Full wwPDB EM Validation Report ⓘ

May 6, 2023 – 01:39 PM EDT

PDB ID	:	8EBW
EMDB ID	:	EMD-28000
Title	:	Initial DNA-lesion (AP) binding by XPC and TFIIH complex2
Authors	:	Kim, J.; Yang, W.
Deposited on	:	2022-08-31
Resolution	:	5.60 Å(reported)
Based on initial model	:	6NMI

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:

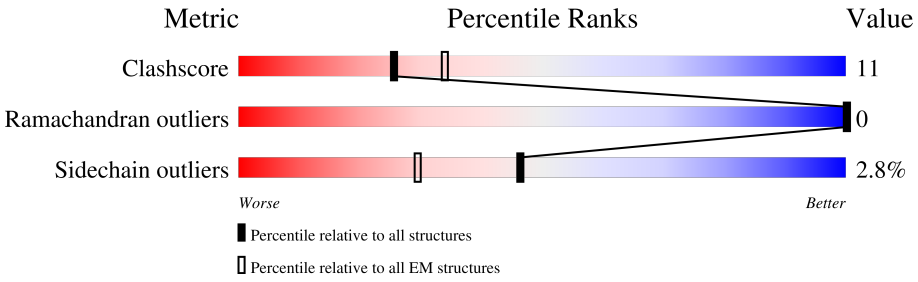
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.60 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	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	782	53% 24% 21%
2	B	768	46% 71% 27%
3	C	548	20% 41% 14% 44%
4	D	462	67% 28%
5	E	417	13% 59% 25% 15%
6	F	308	8% 57% 27% 15%
7	G	71	8% 59% 30% 6% 6%
8	H	950	30% 40% 16% 44%

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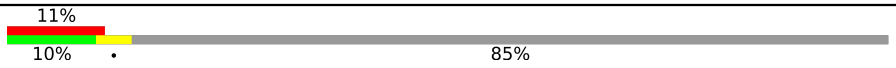
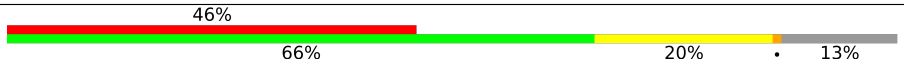
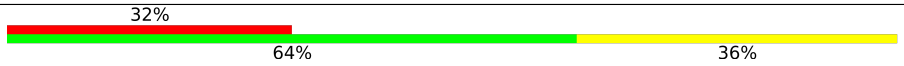
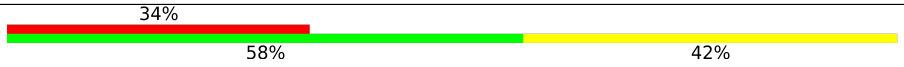
Mol	Chain	Length	Quality of chain
9	I	417	
10	J	172	
11	L	53	
12	M	53	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 30759 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 TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	614	Total	C	N	O	S	0	0
			4955	3163	857	905	30		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	760	Total	C	N	O	S	0	0
			6120	3907	1067	1117	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	761	ASP	-	expression tag	UNP P18074
B	762	TYR	-	expression tag	UNP P18074
B	763	LYS	-	expression tag	UNP P18074
B	764	ASP	-	expression tag	UNP P18074
B	765	ASP	-	expression tag	UNP P18074
B	766	ASP	-	expression tag	UNP P18074
B	767	ASP	-	expression tag	UNP P18074
B	768	LYS	-	expression tag	UNP P18074

- Molecule 3 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	309	Total	C	N	O	S	0	0
			2511	1596	441	461	13		

- Molecule 4 is a protein called General transcription factor IIH subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	446	Total	C	N	O	S	0	0
			3557	2289	620	635	13		

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	355	Total	C	N	O	S	0	0
			2792	1760	483	522	27		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	MET	-	initiating methionine	UNP Q13888
E	-20	GLY	-	expression tag	UNP Q13888
E	-19	SER	-	expression tag	UNP Q13888
E	-18	SER	-	expression tag	UNP Q13888
E	-17	HIS	-	expression tag	UNP Q13888
E	-16	HIS	-	expression tag	UNP Q13888
E	-15	HIS	-	expression tag	UNP Q13888
E	-14	HIS	-	expression tag	UNP Q13888
E	-13	HIS	-	expression tag	UNP Q13888
E	-12	HIS	-	expression tag	UNP Q13888
E	-11	SER	-	expression tag	UNP Q13888
E	-10	SER	-	expression tag	UNP Q13888
E	-9	GLY	-	expression tag	UNP Q13888
E	-8	LEU	-	expression tag	UNP Q13888
E	-7	GLU	-	expression tag	UNP Q13888
E	-6	VAL	-	expression tag	UNP Q13888
E	-5	LEU	-	expression tag	UNP Q13888
E	-4	PHE	-	expression tag	UNP Q13888
E	-3	GLN	-	expression tag	UNP Q13888
E	-2	GLY	-	expression tag	UNP Q13888
E	-1	PRO	-	expression tag	UNP Q13888
E	0	HIS	-	expression tag	UNP Q13888

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	261	Total	C	N	O	S	0	0
			2057	1316	341	381	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	67	Total	C	N	O	S	0	0
			530	342	84	101	3		

- Molecule 8 is a protein called Xeroderma pigmentosum, complementation group C, isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	532	Total	C	N	O	S	0	0
			4364	2790	772	782	20		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	MET	-	initiating methionine	UNP A0A024R2M8
H	-8	ASP	-	expression tag	UNP A0A024R2M8
H	-7	TYR	-	expression tag	UNP A0A024R2M8
H	-6	LYS	-	expression tag	UNP A0A024R2M8
H	-5	ASP	-	expression tag	UNP A0A024R2M8
H	-4	ASP	-	expression tag	UNP A0A024R2M8
H	-3	ASP	-	expression tag	UNP A0A024R2M8
H	-2	ASP	-	expression tag	UNP A0A024R2M8
H	-1	LYS	-	expression tag	UNP A0A024R2M8
H	0	HIS	-	expression tag	UNP A0A024R2M8
H	499	VAL	ALA	conflict	UNP A0A024R2M8

- Molecule 9 is a protein called UV excision repair protein RAD23 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	61	Total	C	N	O	S	0	0
			504	316	95	91	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	410	LEU	-	expression tag	UNP P54727
I	411	GLU	-	expression tag	UNP P54727
I	412	HIS	-	expression tag	UNP P54727
I	413	HIS	-	expression tag	UNP P54727
I	414	HIS	-	expression tag	UNP P54727
I	415	HIS	-	expression tag	UNP P54727
I	416	HIS	-	expression tag	UNP P54727
I	417	HIS	-	expression tag	UNP P54727

- Molecule 10 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	149	Total	C	N	O	S	1	0
			1201	749	194	251	7		

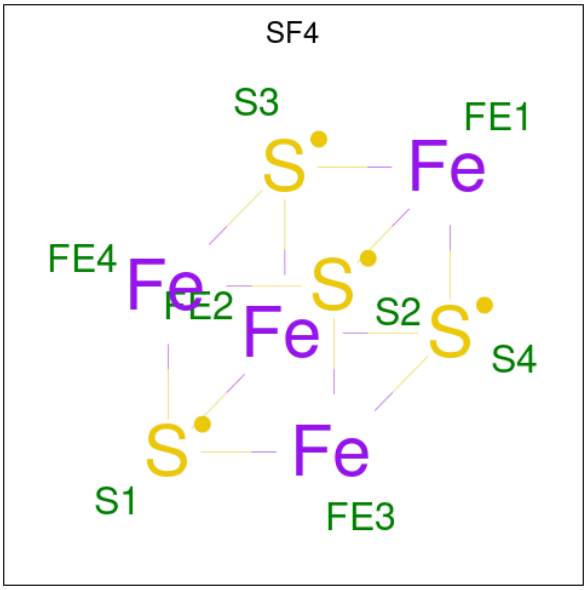
- Molecule 11 is a DNA chain called DNA (Ap).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	53	Total	C	N	O	P	0	0
			1075	510	196	316	53		

- Molecule 12 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	53	Total	C	N	O	P	0	0
			1078	515	190	320	53		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	E	3	Total	Zn	0
			3	3	

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Mol	Chain	Residues	Atoms	AltConf
14	F	2	Total Zn 2 2	0

- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

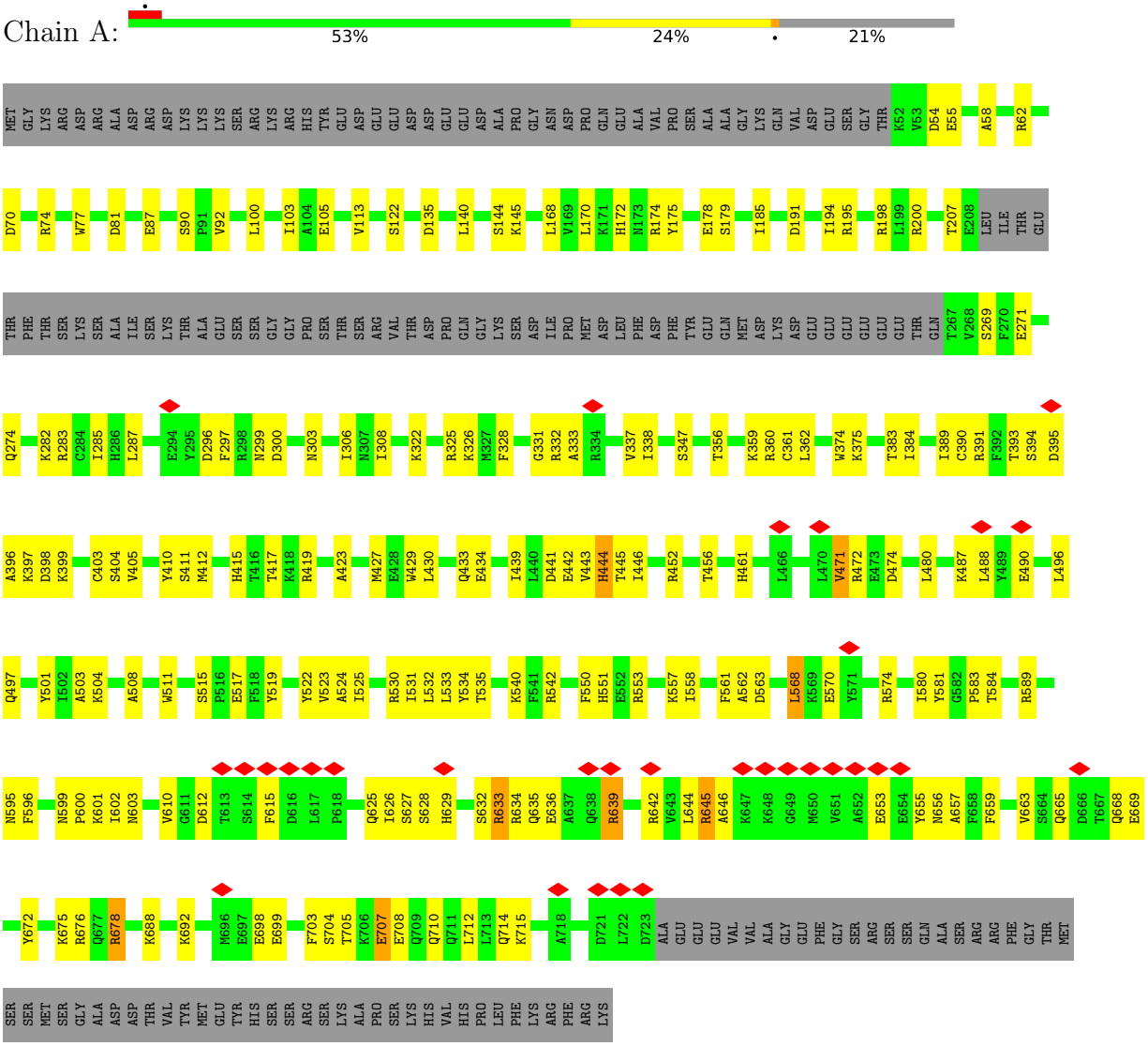
Mol	Chain	Residues	Atoms	AltConf
15	J	2	Total Ca 2 2	0

3 Residue-property plots (i)

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.

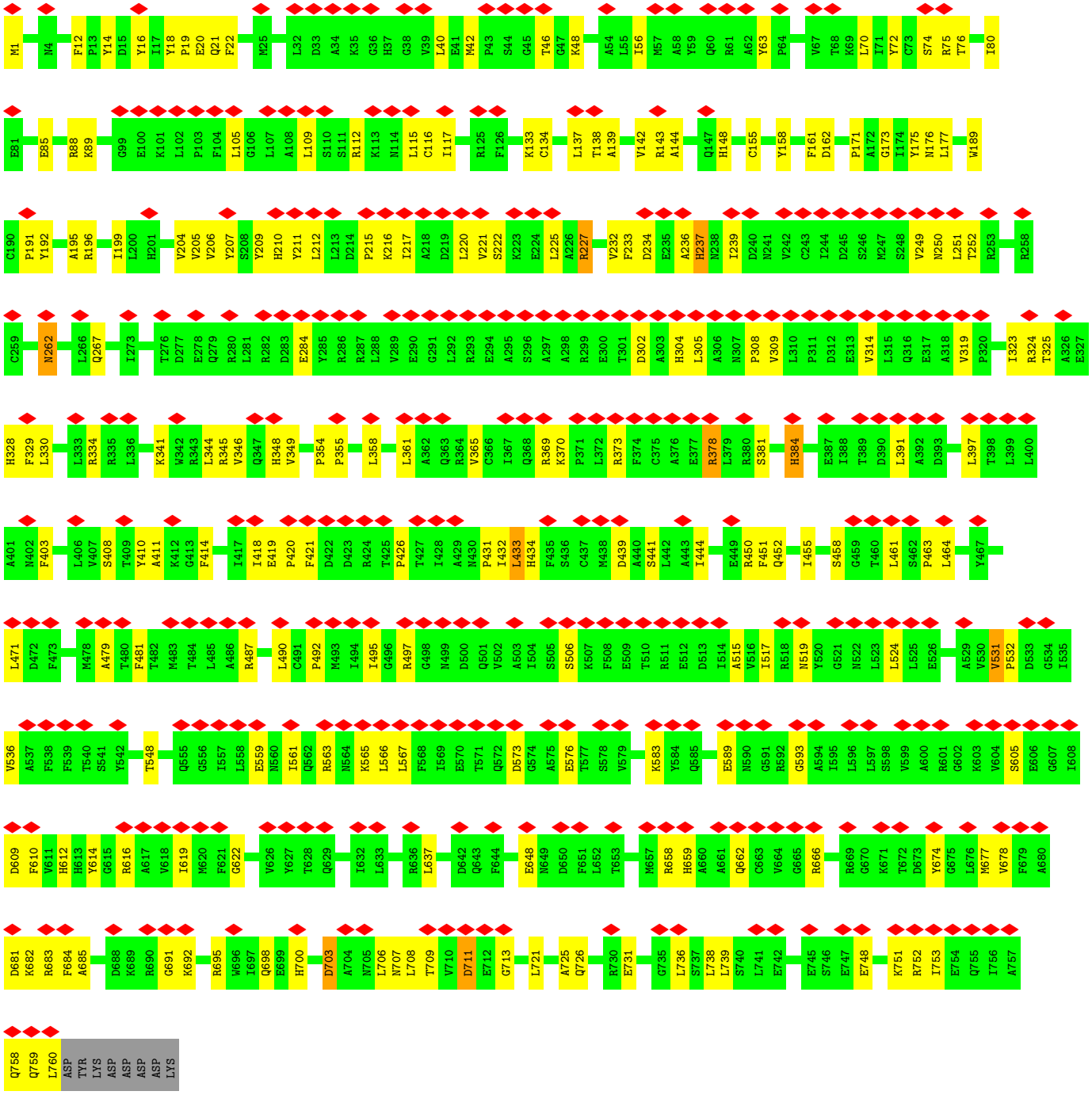
• Molecule 1: TFIIH basal transcription factor complex helicase XPB subunit

Chain A:



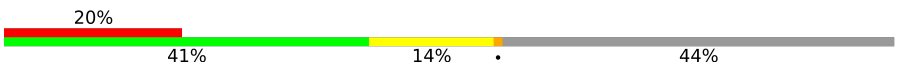
• Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD

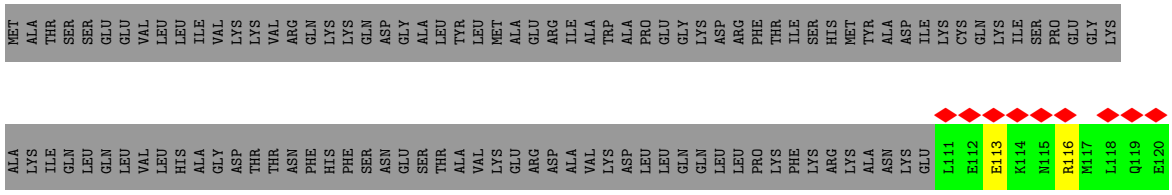
Chain B:

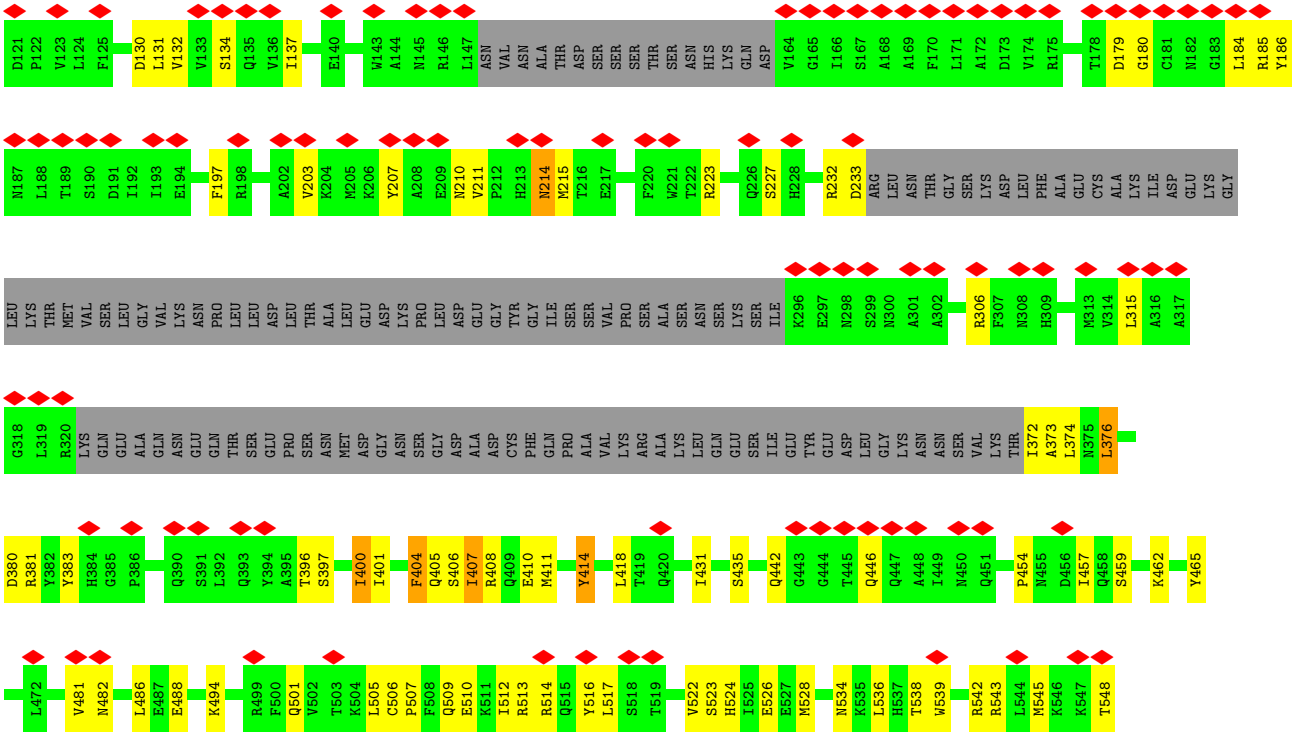


• Molecule 3: General transcription factor IIH subunit 1

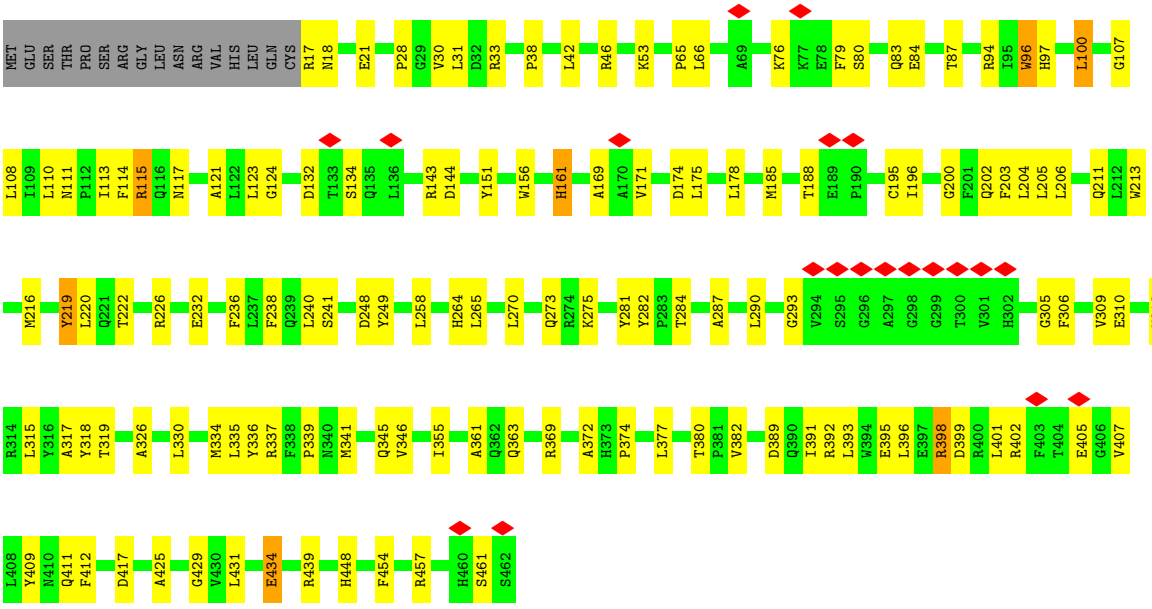
Chain C:



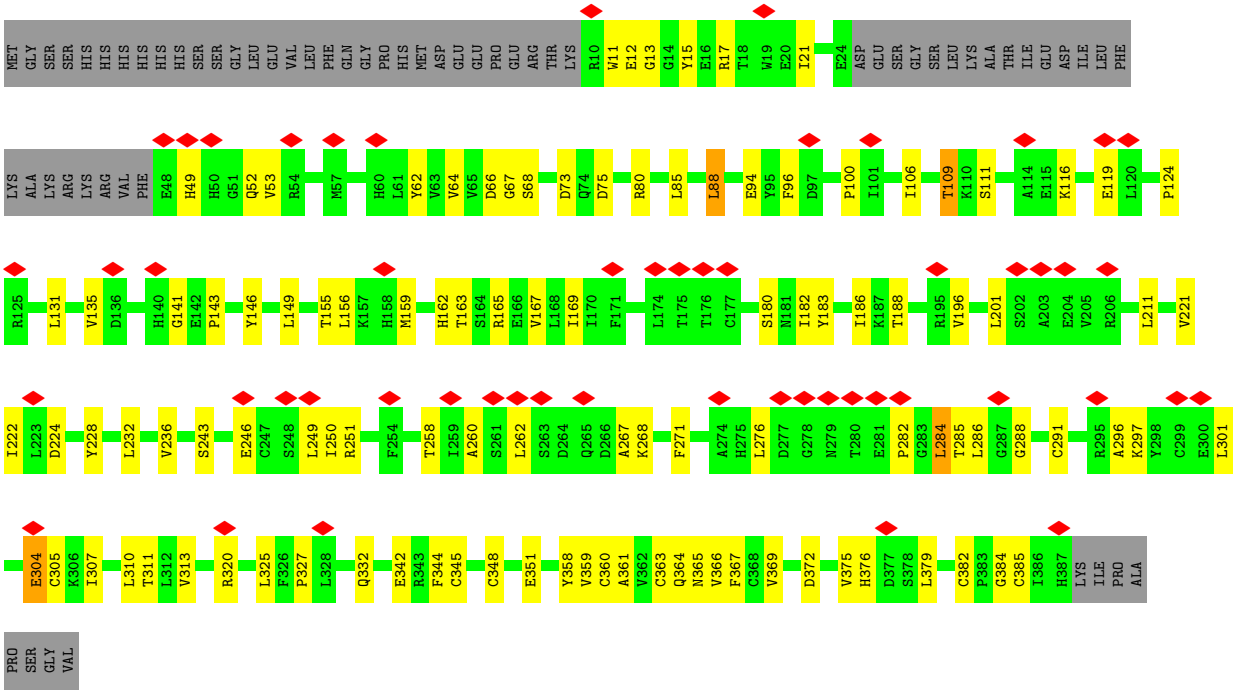




• Molecule 4: General transcription factor IIH subunit 4, p52

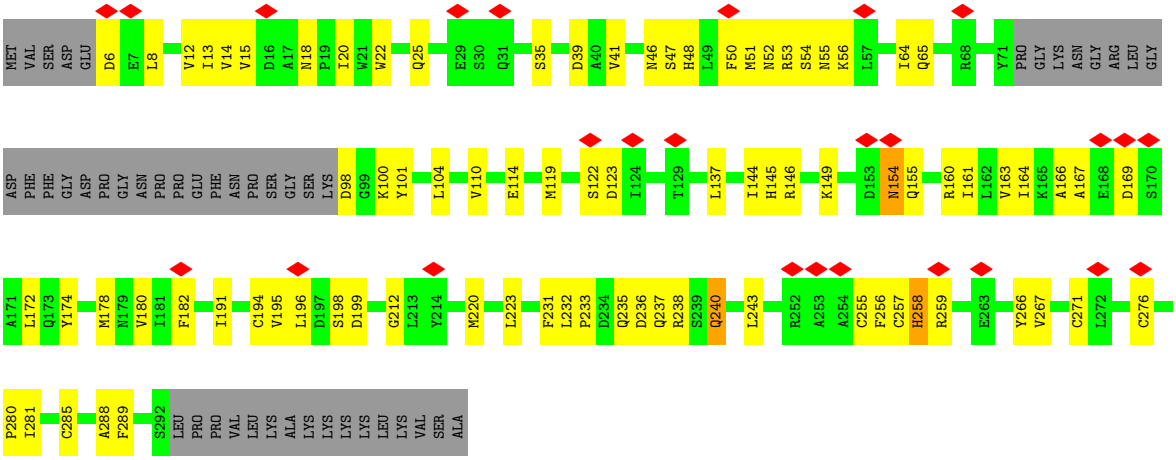


• Molecule 5: General transcription factor IIH subunit 2



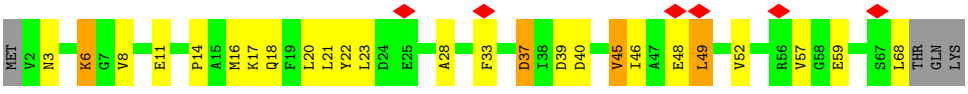
• Molecule 6: General transcription factor IIH subunit 3

Chain F:



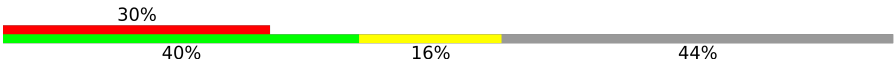
• Molecule 7: General transcription factor IIH subunit 5

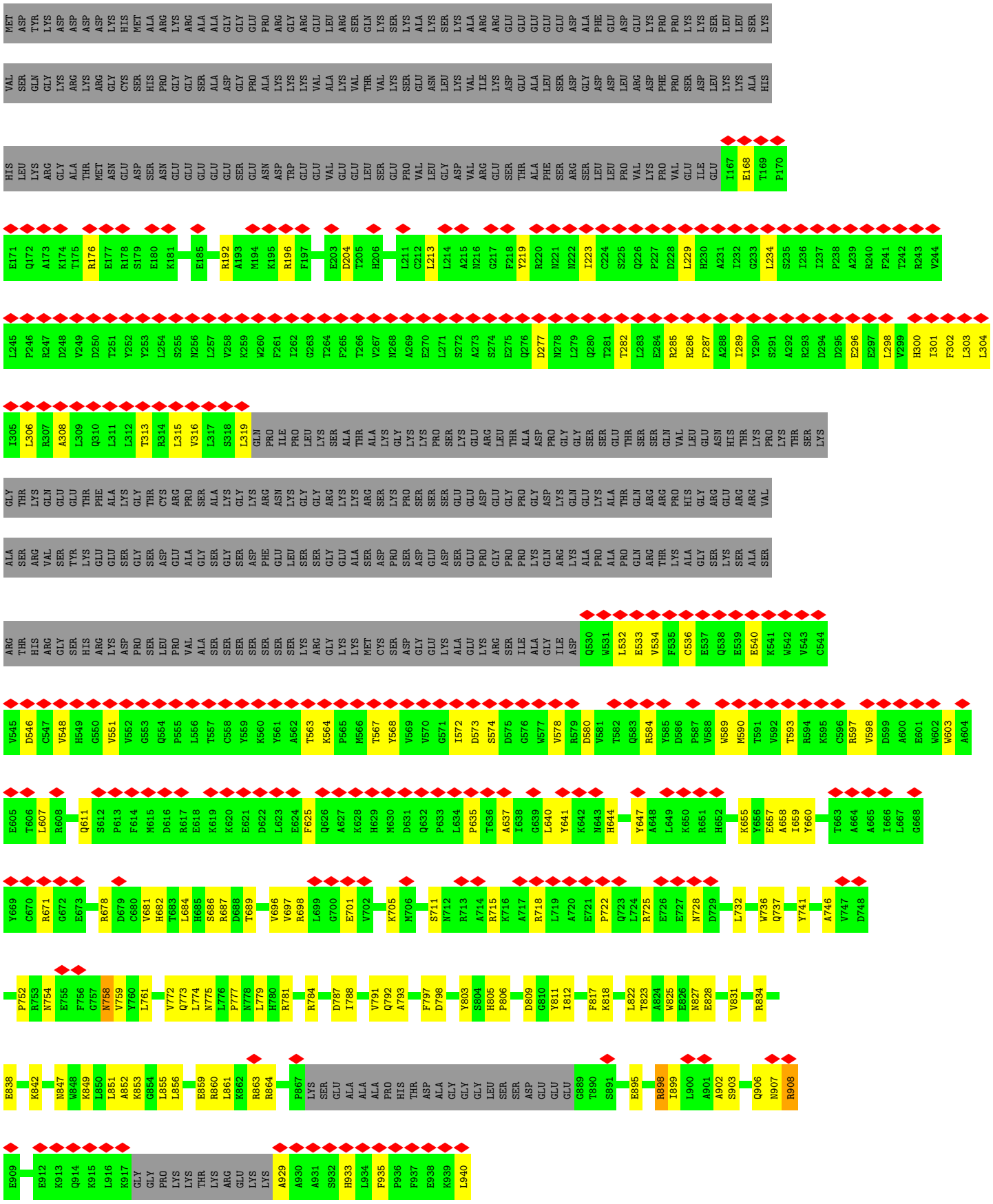
Chain G:



• Molecule 8: Xeroderma pigmentosum, complementation group C, isoform CRA_a

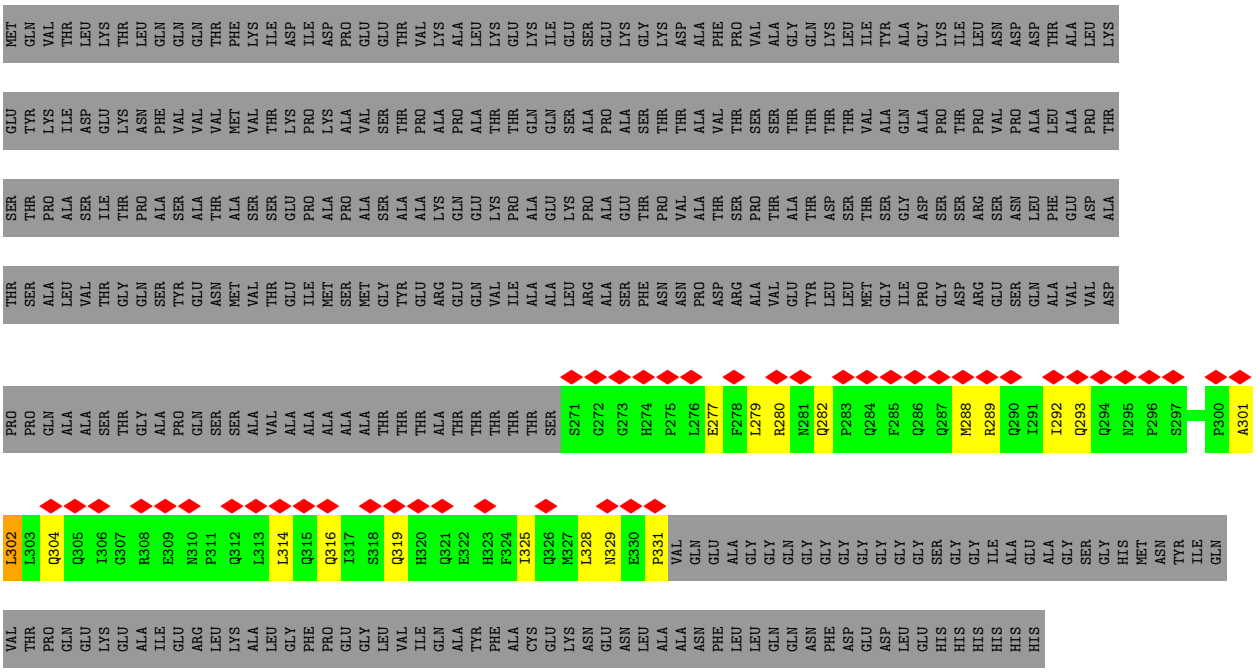
Chain H:




MET ASP TYR LYS ASP ASP ASP ASP LYS HIS MET ALA ARG LYS ARG ALA GLY GLY GLU PRO ARG GLY ARG GLU LEU ARG SER GLN LYS SER LYS ALA LYS SER LYS ALA ARG ARG GLU GLU GLU GLU ASP ALA PHE GLU ASP GLU GLN LYS PRO PRO LYS LYS SER LEU LEU SER LYS
VAL SER GLN GLY LYS ARG LYS ARG GLY CYS SER HIS PRO GLY GLY SER ALA ASP GLY PRO ALA LYS LYS VAL LYS THR VAL LYS SER GLU ASN LEU LYS VAL ILE LYS ASP GLU ALA LEU SER ASP GLY ASP ASP LEU ARG ASP PHE PRO PRO SER ASP LEU LYS LYS ALA HIS
HIS LEU LYS ARG GLY ALA THR MET ASN GLU ASP SER ASN GLU GLU GLU GLU GLU SER GLU ASN ASP TRP GLU GLU VAL GLU GLU LEU SER GLU PRO VAL LEU GLY ASP VAL ARG GLU SER THR ALA PHE SER ARG SER LEU LEU PRO VAL LYS PRO VAL GLU ILE GLU I167 E168 T169 P170
E171 Q172 A173 K174 T175 R176 E177 R178 S179 E180 K181 E185 R192 A193 M194 K195 R196 F197 E203 D204 T205 H206 L211 C212 L213 L214 A215 N216 G217 F218 Y219 R220 N221 N222 I223 C224 S225 Q226 P227 D228 L229 H230 A231 I232 G233 L234 S235 I236 I237 P238 A239 R240 F241 T242 R243 V244
L245 P246 R247 D248 V249 D250 T251 Y252 Y253 L254 S255 N256 L257 V258 K259 W260 F261 I262 G263 T264 F265 T266 V267 N268 A269 E270 L271 S272 A273 S274 E275 Q276 D277 N278 L279 Q280 T281 T282 L283 E284 R285 R286 F287 A288 I289 Y290 S291 A292 R293 D294 D295 E296 E297 L298 V299 H300 I301 F302 L303 L304
I305 L306 R307 A308 L309 Q310 L311 L312 T313 R314 L315 V316 L317 S318 L319 GLN PRO ILE PRO LEU LYS SER ALA THR ALA LYS GLY LYS LYS PRO SER LYS GLU ARG LEU THR ALA ASP PRO GLY GLY SER SER GLU THR SER SER GLN VAL LEU GLU ASN HIS THR LYS PRO LYS THR SER LYS
GLY THR LYS GLN GLU GLU THR PHE ALA LYS GLY THR CYS ARG PRO SER ALA LYS GLY LYS ARG ASN LYS GLY GLY ARG LYS LYS ARG SER LYS PRO SER SER GLU GLU ASP GLU GLY PRO GLY ASP LYS GLN GLU LYS ALA THR GLN ARG ARG PRO HIS GLY ARG GLU ARG ARG VAL
ALA SER ARG VAL SER TYR LYS GLU GLU SER GLY SER ASP GLU ALA GLY SER GLY SER ASP PHE GLU LEU SER SER GLY GLU ALA SER ASP PRO SER ASP GLU ASP SER GLU PRO GLY PRO PRO LYS GLN ARG LYS ALA PRO ALA PRO GLN ARG THR LYS ALA GLY SER LYS SER ALA SER
ARG THR HIS ARG GLY SER HIS ARG LYS ASP PRO SER LEU PRO VAL ALA SER SER SER SER SER SER SER LYS ARG GLY LYS LYS MET CYS SER ASP GLY GLU LYS ALA GLU LYS ARG SER ILE ALA GLY ILE ASP Q530 W531 L532 E533 V534 F535 C536 E537 Q538 E539 E540 K541 W542 V543 C544
V545 D546 C547 V548 H549 G550 V551 V552 G553 Q554 P555 L556 T557 C558 Y559 K560 Y561 A562 T563 K564 P565 M566 T567 Y568 V569 V570 G571 I572 D573 S574 D575 G576 W577 V578 R579 D580 V581 T582 Q583 R584 Y585 D586 P587 V588 W589 M590 T591 V592 T593 R594 K595 C596 R597 V598 D599 A600 E601 W602 W603 A604
E605 T606 L607 R608 Q611 S612 P613 F614 M615 D616 R617 E618 K619 K620 E621 D622 L623 E624 F625 Q626 A627 K628 H629 M630 D631 Q632 P633 L634 P635 T636 A637 I638 G639 L640 Y641 K642 N643 H644 Y647 A648 L649 K650 R651 H652 K655 Y656 E657 A658 I659 Y660 T663 A664 A665 I666 L667 G668
Y669 C670 R671 G672 E673 R678 D679 C680 V681 H682 T683 L684 H685 S686 R687 D688 T689 V696 V697 R698 L699 G700 E701 V702 K705 M706 S711 N712 R713 A714 R715 K716 A717 R718 L719 A720 E721 P722 Q723 L724 R725 E726 E727 N728 D729 L732 W736 Q737 Y741 A746 V747 D748
P752 R753 N754 E755 F756 G757 N758 V759 Y760 L761 V772 Q773 L774 N775 L776 P777 N778 L779 H780 R781 R784 D787 I788 V791 Q792 A793 F797 D798 Y803 S804 H805 P806 D809 G810 Y811 I812 F817 K818 L822 T823 A824 W825 E826 N827 E828 V831 R834
E838 K842 N847 W848 K849 L850 L851 A852 K853 G854 L855 L856 E859 R860 L861 K862 R863 R864 P867 LYS SER GLU ALA ALA ALA PRO HIS THR ASP ALA GLY GLY GLY LEU SER SER ASP GLU GLU GLU GLY T890 S891 E895 R898 I899 L900 A901 A902 S903 Q906 N907 R908
E909 E912 K913 Q914 K915 L916 K917 GLY GLY PRO LYS LYS THR LYS ARG GLU LYS LYS A929 A930 A931 S932 H933 L934 F935 P936 F937 E938 K939 L940

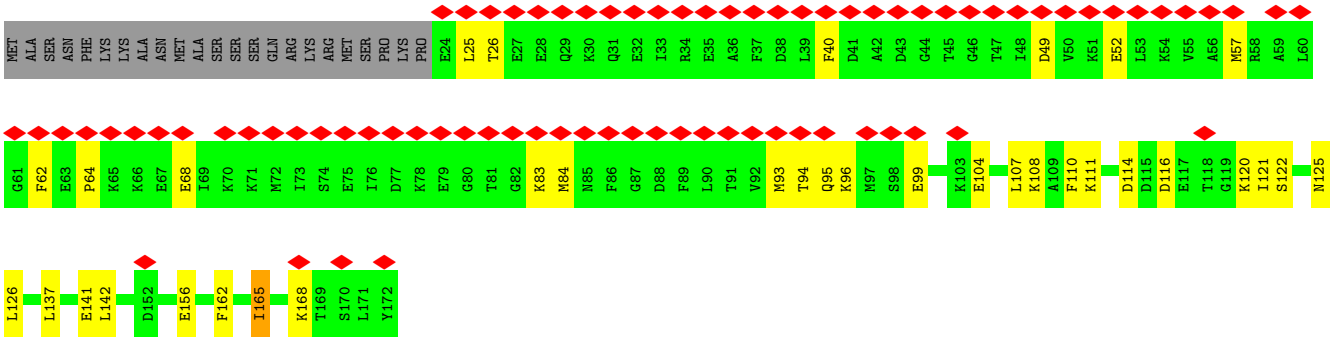
• Molecule 9: UV excision repair protein RAD23 homolog B

Chain I:



• Molecule 10: Centrin-2

Chain J:

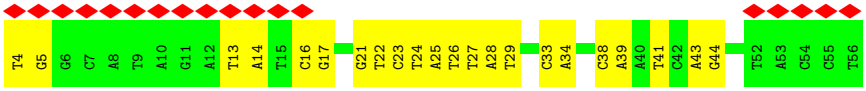


• Molecule 11: DNA (Ap)

Chain L:

• Molecule 12: DNA

Chain M:


T4
G5
G6
C7
A8
T9
A10
G11
A12
T13
A14
T15
C16
G17
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T22
C23
T24
A25
T26
T27
A28
T29
C33
A34
C38
A39
A40
T41
C42
A43
G44
T52
A53
C54
C55
T56

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66841	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 ($e^-/Å^2$)	54.1	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	103000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.245, 1.245, 1.245	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR, SF4, CA, 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	A	0.26	0/5059	0.39	0/6833
2	B	0.24	0/6247	0.38	0/8457
3	C	0.24	0/2564	0.37	0/3460
4	D	0.25	0/3641	0.38	0/4934
5	E	0.24	0/2857	0.39	0/3870
6	F	0.25	0/2093	0.38	0/2833
7	G	0.25	0/536	0.40	0/724
8	H	0.24	0/4467	0.37	0/6041
9	I	0.25	0/515	0.37	0/696
10	J	0.24	0/1211	0.38	0/1605
11	L	0.48	0/1181	0.87	0/1820
12	M	0.48	0/1206	0.89	0/1857
All	All	0.27	0/31577	0.45	0/43130

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4955	0	4997	141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6120	0	6164	134	0
3	C	2511	0	2502	57	0
4	D	3557	0	3596	91	0
5	E	2792	0	2735	75	0
6	F	2057	0	2079	67	0
7	G	530	0	539	23	0
8	H	4364	0	4363	117	0
9	I	504	0	497	10	0
10	J	1201	0	1185	19	0
11	L	1075	0	591	13	0
12	M	1078	0	599	19	0
13	B	8	0	0	0	0
14	E	3	0	0	0	0
14	F	2	0	0	0	0
15	J	2	0	0	0	0
All	All	30759	0	29847	693	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (693) 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:382:CYS:HB3	5:E:385:CYS:SG	2.15	0.86
2:B:349:VAL:HA	2:B:418:ILE:O	1.76	0.84
8:H:711:SER:H	8:H:715:ARG:HE	1.30	0.80
7:G:14:PRO:O	7:G:18:GLN:NE2	2.17	0.76
2:B:622:GLY:HA2	2:B:681:ASP:HB2	1.69	0.75
4:D:407:VAL:HG22	7:G:6:LYS:HB3	1.68	0.75
1:A:444:HIS:O	1:A:472:ARG:NH2	2.20	0.73
6:F:257:CYS:SG	6:F:258:HIS:CD2	2.80	0.73
8:H:773:GLN:NE2	8:H:809:ASP:O	2.23	0.72
1:A:653:GLU:HG2	1:A:655:TYR:H	1.54	0.72
2:B:370:LYS:HA	2:B:373:ARG:HD3	1.71	0.71
4:D:110:LEU:O	4:D:115:ARG:NH2	2.23	0.71
2:B:42:MET:HB3	2:B:48:LYS:HD3	1.72	0.70
1:A:600:PRO:O	1:A:603:ASN:ND2	2.25	0.70
5:E:116:LYS:HE2	5:E:119:GLU:HA	1.72	0.70
5:E:342:GLU:HG2	5:E:344:PHE:H	1.57	0.70
1:A:645:ARG:HD2	1:A:646:ALA:H	1.56	0.70
10:J:57:MET:HB3	10:J:62:PHE:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:MET:HG2	2:B:48:LYS:HB3	1.72	0.69
2:B:56:ILE:HG21	2:B:70:LEU:HD22	1.74	0.69
1:A:639:ARG:HH12	1:A:659:PHE:HE1	1.41	0.68
1:A:672:TYR:OH	12:M:41:DT:OP1	2.12	0.68
1:A:198:ARG:NH2	1:A:207:THR:O	2.26	0.68
7:G:46:ILE:HG22	7:G:48:GLU:H	1.58	0.68
2:B:420:PRO:HA	2:B:431:PRO:HA	1.76	0.68
1:A:563:ASP:H	1:A:627:SER:HB2	1.59	0.67
1:A:553:ARG:NH1	1:A:699:GLU:OE2	2.28	0.67
2:B:506:SER:OG	2:B:683:ARG:NH2	2.27	0.67
1:A:522:TYR:HA	1:A:533:LEU:HD13	1.77	0.67
5:E:375:VAL:HA	5:E:379:LEU:HB3	1.76	0.67
3:C:374:LEU:HD11	6:F:285:CYS:HB2	1.78	0.65
2:B:143:ARG:NH1	2:B:162:ASP:OD2	2.29	0.65
1:A:636:GLU:HG3	1:A:676:ARG:HE	1.59	0.65
4:D:124:GLY:HA2	6:F:100:LYS:HB3	1.79	0.65
8:H:546:ASP:HB3	8:H:551:VAL:HB	1.79	0.65
1:A:306:ILE:HD13	1:A:404:SER:HB3	1.79	0.65
8:H:644:HIS:HB3	8:H:647:TYR:HB2	1.79	0.65
4:D:355:ILE:HD13	4:D:395:GLU:HA	1.79	0.65
8:H:718:ARG:HB3	8:H:725:ARG:HA	1.78	0.64
1:A:394:SER:OG	1:A:412:MET:SD	2.55	0.64
8:H:775:ASN:ND2	8:H:809:ASP:OD1	2.30	0.64
3:C:446:GLN:HB3	5:E:262:LEU:HD12	1.79	0.64
1:A:54:ASP:OD1	1:A:55:GLU:N	2.30	0.64
1:A:168:LEU:HD11	1:A:175:TYR:HB3	1.80	0.64
5:E:186:ILE:HG12	5:E:211:LEU:HD13	1.80	0.64
1:A:54:ASP:OD2	4:D:337:ARG:NH1	2.31	0.64
4:D:411:GLN:NE2	7:G:3:ASN:O	2.31	0.64
2:B:75:ARG:HH22	2:B:662:GLN:HE22	1.46	0.64
8:H:686:SER:HG	8:H:689:THR:HG1	1.35	0.64
2:B:725:ALA:HB1	5:E:221:VAL:HG21	1.80	0.63
1:A:410:TYR:OH	1:A:441:ASP:O	2.17	0.63
6:F:281:ILE:HA	6:F:288:ALA:HA	1.79	0.63
1:A:472:ARG:HG3	1:A:474:ASP:H	1.63	0.63
2:B:515:ALA:O	2:B:519:ASN:ND2	2.32	0.63
2:B:112:ARG:NH1	2:B:134:CYS:SG	2.71	0.63
2:B:609:ASP:OD1	2:B:666:ARG:NH1	2.31	0.63
1:A:361:CYS:HB3	1:A:405:VAL:HG22	1.80	0.63
3:C:381:ARG:NH1	6:F:256:PHE:O	2.32	0.63
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:LEU:HD12	4:D:94:ARG:HD3	1.81	0.62
8:H:895:GLU:OE1	8:H:898:ARG:NH1	2.31	0.62
2:B:479:ALA:HB2	2:B:759:GLN:HG2	1.80	0.62
1:A:274:GLN:NE2	1:A:456:THR:O	2.33	0.62
4:D:405:GLU:HA	7:G:8:VAL:HA	1.80	0.62
4:D:396:LEU:HD22	8:H:908:ARG:HG3	1.81	0.62
2:B:105:LEU:HA	2:B:173:GLY:H	1.65	0.62
2:B:225:LEU:O	2:B:450:ARG:NH2	2.33	0.62
2:B:237:HIS:O	2:B:658:ARG:NH1	2.32	0.62
3:C:512:ILE:O	3:C:516:TYR:N	2.33	0.62
4:D:411:GLN:HE22	7:G:3:ASN:HB3	1.64	0.62
7:G:39:ASP:OD1	7:G:40:ASP:N	2.33	0.62
6:F:52:ASN:ND2	6:F:54:SER:OG	2.33	0.61
5:E:291:CYS:HB3	5:E:296:ALA:H	1.65	0.61
8:H:705:LYS:HB3	8:H:732:LEU:HB2	1.82	0.61
2:B:419:GLU:OE2	2:B:434:HIS:NE2	2.32	0.61
4:D:96:TRP:HB3	4:D:110:LEU:HD23	1.81	0.61
4:D:335:LEU:HD11	4:D:345:GLN:HB2	1.81	0.61
2:B:736:LEU:O	2:B:752:ARG:NH2	2.34	0.61
1:A:634:ARG:NH2	1:A:635:GLN:OE1	2.29	0.61
2:B:691:GLY:HA2	2:B:698:GLN:HE22	1.65	0.61
8:H:196:ARG:NH2	12:M:23:DC:OP1	2.34	0.61
2:B:589:GLU:OE2	2:B:614:TYR:OH	2.19	0.60
2:B:267:GLN:OE1	2:B:334:ARG:NH2	2.33	0.60
2:B:685:ALA:HA	2:B:706:LEU:HD11	1.81	0.60
4:D:113:ILE:O	4:D:117:ASN:ND2	2.27	0.60
6:F:98:ASP:HB2	6:F:100:LYS:HE2	1.83	0.60
8:H:168:GLU:OE2	8:H:176:ARG:NH1	2.34	0.60
8:H:798:ASP:O	8:H:805:HIS:N	2.29	0.60
5:E:365:ASN:HD21	5:E:384:GLY:HA3	1.66	0.60
5:E:375:VAL:HG22	5:E:379:LEU:HD23	1.83	0.60
6:F:65:GLN:NE2	6:F:123:ASP:O	2.34	0.60
2:B:349:VAL:HG22	2:B:419:GLU:HA	1.83	0.60
8:H:637:ALA:HB3	8:H:640:LEU:HG	1.82	0.60
2:B:232:VAL:HA	2:B:455:ILE:HB	1.84	0.60
8:H:793:ALA:HB2	8:H:812:ILE:HG13	1.84	0.60
1:A:515:SER:OG	1:A:517:GLU:OE1	2.18	0.60
6:F:238:ARG:HB3	6:F:243:LEU:HD11	1.84	0.60
2:B:324:ARG:O	2:B:378:ARG:NH1	2.35	0.60
4:D:355:ILE:HG22	4:D:398:ARG:HH11	1.66	0.60
8:H:774:LEU:HD11	8:H:818:LYS:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:PRO:HD3	2:B:411:ALA:HB1	1.84	0.59
3:C:501:GLN:HG3	3:C:505:LEU:HD23	1.83	0.59
1:A:62:ARG:HA	4:D:339:PRO:HG3	1.84	0.59
8:H:711:SER:N	8:H:715:ARG:HE	1.99	0.59
8:H:929:ALA:O	8:H:933:HIS:ND1	2.34	0.59
1:A:532:LEU:HA	1:A:535:THR:HG22	1.85	0.59
4:D:222:THR:O	4:D:226:ARG:NH1	2.35	0.59
1:A:615:PHE:O	1:A:642:ARG:NH1	2.26	0.59
1:A:172:HIS:HB2	1:A:174:ARG:HD3	1.82	0.59
2:B:22:PHE:HD2	2:B:753:ILE:HG21	1.66	0.59
8:H:572:ILE:HG12	8:H:578:VAL:HG22	1.85	0.59
1:A:308:ILE:HB	1:A:384:ILE:HB	1.83	0.59
3:C:512:ILE:HG23	3:C:517:LEU:HB2	1.84	0.59
1:A:337:VAL:O	1:A:488:LEU:N	2.29	0.59
4:D:313:TYR:HB3	4:D:346:VAL:HB	1.84	0.59
6:F:255:CYS:SG	6:F:276:CYS:N	2.76	0.59
4:D:216:MET:HG3	4:D:290:LEU:HD21	1.85	0.58
3:C:523:SER:HB3	5:E:268:LYS:HG2	1.85	0.58
1:A:692:LYS:HE2	8:H:906:GLN:HE21	1.68	0.58
2:B:176:ASN:OD1	2:B:177:LEU:N	2.36	0.58
5:E:361:ALA:O	5:E:364:GLN:NE2	2.36	0.58
2:B:70:LEU:HB3	2:B:204:VAL:HG22	1.85	0.58
4:D:188:THR:OG1	4:D:195:CYS:SG	2.59	0.58
6:F:48:HIS:NE2	6:F:56:LYS:O	2.33	0.58
9:I:316:GLN:OE1	9:I:319:GLN:NE2	2.36	0.58
1:A:471:VAL:HG23	1:A:634:ARG:HB3	1.86	0.58
4:D:206:LEU:O	4:D:211:GLN:NE2	2.37	0.58
4:D:66:LEU:O	4:D:108:LEU:N	2.36	0.58
4:D:30:VAL:HG22	4:D:33:ARG:HH21	1.68	0.58
1:A:584:THR:O	1:A:589:ARG:NH1	2.37	0.58
5:E:372:ASP:OD1	5:E:376:HIS:NE2	2.37	0.58
7:G:17:LYS:NZ	7:G:39:ASP:O	2.32	0.58
2:B:21:GLN:NE2	2:B:46:THR:O	2.37	0.57
2:B:566:LEU:N	2:B:593:GLY:O	2.36	0.57
8:H:781:ARG:HA	8:H:784:ARG:HE	1.67	0.57
2:B:217:ILE:HG23	2:B:220:LEU:HD12	1.86	0.57
2:B:346:VAL:HG12	2:B:348:HIS:H	1.68	0.57
8:H:589:TRP:HA	8:H:593:THR:HB	1.84	0.57
3:C:113:GLU:OE1	3:C:116:ARG:NH2	2.37	0.57
5:E:94:GLU:HG3	5:E:236:VAL:HG11	1.85	0.57
1:A:644:LEU:HD13	1:A:657:ALA:HB1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ALA:HB2	4:D:334:MET:HB3	1.87	0.57
1:A:113:VAL:N	4:D:310:GLU:OE2	2.30	0.56
5:E:250:ILE:O	6:F:267:VAL:N	2.33	0.56
12:M:24:DT:H2"	12:M:25:DA:C8	2.40	0.56
6:F:271:CYS:HB3	6:F:285:CYS:HB3	1.86	0.56
10:J:68:GLU:OE2	10:J:96:LYS:NZ	2.38	0.56
2:B:305:LEU:HD11	2:B:391:LEU:HD13	1.87	0.56
5:E:304:GLU:HA	5:E:311:THR:HA	1.87	0.56
8:H:777:PRO:O	8:H:825:TRP:NE1	2.31	0.56
9:I:292:ILE:HG21	9:I:328:LEU:HD13	1.88	0.56
9:I:325:ILE:O	9:I:329:ASN:ND2	2.29	0.56
3:C:179:ASP:OD2	3:C:185:ARG:NH2	2.39	0.56
4:D:369:ARG:HG3	4:D:382:VAL:HG11	1.88	0.56
4:D:171:VAL:HB	4:D:175:LEU:HD23	1.88	0.56
2:B:85:GLU:HG2	2:B:89:LYS:HE3	1.88	0.56
4:D:161:HIS:HB3	4:D:169:ALA:HB2	1.88	0.56
1:A:633:ARG:HB3	1:A:676:ARG:HA	1.88	0.56
8:H:641:TYR:CD1	8:H:647:TYR:HB3	2.40	0.55
1:A:135:ASP:OD1	1:A:135:ASP:N	2.37	0.55
2:B:369:ARG:O	2:B:408:SER:OG	2.24	0.55
4:D:412:PHE:O	4:D:439:ARG:NH2	2.39	0.55
8:H:567:THR:O	8:H:597:ARG:NH1	2.37	0.55
8:H:678:ARG:HD2	8:H:681:VAL:HB	1.87	0.55
1:A:419:ARG:HA	11:L:24:DG:H5"	1.87	0.55
1:A:584:THR:HG22	1:A:589:ARG:HB2	1.89	0.55
6:F:8:LEU:HD23	6:F:54:SER:HB2	1.88	0.55
7:G:49:LEU:HD13	7:G:52:VAL:HB	1.89	0.55
2:B:616:ARG:NH1	2:B:674:TYR:O	2.39	0.55
1:A:497:GLN:HB3	1:A:504:LYS:HG2	1.89	0.55
4:D:401:LEU:HD21	7:G:57:VAL:HG11	1.88	0.55
1:A:688:LYS:HD2	8:H:935:PHE:HE1	1.71	0.55
5:E:249:LEU:HG	6:F:266:TYR:HB3	1.89	0.55
8:H:298:LEU:HD23	8:H:548:VAL:HG22	1.89	0.55
1:A:496:LEU:HD22	1:A:501:TYR:HD2	1.72	0.55
8:H:296:GLU:O	8:H:300:HIS:ND1	2.27	0.55
8:H:859:GLU:OE2	8:H:863:ARG:NH2	2.40	0.55
9:I:301:ALA:O	9:I:304:GLN:HB3	2.06	0.55
10:J:25:LEU:HD13	10:J:94:THR:HG21	1.89	0.55
1:A:443:VAL:HG12	1:A:480:LEU:HD11	1.89	0.55
4:D:249:TYR:HB2	4:D:281:TYR:CZ	2.42	0.55
1:A:503:ALA:HB2	1:A:646:ALA:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:705:LYS:HD3	8:H:732:LEU:HD12	1.88	0.55
1:A:444:HIS:HD2	1:A:445:THR:HG23	1.72	0.54
2:B:619:ILE:HG12	2:B:678:VAL:HB	1.88	0.54
1:A:714:GLN:HG2	8:H:861:LEU:HD13	1.89	0.54
8:H:213:LEU:HD13	8:H:319:LEU:HD22	1.89	0.54
2:B:40:LEU:HB3	2:B:481:PHE:HE1	1.70	0.54
2:B:506:SER:HB3	2:B:622:GLY:HA3	1.88	0.54
5:E:332:GLN:NE2	5:E:359:VAL:O	2.41	0.54
6:F:280:PRO:O	6:F:289:PHE:N	2.28	0.54
8:H:855:LEU:O	8:H:859:GLU:N	2.29	0.54
12:M:23:DC:H2"	12:M:24:DT:C5	2.43	0.54
1:A:595:ASN:HB3	1:A:602:ILE:HD12	1.89	0.54
5:E:85:LEU:HD12	5:E:135:VAL:HA	1.90	0.54
5:E:285:THR:O	5:E:297:LYS:NZ	2.39	0.54
8:H:590:MET:HB3	8:H:644:HIS:HE2	1.73	0.54
2:B:531:VAL:HG22	2:B:532:PRO:HD2	1.88	0.54
8:H:657:GLU:O	8:H:705:LYS:NZ	2.36	0.54
4:D:53:LYS:NZ	6:F:51:MET:O	2.31	0.54
4:D:270:LEU:HB3	4:D:287:ALA:HB2	1.89	0.54
5:E:251:ARG:HA	6:F:266:TYR:HA	1.89	0.54
3:C:494:LYS:HD2	3:C:536:LEU:HD23	1.89	0.54
7:G:14:PRO:HG2	8:H:899:ILE:HG23	1.90	0.54
3:C:130:ASP:O	3:C:134:SER:OG	2.23	0.53
4:D:46:ARG:HH12	6:F:53:ARG:HE	1.56	0.53
1:A:581:TYR:O	1:A:584:THR:OG1	2.26	0.53
4:D:65:PRO:HB2	4:D:107:GLY:HA3	1.91	0.53
1:A:698:GLU:OE1	1:A:698:GLU:N	2.34	0.53
2:B:517:ILE:HG23	2:B:548:THR:HG23	1.90	0.53
4:D:273:GLN:NE2	4:D:275:LYS:O	2.42	0.53
2:B:115:LEU:HD13	2:B:192:TYR:HA	1.91	0.53
6:F:231:PHE:O	6:F:238:ARG:NH2	2.40	0.53
8:H:852:ALA:HA	8:H:855:LEU:HD12	1.90	0.53
2:B:161:PHE:HB2	2:B:189:TRP:HB3	1.90	0.53
1:A:174:ARG:NE	1:A:271:GLU:OE2	2.38	0.53
3:C:539:TRP:HZ3	3:C:543:ARG:HD2	1.74	0.52
8:H:536:CYS:O	8:H:540:GLU:N	2.43	0.52
10:J:49:ASP:HB2	10:J:52:GLU:HG2	1.90	0.52
4:D:18:ASN:ND2	4:D:21:GLU:OE1	2.42	0.52
5:E:360:CYS:SG	5:E:361:ALA:N	2.83	0.52
6:F:255:CYS:O	6:F:259:ARG:N	2.38	0.52
5:E:284:LEU:HD23	5:E:284:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:ASN:HD22	6:F:64:ILE:HD11	1.74	0.52
11:L:41:DG:H2"	11:L:42:DA:C8	2.43	0.52
3:C:408:ARG:NH2	6:F:123:ASP:OD1	2.42	0.52
5:E:111:SER:HA	5:E:141:GLY:HA3	1.92	0.52
12:M:38:DC:H2"	12:M:39:DA:C8	2.45	0.52
2:B:309:VAL:O	2:B:410:TYR:OH	2.23	0.52
3:C:406:SER:O	3:C:410:GLU:N	2.42	0.52
2:B:1:MET:N	2:B:12:PHE:O	2.38	0.52
3:C:482:ASN:H	3:C:486:LEU:HD12	1.75	0.52
5:E:96:PHE:HD2	5:E:124:PRO:HB3	1.75	0.52
5:E:100:PRO:HG3	5:E:320:ARG:HD2	1.92	0.52
5:E:305:CYS:N	5:E:310:LEU:O	2.37	0.52
1:A:580:ILE:HG23	1:A:584:THR:HG21	1.91	0.52
2:B:323:ILE:HB	2:B:329:PHE:HD1	1.74	0.52
3:C:411:MET:HE3	6:F:35:SER:H	1.74	0.52
9:I:293:GLN:HE22	9:I:331:PRO:HA	1.75	0.52
3:C:376:LEU:HD13	3:C:376:LEU:H	1.75	0.52
3:C:510:GLU:HG2	3:C:513:ARG:HH21	1.74	0.52
8:H:774:LEU:HD21	8:H:818:LYS:HE3	1.91	0.52
1:A:384:ILE:HG23	1:A:389:ILE:HD11	1.92	0.52
1:A:508:ALA:HB2	8:H:935:PHE:CE2	2.45	0.52
2:B:458:SER:HB3	2:B:461:LEU:HD21	1.91	0.52
2:B:637:LEU:HD13	2:B:648:GLU:HB2	1.91	0.51
1:A:540:LYS:HD3	1:A:626:ILE:HG23	1.91	0.51
4:D:87:THR:HG23	4:D:96:TRP:HZ2	1.75	0.51
5:E:201:LEU:HG	5:E:222:ILE:HD12	1.91	0.51
6:F:101:TYR:HB3	6:F:104:LEU:HB2	1.93	0.51
1:A:303:ASN:O	1:A:359:LYS:NZ	2.32	0.51
4:D:238:PHE:O	4:D:241:SER:OG	2.19	0.51
2:B:251:LEU:HD12	2:B:433:LEU:HD22	1.91	0.51
5:E:64:VAL:HB	5:E:169:ILE:HA	1.92	0.51
5:E:167:VAL:HB	5:E:196:VAL:HG22	1.91	0.51
2:B:237:HIS:NE2	2:B:662:GLN:OE1	2.41	0.51
8:H:823:THR:O	8:H:827:ASN:ND2	2.27	0.51
3:C:418:LEU:HD22	4:D:123:LEU:HB3	1.91	0.51
5:E:156:LEU:HA	5:E:159:MET:HG2	1.93	0.51
8:H:788:ILE:HD13	8:H:817:PHE:HB3	1.92	0.51
4:D:38:PRO:HB3	4:D:121:ALA:HB2	1.93	0.51
5:E:149:LEU:HD21	5:E:169:ILE:HD11	1.92	0.51
8:H:684:LEU:HB3	8:H:732:LEU:HB3	1.93	0.51
1:A:525:ILE:HD12	1:A:533:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LYS:HE3	2:B:137:LEU:HD11	1.93	0.51
6:F:236:ASP:OD1	6:F:236:ASP:N	2.42	0.51
8:H:736:TRP:CD1	8:H:737:GLN:HG3	2.46	0.51
1:A:504:LYS:N	1:A:656:ASN:OD1	2.44	0.51
1:A:629:HIS:NE2	12:M:39:DA:O3'	2.38	0.51
2:B:319:VAL:O	2:B:324:ARG:NE	2.39	0.51
5:E:156:LEU:HB3	5:E:165:ARG:HG2	1.92	0.51
8:H:229:LEU:HB3	8:H:304:LEU:HD13	1.93	0.51
8:H:856:LEU:O	8:H:860:ARG:N	2.37	0.51
2:B:199:ILE:HG23	2:B:205:VAL:HG21	1.93	0.50
2:B:284:GLU:OE2	2:B:378:ARG:NH2	2.44	0.50
2:B:439:ASP:OD1	2:B:441:SER:OG	2.25	0.50
8:H:698:ARG:HB2	8:H:701:GLU:HG3	1.94	0.50
1:A:105:GLU:HG3	1:A:122:SER:HB3	1.94	0.50
3:C:431:ILE:O	3:C:435:SER:N	2.44	0.50
4:D:185:MET:HA	4:D:196:ILE:HA	1.93	0.50
4:D:425:ALA:O	4:D:429:GLY:N	2.44	0.50
2:B:561:ILE:HG22	2:B:567:LEU:HD21	1.94	0.50
3:C:373:ALA:HA	5:E:53:VAL:HA	1.94	0.50
3:C:459:SER:HA	3:C:462:LYS:HD2	1.93	0.50
6:F:6:ASP:HB3	6:F:155:GLN:HA	1.92	0.50
12:M:24:DT:H2"	12:M:25:DA:N7	2.27	0.50
2:B:233:PHE:N	2:B:455:ILE:O	2.41	0.50
3:C:131:LEU:HB3	3:C:137:ILE:HG12	1.93	0.50
4:D:399:ASP:O	8:H:908:ARG:NH2	2.45	0.50
4:D:431:LEU:HD21	4:D:434:GLU:HG2	1.94	0.50
6:F:12:VAL:HB	6:F:161:ILE:HA	1.94	0.50
8:H:902:ALA:HA	8:H:906:GLN:HB2	1.92	0.50
4:D:80:SER:O	4:D:84:GLU:N	2.34	0.50
8:H:306:LEU:HB3	8:H:313:THR:HG21	1.93	0.50
1:A:297:PHE:HZ	1:A:356:THR:HG22	1.77	0.50
2:B:681:ASP:HB3	2:B:684:PHE:HD2	1.77	0.49
4:D:28:PRO:HB3	4:D:94:ARG:CZ	2.42	0.49
4:D:202:GLN:HB3	4:D:363:GLN:HE22	1.76	0.49
1:A:87:GLU:HG3	1:A:90:SER:HB2	1.95	0.49
1:A:531:ILE:HA	1:A:534:TYR:CE2	2.47	0.49
2:B:195:ALA:O	2:B:199:ILE:HG13	2.12	0.49
2:B:497:ARG:HH21	2:B:708:LEU:HA	1.76	0.49
8:H:655:LYS:HD2	11:L:35:DA:H5"	1.94	0.49
11:L:23:DT:H2"	11:L:24:DG:C8	2.48	0.49
1:A:322:LYS:O	1:A:326:LYS:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLN:NE2	1:A:434:GLU:O	2.42	0.49
4:D:132:ASP:OD1	4:D:134:SER:OG	2.19	0.49
4:D:174:ASP:O	4:D:178:LEU:N	2.41	0.49
2:B:637:LEU:HD22	2:B:648:GLU:HA	1.94	0.49
8:H:696:VAL:HG23	8:H:741:TYR:HA	1.93	0.49
10:J:110:PHE:O	10:J:114:ASP:N	2.41	0.49
12:M:43:DA:H2"	12:M:44:DG:C8	2.47	0.49
1:A:530:ARG:HA	1:A:533:LEU:HD12	1.95	0.49
2:B:681:ASP:HB3	2:B:684:PHE:CD2	2.48	0.49
5:E:15:TYR:OH	5:E:17:ARG:NE	2.46	0.49
5:E:260:ALA:HB1	5:E:267:ALA:HA	1.95	0.49
1:A:331:GLY:N	5:E:13:GLY:O	2.46	0.49
1:A:534:TYR:HE2	1:A:668:GLN:HE21	1.59	0.49
4:D:213:TRP:CE3	4:D:293:GLY:HA2	2.48	0.49
8:H:907:ASN:OD1	8:H:908:ARG:NH1	2.38	0.49
1:A:511:TRP:HB3	1:A:665:GLN:HG2	1.93	0.49
2:B:410:TYR:HB3	2:B:414:PHE:CE2	2.47	0.49
5:E:52:GLN:NE2	5:E:325:LEU:O	2.46	0.49
5:E:296:ALA:HB2	5:E:307:ILE:HD12	1.95	0.49
11:L:22:DC:H2'	11:L:23:DT:H72	1.95	0.49
2:B:227:ARG:O	2:B:452:GLN:N	2.46	0.49
3:C:505:LEU:HD11	3:C:522:VAL:HG13	1.93	0.49
1:A:563:ASP:N	1:A:627:SER:HB2	2.26	0.48
5:E:344:PHE:HD1	5:E:351:GLU:HA	1.78	0.48
2:B:12:PHE:HE1	2:B:14:TYR:HB2	1.78	0.48
2:B:249:VAL:HG11	2:B:403:PHE:HB2	1.95	0.48
2:B:463:PRO:HG3	2:B:692:LYS:HE3	1.95	0.48
3:C:400:ILE:HD11	6:F:20:ILE:HG12	1.95	0.48
3:C:407:ILE:HD12	6:F:22:TRP:HB2	1.95	0.48
5:E:75:ASP:OD2	5:E:80:ARG:NH2	2.45	0.48
1:A:195:ARG:HB3	1:A:200:ARG:HH21	1.78	0.48
1:A:328:PHE:HD2	5:E:12:GLU:HB3	1.78	0.48
1:A:628:SER:OG	1:A:676:ARG:NH1	2.37	0.48
2:B:711:ASP:OD1	2:B:711:ASP:N	2.44	0.48
6:F:164:ILE:HG22	6:F:194:CYS:HB3	1.95	0.48
2:B:302:ASP:HA	2:B:304:HIS:CE1	2.48	0.48
6:F:18:ASN:ND2	6:F:64:ILE:HD11	2.28	0.48
1:A:557:LYS:HB3	1:A:596:PHE:HZ	1.77	0.48
2:B:209:TYR:OH	2:B:234:ASP:O	2.31	0.48
2:B:464:LEU:HD12	2:B:760:LEU:HD12	1.95	0.48
6:F:235:GLN:HA	6:F:238:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:40:DC:H2"	11:L:41:DG:C8	2.49	0.48
1:A:100:LEU:HD23	1:A:103:ILE:HD11	1.96	0.48
2:B:216:LYS:HA	2:B:308:PRO:HD2	1.94	0.48
4:D:17:ARG:O	4:D:213:TRP:NE1	2.28	0.48
4:D:317:ALA:HB1	4:D:319:THR:HG22	1.96	0.48
8:H:759:VAL:HG23	8:H:791:VAL:HG11	1.95	0.48
1:A:441:ASP:OD1	1:A:442:GLU:N	2.46	0.48
6:F:15:VAL:HG22	6:F:164:ILE:HD11	1.96	0.48
1:A:375:LYS:HD2	1:A:391:ARG:HD3	1.96	0.48
3:C:509:GLN:HG2	3:C:522:VAL:HG11	1.96	0.48
4:D:389:ASP:O	4:D:393:LEU:HG	2.14	0.48
8:H:847:ASN:O	8:H:851:LEU:N	2.45	0.48
1:A:712:LEU:HA	1:A:715:LYS:HD2	1.96	0.48
8:H:303:LEU:HD22	8:H:315:LEU:HB2	1.96	0.48
8:H:659:ILE:HG12	8:H:681:VAL:HG22	1.96	0.48
10:J:137:LEU:HD11	10:J:141:GLU:HG2	1.95	0.48
2:B:74:SER:N	2:B:207:TYR:O	2.47	0.47
2:B:267:GLN:HG3	2:B:330:LEU:HD13	1.96	0.47
5:E:224:ASP:N	5:E:224:ASP:OD1	2.47	0.47
1:A:429:TRP:HE3	1:A:430:LEU:HD12	1.79	0.47
1:A:636:GLU:HG3	1:A:676:ARG:NE	2.27	0.47
6:F:235:GLN:NE2	6:F:236:ASP:OD1	2.46	0.47
7:G:17:LYS:NZ	7:G:37:ASP:OD1	2.43	0.47
1:A:707:GLU:OE1	1:A:708:GLU:N	2.47	0.47
2:B:215:PRO:HB2	2:B:309:VAL:HA	1.96	0.47
8:H:219:TYR:CZ	8:H:223:ILE:HD11	2.48	0.47
8:H:754:ASN:OD1	8:H:758:ASN:N	2.32	0.47
1:A:282:LYS:HE3	1:A:452:ARG:HH22	1.79	0.47
4:D:326:ALA:O	4:D:330:LEU:HG	2.15	0.47
5:E:363:CYS:SG	5:E:365:ASN:ND2	2.87	0.47
8:H:825:TRP:O	8:H:828:GLU:HB3	2.15	0.47
12:M:13:DT:H2"	12:M:14:DA:H5"	1.96	0.47
4:D:200:GLY:O	4:D:204:LEU:HG	2.15	0.47
1:A:678:ARG:HH21	7:G:68:LEU:HD22	1.79	0.47
2:B:252:THR:HG22	2:B:432:ILE:HG12	1.96	0.47
3:C:534:ASN:O	3:C:538:THR:OG1	2.28	0.47
6:F:13:ILE:HG21	6:F:41:VAL:HG13	1.97	0.47
8:H:754:ASN:N	8:H:758:ASN:O	2.36	0.47
1:A:362:LEU:O	1:A:439:ILE:N	2.41	0.47
2:B:495:ILE:HD11	2:B:713:GLY:HA3	1.97	0.47
8:H:580:ASP:OD2	8:H:603:TRP:NE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:VAL:HG13	1:A:669:GLU:HG2	1.97	0.47
2:B:88:ARG:HH22	2:B:176:ASN:HB2	1.80	0.47
2:B:536:VAL:HG21	2:B:610:PHE:CZ	2.50	0.47
4:D:306:PHE:HB2	4:D:318:TYR:HB2	1.97	0.47
1:A:331:GLY:HA2	5:E:13:GLY:HA2	1.97	0.47
1:A:557:LYS:HB3	1:A:596:PHE:CZ	2.50	0.47
4:D:309:VAL:HG22	4:D:315:LEU:HD22	1.96	0.47
4:D:392:ARG:O	4:D:396:LEU:HG	2.15	0.47
6:F:14:VAL:HB	6:F:163:VAL:HG22	1.97	0.47
6:F:110:VAL:O	6:F:114:GLU:HG2	2.15	0.47
8:H:797:PHE:CD1	12:M:26:DT:H2'	2.50	0.47
8:H:899:ILE:O	8:H:903:SER:OG	2.20	0.47
1:A:629:HIS:CD2	1:A:632:SER:HB3	2.50	0.46
8:H:635:PRO:HG3	8:H:647:TYR:CE2	2.50	0.46
10:J:95:GLN:NE2	10:J:99:GLU:OE2	2.48	0.46
4:D:79:PHE:CD2	6:F:240:GLN:HB3	2.50	0.46
6:F:101:TYR:HD2	6:F:104:LEU:H	1.63	0.46
8:H:687:ARG:HG3	8:H:697:VAL:HB	1.98	0.46
8:H:831:VAL:HG22	8:H:834:ARG:HH21	1.79	0.46
2:B:117:ILE:HD11	2:B:191:PRO:HD3	1.97	0.46
4:D:417:ASP:OD1	4:D:417:ASP:N	2.48	0.46
2:B:262:ASN:HD21	2:B:397:LEU:HD22	1.80	0.46
2:B:703:ASP:OD1	2:B:703:ASP:N	2.47	0.46
3:C:184:LEU:HD22	3:C:186:TYR:HE1	1.81	0.46
1:A:393:THR:OG1	1:A:396:ALA:O	2.28	0.46
8:H:567:THR:HA	8:H:593:THR:HG23	1.98	0.46
8:H:584:ARG:HB2	8:H:625:PHE:CE1	2.50	0.46
8:H:838:GLU:HB3	8:H:842:LYS:HE3	1.96	0.46
2:B:487:ARG:NH2	2:B:726:GLN:O	2.48	0.46
6:F:154:ASN:OD1	6:F:154:ASN:N	2.49	0.46
2:B:222:SER:HA	2:B:225:LEU:HD12	1.97	0.46
5:E:66:ASP:HA	5:E:109:THR:HG23	1.96	0.46
5:E:131:LEU:O	5:E:135:VAL:HG23	2.16	0.46
5:E:276:LEU:HD23	5:E:282:PRO:HG3	1.98	0.46
1:A:692:LYS:HE2	8:H:906:GLN:HG3	1.97	0.46
2:B:721:LEU:O	2:B:725:ALA:N	2.49	0.46
4:D:399:ASP:OD1	4:D:399:ASP:N	2.49	0.46
1:A:325:ARG:HD2	5:E:15:TYR:HB2	1.97	0.46
1:A:581:TYR:CD2	1:A:583:PRO:HD2	2.50	0.46
2:B:212:LEU:HD13	2:B:221:VAL:HB	1.98	0.46
3:C:539:TRP:HA	3:C:542:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:457:ARG:O	4:D:461:SER:N	2.40	0.46
1:A:610:VAL:HG12	11:L:21:DG:H5'	1.96	0.45
8:H:635:PRO:HG2	8:H:641:TYR:CZ	2.51	0.45
2:B:139:ALA:HB3	2:B:142:VAL:HB	1.97	0.45
2:B:250:ASN:OD1	2:B:434:HIS:ND1	2.49	0.45
2:B:314:VAL:HG13	2:B:373:ARG:HH21	1.81	0.45
4:D:156:TRP:HZ2	4:D:211:GLN:HB3	1.81	0.45
6:F:233:PRO:O	6:F:238:ARG:NE	2.49	0.45
8:H:907:ASN:OD1	8:H:908:ARG:HD2	2.16	0.45
9:I:289:ARG:HG3	9:I:328:LEU:HA	1.97	0.45
4:D:111:ASN:HB3	4:D:114:PHE:HB3	1.98	0.45
5:E:348:CYS:O	6:F:146:ARG:NH1	2.49	0.45
10:J:40:PHE:CD1	10:J:52:GLU:HB3	2.51	0.45
1:A:191:ASP:OD2	1:A:283:ARG:NE	2.36	0.45
1:A:325:ARG:HG2	5:E:12:GLU:HA	1.98	0.45
1:A:443:VAL:HG13	1:A:446:ILE:HD12	1.97	0.45
3:C:179:ASP:OD1	3:C:180:GLY:N	2.43	0.45
4:D:232:GLU:HB3	4:D:258:LEU:HD21	1.99	0.45
8:H:671:ARG:NH1	12:M:16:DC:H5'	2.31	0.45
2:B:605:SER:O	2:B:662:GLN:NE2	2.47	0.45
3:C:509:GLN:HE21	3:C:522:VAL:HG11	1.82	0.45
6:F:48:HIS:CE1	6:F:55:ASN:HB3	2.51	0.45
8:H:282:THR:O	8:H:286:ARG:HG2	2.17	0.45
1:A:645:ARG:HH11	1:A:646:ALA:N	2.14	0.45
6:F:220:MET:O	6:F:223:LEU:HB3	2.17	0.45
4:D:236:PHE:CE2	4:D:240:LEU:HD11	2.51	0.45
4:D:407:VAL:HA	7:G:6:LYS:HA	1.99	0.45
10:J:57:MET:SD	10:J:64:PRO:HG3	2.56	0.45
7:G:17:LYS:HZ1	7:G:37:ASP:CG	2.20	0.45
8:H:277:ASP:OD2	8:H:285:ARG:NH1	2.49	0.45
8:H:568:TYR:OH	8:H:598:VAL:N	2.50	0.45
2:B:144:ALA:O	2:B:148:HIS:ND1	2.44	0.45
4:D:317:ALA:O	4:D:341:MET:HA	2.16	0.45
1:A:81:ASP:OD2	4:D:336:TYR:OH	2.24	0.44
1:A:140:LEU:O	1:A:144:SER:N	2.40	0.44
1:A:179:SER:HB3	1:A:185:ILE:HD11	1.99	0.44
1:A:550:PHE:HE1	8:H:940:LEU:HD12	1.82	0.44
1:A:703:PHE:CE1	1:A:712:LEU:HB2	2.53	0.44
4:D:156:TRP:NE1	4:D:211:GLN:OE1	2.36	0.44
1:A:77:TRP:NE1	1:A:145:LYS:HD2	2.32	0.44
3:C:414:TYR:OH	6:F:39:ASP:OD1	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:258:THR:N	5:E:288:GLY:O	2.51	0.44
5:E:262:LEU:HD21	5:E:286:LEU:HD22	1.97	0.44
3:C:510:GLU:OE1	3:C:514:ARG:NH2	2.49	0.44
8:H:192:ARG:NH2	12:M:22:DT:OP2	2.50	0.44
8:H:234:LEU:HB2	8:H:308:ALA:HB1	1.98	0.44
1:A:625:GLN:HB2	1:A:639:ARG:NH1	2.31	0.44
2:B:344:LEU:HD12	2:B:418:ILE:HG23	1.99	0.44
2:B:532:PRO:HG2	2:B:616:ARG:HB3	1.99	0.44
4:D:454:PHE:N	4:D:457:ARG:HH21	2.15	0.44
6:F:191:ILE:O	6:F:212:GLY:HA3	2.17	0.44
1:A:347:SER:HA	1:A:374:TRP:CH2	2.52	0.44
1:A:703:PHE:HA	1:A:708:GLU:HB3	1.99	0.44
4:D:265:LEU:HD22	4:D:270:LEU:HD12	1.98	0.44
5:E:345:CYS:SG	5:E:367:PHE:HA	2.58	0.44
9:I:277:GLU:O	9:I:280:ARG:HB2	2.18	0.44
1:A:390:CYS:HB3	1:A:398:ASP:HB2	1.98	0.44
1:A:629:HIS:HD2	1:A:632:SER:HB3	1.82	0.44
4:D:305:GLY:HA3	4:D:372:ALA:O	2.18	0.44
8:H:302:PHE:HD2	8:H:532:LEU:HD12	1.82	0.44
1:A:542:ARG:NH1	1:A:704:SER:HA	2.33	0.44
3:C:232:ARG:HB2	3:C:306:ARG:HH11	1.83	0.44
3:C:383:TYR:HB3	6:F:172:LEU:HA	1.98	0.44
7:G:23:LEU:HD22	7:G:28:ALA:HB3	2.00	0.44
8:H:641:TYR:HD1	8:H:647:TYR:HB3	1.81	0.44
8:H:806:PRO:HB3	12:M:27:DT:O2	2.18	0.44
4:D:248:ASP:HB3	4:D:282:TYR:CE2	2.53	0.44
10:J:84:MET:SD	10:J:84:MET:N	2.91	0.44
1:A:70:ASP:HB3	1:A:74:ARG:HG3	2.00	0.44
1:A:395:ASP:N	1:A:395:ASP:OD1	2.51	0.44
2:B:112:ARG:O	2:B:116:CYS:N	2.51	0.44
2:B:583:LYS:HD2	3:C:315:LEU:HD12	2.00	0.44
2:B:682:LYS:HE3	2:B:707:ASN:HD21	1.83	0.44
8:H:827:ASN:O	8:H:831:VAL:HG23	2.18	0.44
2:B:369:ARG:H	2:B:369:ARG:HG2	1.67	0.43
2:B:748:GLU:HA	2:B:751:LYS:HD2	2.00	0.43
3:C:214:ASN:N	3:C:214:ASN:OD1	2.50	0.43
8:H:722:PRO:HA	8:H:725:ARG:HG3	2.00	0.43
11:L:49:DT:H2"	11:L:50:DG:C8	2.53	0.43
1:A:633:ARG:H	1:A:633:ARG:HG3	1.54	0.43
5:E:232:LEU:O	5:E:236:VAL:HG23	2.18	0.43
10:J:137:LEU:HD23	10:J:142:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:4:DT:H2"	12:M:5:DG:C8	2.53	0.43
2:B:492:PRO:HA	2:B:677:MET:HB2	1.99	0.43
4:D:402:ARG:HD2	7:G:11:GLU:HG3	2.01	0.43
6:F:12:VAL:HG21	6:F:144:ILE:HD11	2.00	0.43
1:A:300:ASP:HB3	1:A:359:LYS:HE3	2.00	0.43
7:G:17:LYS:O	7:G:21:LEU:HG	2.17	0.43
8:H:658:ALA:HB3	8:H:684:LEU:HD13	2.01	0.43
10:J:110:PHE:CZ	10:J:121:ILE:HG13	2.54	0.43
1:A:296:ASP:HB3	1:A:299:ASN:HB2	2.00	0.43
1:A:297:PHE:HD1	1:A:333:ALA:HB2	1.84	0.43
1:A:415:HIS:HB3	1:A:419:ARG:NE	2.34	0.43
2:B:325:THR:HB	2:B:328:HIS:CG	2.53	0.43
12:M:33:DC:H2"	12:M:34:DA:C8	2.53	0.43
1:A:562:ALA:HB3	1:A:568:LEU:HB2	2.00	0.43
10:J:104:GLU:O	10:J:108:LYS:HG3	2.19	0.43
2:B:143:ARG:NH1	2:B:158:TYR:OH	2.51	0.43
2:B:421:PHE:HB2	2:B:426:PRO:HA	2.01	0.43
4:D:143:ARG:HH12	4:D:151:TYR:HB2	1.84	0.43
5:E:62:TYR:OH	5:E:155:THR:HG21	2.18	0.43
5:E:88:LEU:HD22	5:E:131:LEU:HD11	2.00	0.43
5:E:348:CYS:SG	6:F:146:ARG:HD2	2.59	0.43
1:A:472:ARG:HG3	1:A:474:ASP:N	2.31	0.43
1:A:570:GLU:OE2	1:A:574:ARG:NH1	2.28	0.43
3:C:401:ILE:O	3:C:405:GLN:N	2.44	0.43
4:D:87:THR:HG23	4:D:96:TRP:CZ2	2.54	0.43
4:D:361:ALA:HB1	4:D:391:ILE:HG22	2.01	0.43
8:H:803:TYR:HB2	8:H:805:HIS:CE1	2.53	0.43
10:J:120:LYS:HB3	10:J:156:GLU:HG3	1.99	0.43
2:B:196:ARG:HH22	2:B:220:LEU:HD22	1.83	0.43
3:C:522:VAL:HG12	3:C:526:GLU:HG3	2.00	0.43
1:A:390:CYS:HB2	1:A:403:CYS:SG	2.59	0.43
3:C:481:VAL:HG13	3:C:486:LEU:HB2	2.01	0.43
4:D:111:ASN:OD1	4:D:114:PHE:N	2.35	0.43
4:D:216:MET:O	4:D:220:LEU:HG	2.19	0.43
10:J:107:LEU:O	10:J:111:LYS:HG2	2.19	0.43
11:L:14:DT:H2"	11:L:15:DG:N7	2.34	0.43
2:B:589:GLU:O	5:E:183:TYR:OH	2.30	0.42
4:D:76:LYS:HD2	6:F:240:GLN:HA	2.00	0.42
5:E:182:ILE:O	5:E:186:ILE:HG13	2.19	0.42
1:A:100:LEU:HA	1:A:103:ILE:HG12	2.01	0.42
3:C:545:MET:O	3:C:548:THR:OG1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:222:THR:OG1	4:D:226:ARG:NH1	2.44	0.42
5:E:146:TYR:CZ	5:E:180:SER:HB3	2.53	0.42
6:F:167:ALA:O	6:F:198:SER:OG	2.37	0.42
6:F:237:GLN:HA	6:F:240:GLN:NE2	2.34	0.42
8:H:287:PHE:CZ	8:H:301:ILE:HG23	2.54	0.42
11:L:5:DA:H2"	11:L:6:DG:C8	2.54	0.42
1:A:612:ASP:OD1	1:A:612:ASP:N	2.51	0.42
1:A:634:ARG:HG3	1:A:635:GLN:N	2.34	0.42
2:B:109:LEU:HB3	2:B:207:TYR:HB3	2.01	0.42
5:E:271:PHE:HB3	5:E:282:PRO:HB2	2.01	0.42
7:G:45:VAL:HG12	7:G:46:ILE:H	1.84	0.42
8:H:573:ASP:OD1	8:H:574:SER:N	2.47	0.42
2:B:72:TYR:HB3	2:B:206:VAL:HG22	2.01	0.42
2:B:444:ILE:HD13	2:B:471:LEU:HD13	2.01	0.42
4:D:409:TYR:OH	4:D:448:HIS:ND1	2.30	0.42
5:E:66:ASP:OD1	5:E:67:GLY:N	2.52	0.42
1:A:524:ALA:HA	7:G:22:TYR:CE1	2.55	0.42
2:B:490:LEU:HD21	2:B:700:HIS:CG	2.54	0.42
4:D:213:TRP:CD2	4:D:293:GLY:HA2	2.55	0.42
8:H:849:LYS:HG3	8:H:853:LYS:HE3	2.01	0.42
1:A:551:HIS:HB2	1:A:558:ILE:HD11	2.02	0.42
2:B:250:ASN:HA	2:B:433:LEU:O	2.20	0.42
3:C:380:ASP:N	3:C:380:ASP:OD1	2.52	0.42
4:D:80:SER:HA	4:D:83:GLN:HB3	2.00	0.42
4:D:219:TYR:OH	4:D:264:HIS:ND1	2.49	0.42
7:G:16:MET:O	7:G:20:LEU:HG	2.20	0.42
2:B:18:TYR:HB3	2:B:20:GLU:OE1	2.20	0.42
3:C:381:ARG:HD2	6:F:256:PHE:CD1	2.55	0.42
4:D:248:ASP:HB3	4:D:282:TYR:CZ	2.55	0.42
4:D:402:ARG:NH2	8:H:907:ASN:O	2.53	0.42
6:F:46:ASN:O	6:F:50:PHE:HB2	2.20	0.42
8:H:660:TYR:HB3	8:H:682:HIS:ND1	2.35	0.42
8:H:774:LEU:HD13	8:H:822:LEU:HD21	2.02	0.42
1:A:399:LYS:H	1:A:399:LYS:HD2	1.85	0.42
1:A:599:ASN:HD21	1:A:601:LYS:HB2	1.85	0.42
1:A:710:GLN:O	1:A:714:GLN:HG3	2.20	0.42
8:H:590:MET:HB3	8:H:644:HIS:NE2	2.34	0.42
8:H:895:GLU:HA	8:H:898:ARG:NH1	2.35	0.42
9:I:288:MET:HB3	9:I:302:LEU:HD13	2.02	0.42
2:B:354:PRO:N	2:B:355:PRO:HD2	2.35	0.41
3:C:132:VAL:HA	3:C:137:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:320:ARG:HA	6:F:182:PHE:CE2	2.55	0.41
11:L:26:DG:H2'	11:L:27:DG:C8	2.55	0.41
1:A:191:ASP:HB3	1:A:194:ILE:HB	2.01	0.41
2:B:225:LEU:HB3	2:B:451:PHE:HE1	1.84	0.41
3:C:401:ILE:HA	3:C:404:PHE:HB3	2.02	0.41
4:D:96:TRP:HA	4:D:110:LEU:HA	2.02	0.41
5:E:358:TYR:HE1	5:E:369:VAL:HG22	1.85	0.41
8:H:316:VAL:HG21	8:H:533:GLU:HG3	2.01	0.41
11:L:37:DG:C2	12:M:21:DG:C2	3.08	0.41
11:L:41:DG:C2	12:M:17:DG:C2	3.09	0.41
2:B:341:LYS:O	2:B:345:ARG:HG3	2.20	0.41
8:H:718:ARG:HD3	8:H:728:ASN:HB3	2.02	0.41
1:A:519:TYR:O	1:A:523:VAL:HG23	2.20	0.41
1:A:584:THR:HB	1:A:589:ARG:HH11	1.84	0.41
2:B:381:SER:O	2:B:384:HIS:ND1	2.50	0.41
2:B:637:LEU:HB3	2:B:648:GLU:HB3	2.02	0.41
4:D:374:PRO:HA	4:D:377:LEU:HG	2.02	0.41
5:E:162:HIS:CD2	5:E:163:THR:HG23	2.56	0.41
3:C:197:PHE:HE1	3:C:203:VAL:HG12	1.85	0.41
6:F:47:SER:O	6:F:51:MET:HG3	2.20	0.41
8:H:313:THR:HG22	8:H:534:VAL:HG22	2.02	0.41
1:A:283:ARG:HG3	1:A:287:LEU:HD23	2.03	0.41
2:B:76:THR:O	2:B:80:ILE:HG13	2.20	0.41
2:B:134:CYS:O	2:B:138:THR:OG1	2.24	0.41
3:C:372:ILE:HD11	5:E:243:SER:HA	2.02	0.41
3:C:506:CYS:HB3	3:C:507:PRO:HD3	2.03	0.41
5:E:162:HIS:HA	5:E:246:GLU:HB2	2.01	0.41
8:H:772:VAL:HG11	8:H:818:LYS:NZ	2.36	0.41
8:H:860:ARG:O	8:H:864:ARG:HG3	2.21	0.41
1:A:338:ILE:HG12	1:A:488:LEU:HB2	2.03	0.41
2:B:524:LEU:HD23	2:B:561:ILE:HD13	2.01	0.41
2:B:573:ASP:HB3	2:B:576:GLU:HG2	2.02	0.41
2:B:616:ARG:HD3	2:B:616:ARG:HA	1.75	0.41
3:C:233:ASP:OD1	3:C:233:ASP:N	2.53	0.41
4:D:100:LEU:H	4:D:100:LEU:HD13	1.84	0.41
5:E:183:TYR:HA	5:E:186:ILE:HD12	2.02	0.41
8:H:315:LEU:HA	8:H:532:LEU:HD23	2.02	0.41
8:H:607:LEU:O	8:H:611:GLN:HG3	2.21	0.41
1:A:487:LYS:NZ	1:A:490:GLU:OE1	2.45	0.41
6:F:65:GLN:HE22	6:F:123:ASP:H	1.68	0.41
6:F:145:HIS:NE2	6:F:149:LYS:HE3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:635:PRO:HG2	8:H:641:TYR:CE2	2.56	0.41
1:A:524:ALA:HA	7:G:22:TYR:HE1	1.86	0.41
2:B:221:VAL:HG12	2:B:225:LEU:HD11	2.03	0.41
2:B:559:GLU:O	2:B:563:ARG:HG3	2.21	0.41
3:C:207:TYR:CZ	3:C:211:VAL:HG11	2.56	0.41
3:C:373:ALA:HA	5:E:53:VAL:HG12	2.03	0.41
3:C:454:PRO:HD2	3:C:457:ILE:HD12	2.03	0.41
5:E:301:LEU:HD23	5:E:301:LEU:HA	1.92	0.41
6:F:137:LEU:HB3	6:F:180:VAL:HG11	2.02	0.41
6:F:166:ALA:HB2	6:F:196:LEU:HD12	2.02	0.41
6:F:169:ASP:N	6:F:169:ASP:OD1	2.54	0.41
6:F:195:VAL:HG11	6:F:199:ASP:OD1	2.21	0.41
7:G:33:PHE:HE2	7:G:48:GLU:HB3	1.86	0.41
8:H:204:ASP:HB3	9:I:314:LEU:HD23	2.03	0.41
8:H:285:ARG:O	8:H:289:ILE:HG13	2.21	0.41
8:H:660:TYR:HD2	8:H:682:HIS:CE1	2.38	0.41
9:I:279:LEU:HA	9:I:282:GLN:HB2	2.02	0.41
10:J:116:ASP:OD1	10:J:116:ASP:N	2.45	0.41
10:J:162:PHE:O	10:J:165:ILE:HG22	2.20	0.41
12:M:28:DA:H2'	12:M:29:DT:H71	2.03	0.41
1:A:423:ALA:O	1:A:427:MET:HG2	2.21	0.41
1:A:675:LYS:O	1:A:678:ARG:HB2	2.21	0.41
2:B:16:TYR:HB3	2:B:738:LEU:HD11	2.03	0.41
2:B:19:PRO:HB3	2:B:739:LEU:HD11	2.02	0.41
2:B:532:PRO:O	2:B:565:LYS:HE3	2.21	0.41
3:C:223:ARG:O	3:C:227:SER:N	2.54	0.41
3:C:524:HIS:NE2	3:C:528:MET:SD	2.94	0.41
8:H:761:LEU:HD22	8:H:812:ILE:HD11	2.03	0.41
8:H:779:LEU:HB3	8:H:811:TYR:CD1	2.56	0.41
8:H:849:LYS:HE3	8:H:853:LYS:NZ	2.36	0.41
1:A:360:ARG:HH21	1:A:429:TRP:HH2	1.67	0.40
2:B:682:LYS:HE3	2:B:707:ASN:ND2	2.36	0.40
3:C:210:ASN:HB3	3:C:215:MET:HG2	2.03	0.40
3:C:397:SER:O	3:C:400:ILE:HG22	2.21	0.40
6:F:174:TYR:O	6:F:178:MET:HG2	2.21	0.40
8:H:303:LEU:HD13	8:H:532:LEU:HD22	2.03	0.40
8:H:851:LEU:HD21	10:J:126:LEU:HD11	2.02	0.40
10:J:122:SER:OG	10:J:125:ASN:OD1	2.24	0.40
1:A:170:LEU:O	1:A:461:HIS:NE2	2.48	0.40
1:A:178:GLU:HB3	1:A:269:SER:HB3	2.02	0.40
2:B:236:ALA:HB1	2:B:239:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:160:ARG:NH2	6:F:232:LEU:O	2.43	0.40
8:H:792:GLN:HG2	8:H:811:TYR:CD2	2.56	0.40
5:E:73:ASP:HB3	5:E:80:ARG:NE	2.36	0.40
5:E:106:ILE:HD13	5:E:131:LEU:HD21	2.04	0.40
6:F:119:MET:O	6:F:122:SER:OG	2.32	0.40
1:A:297:PHE:HB2	1:A:332:ARG:HA	2.02	0.40
2:B:410:TYR:HB3	2:B:414:PHE:CZ	2.56	0.40
2:B:695:ARG:NH2	2:B:758:GLN:OE1	2.48	0.40
5:E:49:HIS:CE1	5:E:327:PRO:HB3	2.56	0.40
8:H:306:LEU:HD12	8:H:532:LEU:HD13	2.03	0.40
8:H:746:ALA:HA	8:H:752:PRO:HD3	2.03	0.40
8:H:856:LEU:O	8:H:859:GLU:HB3	2.21	0.40
1:A:444:HIS:CD2	1:A:445:THR:HG23	2.53	0.40
1:A:561:PHE:CE1	1:A:639:ARG:HD2	2.57	0.40
2:B:171:PRO:O	2:B:175:TYR:OH	2.29	0.40
2:B:497:ARG:HB2	2:B:709:THR:HG22	2.02	0.40
6:F:25:GLN:HA	6:F:25:GLN:NE2	2.36	0.40
8:H:684:LEU:HD11	8:H:736:TRP:HH2	1.85	0.40
12:M:23:DC:H2"	12:M:24:DT:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	610/782 (78%)	591 (97%)	19 (3%)	0	100	100
2	B	758/768 (99%)	748 (99%)	10 (1%)	0	100	100
3	C	301/548 (55%)	295 (98%)	6 (2%)	0	100	100
4	D	444/462 (96%)	439 (99%)	5 (1%)	0	100	100
5	E	351/417 (84%)	342 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	257/308 (83%)	249 (97%)	8 (3%)	0	100	100
7	G	65/71 (92%)	64 (98%)	1 (2%)	0	100	100
8	H	524/950 (55%)	505 (96%)	19 (4%)	0	100	100
9	I	59/417 (14%)	56 (95%)	3 (5%)	0	100	100
10	J	148/172 (86%)	146 (99%)	2 (1%)	0	100	100
All	All	3517/4895 (72%)	3435 (98%)	82 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	543/688 (79%)	528 (97%)	15 (3%)	43	65
2	B	664/672 (99%)	645 (97%)	19 (3%)	42	64
3	C	277/484 (57%)	267 (96%)	10 (4%)	35	59
4	D	384/399 (96%)	370 (96%)	14 (4%)	35	59
5	E	317/371 (85%)	307 (97%)	10 (3%)	39	61
6	F	233/272 (86%)	230 (99%)	3 (1%)	69	82
7	G	60/64 (94%)	55 (92%)	5 (8%)	11	36
8	H	467/815 (57%)	461 (99%)	6 (1%)	69	82
9	I	57/336 (17%)	56 (98%)	1 (2%)	59	77
10	J	130/152 (86%)	125 (96%)	5 (4%)	33	57
All	All	3132/4253 (74%)	3044 (97%)	88 (3%)	46	65

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	285	ILE

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Mol	Chain	Res	Type
1	A	383	THR
1	A	397	LYS
1	A	411	SER
1	A	417	THR
1	A	444	HIS
1	A	471	VAL
1	A	568	LEU
1	A	633	ARG
1	A	639	ARG
1	A	645	ARG
1	A	678	ARG
1	A	705	THR
1	A	707	GLU
2	B	63	TYR
2	B	155	CYS
2	B	210	HIS
2	B	211	TYR
2	B	227	ARG
2	B	237	HIS
2	B	262	ASN
2	B	358	LEU
2	B	361	LEU
2	B	365	VAL
2	B	378	ARG
2	B	384	HIS
2	B	433	LEU
2	B	531	VAL
2	B	612	HIS
2	B	659	HIS
2	B	703	ASP
2	B	711	ASP
2	B	731	GLU
3	C	214	ASN
3	C	376	LEU
3	C	396	THR
3	C	400	ILE
3	C	404	PHE
3	C	407	ILE
3	C	414	TYR
3	C	442	GLN
3	C	465	TYR
3	C	488	GLU

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Mol	Chain	Res	Type
4	D	42	LEU
4	D	96	TRP
4	D	97	HIS
4	D	100	LEU
4	D	115	ARG
4	D	144	ASP
4	D	161	HIS
4	D	203	PHE
4	D	205	LEU
4	D	219	TYR
4	D	284	THR
4	D	380	THR
4	D	398	ARG
4	D	434	GLU
5	E	11	TRP
5	E	21	ILE
5	E	88	LEU
5	E	109	THR
5	E	188	THR
5	E	228	TYR
5	E	284	LEU
5	E	304	GLU
5	E	313	VAL
5	E	366	VAL
6	F	154	ASN
6	F	240	GLN
6	F	258	HIS
7	G	6	LYS
7	G	37	ASP
7	G	45	VAL
7	G	49	LEU
7	G	59	GLU
8	H	563	THR
8	H	564	LYS
8	H	758	ASN
8	H	787	ASP
8	H	898	ARG
8	H	908	ARG
9	I	302	LEU
10	J	26	THR
10	J	83	LYS
10	J	93	MET

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Mol	Chain	Res	Type
10	J	165	ILE
10	J	168	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	562	GLN
4	D	411	GLN
5	E	332	GLN
5	E	365	ASN
6	F	25	GLN
6	F	52	ASN
6	F	65	GLN
6	F	258	HIS
7	G	18	GLN
9	I	293	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	3DR	L	31	11	8,11,12	6.27	4 (50%)	9,14,17	1.53	2 (22%)
11	3DR	L	30	11	8,11,12	6.25	4 (50%)	9,14,17	1.68	3 (33%)

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	3DR	L	31	11	-	2/3/15/16	0/1/1/1
11	3DR	L	30	11	-	0/3/15/16	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	31	3DR	C2'-C3'	-13.26	1.29	1.52
11	L	30	3DR	C2'-C3'	-12.93	1.30	1.52
11	L	30	3DR	O4'-C4'	-9.93	1.28	1.44
11	L	31	3DR	O4'-C4'	-9.58	1.28	1.44
11	L	31	3DR	C3'-C4'	4.52	1.65	1.53
11	L	30	3DR	C3'-C4'	4.44	1.65	1.53
11	L	31	3DR	O4'-C1'	4.42	1.56	1.42
11	L	30	3DR	O4'-C1'	4.41	1.56	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	31	3DR	O4'-C4'-C3'	3.16	108.38	103.73
11	L	30	3DR	C1'-C2'-C3'	2.73	106.28	103.20
11	L	30	3DR	C2'-C3'-C4'	2.61	108.15	102.75
11	L	30	3DR	C1'-O4'-C4'	-2.56	104.35	108.48
11	L	31	3DR	C2'-C3'-C4'	2.12	107.15	102.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	31	3DR	O4'-C4'-C5'-O5'
11	L	31	3DR	C3'-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 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
13	SF4	B	1000	2	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
13	SF4	B	1000	2	-	-	0/6/5/5

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)

There are no chain breaks in this entry.

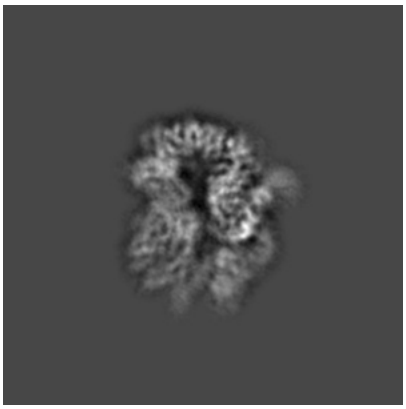
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28000. These allow visual inspection of the internal detail of the map and identification of artifacts.

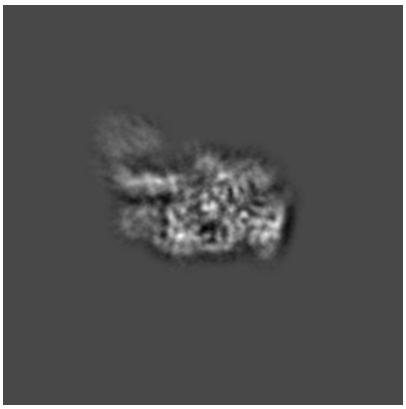
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

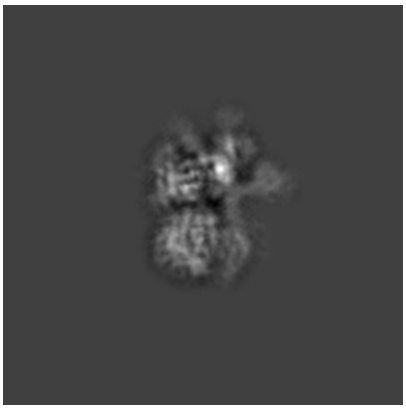
6.1.1 Primary map



X

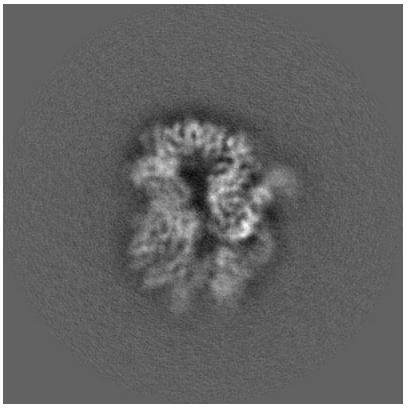


Y

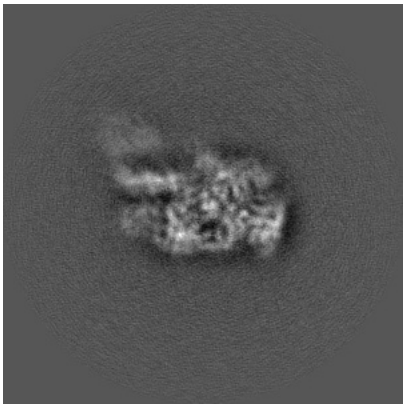


Z

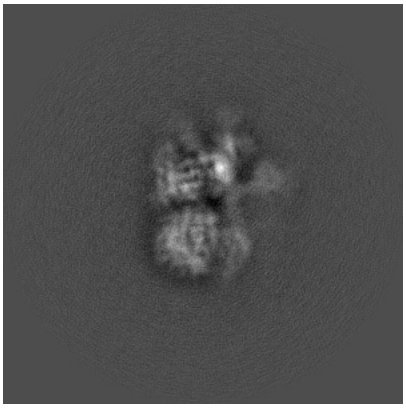
6.1.2 Raw map



X



Y

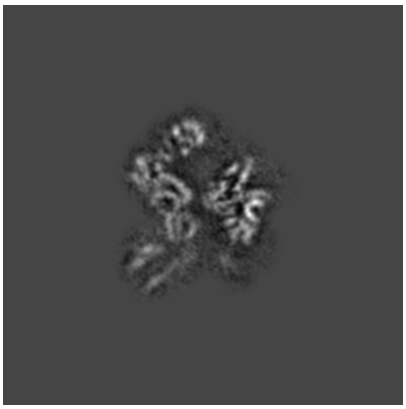


Z

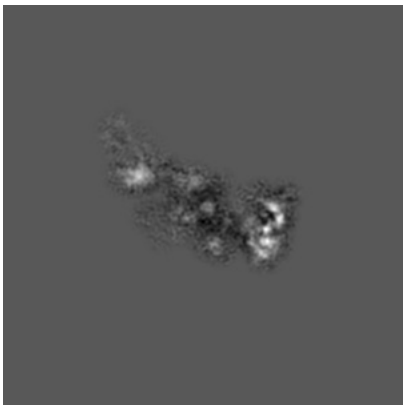
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

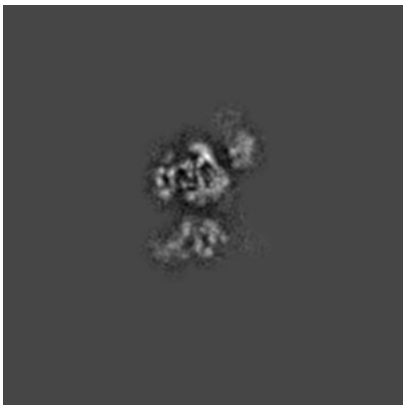
6.2.1 Primary map



X Index: 150

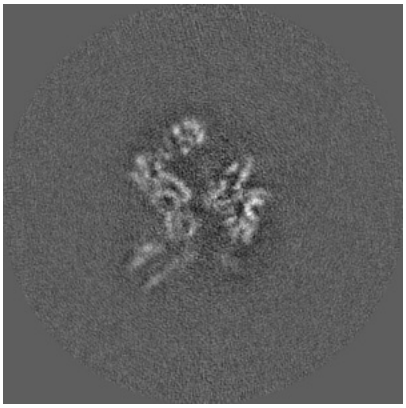


Y Index: 150

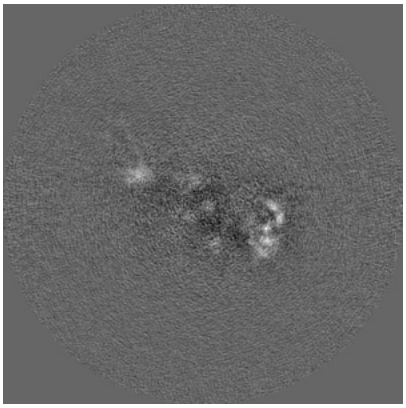


Z Index: 150

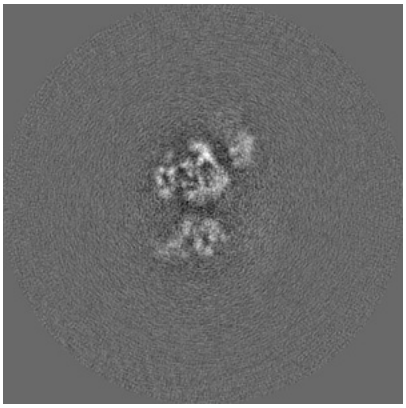
6.2.2 Raw map



X Index: 150



Y Index: 150

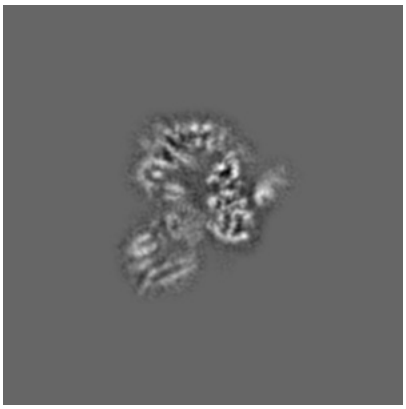


Z Index: 150

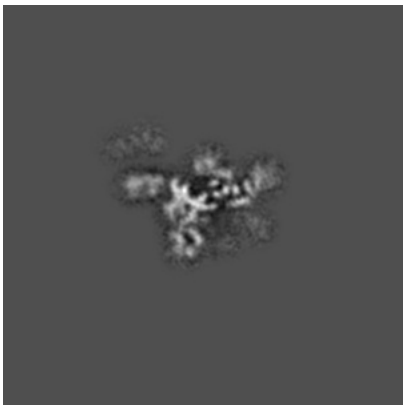
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

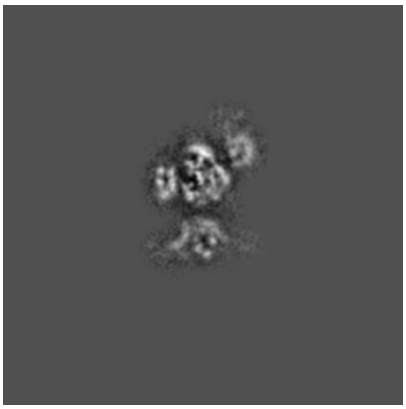
6.3.1 Primary map



X Index: 141

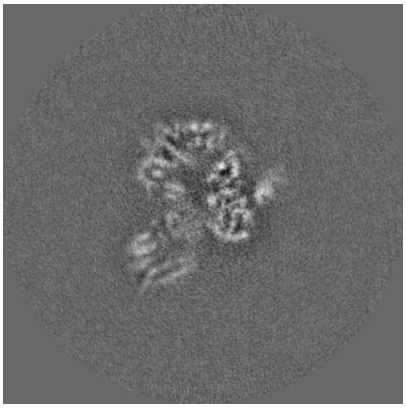


Y Index: 183

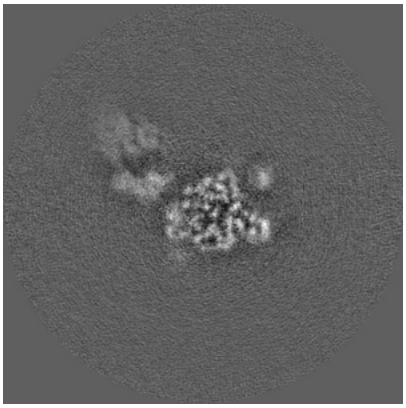


Z Index: 152

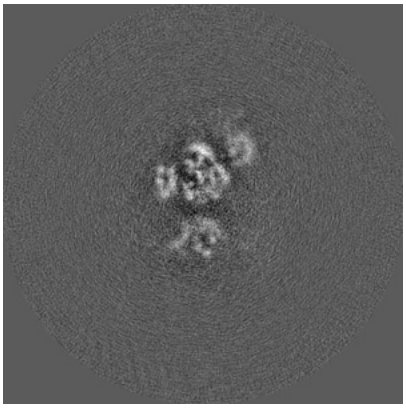
6.3.2 Raw map



X Index: 141



Y Index: 170

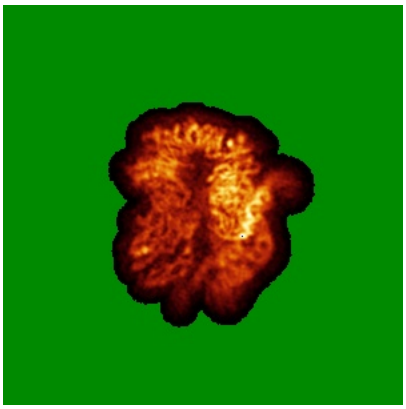


Z Index: 152

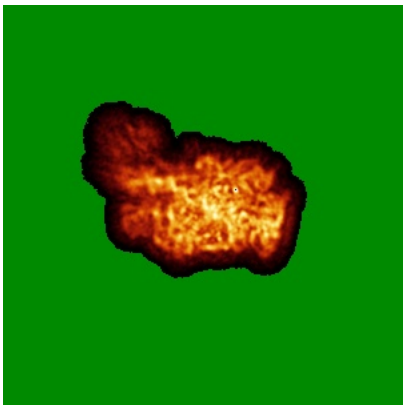
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

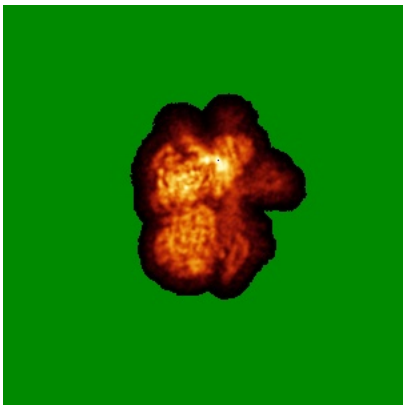
6.4.1 Primary map



X

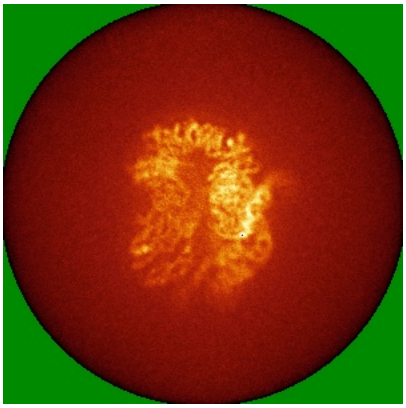


Y

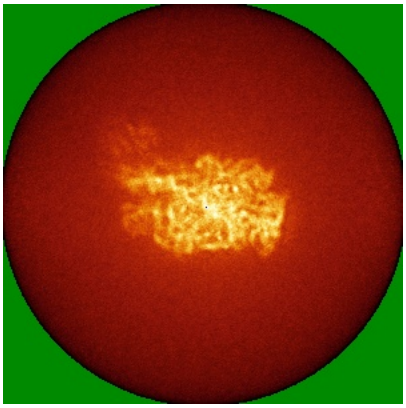


Z

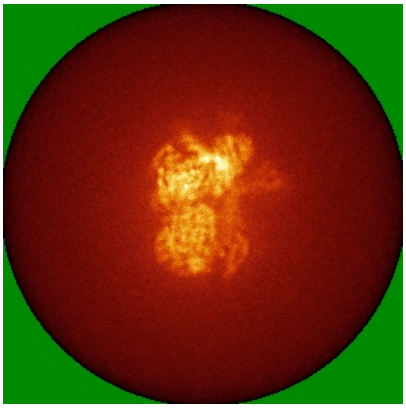
6.4.2 Raw map



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 0.008. 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.

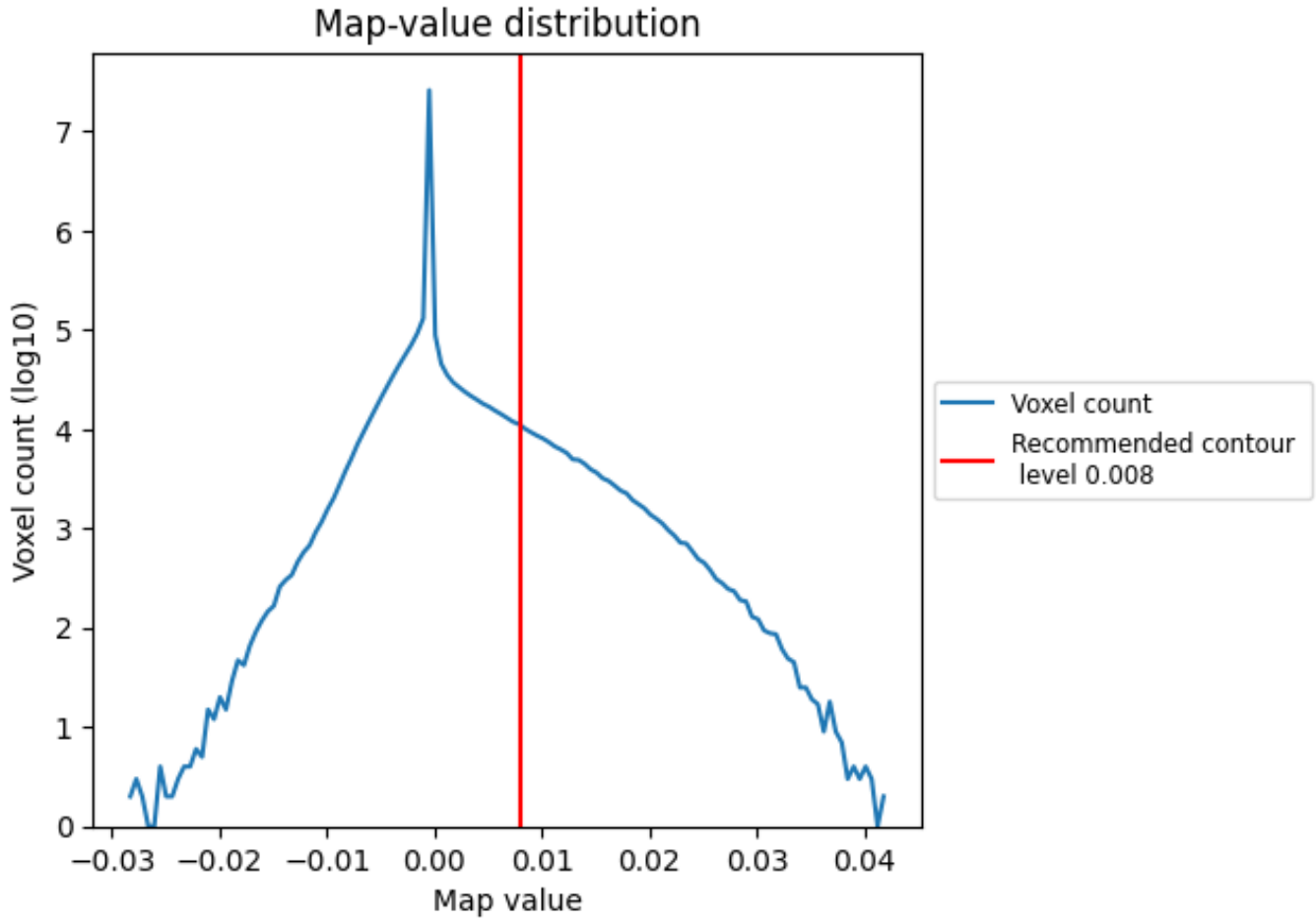
6.6 Mask visualisation (i)

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

7 Map analysis

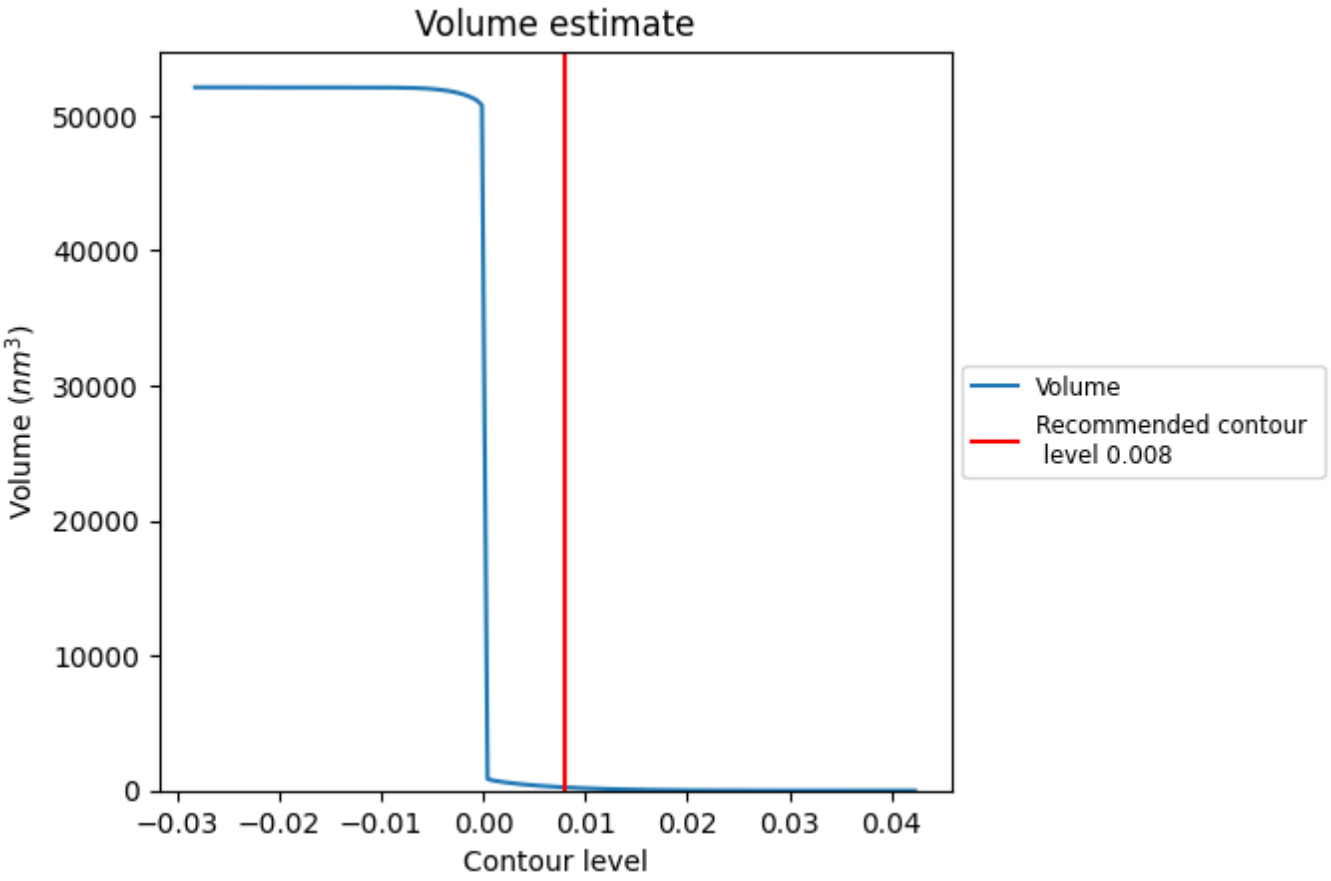
This section contains the results of statistical analysis of the map.

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.

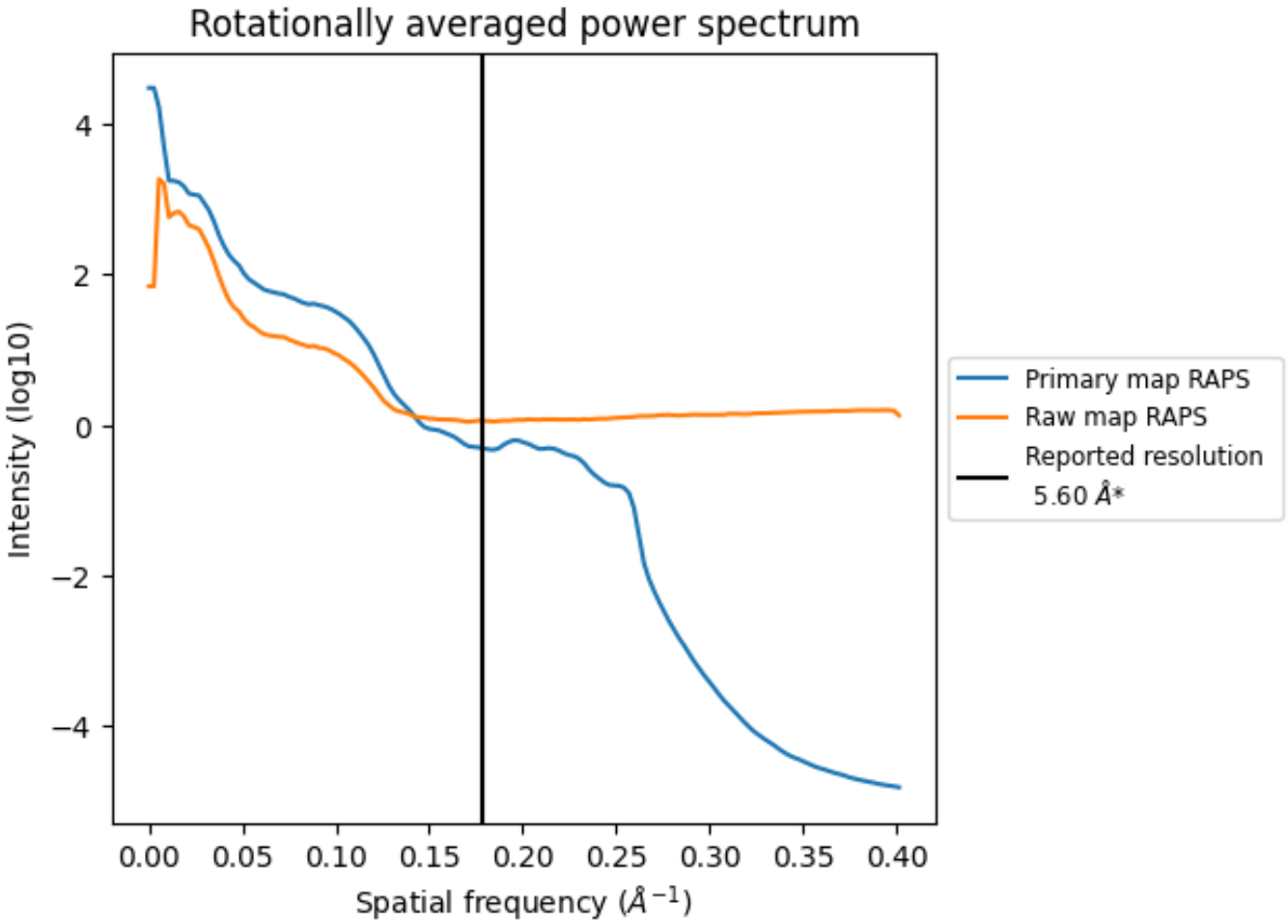
7.2 Volume estimate



The volume at the recommended contour level is 236 nm^3; this corresponds to an approximate mass of 213 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)

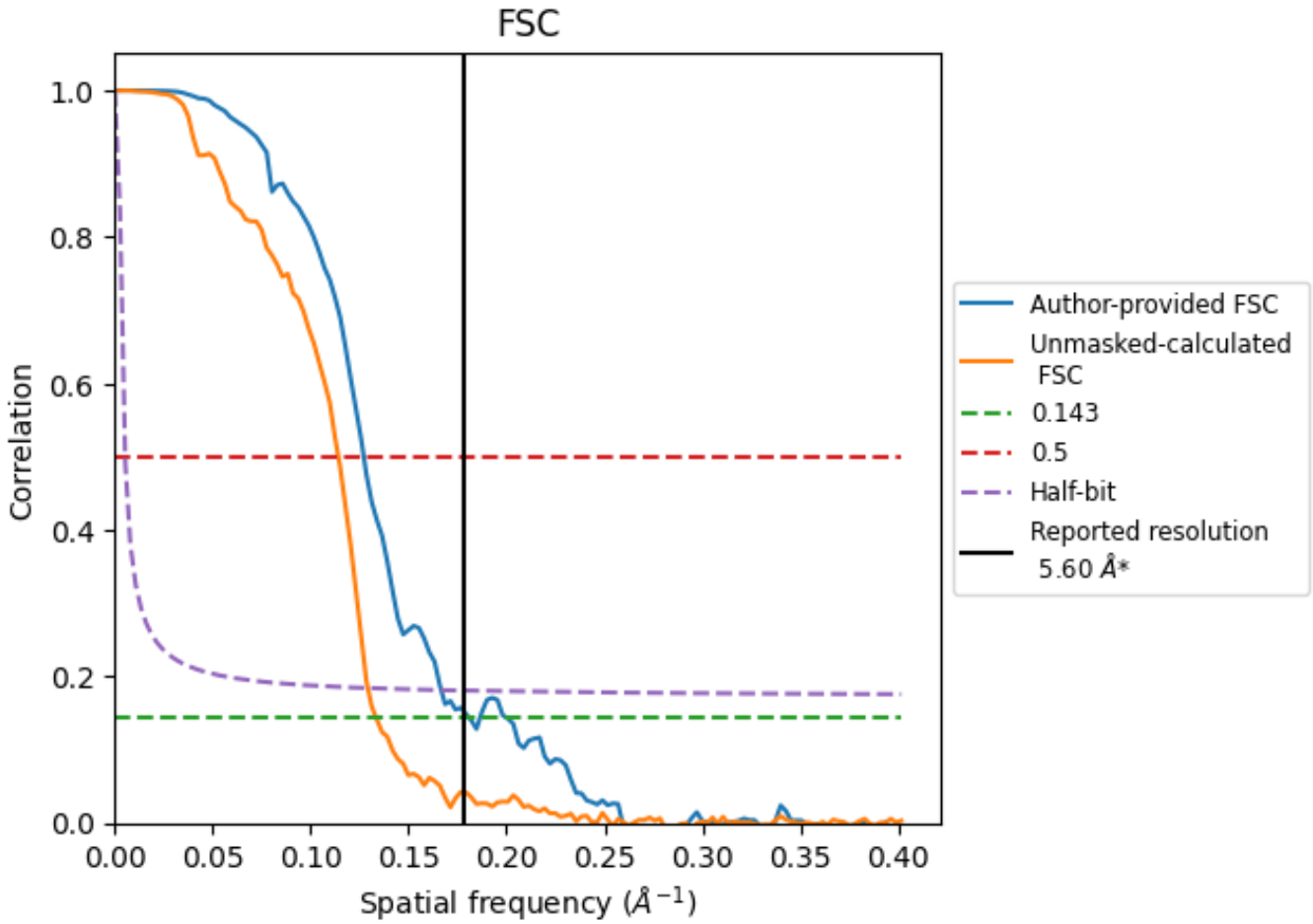


*Reported resolution corresponds to spatial frequency of 0.179 Å^{-1}

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 0.179 Å^{-1}

8.2 Resolution estimates (i)

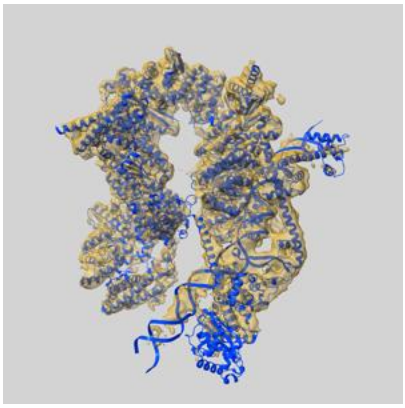
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	5.52	7.86	6.00
Unmasked-calculated*	7.49	8.76	7.74

*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 7.49 differs from the reported value 5.6 by more than 10 %

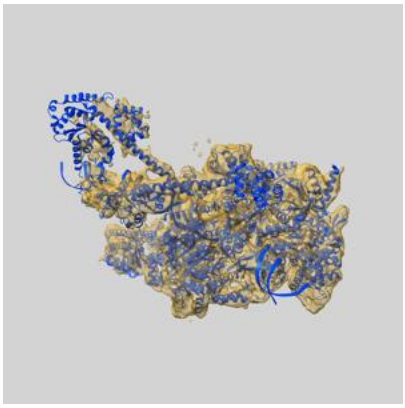
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28000 and PDB model 8EBW. Per-residue inclusion information can be found in section 3 on page 9.

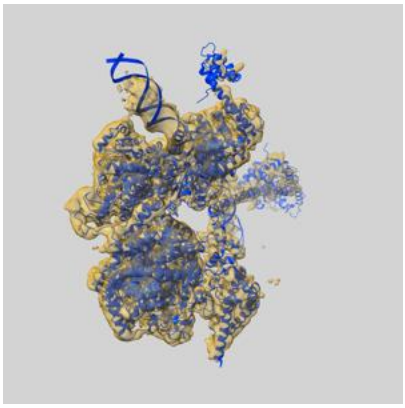
9.1 Map-model overlay



X



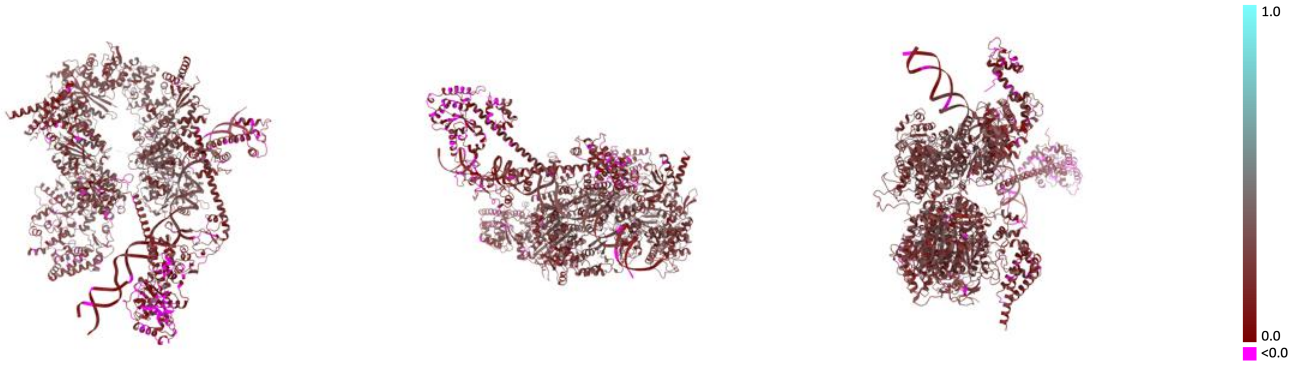
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

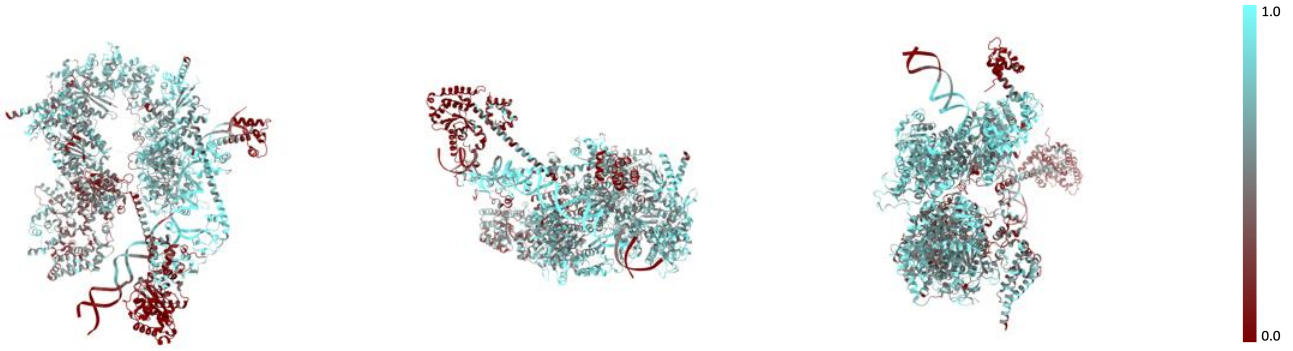
9.2 Q-score mapped to coordinate model (i)



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.

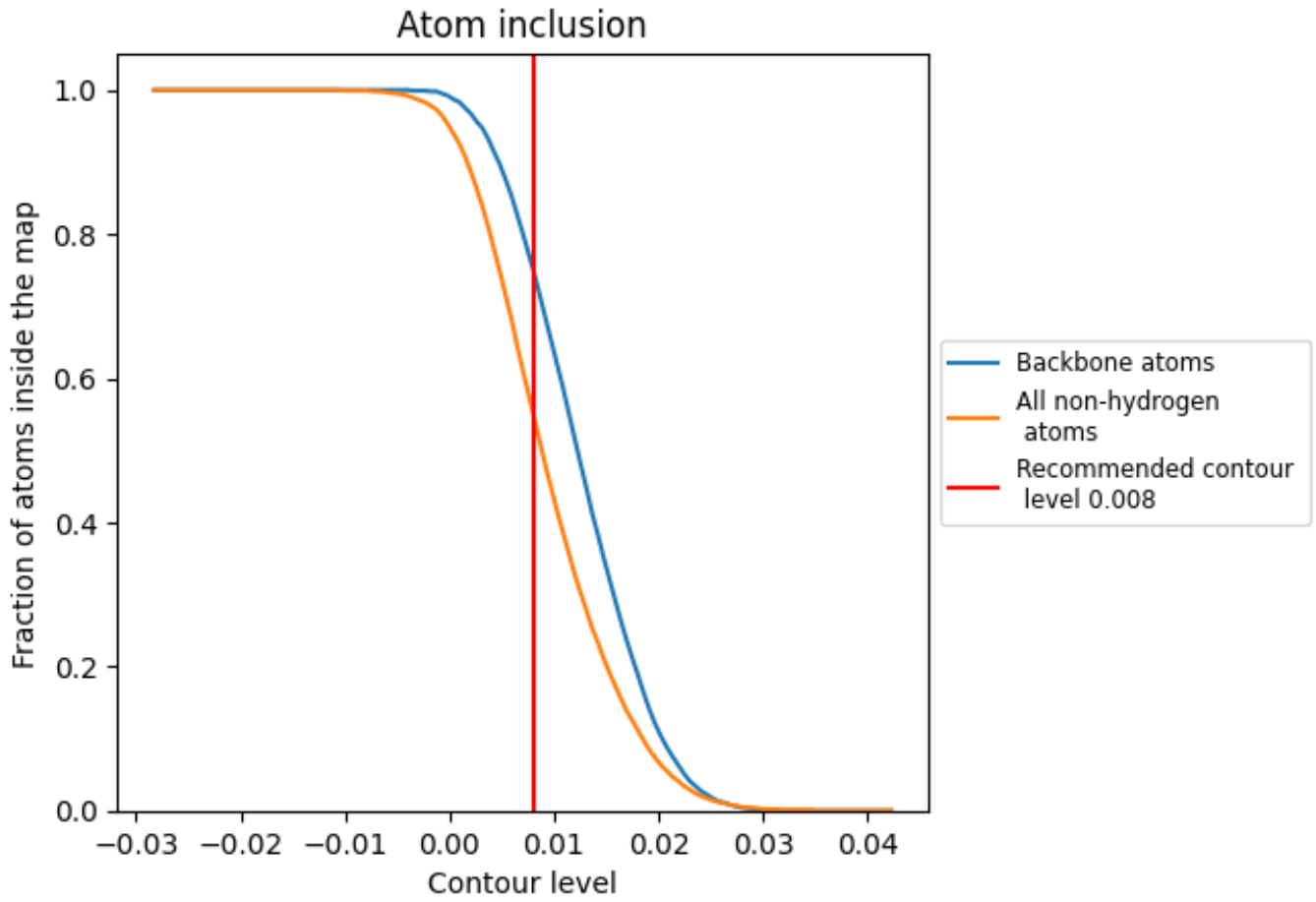
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 55% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5520	0.2080
A	0.6910	0.2640
B	0.4320	0.1970
C	0.5160	0.1880
D	0.7260	0.2490
E	0.6210	0.2490
F	0.6390	0.2530
G	0.6740	0.2460
H	0.3890	0.1330
I	0.2470	0.1080
J	0.4080	0.1330
L	0.5800	0.1750
M	0.6260	0.1830