	2.32	0.43
6:H:10:ILE:CG2	6:H:18:ILE:HD11	2.49	0.43
1:A:594:TYR:HE2	1:A:762:ARG:HH11	1.67	0.42
1:A:830:GLU:HG3	1:A:965:PRO:HB3	1.99	0.42
6:H:225:ASP:HB3	6:H:250:ILE:HD11	2.01	0.42
1:A:188:LEU:CA	1:A:213:THR:O	2.62	0.42
2:B:378:ALA:HA	2:B:379:PRO:HA	1.81	0.42
2:B:137:ASP:OD1	2:B:138:GLU:N	2.45	0.42
5:E:234:PRO:CB	6:H:344:PHE:CZ	2.93	0.42
6:H:275:LEU:O	6:H:277:LYS:N	2.52	0.42
2:B:131:ASP:OD1	2:B:131:ASP:N	2.52	0.42
6:H:311:CYS:SG	6:H:321:ILE:HB	2.60	0.42
1:A:137:VAL:HG22	1:A:286:LEU:HB2	2.00	0.42
1:A:618:TYR:OH	1:A:711:LEU:O	2.31	0.42
1:A:740:THR:HA	1:A:748:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ASP:OD1	2:B:168:ASP:N	2.47	0.42
2:B:407:THR:HG21	2:B:427:THR:HB	2.01	0.42
3:C:108:LEU:H	3:C:108:LEU:HG	1.73	0.42
5:E:44:HIS:HD2	6:H:339:ARG:CG	2.32	0.42
5:E:223:SER:OG	5:E:224:THR:N	2.53	0.42
1:A:421:LEU:HD22	1:A:421:LEU:N	2.33	0.42
5:G:95:ASN:OD1	5:G:95:ASN:N	2.52	0.42
6:H:29:ARG:NH1	6:H:173:TYR:CE2	2.87	0.42
6:H:139:ASP:HA	6:H:142:LYS:HD3	2.01	0.42
4:D:61:CYS:HB2	4:D:69:ARG:HH21	1.85	0.42
6:H:190:LEU:HD12	6:H:191:MET:N	2.34	0.42
6:H:192:ARG:O	6:H:193:HIS:HB2	2.20	0.42
6:H:197:SER:HB3	6:H:200:LYS:HG2	2.01	0.42
6:H:272:GLU:HG3	6:H:273:ASN:N	2.31	0.42
3:C:62:LEU:HD12	3:C:79:VAL:HG22	2.01	0.42
5:F:7:VAL:HG23	5:F:8:GLN:HG3	2.02	0.42
6:H:265:PRO:C	6:H:267:LYS:N	2.73	0.42
1:A:385:ILE:HG21	1:A:421:LEU:HD12	2.02	0.42
6:H:194:LEU:O	6:H:194:LEU:CG	2.67	0.42
6:H:26:TYR:CD1	6:H:29:ARG:HD2	2.55	0.41
6:H:63:HIS:HD2	6:H:137:HIS:O	2.03	0.41
6:H:238:ILE:O	6:H:238:ILE:HG12	2.19	0.41
6:H:252:LYS:HD3	6:H:252:LYS:HA	1.92	0.41
1:A:260:ILE:HG22	1:A:297:SER:HB2	2.01	0.41
1:A:682:ARG:O	1:A:686:LEU:HG	2.20	0.41
6:H:134:THR:CG2	6:H:135:LYS:H	2.21	0.41
6:H:192:ARG:O	6:H:193:HIS:CB	2.68	0.41
6:H:202:LEU:N	6:H:202:LEU:CD1	2.84	0.41
1:A:523:LEU:HD12	1:A:528:VAL:HB	2.02	0.41
6:H:248:ASP:O	6:H:251:GLN:HB2	2.20	0.41
6:H:263:LEU:HD13	6:H:268:TYR:CB	2.50	0.41
6:H:139:ASP:C	6:H:141:CYS:N	2.73	0.41
1:A:579:GLU:O	1:A:707:GLN:NE2	2.51	0.41
5:E:252:ALA:H	6:H:340:LEU:HD21	1.85	0.41
5:G:209:LEU:HD23	5:G:212:LEU:HD12	2.03	0.41
6:H:245:ARG:HD2	6:H:245:ARG:HA	1.90	0.41
1:A:597:PRO:HD2	1:A:766:SER:HA	2.02	0.41
6:H:79:ILE:O	6:H:81:PRO:HD3	2.21	0.41
6:H:212:ILE:HG22	6:H:213:LEU:N	2.35	0.41
6:H:258:GLU:O	6:H:262:ARG:HG2	2.20	0.41
5:E:38:GLN:HE21	5:E:125:GLN:NE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:LEU:C	6:H:351:SER:HA	2.38	0.41
1:A:400:ASN:HD21	1:A:446:THR:HG23	1.85	0.41
1:A:1039:LYS:N	1:A:1039:LYS:HD3	2.33	0.41
4:D:105:TYR:O	4:D:107:LEU:N	2.54	0.41
5:G:162:CYS:SG	5:G:163:ALA:N	2.94	0.41
6:H:302:ASN:C	6:H:302:ASN:ND2	2.74	0.41
6:H:316:PHE:CD1	6:H:317:SER:N	2.88	0.41
1:A:186:ALA:C	1:A:188:LEU:HD23	2.41	0.41
5:F:182:LEU:HD12	5:F:182:LEU:HA	1.95	0.41
5:G:63:ASP:OD1	5:G:63:ASP:N	2.43	0.41
6:H:9:LEU:HD11	6:H:247:VAL:HG21	2.02	0.41
6:H:62:SER:C	6:H:64:LEU:N	2.75	0.41
1:A:367:LYS:HE3	1:A:369:GLN:HE21	1.85	0.40
1:A:1030:GLN:O	1:A:1033:GLU:HB2	2.21	0.40
5:E:40:MET:HE2	5:E:126:LEU:CG	2.51	0.40
5:E:151:LEU:HA	5:E:154:ILE:HD12	2.03	0.40
6:H:17:ALA:HB2	6:H:211:ARG:CG	2.52	0.40
6:H:135:LYS:HA	6:H:138:ASN:CB	2.51	0.40
1:A:323:LYS:HE3	1:A:323:LYS:HB3	1.92	0.40
5:G:14:LYS:HA	5:G:17:GLU:HB2	2.02	0.40
5:G:138:LYS:HB3	5:G:196:THR:HG22	2.02	0.40
6:H:3:ILE:CG2	6:H:6:LEU:HB2	2.48	0.40
6:H:308:LYS:NZ	6:H:308:LYS:CB	2.83	0.40
2:B:35:SER:O	2:B:333:GLN:NE2	2.54	0.40
5:E:159:VAL:HG13	5:E:170:SER:HB3	2.03	0.40
6:H:39:ILE:HA	6:H:42:PHE:HD2	1.86	0.40
6:H:200:LYS:C	6:H:202:LEU:H	2.24	0.40
6:H:284:LEU:C	6:H:286:PRO:HD3	2.42	0.40
5:E:234:PRO:HB2	6:H:344:PHE:HZ	1.84	0.40
5:E:179:ASN:OD1	5:E:179:ASN:N	2.54	0.40
6:H:143:HIS:C	6:H:145:LEU:N	2.75	0.40
6:H:180:MET:O	6:H:181:ALA:C	2.59	0.40
6:H:300:GLU:OE2	6:H:301:PRO:HD2	2.22	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	1003/1107 (91%)	933 (93%)	66 (7%)	4 (0%)	34	71
2	B	425/469 (91%)	398 (94%)	27 (6%)	0	100	100
3	C	141/474 (30%)	131 (93%)	10 (7%)	0	100	100
4	D	64/137 (47%)	49 (77%)	12 (19%)	3 (5%)	2	23
5	E	247/264 (94%)	239 (97%)	8 (3%)	0	100	100
5	F	243/264 (92%)	236 (97%)	7 (3%)	0	100	100
5	G	245/264 (93%)	229 (94%)	16 (6%)	0	100	100
6	H	300/380 (79%)	215 (72%)	63 (21%)	22 (7%)	1	15
All	All	2668/3359 (79%)	2430 (91%)	209 (8%)	29 (1%)	18	51

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	79	GLU
6	H	93	LYS
6	H	271	PRO
6	H	272	GLU
6	H	315	GLN
6	H	337	GLN
6	H	157	SER
6	H	200	LYS
6	H	239	ARG
6	H	254	LYS
6	H	333	GLN
6	H	201	LYS
6	H	264	ASP
1	A	85	PRO
6	H	36	SER
6	H	199	ALA
6	H	240	GLY

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Mol	Chain	Res	Type
6	H	262	ARG
6	H	305	GLU
6	H	317	SER
6	H	334	GLY
1	A	756	THR
1	A	1021	HIS
1	A	1040	GLU
4	D	106	PRO
6	H	216	LEU
4	D	105	TYR
6	H	90	PRO
6	H	231	GLY

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	857/944 (91%)	843 (98%)	14 (2%)	62	79
2	B	367/403 (91%)	364 (99%)	3 (1%)	81	89
3	C	125/413 (30%)	125 (100%)	0	100	100
4	D	59/120 (49%)	58 (98%)	1 (2%)	60	78
5	E	217/230 (94%)	217 (100%)	0	100	100
5	F	216/230 (94%)	215 (100%)	1 (0%)	88	93
5	G	217/230 (94%)	217 (100%)	0	100	100
6	H	232/321 (72%)	212 (91%)	20 (9%)	10	36
All	All	2290/2891 (79%)	2251 (98%)	39 (2%)	62	78

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	190	VAL
1	A	676	LYS

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Mol	Chain	Res	Type
1	A	701	TYR
1	A	889	ARG
1	A	910	ARG
1	A	993	THR
1	A	1019	LEU
1	A	1021	HIS
1	A	1032	ARG
1	A	1038	GLN
1	A	1039	LYS
1	A	1074	ARG
1	A	1098	ARG
2	B	44	ARG
2	B	180	ASP
2	B	220	ASP
4	D	79	GLU
5	F	153	HIS
6	H	6	LEU
6	H	13	VAL
6	H	27	PHE
6	H	67	MET
6	H	135	LYS
6	H	137	HIS
6	H	172	VAL
6	H	204	ILE
6	H	238	ILE
6	H	252	LYS
6	H	274	TRP
6	H	275	LEU
6	H	276	HIS
6	H	287	GLU
6	H	302	ASN
6	H	316	PHE
6	H	325	VAL
6	H	330	LYS
6	H	331	SER
6	H	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	369	GLN

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Mol	Chain	Res	Type
1	A	430	ASN
1	A	558	GLN
1	A	726	GLN
1	A	842	ASN
1	A	865	GLN
1	A	1021	HIS
1	A	1038	GLN
1	A	1043	HIS
1	A	1092	GLN
2	B	21	ASN
2	B	70	GLN
2	B	140	GLN
3	C	116	ASN
5	E	38	GLN
5	E	44	HIS
5	F	65	ASN
5	G	108	GLN
5	G	204	GLN
5	G	246	HIS
6	H	4	GLN
6	H	21	ASN
6	H	63	HIS
6	H	77	ASN
6	H	137	HIS
6	H	193	HIS
6	H	222	GLN
6	H	253	HIS
6	H	273	ASN
6	H	302	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#|Z| > 2$
7	DOC	P	25	8,7	16,19,20	4.81	12 (75%)	20,26,29	1.92	4 (20%)

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
7	DOC	P	25	8,7	-	2/7/18/19	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	25	DOC	C3'-C2'	-8.38	1.31	1.54
7	P	25	DOC	O4'-C4'	-8.26	1.28	1.44
7	P	25	DOC	C2-N3	6.05	1.48	1.36
7	P	25	DOC	O4'-C1'	5.89	1.55	1.42
7	P	25	DOC	C6-C5	5.89	1.48	1.35
7	P	25	DOC	C1'-N1	-5.43	1.34	1.48
7	P	25	DOC	C4-N4	5.39	1.46	1.33
7	P	25	DOC	C4-N3	4.95	1.44	1.34
7	P	25	DOC	C2-N1	3.82	1.48	1.40
7	P	25	DOC	O2-C2	-3.07	1.18	1.23
7	P	25	DOC	C6-N1	2.63	1.44	1.38
7	P	25	DOC	C5-C4	2.29	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	25	DOC	C4'-O4'-C1'	-6.07	104.08	109.81
7	P	25	DOC	C3'-C2'-C1'	3.09	106.35	102.78
7	P	25	DOC	C2'-C3'-C4'	2.22	106.88	102.72
7	P	25	DOC	C6-C5-C4	2.02	120.76	117.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	25	DOC	C3'-C4'-C5'-O5'
7	P	25	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5   Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
11	TTP	A	1203	-	26,30,30	4.24	14 (53%)	39,47,47	2.09	14 (35%)
10	SF4	A	1202	1	0,12,12	-	-	-		

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
11	TTP	A	1203	-	-	3/22/34/34	0/2/2/2
10	SF4	A	1202	1	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1203	TTP	C2'-C3'	-11.63	1.22	1.52
11	A	1203	TTP	C6-C5	8.22	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1203	TTP	O4'-C4'	-7.86	1.27	1.45
11	A	1203	TTP	C2-N3	6.35	1.49	1.38
11	A	1203	TTP	C2-N1	6.12	1.48	1.38
11	A	1203	TTP	C1'-N1	-5.28	1.34	1.48
11	A	1203	TTP	C3'-C4'	4.42	1.65	1.53
11	A	1203	TTP	C6-N1	3.73	1.44	1.38
11	A	1203	TTP	O4'-C1'	3.46	1.50	1.42
11	A	1203	TTP	C4-N3	3.32	1.45	1.38
11	A	1203	TTP	O3'-C3'	2.92	1.49	1.43
11	A	1203	TTP	O4-C4	-2.86	1.18	1.23
11	A	1203	TTP	O2-C2	-2.71	1.18	1.23
11	A	1203	TTP	C4-C5	2.35	1.48	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1203	TTP	C4-N3-C2	-6.10	119.46	127.35
11	A	1203	TTP	C5-C4-N3	4.97	119.55	115.31
11	A	1203	TTP	N3-C2-N1	4.63	121.04	114.89
11	A	1203	TTP	O4-C4-C5	-3.79	120.51	124.90
11	A	1203	TTP	C6-C5-C4	2.74	120.32	118.03
11	A	1203	TTP	C5M-C5-C6	-2.64	119.33	122.85
11	A	1203	TTP	C5-C6-N1	-2.51	120.76	123.34
11	A	1203	TTP	O2-C2-N1	-2.50	119.46	122.79
11	A	1203	TTP	C6-N1-C2	-2.40	118.86	121.30
11	A	1203	TTP	C2'-C1'-N1	-2.28	108.52	113.77
11	A	1203	TTP	O4'-C1'-N1	2.18	111.75	107.86
11	A	1203	TTP	C3'-C2'-C1'	2.13	107.86	102.54
11	A	1203	TTP	PB-O3A-PA	-2.08	125.70	132.83
11	A	1203	TTP	PB-O3B-PG	-2.01	125.92	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1203	TTP	O4'-C4'-C5'-O5'
11	A	1203	TTP	C3'-C4'-C5'-O5'
11	A	1203	TTP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1202	SF4	2	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TTP A 1203

Bond lengths

Bond angles

Torsions

Rings
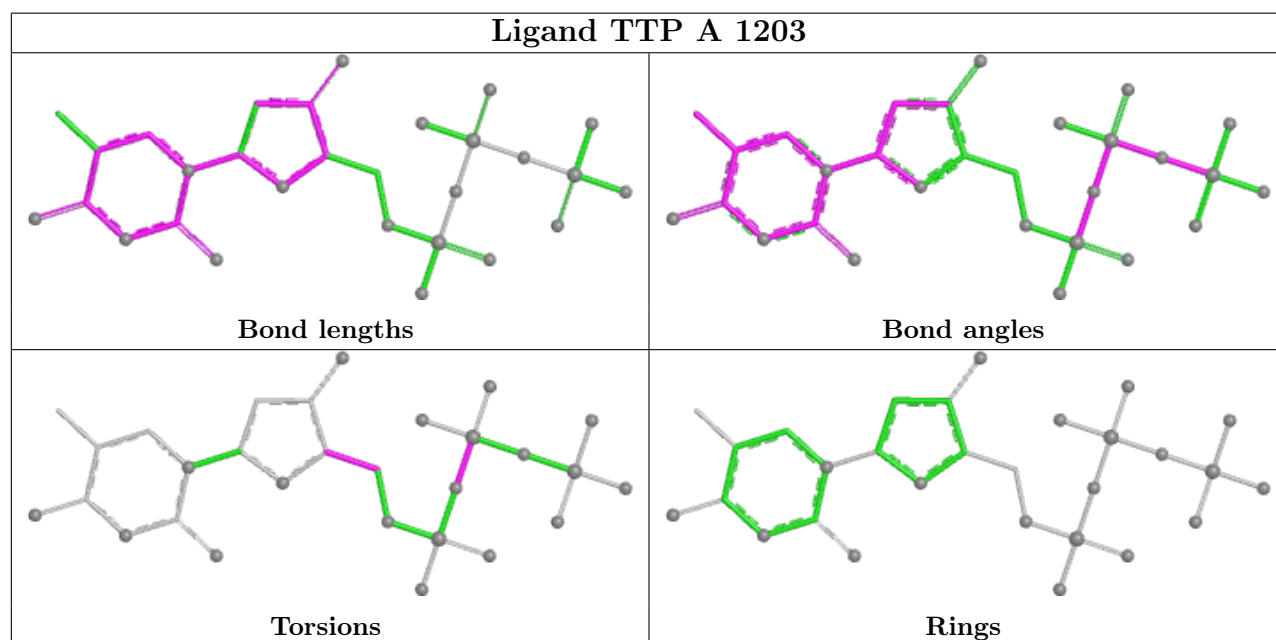
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-10540. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1   Orthogonal projections ⓘ

6.1.1   Primary map

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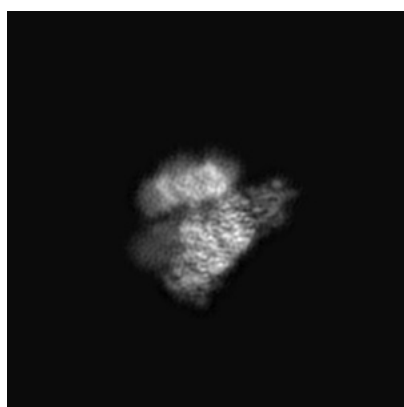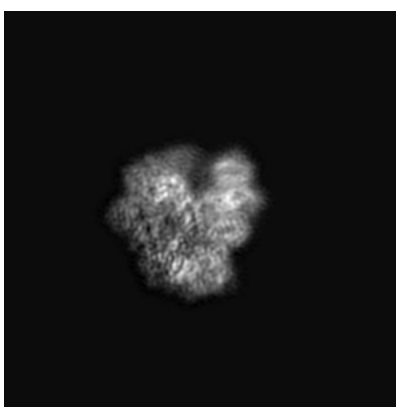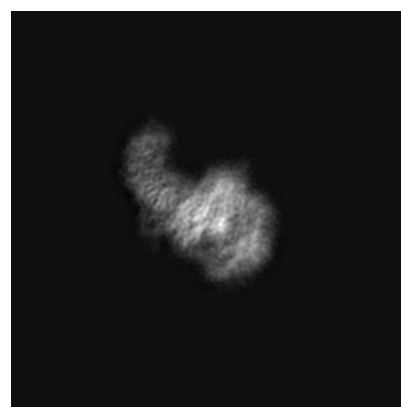
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
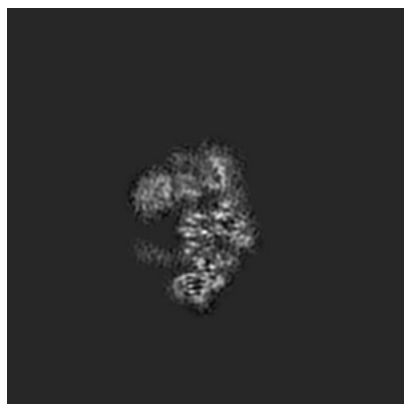
6.2.1   Primary map
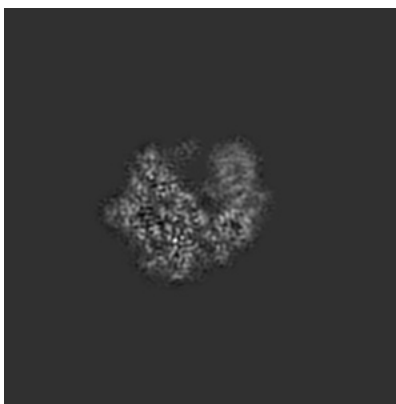
X Index: 200   Y Index: 200   Z Index: 200
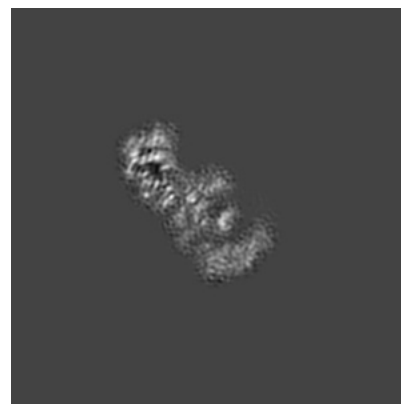
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
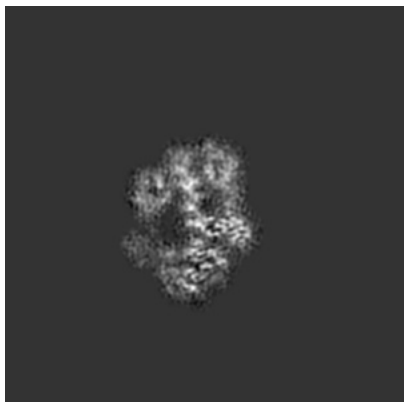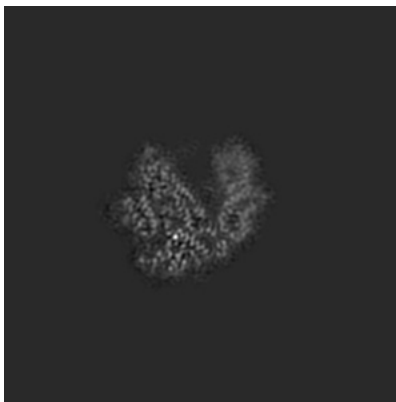
| X Index: 209 | Y Index: 204 | Z Index: 220 |
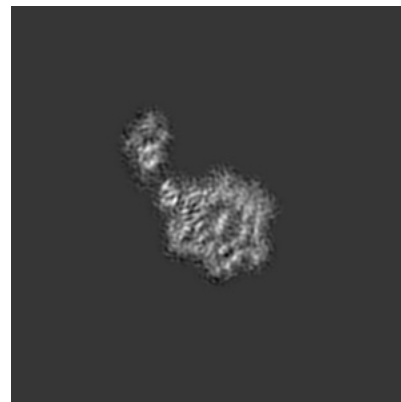
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map
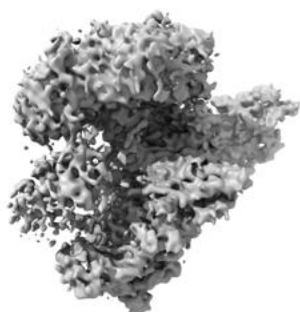
| X | Y | Z |
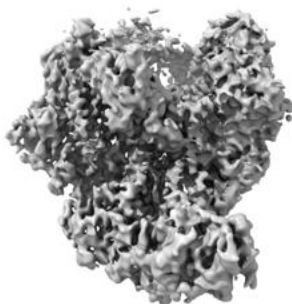
The images above show the 3D surface view of the map at the recommended contour level 0.0073. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

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

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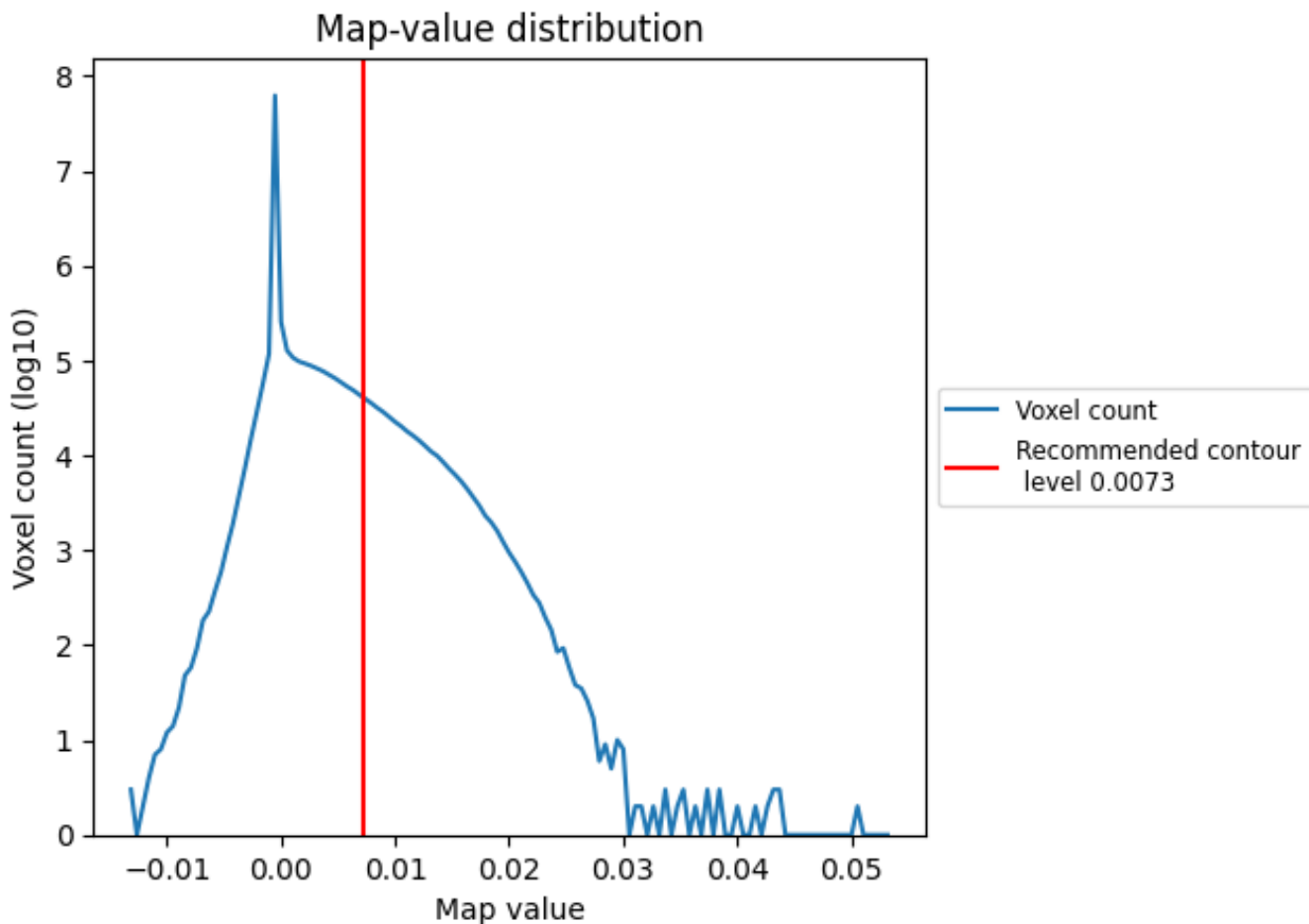
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
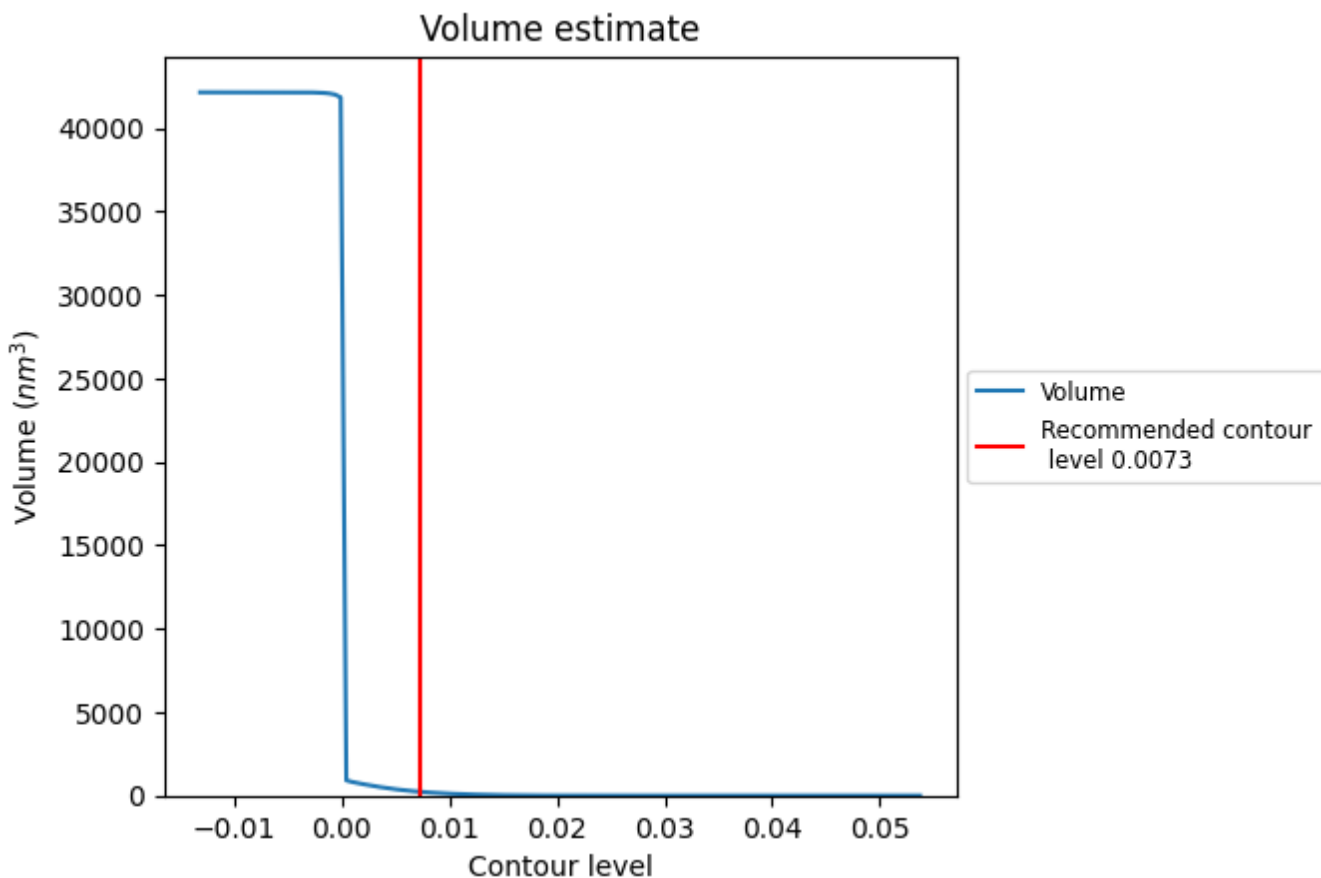
The volume at the recommended contour level is 225 nm^3; this corresponds to an approximate mass of 204 kDa.

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 (i)
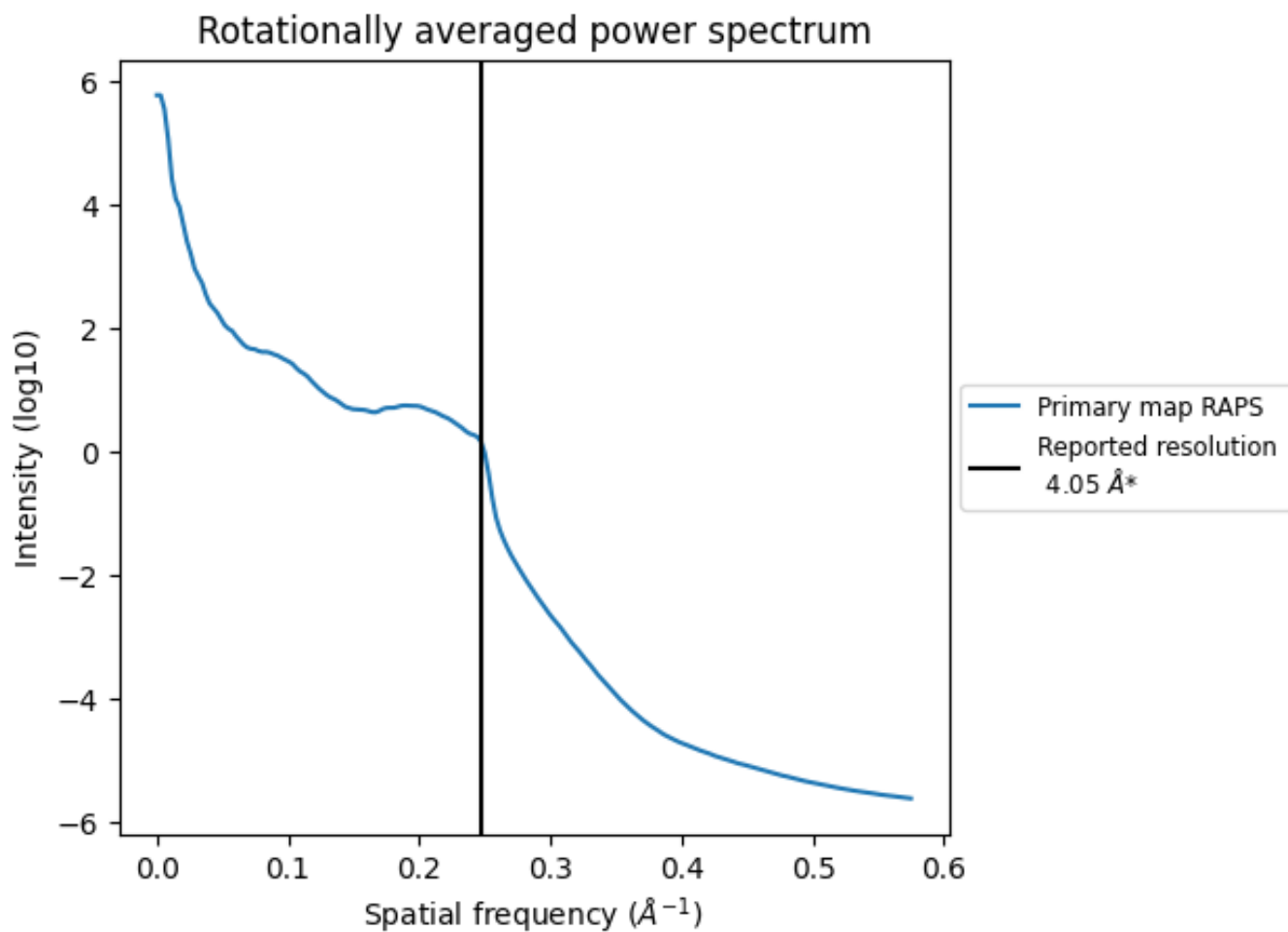
*Reported resolution corresponds to spatial frequency of 0.247 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
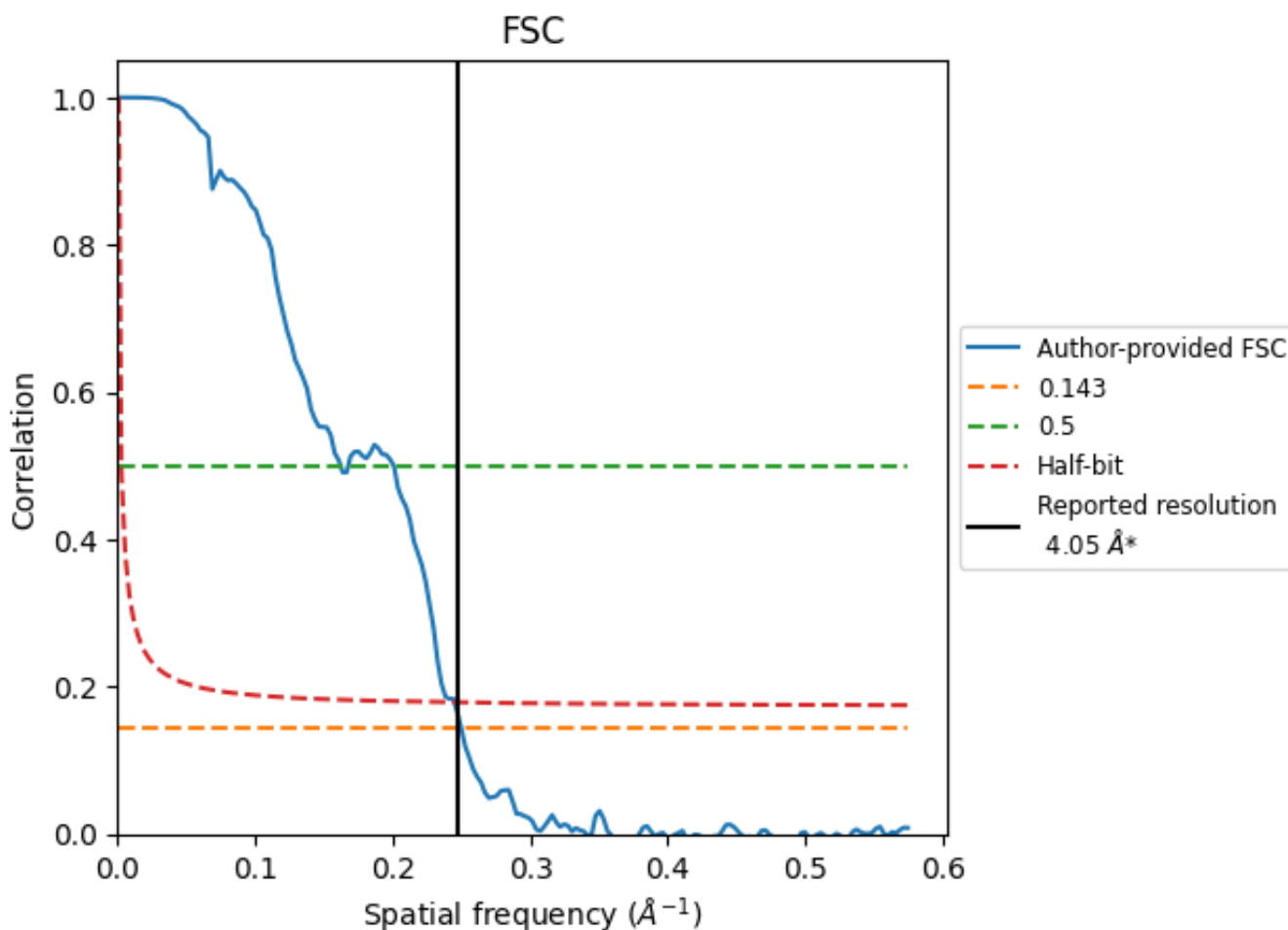
*Reported resolution corresponds to spatial frequency of 0.247 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.00	6.17	4.08
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10540 and PDB model 6TNZ. Per-residue inclusion information can be found in section .

9.1 Map-model overlay ⓘ
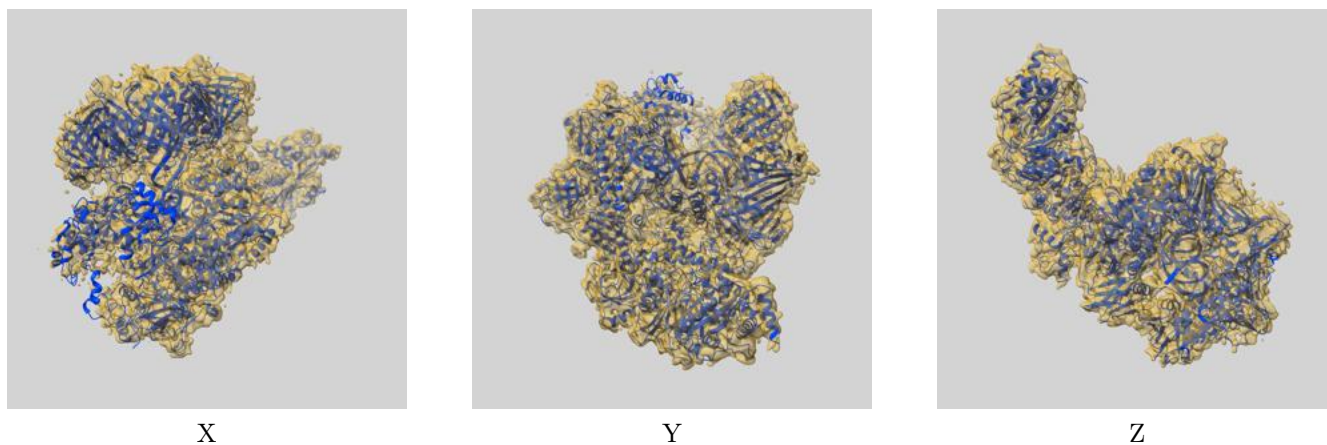
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0073 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 ⓘ

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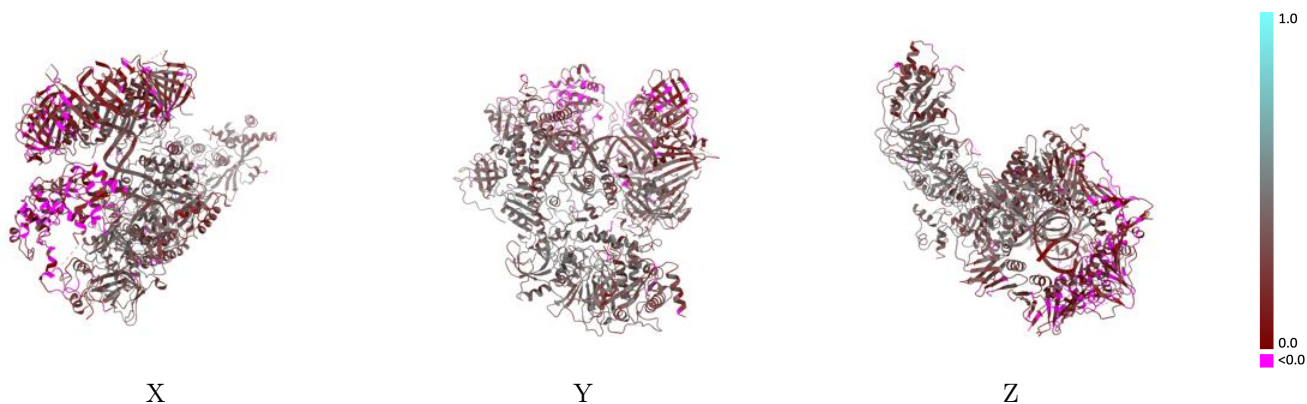
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X　　　　　　　　　　　Y　　　　　　　　　　　Z
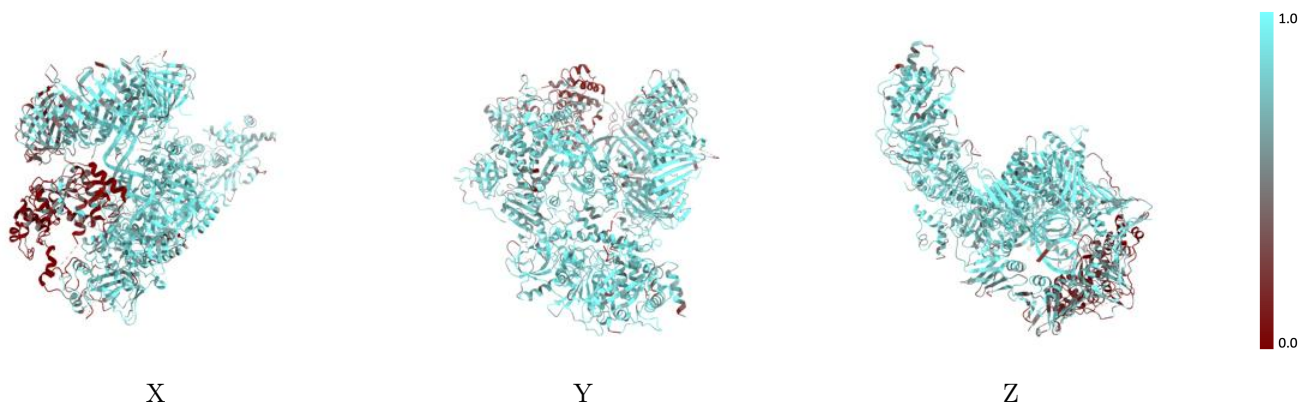
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0073).

9.4 Atom inclusion (i)
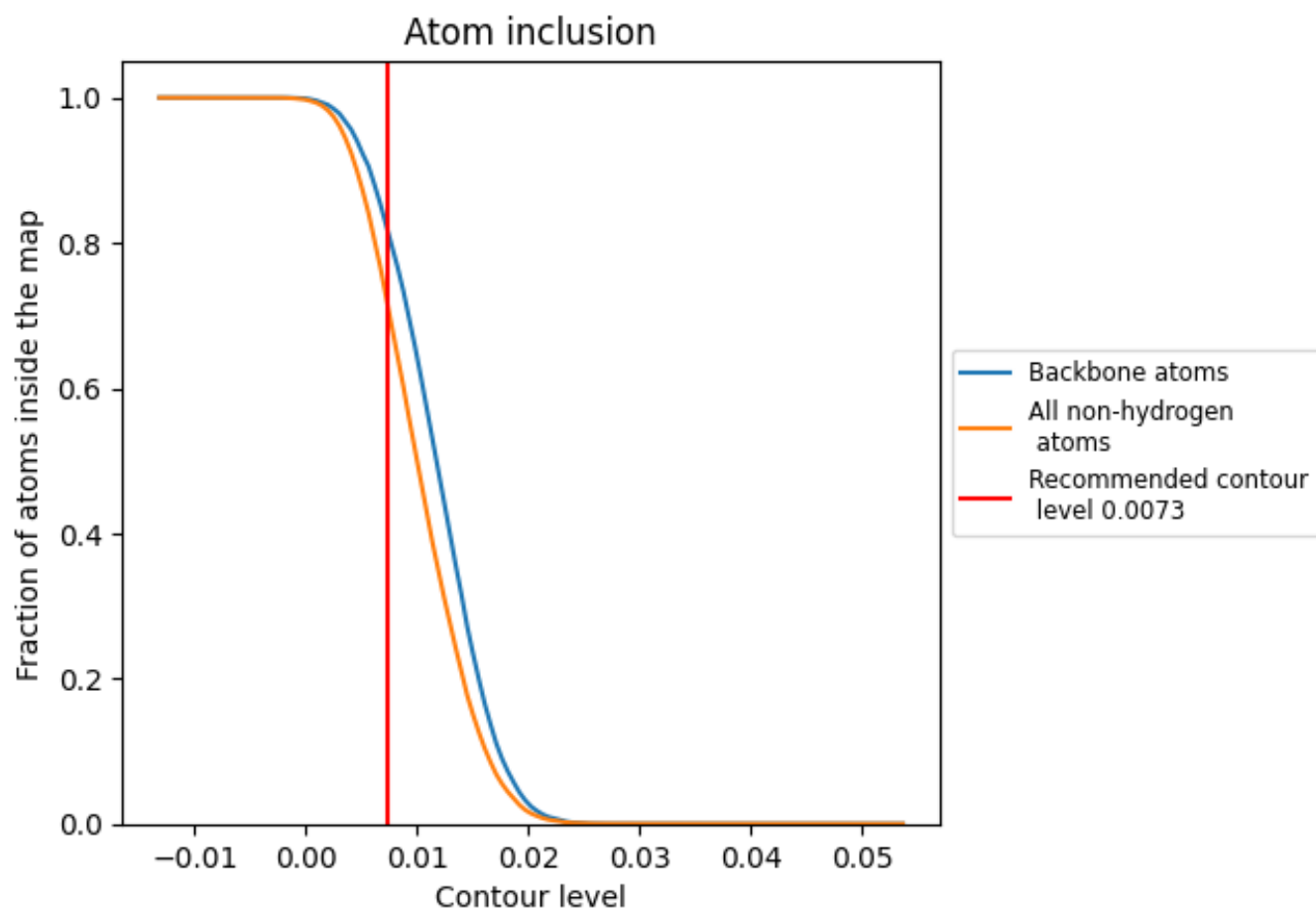
At the recommended contour level, 82% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary   (i)

The table lists the average atom inclusion at the recommended contour level (0.0073) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7201	0.2830
A	0.7894	0.3420
B	0.8132	0.3860
C	0.7574	0.3090
D	0.7955	0.3810
E	0.6216	0.1430
F	0.8232	0.3340
G	0.7697	0.1720
H	0.1817	0.0570
P	0.8806	0.2780
T	0.9189	0.3140

1.0

0.0
<0.0