Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 04:21 am GMT

PDB ID	:	6XTY
EMDB ID	:	EMD-10621
Title	:	CryoEM structure of human CMG bound to AND-1 (CMGA)
Authors	:	Rzechorzek, N.J.; Pellegrini, L.; Chirgadze, D.Y.; Hardwick, S.W.
Deposited on	:	2020-01-16
Resolution	:	6.77 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:

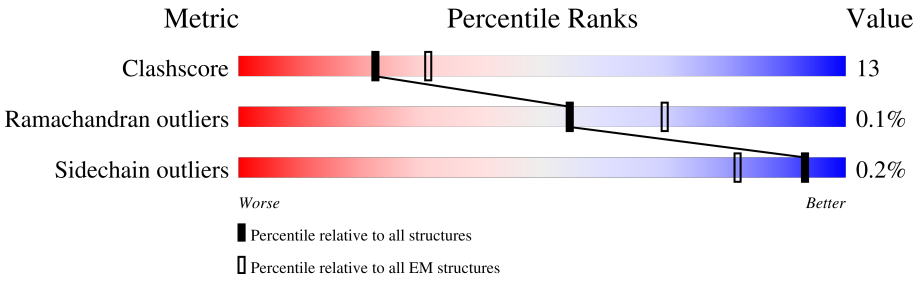
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 6.77 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	2	904	46% 21% 32%
2	3	853	5% 52% 19% 29%
3	4	863	5% 50% 19% 31%
4	5	734	8% 56% 22% 21%
5	6	821	7% 58% 15% 26%
6	7	719	5% 66% 17% 17%
7	A	196	64% 36%
8	B	185	66% 29% 5%

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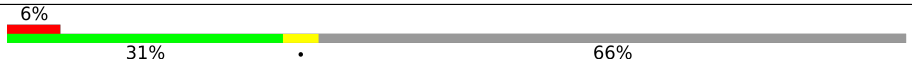
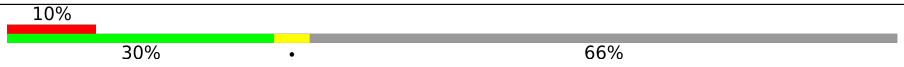
Mol	Chain	Length	Quality of chain
9	C	216	
10	D	223	
11	E	566	
12	F	1171	
12	G	1171	
12	H	1171	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 48821 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	611	4832	3040	863	899	30	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	608	4782	2997	844	916	25	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	598	4784	3016	850	892	26	0	0

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	577	4524	2841	805	843	35	0	0

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	609	4873	3068	862	917	26	0	0

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	598	4727	2960	837	901	29	0	0

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	196	Total	C	N	O	S	0	0
			1613	1016	290	295	12		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	176	Total	C	N	O	S	0	0
			1431	916	242	264	9		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	194	Total	C	N	O	S	0	0
			1552	985	268	293	6		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	203	Total	C	N	O	S	0	0
			1679	1065	290	314	10		

- Molecule 11 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	538	Total	C	N	O	S	0	0
			4380	2785	751	813	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	346	GLN	GLU	variant	UNP O75419

- Molecule 12 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	403	Total	C	N	O	S	3	0
			3213	2038	559	595	21		
12	G	403	Total	C	N	O	S	3	0
			3213	2038	559	595	21		
12	H	403	Total	C	N	O	S	3	0
			3213	2038	559	595	21		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-41	MET	-	initiating methionine	UNP O75717
F	-40	SER	-	expression tag	UNP O75717
F	-39	ALA	-	expression tag	UNP O75717
F	-38	TRP	-	expression tag	UNP O75717
F	-37	SER	-	expression tag	UNP O75717
F	-36	HIS	-	expression tag	UNP O75717
F	-35	PRO	-	expression tag	UNP O75717
F	-34	GLN	-	expression tag	UNP O75717
F	-33	PHE	-	expression tag	UNP O75717
F	-32	GLU	-	expression tag	UNP O75717
F	-31	LYS	-	expression tag	UNP O75717
F	-30	GLY	-	expression tag	UNP O75717
F	-29	GLY	-	expression tag	UNP O75717
F	-28	GLY	-	expression tag	UNP O75717
F	-27	SER	-	expression tag	UNP O75717
F	-26	GLY	-	expression tag	UNP O75717
F	-25	GLY	-	expression tag	UNP O75717
F	-24	GLY	-	expression tag	UNP O75717
F	-23	SER	-	expression tag	UNP O75717
F	-22	GLY	-	expression tag	UNP O75717
F	-21	GLY	-	expression tag	UNP O75717
F	-20	SER	-	expression tag	UNP O75717
F	-19	ALA	-	expression tag	UNP O75717
F	-18	TRP	-	expression tag	UNP O75717
F	-17	SER	-	expression tag	UNP O75717
F	-16	HIS	-	expression tag	UNP O75717
F	-15	PRO	-	expression tag	UNP O75717
F	-14	GLN	-	expression tag	UNP O75717
F	-13	PHE	-	expression tag	UNP O75717
F	-12	GLU	-	expression tag	UNP O75717
F	-11	LYS	-	expression tag	UNP O75717
F	-10	GLU	-	expression tag	UNP O75717
F	-9	ASN	-	expression tag	UNP O75717
F	-8	LEU	-	expression tag	UNP O75717
F	-7	TYR	-	expression tag	UNP O75717
F	-6	PHE	-	expression tag	UNP O75717
F	-5	GLN	-	expression tag	UNP O75717
F	-4	GLY	-	expression tag	UNP O75717
F	-3	SER	-	expression tag	UNP O75717
F	-2	SER	-	expression tag	UNP O75717
F	-1	ALA	-	expression tag	UNP O75717
F	0	THR	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-41	MET	-	initiating methionine	UNP O75717
G	-40	SER	-	expression tag	UNP O75717
G	-39	ALA	-	expression tag	UNP O75717
G	-38	TRP	-	expression tag	UNP O75717
G	-37	SER	-	expression tag	UNP O75717
G	-36	HIS	-	expression tag	UNP O75717
G	-35	PRO	-	expression tag	UNP O75717
G	-34	GLN	-	expression tag	UNP O75717
G	-33	PHE	-	expression tag	UNP O75717
G	-32	GLU	-	expression tag	UNP O75717
G	-31	LYS	-	expression tag	UNP O75717
G	-30	GLY	-	expression tag	UNP O75717
G	-29	GLY	-	expression tag	UNP O75717
G	-28	GLY	-	expression tag	UNP O75717
G	-27	SER	-	expression tag	UNP O75717
G	-26	GLY	-	expression tag	UNP O75717
G	-25	GLY	-	expression tag	UNP O75717
G	-24	GLY	-	expression tag	UNP O75717
G	-23	SER	-	expression tag	UNP O75717
G	-22	GLY	-	expression tag	UNP O75717
G	-21	GLY	-	expression tag	UNP O75717
G	-20	SER	-	expression tag	UNP O75717
G	-19	ALA	-	expression tag	UNP O75717
G	-18	TRP	-	expression tag	UNP O75717
G	-17	SER	-	expression tag	UNP O75717
G	-16	HIS	-	expression tag	UNP O75717
G	-15	PRO	-	expression tag	UNP O75717
G	-14	GLN	-	expression tag	UNP O75717
G	-13	PHE	-	expression tag	UNP O75717
G	-12	GLU	-	expression tag	UNP O75717
G	-11	LYS	-	expression tag	UNP O75717
G	-10	GLU	-	expression tag	UNP O75717
G	-9	ASN	-	expression tag	UNP O75717
G	-8	LEU	-	expression tag	UNP O75717
G	-7	TYR	-	expression tag	UNP O75717
G	-6	PHE	-	expression tag	UNP O75717
G	-5	GLN	-	expression tag	UNP O75717
G	-4	GLY	-	expression tag	UNP O75717
G	-3	SER	-	expression tag	UNP O75717
G	-2	SER	-	expression tag	UNP O75717
G	-1	ALA	-	expression tag	UNP O75717
G	0	THR	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-41	MET	-	initiating methionine	UNP O75717
H	-40	SER	-	expression tag	UNP O75717
H	-39	ALA	-	expression tag	UNP O75717
H	-38	TRP	-	expression tag	UNP O75717
H	-37	SER	-	expression tag	UNP O75717
H	-36	HIS	-	expression tag	UNP O75717
H	-35	PRO	-	expression tag	UNP O75717
H	-34	GLN	-	expression tag	UNP O75717
H	-33	PHE	-	expression tag	UNP O75717
H	-32	GLU	-	expression tag	UNP O75717
H	-31	LYS	-	expression tag	UNP O75717
H	-30	GLY	-	expression tag	UNP O75717
H	-29	GLY	-	expression tag	UNP O75717
H	-28	GLY	-	expression tag	UNP O75717
H	-27	SER	-	expression tag	UNP O75717
H	-26	GLY	-	expression tag	UNP O75717
H	-25	GLY	-	expression tag	UNP O75717
H	-24	GLY	-	expression tag	UNP O75717
H	-23	SER	-	expression tag	UNP O75717
H	-22	GLY	-	expression tag	UNP O75717
H	-21	GLY	-	expression tag	UNP O75717
H	-20	SER	-	expression tag	UNP O75717
H	-19	ALA	-	expression tag	UNP O75717
H	-18	TRP	-	expression tag	UNP O75717
H	-17	SER	-	expression tag	UNP O75717
H	-16	HIS	-	expression tag	UNP O75717
H	-15	PRO	-	expression tag	UNP O75717
H	-14	GLN	-	expression tag	UNP O75717
H	-13	PHE	-	expression tag	UNP O75717
H	-12	GLU	-	expression tag	UNP O75717
H	-11	LYS	-	expression tag	UNP O75717
H	-10	GLU	-	expression tag	UNP O75717
H	-9	ASN	-	expression tag	UNP O75717
H	-8	LEU	-	expression tag	UNP O75717
H	-7	TYR	-	expression tag	UNP O75717
H	-6	PHE	-	expression tag	UNP O75717
H	-5	GLN	-	expression tag	UNP O75717
H	-4	GLY	-	expression tag	UNP O75717
H	-3	SER	-	expression tag	UNP O75717
H	-2	SER	-	expression tag	UNP O75717
H	-1	ALA	-	expression tag	UNP O75717
H	0	THR	-	expression tag	UNP O75717

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

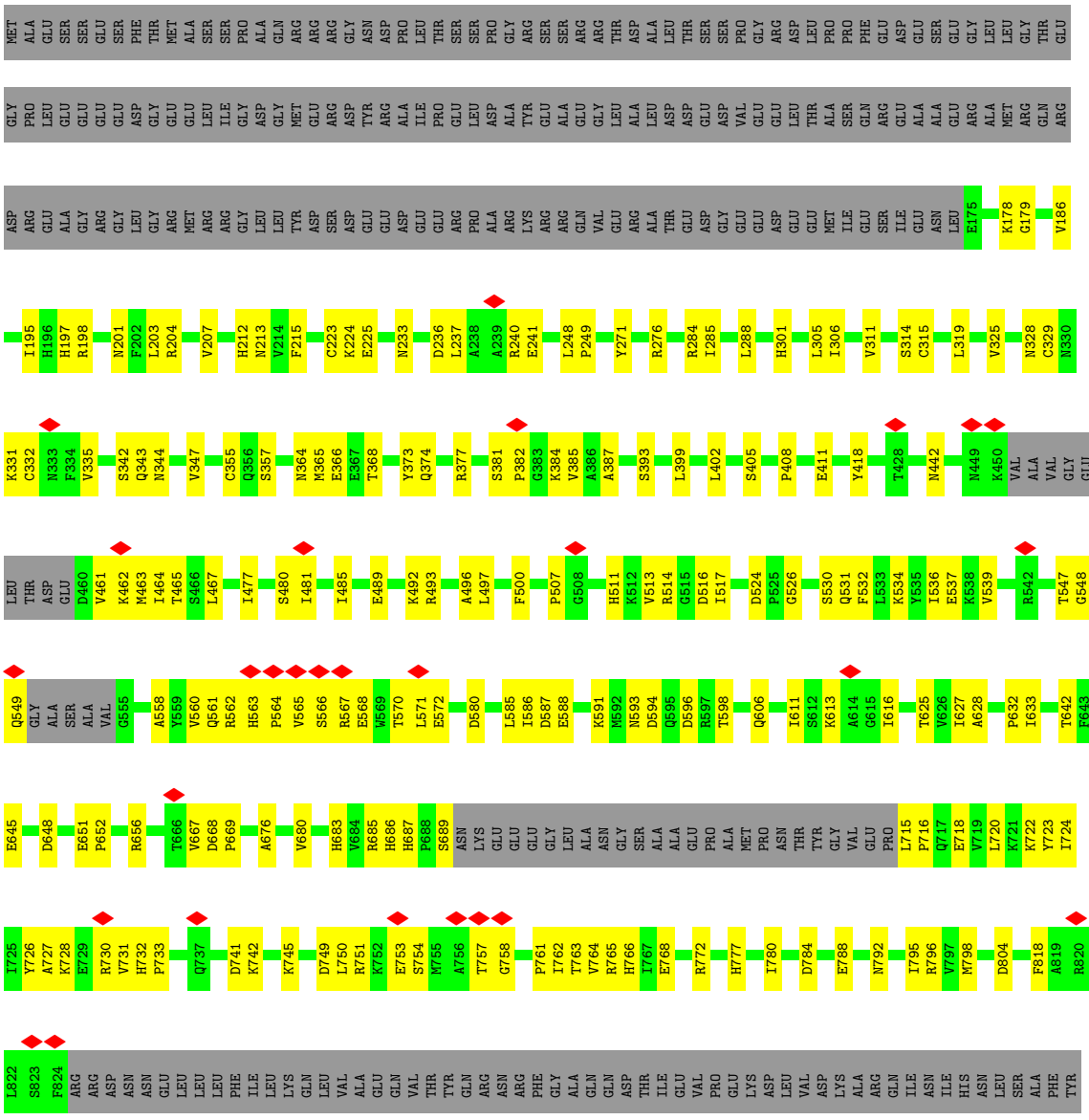
Mol	Chain	Residues	Atoms	AltConf
13	2	1	Total Zn 1 1	0
13	4	1	Total Zn 1 1	0
13	5	1	Total Zn 1 1	0
13	6	1	Total Zn 1 1	0
13	7	1	Total Zn 1 1	0

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.

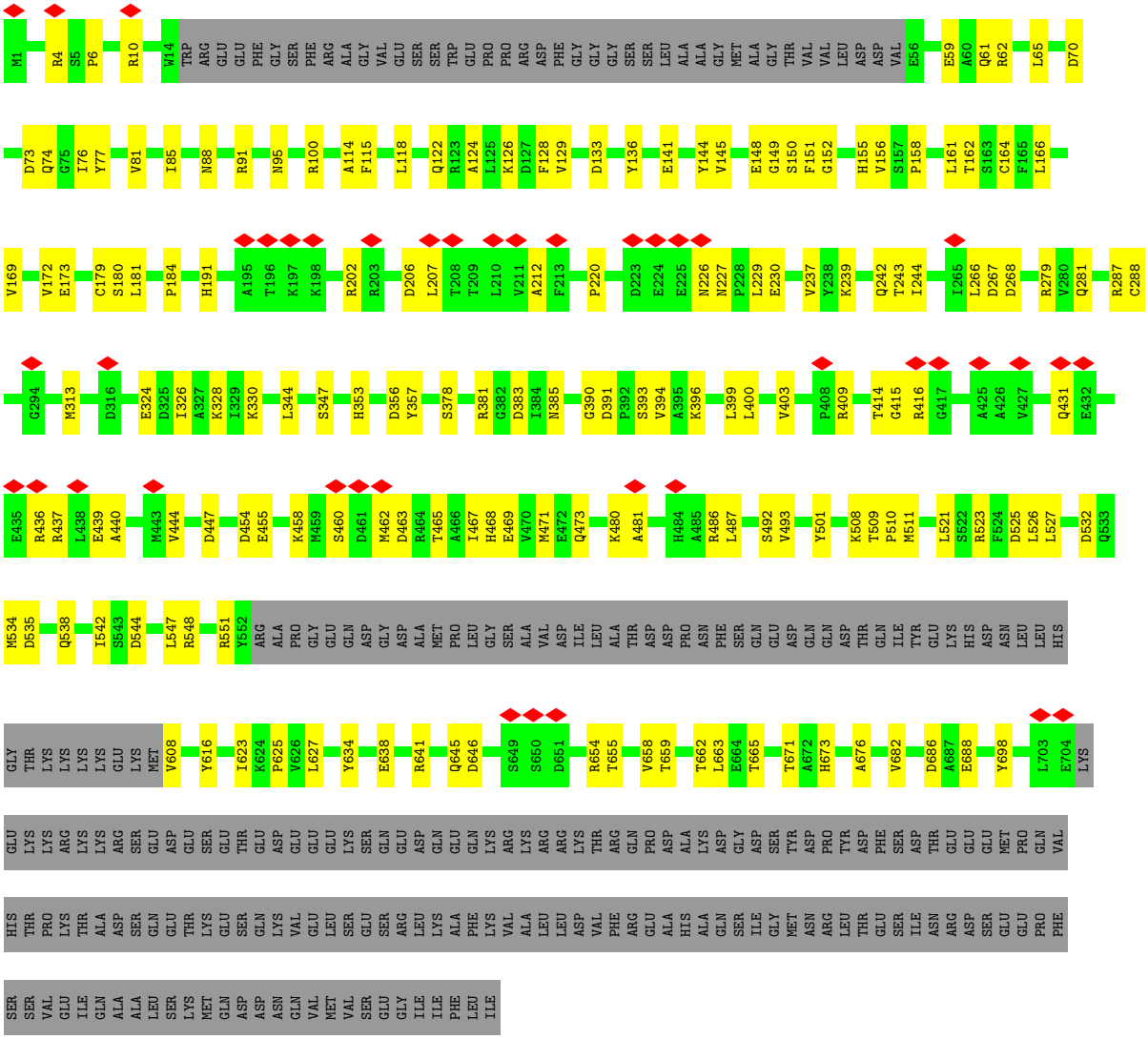
• Molecule 1: DNA replication licensing factor MCM2

Chain 2:



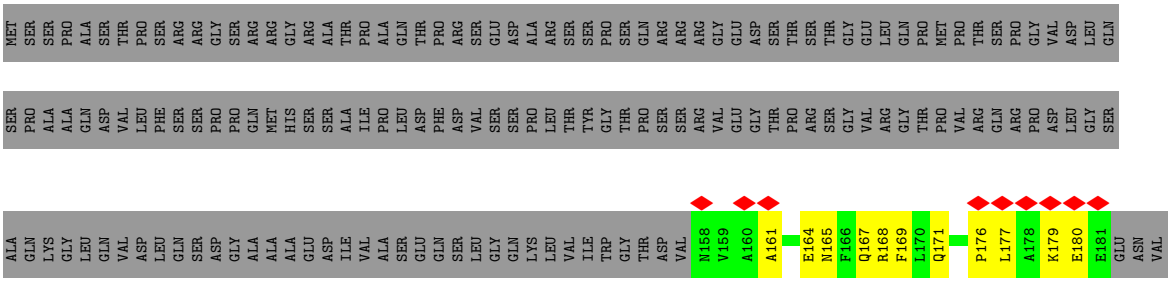
• Molecule 2: DNA replication licensing factor MCM3

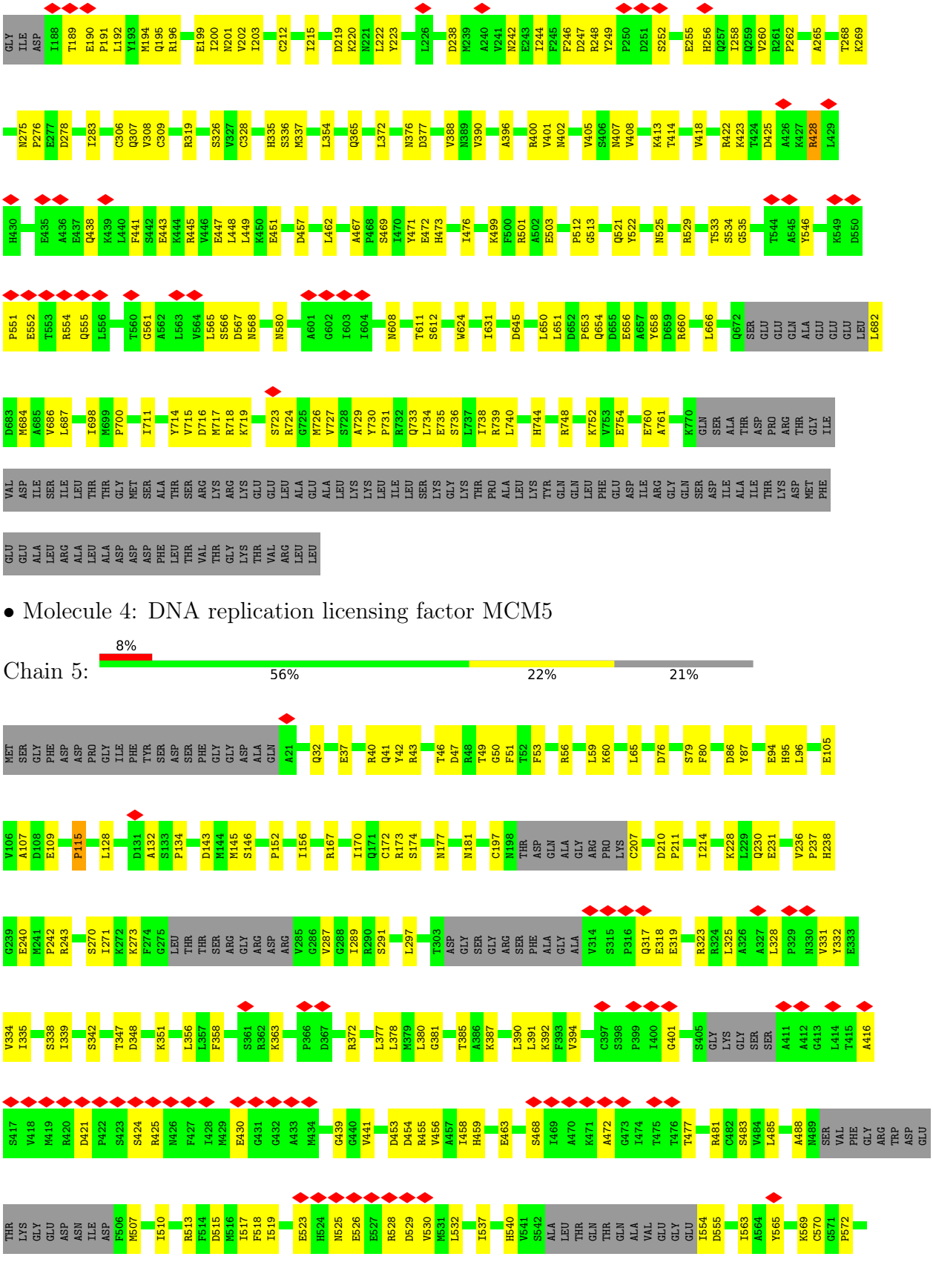
Chain 3:



• Molecule 3: DNA replication licensing factor MCM4

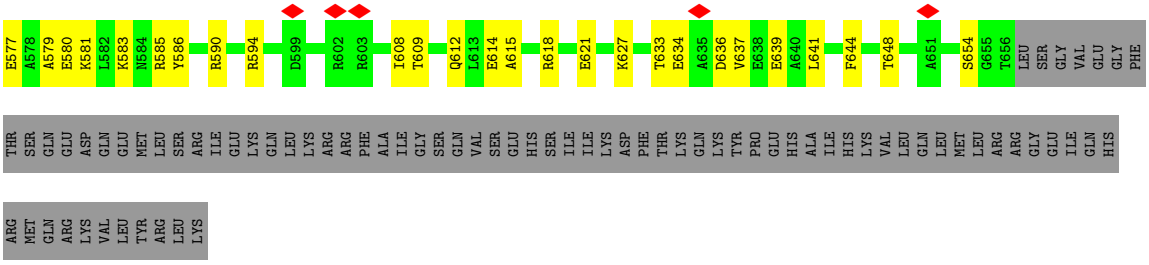
Chain 4:





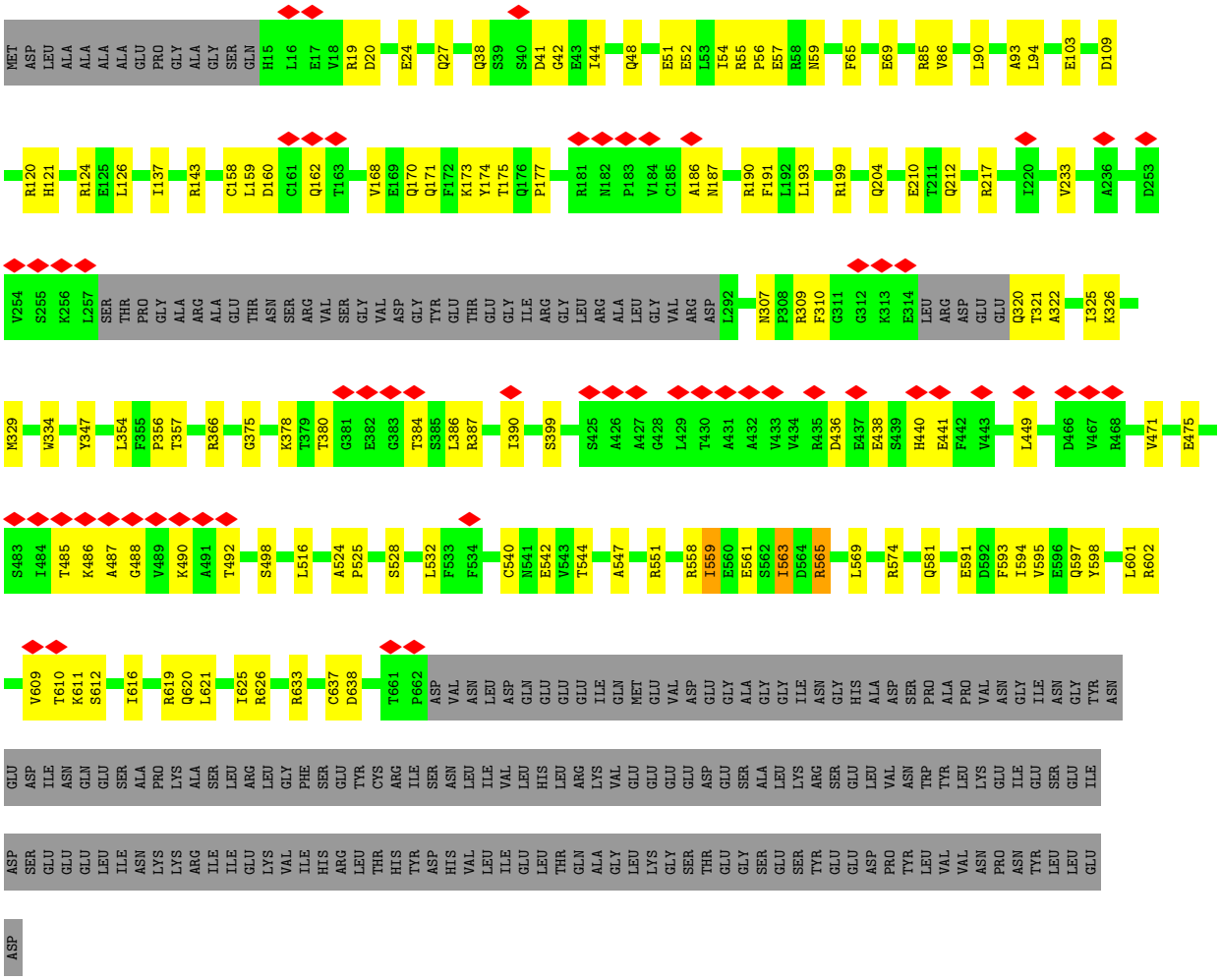
• Molecule 4: DNA replication licensing factor MCM5

Chain 5:



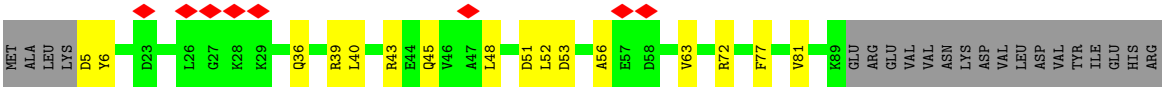
• Molecule 5: DNA replication licensing factor MCM6

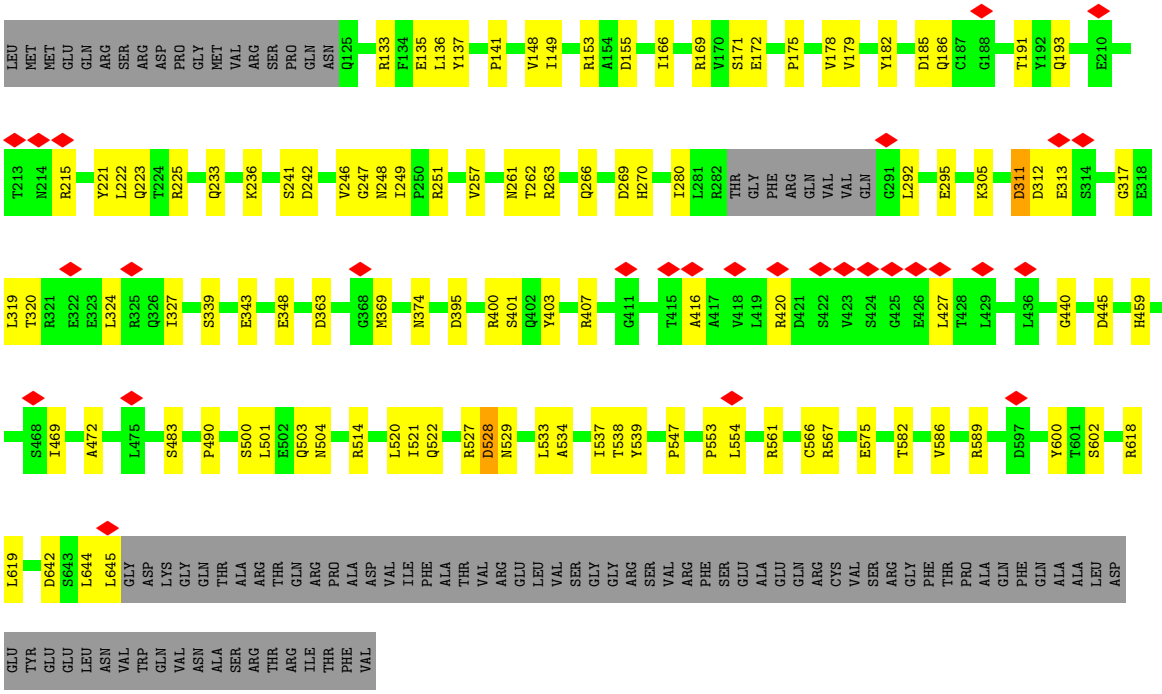
Chain 6:



• Molecule 6: DNA replication licensing factor MCM7

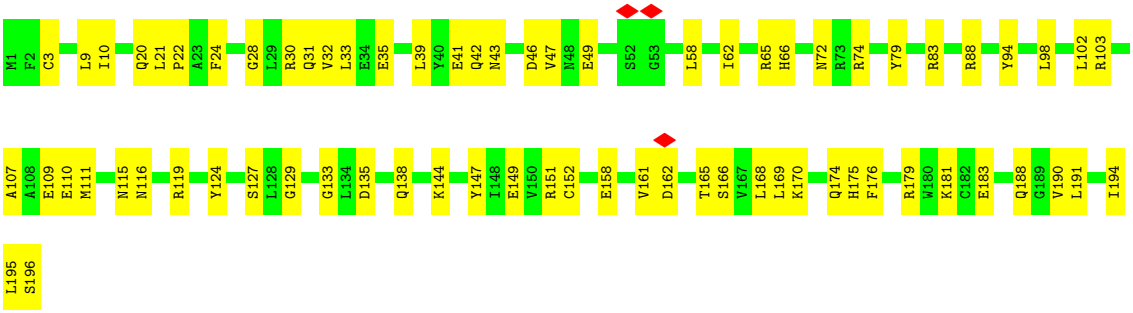
Chain 7:





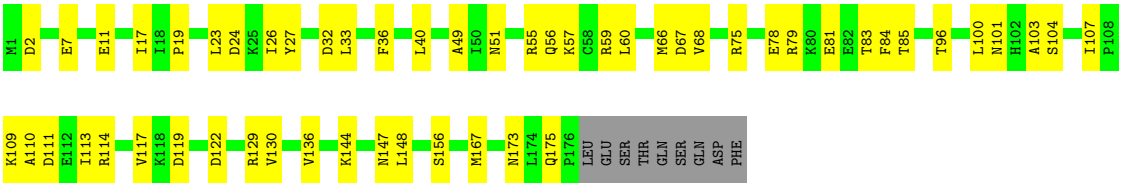
• Molecule 7: DNA replication complex GINS protein PSF1

Chain A:



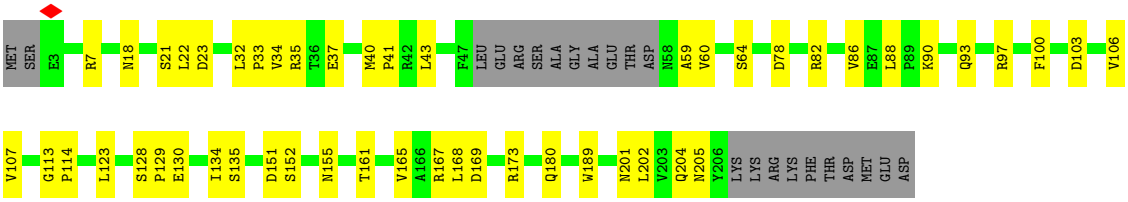
• Molecule 8: DNA replication complex GINS protein PSF2

Chain B:



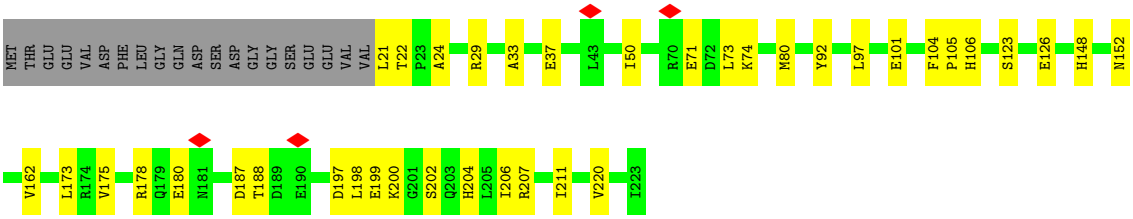
• Molecule 9: DNA replication complex GINS protein PSF3

Chain C:



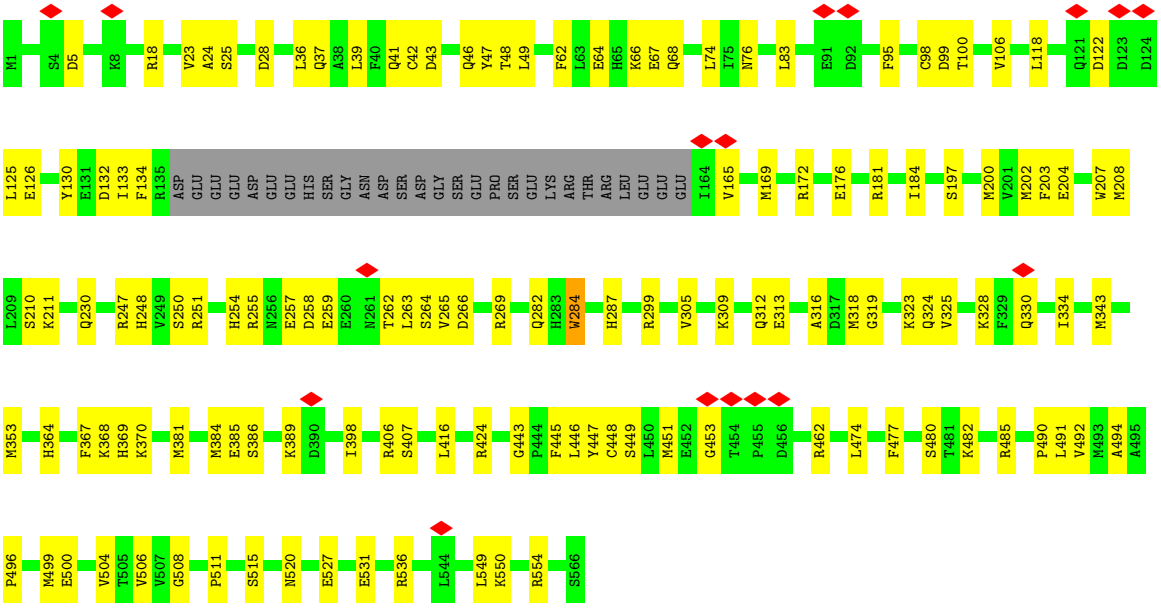
• Molecule 10: DNA replication complex GINS protein SLD5

Chain D:



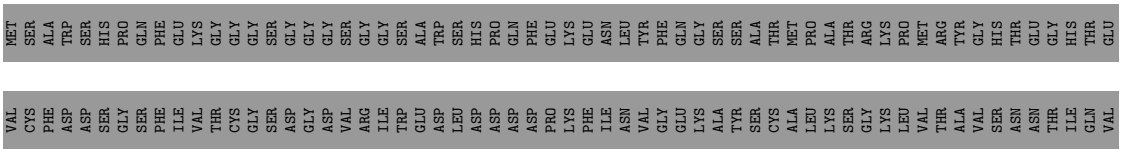
• Molecule 11: Cell division control protein 45 homolog

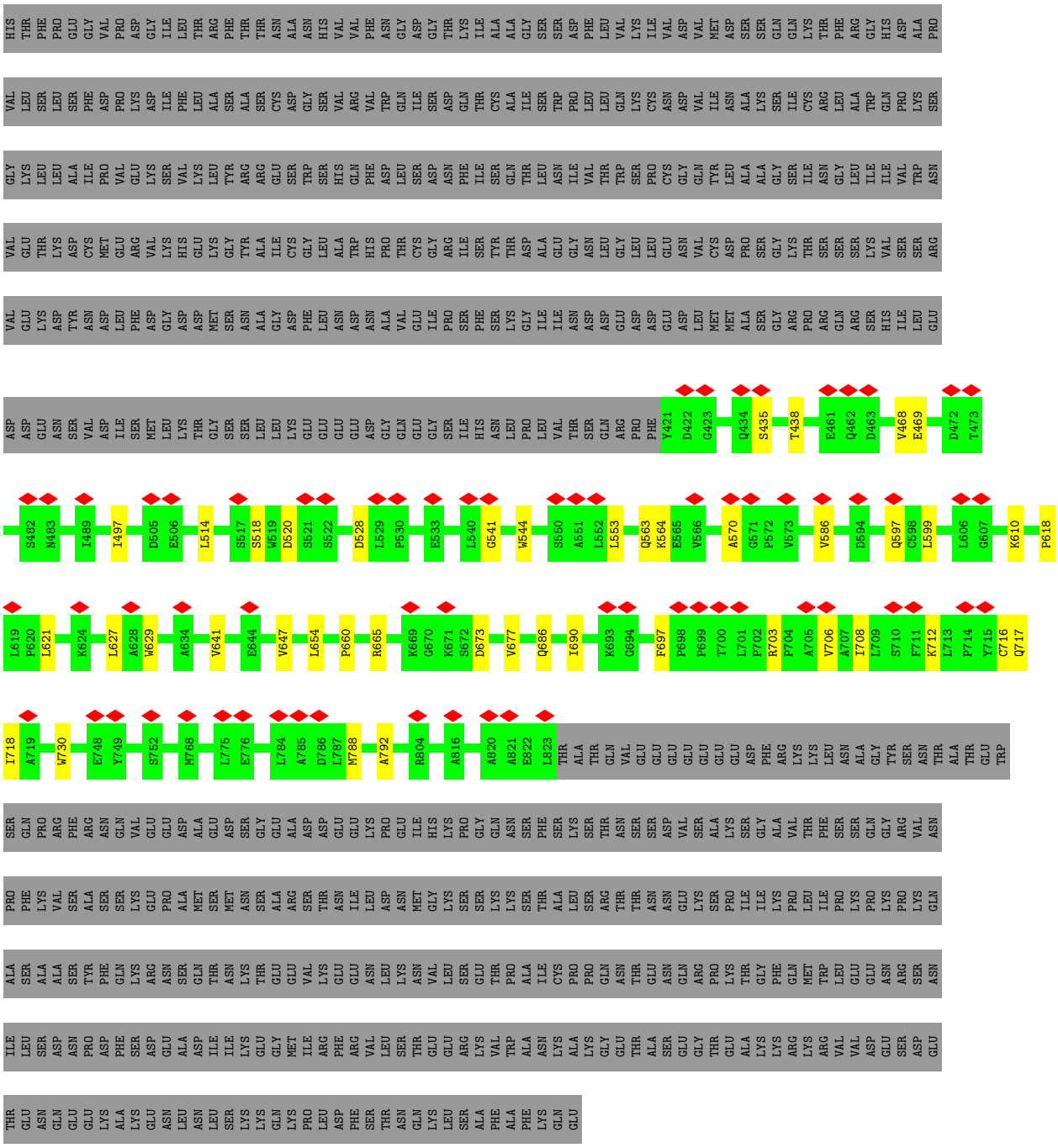
Chain E:



• Molecule 12: WD repeat and HMG-box DNA-binding protein 1

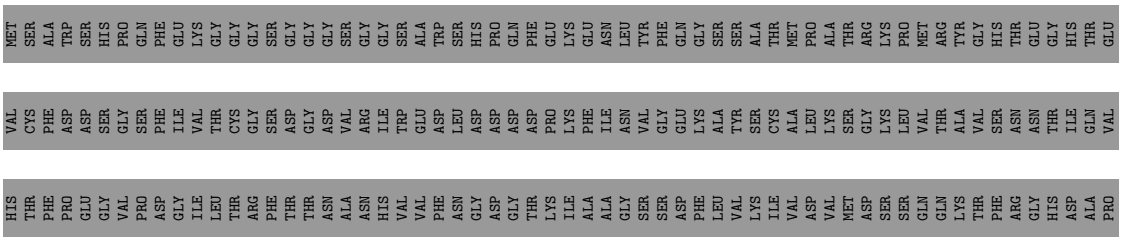
Chain F:

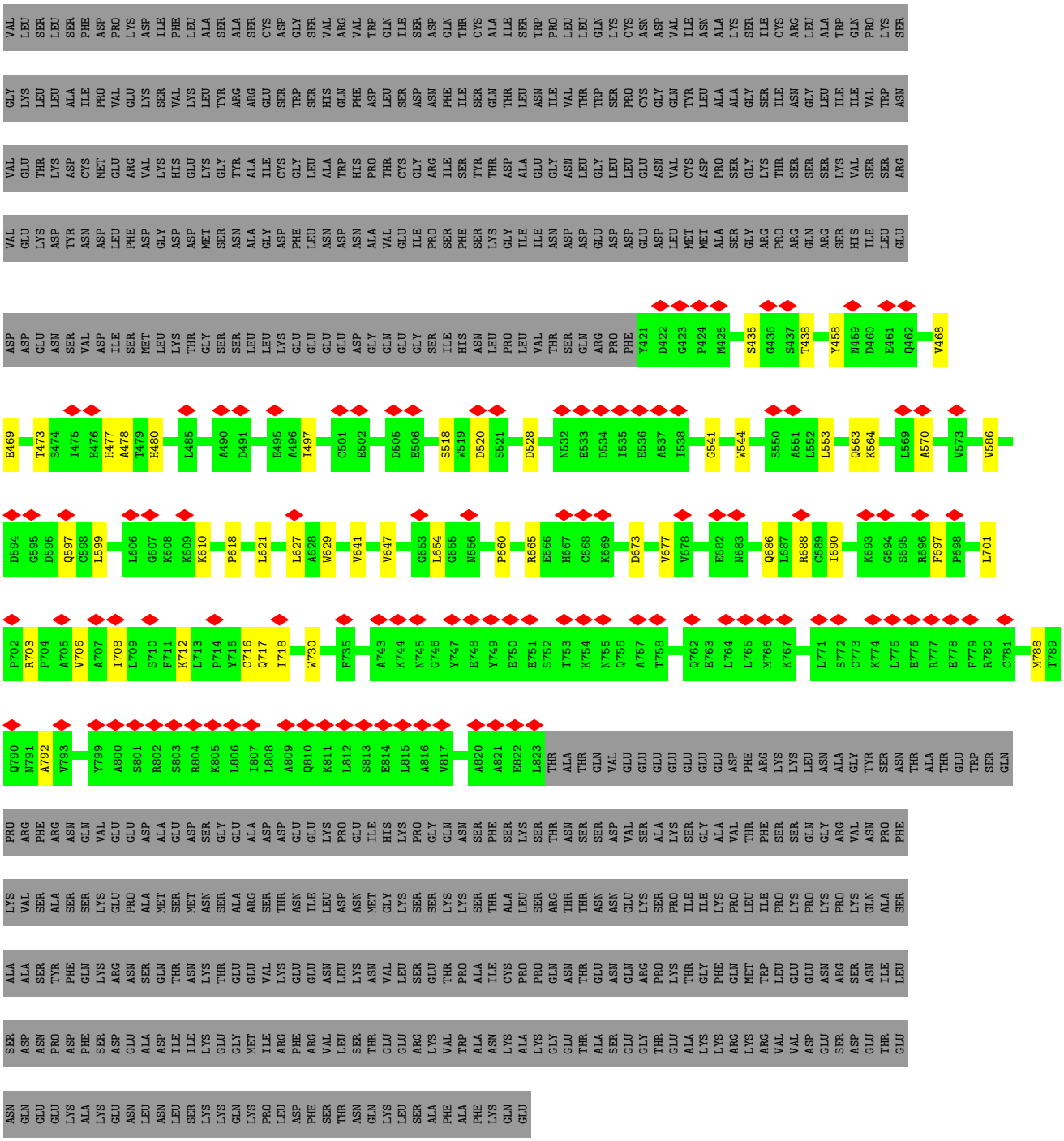




• Molecule 12: WD repeat and HMG-box DNA-binding protein 1

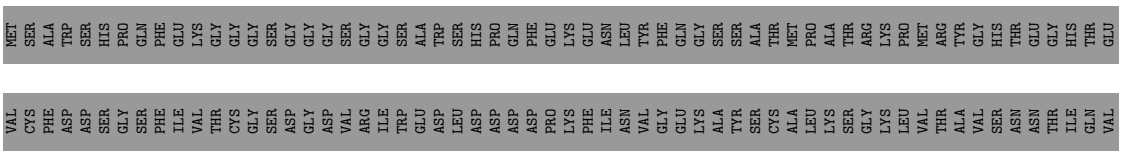
Chain G:

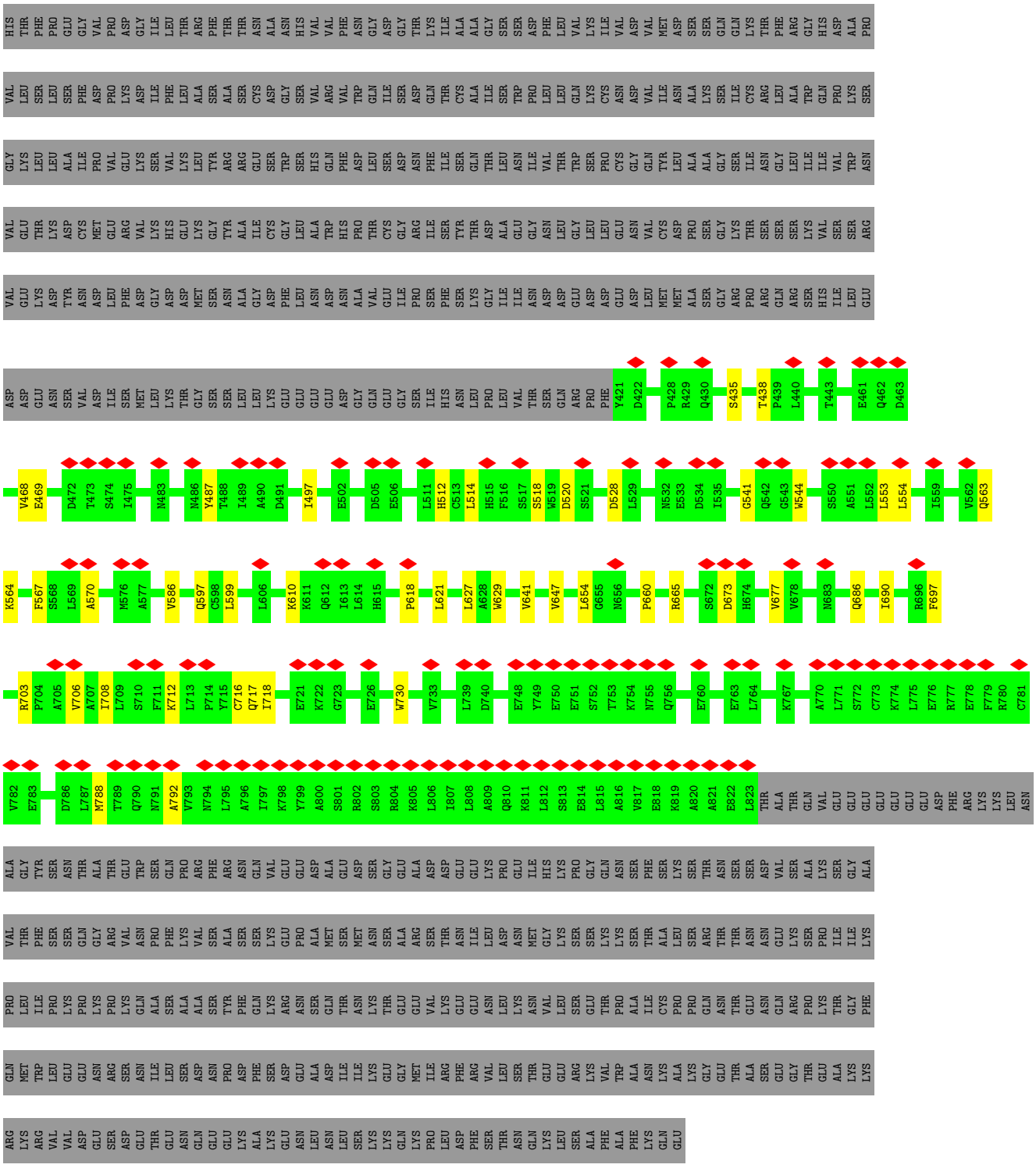




• Molecule 12: WD repeat and HMG-box DNA-binding protein 1

Chain H:




HIS THR PHE PRO GLU GLY VAL PRO ASP GLY ILE LEU THR ARG PHE THR THR ASN ALA ASN HIS VAL VAL PHE ASN GLY ASP GLY THR LYS ILE ALA ALA GLY SER SER ASP PHE LEU VAL LYS ILE VAL ASP VAL MET ASP SER SER GLN GLN LYS THR PHE ARG GLY HIS ASP ALA PRO
VAL LEU SER LEU SER PHE ASP PRO LYS ASP ILE PHE LEU ALA SER ALA SER CYS ASP GLY SER VAL ARG VAL TRP GLN ILE SER ASP GLN THR CYS ALA ILE SER TRP PRO LEU LEU GLN LYS CYS ASN ASP VAL ILE ASN ALA LYS SER ILE CYS ARG LEU ALA TRP GLN PRO LYS SER
GLY LYS LEU LEU ALA ILE PRO VAL GLU LYS SER VAL LYS LEU TYR ARG ARG GLU SER TRP SER HIS GLN PHE ASP LEU SER ASP ASN PHE ILE SER GLN THR LEU ASN ILE VAL THR TRP SER PRO CYS GLY GLN TYR LEU ALA ALA GLY SER ILE ASN GLY LEU ILE ILE VAL THR ASN
VAL GLU THR LYS ASP CYS MET GLU ARG VAL LYS HIS GLU LYS GLY TYR ALA ILE CYS GLY LEU ALA TRP HIS PRO THR CYS GLY ARG ILE SER TYR THR ASP ALA GLU GLY ASN LEU GLY LEU LEU GLU ASN VAL CYS ASP PRO SER GLY LYS THR SER SER LYS VAL SER SER ARG
VAL GLU LYS ASP TYR ASN ASP LEU PHE ASP GLY GLY ASP ASP MET SER ASN ALA GLY ASP PHE LEU ASN ASP GLU ASP ASP ASN ALA VAL GLU ILE PRO SER PHE SER LYS GLY ILE ILE ASN ASP ASP GLU ASP ASP GLU ASP ASN LEU MET MET ALA SER GLY ARG PRO ASP ARG GLN ARG SER HIS ILE LEU GLU
ASP ASP GLU ASN SER VAL ASP ILE SER MET LEU LEU LYS THR GLY SER SER LEU LEU LYS GLU GLU GLU GLU ASP GLY GLN GLU GLY SER ILE HIS ASN LEU PRO LEU VAL THR SER GLN ARG PRO PHE Y421 D422 P428 R429 Q430 S435 T438 P439 L440 T443 E461 Q462 D463
V468 E469 D472 T473 S474 I475 N483 N486 Y487 T488 I489 A490 D491 I497 E502 D505 E506 L511 H512 C513 L514 H515 F516 S517 S518 W519 D520 S521 D528 L529 N532 E533 D534 I535 G541 Q542 G543 W544 S550 A551 L552 L553 L554 I559 V562 Q563
K564 F567 S568 L569 A570 M576 A577 V586 Q597 C598 L599 L606 K610 K611 Q612 I613 L614 H615 P618 L621 L627 A628 W629 V641 V647 L654 G655 N656 P660 R665 S672 D673 H674 V677 V678 N683 Q686 I690 R696 F697
R703 P704 A705 V706 A707 I708 L709 S710 F711 K712 L713 P714 Y715 C716 Q717 I718 E721 K722 G723 E726 W730 V733 L739 D740 E748 Y749 E750 E751 S752 T753 K754 N755 Q756 E760 E763 L764 K767 A770 L771 S772 C773 K774 L775 E776 R777 E778 F779 R780 C781
V782 E783 D786 L787 M788 T789 Q790 N791 A792 V793 N794 L795 A796 I797 K798 Y799 A800 S801 R802 S803 R804 K805 L806 I807 L808 A809 Q810 K811 L812 S813 E814 L815 A816 V817 E818 K819 A820 A821 E822 L823 THR ALA THR GLN VAL GLU GLU GLU GLU GLU GLU GLU GLU ASP PHE ARG LYS LYS LEU ASN
ALA GLY TYR SER ASN THR ALA THR GLU TRP SER GLN PRO ARG PHE ARG ASN GLN VAL GLU GLU ASP ALA GLU ASP SER GLY GLU ALA ASP GLU GLU LYS PRO GLU ILE HIS LYS PRO GLY GLN ASN SER PHE SER LYS SER THR ASN SER SER ASP VAL SER ALA LYS SER GLY ALA
VAL THR PHE SER SER GLN GLY ARG VAL ASN PRO PHE LYS VAL SER ALA SER SER SER LYS GLU PRO ALA MET SER MET ASN SER ALA ARG SER THR ASN ILE LEU ASP ASN MET GLY LYS SER SER LYS LYS SER THR ALA LEU SER ARG THR THR ASN ASN GLU LYS SER PRO ILE ILE LYS
PRO LEU ILE PRO LYS PRO LYS PRO GLN ALA SER ALA ALA SER TYR PHE GLN LYS ARG ASN SER GLN THR ASN LYS THR GLU GLU VAL LYS GLU GLU ASN LEU LYS ASN VAL LEU SER GLU THR PRO ALA ILE CYS PRO PRO GLN ASN THR GLU ASN GLN ARG PRO LYS THR GLY PHE
GLN MET TRP LEU GLU GLU ASN ARG SER ASN ILE LEU SER ASP ASN PRO ASP PHE SER ASP GLU ALA ASP ILE ILE LYS GLU GLY MET ILE ARG PHE ARG VAL LEU SER THR GLU GLU ARG LYS VAL TRP ALA ASN LYS ALA LYS GLY GLU THR ALA SER GLU GLY THR GLU ALA LYS LYS
ARG LYS ARG VAL VAL ASP GLU SER ASP GLU THR GLU ASN GLN GLU GLU LYS ALA LYS GLU ASN LEU ASN SER LYS LYS GLN LYS PRO LEU ASP PHE SER THR ASN GLN LYS LEU SER ALA PHE ALA PHE LYS GLN GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15393	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 ($e^-/Å^2$)	54.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.639	Depositor
Minimum map value	-0.543	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	455.8, 455.8, 455.8	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	2	0.39	0/4923	0.47	0/6648
2	3	0.44	0/4859	0.50	0/6563
3	4	0.49	0/4870	0.52	0/6579
4	5	0.45	0/4590	0.50	0/6171
5	6	0.48	0/4955	0.51	0/6685
6	7	0.46	0/4801	0.50	0/6482
7	A	0.43	0/1645	0.46	0/2210
8	B	0.46	0/1462	0.49	0/1981
9	C	0.46	0/1587	0.49	0/2143
10	D	0.47	0/1711	0.48	0/2305
11	E	0.46	0/4472	0.48	0/6037
12	F	0.24	0/3293	0.42	0/4462
12	G	0.24	0/3293	0.42	0/4462
12	H	0.24	0/3293	0.42	0/4462
All	All	0.42	0/49754	0.48	0/67190

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	2	4832	0	4839	242	0
2	3	4782	0	4826	152	0
3	4	4784	0	4825	137	0
4	5	4524	0	4608	209	0
5	6	4873	0	4901	149	0
6	7	4727	0	4758	119	0
7	A	1613	0	1606	82	0
8	B	1431	0	1456	100	0
9	C	1552	0	1504	43	0
10	D	1679	0	1700	30	0
11	E	4380	0	4331	234	0
12	F	3213	0	3168	29	0
12	G	3213	0	3168	93	0
12	H	3213	0	3168	31	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
All	All	48821	0	48858	1228	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 (1228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:562:ARG:HH21	5:6:440:HIS:CD2	1.19	1.58
1:2:377:ARG:CG	1:2:565:VAL:HG22	1.33	1.57
8:B:59:ARG:CZ	12:G:703:ARG:HD2	1.20	1.57
1:2:377:ARG:CD	1:2:565:VAL:HG22	1.33	1.56
2:3:416:ARG:CG	4:5:456:VAL:HG11	1.31	1.55
1:2:511:HIS:CE1	4:5:342:SER:HB2	1.41	1.54
11:E:210:SER:HB2	12:G:473:THR:CG2	1.37	1.52
1:2:377:ARG:HG3	1:2:565:VAL:CG2	1.31	1.51
1:2:549:GLN:HG2	5:6:471:VAL:CG1	1.41	1.49
1:2:549:GLN:CG	5:6:471:VAL:HG11	1.43	1.46
3:4:521:GLN:NE2	6:7:464:GLN:HG2	1.29	1.45
11:E:254:HIS:CE1	12:G:458:TYR:CZ	1.79	1.44
1:2:549:GLN:CG	5:6:471:VAL:CG1	1.93	1.42
8:B:59:ARG:CZ	12:G:703:ARG:CD	1.98	1.40
3:4:568:ASN:ND2	5:6:217:ARG:NH2	1.69	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:314:SER:HB3	1:2:563:HIS:NE2	1.33	1.38
11:E:254:HIS:HE1	12:G:458:TYR:CZ	1.03	1.37
5:6:357:THR:HA	5:6:551:ARG:NH1	1.05	1.36
11:E:255:ARG:O	12:G:701:LEU:CD1	1.72	1.35
1:2:549:GLN:CD	5:6:471:VAL:CG1	1.90	1.34
4:5:86:ASP:OD2	11:E:334:ILE:CG2	1.76	1.33
1:2:549:GLN:OE1	5:6:471:VAL:CG1	1.76	1.32
11:E:210:SER:CB	12:G:473:THR:CG2	2.06	1.31
1:2:580:ASP:HB3	4:5:238:HIS:NE2	1.43	1.31
11:E:255:ARG:O	12:G:701:LEU:HD11	1.16	1.31
1:2:549:GLN:CD	5:6:471:VAL:HG11	0.93	1.30
8:B:111:ASP:OD1	11:E:265:VAL:N	1.61	1.30
1:2:276:ARG:NH2	11:E:318:MET:O	1.66	1.29
1:2:549:GLN:OE1	5:6:471:VAL:HG11	1.20	1.29
1:2:562:ARG:NH2	5:6:440:HIS:CD2	2.00	1.28
1:2:377:ARG:CG	1:2:565:VAL:CG2	1.94	1.28
5:6:357:THR:CA	5:6:551:ARG:NH1	1.99	1.26
8:B:59:ARG:NE	12:G:703:ARG:HD2	1.52	1.24
5:6:357:THR:CA	5:6:551:ARG:HH11	1.49	1.24
11:E:210:SER:CB	12:G:473:THR:HG23	1.67	1.23
2:3:416:ARG:HG2	4:5:456:VAL:CG1	1.68	1.22
2:3:487:LEU:CD2	6:7:241:SER:OG	1.88	1.20
1:2:765:ARG:NH2	4:5:385:THR:HG21	1.55	1.20
11:E:257:GLU:OE1	12:G:701:LEU:HD12	1.33	1.20
1:2:561:GLN:HE21	5:6:488:GLY:CA	1.54	1.20
8:B:59:ARG:NH1	12:G:703:ARG:CD	2.04	1.19
8:B:59:ARG:NH2	12:G:703:ARG:HB3	1.54	1.19
2:3:444:VAL:HG12	6:7:246:VAL:O	1.40	1.18
1:2:511:HIS:CE1	4:5:342:SER:CB	2.25	1.18
3:4:568:ASN:ND2	5:6:217:ARG:HH21	1.28	1.17
1:2:606:GLN:HE22	4:5:392:LYS:CE	1.57	1.17
1:2:561:GLN:CG	5:6:487:ALA:O	1.92	1.17
4:5:80:PHE:HD1	11:E:367:PHE:CE1	1.62	1.17
4:5:80:PHE:CD1	11:E:367:PHE:CE1	2.31	1.17
1:2:526:GLY:HA2	5:6:619:ARG:CZ	1.74	1.16
11:E:254:HIS:HE1	12:G:458:TYR:CE1	1.54	1.16
3:4:555:GLN:OE1	5:6:143:ARG:NH1	1.74	1.16
1:2:314:SER:CB	1:2:563:HIS:NE2	2.09	1.16
3:4:568:ASN:HD22	5:6:217:ARG:NH2	1.26	1.16
11:E:251:ARG:HD3	12:G:480:HIS:HB2	1.28	1.14
2:3:487:LEU:HD21	6:7:241:SER:OG	1.41	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:606:GLN:HE22	4:5:392:LYS:HE3	1.10	1.11
1:2:561:GLN:HG3	5:6:487:ALA:O	1.47	1.11
4:5:42:TYR:HA	11:E:367:PHE:CE2	1.84	1.11
1:2:377:ARG:HD3	1:2:565:VAL:HG22	1.29	1.11
1:2:561:GLN:HE21	5:6:488:GLY:HA2	1.10	1.10
4:5:86:ASP:OD2	11:E:334:ILE:HG22	1.36	1.09
4:5:56:ARG:NH2	8:B:119:ASP:OD1	1.85	1.09
8:B:40:LEU:HD21	12:G:688:ARG:CD	1.83	1.09
2:3:416:ARG:CB	4:5:456:VAL:HG11	1.82	1.08
8:B:59:ARG:NH1	12:G:703:ARG:HD3	1.61	1.08
2:3:416:ARG:CG	4:5:456:VAL:CG1	2.28	1.07
1:2:562:ARG:NH2	5:6:440:HIS:NE2	2.02	1.07
11:E:210:SER:HB2	12:G:473:THR:HG21	1.10	1.07
3:4:521:GLN:NE2	6:7:464:GLN:CG	2.18	1.06
4:5:86:ASP:OD2	11:E:334:ILE:HG21	1.56	1.05
8:B:40:LEU:HD11	12:G:688:ARG:CZ	1.87	1.05
1:2:377:ARG:HG3	1:2:565:VAL:HG21	1.06	1.04
1:2:271:TYR:OH	11:E:313:GLU:OE1	1.75	1.03
4:5:43:ARG:HH21	11:E:266:ASP:CG	1.63	1.01
1:2:377:ARG:CD	1:2:565:VAL:CG2	2.27	1.01
4:5:86:ASP:CG	11:E:334:ILE:HG22	1.80	1.01
2:3:462:MET:O	6:7:407:ARG:NH1	1.94	1.00
11:E:259:GLU:OE2	12:G:701:LEU:C	1.98	1.00
1:2:271:TYR:CE1	11:E:313:GLU:OE1	2.14	1.00
8:B:111:ASP:OD2	11:E:264:SER:OG	1.80	0.99
3:4:521:GLN:HE21	6:7:464:GLN:HG2	1.23	0.99
1:2:562:ARG:HH21	5:6:440:HIS:HD2	1.07	0.99
1:2:564:PRO:HA	5:6:441:GLU:CD	1.80	0.98
1:2:549:GLN:HG2	5:6:471:VAL:HG12	1.01	0.98
4:5:86:ASP:CG	11:E:334:ILE:CG2	2.32	0.98
2:3:439:GLU:OE1	4:5:472:ALA:O	1.82	0.98
8:B:59:ARG:NH2	12:G:703:ARG:CB	2.28	0.97
2:3:465:THR:CG2	6:7:407:ARG:HG2	1.94	0.96
11:E:254:HIS:CE1	12:G:458:TYR:CE1	2.14	0.96
1:2:511:HIS:HE1	4:5:342:SER:HB2	1.29	0.96
8:B:40:LEU:HD11	12:G:688:ARG:NH2	1.81	0.95
4:5:43:ARG:NE	11:E:266:ASP:OD1	1.98	0.95
1:2:549:GLN:OE1	5:6:471:VAL:CG2	2.15	0.94
4:5:42:TYR:HE1	11:E:367:PHE:HB3	1.29	0.94
1:2:561:GLN:HG2	5:6:487:ALA:O	1.68	0.94
11:E:259:GLU:OE2	12:G:701:LEU:CB	2.17	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:416:ARG:HG2	4:5:456:VAL:HG11	0.93	0.93
8:B:56:GLN:OE1	11:E:211:LYS:O	1.87	0.93
11:E:257:GLU:OE1	12:G:701:LEU:CD1	2.17	0.92
4:5:46:THR:HG21	11:E:406:ARG:O	1.69	0.92
1:2:765:ARG:HH21	4:5:385:THR:HG21	1.26	0.91
4:5:40:ARG:NH2	8:B:119:ASP:OD2	2.03	0.91
1:2:561:GLN:NE2	5:6:488:GLY:HA2	1.85	0.91
1:2:606:GLN:NE2	4:5:392:LYS:CE	2.34	0.91
1:2:511:HIS:NE2	4:5:342:SER:HB2	1.86	0.90
8:B:111:ASP:OD1	11:E:264:SER:HA	1.70	0.90
1:2:561:GLN:NE2	5:6:488:GLY:CA	2.34	0.90
1:2:271:TYR:CZ	11:E:313:GLU:OE1	2.24	0.90
8:B:59:ARG:HH21	12:G:703:ARG:HB3	1.31	0.90
8:B:111:ASP:OD1	11:E:264:SER:CA	2.19	0.90
1:2:549:GLN:HB3	5:6:475:GLU:OE2	1.73	0.89
3:4:568:ASN:HD22	5:6:217:ARG:CZ	1.85	0.89
7:A:166:SER:O	11:E:68:GLN:HG2	1.72	0.89
11:E:207:TRP:CZ2	12:G:478:ALA:O	2.25	0.88
11:E:259:GLU:OE2	12:G:701:LEU:HB3	1.72	0.88
1:2:549:GLN:OE1	5:6:471:VAL:HG21	1.71	0.88
1:2:606:GLN:NE2	4:5:392:LYS:HE3	1.88	0.87
2:3:487:LEU:HD23	6:7:241:SER:OG	1.72	0.87
1:2:526:GLY:CA	5:6:619:ARG:CZ	2.51	0.87
3:4:555:GLN:HE22	5:6:143:ARG:HH22	1.23	0.87
4:5:42:TYR:CE1	11:E:367:PHE:CB	2.58	0.87
5:6:356:PRO:O	5:6:551:ARG:NH1	2.07	0.86
11:E:255:ARG:O	12:G:701:LEU:HD13	1.73	0.86
3:4:521:GLN:HE21	6:7:464:GLN:CG	1.81	0.85
2:3:444:VAL:CG1	6:7:246:VAL:O	2.24	0.85
8:B:110:ALA:HB3	11:E:264:SER:HB2	1.59	0.85
3:4:568:ASN:ND2	5:6:217:ARG:CZ	2.40	0.85
1:2:606:GLN:HE22	4:5:392:LYS:NZ	1.74	0.85
4:5:80:PHE:CE1	11:E:367:PHE:CE1	2.65	0.85
3:4:521:GLN:HE22	6:7:464:GLN:HG2	1.32	0.84
1:2:314:SER:HB3	1:2:563:HIS:CD2	2.14	0.83
1:2:606:GLN:NE2	4:5:392:LYS:NZ	2.26	0.83
8:B:111:ASP:OD1	11:E:264:SER:C	2.16	0.83
4:5:42:TYR:CE1	11:E:367:PHE:HB3	2.13	0.83
4:5:42:TYR:CD1	11:E:367:PHE:CD2	2.65	0.83
1:2:656:ARG:NH2	4:5:385:THR:OG1	2.13	0.81
1:2:765:ARG:HH22	4:5:385:THR:HG21	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:555:GLN:NE2	5:6:143:ARG:HH22	1.78	0.81
4:5:42:TYR:HE1	11:E:367:PHE:CB	1.92	0.81
1:2:377:ARG:CG	1:2:565:VAL:HG21	1.88	0.81
1:2:564:PRO:HA	5:6:441:GLU:OE2	1.80	0.80
8:B:59:ARG:NH1	12:G:703:ARG:HD2	1.80	0.80
4:5:42:TYR:HA	11:E:367:PHE:HE2	1.46	0.80
3:4:512:PRO:HB2	6:7:600:TYR:CE2	2.17	0.80
11:E:207:TRP:HZ2	12:G:478:ALA:O	1.63	0.79
2:3:416:ARG:HG3	4:5:456:VAL:HG11	1.59	0.79
2:3:416:ARG:CB	4:5:456:VAL:CG1	2.56	0.79
5:6:159:LEU:HB3	5:6:187:ASN:HD21	1.48	0.79
8:B:129:ARG:NH2	9:C:151:ASP:OD2	2.16	0.79
9:C:34:VAL:HG12	9:C:86:VAL:HG12	1.65	0.79
8:B:109:LYS:HG3	11:E:262:THR:HB	1.63	0.78
7:A:98:LEU:H	7:A:103:ARG:HH21	1.31	0.78
1:2:561:GLN:HE21	5:6:488:GLY:HA3	1.45	0.78
1:2:765:ARG:HH21	4:5:385:THR:CG2	1.96	0.78
8:B:40:LEU:HD21	12:G:688:ARG:HD3	1.65	0.78
1:2:271:TYR:HE1	11:E:313:GLU:OE1	1.63	0.78
3:4:731:PRO:HD2	5:6:399:SER:OG	1.84	0.77
12:F:716:CYS:H	12:G:563:GLN:HE22	1.31	0.77
1:2:562:ARG:CZ	5:6:440:HIS:NE2	2.48	0.77
11:E:210:SER:HB2	12:G:473:THR:HG22	1.59	0.77
1:2:549:GLN:OE1	5:6:471:VAL:CB	2.31	0.77
1:2:224:LYS:O	11:E:312:GLN:HB3	1.84	0.77
11:E:389:LYS:HZ1	11:E:462:ARG:HD2	1.50	0.77
12:F:563:GLN:HE22	12:H:716:CYS:H	1.31	0.77
12:G:716:CYS:H	12:H:563:GLN:HE22	1.31	0.77
2:3:4:ARG:NH1	9:C:107:VAL:HA	2.00	0.77
8:B:56:GLN:OE1	11:E:211:LYS:C	2.21	0.77
11:E:210:SER:OG	12:G:473:THR:HG23	1.85	0.76
11:E:257:GLU:HB2	12:G:458:TYR:HE1	1.49	0.76
1:2:561:GLN:HE22	1:2:564:PRO:HD3	1.49	0.76
3:4:161:ALA:O	3:4:165:ASN:ND2	2.18	0.76
8:B:59:ARG:NH2	12:G:703:ARG:CG	2.49	0.76
3:4:469:SER:HB3	6:7:369:MET:SD	2.25	0.75
1:2:377:ARG:HD2	1:2:565:VAL:HG22	1.65	0.75
4:5:43:ARG:NH2	11:E:266:ASP:CG	2.39	0.75
4:5:43:ARG:NH2	11:E:266:ASP:OD1	2.20	0.75
4:5:80:PHE:CE1	11:E:367:PHE:CZ	2.75	0.75
1:2:377:ARG:CB	1:2:565:VAL:CG2	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:100:ARG:NH2	2:3:150:SER:O	2.20	0.74
5:6:380:THR:HG1	5:6:384:THR:HG1	1.31	0.74
1:2:667:VAL:HG12	5:6:602:ARG:HH21	1.51	0.74
8:B:59:ARG:CZ	12:G:703:ARG:CG	2.65	0.74
7:A:170:LYS:NZ	11:E:64:GLU:OE2	2.16	0.74
5:6:356:PRO:C	5:6:551:ARG:HH12	1.91	0.74
8:B:40:LEU:HD11	12:G:688:ARG:NE	2.02	0.74
4:5:80:PHE:HD1	11:E:367:PHE:CD1	2.05	0.74
3:4:191:PRO:HB2	3:4:194:MET:HB2	1.70	0.73
8:B:7:GLU:OE1	9:C:189:TRP:NE1	2.21	0.73
2:3:658:VAL:HG23	2:3:662:THR:HG21	1.71	0.73
2:3:416:ARG:HB3	4:5:456:VAL:CG1	2.18	0.73
11:E:99:ASP:OD1	11:E:100:THR:N	2.22	0.73
3:4:521:GLN:HE21	6:7:464:GLN:CD	1.92	0.72
1:2:580:ASP:CB	4:5:238:HIS:NE2	2.39	0.72
8:B:109:LYS:CG	11:E:262:THR:HB	2.18	0.72
1:2:377:ARG:HG3	1:2:565:VAL:CB	2.16	0.72
1:2:561:GLN:NE2	5:6:488:GLY:HA3	2.02	0.72
8:B:111:ASP:CG	11:E:264:SER:HG	1.92	0.72
7:A:179:ARG:NH2	7:A:183:GLU:OE2	2.23	0.72
5:6:187:ASN:ND2	5:6:190:ARG:O	2.23	0.72
8:B:40:LEU:HD21	12:G:688:ARG:NE	2.04	0.72
7:A:195:LEU:HD22	11:E:41:GLN:HE22	1.55	0.72
1:2:526:GLY:HA2	5:6:619:ARG:NH2	2.05	0.71
8:B:59:ARG:NH2	12:G:703:ARG:HD2	2.01	0.71
4:5:537:ILE:HA	4:5:540:HIS:HB3	1.71	0.71
5:6:27:GLN:HG3	5:6:93:ALA:HB2	1.73	0.71
5:6:307:ASN:O	5:6:309:ARG:NH1	2.23	0.71
5:6:54:ILE:HD11	5:6:103:GLU:HB2	1.71	0.71
2:3:347:SER:HG	2:3:608:VAL:N	1.88	0.71
11:E:210:SER:CB	12:G:473:THR:HG21	1.97	0.71
11:E:257:GLU:HB2	12:G:458:TYR:CE1	2.25	0.70
3:4:555:GLN:CD	5:6:143:ARG:HH12	1.94	0.70
7:A:176:PHE:CE1	11:E:41:GLN:HG2	2.25	0.70
4:5:43:ARG:CZ	11:E:266:ASP:OD1	2.40	0.70
5:6:310:PHE:CZ	5:6:574:ARG:HG2	2.27	0.70
2:3:230:GLU:OE1	6:7:72:ARG:NH2	2.25	0.70
4:5:79:SER:OG	11:E:368:LYS:HB3	1.91	0.69
11:E:287:HIS:HB2	11:E:325:VAL:HG12	1.73	0.69
3:4:568:ASN:HD22	5:6:217:ARG:HH21	0.75	0.69
7:A:147:TYR:HE2	11:E:46:GLN:HG2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:818:PHE:HA	1:2:821:TYR:HB3	1.75	0.69
7:A:151:ARG:CZ	11:E:398:ILE:HG23	2.23	0.69
11:E:210:SER:HB3	12:G:473:THR:HG23	1.70	0.69
1:2:377:ARG:CB	1:2:565:VAL:HG22	2.19	0.69
2:3:4:ARG:NH1	9:C:106:VAL:O	2.26	0.69
8:B:40:LEU:CD2	12:G:688:ARG:HD3	2.22	0.69
1:2:325:VAL:HA	1:2:368:THR:HG23	1.74	0.68
1:2:754:SER:HB2	1:2:761:PRO:HB3	1.75	0.68
11:E:257:GLU:CD	12:G:701:LEU:HD12	2.14	0.68
11:E:263:LEU:HD23	11:E:269:ARG:HH21	1.57	0.68
1:2:580:ASP:HB3	4:5:238:HIS:CD2	2.28	0.68
2:3:534:MET:CE	4:5:594:ARG:HG2	2.24	0.68
1:2:224:LYS:HB3	11:E:312:GLN:HB2	1.75	0.68
11:E:257:GLU:CB	12:G:458:TYR:HE1	2.06	0.68
3:4:219:ASP:OD1	3:4:220:LYS:N	2.26	0.68
1:2:593:ASN:ND2	1:2:596:ASP:OD2	2.27	0.68
5:6:390:ILE:O	5:6:498:SER:OG	2.12	0.68
3:4:335:HIS:O	3:4:335:HIS:ND1	2.27	0.68
2:3:416:ARG:HG2	4:5:456:VAL:CB	2.24	0.68
3:4:546:TYR:CE2	6:7:472:ALA:HB1	2.29	0.68
1:2:526:GLY:HA2	5:6:619:ARG:NE	2.09	0.67
4:5:47:ASP:HB2	11:E:406:ARG:HH22	1.58	0.67
11:E:251:ARG:HD3	12:G:480:HIS:CB	2.18	0.67
7:A:176:PHE:HB2	11:E:47:TYR:CE1	2.30	0.67
8:B:40:LEU:CD2	12:G:688:ARG:CD	2.68	0.67
2:3:444:VAL:O	6:7:246:VAL:HB	1.95	0.67
4:5:42:TYR:OH	11:E:368:LYS:NZ	2.25	0.67
1:2:507:PRO:HD3	1:2:513:VAL:HG12	1.77	0.67
4:5:80:PHE:CD1	11:E:367:PHE:CZ	2.83	0.67
1:2:549:GLN:CG	5:6:471:VAL:HG12	1.84	0.67
3:4:388:VAL:HG12	3:4:423:LYS:HG2	1.76	0.67
5:6:20:ASP:OD1	5:6:85:ARG:NH2	2.28	0.67
2:3:70:ASP:OD2	2:3:77:TYR:N	2.26	0.67
4:5:79:SER:CB	11:E:368:LYS:HB3	2.24	0.67
1:2:757:THR:HG22	1:2:758:GLY:H	1.60	0.66
2:3:645:GLN:OE1	2:3:654:ARG:NH2	2.29	0.66
11:E:447:TYR:OH	11:E:554:ARG:NH2	2.28	0.66
7:A:144:LYS:NZ	8:B:11:GLU:OE2	2.28	0.66
1:2:204:ARG:O	1:2:213:ASN:ND2	2.28	0.66
3:4:726:MET:HG3	3:4:727:VAL:H	1.59	0.66
7:A:149:GLU:OE2	7:A:174:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:56:GLN:OE1	11:E:211:LYS:HB3	1.96	0.66
1:2:328:ASN:HD22	1:2:364:ASN:HB2	1.60	0.66
10:D:202:SER:HG	10:D:204:HIS:HE2	1.43	0.66
2:3:91:ARG:NH2	2:3:268:ASP:OD1	2.28	0.66
1:2:198:ARG:NH2	1:2:241:GLU:OE2	2.29	0.66
2:3:465:THR:HG22	6:7:407:ARG:HG2	1.76	0.66
1:2:301:HIS:HB3	1:2:306:ILE:HD11	1.77	0.66
4:5:132:ALA:HA	11:E:328:LYS:HD2	1.78	0.66
8:B:23:LEU:HB3	8:B:36:PHE:HD2	1.61	0.66
7:A:74:ARG:NH2	9:C:18:ASN:O	2.29	0.66
8:B:111:ASP:CG	11:E:264:SER:OG	2.34	0.66
1:2:365:MET:HB2	4:5:273:LYS:HZ1	1.59	0.65
2:3:465:THR:HG21	6:7:407:ARG:HG2	1.76	0.65
3:4:400:ARG:HG2	3:4:408:VAL:HG12	1.76	0.65
10:D:71:GLU:OE1	10:D:73:LEU:N	2.25	0.65
2:3:151:PHE:H	2:3:155:HIS:HE1	1.43	0.65
4:5:441:VAL:HG22	4:5:483:SER:HB2	1.78	0.65
10:D:22:THR:HG22	10:D:24:ALA:H	1.60	0.65
11:E:257:GLU:CB	12:G:458:TYR:CE1	2.80	0.65
3:4:246:PHE:HA	3:4:249:TYR:CD2	2.32	0.65
5:6:310:PHE:HZ	5:6:574:ARG:HG2	1.61	0.65
11:E:323:LYS:HG3	11:E:324:GLN:HE21	1.61	0.65
11:E:448:CYS:SG	11:E:449:SER:N	2.70	0.65
1:2:514:ARG:O	1:2:772:ARG:NH1	2.30	0.65
1:2:733:PRO:HA	1:2:784:ASP:HB3	1.79	0.65
3:4:568:ASN:HD21	5:6:217:ARG:NH2	1.89	0.65
5:6:558:ARG:HB3	5:6:561:GLU:HB2	1.79	0.65
2:3:544:ASP:OD2	2:3:548:ARG:NH2	2.31	0.64
4:5:416:ALA:HA	4:5:430:GLU:O	1.97	0.64
2:3:152:GLY:HA3	9:C:103:ASP:HB2	1.77	0.64
8:B:51:ASN:ND2	10:D:80:MET:SD	2.70	0.64
2:3:381:ARG:NH2	2:3:385:ASN:OD1	2.28	0.64
7:A:175:HIS:HA	11:E:48:THR:HA	1.78	0.64
4:5:115:PRO:HA	8:B:130:VAL:HG22	1.79	0.64
4:5:167:ARG:HH11	4:5:181:ASN:HA	1.63	0.64
5:6:436:ASP:O	5:6:440:HIS:N	2.31	0.64
11:E:28:ASP:OD1	11:E:197:SER:OG	2.15	0.64
2:3:61:GLN:HG3	2:3:124:ALA:HB2	1.79	0.64
4:5:47:ASP:CB	11:E:406:ARG:HH22	2.11	0.64
4:5:42:TYR:OH	11:E:368:LYS:HG2	1.97	0.64
4:5:53:PHE:HZ	8:B:114:ARG:HG2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:416:ALA:HB3	6:7:469:ILE:HD11	1.80	0.64
4:5:421:ASP:HB3	4:5:424:SER:OG	1.98	0.64
9:C:35:ARG:NH1	9:C:37:GLU:OE2	2.30	0.64
3:4:471:TYR:HD2	3:4:658:TYR:HE1	1.46	0.63
3:4:555:GLN:OE1	5:6:143:ARG:CZ	2.44	0.63
12:G:654:LEU:HD12	12:H:610:LYS:HG2	1.80	0.63
7:A:176:PHE:HB3	11:E:47:TYR:H	1.63	0.63
1:2:377:ARG:HG3	1:2:565:VAL:CG1	2.27	0.63
1:2:485:ILE:HD11	1:2:531:GLN:HB2	1.80	0.63
11:E:259:GLU:OE2	12:G:701:LEU:O	2.16	0.63
3:4:425:ASP:HB3	3:4:428:ARG:HG3	1.81	0.63
7:A:175:HIS:ND1	11:E:48:THR:HG23	2.14	0.63
8:B:55:ARG:HH21	11:E:43:ASP:HA	1.63	0.63
1:2:402:LEU:O	1:2:405:SER:OG	2.12	0.63
12:F:654:LEU:HD12	12:G:610:LYS:HG2	1.80	0.63
8:B:175:GLN:HB2	10:D:188:THR:HG21	1.80	0.63
4:5:80:PHE:HE1	11:E:367:PHE:CZ	2.16	0.63
4:5:42:TYR:CE1	11:E:367:PHE:HB2	2.33	0.62
5:6:187:ASN:HB2	5:6:190:ARG:HB2	1.80	0.62
7:A:111:MET:O	7:A:115:ASN:ND2	2.29	0.62
7:A:174:GLN:HG3	11:E:49:LEU:HB3	1.80	0.62
10:D:21:LEU:HD21	10:D:29:ARG:HH12	1.63	0.62
3:4:365:GLN:NE2	6:7:266:GLN:OE1	2.33	0.62
2:3:162:THR:OG1	2:3:164:CYS:SG	2.54	0.62
12:F:610:LYS:HG2	12:H:654:LEU:HD12	1.80	0.62
1:2:500:PHE:O	1:2:728:LYS:NZ	2.33	0.62
2:3:416:ARG:HG2	4:5:456:VAL:CG2	2.29	0.62
12:G:518:SER:OG	12:G:520:ASP:OD1	2.17	0.62
1:2:567:ARG:HD2	5:6:440:HIS:HD2	1.64	0.62
1:2:377:ARG:HD3	1:2:565:VAL:CG2	2.15	0.62
5:6:594:ILE:HD13	5:6:625:ILE:HG22	1.82	0.62
2:3:416:ARG:HG2	4:5:456:VAL:HG21	1.81	0.62
1:2:489:GLU:HA	1:2:492:LYS:HD2	1.81	0.62
9:C:7:ARG:NH2	9:C:23:ASP:OD2	2.33	0.62
1:2:667:VAL:HG12	5:6:602:ARG:NH2	2.14	0.62
8:B:40:LEU:HD21	12:G:688:ARG:HD2	1.75	0.62
4:5:42:TYR:CD1	11:E:367:PHE:CG	2.87	0.61
4:5:65:LEU:HD11	9:C:155:ASN:O	1.99	0.61
4:5:347:THR:O	4:5:351:LYS:N	2.32	0.61
1:2:314:SER:HB2	1:2:565:VAL:CG2	2.30	0.61
2:3:115:PHE:CZ	2:3:287:ARG:HD3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:518:SER:OG	12:F:520:ASP:OD1	2.17	0.61
3:4:402:ASN:HB2	3:4:405:VAL:HG22	1.83	0.61
1:2:683:HIS:CE1	5:6:386:LEU:HD13	2.35	0.61
1:2:742:LYS:HD2	1:2:788:GLU:HG3	1.82	0.61
1:2:314:SER:CB	1:2:563:HIS:CD2	2.79	0.61
3:4:719:LYS:HE2	5:6:542:GLU:OE2	2.01	0.61
4:5:86:ASP:CG	11:E:334:ILE:HG21	2.13	0.61
6:7:56:ALA:HB2	6:7:63:VAL:HG21	1.82	0.61
6:7:520:LEU:HD23	6:7:644:LEU:HD11	1.82	0.61
3:4:469:SER:CB	6:7:369:MET:SD	2.88	0.60
6:7:222:LEU:HD12	6:7:223:GLN:H	1.66	0.60
12:H:518:SER:OG	12:H:520:ASP:OD1	2.17	0.60
7:A:174:GLN:O	11:E:49:LEU:N	2.32	0.60
5:6:124:ARG:NH2	5:6:210:GLU:OE2	2.34	0.60
6:7:171:SER:OG	6:7:172:GLU:N	2.35	0.60
2:3:440:ALA:CB	6:7:247:GLY:HA2	2.30	0.60
4:5:43:ARG:HD3	8:B:114:ARG:HD3	1.84	0.60
4:5:174:SER:OG	4:5:207:CYS:SG	2.60	0.60
4:5:231:GLU:OE2	4:5:243:ARG:N	2.28	0.60
5:6:109:ASP:OD1	5:6:109:ASP:N	2.34	0.60
6:7:52:LEU:HD12	6:7:141:PRO:HD3	1.84	0.60
3:4:306:CYS:SG	3:4:308:VAL:N	2.67	0.60
5:6:159:LEU:HB3	5:6:187:ASN:ND2	2.16	0.60
2:3:465:THR:CB	6:7:407:ARG:HG2	2.30	0.60
8:B:56:GLN:OE1	11:E:211:LYS:CA	2.50	0.60
2:3:534:MET:HE3	4:5:594:ARG:HG2	1.83	0.60
3:4:718:ARG:NH1	3:4:729:ALA:O	2.31	0.60
11:E:210:SER:OG	12:G:473:THR:CG2	2.45	0.60
1:2:314:SER:HB2	1:2:565:VAL:HG23	1.84	0.59
1:2:329:CYS:HB3	1:2:332:CYS:SG	2.41	0.59
1:2:562:ARG:NH2	5:6:440:HIS:HD2	1.73	0.59
4:5:80:PHE:CD1	11:E:367:PHE:HE1	2.16	0.59
5:6:52:GLU:OE2	5:6:55:ARG:NH1	2.35	0.59
1:2:549:GLN:OE1	5:6:471:VAL:HG13	1.93	0.59
1:2:563:HIS:HD2	1:2:565:VAL:H	1.49	0.59
2:3:212:ALA:HB2	2:3:287:ARG:HH22	1.67	0.59
4:5:528:ARG:O	4:5:532:LEU:HG	2.02	0.59
6:7:374:ASN:HB3	6:7:483:SER:HB3	1.84	0.59
1:2:343:GLN:HA	4:5:287:VAL:HG11	1.84	0.59
2:3:6:PRO:HD2	2:3:149:GLY:O	2.02	0.59
5:6:611:LYS:NZ	5:6:612:SER:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:43:ASN:O	7:A:47:VAL:HG23	2.02	0.59
12:G:641:VAL:HG21	12:G:677:VAL:HG21	1.84	0.59
2:3:663:LEU:HD23	6:7:537:ILE:HD12	1.83	0.59
7:A:135:ASP:OD2	7:A:138:GLN:NE2	2.32	0.59
12:H:641:VAL:HG21	12:H:677:VAL:HG21	1.84	0.59
2:3:173:GLU:HG3	2:3:281:GLN:HG2	1.83	0.59
4:5:42:TYR:HD1	11:E:367:PHE:CD2	2.20	0.59
1:2:477:ILE:O	1:2:480:SER:OG	2.19	0.59
1:2:514:ARG:NH2	1:2:516:ASP:O	2.36	0.59
2:3:173:GLU:N	2:3:173:GLU:OE1	2.36	0.59
2:3:447:ASP:HB3	6:7:246:VAL:CG1	2.33	0.59
3:4:476:ILE:CD1	3:4:650:LEU:HD11	2.32	0.59
2:3:344:LEU:HD11	2:3:616:TYR:HE2	1.67	0.59
3:4:247:ASP:HB2	3:4:248:ARG:HD2	1.85	0.59
2:3:141:GLU:OE1	2:3:237:VAL:HG11	2.03	0.59
4:5:51:PHE:CE1	11:E:266:ASP:HB3	2.38	0.59
4:5:507:MET:HB2	4:5:510:ILE:HG22	1.83	0.59
6:7:403:TYR:OH	6:7:445:ASP:OD2	2.19	0.59
1:2:384:LYS:HG2	1:2:385:VAL:HG23	1.85	0.58
4:5:42:TYR:HA	11:E:367:PHE:CD2	2.37	0.58
11:E:257:GLU:HG2	11:E:258:ASP:N	2.18	0.58
1:2:463:MET:O	1:2:467:LEU:HG	2.03	0.58
1:2:762:ILE:HG23	1:2:766:HIS:HB2	1.85	0.58
6:7:324:LEU:HA	6:7:327:ILE:HG22	1.84	0.58
9:C:106:VAL:O	9:C:167:ARG:NH2	2.36	0.58
2:3:447:ASP:CB	6:7:246:VAL:HG12	2.34	0.58
5:6:598:TYR:HB2	5:6:621:LEU:HD13	1.84	0.58
7:A:149:GLU:CD	11:E:47:TYR:HH	2.06	0.58
9:C:204:GLN:N	9:C:204:GLN:OE1	2.36	0.58
10:D:175:VAL:HG12	10:D:220:VAL:HG12	1.83	0.58
12:F:641:VAL:HG21	12:F:677:VAL:HG21	1.84	0.58
1:2:377:ARG:HD2	1:2:565:VAL:HA	1.85	0.58
6:7:311:ASP:O	6:7:313:GLU:HG2	2.04	0.58
1:2:580:ASP:OD2	4:5:238:HIS:CD2	2.57	0.58
4:5:47:ASP:HB2	11:E:406:ARG:NH2	2.18	0.58
10:D:29:ARG:HE	10:D:50:ILE:HD11	1.68	0.58
1:2:314:SER:CB	1:2:565:VAL:HG23	2.34	0.58
2:3:440:ALA:CB	6:7:247:GLY:CA	2.82	0.58
3:4:566:SER:OG	3:4:567:ASP:N	2.35	0.58
1:2:377:ARG:NH2	1:2:393:SER:OG	2.37	0.57
3:4:278:ASP:HB3	3:4:283:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:536:ARG:HE	11:E:550:LYS:HE2	1.69	0.57
1:2:315:CYS:HB2	1:2:374:GLN:HE21	1.69	0.57
1:2:731:VAL:O	1:2:732:HIS:ND1	2.36	0.57
3:4:428:ARG:HH11	3:4:428:ARG:HB3	1.69	0.57
3:4:546:TYR:CE2	6:7:472:ALA:CB	2.87	0.57
6:7:567:ARG:O	6:7:618:ARG:NH1	2.37	0.57
8:B:57:LYS:NZ	11:E:211:LYS:NZ	2.53	0.57
1:2:763:THR:HG22	1:2:764:VAL:H	1.69	0.57
4:5:439:GLY:N	4:5:481:ARG:O	2.37	0.57
11:E:385:GLU:OE1	11:E:462:ARG:NE	2.37	0.57
4:5:60:LYS:NZ	8:B:122:ASP:OD2	2.23	0.57
1:2:517:ILE:O	1:2:625:THR:OG1	2.21	0.57
6:7:178:VAL:HG12	6:7:179:VAL:HG23	1.87	0.57
10:D:37:GLU:HG3	10:D:92:TYR:HE1	1.70	0.57
1:2:224:LYS:HB3	11:E:312:GLN:CB	2.35	0.57
2:3:447:ASP:HB3	6:7:246:VAL:HG12	1.87	0.57
3:4:555:GLN:HE22	5:6:143:ARG:NH2	1.98	0.57
8:B:78:GLU:OE1	8:B:85:THR:OG1	2.22	0.56
2:3:527:LEU:HD23	2:3:655:THR:HB	1.87	0.56
7:A:168:LEU:CD2	11:E:64:GLU:HB3	2.35	0.56
8:B:2:ASP:N	8:B:2:ASP:OD1	2.35	0.56
2:3:385:ASN:HD22	2:3:493:VAL:H	1.54	0.56
2:3:509:THR:HG23	2:3:511:MET:H	1.71	0.56
7:A:194:ILE:HG13	7:A:195:LEU:H	1.70	0.56
9:C:168:LEU:O	9:C:173:ARG:NH1	2.38	0.56
9:C:169:ASP:OD1	9:C:169:ASP:N	2.37	0.56
10:D:123:SER:HB3	10:D:126:GLU:HG3	1.88	0.56
4:5:325:LEU:HA	4:5:328:LEU:HD23	1.86	0.56
6:7:459:HIS:O	6:7:514:ARG:NH1	2.32	0.56
11:E:207:TRP:CE2	12:G:478:ALA:O	2.58	0.56
1:2:325:VAL:HG11	1:2:347:VAL:HG11	1.88	0.56
1:2:377:ARG:HD2	1:2:565:VAL:HG13	1.88	0.56
1:2:562:ARG:NE	5:6:440:HIS:NE2	2.53	0.56
2:3:73:ASP:OD1	2:3:74:GLN:N	2.37	0.56
6:7:40:LEU:HD23	6:7:45:GLN:HB3	1.87	0.56
4:5:586:TYR:CZ	4:5:590:ARG:HD2	2.40	0.56
2:3:393:SER:CB	4:5:609:THR:HB	2.36	0.56
2:3:465:THR:HB	6:7:407:ARG:HG2	1.88	0.56
3:4:199:GLU:HA	3:4:202:VAL:HG12	1.88	0.56
4:5:172:CYS:HB3	4:5:177:ASN:H	1.70	0.56
4:5:377:LEU:HB2	4:5:485:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:55:ARG:O	11:E:42:CYS:SG	2.63	0.56
2:3:409:ARG:NH2	2:3:447:ASP:O	2.24	0.56
2:3:616:TYR:OH	2:3:676:ALA:O	2.21	0.56
6:7:169:ARG:HH11	6:7:236:LYS:HD3	1.71	0.56
11:E:282:GLN:O	11:E:330:GLN:NE2	2.39	0.56
1:2:765:ARG:HG3	1:2:765:ARG:O	2.06	0.55
6:7:363:ASP:OD1	6:7:363:ASP:N	2.37	0.55
8:B:110:ALA:HB3	11:E:264:SER:CB	2.34	0.55
3:4:533:THR:HG22	3:4:534:SER:H	1.70	0.55
4:5:170:ILE:HG22	4:5:214:ILE:HD13	1.87	0.55
11:E:259:GLU:OE2	12:G:701:LEU:CA	2.53	0.55
2:3:662:THR:O	2:3:665:THR:HG22	2.06	0.55
3:4:390:VAL:HG23	3:4:418:VAL:HG23	1.87	0.55
3:4:654:GLN:HG3	6:7:589:ARG:HH21	1.70	0.55
3:4:476:ILE:HD11	3:4:650:LEU:HD11	1.89	0.55
3:4:457:ASP:N	3:4:457:ASP:OD1	2.38	0.55
5:6:601:LEU:HG	5:6:616:ILE:HD13	1.88	0.55
3:4:328:CYS:SG	3:4:336:SER:OG	2.65	0.55
3:4:405:VAL:HG23	3:4:407:ASN:H	1.72	0.55
4:5:372:ARG:HB2	4:5:618:ARG:NH2	2.22	0.55
4:5:633:THR:OG1	4:5:634:GLU:N	2.38	0.55
9:C:90:LYS:HA	9:C:93:GLN:HB2	1.89	0.55
11:E:230:GLN:NE2	11:E:381:MET:SD	2.79	0.55
2:3:460:SER:OG	2:3:463:ASP:OD2	2.25	0.55
3:4:189:THR:HB	3:4:195:GLN:HE22	1.71	0.55
4:5:565:TYR:CE1	4:5:569:LYS:HG3	2.41	0.55
5:6:174:TYR:OH	5:6:193:LEU:HD22	2.06	0.55
8:B:59:ARG:CD	12:G:703:ARG:HD2	2.36	0.55
12:G:665:ARG:NH1	12:G:673:ASP:O	2.40	0.55
7:A:62:ILE:O	7:A:66:HIS:N	2.34	0.55
11:E:515:SER:O	11:E:515:SER:OG	2.25	0.55
2:3:267:ASP:OD2	2:3:268:ASP:N	2.40	0.55
3:4:200:ILE:HG21	3:4:258:ILE:HD11	1.87	0.55
6:7:269:ASP:OD1	6:7:270:HIS:N	2.40	0.55
11:E:259:GLU:CD	12:G:701:LEU:HB3	2.26	0.55
2:3:244:ILE:HD13	2:3:266:LEU:HD11	1.89	0.54
3:4:716:ASP:OD1	3:4:717:MET:N	2.39	0.54
11:E:443:GLY:O	11:E:485:ARG:NH2	2.39	0.54
1:2:377:ARG:HB2	1:2:565:VAL:CG2	2.37	0.54
1:2:580:ASP:OD2	4:5:238:HIS:HD2	1.88	0.54
3:4:354:LEU:HD13	3:4:372:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:170:GLN:OE1	5:6:170:GLN:N	2.40	0.54
1:2:680:VAL:HG11	5:6:591:GLU:HG3	1.88	0.54
8:B:24:ASP:OD1	8:B:24:ASP:N	2.36	0.54
12:H:665:ARG:NH1	12:H:673:ASP:O	2.40	0.54
1:2:765:ARG:HH21	4:5:385:THR:CB	2.20	0.54
10:D:106:HIS:NE2	10:D:162:VAL:O	2.39	0.54
12:F:665:ARG:NH1	12:F:673:ASP:O	2.40	0.54
2:3:471:MET:HE2	2:3:523:ARG:HB3	1.89	0.54
4:5:380:LEU:HA	4:5:488:ALA:HB3	1.88	0.54
4:5:37:GLU:OE1	4:5:41:GLN:NE2	2.40	0.54
6:7:5:ASP:OD1	6:7:6:TYR:N	2.36	0.54
6:7:500:SER:O	6:7:504:ASN:ND2	2.41	0.54
2:3:534:MET:HE2	4:5:594:ARG:HG2	1.90	0.54
6:7:135:GLU:HG3	6:7:137:TYR:CZ	2.43	0.54
3:4:748:ARG:HH22	3:4:754:GLU:HG2	1.74	0.53
4:5:634:GLU:HA	4:5:637:VAL:HG12	1.91	0.53
5:6:320:GLN:O	5:6:581:GLN:NE2	2.41	0.53
7:A:129:GLY:H	7:A:133:GLY:HA2	1.73	0.53
1:2:276:ARG:HH21	11:E:318:MET:C	2.03	0.53
1:2:570:THR:OG1	1:2:571:LEU:N	2.41	0.53
5:6:109:ASP:OD2	5:6:199:ARG:NH2	2.42	0.53
6:7:445:ASP:OD1	6:7:445:ASP:N	2.33	0.53
6:7:521:ILE:HG13	6:7:522:GLN:H	1.73	0.53
5:6:171:GLN:H	5:6:175:THR:HG21	1.74	0.53
6:7:186:GLN:HE21	6:7:215:ARG:HH11	1.55	0.53
12:F:599:LEU:HD22	12:F:621:LEU:HD11	1.90	0.53
1:2:765:ARG:NH2	4:5:385:THR:CG2	2.46	0.53
2:3:469:GLU:HA	2:3:473:GLN:OE1	2.08	0.53
6:7:51:ASP:OD1	6:7:52:LEU:N	2.41	0.53
10:D:178:ARG:NE	10:D:180:GLU:OE2	2.39	0.53
12:H:468:VAL:HG21	12:H:497:ILE:HD13	1.90	0.53
1:2:366:GLU:N	1:2:366:GLU:OE2	2.42	0.53
2:3:191:HIS:HB3	2:3:229:LEU:HD22	1.89	0.53
11:E:496:PRO:HA	11:E:504:VAL:HG12	1.90	0.53
4:5:156:ILE:HD12	4:5:230:GLN:HB2	1.90	0.53
6:7:528:ASP:N	6:7:528:ASP:OD1	2.42	0.53
12:G:599:LEU:HD22	12:G:621:LEU:HD11	1.90	0.53
12:H:712:LYS:HE3	12:H:718:ILE:HD13	1.91	0.53
3:4:501:ARG:O	3:4:739:ARG:NH2	2.41	0.53
12:F:597:GLN:HB3	12:F:599:LEU:HD13	1.91	0.53
1:2:792:ASN:O	1:2:796:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:390:GLY:O	2:3:396:LYS:NZ	2.41	0.53
4:5:380:LEU:HD23	4:5:381:GLY:N	2.23	0.53
8:B:57:LYS:NZ	11:E:211:LYS:HZ1	2.07	0.53
8:B:136:VAL:HG13	8:B:167:MET:HE1	1.91	0.53
12:H:597:GLN:HB3	12:H:599:LEU:HD13	1.91	0.53
12:H:599:LEU:HD22	12:H:621:LEU:HD11	1.90	0.53
1:2:687:HIS:O	1:2:689:SER:N	2.41	0.53
3:4:179:LYS:HG3	3:4:180:GLU:HG2	1.91	0.53
12:G:468:VAL:HG21	12:G:497:ILE:HD13	1.90	0.53
1:2:225:GLU:OE2	11:E:312:GLN:NE2	2.42	0.53
11:E:386:SER:O	11:E:389:LYS:NZ	2.32	0.53
12:G:597:GLN:HB3	12:G:599:LEU:HD13	1.91	0.53
4:5:43:ARG:CD	8:B:114:ARG:HD3	2.39	0.52
2:3:437:ARG:HH11	6:7:249:ILE:HD12	1.72	0.52
4:5:79:SER:HB2	11:E:367:PHE:O	2.10	0.52
4:5:172:CYS:SG	4:5:173:ARG:N	2.82	0.52
5:6:559:ILE:H	5:6:559:ILE:HD12	1.74	0.52
8:B:144:LYS:HE2	10:D:204:HIS:CE1	2.44	0.52
12:G:712:LYS:HE3	12:G:718:ILE:HD13	1.91	0.52
1:2:804:ASP:N	1:2:804:ASP:OD1	2.35	0.52
4:5:526:GLU:HA	4:5:529:ASP:HB2	1.91	0.52
1:2:606:GLN:NE2	4:5:392:LYS:HZ1	2.06	0.52
2:3:440:ALA:HB2	6:7:247:GLY:HA2	1.92	0.52
6:7:223:GLN:HE21	6:7:225:ARG:HB2	1.74	0.52
11:E:25:SER:OG	11:E:384:MET:SD	2.66	0.52
2:3:627:LEU:HA	2:3:682:VAL:HG22	1.91	0.52
3:4:199:GLU:O	3:4:203:ILE:HG12	2.10	0.52
10:D:187:ASP:OD1	10:D:188:THR:N	2.38	0.52
12:F:468:VAL:HG21	12:F:497:ILE:HD13	1.91	0.52
5:6:525:PRO:O	5:6:528:SER:OG	2.22	0.52
2:3:133:ASP:OD1	2:3:136:TYR:N	2.34	0.52
3:4:448:LEU:O	3:4:451:GLU:HG3	2.09	0.52
4:5:96:LEU:HD22	4:5:297:LEU:HD22	1.91	0.52
8:B:144:LYS:HE2	10:D:204:HIS:HE1	1.75	0.52
5:6:321:THR:OG1	5:6:322:ALA:N	2.42	0.52
7:A:161:VAL:HG13	7:A:181:LYS:NZ	2.25	0.52
12:F:712:LYS:HE3	12:F:718:ILE:HD13	1.91	0.52
2:3:634:TYR:OH	2:3:688:GLU:OE1	2.14	0.52
2:3:638:GLU:OE1	2:3:641:ARG:NH2	2.35	0.52
4:5:332:TYR:HE2	4:5:351:LYS:HE2	1.75	0.51
4:5:585:ARG:HG2	4:5:641:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:59:ARG:NE	12:G:703:ARG:CD	2.46	0.51
1:2:644:SER:OG	1:2:651:GLU:OE1	2.25	0.51
3:4:167:GLN:HG2	3:4:244:ILE:HD11	1.92	0.51
10:D:199:GLU:HG3	10:D:200:LYS:H	1.75	0.51
1:2:777:HIS:HA	1:2:780:ILE:HG22	1.92	0.51
4:5:53:PHE:CZ	8:B:114:ARG:HG2	2.44	0.51
6:7:257:VAL:HG13	6:7:261:ASN:HB2	1.93	0.51
11:E:28:ASP:OD2	11:E:76:ASN:ND2	2.36	0.51
11:E:368:LYS:O	11:E:369:HIS:ND1	2.44	0.51
1:2:558:ALA:HB3	1:2:611:ILE:HD13	1.93	0.51
2:3:673:HIS:HD2	2:3:686:ASP:HA	1.74	0.51
4:5:319:GLU:O	4:5:323:ARG:HG2	2.10	0.51
5:6:609:VAL:HG22	5:6:610:THR:HG23	1.93	0.51
7:A:39:LEU:HD22	7:A:65:ARG:HG2	1.93	0.51
4:5:87:TYR:HB3	4:5:95:HIS:CE1	2.45	0.51
7:A:158:GLU:HG3	7:A:166:SER:HB3	1.92	0.51
8:B:100:LEU:O	8:B:104:SER:HB2	2.10	0.51
4:5:236:VAL:HG21	4:5:242:PRO:HG3	1.93	0.51
6:7:280:ILE:HD12	6:7:295:GLU:HG3	1.92	0.51
8:B:103:ALA:O	8:B:107:ILE:HG12	2.11	0.51
2:3:88:ASN:HA	2:3:136:TYR:OH	2.10	0.51
3:4:171:GLN:HE21	3:4:244:ILE:HD12	1.76	0.51
11:E:98:CYS:HB2	11:E:118:LEU:HD12	1.93	0.51
11:E:451:MET:HG2	11:E:453:GLY:H	1.76	0.50
2:3:623:ILE:HG22	2:3:625:PRO:HD3	1.92	0.50
4:5:143:ASP:OD1	4:5:143:ASP:N	2.45	0.50
4:5:590:ARG:HG2	4:5:608:ILE:HG21	1.94	0.50
8:B:56:GLN:OE1	11:E:211:LYS:CB	2.59	0.50
1:2:377:ARG:CB	1:2:565:VAL:HG21	2.38	0.50
4:5:590:ARG:HG2	4:5:608:ILE:CG2	2.42	0.50
5:6:19:ARG:NH1	5:6:24:GLU:OE2	2.45	0.50
7:A:109:GLU:OE2	7:A:109:GLU:N	2.40	0.50
9:C:100:PHE:CE1	9:C:107:VAL:HG11	2.47	0.50
11:E:527:GLU:O	11:E:531:GLU:HG3	2.11	0.50
1:2:276:ARG:HE	11:E:319:GLY:HA3	1.76	0.50
4:5:387:LYS:O	4:5:391:LEU:HG	2.12	0.50
6:7:317:GLY:HA2	6:7:561:ARG:HE	1.76	0.50
1:2:315:CYS:SG	1:2:408:PRO:HD3	2.51	0.50
2:3:122:GLN:HG2	2:3:145:VAL:HG12	1.94	0.50
2:3:151:PHE:H	2:3:155:HIS:CE1	2.27	0.50
3:4:568:ASN:HD22	5:6:217:ARG:NE	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:338:SER:O	4:5:338:SER:OG	2.27	0.50
5:6:485:THR:HG23	5:6:490:LYS:HE2	1.94	0.50
8:B:49:ALA:HB1	8:B:60:LEU:HD21	1.93	0.50
11:E:5:ASP:OD1	11:E:5:ASP:N	2.45	0.50
4:5:390:LEU:O	4:5:394:VAL:HG23	2.11	0.50
6:7:36:GLN:HE22	6:7:39:ARG:CZ	2.25	0.50
9:C:128:SER:OG	9:C:129:PRO:HD2	2.12	0.50
1:2:462:LYS:HG3	1:2:463:MET:SD	2.51	0.50
3:4:656:GLU:O	3:4:660:ARG:HG3	2.10	0.50
1:2:548:GLY:N	1:2:587:ASP:O	2.44	0.49
1:2:676:ALA:HB3	5:6:595:VAL:HG23	1.94	0.49
3:4:698:ILE:HG22	3:4:700:PRO:HD3	1.92	0.49
4:5:47:ASP:H	11:E:406:ARG:NH2	2.10	0.49
6:7:153:ARG:HH12	6:7:251:ARG:NH1	2.10	0.49
1:2:560:VAL:H	1:2:613:LYS:HE2	1.77	0.49
2:3:85:ILE:HD11	2:3:129:VAL:HG23	1.93	0.49
4:5:453:ASP:OD2	4:5:454:ASP:N	2.45	0.49
7:A:58:LEU:HD23	9:C:41:PRO:HG2	1.94	0.49
2:3:81:VAL:HG21	2:3:128:PHE:HE2	1.77	0.49
3:4:396:ALA:HB2	3:4:414:THR:HG22	1.93	0.49
4:5:380:LEU:HD22	4:5:519:ILE:HD12	1.94	0.49
2:3:179:CYS:HB3	2:3:242:GLN:NE2	2.28	0.49
2:3:462:MET:HB3	6:7:407:ARG:HH11	1.78	0.49
3:4:580:ASN:N	3:4:580:ASN:OD1	2.45	0.49
7:A:88:ARG:NH2	10:D:101:GLU:OE1	2.45	0.49
7:A:149:GLU:OE2	11:E:37:GLN:NE2	2.45	0.49
1:2:642:THR:HG23	1:2:645:GLU:HG2	1.94	0.49
1:2:741:ASP:O	1:2:745:LYS:NZ	2.30	0.49
3:4:376:ASN:OD1	3:4:377:ASP:N	2.45	0.49
3:4:401:VAL:HG12	3:4:407:ASN:O	2.11	0.49
3:4:512:PRO:HB2	6:7:600:TYR:HE2	1.73	0.49
4:5:42:TYR:HD1	11:E:367:PHE:CG	2.30	0.49
6:7:153:ARG:HH12	6:7:251:ARG:HH12	1.60	0.49
8:B:26:ILE:HG13	8:B:33:LEU:HB2	1.93	0.49
9:C:78:ASP:CG	9:C:82:ARG:H	2.13	0.49
1:2:248:LEU:HD21	1:2:285:ILE:HD13	1.95	0.49
1:2:314:SER:OG	1:2:563:HIS:CD2	2.66	0.49
1:2:462:LYS:O	1:2:465:THR:OG1	2.31	0.49
1:2:526:GLY:N	5:6:619:ARG:NH1	2.61	0.49
3:4:319:ARG:HG2	6:7:221:TYR:CE2	2.48	0.49
4:5:614:GLU:HG2	4:5:618:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:357:THR:HA	5:6:551:ARG:HH11	0.67	0.49
7:A:194:ILE:HG13	7:A:195:LEU:N	2.27	0.49
8:B:109:LYS:HG2	11:E:262:THR:HB	1.94	0.49
1:2:373:TYR:CE1	4:5:289:ILE:HD11	2.47	0.49
3:4:740:LEU:HB3	3:4:761:ALA:HB1	1.94	0.49
4:5:134:PRO:HB2	4:5:152:PRO:HD3	1.93	0.49
5:6:159:LEU:O	5:6:162:GLN:NE2	2.45	0.49
11:E:477:PHE:O	11:E:480:SER:N	2.43	0.49
1:2:314:SER:CA	1:2:563:HIS:NE2	2.75	0.49
1:2:547:THR:OG1	1:2:588:GLU:OE1	2.30	0.49
7:A:10:ILE:HD12	9:C:22:LEU:HD22	1.95	0.49
7:A:162:ASP:OD2	7:A:181:LYS:NZ	2.39	0.49
7:A:195:LEU:HD22	11:E:41:GLN:NE2	2.26	0.49
1:2:633:ILE:HB	1:2:648:ASP:OD2	2.12	0.49
4:5:515:ASP:OD1	4:5:515:ASP:N	2.42	0.49
5:6:378:LYS:HB2	5:6:386:LEU:HD12	1.95	0.49
6:7:521:ILE:HG13	6:7:522:GLN:N	2.27	0.49
11:E:172:ARG:O	11:E:176:GLU:HG3	2.13	0.49
1:2:750:LEU:HD21	1:2:762:ILE:HG12	1.94	0.49
2:3:226:ASN:OD1	2:3:227:ASN:N	2.45	0.49
2:3:467:ILE:HG22	2:3:471:MET:HG3	1.94	0.49
3:4:190:GLU:O	3:4:192:LEU:N	2.45	0.49
3:4:723:SER:OG	3:4:724:ARG:NH1	2.46	0.49
4:5:356:LEU:HD13	4:5:377:LEU:HD12	1.95	0.49
1:2:381:SER:HB3	1:2:384:LYS:HE2	1.94	0.48
6:7:500:SER:H	6:7:503:GLN:NE2	2.11	0.48
11:E:257:GLU:HG2	11:E:258:ASP:H	1.77	0.48
1:2:178:LYS:HD3	1:2:179:GLY:N	2.28	0.48
2:3:436:ARG:NH1	2:3:481:ALA:HB3	2.28	0.48
2:3:646:ASP:N	2:3:646:ASP:OD1	2.44	0.48
3:4:242:ASN:O	3:4:249:TYR:OH	2.16	0.48
5:6:86:VAL:O	5:6:90:LEU:HG	2.13	0.48
1:2:500:PHE:CZ	1:2:724:ILE:HG22	2.48	0.48
3:4:682:LEU:HG	3:4:686:VAL:HG11	1.94	0.48
4:5:156:ILE:HG22	4:5:228:LYS:HB3	1.94	0.48
1:2:207:VAL:O	1:2:240:ARG:NH2	2.46	0.48
4:5:51:PHE:CZ	11:E:266:ASP:HB3	2.47	0.48
5:6:160:ASP:OD2	5:6:186:ALA:N	2.29	0.48
10:D:197:ASP:OD1	10:D:197:ASP:N	2.46	0.48
2:3:458:LYS:NZ	4:5:459:HIS:HD2	2.12	0.48
4:5:47:ASP:CB	11:E:406:ARG:NH2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:265:VAL:HG13	11:E:266:ASP:OD2	2.14	0.48
11:E:490:PRO:HD3	11:E:511:PRO:HG3	1.94	0.48
1:2:377:ARG:CG	1:2:565:VAL:CG1	2.90	0.48
1:2:594:ASP:O	1:2:598:THR:HG23	2.13	0.48
2:3:462:MET:CB	6:7:407:ARG:HH11	2.27	0.48
2:3:501:TYR:OH	2:3:508:LYS:NZ	2.47	0.48
7:A:83:ARG:NH2	7:A:110:GLU:OE1	2.46	0.48
11:E:126:GLU:N	11:E:126:GLU:OE1	2.47	0.48
4:5:115:PRO:HA	8:B:130:VAL:CG2	2.44	0.48
11:E:257:GLU:HB3	12:G:458:TYR:CE1	2.49	0.48
2:3:95:ASN:HA	2:3:148:GLU:O	2.14	0.48
12:F:528:ASP:H	12:H:717:GLN:HE21	1.62	0.48
1:2:207:VAL:HA	1:2:212:HIS:O	2.14	0.48
2:3:10:ARG:NH1	9:C:90:LYS:HB2	2.29	0.48
7:A:168:LEU:HD22	11:E:64:GLU:HB3	1.94	0.48
12:G:686:GLN:HB2	12:G:708:ILE:HG23	1.96	0.48
1:2:385:VAL:O	1:2:387:ALA:N	2.46	0.48
11:E:74:LEU:HD11	11:E:95:PHE:HD1	1.79	0.48
1:2:720:LEU:O	1:2:724:ILE:HG23	2.14	0.47
2:3:400:LEU:HD12	2:3:454:ASP:HB3	1.95	0.47
7:A:124:TYR:O	7:A:127:SER:OG	2.26	0.47
11:E:389:LYS:NZ	11:E:462:ARG:HD2	2.23	0.47
12:F:686:GLN:HB2	12:F:708:ILE:HG23	1.96	0.47
3:4:624:TRP:CE2	3:4:651:LEU:HD21	2.49	0.47
5:6:44:ILE:H	5:6:44:ILE:HD12	1.79	0.47
5:6:637:CYS:SG	5:6:638:ASP:N	2.86	0.47
7:A:149:GLU:OE1	11:E:41:GLN:NE2	2.47	0.47
11:E:133:ILE:O	11:E:181:ARG:HD2	2.13	0.47
10:D:104:PHE:CD2	10:D:105:PRO:HD3	2.49	0.47
11:E:343:MET:SD	11:E:343:MET:N	2.87	0.47
1:2:586:ILE:HB	1:2:628:ALA:HB2	1.96	0.47
2:3:447:ASP:CB	6:7:246:VAL:CG1	2.93	0.47
3:4:714:TYR:HB2	3:4:734:LEU:HD13	1.96	0.47
4:5:76:ASP:OD1	11:E:368:LYS:HD3	2.14	0.47
6:7:420:ARG:HG2	6:7:427:LEU:HG	1.96	0.47
7:A:83:ARG:HH21	7:A:110:GLU:CD	2.18	0.47
10:D:175:VAL:HG11	10:D:198:LEU:HD13	1.95	0.47
12:F:717:GLN:HE21	12:G:528:ASP:H	1.62	0.47
12:G:788:MET:HB3	12:G:792:ALA:HB3	1.96	0.47
1:2:343:GLN:NE2	1:2:399:LEU:HD11	2.30	0.47
3:4:521:GLN:O	3:4:525:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:80:PHE:CE1	11:E:367:PHE:HE1	2.30	0.47
8:B:57:LYS:HZ2	11:E:211:LYS:NZ	2.12	0.47
12:G:717:GLN:HE21	12:H:528:ASP:H	1.62	0.47
3:4:306:CYS:HB2	3:4:337:MET:SD	2.55	0.47
4:5:40:ARG:NH2	8:B:75:ARG:NH1	2.63	0.47
4:5:237:PRO:HG2	4:5:240:GLU:OE1	2.15	0.47
5:6:375:GLY:O	5:6:633:ARG:NH2	2.48	0.47
8:B:55:ARG:NE	11:E:42:CYS:O	2.27	0.47
8:B:55:ARG:HA	11:E:42:CYS:SG	2.54	0.47
12:F:788:MET:HB3	12:F:792:ALA:HB3	1.96	0.47
2:3:391:ASP:HB2	2:3:532:ASP:HB2	1.97	0.47
4:5:380:LEU:N	4:5:518:PHE:O	2.48	0.47
7:A:161:VAL:HA	7:A:181:LYS:HZ2	1.80	0.47
7:A:165:THR:HB	11:E:18:ARG:HH22	1.79	0.47
8:B:17:ILE:HG22	8:B:60:LEU:HD23	1.96	0.47
11:E:36:LEU:HD22	11:E:202:MET:HE3	1.97	0.47
11:E:133:ILE:HG13	11:E:181:ARG:HG3	1.97	0.47
12:H:788:MET:HB3	12:H:792:ALA:HB3	1.96	0.47
4:5:577:GLU:HA	4:5:580:GLU:OE2	2.14	0.47
6:7:642:ASP:C	6:7:644:LEU:H	2.18	0.47
1:2:526:GLY:CA	5:6:619:ARG:NH1	2.77	0.47
3:4:265:ALA:O	3:4:422:ARG:NH1	2.48	0.47
3:4:726:MET:HG3	3:4:727:VAL:N	2.28	0.47
4:5:519:ILE:HD12	4:5:654:SER:OG	2.15	0.47
5:6:120:ARG:O	5:6:121:HIS:ND1	2.48	0.47
1:2:276:ARG:NE	11:E:319:GLY:O	2.48	0.47
2:3:436:ARG:HH12	2:3:481:ALA:HB3	1.80	0.47
3:4:513:GLY:HA3	6:7:602:SER:HB2	1.97	0.47
6:7:554:LEU:H	6:7:554:LEU:HD12	1.80	0.47
11:E:491:LEU:HD23	11:E:492:VAL:N	2.30	0.47
1:2:481:ILE:HD11	1:2:496:ALA:HB2	1.97	0.46
4:5:49:THR:CG2	11:E:407:SER:CB	2.92	0.46
4:5:94:GLU:HG3	4:5:95:HIS:HD2	1.79	0.46
11:E:250:SER:O	11:E:254:HIS:HB3	2.15	0.46
12:H:686:GLN:HB2	12:H:708:ILE:HG23	1.96	0.46
1:2:186:VAL:HG13	1:2:195:ILE:HD12	1.97	0.46
2:3:184:PRO:HA	2:3:239:LYS:O	2.15	0.46
2:3:326:ILE:HG12	2:3:330:LYS:HE3	1.98	0.46
4:5:525:ASN:O	4:5:529:ASP:N	2.43	0.46
4:5:608:ILE:HD12	4:5:612:GLN:OE1	2.15	0.46
5:6:56:PRO:O	5:6:57:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:173:LYS:HG2	5:6:174:TYR:H	1.80	0.46
1:2:355:CYS:SG	1:2:357:SER:OG	2.59	0.46
1:2:526:GLY:N	5:6:619:ARG:CZ	2.78	0.46
2:3:655:THR:OG1	2:3:698:TYR:O	2.24	0.46
4:5:50:GLY:HA2	8:B:101:ASN:HD21	1.80	0.46
7:A:147:TYR:CE2	11:E:46:GLN:HG2	2.44	0.46
7:A:94:TYR:CE2	9:C:202:LEU:HD11	2.50	0.46
9:C:88:LEU:HD22	9:C:123:LEU:HD23	1.97	0.46
1:2:566:SER:OG	1:2:568:GLU:HG2	2.16	0.46
11:E:181:ARG:HA	11:E:184:ILE:HG22	1.97	0.46
12:H:586:VAL:HG11	12:H:627:LEU:HD22	1.98	0.46
1:2:587:ASP:OD1	1:2:588:GLU:N	2.49	0.46
1:2:751:ARG:HD3	4:5:532:LEU:HD13	1.97	0.46
2:3:151:PHE:N	2:3:155:HIS:HE1	2.13	0.46
3:4:730:TYR:HB3	5:6:399:SER:CB	2.45	0.46
4:5:115:PRO:CA	8:B:130:VAL:HG22	2.44	0.46
8:B:81:GLU:HG3	8:B:83:THR:H	1.81	0.46
10:D:71:GLU:OE1	10:D:74:LYS:N	2.44	0.46
1:2:284:ARG:HD2	1:2:442:ASN:O	2.15	0.46
1:2:288:LEU:HD21	1:2:305:LEU:HD23	1.96	0.46
2:3:431:GLN:HA	4:5:425:ARG:NH2	2.31	0.46
4:5:32:GLN:NE2	4:5:105:GLU:OE2	2.48	0.46
4:5:49:THR:OG1	4:5:50:GLY:N	2.49	0.46
1:2:463:MET:SD	1:2:463:MET:N	2.88	0.46
7:A:176:PHE:CB	11:E:47:TYR:CE1	2.99	0.46
8:B:57:LYS:HZ2	11:E:211:LYS:HZ1	1.64	0.46
10:D:104:PHE:CG	10:D:105:PRO:HD3	2.51	0.46
2:3:202:ARG:NH2	2:3:220:PRO:HG3	2.31	0.46
2:3:324:GLU:HG2	2:3:328:LYS:HE3	1.98	0.46
2:3:547:LEU:O	2:3:551:ARG:HG3	2.15	0.46
4:5:109:GLU:HB3	8:B:79:ARG:CZ	2.45	0.46
4:5:401:GLY:HA2	4:5:441:VAL:O	2.16	0.46
4:5:468:SER:HB3	4:5:477:THR:HG22	1.98	0.46
4:5:570:CYS:SG	4:5:572:PRO:HD3	2.56	0.46
5:6:187:ASN:OD1	5:6:187:ASN:N	2.49	0.46
7:A:149:GLU:CD	11:E:47:TYR:OH	2.53	0.46
10:D:37:GLU:HG3	10:D:92:TYR:CE1	2.50	0.46
12:F:586:VAL:HG11	12:F:627:LEU:HD22	1.98	0.46
1:2:750:LEU:HB2	1:2:818:PHE:CE2	2.51	0.45
2:3:673:HIS:CD2	2:3:686:ASP:HA	2.50	0.45
3:4:164:GLU:O	3:4:168:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:258:ILE:HD12	3:4:258:ILE:HA	1.77	0.45
3:4:438:GLN:HG2	3:4:441:PHE:CE2	2.51	0.45
4:5:378:LEU:HD23	4:5:517:ILE:HD12	1.98	0.45
12:G:618:PRO:HB2	12:H:570:ALA:HB1	1.98	0.45
2:3:148:GLU:HG2	2:3:149:GLY:N	2.32	0.45
3:4:171:GLN:NE2	3:4:244:ILE:HD12	2.32	0.45
7:A:175:HIS:ND1	11:E:48:THR:CG2	2.77	0.45
8:B:96:THR:HG21	8:B:117:VAL:HG21	1.97	0.45
1:2:726:TYR:CE2	1:2:730:ARG:HD2	2.50	0.45
2:3:206:ASP:HB2	6:7:292:LEU:HD12	1.99	0.45
2:3:535:ASP:HB3	2:3:538:GLN:HE22	1.82	0.45
4:5:210:ASP:OD1	4:5:210:ASP:N	2.43	0.45
4:5:615:ALA:HA	4:5:618:ARG:HG2	1.98	0.45
8:B:27:TYR:HA	8:B:32:ASP:OD1	2.16	0.45
8:B:156:SER:O	8:B:156:SER:OG	2.28	0.45
1:2:223:CYS:O	11:E:316:ALA:HB2	2.17	0.45
1:2:585:LEU:HD23	1:2:627:ILE:HB	1.98	0.45
3:4:191:PRO:O	3:4:195:GLN:N	2.44	0.45
4:5:145:MET:O	4:5:146:SER:OG	2.24	0.45
6:7:223:GLN:HG2	6:7:225:ARG:H	1.81	0.45
7:A:9:LEU:HB3	7:A:79:TYR:CD2	2.51	0.45
11:E:132:ASP:OD2	11:E:132:ASP:N	2.50	0.45
11:E:208:MET:O	12:G:477:HIS:HB3	2.16	0.45
12:F:570:ALA:HB1	12:H:618:PRO:HB2	1.98	0.45
1:2:377:ARG:HD2	1:2:565:VAL:CB	2.46	0.45
2:3:152:GLY:HA3	9:C:103:ASP:CB	2.45	0.45
3:4:222:LEU:HD12	3:4:223:TYR:N	2.32	0.45
4:5:335:ILE:O	4:5:339:ILE:HG23	2.16	0.45
4:5:463:GLU:HG3	4:5:513:ARG:CZ	2.46	0.45
6:7:534:ALA:O	6:7:538:THR:HG23	2.16	0.45
1:2:276:ARG:CZ	11:E:318:MET:O	2.53	0.45
2:3:279:ARG:HB3	2:3:313:MET:HE3	1.99	0.45
6:7:148:VAL:HG12	6:7:149:ILE:H	1.81	0.45
6:7:539:TYR:CG	6:7:547:PRO:HG3	2.51	0.45
11:E:39:LEU:HD23	11:E:39:LEU:HA	1.80	0.45
1:2:203:LEU:HD23	1:2:215:PHE:CD2	2.52	0.45
3:4:201:ASN:OD1	3:4:252:SER:OG	2.18	0.45
7:A:20:GLN:NE2	9:C:205:ASN:OD1	2.49	0.45
8:B:59:ARG:HH11	12:G:703:ARG:HD3	1.68	0.45
11:E:130:TYR:HE1	11:E:134:PHE:HD2	1.64	0.45
12:F:618:PRO:HB2	12:G:570:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:319:LEU:HD13	4:5:289:ILE:HG21	1.99	0.45
3:4:533:THR:HG22	3:4:534:SER:N	2.31	0.45
3:4:555:GLN:NE2	5:6:438:GLU:OE2	2.50	0.45
3:4:730:TYR:H	3:4:733:GLN:NE2	2.15	0.45
4:5:358:PHE:CE1	4:5:563:ILE:HG12	2.52	0.45
4:5:526:GLU:O	4:5:530:VAL:HG23	2.17	0.45
7:A:46:ASP:HA	7:A:49:GLU:HB3	1.98	0.45
10:D:29:ARG:NE	10:D:50:ILE:HD11	2.31	0.45
1:2:377:ARG:CD	1:2:565:VAL:CB	2.93	0.45
1:2:562:ARG:NH1	1:2:567:ARG:O	2.50	0.45
1:2:651:GLU:HB3	1:2:652:PRO:HD3	1.99	0.45
4:5:581:LYS:HG3	4:5:634:GLU:HG2	1.99	0.45
6:7:236:LYS:HE3	6:7:236:LYS:HB3	1.80	0.45
6:7:575:GLU:CD	6:7:575:GLU:H	2.20	0.45
1:2:530:SER:O	1:2:534:LYS:HG2	2.17	0.45
2:3:91:ARG:HB3	2:3:144:TYR:HB2	1.99	0.45
4:5:65:LEU:CD2	9:C:152:SER:HA	2.46	0.45
6:7:182:TYR:HE2	6:7:193:GLN:HG2	1.82	0.45
11:E:203:PHE:HE2	11:E:248:HIS:CD2	2.35	0.45
5:6:569:LEU:HD23	5:6:569:LEU:HA	1.78	0.44
6:7:48:LEU:HD23	6:7:136:LEU:HD12	2.00	0.44
8:B:55:ARG:CA	11:E:42:CYS:SG	3.05	0.44
2:3:126:LYS:HA	2:3:129:VAL:HG12	1.98	0.44
2:3:158:PRO:HD3	2:3:172:VAL:HG13	2.00	0.44
11:E:474:LEU:HD12	11:E:474:LEU:HA	1.81	0.44
12:G:690:ILE:HD13	12:G:706:VAL:HA	1.99	0.44
1:2:365:MET:SD	4:5:270:SER:HB2	2.58	0.44
1:2:493:ARG:O	1:2:497:LEU:HG	2.16	0.44
1:2:532:PHE:O	1:2:536:ILE:HG12	2.17	0.44
1:2:795:ILE:O	1:2:798:MET:HG3	2.17	0.44
3:4:306:CYS:SG	3:4:307:GLN:N	2.89	0.44
4:5:40:ARG:NH2	8:B:75:ARG:HH12	2.15	0.44
4:5:636:ASP:O	4:5:639:GLU:HG3	2.17	0.44
5:6:616:ILE:HG23	5:6:620:GLN:HG3	1.98	0.44
6:7:153:ARG:HB2	6:7:155:ASP:OD2	2.17	0.44
7:A:174:GLN:NE2	11:E:37:GLN:HE22	2.16	0.44
12:G:586:VAL:HG11	12:G:627:LEU:HD22	1.98	0.44
12:H:438:THR:HG22	12:H:697:PHE:HB2	2.00	0.44
3:4:238:ASP:OD2	3:4:260:VAL:HG12	2.17	0.44
8:B:66:MET:HG2	8:B:113:ILE:HD13	1.99	0.44
12:G:438:THR:HG22	12:G:697:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:627:LEU:HD23	2:3:682:VAL:HG21	2.00	0.44
4:5:86:ASP:CB	11:E:334:ILE:HG21	2.48	0.44
4:5:363:LYS:NZ	4:5:621:GLU:OE2	2.42	0.44
4:5:579:ALA:O	4:5:583:LYS:HG3	2.17	0.44
6:7:501:LEU:C	6:7:503:GLN:H	2.21	0.44
7:A:98:LEU:N	7:A:103:ARG:HH21	2.08	0.44
8:B:67:ASP:OD1	8:B:68:VAL:N	2.51	0.44
11:E:62:PHE:O	11:E:66:LYS:HB3	2.17	0.44
2:3:59:GLU:OE1	2:3:62:ARG:NH2	2.51	0.44
2:3:378:SER:OG	6:7:343:GLU:OE2	2.30	0.44
3:4:220:LYS:HE2	3:4:220:LYS:HB3	1.81	0.44
5:6:347:TYR:OH	5:6:366:ARG:HB3	2.18	0.44
6:7:43:ARG:HH22	6:7:133:ARG:HH11	1.66	0.44
6:7:566:CYS:SG	6:7:619:LEU:HA	2.57	0.44
6:7:582:THR:O	6:7:586:VAL:HG23	2.17	0.44
9:C:40:MET:HB3	9:C:60:VAL:HB	1.99	0.44
10:D:173:LEU:HD13	10:D:211:ILE:HD12	1.99	0.44
11:E:299:ARG:HG2	11:E:353:MET:HG2	1.99	0.44
4:5:197:CYS:HB2	4:5:211:PRO:HG3	2.00	0.44
12:H:690:ILE:HD13	12:H:706:VAL:HA	1.99	0.44
1:2:720:LEU:HA	1:2:723:TYR:HB3	1.99	0.44
3:4:255:GLU:HG2	3:4:256:HIS:N	2.32	0.44
5:6:126:LEU:HD21	5:6:137:ILE:HD11	2.00	0.44
10:D:152:ASN:N	10:D:152:ASN:OD1	2.49	0.44
12:F:438:THR:HG22	12:F:697:PHE:HB2	2.00	0.44
1:2:306:ILE:HD12	1:2:418:TYR:HB2	2.00	0.44
1:2:377:ARG:HD2	1:2:565:VAL:CA	2.48	0.44
2:3:166:LEU:HD11	2:3:288:CYS:HB3	2.00	0.44
2:3:487:LEU:HD21	6:7:241:SER:HG	1.68	0.44
3:4:476:ILE:HD11	3:4:650:LEU:CD1	2.48	0.44
4:5:317:GLN:NE2	4:5:318:GLU:HG2	2.33	0.44
4:5:614:GLU:HG2	4:5:618:ARG:HH12	1.83	0.44
5:6:354:LEU:HD12	5:6:354:LEU:HA	1.81	0.44
12:F:690:ILE:HD13	12:F:706:VAL:HA	1.99	0.44
1:2:500:PHE:HE1	1:2:727:ALA:HB3	1.83	0.43
1:2:564:PRO:CA	5:6:441:GLU:CD	2.62	0.43
3:4:413:LYS:HB3	3:4:413:LYS:HE2	1.76	0.43
4:5:43:ARG:NH2	8:B:111:ASP:OD2	2.51	0.43
6:7:233:GLN:HG2	6:7:262:THR:HG22	2.00	0.43
6:7:248:ASN:OD1	6:7:249:ILE:N	2.49	0.43
7:A:176:PHE:HB2	11:E:47:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:567:ARG:HD2	5:6:440:HIS:CD2	2.49	0.43
2:3:118:LEU:HA	2:3:118:LEU:HD23	1.69	0.43
2:3:207:LEU:HD23	2:3:207:LEU:HA	1.82	0.43
3:4:268:THR:HG22	3:4:269:LYS:HG3	2.00	0.43
3:4:534:SER:OG	3:4:535:GLY:N	2.52	0.43
4:5:331:VAL:HG11	4:5:627:LYS:HG2	1.99	0.43
5:6:565:ARG:C	5:6:565:ARG:HD2	2.38	0.43
6:7:148:VAL:HG12	6:7:149:ILE:N	2.33	0.43
7:A:30:ARG:HH21	7:A:31:GLN:HG3	1.83	0.43
7:A:144:LYS:HD2	7:A:144:LYS:HA	1.75	0.43
1:2:332:CYS:HB3	1:2:355:CYS:SG	2.58	0.43
1:2:399:LEU:HA	1:2:399:LEU:HD23	1.69	0.43
1:2:536:ILE:HA	1:2:539:VAL:HG12	1.99	0.43
2:3:525:ASP:OD2	2:3:665:THR:OG1	2.36	0.43
3:4:711:ILE:O	3:4:715:VAL:HG23	2.19	0.43
5:6:168:VAL:HB	5:6:177:PRO:HG3	1.99	0.43
7:A:28:GLY:O	7:A:32:VAL:HG13	2.18	0.43
12:G:541:GLY:HA3	12:G:544:TRP:CE2	2.53	0.43
1:2:382:PRO:HB3	5:6:492:THR:O	2.19	0.43
1:2:384:LYS:HE2	1:2:384:LYS:HB3	1.80	0.43
1:2:549:GLN:CD	5:6:471:VAL:CB	2.77	0.43
2:3:447:ASP:HB3	6:7:246:VAL:HG11	2.01	0.43
5:6:387:ARG:O	5:6:626:ARG:NH1	2.50	0.43
11:E:210:SER:CB	12:G:473:THR:HG22	2.28	0.43
3:4:169:PHE:CZ	3:4:215:ILE:HG22	2.54	0.43
9:C:35:ARG:HA	9:C:64:SER:O	2.18	0.43
9:C:93:GLN:O	9:C:97:ARG:NH1	2.51	0.43
9:C:161:THR:HG21	9:C:180:GLN:NE2	2.34	0.43
11:E:445:PHE:HD1	11:E:446:LEU:O	2.01	0.43
12:G:641:VAL:HG22	12:G:647:VAL:HG22	2.01	0.43
1:2:248:LEU:HB3	1:2:249:PRO:HD3	2.00	0.43
3:4:611:THR:OG1	3:4:612:SER:N	2.52	0.43
5:6:390:ILE:HG22	5:6:626:ARG:HD2	2.00	0.43
6:7:155:ASP:OD2	6:7:155:ASP:N	2.44	0.43
6:7:182:TYR:OH	6:7:193:GLN:NE2	2.51	0.43
7:A:188:GLN:O	9:C:202:LEU:HG	2.19	0.43
9:C:32:LEU:HA	9:C:33:PRO:HD3	1.90	0.43
9:C:78:ASP:OD1	9:C:82:ARG:N	2.38	0.43
11:E:106:VAL:HG11	11:E:133:ILE:HG21	2.00	0.43
11:E:125:LEU:HD23	11:E:125:LEU:HA	1.86	0.43
12:H:641:VAL:HG22	12:H:647:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:749:ASP:O	1:2:753:GLU:HG2	2.19	0.43
3:4:238:ASP:O	3:4:242:ASN:ND2	2.52	0.43
3:4:551:PRO:HG2	3:4:552:GLU:OE1	2.19	0.43
6:7:185:ASP:OD1	6:7:185:ASP:N	2.49	0.43
7:A:176:PHE:CB	11:E:47:TYR:CD1	3.02	0.43
1:2:757:THR:HG22	1:2:758:GLY:N	2.30	0.43
2:3:486:ARG:O	6:7:242:ASP:OD1	2.36	0.43
3:4:276:PRO:HB3	6:7:175:PRO:HB3	2.00	0.43
4:5:51:PHE:CD2	8:B:114:ARG:NH2	2.86	0.43
10:D:33:ALA:O	10:D:37:GLU:HG2	2.18	0.43
11:E:305:VAL:HG12	11:E:309:LYS:NZ	2.33	0.43
2:3:521:LEU:HD12	2:3:521:LEU:HA	1.77	0.43
2:3:437:ARG:NH1	6:7:249:ILE:HD12	2.22	0.43
3:4:561:GLY:O	3:4:565:LEU:HG	2.19	0.43
4:5:50:GLY:HA2	8:B:101:ASN:ND2	2.34	0.43
4:5:555:ASP:OD1	4:5:555:ASP:N	2.52	0.43
5:6:532:LEU:HD12	5:6:532:LEU:HA	1.91	0.43
7:A:41:GLU:HG3	7:A:42:GLN:N	2.34	0.43
8:B:40:LEU:CD2	12:G:688:ARG:NE	2.79	0.43
11:E:259:GLU:OE2	12:G:701:LEU:HB2	2.12	0.43
1:2:723:TYR:OH	1:2:780:ILE:O	2.37	0.42
3:4:326:SER:O	3:4:326:SER:OG	2.36	0.42
4:5:523:GLU:HB2	4:5:528:ARG:HD2	2.01	0.42
8:B:148:LEU:HD23	8:B:148:LEU:HA	1.79	0.42
11:E:36:LEU:HD12	11:E:36:LEU:HA	1.63	0.42
11:E:499:MET:SD	11:E:500:GLU:N	2.92	0.42
11:E:508:GLY:O	11:E:520:ASN:ND2	2.45	0.42
12:F:541:GLY:HA3	12:F:544:TRP:CE2	2.53	0.42
4:5:238:HIS:O	4:5:238:HIS:CG	2.72	0.42
4:5:348:ASP:HA	4:5:351:LYS:HB2	2.00	0.42
5:6:329:MET:HE2	5:6:334:TRP:HE3	1.84	0.42
7:A:33:LEU:HD13	10:D:148:HIS:HB2	2.01	0.42
11:E:200:MET:O	11:E:204:GLU:HG2	2.19	0.42
2:3:671:THR:HG22	2:3:682:VAL:HG11	1.99	0.42
3:4:212:CYS:HB3	3:4:262:PRO:HB3	2.01	0.42
4:5:43:ARG:HH22	8:B:111:ASP:CG	2.23	0.42
5:6:326:LYS:HA	5:6:329:MET:HG3	2.00	0.42
5:6:544:THR:O	5:6:547:ALA:N	2.52	0.42
1:2:315:CYS:H	1:2:563:HIS:CE1	2.38	0.42
1:2:526:GLY:CA	5:6:619:ARG:NH2	2.77	0.42
2:3:74:GLN:HG3	2:3:76:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:356:ASP:OD1	2:3:357:TYR:N	2.53	0.42
2:3:383:ASP:HB3	2:3:492:SER:HB3	2.02	0.42
4:5:644:PHE:O	4:5:648:THR:HG22	2.19	0.42
7:A:31:GLN:O	7:A:35:GLU:HG2	2.19	0.42
8:B:19:PRO:HD2	8:B:40:LEU:O	2.19	0.42
9:C:40:MET:HE1	9:C:43:LEU:HD12	2.00	0.42
1:2:534:LYS:O	1:2:537:GLU:HB3	2.19	0.42
2:3:394:VAL:HG12	2:3:394:VAL:O	2.19	0.42
2:3:415:GLY:HA3	2:3:455:GLU:O	2.19	0.42
3:4:255:GLU:OE1	3:4:255:GLU:N	2.50	0.42
3:4:443:GLU:O	3:4:447:GLU:HG3	2.19	0.42
3:4:529:ARG:HA	3:4:529:ARG:HD2	1.83	0.42
7:A:190:VAL:HG12	7:A:191:LEU:HD12	2.01	0.42
12:H:541:GLY:HA3	12:H:544:TRP:CE2	2.53	0.42
2:3:465:THR:HG22	6:7:407:ARG:CG	2.47	0.42
3:4:654:GLN:N	3:4:654:GLN:OE1	2.53	0.42
4:5:46:THR:HG21	11:E:406:ARG:HB3	2.02	0.42
7:A:3:CYS:SG	7:A:72:ASN:ND2	2.92	0.42
12:F:641:VAL:HG22	12:F:647:VAL:HG22	2.01	0.42
1:2:315:CYS:HB2	1:2:374:GLN:NE2	2.35	0.42
1:2:561:GLN:HB3	1:2:572:GLU:HG2	2.01	0.42
3:4:196:ARG:O	3:4:200:ILE:HG12	2.20	0.42
3:4:306:CYS:HB3	3:4:309:CYS:SG	2.59	0.42
3:4:684:MET:O	3:4:687:LEU:N	2.53	0.42
5:6:38:GLN:CD	5:6:42:GLY:HA2	2.40	0.42
5:6:449:LEU:HD23	5:6:449:LEU:HA	1.74	0.42
7:A:151:ARG:NH2	11:E:398:ILE:HG23	2.35	0.42
11:E:122:ASP:OD1	11:E:122:ASP:N	2.53	0.42
11:E:207:TRP:NE1	12:G:478:ALA:O	2.52	0.42
1:2:668:ASP:HA	1:2:669:PRO:HD3	1.95	0.42
1:2:723:TYR:CE1	1:2:727:ALA:HB2	2.55	0.42
2:3:353:HIS:HB3	2:3:542:ILE:HG12	2.02	0.42
2:3:399:LEU:O	2:3:403:VAL:HG23	2.20	0.42
3:4:467:ALA:HB2	3:4:522:TYR:CD2	2.55	0.42
3:4:735:GLU:O	3:4:738:ILE:HB	2.19	0.42
4:5:348:ASP:OD1	4:5:351:LYS:HD2	2.19	0.42
6:7:395:ASP:OD1	6:7:401:SER:OG	2.24	0.42
7:A:151:ARG:CZ	11:E:398:ILE:CG2	2.97	0.42
8:B:81:GLU:HG2	8:B:85:THR:HG22	2.01	0.42
9:C:113:GLY:HA3	9:C:114:PRO:HA	1.81	0.42
11:E:494:ALA:HB2	11:E:506:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:536:ARG:HH21	11:E:550:LYS:HE2	1.84	0.42
12:G:660:PRO:HG2	12:H:553:LEU:HD21	2.02	0.42
1:2:197:HIS:CE1	1:2:201:ASN:HD21	2.37	0.42
1:2:685:ARG:HG3	1:2:686:HIS:CE1	2.55	0.42
1:2:762:ILE:HA	1:2:766:HIS:ND1	2.34	0.42
2:3:81:VAL:HG21	2:3:128:PHE:CE2	2.53	0.42
2:3:462:MET:HB3	6:7:407:ARG:NH1	2.35	0.42
5:6:48:GLN:HA	5:6:51:GLU:HG2	2.01	0.42
5:6:94:LEU:HD12	5:6:94:LEU:HA	1.84	0.42
5:6:593:PHE:O	5:6:597:GLN:HG2	2.20	0.42
7:A:174:GLN:CG	11:E:49:LEU:HB3	2.50	0.42
9:C:201:ASN:HA	9:C:204:GLN:CD	2.40	0.42
12:F:660:PRO:HG2	12:G:553:LEU:HD21	2.02	0.42
12:H:469:GLU:OE2	12:H:703:ARG:NH2	2.53	0.42
1:2:314:SER:HB2	1:2:565:VAL:HG21	2.00	0.42
1:2:331:LYS:HD2	1:2:357:SER:HB3	2.01	0.42
6:7:269:ASP:OD2	6:7:305:LYS:HE3	2.19	0.42
9:C:130:GLU:OE1	9:C:130:GLU:N	2.33	0.42
11:E:482:LYS:HD3	11:E:482:LYS:HA	1.88	0.42
1:2:524:ASP:HA	1:2:632:PRO:HG3	2.01	0.41
3:4:608:ASN:ND2	5:6:212:GLN:NE2	2.68	0.41
6:7:77:PHE:O	6:7:81:VAL:HG23	2.20	0.41
10:D:206:ILE:HG22	10:D:207:ARG:N	2.34	0.41
12:F:730:TRP:HZ2	12:G:564:LYS:HD2	1.85	0.41
12:H:487:TYR:HH	12:H:512:HIS:HD1	1.68	0.41
4:5:455:ARG:O	4:5:458:ILE:HG22	2.20	0.41
5:6:41:ASP:N	5:6:41:ASP:OD1	2.53	0.41
12:F:469:GLU:OE2	12:F:703:ARG:NH2	2.52	0.41
12:F:553:LEU:HD21	12:H:660:PRO:HG2	2.02	0.41
2:3:416:ARG:HB3	4:5:456:VAL:HG11	1.74	0.41
2:3:509:THR:OG1	2:3:510:PRO:HD2	2.20	0.41
3:4:445:ARG:O	3:4:449:LEU:HG	2.20	0.41
4:5:59:LEU:HD22	4:5:107:ALA:HB2	2.02	0.41
5:6:120:ARG:HG2	5:6:121:HIS:H	1.86	0.41
11:E:83:LEU:HA	11:E:83:LEU:HD12	1.86	0.41
12:G:469:GLU:OE2	12:G:703:ARG:NH2	2.53	0.41
1:2:588:GLU:HB3	1:2:591:LYS:HD2	2.02	0.41
3:4:551:PRO:O	3:4:554:ARG:HD3	2.21	0.41
5:6:486:LYS:HD3	5:6:486:LYS:HA	1.74	0.41
7:A:21:LEU:HD12	7:A:22:PRO:HD2	2.01	0.41
7:A:98:LEU:HB3	7:A:102:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:151:ARG:NH1	11:E:398:ILE:HG23	2.35	0.41
7:A:161:VAL:HG13	7:A:181:LYS:HZ2	1.84	0.41
1:2:203:LEU:HD23	1:2:203:LEU:HA	1.90	0.41
1:2:342:SER:OG	1:2:344:ASN:OD1	2.29	0.41
1:2:464:ILE:HD13	1:2:467:LEU:HD12	2.01	0.41
2:3:281:GLN:HG3	2:3:313:MET:HG3	2.02	0.41
3:4:275:ASN:OD1	6:7:263:ARG:NH2	2.41	0.41
3:4:503:GLU:HB3	3:4:612:SER:HB3	2.02	0.41
3:4:744:HIS:CE1	3:4:760:GLU:HG2	2.55	0.41
4:5:334:VAL:HG22	4:5:554:ILE:HG13	2.02	0.41
6:7:533:LEU:O	6:7:537:ILE:HG13	2.20	0.41
6:7:645:LEU:HD23	6:7:645:LEU:HA	1.91	0.41
7:A:195:LEU:CD2	11:E:41:GLN:OE1	2.69	0.41
9:C:88:LEU:HD13	9:C:134:ILE:HD11	2.02	0.41
11:E:67:GLU:OE2	11:E:67:GLU:N	2.53	0.41
12:H:435:SER:HB3	12:H:629:TRP:CD1	2.56	0.41
5:6:65:PHE:O	5:6:69:GLU:HG3	2.19	0.41
5:6:322:ALA:O	5:6:326:LYS:HB2	2.21	0.41
6:7:166:ILE:HA	6:7:269:ASP:O	2.20	0.41
7:A:24:PHE:CG	7:A:107:ALA:HB2	2.55	0.41
9:C:165:VAL:HA	9:C:168:LEU:HD13	2.02	0.41
11:E:254:HIS:O	11:E:254:HIS:ND1	2.54	0.41
11:E:416:LEU:HD23	11:E:416:LEU:HA	1.88	0.41
12:F:435:SER:HB3	12:F:629:TRP:CD1	2.56	0.41
12:G:730:TRP:HZ2	12:H:564:LYS:HD2	1.85	0.41
4:5:167:ARG:NH1	4:5:181:ASN:HD22	2.18	0.41
6:7:182:TYR:HB2	6:7:191:THR:HG23	2.03	0.41
7:A:151:ARG:NH2	11:E:398:ILE:CG2	2.84	0.41
7:A:165:THR:HB	11:E:18:ARG:NH2	2.35	0.41
8:B:111:ASP:CG	11:E:264:SER:HA	2.39	0.41
1:2:377:ARG:NH1	1:2:377:ARG:HB3	2.36	0.41
1:2:606:GLN:NE2	4:5:392:LYS:HZ2	2.15	0.41
1:2:718:GLU:HG3	1:2:722:LYS:NZ	2.36	0.41
2:3:468:HIS:O	2:3:523:ARG:NH2	2.50	0.41
3:4:176:PRO:O	3:4:177:LEU:HD23	2.21	0.41
5:6:158:CYS:HA	5:6:191:PHE:HD1	1.86	0.41
5:6:357:THR:CA	5:6:551:ARG:HH12	2.00	0.41
6:7:135:GLU:HG3	6:7:137:TYR:OH	2.21	0.41
7:A:116:ASN:OD1	7:A:119:ARG:NH2	2.53	0.41
7:A:194:ILE:O	7:A:196:SER:N	2.53	0.41
1:2:311:VAL:HG22	1:2:411:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:616:ILE:HD12	1:2:616:ILE:HA	1.77	0.41
1:2:765:ARG:HD3	1:2:768:GLU:OE1	2.20	0.41
2:3:156:VAL:HG21	2:3:161:LEU:HD13	2.03	0.41
3:4:472:GLU:HG3	3:4:473:HIS:H	1.86	0.41
4:5:46:THR:CG2	11:E:406:ARG:O	2.56	0.41
4:5:529:ASP:HA	4:5:532:LEU:HD12	2.03	0.41
5:6:325:ILE:O	5:6:329:MET:HG2	2.20	0.41
6:7:348:GLU:OE2	6:7:348:GLU:N	2.36	0.41
7:A:152:CYS:SG	7:A:169:LEU:HG	2.61	0.41
7:A:176:PHE:CG	11:E:47:TYR:CE1	3.09	0.41
8:B:84:PHE:O	8:B:147:ASN:ND2	2.48	0.41
8:B:173:ASN:OD1	9:C:135:SER:OG	2.28	0.41
11:E:364:HIS:CD2	11:E:370:LYS:HD2	2.56	0.41
1:2:233:ASN:HB3	1:2:236:ASP:OD1	2.21	0.41
1:2:715:LEU:HA	1:2:716:PRO:HD3	1.91	0.41
1:2:726:TYR:CZ	1:2:730:ARG:HD2	2.56	0.41
2:3:480:LYS:HD3	2:3:480:LYS:HA	1.80	0.41
3:4:631:ILE:HG13	3:4:631:ILE:O	2.20	0.41
5:6:59:ASN:OD1	5:6:59:ASN:N	2.53	0.41
5:6:187:ASN:HD22	5:6:190:ARG:HB2	1.86	0.41
5:6:516:LEU:HD12	5:6:516:LEU:HA	1.90	0.41
8:B:40:LEU:CD1	12:G:688:ARG:NE	2.77	0.41
11:E:23:VAL:HG12	11:E:24:ALA:O	2.21	0.41
12:G:435:SER:HB3	12:G:629:TRP:CD1	2.56	0.41
1:2:328:ASN:HA	1:2:335:VAL:HA	2.03	0.40
2:3:526:LEU:HD23	2:3:526:LEU:HA	1.85	0.40
3:4:499:LYS:HB3	3:4:499:LYS:HE3	1.83	0.40
4:5:507:MET:SD	4:5:507:MET:N	2.94	0.40
6:7:427:LEU:HD12	6:7:427:LEU:H	1.85	0.40
7:A:43:ASN:HB2	7:A:65:ARG:HD3	2.02	0.40
11:E:284:TRP:HE1	11:E:424:ARG:NH2	2.20	0.40
2:3:114:ALA:HB2	2:3:169:VAL:HG23	2.03	0.40
2:3:509:THR:HG23	2:3:511:MET:N	2.35	0.40
3:4:462:LEU:HD23	3:4:462:LEU:HA	1.90	0.40
4:5:42:TYR:CD1	11:E:367:PHE:CB	3.04	0.40
4:5:128:LEU:O	4:5:128:LEU:HD12	2.21	0.40
4:5:271:ILE:HG12	4:5:291:SER:O	2.21	0.40
5:6:204:GLN:HB2	5:6:233:VAL:HG22	2.04	0.40
8:B:60:LEU:HD23	8:B:60:LEU:HA	1.93	0.40
9:C:40:MET:O	9:C:59:ALA:HA	2.21	0.40
2:3:414:THR:HA	2:3:454:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:659:THR:O	2:3:662:THR:HG22	2.22	0.40
3:4:471:TYR:HD2	3:4:658:TYR:CE1	2.32	0.40
5:6:524:ALA:HB3	5:6:525:PRO:HD3	2.02	0.40
6:7:400:ARG:O	6:7:440:GLY:HA3	2.21	0.40
9:C:21:SER:O	9:C:21:SER:OG	2.39	0.40
12:H:554:LEU:HD22	12:H:567:PHE:CE1	2.57	0.40
2:3:65:LEU:HD12	2:3:65:LEU:HA	1.94	0.40
2:3:180:SER:OG	2:3:181:LEU:N	2.54	0.40
2:3:242:GLN:HG2	2:3:243:THR:H	1.86	0.40
3:4:752:LYS:HE2	3:4:752:LYS:HB3	1.86	0.40
4:5:49:THR:CG2	11:E:407:SER:HB2	2.51	0.40
7:A:124:TYR:CE2	10:D:97:LEU:HD11	2.56	0.40
12:F:497:ILE:HB	12:F:514:LEU:HB2	2.03	0.40
1:2:236:ASP:OD2	1:2:237:LEU:N	2.54	0.40
1:2:461:VAL:O	1:2:464:ILE:N	2.54	0.40
3:4:645:ASP:HB2	3:4:736:SER:OG	2.22	0.40
3:4:666:LEU:HD23	3:4:666:LEU:HA	1.93	0.40
6:7:51:ASP:OD1	6:7:53:ASP:N	2.45	0.40
6:7:339:SER:HB3	6:7:553:PRO:HA	2.03	0.40
7:A:94:TYR:HE2	9:C:202:LEU:HD11	1.87	0.40
11:E:165:VAL:HG22	11:E:169:MET:HG3	2.03	0.40
11:E:549:LEU:HD12	11:E:549:LEU:HA	1.88	0.40
12:F:564:LYS:HD2	12:H:730:TRP:HZ2	1.85	0.40
12:H:497:ILE:HB	12:H:514:LEU:HB2	2.03	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	2	603/904 (67%)	523 (87%)	80 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3	602/853 (71%)	532 (88%)	70 (12%)	0	100	100
3	4	592/863 (69%)	507 (86%)	84 (14%)	1 (0%)	47	81
4	5	563/734 (77%)	503 (89%)	59 (10%)	1 (0%)	47	81
5	6	603/821 (73%)	538 (89%)	62 (10%)	3 (0%)	29	69
6	7	592/719 (82%)	528 (89%)	63 (11%)	1 (0%)	47	81
7	A	194/196 (99%)	170 (88%)	24 (12%)	0	100	100
8	B	174/185 (94%)	161 (92%)	13 (8%)	0	100	100
9	C	190/216 (88%)	173 (91%)	17 (9%)	0	100	100
10	D	201/223 (90%)	186 (92%)	15 (8%)	0	100	100
11	E	534/566 (94%)	480 (90%)	54 (10%)	0	100	100
12	F	404/1171 (34%)	396 (98%)	8 (2%)	0	100	100
12	G	404/1171 (34%)	396 (98%)	8 (2%)	0	100	100
12	H	404/1171 (34%)	396 (98%)	8 (2%)	0	100	100
All	All	6060/9793 (62%)	5489 (91%)	565 (9%)	6 (0%)	54	86

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	540	CYS
3	4	653	PRO
4	5	115	PRO
5	6	559	ILE
5	6	563	ILE
6	7	490	PRO

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	2	535/781 (68%)	535 (100%)	0	100	100
2	3	527/742 (71%)	527 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	4	530/753 (70%)	529 (100%)	1 (0%)	93 96
4	5	494/625 (79%)	494 (100%)	0	100 100
5	6	545/724 (75%)	543 (100%)	2 (0%)	91 94
6	7	514/619 (83%)	507 (99%)	7 (1%)	67 80
7	A	174/174 (100%)	174 (100%)	0	100 100
8	B	160/169 (95%)	160 (100%)	0	100 100
9	C	167/186 (90%)	167 (100%)	0	100 100
10	D	188/205 (92%)	188 (100%)	0	100 100
11	E	491/517 (95%)	489 (100%)	2 (0%)	91 94
12	F	350/1017 (34%)	350 (100%)	0	100 100
12	G	350/1017 (34%)	350 (100%)	0	100 100
12	H	350/1017 (34%)	350 (100%)	0	100 100
All	All	5375/8546 (63%)	5363 (100%)	12 (0%)	93 96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	428	ARG
5	6	563	ILE
5	6	565	ARG
6	7	311	ASP
6	7	312	ASP
6	7	319	LEU
6	7	320	THR
6	7	527	ARG
6	7	528	ASP
6	7	529	ASN
11	E	247	ARG
11	E	284	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	180	HIS
1	2	196	HIS
1	2	197	HIS
1	2	201	ASN

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Mol	Chain	Res	Type
1	2	206	HIS
1	2	282	HIS
1	2	328	ASN
1	2	511	HIS
1	2	561	GLN
1	2	601	HIS
1	2	606	GLN
1	2	607	GLN
2	3	112	ASN
2	3	139	GLN
2	3	155	HIS
2	3	191	HIS
2	3	513	ASN
3	4	165	ASN
3	4	171	GLN
3	4	195	GLN
3	4	214	HIS
3	4	332	HIS
3	4	342	ASN
3	4	415	HIS
3	4	521	GLN
3	4	525	ASN
3	4	568	ASN
3	4	594	GLN
3	4	633	ASN
3	4	733	GLN
3	4	744	HIS
4	5	95	HIS
4	5	181	ASN
4	5	244	HIS
4	5	376	ASN
4	5	426	ASN
4	5	459	HIS
5	6	212	GLN
5	6	342	GLN
5	6	349	ASN
6	7	30	GLN
6	7	36	GLN
6	7	186	GLN
6	7	223	GLN
6	7	503	GLN
6	7	504	ASN

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Mol	Chain	Res	Type
6	7	529	ASN
6	7	543	HIS
7	A	20	GLN
7	A	72	ASN
8	B	51	ASN
8	B	56	GLN
8	B	102	HIS
9	C	136	GLN
9	C	155	ASN
9	C	177	GLN
10	D	78	HIS
11	E	15	GLN
11	E	37	GLN
11	E	248	HIS
11	E	253	ASN
11	E	324	GLN
11	E	364	HIS
12	F	515	HIS
12	F	563	GLN
12	F	717	GLN
12	G	515	HIS
12	G	563	GLN
12	G	717	GLN
12	H	515	HIS
12	H	563	GLN
12	H	717	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

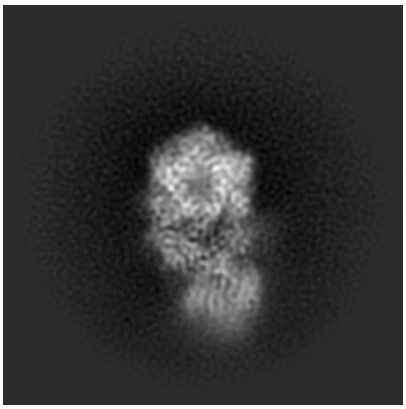
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10621. These allow visual inspection of the internal detail of the map and identification of artifacts.

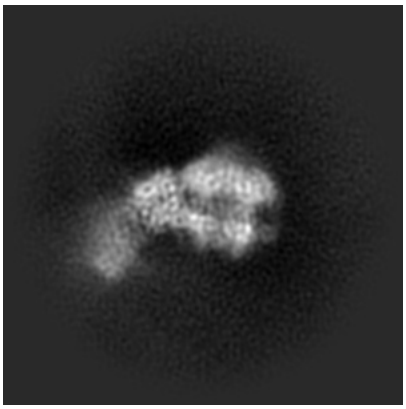
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

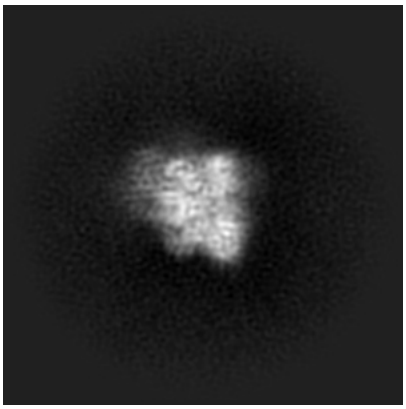
6.1.1 Primary map



X

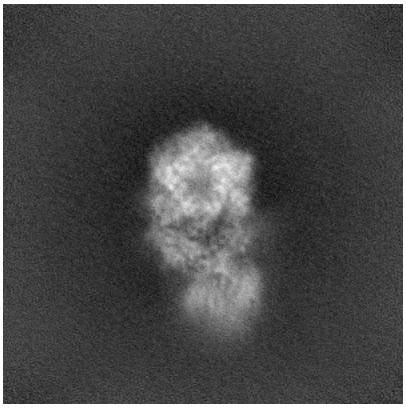


Y

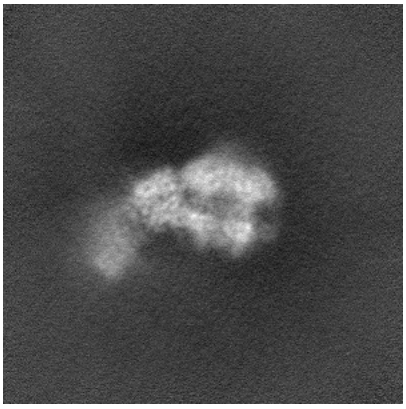


Z

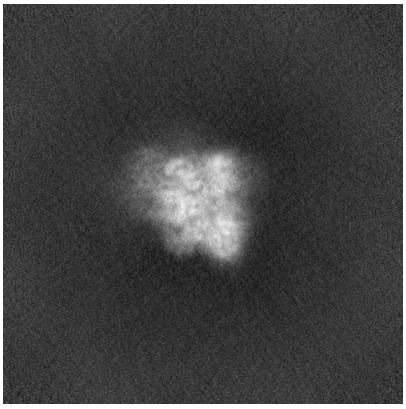
6.1.2 Raw map



X



Y

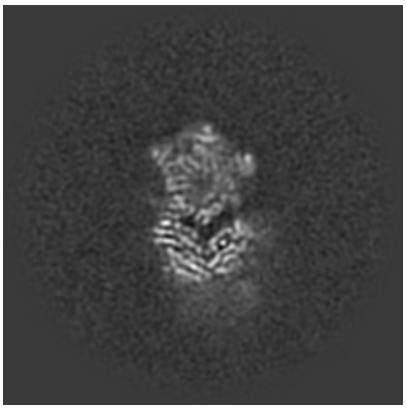


Z

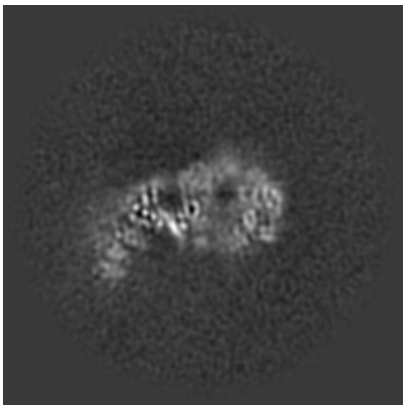
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

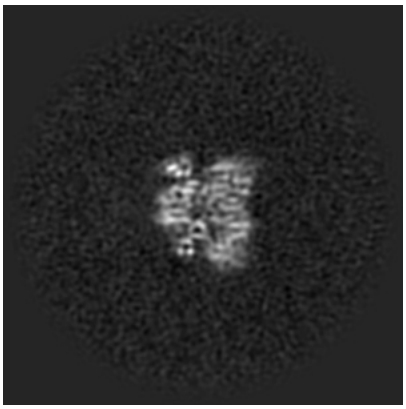
6.2.1 Primary map



X Index: 215

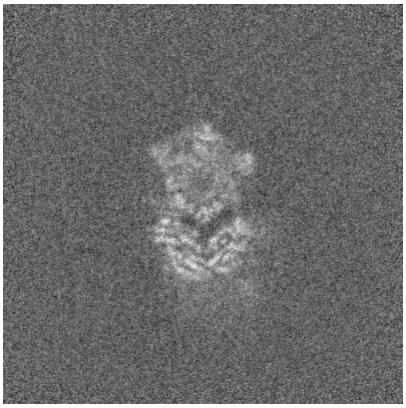


Y Index: 215

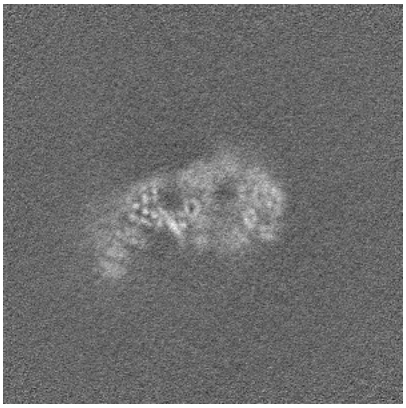


Z Index: 215

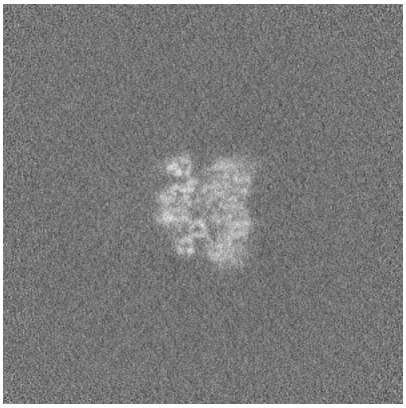
6.2.2 Raw map



X Index: 215



Y Index: 215

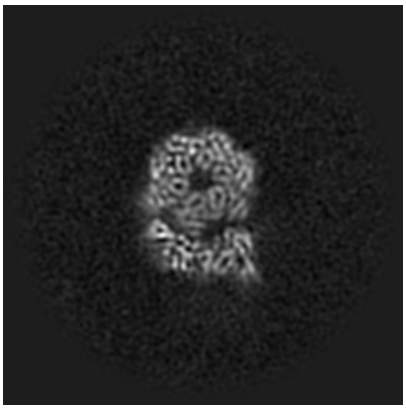


Z Index: 215

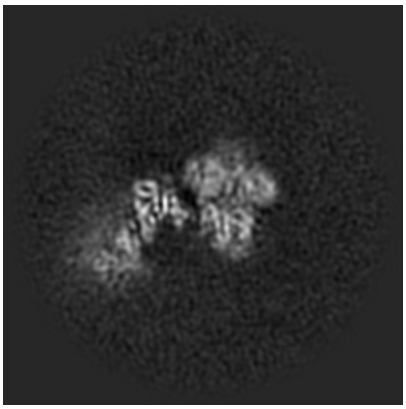
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

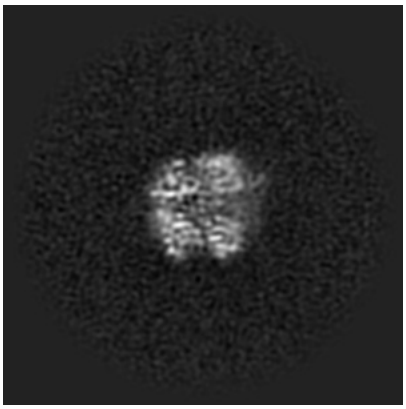
6.3.1 Primary map



X Index: 233

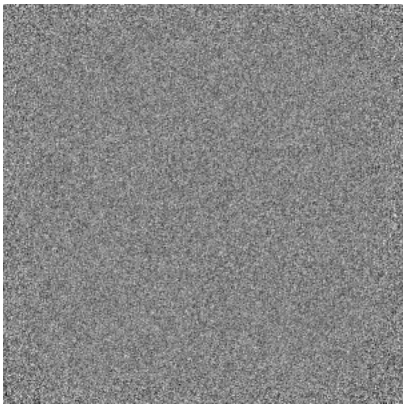


Y Index: 236

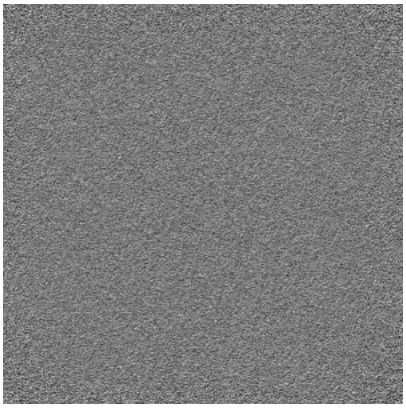


Z Index: 254

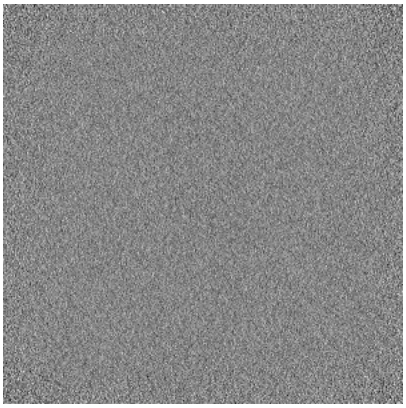
6.3.2 Raw map



X Index: 0



Y Index: 0

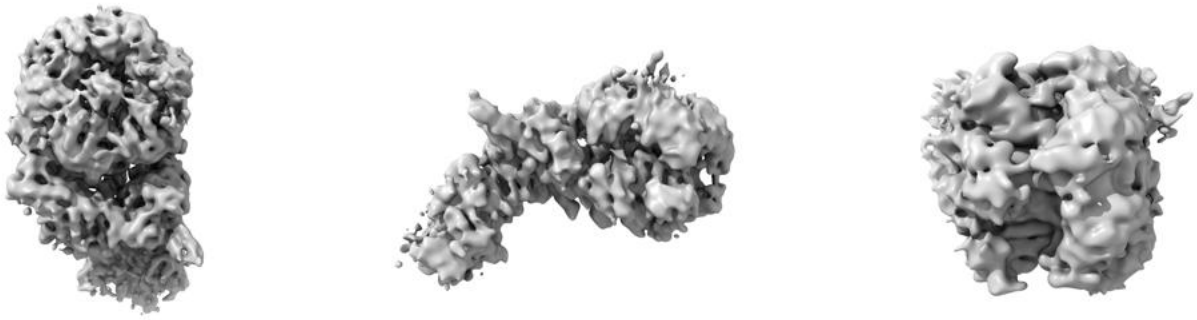


Z Index: 0

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

6.4 Orthogonal surface views (i)

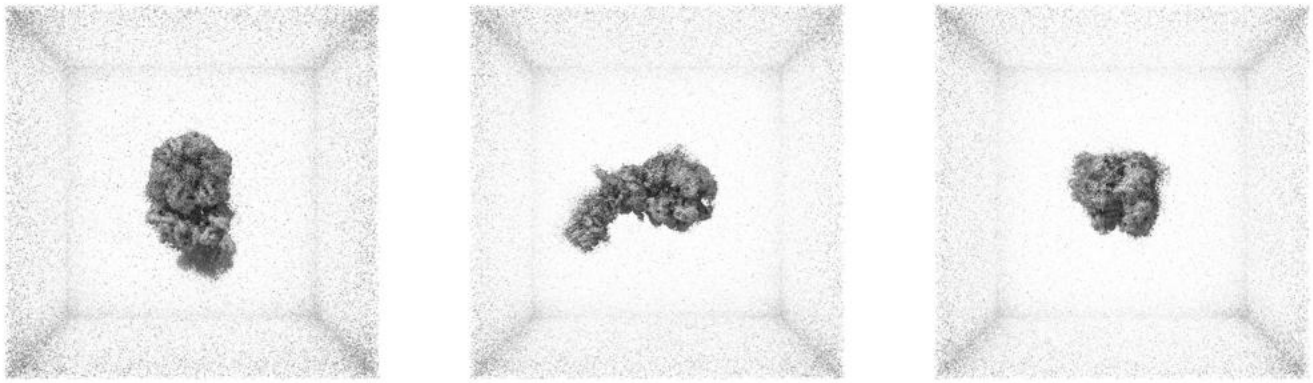
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

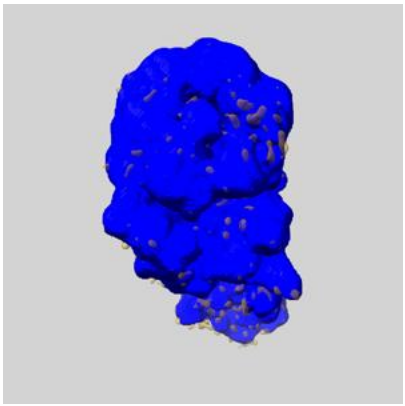
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

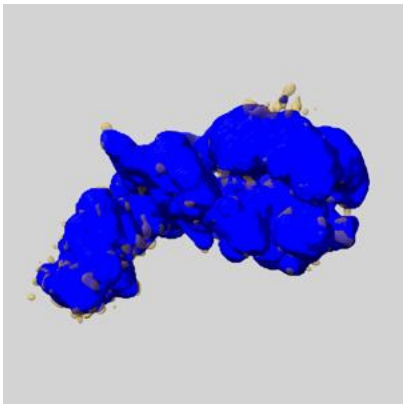
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

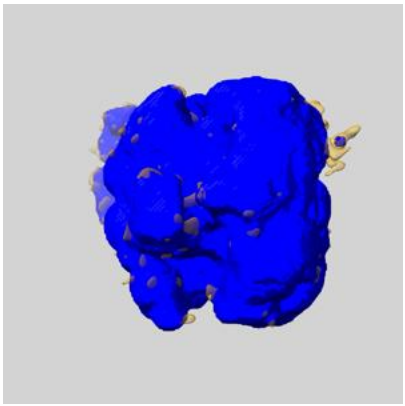
6.5.1 emd_10621_msk_1.map (i)



X



Y

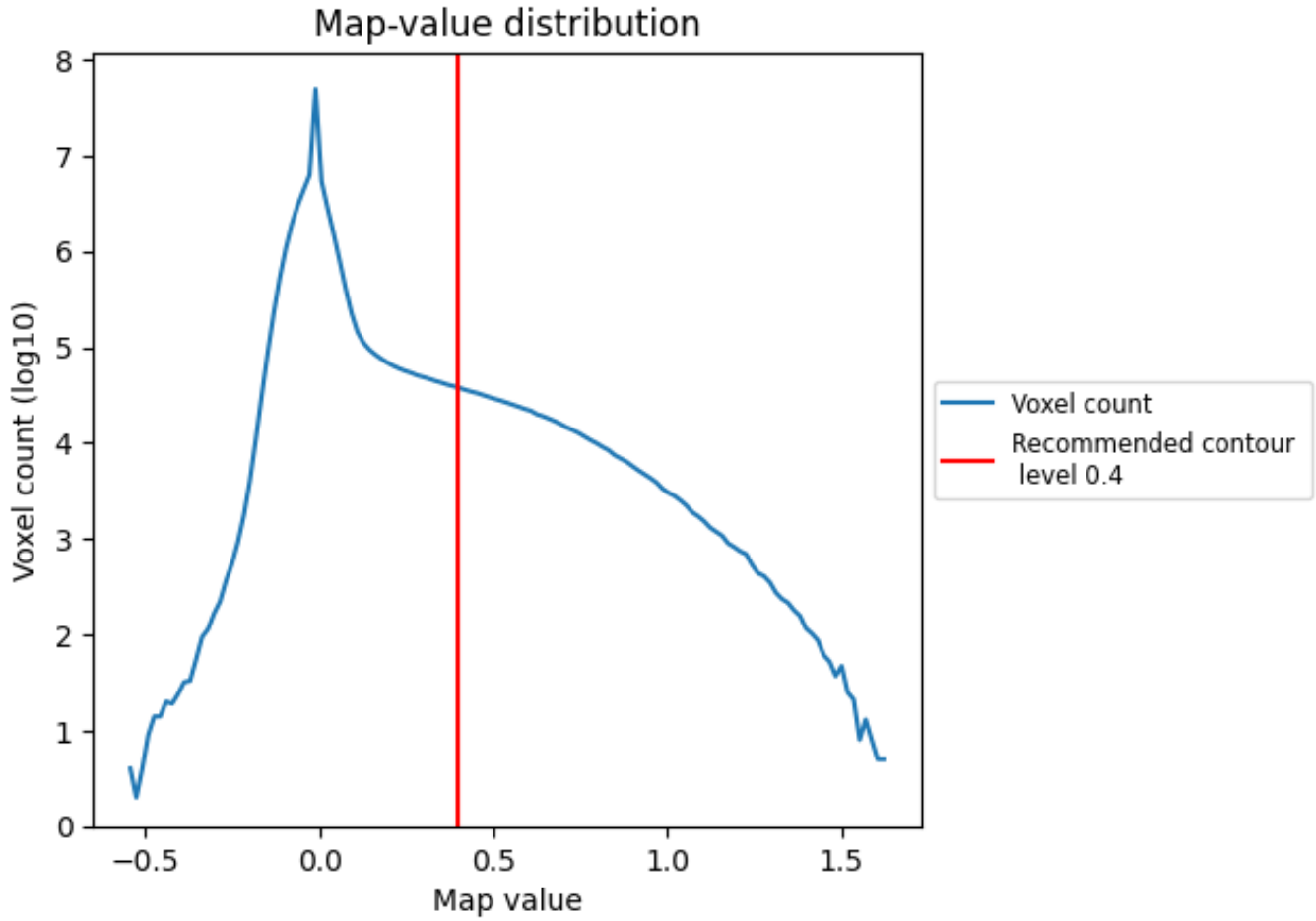


Z

7 Map analysis

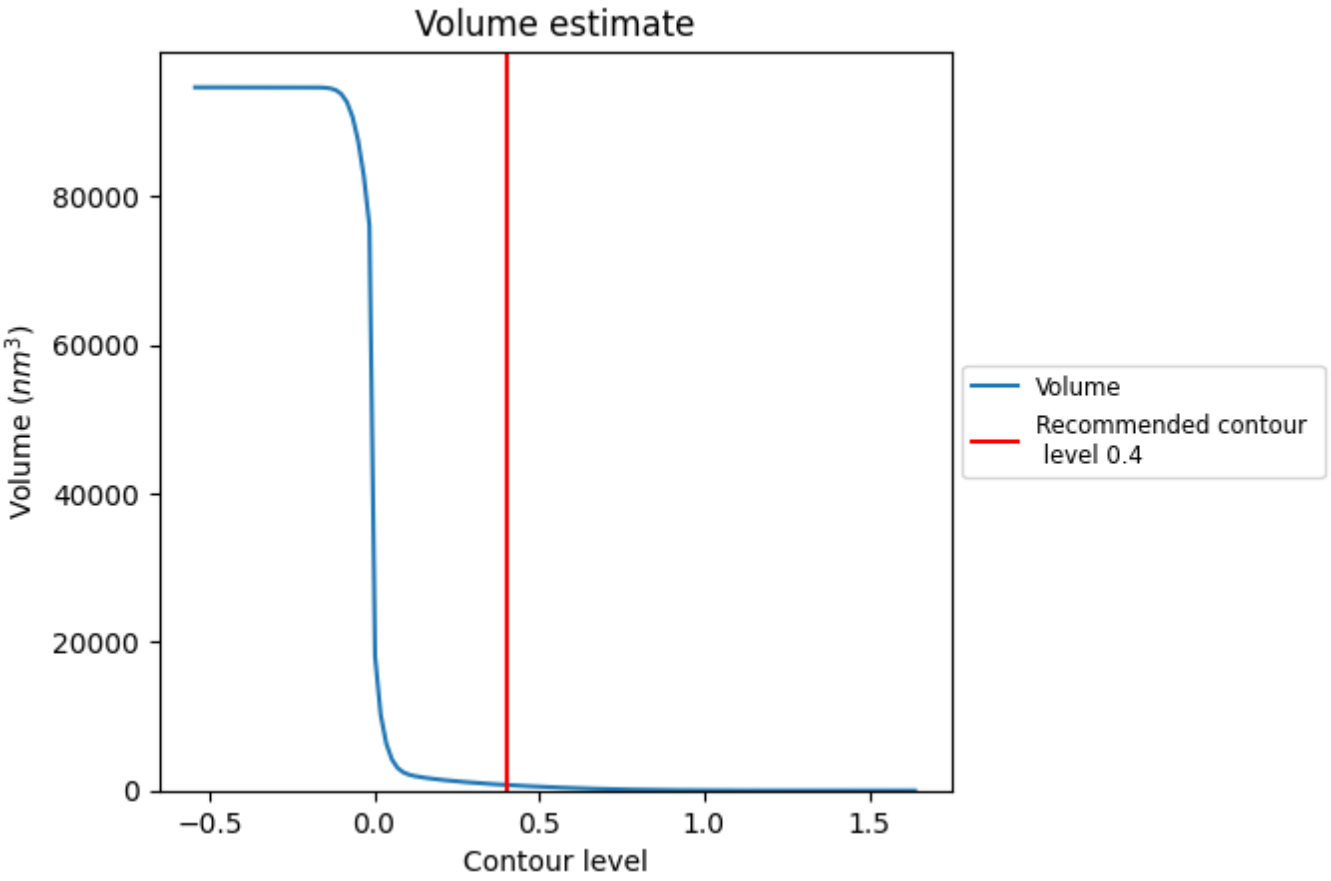
This section contains the results of statistical analysis of the map.

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.

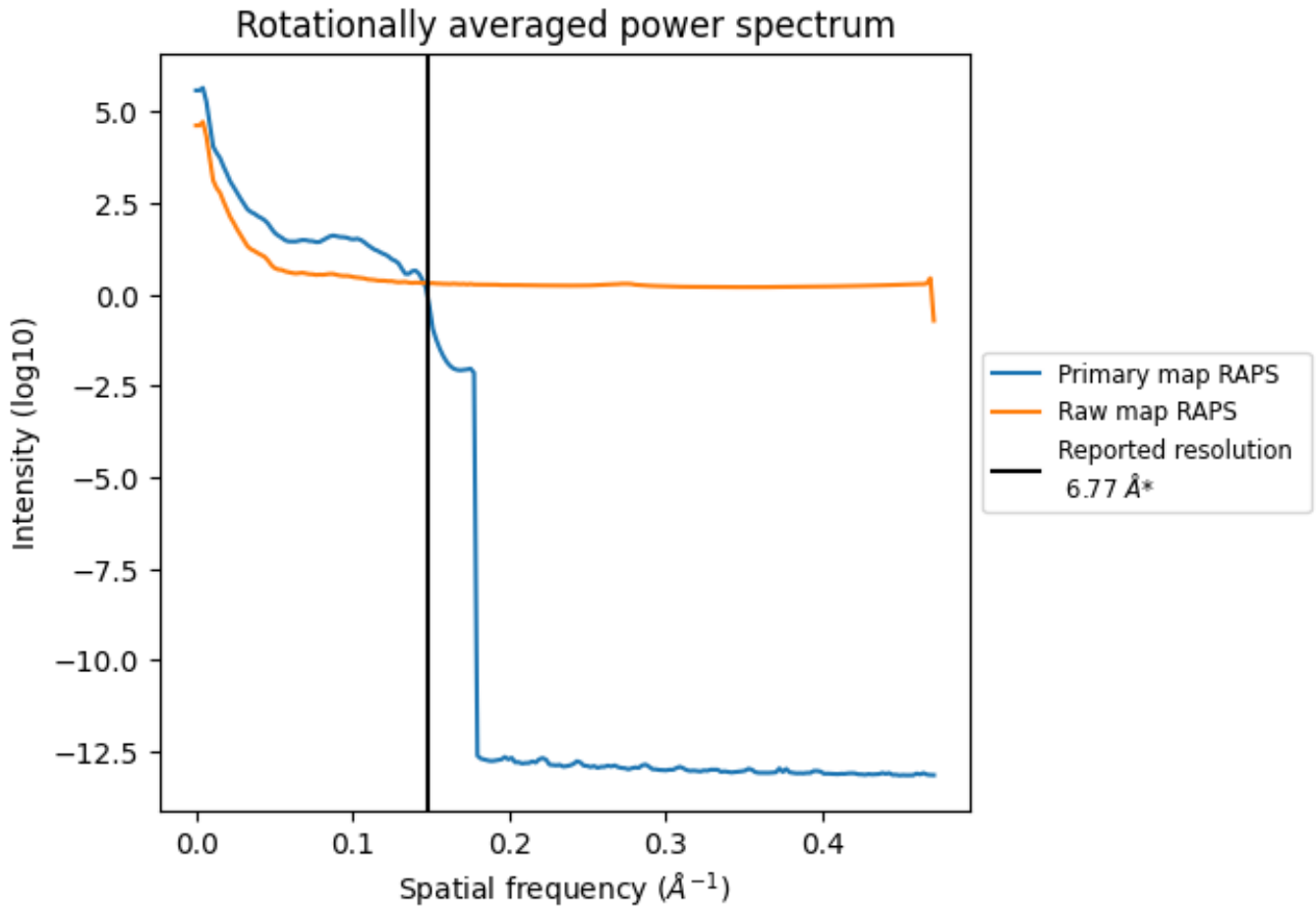
7.2 Volume estimate



The volume at the recommended contour level is 757 nm^3; this corresponds to an approximate mass of 683 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)

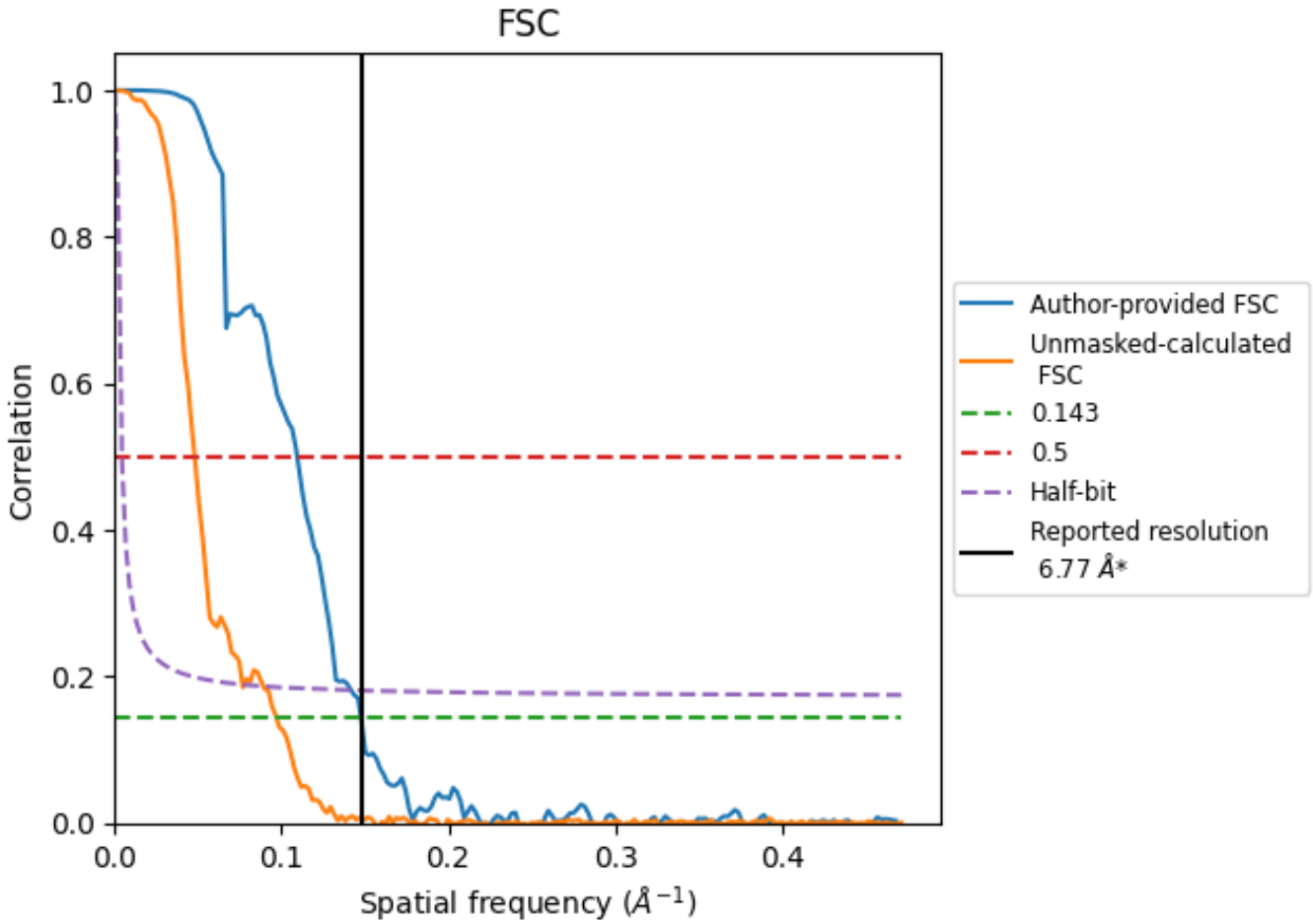


*Reported resolution corresponds to spatial frequency of 0.148 Å^{-1}

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 0.148 Å^{-1}

8.2 Resolution estimates (i)

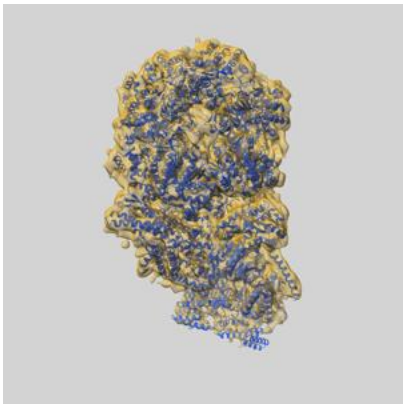
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.77	-	-
Author-provided FSC curve	6.78	9.14	7.05
Unmasked-calculated*	10.31	20.88	13.05

*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 10.31 differs from the reported value 6.77 by more than 10 %

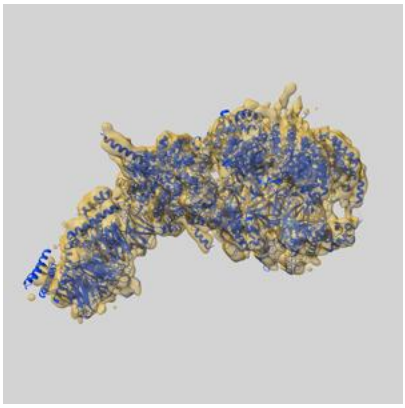
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10621 and PDB model 6XTY. Per-residue inclusion information can be found in section 3 on page 10.

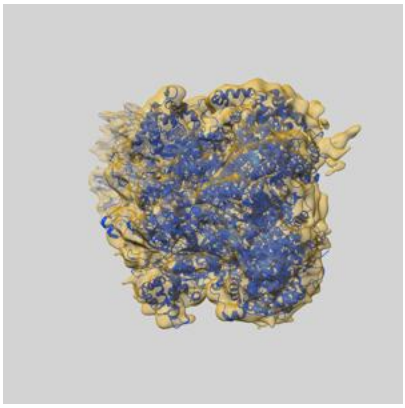
9.1 Map-model overlay



X



Y



Z

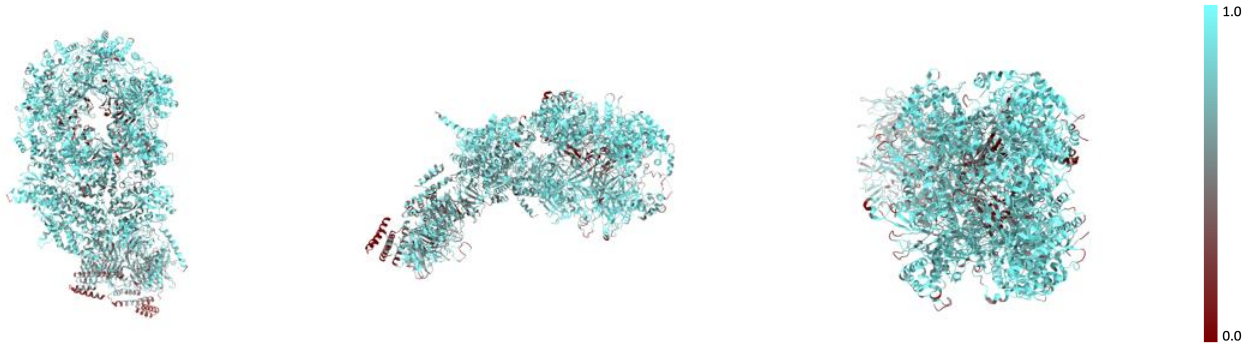
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

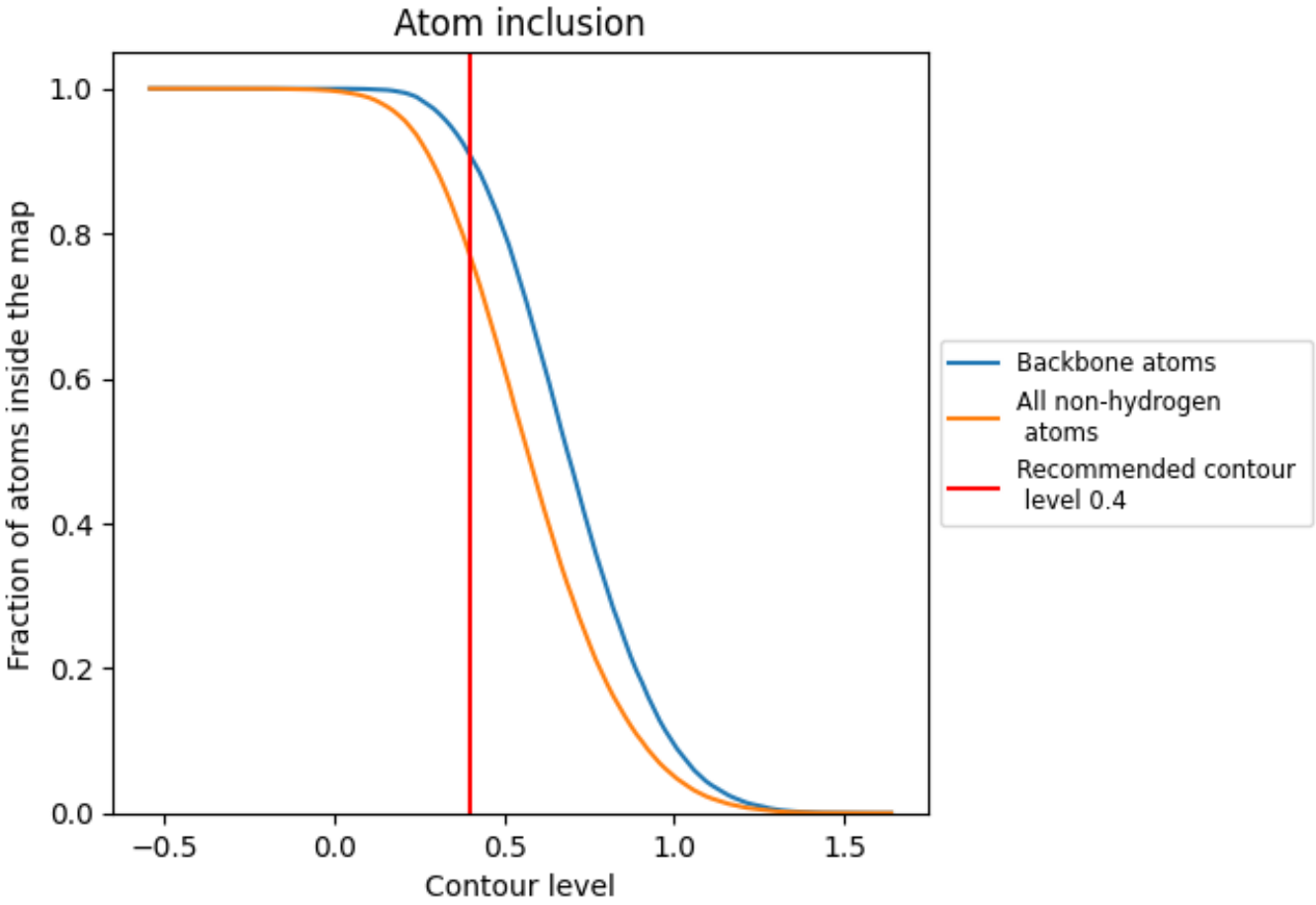
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 77% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7679	0.1270
2	0.8099	0.1330
3	0.8100	0.1200
4	0.8168	0.1280
5	0.7611	0.1260
6	0.8175	0.1210
7	0.8258	0.1250
A	0.8327	0.1430
B	0.8009	0.1520
C	0.8154	0.1420
D	0.8354	0.1380
E	0.7983	0.1410
F	0.6676	0.1200
G	0.5649	0.1270
H	0.5745	0.0990