



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:35 PM UTC

PDB ID : 6TRE / pdb_00006tre
EMDB ID : EMD-10560
Title : Structure of the RBM3/collar region of the Salmonella flagella MS-ring protein
FliF with 32-fold symmetry applied
Authors : Johnson, S.; Fong, Y.H.; Deme, J.C.; Furlong, E.J.; Kuhlen, L.; Lea, S.M.
Deposited on : 2019-12-18
Resolution : 3.30 Å(reported)
Based on initial model : 6SD1

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:

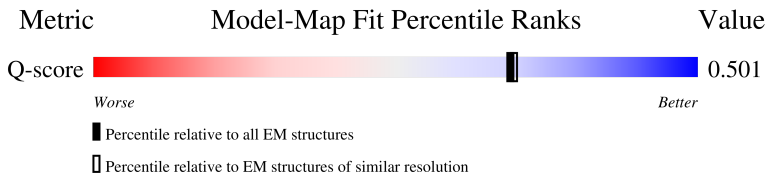
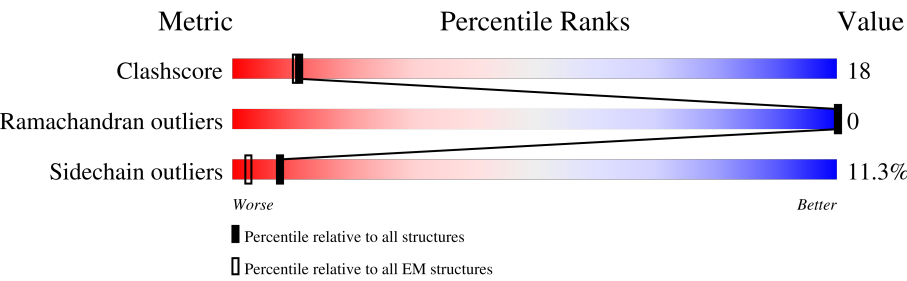
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.30 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.



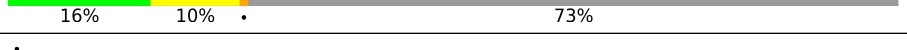
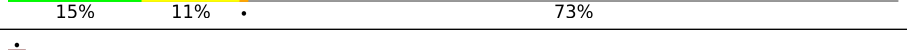
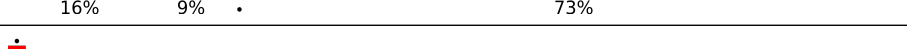
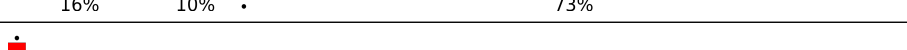
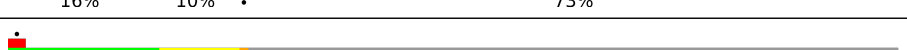
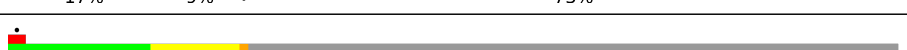
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	1	560	16% 10% 73%
1	2	560	16% 10% 73%
1	3	560	16% 10% 73%
1	4	560	16% 9% 73%

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Mol	Chain	Length	Quality of chain
1	5	560	
1	6	560	
1	A	560	
1	B	560	
1	C	560	
1	D	560	
1	E	560	
1	F	560	
1	G	560	
1	H	560	
1	I	560	
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	U	560	
1	V	560	
1	W	560	

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Mol	Chain	Length	Quality of chain
1	X	560	16%9% 73%
1	Y	560	16%10% 73%
1	Z	560	15%10% 73%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 38176 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 Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	B	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	C	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	D	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	E	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	F	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	G	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	H	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	I	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	J	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	K	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	L	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	M	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	N	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	O	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	P	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	Q	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		

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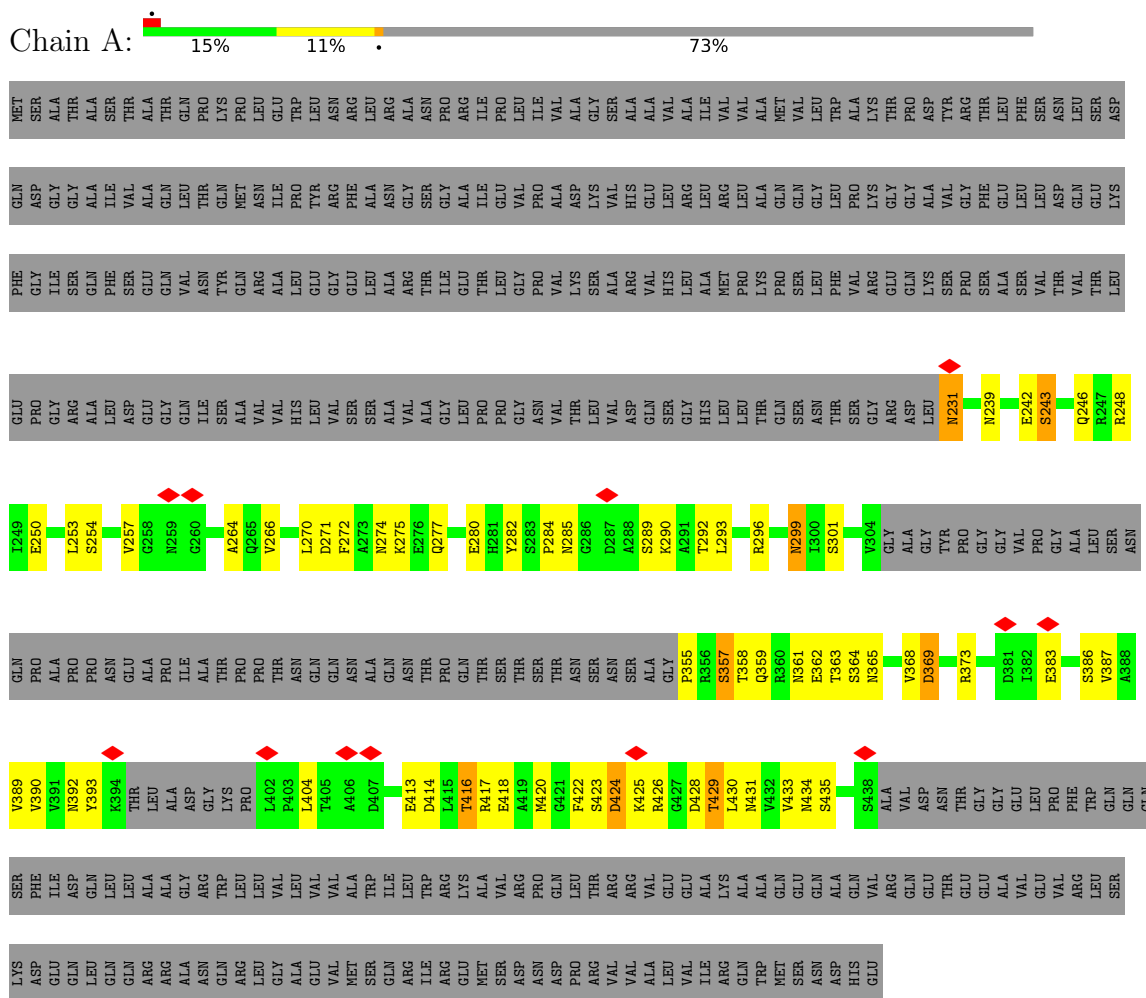
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	S	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	T	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	U	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	V	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	W	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	X	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	Y	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	Z	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	1	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	2	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	3	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	4	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	5	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	6	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		

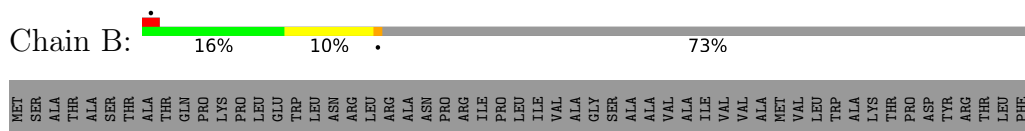
3 Residue-property plots

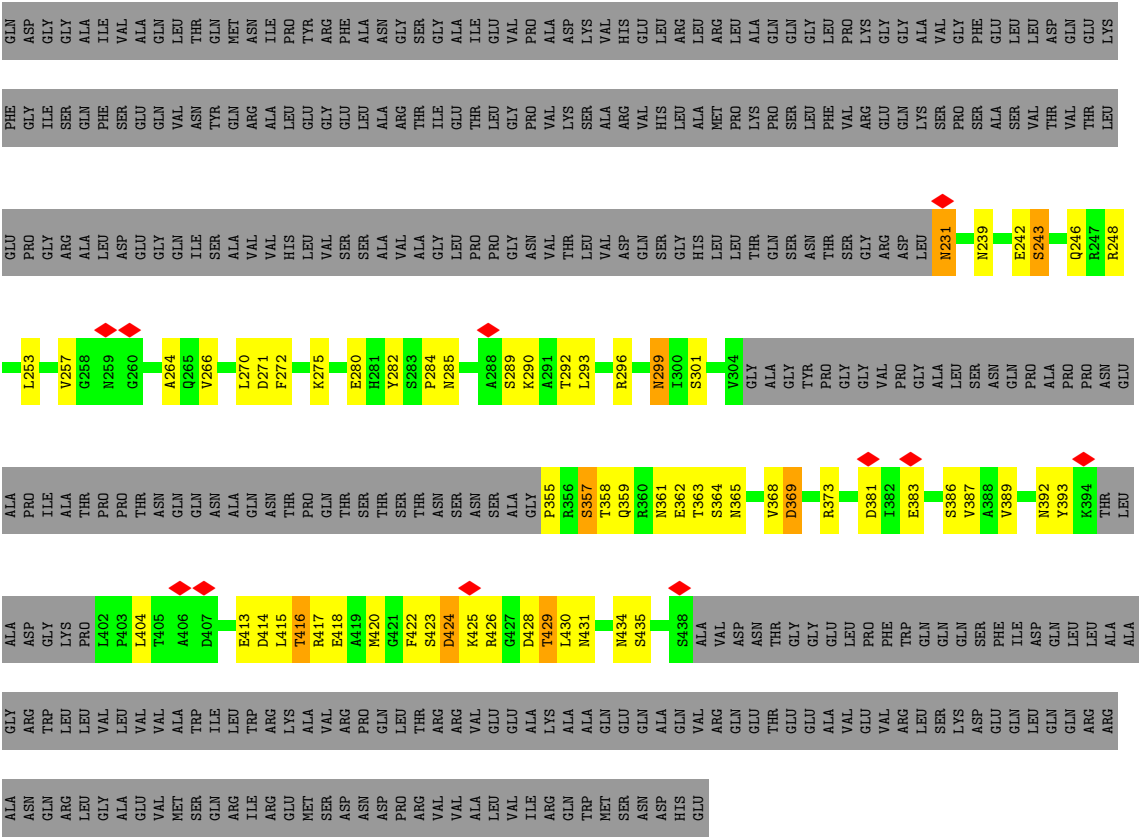
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flagellar M-ring protein

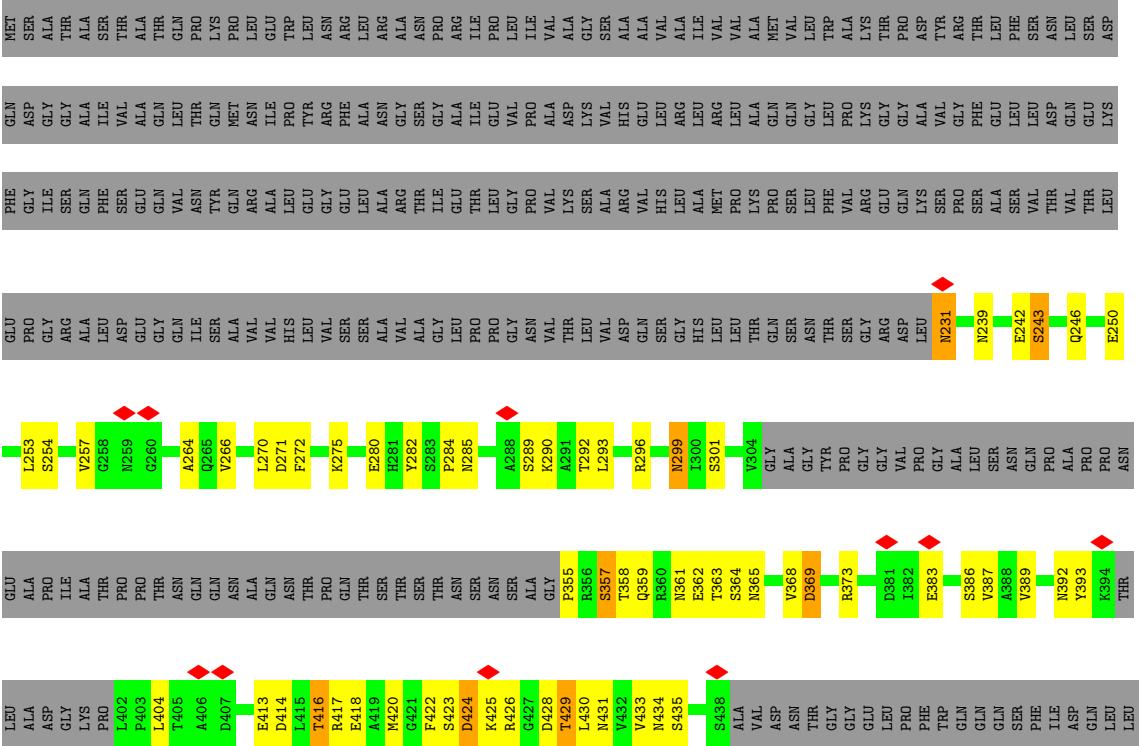


• Molecule 1: Flagellar M-ring protein

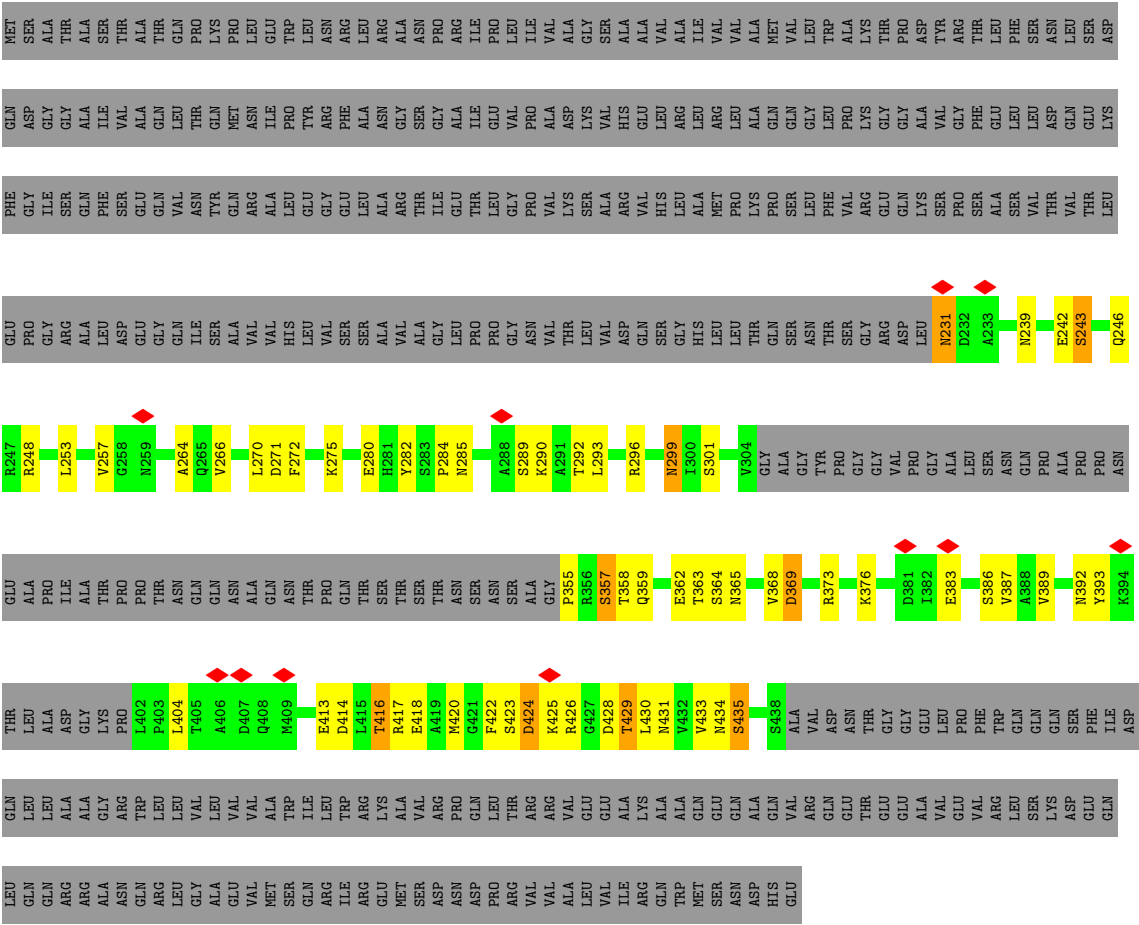




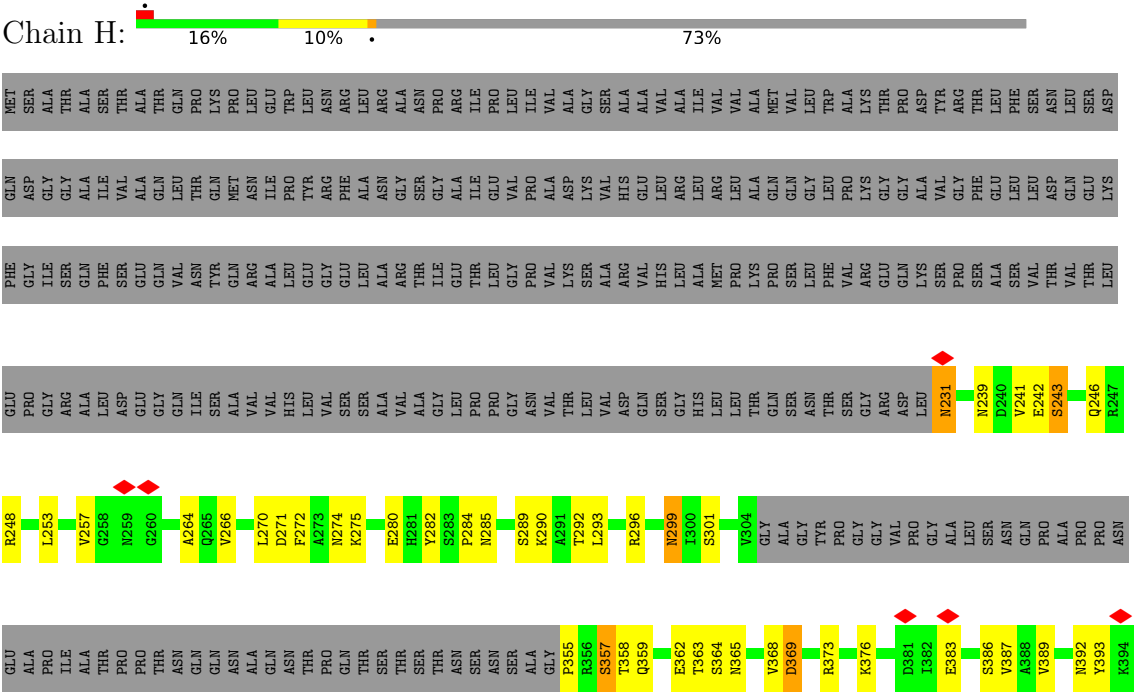
• Molecule 1: Flagellar M-ring protein



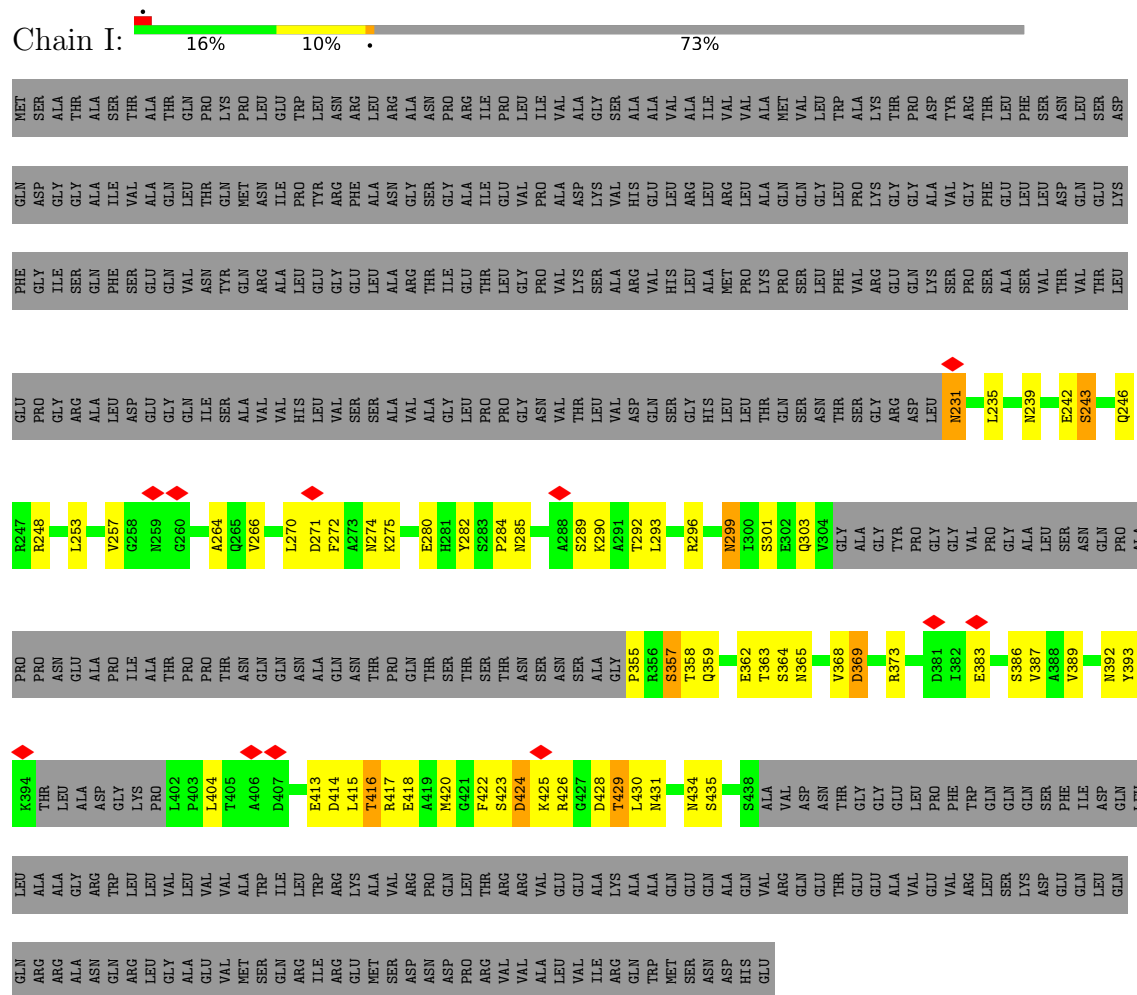




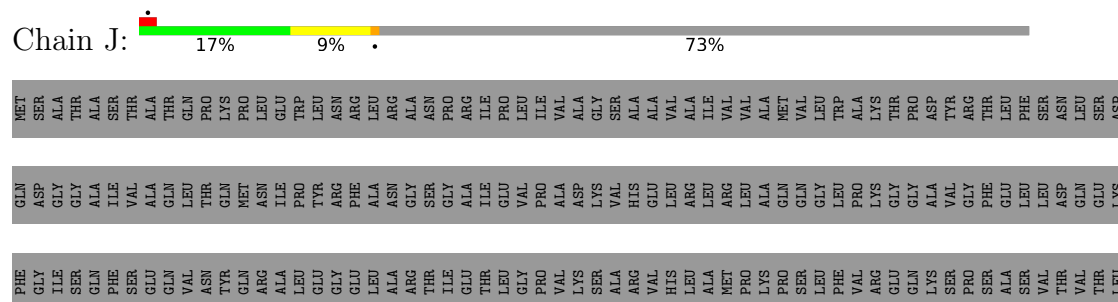
● Molecule 1: Flagellar M-ring protein

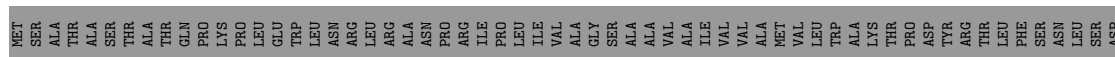


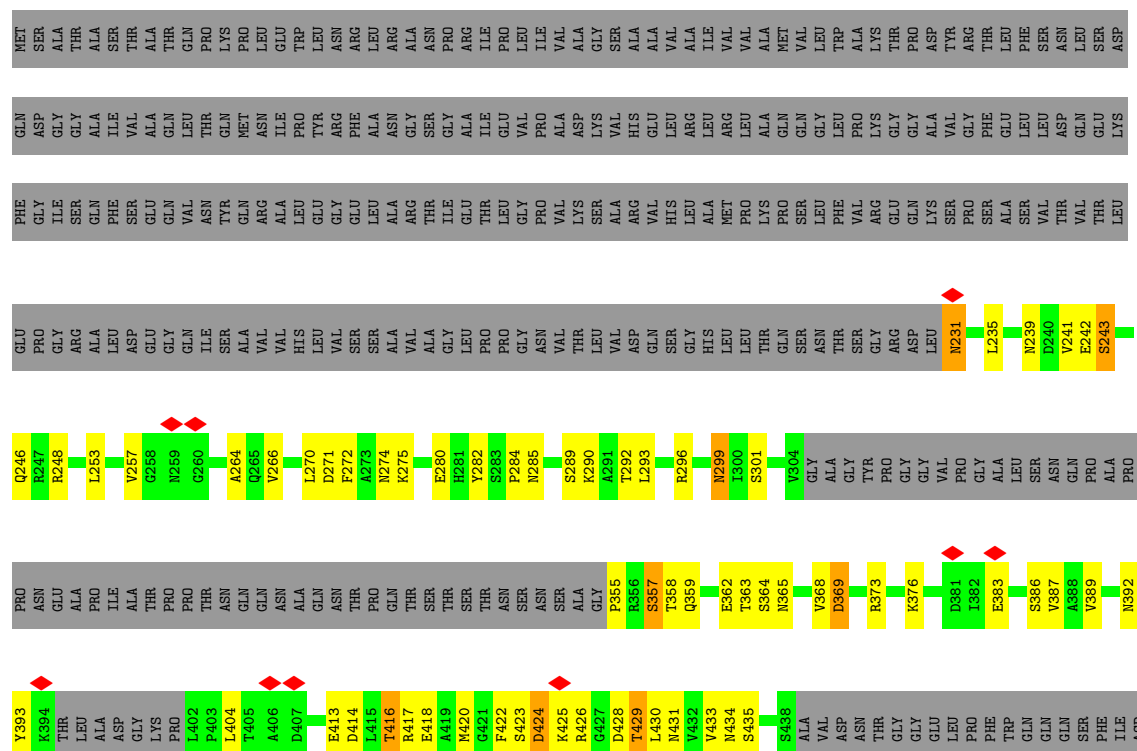
- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein







[illegible]

- Molecule 1: Flagellar M-ring protein

[illegible]

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

GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	ALA	VAL	VAL	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	LEU	THR	LEU	VAL	VAL	ASP	GLN	SER	GLY	HIS	LEU	LEU	THR	THR	SER	GLY	ARG	ASP	ASP	LEU	M231	M235	M239	E242	S243
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R247 R248 L253 Q257 Q258 Q259 Q260 Q264 Q265 Q266 L270 L271 Q272 Q273 Q274 Q275 Q280 Q281 Q282 Q283 Q284 Q285 Q286 Q288 Q289 Q290 Q291 Q292 Q293 L293 Q296 Q299 Q303 Q304
 GLY ALA ALA GLY TYR PRO PRO GLY GLY VAL VAL PRO PRO GLY ALA ALA LEU SER ASN GLN PRO PRO PRO

ASN	GLU	ALA	PRO	ILE	ALA	ALA	THR	PRO	PRO	PRO	THR	ASN	GLN	GLN	ASN	ALA	GLN	ASN	THR	THR	THR	THR	THR	ASN	SER	ASN	SER	ALA	GLY	P355	R356	S357	T358	E362	T363	N365	V368	D369	R373	D381	I382	E383	S386	V387	A389	N392	Y393	K394	THR
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ALA	ASP	GLY	LYS	PRO	L402	P403	L404	T405	A406	D407	E413	D414	T415	T416	R417	E418	A419	M420	G421	F422	S423	D424	K425	R426	D427	D428	T429	L430	M434	S435	S438	ALA	VAL	ASP	ASN	THR	GLY	GLY	GLU	LEU	LEU	PRO	TRP	GLN	GLN	GLN	SER	PHE	ILE	ILE	ASP	GLN	LEU	LEU	ALA
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ARG	TRP	LEU	VAL	VAL	VAL	ALA	TRP	ILE	LEU	TRP	ARG	LYS	ALA	VAL	VAL	ARG	PRO	GLN	LEU	THR	LEU	ARG	ARG	VAL	GLU	GLU	ALA	LYS	ALA	ALA	GLN	VAL	GLN	GLN	GLN	VAL	ARG	GLN	GLU	THR	THR	GLU	GLU	GLY	GLY	ALA	ALA	SER	LEU	ARG	LYS	ASP	GLY	GLN	LEU	GLN	GLN	ARG	ARG	ALA
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ASN	GLN	ARG	LEU	GLY	ALA	GLU	VAL	MET	SER	GLN	ARG	ILE	ARG	GLU	MET	SER	ASP	ASN	ASN	PRO	ARG	VAL	VAL	ALA	LEU	VAL	ILE	ARG	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU
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- Molecule 1: Flagellar M-ring protein



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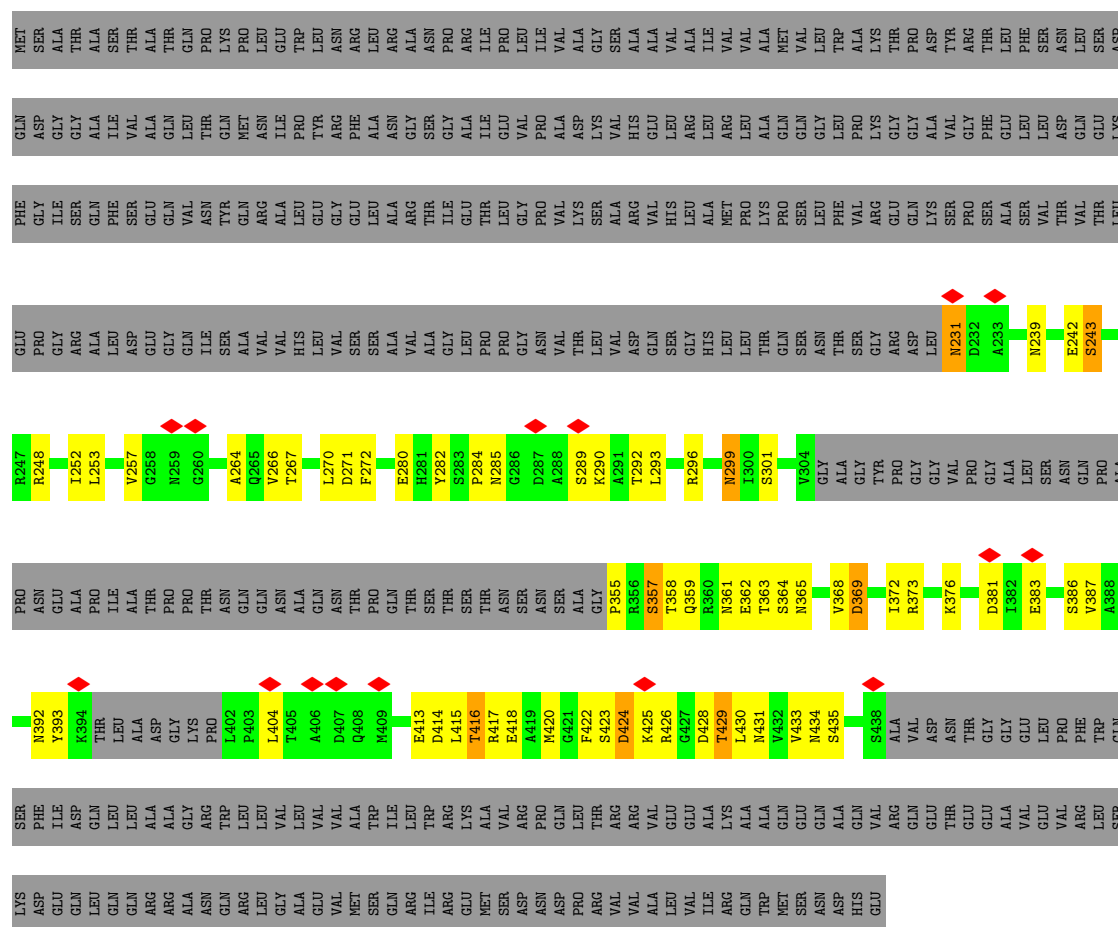
GLN	ASP	GLY	GLY	ALA	ILE	VAL	ALA	ALA	LEU	THR	GLN	MET	ASN	ILE	PRO	TYR	ARG	PHE	ALA	ASN	GLY	SER	GLY	ILE	GLU	VAL	PRO	ALA	ASP	LYS	VAL	HIS	GLU	GLU	LEU	ARG	LEU	ARG	LEU	LEU	LEU	LYS	GLY	GLY	VAL	VAL	PHE	GLU	LEU	LEU	ASP	GLN	GLU	LYS
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ARG
GLJ
GLN
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THR

GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	ALA	VAL	VAL	GLY	LEU	PRO	PRO	ASN	GLY	VAL	THR	LEU	VAL	ASP	GLN	SER	GLY	HIS	LEU	LEU	THR	GLN	SER	ASN	THR	SER	GLY	ARG	ASP	LEU	LEU	N231	N239	E242	S243	Q246	E247
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C32	Depositor
Number of particles used	33026	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	355.104, 355.104, 355.104	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.44	0/1205	0.54	0/1624
1	2	0.44	0/1205	0.54	0/1624
1	3	0.44	0/1205	0.54	0/1624
1	4	0.44	0/1205	0.54	0/1624
1	5	0.44	0/1205	0.54	0/1624
1	6	0.44	0/1205	0.54	0/1624
1	A	0.44	0/1205	0.54	0/1624
1	B	0.44	0/1205	0.54	0/1624
1	C	0.44	0/1205	0.54	0/1624
1	D	0.44	0/1205	0.54	0/1624
1	E	0.44	0/1205	0.54	0/1624
1	F	0.44	0/1205	0.54	0/1624
1	G	0.44	0/1205	0.54	0/1624
1	H	0.44	0/1205	0.54	0/1624
1	I	0.44	0/1205	0.54	0/1624
1	J	0.44	0/1205	0.54	0/1624
1	K	0.44	0/1205	0.54	0/1624
1	L	0.44	0/1205	0.54	0/1624
1	M	0.44	0/1205	0.54	0/1624
1	N	0.44	0/1205	0.54	0/1624
1	O	0.44	0/1205	0.54	0/1624
1	P	0.44	0/1205	0.54	0/1624
1	Q	0.44	0/1205	0.54	0/1624
1	R	0.44	0/1205	0.54	0/1624
1	S	0.44	0/1205	0.54	0/1624
1	T	0.44	0/1205	0.54	0/1624
1	U	0.44	0/1205	0.54	0/1624
1	V	0.44	0/1205	0.54	0/1624
1	W	0.44	0/1205	0.54	0/1624
1	X	0.44	0/1205	0.54	0/1624
1	Y	0.44	0/1205	0.54	0/1624
1	Z	0.44	0/1205	0.54	0/1624
All	All	0.44	0/38560	0.54	0/51968

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	1	1193	0	1173	51	0
1	2	1193	0	1173	52	0
1	3	1193	0	1173	53	0
1	4	1193	0	1173	50	0
1	5	1193	0	1173	52	0
1	6	1193	0	1173	54	0
1	A	1193	0	1173	54	0
1	B	1193	0	1173	47	0
1	C	1193	0	1173	49	0
1	D	1193	0	1173	48	0
1	E	1193	0	1173	50	0
1	F	1193	0	1173	51	0
1	G	1193	0	1173	48	0
1	H	1193	0	1173	51	0
1	I	1193	0	1173	55	0
1	J	1193	0	1173	49	0
1	K	1193	0	1173	50	0
1	L	1193	0	1173	62	0
1	M	1193	0	1173	52	0
1	N	1193	0	1173	46	0
1	O	1193	0	1173	51	0
1	P	1193	0	1173	55	0
1	Q	1193	0	1173	57	0
1	R	1193	0	1173	56	0
1	S	1193	0	1173	56	0
1	T	1193	0	1173	52	0
1	U	1193	0	1173	57	0
1	V	1193	0	1173	54	0
1	W	1193	0	1173	47	0
1	X	1193	0	1173	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1193	0	1173	55	0
1	Z	1193	0	1173	50	0
All	All	38176	0	37536	1385	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 18.

All (1385) 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:L:415:LEU:HD11	1:M:433:VAL:HG21	1.62	0.82
1:Y:292:THR:HG21	1:Z:282:TYR:HB3	1.58	0.82
1:X:369:ASP:OD1	1:X:369:ASP:N	2.14	0.81
1:Y:369:ASP:N	1:Y:369:ASP:OD1	2.14	0.81
1:Z:369:ASP:OD1	1:Z:369:ASP:N	2.14	0.81
1:W:369:ASP:OD1	1:W:369:ASP:N	2.14	0.81
1:V:369:ASP:N	1:V:369:ASP:OD1	2.14	0.80
1:I:369:ASP:OD1	1:I:369:ASP:N	2.14	0.80
1:U:369:ASP:OD1	1:U:369:ASP:N	2.14	0.80
1:4:415:LEU:HD11	1:5:433:VAL:HG21	1.64	0.80
1:T:369:ASP:N	1:T:369:ASP:OD1	2.14	0.80
1:2:369:ASP:N	1:2:369:ASP:OD1	2.14	0.80
1:4:418:GLU:HG3	1:5:431:ASN:HB3	1.61	0.80
1:3:369:ASP:OD1	1:3:369:ASP:N	2.14	0.80
1:S:369:ASP:OD1	1:S:369:ASP:N	2.14	0.79
1:Q:369:ASP:N	1:Q:369:ASP:OD1	2.14	0.79
1:4:369:ASP:N	1:4:369:ASP:OD1	2.14	0.79
1:R:369:ASP:OD1	1:R:369:ASP:N	2.14	0.79
1:P:369:ASP:OD1	1:P:369:ASP:N	2.14	0.78
1:5:369:ASP:OD1	1:5:369:ASP:N	2.14	0.78
1:A:369:ASP:OD1	1:A:369:ASP:N	2.14	0.78
1:J:369:ASP:N	1:J:369:ASP:OD1	2.14	0.78
1:F:369:ASP:OD1	1:F:369:ASP:N	2.14	0.78
1:K:369:ASP:OD1	1:K:369:ASP:N	2.14	0.78
1:O:369:ASP:N	1:O:369:ASP:OD1	2.14	0.78
1:P:373:ARG:HH21	1:Q:275:LYS:HD3	1.47	0.78
1:B:369:ASP:OD1	1:B:369:ASP:N	2.14	0.78
1:6:369:ASP:OD1	1:6:369:ASP:N	2.14	0.78
1:L:369:ASP:N	1:L:369:ASP:OD1	2.14	0.77
1:N:369:ASP:OD1	1:N:369:ASP:N	2.14	0.77
1:I:369:ASP:OD1	1:I:369:ASP:N	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ASP:N	1:C:369:ASP:OD1	2.14	0.77
1:M:369:ASP:OD1	1:M:369:ASP:N	2.14	0.77
1:L:418:GLU:OE1	1:M:429:THR:OG1	2.02	0.77
1:H:369:ASP:N	1:H:369:ASP:OD1	2.14	0.77
1:D:369:ASP:OD1	1:D:369:ASP:N	2.14	0.77
1:E:418:GLU:OE1	1:F:429:THR:OG1	2.03	0.77
1:E:369:ASP:N	1:E:369:ASP:OD1	2.14	0.76
1:G:369:ASP:OD1	1:G:369:ASP:N	2.14	0.75
1:Y:373:ARG:HH21	1:Z:275:LYS:HD3	1.49	0.75
1:H:373:ARG:HH21	1:I:275:LYS:HD3	1.51	0.74
1:L:418:GLU:HG3	1:M:431:ASN:HB3	1.69	0.73
1:4:418:GLU:HG3	1:5:431:ASN:CB	2.18	0.73
1:S:373:ARG:HH21	1:T:275:LYS:HD3	1.52	0.72
1:1:418:GLU:HG3	1:2:431:ASN:HB3	1.72	0.72
1:F:239:ASN:O	1:F:243:SER:OG	2.08	0.72
1:E:239:ASN:O	1:E:243:SER:OG	2.08	0.71
1:K:303:GLN:HA	1:L:357:SER:HA	1.71	0.71
1:G:239:ASN:O	1:G:243:SER:OG	2.08	0.71
1:K:239:ASN:O	1:K:243:SER:OG	2.08	0.71
1:L:239:ASN:O	1:L:243:SER:OG	2.08	0.71
1:4:418:GLU:OE1	1:5:429:THR:OG1	2.08	0.71
1:M:239:ASN:O	1:M:243:SER:OG	2.08	0.71
1:U:239:ASN:O	1:U:243:SER:OG	2.08	0.71
1:6:239:ASN:O	1:6:243:SER:OG	2.08	0.71
1:D:239:ASN:O	1:D:243:SER:OG	2.08	0.71
1:X:239:ASN:O	1:X:243:SER:OG	2.08	0.71
1:B:239:ASN:O	1:B:243:SER:OG	2.08	0.71
1:J:239:ASN:O	1:J:243:SER:OG	2.08	0.71
1:5:239:ASN:O	1:5:243:SER:OG	2.08	0.71
1:A:239:ASN:O	1:A:243:SER:OG	2.08	0.71
1:T:239:ASN:O	1:T:243:SER:OG	2.08	0.71
1:Y:239:ASN:O	1:Y:243:SER:OG	2.08	0.71
1:2:418:GLU:OE1	1:3:429:THR:OG1	2.08	0.71
1:Q:290:LYS:HA	1:R:284:PRO:HB3	1.72	0.71
1:U:373:ARG:HH21	1:V:275:LYS:HD3	1.55	0.71
1:H:239:ASN:O	1:H:243:SER:OG	2.08	0.70
1:Q:239:ASN:O	1:Q:243:SER:OG	2.08	0.70
1:P:239:ASN:O	1:P:243:SER:OG	2.08	0.70
1:2:239:ASN:O	1:2:243:SER:OG	2.08	0.70
1:I:239:ASN:O	1:I:243:SER:OG	2.08	0.70
1:O:239:ASN:O	1:O:243:SER:OG	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:239:ASN:O	1:W:243:SER:OG	2.08	0.70
1:O:248:ARG:NH2	1:P:242:GLU:OE1	2.24	0.70
1:R:239:ASN:O	1:R:243:SER:OG	2.08	0.70
1:V:239:ASN:O	1:V:243:SER:OG	2.08	0.70
1:1:239:ASN:O	1:1:243:SER:OG	2.08	0.70
1:C:239:ASN:O	1:C:243:SER:OG	2.08	0.70
1:Z:239:ASN:O	1:Z:243:SER:OG	2.08	0.70
1:4:239:ASN:O	1:4:243:SER:OG	2.08	0.70
1:N:239:ASN:O	1:N:243:SER:OG	2.08	0.70
1:3:239:ASN:O	1:3:243:SER:OG	2.08	0.70
1:S:239:ASN:O	1:S:243:SER:OG	2.08	0.69
1:Q:373:ARG:HH21	1:R:275:LYS:HD3	1.55	0.69
1:Z:418:GLU:OE1	1:1:429:THR:OG1	2.11	0.69
1:K:290:LYS:HA	1:L:284:PRO:HB3	1.74	0.68
1:O:418:GLU:OE1	1:P:429:THR:OG1	2.12	0.68
1:R:373:ARG:HH21	1:S:275:LYS:HD3	1.58	0.67
1:D:418:GLU:HG3	1:E:431:ASN:HB3	1.76	0.67
1:U:248:ARG:NH2	1:V:242:GLU:OE1	2.28	0.67
1:U:426:ARG:NH2	1:U:428:ASP:OD2	2.28	0.67
1:D:415:LEU:HD11	1:E:433:VAL:HG21	1.77	0.67
1:E:426:ARG:NH2	1:E:428:ASP:OD2	2.28	0.67
1:M:426:ARG:NH2	1:M:428:ASP:OD2	2.28	0.67
1:Z:426:ARG:NH2	1:Z:428:ASP:OD2	2.28	0.67
1:5:418:GLU:OE1	1:6:429:THR:OG1	2.13	0.67
1:X:248:ARG:NH2	1:Y:242:GLU:OE1	2.28	0.67
1:I:373:ARG:HH21	1:J:275:LYS:HD3	1.61	0.66
1:F:426:ARG:NH2	1:F:428:ASP:OD2	2.28	0.66
1:5:426:ARG:NH2	1:5:428:ASP:OD2	2.28	0.66
1:N:426:ARG:NH2	1:N:428:ASP:OD2	2.28	0.66
1:E:415:LEU:HD11	1:F:433:VAL:HG21	1.78	0.66
1:V:426:ARG:NH2	1:V:428:ASP:OD2	2.28	0.66
1:1:426:ARG:NH2	1:1:428:ASP:OD2	2.28	0.66
1:6:426:ARG:NH2	1:6:428:ASP:OD2	2.28	0.66
1:G:426:ARG:NH2	1:G:428:ASP:OD2	2.28	0.65
1:O:426:ARG:NH2	1:O:428:ASP:OD2	2.28	0.65
1:A:282:TYR:HB3	1:6:292:THR:HG21	1.78	0.65
1:H:426:ARG:NH2	1:H:428:ASP:OD2	2.28	0.65
1:A:426:ARG:NH2	1:A:428:ASP:OD2	2.28	0.65
1:4:248:ARG:NH2	1:5:242:GLU:OE1	2.29	0.65
1:R:290:LYS:HA	1:S:284:PRO:HB3	1.77	0.65
1:Q:426:ARG:NH2	1:Q:428:ASP:OD2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:426:ARG:NH2	1:W:428:ASP:OD2	2.28	0.65
1:2:426:ARG:NH2	1:2:428:ASP:OD2	2.28	0.65
1:P:426:ARG:NH2	1:P:428:ASP:OD2	2.28	0.65
1:U:418:GLU:HG3	1:V:431:ASN:HB3	1.78	0.65
1:D:418:GLU:OE1	1:E:429:THR:OG1	2.14	0.64
1:I:426:ARG:NH2	1:I:428:ASP:OD2	2.28	0.64
1:L:418:GLU:HG3	1:M:431:ASN:CB	2.25	0.64
1:A:275:LYS:HD3	1:6:373:ARG:HH21	1.61	0.64
1:U:411:GLN:NE2	1:V:435:SER:OG	2.30	0.64
1:B:426:ARG:NH2	1:B:428:ASP:OD2	2.28	0.64
1:P:373:ARG:HH21	1:Q:275:LYS:CD	2.10	0.64
1:5:415:LEU:HD11	1:6:433:VAL:HG21	1.79	0.64
1:C:426:ARG:NH2	1:C:428:ASP:OD2	2.28	0.64
1:S:248:ARG:NH2	1:T:242:GLU:OE1	2.31	0.64
1:X:373:ARG:HH21	1:Y:275:LYS:HD3	1.62	0.64
1:U:292:THR:HG21	1:V:282:TYR:HB3	1.79	0.64
1:D:426:ARG:NH2	1:D:428:ASP:OD2	2.28	0.64
1:J:426:ARG:NH2	1:J:428:ASP:OD2	2.28	0.64
1:R:426:ARG:NH2	1:R:428:ASP:OD2	2.28	0.63
1:F:418:GLU:HG3	1:G:431:ASN:HB3	1.80	0.63
1:X:426:ARG:NH2	1:X:428:ASP:OD2	2.28	0.63
1:3:373:ARG:HH21	1:4:275:LYS:HD3	1.63	0.63
1:2:248:ARG:NH2	1:3:242:GLU:OE1	2.30	0.63
1:3:426:ARG:NH2	1:3:428:ASP:OD2	2.28	0.63
1:K:373:ARG:HH21	1:L:275:LYS:HD3	1.63	0.63
1:A:274:ASN:HB2	1:6:376:LYS:HB3	1.78	0.63
1:1:248:ARG:NH2	1:2:242:GLU:OE1	2.32	0.63
1:D:392:ASN:OD1	1:D:393:TYR:N	2.32	0.63
1:F:392:ASN:OD1	1:F:393:TYR:N	2.32	0.63
1:I:392:ASN:OD1	1:I:393:TYR:N	2.32	0.62
1:K:392:ASN:OD1	1:K:393:TYR:N	2.32	0.62
1:U:290:LYS:HA	1:V:284:PRO:HB3	1.80	0.62
1:5:392:ASN:OD1	1:5:393:TYR:N	2.32	0.62
1:A:392:ASN:OD1	1:A:393:TYR:N	2.32	0.62
1:H:392:ASN:OD1	1:H:393:TYR:N	2.32	0.62
1:S:292:THR:HG21	1:T:282:TYR:HB3	1.81	0.62
1:B:392:ASN:OD1	1:B:393:TYR:N	2.32	0.62
1:G:392:ASN:OD1	1:G:393:TYR:N	2.32	0.62
1:N:392:ASN:OD1	1:N:393:TYR:N	2.32	0.62
1:J:373:ARG:HH21	1:K:275:LYS:HD3	1.63	0.62
1:M:392:ASN:OD1	1:M:393:TYR:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ASN:OD1	1:C:393:TYR:N	2.32	0.62
1:S:426:ARG:NH2	1:S:428:ASP:OD2	2.28	0.62
1:U:392:ASN:OD1	1:U:393:TYR:N	2.32	0.62
1:K:426:ARG:NH2	1:K:428:ASP:OD2	2.28	0.62
1:S:290:LYS:HA	1:T:284:PRO:HB3	1.81	0.62
1:S:392:ASN:OD1	1:S:393:TYR:N	2.32	0.62
1:W:392:ASN:OD1	1:W:393:TYR:N	2.32	0.62
1:Y:373:ARG:HH21	1:Z:275:LYS:CD	2.12	0.62
1:P:392:ASN:OD1	1:P:393:TYR:N	2.32	0.62
1:Q:392:ASN:OD1	1:Q:393:TYR:N	2.32	0.62
1:2:392:ASN:OD1	1:2:393:TYR:N	2.32	0.62
1:L:392:ASN:OD1	1:L:393:TYR:N	2.32	0.61
1:Y:392:ASN:OD1	1:Y:393:TYR:N	2.32	0.61
1:4:392:ASN:OD1	1:4:393:TYR:N	2.32	0.61
1:Y:426:ARG:NH2	1:Y:428:ASP:OD2	2.28	0.61
1:E:392:ASN:OD1	1:E:393:TYR:N	2.32	0.61
1:H:292:THR:HG21	1:I:282:TYR:HB3	1.83	0.61
1:J:392:ASN:OD1	1:J:393:TYR:N	2.32	0.61
1:1:392:ASN:OD1	1:1:393:TYR:N	2.32	0.61
1:6:392:ASN:OD1	1:6:393:TYR:N	2.32	0.61
1:3:392:ASN:OD1	1:3:393:TYR:N	2.32	0.61
1:4:426:ARG:NH2	1:4:428:ASP:OD2	2.28	0.61
1:Q:387:VAL:HG21	1:Q:420:MET:HG2	1.83	0.61
1:H:248:ARG:NH2	1:I:242:GLU:OE1	2.33	0.61
1:R:392:ASN:OD1	1:R:393:TYR:N	2.32	0.61
1:T:392:ASN:OD1	1:T:393:TYR:N	2.32	0.61
1:U:387:VAL:HG21	1:U:420:MET:HG2	1.83	0.61
1:3:292:THR:HG21	1:4:282:TYR:HB3	1.82	0.61
1:V:392:ASN:OD1	1:V:393:TYR:N	2.32	0.61
1:E:387:VAL:HG21	1:E:420:MET:HG2	1.83	0.61
1:F:387:VAL:HG21	1:F:420:MET:HG2	1.83	0.61
1:R:387:VAL:HG21	1:R:420:MET:HG2	1.83	0.61
1:V:387:VAL:HG21	1:V:420:MET:HG2	1.83	0.61
1:X:392:ASN:OD1	1:X:393:TYR:N	2.32	0.61
1:T:387:VAL:HG21	1:T:420:MET:HG2	1.83	0.60
1:D:387:VAL:HG21	1:D:420:MET:HG2	1.83	0.60
1:W:387:VAL:HG21	1:W:420:MET:HG2	1.83	0.60
1:P:387:VAL:HG21	1:P:420:MET:HG2	1.83	0.60
1:S:387:VAL:HG21	1:S:420:MET:HG2	1.83	0.60
1:Y:387:VAL:HG21	1:Y:420:MET:HG2	1.83	0.60
1:C:387:VAL:HG21	1:C:420:MET:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ARG:NH2	1:E:242:GLU:OE1	2.34	0.60
1:M:373:ARG:HH21	1:N:275:LYS:HD3	1.66	0.60
1:O:392:ASN:OD1	1:O:393:TYR:N	2.32	0.60
1:Z:392:ASN:OD1	1:Z:393:TYR:N	2.32	0.60
1:6:296:ARG:NH2	1:6:362:GLU:OE2	2.35	0.60
1:E:248:ARG:NH2	1:F:242:GLU:OE1	2.33	0.60
1:G:387:VAL:HG21	1:G:420:MET:HG2	1.83	0.60
1:N:418:GLU:OE1	1:O:429:THR:OG1	2.18	0.60
1:T:426:ARG:NH2	1:T:428:ASP:OD2	2.28	0.60
1:X:387:VAL:HG21	1:X:420:MET:HG2	1.83	0.60
1:Z:387:VAL:HG21	1:Z:420:MET:HG2	1.83	0.60
1:5:296:ARG:NH2	1:5:362:GLU:OE2	2.35	0.60
1:5:387:VAL:HG21	1:5:420:MET:HG2	1.83	0.60
1:6:387:VAL:HG21	1:6:420:MET:HG2	1.83	0.60
1:A:387:VAL:HG21	1:A:420:MET:HG2	1.83	0.60
1:P:292:THR:HG21	1:Q:282:TYR:HB3	1.84	0.60
1:4:296:ARG:NH2	1:4:362:GLU:OE2	2.35	0.60
1:A:296:ARG:NH2	1:A:362:GLU:OE2	2.35	0.60
1:B:387:VAL:HG21	1:B:420:MET:HG2	1.83	0.60
1:F:292:THR:HG21	1:G:282:TYR:HB3	1.83	0.60
1:K:299:ASN:HA	1:L:361:ASN:HA	1.84	0.60
1:L:248:ARG:NH2	1:M:242:GLU:OE1	2.35	0.60
1:O:387:VAL:HG21	1:O:420:MET:HG2	1.83	0.60
1:1:387:VAL:HG21	1:1:420:MET:HG2	1.83	0.60
1:B:296:ARG:NH2	1:B:362:GLU:OE2	2.35	0.60
1:L:426:ARG:NH2	1:L:428:ASP:OD2	2.28	0.60
1:1:415:LEU:HD11	1:2:433:VAL:HG21	1.84	0.60
1:3:296:ARG:NH2	1:3:362:GLU:OE2	2.35	0.60
1:H:387:VAL:HG21	1:H:420:MET:HG2	1.83	0.60
1:I:387:VAL:HG21	1:I:420:MET:HG2	1.83	0.60
1:4:387:VAL:HG21	1:4:420:MET:HG2	1.83	0.60
1:2:296:ARG:NH2	1:2:362:GLU:OE2	2.35	0.59
1:J:387:VAL:HG21	1:J:420:MET:HG2	1.83	0.59
1:N:387:VAL:HG21	1:N:420:MET:HG2	1.83	0.59
1:Z:299:ASN:N	1:Z:299:ASN:OD1	2.35	0.59
1:J:292:THR:HG21	1:K:282:TYR:HB3	1.84	0.59
1:K:387:VAL:HG21	1:K:420:MET:HG2	1.83	0.59
1:Y:299:ASN:OD1	1:Y:299:ASN:N	2.35	0.59
1:1:296:ARG:NH2	1:1:362:GLU:OE2	2.35	0.59
1:1:299:ASN:OD1	1:1:299:ASN:N	2.35	0.59
1:2:299:ASN:OD1	1:2:299:ASN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:387:VAL:HG21	1:L:420:MET:HG2	1.83	0.59
1:T:373:ARG:HH21	1:U:275:LYS:HD3	1.67	0.59
1:X:299:ASN:N	1:X:299:ASN:OD1	2.35	0.59
1:1:292:THR:HG21	1:2:282:TYR:HB3	1.83	0.59
1:1:373:ARG:HH21	1:2:275:LYS:HD3	1.66	0.59
1:2:387:VAL:HG21	1:2:420:MET:HG2	1.83	0.59
1:3:299:ASN:N	1:3:299:ASN:OD1	2.35	0.59
1:4:299:ASN:OD1	1:4:299:ASN:N	2.35	0.59
1:W:373:ARG:HH21	1:X:275:LYS:HD3	1.67	0.59
1:3:387:VAL:HG21	1:3:420:MET:HG2	1.83	0.59
1:V:248:ARG:NH2	1:W:242:GLU:OE1	2.35	0.59
1:Z:296:ARG:NH2	1:Z:362:GLU:OE2	2.35	0.59
1:M:387:VAL:HG21	1:M:420:MET:HG2	1.83	0.59
1:V:299:ASN:OD1	1:V:299:ASN:N	2.35	0.59
1:W:299:ASN:OD1	1:W:299:ASN:N	2.35	0.59
1:5:299:ASN:N	1:5:299:ASN:OD1	2.35	0.59
1:Q:296:ARG:NH2	1:Q:362:GLU:OE2	2.35	0.59
1:U:299:ASN:N	1:U:299:ASN:OD1	2.35	0.59
1:Y:296:ARG:NH2	1:Y:362:GLU:OE2	2.35	0.59
1:A:299:ASN:OD1	1:A:299:ASN:N	2.35	0.59
1:J:296:ARG:NH2	1:J:362:GLU:OE2	2.35	0.59
1:K:296:ARG:NH2	1:K:362:GLU:OE2	2.35	0.59
1:L:296:ARG:NH2	1:L:362:GLU:OE2	2.35	0.59
1:X:296:ARG:NH2	1:X:362:GLU:OE2	2.35	0.59
1:6:299:ASN:OD1	1:6:299:ASN:N	2.35	0.59
1:I:296:ARG:NH2	1:I:362:GLU:OE2	2.35	0.59
1:N:296:ARG:NH2	1:N:362:GLU:OE2	2.35	0.59
1:5:418:GLU:HG3	1:6:431:ASN:HB3	1.83	0.59
1:H:296:ARG:NH2	1:H:362:GLU:OE2	2.35	0.58
1:M:296:ARG:NH2	1:M:362:GLU:OE2	2.35	0.58
1:O:296:ARG:NH2	1:O:362:GLU:OE2	2.35	0.58
1:P:296:ARG:NH2	1:P:362:GLU:OE2	2.34	0.58
1:R:296:ARG:NH2	1:R:362:GLU:OE2	2.35	0.58
1:T:299:ASN:OD1	1:T:299:ASN:N	2.35	0.58
1:B:299:ASN:OD1	1:B:299:ASN:N	2.35	0.58
1:V:296:ARG:NH2	1:V:362:GLU:OE2	2.35	0.58
1:W:296:ARG:NH2	1:W:362:GLU:OE2	2.35	0.58
1:S:296:ARG:NH2	1:S:362:GLU:OE2	2.35	0.58
1:S:299:ASN:N	1:S:299:ASN:OD1	2.35	0.58
1:2:418:GLU:HG3	1:3:431:ASN:HB3	1.84	0.58
1:B:418:GLU:OE1	1:C:429:THR:OG1	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:296:ARG:NH2	1:U:362:GLU:OE2	2.35	0.58
1:Y:418:GLU:HG3	1:Z:431:ASN:HB3	1.86	0.58
1:B:248:ARG:NH2	1:C:242:GLU:OE1	2.37	0.58
1:C:299:ASN:OD1	1:C:299:ASN:N	2.35	0.58
1:R:299:ASN:OD1	1:R:299:ASN:N	2.35	0.58
1:T:296:ARG:NH2	1:T:362:GLU:OE2	2.35	0.58
1:U:418:GLU:OE1	1:V:429:THR:OG1	2.22	0.58
1:E:296:ARG:NH2	1:E:362:GLU:OE2	2.35	0.58
1:Q:299:ASN:OD1	1:Q:299:ASN:N	2.35	0.58
1:D:296:ARG:NH2	1:D:362:GLU:OE2	2.35	0.58
1:F:296:ARG:NH2	1:F:362:GLU:OE2	2.35	0.58
1:G:296:ARG:NH2	1:G:362:GLU:OE2	2.35	0.58
1:G:376:LYS:HB3	1:H:274:ASN:HB2	1.86	0.58
1:Q:373:ARG:HH21	1:R:275:LYS:CD	2.16	0.58
1:E:418:GLU:HG3	1:F:431:ASN:HB3	1.85	0.58
1:2:415:LEU:HD11	1:3:433:VAL:HG21	1.86	0.58
1:C:296:ARG:NH2	1:C:362:GLU:OE2	2.35	0.58
1:D:418:GLU:HG3	1:E:431:ASN:CB	2.33	0.58
1:D:299:ASN:N	1:D:299:ASN:OD1	2.35	0.57
1:E:299:ASN:OD1	1:E:299:ASN:N	2.35	0.57
1:I:248:ARG:NH2	1:J:242:GLU:OE1	2.38	0.57
1:W:418:GLU:OE1	1:X:429:THR:OG1	2.22	0.57
1:P:299:ASN:N	1:P:299:ASN:OD1	2.35	0.57
1:V:418:GLU:OE1	1:W:429:THR:OG1	2.23	0.57
1:F:299:ASN:N	1:F:299:ASN:OD1	2.35	0.57
1:Q:292:THR:HG21	1:R:282:TYR:HB3	1.87	0.57
1:I:290:LYS:HA	1:J:284:PRO:HB3	1.87	0.56
1:K:418:GLU:OE1	1:L:429:THR:OG1	2.20	0.56
1:1:418:GLU:OE1	1:2:429:THR:OG1	2.22	0.56
1:G:299:ASN:OD1	1:G:299:ASN:N	2.35	0.56
1:O:299:ASN:OD1	1:O:299:ASN:N	2.35	0.56
1:R:415:LEU:HD22	1:S:388:ALA:HB1	1.87	0.56
1:U:369:ASP:HA	1:V:280:GLU:O	2.05	0.56
1:J:271:ASP:HB2	1:J:383:GLU:HG3	1.88	0.56
1:N:299:ASN:N	1:N:299:ASN:OD1	2.35	0.56
1:O:271:ASP:HB2	1:O:383:GLU:HG3	1.88	0.56
1:I:271:ASP:HB2	1:I:383:GLU:HG3	1.88	0.56
1:K:271:ASP:HB2	1:K:383:GLU:HG3	1.88	0.56
1:P:271:ASP:HB2	1:P:383:GLU:HG3	1.88	0.56
1:Q:271:ASP:HB2	1:Q:383:GLU:HG3	1.88	0.56
1:J:299:ASN:OD1	1:J:299:ASN:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:271:ASP:HB2	1:N:383:GLU:HG3	1.88	0.56
1:B:373:ARG:HH21	1:C:275:LYS:HD3	1.71	0.56
1:C:292:THR:HG21	1:D:282:TYR:HB3	1.85	0.56
1:E:271:ASP:HB2	1:E:383:GLU:HG3	1.88	0.56
1:G:271:ASP:HB2	1:G:383:GLU:HG3	1.88	0.56
1:H:299:ASN:OD1	1:H:299:ASN:N	2.35	0.56
1:L:271:ASP:HB2	1:L:383:GLU:HG3	1.88	0.56
1:M:271:ASP:HB2	1:M:383:GLU:HG3	1.88	0.56
1:R:271:ASP:HB2	1:R:383:GLU:HG3	1.88	0.56
1:U:271:ASP:HB2	1:U:383:GLU:HG3	1.88	0.56
1:H:271:ASP:HB2	1:H:383:GLU:HG3	1.88	0.56
1:K:266:VAL:HG22	1:K:387:VAL:HG22	1.88	0.56
1:T:271:ASP:HB2	1:T:383:GLU:HG3	1.88	0.56
1:V:271:ASP:HB2	1:V:383:GLU:HG3	1.88	0.56
1:4:266:VAL:HG22	1:4:387:VAL:HG22	1.88	0.56
1:B:266:VAL:HG22	1:B:387:VAL:HG22	1.88	0.56
1:D:271:ASP:HB2	1:D:383:GLU:HG3	1.88	0.56
1:K:299:ASN:N	1:K:299:ASN:OD1	2.35	0.56
1:L:299:ASN:OD1	1:L:299:ASN:N	2.35	0.56
1:M:299:ASN:OD1	1:M:299:ASN:N	2.35	0.56
1:3:266:VAL:HG22	1:3:387:VAL:HG22	1.88	0.56
1:B:418:GLU:HG3	1:C:431:ASN:HB3	1.88	0.56
1:C:271:ASP:HB2	1:C:383:GLU:HG3	1.88	0.56
1:G:266:VAL:HG22	1:G:387:VAL:HG22	1.88	0.56
1:L:266:VAL:HG22	1:L:387:VAL:HG22	1.88	0.56
1:S:271:ASP:HB2	1:S:383:GLU:HG3	1.88	0.56
1:W:271:ASP:HB2	1:W:383:GLU:HG3	1.88	0.56
1:C:266:VAL:HG22	1:C:387:VAL:HG22	1.88	0.55
1:F:271:ASP:HB2	1:F:383:GLU:HG3	1.88	0.55
1:I:299:ASN:N	1:I:299:ASN:OD1	2.35	0.55
1:J:231:ASN:N	1:J:231:ASN:OD1	2.40	0.55
1:N:231:ASN:OD1	1:N:231:ASN:N	2.40	0.55
1:F:266:VAL:HG22	1:F:387:VAL:HG22	1.88	0.55
1:K:231:ASN:OD1	1:K:231:ASN:N	2.40	0.55
1:L:231:ASN:N	1:L:231:ASN:OD1	2.40	0.55
1:M:231:ASN:OD1	1:M:231:ASN:N	2.40	0.55
1:O:231:ASN:N	1:O:231:ASN:OD1	2.40	0.55
1:X:271:ASP:HB2	1:X:383:GLU:HG3	1.88	0.55
1:Y:271:ASP:HB2	1:Y:383:GLU:HG3	1.88	0.55
1:5:271:ASP:HB2	1:5:383:GLU:HG3	1.88	0.55
1:6:271:ASP:HB2	1:6:383:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLU:OE1	1:6:248:ARG:NH2	2.39	0.55
1:B:271:ASP:HB2	1:B:383:GLU:HG3	1.88	0.55
1:H:266:VAL:HG22	1:H:387:VAL:HG22	1.88	0.55
1:I:231:ASN:OD1	1:I:231:ASN:N	2.40	0.55
1:P:231:ASN:OD1	1:P:231:ASN:N	2.40	0.55
1:R:373:ARG:HH21	1:S:275:LYS:CD	2.19	0.55
1:S:373:ARG:HH21	1:T:275:LYS:CD	2.19	0.55
1:W:266:VAL:HG22	1:W:387:VAL:HG22	1.88	0.55
1:X:266:VAL:HG22	1:X:387:VAL:HG22	1.88	0.55
1:4:271:ASP:HB2	1:4:383:GLU:HG3	1.88	0.55
1:A:250:GLU:O	1:A:254:SER:OG	2.20	0.55
1:P:266:VAL:HG22	1:P:387:VAL:HG22	1.88	0.55
1:Q:266:VAL:HG22	1:Q:387:VAL:HG22	1.88	0.55
1:W:290:LYS:HA	1:X:284:PRO:HB3	1.88	0.55
1:Z:250:GLU:O	1:Z:254:SER:OG	2.19	0.55
1:Z:271:ASP:HB2	1:Z:383:GLU:HG3	1.88	0.55
1:H:231:ASN:OD1	1:H:231:ASN:N	2.40	0.55
1:J:266:VAL:HG22	1:J:387:VAL:HG22	1.88	0.55
1:X:404:LEU:H	1:X:434:ASN:ND2	2.05	0.55
1:X:418:GLU:OE1	1:Y:429:THR:OG1	2.23	0.55
1:1:271:ASP:HB2	1:1:383:GLU:HG3	1.88	0.55
1:2:266:VAL:HG22	1:2:387:VAL:HG22	1.88	0.55
1:5:266:VAL:HG22	1:5:387:VAL:HG22	1.88	0.55
1:A:266:VAL:HG22	1:A:387:VAL:HG22	1.88	0.55
1:A:404:LEU:H	1:A:434:ASN:ND2	2.05	0.55
1:M:266:VAL:HG22	1:M:387:VAL:HG22	1.88	0.55
1:R:266:VAL:HG22	1:R:387:VAL:HG22	1.88	0.55
1:V:373:ARG:HH21	1:W:275:LYS:HD3	1.72	0.55
1:1:418:GLU:HG3	1:2:431:ASN:CB	2.36	0.55
1:3:271:ASP:HB2	1:3:383:GLU:HG3	1.88	0.55
1:A:271:ASP:HB2	1:A:383:GLU:HG3	1.88	0.55
1:C:373:ARG:HH21	1:D:275:LYS:HD3	1.70	0.55
1:E:404:LEU:H	1:E:434:ASN:ND2	2.05	0.55
1:N:404:LEU:H	1:N:434:ASN:ND2	2.05	0.55
1:O:404:LEU:H	1:O:434:ASN:ND2	2.05	0.55
1:S:404:LEU:H	1:S:434:ASN:ND2	2.05	0.55
1:W:404:LEU:H	1:W:434:ASN:ND2	2.05	0.55
1:Y:266:VAL:HG22	1:Y:387:VAL:HG22	1.88	0.55
1:2:231:ASN:OD1	1:2:231:ASN:N	2.40	0.55
1:2:404:LEU:H	1:2:434:ASN:ND2	2.05	0.55
1:6:404:LEU:H	1:6:434:ASN:ND2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:VAL:HG22	1:E:387:VAL:HG22	1.88	0.55
1:J:404:LEU:H	1:J:434:ASN:ND2	2.05	0.55
1:Q:404:LEU:H	1:Q:434:ASN:ND2	2.05	0.55
1:Y:404:LEU:H	1:Y:434:ASN:ND2	2.05	0.55
1:3:231:ASN:OD1	1:3:231:ASN:N	2.40	0.55
1:4:404:LEU:H	1:4:434:ASN:ND2	2.05	0.55
1:5:404:LEU:H	1:5:434:ASN:ND2	2.05	0.55
1:D:266:VAL:HG22	1:D:387:VAL:HG22	1.88	0.55
1:K:404:LEU:H	1:K:434:ASN:ND2	2.05	0.55
1:T:404:LEU:H	1:T:434:ASN:ND2	2.05	0.55
1:V:266:VAL:HG22	1:V:387:VAL:HG22	1.88	0.55
1:2:271:ASP:HB2	1:2:383:GLU:HG3	1.88	0.55
1:3:404:LEU:H	1:3:434:ASN:ND2	2.05	0.55
1:4:231:ASN:N	1:4:231:ASN:OD1	2.40	0.55
1:D:404:LEU:H	1:D:434:ASN:ND2	2.05	0.55
1:O:266:VAL:HG22	1:O:387:VAL:HG22	1.88	0.55
1:R:248:ARG:NH2	1:S:242:GLU:OE1	2.40	0.55
1:5:231:ASN:OD1	1:5:231:ASN:N	2.40	0.55
1:F:404:LEU:H	1:F:434:ASN:ND2	2.05	0.54
1:G:231:ASN:N	1:G:231:ASN:OD1	2.40	0.54
1:I:404:LEU:H	1:I:434:ASN:ND2	2.05	0.54
1:K:292:THR:HG21	1:L:282:TYR:HB3	1.89	0.54
1:P:404:LEU:H	1:P:434:ASN:ND2	2.05	0.54
1:R:404:LEU:H	1:R:434:ASN:ND2	2.05	0.54
1:1:404:LEU:H	1:1:434:ASN:ND2	2.05	0.54
1:E:231:ASN:N	1:E:231:ASN:OD1	2.40	0.54
1:P:373:ARG:NH2	1:Q:275:LYS:HD3	2.18	0.54
1:S:266:VAL:HG22	1:S:387:VAL:HG22	1.88	0.54
1:V:404:LEU:H	1:V:434:ASN:ND2	2.05	0.54
1:6:231:ASN:N	1:6:231:ASN:OD1	2.40	0.54
1:B:404:LEU:H	1:B:434:ASN:ND2	2.05	0.54
1:F:231:ASN:OD1	1:F:231:ASN:N	2.40	0.54
1:F:373:ARG:HH21	1:G:275:LYS:HD3	1.71	0.54
1:Z:266:VAL:HG22	1:Z:387:VAL:HG22	1.88	0.54
1:6:266:VAL:HG22	1:6:387:VAL:HG22	1.88	0.54
1:C:231:ASN:OD1	1:C:231:ASN:N	2.40	0.54
1:D:231:ASN:OD1	1:D:231:ASN:N	2.40	0.54
1:M:404:LEU:H	1:M:434:ASN:ND2	2.05	0.54
1:Z:404:LEU:H	1:Z:434:ASN:ND2	2.05	0.54
1:A:231:ASN:OD1	1:A:231:ASN:N	2.40	0.54
1:B:231:ASN:OD1	1:B:231:ASN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:VAL:HG22	1:I:387:VAL:HG22	1.88	0.54
1:1:266:VAL:HG22	1:1:387:VAL:HG22	1.88	0.54
1:4:411:GLN:NE2	1:5:435:SER:OG	2.40	0.54
1:N:266:VAL:HG22	1:N:387:VAL:HG22	1.88	0.54
1:U:404:LEU:H	1:U:434:ASN:ND2	2.05	0.54
1:Z:248:ARG:NH2	1:1:242:GLU:OE1	2.40	0.54
1:E:364:SER:O	1:E:365:ASN:ND2	2.41	0.54
1:H:373:ARG:HH21	1:I:275:LYS:CD	2.20	0.54
1:H:404:LEU:H	1:H:434:ASN:ND2	2.05	0.54
1:L:404:LEU:H	1:L:434:ASN:ND2	2.05	0.54
1:S:418:GLU:OE1	1:T:429:THR:OG1	2.24	0.54
1:5:364:SER:O	1:5:365:ASN:ND2	2.41	0.54
1:C:404:LEU:H	1:C:434:ASN:ND2	2.05	0.54
1:F:364:SER:O	1:F:365:ASN:ND2	2.41	0.54
1:U:364:SER:O	1:U:365:ASN:ND2	2.41	0.54
1:Z:364:SER:O	1:Z:365:ASN:ND2	2.41	0.54
1:1:364:SER:O	1:1:365:ASN:ND2	2.41	0.54
1:6:364:SER:O	1:6:365:ASN:ND2	2.41	0.54
1:G:404:LEU:H	1:G:434:ASN:ND2	2.05	0.53
1:Q:373:ARG:NH2	1:R:275:LYS:HD3	2.23	0.53
1:T:364:SER:O	1:T:365:ASN:ND2	2.41	0.53
1:U:266:VAL:HG22	1:U:387:VAL:HG22	1.88	0.53
1:A:364:SER:O	1:A:365:ASN:ND2	2.41	0.53
1:D:364:SER:O	1:D:365:ASN:ND2	2.41	0.53
1:M:292:THR:HG21	1:N:282:TYR:HB3	1.90	0.53
1:P:364:SER:O	1:P:365:ASN:ND2	2.41	0.53
1:V:364:SER:O	1:V:365:ASN:ND2	2.41	0.53
1:2:364:SER:O	1:2:365:ASN:ND2	2.41	0.53
1:J:364:SER:O	1:J:365:ASN:ND2	2.41	0.53
1:R:364:SER:O	1:R:365:ASN:ND2	2.41	0.53
1:Y:364:SER:O	1:Y:365:ASN:ND2	2.41	0.53
1:I:364:SER:O	1:I:365:ASN:ND2	2.41	0.53
1:K:364:SER:O	1:K:365:ASN:ND2	2.41	0.53
1:O:364:SER:O	1:O:365:ASN:ND2	2.41	0.53
1:Q:364:SER:O	1:Q:365:ASN:ND2	2.41	0.53
1:T:266:VAL:HG22	1:T:387:VAL:HG22	1.88	0.53
1:3:364:SER:O	1:3:365:ASN:ND2	2.41	0.53
1:4:364:SER:O	1:4:365:ASN:ND2	2.41	0.53
1:M:364:SER:O	1:M:365:ASN:ND2	2.41	0.53
1:G:364:SER:O	1:G:365:ASN:ND2	2.41	0.53
1:H:364:SER:O	1:H:365:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:364:SER:O	1:L:365:ASN:ND2	2.41	0.53
1:S:364:SER:O	1:S:365:ASN:ND2	2.41	0.53
1:W:364:SER:O	1:W:365:ASN:ND2	2.41	0.53
1:G:373:ARG:HH21	1:H:275:LYS:HD3	1.74	0.53
1:K:369:ASP:HA	1:L:280:GLU:O	2.08	0.53
1:N:364:SER:O	1:N:365:ASN:ND2	2.41	0.53
1:S:418:GLU:HG3	1:T:431:ASN:HB3	1.90	0.53
1:B:364:SER:O	1:B:365:ASN:ND2	2.41	0.53
1:C:364:SER:O	1:C:365:ASN:ND2	2.41	0.53
1:I:231:ASN:N	1:I:231:ASN:OD1	2.40	0.53
1:G:248:ARG:NH2	1:H:242:GLU:OE1	2.41	0.53
1:Z:231:ASN:OD1	1:Z:231:ASN:N	2.40	0.53
1:3:373:ARG:HH21	1:4:275:LYS:CD	2.22	0.53
1:X:364:SER:O	1:X:365:ASN:ND2	2.41	0.53
1:Y:231:ASN:OD1	1:Y:231:ASN:N	2.40	0.53
1:A:373:ARG:HH21	1:B:275:LYS:HD3	1.74	0.52
1:S:369:ASP:HA	1:T:280:GLU:O	2.09	0.52
1:A:433:VAL:HG21	1:6:415:LEU:HD11	1.91	0.52
1:K:248:ARG:NH2	1:L:242:GLU:OE1	2.43	0.52
1:W:231:ASN:OD1	1:W:231:ASN:N	2.40	0.52
1:X:231:ASN:N	1:X:231:ASN:OD1	2.40	0.52
1:Y:373:ARG:NH2	1:Z:275:LYS:NZ	2.57	0.52
1:Q:231:ASN:N	1:Q:231:ASN:OD1	2.40	0.52
1:V:231:ASN:N	1:V:231:ASN:OD1	2.40	0.52
1:X:292:THR:HG21	1:Y:282:TYR:HB3	1.91	0.52
1:R:231:ASN:OD1	1:R:231:ASN:N	2.40	0.52
1:S:231:ASN:OD1	1:S:231:ASN:N	2.40	0.52
1:T:231:ASN:OD1	1:T:231:ASN:N	2.40	0.52
1:U:231:ASN:OD1	1:U:231:ASN:N	2.40	0.52
1:4:415:LEU:HD21	1:5:433:VAL:HG22	1.91	0.52
1:5:418:GLU:HG3	1:6:431:ASN:CB	2.39	0.52
1:R:415:LEU:CD2	1:S:388:ALA:HB1	2.40	0.52
1:C:389:VAL:HG21	1:C:416:THR:HG21	1.92	0.51
1:F:250:GLU:O	1:F:254:SER:OG	2.19	0.51
1:A:389:VAL:HG21	1:A:416:THR:HG21	1.92	0.51
1:R:418:GLU:OE1	1:S:429:THR:OG1	2.27	0.51
1:4:389:VAL:HG21	1:4:416:THR:HG21	1.92	0.51
1:6:389:VAL:HG21	1:6:416:THR:HG21	1.92	0.51
1:D:389:VAL:HG21	1:D:416:THR:HG21	1.92	0.51
1:F:389:VAL:HG21	1:F:416:THR:HG21	1.92	0.51
1:A:248:ARG:NH2	1:B:242:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:373:ARG:HH21	1:P:275:LYS:HD3	1.74	0.51
1:5:389:VAL:HG21	1:5:416:THR:HG21	1.92	0.51
1:B:389:VAL:HG21	1:B:416:THR:HG21	1.92	0.51
1:E:389:VAL:HG21	1:E:416:THR:HG21	1.92	0.51
1:Y:373:ARG:NH2	1:Z:275:LYS:HD3	2.23	0.51
1:L:292:THR:HG21	1:M:282:TYR:HB3	1.92	0.51
1:G:389:VAL:HG21	1:G:416:THR:HG21	1.92	0.51
1:I:418:GLU:OE1	1:J:429:THR:OG1	2.27	0.51
1:R:389:VAL:HG21	1:R:416:THR:HG21	1.92	0.51
1:S:389:VAL:HG21	1:S:416:THR:HG21	1.92	0.51
1:2:389:VAL:HG21	1:2:416:THR:HG21	1.92	0.51
1:H:389:VAL:HG21	1:H:416:THR:HG21	1.92	0.51
1:1:411:GLN:NE2	1:2:435:SER:OG	2.39	0.51
1:A:418:GLU:HG3	1:B:431:ASN:HB3	1.93	0.51
1:3:389:VAL:HG21	1:3:416:THR:HG21	1.92	0.51
1:N:248:ARG:NH2	1:O:242:GLU:OE1	2.44	0.51
1:Q:389:VAL:HG21	1:Q:416:THR:HG21	1.92	0.51
1:Q:303:GLN:HA	1:R:357:SER:HA	1.92	0.50
1:T:389:VAL:HG21	1:T:416:THR:HG21	1.92	0.50
1:H:369:ASP:HA	1:I:280:GLU:O	2.12	0.50
1:Z:389:VAL:HG21	1:Z:416:THR:HG21	1.92	0.50
1:1:389:VAL:HG21	1:1:416:THR:HG21	1.92	0.50
1:B:292:THR:HG21	1:C:282:TYR:HB3	1.93	0.50
1:I:389:VAL:HG21	1:I:416:THR:HG21	1.92	0.50
1:Q:415:LEU:HD22	1:R:388:ALA:HB1	1.93	0.50
1:5:248:ARG:NH2	1:6:242:GLU:OE1	2.44	0.50
1:A:292:THR:HG21	1:B:282:TYR:HB3	1.94	0.50
1:R:292:THR:HG21	1:S:282:TYR:HB3	1.94	0.50
1:P:389:VAL:HG21	1:P:416:THR:HG21	1.92	0.50
1:J:357:SER:O	1:J:357:SER:OG	2.29	0.50
1:J:389:VAL:HG21	1:J:416:THR:HG21	1.92	0.50
1:K:389:VAL:HG21	1:K:416:THR:HG21	1.92	0.50
1:L:389:VAL:HG21	1:L:416:THR:HG21	1.92	0.50
1:W:292:THR:HG21	1:X:282:TYR:HB3	1.93	0.50
1:Y:373:ARG:HH21	1:Z:275:LYS:CE	2.24	0.50
1:L:373:ARG:HH21	1:M:275:LYS:HD3	1.77	0.50
1:U:389:VAL:HG21	1:U:416:THR:HG21	1.92	0.50
1:Y:389:VAL:HG21	1:Y:416:THR:HG21	1.92	0.50
1:M:389:VAL:HG21	1:M:416:THR:HG21	1.92	0.50
1:P:376:LYS:HB3	1:Q:274:ASN:HB2	1.93	0.50
1:U:303:GLN:HA	1:V:357:SER:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:389:VAL:HG21	1:X:416:THR:HG21	1.92	0.50
1:N:357:SER:O	1:N:357:SER:OG	2.29	0.50
1:R:373:ARG:NH2	1:S:275:LYS:HD3	2.25	0.49
1:W:389:VAL:HG21	1:W:416:THR:HG21	1.92	0.49
1:E:418:GLU:HG3	1:F:431:ASN:CB	2.42	0.49
1:F:415:LEU:HD11	1:G:433:VAL:HG21	1.94	0.49
1:F:418:GLU:OE1	1:G:429:THR:OG1	2.30	0.49
1:J:373:ARG:HH21	1:K:275:LYS:CD	2.25	0.49
1:O:357:SER:O	1:O:357:SER:OG	2.29	0.49
1:N:389:VAL:HG21	1:N:416:THR:HG21	1.92	0.49
1:O:389:VAL:HG21	1:O:416:THR:HG21	1.92	0.49
1:V:389:VAL:HG21	1:V:416:THR:HG21	1.92	0.49
1:O:376:LYS:HB3	1:P:274:ASN:HB2	1.93	0.49
1:A:431:ASN:HB3	1:6:418:GLU:HG3	1.94	0.49
1:M:250:GLU:O	1:M:254:SER:OG	2.19	0.49
1:W:414:ASP:O	1:W:418:GLU:HG2	2.13	0.49
1:L:414:ASP:O	1:L:418:GLU:HG2	2.13	0.49
1:M:414:ASP:O	1:M:418:GLU:HG2	2.13	0.49
1:P:241:VAL:CG2	1:Q:235:LEU:HD11	2.43	0.49
1:P:357:SER:O	1:P:357:SER:OG	2.29	0.49
1:Y:369:ASP:HA	1:Z:280:GLU:O	2.13	0.49
1:I:414:ASP:O	1:I:418:GLU:HG2	2.13	0.49
1:J:414:ASP:O	1:J:418:GLU:HG2	2.13	0.49
1:K:414:ASP:O	1:K:418:GLU:HG2	2.13	0.49
1:V:414:ASP:O	1:V:418:GLU:HG2	2.13	0.49
1:X:414:ASP:O	1:X:418:GLU:HG2	2.13	0.49
1:N:414:ASP:O	1:N:418:GLU:HG2	2.13	0.48
1:U:414:ASP:O	1:U:418:GLU:HG2	2.13	0.48
1:B:357:SER:O	1:B:357:SER:OG	2.29	0.48
1:H:414:ASP:O	1:H:418:GLU:HG2	2.13	0.48
1:I:373:ARG:HH21	1:J:275:LYS:CD	2.25	0.48
1:O:241:VAL:HG22	1:P:235:LEU:HD21	1.95	0.48
1:I:292:THR:HG21	1:J:282:TYR:HB3	1.94	0.48
1:Y:414:ASP:O	1:Y:418:GLU:HG2	2.13	0.48
1:C:357:SER:O	1:C:357:SER:OG	2.29	0.48
1:D:357:SER:O	1:D:357:SER:OG	2.29	0.48
1:O:414:ASP:O	1:O:418:GLU:HG2	2.13	0.48
1:T:414:ASP:O	1:T:418:GLU:HG2	2.13	0.48
1:Z:414:ASP:O	1:Z:418:GLU:HG2	2.13	0.48
1:A:280:GLU:O	1:6:369:ASP:HA	2.14	0.48
1:A:414:ASP:O	1:A:418:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ASP:O	1:B:418:GLU:HG2	2.13	0.48
1:Q:369:ASP:HA	1:R:280:GLU:O	2.13	0.48
1:X:290:LYS:HA	1:Y:284:PRO:HB3	1.95	0.48
1:5:357:SER:O	1:5:357:SER:OG	2.29	0.48
1:6:357:SER:O	1:6:357:SER:OG	2.29	0.48
1:A:357:SER:O	1:A:357:SER:OG	2.29	0.48
1:C:414:ASP:O	1:C:418:GLU:HG2	2.13	0.48
1:E:357:SER:O	1:E:357:SER:OG	2.29	0.48
1:1:414:ASP:O	1:1:418:GLU:HG2	2.13	0.48
1:6:414:ASP:O	1:6:418:GLU:HG2	2.13	0.48
1:D:414:ASP:O	1:D:418:GLU:HG2	2.13	0.48
1:E:248:ARG:NH1	1:F:267:THR:HG23	2.29	0.48
1:2:414:ASP:O	1:2:418:GLU:HG2	2.13	0.48
1:4:357:SER:O	1:4:357:SER:OG	2.29	0.48
1:4:363:THR:HG22	1:4:364:SER:H	1.78	0.48
1:5:414:ASP:O	1:5:418:GLU:HG2	2.13	0.48
1:G:414:ASP:O	1:G:418:GLU:HG2	2.13	0.48
1:I:369:ASP:HA	1:J:280:GLU:O	2.14	0.48
1:K:290:LYS:HA	1:L:284:PRO:CB	2.44	0.48
1:P:414:ASP:O	1:P:418:GLU:HG2	2.13	0.48
1:Q:414:ASP:O	1:Q:418:GLU:HG2	2.13	0.48
1:T:290:LYS:HA	1:U:284:PRO:HB3	1.95	0.48
1:2:363:THR:HG22	1:2:364:SER:H	1.79	0.48
1:S:414:ASP:O	1:S:418:GLU:HG2	2.13	0.48
1:X:413:GLU:HG2	1:X:417:ARG:HH12	1.79	0.48
1:Z:363:THR:HG22	1:Z:364:SER:H	1.79	0.48
1:Z:413:GLU:HG2	1:Z:417:ARG:HH12	1.79	0.48
1:1:363:THR:HG22	1:1:364:SER:H	1.79	0.48
1:4:414:ASP:O	1:4:418:GLU:HG2	2.13	0.48
1:E:414:ASP:O	1:E:418:GLU:HG2	2.13	0.48
1:3:357:SER:O	1:3:357:SER:OG	2.29	0.48
1:3:414:ASP:O	1:3:418:GLU:HG2	2.13	0.48
1:F:414:ASP:O	1:F:418:GLU:HG2	2.13	0.47
1:F:418:GLU:HG3	1:G:431:ASN:CB	2.43	0.47
1:N:417:ARG:HG3	1:N:422:PHE:CB	2.45	0.47
1:S:424:ASP:N	1:S:424:ASP:OD1	2.48	0.47
1:T:413:GLU:HG2	1:T:417:ARG:HH12	1.79	0.47
1:V:413:GLU:HG2	1:V:417:ARG:HH12	1.79	0.47
1:V:424:ASP:OD1	1:V:424:ASP:N	2.47	0.47
1:2:413:GLU:HG2	1:2:417:ARG:HH12	1.79	0.47
1:3:363:THR:HG22	1:3:364:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:SER:O	1:F:357:SER:OG	2.29	0.47
1:L:363:THR:HG22	1:L:364:SER:H	1.79	0.47
1:M:417:ARG:HG3	1:M:422:PHE:CB	2.45	0.47
1:R:414:ASP:O	1:R:418:GLU:HG2	2.13	0.47
1:C:417:ARG:HG3	1:C:422:PHE:CB	2.45	0.47
1:D:413:GLU:HG2	1:D:417:ARG:HH12	1.79	0.47
1:G:413:GLU:HG2	1:G:417:ARG:HH12	1.79	0.47
1:I:413:GLU:HG2	1:I:417:ARG:HH12	1.79	0.47
1:L:413:GLU:HG2	1:L:417:ARG:HH12	1.79	0.47
1:L:417:ARG:HG3	1:L:422:PHE:CB	2.44	0.47
1:N:413:GLU:HG2	1:N:417:ARG:HH12	1.79	0.47
1:O:417:ARG:HG3	1:O:422:PHE:CB	2.45	0.47
1:P:413:GLU:HG2	1:P:417:ARG:HH12	1.79	0.47
1:R:357:SER:O	1:R:357:SER:OG	2.29	0.47
1:R:417:ARG:HG3	1:R:422:PHE:CB	2.45	0.47
1:U:424:ASP:OD1	1:U:424:ASP:N	2.47	0.47
1:4:413:GLU:HG2	1:4:417:ARG:HH12	1.79	0.47
1:B:413:GLU:HG2	1:B:417:ARG:HH12	1.79	0.47
1:C:413:GLU:HG2	1:C:417:ARG:HH12	1.79	0.47
1:D:417:ARG:HG3	1:D:422:PHE:CB	2.45	0.47
1:E:413:GLU:HG2	1:E:417:ARG:HH12	1.79	0.47
1:E:417:ARG:HG3	1:E:422:PHE:CB	2.45	0.47
1:G:363:THR:HG22	1:G:364:SER:H	1.78	0.47
1:M:363:THR:HG22	1:M:364:SER:H	1.79	0.47
1:P:417:ARG:HG3	1:P:422:PHE:CB	2.45	0.47
1:Q:417:ARG:HG3	1:Q:422:PHE:CB	2.45	0.47
1:R:413:GLU:HG2	1:R:417:ARG:HH12	1.79	0.47
1:R:424:ASP:OD1	1:R:424:ASP:N	2.47	0.47
1:S:417:ARG:HG3	1:S:422:PHE:CB	2.45	0.47
1:T:418:GLU:OE1	1:U:429:THR:OG1	2.29	0.47
1:X:418:GLU:HG3	1:Y:431:ASN:HB3	1.97	0.47
1:Y:363:THR:HG22	1:Y:364:SER:H	1.79	0.47
1:2:418:GLU:HG3	1:3:431:ASN:CB	2.44	0.47
1:5:363:THR:HG22	1:5:364:SER:H	1.79	0.47
1:B:417:ARG:HG3	1:B:422:PHE:CB	2.45	0.47
1:C:363:THR:HG22	1:C:364:SER:H	1.79	0.47
1:F:413:GLU:HG2	1:F:417:ARG:HH12	1.79	0.47
1:H:290:LYS:HA	1:I:284:PRO:HB3	1.97	0.47
1:H:363:THR:HG22	1:H:364:SER:H	1.79	0.47
1:H:417:ARG:HG3	1:H:422:PHE:CB	2.45	0.47
1:J:413:GLU:HG2	1:J:417:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:417:ARG:HG3	1:V:422:PHE:CB	2.45	0.47
1:X:424:ASP:N	1:X:424:ASP:OD1	2.47	0.47
1:5:413:GLU:HG2	1:5:417:ARG:HH12	1.79	0.47
1:6:417:ARG:HG3	1:6:422:PHE:CB	2.44	0.47
1:A:417:ARG:HG3	1:A:422:PHE:CB	2.45	0.47
1:B:363:THR:HG22	1:B:364:SER:H	1.79	0.47
1:G:357:SER:O	1:G:357:SER:OG	2.29	0.47
1:I:363:THR:HG22	1:I:364:SER:H	1.79	0.47
1:K:413:GLU:HG2	1:K:417:ARG:HH12	1.79	0.47
1:S:373:ARG:NH2	1:T:275:LYS:HD3	2.25	0.47
1:A:413:GLU:HG2	1:A:417:ARG:HH12	1.79	0.47
1:B:415:LEU:HD11	1:C:433:VAL:HG21	1.97	0.47
1:D:285:ASN:ND2	1:D:368:VAL:HG12	2.30	0.47
1:F:417:ARG:HG3	1:F:422:PHE:CB	2.45	0.47
1:H:241:VAL:HG22	1:I:235:LEU:HD21	1.96	0.47
1:H:357:SER:O	1:H:357:SER:OG	2.29	0.47
1:K:285:ASN:ND2	1:K:368:VAL:HG12	2.30	0.47
1:K:417:ARG:HG3	1:K:422:PHE:CB	2.45	0.47
1:M:413:GLU:HG2	1:M:417:ARG:HH12	1.79	0.47
1:O:363:THR:HG22	1:O:364:SER:H	1.79	0.47
1:P:363:THR:HG22	1:P:364:SER:H	1.79	0.47
1:Q:363:THR:HG22	1:Q:364:SER:H	1.79	0.47
1:Q:413:GLU:HG2	1:Q:417:ARG:HH12	1.79	0.47
1:Q:418:GLU:OE1	1:R:429:THR:OG1	2.32	0.47
1:R:250:GLU:O	1:R:254:SER:OG	2.20	0.47
1:S:285:ASN:ND2	1:S:368:VAL:HG12	2.30	0.47
1:U:363:THR:HG22	1:U:364:SER:H	1.79	0.47
1:V:363:THR:HG22	1:V:364:SER:H	1.79	0.47
1:W:417:ARG:HG3	1:W:422:PHE:CB	2.45	0.47
1:W:424:ASP:OD1	1:W:424:ASP:N	2.47	0.47
1:X:417:ARG:HG3	1:X:422:PHE:CB	2.45	0.47
1:Z:417:ARG:HG3	1:Z:422:PHE:CB	2.45	0.47
1:1:357:SER:O	1:1:357:SER:OG	2.29	0.47
1:1:424:ASP:N	1:1:424:ASP:OD1	2.47	0.47
1:2:285:ASN:ND2	1:2:368:VAL:HG12	2.30	0.47
1:3:413:GLU:HG2	1:3:417:ARG:HH12	1.79	0.47
1:4:417:ARG:HG3	1:4:422:PHE:CB	2.45	0.47
1:6:413:GLU:HG2	1:6:417:ARG:HH12	1.79	0.47
1:H:413:GLU:HG2	1:H:417:ARG:HH12	1.79	0.47
1:I:285:ASN:ND2	1:I:368:VAL:HG12	2.30	0.47
1:I:417:ARG:HG3	1:I:422:PHE:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:363:THR:HG22	1:J:364:SER:H	1.79	0.47
1:T:357:SER:O	1:T:357:SER:OG	2.29	0.47
1:V:285:ASN:ND2	1:V:368:VAL:HG12	2.30	0.47
1:W:250:GLU:O	1:W:254:SER:OG	2.20	0.47
1:Y:285:ASN:ND2	1:Y:368:VAL:HG12	2.30	0.47
1:Y:417:ARG:HG3	1:Y:422:PHE:CB	2.45	0.47
1:1:413:GLU:HG2	1:1:417:ARG:HH12	1.79	0.47
1:5:285:ASN:ND2	1:5:368:VAL:HG12	2.30	0.47
1:5:417:ARG:HG3	1:5:422:PHE:CB	2.45	0.47
1:A:418:GLU:OE1	1:B:429:THR:OG1	2.31	0.47
1:C:250:GLU:O	1:C:254:SER:OG	2.20	0.47
1:F:285:ASN:ND2	1:F:368:VAL:HG12	2.30	0.47
1:F:363:THR:HG22	1:F:364:SER:H	1.79	0.47
1:G:285:ASN:ND2	1:G:368:VAL:HG12	2.30	0.47
1:K:363:THR:HG22	1:K:364:SER:H	1.79	0.47
1:N:285:ASN:ND2	1:N:368:VAL:HG12	2.30	0.47
1:O:413:GLU:HG2	1:O:417:ARG:HH12	1.79	0.47
1:P:285:ASN:ND2	1:P:368:VAL:HG12	2.30	0.47
1:Q:424:ASP:OD1	1:Q:424:ASP:N	2.47	0.47
1:A:285:ASN:ND2	1:A:368:VAL:HG12	2.30	0.47
1:F:424:ASP:OD1	1:F:424:ASP:N	2.47	0.47
1:J:417:ARG:HG3	1:J:422:PHE:CB	2.45	0.47
1:R:363:THR:HG22	1:R:364:SER:H	1.79	0.47
1:S:413:GLU:HG2	1:S:417:ARG:HH12	1.79	0.47
1:T:424:ASP:OD1	1:T:424:ASP:N	2.48	0.47
1:U:417:ARG:HG3	1:U:422:PHE:CB	2.45	0.47
1:3:417:ARG:HG3	1:3:422:PHE:CB	2.45	0.47
1:L:290:LYS:HA	1:M:284:PRO:HB3	1.96	0.46
1:M:285:ASN:ND2	1:M:368:VAL:HG12	2.30	0.46
1:U:285:ASN:ND2	1:U:368:VAL:HG12	2.30	0.46
1:W:363:THR:HG22	1:W:364:SER:H	1.79	0.46
1:W:413:GLU:HG2	1:W:417:ARG:HH12	1.79	0.46
1:X:285:ASN:ND2	1:X:368:VAL:HG12	2.30	0.46
1:X:363:THR:HG22	1:X:364:SER:H	1.79	0.46
1:Y:357:SER:O	1:Y:357:SER:OG	2.29	0.46
1:1:285:ASN:ND2	1:1:368:VAL:HG12	2.30	0.46
1:4:285:ASN:ND2	1:4:368:VAL:HG12	2.30	0.46
1:A:363:THR:HG22	1:A:364:SER:H	1.79	0.46
1:B:285:ASN:ND2	1:B:368:VAL:HG12	2.30	0.46
1:N:363:THR:HG22	1:N:364:SER:H	1.79	0.46
1:R:285:ASN:ND2	1:R:368:VAL:HG12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:363:THR:HG22	1:S:364:SER:H	1.79	0.46
1:T:417:ARG:HG3	1:T:422:PHE:CB	2.45	0.46
1:U:357:SER:O	1:U:357:SER:OG	2.29	0.46
1:U:413:GLU:HG2	1:U:417:ARG:HH12	1.79	0.46
1:X:357:SER:O	1:X:357:SER:OG	2.29	0.46
1:1:417:ARG:HG3	1:1:422:PHE:CB	2.45	0.46
1:D:363:THR:HG22	1:D:364:SER:H	1.79	0.46
1:G:417:ARG:HG3	1:G:422:PHE:CB	2.45	0.46
1:H:285:ASN:ND2	1:H:368:VAL:HG12	2.30	0.46
1:I:357:SER:O	1:I:357:SER:OG	2.29	0.46
1:Q:415:LEU:CD2	1:R:388:ALA:HB1	2.46	0.46
1:T:363:THR:HG22	1:T:364:SER:H	1.79	0.46
1:T:373:ARG:HH21	1:U:275:LYS:CD	2.26	0.46
1:W:248:ARG:NH2	1:X:242:GLU:OE1	2.47	0.46
1:Y:413:GLU:HG2	1:Y:417:ARG:HH12	1.79	0.46
1:D:424:ASP:OD1	1:D:424:ASP:N	2.48	0.46
1:E:363:THR:HG22	1:E:364:SER:H	1.79	0.46
1:F:248:ARG:NH2	1:G:242:GLU:OE1	2.49	0.46
1:T:292:THR:HG21	1:U:282:TYR:HB3	1.97	0.46
1:6:363:THR:HG22	1:6:364:SER:N	2.31	0.46
1:A:363:THR:HG22	1:A:364:SER:N	2.31	0.46
1:T:285:ASN:ND2	1:T:368:VAL:HG12	2.30	0.46
1:W:363:THR:HG22	1:W:364:SER:N	2.31	0.46
1:X:241:VAL:HG22	1:Y:235:LEU:HD21	1.98	0.46
1:4:246:GLN:HG3	1:4:264:ALA:O	2.15	0.46
1:5:246:GLN:HG3	1:5:264:ALA:O	2.16	0.46
1:6:363:THR:HG22	1:6:364:SER:H	1.79	0.46
1:B:363:THR:HG22	1:B:364:SER:N	2.31	0.46
1:C:424:ASP:OD1	1:C:424:ASP:N	2.47	0.46
1:E:246:GLN:HG3	1:E:264:ALA:O	2.15	0.46
1:F:246:GLN:HG3	1:F:264:ALA:O	2.15	0.46
1:Q:285:ASN:ND2	1:Q:368:VAL:HG12	2.30	0.46
1:S:363:THR:HG22	1:S:364:SER:N	2.31	0.46
1:T:246:GLN:HG3	1:T:264:ALA:O	2.15	0.46
1:Z:285:ASN:ND2	1:Z:368:VAL:HG12	2.30	0.46
1:2:417:ARG:HG3	1:2:422:PHE:CB	2.45	0.46
1:G:418:GLU:OE1	1:H:429:THR:OG1	2.33	0.46
1:O:246:GLN:HG3	1:O:264:ALA:O	2.15	0.46
1:T:363:THR:HG22	1:T:364:SER:N	2.31	0.46
1:V:363:THR:HG22	1:V:364:SER:N	2.31	0.46
1:X:363:THR:HG22	1:X:364:SER:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:363:THR:HG22	1:Z:364:SER:N	2.31	0.46
1:1:363:THR:HG22	1:1:364:SER:N	2.31	0.46
1:3:285:ASN:ND2	1:3:368:VAL:HG12	2.30	0.46
1:5:363:THR:HG22	1:5:364:SER:N	2.31	0.46
1:6:246:GLN:HG3	1:6:264:ALA:O	2.15	0.46
1:A:246:GLN:HG3	1:A:264:ALA:O	2.15	0.46
1:A:424:ASP:OD1	1:A:424:ASP:N	2.47	0.46
1:C:285:ASN:ND2	1:C:368:VAL:HG12	2.30	0.46
1:C:363:THR:HG22	1:C:364:SER:N	2.31	0.46
1:E:285:ASN:ND2	1:E:368:VAL:HG12	2.30	0.46
1:L:285:ASN:ND2	1:L:368:VAL:HG12	2.30	0.46
1:Q:246:GLN:HG3	1:Q:264:ALA:O	2.15	0.46
1:Q:248:ARG:NH2	1:R:242:GLU:OE1	2.49	0.46
1:S:246:GLN:HG3	1:S:264:ALA:O	2.16	0.46
1:U:270:LEU:HB2	1:U:272:PHE:CE2	2.51	0.46
1:W:285:ASN:ND2	1:W:368:VAL:HG12	2.30	0.46
1:X:270:LEU:HB2	1:X:272:PHE:CE2	2.51	0.46
1:X:369:ASP:HA	1:Y:280:GLU:O	2.16	0.46
1:Y:363:THR:HG22	1:Y:364:SER:N	2.31	0.46
1:2:363:THR:HG22	1:2:364:SER:N	2.31	0.46
1:2:373:ARG:HH21	1:3:275:LYS:HD3	1.81	0.46
1:4:363:THR:HG22	1:4:364:SER:N	2.31	0.46
1:5:270:LEU:HB2	1:5:272:PHE:CE2	2.51	0.46
1:D:246:GLN:HG3	1:D:264:ALA:O	2.15	0.46
1:G:424:ASP:OD1	1:G:424:ASP:N	2.47	0.46
1:J:246:GLN:HG3	1:J:264:ALA:O	2.16	0.46
1:J:285:ASN:ND2	1:J:368:VAL:HG12	2.30	0.46
1:N:246:GLN:HG3	1:N:264:ALA:O	2.15	0.46
1:P:246:GLN:HG3	1:P:264:ALA:O	2.15	0.46
1:Q:270:LEU:HB2	1:Q:272:PHE:CE2	2.51	0.46
1:R:363:THR:HG22	1:R:364:SER:N	2.31	0.46
1:U:363:THR:HG22	1:U:364:SER:N	2.31	0.46
1:Y:270:LEU:HB2	1:Y:272:PHE:CE2	2.51	0.46
1:3:290:LYS:HA	1:4:284:PRO:HB3	1.98	0.46
1:4:270:LEU:HB2	1:4:272:PHE:CE2	2.51	0.46
1:5:424:ASP:OD1	1:5:424:ASP:N	2.47	0.46
1:6:285:ASN:ND2	1:6:368:VAL:HG12	2.30	0.46
1:B:270:LEU:HB2	1:B:272:PHE:CE2	2.51	0.46
1:H:424:ASP:OD1	1:H:424:ASP:N	2.47	0.46
1:I:246:GLN:HG3	1:I:264:ALA:O	2.15	0.46
1:J:363:THR:HG22	1:J:364:SER:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:246:GLN:HG3	1:K:264:ALA:O	2.15	0.46
1:M:363:THR:HG22	1:M:364:SER:N	2.31	0.46
1:M:373:ARG:HH21	1:N:275:LYS:CD	2.27	0.46
1:R:246:GLN:HG3	1:R:264:ALA:O	2.15	0.46
1:U:246:GLN:HG3	1:U:264:ALA:O	2.15	0.46
1:V:270:LEU:HB2	1:V:272:PHE:CE2	2.51	0.46
1:Y:290:LYS:HA	1:Z:284:PRO:HB3	1.97	0.46
1:3:246:GLN:HG3	1:3:264:ALA:O	2.16	0.46
1:G:246:GLN:HG3	1:G:264:ALA:O	2.16	0.45
1:H:246:GLN:HG3	1:H:264:ALA:O	2.15	0.45
1:I:424:ASP:N	1:I:424:ASP:OD1	2.47	0.45
1:K:363:THR:HG22	1:K:364:SER:N	2.31	0.45
1:L:363:THR:HG22	1:L:364:SER:N	2.31	0.45
1:W:270:LEU:HB2	1:W:272:PHE:CE2	2.51	0.45
1:X:246:GLN:HG3	1:X:264:ALA:O	2.15	0.45
1:Y:246:GLN:HG3	1:Y:264:ALA:O	2.16	0.45
1:Z:246:GLN:HG3	1:Z:264:ALA:O	2.15	0.45
1:Z:270:LEU:HB2	1:Z:272:PHE:CE2	2.51	0.45
1:C:270:LEU:HB2	1:C:272:PHE:CE2	2.51	0.45
1:E:424:ASP:OD1	1:E:424:ASP:N	2.47	0.45
1:L:255:PRO:O	1:M:437:PHE:HA	2.16	0.45
1:N:363:THR:HG22	1:N:364:SER:N	2.31	0.45
1:O:285:ASN:ND2	1:O:368:VAL:HG12	2.30	0.45
1:Q:363:THR:HG22	1:Q:364:SER:N	2.31	0.45
1:R:270:LEU:HB2	1:R:272:PHE:CE2	2.51	0.45
1:V:246:GLN:HG3	1:V:264:ALA:O	2.15	0.45
1:W:246:GLN:HG3	1:W:264:ALA:O	2.15	0.45
1:Z:424:ASP:OD1	1:Z:424:ASP:N	2.47	0.45
1:1:246:GLN:HG3	1:1:264:ALA:O	2.15	0.45
1:3:363:THR:HG22	1:3:364:SER:N	2.31	0.45
1:B:424:ASP:N	1:B:424:ASP:OD1	2.47	0.45
1:D:363:THR:HG22	1:D:364:SER:N	2.31	0.45
1:I:363:THR:HG22	1:I:364:SER:N	2.31	0.45
1:L:246:GLN:HG3	1:L:264:ALA:O	2.16	0.45
1:O:363:THR:HG22	1:O:364:SER:N	2.31	0.45
1:O:418:GLU:HG3	1:P:431:ASN:HB3	1.99	0.45
1:S:270:LEU:HB2	1:S:272:PHE:CE2	2.51	0.45
1:T:270:LEU:HB2	1:T:272:PHE:CE2	2.51	0.45
1:1:270:LEU:HB2	1:1:272:PHE:CE2	2.51	0.45
1:2:246:GLN:HG3	1:2:264:ALA:O	2.15	0.45
1:6:270:LEU:HB2	1:6:272:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:357:SER:O	1:K:357:SER:OG	2.29	0.45
1:G:363:THR:HG22	1:G:364:SER:N	2.31	0.45
1:K:424:ASP:OD1	1:K:424:ASP:N	2.47	0.45
1:L:415:LEU:HD21	1:M:433:VAL:HG22	1.99	0.45
1:N:270:LEU:HB2	1:N:272:PHE:CE2	2.51	0.45
1:P:270:LEU:HB2	1:P:272:PHE:CE2	2.51	0.45
1:P:363:THR:HG22	1:P:364:SER:N	2.31	0.45
1:1:369:ASP:HA	1:2:280:GLU:O	2.17	0.45
1:A:270:LEU:HB2	1:A:272:PHE:CE2	2.51	0.45
1:B:246:GLN:HG3	1:B:264:ALA:O	2.16	0.45
1:C:246:GLN:HG3	1:C:264:ALA:O	2.16	0.45
1:H:363:THR:HG22	1:H:364:SER:N	2.31	0.45
1:3:270:LEU:HB2	1:3:272:PHE:CE2	2.51	0.45
1:4:255:PRO:O	1:5:437:PHE:HA	2.17	0.45
1:B:239:ASN:HA	1:B:242:GLU:HG2	1.99	0.45
1:J:270:LEU:HB2	1:J:272:PHE:CE2	2.51	0.45
1:M:246:GLN:HG3	1:M:264:ALA:O	2.15	0.45
1:M:424:ASP:OD1	1:M:424:ASP:N	2.47	0.45
1:P:248:ARG:NH2	1:Q:242:GLU:OE1	2.50	0.45
1:T:239:ASN:HA	1:T:242:GLU:HG2	1.99	0.45
1:A:239:ASN:HA	1:A:242:GLU:HG2	1.99	0.45
1:A:277:GLN:HA	1:6:372:ILE:O	2.17	0.45
1:C:239:ASN:HA	1:C:242:GLU:HG2	1.99	0.45
1:C:418:GLU:OE1	1:D:429:THR:OG1	2.35	0.45
1:D:239:ASN:HA	1:D:242:GLU:HG2	1.99	0.45
1:E:363:THR:HG22	1:E:364:SER:N	2.31	0.45
1:F:270:LEU:HB2	1:F:272:PHE:CE2	2.51	0.45
1:I:270:LEU:HB2	1:I:272:PHE:CE2	2.51	0.45
1:K:239:ASN:HA	1:K:242:GLU:HG2	1.99	0.45
1:L:357:SER:O	1:L:357:SER:OG	2.29	0.45
1:M:270:LEU:HB2	1:M:272:PHE:CE2	2.51	0.45
1:M:355:PRO:O	1:M:357:SER:N	2.50	0.45
1:S:239:ASN:HA	1:S:242:GLU:HG2	1.99	0.45
1:6:424:ASP:N	1:6:424:ASP:OD1	2.47	0.45
1:A:431:ASN:CB	1:6:418:GLU:HG3	2.47	0.45
1:E:270:LEU:HB2	1:E:272:PHE:CE2	2.51	0.45
1:J:239:ASN:HA	1:J:242:GLU:HG2	1.99	0.45
1:J:355:PRO:O	1:J:357:SER:N	2.50	0.45
1:L:239:ASN:HA	1:L:242:GLU:HG2	1.99	0.45
1:L:303:GLN:HA	1:M:357:SER:HA	1.98	0.45
1:P:355:PRO:O	1:P:357:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:253:LEU:HA	1:S:253:LEU:HD23	1.82	0.45
1:V:418:GLU:HG3	1:W:431:ASN:HB3	1.99	0.45
1:1:239:ASN:HA	1:1:242:GLU:HG2	1.99	0.45
1:6:239:ASN:HA	1:6:242:GLU:HG2	1.99	0.45
1:F:363:THR:HG22	1:F:364:SER:N	2.31	0.45
1:G:355:PRO:O	1:G:357:SER:N	2.50	0.45
1:U:239:ASN:HA	1:U:242:GLU:HG2	1.99	0.45
1:W:373:ARG:HH21	1:X:275:LYS:CD	2.28	0.45
1:3:418:GLU:OE1	1:4:429:THR:OG1	2.32	0.45
1:3:424:ASP:N	1:3:424:ASP:OD1	2.47	0.45
1:4:424:ASP:OD1	1:4:424:ASP:N	2.48	0.45
1:D:270:LEU:HB2	1:D:272:PHE:CE2	2.51	0.44
1:K:270:LEU:HB2	1:K:272:PHE:CE2	2.51	0.44
1:M:239:ASN:HA	1:M:242:GLU:HG2	1.99	0.44
1:S:355:PRO:O	1:S:357:SER:N	2.50	0.44
1:Z:239:ASN:HA	1:Z:242:GLU:HG2	1.99	0.44
1:2:239:ASN:HA	1:2:242:GLU:HG2	1.99	0.44
1:2:270:LEU:HB2	1:2:272:PHE:CE2	2.51	0.44
1:H:253:LEU:HD23	1:H:253:LEU:HA	1.82	0.44
1:I:239:ASN:HA	1:I:242:GLU:HG2	1.99	0.44
1:A:429:THR:OG1	1:6:418:GLU:OE1	2.35	0.44
1:D:355:PRO:O	1:D:357:SER:N	2.50	0.44
1:G:270:LEU:HB2	1:G:272:PHE:CE2	2.51	0.44
1:H:270:LEU:HB2	1:H:272:PHE:CE2	2.51	0.44
1:K:373:ARG:HH21	1:L:275:LYS:CD	2.29	0.44
1:O:270:LEU:HB2	1:O:272:PHE:CE2	2.51	0.44
1:Q:355:PRO:O	1:Q:357:SER:N	2.50	0.44
1:R:239:ASN:HA	1:R:242:GLU:HG2	1.99	0.44
1:E:239:ASN:HA	1:E:242:GLU:HG2	1.99	0.44
1:I:415:LEU:HD22	1:J:388:ALA:HB1	1.99	0.44
1:L:270:LEU:HB2	1:L:272:PHE:CE2	2.51	0.44
1:N:239:ASN:HA	1:N:242:GLU:HG2	1.99	0.44
1:O:355:PRO:O	1:O:357:SER:N	2.50	0.44
1:R:369:ASP:HA	1:S:280:GLU:O	2.17	0.44
1:S:411:GLN:NE2	1:T:435:SER:OG	2.42	0.44
1:V:355:PRO:O	1:V:357:SER:N	2.50	0.44
1:2:271:ASP:HB2	1:2:383:GLU:CG	2.48	0.44
1:3:239:ASN:HA	1:3:242:GLU:HG2	1.99	0.44
1:3:271:ASP:HB2	1:3:383:GLU:CG	2.48	0.44
1:C:271:ASP:HB2	1:C:383:GLU:CG	2.48	0.44
1:C:280:GLU:HG2	1:C:282:TYR:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ASP:HB2	1:D:383:GLU:CG	2.48	0.44
1:H:355:PRO:O	1:H:357:SER:N	2.50	0.44
1:H:376:LYS:HB3	1:I:274:ASN:HB2	1.98	0.44
1:I:355:PRO:O	1:I:357:SER:N	2.50	0.44
1:J:424:ASP:OD1	1:J:424:ASP:N	2.47	0.44
1:K:355:PRO:O	1:K:357:SER:N	2.50	0.44
1:L:355:PRO:O	1:L:357:SER:N	2.50	0.44
1:O:415:LEU:HD11	1:P:433:VAL:HG21	1.99	0.44
1:Q:280:GLU:HG2	1:Q:282:TYR:HE2	1.83	0.44
1:Q:299:ASN:HA	1:R:361:ASN:HA	2.00	0.44
1:S:280:GLU:HG2	1:S:282:TYR:HE2	1.83	0.44
1:V:239:ASN:HA	1:V:242:GLU:HG2	1.99	0.44
1:Y:239:ASN:HA	1:Y:242:GLU:HG2	1.99	0.44
1:2:424:ASP:OD1	1:2:424:ASP:N	2.47	0.44
1:E:271:ASP:HB2	1:E:383:GLU:CG	2.48	0.44
1:F:355:PRO:O	1:F:357:SER:N	2.50	0.44
1:L:253:LEU:HD23	1:L:253:LEU:HA	1.82	0.44
1:L:424:ASP:OD1	1:L:424:ASP:N	2.47	0.44
1:N:355:PRO:O	1:N:357:SER:N	2.50	0.44
1:P:424:ASP:OD1	1:P:424:ASP:N	2.47	0.44
1:U:280:GLU:HG2	1:U:282:TYR:HE2	1.83	0.44
1:V:271:ASP:HB2	1:V:383:GLU:CG	2.48	0.44
1:1:271:ASP:HB2	1:1:383:GLU:CG	2.48	0.44
1:1:355:PRO:O	1:1:357:SER:N	2.50	0.44
1:4:271:ASP:HB2	1:4:383:GLU:CG	2.48	0.44
1:A:280:GLU:HG2	1:A:282:TYR:HE2	1.83	0.44
1:B:271:ASP:HB2	1:B:383:GLU:CG	2.48	0.44
1:E:355:PRO:O	1:E:357:SER:N	2.50	0.44
1:H:239:ASN:HA	1:H:242:GLU:HG2	1.99	0.44
1:M:280:GLU:HG2	1:M:282:TYR:HE2	1.83	0.44
1:N:418:GLU:HG3	1:O:431:ASN:HB3	2.00	0.44
1:N:424:ASP:OD1	1:N:424:ASP:N	2.47	0.44
1:O:280:GLU:HG2	1:O:282:TYR:HE2	1.83	0.44
1:O:424:ASP:OD1	1:O:424:ASP:N	2.47	0.44
1:T:355:PRO:O	1:T:357:SER:N	2.50	0.44
1:U:355:PRO:O	1:U:357:SER:N	2.50	0.44
1:W:271:ASP:HB2	1:W:383:GLU:CG	2.48	0.44
1:W:280:GLU:HG2	1:W:282:TYR:HE2	1.83	0.44
1:Z:355:PRO:O	1:Z:357:SER:N	2.50	0.44
1:4:248:ARG:NH1	1:5:267:THR:HG23	2.32	0.44
1:5:239:ASN:HA	1:5:242:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:355:PRO:O	1:5:357:SER:N	2.50	0.44
1:B:355:PRO:O	1:B:357:SER:N	2.50	0.44
1:E:280:GLU:HG2	1:E:282:TYR:HE2	1.83	0.44
1:K:280:GLU:HG2	1:K:282:TYR:HE2	1.83	0.44
1:K:302:GLU:O	1:L:358:THR:N	2.51	0.44
1:O:239:ASN:HA	1:O:242:GLU:HG2	1.99	0.44
1:R:355:PRO:O	1:R:357:SER:N	2.50	0.44
1:U:271:ASP:HB2	1:U:383:GLU:CG	2.48	0.44
1:X:355:PRO:O	1:X:357:SER:N	2.50	0.44
1:Y:280:GLU:HG2	1:Y:282:TYR:HE2	1.83	0.44
1:Z:280:GLU:HG2	1:Z:282:TYR:HE2	1.83	0.44
1:G:239:ASN:HA	1:G:242:GLU:HG2	1.99	0.44
1:L:248:ARG:NH1	1:M:267:THR:HG23	2.33	0.44
1:M:357:SER:O	1:M:357:SER:OG	2.29	0.44
1:O:271:ASP:HB2	1:O:383:GLU:CG	2.48	0.44
1:2:280:GLU:HG2	1:2:282:TYR:HE2	1.83	0.44
1:4:418:GLU:HG3	1:5:431:ASN:HB2	1.99	0.44
1:5:280:GLU:HG2	1:5:282:TYR:HE2	1.83	0.44
1:I:280:GLU:HG2	1:I:282:TYR:HE2	1.83	0.43
1:I:299:ASN:HA	1:J:361:ASN:HA	2.00	0.43
1:X:271:ASP:HB2	1:X:383:GLU:CG	2.48	0.43
1:Z:373:ARG:HH21	1:1:275:LYS:HD3	1.82	0.43
1:4:355:PRO:O	1:4:357:SER:N	2.50	0.43
1:P:239:ASN:HA	1:P:242:GLU:HG2	1.99	0.43
1:Q:239:ASN:HA	1:Q:242:GLU:HG2	1.99	0.43
1:W:239:ASN:HA	1:W:242:GLU:HG2	1.99	0.43
1:X:239:ASN:HA	1:X:242:GLU:HG2	1.99	0.43
1:X:280:GLU:HG2	1:X:282:TYR:HE2	1.83	0.43
1:Y:253:LEU:HD23	1:Y:253:LEU:HA	1.82	0.43
1:2:355:PRO:O	1:2:357:SER:N	2.50	0.43
1:4:280:GLU:HG2	1:4:282:TYR:HE2	1.83	0.43
1:6:355:PRO:O	1:6:357:SER:N	2.50	0.43
1:F:239:ASN:HA	1:F:242:GLU:HG2	1.99	0.43
1:H:280:GLU:HG2	1:H:282:TYR:HE2	1.83	0.43
1:H:373:ARG:NH2	1:I:275:LYS:HD3	2.26	0.43
1:Y:355:PRO:O	1:Y:357:SER:N	2.50	0.43
1:1:280:GLU:HG2	1:1:282:TYR:HE2	1.83	0.43
1:A:271:ASP:HB2	1:A:383:GLU:CG	2.48	0.43
1:F:280:GLU:HG2	1:F:282:TYR:HE2	1.83	0.43
1:G:280:GLU:HG2	1:G:282:TYR:HE2	1.83	0.43
1:T:271:ASP:HB2	1:T:383:GLU:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:418:GLU:HB2	1:V:388:ALA:HB2	2.01	0.43
1:W:253:LEU:HA	1:W:253:LEU:HD23	1.82	0.43
1:3:280:GLU:HG2	1:3:282:TYR:HE2	1.83	0.43
1:3:355:PRO:O	1:3:357:SER:N	2.50	0.43
1:4:239:ASN:HA	1:4:242:GLU:HG2	1.99	0.43
1:5:250:GLU:O	1:5:254:SER:OG	2.19	0.43
1:5:271:ASP:HB2	1:5:383:GLU:CG	2.48	0.43
1:A:355:PRO:O	1:A:357:SER:N	2.50	0.43
1:J:280:GLU:HG2	1:J:282:TYR:HE2	1.83	0.43
1:L:271:ASP:HB2	1:L:383:GLU:CG	2.48	0.43
1:Z:271:ASP:HB2	1:Z:383:GLU:CG	2.48	0.43
1:6:271:ASP:HB2	1:6:383:GLU:CG	2.48	0.43
1:C:355:PRO:O	1:C:357:SER:N	2.50	0.43
1:D:292:THR:HG21	1:E:282:TYR:HB3	1.99	0.43
1:K:271:ASP:HB2	1:K:383:GLU:CG	2.48	0.43
1:N:250:GLU:O	1:N:254:SER:OG	2.20	0.43
1:V:280:GLU:HG2	1:V:282:TYR:HE2	1.83	0.43
1:W:355:PRO:O	1:W:357:SER:N	2.50	0.43
1:X:373:ARG:HH21	1:Y:275:LYS:CD	2.30	0.43
1:1:376:LYS:HB3	1:2:274:ASN:HB2	2.01	0.43
1:B:280:GLU:HG2	1:B:282:TYR:HE2	1.83	0.43
1:L:280:GLU:HG2	1:L:282:TYR:HE2	1.83	0.43
1:D:280:GLU:HG2	1:D:282:TYR:HE2	1.83	0.43
1:G:292:THR:HG21	1:H:282:TYR:HB3	1.99	0.43
1:N:271:ASP:HB2	1:N:383:GLU:CG	2.48	0.43
1:N:280:GLU:HG2	1:N:282:TYR:HE2	1.83	0.43
1:P:280:GLU:HG2	1:P:282:TYR:HE2	1.83	0.43
1:P:369:ASP:HA	1:Q:280:GLU:O	2.18	0.43
1:T:248:ARG:NH2	1:U:242:GLU:OE1	2.50	0.43
1:U:253:LEU:HA	1:U:253:LEU:HD23	1.82	0.43
1:5:253:LEU:HD23	1:5:253:LEU:HA	1.82	0.43
1:6:280:GLU:HG2	1:6:282:TYR:HE2	1.83	0.43
1:J:271:ASP:HB2	1:J:383:GLU:CG	2.48	0.43
1:S:271:ASP:HB2	1:S:383:GLU:CG	2.48	0.43
1:T:280:GLU:HG2	1:T:282:TYR:HE2	1.83	0.43
1:V:292:THR:HG21	1:W:282:TYR:HB3	2.00	0.43
1:1:253:LEU:HA	1:1:253:LEU:HD23	1.82	0.43
1:R:280:GLU:HG2	1:R:282:TYR:HE2	1.83	0.43
1:V:253:LEU:HD23	1:V:253:LEU:HA	1.82	0.43
1:W:303:GLN:HA	1:X:357:SER:HA	2.00	0.43
1:5:248:ARG:NH1	1:6:267:THR:HG23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ARG:HH21	1:D:275:LYS:CD	2.32	0.42
1:O:303:GLN:HA	1:P:357:SER:HA	2.01	0.42
1:Q:271:ASP:HB2	1:Q:383:GLU:CG	2.48	0.42
1:Y:424:ASP:OD1	1:Y:424:ASP:N	2.47	0.42
1:D:373:ARG:HH21	1:E:275:LYS:HD3	1.84	0.42
1:I:271:ASP:HB2	1:I:383:GLU:CG	2.48	0.42
1:U:415:LEU:HD11	1:V:433:VAL:HG21	2.00	0.42
1:Y:271:ASP:HB2	1:Y:383:GLU:CG	2.48	0.42
1:Y:373:ARG:HH21	1:Z:275:LYS:NZ	2.17	0.42
1:A:275:LYS:CD	1:6:373:ARG:HH21	2.31	0.42
1:G:293:LEU:HD22	1:G:296:ARG:HB2	2.02	0.42
1:T:293:LEU:HD22	1:T:296:ARG:HB2	2.02	0.42
1:E:293:LEU:HD22	1:E:296:ARG:HB2	2.02	0.42
1:G:271:ASP:HB2	1:G:383:GLU:CG	2.48	0.42
1:M:271:ASP:HB2	1:M:383:GLU:CG	2.48	0.42
1:V:293:LEU:HD22	1:V:296:ARG:HB2	2.02	0.42
1:X:293:LEU:HD22	1:X:296:ARG:HB2	2.02	0.42
1:X:376:LYS:HB3	1:Y:274:ASN:HB2	2.01	0.42
1:3:373:ARG:HH21	1:4:275:LYS:CE	2.32	0.42
1:B:293:LEU:HD22	1:B:296:ARG:HB2	2.02	0.42
1:E:404:LEU:H	1:E:434:ASN:HD21	1.68	0.42
1:H:271:ASP:HB2	1:H:383:GLU:CG	2.48	0.42
1:I:293:LEU:HD22	1:I:296:ARG:HB2	2.02	0.42
1:P:241:VAL:HG22	1:Q:235:LEU:HD21	2.01	0.42
1:P:271:ASP:HB2	1:P:383:GLU:CG	2.48	0.42
1:R:271:ASP:HB2	1:R:383:GLU:CG	2.48	0.42
1:W:293:LEU:HD22	1:W:296:ARG:HB2	2.02	0.42
1:Y:293:LEU:HD22	1:Y:296:ARG:HB2	2.02	0.42
1:1:293:LEU:HD22	1:1:296:ARG:HB2	2.02	0.42
1:A:390:VAL:HG13	1:6:252:ILE:HD11	2.02	0.42
1:C:293:LEU:HD22	1:C:296:ARG:HB2	2.02	0.42
1:D:293:LEU:HD22	1:D:296:ARG:HB2	2.02	0.42
1:J:293:LEU:HD22	1:J:296:ARG:HB2	2.02	0.42
1:K:293:LEU:HD22	1:K:296:ARG:HB2	2.02	0.42
1:N:293:LEU:HD22	1:N:296:ARG:HB2	2.02	0.42
1:R:293:LEU:HD22	1:R:296:ARG:HB2	2.02	0.42
1:U:293:LEU:HD22	1:U:296:ARG:HB2	2.02	0.42
1:U:373:ARG:HH21	1:V:275:LYS:CD	2.26	0.42
1:3:293:LEU:HD22	1:3:296:ARG:HB2	2.02	0.42
1:6:293:LEU:HD22	1:6:296:ARG:HB2	2.02	0.42
1:F:293:LEU:HD22	1:F:296:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:LEU:HD22	1:H:296:ARG:HB2	2.02	0.42
1:H:404:LEU:H	1:H:434:ASN:HD21	1.68	0.42
1:I:373:ARG:NH2	1:J:275:LYS:HD3	2.31	0.42
1:K:404:LEU:H	1:K:434:ASN:HD21	1.68	0.42
1:L:293:LEU:HD22	1:L:296:ARG:HB2	2.02	0.42
1:P:293:LEU:HD22	1:P:296:ARG:HB2	2.02	0.42
1:U:290:LYS:HA	1:V:284:PRO:CB	2.48	0.42
1:E:301:SER:HB3	1:E:359:GLN:HB3	2.02	0.42
1:F:301:SER:HB3	1:F:359:GLN:HB3	2.02	0.42
1:L:250:GLU:O	1:L:254:SER:OG	2.20	0.42
1:M:290:LYS:HA	1:N:284:PRO:HB3	2.02	0.42
1:Z:293:LEU:HD22	1:Z:296:ARG:HB2	2.02	0.42
1:1:417:ARG:HG3	1:1:422:PHE:HB3	2.02	0.42
1:2:293:LEU:HD22	1:2:296:ARG:HB2	2.02	0.42
1:2:301:SER:HB3	1:2:359:GLN:HB3	2.02	0.42
1:4:293:LEU:HD22	1:4:296:ARG:HB2	2.02	0.42
1:5:293:LEU:HD22	1:5:296:ARG:HB2	2.02	0.42
1:5:417:ARG:HG3	1:5:422:PHE:HB3	2.02	0.42
1:H:253:LEU:O	1:H:257:VAL:HG22	2.20	0.42
1:M:293:LEU:HD22	1:M:296:ARG:HB2	2.02	0.42
1:N:404:LEU:H	1:N:434:ASN:HD21	1.68	0.42
1:O:293:LEU:HD22	1:O:296:ARG:HB2	2.02	0.42
1:S:293:LEU:HD22	1:S:296:ARG:HB2	2.02	0.42
1:Z:417:ARG:HG3	1:Z:422:PHE:HB3	2.02	0.42
1:2:417:ARG:HG3	1:2:422:PHE:HB3	2.02	0.42
1:3:253:LEU:HD23	1:3:253:LEU:HA	1.82	0.42
1:3:301:SER:HB3	1:3:359:GLN:HB3	2.02	0.42
1:6:417:ARG:HG3	1:6:422:PHE:HB3	2.02	0.42
1:A:293:LEU:HD22	1:A:296:ARG:HB2	2.02	0.42
1:A:417:ARG:HG3	1:A:422:PHE:HB3	2.02	0.42
1:C:253:LEU:HD23	1:C:253:LEU:HA	1.82	0.42
1:F:411:GLN:NE2	1:G:435:SER:OG	2.45	0.42
1:G:416:THR:O	1:G:420:MET:HG3	2.20	0.42
1:I:253:LEU:O	1:I:257:VAL:HG22	2.20	0.42
1:J:253:LEU:O	1:J:257:VAL:HG22	2.20	0.42
1:Q:293:LEU:HD22	1:Q:296:ARG:HB2	2.02	0.42
1:Y:415:LEU:HD11	1:Z:433:VAL:HG21	2.02	0.42
1:Z:253:LEU:O	1:Z:257:VAL:HG22	2.20	0.42
1:4:417:ARG:HG3	1:4:422:PHE:HB3	2.02	0.42
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.82	0.41
1:B:404:LEU:H	1:B:434:ASN:HD21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ARG:NH1	1:E:267:THR:HG23	2.35	0.41
1:D:301:SER:HB3	1:D:359:GLN:HB3	2.02	0.41
1:F:416:THR:O	1:F:420:MET:HG3	2.20	0.41
1:G:301:SER:HB3	1:G:359:GLN:HB3	2.02	0.41
1:G:404:LEU:H	1:G:434:ASN:HD21	1.68	0.41
1:O:369:ASP:HA	1:P:280:GLU:O	2.20	0.41
1:X:253:LEU:O	1:X:257:VAL:HG22	2.20	0.41
1:Y:253:LEU:O	1:Y:257:VAL:HG22	2.20	0.41
1:Z:416:THR:O	1:Z:420:MET:HG3	2.20	0.41
1:1:253:LEU:O	1:1:257:VAL:HG22	2.20	0.41
1:1:415:LEU:HD21	1:2:433:VAL:HG22	2.03	0.41
1:2:248:ARG:NH1	1:3:267:THR:HG23	2.35	0.41
1:2:253:LEU:O	1:2:257:VAL:HG22	2.20	0.41
1:3:253:LEU:O	1:3:257:VAL:HG22	2.20	0.41
1:4:301:SER:HB3	1:4:359:GLN:HB3	2.02	0.41
1:E:416:THR:O	1:E:420:MET:HG3	2.20	0.41
1:G:253:LEU:O	1:G:257:VAL:HG22	2.20	0.41
1:J:253:LEU:HD23	1:J:253:LEU:HA	1.82	0.41
1:K:253:LEU:O	1:K:257:VAL:HG22	2.20	0.41
1:L:404:LEU:H	1:L:434:ASN:HD21	1.68	0.41
1:M:253:LEU:O	1:M:257:VAL:HG22	2.20	0.41
1:N:248:ARG:NH1	1:O:267:THR:HG23	2.35	0.41
1:Q:357:SER:O	1:Q:357:SER:OG	2.29	0.41
1:V:301:SER:HB3	1:V:359:GLN:HB3	2.02	0.41
1:X:416:THR:O	1:X:420:MET:HG3	2.20	0.41
1:Y:416:THR:O	1:Y:420:MET:HG3	2.20	0.41
1:1:301:SER:HB3	1:1:359:GLN:HB3	2.02	0.41
1:3:417:ARG:HG3	1:3:422:PHE:HB3	2.02	0.41
1:4:253:LEU:O	1:4:257:VAL:HG22	2.20	0.41
1:F:253:LEU:O	1:F:257:VAL:HG22	2.20	0.41
1:H:416:THR:O	1:H:420:MET:HG3	2.20	0.41
1:H:418:GLU:OE1	1:I:429:THR:OG1	2.37	0.41
1:I:404:LEU:H	1:I:434:ASN:HD21	1.68	0.41
1:L:253:LEU:O	1:L:257:VAL:HG22	2.20	0.41
1:S:241:VAL:HG22	1:T:235:LEU:HD21	2.02	0.41
1:T:253:LEU:O	1:T:257:VAL:HG22	2.20	0.41
1:U:301:SER:HB3	1:U:359:GLN:HB3	2.02	0.41
1:V:417:ARG:HG3	1:V:422:PHE:HB3	2.02	0.41
1:W:253:LEU:O	1:W:257:VAL:HG22	2.20	0.41
1:W:417:ARG:HG3	1:W:422:PHE:HB3	2.02	0.41
1:3:373:ARG:NH2	1:4:275:LYS:HD3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ARG:HG3	1:B:422:PHE:HB3	2.02	0.41
1:C:301:SER:HB3	1:C:359:GLN:HB3	2.02	0.41
1:D:416:THR:O	1:D:420:MET:HG3	2.20	0.41
1:F:271:ASP:HB2	1:F:383:GLU:CG	2.48	0.41
1:H:301:SER:HB3	1:H:359:GLN:HB3	2.02	0.41
1:I:416:THR:O	1:I:420:MET:HG3	2.20	0.41
1:K:415:LEU:HD22	1:L:388:ALA:HB1	2.02	0.41
1:M:301:SER:HB3	1:M:359:GLN:HB3	2.02	0.41
1:Q:416:THR:O	1:Q:420:MET:HG3	2.20	0.41
1:R:416:THR:O	1:R:420:MET:HG3	2.20	0.41
1:U:253:LEU:O	1:U:257:VAL:HG22	2.20	0.41
1:Y:284:PRO:O	1:Y:290:LYS:HE2	2.21	0.41
1:Y:417:ARG:HG3	1:Y:422:PHE:HB3	2.02	0.41
1:Z:284:PRO:O	1:Z:290:LYS:HE2	2.21	0.41
1:1:416:THR:O	1:1:420:MET:HG3	2.20	0.41
1:5:253:LEU:O	1:5:257:VAL:HG22	2.20	0.41
1:5:292:THR:HG21	1:6:282:TYR:HB3	2.02	0.41
1:5:404:LEU:H	1:5:434:ASN:HD21	1.68	0.41
1:L:417:ARG:HG3	1:L:422:PHE:HB3	2.02	0.41
1:N:253:LEU:HA	1:N:253:LEU:HD23	1.82	0.41
1:N:301:SER:HB3	1:N:359:GLN:HB3	2.02	0.41
1:Q:253:LEU:HA	1:Q:253:LEU:HD23	1.82	0.41
1:Q:284:PRO:O	1:Q:290:LYS:HE2	2.21	0.41
1:S:253:LEU:O	1:S:257:VAL:HG22	2.20	0.41
1:U:417:ARG:HG3	1:U:422:PHE:HB3	2.02	0.41
1:V:253:LEU:O	1:V:257:VAL:HG22	2.20	0.41
1:W:284:PRO:O	1:W:290:LYS:HE2	2.21	0.41
1:W:301:SER:HB3	1:W:359:GLN:HB3	2.02	0.41
1:W:416:THR:O	1:W:420:MET:HG3	2.20	0.41
1:X:284:PRO:O	1:X:290:LYS:HE2	2.21	0.41
1:X:417:ARG:HG3	1:X:422:PHE:HB3	2.02	0.41
1:3:418:GLU:HG3	1:4:431:ASN:HB3	2.03	0.41
1:5:301:SER:HB3	1:5:359:GLN:HB3	2.02	0.41
1:C:416:THR:O	1:C:420:MET:HG3	2.20	0.41
1:C:417:ARG:HG3	1:C:422:PHE:HB3	2.02	0.41
1:D:404:LEU:H	1:D:434:ASN:HD21	1.68	0.41
1:D:417:ARG:HG3	1:D:422:PHE:HB3	2.02	0.41
1:E:253:LEU:HA	1:E:253:LEU:HD23	1.82	0.41
1:E:373:ARG:HH21	1:F:275:LYS:HD3	1.85	0.41
1:K:417:ARG:HG3	1:K:422:PHE:HB3	2.02	0.41
1:L:301:SER:HB3	1:L:359:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:253:LEU:O	1:N:257:VAL:HG22	2.20	0.41
1:N:415:LEU:HD11	1:O:433:VAL:HG21	2.02	0.41
1:O:404:LEU:H	1:O:434:ASN:HD21	1.68	0.41
1:P:241:VAL:HG23	1:Q:235:LEU:HD11	2.02	0.41
1:T:301:SER:HB3	1:T:359:GLN:HB3	2.02	0.41
1:2:303:GLN:HA	1:3:357:SER:HA	2.03	0.41
1:E:253:LEU:O	1:E:257:VAL:HG22	2.20	0.41
1:E:417:ARG:HG3	1:E:422:PHE:HB3	2.02	0.41
1:F:404:LEU:H	1:F:434:ASN:HD21	1.68	0.41
1:I:303:GLN:HA	1:J:357:SER:HA	2.02	0.41
1:J:416:THR:O	1:J:420:MET:HG3	2.20	0.41
1:L:416:THR:O	1:L:420:MET:HG3	2.20	0.41
1:P:417:ARG:HG3	1:P:422:PHE:HB3	2.02	0.41
1:R:253:LEU:O	1:R:257:VAL:HG22	2.20	0.41
1:R:284:PRO:O	1:R:290:LYS:HE2	2.21	0.41
1:S:416:THR:O	1:S:420:MET:HG3	2.20	0.41
1:T:416:THR:O	1:T:420:MET:HG3	2.20	0.41
1:U:284:PRO:O	1:U:290:LYS:HE2	2.21	0.41
1:Z:301:SER:HB3	1:Z:359:GLN:HB3	2.02	0.41
1:F:417:ARG:HG3	1:F:422:PHE:HB3	2.02	0.41
1:K:416:THR:O	1:K:420:MET:HG3	2.20	0.41
1:L:415:LEU:HD11	1:M:433:VAL:CG2	2.43	0.41
1:M:416:THR:O	1:M:420:MET:HG3	2.20	0.41
1:O:417:ARG:HG3	1:O:422:PHE:HB3	2.02	0.41
1:V:284:PRO:O	1:V:290:LYS:HE2	2.21	0.41
1:1:284:PRO:O	1:1:290:LYS:HE2	2.21	0.41
1:2:416:THR:O	1:2:420:MET:HG3	2.20	0.41
1:6:253:LEU:O	1:6:257:VAL:HG22	2.20	0.41
1:A:253:LEU:O	1:A:257:VAL:HG22	2.20	0.41
1:B:416:THR:O	1:B:420:MET:HG3	2.20	0.41
1:C:404:LEU:H	1:C:434:ASN:HD21	1.68	0.41
1:C:418:GLU:HG3	1:D:431:ASN:HB3	2.03	0.41
1:D:253:LEU:O	1:D:257:VAL:HG22	2.20	0.41
1:F:235:LEU:HD23	1:F:235:LEU:HA	1.96	0.41
1:G:253:LEU:HA	1:G:253:LEU:HD23	1.82	0.41
1:G:284:PRO:O	1:G:290:LYS:HE2	2.21	0.41
1:H:418:GLU:HG3	1:I:431:ASN:HB3	2.03	0.41
1:I:301:SER:HB3	1:I:359:GLN:HB3	2.02	0.41
1:M:404:LEU:H	1:M:434:ASN:HD21	1.68	0.41
1:M:417:ARG:HG3	1:M:422:PHE:HB3	2.02	0.41
1:N:417:ARG:HG3	1:N:422:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:253:LEU:O	1:O:257:VAL:HG22	2.20	0.41
1:O:301:SER:HB3	1:O:359:GLN:HB3	2.02	0.41
1:P:253:LEU:O	1:P:257:VAL:HG22	2.20	0.41
1:P:284:PRO:O	1:P:290:LYS:HE2	2.21	0.41
1:P:416:THR:O	1:P:420:MET:HG3	2.20	0.41
1:S:284:PRO:O	1:S:290:LYS:HE2	2.21	0.41
1:T:284:PRO:O	1:T:290:LYS:HE2	2.21	0.41
1:T:415:LEU:HD22	1:U:388:ALA:HB1	2.03	0.41
1:U:367:GLU:HB3	1:V:282:TYR:CE1	2.56	0.41
1:U:416:THR:O	1:U:420:MET:HG3	2.20	0.41
1:V:416:THR:O	1:V:420:MET:HG3	2.20	0.41
1:W:404:LEU:H	1:W:434:ASN:HD21	1.68	0.41
1:X:301:SER:HB3	1:X:359:GLN:HB3	2.02	0.41
1:2:284:PRO:O	1:2:290:LYS:HE2	2.21	0.41
1:B:301:SER:HB3	1:B:359:GLN:HB3	2.02	0.41
1:E:284:PRO:O	1:E:290:LYS:HE2	2.21	0.41
1:F:284:PRO:O	1:F:290:LYS:HE2	2.21	0.41
1:J:417:ARG:HG3	1:J:422:PHE:HB3	2.02	0.41
1:N:416:THR:O	1:N:420:MET:HG3	2.20	0.41
1:Q:417:ARG:HG3	1:Q:422:PHE:HB3	2.02	0.41
1:6:301:SER:HB3	1:6:359:GLN:HB3	2.02	0.41
1:A:416:THR:O	1:A:420:MET:HG3	2.20	0.40
1:B:253:LEU:O	1:B:257:VAL:HG22	2.20	0.40
1:O:284:PRO:O	1:O:290:LYS:HE2	2.21	0.40
1:O:292:THR:HG21	1:P:282:TYR:HB3	2.03	0.40
1:O:416:THR:O	1:O:420:MET:HG3	2.20	0.40
1:Q:253:LEU:O	1:Q:257:VAL:HG22	2.20	0.40
1:Q:404:LEU:H	1:Q:434:ASN:HD21	1.68	0.40
1:R:417:ARG:HG3	1:R:422:PHE:HB3	2.02	0.40
1:S:417:ARG:HG3	1:S:422:PHE:HB3	2.02	0.40
1:U:241:VAL:HG22	1:V:235:LEU:HD21	2.03	0.40
1:U:299:ASN:HA	1:V:361:ASN:HA	2.03	0.40
1:1:404:LEU:H	1:1:434:ASN:HD21	1.68	0.40
1:3:284:PRO:O	1:3:290:LYS:HE2	2.21	0.40
1:A:284:PRO:O	1:A:290:LYS:HE2	2.21	0.40
1:A:404:LEU:H	1:A:434:ASN:HD21	1.68	0.40
1:K:301:SER:HB3	1:K:359:GLN:HB3	2.02	0.40
1:L:411:GLN:NE2	1:M:435:SER:OG	2.49	0.40
1:N:284:PRO:O	1:N:290:LYS:HE2	2.21	0.40
1:P:301:SER:HB3	1:P:359:GLN:HB3	2.02	0.40
1:S:301:SER:HB3	1:S:359:GLN:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:417:ARG:HG3	1:T:422:PHE:HB3	2.02	0.40
1:3:250:GLU:O	1:3:254:SER:OG	2.20	0.40
1:D:284:PRO:O	1:D:290:LYS:HE2	2.21	0.40
1:G:417:ARG:HG3	1:G:422:PHE:HB3	2.02	0.40
1:O:253:LEU:HD23	1:O:253:LEU:HA	1.82	0.40
1:S:357:SER:O	1:S:357:SER:OG	2.29	0.40
1:Z:404:LEU:H	1:Z:434:ASN:HD21	1.68	0.40
1:2:404:LEU:H	1:2:434:ASN:HD21	1.68	0.40
1:3:385:LEU:N	1:3:428:ASP:OD1	2.51	0.40
1:3:416:THR:O	1:3:420:MET:HG3	2.20	0.40
1:4:284:PRO:O	1:4:290:LYS:HE2	2.21	0.40
1:6:404:LEU:H	1:6:434:ASN:HD21	1.68	0.40
1:6:416:THR:O	1:6:420:MET:HG3	2.20	0.40
1:A:301:SER:HB3	1:A:359:GLN:HB3	2.02	0.40
1:A:361:ASN:OD1	1:A:361:ASN:N	2.55	0.40
1:B:284:PRO:O	1:B:290:LYS:HE2	2.21	0.40
1:B:361:ASN:OD1	1:B:361:ASN:N	2.55	0.40
1:C:361:ASN:OD1	1:C:361:ASN:N	2.55	0.40
1:H:417:ARG:HG3	1:H:422:PHE:HB3	2.02	0.40
1:I:417:ARG:HG3	1:I:422:PHE:HB3	2.02	0.40
1:J:404:LEU:H	1:J:434:ASN:HD21	1.68	0.40
1:L:385:LEU:N	1:L:428:ASP:OD1	2.51	0.40
1:N:373:ARG:HH21	1:O:275:LYS:HD3	1.86	0.40
1:P:373:ARG:HH21	1:Q:275:LYS:CE	2.34	0.40
1:S:404:LEU:H	1:S:434:ASN:HD21	1.68	0.40
1:T:404:LEU:H	1:T:434:ASN:HD21	1.68	0.40
1:Y:301:SER:HB3	1:Y:359:GLN:HB3	2.02	0.40
1:Z:244:ARG:HD2	1:1:235:LEU:HD22	2.03	0.40
1:Z:415:LEU:HD22	1:1:388:ALA:HB1	2.04	0.40
1:3:404:LEU:H	1:3:434:ASN:HD21	1.68	0.40
1:6:284:PRO:O	1:6:290:LYS:HE2	2.21	0.40
1:6:361:ASN:OD1	1:6:361:ASN:N	2.55	0.40
1:B:290:LYS:HA	1:C:284:PRO:HB3	2.04	0.40
1:C:253:LEU:O	1:C:257:VAL:HG22	2.20	0.40
1:C:284:PRO:O	1:C:290:LYS:HE2	2.21	0.40
1:D:361:ASN:OD1	1:D:361:ASN:N	2.55	0.40
1:H:284:PRO:O	1:H:290:LYS:HE2	2.21	0.40
1:J:373:ARG:HH21	1:K:275:LYS:CE	2.35	0.40
1:J:418:GLU:HG3	1:K:431:ASN:HB3	2.04	0.40
1:P:404:LEU:H	1:P:434:ASN:HD21	1.68	0.40
1:R:404:LEU:H	1:R:434:ASN:HD21	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:361:ASN:OD1	1:5:361:ASN:N	2.55	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	1	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	2	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	3	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	4	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	5	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	6	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	A	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	B	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	C	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	D	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	E	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	F	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	G	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	H	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	I	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	J	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	K	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	L	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	M	145/560 (26%)	130 (90%)	15 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	O	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	P	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	Q	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	R	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	S	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	T	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	U	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	V	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	W	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	X	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	Y	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
1	Z	145/560 (26%)	130 (90%)	15 (10%)	0	100	100
All	All	4640/17920 (26%)	4160 (90%)	480 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	2	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	3	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	4	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	5	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	6	134/467 (29%)	118 (88%)	16 (12%)	5	20
1	A	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	B	134/467 (29%)	118 (88%)	16 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	D	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	E	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	F	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	G	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	H	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	I	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	J	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	K	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	L	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	M	134/467 (29%)	118 (88%)	16 (12%)	5	20
1	N	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	O	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	P	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	Q	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	R	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	S	134/467 (29%)	118 (88%)	16 (12%)	5	20
1	T	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	U	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	V	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	W	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	X	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	Y	134/467 (29%)	119 (89%)	15 (11%)	6	22
1	Z	134/467 (29%)	118 (88%)	16 (12%)	5	20
All	All	4288/14944 (29%)	3803 (89%)	485 (11%)	8	21

All (485) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	243	SER
1	A	289	SER
1	A	299	ASN
1	A	357	SER

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Mol	Chain	Res	Type
1	A	358	THR
1	A	369	ASP
1	A	386	SER
1	A	416	THR
1	A	423	SER
1	A	424	ASP
1	A	425	LYS
1	A	429	THR
1	A	430	LEU
1	A	435	SER
1	B	231	ASN
1	B	243	SER
1	B	289	SER
1	B	299	ASN
1	B	357	SER
1	B	358	THR
1	B	369	ASP
1	B	381	ASP
1	B	386	SER
1	B	416	THR
1	B	423	SER
1	B	424	ASP
1	B	425	LYS
1	B	429	THR
1	B	430	LEU
1	B	435	SER
1	C	231	ASN
1	C	243	SER
1	C	289	SER
1	C	299	ASN
1	C	357	SER
1	C	358	THR
1	C	369	ASP
1	C	386	SER
1	C	416	THR
1	C	423	SER
1	C	424	ASP
1	C	425	LYS
1	C	429	THR
1	C	430	LEU
1	C	435	SER
1	D	231	ASN

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Mol	Chain	Res	Type
1	D	243	SER
1	D	289	SER
1	D	299	ASN
1	D	357	SER
1	D	358	THR
1	D	369	ASP
1	D	386	SER
1	D	416	THR
1	D	423	SER
1	D	424	ASP
1	D	425	LYS
1	D	429	THR
1	D	430	LEU
1	D	435	SER
1	E	231	ASN
1	E	243	SER
1	E	289	SER
1	E	299	ASN
1	E	357	SER
1	E	358	THR
1	E	369	ASP
1	E	386	SER
1	E	416	THR
1	E	423	SER
1	E	424	ASP
1	E	425	LYS
1	E	429	THR
1	E	430	LEU
1	E	435	SER
1	F	231	ASN
1	F	243	SER
1	F	289	SER
1	F	299	ASN
1	F	357	SER
1	F	358	THR
1	F	369	ASP
1	F	386	SER
1	F	416	THR
1	F	423	SER
1	F	424	ASP
1	F	425	LYS
1	F	429	THR

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Mol	Chain	Res	Type
1	F	430	LEU
1	F	435	SER
1	G	231	ASN
1	G	243	SER
1	G	289	SER
1	G	299	ASN
1	G	357	SER
1	G	358	THR
1	G	369	ASP
1	G	386	SER
1	G	416	THR
1	G	423	SER
1	G	424	ASP
1	G	425	LYS
1	G	429	THR
1	G	430	LEU
1	G	435	SER
1	H	231	ASN
1	H	243	SER
1	H	289	SER
1	H	299	ASN
1	H	357	SER
1	H	358	THR
1	H	369	ASP
1	H	386	SER
1	H	416	THR
1	H	423	SER
1	H	424	ASP
1	H	425	LYS
1	H	429	THR
1	H	430	LEU
1	H	435	SER
1	I	231	ASN
1	I	243	SER
1	I	289	SER
1	I	299	ASN
1	I	357	SER
1	I	358	THR
1	I	369	ASP
1	I	386	SER
1	I	416	THR
1	I	423	SER

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Mol	Chain	Res	Type
1	I	424	ASP
1	I	425	LYS
1	I	429	THR
1	I	430	LEU
1	I	435	SER
1	J	231	ASN
1	J	243	SER
1	J	289	SER
1	J	299	ASN
1	J	357	SER
1	J	358	THR
1	J	369	ASP
1	J	386	SER
1	J	416	THR
1	J	423	SER
1	J	424	ASP
1	J	425	LYS
1	J	429	THR
1	J	430	LEU
1	J	435	SER
1	K	231	ASN
1	K	243	SER
1	K	289	SER
1	K	299	ASN
1	K	357	SER
1	K	358	THR
1	K	369	ASP
1	K	386	SER
1	K	416	THR
1	K	423	SER
1	K	424	ASP
1	K	425	LYS
1	K	429	THR
1	K	430	LEU
1	K	435	SER
1	L	231	ASN
1	L	243	SER
1	L	289	SER
1	L	299	ASN
1	L	357	SER
1	L	358	THR
1	L	369	ASP

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Mol	Chain	Res	Type
1	L	386	SER
1	L	416	THR
1	L	423	SER
1	L	424	ASP
1	L	425	LYS
1	L	429	THR
1	L	430	LEU
1	L	435	SER
1	M	231	ASN
1	M	243	SER
1	M	289	SER
1	M	299	ASN
1	M	357	SER
1	M	358	THR
1	M	369	ASP
1	M	381	ASP
1	M	386	SER
1	M	416	THR
1	M	423	SER
1	M	424	ASP
1	M	425	LYS
1	M	429	THR
1	M	430	LEU
1	M	435	SER
1	N	231	ASN
1	N	243	SER
1	N	289	SER
1	N	299	ASN
1	N	357	SER
1	N	358	THR
1	N	369	ASP
1	N	386	SER
1	N	416	THR
1	N	423	SER
1	N	424	ASP
1	N	425	LYS
1	N	429	THR
1	N	430	LEU
1	N	435	SER
1	O	231	ASN
1	O	243	SER
1	O	289	SER

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Mol	Chain	Res	Type
1	O	299	ASN
1	O	357	SER
1	O	358	THR
1	O	369	ASP
1	O	386	SER
1	O	416	THR
1	O	423	SER
1	O	424	ASP
1	O	425	LYS
1	O	429	THR
1	O	430	LEU
1	O	435	SER
1	P	231	ASN
1	P	243	SER
1	P	289	SER
1	P	299	ASN
1	P	357	SER
1	P	358	THR
1	P	369	ASP
1	P	386	SER
1	P	416	THR
1	P	423	SER
1	P	424	ASP
1	P	425	LYS
1	P	429	THR
1	P	430	LEU
1	P	435	SER
1	Q	231	ASN
1	Q	243	SER
1	Q	289	SER
1	Q	299	ASN
1	Q	357	SER
1	Q	358	THR
1	Q	369	ASP
1	Q	386	SER
1	Q	416	THR
1	Q	423	SER
1	Q	424	ASP
1	Q	425	LYS
1	Q	429	THR
1	Q	430	LEU
1	Q	435	SER

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Mol	Chain	Res	Type
1	R	231	ASN
1	R	243	SER
1	R	289	SER
1	R	299	ASN
1	R	357	SER
1	R	358	THR
1	R	369	ASP
1	R	386	SER
1	R	416	THR
1	R	423	SER
1	R	424	ASP
1	R	425	LYS
1	R	429	THR
1	R	430	LEU
1	R	435	SER
1	S	231	ASN
1	S	243	SER
1	S	289	SER
1	S	299	ASN
1	S	357	SER
1	S	358	THR
1	S	369	ASP
1	S	381	ASP
1	S	386	SER
1	S	416	THR
1	S	423	SER
1	S	424	ASP
1	S	425	LYS
1	S	429	THR
1	S	430	LEU
1	S	435	SER
1	T	231	ASN
1	T	243	SER
1	T	289	SER
1	T	299	ASN
1	T	357	SER
1	T	358	THR
1	T	369	ASP
1	T	386	SER
1	T	416	THR
1	T	423	SER
1	T	424	ASP

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Mol	Chain	Res	Type
1	T	425	LYS
1	T	429	THR
1	T	430	LEU
1	T	435	SER
1	U	231	ASN
1	U	243	SER
1	U	289	SER
1	U	299	ASN
1	U	357	SER
1	U	358	THR
1	U	369	ASP
1	U	386	SER
1	U	416	THR
1	U	423	SER
1	U	424	ASP
1	U	425	LYS
1	U	429	THR
1	U	430	LEU
1	U	435	SER
1	V	231	ASN
1	V	243	SER
1	V	289	SER
1	V	299	ASN
1	V	357	SER
1	V	358	THR
1	V	369	ASP
1	V	386	SER
1	V	416	THR
1	V	423	SER
1	V	424	ASP
1	V	425	LYS
1	V	429	THR
1	V	430	LEU
1	V	435	SER
1	W	231	ASN
1	W	243	SER
1	W	289	SER
1	W	299	ASN
1	W	357	SER
1	W	358	THR
1	W	369	ASP
1	W	386	SER

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Mol	Chain	Res	Type
1	W	416	THR
1	W	423	SER
1	W	424	ASP
1	W	425	LYS
1	W	429	THR
1	W	430	LEU
1	W	435	SER
1	X	231	ASN
1	X	243	SER
1	X	289	SER
1	X	299	ASN
1	X	357	SER
1	X	358	THR
1	X	369	ASP
1	X	386	SER
1	X	416	THR
1	X	423	SER
1	X	424	ASP
1	X	425	LYS
1	X	429	THR
1	X	430	LEU
1	X	435	SER
1	Y	231	ASN
1	Y	243	SER
1	Y	289	SER
1	Y	299	ASN
1	Y	357	SER
1	Y	358	THR
1	Y	369	ASP
1	Y	386	SER
1	Y	416	THR
1	Y	423	SER
1	Y	424	ASP
1	Y	425	LYS
1	Y	429	THR
1	Y	430	LEU
1	Y	435	SER
1	Z	231	ASN
1	Z	243	SER
1	Z	289	SER
1	Z	299	ASN
1	Z	357	SER

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Mol	Chain	Res	Type
1	Z	358	THR
1	Z	369	ASP
1	Z	381	ASP
1	Z	386	SER
1	Z	416	THR
1	Z	423	SER
1	Z	424	ASP
1	Z	425	LYS
1	Z	429	THR
1	Z	430	LEU
1	Z	435	SER
1	1	231	ASN
1	1	243	SER
1	1	289	SER
1	1	299	ASN
1	1	357	SER
1	1	358	THR
1	1	369	ASP
1	1	386	SER
1	1	416	THR
1	1	423	SER
1	1	424	ASP
1	1	425	LYS
1	1	429	THR
1	1	430	LEU
1	1	435	SER
1	2	231	ASN
1	2	243	SER
1	2	289	SER
1	2	299	ASN
1	2	357	SER
1	2	358	THR
1	2	369	ASP
1	2	386	SER
1	2	416	THR
1	2	423	SER
1	2	424	ASP
1	2	425	LYS
1	2	429	THR
1	2	430	LEU
1	2	435	SER
1	3	231	ASN

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Mol	Chain	Res	Type
1	3	243	SER
1	3	289	SER
1	3	299	ASN
1	3	357	SER
1	3	358	THR
1	3	369	ASP
1	3	386	SER
1	3	416	THR
1	3	423	SER
1	3	424	ASP
1	3	425	LYS
1	3	429	THR
1	3	430	LEU
1	3	435	SER
1	4	231	ASN
1	4	243	SER
1	4	289	SER
1	4	299	ASN
1	4	357	SER
1	4	358	THR
1	4	369	ASP
1	4	386	SER
1	4	416	THR
1	4	423	SER
1	4	424	ASP
1	4	425	LYS
1	4	429	THR
1	4	430	LEU
1	4	435	SER
1	5	231	ASN
1	5	243	SER
1	5	289	SER
1	5	299	ASN
1	5	357	SER
1	5	358	THR
1	5	369	ASP
1	5	386	SER
1	5	416	THR
1	5	423	SER
1	5	424	ASP
1	5	425	LYS
1	5	429	THR

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Mol	Chain	Res	Type
1	5	430	LEU
1	5	435	SER
1	6	231	ASN
1	6	243	SER
1	6	289	SER
1	6	299	ASN
1	6	357	SER
1	6	358	THR
1	6	369	ASP
1	6	381	ASP
1	6	386	SER
1	6	416	THR
1	6	423	SER
1	6	424	ASP
1	6	425	LYS
1	6	429	THR
1	6	430	LEU
1	6	435	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	285	ASN
1	A	365	ASN
1	A	374	HIS
1	B	231	ASN
1	B	285	ASN
1	B	365	ASN
1	B	374	HIS
1	C	231	ASN
1	C	281	HIS
1	C	285	ASN
1	C	365	ASN
1	C	374	HIS
1	D	231	ASN
1	D	281	HIS
1	D	285	ASN
1	D	365	ASN
1	D	431	ASN
1	D	434	ASN
1	E	231	ASN

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Mol	Chain	Res	Type
1	E	274	ASN
1	E	285	ASN
1	E	365	ASN
1	E	374	HIS
1	E	431	ASN
1	E	434	ASN
1	F	231	ASN
1	F	281	HIS
1	F	365	ASN
1	F	374	HIS
1	F	431	ASN
1	F	434	ASN
1	G	231	ASN
1	G	285	ASN
1	G	365	ASN
1	G	374	HIS
1	G	434	ASN
1	H	231	ASN
1	H	281	HIS
1	H	285	ASN
1	H	365	ASN
1	H	434	ASN
1	I	231	ASN
1	I	285	ASN
1	I	365	ASN
1	I	374	HIS
1	I	431	ASN
1	J	231	ASN
1	J	274	ASN
1	J	281	HIS
1	J	285	ASN
1	J	365	ASN
1	J	374	HIS
1	J	431	ASN
1	K	231	ASN
1	K	281	HIS
1	K	285	ASN
1	K	365	ASN
1	K	374	HIS
1	K	431	ASN
1	L	231	ASN
1	L	285	ASN

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Mol	Chain	Res	Type
1	L	365	ASN
1	L	374	HIS
1	L	411	GLN
1	L	431	ASN
1	M	231	ASN
1	M	281	HIS
1	M	285	ASN
1	M	365	ASN
1	M	374	HIS
1	M	431	ASN
1	M	434	ASN
1	N	231	ASN
1	N	274	ASN
1	N	281	HIS
1	N	365	ASN
1	N	431	ASN
1	N	434	ASN
1	O	231	ASN
1	O	281	HIS
1	O	365	ASN
1	O	374	HIS
1	P	231	ASN
1	P	281	HIS
1	P	285	ASN
1	P	365	ASN
1	P	374	HIS
1	Q	231	ASN
1	Q	281	HIS
1	Q	365	ASN
1	Q	374	HIS
1	Q	431	ASN
1	R	231	ASN
1	R	281	HIS
1	R	285	ASN
1	R	365	ASN
1	R	374	HIS
1	R	431	ASN
1	R	434	ASN
1	S	231	ASN
1	S	269	GLN
1	S	281	HIS
1	S	285	ASN

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Mol	Chain	Res	Type
1	S	365	ASN
1	S	374	HIS
1	S	431	ASN
1	T	231	ASN
1	T	274	ASN
1	T	285	ASN
1	T	365	ASN
1	T	374	HIS
1	T	431	ASN
1	T	434	ASN
1	U	231	ASN
1	U	281	HIS
1	U	365	ASN
1	U	374	HIS
1	U	411	GLN
1	U	431	ASN
1	U	434	ASN
1	V	231	ASN
1	V	285	ASN
1	V	365	ASN
1	V	431	ASN
1	V	434	ASN
1	W	231	ASN
1	W	281	HIS
1	W	365	ASN
1	W	374	HIS
1	W	434	ASN
1	X	231	ASN
1	X	281	HIS
1	X	285	ASN
1	X	365	ASN
1	X	434	ASN
1	Y	231	ASN
1	Y	274	ASN
1	Y	285	ASN
1	Y	365	ASN
1	Y	374	HIS
1	Y	431	ASN
1	Y	434	ASN
1	Z	231	ASN
1	Z	365	ASN
1	1	231	ASN

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Mol	Chain	Res	Type
1	1	274	ASN
1	1	281	HIS
1	1	365	ASN
1	1	374	HIS
1	1	411	GLN
1	2	231	ASN
1	2	285	ASN
1	2	365	ASN
1	3	231	ASN
1	3	281	HIS
1	3	285	ASN
1	3	365	ASN
1	3	374	HIS
1	3	434	ASN
1	4	231	ASN
1	4	281	HIS
1	4	365	ASN
1	4	374	HIS
1	4	411	GLN
1	5	231	ASN
1	5	285	ASN
1	5	365	ASN
1	5	374	HIS
1	5	431	ASN
1	6	231	ASN
1	6	281	HIS
1	6	365	ASN
1	6	374	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

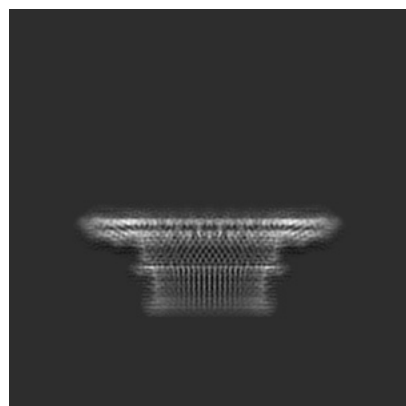
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10560. These allow visual inspection of the internal detail of the map and identification of artifacts.

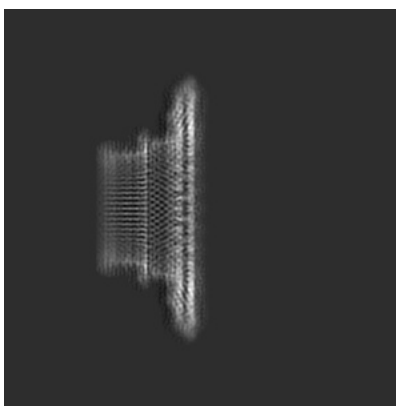
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

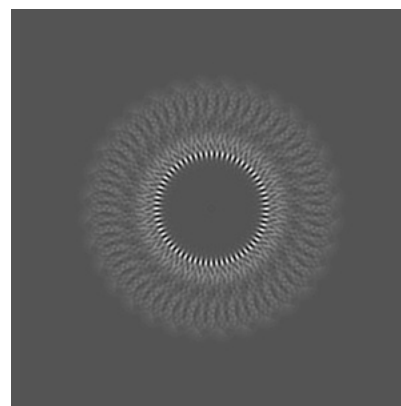
6.1.1 Primary map



X

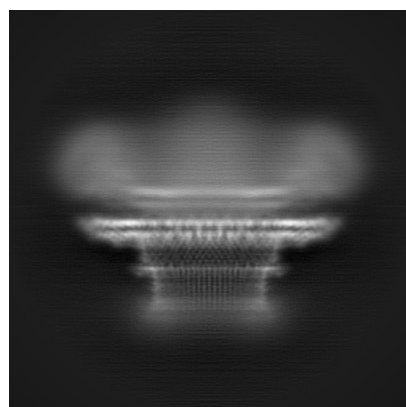


Y

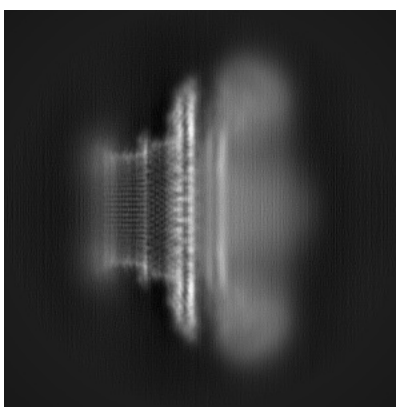


Z

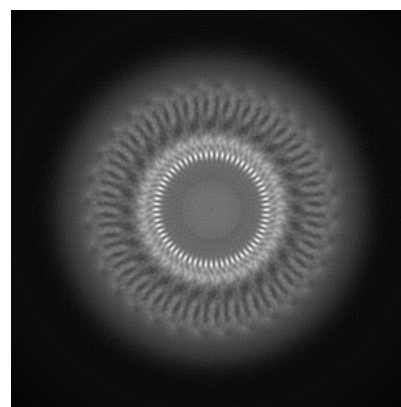
6.1.2 Raw map



X



Y

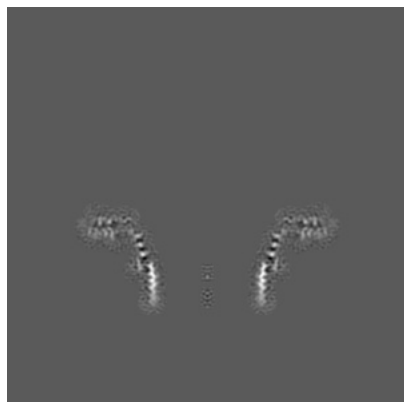


Z

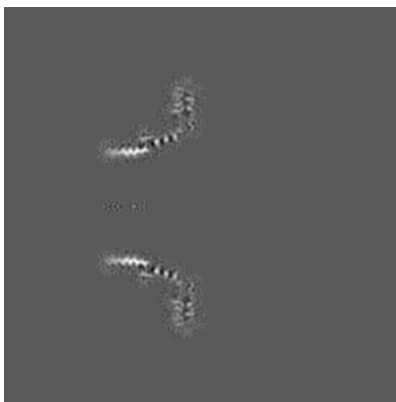
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

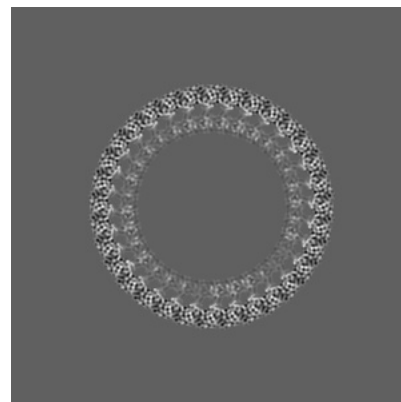
6.2.1 Primary map



X Index: 216

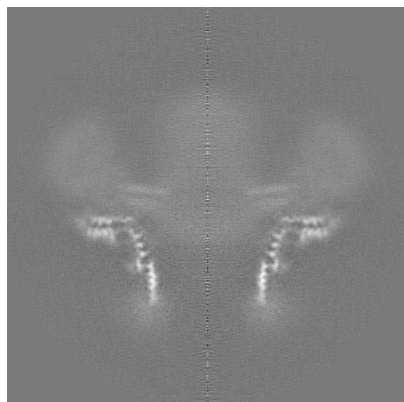


Y Index: 216

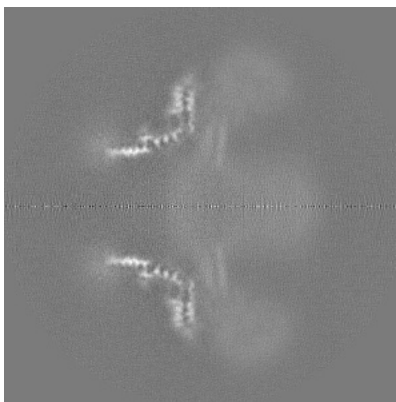


Z Index: 216

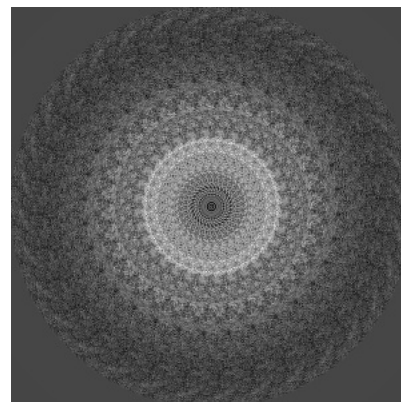
6.2.2 Raw map



X Index: 216



Y Index: 216



Z Index: 216

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

6.3 Largest variance slices [i](#)

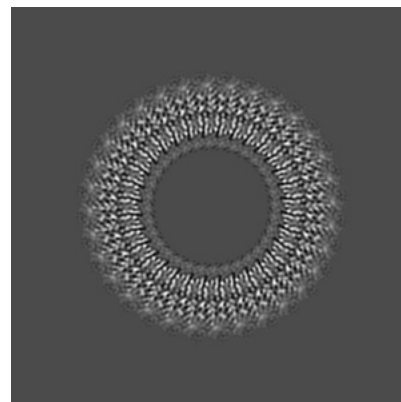
6.3.1 Primary map



X Index: 159

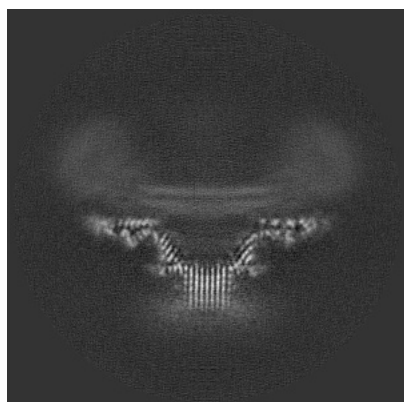


Y Index: 159

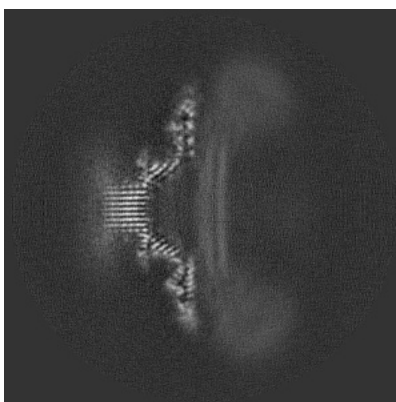


Z Index: 190

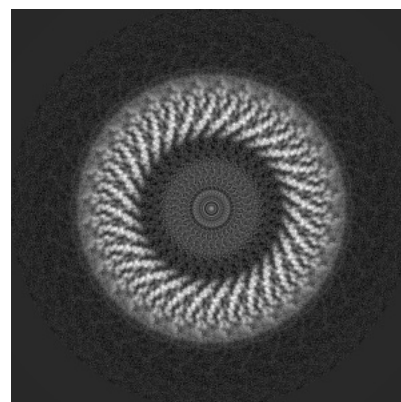
6.3.2 Raw map



X Index: 274



Y Index: 158

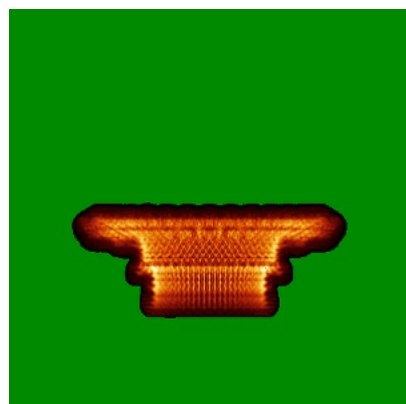


Z Index: 201

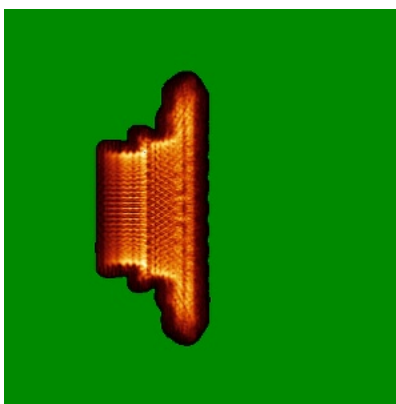
The images above show the largest variance slices of the map in three orthogonal directions.

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

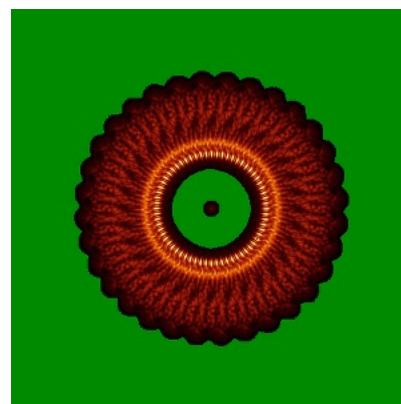
6.4.1 Primary map



X

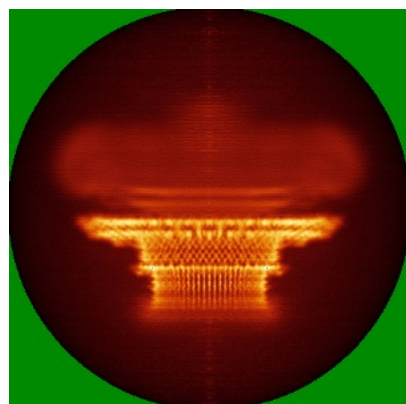


Y

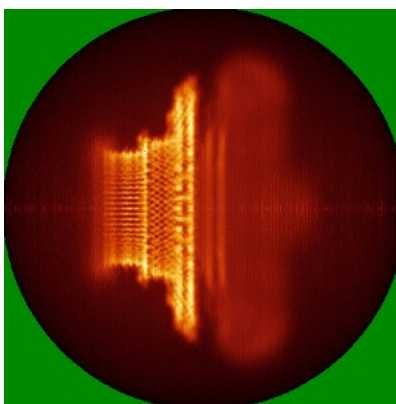


Z

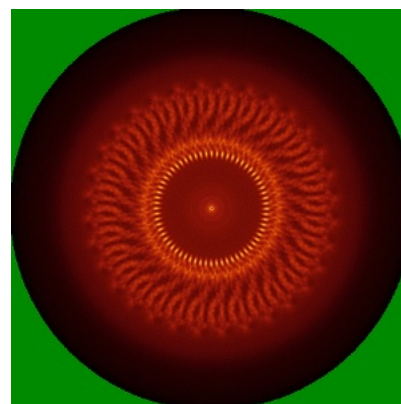
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

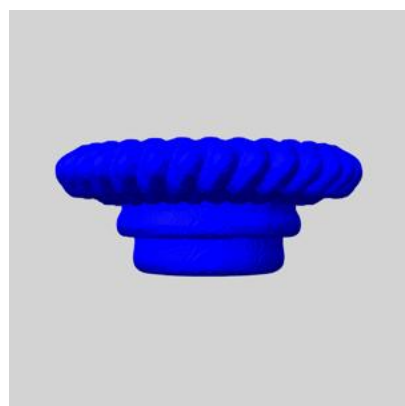
6.6 Mask visualisation [i](#)

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

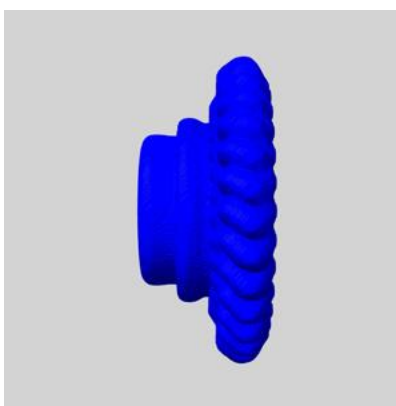
A mask typically either:

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

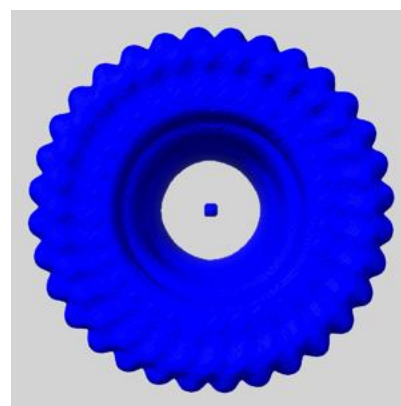
6.6.1 emd_10560_msk_1.map [i](#)



X



Y

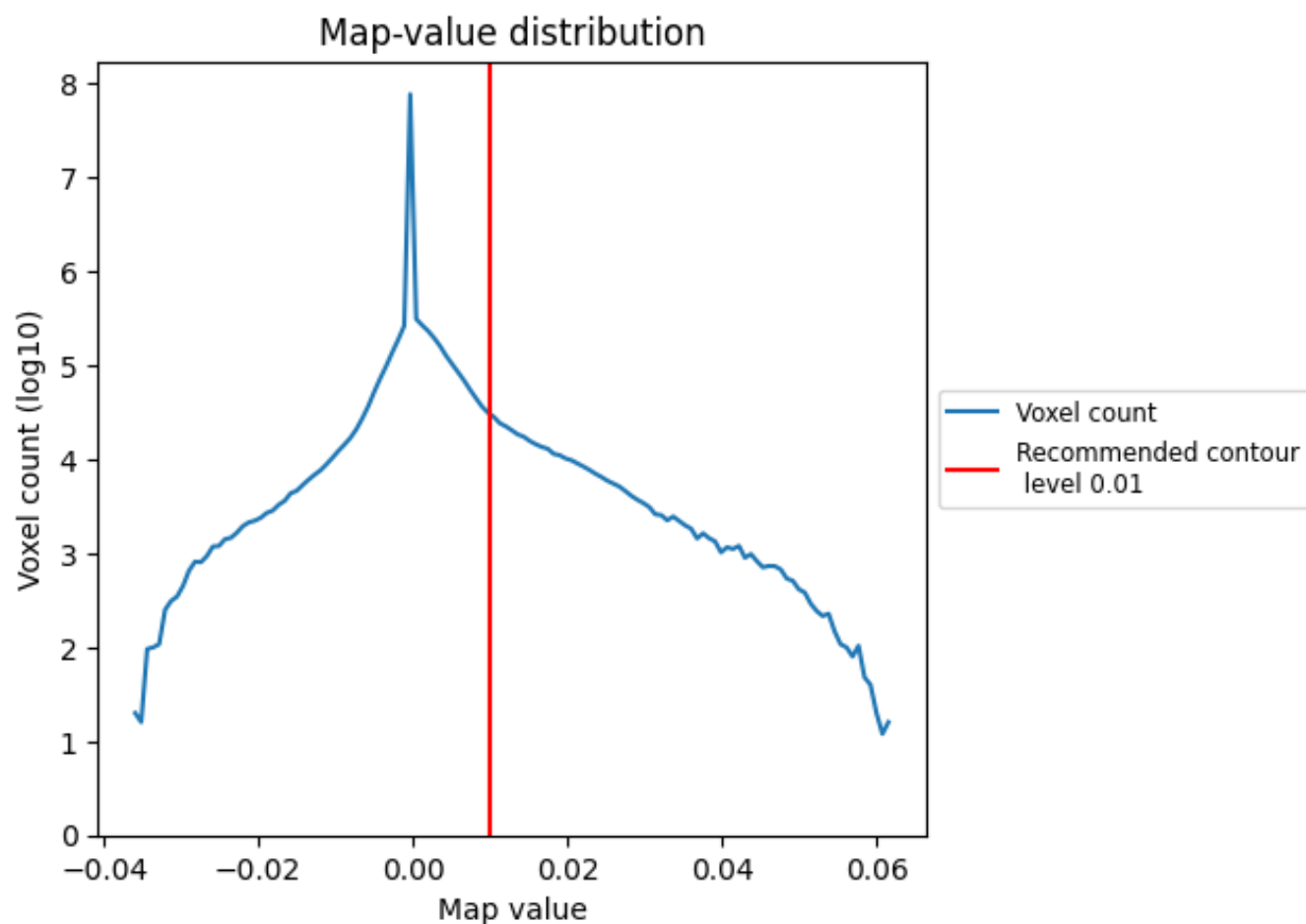


Z

7 Map analysis [i](#)

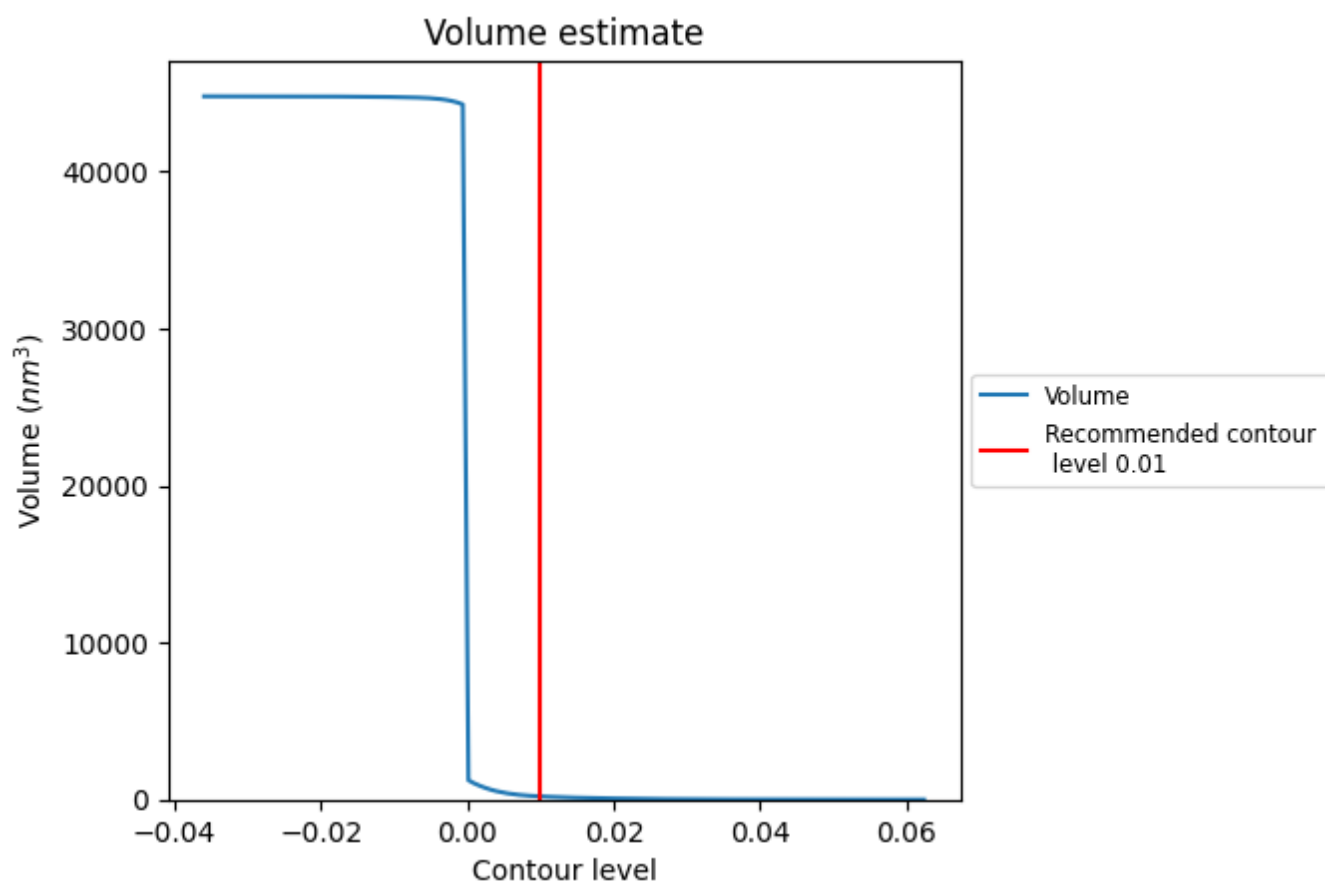
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

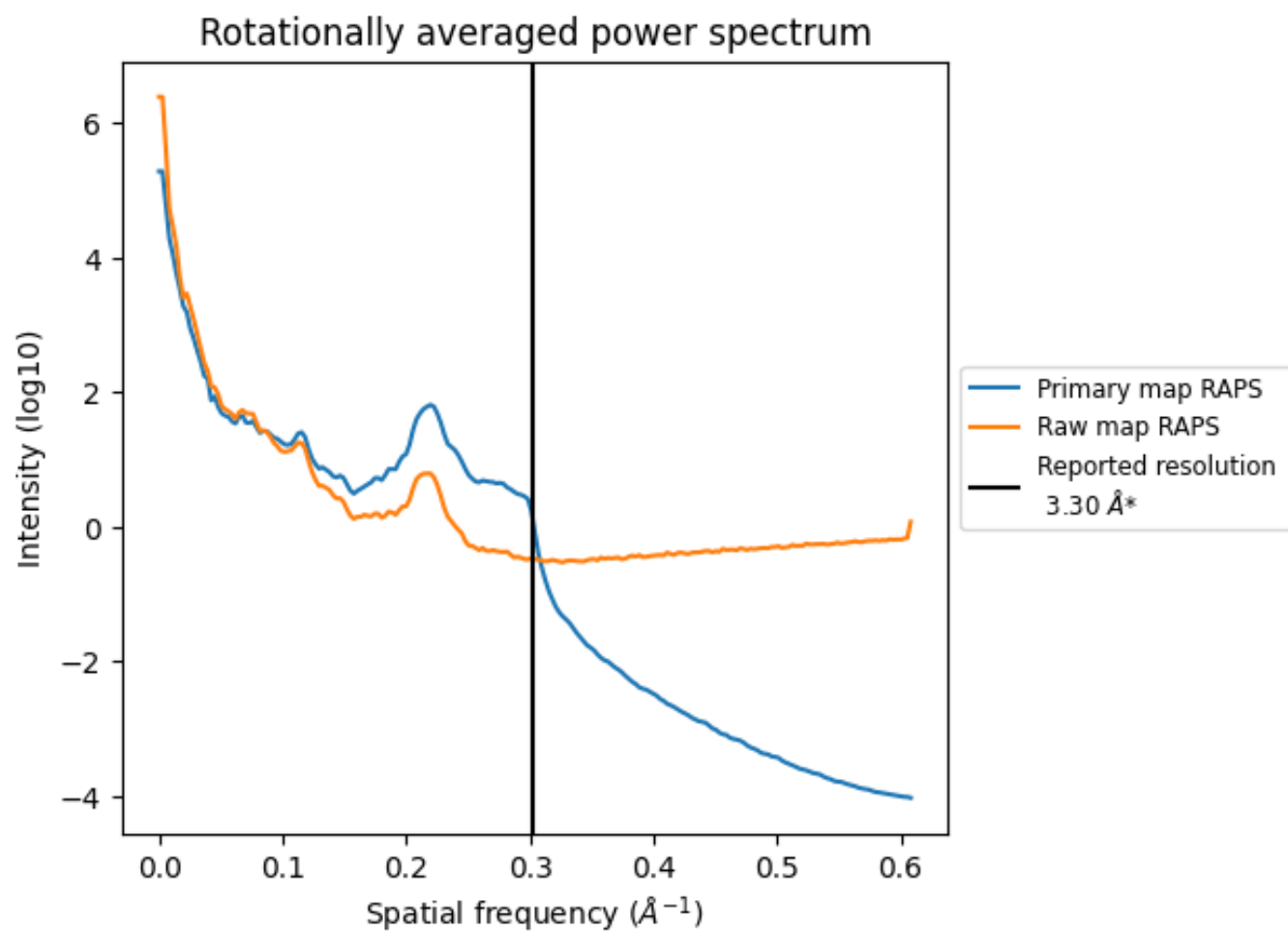
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 181 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

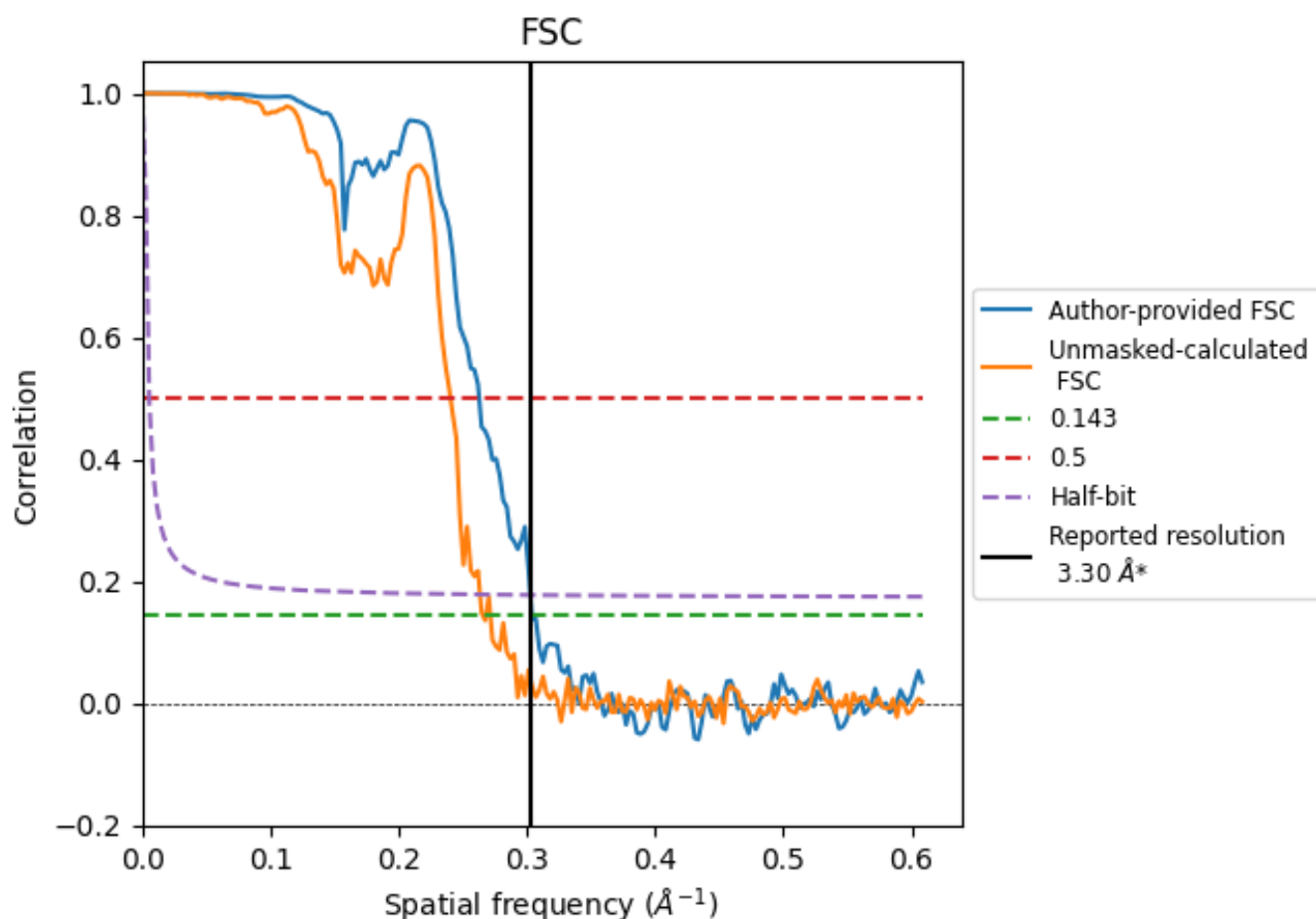


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

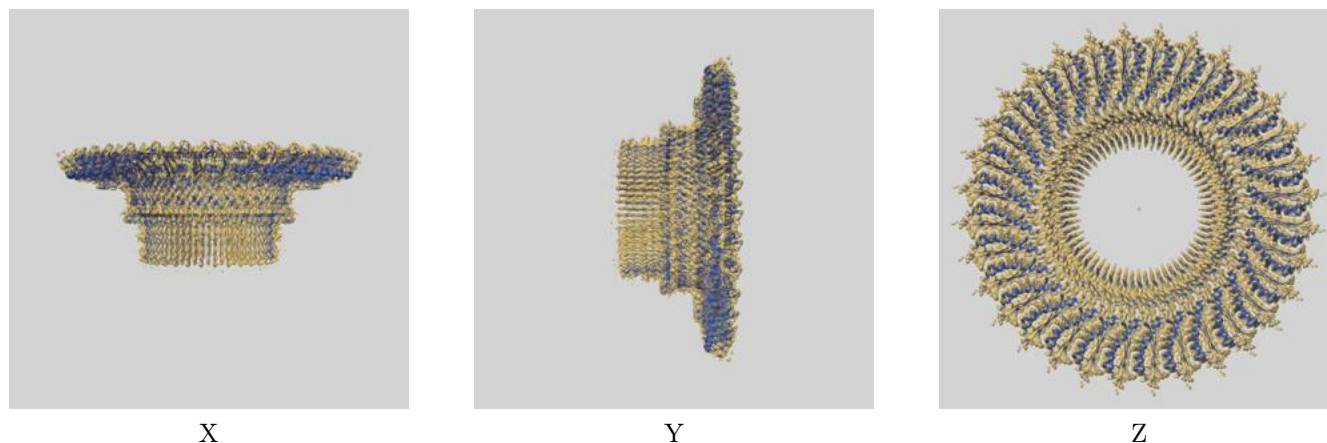
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.81	3.30
Unmasked-calculated*	3.76	4.16	3.80

*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 3.76 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

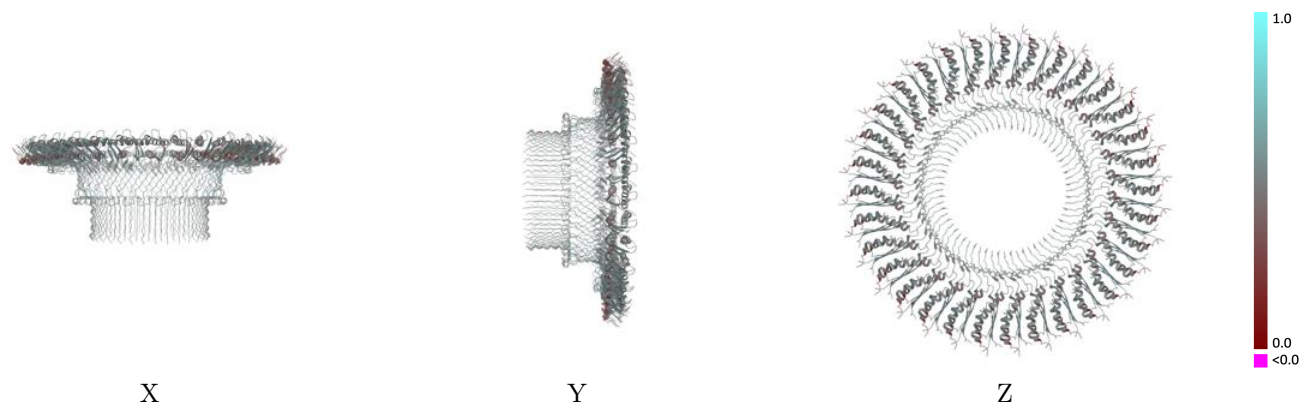
This section contains information regarding the fit between EMDB map EMD-10560 and PDB model 6TRE. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

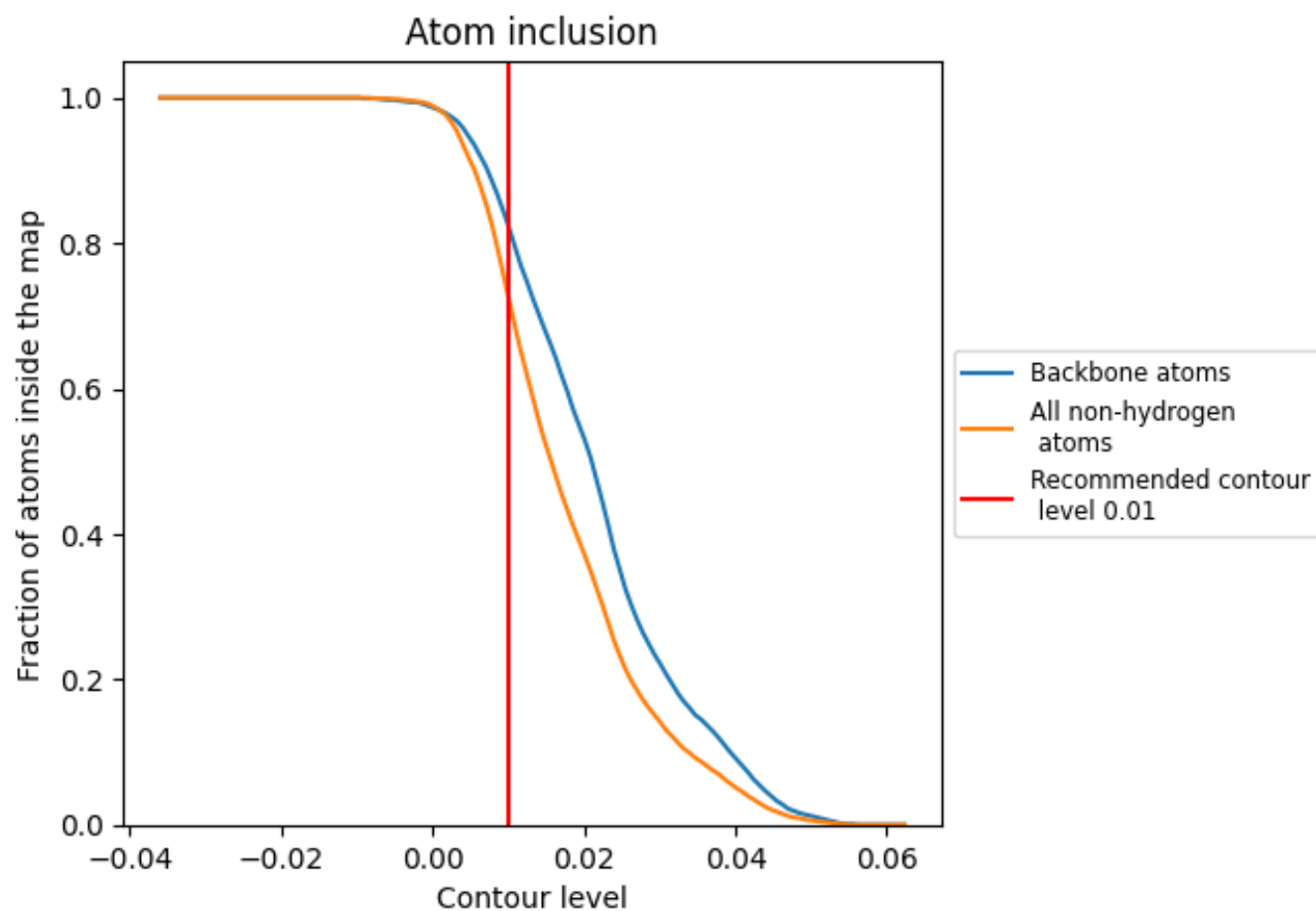


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 73% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7270	 0.5010
1	 0.7350	 0.5040
2	 0.7340	 0.5040
3	 0.7290	 0.5000
4	 0.7120	 0.4990
5	 0.7160	 0.4940
6	 0.7080	 0.4850
A	 0.7200	 0.4970
B	 0.7260	 0.5050
C	 0.7220	 0.5050
D	 0.7170	 0.5060
E	 0.7330	 0.5080
F	 0.7180	 0.5020
G	 0.7280	 0.5000
H	 0.7400	 0.5090
I	 0.7340	 0.5060
J	 0.7290	 0.5000
K	 0.7320	 0.5000
L	 0.7330	 0.5000
M	 0.7400	 0.5080
N	 0.7260	 0.5040
O	 0.7300	 0.5020
P	 0.7320	 0.5040
Q	 0.7100	 0.4750
R	 0.7150	 0.4830
S	 0.7160	 0.4900
T	 0.7400	 0.5030
U	 0.7240	 0.4970
V	 0.7370	 0.5060
W	 0.7430	 0.5060
X	 0.7330	 0.5070
Y	 0.7310	 0.5050
Z	 0.7290	 0.5040

