Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 03:46 AM EST

PDB ID	:	6VXK
EMDB ID	:	EMD-21442
Title	:	Cryo-EM Structure of the full-length A39R/PlexinC1 complex
Authors	:	Kuo, Y.-C.; Chen, H.; Shang, G.; Uchikawa, E.; Tian, H.; Bai, X.; Zhang, X.
Deposited on	:	2020-02-22
Resolution	:	3.10 Å(reported)
Based on initial model	:	3NVN

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

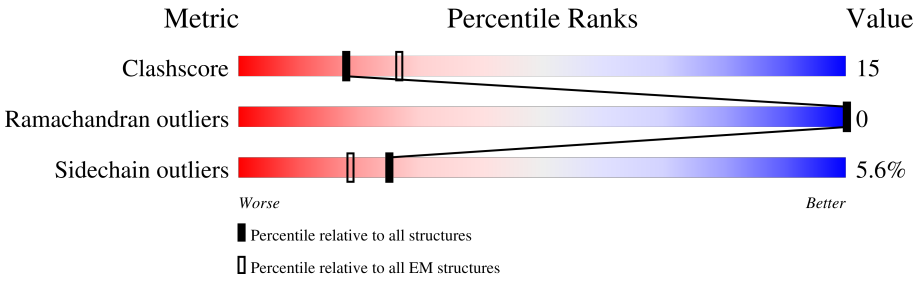
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	398	64% 30% • 5%
1	C	398	64% 29% • 5%
2	B	1545	32% 15% • 52%
2	D	1545	32% 16% • 52%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17418 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 Semaphorin-like protein 139.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			3022	1926	500	585	11		
1	C	380	Total	C	N	O	S	0	0
			3022	1926	500	585	11		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLU	-	expression tag	UNP Q8JL80
A	13	LEU	-	expression tag	UNP Q8JL80
A	14	GLU	-	expression tag	UNP Q8JL80
A	400	GLY	-	expression tag	UNP Q8JL80
A	401	THR	-	expression tag	UNP Q8JL80
A	402	HIS	-	expression tag	UNP Q8JL80
A	403	HIS	-	expression tag	UNP Q8JL80
A	404	HIS	-	expression tag	UNP Q8JL80
A	405	HIS	-	expression tag	UNP Q8JL80
A	406	HIS	-	expression tag	UNP Q8JL80
A	407	HIS	-	expression tag	UNP Q8JL80
A	408	HIS	-	expression tag	UNP Q8JL80
A	409	HIS	-	expression tag	UNP Q8JL80
C	12	GLU	-	expression tag	UNP Q8JL80
C	13	LEU	-	expression tag	UNP Q8JL80
C	14	GLU	-	expression tag	UNP Q8JL80
C	400	GLY	-	expression tag	UNP Q8JL80
C	401	THR	-	expression tag	UNP Q8JL80
C	402	HIS	-	expression tag	UNP Q8JL80
C	403	HIS	-	expression tag	UNP Q8JL80
C	404	HIS	-	expression tag	UNP Q8JL80
C	405	HIS	-	expression tag	UNP Q8JL80
C	406	HIS	-	expression tag	UNP Q8JL80
C	407	HIS	-	expression tag	UNP Q8JL80
C	408	HIS	-	expression tag	UNP Q8JL80
C	409	HIS	-	expression tag	UNP Q8JL80

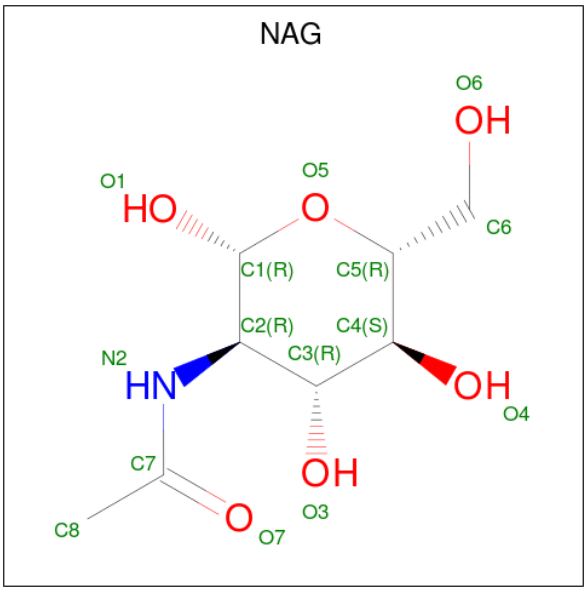
- Molecule 2 is a protein called Plexin-C1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	747	Total	C	N	O	S	0	0
			5561	3496	971	1056	38		
2	D	747	Total	C	N	O	S	0	0
			5561	3496	971	1056	38		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1569	GLY	-	expression tag	UNP O60486
B	1570	THR	-	expression tag	UNP O60486
B	1571	SER	-	expression tag	UNP O60486
B	1572	SER	-	expression tag	UNP O60486
B	1573	GLY	-	expression tag	UNP O60486
B	1574	LEU	-	expression tag	UNP O60486
B	1575	GLU	-	expression tag	UNP O60486
B	1576	VAL	-	expression tag	UNP O60486
B	1577	LEU	-	expression tag	UNP O60486
B	1578	PHE	-	expression tag	UNP O60486
B	1579	GLN	-	expression tag	UNP O60486
D	1569	GLY	-	expression tag	UNP O60486
D	1570	THR	-	expression tag	UNP O60486
D	1571	SER	-	expression tag	UNP O60486
D	1572	SER	-	expression tag	UNP O60486
D	1573	GLY	-	expression tag	UNP O60486
D	1574	LEU	-	expression tag	UNP O60486
D	1575	GLU	-	expression tag	UNP O60486
D	1576	VAL	-	expression tag	UNP O60486
D	1577	LEU	-	expression tag	UNP O60486
D	1578	PHE	-	expression tag	UNP O60486
D	1579	GLN	-	expression tag	UNP O60486

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 112 64 8 40	0
3	B	1	Total C N O 112 64 8 40	0
3	B	1	Total C N O 112 64 8 40	0
3	B	1	Total C N O 112 64 8 40	0
3	B	1	Total C N O 112 64 8 40	0
3	B	1	Total C N O 112 64 8 40	0
3	B	1	Total C N O 112 64 8 40	0
3	B	1	Total C N O 112 64 8 40	0
3	C	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 112 64 8 40	0
3	D	1	Total C N O 112 64 8 40	0
3	D	1	Total C N O 112 64 8 40	0
3	D	1	Total C N O 112 64 8 40	0

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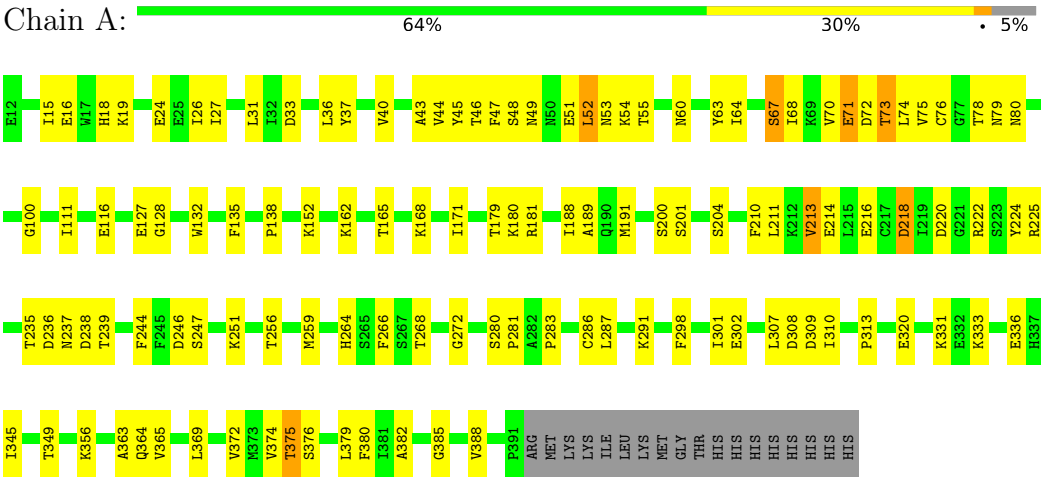
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			112	64	8	40	
3	D	1	Total	C	N	O	0
			112	64	8	40	
3	D	1	Total	C	N	O	0
			112	64	8	40	
3	D	1	Total	C	N	O	0
			112	64	8	40	

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.

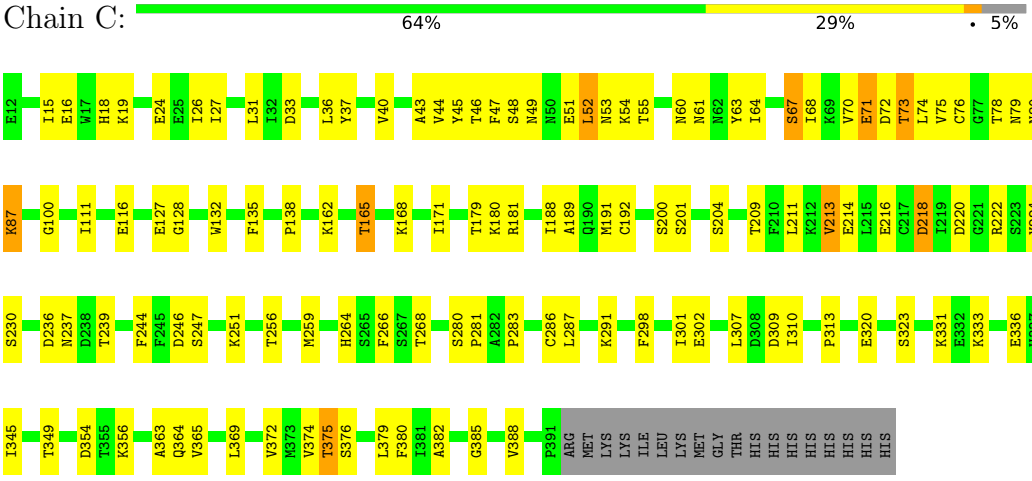
• Molecule 1: Semaphorin-like protein 139

Chain A:



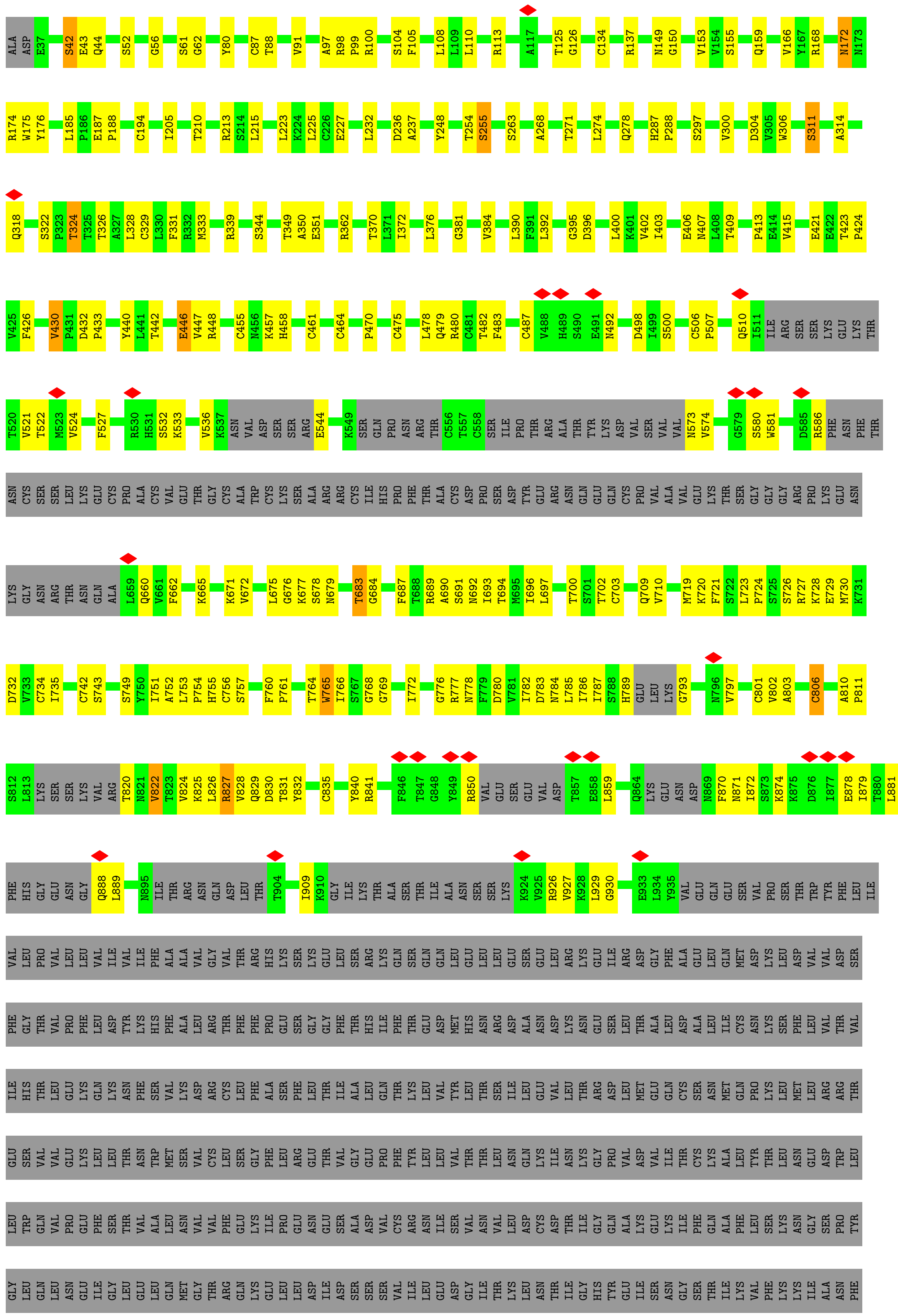
• Molecule 1: Semaphorin-like protein 139

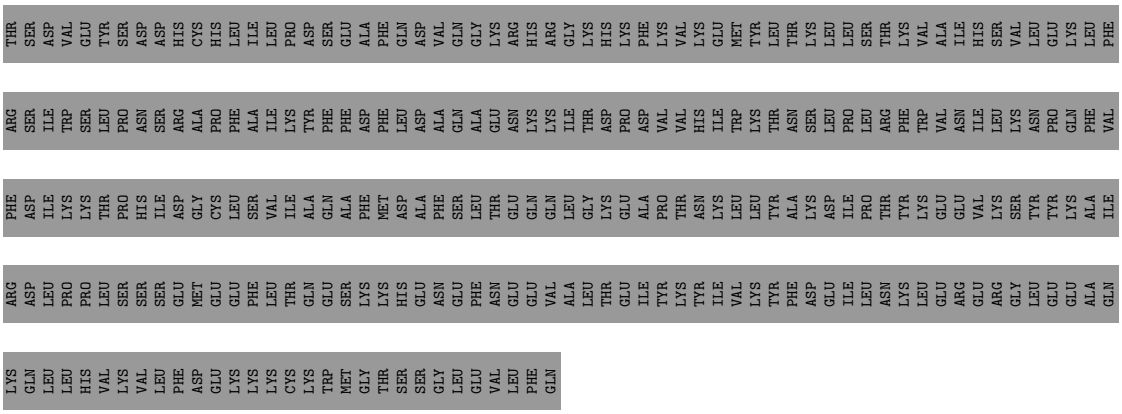
Chain C:



• Molecule 2: Plexin-C1

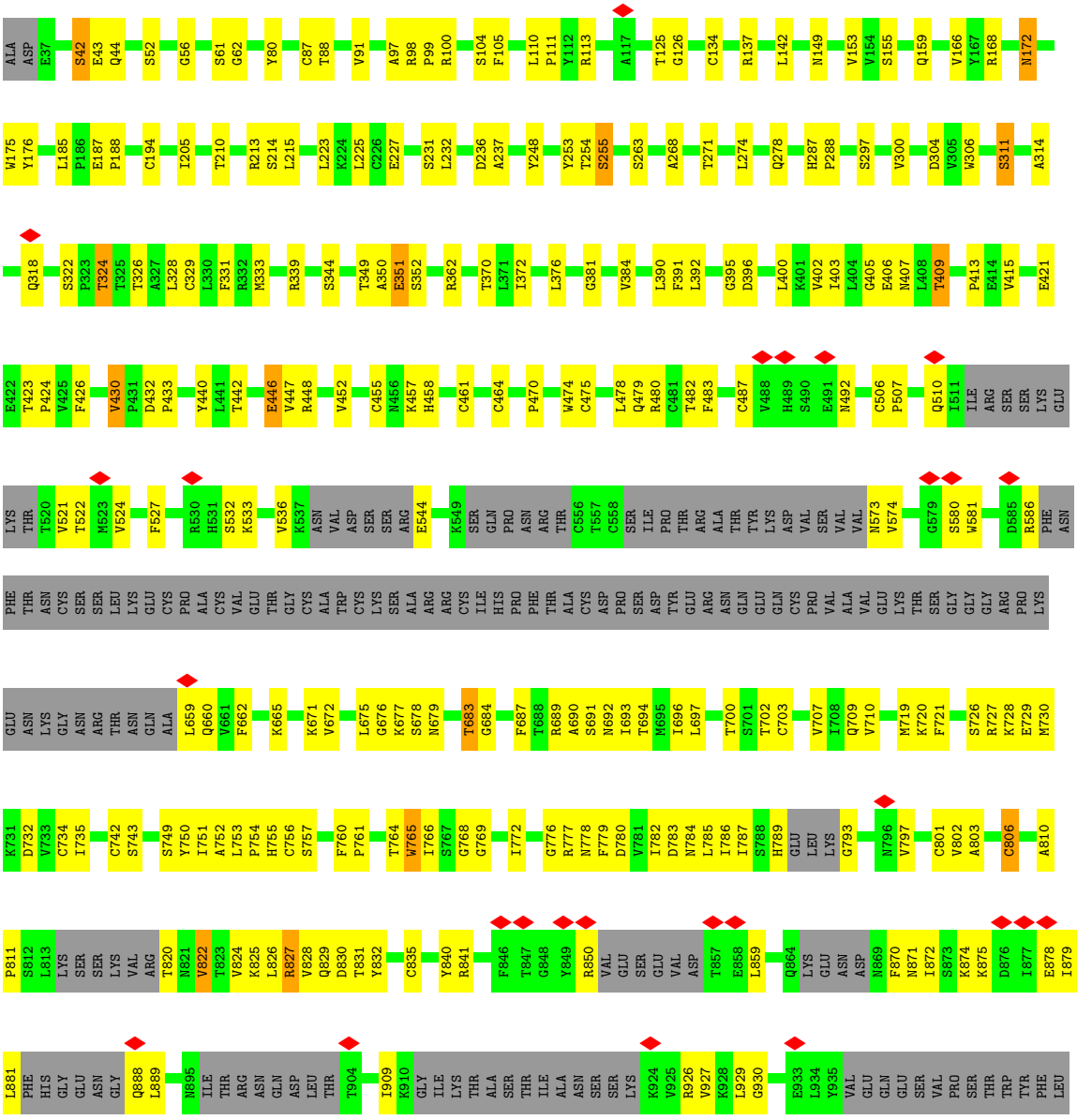
Chain B:

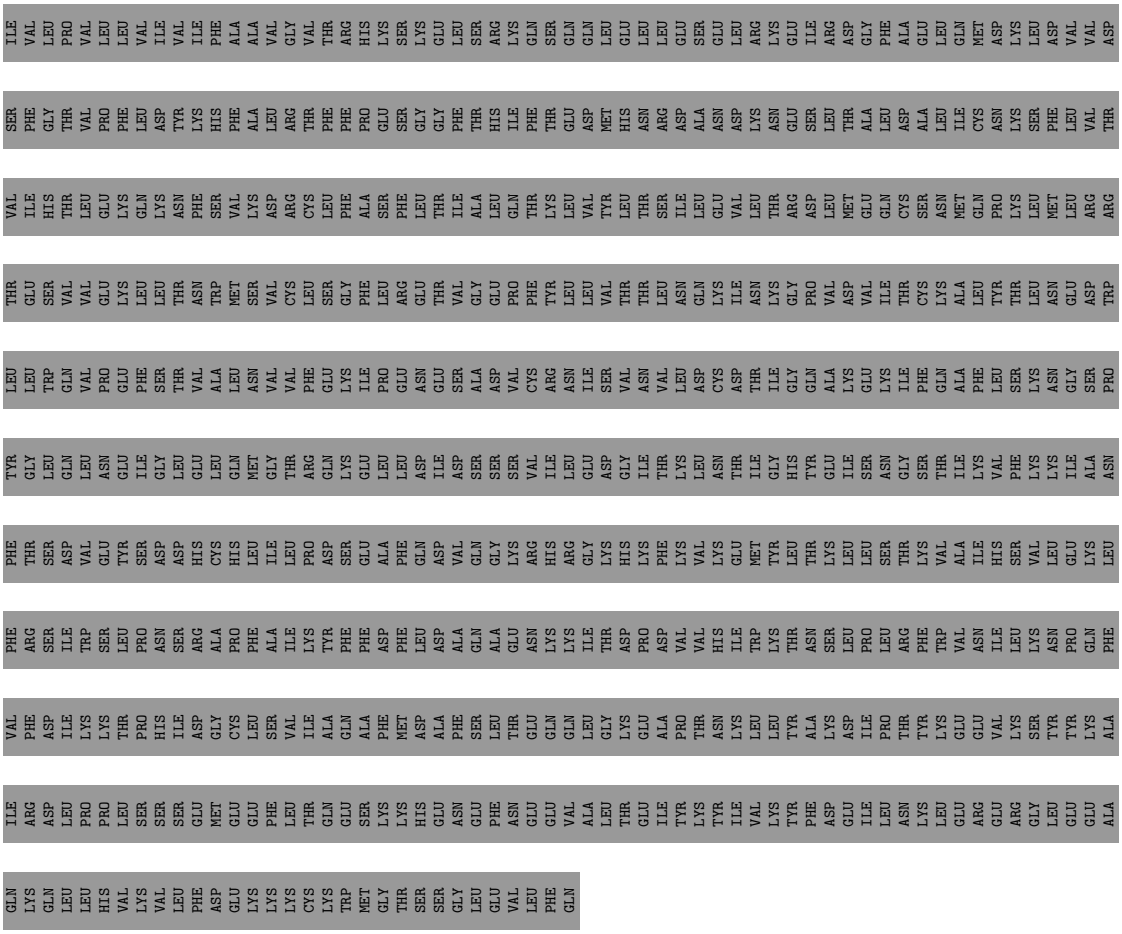

ALA ASP E37 S42 E43 Q44 S52 G56 S61 G62 Y80 C87 T88 V91 A97 R98 P99 R100 S104 F105 L108 L109 L110 R113 A117 T125 G126 C134 R137 N149 G150 V153 V154 S155 Q159 V166 Y167 R168 N172 N173
R174 W175 Y176 L185 P186 E187 P188 C194 I205 T210 R213 S214 L215 L223 K224 L225 C226 E227 L232 D236 A237 Y248 T254 S255 S263 A268 T271 L274 Q278 H287 P288 S297 V300 D304 V305 W306 S311 A314
Q318 S322 P323 T324 T325 T326 A327 L328 C329 L330 F331 R332 M333 R339 S344 T349 A350 E351 R362 T370 L371 I372 L376 G381 V384 L390 F391 L392 G395 D396 L400 K401 V402 I403 E406 N407 L408 T409 P413 E414 V415 E421 E422 T423 P424
V425 F426 V430 P431 D432 P433 Y440 L441 T442 E446 V447 R448 C455 N456 K457 H458 C461 C464 P470 C475 L478 Q479 R480 C481 T482 F483 C487 V488 H489 S490 E491 N492 D498 I499 S500 C506 P507 Q510 I511 ILE ARG SER SER LYS GLU LYS THR
T520 V521 T522 M523 V524 F527 R530 H531 S532 K533 V536 K537 ASN VAL ASP SER SER ARG E544 K549 SER GLN PRO ASN ARG THR C556 T557 C558 SER ILE PRO THR ARG ALA THR TYR LYS ASP VAL SER VAL VAL N573 V574 G579 S580 W581 D585 R586 PHE ASN PHE THR
ASN CYS SER SER LEU LYS GLU CYS PRO ALA CYS VAL GLU THR GLY CYS ALA TRP CYS LYS SER ALA ARG ARG CYS ILE HIS PRO PHE THR ALA CYS ASP PRO SER ASP TYR GLU ARG ASN GLN GLU GLN CYS PRO VAL ALA VAL GLU LYS THR SER GLY GLY GLY ARG PRO LYS GLU ASN
LYS GLY ASN ARG THR ASN GLN ALA L659 Q660 V661 F662 K665 K671 V672 L675 G676 K677 S678 N679 T683 G684 F687 T688 R689 A690 S691 N692 I693 T694 M695 I696 L697 T700 S701 T702 C703 Q709 V710 M719 K720 F721 S722 L723 P724 S725 S726 R727 K728 E729 M730 K731
D732 V733 C734 I735 C742 S743 S749 Y750 I751 A752 L753 P754 H755 C756 S757 F760 P761 T764 W765 I766 S767 G768 G769 I772 G776 R777 N778 F779 D780 V781 I782 D783 N784 L785 I786 I787 S788 H789 GLU LEU LYS G793 N796 V797 C801 V802 A803 C806 A810 P811
S812 L813 LYS SER SER LYS VAL ARG T820 N821 V822 T823 V824 K825 L826 R827 V828 Q829 D830 T831 Y832 C835 Y840 R841 F846 T847 G848 Y849 R850 VAL GLU SER GLU VAL ASP T857 E858 L859 Q864 LYS GLU ASN ASP N869 F870 N871 I872 S873 K874 K875 D876 I877 E878 I879 T880 L881
PHE HIS GLY GLU ASN GLY Q888 L889 N895 ILE THR ARG ASN GLN ASP LEU THR T904 I909 K910 GLY ILE LYS THR ALA SER THR ILE ALA ASN SER SER LYS K924 V925 R926 V927 K928 L929 G930 E933 L934 Y935 VAL GLU GLN GLU SER VAL PRO SER THR TRP TYR PHE LEU ILE
VAL LEU PRO VAL LEU LEU VAL ILE VAL ILE PHE ALA ALA VAL GLY VAL THR ARG HIS LYS SER LYS GLU LEU SER ARG LYS GLN SER GLN GLN LEU GLU LEU LEU GLU SER GLU LEU ARG LYS GLU ILE ARG ASP GLY PHE ALA GLU LEU GLN MET ASP LYS LEU ASP VAL VAL ASP SER
PHE GLY THR VAL PRO PHE LEU ASP TYR LYS HIS PHE ALA LEU ARG THR PHE PHE PRO GLU SER GLY GLY PHE THR HIS ILE PHE THR GLU ASP MET HIS ASN ARG ASP ALA ASN ASP LYS ASN GLU SER LEU THR ALA LEU ASP ALA LEU ILE CYS ASN LYS SER PHE LEU VAL THR VAL
ILE HIS THR LEU GLU LYS GLN LYS ASN PHE SER VAL LYS ASP ARG CYS LEU PHE ALA SER PHE LEU THR ILE ALA LEU GLN THR LYS LEU VAL TYR LEU THR SER ILE LEU GLU VAL LEU THR ARG ASP LEU MET GLU GLN CYS SER ASN MET GLN PRO LYS LEU MET LEU ARG ARG THR
GLU SER VAL VAL GLU LYS LEU LEU THR ASN TRP MET SER VAL CYS LEU SER GLY PHE LEU ARG GLU THR VAL GLY GLU PRO PHE TYR LEU LEU VAL THR THR LEU ASN GLN LYS ILE ASN LYS GLY PRO VAL ASP VAL ILE THR CYS LYS ALA LEU TYR THR LEU ASN GLU ASP TRP LEU
LEU TRP GLN VAL PRO GLU PHE SER THR VAL ALA LEU ASN VAL VAL PHE GLU LYS ILE PRO GLU ASN GLU SER ALA ASP VAL CYS ARG ASN ILE SER VAL ASN VAL LEU ASP CYS ASP THR ILE GLY GLN ALA LYS GLU LYS ILE PHE GLN ALA PHE LEU SER LYS ASN GLY SER PRO TYR
GLY LEU GLN LEU ASN GLU ILE GLY LEU GLU LEU GLN MET GLY THR ARG GLN LYS GLU LEU LEU ASP ILE ASP SER SER SER VAL ILE LEU GLU ASP GLY ILE THR LYS LEU ASN THR ILE GLY HIS TYR GLU ILE SER ASN GLY SER THR ILE LYS VAL PHE LYS LYS ILE ALA ASN PHE



• Molecule 2: Plexin-C1

Chain D:




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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	143750	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 ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/3093	0.53	0/4195
1	C	0.67	0/3093	0.53	0/4195
2	B	0.52	0/5663	0.52	1/7689 (0.0%)
2	D	0.52	0/5663	0.52	1/7689 (0.0%)
All	All	0.58	0/17512	0.53	2/23768 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	806	CYS	CA-CB-SG	6.76	126.17	114.00
2	B	806	CYS	CA-CB-SG	6.74	126.13	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	0	2956	88	0
1	C	3022	0	2956	86	0
2	B	5561	0	5301	167	0
2	D	5561	0	5301	174	0
3	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	112	0	104	4	0
3	C	14	0	13	0	0
3	D	112	0	104	4	0
All	All	17418	0	16748	511	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 15.

All (511) 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)
2:D:507:PRO:HA	2:D:524:VAL:O	1.45	1.14
2:B:507:PRO:HA	2:B:524:VAL:O	1.45	1.12
2:D:536:VAL:O	2:D:544:GLU:HA	1.62	0.99
2:B:536:VAL:O	2:B:544:GLU:HA	1.62	0.99
2:B:783:ASP:H	2:B:828:VAL:HG12	1.43	0.82
2:D:783:ASP:H	2:D:828:VAL:HG12	1.43	0.82
2:B:402:VAL:HG12	2:B:413:PRO:HB3	1.71	0.73
2:D:402:VAL:HG12	2:D:413:PRO:HB3	1.71	0.72
2:B:446:GLU:OE1	2:B:448:ARG:NH2	2.23	0.71
2:D:510:GLN:O	2:D:521:VAL:HA	1.91	0.71
2:B:510:GLN:O	2:B:521:VAL:HA	1.90	0.71
1:C:36:LEU:HB3	1:C:47:PHE:HB3	1.73	0.71
1:A:345:ILE:HD11	1:A:369:LEU:HD22	1.73	0.70
2:B:430:VAL:HG23	2:B:440:TYR:HB2	1.73	0.70
1:C:345:ILE:HD11	1:C:369:LEU:HD22	1.73	0.70
2:D:430:VAL:HG23	2:D:440:TYR:HB2	1.73	0.70
1:C:44:VAL:HG21	1:C:75:VAL:HG11	1.74	0.69
1:C:331:LYS:HB2	1:C:374:VAL:HG11	1.73	0.69
2:D:446:GLU:OE1	2:D:448:ARG:NH2	2.23	0.69
1:A:36:LEU:HB3	1:A:47:PHE:HB3	1.73	0.69
1:A:331:LYS:HB2	1:A:374:VAL:HG11	1.73	0.69
1:A:44:VAL:HG21	1:A:75:VAL:HG11	1.74	0.67
2:B:98:ARG:NH1	2:B:395:GLY:O	2.28	0.67
1:A:216:GLU:HB2	1:A:310:ILE:HD11	1.77	0.66
2:B:44:GLN:HE21	2:B:88:THR:HA	1.59	0.66
2:D:827:ARG:HH21	2:D:830:ASP:H	1.43	0.66
1:C:216:GLU:HB2	1:C:310:ILE:HD11	1.77	0.66
2:B:311:SER:HB2	2:B:326:THR:HG22	1.78	0.66
2:D:98:ARG:NH1	2:D:395:GLY:O	2.28	0.66
1:A:73:THR:O	1:A:73:THR:OG1	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:GLN:HE21	2:D:88:THR:HA	1.59	0.65
1:A:214:GLU:OE2	1:C:181:ARG:NH2	2.27	0.65
1:C:60:ASN:HD22	1:C:80:ASN:HB2	1.61	0.65
2:D:311:SER:HB2	2:D:326:THR:HG22	1.78	0.65
2:B:827:ARG:HH21	2:B:830:ASP:H	1.43	0.65
2:D:784:ASN:HD21	2:D:827:ARG:HH11	1.45	0.65
1:A:60:ASN:HD22	1:A:80:ASN:HB2	1.60	0.65
2:D:700:THR:HG22	2:D:702:THR:H	1.62	0.65
2:B:784:ASN:HD21	2:B:827:ARG:HH11	1.45	0.64
1:A:283:PRO:HB3	1:A:301:ILE:HD13	1.79	0.64
2:D:175:TRP:O	2:D:210:THR:OG1	2.12	0.64
1:A:369:LEU:HD23	1:A:382:ALA:HB2	1.79	0.64
1:C:369:LEU:HD23	1:C:382:ALA:HB2	1.79	0.64
2:B:700:THR:HG22	2:B:702:THR:H	1.63	0.64
1:C:283:PRO:HB3	1:C:301:ILE:HD13	1.79	0.64
1:C:127:GLU:HB3	2:D:350:ALA:HB1	1.80	0.64
1:A:116:GLU:HB2	1:A:138:PRO:HG2	1.79	0.63
2:D:766:ILE:N	2:D:841:ARG:O	2.25	0.63
1:C:116:GLU:HB2	1:C:138:PRO:HG2	1.79	0.63
2:B:205:ILE:HD12	2:B:223:LEU:HD23	1.80	0.63
1:C:48:SER:O	1:C:51:GLU:HB2	1.98	0.63
1:A:24:GLU:OE2	1:A:45:TYR:OH	2.16	0.63
2:D:726:SER:OG	2:D:727:ARG:N	2.32	0.63
1:A:48:SER:O	1:A:51:GLU:HB2	1.98	0.62
1:A:181:ARG:HD2	1:C:225:ARG:NH2	2.14	0.62
2:B:766:ILE:N	2:B:841:ARG:O	2.25	0.62
1:A:333:LYS:HE3	1:A:341:ARG:HH21	1.64	0.62
2:D:780:ASP:N	2:D:780:ASP:OD1	2.30	0.62
2:B:726:SER:OG	2:B:727:ARG:N	2.32	0.62
2:B:780:ASP:OD1	2:B:780:ASP:N	2.30	0.62
1:C:333:LYS:HE3	1:C:341:ARG:HH21	1.64	0.62
1:C:24:GLU:OE2	1:C:45:TYR:OH	2.16	0.62
1:C:236:ASP:OD2	1:C:338:ARG:NH2	2.32	0.62
2:D:104:SER:OG	2:D:105:PHE:N	2.32	0.61
2:D:205:ILE:HD12	2:D:223:LEU:HD23	1.80	0.61
2:D:442:THR:HG23	2:D:447:VAL:HG22	1.82	0.61
2:B:442:THR:HG23	2:B:447:VAL:HG22	1.82	0.61
1:C:247:SER:OG	1:C:251:LYS:O	2.18	0.61
1:A:236:ASP:OD2	1:A:338:ARG:NH2	2.32	0.61
2:D:227:GLU:OE1	2:D:227:GLU:N	2.33	0.61
2:B:475:CYS:O	2:B:479:GLN:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:HIS:ND1	2:D:324:THR:O	2.34	0.61
1:A:247:SER:OG	1:A:251:LYS:O	2.18	0.61
2:D:660:GLN:NE2	2:D:689:ARG:O	2.34	0.60
2:D:889:LEU:HA	2:D:909:ILE:HG12	1.83	0.60
2:B:660:GLN:NE2	2:B:689:ARG:O	2.34	0.60
2:D:324:THR:O	2:D:324:THR:OG1	2.19	0.60
2:B:104:SER:OG	2:B:105:PHE:N	2.32	0.60
2:B:175:TRP:O	2:B:210:THR:OG1	2.12	0.60
1:C:70:VAL:HG23	1:C:71:GLU:H	1.67	0.60
2:D:475:CYS:O	2:D:479:GLN:N	2.34	0.60
1:A:246:ASP:OD1	1:A:247:SER:N	2.34	0.60
1:C:246:ASP:OD1	1:C:247:SER:N	2.34	0.60
2:B:287:HIS:ND1	2:B:324:THR:O	2.34	0.60
1:C:73:THR:O	1:C:73:THR:OG1	2.14	0.59
2:D:789:HIS:O	2:D:793:GLY:N	2.36	0.59
2:B:889:LEU:HA	2:B:909:ILE:HG12	1.83	0.59
2:D:42:SER:OG	2:D:43:GLU:N	2.35	0.59
1:A:70:VAL:HG23	1:A:71:GLU:H	1.67	0.59
2:B:42:SER:OG	2:B:43:GLU:N	2.35	0.58
1:A:225:ARG:NH2	1:C:181:ARG:HD2	2.19	0.58
2:B:789:HIS:O	2:B:793:GLY:N	2.36	0.58
2:D:700:THR:OG1	2:D:729:GLU:OE2	2.16	0.58
1:A:309:ASP:OD1	1:A:310:ILE:N	2.35	0.58
2:B:227:GLU:OE1	2:B:227:GLU:N	2.33	0.58
1:A:60:ASN:OD1	1:A:60:ASN:N	2.38	0.57
2:B:324:THR:O	2:B:324:THR:OG1	2.19	0.57
1:C:309:ASP:OD1	1:C:310:ILE:N	2.35	0.57
2:B:172:ASN:OD1	2:B:172:ASN:N	2.36	0.57
2:D:172:ASN:OD1	2:D:172:ASN:N	2.36	0.57
1:A:266:PHE:HA	1:A:307:LEU:HD11	1.87	0.57
1:C:220:ASP:OD1	1:C:222:ARG:NH2	2.38	0.57
2:D:44:GLN:N	2:D:44:GLN:OE1	2.38	0.57
2:B:784:ASN:ND2	2:B:827:ARG:HH11	2.02	0.57
1:A:127:GLU:HB3	2:B:350:ALA:HB1	1.87	0.56
1:A:220:ASP:OD1	1:A:222:ARG:NH2	2.38	0.56
2:B:44:GLN:N	2:B:44:GLN:OE1	2.38	0.56
2:D:696:ILE:HB	2:D:734:CYS:SG	2.46	0.56
2:B:730:MET:HA	2:B:749:SER:HA	1.87	0.56
1:C:333:LYS:NZ	1:C:354:ASP:OD2	2.26	0.56
2:B:696:ILE:HB	2:B:734:CYS:SG	2.46	0.56
1:C:132:TRP:NE1	1:C:191:MET:SD	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:784:ASN:ND2	2:D:827:ARG:HH11	2.02	0.56
1:A:132:TRP:NE1	1:A:191:MET:SD	2.78	0.56
1:C:266:PHE:HA	1:C:307:LEU:HD11	1.87	0.55
2:B:326:THR:HG21	2:B:376:LEU:H	1.71	0.55
2:D:326:THR:HG21	2:D:376:LEU:H	1.71	0.55
2:B:766:ILE:HA	2:B:840:TYR:HB3	1.88	0.55
2:D:421:GLU:N	2:D:421:GLU:OE1	2.40	0.55
2:B:784:ASN:HD21	2:B:827:ARG:HD3	1.72	0.55
2:D:300:VAL:HG22	2:D:381:GLY:HA3	1.89	0.55
2:D:783:ASP:HB2	2:D:828:VAL:HA	1.89	0.55
2:D:785:LEU:HD11	2:D:824:VAL:HB	1.89	0.55
1:C:46:THR:OG1	1:C:53:ASN:O	2.24	0.55
2:D:730:MET:HA	2:D:749:SER:HA	1.88	0.55
2:B:783:ASP:HB2	2:B:828:VAL:HA	1.89	0.55
1:C:60:ASN:OD1	1:C:60:ASN:N	2.37	0.55
2:B:421:GLU:OE1	2:B:421:GLU:N	2.40	0.55
2:B:786:ILE:HG13	2:B:832:TYR:HE1	1.72	0.55
1:C:44:VAL:HG22	1:C:64:ILE:HG21	1.89	0.54
1:C:375:THR:OG1	1:C:376:SER:N	2.41	0.54
2:D:784:ASN:HD21	2:D:827:ARG:HD3	1.72	0.54
1:A:222:ARG:NH1	1:A:320:GLU:OE1	2.41	0.54
2:B:110:LEU:HD11	2:B:166:VAL:HG13	1.90	0.54
2:D:766:ILE:HA	2:D:840:TYR:HB3	1.88	0.54
2:D:786:ILE:HG13	2:D:832:TYR:HE1	1.72	0.54
2:B:660:GLN:OE1	2:B:660:GLN:N	2.39	0.54
2:D:52:SER:OG	2:D:56:GLY:O	2.25	0.54
2:D:110:LEU:HD11	2:D:166:VAL:HG13	1.90	0.54
2:D:820:THR:N	2:D:840:TYR:O	2.41	0.54
2:D:827:ARG:HA	2:D:831:THR:O	2.08	0.54
1:C:45:TYR:CE2	1:C:54:LYS:HB2	2.43	0.53
2:D:660:GLN:OE1	2:D:660:GLN:N	2.40	0.53
2:B:785:LEU:HD11	2:B:824:VAL:HB	1.89	0.53
2:D:403:ILE:HD13	2:D:470:PRO:HD3	1.90	0.53
2:B:300:VAL:HG22	2:B:381:GLY:HA3	1.89	0.53
2:B:573:ASN:HA	2:B:586:ARG:HA	1.90	0.53
2:D:573:ASN:HA	2:D:586:ARG:HA	1.90	0.53
1:C:222:ARG:NH1	1:C:320:GLU:OE1	2.41	0.53
1:A:44:VAL:HG22	1:A:64:ILE:HG21	1.89	0.53
2:B:403:ILE:HD13	2:B:470:PRO:HD3	1.90	0.53
1:A:375:THR:OG1	1:A:376:SER:N	2.41	0.53
2:B:820:THR:N	2:B:840:TYR:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD23	1:A:291:LYS:HB3	1.91	0.53
1:C:228:ILE:HD11	1:C:246:ASP:HB2	1.90	0.53
2:B:785:LEU:HD12	2:B:786:ILE:H	1.74	0.53
2:D:785:LEU:HD12	2:D:786:ILE:H	1.74	0.53
1:A:45:TYR:CE2	1:A:54:LYS:HB2	2.43	0.53
2:B:52:SER:OG	2:B:56:GLY:O	2.25	0.53
2:B:782:ILE:HD11	2:B:826:LEU:HD13	1.91	0.53
3:B:1608:NAG:H83	3:B:1608:NAG:H3	1.91	0.53
2:D:98:ARG:HH11	2:D:424:PRO:HB3	1.74	0.53
2:D:782:ILE:HD11	2:D:826:LEU:HD13	1.91	0.53
1:C:220:ASP:HB2	1:C:222:ARG:HE	1.73	0.52
2:B:492:ASN:OD1	2:B:492:ASN:N	2.42	0.52
2:B:536:VAL:O	2:B:544:GLU:CA	2.48	0.52
2:D:390:LEU:HB2	2:D:402:VAL:HG22	1.91	0.52
1:C:287:LEU:HD23	1:C:291:LYS:HB3	1.91	0.52
2:B:827:ARG:HA	2:B:831:THR:O	2.08	0.52
1:A:46:THR:OG1	1:A:53:ASN:O	2.24	0.52
1:A:220:ASP:HB2	1:A:222:ARG:HE	1.73	0.52
2:D:678:SER:OG	2:D:679:ASN:OD1	2.25	0.52
3:D:1604:NAG:O7	3:D:1604:NAG:O3	2.25	0.52
3:D:1608:NAG:H83	3:D:1608:NAG:H3	1.91	0.52
2:B:44:GLN:NE2	2:B:87:CYS:O	2.43	0.52
2:B:765:TRP:HZ3	2:B:930:GLY:HA3	1.75	0.52
2:D:44:GLN:NE2	2:D:87:CYS:O	2.43	0.52
2:D:675:LEU:HD12	2:D:753:LEU:HD21	1.92	0.52
2:D:824:VAL:HG23	2:D:835:CYS:HB2	1.92	0.52
1:A:228:ILE:HD11	1:A:246:ASP:HB2	1.90	0.52
2:B:870:PHE:HB2	2:B:872:ILE:HD11	1.92	0.52
2:D:492:ASN:OD1	2:D:492:ASN:N	2.42	0.52
2:D:870:PHE:HB2	2:D:872:ILE:HD11	1.92	0.52
2:B:98:ARG:HH11	2:B:424:PRO:HB3	1.74	0.52
2:B:268:ALA:HB3	2:B:274:LEU:HB3	1.91	0.51
2:D:761:PRO:HG2	2:D:772:ILE:HD13	1.92	0.51
1:A:27:ILE:HD13	1:A:63:TYR:HB3	1.92	0.51
2:B:824:VAL:HG23	2:B:835:CYS:HB2	1.92	0.51
1:C:19:LYS:HA	1:C:385:GLY:HA3	1.93	0.51
1:C:27:ILE:HD13	1:C:63:TYR:HB3	1.92	0.51
2:B:344:SER:HB2	2:B:349:THR:OG1	2.11	0.51
2:B:761:PRO:HG2	2:B:772:ILE:HD13	1.92	0.51
2:D:268:ALA:HB3	2:D:274:LEU:HB3	1.91	0.51
1:A:298:PHE:HA	1:A:301:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:700:THR:OG1	2:B:729:GLU:OE2	2.16	0.51
2:B:580:SER:HG	2:B:581:TRP:HD1	1.57	0.51
2:B:675:LEU:HD12	2:B:753:LEU:HD21	1.92	0.51
1:C:16:GLU:OE1	1:C:18:HIS:NE2	2.43	0.51
2:B:390:LEU:HB2	2:B:402:VAL:HG22	1.91	0.51
2:D:765:TRP:HZ3	2:D:930:GLY:HA3	1.75	0.51
2:D:872:ILE:HD12	2:D:872:ILE:H	1.75	0.51
2:B:694:THR:HG22	2:B:709:GLN:HE22	1.76	0.50
2:B:872:ILE:HD12	2:B:872:ILE:H	1.75	0.50
1:C:349:THR:OG1	1:C:364:GLN:OE1	2.29	0.50
1:A:16:GLU:OE1	1:A:18:HIS:NE2	2.43	0.50
2:D:344:SER:HB2	2:D:349:THR:OG1	2.11	0.50
1:C:79:ASN:OD1	1:C:84:LYS:HB3	2.11	0.50
1:C:298:PHE:HA	1:C:301:ILE:HG22	1.93	0.50
1:A:72:ASP:HB2	1:A:87:LYS:HD2	1.93	0.50
1:A:79:ASN:OD1	1:A:84:LYS:HB3	2.11	0.50
1:A:349:THR:OG1	1:A:364:GLN:OE1	2.29	0.50
1:C:72:ASP:HB2	1:C:87:LYS:HD2	1.93	0.50
1:A:19:LYS:HA	1:A:385:GLY:HA3	1.93	0.50
2:B:820:THR:O	2:B:840:TYR:N	2.41	0.50
2:D:91:VAL:HG22	2:D:105:PHE:HZ	1.77	0.50
2:D:871:ASN:HB3	3:D:1608:NAG:O5	2.11	0.50
2:B:802:VAL:HG22	2:B:803:ALA:H	1.77	0.49
1:C:236:ASP:OD1	1:C:236:ASP:N	2.43	0.49
2:D:755:HIS:CE1	2:D:777:ARG:HB2	2.47	0.49
2:D:802:VAL:HG22	2:D:803:ALA:H	1.77	0.49
2:B:678:SER:OG	2:B:679:ASN:OD1	2.25	0.49
2:D:694:THR:HG22	2:D:709:GLN:HE22	1.76	0.49
2:D:407:ASN:OD1	2:D:407:ASN:N	2.36	0.49
2:D:580:SER:HG	2:D:581:TRP:HD1	1.59	0.49
2:B:532:SER:OG	2:B:533:LYS:N	2.46	0.49
2:D:879:ILE:HA	2:D:926:ARG:O	2.12	0.49
1:A:218:ASP:OD1	1:A:218:ASP:N	2.45	0.49
2:B:871:ASN:HB3	3:B:1608:NAG:O5	2.11	0.49
2:B:764:THR:O	2:B:840:TYR:HA	2.13	0.49
1:C:224:TYR:OH	1:C:320:GLU:OE2	2.20	0.49
2:B:879:ILE:HA	2:B:926:ARG:O	2.12	0.49
1:A:60:ASN:ND2	1:A:80:ASN:HB2	2.28	0.49
2:B:755:HIS:CE1	2:B:777:ARG:HB2	2.47	0.48
2:D:764:THR:O	2:D:840:TYR:HA	2.13	0.48
1:A:236:ASP:N	1:A:236:ASP:OD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ASP:N	1:C:218:ASP:OD1	2.45	0.48
1:C:372:VAL:HG22	1:C:380:PHE:HD1	1.78	0.48
2:D:532:SER:OG	2:D:533:LYS:N	2.46	0.48
2:D:679:ASN:HB3	2:D:720:LYS:HE2	1.94	0.48
2:D:697:LEU:HA	2:D:732:ASP:O	2.13	0.48
2:B:697:LEU:HA	2:B:732:ASP:O	2.13	0.48
2:D:457:LYS:HE3	2:D:458:HIS:CE1	2.49	0.48
1:A:372:VAL:HG22	1:A:380:PHE:HD1	1.78	0.48
2:B:407:ASN:OD1	2:B:407:ASN:N	2.36	0.48
2:B:679:ASN:HB3	2:B:720:LYS:HE2	1.94	0.48
1:C:33:ASP:N	1:C:33:ASP:OD2	2.47	0.48
1:A:264:HIS:CE1	1:A:268:THR:HG21	2.49	0.48
2:B:874:LYS:HG2	2:B:889:LEU:HD22	1.96	0.48
1:C:264:HIS:CE1	1:C:268:THR:HG21	2.49	0.48
2:D:660:GLN:HE21	2:D:689:ARG:HB3	1.78	0.48
2:D:761:PRO:HD2	2:D:772:ILE:HG23	1.94	0.48
1:A:201:SER:OG	2:B:215:LEU:O	2.17	0.48
2:B:91:VAL:HG22	2:B:105:PHE:HZ	1.77	0.48
1:C:201:SER:OG	2:D:215:LEU:O	2.22	0.48
1:A:181:ARG:NH2	1:C:214:GLU:OE2	2.38	0.48
2:B:457:LYS:HE3	2:B:458:HIS:CE1	2.49	0.47
1:C:26:ILE:HD13	1:C:40:VAL:HG23	1.96	0.47
1:C:60:ASN:ND2	1:C:80:ASN:HB2	2.28	0.47
1:C:280:SER:OG	1:C:281:PRO:HD3	2.14	0.47
1:A:168:LYS:HE2	1:A:286:CYS:SG	2.55	0.47
1:A:280:SER:OG	1:A:281:PRO:HD3	2.14	0.47
2:B:761:PRO:HD2	2:B:772:ILE:HG23	1.94	0.47
3:B:1604:NAG:O7	3:B:1604:NAG:O3	2.25	0.47
2:D:536:VAL:O	2:D:544:GLU:CA	2.48	0.47
2:D:874:LYS:HG2	2:D:889:LEU:HD22	1.96	0.47
1:A:216:GLU:HG3	1:A:218:ASP:OD1	2.15	0.47
1:A:235:THR:OG1	1:A:238:ASP:O	2.20	0.47
2:B:765:TRP:O	2:B:768:GLY:N	2.45	0.47
1:C:68:ILE:HG21	1:C:111:ILE:HG12	1.96	0.47
1:A:26:ILE:HD13	1:A:40:VAL:HG23	1.96	0.47
1:A:37:TYR:CE1	1:A:46:THR:HG22	2.50	0.47
2:B:324:THR:HB	2:B:372:ILE:HG21	1.97	0.47
2:B:676:GLY:O	2:B:829:GLN:HG3	2.15	0.47
2:B:660:GLN:HE21	2:B:689:ARG:HB3	1.78	0.47
2:B:536:VAL:HG12	2:B:574:VAL:HG13	1.96	0.47
1:C:37:TYR:CE1	1:C:46:THR:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LYS:HE2	1:C:286:CYS:SG	2.55	0.47
2:D:671:LYS:NZ	2:D:780:ASP:OD2	2.48	0.47
2:D:676:GLY:O	2:D:829:GLN:HG3	2.15	0.47
2:D:765:TRP:O	2:D:768:GLY:N	2.45	0.47
2:B:99:PRO:HG2	2:B:314:ALA:HB3	1.97	0.47
2:B:580:SER:OG	2:B:581:TRP:HD1	1.98	0.47
2:B:671:LYS:NZ	2:B:780:ASP:OD2	2.48	0.47
2:B:98:ARG:NH2	2:B:318:GLN:OE1	2.46	0.47
2:B:475:CYS:O	2:B:479:GLN:CA	2.63	0.46
2:D:99:PRO:HG2	2:D:314:ALA:HB3	1.97	0.46
2:D:426:PHE:HB3	2:D:442:THR:HB	1.97	0.46
2:D:580:SER:OG	2:D:581:TRP:HD1	1.98	0.46
1:C:216:GLU:HG3	1:C:218:ASP:OD1	2.15	0.46
2:B:841:ARG:HB2	2:B:870:PHE:CZ	2.51	0.46
2:D:475:CYS:O	2:D:479:GLN:CA	2.63	0.46
2:D:841:ARG:HB2	2:D:870:PHE:CZ	2.51	0.46
1:A:33:ASP:OD2	1:A:33:ASP:N	2.47	0.46
2:B:108:LEU:HD23	2:B:108:LEU:HA	1.66	0.46
1:A:68:ILE:HG21	1:A:111:ILE:HG12	1.96	0.46
2:D:324:THR:HB	2:D:372:ILE:HG21	1.97	0.46
2:D:153:VAL:HG21	2:D:215:LEU:HD12	1.98	0.46
2:D:536:VAL:HG12	2:D:574:VAL:HG13	1.96	0.46
2:B:426:PHE:HB3	2:B:442:THR:HB	1.97	0.46
1:C:40:VAL:HG12	1:C:43:ALA:O	2.16	0.46
1:A:40:VAL:HG12	1:A:43:ALA:O	2.16	0.46
2:B:787:ILE:HG22	2:B:822:VAL:HG21	1.98	0.46
1:C:15:ILE:HA	1:C:388:VAL:O	2.16	0.45
2:D:751:ILE:HD13	2:D:751:ILE:HA	1.85	0.45
2:B:236:ASP:OD1	2:B:237:ALA:N	2.47	0.45
2:B:248:TYR:OH	2:B:278:GLN:NE2	2.49	0.45
2:D:446:GLU:HB2	2:D:448:ARG:HH21	1.82	0.45
1:C:349:THR:HG23	1:C:363:ALA:O	2.17	0.45
2:D:827:ARG:NH2	2:D:830:ASP:H	2.13	0.45
1:A:15:ILE:HA	1:A:388:VAL:O	2.16	0.45
2:B:287:HIS:CG	2:B:288:PRO:HD2	2.52	0.45
1:C:372:VAL:HG22	1:C:380:PHE:CD1	2.52	0.45
2:D:797:VAL:HB	2:D:811:PRO:HG3	1.98	0.45
2:B:665:LYS:N	2:B:683:THR:O	2.50	0.45
2:B:850:ARG:HA	2:B:859:LEU:HA	1.99	0.45
1:C:216:GLU:O	1:C:313:PRO:HD3	2.17	0.45
2:B:153:VAL:HG21	2:B:215:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:SER:HB2	2:B:306:TRP:HZ2	1.82	0.45
2:D:406:GLU:HG2	2:D:407:ASN:N	2.32	0.45
2:D:820:THR:O	2:D:840:TYR:N	2.41	0.45
2:B:754:PRO:HB3	2:B:778:ASN:O	2.17	0.45
2:B:769:GLY:N	2:B:810:ALA:O	2.43	0.45
2:D:98:ARG:NH2	2:D:318:GLN:OE1	2.46	0.45
2:D:248:TYR:OH	2:D:278:GLN:NE2	2.49	0.45
2:D:297:SER:HB2	2:D:306:TRP:HZ2	1.82	0.45
1:A:188:ILE:HG22	1:A:213:VAL:HG23	1.99	0.45
1:A:216:GLU:O	1:A:313:PRO:HD3	2.17	0.45
2:B:446:GLU:HB2	2:B:448:ARG:HH21	1.82	0.45
2:D:850:ARG:HA	2:D:859:LEU:HA	1.99	0.45
2:D:874:LYS:HZ1	2:D:888:GLN:N	2.15	0.45
2:B:797:VAL:HB	2:B:811:PRO:HG3	1.98	0.44
1:A:239:THR:O	1:A:259:MET:HB2	2.17	0.44
2:B:406:GLU:HG2	2:B:407:ASN:N	2.32	0.44
1:C:179:THR:OG1	1:C:180:LYS:N	2.50	0.44
2:D:287:HIS:CG	2:D:288:PRO:HD2	2.52	0.44
2:D:754:PRO:HB3	2:D:778:ASN:O	2.17	0.44
2:B:735:ILE:O	2:B:743:SER:OG	2.31	0.44
1:A:349:THR:HG23	1:A:363:ALA:O	2.17	0.44
2:D:665:LYS:N	2:D:683:THR:O	2.50	0.44
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.66	0.44
1:A:372:VAL:HG22	1:A:380:PHE:CD1	2.52	0.44
2:B:225:LEU:HD11	2:B:232:LEU:HD22	1.99	0.44
2:B:874:LYS:HZ1	2:B:888:GLN:N	2.15	0.44
2:D:80:TYR:CD2	2:D:87:CYS:HB3	2.53	0.44
2:D:787:ILE:HG22	2:D:822:VAL:HG21	1.98	0.44
1:C:76:CYS:HA	1:C:85:CYS:HA	1.99	0.44
2:D:405:GLY:N	2:D:409:THR:O	2.41	0.44
2:D:735:ILE:O	2:D:743:SER:OG	2.31	0.44
2:B:482:THR:OG1	2:B:483:PHE:N	2.51	0.44
2:D:351:GLU:OE2	2:D:352:SER:OG	2.29	0.44
2:B:168:ARG:HD3	2:B:175:TRP:CZ2	2.53	0.44
2:B:874:LYS:HE2	2:B:874:LYS:HB3	1.74	0.44
1:C:239:THR:O	1:C:259:MET:HB2	2.17	0.44
2:D:225:LEU:HD11	2:D:232:LEU:HD22	1.99	0.44
1:C:188:ILE:HG22	1:C:213:VAL:HG23	1.99	0.43
2:D:827:ARG:O	2:D:827:ARG:HG3	2.18	0.43
2:D:187:GLU:N	2:D:188:PRO:HD3	2.33	0.43
2:B:187:GLU:N	2:B:188:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:482:THR:OG1	2:D:483:PHE:N	2.51	0.43
2:B:691:SER:OG	2:B:692:ASN:N	2.51	0.43
2:B:723:LEU:HA	2:B:724:PRO:HD3	1.89	0.43
2:D:176:TYR:CZ	2:D:271:THR:HG23	2.53	0.43
2:D:734:CYS:HB2	2:D:742:CYS:HB3	1.47	0.43
2:B:185:LEU:HA	2:B:185:LEU:HD23	1.67	0.43
1:A:19:LYS:HB3	1:A:19:LYS:HE2	1.80	0.43
2:B:80:TYR:CD2	2:B:87:CYS:HB3	2.53	0.43
2:B:176:TYR:CZ	2:B:271:THR:HG23	2.53	0.43
2:B:752:ALA:HB3	2:B:778:ASN:ND2	2.33	0.43
2:D:168:ARG:HD3	2:D:175:TRP:CZ2	2.53	0.43
2:D:248:TYR:CZ	2:D:263:SER:HB2	2.54	0.43
1:A:179:THR:OG1	1:A:180:LYS:N	2.50	0.43
2:D:687:PHE:CD2	2:D:719:MET:HG2	2.54	0.43
2:D:694:THR:HG22	2:D:709:GLN:NE2	2.34	0.43
2:B:254:THR:OG1	2:B:255:SER:N	2.52	0.43
2:B:248:TYR:CZ	2:B:263:SER:HB2	2.54	0.43
2:B:757:SER:OG	2:B:776:GLY:HA2	2.19	0.43
2:D:304:ASP:OD1	2:D:304:ASP:N	2.51	0.43
2:D:691:SER:OG	2:D:692:ASN:N	2.51	0.43
2:D:752:ALA:HB3	2:D:778:ASN:ND2	2.33	0.43
1:A:76:CYS:HA	1:A:85:CYS:HA	1.99	0.42
1:A:171:ILE:HG13	1:A:189:ALA:HB3	2.01	0.42
1:A:298:PHE:CE2	1:A:302:GLU:HG3	2.54	0.42
2:D:61:SER:OG	2:D:62:GLY:N	2.52	0.42
2:D:874:LYS:HE2	2:D:874:LYS:HB3	1.74	0.42
1:A:127:GLU:HG3	1:A:128:GLY:H	1.84	0.42
2:D:306:TRP:HB2	2:D:333:MET:SD	2.60	0.42
2:B:304:ASP:OD1	2:B:304:ASP:N	2.51	0.42
2:B:400:LEU:HB3	2:B:415:VAL:HA	2.01	0.42
2:D:231:SER:HG	2:D:253:TYR:HD2	1.65	0.42
2:D:254:THR:OG1	2:D:255:SER:N	2.52	0.42
2:D:328:LEU:HD22	2:D:392:LEU:HD21	2.02	0.42
2:D:786:ILE:HG13	2:D:832:TYR:CE1	2.53	0.42
1:A:67:SER:HB3	1:A:75:VAL:HG22	2.01	0.42
2:B:728:LYS:HE3	2:B:752:ALA:HB2	2.01	0.42
2:B:827:ARG:HG3	2:B:827:ARG:O	2.18	0.42
2:D:396:ASP:OD1	2:D:396:ASP:N	2.53	0.42
2:D:659:LEU:HD23	2:D:659:LEU:HA	1.88	0.42
2:B:126:GLY:HA2	2:B:134:CYS:HA	2.01	0.42
2:B:461:CYS:O	2:B:464:CYS:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:THR:HG22	2:B:709:GLN:NE2	2.34	0.42
1:C:31:LEU:HD11	1:C:375:THR:HG22	2.02	0.42
1:C:171:ILE:HG13	1:C:189:ALA:HB3	2.01	0.42
2:D:126:GLY:HA2	2:D:134:CYS:HA	2.01	0.42
2:D:665:LYS:H	2:D:684:GLY:HA2	1.85	0.42
2:D:690:ALA:HB3	2:D:693:ILE:HD11	2.02	0.42
2:B:753:LEU:HD23	2:B:753:LEU:HA	1.80	0.42
1:C:127:GLU:HG3	1:C:128:GLY:H	1.84	0.42
1:C:336:GLU:OE1	1:C:356:LYS:HD2	2.19	0.42
2:D:478:LEU:HG	2:D:480:ARG:HB2	2.01	0.42
2:D:757:SER:OG	2:D:776:GLY:HA2	2.19	0.42
1:A:68:ILE:HD13	1:A:111:ILE:HD11	2.02	0.42
1:A:152:LYS:HA	1:A:152:LYS:HD3	1.88	0.42
1:A:336:GLU:OE1	1:A:356:LYS:HD2	2.19	0.42
2:B:306:TRP:HB2	2:B:333:MET:SD	2.60	0.42
2:B:396:ASP:OD1	2:B:396:ASP:N	2.53	0.42
2:D:185:LEU:HA	2:D:185:LEU:HD23	1.67	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.79	0.42
1:A:100:GLY:HA3	1:A:135:PHE:CZ	2.55	0.42
2:B:61:SER:OG	2:B:62:GLY:N	2.52	0.42
2:D:236:ASP:OD1	2:D:237:ALA:N	2.47	0.42
2:D:384:VAL:HG13	2:D:470:PRO:HB2	2.00	0.42
2:B:328:LEU:HD22	2:B:392:LEU:HD21	2.02	0.42
2:B:687:PHE:CD2	2:B:719:MET:HG2	2.54	0.42
1:C:189:ALA:HA	1:C:211:LEU:O	2.19	0.42
1:C:298:PHE:CE2	1:C:302:GLU:HG3	2.54	0.42
2:D:227:GLU:H	2:D:227:GLU:CD	2.22	0.42
2:D:728:LYS:HE3	2:D:752:ALA:HB2	2.01	0.42
1:A:189:ALA:HA	1:A:211:LEU:O	2.19	0.42
2:B:384:VAL:HG13	2:B:470:PRO:HB2	2.00	0.42
1:A:37:TYR:CD1	1:A:46:THR:HG22	2.54	0.41
2:B:326:THR:HB	2:B:376:LEU:HB2	2.03	0.41
2:B:432:ASP:HA	2:B:433:PRO:HD3	1.90	0.41
2:B:478:LEU:HG	2:B:480:ARG:HB2	2.02	0.41
2:B:825:LYS:HE3	2:B:825:LYS:HB2	1.82	0.41
1:C:37:TYR:CD1	1:C:46:THR:HG22	2.54	0.41
2:D:825:LYS:HB2	2:D:825:LYS:HE3	1.82	0.41
2:B:97:ALA:HB3	2:B:100:ARG:HD2	2.01	0.41
2:B:339:ARG:NH1	2:B:362:ARG:O	2.53	0.41
1:C:67:SER:HB3	1:C:75:VAL:HG22	2.01	0.41
2:D:248:TYR:CE1	2:D:263:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:339:ARG:NH1	2:D:362:ARG:O	2.53	0.41
2:D:400:LEU:HB3	2:D:415:VAL:HA	2.01	0.41
2:D:475:CYS:O	2:D:479:GLN:HA	2.20	0.41
2:D:662:PHE:HZ	2:D:689:ARG:O	2.04	0.41
2:B:475:CYS:O	2:B:479:GLN:HA	2.20	0.41
1:C:68:ILE:HD13	1:C:111:ILE:HD11	2.02	0.41
2:D:474:TRP:NE1	2:D:479:GLN:OE1	2.52	0.41
1:A:162:LYS:HE3	1:A:162:LYS:HB3	1.86	0.41
1:A:191:MET:HE2	1:A:210:PHE:CD2	2.56	0.41
2:D:142:LEU:HD23	2:D:142:LEU:HA	1.78	0.41
2:D:461:CYS:O	2:D:464:CYS:N	2.51	0.41
2:D:769:GLY:N	2:D:810:ALA:O	2.43	0.41
2:B:166:VAL:HA	2:B:176:TYR:O	2.21	0.41
2:B:710:VAL:HG22	2:B:721:PHE:CZ	2.55	0.41
1:A:31:LEU:HD11	1:A:375:THR:HG22	2.02	0.41
2:B:672:VAL:HG23	2:B:677:LYS:HB2	2.03	0.41
1:C:100:GLY:HA3	1:C:135:PHE:CZ	2.55	0.41
2:D:97:ALA:HB3	2:D:100:ARG:HD2	2.01	0.41
1:A:211:LEU:HG	1:A:301:ILE:HD11	2.03	0.41
1:A:287:LEU:HB3	1:A:291:LYS:HB2	2.03	0.41
2:B:159:GLN:OE1	2:B:159:GLN:N	2.48	0.41
2:B:662:PHE:HZ	2:B:689:ARG:O	2.04	0.41
2:B:690:ALA:HB3	2:B:693:ILE:HD11	2.02	0.41
2:B:764:THR:HG22	2:B:765:TRP:N	2.36	0.41
2:D:149:ASN:O	2:D:214:SER:HA	2.21	0.41
1:A:301:ILE:HD12	1:A:301:ILE:HA	1.80	0.41
2:B:406:GLU:HG2	2:B:407:ASN:H	1.85	0.41
2:D:166:VAL:HA	2:D:176:TYR:O	2.21	0.41
2:D:329:CYS:HB3	2:D:331:PHE:CE1	2.56	0.41
2:D:406:GLU:HG2	2:D:407:ASN:H	1.85	0.41
2:D:710:VAL:HG22	2:D:721:PHE:CZ	2.55	0.41
1:A:222:ARG:H	1:A:222:ARG:HG2	1.66	0.41
2:B:248:TYR:CE1	2:B:263:SER:HB2	2.55	0.41
2:B:255:SER:OG	3:B:1604:NAG:N2	2.54	0.41
2:B:329:CYS:HB3	2:B:331:PHE:CE1	2.56	0.41
2:B:734:CYS:HB2	2:B:742:CYS:HB3	1.47	0.41
2:B:751:ILE:HD13	2:B:751:ILE:HA	1.85	0.41
2:B:878:GLU:O	2:B:927:VAL:HA	2.21	0.41
1:C:87:LYS:HA	1:C:87:LYS:HD3	1.66	0.41
1:C:200:SER:O	1:C:204:SER:HB2	2.21	0.41
2:D:159:GLN:OE1	2:D:159:GLN:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:432:ASP:HA	2:D:433:PRO:HD3	1.90	0.41
2:D:878:GLU:O	2:D:927:VAL:HA	2.21	0.41
1:A:200:SER:O	1:A:204:SER:HB2	2.21	0.41
2:B:185:LEU:O	2:B:187:GLU:N	2.50	0.41
2:B:728:LYS:H	2:B:728:LYS:HG3	1.74	0.41
1:C:222:ARG:H	1:C:222:ARG:HG2	1.66	0.41
2:B:172:ASN:HD21	2:B:174:ARG:HE	1.69	0.40
1:C:211:LEU:HG	1:C:301:ILE:HD11	2.03	0.40
2:D:726:SER:HB3	2:D:750:TYR:CE2	2.56	0.40
2:D:779:PHE:HD1	2:D:779:PHE:HA	1.74	0.40
2:D:875:LYS:HE2	2:D:875:LYS:HB2	1.86	0.40
2:B:149:ASN:OD1	2:B:150:GLY:N	2.49	0.40
1:C:251:LYS:N	1:C:323:SER:HB3	2.37	0.40
2:D:326:THR:HB	2:D:376:LEU:HB2	2.02	0.40
2:B:665:LYS:H	2:B:684:GLY:HA2	1.85	0.40
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.79	0.40
1:C:61:ASN:ND2	1:C:80:ASN:HD22	2.18	0.40
1:C:162:LYS:NZ	1:C:165:THR:O	2.52	0.40
2:D:110:LEU:HA	2:D:111:PRO:HD3	1.86	0.40
2:B:413:PRO:HD2	2:B:703:CYS:SG	2.62	0.40
1:C:192:CYS:N	1:C:209:THR:OG1	2.45	0.40
1:C:287:LEU:HB3	1:C:291:LYS:HB2	2.03	0.40
2:D:391:PHE:CZ	2:D:452:VAL:HB	2.57	0.40
2:D:672:VAL:HG23	2:D:677:LYS:HB2	2.03	0.40
1:A:224:TYR:OH	1:A:320:GLU:OE2	2.20	0.40
1:A:272:GLY:HA2	1:A:308:ASP:HB2	2.03	0.40
2:B:498:ASP:OD1	2:B:500:SER:N	2.53	0.40
2:D:255:SER:OG	3:D:1604:NAG:N2	2.54	0.40
2:D:413:PRO:HD2	2:D:703:CYS:SG	2.62	0.40
2:D:696:ILE:HG12	2:D:707:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/398 (95%)	341 (90%)	37 (10%)	0	100	100
1	C	378/398 (95%)	342 (90%)	36 (10%)	0	100	100
2	B	721/1545 (47%)	642 (89%)	79 (11%)	0	100	100
2	D	721/1545 (47%)	642 (89%)	79 (11%)	0	100	100
All	All	2198/3886 (57%)	1967 (90%)	231 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/358 (95%)	320 (94%)	19 (6%)	21	52
1	C	339/358 (95%)	320 (94%)	19 (6%)	21	52
2	B	587/1370 (43%)	554 (94%)	33 (6%)	21	52
2	D	587/1370 (43%)	554 (94%)	33 (6%)	21	52
All	All	1852/3456 (54%)	1748 (94%)	104 (6%)	25	52

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	52	LEU
1	A	55	THR
1	A	67	SER
1	A	71	GLU
1	A	73	THR
1	A	74	LEU
1	A	78	THR
1	A	87	LYS
1	A	165	THR

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Mol	Chain	Res	Type
1	A	213	VAL
1	A	218	ASP
1	A	230	SER
1	A	237	ASN
1	A	244	PHE
1	A	256	THR
1	A	365	VAL
1	A	375	THR
1	A	379	LEU
2	B	42	SER
2	B	113	ARG
2	B	125	THR
2	B	137	ARG
2	B	155	SER
2	B	172	ASN
2	B	194	CYS
2	B	213	ARG
2	B	255	SER
2	B	311	SER
2	B	322	SER
2	B	324	THR
2	B	351	GLU
2	B	370	THR
2	B	409	THR
2	B	423	THR
2	B	430	VAL
2	B	446	GLU
2	B	455	CYS
2	B	487	CYS
2	B	506	CYS
2	B	522	THR
2	B	527	PHE
2	B	683	THR
2	B	756	CYS
2	B	760	PHE
2	B	765	TRP
2	B	801	CYS
2	B	806	CYS
2	B	822	VAL
2	B	827	ARG
2	B	881	LEU
2	B	929	LEU

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Mol	Chain	Res	Type
1	C	49	ASN
1	C	52	LEU
1	C	55	THR
1	C	67	SER
1	C	71	GLU
1	C	73	THR
1	C	74	LEU
1	C	78	THR
1	C	87	LYS
1	C	165	THR
1	C	213	VAL
1	C	218	ASP
1	C	230	SER
1	C	237	ASN
1	C	244	PHE
1	C	256	THR
1	C	365	VAL
1	C	375	THR
1	C	379	LEU
2	D	42	SER
2	D	113	ARG
2	D	125	THR
2	D	137	ARG
2	D	155	SER
2	D	172	ASN
2	D	194	CYS
2	D	213	ARG
2	D	255	SER
2	D	311	SER
2	D	322	SER
2	D	324	THR
2	D	351	GLU
2	D	370	THR
2	D	409	THR
2	D	423	THR
2	D	430	VAL
2	D	446	GLU
2	D	455	CYS
2	D	487	CYS
2	D	506	CYS
2	D	522	THR
2	D	527	PHE

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Mol	Chain	Res	Type
2	D	683	THR
2	D	756	CYS
2	D	760	PHE
2	D	765	TRP
2	D	801	CYS
2	D	806	CYS
2	D	822	VAL
2	D	827	ARG
2	D	881	LEU
2	D	929	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	80	ASN
1	A	264	HIS
1	A	295	HIS
2	B	67	GLN
2	B	218	GLN
2	B	278	GLN
2	B	353	HIS
2	B	458	HIS
2	B	670	GLN
2	B	718	HIS
2	B	784	ASN
2	B	794	ASN
2	B	829	GLN
1	C	59	ASN
1	C	80	ASN
1	C	264	HIS
1	C	295	HIS
2	D	67	GLN
2	D	218	GLN
2	D	278	GLN
2	D	353	HIS
2	D	458	HIS
2	D	670	GLN
2	D	718	HIS
2	D	784	ASN
2	D	794	ASN
2	D	829	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

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	1603	2	14,14,15	0.20	0	17,19,21	0.51	0
3	NAG	B	1601	2	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	D	1602	2	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	D	1605	2	14,14,15	0.17	0	17,19,21	0.49	0
3	NAG	B	1607	2	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
3	NAG	B	1606	2	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	D	1601	2	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	B	1604	2	14,14,15	0.35	0	17,19,21	0.55	0
3	NAG	B	1602	2	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	D	1606	2	14,14,15	0.34	0	17,19,21	0.58	0
3	NAG	A	501	1	14,14,15	0.15	0	17,19,21	0.55	0
3	NAG	B	1605	2	14,14,15	0.16	0	17,19,21	0.50	0
3	NAG	D	1604	2	14,14,15	0.35	0	17,19,21	0.55	0
3	NAG	D	1607	2	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
3	NAG	B	1603	2	14,14,15	0.21	0	17,19,21	0.51	0
3	NAG	B	1608	2	14,14,15	0.31	0	17,19,21	1.23	1 (5%)
3	NAG	D	1608	2	14,14,15	0.31	0	17,19,21	1.23	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	501	1	14,14,15	0.15	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1603	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1601	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1602	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1605	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1607	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1606	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1601	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1604	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1602	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1606	2	-	0/6/23/26	0/1/1/1
3	NAG	A	501	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1605	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1604	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1607	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1603	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1608	2	-	5/6/23/26	0/1/1/1
3	NAG	D	1608	2	-	5/6/23/26	0/1/1/1
3	NAG	C	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1608	NAG	C2-N2-C7	4.25	128.96	122.90
3	D	1608	NAG	C2-N2-C7	4.25	128.96	122.90
3	D	1607	NAG	C1-O5-C5	2.42	115.48	112.19
3	B	1607	NAG	C1-O5-C5	2.41	115.45	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C4-C5-C6-O6
3	C	501	NAG	C4-C5-C6-O6
3	B	1601	NAG	C4-C5-C6-O6
3	D	1601	NAG	C4-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	C	501	NAG	O5-C5-C6-O6
3	B	1602	NAG	C4-C5-C6-O6
3	D	1602	NAG	C4-C5-C6-O6
3	B	1601	NAG	O5-C5-C6-O6
3	D	1601	NAG	O5-C5-C6-O6
3	B	1607	NAG	O5-C5-C6-O6
3	D	1607	NAG	O5-C5-C6-O6
3	B	1608	NAG	C4-C5-C6-O6
3	D	1608	NAG	C4-C5-C6-O6
3	B	1602	NAG	O5-C5-C6-O6
3	B	1608	NAG	O5-C5-C6-O6
3	D	1602	NAG	O5-C5-C6-O6
3	D	1608	NAG	O5-C5-C6-O6
3	B	1603	NAG	C4-C5-C6-O6
3	D	1603	NAG	C4-C5-C6-O6
3	B	1604	NAG	C1-C2-N2-C7
3	D	1604	NAG	C1-C2-N2-C7
3	B	1607	NAG	C4-C5-C6-O6
3	D	1607	NAG	C4-C5-C6-O6
3	B	1608	NAG	C8-C7-N2-C2
3	B	1608	NAG	O7-C7-N2-C2
3	D	1608	NAG	C8-C7-N2-C2
3	D	1608	NAG	O7-C7-N2-C2
3	B	1603	NAG	O5-C5-C6-O6
3	D	1603	NAG	O5-C5-C6-O6
3	B	1605	NAG	O5-C5-C6-O6
3	D	1605	NAG	O5-C5-C6-O6
3	B	1604	NAG	C3-C2-N2-C7
3	B	1608	NAG	C3-C2-N2-C7
3	D	1604	NAG	C3-C2-N2-C7
3	D	1608	NAG	C3-C2-N2-C7
3	B	1604	NAG	O5-C5-C6-O6
3	D	1604	NAG	O5-C5-C6-O6
3	B	1604	NAG	C4-C5-C6-O6
3	D	1604	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1604	NAG	2	0
3	D	1604	NAG	2	0
3	B	1608	NAG	2	0
3	D	1608	NAG	2	0

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.

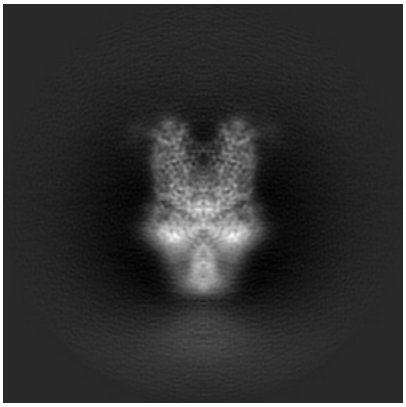
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21442. These allow visual inspection of the internal detail of the map and identification of artifacts.

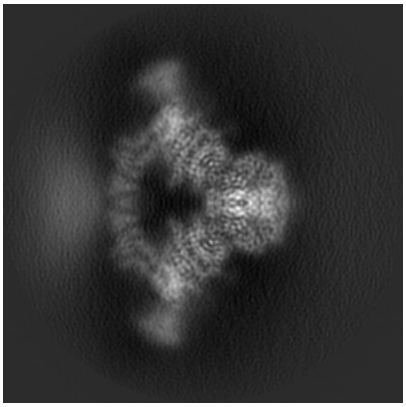
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

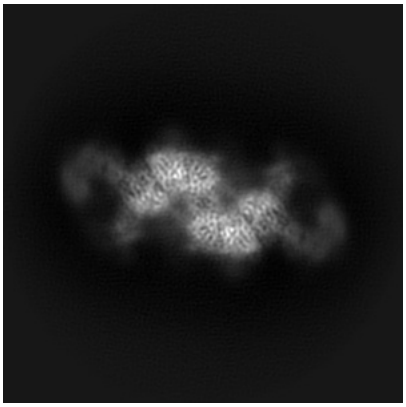
6.1.1 Primary map



X



Y

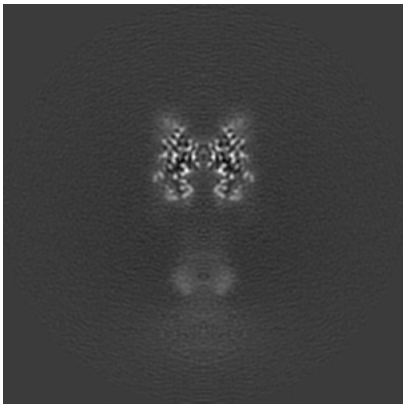


Z

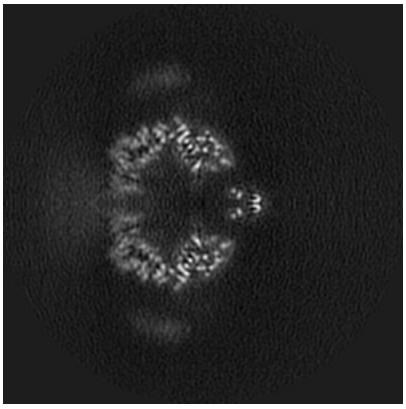
The images above show the map projected in three orthogonal directions.

6.2 Central slices

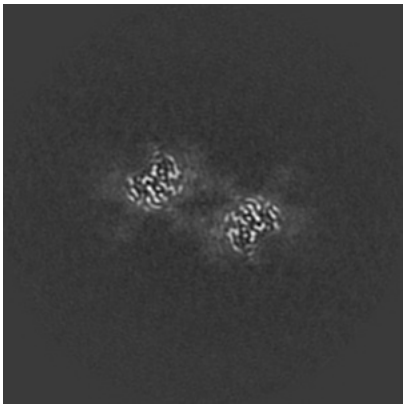
6.2.1 Primary map



X Index: 180



Y Index: 180

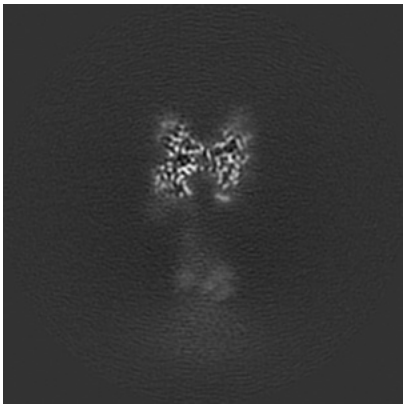


Z Index: 180

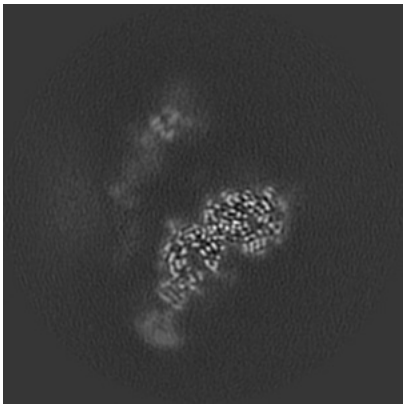
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

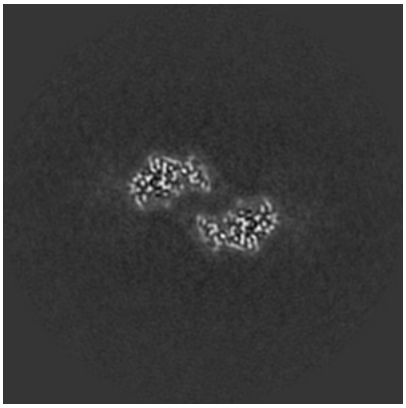
6.3.1 Primary map



X Index: 185



Y Index: 206



Z Index: 187

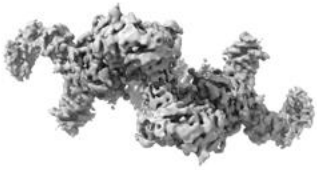
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

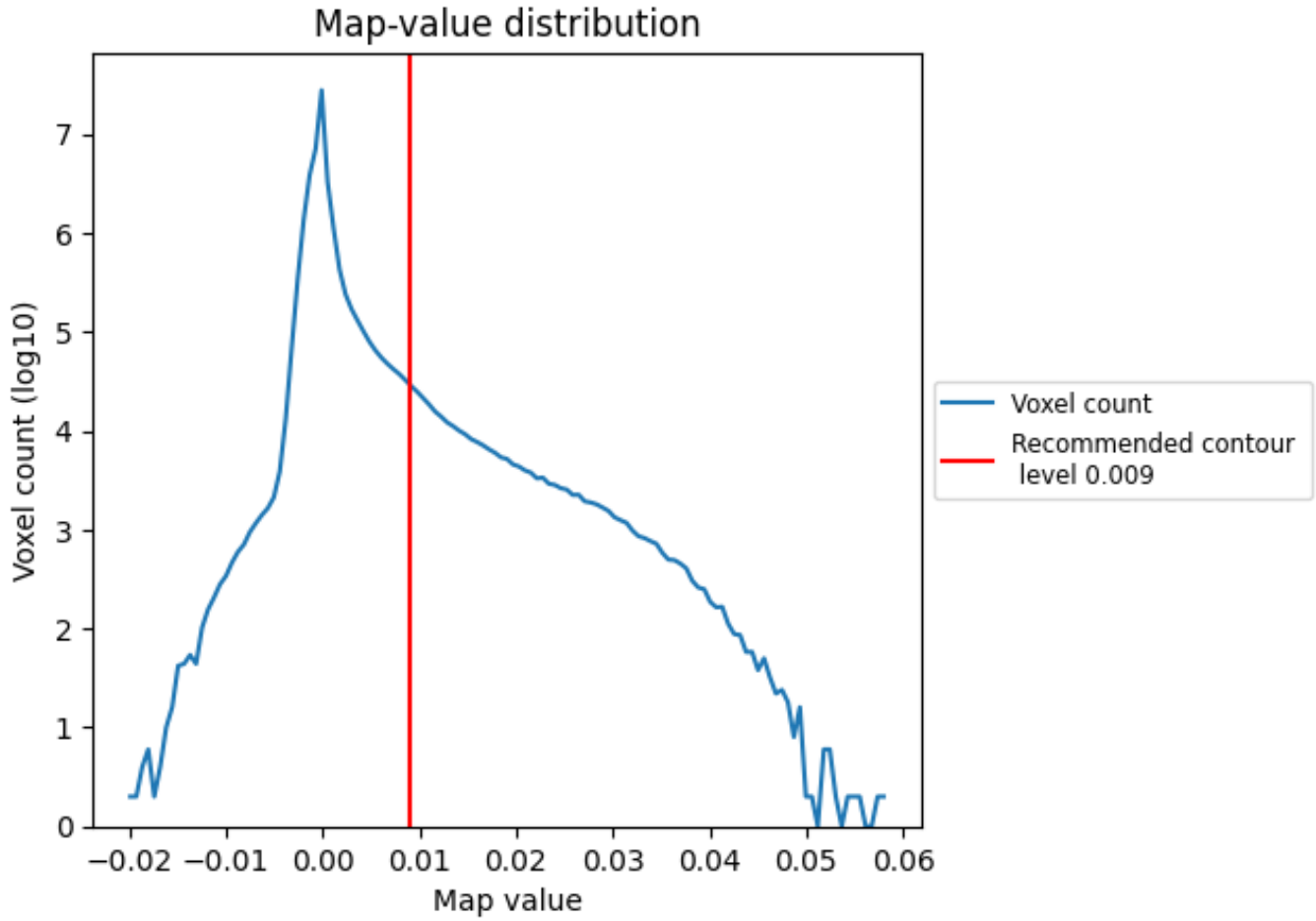
6.5 Mask visualisation (i)

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

7 Map analysis

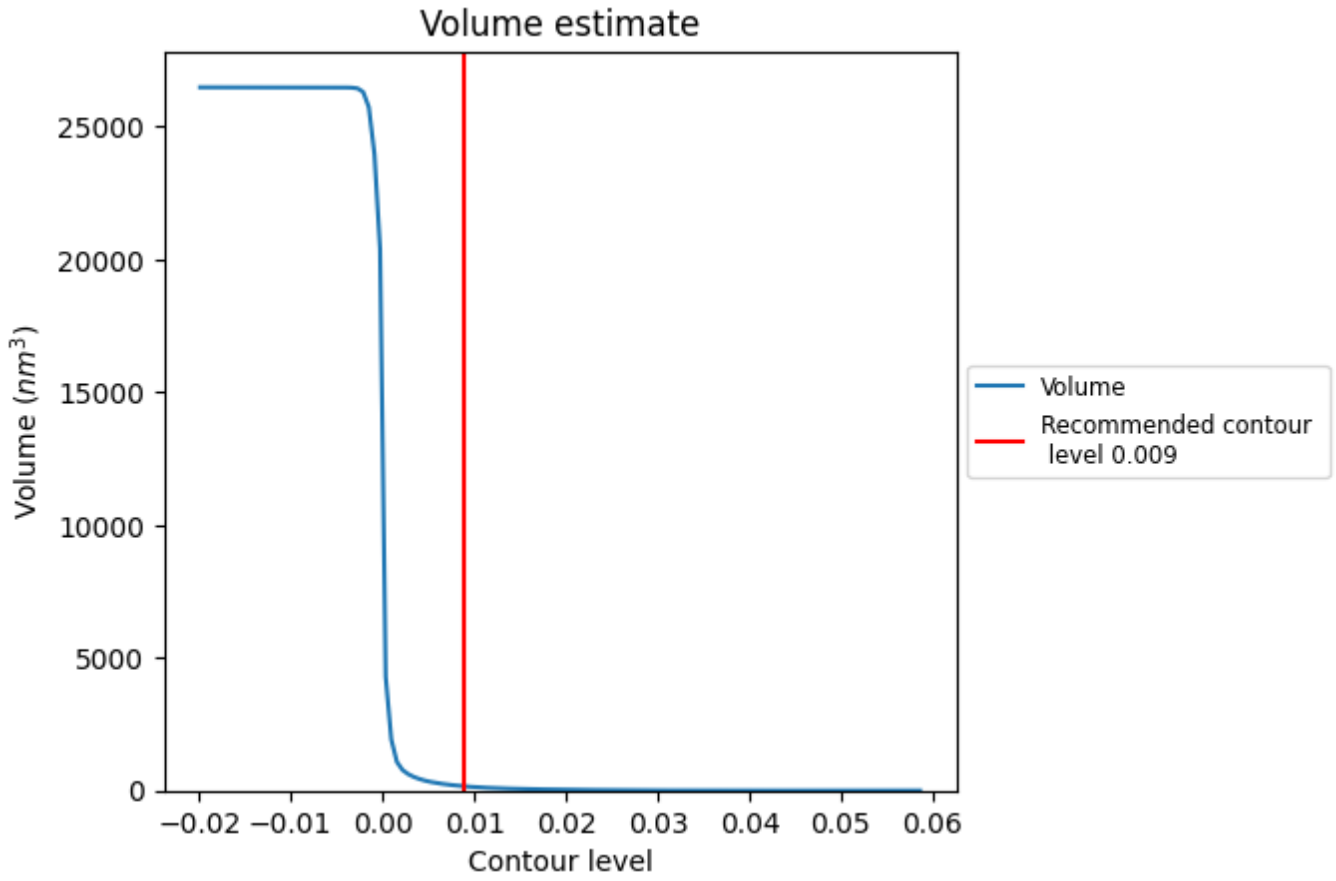
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

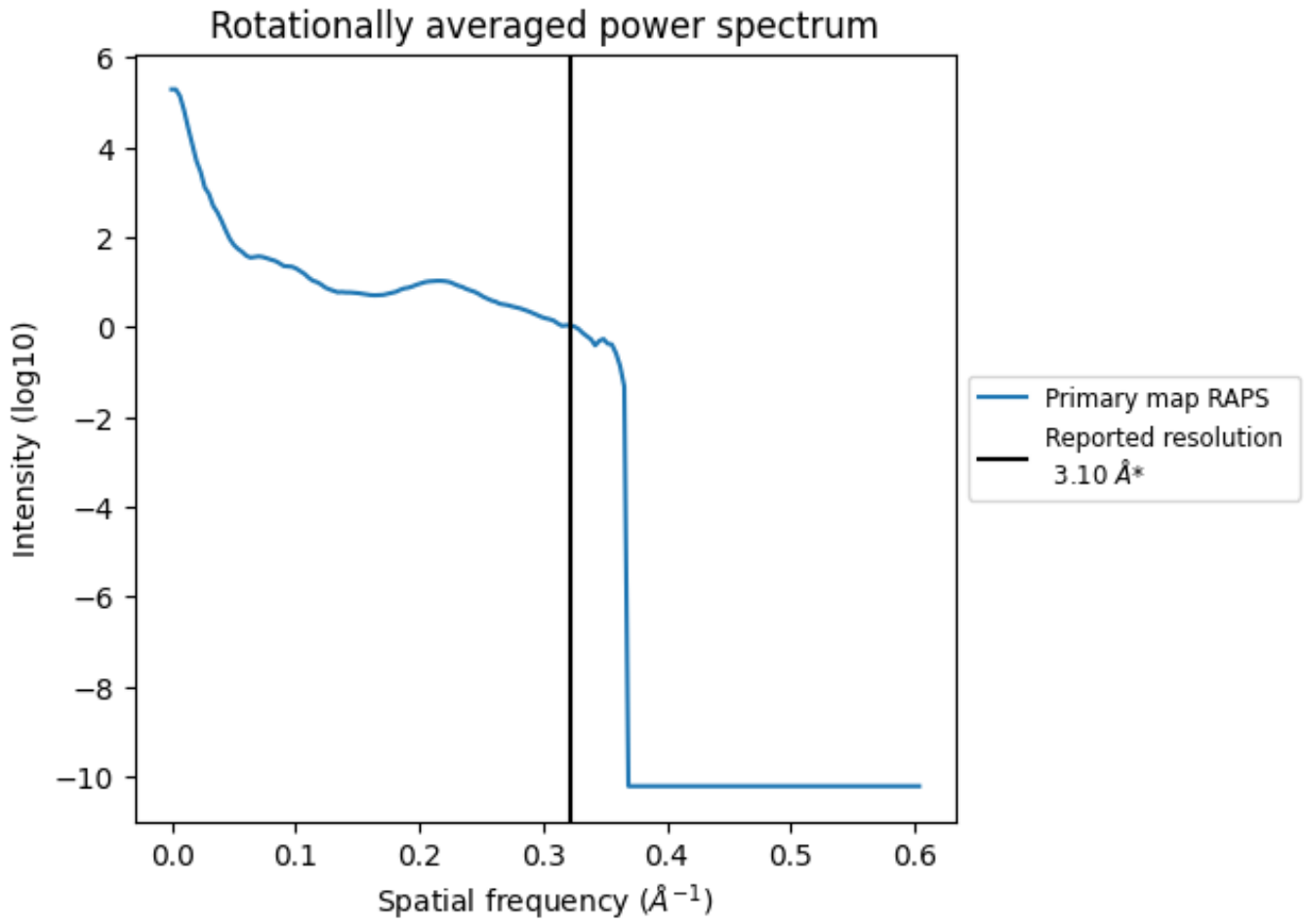
7.2 Volume estimate



The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 143 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 0.323 Å^{-1}

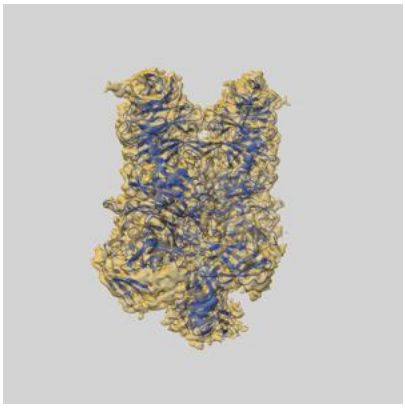
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

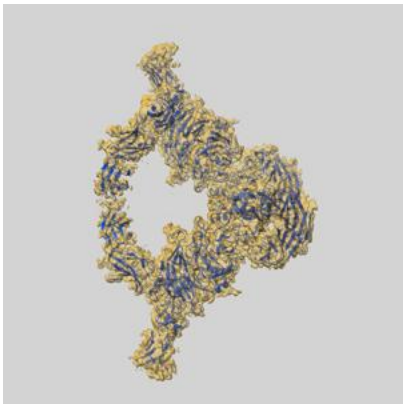
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21442 and PDB model 6VXK. Per-residue inclusion information can be found in section 3 on page 7.

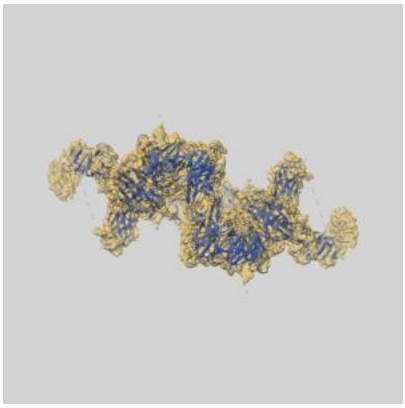
9.1 Map-model overlay



X



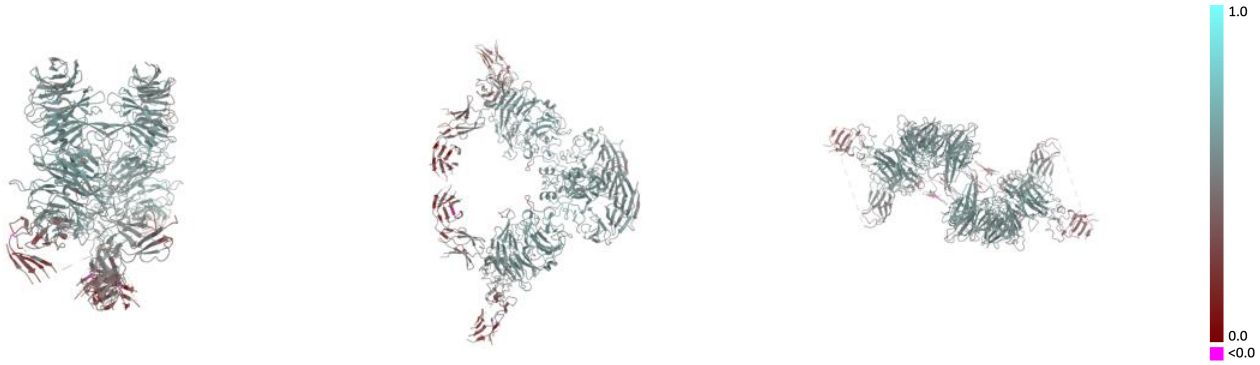
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

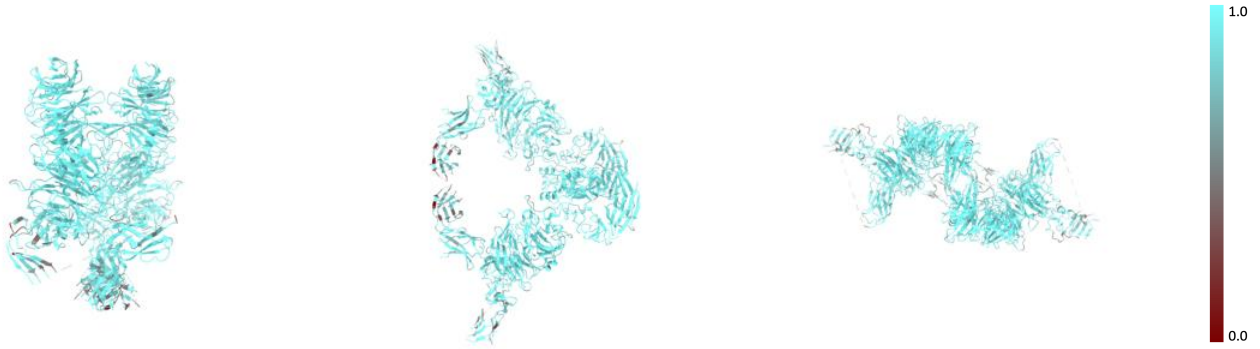
9.2 Q-score mapped to coordinate model (i)



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.

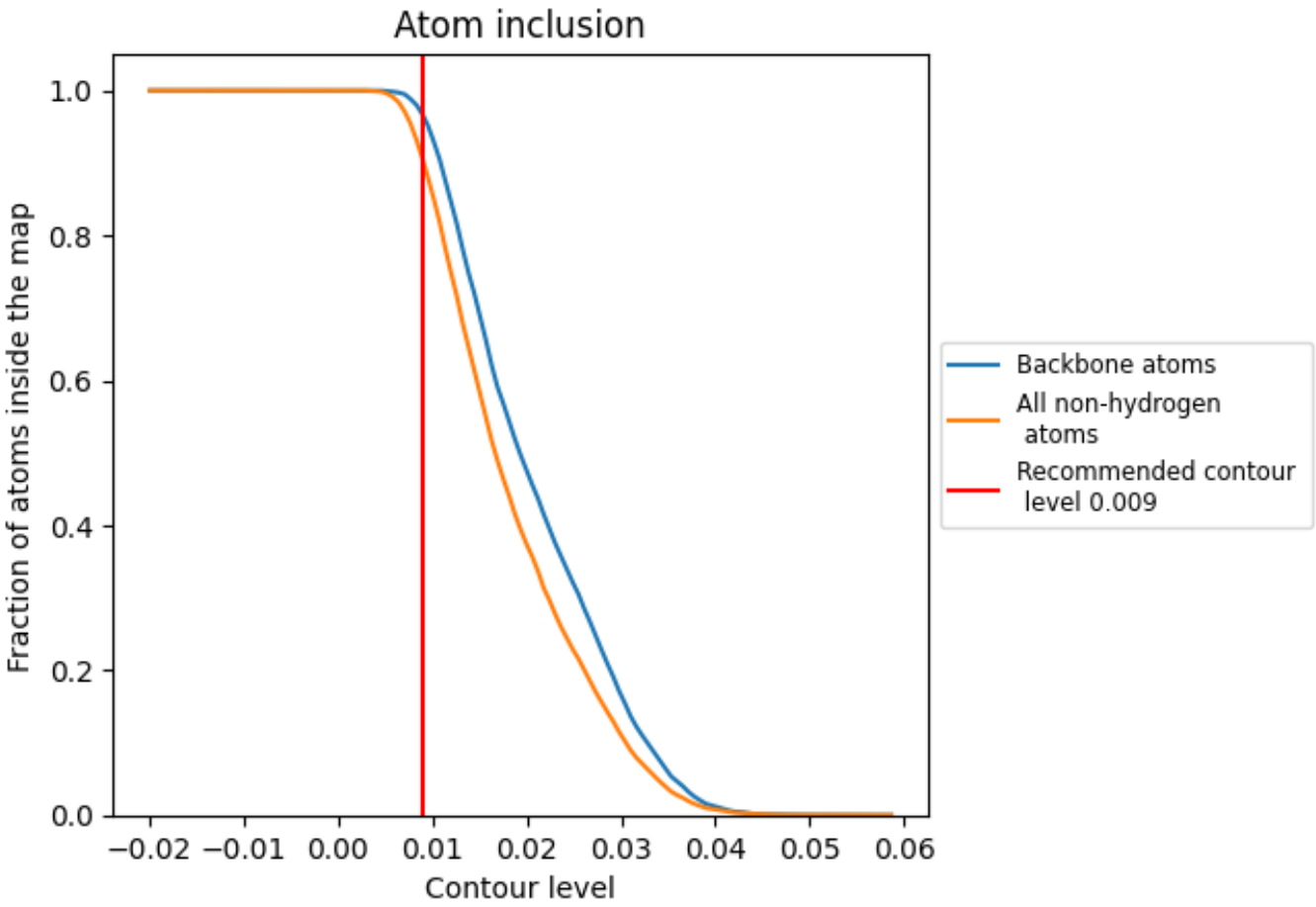
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9046	0.5120
A	0.9393	0.5510
B	0.8862	0.4920
C	0.9386	0.5500
D	0.8862	0.4910