



Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 02:45 PM JST

PDB ID : 8Z5S / pdb_00008z5s
EMDB ID : EMD-39780
Title : Cryo-EM structure of the proximal rod-export apparatus of the polar flagellar motor
Authors : Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2024-04-18
Resolution : 3.03 Å(reported)
Based on initial model : .

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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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

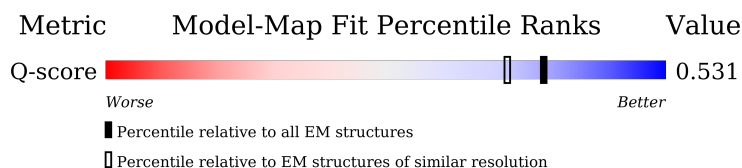
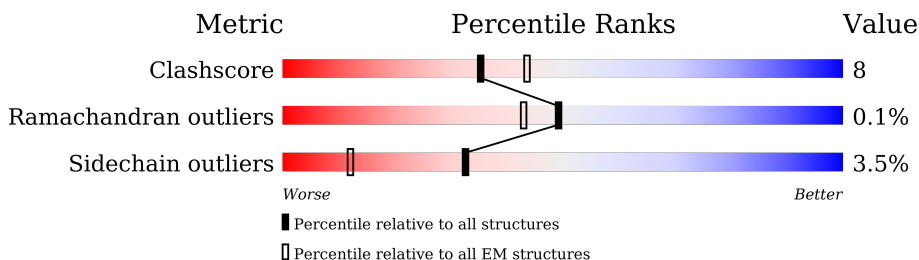
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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.



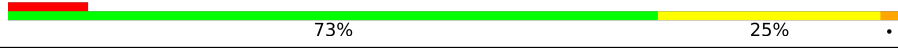
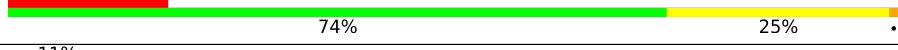
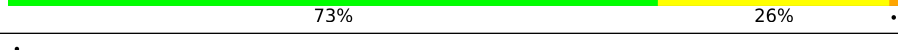
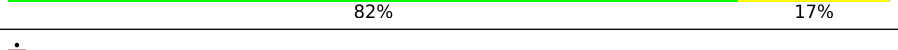
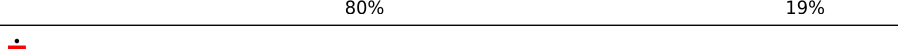
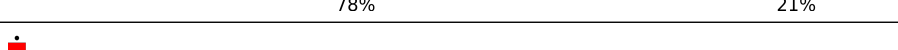
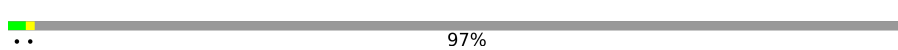
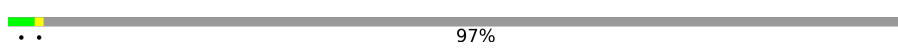
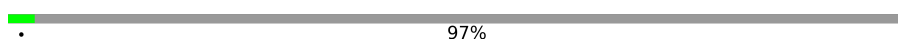
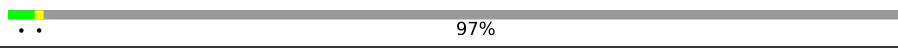
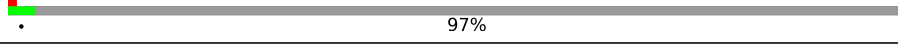
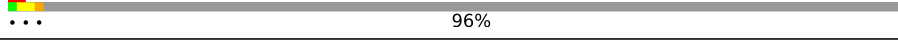
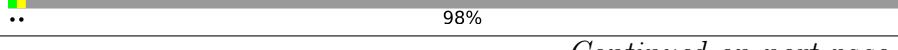
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13929 (2.53 - 3.53)

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	289	
1	2	289	
1	3	289	
1	y	289	

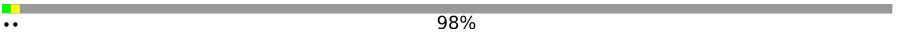
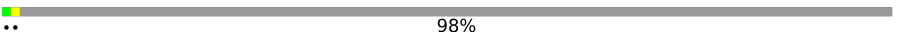
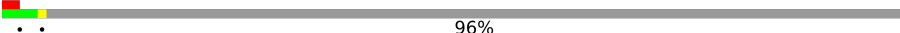
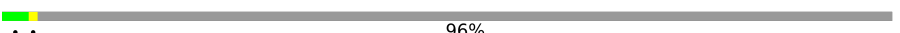
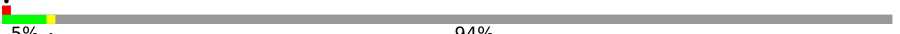
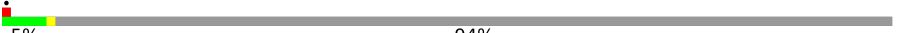
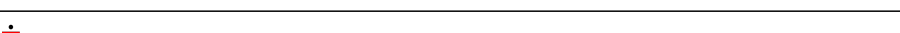
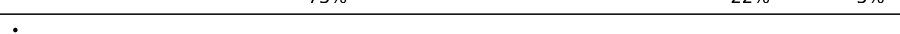
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Mol	Chain	Length	Quality of chain
1	z	289	
2	4	89	
2	5	89	
2	6	89	
2	7	89	
3	m	249	
3	n	249	
3	o	249	
3	p	249	
3	q	249	
4	r	103	
4	s	103	
4	t	103	
4	u	103	
4	v	103	
4	w	103	
5	x	376	
6	8	260	
7	AA	580	
7	AB	580	
7	AC	580	
7	AD	580	
7	AE	580	
7	AF	580	
7	AG	580	

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Mol	Chain	Length	Quality of chain
7	AH	580	 98%
7	AI	580	 98%
7	AJ	580	 96%
7	AK	580	 96%
7	AL	580	 5% 94%
7	AM	580	 5% 94%
7	AN	580	 5% 94%
7	AO	580	 94%
8	b	131	 69% 14% 17%
8	c	131	 8% 66% 16% 18%
8	d	131	 69% 14% 17%
8	e	131	 66% 16% 18%
8	f	131	 68% 15% 18%
9	g	137	 79% 16% 5%
9	h	137	 73% 22% 5%
9	i	137	 67% 24% 5%
9	j	137	 81% 13% 5%
9	k	137	 75% 20% 5%
9	l	137	 75% 18% 5%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 38700 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 biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	207	Total	C	N	O	S	0	0
			1599	1055	243	282	19		
1	2	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
1	3	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
1	y	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
1	z	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	26	SER	THR	conflict	UNP A0A1W6TTE6
1	204	ASP	GLU	conflict	UNP A0A1W6TTE6
2	26	SER	THR	conflict	UNP A0A1W6TTE6
2	204	ASP	GLU	conflict	UNP A0A1W6TTE6
3	26	SER	THR	conflict	UNP A0A1W6TTE6
3	204	ASP	GLU	conflict	UNP A0A1W6TTE6
y	26	SER	THR	conflict	UNP A0A1W6TTE6
y	204	ASP	GLU	conflict	UNP A0A1W6TTE6
z	26	SER	THR	conflict	UNP A0A1W6TTE6
z	204	ASP	GLU	conflict	UNP A0A1W6TTE6

- Molecule 2 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
2	5	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
2	6	89	Total	C	N	O	S	0	0
			722	489	107	117	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	89	Total	C	N	O	S	0	0
			722	489	107	117	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	34	ILE	VAL	conflict	UNP A0A0H0YAF4
5	34	ILE	VAL	conflict	UNP A0A0H0YAF4
6	34	ILE	VAL	conflict	UNP A0A0H0YAF4
7	34	ILE	VAL	conflict	UNP A0A0H0YAF4

- Molecule 3 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	m	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
3	n	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
3	o	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
3	p	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
3	q	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		

- Molecule 4 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	r	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
4	s	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
4	t	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
4	u	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
4	v	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
4	w	40	Total	C	N	O	S	0	0
			311	194	53	61	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
s	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
t	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
u	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
v	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
w	3	VAL	ILE	conflict	UNP A0A0H0Y9C1

- Molecule 5 is a protein called Flagellar biosynthetic protein FlhB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	x	71	Total	C	N	O	S	0	0
			552	370	83	95	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	87	THR	SER	conflict	UNP A0A0H0YB55

- Molecule 6 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	242	Total	C	N	O	S	0	0
			1896	1265	295	315	21		

- Molecule 7 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AA	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AB	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AC	20	Total	C	N	O	S	0	0
			139	84	24	30	1		
7	AD	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AE	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AF	23	Total	C	N	O	S	0	0
			158	97	27	33	1		
7	AG	11	Total	C	N	O		0	0
			73	46	13	14			
7	AH	11	Total	C	N	O		0	0
			73	46	13	14			

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	11	Total	C	N	O		0	0
			73	46	13	14			
7	AJ	24	Total	C	N	O	S	0	0
			163	100	28	34	1		
7	AK	25	Total	C	N	O	S	0	0
			169	104	29	35	1		
7	AL	32	Total	C	N	O	S	0	0
			220	134	38	46	2		
7	AM	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AN	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AO	32	Total	C	N	O	S	0	0
			220	134	38	46	2		

- Molecule 8 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	109	Total	C	N	O	S	0	0
			845	523	155	166	1		
8	c	107	Total	C	N	O	S	0	0
			835	518	153	163	1		
8	d	109	Total	C	N	O	S	0	0
			845	523	155	166	1		
8	e	108	Total	C	N	O	S	0	0
			837	519	154	163	1		
8	f	108	Total	C	N	O	S	0	0
			837	519	154	163	1		

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgC.

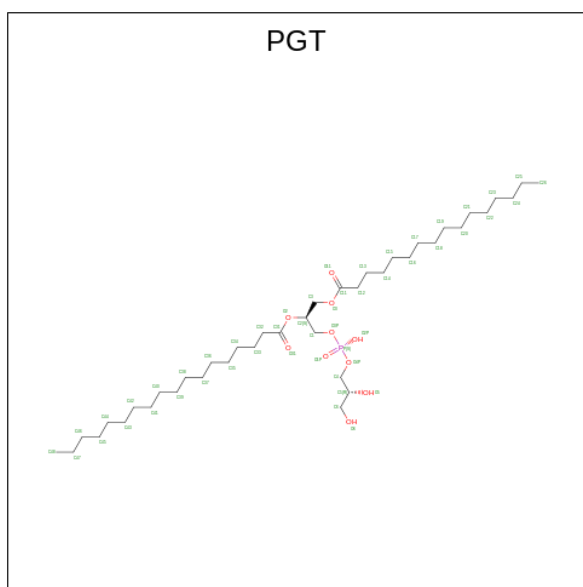
Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	h	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	i	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	j	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	k	130	Total	C	N	O	S	0	0
			983	605	168	203	7		

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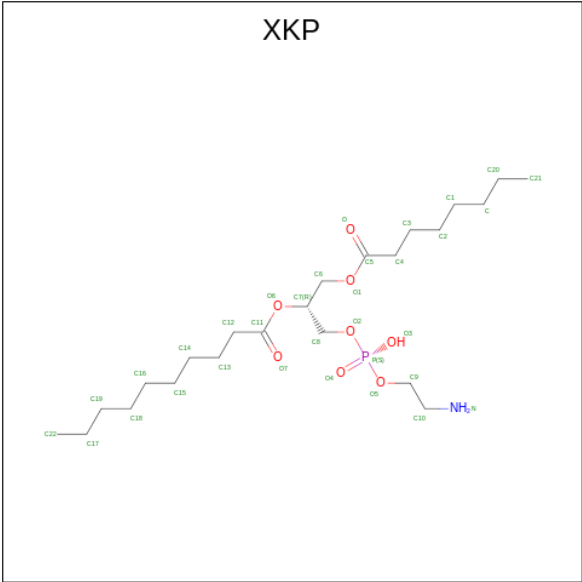
Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	130	Total	C	N	O	S	0	0
			983	605	168	203	7		

- Molecule 10 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	2	1	Total	C	O	P	0
			51	40	10	1	
10	t	1	Total	C	O	P	0
			51	40	10	1	
10	v	1	Total	C	O	P	0
			51	40	10	1	
10	e	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 11 is (11R,14S)-17-amino-14-hydroxy-8,14-dioxo-9,13,15-trioxa-14lambda 5 -phosphahaheptadecan-11-yl decanoate (CCD ID: XKP) (formula: C₂₃H₄₆NO₈P) (labeled as "Ligand of Interest" by depositor).

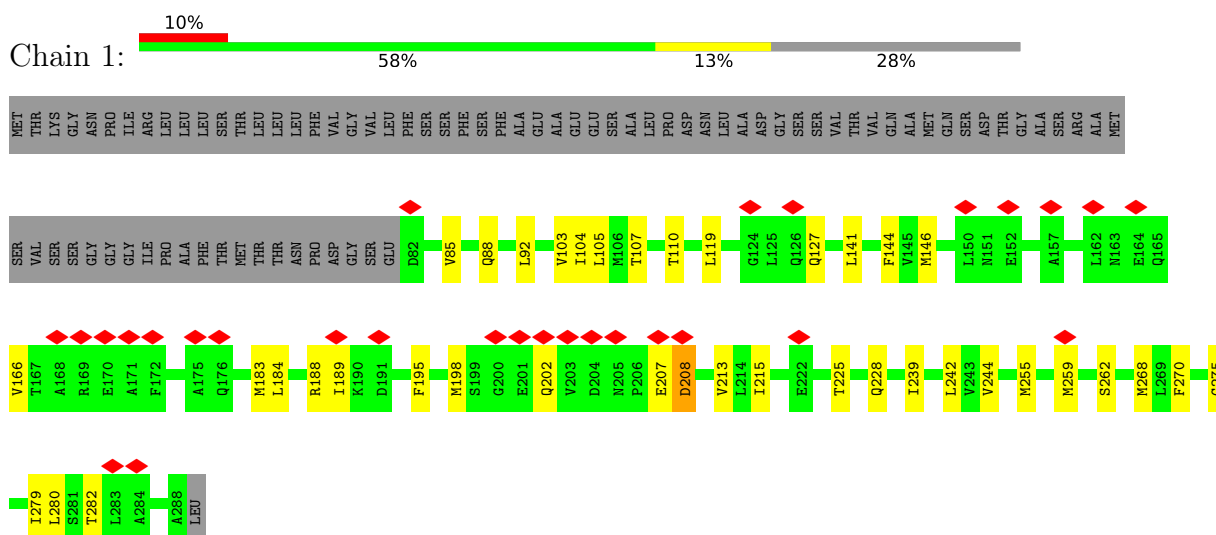


Mol	Chain	Residues	Atoms					AltConf
11	s	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	t	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	u	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	v	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	e	1	Total	C	N	O	P	0
			32	22	1	8	1	

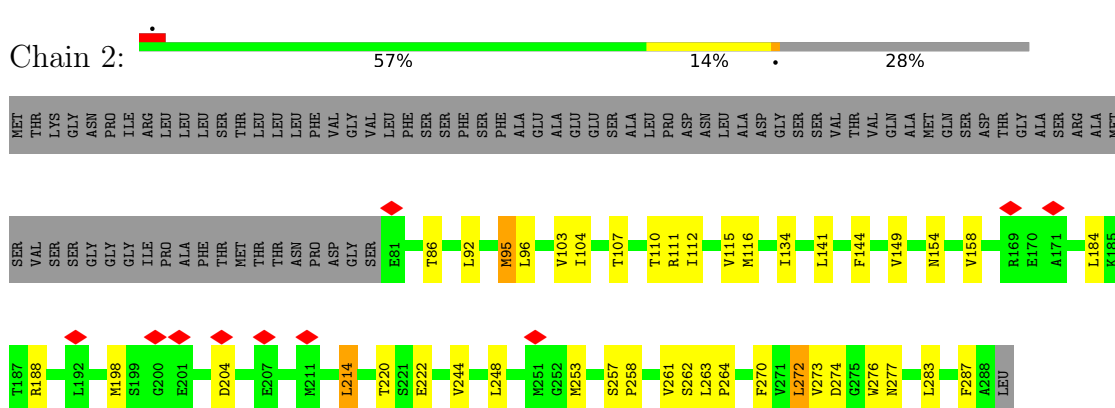
3 Residue-property plots

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.

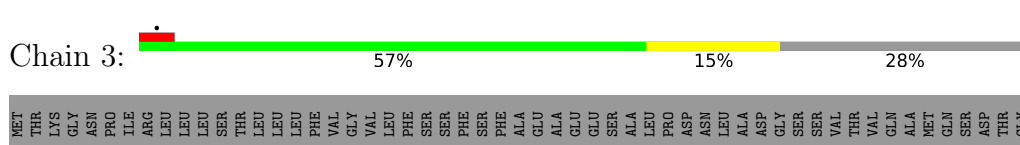
• Molecule 1: Flagellar biosynthetic protein FlpP

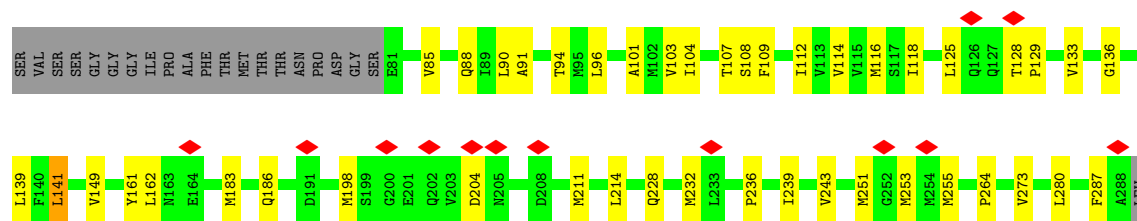


• Molecule 1: Flagellar biosynthetic protein FlpP

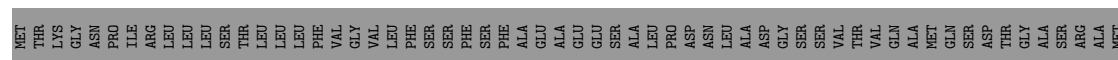


• Molecule 1: Flagellar biosynthetic protein FlpP

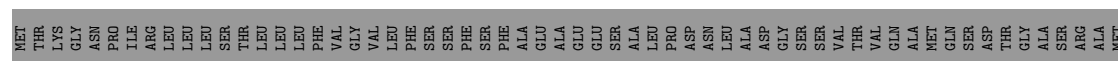




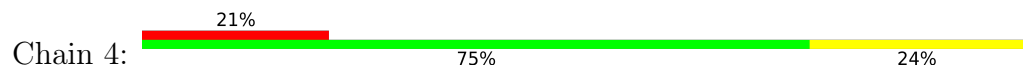
• Molecule 1: Flagellar biosynthetic protein FliP



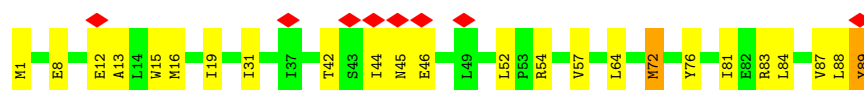
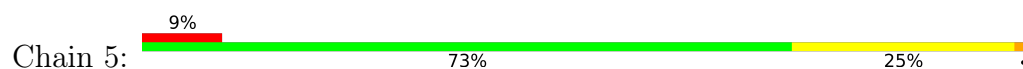
• Molecule 1: Flagellar biosynthetic protein FliP



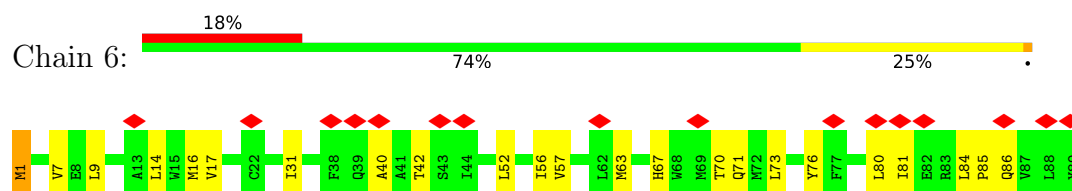
• Molecule 2: Flagellar biosynthetic protein FliQ



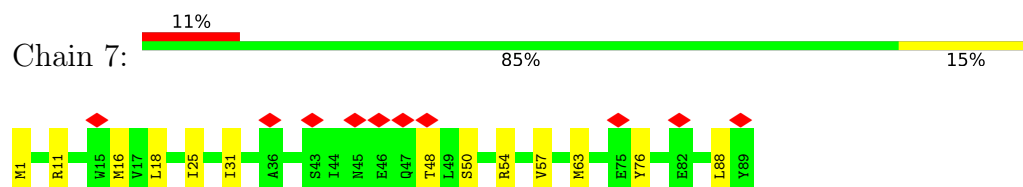
• Molecule 2: Flagellar biosynthetic protein FliQ



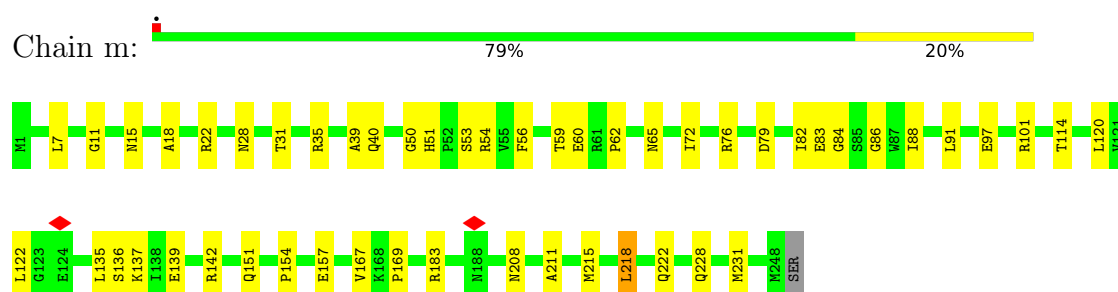
- Molecule 2: Flagellar biosynthetic protein FliQ



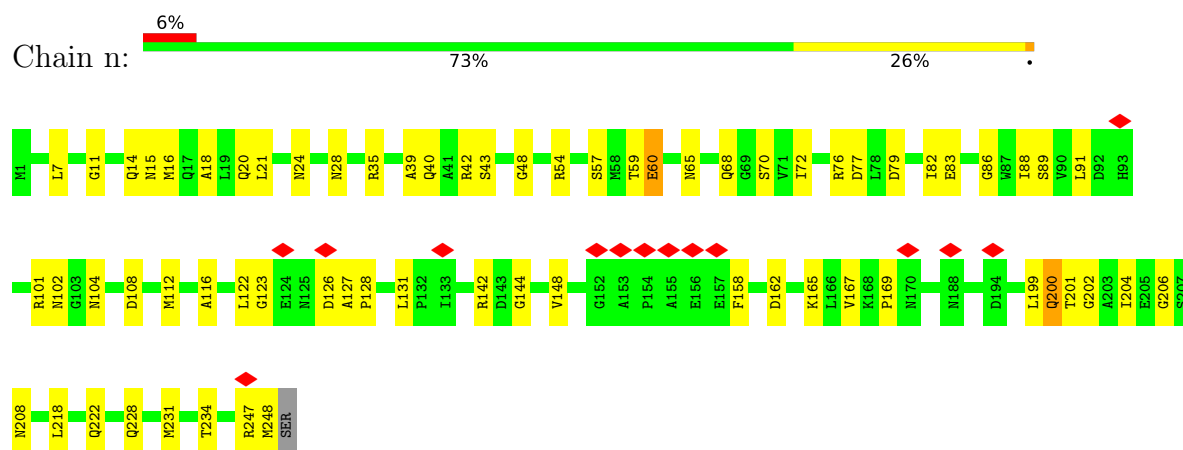
- Molecule 2: Flagellar biosynthetic protein FliQ



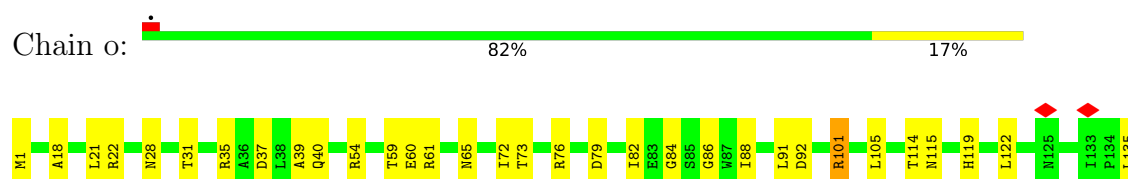
- Molecule 3: Flagellar basal-body rod protein FlgF



- Molecule 3: Flagellar basal-body rod protein FlgF

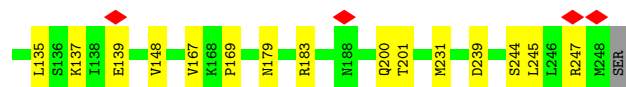
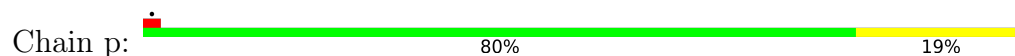


- Molecule 3: Flagellar basal-body rod protein FlgF

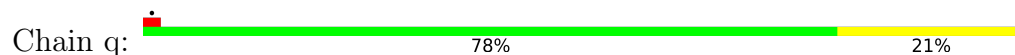




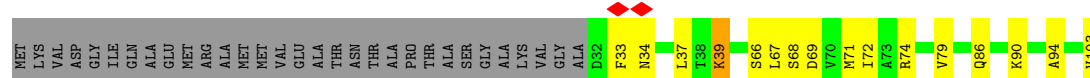
- Molecule 3: Flagellar basal-body rod protein FlgF



- Molecule 3: Flagellar basal-body rod protein FlgF



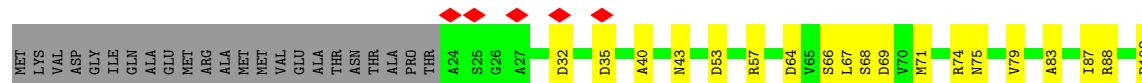
- Molecule 4: Flagellar hook-basal body complex protein FliE



- Molecule 4: Flagellar hook-basal body complex protein FliE

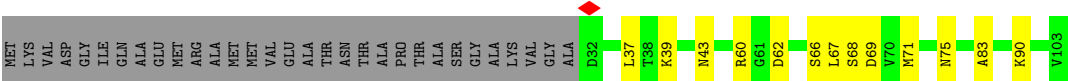


- Molecule 4: Flagellar hook-basal body complex protein FliE

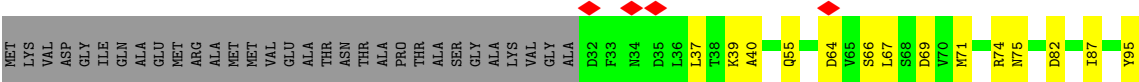


V103

• Molecule 4: Flagellar hook-basal body complex protein FliE

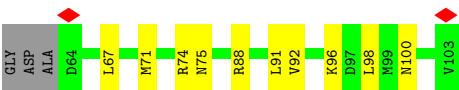
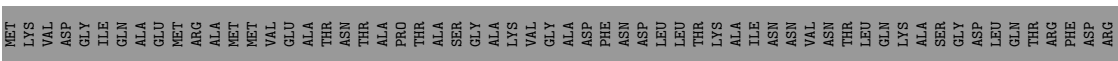


• Molecule 4: Flagellar hook-basal body complex protein FliE

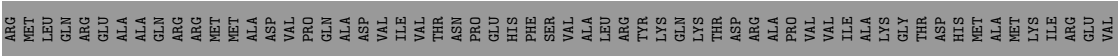
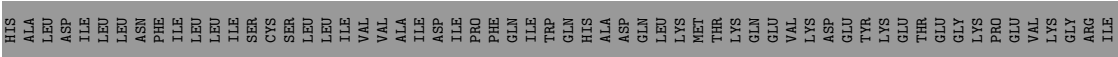
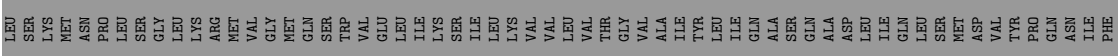
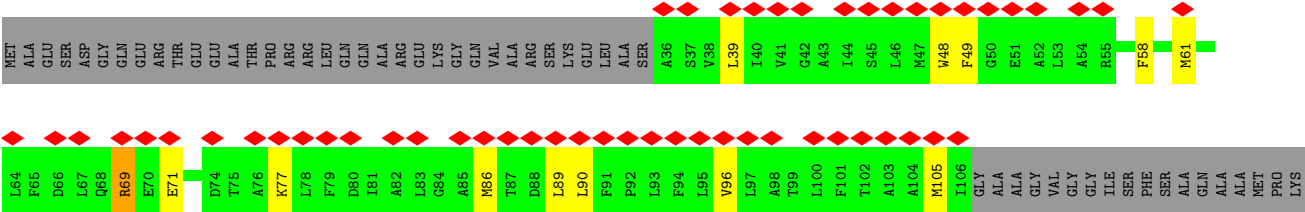


V103

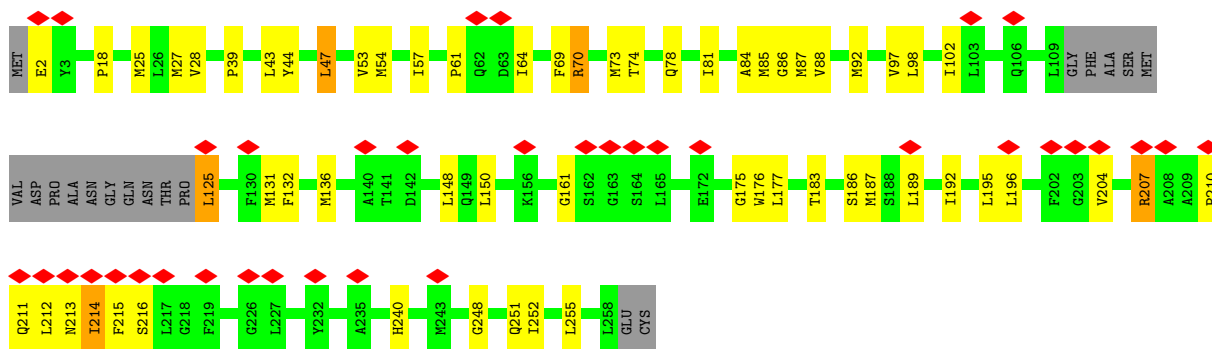
• Molecule 4: Flagellar hook-basal body complex protein FliE



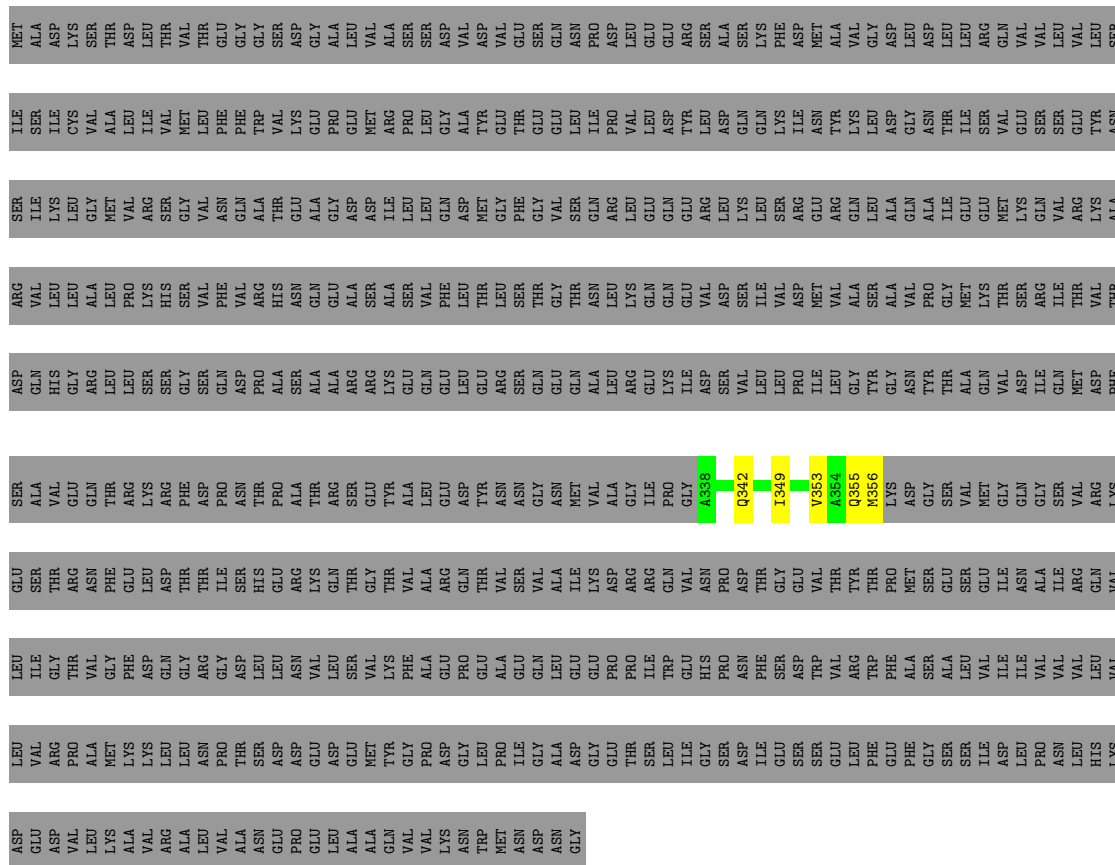
• Molecule 5: Flagellar biosynthetic protein FlhB



- Molecule 6: Flagellar biosynthetic protein FliR



- Molecule 7: Flagellar M-ring protein



- Molecule 7: Flagellar M-ring protein

97%

- Molecule 7: Flagellar M-ring protein

97%

[illegible]

- Molecule 7: Flagellar M-ring protein

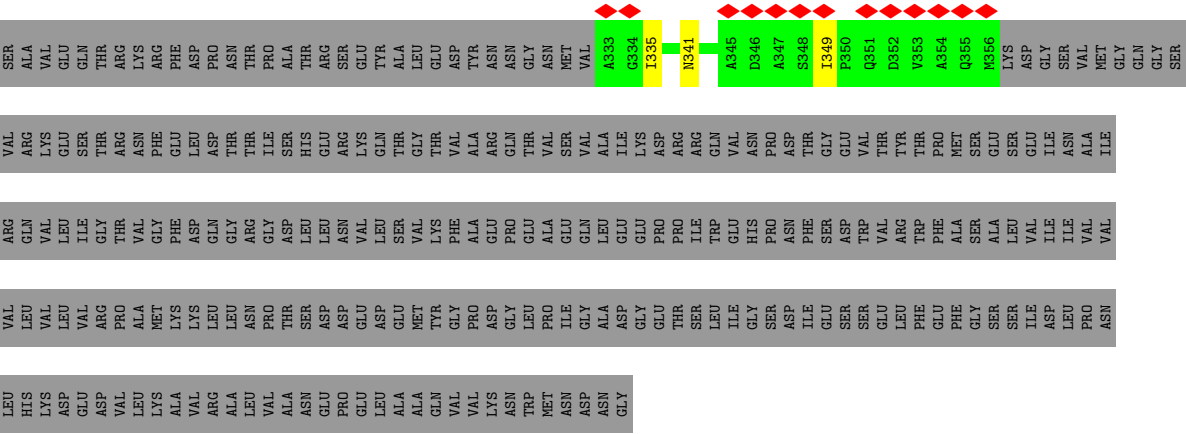
Chain AI: 98%

[illegible]

- Molecule 7: Flagellar M-ring protein

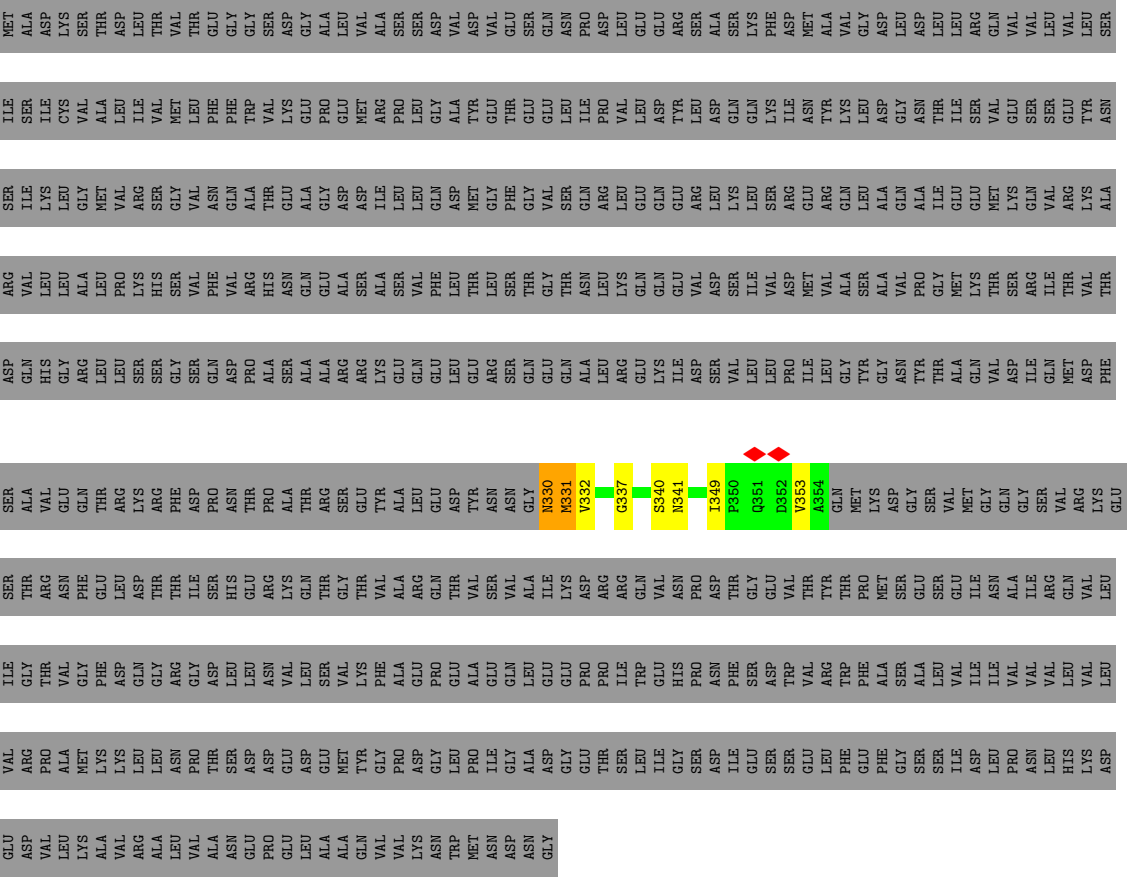
Chain AJ: 96%

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



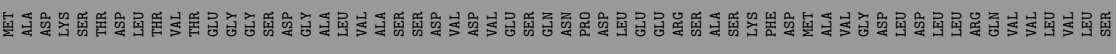
● Molecule 7: Flagellar M-ring protein

Chain AK: .. 96%



● Molecule 7: Flagellar M-ring protein

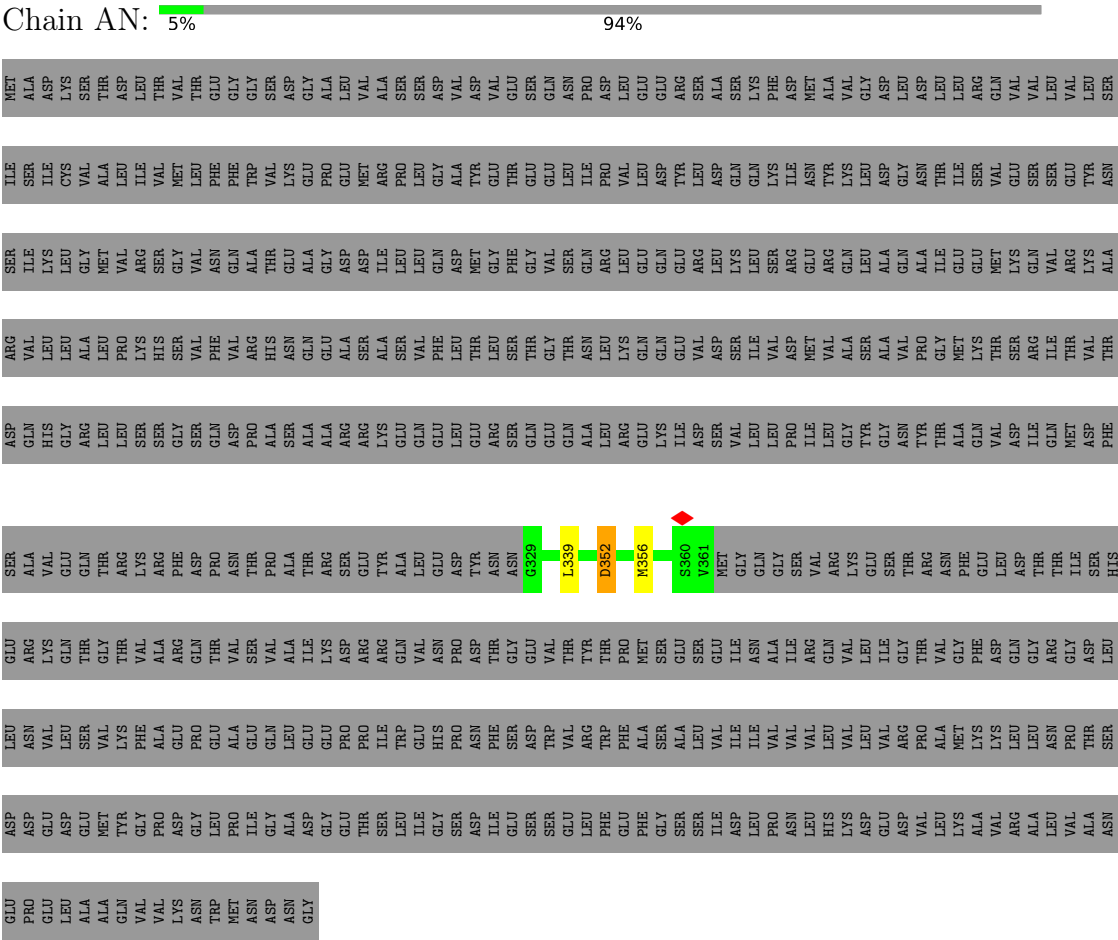
Chain AL: 5% .



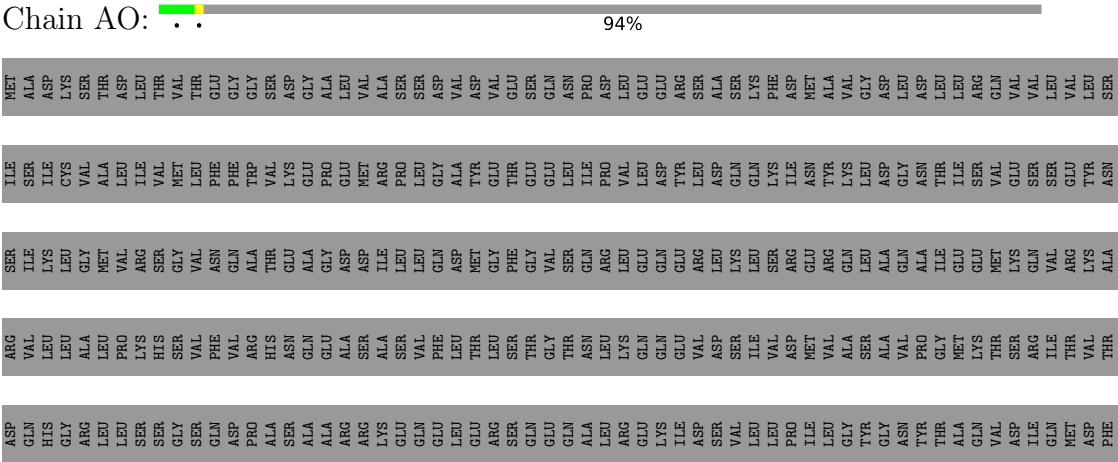


ALA
LEU
VAL
ALA
ASN
GLU
PRO
GLU
LEU
ALA
ALA
GLN
VAL
VAL
LYS
ASN
TRP
MET
ASN
ASP
ASN
GLY

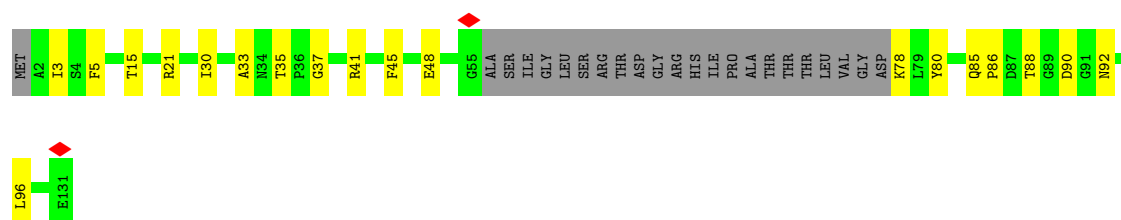
● Molecule 7: Flagellar M-ring protein



● Molecule 7: Flagellar M-ring protein



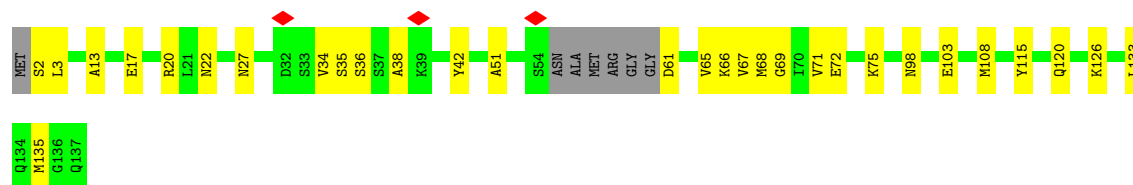
Chain f:



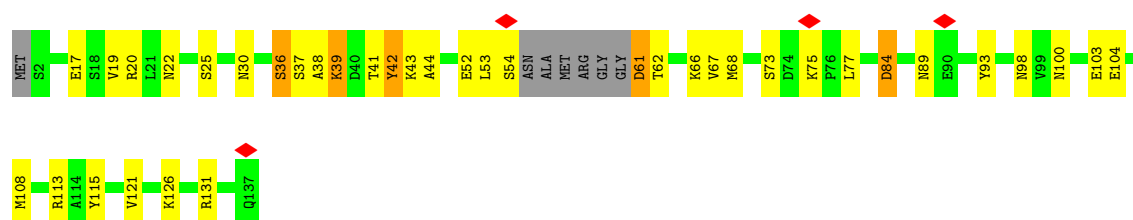
Chain g: 79% 16% 5%



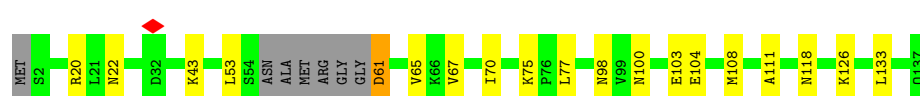
Chain h: 73% 22% 5%



Chain i: 67% 24% 5%



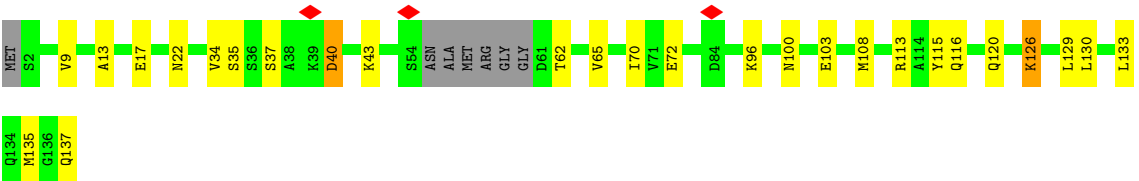
Chain j: 81% 13% 5%



WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 9: Flagellar basal-body rod protein FlgC



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.875	Depositor
Minimum map value	-2.095	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	744.0, 744.0, 744.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/1628	0.30	0/2209
1	2	0.16	0/1637	0.33	0/2221
1	3	0.10	0/1637	0.26	0/2221
1	y	0.10	0/1637	0.27	0/2221
1	z	0.11	0/1637	0.28	0/2221
2	4	0.12	0/739	0.31	0/1005
2	5	0.16	0/739	0.34	0/1005
2	6	0.28	0/739	0.49	0/1005
2	7	0.16	0/739	0.33	0/1005
3	m	0.11	0/1905	0.26	0/2572
3	n	0.13	0/1905	0.26	0/2572
3	o	0.10	0/1905	0.26	0/2572
3	p	0.11	0/1905	0.26	0/2572
3	q	0.10	0/1905	0.25	0/2572
4	r	0.32	0/564	0.43	0/759
4	s	0.08	0/609	0.20	0/819
4	t	0.07	0/609	0.17	0/819
4	u	0.07	0/564	0.16	0/759
4	v	0.07	0/564	0.18	0/759
4	w	0.09	0/313	0.19	0/420
5	x	0.08	0/562	0.19	0/760
6	8	0.09	0/1941	0.25	0/2631
7	AA	0.35	0/137	0.45	0/188
7	AB	0.29	0/137	0.43	0/188
7	AC	0.14	0/141	0.31	0/193
7	AD	0.30	0/137	0.46	0/188
7	AE	0.12	0/137	0.28	0/188
7	AF	0.92	0/161	1.23	0/221
7	AG	0.16	0/75	0.32	0/103
7	AH	0.20	0/75	0.42	0/103
7	AI	0.94	0/75	1.34	0/103
7	AJ	0.37	0/166	0.57	0/228

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	AK	0.31	0/172	0.70	0/237
7	AL	0.39	0/223	0.62	0/304
7	AM	0.20	0/227	0.44	0/309
7	AN	0.23	0/227	0.49	0/309
7	AO	0.16	0/223	0.40	0/304
8	b	0.22	0/856	0.36	0/1151
8	c	0.22	0/846	0.30	0/1138
8	d	0.23	0/856	0.31	0/1151
8	e	0.19	0/848	0.31	0/1140
8	f	0.22	0/848	0.35	0/1140
9	g	0.11	0/996	0.26	0/1348
9	h	0.10	0/996	0.26	0/1348
9	i	0.30	0/996	0.46	0/1348
9	j	0.10	0/996	0.24	0/1348
9	k	0.11	0/996	0.28	0/1348
9	l	0.13	0/996	0.30	0/1348
All	All	0.17	0/38926	0.32	0/52673

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	188	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1599	0	1685	27	0
1	2	1608	0	1691	32	0
1	3	1608	0	1691	34	0
1	y	1608	0	1691	26	0
1	z	1608	0	1691	36	0
2	4	722	0	768	16	0
2	5	722	0	768	19	0
2	6	722	0	768	15	0
2	7	722	0	768	10	0
3	m	1879	0	1864	31	0
3	n	1879	0	1864	46	0
3	o	1879	0	1864	24	0
3	p	1879	0	1864	30	0
3	q	1879	0	1864	37	0
4	r	560	0	561	12	0
4	s	605	0	609	11	0
4	t	605	0	609	19	0
4	u	560	0	561	10	0
4	v	560	0	561	21	0
4	w	311	0	320	8	0
5	x	552	0	577	13	0
6	8	1896	0	1968	44	0
7	AA	135	0	128	3	0
7	AB	135	0	128	2	0
7	AC	139	0	131	0	0
7	AD	135	0	128	2	0
7	AE	135	0	128	2	0
7	AF	158	0	152	13	0
7	AG	73	0	72	4	0
7	AH	73	0	72	4	0
7	AI	73	0	72	8	0
7	AJ	163	0	157	4	0
7	AK	169	0	164	5	0
7	AL	220	0	215	3	0
7	AM	224	0	218	4	0
7	AN	224	0	218	2	0
7	AO	220	0	215	3	0
8	b	845	0	833	12	0
8	c	835	0	825	19	0
8	d	845	0	833	11	0
8	e	837	0	829	15	0
8	f	837	0	829	14	0
9	g	983	0	958	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	h	983	0	958	23	0
9	i	983	0	958	30	0
9	j	983	0	958	12	0
9	k	983	0	958	20	0
9	l	983	0	958	23	0
10	2	51	0	78	10	0
10	e	51	0	78	4	0
10	t	51	0	78	15	0
10	v	51	0	78	12	0
11	e	32	0	0	1	0
11	s	32	0	0	1	0
11	t	32	0	0	2	0
11	u	32	0	0	3	0
11	v	32	0	0	6	0
All	All	38700	0	39014	610	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 8.

All (610) 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)
4:v:40:ALA:HB2	11:v:201:XKP:O	1.46	1.15
9:i:52:GLU:HG3	9:i:52:GLU:O	1.47	1.06
9:i:52:GLU:O	9:i:52:GLU:CG	2.15	0.94
1:z:96:LEU:HD21	10:e:202:PGT:H222	1.52	0.90
4:t:87:ILE:HD11	10:t:202:PGT:H182	1.55	0.86
10:v:202:PGT:H31	8:f:5:PHE:CE2	2.11	0.85
1:z:96:LEU:CD2	10:e:202:PGT:H222	2.07	0.84
4:v:40:ALA:CB	11:v:201:XKP:O	2.23	0.84
1:y:82:ASP:HB3	1:y:167:THR:HG23	1.62	0.80
4:v:37:LEU:HD23	11:v:201:XKP:C	2.16	0.76
1:1:92:LEU:HB2	10:t:202:PGT:H221	1.68	0.75
4:t:87:ILE:HD12	10:t:202:PGT:H352	1.67	0.75
4:t:43:ASN:HD21	10:t:202:PGT:H11	1.49	0.75
4:t:87:ILE:HD13	11:t:201:XKP:C20	2.18	0.74
3:n:102:ASN:HD21	3:n:116:ALA:HB3	1.55	0.72
3:n:54:ARG:NH1	8:c:86:PRO:O	2.24	0.71
2:4:25:ILE:HG13	2:5:52:LEU:HD12	1.73	0.71
4:s:98:LEU:HD21	6:8:47:LEU:HD21	1.72	0.69
4:v:103:VAL:O	1:y:120:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:22:ARG:HE	3:m:39:ALA:HB3	1.58	0.69
7:AL:341:ASN:ND2	8:c:88:THR:OG1	2.26	0.68
9:l:40:ASP:N	9:l:40:ASP:OD1	2.26	0.68
4:r:103:VAL:HG23	1:z:113:VAL:HG13	1.76	0.68
7:AF:335:ILE:HG13	7:AF:338:ALA:HB2	1.74	0.68
8:e:5:PHE:CE2	10:e:202:PGT:H32	2.28	0.68
6:8:92:MET:HE2	6:8:248:GLY:HA3	1.77	0.67
3:q:86:GLY:O	3:q:101:ARG:NH1	2.28	0.67
3:n:43:SER:HB2	9:i:36:SER:HB2	1.77	0.67
2:5:54:ARG:NH1	2:7:48:THR:OG1	2.28	0.67
4:t:43:ASN:ND2	10:t:202:PGT:H11	2.10	0.67
3:n:24:ASN:O	3:n:28:ASN:ND2	2.24	0.66
1:2:244:VAL:HG11	1:2:262:SER:HB2	1.78	0.66
7:AA:355:GLN:O	7:AA:356:MET:HB3	1.94	0.66
3:o:65:ASN:O	3:o:208:ASN:ND2	2.29	0.66
1:2:141:LEU:HG	1:z:198:MET:HE1	1.78	0.66
9:i:53:LEU:O	9:i:54:SER:C	2.38	0.65
9:j:75:LYS:O	9:j:98:ASN:ND2	2.29	0.65
1:y:103:VAL:O	1:y:107:THR:OG1	2.15	0.65
3:o:54:ARG:HE	9:h:22:ASN:HD22	1.45	0.65
3:o:135:LEU:HD13	3:o:138:ILE:HD11	1.78	0.64
1:1:239:ILE:HG23	2:6:17:VAL:HG12	1.79	0.64
2:6:9:LEU:HD21	2:6:80:LEU:HD21	1.80	0.64
1:3:198:MET:HE2	1:y:144:PHE:HB2	1.80	0.64
1:z:244:VAL:HG11	1:z:262:SER:HB3	1.79	0.64
3:n:83:GLU:OE2	3:n:142:ARG:NH1	2.30	0.64
6:8:186:SER:HA	6:8:189:LEU:HD23	1.80	0.63
1:2:184:LEU:HG	1:2:214:LEU:HD11	1.81	0.63
2:7:50:SER:O	2:7:54:ARG:NH1	2.31	0.63
7:AI:335:ILE:HG13	7:AI:338:ALA:HB2	1.78	0.63
3:n:54:ARG:NH2	8:c:85:GLN:OE1	2.31	0.63
1:1:85:VAL:HA	1:1:88:GLN:HE21	1.63	0.63
1:1:183:MET:HE1	1:1:215:ILE:HG12	1.80	0.63
3:n:231:MET:HE2	9:i:108:MET:HE2	1.79	0.63
9:i:43:LYS:HG2	9:i:77:LEU:HD21	1.80	0.63
3:m:91:LEU:HD23	3:m:122:LEU:HD21	1.80	0.62
3:p:137:LYS:NZ	3:p:139:GLU:OE2	2.33	0.62
8:f:30:ILE:HG23	8:f:96:LEU:HD11	1.80	0.62
1:2:103:VAL:O	1:2:107:THR:OG1	2.18	0.62
3:m:11:GLY:O	3:m:15:ASN:ND2	2.31	0.62
7:AI:334:GLY:O	7:AI:335:ILE:C	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:61:ASP:OD1	9:i:61:ASP:N	2.33	0.62
1:z:103:VAL:O	1:z:107:THR:OG1	2.17	0.61
8:d:35:THR:O	8:d:92:ASN:ND2	2.33	0.61
4:w:71:MET:O	4:w:75:ASN:ND2	2.30	0.61
7:AH:335:ILE:HB	7:AH:338:ALA:HB2	1.82	0.61
1:1:104:ILE:O	1:1:110:THR:OG1	2.19	0.61
1:1:141:LEU:HD11	1:1:280:LEU:HD22	1.82	0.61
10:2:301:PGT:H321	10:2:301:PGT:H132	1.83	0.61
2:4:59:LEU:HD13	5:x:90:LEU:HD22	1.82	0.61
3:p:231:MET:HE2	9:k:108:MET:HE2	1.83	0.61
1:1:244:VAL:HG11	1:1:262:SER:HB3	1.81	0.61
2:4:1:MET:SD	2:4:1:MET:N	2.73	0.61
9:h:17:GLU:OE1	9:h:20:ARG:NH2	2.32	0.61
2:7:31:ILE:HG13	2:7:57:VAL:HG11	1.81	0.60
3:p:11:GLY:O	3:p:15:ASN:ND2	2.30	0.60
1:3:91:ALA:HA	10:v:202:PGT:H452	1.83	0.60
3:n:76:ARG:NH1	3:n:79:ASP:OD1	2.34	0.60
1:y:88:GLN:OE1	1:y:161:TYR:OH	2.14	0.60
3:q:40:GLN:NE2	9:l:35:SER:OG	2.35	0.60
7:AI:335:ILE:HD12	9:h:71:VAL:HG23	1.82	0.60
3:n:54:ARG:HE	9:i:22:ASN:HD22	1.49	0.60
3:p:54:ARG:HE	9:k:22:ASN:HD22	1.48	0.60
3:q:44:MET:HA	9:l:37:SER:HB3	1.84	0.60
8:e:15:THR:HG23	8:e:45:PHE:HZ	1.67	0.60
4:t:75:ASN:HD22	9:h:135:MET:HE2	1.66	0.60
1:y:112:ILE:HG23	1:y:283:LEU:HD23	1.84	0.60
9:i:100:ASN:HD22	9:i:103:GLU:H	1.49	0.60
9:k:75:LYS:O	9:k:98:ASN:ND2	2.34	0.60
3:q:65:ASN:O	3:q:208:ASN:ND2	2.34	0.59
1:2:95:MET:HB3	10:2:301:PGT:H252	1.84	0.59
3:m:86:GLY:O	3:m:101:ARG:NH1	2.35	0.59
4:u:71:MET:HE3	9:j:133:LEU:HD23	1.83	0.59
4:t:87:ILE:HD11	10:t:202:PGT:C18	2.28	0.59
3:p:54:ARG:NH1	8:f:86:PRO:O	2.36	0.59
9:l:113:ARG:NH2	9:l:116:GLN:OE1	2.36	0.59
1:1:92:LEU:HD13	10:t:202:PGT:C19	2.32	0.59
3:q:102:ASN:HD21	3:q:116:ALA:HB3	1.66	0.59
7:AF:350:PRO:HA	7:AF:353:VAL:HG22	1.83	0.59
3:m:54:ARG:HE	9:j:22:ASN:HD22	1.51	0.59
3:o:91:LEU:HD23	3:o:122:LEU:HD21	1.85	0.59
8:d:108:ILE:HD11	9:h:126:LYS:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:31:ILE:HG13	2:4:57:VAL:HG21	1.85	0.58
3:m:50:GLY:O	7:AH:341:ASN:ND2	2.36	0.58
8:f:35:THR:O	8:f:92:ASN:ND2	2.37	0.58
9:j:61:ASP:N	9:j:61:ASP:OD1	2.35	0.58
4:s:90:LYS:HE3	4:w:74:ARG:HH21	1.68	0.58
3:o:22:ARG:HE	3:o:39:ALA:HB3	1.69	0.58
1:z:183:MET:HE1	1:z:215:ILE:HG12	1.86	0.58
8:f:41:ARG:HG2	8:f:78:LYS:HE2	1.85	0.58
6:8:70:ARG:HA	6:8:73:MET:HE2	1.85	0.57
2:4:54:ARG:NH1	2:5:46:GLU:OE2	2.38	0.57
3:m:54:ARG:NH1	8:e:86:PRO:O	2.35	0.57
1:y:248:LEU:HD11	1:y:261:VAL:HG11	1.86	0.57
7:AG:335:ILE:HB	7:AG:338:ALA:HB2	1.86	0.57
3:q:22:ARG:HE	3:q:39:ALA:HB3	1.68	0.57
11:t:201:XKP:C1	10:t:202:PGT:H191	2.35	0.57
7:AO:335:ILE:O	7:AO:340:SER:OG	2.14	0.57
3:n:104:ASN:HB3	3:n:116:ALA:HB2	1.87	0.57
3:n:48:GLY:O	7:AJ:341:ASN:ND2	2.38	0.57
3:o:86:GLY:O	3:o:101:ARG:NH1	2.37	0.57
3:q:54:ARG:NH1	8:b:86:PRO:O	2.38	0.57
4:u:68:SER:OG	8:d:20:GLU:OE2	2.20	0.57
4:v:66:SER:OG	4:v:69:ASP:OD1	2.23	0.57
3:o:40:GLN:NE2	9:h:35:SER:OG	2.38	0.57
3:o:40:GLN:NE2	3:o:60:GLU:OE2	2.35	0.57
6:8:187:MET:HE2	6:8:240:HIS:HB3	1.86	0.57
9:k:61:ASP:OD1	9:k:61:ASP:N	2.38	0.57
1:3:239:ILE:HG23	5:x:89:LEU:HD22	1.87	0.57
7:AK:331:MET:HE3	9:g:52:GLU:HB2	1.87	0.57
7:AN:352:ASP:OD1	7:AN:352:ASP:N	2.38	0.57
9:g:75:LYS:O	9:g:98:ASN:ND2	2.33	0.57
9:l:34:VAL:HG12	9:l:96:LYS:HG2	1.87	0.57
9:h:61:ASP:OD1	9:h:61:ASP:N	2.36	0.56
1:1:228:GLN:HA	6:8:136:MET:HE1	1.85	0.56
1:3:136:GLY:HA3	6:8:87:MET:HE2	1.87	0.56
2:5:31:ILE:HG13	2:5:57:VAL:HG21	1.88	0.56
3:m:83:GLU:OE2	3:m:142:ARG:NH2	2.39	0.56
3:m:231:MET:HE2	9:j:108:MET:HE2	1.87	0.56
3:p:82:ILE:HD11	3:p:88:ILE:HG13	1.88	0.56
4:v:37:LEU:CD2	11:v:201:XKP:C	2.83	0.56
7:AI:335:ILE:HD11	9:h:69:GLY:HA3	1.86	0.56
9:i:17:GLU:OE1	9:i:20:ARG:NH2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:231:MET:HE2	9:h:108:MET:HE2	1.87	0.56
3:q:54:ARG:HE	9:l:22:ASN:HD22	1.53	0.56
1:2:144:PHE:HB2	1:z:198:MET:HE2	1.86	0.56
3:n:126:ASP:OD1	3:n:165:LYS:NZ	2.31	0.56
3:p:86:GLY:O	3:p:101:ARG:NH1	2.39	0.56
1:y:220:THR:HG23	1:z:276:TRP:HB3	1.88	0.55
4:t:68:SER:OG	8:c:20:GLU:OE2	2.24	0.55
7:AF:350:PRO:O	7:AF:351:GLN:C	2.50	0.55
1:1:92:LEU:HD13	10:t:202:PGT:H192	1.88	0.55
3:p:76:ARG:NH1	3:p:79:ASP:OD1	2.39	0.55
7:AH:335:ILE:HD12	7:AN:356:MET:HE1	1.88	0.55
9:g:20:ARG:HH21	9:g:111:ALA:HA	1.71	0.55
1:1:103:VAL:O	1:1:107:THR:HG22	2.06	0.55
1:2:115:VAL:HG11	1:2:283:LEU:HD11	1.87	0.55
2:6:40:ALA:HA	6:8:211:GLN:HG3	1.87	0.55
4:r:72:ILE:HG12	9:k:135:MET:HE1	1.89	0.55
2:5:13:ALA:HB1	1:z:239:ILE:HD11	1.89	0.55
4:w:67:LEU:HD12	9:g:129:LEU:HD22	1.88	0.55
3:p:244:SER:HA	3:p:247:ARG:HG3	1.89	0.55
1:1:268:MET:HE1	2:7:1:MET:HG3	1.88	0.55
2:6:84:LEU:N	2:6:85:PRO:HD2	2.21	0.55
3:p:91:LEU:HD23	3:p:122:LEU:HD21	1.89	0.55
1:z:104:ILE:O	1:z:110:THR:OG1	2.24	0.55
9:k:3:LEU:HD21	9:k:128:MET:HE3	1.89	0.55
1:3:103:VAL:O	1:3:107:THR:OG1	2.23	0.54
1:3:112:ILE:HD13	1:3:141:LEU:HB3	1.89	0.54
4:u:66:SER:OG	4:u:69:ASP:OD1	2.25	0.54
7:AD:348:SER:HB2	7:AD:356:MET:HE3	1.89	0.54
3:m:154:PRO:HG2	3:m:157:GLU:HG3	1.89	0.54
7:AF:352:ASP:O	7:AF:353:VAL:C	2.51	0.54
9:g:108:MET:HE2	9:i:121:VAL:HG22	1.89	0.54
9:k:3:LEU:HB3	9:k:129:LEU:HD21	1.89	0.54
9:k:43:LYS:HG2	9:k:77:LEU:HD21	1.90	0.54
2:4:6:PHE:HB2	1:z:268:MET:HE2	1.89	0.54
1:3:198:MET:HE1	1:y:141:LEU:HD22	1.90	0.54
3:p:18:ALA:HB2	3:p:59:THR:HG21	1.90	0.54
8:c:30:ILE:HG23	8:c:96:LEU:HD11	1.89	0.54
1:3:239:ILE:HD12	5:x:89:LEU:HD22	1.90	0.54
9:g:84:ASP:OD1	9:i:73:SER:OG	2.23	0.54
3:q:248:MET:HG2	9:l:126:LYS:HD3	1.91	0.53
9:g:9:VAL:HG21	9:g:62:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:231:MET:HE2	9:l:108:MET:HE2	1.89	0.53
4:t:66:SER:OG	4:t:69:ASP:OD1	2.26	0.53
3:m:65:ASN:O	3:m:208:ASN:ND2	2.36	0.53
4:r:94:ALA:HA	1:z:100:PRO:HG3	1.90	0.53
4:s:26:GLY:HA3	6:8:54:MET:HE2	1.90	0.53
3:o:76:ARG:NH1	3:o:79:ASP:OD1	2.39	0.53
4:t:71:MET:HE3	9:h:133:LEU:HA	1.89	0.53
7:AI:339:LEU:HD11	9:h:72:GLU:HG3	1.91	0.53
7:AJ:335:ILE:HG22	9:g:87:LEU:HD11	1.89	0.53
8:d:31:ALA:HA	9:j:118:ASN:HD21	1.73	0.53
8:c:85:GLN:HE21	9:i:19:VAL:HG22	1.73	0.53
8:e:36:PRO:HB3	8:e:90:ASP:HB2	1.91	0.53
4:v:71:MET:HE3	9:l:133:LEU:HD23	1.91	0.53
6:8:64:ILE:HG22	6:8:70:ARG:HG2	1.91	0.53
8:f:37:GLY:N	8:f:90:ASP:O	2.42	0.53
1:3:85:VAL:HG13	8:b:3:ILE:HA	1.90	0.52
2:5:81:ILE:HG13	1:z:278:LEU:HD21	1.91	0.52
1:3:125:LEU:HB3	1:3:128:THR:HB	1.91	0.52
6:8:97:VAL:HG22	6:8:131:MET:HB2	1.90	0.52
3:m:18:ALA:HB2	3:m:59:THR:HG21	1.90	0.52
3:n:82:ILE:HD11	3:n:88:ILE:HG13	1.92	0.52
8:b:128:ILE:HG13	8:b:129:LYS:HG3	1.91	0.52
1:1:92:LEU:HD13	10:t:202:PGT:C20	2.40	0.52
3:q:77:ASP:OD1	3:q:77:ASP:N	2.43	0.52
7:AM:340:SER:HA	7:AM:349:ILE:HD11	1.90	0.52
1:y:208:ASP:OD1	1:y:208:ASP:N	2.42	0.52
8:e:41:ARG:NH2	8:e:80:TYR:OH	2.38	0.52
2:5:81:ILE:HG21	1:z:278:LEU:HD11	1.91	0.52
3:n:42:ARG:NH1	7:AE:351:GLN:O	2.38	0.52
6:8:150:LEU:HD13	6:8:252:ILE:HG21	1.92	0.52
1:2:248:LEU:HD11	1:2:261:VAL:HG11	1.92	0.52
10:v:202:PGT:H262	1:y:96:LEU:HD23	1.91	0.52
3:o:18:ALA:HB2	3:o:59:THR:HG21	1.91	0.51
6:8:28:VAL:HB	6:8:86:GLY:HA3	1.91	0.51
1:2:112:ILE:HD13	1:2:141:LEU:HB3	1.92	0.51
3:n:86:GLY:O	3:n:101:ARG:NH1	2.44	0.51
4:v:87:ILE:HD11	10:v:202:PGT:H181	1.92	0.51
4:v:87:ILE:HD11	10:v:202:PGT:C18	2.39	0.51
9:l:9:VAL:HG21	9:l:62:THR:HB	1.92	0.51
3:n:70:SER:O	3:n:206:GLY:N	2.30	0.51
3:o:82:ILE:HD11	3:o:88:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:198:MET:HE2	6:8:53:VAL:HG11	1.92	0.51
1:3:139:LEU:HD21	4:w:98:LEU:HD13	1.93	0.51
3:q:84:GLY:O	3:q:101:ARG:NH2	2.42	0.51
7:AF:347:ALA:O	7:AF:353:VAL:HG13	2.10	0.51
1:3:255:MET:HB2	6:8:214:ILE:HG12	1.93	0.51
3:o:84:GLY:O	3:o:101:ARG:NH2	2.43	0.51
4:s:74:ARG:NH2	8:c:119:SER:OG	2.44	0.51
4:s:87:ILE:HD12	11:s:201:XKP:C3	2.41	0.51
7:AI:339:LEU:HD11	9:h:72:GLU:CG	2.41	0.51
1:1:282:THR:HG21	2:6:81:ILE:HG23	1.93	0.51
1:2:112:ILE:HG22	1:2:116:MET:HE2	1.93	0.51
3:q:14:GLN:HG3	3:q:58:MET:HA	1.92	0.51
10:v:202:PGT:H162	8:f:3:ILE:HG21	1.92	0.51
3:o:1:MET:HG3	3:o:239:ASP:HB2	1.93	0.50
2:6:52:LEU:HB2	2:7:25:ILE:HG21	1.94	0.50
3:m:56:PHE:HZ	8:e:88:THR:HG22	1.74	0.50
4:v:40:ALA:CA	11:v:201:XKP:O	2.59	0.50
7:AH:342:GLN:HG3	7:AH:343:PRO:HD2	1.92	0.50
8:b:35:THR:O	8:b:92:ASN:ND2	2.44	0.50
10:2:301:PGT:H211	11:u:201:XKP:C2	2.42	0.50
6:8:81:ILE:HG22	6:8:85:MET:HE1	1.94	0.50
7:AG:336:PRO:HG2	7:AO:352:ASP:HB3	1.92	0.50
3:q:51:HIS:HB3	9:l:70:ILE:HD13	1.93	0.50
5:x:39:LEU:HD22	6:8:204:VAL:HG23	1.93	0.50
7:AK:330:ASN:N	7:AK:330:ASN:HD22	2.10	0.50
8:c:104:MET:SD	9:i:126:LYS:NZ	2.80	0.50
3:n:21:LEU:HD23	3:n:39:ALA:HB2	1.94	0.50
7:AF:347:ALA:HA	7:AF:353:VAL:CG1	2.42	0.50
1:2:276:TRP:HB3	1:z:220:THR:HG23	1.93	0.50
7:AK:353:VAL:HG21	9:g:71:VAL:HG11	1.94	0.50
1:3:183:MET:HE1	1:3:211:MET:HG3	1.92	0.50
9:i:37:SER:O	9:i:38:ALA:HB3	2.11	0.50
1:1:104:ILE:HD12	6:8:44:TYR:HE2	1.77	0.50
4:u:83:ALA:HB2	8:d:128:ILE:HD13	1.94	0.50
4:s:99:MET:HA	6:8:43:LEU:HD21	1.95	0.49
4:u:60:ARG:NH1	4:u:62:ASP:OD1	2.45	0.49
1:z:142:THR:HA	1:z:145:VAL:HG22	1.93	0.49
3:p:247:ARG:HG2	9:l:120:GLN:HE22	1.77	0.49
2:4:5:MET:SD	2:4:83:ARG:NH2	2.85	0.49
3:m:53:SER:OG	8:e:85:GLN:NE2	2.34	0.49
3:q:35:ARG:NH1	3:q:101:ARG:HD3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:112:ILE:HG23	1:2:283:LEU:HD23	1.94	0.49
1:1:195:PHE:HB3	1:1:213:VAL:HG22	1.95	0.49
1:y:144:PHE:O	1:y:147:SER:OG	2.27	0.49
1:2:116:MET:HE3	1:2:134:ILE:HG23	1.94	0.49
3:p:84:GLY:O	3:p:101:ARG:NH2	2.32	0.49
4:v:39:LYS:HD3	11:v:201:XKP:O4	2.12	0.49
4:r:71:MET:HE3	9:k:133:LEU:HD23	1.95	0.49
9:h:75:LYS:O	9:h:98:ASN:ND2	2.43	0.49
8:f:33:ALA:O	8:f:92:ASN:ND2	2.45	0.49
1:2:253:MET:HA	1:z:249:MET:HE3	1.95	0.49
2:6:1:MET:SD	2:6:1:MET:N	2.70	0.48
3:p:200:GLN:NE2	3:p:201:THR:O	2.45	0.48
1:1:184:LEU:HD11	1:1:207:GLU:HA	1.95	0.48
7:AL:353:VAL:HG21	9:h:71:VAL:HG11	1.94	0.48
3:q:40:GLN:NE2	3:q:60:GLU:OE2	2.40	0.48
5:x:49:PHE:HB3	5:x:96:VAL:HG22	1.95	0.48
8:c:97:ASP:OD1	9:i:115:TYR:OH	2.32	0.48
3:m:35:ARG:NH1	3:m:101:ARG:HD3	2.29	0.48
3:n:89:SER:HB3	3:n:122:LEU:HD12	1.95	0.48
3:p:22:ARG:HE	3:p:39:ALA:HB3	1.78	0.48
1:3:236:PRO:HB2	5:x:61:MET:HG2	1.95	0.48
1:y:82:ASP:OD1	1:y:82:ASP:N	2.45	0.48
1:y:183:MET:HE1	1:y:215:ILE:HG12	1.95	0.48
6:8:183:THR:HG22	6:8:187:MET:HE3	1.95	0.48
9:g:61:ASP:N	9:g:61:ASP:OD1	2.45	0.48
1:z:111:ARG:NE	1:z:222:GLU:OE1	2.44	0.48
8:d:39:LYS:NZ	8:d:91:GLY:O	2.40	0.48
1:1:119:LEU:HD21	1:1:270:PHE:CE1	2.49	0.47
2:5:8:GLU:HG2	2:5:83:ARG:NH2	2.29	0.47
3:n:40:GLN:NE2	3:n:60:GLU:OE2	2.39	0.47
3:m:76:ARG:NH1	3:m:79:ASP:OD1	2.44	0.47
1:y:149:VAL:HG23	1:y:178:PRO:HB2	1.96	0.47
9:h:13:ALA:O	9:h:17:GLU:HG2	2.14	0.47
3:n:14:GLN:HB3	3:n:59:THR:HG23	1.95	0.47
2:5:42:THR:HG23	2:5:44:ILE:HG12	1.96	0.47
4:u:39:LYS:HE3	11:u:201:XKP:C8	2.44	0.47
8:f:85:GLN:OE1	9:k:22:ASN:ND2	2.47	0.47
4:s:71:MET:SD	4:s:74:ARG:NH1	2.85	0.47
4:w:92:VAL:HG13	6:8:27:MET:HE1	1.96	0.47
8:d:30:ILE:HG23	8:d:96:LEU:HD11	1.97	0.47
1:2:154:ASN:HA	1:2:158:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:248:MET:HA	9:i:126:LYS:HD3	1.96	0.47
4:u:71:MET:O	4:u:75:ASN:ND2	2.28	0.47
4:w:88:ARG:HH11	4:w:92:VAL:HG21	1.80	0.47
8:b:9:LEU:HD12	8:b:120:LYS:HB3	1.97	0.47
8:c:24:GLU:OE2	9:h:2:SER:N	2.47	0.47
1:2:264:PRO:HG3	1:z:234:PHE:CG	2.50	0.47
3:m:114:THR:HG22	3:m:120:LEU:HD13	1.96	0.47
3:o:35:ARG:NH1	3:o:101:ARG:HD3	2.30	0.47
8:b:30:ILE:HG23	8:b:96:LEU:HD11	1.96	0.47
1:1:105:LEU:HD23	6:8:44:TYR:HB3	1.97	0.47
4:r:39:LYS:HD2	11:e:201:XKP:O2	2.15	0.47
8:f:21:ARG:NH1	8:f:48:GLU:OE1	2.48	0.47
1:2:258:PRO:HA	1:2:261:VAL:HG12	1.98	0.46
2:5:87:VAL:C	2:5:89:TYR:H	2.23	0.46
3:o:21:LEU:HD23	3:o:39:ALA:HB2	1.97	0.46
4:v:87:ILE:CG2	10:v:202:PGT:H392	2.45	0.46
7:AF:349:ILE:O	7:AF:350:PRO:C	2.58	0.46
7:AM:341:ASN:ND2	8:f:88:THR:OG1	2.48	0.46
8:e:43:LEU:HG	8:e:48:GLU:HG3	1.96	0.46
9:i:84:ASP:OD1	9:i:84:ASP:N	2.32	0.46
7:AK:340:SER:HA	7:AK:349:ILE:HD11	1.97	0.46
4:s:90:LYS:HG3	4:w:74:ARG:HE	1.80	0.46
1:z:81:GLU:O	1:z:169:ARG:NH2	2.49	0.46
8:c:35:THR:O	8:c:92:ASN:ND2	2.48	0.46
9:j:20:ARG:HH21	9:j:111:ALA:HA	1.79	0.46
1:3:264:PRO:HG2	6:8:196:LEU:HD11	1.98	0.46
4:s:103:VAL:HG11	6:8:43:LEU:HB2	1.98	0.46
4:t:40:ALA:HB1	10:t:202:PGT:H342	1.97	0.46
9:h:66:LYS:HE3	9:h:68:MET:SD	2.56	0.46
9:j:100:ASN:O	9:j:104:GLU:HG2	2.16	0.46
3:p:51:HIS:HB3	9:k:70:ILE:HD13	1.97	0.46
1:1:208:ASP:OD1	1:1:208:ASP:N	2.49	0.46
10:2:301:PGT:H31	8:d:5:PHE:CE2	2.50	0.46
3:o:28:ASN:O	3:o:31:THR:OG1	2.34	0.46
1:y:141:LEU:HD11	1:y:280:LEU:HD22	1.98	0.46
6:8:85:MET:HG3	6:8:252:ILE:HG23	1.98	0.46
8:d:15:THR:HG23	8:d:45:PHE:HZ	1.81	0.46
9:j:100:ASN:HB3	9:j:103:GLU:HG2	1.98	0.46
3:p:28:ASN:O	3:p:31:THR:OG1	2.32	0.46
1:2:186:GLN:NE2	1:2:287:PHE:O	2.49	0.46
3:n:91:LEU:HD21	3:n:128:PRO:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:9:MET:HE3	3:p:9:MET:HB3	1.82	0.46
7:AI:342:GLN:O	7:AI:343:PRO:C	2.59	0.46
2:6:16:MET:HE1	2:6:76:TYR:HB2	1.97	0.46
3:p:131:LEU:HD23	3:p:148:VAL:HG11	1.97	0.46
1:3:128:THR:HG22	6:8:98:LEU:HG	1.98	0.45
6:8:25:MET:HE1	6:8:148:LEU:HD23	1.98	0.45
3:n:91:LEU:HD23	3:n:122:LEU:HD21	1.98	0.45
7:AF:344:PRO:O	7:AF:345:ALA:C	2.57	0.45
1:2:263:LEU:HD23	1:z:234:PHE:HE2	1.80	0.45
10:2:301:PGT:H122	10:2:301:PGT:H32	1.48	0.45
4:t:53:ASP:OD2	4:t:57:ARG:NH1	2.50	0.45
8:e:30:ILE:HG23	8:e:96:LEU:HD11	1.98	0.45
2:5:19:ILE:HG21	2:5:72:MET:HE1	1.98	0.45
4:v:82:ASP:OD1	8:b:126:LYS:HE2	2.16	0.45
1:y:183:MET:HE2	1:y:214:LEU:HG	1.98	0.45
6:8:74:THR:O	6:8:78:GLN:HG2	2.17	0.45
8:b:39:LYS:NZ	8:b:91:GLY:O	2.42	0.45
9:i:39:LYS:HA	9:i:39:LYS:HD3	1.74	0.45
3:n:57:SER:HB3	9:i:30:ASN:OD1	2.17	0.45
3:q:18:ALA:HB2	3:q:59:THR:HG21	1.99	0.45
7:AF:336:PRO:HG2	7:AM:352:ASP:HB3	1.98	0.45
9:i:52:GLU:O	9:i:53:LEU:C	2.59	0.45
1:3:90:LEU:O	1:3:94:THR:OG1	2.34	0.45
1:3:116:MET:HE3	6:8:177:LEU:HD22	1.98	0.45
4:v:87:ILE:HD12	10:v:202:PGT:H351	1.98	0.45
1:2:204:ASP:OD1	1:2:204:ASP:N	2.49	0.45
9:h:27:ASN:OD1	9:h:42:TYR:OH	2.27	0.45
1:1:144:PHE:HD2	1:2:198:MET:HE3	1.82	0.45
2:6:31:ILE:HG13	2:6:57:VAL:HG11	1.99	0.45
3:p:114:THR:HG22	3:p:120:LEU:HD13	1.99	0.45
3:q:244:SER:HA	3:q:247:ARG:HB2	1.98	0.45
4:r:68:SER:OG	8:e:20:GLU:OE2	2.34	0.45
4:r:86:GLN:O	4:r:90:LYS:HG2	2.17	0.45
1:z:116:MET:SD	1:z:134:ILE:HG23	2.57	0.45
1:3:108:SER:HB2	1:3:287:PHE:CZ	2.51	0.44
2:5:1:MET:HE2	2:5:87:VAL:HG11	1.98	0.44
3:n:18:ALA:HB2	3:n:59:THR:HG21	1.98	0.44
3:p:21:LEU:HD23	3:p:39:ALA:HB2	1.98	0.44
7:AJ:341:ASN:HD21	8:c:86:PRO:HG3	1.82	0.44
7:AM:331:MET:HE2	7:AM:331:MET:HB3	1.87	0.44
8:c:26:ILE:HG21	8:c:103:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:251:MET:HE2	5:x:39:LEU:HD23	1.99	0.44
2:5:87:VAL:C	2:5:89:TYR:N	2.74	0.44
3:m:137:LYS:NZ	3:m:139:GLU:OE2	2.48	0.44
3:n:167:VAL:HG12	3:n:169:PRO:HD3	1.98	0.44
10:t:202:PGT:H31	8:c:5:PHE:CE2	2.52	0.44
1:z:125:LEU:HD22	1:z:263:LEU:HD11	1.98	0.44
7:AF:339:LEU:HD11	9:l:72:GLU:HG3	1.99	0.44
6:8:18:PRO:HB3	6:8:57:ILE:HD13	2.00	0.44
3:n:54:ARG:HE	9:i:22:ASN:ND2	2.15	0.44
3:n:131:LEU:HD23	3:n:148:VAL:HG11	1.99	0.44
6:8:215:PHE:HD2	6:8:216:SER:H	1.66	0.44
3:q:82:ILE:HD11	3:q:88:ILE:HG13	2.00	0.44
4:s:48:GLN:HE21	4:s:81:PHE:HB2	1.81	0.44
4:v:67:LEU:HD12	9:l:129:LEU:HD22	1.99	0.44
8:b:85:GLN:OE1	9:l:22:ASN:ND2	2.51	0.44
2:6:63:MET:HG2	2:7:11:ARG:HA	1.98	0.44
3:o:105:LEU:HA	3:o:115:ASN:HA	2.00	0.44
3:q:46:ALA:HA	7:AA:349:ILE:HG12	1.99	0.44
4:w:96:LYS:O	4:w:100:ASN:ND2	2.45	0.44
5:x:71:GLU:HA	5:x:77:LYS:HD2	1.99	0.44
3:p:40:GLN:HG2	3:p:62:PRO:HD3	1.99	0.44
7:AF:348:SER:O	7:AF:349:ILE:HB	2.17	0.44
9:i:66:LYS:HE3	9:i:68:MET:HG2	1.99	0.44
3:m:211:ALA:O	3:m:215:MET:HG2	2.18	0.44
3:q:21:LEU:HD23	3:q:39:ALA:HB2	2.00	0.44
3:q:37:ASP:OD1	3:q:176:LYS:NZ	2.42	0.44
7:AA:353:VAL:O	7:AA:356:MET:HG2	2.18	0.44
10:e:202:PGT:H432	10:e:202:PGT:H462	1.63	0.44
2:4:20:MET:HE1	2:4:69:MET:HB3	2.00	0.43
3:q:91:LEU:HD21	3:q:128:PRO:HG3	1.98	0.43
4:v:64:ASP:OD1	4:v:64:ASP:N	2.48	0.43
8:b:21:ARG:NH1	8:b:48:GLU:OE1	2.51	0.43
2:5:8:GLU:HG2	2:5:83:ARG:HH22	1.82	0.43
2:6:67:HIS:HD2	2:7:11:ARG:HH22	1.65	0.43
1:y:238:LEU:HD11	1:z:261:VAL:HG13	2.00	0.43
9:k:39:LYS:HD2	9:k:39:LYS:HA	1.85	0.43
2:5:12:GLU:OE1	2:5:83:ARG:NH1	2.50	0.43
3:m:51:HIS:HB3	9:j:70:ILE:HD13	1.99	0.43
10:t:202:PGT:H122	10:t:202:PGT:H32	1.78	0.43
1:y:204:ASP:OD1	1:y:204:ASP:N	2.46	0.43
3:m:54:ARG:HE	9:j:22:ASN:ND2	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:15:ASN:ND2	3:n:228:GLN:HE22	2.16	0.43
1:y:108:SER:HB2	1:y:287:PHE:CZ	2.53	0.43
9:g:100:ASN:O	9:g:104:GLU:HG2	2.18	0.43
3:o:92:ASP:OD1	3:o:92:ASP:N	2.46	0.43
3:o:154:PRO:HG2	3:o:157:GLU:HG3	1.99	0.43
4:v:55:GLN:NE2	4:v:74:ARG:HE	2.16	0.43
8:e:35:THR:O	8:e:92:ASN:ND2	2.52	0.43
1:2:92:LEU:HD13	10:2:301:PGT:C21	2.48	0.43
3:m:97:GLU:O	3:m:183:ARG:NH1	2.52	0.43
4:t:88:ARG:HB2	10:t:202:PGT:H422	1.99	0.43
8:e:41:ARG:HD3	8:e:78:LYS:HD2	2.00	0.43
3:q:91:LEU:HD23	3:q:122:LEU:HD21	2.01	0.43
8:b:33:ALA:O	8:b:92:ASN:ND2	2.51	0.43
9:k:100:ASN:HB3	9:k:103:GLU:HG2	1.99	0.43
3:m:218:LEU:O	3:m:222:GLN:HG3	2.18	0.43
3:q:238:MET:HE3	9:l:115:TYR:CG	2.53	0.43
6:8:132:PHE:O	6:8:136:MET:HG2	2.19	0.43
8:b:36:PRO:HB3	8:b:90:ASP:HB2	2.01	0.43
8:f:15:THR:HG23	8:f:45:PHE:HZ	1.84	0.43
1:1:255:MET:HG2	1:2:257:SER:HA	2.01	0.43
1:3:114:VAL:O	1:3:118:ILE:HG12	2.17	0.43
2:4:81:ILE:HG13	1:y:278:LEU:HD21	2.01	0.43
3:m:136:SER:HB2	3:m:151:GLN:HA	2.00	0.43
3:n:77:ASP:OD1	3:n:77:ASP:N	2.51	0.43
3:q:43:SER:O	9:l:37:SER:N	2.52	0.43
1:z:203:VAL:HG11	1:z:209:VAL:HG12	1.99	0.43
7:AE:343:PRO:HG3	8:c:80:TYR:CZ	2.54	0.43
8:d:36:PRO:HB3	8:d:90:ASP:HB2	2.01	0.43
9:i:75:LYS:HB2	9:i:98:ASN:HD22	1.84	0.43
1:1:275:GLY:O	1:1:279:ILE:HG12	2.19	0.43
2:5:84:LEU:HD11	1:z:229:ILE:HG12	2.01	0.43
4:t:64:ASP:OD1	4:t:64:ASP:N	2.46	0.43
1:y:195:PHE:HB3	1:y:213:VAL:HG13	2.01	0.43
2:7:16:MET:HE1	2:7:76:TYR:HB2	2.01	0.42
6:8:207:ARG:HH12	6:8:210:PRO:HA	1.84	0.42
9:l:13:ALA:O	9:l:17:GLU:HG2	2.19	0.42
1:3:204:ASP:OD1	1:3:204:ASP:N	2.52	0.42
1:3:228:GLN:O	1:3:232:MET:HG2	2.18	0.42
4:u:43:ASN:ND2	11:u:201:XKP:C8	2.82	0.42
9:i:100:ASN:O	9:i:104:GLU:HG2	2.19	0.42
1:2:92:LEU:HD11	10:2:301:PGT:H192	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:243:VAL:HG21	5:x:89:LEU:HD11	2.01	0.42
3:o:238:MET:HE3	9:h:115:TYR:CG	2.54	0.42
3:q:54:ARG:HE	9:l:22:ASN:ND2	2.17	0.42
6:8:176:TRP:HE1	6:8:251:GLN:HG2	1.83	0.42
2:4:49:LEU:HD23	2:4:49:LEU:H	1.84	0.42
3:p:245:LEU:HG	9:k:119:VAL:HG13	2.00	0.42
7:AL:338:ALA:HB1	9:h:103:GLU:HB2	2.01	0.42
9:i:44:ALA:O	9:i:73:SER:N	2.46	0.42
1:3:101:ALA:HB2	4:v:95:TYR:OH	2.19	0.42
3:n:200:GLN:NE2	3:n:201:THR:O	2.53	0.42
9:k:126:LYS:HE2	9:k:126:LYS:HB3	1.86	0.42
2:5:15:TRP:HE3	2:7:63:MET:HE1	1.85	0.42
2:6:70:THR:O	2:6:71:GLN:C	2.63	0.42
4:r:71:MET:HE3	9:k:133:LEU:HA	2.01	0.42
1:z:110:THR:HG21	1:z:219:ILE:HD11	2.01	0.42
6:8:84:ALA:HB1	6:8:255:LEU:HD13	2.01	0.42
9:g:127:GLN:O	9:g:131:ARG:HG2	2.20	0.42
9:i:41:THR:O	9:i:42:TYR:C	2.62	0.42
3:q:210:ASN:O	3:q:214:GLU:HG2	2.20	0.42
1:y:167:THR:HG22	1:y:169:ARG:H	1.84	0.42
1:z:166:VAL:HB	1:z:170:GLU:HB2	2.00	0.42
7:AO:333:ALA:HB3	7:AO:356:MET:HB3	2.02	0.42
9:h:36:SER:OG	9:h:38:ALA:O	2.27	0.42
1:2:92:LEU:HD11	10:2:301:PGT:H171	2.02	0.42
1:2:272:LEU:HD12	1:2:273:VAL:HG23	2.02	0.42
2:4:17:VAL:HG23	1:y:243:VAL:HG23	2.01	0.42
2:4:21:VAL:O	2:4:25:ILE:HG12	2.20	0.42
3:n:40:GLN:HE21	3:n:60:GLU:CD	2.27	0.42
4:r:33:PHE:HE1	1:z:154:ASN:HB2	1.84	0.42
4:r:66:SER:OG	4:r:69:ASP:OD1	2.38	0.42
7:AK:337:GLY:O	7:AK:341:ASN:ND2	2.53	0.42
1:3:280:LEU:HD11	6:8:175:GLY:HA2	2.02	0.42
3:m:53:SER:HG	8:e:85:GLN:HE21	1.61	0.42
3:n:35:ARG:NH1	3:n:101:ARG:HD3	2.34	0.42
3:o:37:ASP:HB3	3:o:61:ARG:HD2	2.02	0.42
3:p:54:ARG:HE	9:k:22:ASN:ND2	2.14	0.42
4:r:71:MET:HA	4:r:74:ARG:HG2	2.02	0.42
10:v:202:PGT:H262	1:y:96:LEU:CD2	2.49	0.42
7:AD:346:ASP:OD1	8:d:39:LYS:NZ	2.44	0.42
7:AF:342:GLN:O	7:AF:343:PRO:C	2.61	0.42
1:3:162:LEU:HD21	6:8:69:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:80:LEU:HA	2:4:83:ARG:HG2	2.01	0.42
2:5:16:MET:HE2	2:5:76:TYR:HB2	2.02	0.42
3:p:87:TRP:HB3	3:p:99:LEU:HB3	2.01	0.42
3:q:76:ARG:NH1	3:q:79:ASP:OD1	2.47	0.42
3:q:97:GLU:O	3:q:183:ARG:NH1	2.53	0.42
4:t:83:ALA:HB2	8:c:128:ILE:HD13	2.02	0.42
5:x:105:MET:HE2	5:x:105:MET:HB3	1.98	0.42
1:3:255:MET:HE3	6:8:214:ILE:HG12	2.01	0.41
3:m:84:GLY:O	3:m:101:ARG:NH2	2.31	0.41
3:n:123:GLY:N	3:n:127:ALA:O	2.53	0.41
3:n:218:LEU:O	3:n:222:GLN:HG3	2.20	0.41
7:AB:343:PRO:HG3	8:f:80:TYR:CZ	2.55	0.41
9:l:100:ASN:HB3	9:l:103:GLU:HG2	2.01	0.41
2:4:8:GLU:OE1	2:4:83:ARG:NH2	2.53	0.41
3:m:82:ILE:HD11	3:m:88:ILE:HG13	2.02	0.41
3:n:65:ASN:O	3:n:208:ASN:ND2	2.51	0.41
5:x:77:LYS:HE3	5:x:77:LYS:HB2	1.89	0.41
1:z:183:MET:HB2	1:z:214:LEU:HD21	2.02	0.41
1:2:274:ASP:OD2	1:2:277:ASN:ND2	2.52	0.41
3:m:28:ASN:O	3:m:31:THR:OG1	2.37	0.41
3:m:167:VAL:HG12	3:m:169:PRO:HD3	2.03	0.41
3:n:142:ARG:HH12	3:n:200:GLN:HG2	1.86	0.41
3:q:81:THR:HG23	3:q:200:GLN:HB3	2.03	0.41
10:v:202:PGT:H31	8:f:5:PHE:HE2	1.76	0.41
6:8:88:VAL:HG12	6:8:92:MET:HE3	2.02	0.41
6:8:207:ARG:HD3	6:8:207:ARG:O	2.20	0.41
10:2:301:PGT:H392	4:u:37:LEU:HD11	2.01	0.41
1:3:88:GLN:OE1	1:3:161:TYR:OH	2.29	0.41
3:n:11:GLY:O	3:n:15:ASN:ND2	2.45	0.41
7:AB:353:VAL:HG21	9:k:38:ALA:HB2	2.01	0.41
9:k:96:LYS:HE3	9:k:96:LYS:HB3	1.89	0.41
1:1:188:ARG:NH1	1:1:225:THR:OG1	2.46	0.41
1:3:104:ILE:HG22	1:3:109:PHE:CD2	2.56	0.41
1:3:253:MET:H	1:3:253:MET:HG2	1.69	0.41
3:n:16:MET:O	3:n:20:GLN:HG3	2.20	0.41
3:q:14:GLN:HB3	3:q:59:THR:HG23	2.01	0.41
7:AF:346:ASP:HB3	7:AF:347:ALA:H	1.61	0.41
8:c:32:GLN:NE2	9:h:51:ALA:HB2	2.35	0.41
1:2:96:LEU:HD21	10:2:301:PGT:H222	2.02	0.41
1:3:273:VAL:HG22	5:x:58:PHE:CE2	2.56	0.41
3:n:68:GLN:OE1	3:n:101:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:v:87:ILE:HG21	10:v:202:PGT:H392	2.01	0.41
6:8:61:PRO:HG3	6:8:161:GLY:HA3	2.03	0.41
9:j:43:LYS:HG2	9:j:77:LEU:HD21	2.02	0.41
2:4:44:ILE:HG22	2:4:46:GLU:H	1.86	0.41
3:p:1:MET:HG3	3:p:239:ASP:HB2	2.03	0.41
3:q:248:MET:HE3	9:l:130:LEU:HD11	2.03	0.41
4:t:87:ILE:CD1	10:t:202:PGT:H182	2.38	0.41
4:t:102:PRO:HG2	6:8:39:PRO:HD2	2.01	0.41
1:z:184:LEU:O	1:z:187:THR:HG22	2.21	0.41
6:8:213:ASN:HB2	6:8:215:PHE:CE1	2.55	0.41
1:1:189:ILE:HD12	1:1:189:ILE:H	1.85	0.41
2:6:73:LEU:HD13	2:6:73:LEU:HA	1.97	0.41
3:p:77:ASP:OD1	3:p:77:ASP:N	2.53	0.41
3:p:108:ASP:OD1	3:p:112:MET:N	2.54	0.41
3:p:179:ASN:HD21	3:p:183:ARG:HH21	1.69	0.41
4:t:79:VAL:HG11	8:c:124:LEU:HD23	2.03	0.41
4:v:75:ASN:HD22	9:l:135:MET:HE2	1.85	0.41
10:v:202:PGT:H461	10:v:202:PGT:H432	1.47	0.41
7:AG:343:PRO:HA	7:AG:344:PRO:HD3	1.92	0.41
7:AI:335:ILE:O	7:AI:336:PRO:C	2.61	0.41
7:AJ:341:ASN:ND2	8:c:86:PRO:HG3	2.36	0.41
9:i:89:ASN:OD1	9:i:93:TYR:N	2.51	0.41
1:2:104:ILE:O	1:2:110:THR:OG1	2.38	0.41
1:3:128:THR:HB	1:3:129:PRO:HD3	2.03	0.41
2:6:81:ILE:HA	2:6:84:LEU:HD13	2.02	0.41
3:n:231:MET:HA	3:n:234:THR:HG22	2.03	0.41
3:q:83:GLU:OE1	3:q:142:ARG:NH2	2.54	0.41
4:r:79:VAL:HG11	8:e:124:LEU:HD23	2.03	0.41
4:v:71:MET:SD	4:v:74:ARG:HD3	2.61	0.41
7:AG:339:LEU:HD11	9:k:72:GLU:HG3	2.03	0.41
9:i:53:LEU:N	9:i:53:LEU:HD23	2.36	0.41
1:2:270:PHE:HE2	1:2:276:TRP:CD1	2.38	0.40
3:n:108:ASP:OD1	3:n:112:MET:N	2.54	0.40
3:o:167:VAL:HG12	3:o:169:PRO:HD3	2.04	0.40
3:q:245:LEU:O	9:l:126:LYS:NZ	2.53	0.40
5:x:69:ARG:CZ	5:x:69:ARG:H	2.34	0.40
1:2:96:LEU:HB3	4:u:90:LYS:HB3	2.03	0.40
1:3:186:GLN:HE22	1:3:287:PHE:HA	1.85	0.40
3:m:40:GLN:HG2	3:m:62:PRO:HD3	2.01	0.40
3:n:247:ARG:NE	9:h:120:GLN:HE22	2.18	0.40
3:o:115:ASN:OD1	3:o:119:HIS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:10:SER:O	3:q:14:GLN:HG2	2.22	0.40
1:y:254:MET:HB2	1:z:254:MET:SD	2.61	0.40
1:1:242:LEU:HD13	6:8:125:LEU:HD12	2.01	0.40
1:2:111:ARG:NE	1:2:222:GLU:OE1	2.50	0.40
2:5:84:LEU:HD13	1:z:232:MET:HG3	2.04	0.40
2:6:56:ILE:HG12	2:7:18:LEU:HD11	2.04	0.40
3:m:15:ASN:ND2	3:m:228:GLN:HE22	2.18	0.40
3:n:7:LEU:HD23	9:i:25:SER:HB2	2.04	0.40
3:n:76:ARG:O	3:n:202:GLY:HA2	2.20	0.40
3:n:144:GLY:HA2	3:n:199:LEU:HD12	2.03	0.40
3:q:2:ASP:C	3:q:4:ALA:H	2.29	0.40
4:t:71:MET:SD	4:t:74:ARG:HD3	2.61	0.40
1:z:152:GLU:CD	1:z:178:PRO:HB3	2.46	0.40
3:p:167:VAL:HG12	3:p:169:PRO:HD3	2.04	0.40
2:4:14:LEU:HA	2:4:17:VAL:HG12	2.03	0.40
4:s:57:ARG:HB3	4:s:65:VAL:HG21	2.02	0.40
1:z:86:THR:HG22	8:e:127:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	205/289 (71%)	202 (98%)	3 (2%)	0	100	100
1	2	206/289 (71%)	203 (98%)	3 (2%)	0	100	100
1	3	206/289 (71%)	204 (99%)	2 (1%)	0	100	100
1	y	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
1	z	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
2	4	87/89 (98%)	87 (100%)	0	0	100	100
2	5	87/89 (98%)	86 (99%)	0	1 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
2	7	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
3	m	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
3	n	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
3	o	246/249 (99%)	241 (98%)	5 (2%)	0	100	100
3	p	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
3	q	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
4	r	70/103 (68%)	70 (100%)	0	0	100	100
4	s	78/103 (76%)	78 (100%)	0	0	100	100
4	t	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
4	u	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
4	v	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
4	w	38/103 (37%)	38 (100%)	0	0	100	100
5	x	69/376 (18%)	69 (100%)	0	0	100	100
6	8	238/260 (92%)	232 (98%)	6 (2%)	0	100	100
7	AA	17/580 (3%)	17 (100%)	0	0	100	100
7	AB	17/580 (3%)	15 (88%)	2 (12%)	0	100	100
7	AC	18/580 (3%)	18 (100%)	0	0	100	100
7	AD	17/580 (3%)	17 (100%)	0	0	100	100
7	AE	17/580 (3%)	17 (100%)	0	0	100	100
7	AF	21/580 (4%)	14 (67%)	6 (29%)	1 (5%)	2	9
7	AG	9/580 (2%)	7 (78%)	2 (22%)	0	100	100
7	AH	9/580 (2%)	9 (100%)	0	0	100	100
7	AI	9/580 (2%)	8 (89%)	1 (11%)	0	100	100
7	AJ	22/580 (4%)	18 (82%)	4 (18%)	0	100	100
7	AK	23/580 (4%)	23 (100%)	0	0	100	100
7	AL	30/580 (5%)	26 (87%)	4 (13%)	0	100	100
7	AM	31/580 (5%)	31 (100%)	0	0	100	100
7	AN	31/580 (5%)	31 (100%)	0	0	100	100
7	AO	30/580 (5%)	30 (100%)	0	0	100	100
8	b	105/131 (80%)	104 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c	103/131 (79%)	102 (99%)	1 (1%)	0	100	100
8	d	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
8	e	104/131 (79%)	104 (100%)	0	0	100	100
8	f	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
9	g	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
9	h	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
9	i	126/137 (92%)	122 (97%)	3 (2%)	1 (1%)	16	46
9	j	126/137 (92%)	125 (99%)	1 (1%)	0	100	100
9	k	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
9	l	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
All	All	4896/14477 (34%)	4795 (98%)	98 (2%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	5	88	LEU
9	i	42	TYR
7	AF	349	ILE

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	181/247 (73%)	175 (97%)	6 (3%)	33	64
1	2	182/247 (74%)	176 (97%)	6 (3%)	33	64
1	3	182/247 (74%)	177 (97%)	5 (3%)	39	68
1	y	182/247 (74%)	175 (96%)	7 (4%)	29	60
1	z	182/247 (74%)	175 (96%)	7 (4%)	29	60
2	4	80/80 (100%)	77 (96%)	3 (4%)	29	60
2	5	80/80 (100%)	76 (95%)	4 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	6	80/80 (100%)	75 (94%)	5 (6%)	16	45
2	7	80/80 (100%)	79 (99%)	1 (1%)	61	79
3	m	204/205 (100%)	199 (98%)	5 (2%)	42	69
3	n	204/205 (100%)	198 (97%)	6 (3%)	37	67
3	o	204/205 (100%)	198 (97%)	6 (3%)	37	67
3	p	204/205 (100%)	202 (99%)	2 (1%)	68	81
3	q	204/205 (100%)	200 (98%)	4 (2%)	48	73
4	r	63/84 (75%)	59 (94%)	4 (6%)	16	45
4	s	66/84 (79%)	64 (97%)	2 (3%)	36	66
4	t	66/84 (79%)	63 (96%)	3 (4%)	24	56
4	u	63/84 (75%)	62 (98%)	1 (2%)	55	76
4	v	63/84 (75%)	63 (100%)	0	100	100
4	w	36/84 (43%)	35 (97%)	1 (3%)	38	67
5	x	58/317 (18%)	55 (95%)	3 (5%)	21	51
6	8	204/218 (94%)	194 (95%)	10 (5%)	22	53
7	AA	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AB	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AC	15/500 (3%)	15 (100%)	0	100	100
7	AD	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AE	15/500 (3%)	15 (100%)	0	100	100
7	AF	17/500 (3%)	13 (76%)	4 (24%)	1	4
7	AG	8/500 (2%)	8 (100%)	0	100	100
7	AH	8/500 (2%)	7 (88%)	1 (12%)	4	18
7	AI	8/500 (2%)	8 (100%)	0	100	100
7	AJ	17/500 (3%)	16 (94%)	1 (6%)	18	47
7	AK	18/500 (4%)	15 (83%)	3 (17%)	2	10
7	AL	24/500 (5%)	23 (96%)	1 (4%)	26	58
7	AM	24/500 (5%)	24 (100%)	0	100	100
7	AN	24/500 (5%)	22 (92%)	2 (8%)	10	34
7	AO	24/500 (5%)	23 (96%)	1 (4%)	26	58
8	b	89/106 (84%)	88 (99%)	1 (1%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	c	88/106 (83%)	86 (98%)	2 (2%)	44	70
8	d	89/106 (84%)	86 (97%)	3 (3%)	32	63
8	e	88/106 (83%)	85 (97%)	3 (3%)	32	63
8	f	88/106 (83%)	88 (100%)	0	100	100
9	g	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	h	111/115 (96%)	107 (96%)	4 (4%)	31	62
9	i	111/115 (96%)	103 (93%)	8 (7%)	13	40
9	j	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	k	111/115 (96%)	105 (95%)	6 (5%)	20	50
9	l	111/115 (96%)	106 (96%)	5 (4%)	24	56
All	All	4223/12339 (34%)	4074 (96%)	149 (4%)	32	62

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	127	GLN
1	1	146	MET
1	1	166	VAL
1	1	202	GLN
1	1	208	ASP
1	1	259	MET
1	2	86	THR
1	2	95	MET
1	2	149	VAL
1	2	214	LEU
1	2	220	THR
1	2	272	LEU
1	3	96	LEU
1	3	133	VAL
1	3	141	LEU
1	3	149	VAL
1	3	214	LEU
2	4	1	MET
2	4	16	MET
2	4	55	LEU
2	5	45	ASN
2	5	64	LEU
2	5	72	MET

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Mol	Chain	Res	Type
2	5	89	TYR
2	6	1	MET
2	6	7	VAL
2	6	14	LEU
2	6	42	THR
2	6	86	GLN
2	7	88	LEU
3	m	7	LEU
3	m	60	GLU
3	m	72	ILE
3	m	135	LEU
3	m	218	LEU
3	n	60	GLU
3	n	72	ILE
3	n	158	PHE
3	n	162	ASP
3	n	200	GLN
3	n	204	ILE
3	o	72	ILE
3	o	73	THR
3	o	101	ARG
3	o	114	THR
3	o	158	PHE
3	o	229	VAL
3	p	72	ILE
3	p	135	LEU
3	q	72	ILE
3	q	73	THR
3	q	135	LEU
3	q	204	ILE
4	r	34	ASN
4	r	37	LEU
4	r	39	LYS
4	r	67	LEU
4	s	67	LEU
4	s	98	LEU
4	t	32	ASP
4	t	35	ASP
4	t	67	LEU
4	u	67	LEU
4	w	91	LEU
5	x	48	TRP

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Mol	Chain	Res	Type
5	x	69	ARG
5	x	86	MET
1	y	86	THR
1	y	99	LEU
1	y	113	VAL
1	y	141	LEU
1	y	254	MET
1	y	261	VAL
1	y	283	LEU
1	z	86	THR
1	z	87	LEU
1	z	113	VAL
1	z	128	THR
1	z	184	LEU
1	z	192	LEU
1	z	272	LEU
6	8	2	GLU
6	8	47	LEU
6	8	70	ARG
6	8	102	ILE
6	8	125	LEU
6	8	192	ILE
6	8	195	LEU
6	8	207	ARG
6	8	212	LEU
6	8	214	ILE
7	AA	342	GLN
7	AB	342	GLN
7	AD	349	ILE
7	AF	346	ASP
7	AF	351	GLN
7	AF	352	ASP
7	AF	355	GLN
7	AH	342	GLN
7	AJ	349	ILE
7	AK	330	ASN
7	AK	331	MET
7	AK	332	VAL
7	AL	339	LEU
7	AN	339	LEU
7	AN	352	ASP
7	AO	330	ASN

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Mol	Chain	Res	Type
8	b	9	LEU
8	c	6	ASP
8	c	87	ASP
8	d	4	SER
8	d	6	ASP
8	d	7	ASN
8	e	6	ASP
8	e	7	ASN
8	e	88	THR
9	g	23	THR
9	g	39	LYS
9	g	53	LEU
9	g	65	VAL
9	g	134	GLN
9	h	3	LEU
9	h	34	VAL
9	h	65	VAL
9	h	67	VAL
9	i	36	SER
9	i	39	LYS
9	i	61	ASP
9	i	62	THR
9	i	67	VAL
9	i	84	ASP
9	i	113	ARG
9	i	131	ARG
9	j	53	LEU
9	j	61	ASP
9	j	65	VAL
9	j	67	VAL
9	j	126	LYS
9	k	14	MET
9	k	40	ASP
9	k	53	LEU
9	k	65	VAL
9	k	113	ARG
9	k	134	GLN
9	l	40	ASP
9	l	43	LYS
9	l	65	VAL
9	l	126	LYS
9	l	137	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	88	GLN
1	1	127	GLN
1	1	228	GLN
1	2	127	GLN
1	3	186	GLN
1	3	205	ASN
2	4	47	GLN
2	4	71	GLN
2	6	47	GLN
2	6	67	HIS
2	7	39	GLN
2	7	67	HIS
3	m	179	ASN
3	m	200	GLN
3	m	228	GLN
3	n	15	ASN
3	n	24	ASN
3	n	102	ASN
3	n	188	ASN
3	n	200	GLN
3	o	40	GLN
3	o	102	ASN
3	o	200	GLN
3	p	14	GLN
3	p	119	HIS
3	p	179	ASN
3	p	200	GLN
3	p	228	GLN
3	q	15	ASN
3	q	20	GLN
3	q	40	GLN
3	q	102	ASN
3	q	200	GLN
4	r	42	ASN
4	r	86	GLN
4	s	45	ASN
4	s	86	GLN
4	s	89	ASN
4	t	45	ASN
4	t	75	ASN
4	t	86	GLN

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Mol	Chain	Res	Type
4	u	43	ASN
4	u	86	GLN
4	v	55	GLN
4	v	75	ASN
1	y	186	GLN
1	z	126	GLN
1	z	127	GLN
1	z	165	GLN
6	8	90	GLN
6	8	106	GLN
6	8	182	GLN
6	8	199	ASN
6	8	211	GLN
7	AH	342	GLN
7	AK	330	ASN
7	AL	341	ASN
7	AL	351	GLN
7	AM	341	ASN
7	AN	342	GLN
7	AO	330	ASN
7	AO	355	GLN
8	b	50	GLN
8	c	32	GLN
8	c	106	ASN
8	c	110	HIS
8	d	14	HIS
8	d	105	GLN
8	d	106	ASN
8	d	107	GLN
8	d	110	HIS
8	e	85	GLN
8	e	101	ASN
8	e	107	GLN
8	e	110	HIS
8	f	14	HIS
8	f	34	ASN
8	f	50	GLN
8	f	107	GLN
8	f	110	HIS
9	g	100	ASN
9	g	118	ASN
9	g	134	GLN

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Mol	Chain	Res	Type
9	h	127	GLN
9	i	22	ASN
9	i	46	HIS
9	i	100	ASN
9	i	118	ASN
9	j	22	ASN
9	j	118	ASN
9	k	22	ASN
9	k	100	ASN
9	k	120	GLN
9	l	22	ASN
9	l	100	ASN
9	l	120	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	XKP	t	201	-	31,31,32	0.36	0	34,36,37	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	XKP	s	201	-	31,31,32	0.37	0	34,36,37	0.35	0
11	XKP	e	201	-	31,31,32	0.36	0	34,36,37	0.43	0
10	PGT	v	202	-	50,50,50	0.30	0	53,56,56	0.38	0
11	XKP	u	201	-	31,31,32	0.38	0	34,36,37	0.43	0
10	PGT	2	301	-	50,50,50	0.31	0	53,56,56	0.47	0
11	XKP	v	201	-	31,31,32	0.37	0	34,36,37	0.49	0
10	PGT	t	202	-	50,50,50	0.30	0	53,56,56	0.37	0
10	PGT	e	202	-	50,50,50	0.33	0	53,56,56	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	XKP	t	201	-	-	25/35/35/36	-
11	XKP	s	201	-	-	20/35/35/36	-
11	XKP	e	201	-	-	17/35/35/36	-
10	PGT	v	202	-	-	39/55/55/55	-
11	XKP	u	201	-	-	18/35/35/36	-
10	PGT	2	301	-	-	34/55/55/55	-
11	XKP	v	201	-	-	20/35/35/36	-
10	PGT	t	202	-	-	37/55/55/55	-
10	PGT	e	202	-	-	32/55/55/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (242) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	2	301	PGT	C32-C31-O2-C2
10	2	301	PGT	C1-O3P-P-O1P
10	2	301	PGT	C4-O4P-P-O3P
10	2	301	PGT	C4-O4P-P-O1P
10	2	301	PGT	C5-C4-O4P-P
10	t	202	PGT	C4-O4P-P-O2P
10	t	202	PGT	C4-C5-C6-O6
10	v	202	PGT	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
10	v	202	PGT	C1-O3P-P-O1P
10	v	202	PGT	O11-C11-O3-C3
10	v	202	PGT	C12-C11-O3-C3
10	e	202	PGT	O31-C31-O2-C2
10	e	202	PGT	C4-O4P-P-O1P
10	e	202	PGT	C4-O4P-P-O2P
10	e	202	PGT	C4-C5-C6-O6
10	e	202	PGT	O5-C5-C6-O6
11	s	201	XKP	C12-C11-O6-C7
11	s	201	XKP	O7-C11-O6-C7
11	s	201	XKP	N-C10-C9-O5
11	s	201	XKP	C8-O2-P-O3
11	s	201	XKP	C9-O5-P-O3
11	s	201	XKP	C9-O5-P-O4
11	t	201	XKP	C12-C11-O6-C7
11	t	201	XKP	O7-C11-O6-C7
11	t	201	XKP	N-C10-C9-O5
11	t	201	XKP	C8-O2-P-O3
11	t	201	XKP	C8-O2-P-O4
11	t	201	XKP	C8-O2-P-O5
11	t	201	XKP	C9-O5-P-O2
11	t	201	XKP	C9-O5-P-O3
11	t	201	XKP	C9-O5-P-O4
11	u	201	XKP	C12-C11-O6-C7
11	u	201	XKP	C8-O2-P-O3
11	u	201	XKP	C8-O2-P-O4
11	u	201	XKP	C8-O2-P-O5
11	u	201	XKP	C9-O5-P-O4
11	v	201	XKP	O7-C11-O6-C7
11	e	201	XKP	N-C10-C9-O5
11	e	201	XKP	C9-O5-P-O2
11	e	201	XKP	C9-O5-P-O3
10	2	301	PGT	O11-C11-O3-C3
10	t	202	PGT	O11-C11-O3-C3
10	2	301	PGT	C12-C11-O3-C3
10	t	202	PGT	C12-C11-O3-C3
10	e	202	PGT	O11-C11-O3-C3
10	2	301	PGT	O31-C31-O2-C2
10	v	202	PGT	O31-C31-O2-C2
11	u	201	XKP	O7-C11-O6-C7
10	e	202	PGT	C12-C11-O3-C3
10	e	202	PGT	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
11	v	201	XKP	C12-C11-O6-C7
10	t	202	PGT	C39-C40-C41-C42
11	s	201	XKP	C15-C16-C18-C19
11	s	201	XKP	O-C5-O1-C6
10	2	301	PGT	C43-C44-C45-C46
10	v	202	PGT	O4P-C4-C5-O5
11	s	201	XKP	C4-C5-O1-C6
10	t	202	PGT	C32-C31-O2-C2
10	t	202	PGT	C16-C17-C18-C19
10	e	202	PGT	C43-C44-C45-C46
10	2	301	PGT	C15-C16-C17-C18
10	e	202	PGT	C39-C40-C41-C42
11	t	201	XKP	C-C1-C2-C3
10	v	202	PGT	C43-C44-C45-C46
11	t	201	XKP	C4-C5-O1-C6
10	v	202	PGT	C11-C12-C13-C14
10	2	301	PGT	O4P-C4-C5-C6
10	t	202	PGT	O31-C31-O2-C2
11	e	201	XKP	C1-C2-C3-C4
11	t	201	XKP	O-C5-O1-C6
11	e	201	XKP	C11-C12-C13-C14
11	t	201	XKP	C11-C12-C13-C14
10	2	301	PGT	C11-C12-C13-C14
11	s	201	XKP	C2-C3-C4-C5
11	s	201	XKP	C11-C12-C13-C14
11	v	201	XKP	C2-C3-C4-C5
11	t	201	XKP	C2-C3-C4-C5
10	t	202	PGT	C14-C15-C16-C17
10	t	202	PGT	C31-C32-C33-C34
10	2	301	PGT	C1-O3P-P-O4P
10	t	202	PGT	C4-O4P-P-O3P
10	v	202	PGT	C1-O3P-P-O4P
10	v	202	PGT	C4-O4P-P-O3P
10	e	202	PGT	C4-O4P-P-O3P
11	s	201	XKP	C9-O5-P-O2
11	v	201	XKP	C8-O2-P-O5
11	s	201	XKP	C12-C13-C14-C15
10	v	202	PGT	C41-C42-C43-C44
11	s	201	XKP	C-C1-C2-C3
11	u	201	XKP	C1-C2-C3-C4
10	v	202	PGT	C32-C33-C34-C35
10	t	202	PGT	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
10	v	202	PGT	C36-C37-C38-C39
10	e	202	PGT	C15-C16-C17-C18
10	2	301	PGT	C39-C40-C41-C42
10	t	202	PGT	C43-C44-C45-C46
10	e	202	PGT	C12-C13-C14-C15
11	s	201	XKP	C13-C14-C15-C16
11	t	201	XKP	C14-C15-C16-C18
11	e	201	XKP	C14-C15-C16-C18
10	e	202	PGT	C42-C43-C44-C45
10	e	202	PGT	C22-C23-C24-C25
10	2	301	PGT	C41-C42-C43-C44
10	e	202	PGT	C37-C38-C39-C40
11	u	201	XKP	C15-C16-C18-C19
11	e	201	XKP	O7-C11-O6-C7
11	e	201	XKP	C12-C11-O6-C7
10	e	202	PGT	C19-C20-C21-C22
10	2	301	PGT	C21-C22-C23-C24
10	v	202	PGT	C20-C21-C22-C23
10	v	202	PGT	C22-C23-C24-C25
10	e	202	PGT	C36-C37-C38-C39
11	v	201	XKP	C14-C15-C16-C18
10	2	301	PGT	C13-C14-C15-C16
10	v	202	PGT	C14-C15-C16-C17
11	t	201	XKP	C15-C16-C18-C19
10	v	202	PGT	C38-C39-C40-C41
11	u	201	XKP	C13-C14-C15-C16
11	s	201	XKP	C20-C-C1-C2
11	u	201	XKP	C2-C3-C4-C5
10	2	301	PGT	C42-C43-C44-C45
10	t	202	PGT	C36-C37-C38-C39
10	e	202	PGT	C33-C34-C35-C36
10	2	301	PGT	O4P-C4-C5-O5
10	v	202	PGT	C44-C45-C46-C47
10	v	202	PGT	C19-C20-C21-C22
10	v	202	PGT	O4P-C4-C5-C6
10	t	202	PGT	C13-C14-C15-C16
11	e	201	XKP	C2-C3-C4-C5
10	2	301	PGT	C23-C24-C25-C26
10	t	202	PGT	C23-C24-C25-C26
10	t	202	PGT	C37-C38-C39-C40
11	u	201	XKP	C4-C5-O1-C6
10	v	202	PGT	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
10	t	202	PGT	C41-C42-C43-C44
11	u	201	XKP	C11-C12-C13-C14
11	v	201	XKP	C4-C5-O1-C6
11	u	201	XKP	C20-C-C1-C2
11	e	201	XKP	C12-C13-C14-C15
10	v	202	PGT	C16-C17-C18-C19
11	v	201	XKP	C-C1-C2-C3
10	t	202	PGT	C12-C13-C14-C15
11	s	201	XKP	C8-O2-P-O5
11	u	201	XKP	C9-O5-P-O2
10	e	202	PGT	C31-C32-C33-C34
10	t	202	PGT	C42-C43-C44-C45
10	2	301	PGT	C32-C33-C34-C35
11	u	201	XKP	O-C5-O1-C6
11	t	201	XKP	O1-C6-C7-C8
10	v	202	PGT	C45-C46-C47-C48
10	2	301	PGT	C33-C34-C35-C36
10	e	202	PGT	C32-C33-C34-C35
11	e	201	XKP	C-C1-C2-C3
10	e	202	PGT	C38-C39-C40-C41
11	v	201	XKP	O-C5-O1-C6
10	v	202	PGT	C15-C16-C17-C18
11	u	201	XKP	C-C1-C2-C3
10	t	202	PGT	C35-C36-C37-C38
10	t	202	PGT	C33-C34-C35-C36
11	t	201	XKP	C1-C-C20-C21
10	t	202	PGT	C32-C33-C34-C35
10	v	202	PGT	C13-C14-C15-C16
11	v	201	XKP	C15-C16-C18-C19
10	t	202	PGT	C19-C20-C21-C22
10	2	301	PGT	C1-C2-C3-O3
10	e	202	PGT	C1-C2-C3-O3
10	e	202	PGT	C45-C46-C47-C48
10	2	301	PGT	C19-C20-C21-C22
10	t	202	PGT	C22-C23-C24-C25
10	e	202	PGT	O2-C2-C3-O3
11	t	201	XKP	O1-C6-C7-O6
11	v	201	XKP	O1-C6-C7-O6
10	v	202	PGT	C40-C41-C42-C43
10	v	202	PGT	C17-C18-C19-C20
10	t	202	PGT	C34-C35-C36-C37
10	e	202	PGT	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
11	v	201	XKP	C6-C7-C8-O2
11	s	201	XKP	C14-C15-C16-C18
10	e	202	PGT	C34-C35-C36-C37
10	v	202	PGT	C12-C13-C14-C15
11	v	201	XKP	O1-C6-C7-C8
11	e	201	XKP	C16-C18-C19-C17
10	2	301	PGT	O2-C2-C3-O3
10	v	202	PGT	O2-C2-C3-O3
10	e	202	PGT	C14-C15-C16-C17
10	t	202	PGT	C5-C4-O4P-P
11	t	201	XKP	C1-C2-C3-C4
10	2	301	PGT	C1-O3P-P-O2P
10	t	202	PGT	C4-O4P-P-O1P
10	v	202	PGT	C1-O3P-P-O2P
10	v	202	PGT	C4-O4P-P-O1P
11	s	201	XKP	C8-O2-P-O4
11	v	201	XKP	C8-O2-P-O4
11	e	201	XKP	C9-O5-P-O4
10	2	301	PGT	C22-C23-C24-C25
11	e	201	XKP	C10-C9-O5-P
10	2	301	PGT	O3P-C1-C2-O2
11	v	201	XKP	O6-C7-C8-O2
10	v	202	PGT	C1-C2-C3-O3
10	t	202	PGT	O2-C2-C3-O3
11	s	201	XKP	C7-C8-O2-P
11	v	201	XKP	C13-C14-C15-C16
10	t	202	PGT	O5-C5-C6-O6
10	2	301	PGT	C16-C17-C18-C19
11	u	201	XKP	C1-C-C20-C21
10	t	202	PGT	C21-C22-C23-C24
11	v	201	XKP	C9-O5-P-O2
11	t	201	XKP	C16-C18-C19-C17
10	2	301	PGT	C38-C39-C40-C41
11	t	201	XKP	O6-C7-C8-O2
10	2	301	PGT	C17-C18-C19-C20
10	t	202	PGT	C2-C1-O3P-P
10	v	202	PGT	C37-C38-C39-C40
11	v	201	XKP	C20-C-C1-C2
11	t	201	XKP	C12-C13-C14-C15
10	2	301	PGT	O3P-C1-C2-C3
11	t	201	XKP	C6-C7-C8-O2
10	v	202	PGT	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
11	v	201	XKP	C12-C13-C14-C15
10	v	202	PGT	C5-C4-O4P-P
10	v	202	PGT	C39-C40-C41-C42
10	v	202	PGT	O3-C11-C12-C13
10	t	202	PGT	C1-C2-C3-O3
10	t	202	PGT	O2-C31-C32-C33
10	2	301	PGT	C37-C38-C39-C40
11	v	201	XKP	C1-C-C20-C21
10	v	202	PGT	C42-C43-C44-C45
10	e	202	PGT	O4P-C4-C5-C6
10	2	301	PGT	C40-C41-C42-C43
11	e	201	XKP	C1-C-C20-C21
10	v	202	PGT	O11-C11-C12-C13
11	e	201	XKP	C15-C16-C18-C19
11	e	201	XKP	C20-C-C1-C2
10	t	202	PGT	O31-C31-C32-C33
10	t	202	PGT	C1-O3P-P-O1P
11	u	201	XKP	C9-O5-P-O3
11	v	201	XKP	C9-O5-P-O4
10	e	202	PGT	C18-C19-C20-C21
10	t	202	PGT	C20-C21-C22-C23
11	t	201	XKP	C7-C8-O2-P
10	e	202	PGT	O4P-C4-C5-O5
10	e	202	PGT	O3-C11-C12-C13

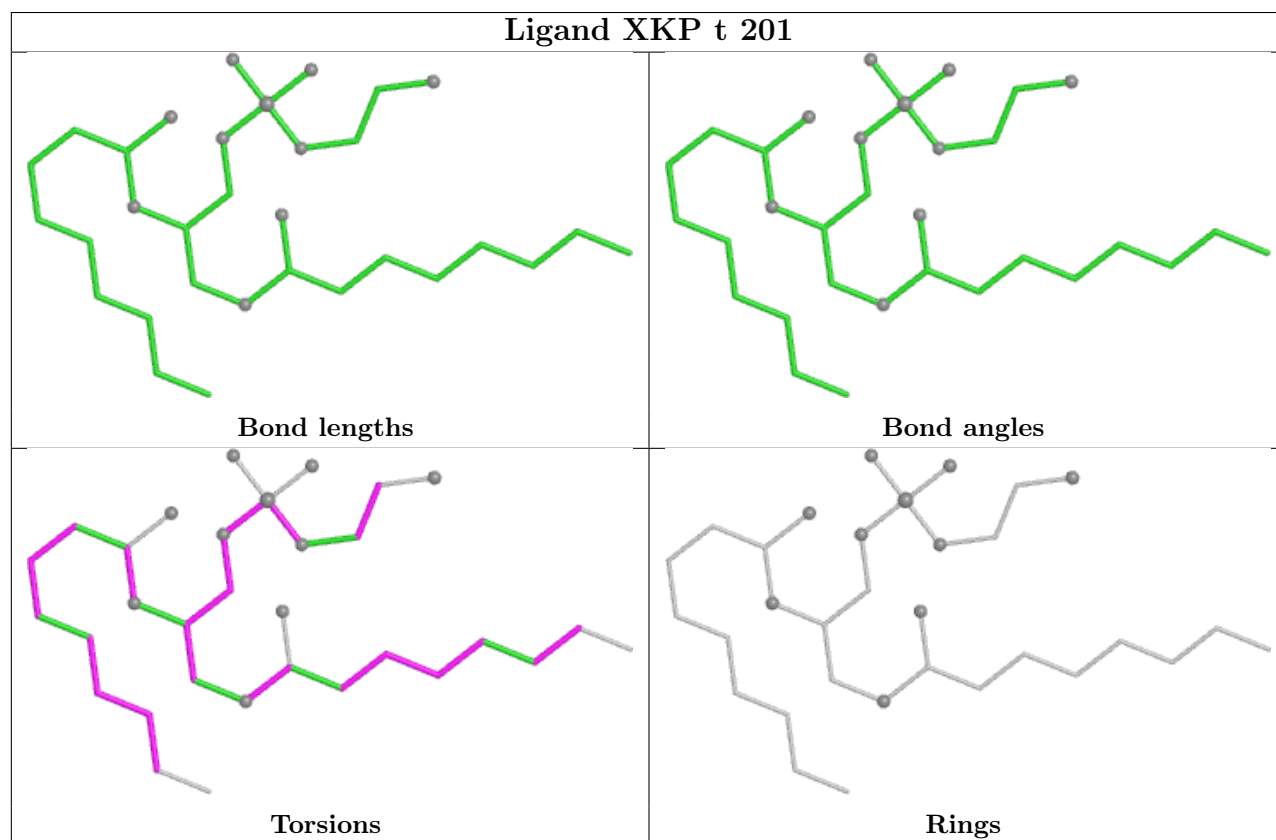
There are no ring outliers.

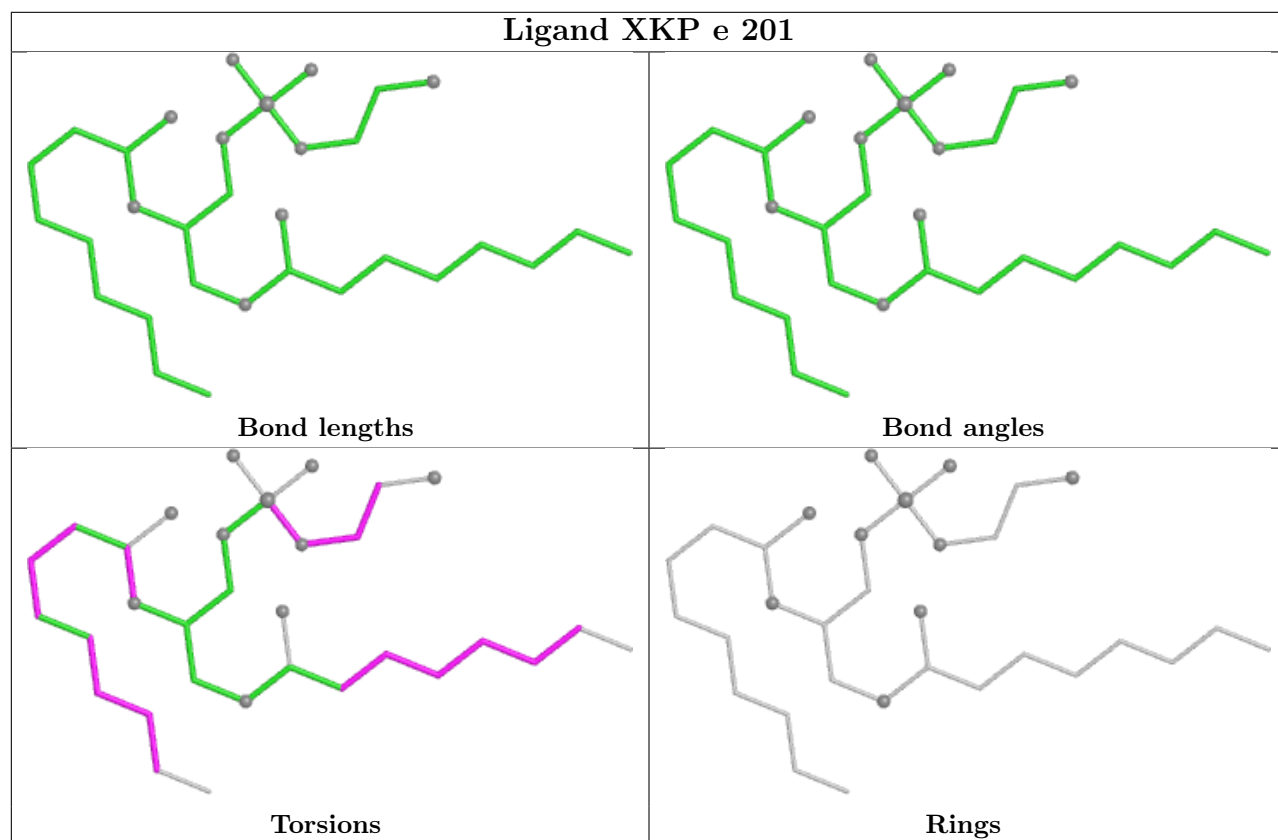
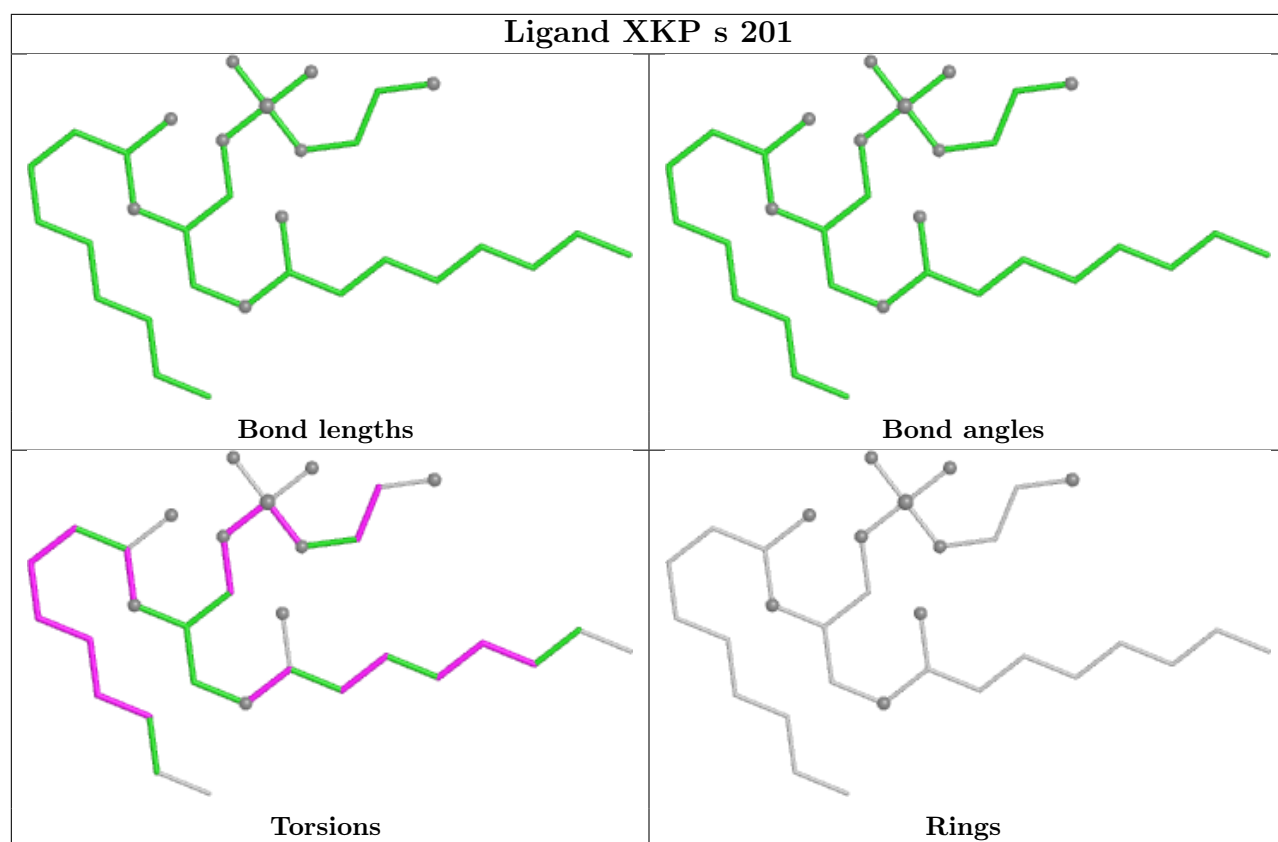
9 monomers are involved in 52 short contacts:

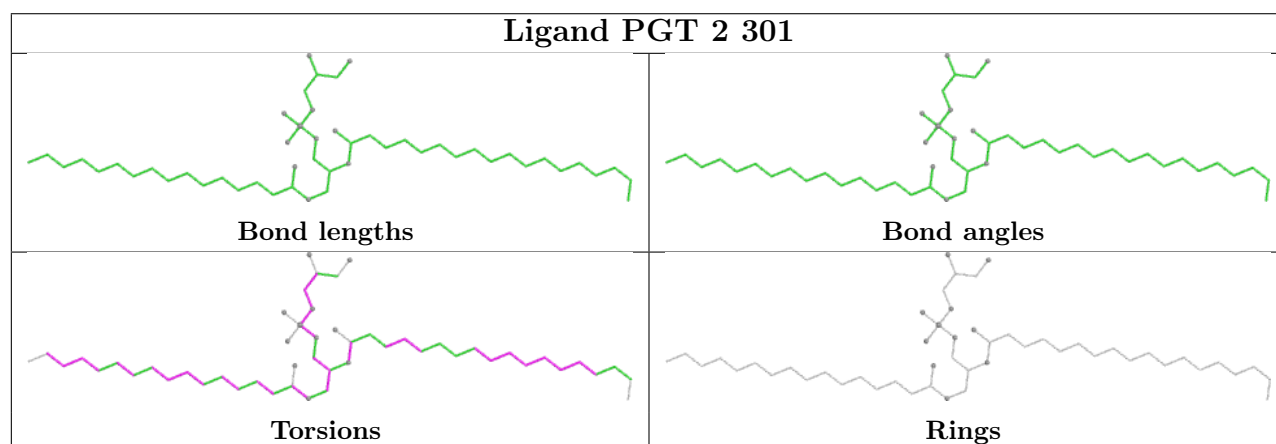
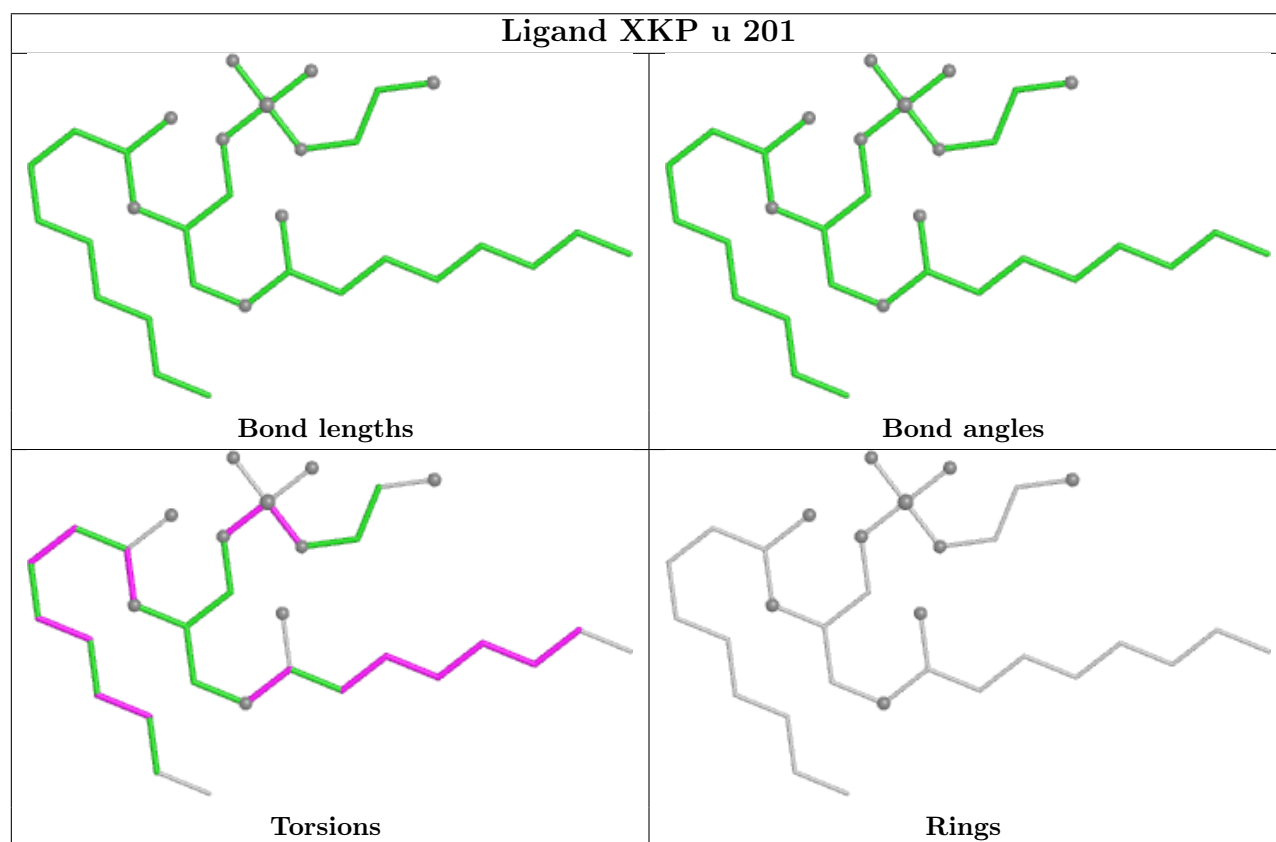
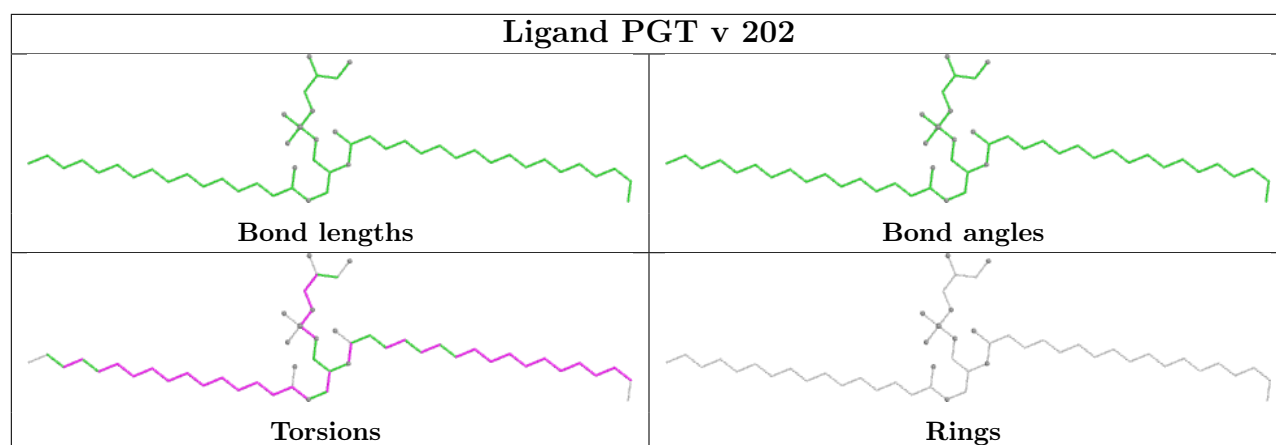
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	t	201	XKP	2	0
11	s	201	XKP	1	0
11	e	201	XKP	1	0
10	v	202	PGT	12	0
11	u	201	XKP	3	0
10	2	301	PGT	10	0
11	v	201	XKP	6	0
10	t	202	PGT	15	0
10	e	202	PGT	4	0

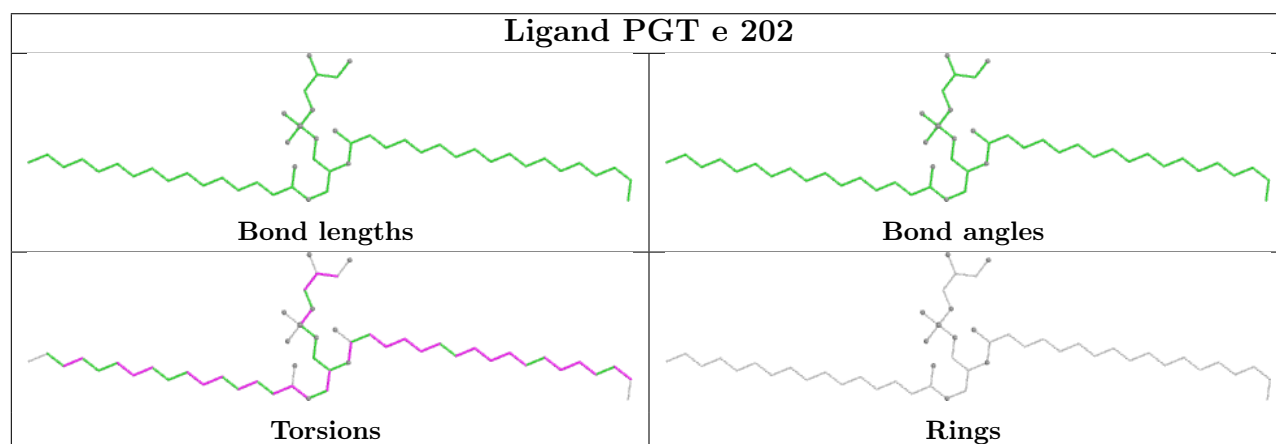
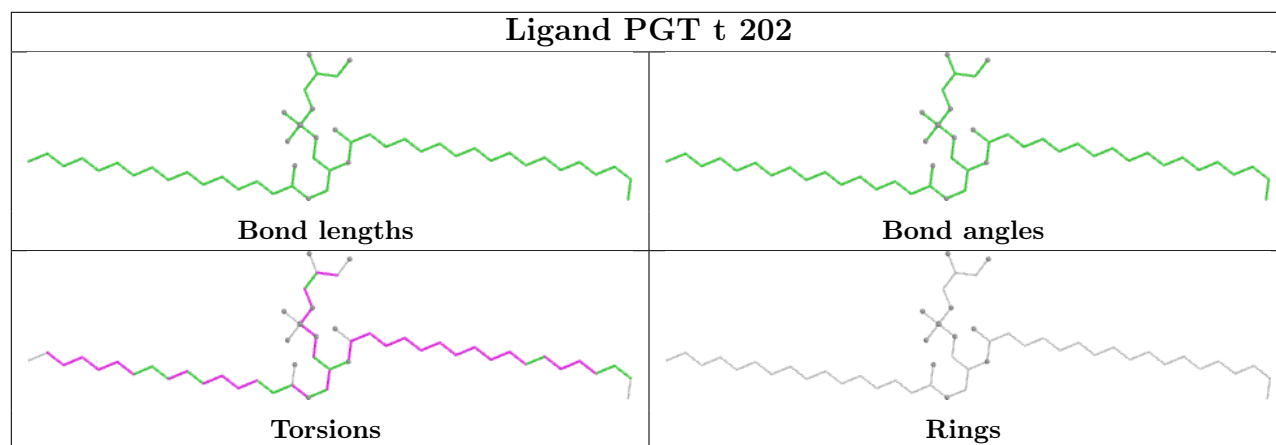
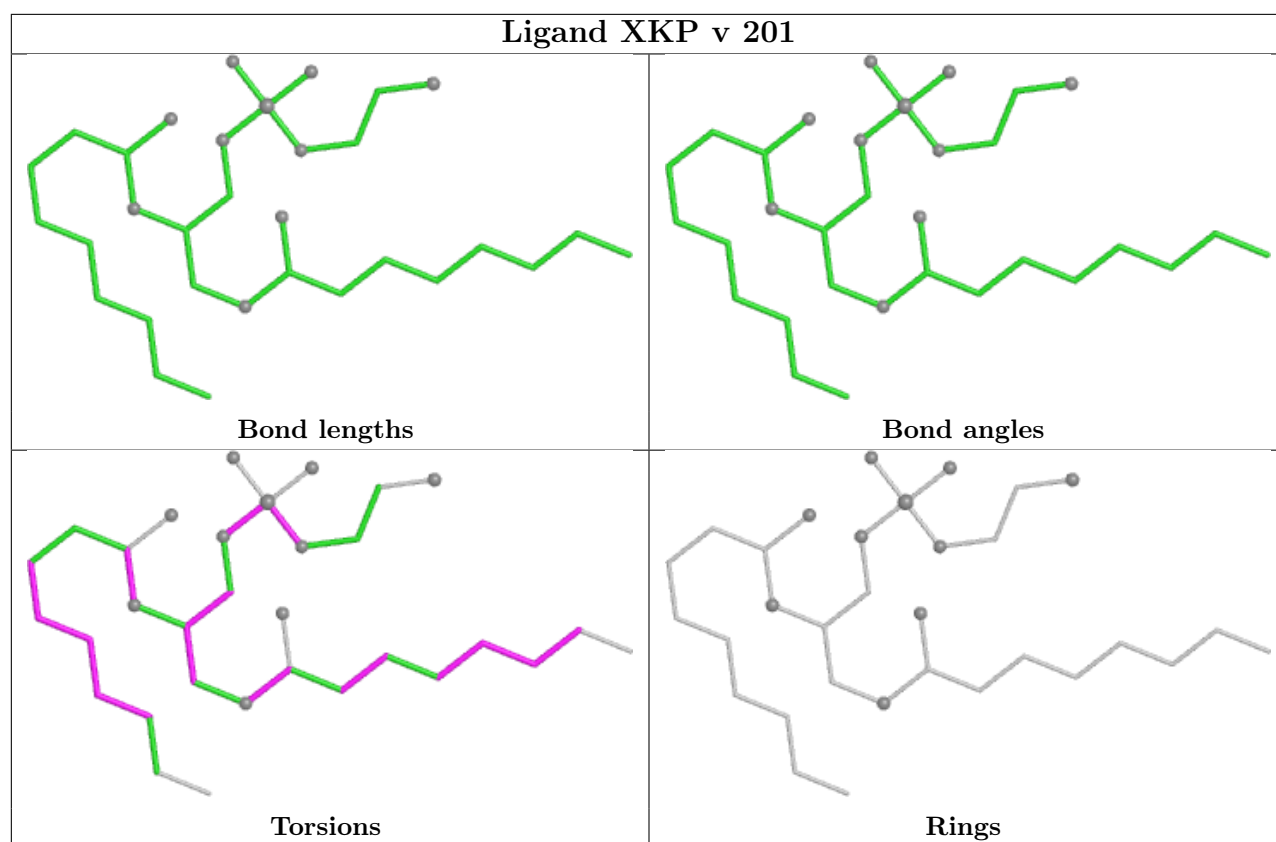
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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









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.

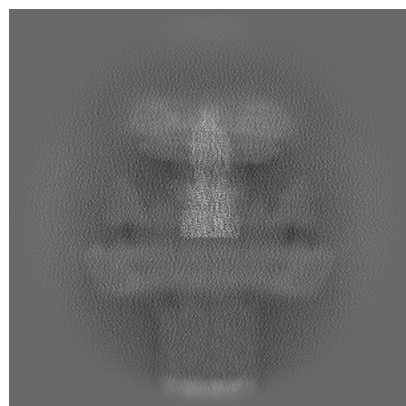
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39780. These allow visual inspection of the internal detail of the map and identification of artifacts.

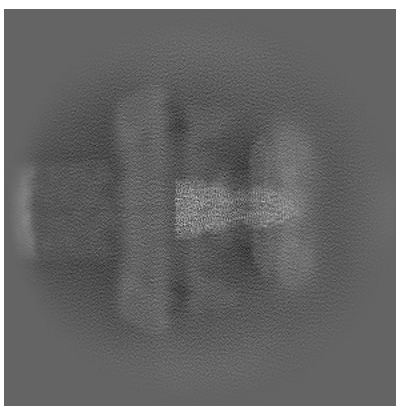
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

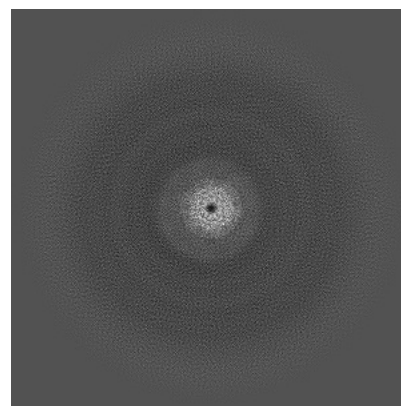
6.1.1 Primary map



X

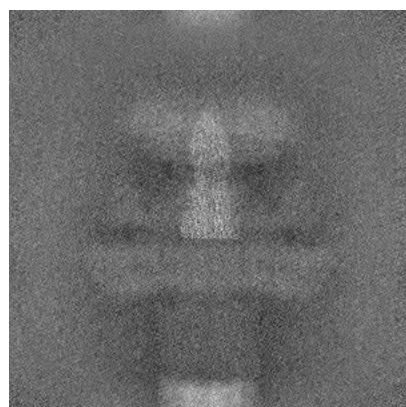


Y

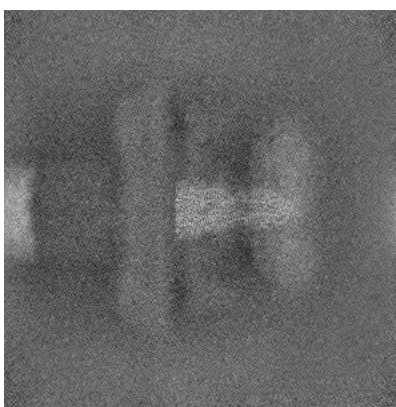


Z

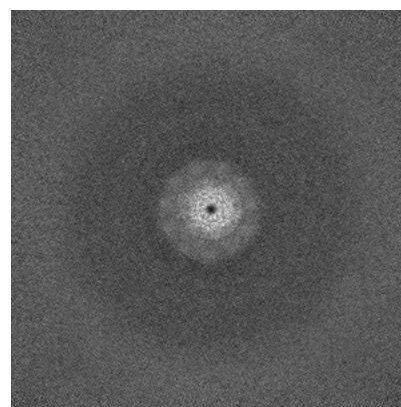
6.1.2 Raw map



X



Y

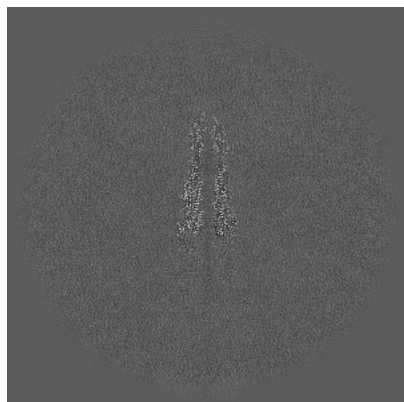


Z

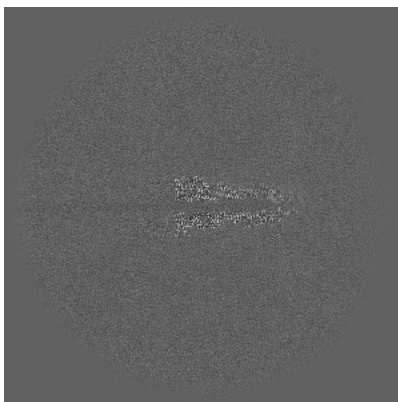
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

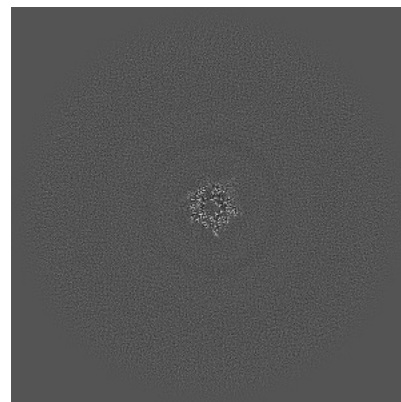
6.2.1 Primary map



X Index: 310

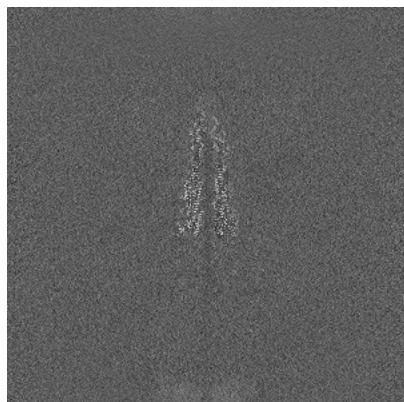


Y Index: 310

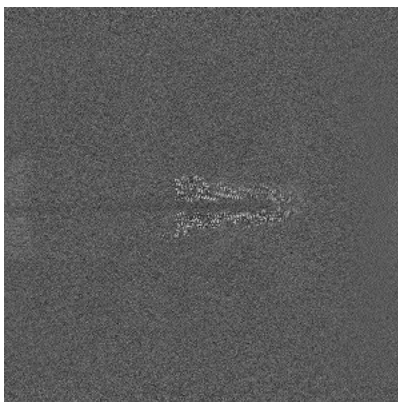


Z Index: 310

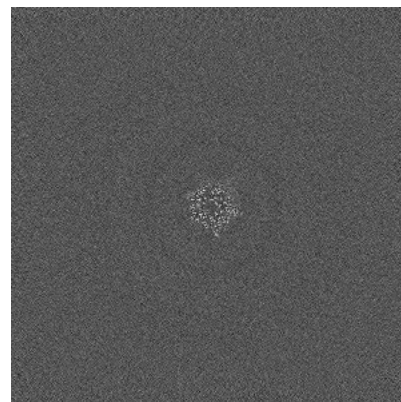
6.2.2 Raw map



X Index: 310



Y Index: 310

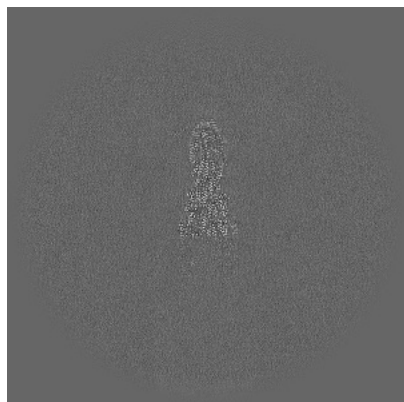


Z Index: 310

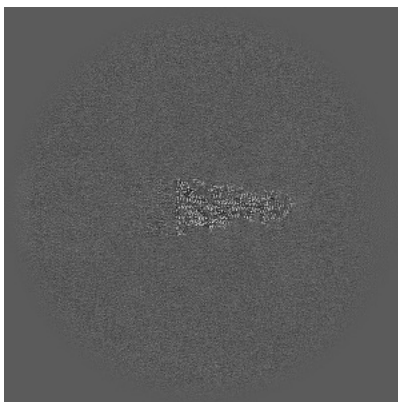
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

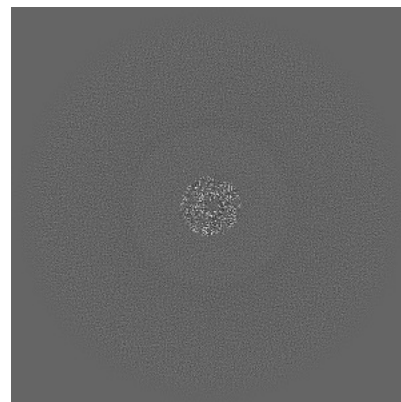
6.3.1 Primary map



X Index: 297

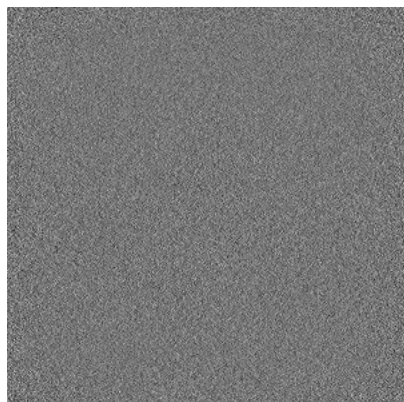


Y Index: 296

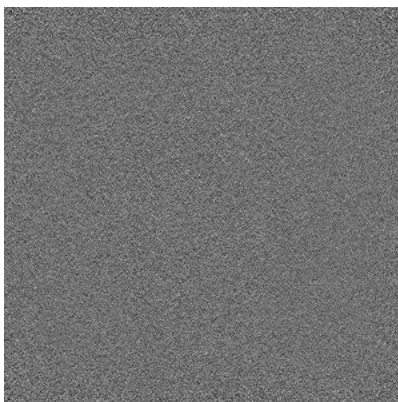


Z Index: 276

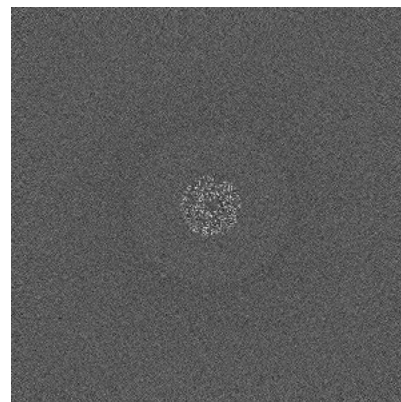
6.3.2 Raw map



X Index: 0



Y Index: 0

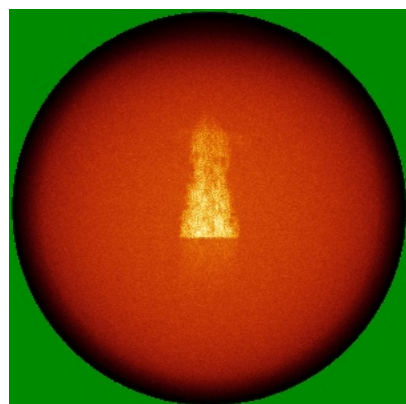


Z Index: 276

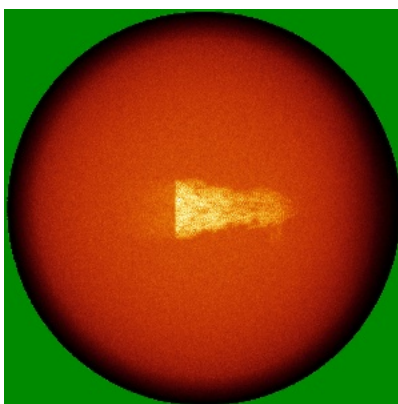
The images above show the largest variance slices of the map in three orthogonal directions.

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

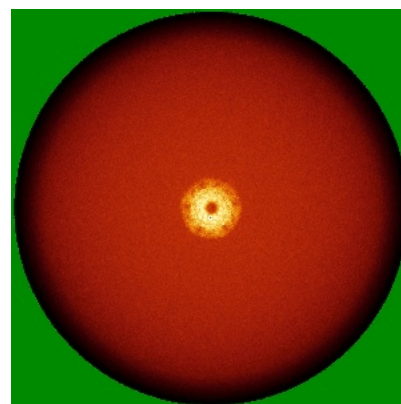
6.4.1 Primary map



X

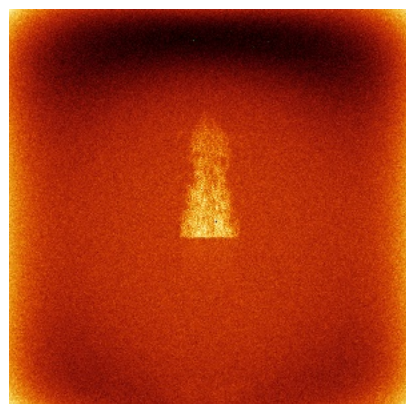


Y

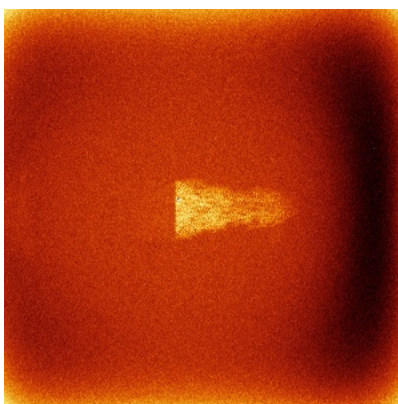


Z

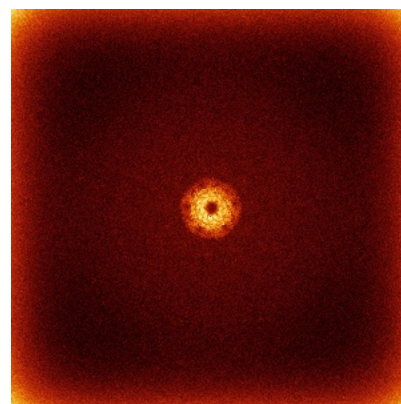
6.4.2 Raw map



X



Y

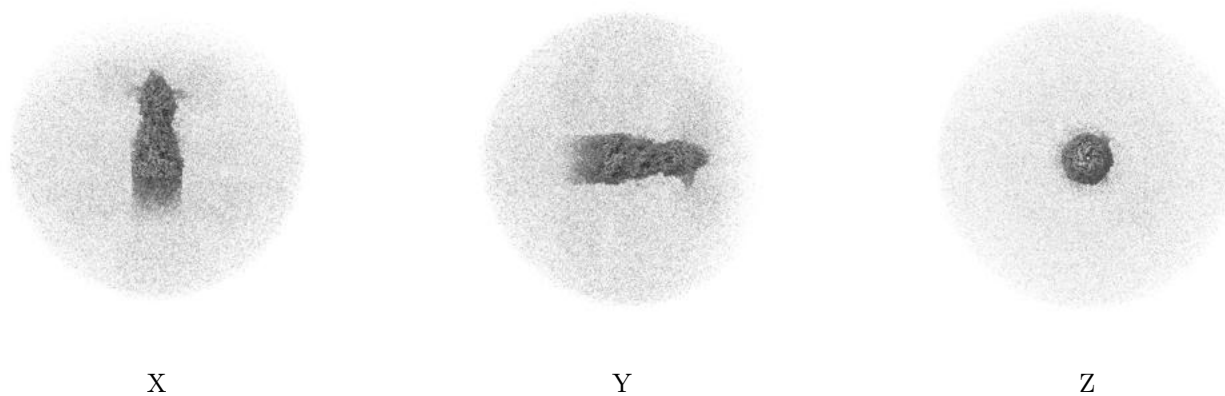


Z

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

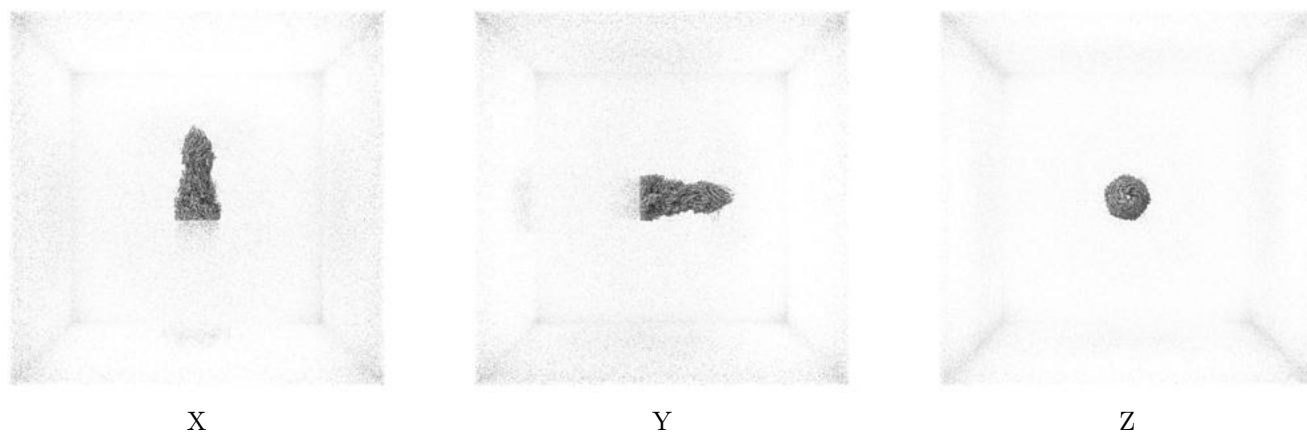
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

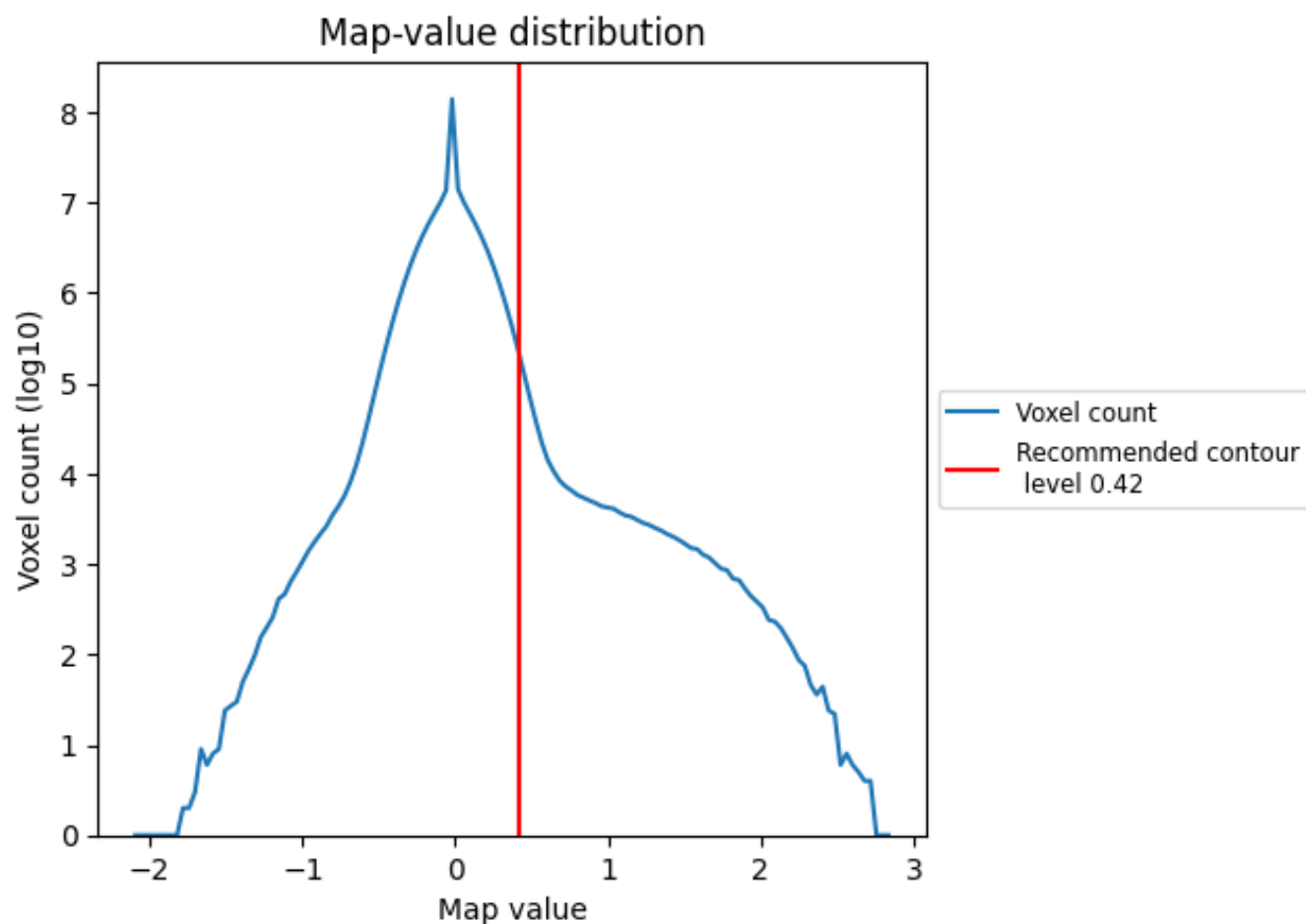
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

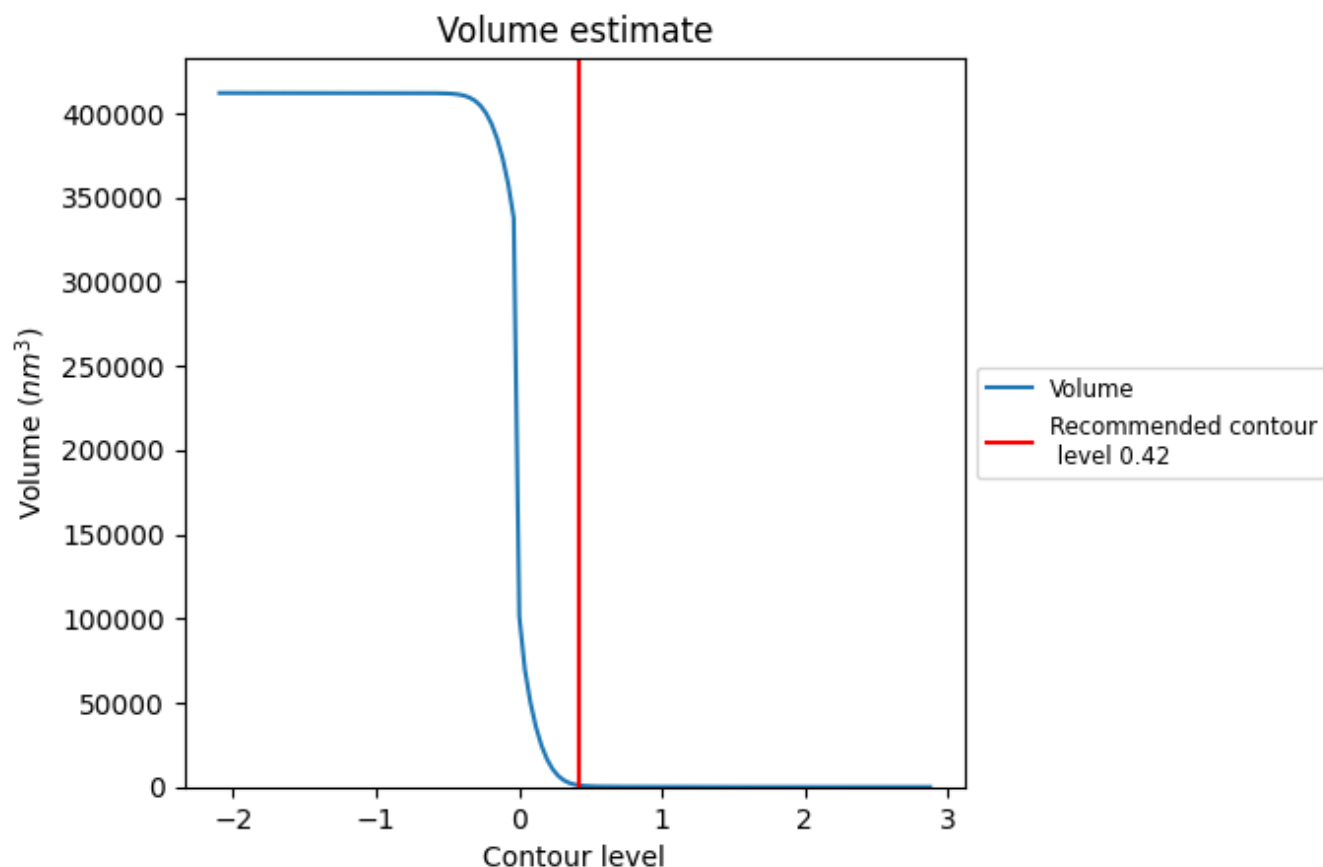
This section contains the results of statistical analysis of the map.

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.

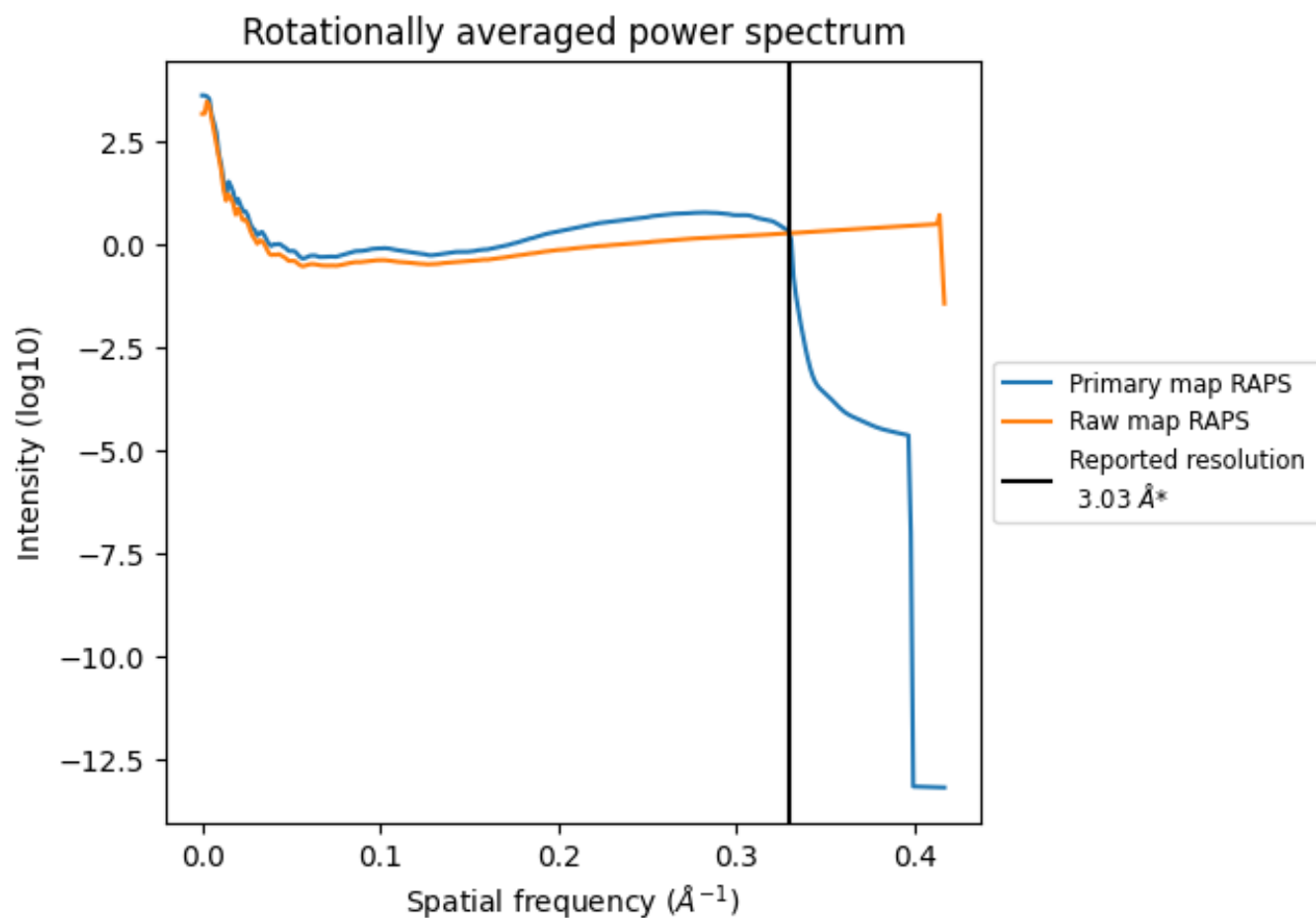
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 972 nm^3 ; this corresponds to an approximate mass of 878 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 ⓘ

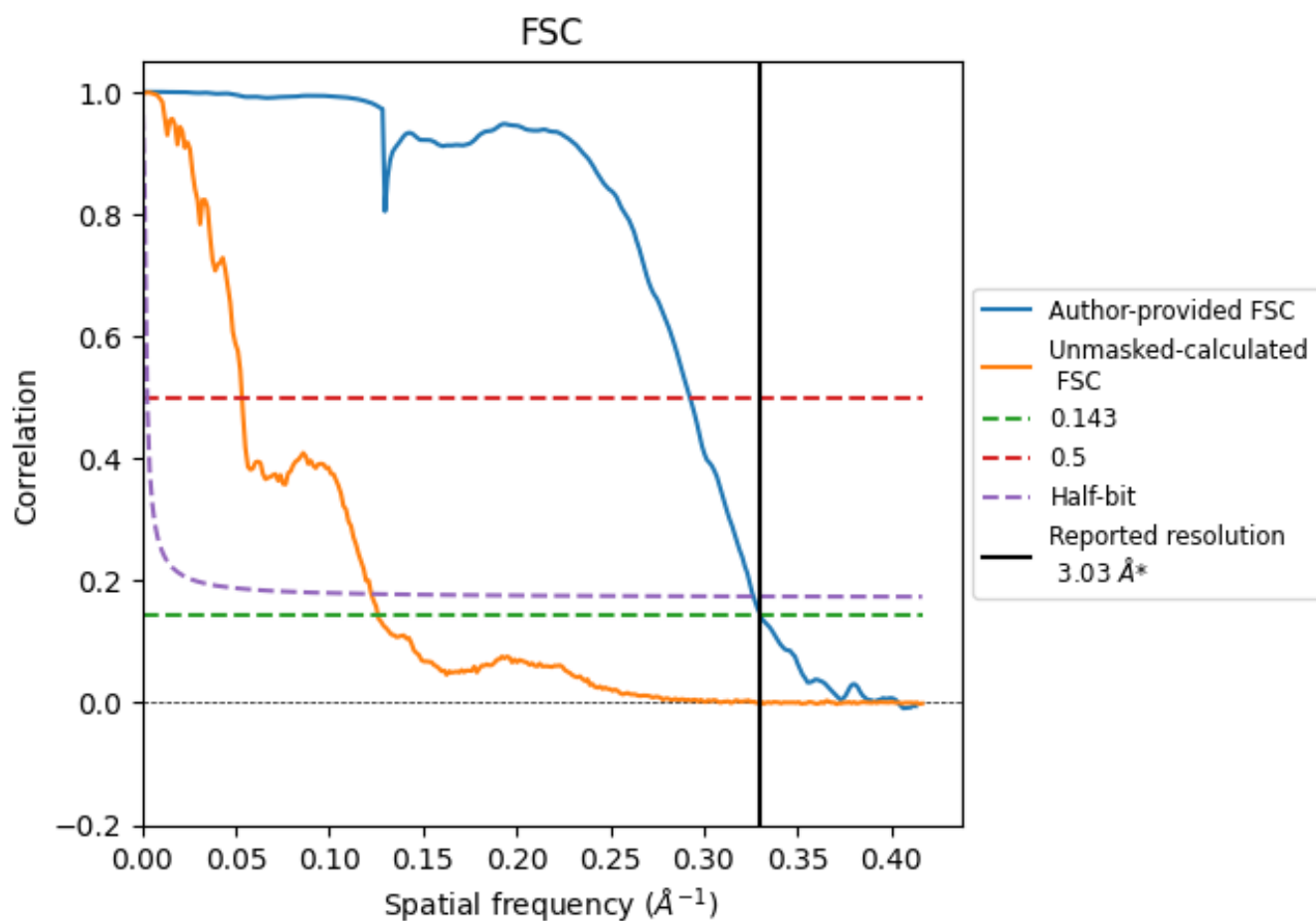


*Reported resolution corresponds to spatial frequency of 0.330 $\text{\AA}^{-1}$

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 0.330 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

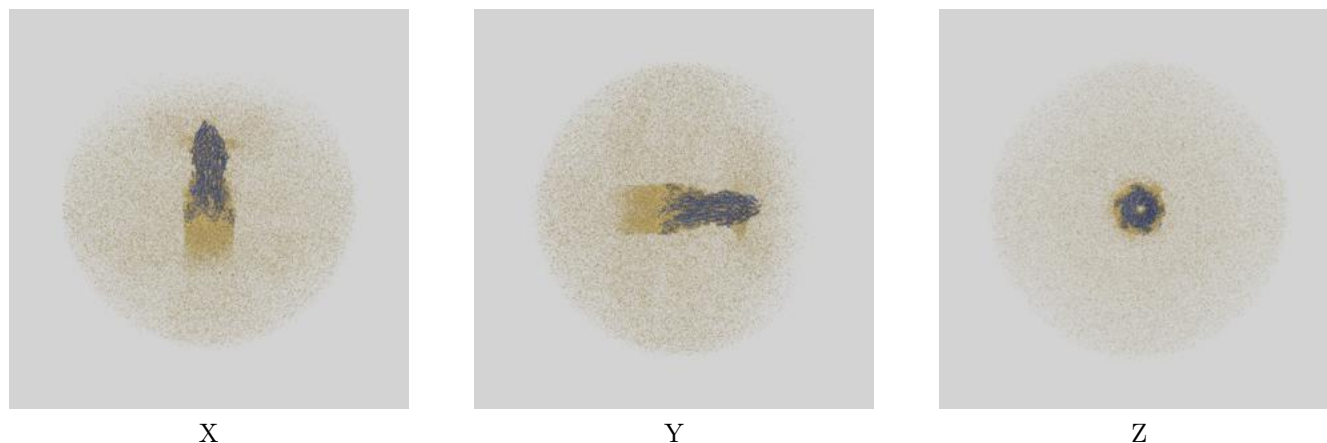
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.42	3.06
Unmasked-calculated*	7.94	18.76	8.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.94 differs from the reported value 3.03 by more than 10 %

9 Map-model fit [i](#)

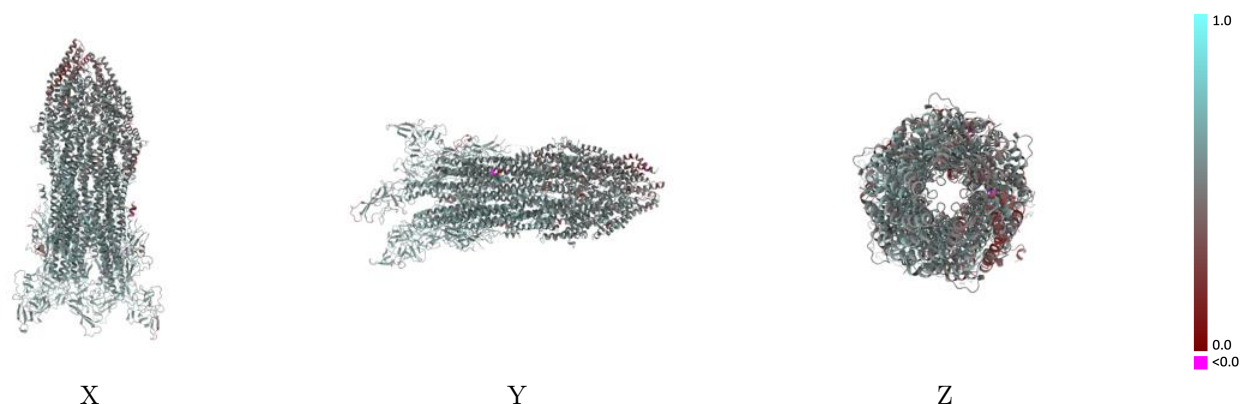
This section contains information regarding the fit between EMDB map EMD-39780 and PDB model 8Z5S. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



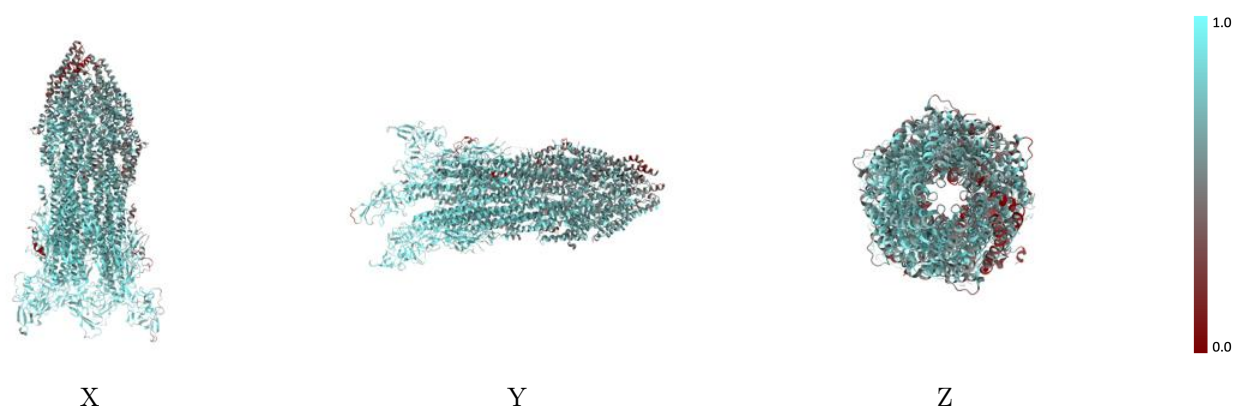
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



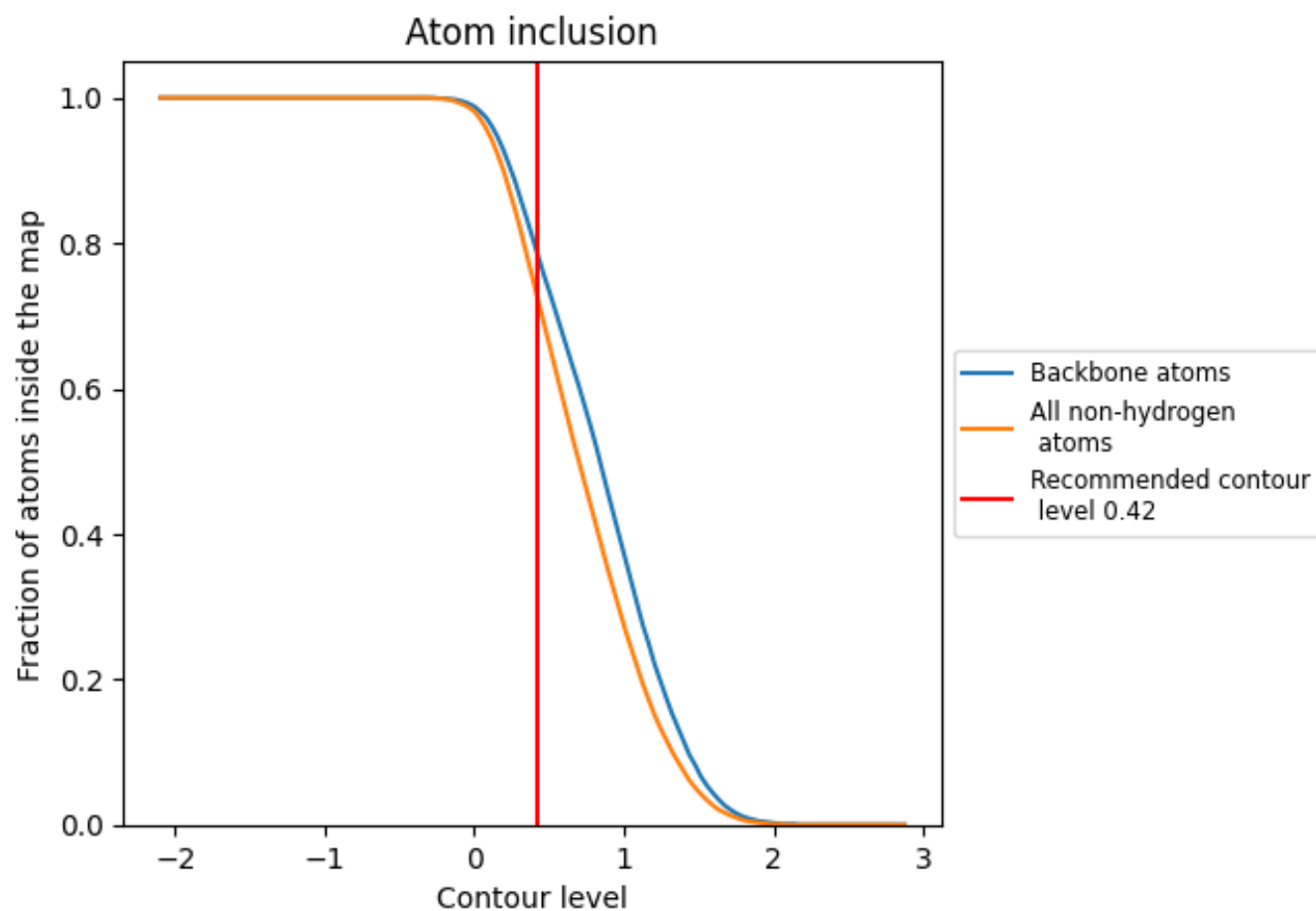
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7270	 0.5310
1	 0.6080	 0.4950
2	 0.6940	 0.5170
3	 0.6770	 0.5050
4	 0.5410	 0.4620
5	 0.6410	 0.4880
6	 0.5880	 0.4760
7	 0.6130	 0.4910
8	 0.6090	 0.4830
AA	 0.7330	 0.5090
AB	 0.7780	 0.5510
AC	 0.7700	 0.5490
AD	 0.7560	 0.5690
AE	 0.6220	 0.5130
AF	 0.3990	 0.4030
AG	 0.7940	 0.5320
AH	 0.7940	 0.5470
AI	 0.6850	 0.4850
AJ	 0.3370	 0.4000
AK	 0.7340	 0.5370
AL	 0.6640	 0.4930
AM	 0.6920	 0.5050
AN	 0.7720	 0.5490
AO	 0.7730	 0.5520
b	 0.7970	 0.5610
c	 0.7330	 0.5200
d	 0.7890	 0.5640
e	 0.8110	 0.5720
f	 0.8190	 0.5720
g	 0.7630	 0.5440
h	 0.8030	 0.5560
i	 0.7700	 0.5380
j	 0.8250	 0.5670
k	 0.8220	 0.5600
l	 0.8060	 0.5550



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Chain	Atom inclusion	Q-score
m	 0.8210	 0.5650
n	 0.7430	 0.5330
o	 0.8120	 0.5620
p	 0.8090	 0.5610
q	 0.7740	 0.5480
r	 0.7330	 0.5470
s	 0.6670	 0.5070
t	 0.6880	 0.5290
u	 0.7480	 0.5500
v	 0.7400	 0.5560
w	 0.7480	 0.5480
x	 0.2790	 0.3340
y	 0.7330	 0.5340
z	 0.7410	 0.5360