



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:30 AM UTC

PDB ID : 6DUZ / pdb_00006duz
EMDB ID : EMD-8913
Title : Structure of the periplasmic domains of PrgH and PrgK from the assembled Salmonella type III secretion injectisome needle complex
Authors : Hu, J.; Worrall, L.J.; Vuckovic, M.; Atkinson, C.E.; Strynadka, N.C.J.
Deposited on : 2018-06-22
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

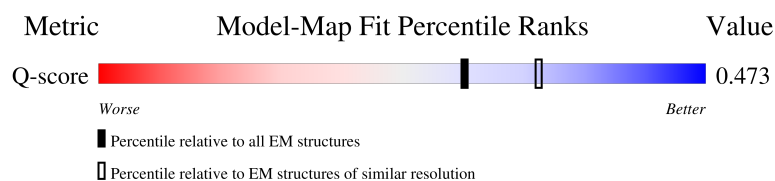
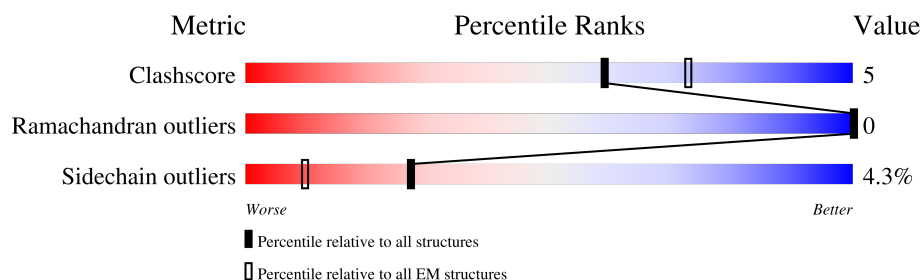
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



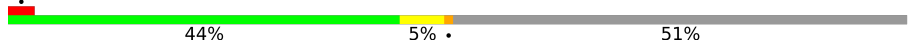
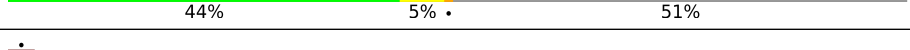
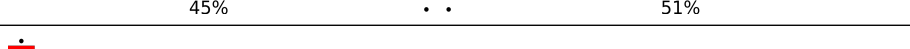
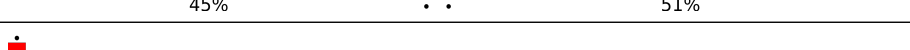
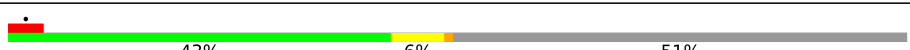
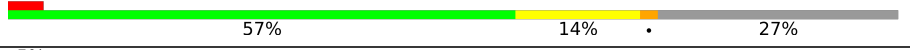
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	A	392	 44% 5% 51%
1	B	392	 45% 5% 51%
1	C	392	 45% 5% 51%
1	D	392	 45% 5% 51%

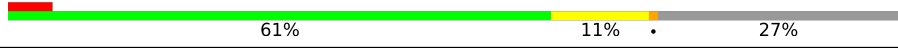
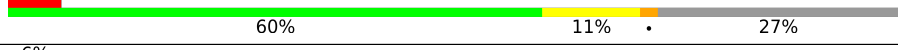
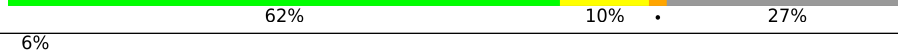
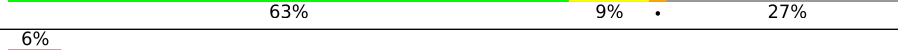
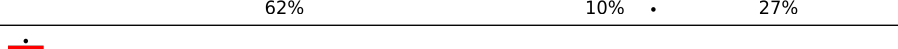
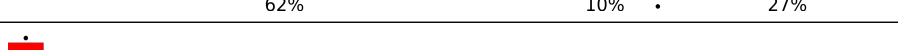
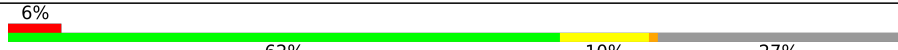
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Mol	Chain	Length	Quality of chain
1	E	392	
1	F	392	
1	G	392	
1	H	392	
1	I	392	
1	J	392	
1	K	392	
1	L	392	
1	M	392	
1	N	392	
1	O	392	
1	P	392	
1	Q	392	
1	R	392	
1	S	392	
1	T	392	
1	U	392	
1	V	392	
1	W	392	
1	X	392	
2	Y	252	
2	Z	252	
2	a	252	
2	b	252	
2	c	252	

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Mol	Chain	Length	Quality of chain
2	d	252	
2	e	252	
2	f	252	
2	g	252	
2	h	252	
2	i	252	
2	j	252	
2	k	252	
2	l	252	
2	m	252	
2	n	252	
2	o	252	
2	p	252	
2	q	252	
2	r	252	
2	s	252	
2	t	252	
2	u	252	
2	v	252	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 72744 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 Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	B	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	C	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	D	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	E	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	F	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	G	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	H	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	I	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	J	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	K	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	L	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	M	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	N	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	O	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	P	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
1	Q	194	Total 1600	C 1011	N 288	O 297	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
1	S	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
1	T	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
1	U	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
1	V	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
1	W	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
1	X	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		

- Molecule 2 is a protein called Lipoprotein PrgK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	Z	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	a	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	b	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	c	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	d	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	e	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	f	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	g	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	h	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	i	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		
2	j	184	Total	C	N	O	S	0	0
			1431	901	250	277	3		

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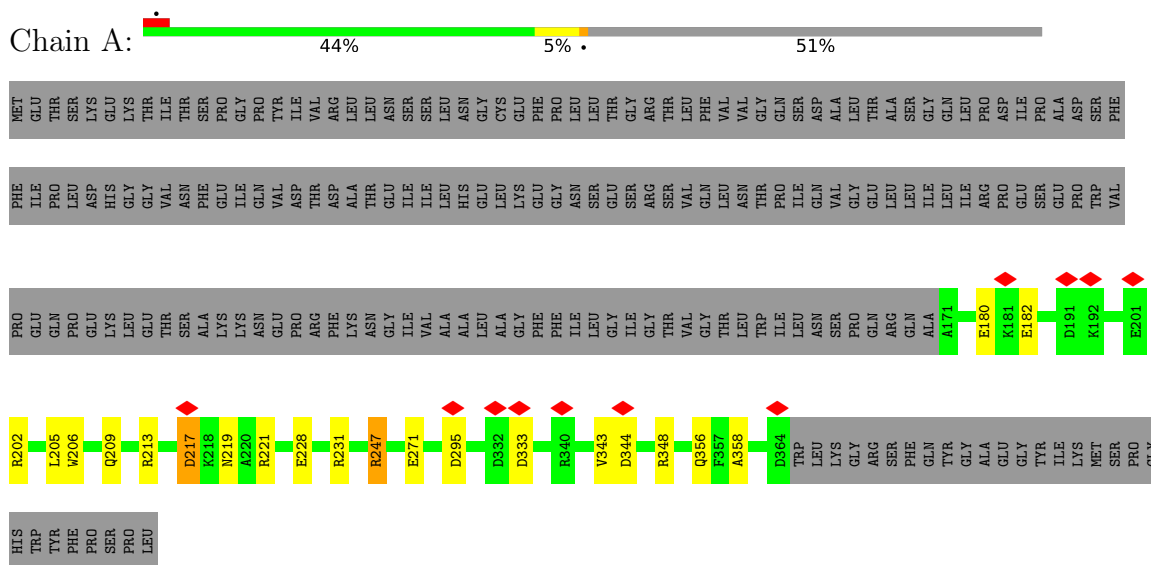
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	l	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	m	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	n	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	o	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	p	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	q	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	r	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	s	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	t	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	u	184	Total 1431	C 901	N 250	O 277	S 3	0	0
2	v	184	Total 1431	C 901	N 250	O 277	S 3	0	0

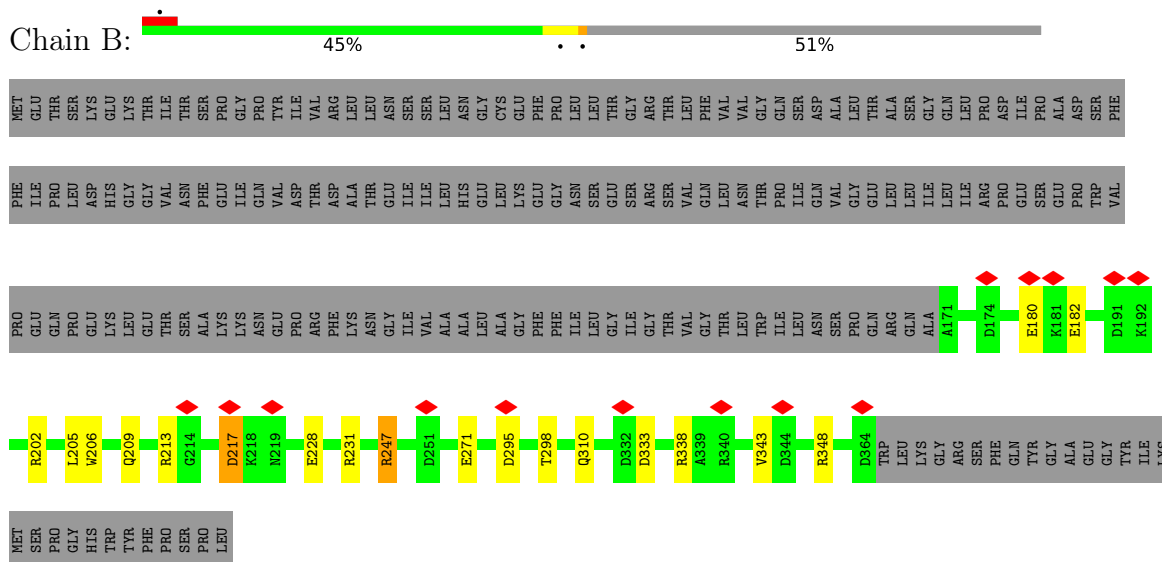
3 Residue-property plots

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: Protein PrgH



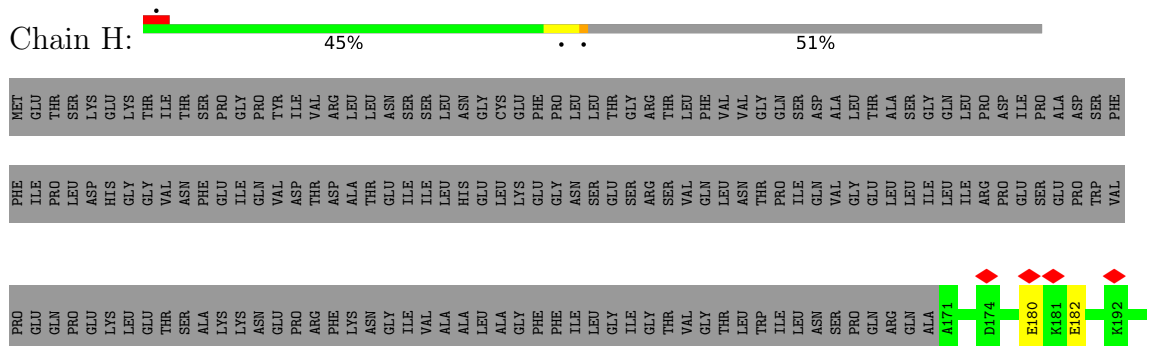
• Molecule 1: Protein PrgH

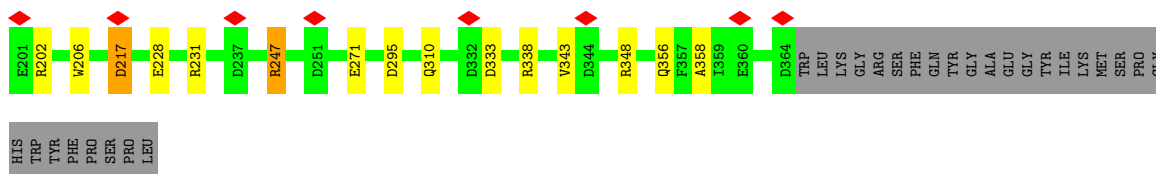


Chain C: 45% 51%

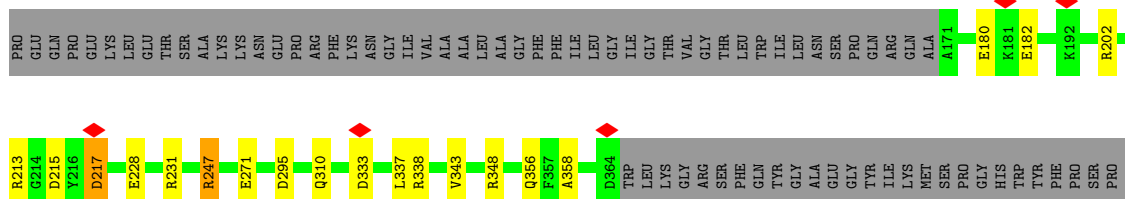
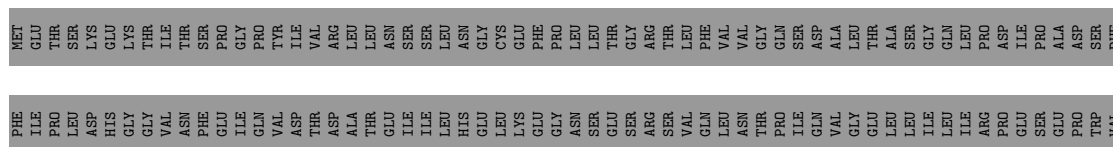


Chain F:

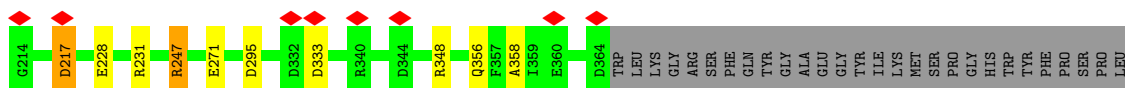
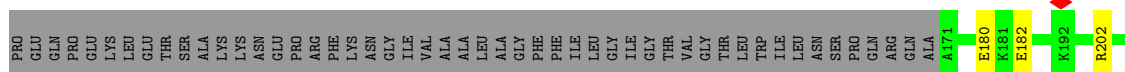
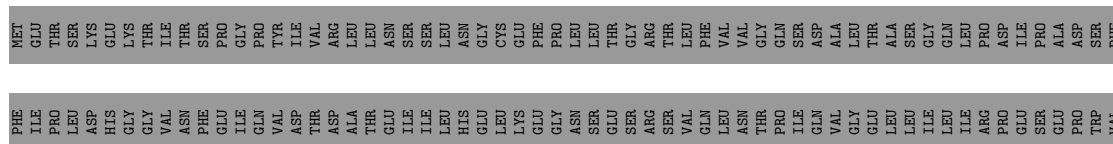




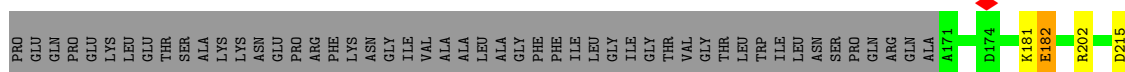
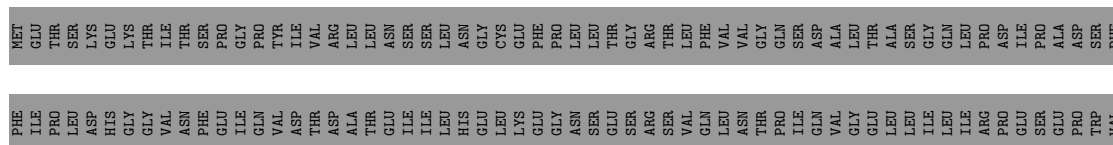
- Molecule 1: Protein PrgH

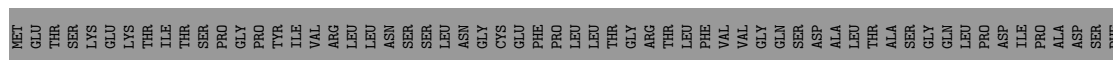


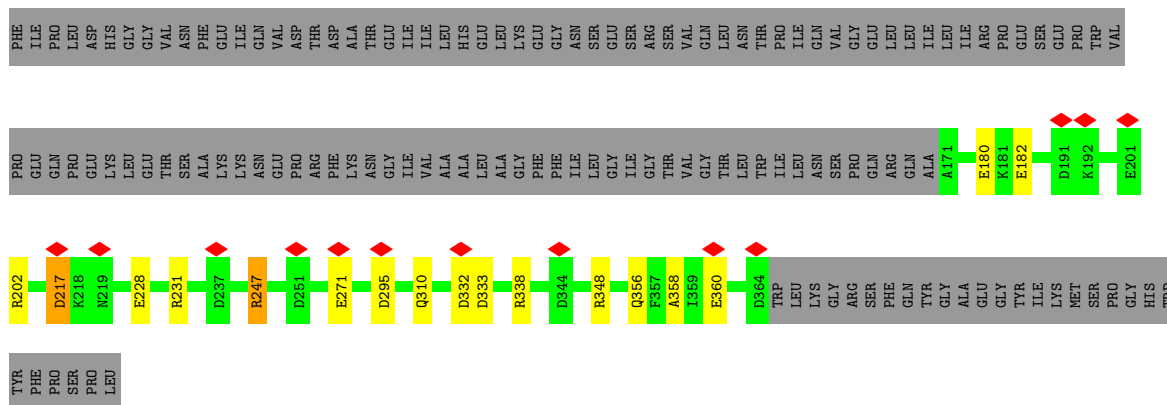
- Molecule 1: Protein PrgH



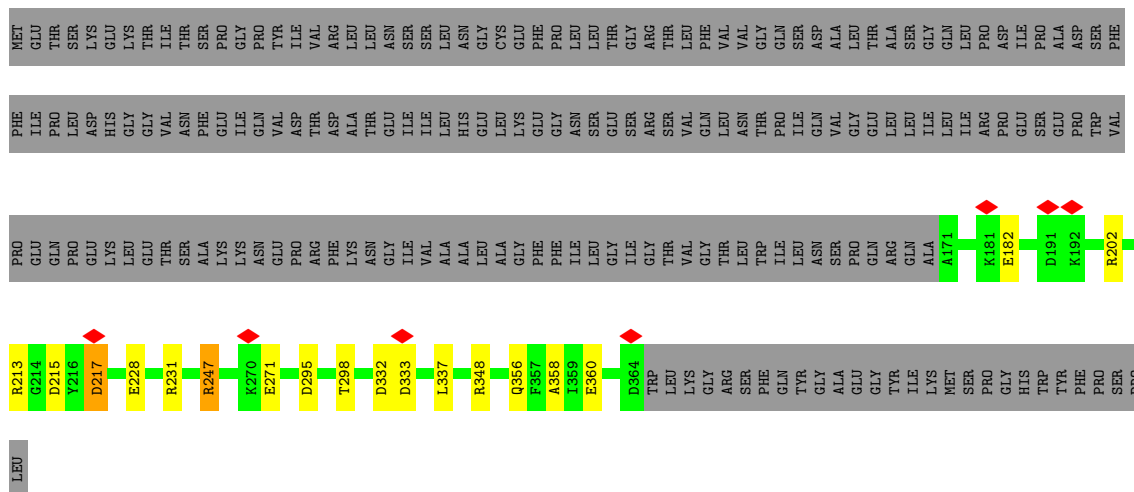
- Molecule 1: Protein PrgH



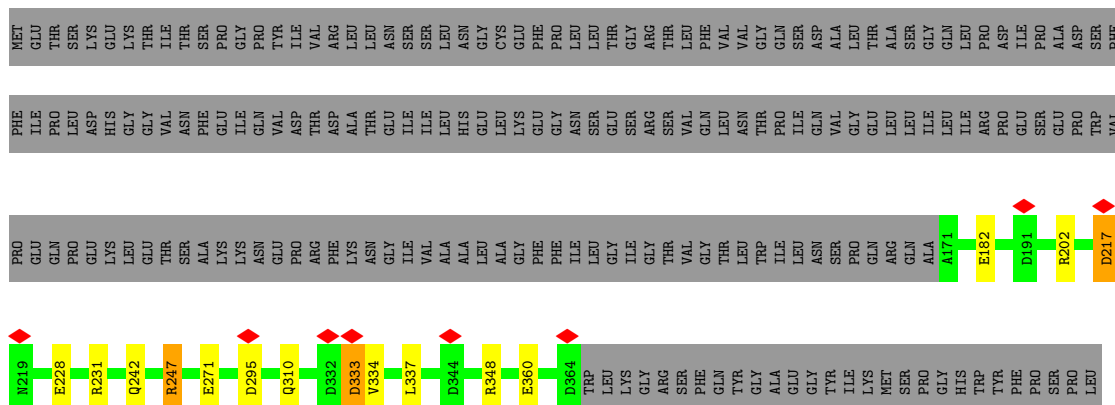




- Molecule 1: Protein PrgH



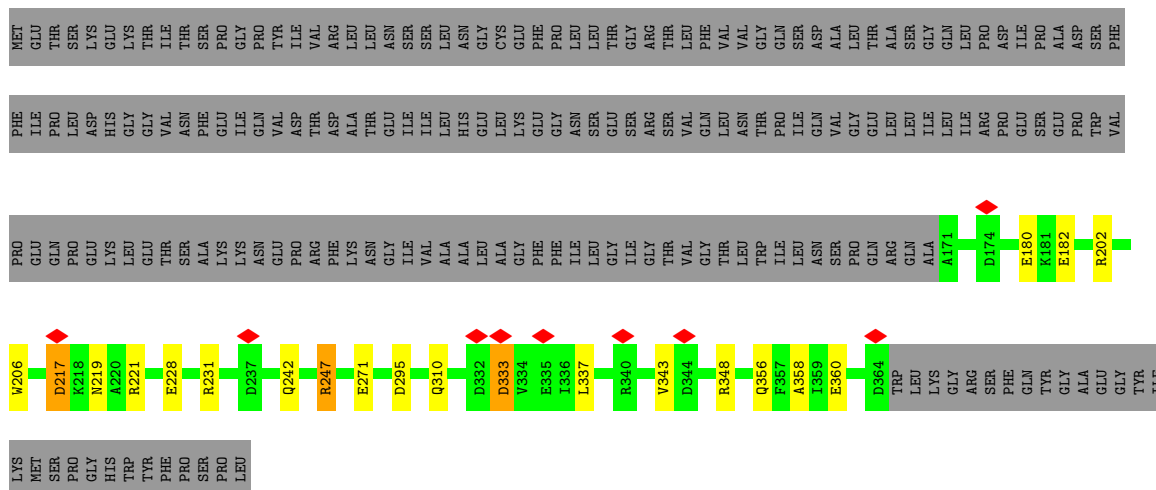
- Molecule 1: Protein PrgH



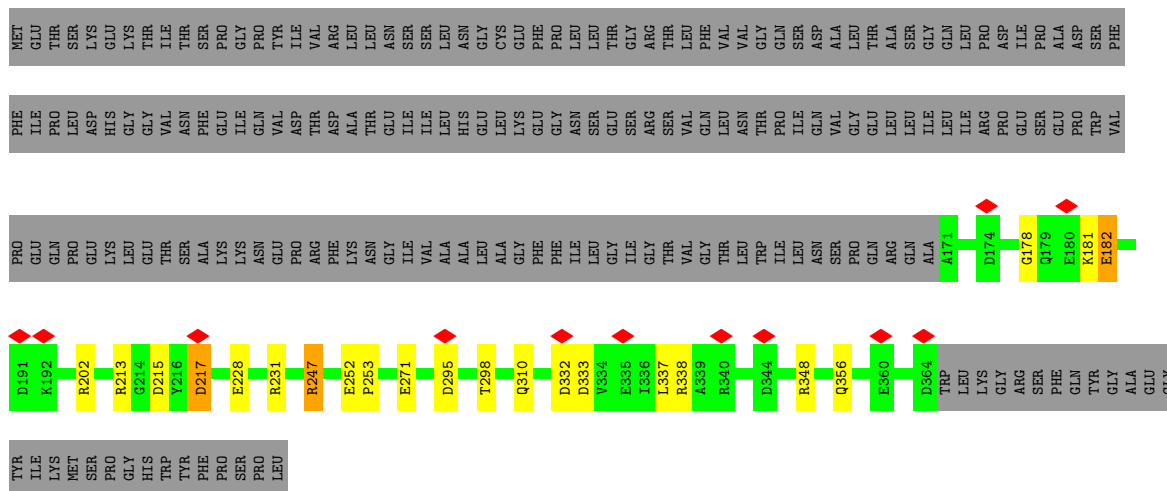
- Molecule 1: Protein PrgH



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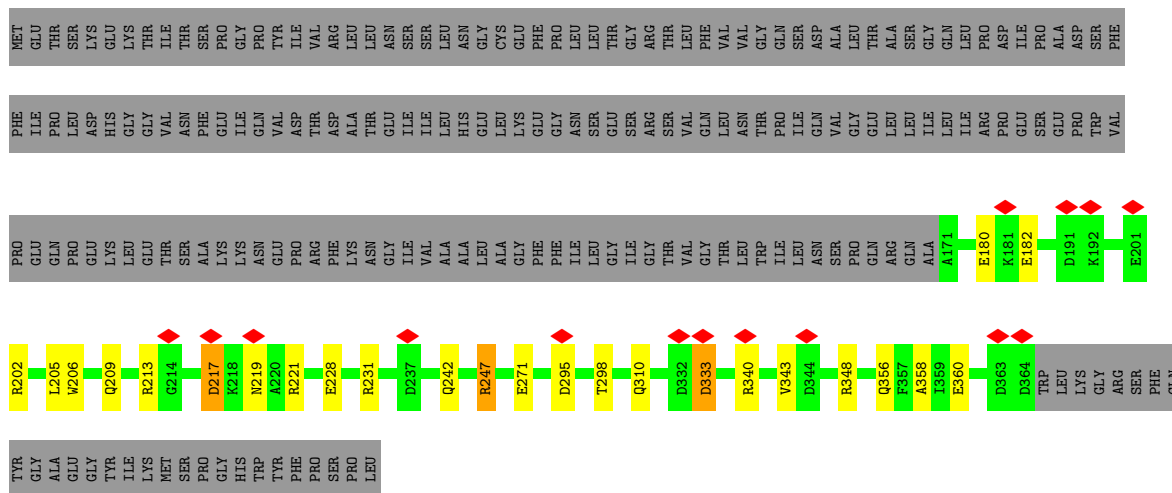


- Molecule 1: Protein PrgH

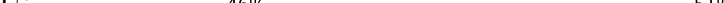


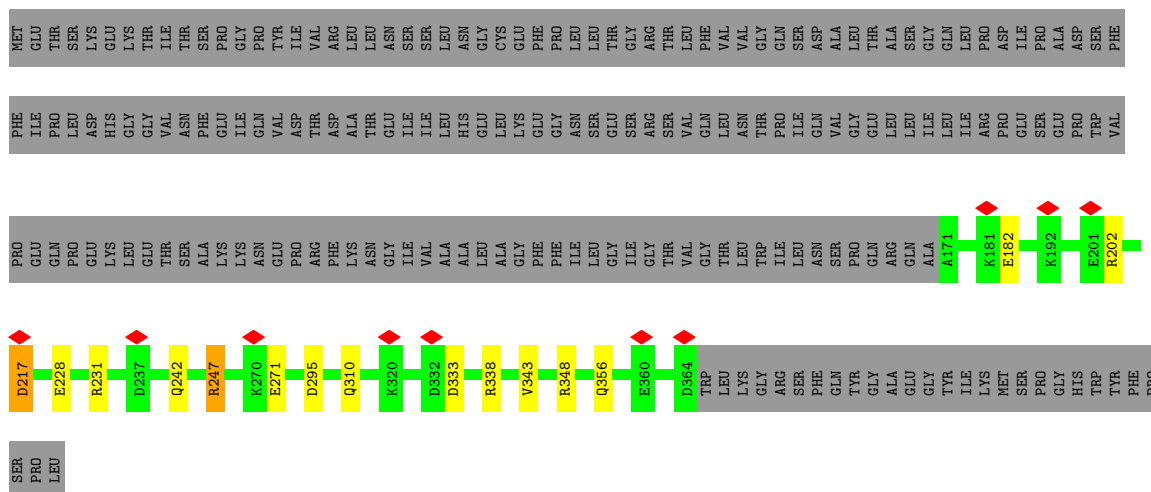
- Molecule 1: Protein PrgH

Chain T: 43% 6% 51%

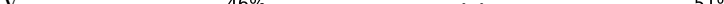


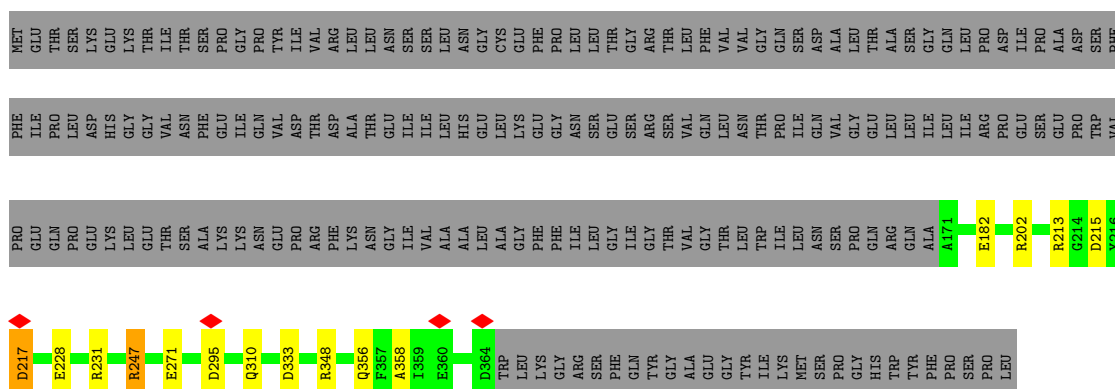
- Molecule 1: Protein PrgH

Chain U:  46% 51%

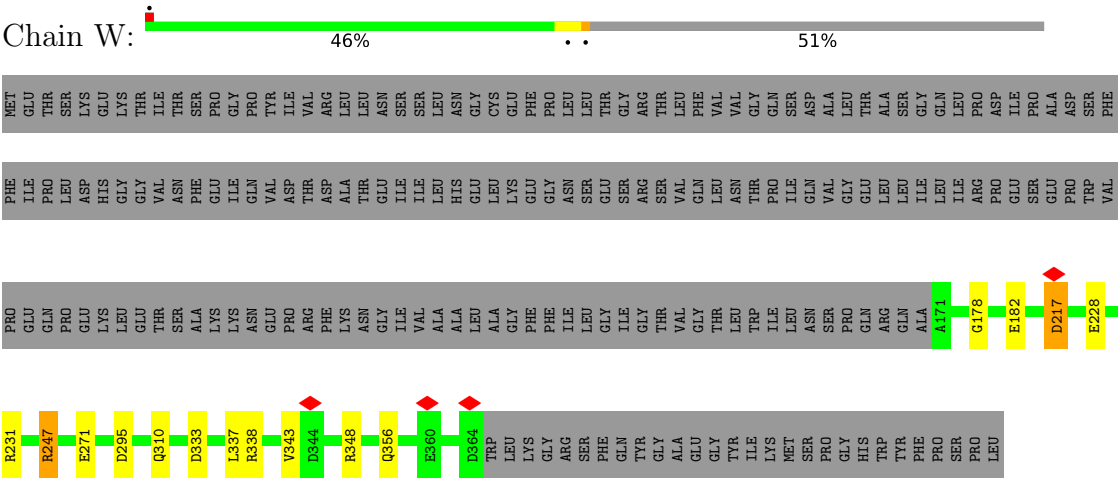


- Molecule 1: Protein PrgH

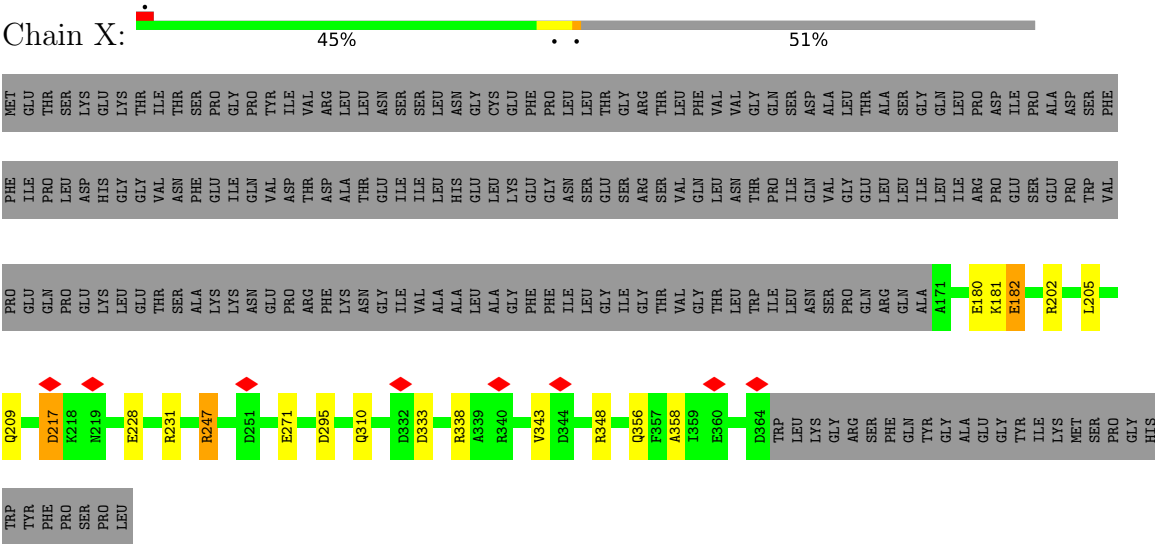
Chain V:  46% 51%



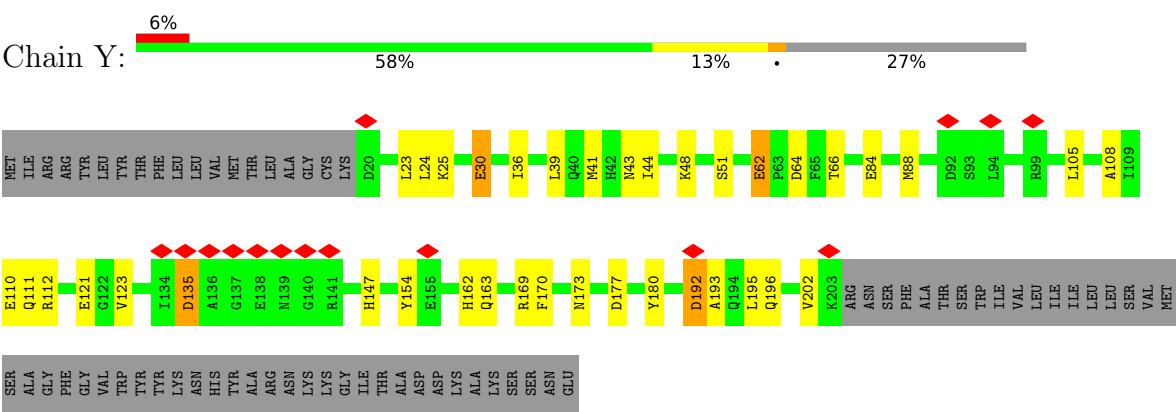
• Molecule 1: Protein PrgH



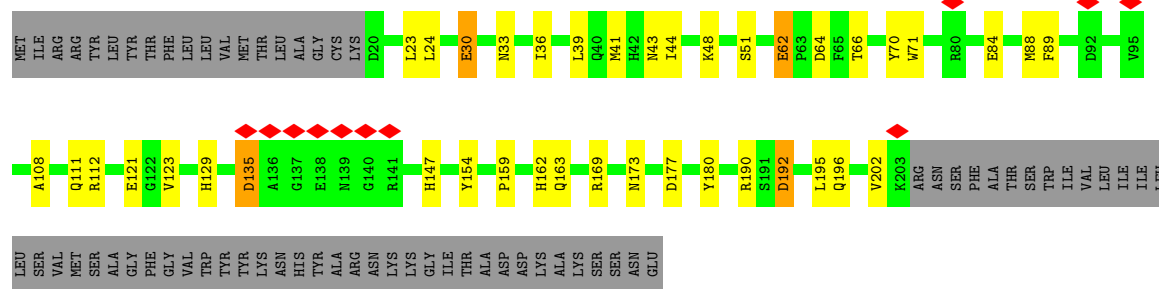
• Molecule 1: Protein PrgH



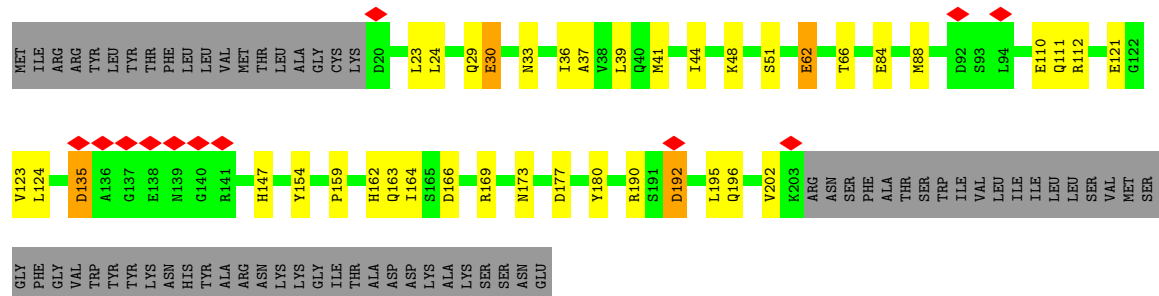
• Molecule 2: Lipoprotein PrgK



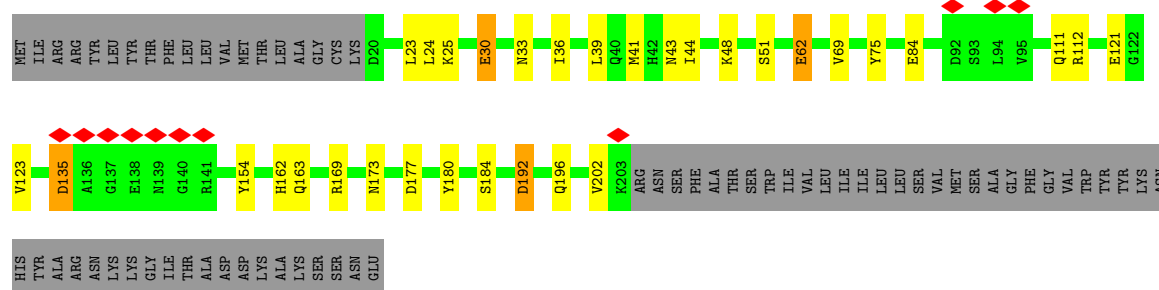
• Molecule 2: Lipoprotein PrgK



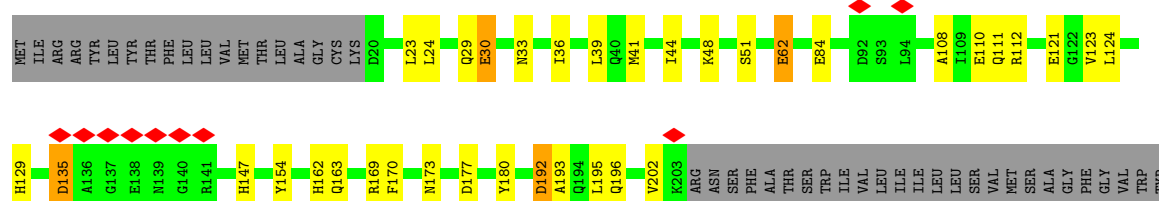
• Molecule 2: Lipoprotein PrgK



• Molecule 2: Lipoprotein PrgK



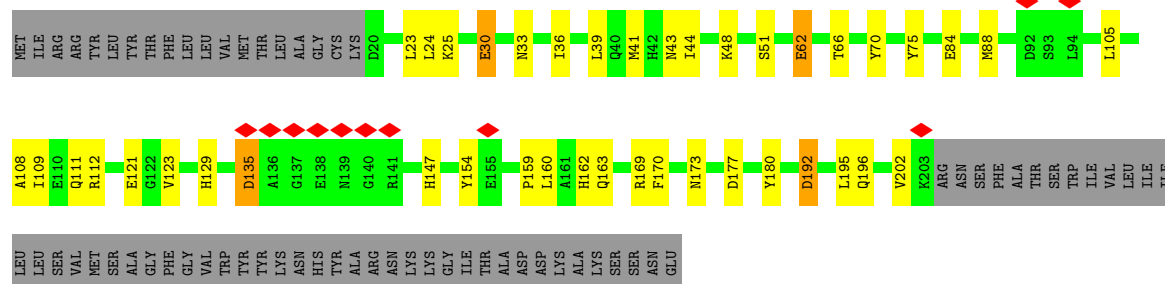
• Molecule 2: Lipoprotein PrgK



TYR
LYS
ASN
HIS
TYR
ALA
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
GLY
ALA
LYS
SER
SER
ASN
GLU

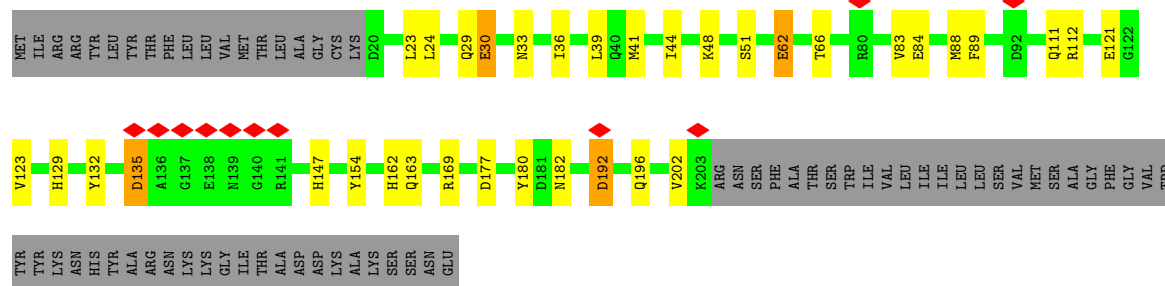
• Molecule 2: Lipoprotein PrgK

Chain d:



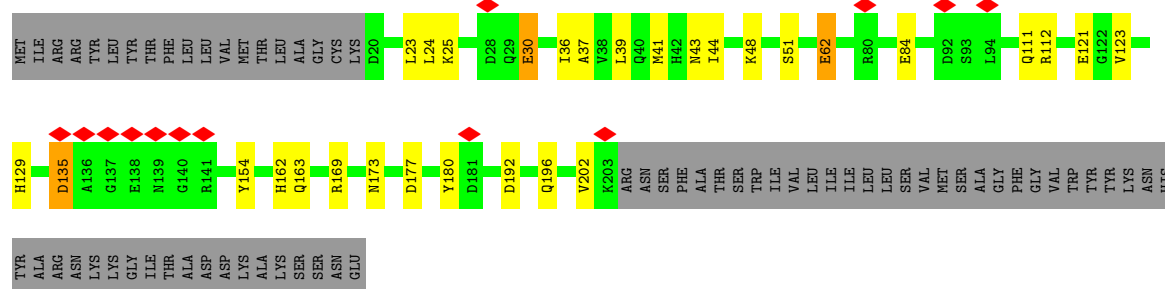
• Molecule 2: Lipoprotein PrgK

Chain e:



• Molecule 2: Lipoprotein PrgK

Chain f:

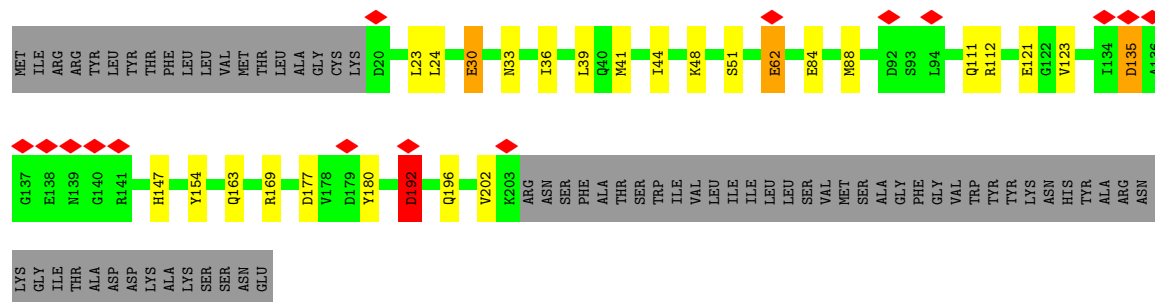


• Molecule 2: Lipoprotein PrgK

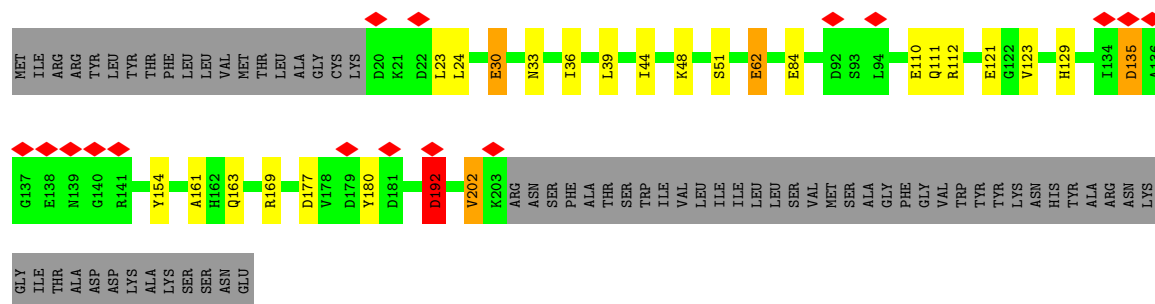
Chain g:



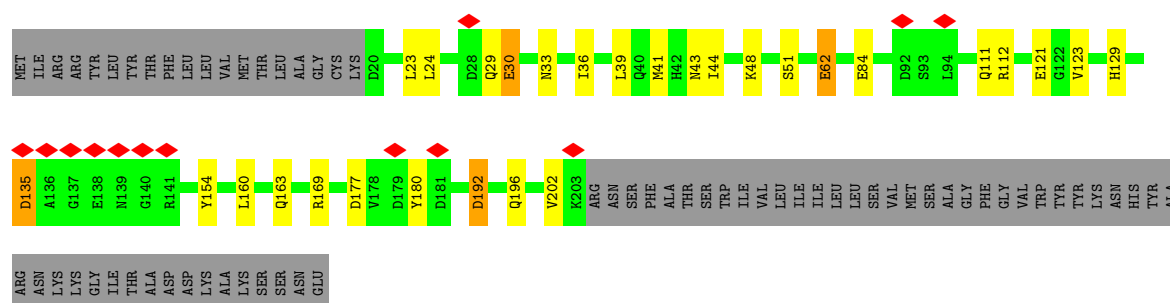
- Molecule 2: Lipoprotein PrgK



- Molecule 2: Lipoprotein PrgK

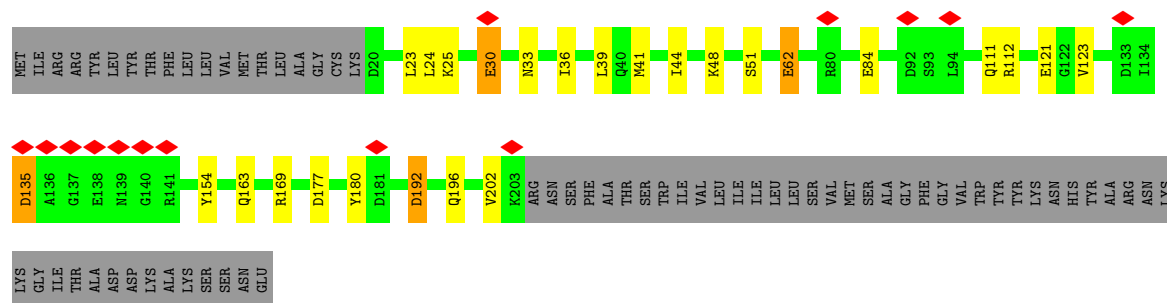


- Molecule 2: Lipoprotein PrgK



- Molecule 2: Lipoprotein PrgK





• Molecule 2: Lipoprotein PrgK



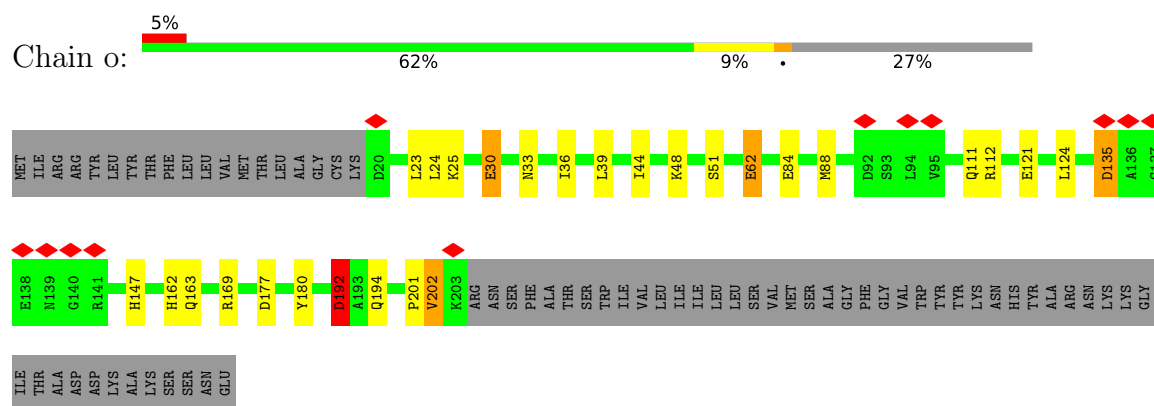
• Molecule 2: Lipoprotein PrgK



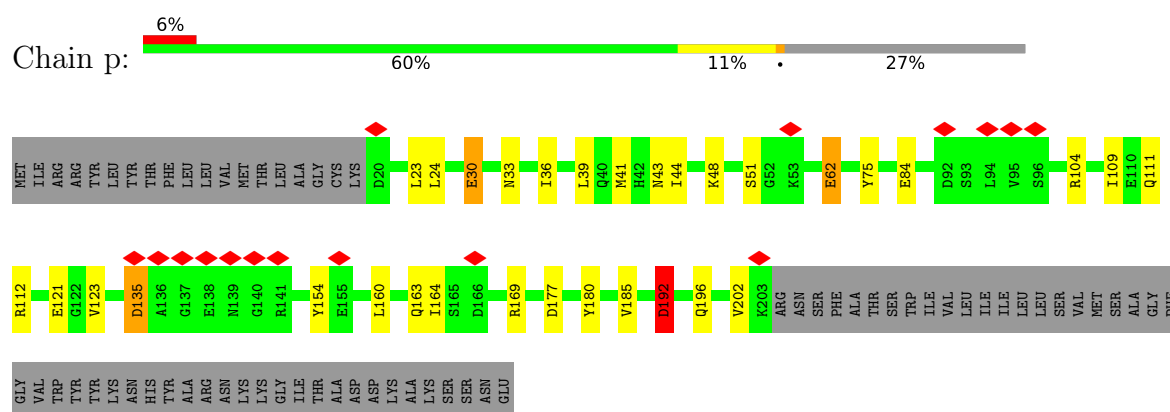
• Molecule 2: Lipoprotein PrgK



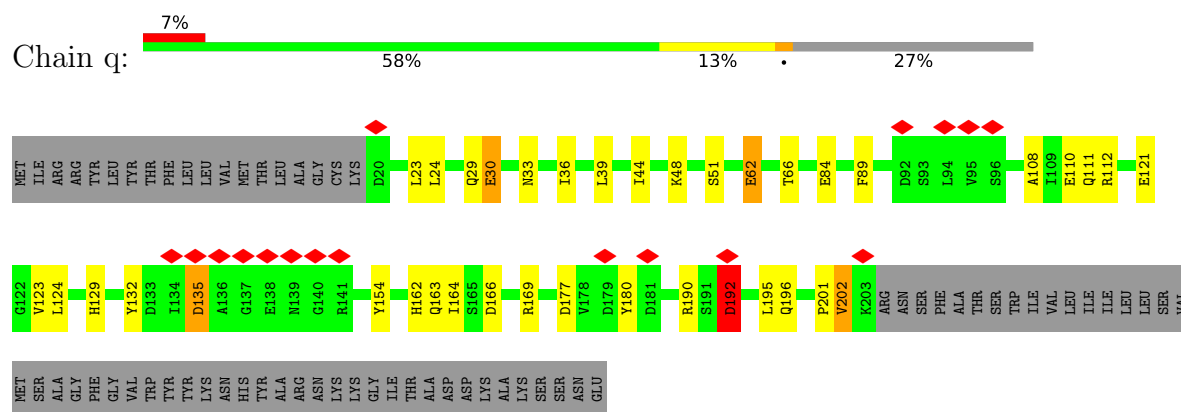
• Molecule 2: Lipoprotein PrgK



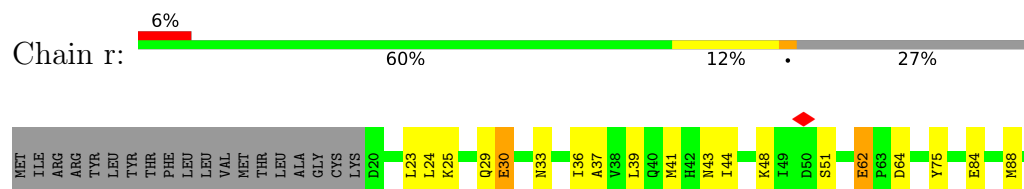
• Molecule 2: Lipoprotein PrgK

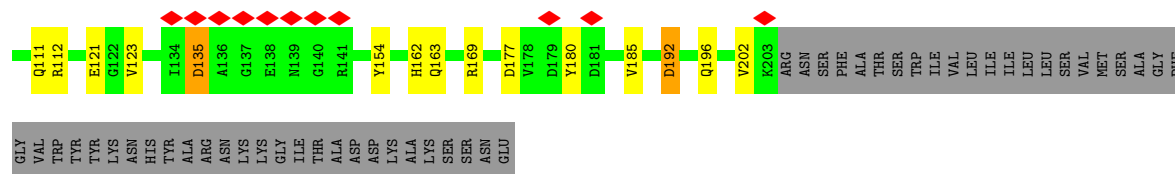


• Molecule 2: Lipoprotein PrgK

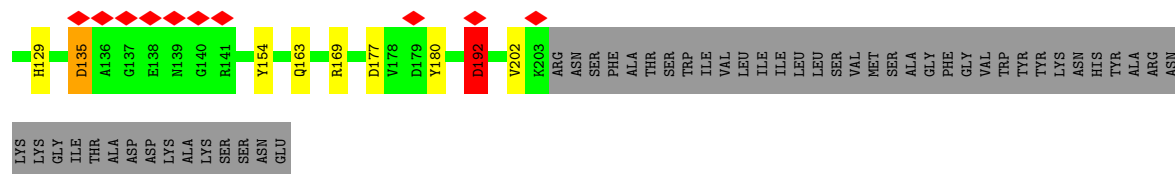


• Molecule 2: Lipoprotein PrgK

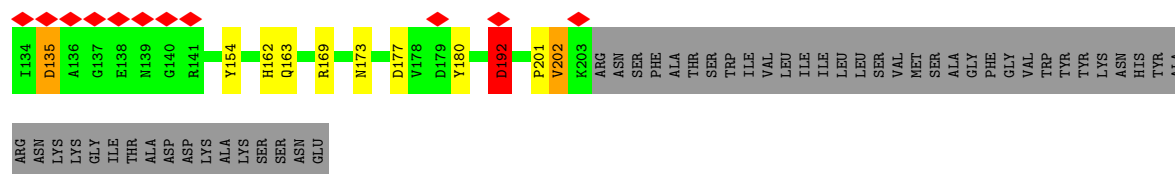




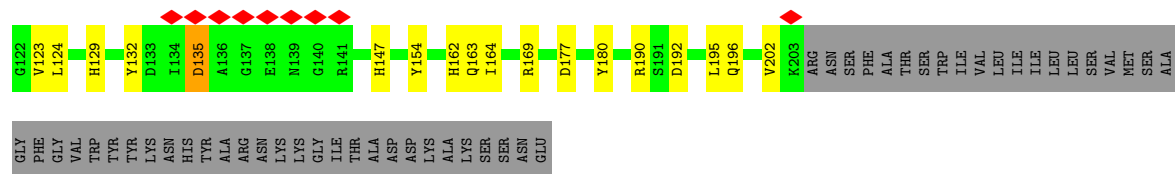
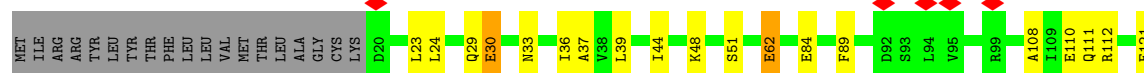
• Molecule 2: Lipoprotein PrgK



• Molecule 2: Lipoprotein PrgK

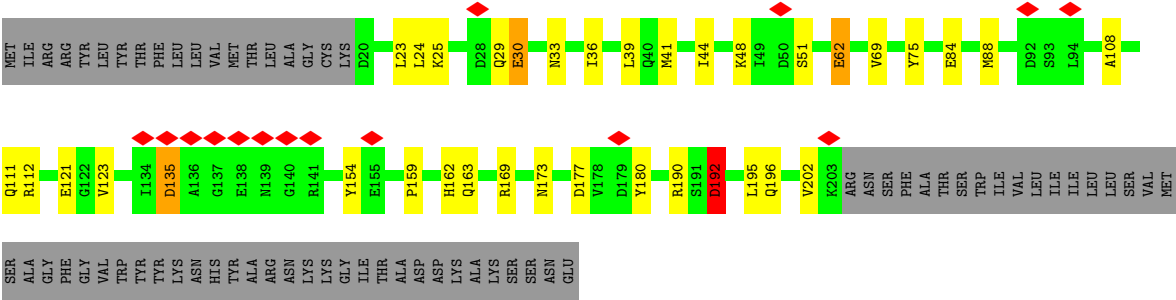


• Molecule 2: Lipoprotein PrgK



• Molecule 2: Lipoprotein PrgK





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C24	Depositor
Number of particles used	58000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.448	Depositor
Minimum map value	-0.905	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	525.0, 525.0, 525.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.75, 1.75, 1.75	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	A	0.26	0/1632	0.54	0/2204
1	B	0.26	0/1632	0.54	0/2204
1	C	0.26	0/1632	0.54	0/2204
1	D	0.26	0/1632	0.54	0/2204
1	E	0.26	0/1632	0.54	0/2204
1	F	0.26	0/1632	0.54	0/2204
1	G	0.26	0/1632	0.54	0/2204
1	H	0.26	0/1632	0.54	0/2204
1	I	0.26	0/1632	0.54	0/2204
1	J	0.26	0/1632	0.54	0/2204
1	K	0.26	0/1632	0.54	0/2204
1	L	0.26	0/1632	0.54	0/2204
1	M	0.26	0/1632	0.54	0/2204
1	N	0.26	0/1632	0.54	0/2204
1	O	0.26	0/1632	0.54	0/2204
1	P	0.26	0/1632	0.54	0/2204
1	Q	0.26	0/1632	0.54	0/2204
1	R	0.26	0/1632	0.54	0/2204
1	S	0.26	0/1632	0.54	0/2204
1	T	0.26	0/1632	0.54	0/2204
1	U	0.26	0/1632	0.54	0/2204
1	V	0.26	0/1632	0.54	0/2204
1	W	0.26	0/1632	0.54	0/2204
1	X	0.26	0/1632	0.54	0/2204
2	Y	0.29	0/1458	0.61	3/1979 (0.2%)
2	Z	0.29	0/1458	0.61	3/1979 (0.2%)
2	a	0.29	0/1458	0.60	3/1979 (0.2%)
2	b	0.29	0/1458	0.61	3/1979 (0.2%)
2	c	0.29	0/1458	0.61	3/1979 (0.2%)
2	d	0.29	0/1458	0.61	3/1979 (0.2%)
2	e	0.29	0/1458	0.60	3/1979 (0.2%)
2	f	0.29	0/1458	0.61	2/1979 (0.1%)
2	g	0.29	0/1458	0.61	2/1979 (0.1%)
2	h	0.29	0/1458	0.61	3/1979 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	i	0.29	0/1458	0.61	3/1979 (0.2%)
2	j	0.29	0/1458	0.61	3/1979 (0.2%)
2	k	0.29	0/1458	0.61	2/1979 (0.1%)
2	l	0.29	0/1458	0.61	3/1979 (0.2%)
2	m	0.29	0/1458	0.60	3/1979 (0.2%)
2	n	0.29	0/1458	0.61	3/1979 (0.2%)
2	o	0.29	0/1458	0.61	3/1979 (0.2%)
2	p	0.29	0/1458	0.61	3/1979 (0.2%)
2	q	0.29	0/1458	0.61	3/1979 (0.2%)
2	r	0.29	0/1458	0.61	3/1979 (0.2%)
2	s	0.29	0/1458	0.60	3/1979 (0.2%)
2	t	0.29	0/1458	0.61	3/1979 (0.2%)
2	u	0.29	0/1458	0.61	2/1979 (0.1%)
2	v	0.29	0/1458	0.61	3/1979 (0.2%)
All	All	0.28	0/74160	0.57	68/100392 (0.1%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	p	62	GLU	CA-CB-CG	5.78	125.66	114.10
2	r	62	GLU	CA-CB-CG	5.77	125.64	114.10
2	g	62	GLU	CA-CB-CG	5.76	125.62	114.10
2	k	62	GLU	CA-CB-CG	5.75	125.60	114.10
2	l	62	GLU	CA-CB-CG	5.75	125.60	114.10
2	Y	62	GLU	CA-CB-CG	5.75	125.59	114.10
2	a	62	GLU	CA-CB-CG	5.75	125.59	114.10
2	f	62	GLU	CA-CB-CG	5.75	125.59	114.10
2	b	62	GLU	CA-CB-CG	5.74	125.59	114.10
2	d	62	GLU	CA-CB-CG	5.74	125.58	114.10
2	e	62	GLU	CA-CB-CG	5.74	125.58	114.10
2	u	62	GLU	CA-CB-CG	5.74	125.58	114.10
2	c	62	GLU	CA-CB-CG	5.74	125.57	114.10
2	q	62	GLU	CA-CB-CG	5.74	125.57	114.10
2	o	62	GLU	CA-CB-CG	5.72	125.55	114.10
2	t	62	GLU	CA-CB-CG	5.72	125.54	114.10
2	Z	62	GLU	CA-CB-CG	5.72	125.53	114.10
2	s	62	GLU	CA-CB-CG	5.72	125.53	114.10
2	m	62	GLU	CA-CB-CG	5.71	125.53	114.10
2	i	62	GLU	CA-CB-CG	5.71	125.52	114.10
2	v	62	GLU	CA-CB-CG	5.71	125.52	114.10
2	n	62	GLU	CA-CB-CG	5.71	125.52	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	62	GLU	CA-CB-CG	5.71	125.51	114.10
2	h	62	GLU	CA-CB-CG	5.69	125.48	114.10
2	d	30	GLU	CA-CB-CG	5.30	124.71	114.10
2	k	30	GLU	CA-CB-CG	5.29	124.69	114.10
2	h	30	GLU	CA-CB-CG	5.28	124.66	114.10
2	t	30	GLU	CA-CB-CG	5.27	124.64	114.10
2	b	30	GLU	CA-CB-CG	5.26	124.62	114.10
2	f	30	GLU	CA-CB-CG	5.26	124.62	114.10
2	Y	30	GLU	CA-CB-CG	5.26	124.62	114.10
2	Z	30	GLU	CA-CB-CG	5.26	124.62	114.10
2	o	30	GLU	CA-CB-CG	5.26	124.62	114.10
2	c	30	GLU	CA-CB-CG	5.26	124.61	114.10
2	g	30	GLU	CA-CB-CG	5.26	124.61	114.10
2	n	30	GLU	CA-CB-CG	5.26	124.61	114.10
2	r	30	GLU	CA-CB-CG	5.25	124.61	114.10
2	u	30	GLU	CA-CB-CG	5.25	124.61	114.10
2	i	30	GLU	CA-CB-CG	5.25	124.60	114.10
2	v	30	GLU	CA-CB-CG	5.25	124.60	114.10
2	j	30	GLU	CA-CB-CG	5.25	124.60	114.10
2	m	30	GLU	CA-CB-CG	5.25	124.59	114.10
2	a	30	GLU	CA-CB-CG	5.24	124.58	114.10
2	l	30	GLU	CA-CB-CG	5.23	124.57	114.10
2	s	30	GLU	CA-CB-CG	5.23	124.56	114.10
2	q	30	GLU	CA-CB-CG	5.23	124.55	114.10
2	p	30	GLU	CA-CB-CG	5.22	124.55	114.10
2	e	30	GLU	CA-CB-CG	5.22	124.54	114.10
2	c	192	ASP	CA-CB-CG	5.10	117.70	112.60
2	d	192	ASP	CA-CB-CG	5.10	117.70	112.60
2	v	192	ASP	CA-CB-CG	5.10	117.70	112.60
2	h	192	ASP	CA-CB-CG	5.09	117.69	112.60
2	l	192	ASP	CA-CB-CG	5.09	117.69	112.60
2	n	192	ASP	CA-CB-CG	5.07	117.67	112.60
2	i	192	ASP	CA-CB-CG	5.06	117.66	112.60
2	Z	192	ASP	CA-CB-CG	5.06	117.66	112.60
2	Y	192	ASP	CA-CB-CG	5.06	117.66	112.60
2	r	192	ASP	CA-CB-CG	5.06	117.66	112.60
2	s	192	ASP	CA-CB-CG	5.05	117.65	112.60
2	e	192	ASP	CA-CB-CG	5.04	117.64	112.60
2	p	192	ASP	CA-CB-CG	5.04	117.64	112.60
2	a	192	ASP	CA-CB-CG	5.04	117.64	112.60
2	q	192	ASP	CA-CB-CG	5.04	117.64	112.60
2	m	192	ASP	CA-CB-CG	5.03	117.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	192	ASP	CA-CB-CG	5.03	117.63	112.60
2	t	192	ASP	CA-CB-CG	5.01	117.61	112.60
2	j	192	ASP	CA-CB-CG	5.01	117.61	112.60
2	o	192	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1600	0	1580	22	0
1	B	1600	0	1580	16	0
1	C	1600	0	1580	16	0
1	D	1600	0	1580	15	0
1	E	1600	0	1580	18	0
1	F	1600	0	1580	24	0
1	G	1600	0	1580	15	0
1	H	1600	0	1580	14	0
1	I	1600	0	1580	16	0
1	J	1600	0	1580	10	0
1	K	1600	0	1580	17	0
1	L	1600	0	1580	23	0
1	M	1600	0	1580	14	0
1	N	1600	0	1580	14	0
1	O	1600	0	1580	15	0
1	P	1600	0	1580	14	0
1	Q	1600	0	1580	20	0
1	R	1600	0	1580	24	0
1	S	1600	0	1580	20	0
1	T	1600	0	1580	27	0
1	U	1600	0	1580	11	0
1	V	1600	0	1580	12	0
1	W	1600	0	1580	11	0
1	X	1600	0	1580	17	0
2	Y	1431	0	1424	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	1431	0	1424	34	0
2	a	1431	0	1424	31	0
2	b	1431	0	1424	26	0
2	c	1431	0	1424	30	0
2	d	1431	0	1424	45	0
2	e	1431	0	1424	29	0
2	f	1431	0	1424	22	0
2	g	1431	0	1424	23	0
2	h	1431	0	1424	19	0
2	i	1431	0	1424	17	0
2	j	1431	0	1424	18	0
2	k	1431	0	1424	17	0
2	l	1431	0	1424	19	0
2	m	1431	0	1424	21	0
2	n	1431	0	1424	23	0
2	o	1431	0	1424	20	0
2	p	1431	0	1424	25	0
2	q	1431	0	1424	29	0
2	r	1431	0	1424	27	0
2	s	1431	0	1424	19	0
2	t	1431	0	1424	25	0
2	u	1431	0	1424	26	0
2	v	1431	0	1424	29	0
All	All	72744	0	72096	670	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 5.

All (670) 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:A:180:GLU:OE1	2:Y:196:GLN:NE2	1.68	1.26
1:T:180:GLU:OE1	2:r:196:GLN:NE2	1.80	1.13
1:B:180:GLU:OE1	2:Z:196:GLN:NE2	1.86	1.08
1:F:180:GLU:OE1	2:d:196:GLN:NE2	1.92	1.02
1:D:180:GLU:OE1	2:b:196:GLN:NE2	1.96	0.97
1:H:180:GLU:OE1	2:f:196:GLN:NE2	1.98	0.95
1:A:202:ARG:HH21	2:Y:41:MET:HG3	1.31	0.95
1:T:202:ARG:HH21	2:r:41:MET:HG3	1.32	0.94
1:C:180:GLU:OE1	2:a:196:GLN:NE2	2.01	0.93
2:d:112:ARG:NH1	2:e:84:GLU:HG2	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:112:ARG:NH1	2:d:84:GLU:HG2	1.84	0.92
1:Q:332:ASP:OD2	1:R:360:GLU:OE2	1.90	0.89
2:Y:112:ARG:NH1	2:Z:84:GLU:HG2	1.90	0.87
2:d:173:ASN:HB2	2:e:147:HIS:HB3	1.58	0.85
1:C:343:VAL:HG11	2:Z:162:HIS:CE1	2.14	0.83
1:Q:202:ARG:NH1	2:o:192:ASP:O	2.12	0.82
1:G:180:GLU:OE1	2:e:196:GLN:NE2	2.11	0.82
1:L:180:GLU:OE1	2:j:196:GLN:NE2	2.13	0.81
1:E:180:GLU:OE1	2:c:196:GLN:NE2	2.11	0.80
1:F:206:TRP:CE3	2:d:43:ASN:HB2	2.17	0.79
1:K:202:ARG:NH1	2:i:192:ASP:O	2.16	0.79
1:K:332:ASP:OD2	1:L:360:GLU:OE2	1.99	0.79
1:A:209:GLN:OE1	2:v:195:LEU:HD22	1.82	0.79
1:F:202:ARG:HH21	2:d:41:MET:HG3	1.48	0.77
1:T:202:ARG:NH2	2:r:41:MET:HG3	1.99	0.77
2:c:196:GLN:O	2:d:66:THR:HG21	1.86	0.76
1:B:202:ARG:HH21	2:Z:41:MET:HG3	1.50	0.76
1:A:206:TRP:CE3	2:Y:43:ASN:HB2	2.21	0.75
2:g:112:ARG:NH1	2:h:84:GLU:HG2	2.02	0.74
1:T:206:TRP:CE3	2:r:43:ASN:HB2	2.22	0.74
1:A:202:ARG:NH2	2:Y:41:MET:HG3	2.03	0.74
2:Y:173:ASN:HB2	2:Z:147:HIS:HB3	1.71	0.73
1:D:202:ARG:HH21	2:b:41:MET:HG3	1.52	0.72
2:p:112:ARG:NE	2:q:110:GLU:OE2	2.23	0.72
1:F:202:ARG:NH2	2:d:41:MET:HG3	2.04	0.71
1:K:338:ARG:HH12	1:L:358:ALA:HB1	1.55	0.71
2:Y:108:ALA:HB2	2:Z:88:MET:SD	2.31	0.71
1:R:180:GLU:OE1	2:p:196:GLN:NE2	2.23	0.70
1:D:343:VAL:HG11	2:a:162:HIS:CE1	2.25	0.70
2:u:112:ARG:NH1	2:v:84:GLU:HG2	2.07	0.70
1:X:180:GLU:OE1	2:v:196:GLN:NE2	2.21	0.70
1:M:180:GLU:OE1	2:k:196:GLN:NE2	2.23	0.69
1:L:228:GLU:OE2	1:L:231:ARG:NH2	2.22	0.69
1:S:228:GLU:OE2	1:S:231:ARG:NH2	2.22	0.68
1:X:228:GLU:OE2	1:X:231:ARG:NH2	2.22	0.68
1:Q:228:GLU:OE2	1:Q:231:ARG:NH2	2.22	0.68
1:K:228:GLU:OE2	1:K:231:ARG:NH2	2.22	0.67
2:c:173:ASN:HB2	2:d:147:HIS:HB3	1.77	0.67
1:E:228:GLU:OE2	1:E:231:ARG:NH2	2.22	0.67
1:F:228:GLU:OE2	1:F:231:ARG:NH2	2.22	0.67
1:V:215:ASP:HB2	2:t:202:VAL:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:ARG:HH21	2:f:41:MET:HG3	1.60	0.67
1:D:206:TRP:CE3	2:b:43:ASN:HB2	2.29	0.67
1:P:202:ARG:NH1	2:n:192:ASP:O	2.28	0.67
1:I:228:GLU:OE2	1:I:231:ARG:NH2	2.22	0.66
1:M:228:GLU:OE2	1:M:231:ARG:NH2	2.22	0.66
2:Y:84:GLU:HG2	2:v:112:ARG:NH1	2.10	0.66
1:Q:182:GLU:OE2	1:R:221:ARG:HD2	1.95	0.66
1:J:228:GLU:OE2	1:J:231:ARG:NH2	2.22	0.66
1:O:228:GLU:OE2	1:O:231:ARG:NH2	2.22	0.66
2:Z:112:ARG:NH1	2:a:84:GLU:HG2	2.10	0.66
2:g:173:ASN:HB2	2:h:147:HIS:HB3	1.78	0.66
1:P:337:LEU:HD21	2:n:160:LEU:HD12	1.78	0.66
1:V:228:GLU:OE2	1:V:231:ARG:NH2	2.22	0.65
2:a:124:LEU:HD22	2:b:75:TYR:CE1	2.31	0.65
1:C:228:GLU:OE2	1:C:231:ARG:NH2	2.22	0.65
1:O:202:ARG:NH1	2:m:192:ASP:O	2.29	0.65
2:c:112:ARG:HH12	2:d:84:GLU:HG2	1.57	0.65
1:P:333:ASP:OD2	2:n:185:VAL:O	2.15	0.65
1:K:182:GLU:OE2	1:L:221:ARG:HD2	1.96	0.65
1:D:209:GLN:OE1	2:a:195:LEU:HD22	1.96	0.65
1:D:228:GLU:OE2	1:D:231:ARG:NH2	2.22	0.65
1:G:228:GLU:OE2	1:G:231:ARG:NH2	2.22	0.65
2:c:108:ALA:HB2	2:d:88:MET:SD	2.38	0.64
1:P:228:GLU:OE2	1:P:231:ARG:NH2	2.22	0.64
1:A:228:GLU:OE2	1:A:231:ARG:NH2	2.22	0.64
1:H:228:GLU:OE2	1:H:231:ARG:NH2	2.22	0.64
1:Q:338:ARG:HH12	1:R:358:ALA:HB1	1.62	0.64
1:Q:215:ASP:HB2	2:o:202:VAL:HG13	1.79	0.64
1:N:228:GLU:OE2	1:N:231:ARG:NH2	2.22	0.63
1:D:202:ARG:NH2	2:b:41:MET:HG3	2.13	0.63
2:n:112:ARG:NH1	2:o:84:GLU:HG2	2.14	0.63
1:T:228:GLU:OE2	1:T:231:ARG:NH2	2.22	0.63
1:A:247:ARG:HG2	1:A:247:ARG:HH11	1.64	0.62
1:E:247:ARG:HH11	1:E:247:ARG:HG2	1.64	0.62
1:U:247:ARG:HG2	1:U:247:ARG:HH11	1.64	0.62
2:Y:196:GLN:O	2:Z:66:THR:HG21	1.98	0.62
1:B:247:ARG:HH11	1:B:247:ARG:HG2	1.65	0.62
1:V:247:ARG:HH11	1:V:247:ARG:HG2	1.65	0.62
1:W:228:GLU:OE2	1:W:231:ARG:NH2	2.22	0.62
1:X:247:ARG:HH11	1:X:247:ARG:HG2	1.65	0.62
1:B:228:GLU:OE2	1:B:231:ARG:NH2	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ARG:HG2	1:C:247:ARG:HH11	1.65	0.62
1:D:247:ARG:HG2	1:D:247:ARG:HH11	1.65	0.62
1:G:247:ARG:HH11	1:G:247:ARG:HG2	1.65	0.62
1:W:247:ARG:HG2	1:W:247:ARG:HH11	1.65	0.62
1:I:247:ARG:HG2	1:I:247:ARG:HH11	1.65	0.62
1:J:247:ARG:HG2	1:J:247:ARG:HH11	1.65	0.62
1:K:247:ARG:HG2	1:K:247:ARG:HH11	1.65	0.62
1:L:247:ARG:HH11	1:L:247:ARG:HG2	1.65	0.62
1:P:333:ASP:HB3	2:n:164:ILE:HD11	1.82	0.62
1:F:247:ARG:HG2	1:F:247:ARG:HH11	1.65	0.62
1:H:247:ARG:HG2	1:H:247:ARG:HH11	1.65	0.62
1:M:247:ARG:HG2	1:M:247:ARG:HH11	1.65	0.62
2:f:112:ARG:NH1	2:g:84:GLU:HG2	2.14	0.62
1:N:247:ARG:HH11	1:N:247:ARG:HG2	1.65	0.62
1:N:338:ARG:HH12	1:O:358:ALA:HB1	1.65	0.62
1:Q:247:ARG:HH11	1:Q:247:ARG:HG2	1.65	0.62
1:O:247:ARG:HG2	1:O:247:ARG:HH11	1.65	0.62
1:R:228:GLU:OE2	1:R:231:ARG:NH2	2.22	0.62
1:R:247:ARG:HG2	1:R:247:ARG:HH11	1.65	0.62
1:S:247:ARG:HH11	1:S:247:ARG:HG2	1.65	0.62
1:T:247:ARG:HG2	1:T:247:ARG:HH11	1.65	0.62
2:d:39:LEU:HD22	2:d:44:ILE:HD11	1.82	0.62
2:c:39:LEU:HD22	2:c:44:ILE:HD11	1.82	0.62
1:P:247:ARG:HG2	1:P:247:ARG:HH11	1.65	0.61
2:b:39:LEU:HD22	2:b:44:ILE:HD11	1.83	0.61
2:e:39:LEU:HD22	2:e:44:ILE:HD11	1.82	0.61
2:v:39:LEU:HD22	2:v:44:ILE:HD11	1.82	0.61
2:a:39:LEU:HD22	2:a:44:ILE:HD11	1.82	0.61
2:t:39:LEU:HD22	2:t:44:ILE:HD11	1.82	0.61
2:u:39:LEU:HD22	2:u:44:ILE:HD11	1.83	0.61
2:Z:39:LEU:HD22	2:Z:44:ILE:HD11	1.82	0.61
2:s:39:LEU:HD22	2:s:44:ILE:HD11	1.82	0.61
2:Y:39:LEU:HD22	2:Y:44:ILE:HD11	1.82	0.61
2:f:39:LEU:HD22	2:f:44:ILE:HD11	1.82	0.61
2:g:39:LEU:HD22	2:g:44:ILE:HD11	1.82	0.61
2:l:112:ARG:NH1	2:m:84:GLU:HG2	2.14	0.61
2:r:39:LEU:HD22	2:r:44:ILE:HD11	1.82	0.61
1:K:310:GLN:NE2	1:L:356:GLN:OE1	2.33	0.61
2:h:39:LEU:HD22	2:h:44:ILE:HD11	1.82	0.61
2:j:39:LEU:HD22	2:j:44:ILE:HD11	1.82	0.61
2:k:39:LEU:HD22	2:k:44:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:39:LEU:HD22	2:q:44:ILE:HD11	1.82	0.61
1:U:228:GLU:OE2	1:U:231:ARG:NH2	2.22	0.61
2:i:39:LEU:HD22	2:i:44:ILE:HD11	1.82	0.61
2:p:39:LEU:HD22	2:p:44:ILE:HD11	1.82	0.61
1:C:344:ASP:OD1	2:Z:159:PRO:HG3	2.01	0.60
1:O:215:ASP:HB2	2:m:202:VAL:HG13	1.83	0.60
2:l:39:LEU:HD22	2:l:44:ILE:HD11	1.82	0.60
1:C:343:VAL:HG11	2:Z:162:HIS:NE2	2.16	0.60
1:Q:181:LYS:HE2	1:R:219:ASN:HD21	1.66	0.60
2:d:108:ALA:HB2	2:e:88:MET:SD	2.42	0.60
2:o:39:LEU:HD22	2:o:44:ILE:HD11	1.82	0.60
1:T:209:GLN:OE1	2:q:195:LEU:HD22	2.00	0.60
2:m:39:LEU:HD22	2:m:44:ILE:HD11	1.82	0.60
2:n:39:LEU:HD22	2:n:44:ILE:HD11	1.82	0.60
1:A:356:GLN:OE1	1:X:310:GLN:NE2	2.34	0.60
1:S:182:GLU:OE2	1:T:221:ARG:HD2	2.03	0.59
2:p:112:ARG:HG2	2:q:129:HIS:HE1	1.67	0.59
1:A:343:VAL:HG11	2:v:162:HIS:CE1	2.37	0.59
1:C:247:ARG:NH1	1:C:348:ARG:O	2.36	0.59
1:N:310:GLN:NE2	1:O:356:GLN:OE1	2.35	0.59
1:L:247:ARG:NH1	1:L:348:ARG:O	2.36	0.59
1:W:247:ARG:NH1	1:W:348:ARG:O	2.36	0.59
2:Y:112:ARG:HH12	2:Z:84:GLU:HG2	1.65	0.59
1:F:247:ARG:NH1	1:F:348:ARG:O	2.36	0.59
1:G:247:ARG:NH1	1:G:348:ARG:O	2.36	0.59
1:M:247:ARG:NH1	1:M:348:ARG:O	2.36	0.59
1:P:247:ARG:NH1	1:P:348:ARG:O	2.36	0.59
1:X:247:ARG:NH1	1:X:348:ARG:O	2.36	0.59
1:O:247:ARG:NH1	1:O:348:ARG:O	2.36	0.59
1:S:247:ARG:NH1	1:S:348:ARG:O	2.36	0.59
1:B:247:ARG:NH1	1:B:348:ARG:O	2.36	0.58
1:E:247:ARG:NH1	1:E:348:ARG:O	2.36	0.58
1:K:247:ARG:NH1	1:K:348:ARG:O	2.36	0.58
2:p:104:ARG:HE	2:q:89:PHE:HE1	1.50	0.58
1:Q:247:ARG:NH1	1:Q:348:ARG:O	2.36	0.58
2:Z:173:ASN:HB2	2:a:147:HIS:HB3	1.84	0.58
1:I:247:ARG:NH1	1:I:348:ARG:O	2.36	0.58
1:N:247:ARG:NH1	1:N:348:ARG:O	2.36	0.58
1:H:247:ARG:NH1	1:H:348:ARG:O	2.36	0.58
1:J:247:ARG:NH1	1:J:348:ARG:O	2.36	0.58
1:D:247:ARG:NH1	1:D:348:ARG:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:310:GLN:NE2	1:Q:356:GLN:OE1	2.36	0.58
1:T:247:ARG:NH1	1:T:348:ARG:O	2.36	0.58
1:U:202:ARG:NH1	2:s:192:ASP:O	2.36	0.58
1:E:298:THR:HG21	1:F:242:GLN:HE22	1.69	0.58
1:V:247:ARG:NH1	1:V:348:ARG:O	2.36	0.58
1:Q:338:ARG:HH12	1:R:358:ALA:CB	2.17	0.58
1:R:247:ARG:NH1	1:R:348:ARG:O	2.36	0.58
1:U:247:ARG:NH1	1:U:348:ARG:O	2.36	0.58
1:B:206:TRP:CE3	2:Z:43:ASN:HB2	2.39	0.58
2:u:124:LEU:HD22	2:v:75:TYR:CE1	2.37	0.57
1:V:202:ARG:NH1	2:t:192:ASP:O	2.37	0.57
2:d:109:ILE:HD11	2:e:132:TYR:CD2	2.40	0.57
1:A:247:ARG:NH1	1:A:348:ARG:O	2.36	0.57
1:B:310:GLN:NE2	1:C:356:GLN:OE1	2.36	0.57
2:d:112:ARG:HH12	2:e:84:GLU:HG2	1.69	0.57
2:j:112:ARG:NH1	2:k:84:GLU:HG2	2.19	0.57
1:K:338:ARG:HH12	1:L:358:ALA:CB	2.17	0.57
1:F:209:GLN:OE1	2:c:195:LEU:HD22	2.05	0.57
1:C:202:ARG:HH21	2:a:41:MET:HG3	1.68	0.57
1:G:343:VAL:HG11	2:d:162:HIS:CE1	2.40	0.57
2:k:112:ARG:HG2	2:l:129:HIS:HE1	1.68	0.56
1:A:205:LEU:HD11	2:v:190:ARG:NH2	2.21	0.56
1:X:343:VAL:HG11	2:u:162:HIS:CE1	2.40	0.56
2:a:173:ASN:HD21	2:b:184:SER:CB	2.18	0.56
2:m:112:ARG:HG2	2:n:129:HIS:HE1	1.71	0.56
2:t:109:ILE:HD11	2:u:132:TYR:CD2	2.40	0.56
2:t:104:ARG:HE	2:u:89:PHE:HE1	1.54	0.56
1:N:202:ARG:NH1	2:l:192:ASP:O	2.38	0.56
2:Z:196:GLN:O	2:a:66:THR:HG21	2.05	0.56
2:t:112:ARG:NH1	2:u:84:GLU:HG2	2.21	0.56
2:u:108:ALA:HB2	2:v:88:MET:SD	2.46	0.56
2:s:37:ALA:HB2	2:t:69:VAL:HG12	1.87	0.56
1:Q:310:GLN:NE2	1:R:356:GLN:OE1	2.39	0.56
2:a:29:GLN:NE2	2:b:25:LYS:H	2.04	0.56
1:K:181:LYS:HE2	1:L:219:ASN:HD21	1.71	0.55
1:J:180:GLU:OE1	2:h:196:GLN:NE2	2.35	0.55
2:a:37:ALA:HB2	2:b:69:VAL:HG12	1.89	0.55
1:F:310:GLN:NE2	1:G:356:GLN:OE1	2.39	0.55
2:t:112:ARG:NE	2:u:110:GLU:OE2	2.38	0.55
2:l:196:GLN:O	2:m:66:THR:HG21	2.06	0.55
1:B:202:ARG:NH2	2:Z:41:MET:HG3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:TRP:CE3	2:f:43:ASN:HB2	2.42	0.55
1:I:180:GLU:OE1	2:g:196:GLN:NE2	2.35	0.55
2:f:196:GLN:O	2:g:66:THR:HG21	2.06	0.55
2:q:112:ARG:NH1	2:r:84:GLU:HG2	2.21	0.55
1:Q:213:ARG:HD3	2:o:201:PRO:HB3	1.89	0.55
1:G:202:ARG:HH21	2:e:41:MET:HG3	1.71	0.54
1:S:338:ARG:HH12	1:T:358:ALA:HB1	1.71	0.54
2:j:135:ASP:OD1	2:j:135:ASP:N	2.41	0.54
2:c:135:ASP:OD1	2:c:135:ASP:N	2.41	0.54
2:e:135:ASP:OD1	2:e:135:ASP:N	2.41	0.54
2:h:135:ASP:OD1	2:h:135:ASP:N	2.41	0.54
1:P:334:VAL:HG22	2:n:164:ILE:CG2	2.38	0.54
2:i:84:GLU:OE1	2:i:111:GLN:NE2	2.41	0.54
2:l:135:ASP:OD1	2:l:135:ASP:N	2.41	0.54
2:m:135:ASP:OD1	2:m:135:ASP:N	2.41	0.54
1:V:213:ARG:HD3	2:t:201:PRO:HB3	1.90	0.54
2:Y:84:GLU:OE1	2:Y:111:GLN:NE2	2.41	0.54
2:o:84:GLU:OE1	2:o:111:GLN:NE2	2.41	0.54
2:q:84:GLU:OE1	2:q:111:GLN:NE2	2.41	0.54
2:t:84:GLU:OE1	2:t:111:GLN:NE2	2.41	0.54
2:Z:84:GLU:OE1	2:Z:111:GLN:NE2	2.41	0.54
2:a:135:ASP:OD1	2:a:135:ASP:N	2.41	0.54
2:f:135:ASP:N	2:f:135:ASP:OD1	2.41	0.54
2:o:135:ASP:OD1	2:o:135:ASP:N	2.41	0.54
2:u:84:GLU:OE1	2:u:111:GLN:NE2	2.41	0.54
1:Q:298:THR:HG21	1:R:242:GLN:HE22	1.73	0.54
2:c:84:GLU:OE1	2:c:111:GLN:NE2	2.41	0.54
2:g:135:ASP:OD1	2:g:135:ASP:N	2.41	0.54
2:j:84:GLU:OE1	2:j:111:GLN:NE2	2.41	0.54
2:k:135:ASP:N	2:k:135:ASP:OD1	2.41	0.54
2:l:84:GLU:OE1	2:l:111:GLN:NE2	2.41	0.54
2:m:84:GLU:OE1	2:m:111:GLN:NE2	2.41	0.54
1:H:343:VAL:HG11	2:e:162:HIS:CE1	2.43	0.54
2:Z:135:ASP:N	2:Z:135:ASP:OD1	2.41	0.54
2:a:173:ASN:HD21	2:b:184:SER:HB3	1.72	0.54
2:f:84:GLU:OE1	2:f:111:GLN:NE2	2.41	0.54
2:n:84:GLU:OE1	2:n:111:GLN:NE2	2.41	0.54
2:p:84:GLU:OE1	2:p:111:GLN:NE2	2.41	0.54
2:v:135:ASP:OD1	2:v:135:ASP:N	2.41	0.54
1:L:310:GLN:NE2	1:M:356:GLN:OE1	2.40	0.53
2:b:84:GLU:OE1	2:b:111:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LEU:HD11	2:a:190:ARG:NH2	2.23	0.53
2:d:135:ASP:N	2:d:135:ASP:OD1	2.41	0.53
2:h:84:GLU:OE1	2:h:111:GLN:NE2	2.41	0.53
2:r:84:GLU:OE1	2:r:111:GLN:NE2	2.41	0.53
2:s:84:GLU:OE1	2:s:111:GLN:NE2	2.41	0.53
2:v:84:GLU:OE1	2:v:111:GLN:NE2	2.41	0.53
1:L:202:ARG:HH21	2:j:41:MET:HG3	1.74	0.53
1:S:332:ASP:OD2	1:T:360:GLU:OE2	2.26	0.53
2:e:84:GLU:OE1	2:e:111:GLN:NE2	2.41	0.53
2:p:135:ASP:N	2:p:135:ASP:OD1	2.41	0.53
1:O:213:ARG:HD3	2:m:201:PRO:HB3	1.91	0.53
2:Y:135:ASP:OD1	2:Y:135:ASP:N	2.41	0.53
2:c:169:ARG:NH1	2:c:180:TYR:OH	2.42	0.53
2:g:84:GLU:OE1	2:g:111:GLN:NE2	2.41	0.53
2:r:135:ASP:OD1	2:r:135:ASP:N	2.41	0.53
2:t:135:ASP:OD1	2:t:135:ASP:N	2.41	0.53
2:i:135:ASP:N	2:i:135:ASP:OD1	2.41	0.53
1:E:182:GLU:OE2	1:F:221:ARG:HD2	2.09	0.53
2:a:169:ARG:NH1	2:a:180:TYR:OH	2.42	0.53
2:j:169:ARG:NH1	2:j:180:TYR:OH	2.42	0.53
2:k:112:ARG:NE	2:l:110:GLU:OE2	2.41	0.53
2:d:84:GLU:OE1	2:d:111:GLN:NE2	2.41	0.53
2:k:84:GLU:OE1	2:k:111:GLN:NE2	2.41	0.53
1:T:343:VAL:HG11	2:q:162:HIS:CE1	2.43	0.53
2:a:84:GLU:OE1	2:a:111:GLN:NE2	2.41	0.53
2:c:193:ALA:HA	2:d:70:TYR:CE2	2.44	0.53
2:e:169:ARG:NH1	2:e:180:TYR:OH	2.42	0.53
2:m:169:ARG:NH1	2:m:180:TYR:OH	2.42	0.53
1:S:310:GLN:NE2	1:T:356:GLN:OE1	2.42	0.53
1:R:333:ASP:OD2	2:p:185:VAL:O	2.27	0.52
2:v:169:ARG:NH1	2:v:180:TYR:OH	2.42	0.52
1:O:332:ASP:OD2	1:P:360:GLU:OE2	2.26	0.52
2:n:135:ASP:N	2:n:135:ASP:OD1	2.41	0.52
2:Z:169:ARG:NH1	2:Z:180:TYR:OH	2.42	0.52
1:E:298:THR:HG21	1:F:242:GLN:NE2	2.25	0.52
2:b:135:ASP:N	2:b:135:ASP:OD1	2.41	0.52
2:g:169:ARG:NH1	2:g:180:TYR:OH	2.42	0.52
2:p:169:ARG:NH1	2:p:180:TYR:OH	2.42	0.52
2:r:112:ARG:NH1	2:s:84:GLU:HG2	2.24	0.52
2:Y:169:ARG:NH1	2:Y:180:TYR:OH	2.42	0.52
2:d:170:PHE:HZ	2:e:129:HIS:CD2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:169:ARG:NH1	2:l:180:TYR:OH	2.42	0.52
2:o:169:ARG:NH1	2:o:180:TYR:OH	2.42	0.52
2:Y:147:HIS:HB3	2:v:173:ASN:HB2	1.92	0.52
2:q:135:ASP:OD1	2:q:135:ASP:N	2.41	0.52
2:u:29:GLN:NE2	2:v:25:LYS:H	2.07	0.52
2:u:135:ASP:N	2:u:135:ASP:OD1	2.41	0.52
2:r:169:ARG:NH1	2:r:180:TYR:OH	2.42	0.52
1:A:358:ALA:HB1	1:X:338:ARG:HH12	1.74	0.52
2:b:169:ARG:NH1	2:b:180:TYR:OH	2.42	0.52
2:t:169:ARG:NH1	2:t:180:TYR:OH	2.42	0.52
1:K:182:GLU:OE2	1:L:221:ARG:CD	2.57	0.52
2:f:112:ARG:NE	2:g:110:GLU:OE2	2.42	0.52
2:d:170:PHE:CZ	2:e:129:HIS:CD2	2.98	0.51
2:s:112:ARG:HG2	2:t:129:HIS:HE1	1.74	0.51
2:s:135:ASP:N	2:s:135:ASP:OD1	2.41	0.51
1:L:337:LEU:HD21	2:j:160:LEU:HD12	1.92	0.51
2:o:112:ARG:NH1	2:p:84:GLU:HG2	2.25	0.51
2:q:169:ARG:NH1	2:q:180:TYR:OH	2.42	0.51
1:U:343:VAL:HG11	2:r:162:HIS:CE1	2.45	0.51
2:a:112:ARG:NH1	2:b:84:GLU:HG2	2.26	0.51
2:u:169:ARG:NH1	2:u:180:TYR:OH	2.42	0.51
1:I:202:ARG:NH1	2:g:192:ASP:O	2.42	0.51
1:I:343:VAL:HG11	2:f:162:HIS:CE1	2.46	0.51
2:h:112:ARG:HG2	2:i:129:HIS:HE1	1.75	0.51
1:S:182:GLU:OE2	1:T:221:ARG:CD	2.58	0.51
1:G:343:VAL:HG11	2:d:162:HIS:NE2	2.25	0.51
2:d:109:ILE:HD11	2:e:132:TYR:HD2	1.75	0.51
2:d:169:ARG:NH1	2:d:180:TYR:OH	2.42	0.51
2:g:108:ALA:HB2	2:h:88:MET:SD	2.51	0.51
2:s:169:ARG:NH1	2:s:180:TYR:OH	2.42	0.51
1:K:298:THR:HG21	1:L:242:GLN:HE22	1.76	0.50
2:i:169:ARG:NH1	2:i:180:TYR:OH	2.42	0.50
1:R:202:ARG:HH21	2:p:41:MET:HG3	1.75	0.50
2:n:169:ARG:NH1	2:n:180:TYR:OH	2.42	0.50
1:T:298:THR:HG21	1:U:242:GLN:NE2	2.27	0.50
2:b:112:ARG:NE	2:c:110:GLU:OE2	2.42	0.50
2:l:112:ARG:NE	2:m:110:GLU:OE2	2.42	0.50
2:e:112:ARG:NH1	2:f:84:GLU:HG2	2.26	0.50
1:F:343:VAL:HG11	2:c:162:HIS:CE1	2.47	0.50
2:b:112:ARG:NH1	2:c:84:GLU:HG2	2.27	0.50
1:T:333:ASP:OD2	2:r:185:VAL:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:310:GLN:NE2	1:X:356:GLN:OE1	2.46	0.49
2:f:169:ARG:NH1	2:f:180:TYR:OH	2.42	0.49
1:L:206:TRP:CE3	2:j:43:ASN:HB2	2.48	0.49
2:Y:193:ALA:HA	2:Z:70:TYR:CZ	2.47	0.49
2:t:173:ASN:HB2	2:u:147:HIS:HB3	1.93	0.49
1:E:332:ASP:OD2	1:F:360:GLU:OE2	2.31	0.49
1:H:202:ARG:NH2	2:f:41:MET:HG3	2.26	0.49
1:S:202:ARG:NH1	2:q:192:ASP:O	2.46	0.49
2:k:169:ARG:NH1	2:k:180:TYR:OH	2.42	0.49
1:T:340:ARG:CZ	2:q:166:ASP:OD2	2.60	0.49
2:d:173:ASN:HD22	2:e:182:ASN:C	2.21	0.49
1:A:206:TRP:CD2	2:Y:43:ASN:HB2	2.47	0.49
2:c:193:ALA:HA	2:d:70:TYR:CZ	2.48	0.49
1:T:217:ASP:OD1	1:T:217:ASP:N	2.46	0.49
1:W:217:ASP:OD1	1:W:217:ASP:N	2.46	0.49
2:Z:112:ARG:NE	2:a:110:GLU:OE2	2.42	0.49
2:q:29:GLN:NE2	2:r:25:LYS:H	2.11	0.49
1:S:217:ASP:OD1	1:S:217:ASP:N	2.46	0.49
1:A:213:ARG:HH21	2:Y:64:ASP:CG	2.21	0.48
1:I:310:GLN:NE2	1:J:356:GLN:OE1	2.45	0.48
1:I:338:ARG:HH12	1:J:358:ALA:HB1	1.78	0.48
1:J:202:ARG:NH1	2:h:192:ASP:O	2.45	0.48
1:P:217:ASP:N	1:P:217:ASP:OD1	2.46	0.48
2:p:112:ARG:HG2	2:q:129:HIS:CE1	2.47	0.48
1:N:332:ASP:OD2	1:O:360:GLU:OE2	2.31	0.48
2:Y:105:LEU:HD13	2:Z:89:PHE:CE2	2.48	0.48
1:A:221:ARG:HD2	1:X:182:GLU:OE2	2.13	0.48
1:V:217:ASP:OD1	1:V:217:ASP:N	2.46	0.48
1:F:337:LEU:HD21	2:d:160:LEU:HD12	1.96	0.48
1:B:217:ASP:OD1	1:B:217:ASP:N	2.46	0.48
1:B:343:VAL:HG11	2:Y:162:HIS:CE1	2.49	0.48
1:Q:217:ASP:OD1	1:Q:217:ASP:N	2.46	0.48
2:Z:112:ARG:HH12	2:a:84:GLU:HG2	1.79	0.48
1:C:217:ASP:OD1	1:C:217:ASP:N	2.46	0.48
1:X:217:ASP:N	1:X:217:ASP:OD1	2.46	0.48
1:A:344:ASP:OD1	2:v:159:PRO:HG3	2.13	0.48
1:L:217:ASP:OD1	1:L:217:ASP:N	2.46	0.48
1:S:181:LYS:HE2	1:T:219:ASN:HD21	1.78	0.48
2:d:105:LEU:HD13	2:e:89:PHE:CE2	2.49	0.48
1:B:338:ARG:HH12	1:C:358:ALA:HB1	1.78	0.48
1:G:344:ASP:OD1	2:d:159:PRO:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217:ASP:OD1	1:O:217:ASP:N	2.46	0.48
1:R:337:LEU:HD21	2:p:160:LEU:HD12	1.95	0.48
2:d:196:GLN:O	2:e:66:THR:HG21	2.14	0.48
1:F:359:ILE:HD12	2:c:162:HIS:ND1	2.29	0.48
1:U:217:ASP:N	1:U:217:ASP:OD1	2.46	0.48
1:A:217:ASP:OD1	1:A:217:ASP:N	2.46	0.47
1:C:209:GLN:OE1	2:Z:195:LEU:HD22	2.14	0.47
1:T:205:LEU:HD11	2:q:190:ARG:NH2	2.29	0.47
2:h:169:ARG:NH1	2:h:180:TYR:OH	2.42	0.47
1:M:217:ASP:OD1	1:M:217:ASP:N	2.46	0.47
1:R:310:GLN:NE2	1:S:356:GLN:OE1	2.47	0.47
1:D:217:ASP:OD1	1:D:217:ASP:N	2.46	0.47
1:G:217:ASP:OD1	1:G:217:ASP:N	2.46	0.47
1:R:217:ASP:OD1	1:R:217:ASP:N	2.46	0.47
1:E:310:GLN:NE2	1:F:356:GLN:OE1	2.47	0.47
1:F:217:ASP:OD1	1:F:217:ASP:N	2.46	0.47
1:D:310:GLN:NE2	1:E:356:GLN:OE1	2.48	0.47
1:H:217:ASP:OD1	1:H:217:ASP:N	2.46	0.47
1:K:217:ASP:OD1	1:K:217:ASP:N	2.46	0.47
2:s:33:ASN:ND2	2:t:23:LEU:O	2.46	0.47
1:B:205:LEU:HD13	2:Z:71:TRP:CZ2	2.50	0.47
1:V:310:GLN:NE2	1:W:356:GLN:OE1	2.47	0.47
1:W:338:ARG:HH12	1:X:358:ALA:HB1	1.79	0.47
2:i:112:ARG:HG2	2:j:129:HIS:HE1	1.80	0.47
1:E:359:ILE:HD12	2:b:162:HIS:ND1	2.30	0.47
1:M:338:ARG:HH12	1:N:358:ALA:HB1	1.80	0.47
2:Y:66:THR:HG21	2:v:196:GLN:O	2.14	0.47
2:o:124:LEU:HD22	2:p:75:TYR:CE1	2.50	0.47
2:m:112:ARG:NE	2:n:110:GLU:OE2	2.47	0.47
1:G:338:ARG:HH12	1:H:358:ALA:HB1	1.80	0.47
1:N:217:ASP:N	1:N:217:ASP:OD1	2.46	0.47
1:Q:182:GLU:OE2	1:R:221:ARG:CD	2.62	0.47
1:W:343:VAL:HG11	2:t:162:HIS:CE1	2.50	0.47
1:S:298:THR:HG21	1:T:242:GLN:HE22	1.80	0.46
1:U:310:GLN:NE2	1:V:356:GLN:OE1	2.48	0.46
1:I:217:ASP:N	1:I:217:ASP:OD1	2.46	0.46
2:a:33:ASN:ND2	2:b:23:LEU:O	2.46	0.46
1:T:206:TRP:CD2	2:r:43:ASN:HB2	2.50	0.46
2:d:173:ASN:ND2	2:e:182:ASN:O	2.47	0.46
1:B:209:GLN:OE1	2:Y:195:LEU:HD22	2.16	0.46
1:S:215:ASP:HB2	2:q:202:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:88:MET:SD	2:v:108:ALA:HB2	2.55	0.46
1:G:310:GLN:NE2	1:H:356:GLN:OE1	2.48	0.46
1:I:337:LEU:HD21	2:g:160:LEU:HD12	1.98	0.46
1:J:217:ASP:OD1	1:J:217:ASP:N	2.46	0.46
1:B:213:ARG:HH21	2:Z:64:ASP:CG	2.24	0.46
1:M:310:GLN:NE2	1:N:356:GLN:OE1	2.48	0.46
1:O:337:LEU:HD21	2:m:160:LEU:HD12	1.97	0.46
1:P:333:ASP:HB3	2:n:164:ILE:CD1	2.45	0.46
1:T:310:GLN:NE2	1:U:356:GLN:OE1	2.49	0.46
2:p:196:GLN:O	2:q:66:THR:HG21	2.15	0.46
1:E:217:ASP:OD1	1:E:217:ASP:N	2.46	0.46
1:E:338:ARG:HH12	1:F:358:ALA:HB1	1.82	0.45
1:M:332:ASP:OD2	1:N:360:GLU:OE2	2.33	0.45
2:s:33:ASN:OD1	2:s:48:LYS:NZ	2.50	0.45
2:s:112:ARG:NE	2:t:110:GLU:OE2	2.49	0.45
1:F:343:VAL:HG11	2:c:162:HIS:NE2	2.31	0.45
1:H:310:GLN:NE2	1:I:356:GLN:OE1	2.49	0.45
2:e:33:ASN:OD1	2:e:48:LYS:NZ	2.50	0.45
2:h:33:ASN:OD1	2:h:48:LYS:NZ	2.50	0.45
2:q:108:ALA:HB2	2:r:88:MET:SD	2.56	0.45
2:r:33:ASN:OD1	2:r:48:LYS:NZ	2.50	0.45
1:G:359:ILE:HD12	2:d:162:HIS:ND1	2.31	0.45
1:I:215:ASP:HB2	2:g:202:VAL:HG13	1.98	0.45
2:i:33:ASN:OD1	2:i:48:LYS:NZ	2.50	0.45
2:n:108:ALA:HB2	2:o:88:MET:SD	2.57	0.45
1:I:213:ARG:HD3	2:g:201:PRO:HB3	1.99	0.45
1:K:337:LEU:HD23	2:i:161:ALA:HA	1.98	0.45
1:W:337:LEU:HD22	2:u:164:ILE:HD12	1.99	0.45
2:l:33:ASN:OD1	2:l:48:LYS:NZ	2.50	0.45
2:p:33:ASN:OD1	2:p:48:LYS:NZ	2.50	0.45
1:E:202:ARG:HH21	2:c:41:MET:HG3	1.82	0.44
1:T:202:ARG:NH2	2:r:41:MET:CG	2.77	0.44
2:a:36:ILE:HD11	2:a:48:LYS:HB2	2.00	0.44
2:g:33:ASN:OD1	2:g:48:LYS:NZ	2.50	0.44
2:h:36:ILE:HD11	2:h:48:LYS:HB2	1.99	0.44
2:j:33:ASN:OD1	2:j:48:LYS:NZ	2.50	0.44
2:k:33:ASN:OD1	2:k:48:LYS:NZ	2.50	0.44
2:n:33:ASN:OD1	2:n:48:LYS:NZ	2.50	0.44
2:q:33:ASN:OD1	2:q:48:LYS:NZ	2.50	0.44
2:a:33:ASN:OD1	2:a:48:LYS:NZ	2.50	0.44
2:c:36:ILE:HD11	2:c:48:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:170:PHE:CZ	2:d:129:HIS:CD2	3.06	0.44
2:f:36:ILE:HD11	2:f:48:LYS:HB2	2.00	0.44
2:k:112:ARG:HG2	2:l:129:HIS:CE1	2.52	0.44
2:n:173:ASN:HB2	2:o:147:HIS:HB3	1.99	0.44
1:K:215:ASP:HB2	2:i:202:VAL:HG13	1.99	0.44
1:S:213:ARG:HD3	2:q:201:PRO:HB3	1.99	0.44
2:Y:36:ILE:HD11	2:Y:48:LYS:HB2	2.00	0.44
1:C:337:LEU:HD22	2:a:164:ILE:HD12	2.00	0.44
1:Q:206:TRP:CZ3	2:o:194:GLN:NE2	2.85	0.44
2:c:29:GLN:NE2	2:d:25:LYS:O	2.50	0.44
2:d:36:ILE:HD11	2:d:48:LYS:HB2	2.00	0.44
2:j:36:ILE:HD11	2:j:48:LYS:HB2	2.00	0.44
2:m:33:ASN:OD1	2:m:48:LYS:NZ	2.50	0.44
2:n:23:LEU:HD12	2:n:24:LEU:HG	1.99	0.44
1:D:344:ASP:OD1	2:a:159:PRO:HG3	2.17	0.44
1:L:202:ARG:NH2	2:j:41:MET:HG3	2.32	0.44
1:N:180:GLU:OE1	2:l:196:GLN:NE2	2.40	0.44
2:e:36:ILE:HD11	2:e:48:LYS:HB2	2.00	0.44
2:h:112:ARG:NH1	2:i:84:GLU:HG2	2.32	0.44
2:m:23:LEU:HD12	2:m:24:LEU:HG	2.00	0.44
2:v:177:ASP:OD1	2:v:177:ASP:N	2.51	0.44
2:p:109:ILE:HD11	2:q:132:TYR:CD2	2.53	0.44
2:r:177:ASP:OD1	2:r:177:ASP:N	2.51	0.44
1:A:202:ARG:NH2	2:Y:41:MET:CG	2.77	0.44
1:B:298:THR:HG21	1:C:242:GLN:HE22	1.82	0.44
1:N:338:ARG:HH12	1:O:358:ALA:CB	2.29	0.44
1:W:178:GLY:HA3	2:u:196:GLN:OE1	2.17	0.44
2:Y:23:LEU:HD12	2:Y:24:LEU:HG	2.00	0.44
2:Y:177:ASP:OD1	2:Y:177:ASP:N	2.51	0.44
2:u:36:ILE:HD11	2:u:48:LYS:HB2	1.99	0.44
1:S:298:THR:HG21	1:T:242:GLN:NE2	2.33	0.44
2:a:23:LEU:HD12	2:a:24:LEU:HG	2.00	0.44
2:c:170:PHE:HZ	2:d:129:HIS:CD2	2.35	0.44
2:o:23:LEU:HD12	2:o:24:LEU:HG	2.00	0.44
2:q:177:ASP:OD1	2:q:177:ASP:N	2.51	0.44
2:Z:177:ASP:N	2:Z:177:ASP:OD1	2.51	0.43
2:c:23:LEU:HD12	2:c:24:LEU:HG	2.00	0.43
2:l:36:ILE:HD11	2:l:48:LYS:HB2	2.00	0.43
2:q:29:GLN:HE21	2:r:24:LEU:HA	1.83	0.43
2:r:112:ARG:HG2	2:s:129:HIS:HE1	1.83	0.43
2:u:177:ASP:N	2:u:177:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:23:LEU:HD12	2:b:24:LEU:HG	2.00	0.43
2:l:23:LEU:HD12	2:l:24:LEU:HG	2.00	0.43
2:p:177:ASP:N	2:p:177:ASP:OD1	2.51	0.43
2:v:23:LEU:HD12	2:v:24:LEU:HG	2.00	0.43
2:Z:23:LEU:HD12	2:Z:24:LEU:HG	2.00	0.43
2:b:36:ILE:HD11	2:b:48:LYS:HB2	2.00	0.43
2:e:23:LEU:HD12	2:e:24:LEU:HG	2.00	0.43
2:g:112:ARG:HH12	2:h:84:GLU:HG2	1.82	0.43
2:h:112:ARG:NE	2:i:110:GLU:OE2	2.49	0.43
2:u:23:LEU:HD12	2:u:24:LEU:HG	2.00	0.43
1:A:205:LEU:HD11	2:v:190:ARG:HH22	1.83	0.43
1:S:337:LEU:HD22	2:q:164:ILE:HD12	2.00	0.43
2:g:36:ILE:HD11	2:g:48:LYS:HB2	2.00	0.43
2:o:177:ASP:OD1	2:o:177:ASP:N	2.51	0.43
2:p:23:LEU:HD12	2:p:24:LEU:HG	2.00	0.43
2:r:37:ALA:HB2	2:s:69:VAL:HG12	2.00	0.43
2:s:36:ILE:HD11	2:s:48:LYS:HB2	2.00	0.43
1:J:202:ARG:HH21	2:h:41:MET:HG3	1.84	0.43
2:a:173:ASN:OD1	2:b:184:SER:OG	2.36	0.43
2:c:177:ASP:OD1	2:c:177:ASP:N	2.51	0.43
2:d:23:LEU:HD12	2:d:24:LEU:HG	2.00	0.43
2:i:23:LEU:HD12	2:i:24:LEU:HG	2.00	0.43
2:i:112:ARG:NH1	2:j:84:GLU:HG2	2.33	0.43
2:s:177:ASP:OD1	2:s:177:ASP:N	2.51	0.43
1:B:298:THR:HG21	1:C:242:GLN:NE2	2.34	0.43
2:a:177:ASP:N	2:a:177:ASP:OD1	2.51	0.43
2:e:177:ASP:OD1	2:e:177:ASP:N	2.51	0.43
2:t:23:LEU:HD12	2:t:24:LEU:HG	1.99	0.43
1:R:247:ARG:HG2	1:R:247:ARG:NH1	2.33	0.43
2:d:177:ASP:OD1	2:d:177:ASP:N	2.51	0.43
2:f:177:ASP:OD1	2:f:177:ASP:N	2.51	0.43
2:h:23:LEU:HD12	2:h:24:LEU:HG	2.00	0.43
2:n:36:ILE:HD11	2:n:48:LYS:HB2	2.00	0.43
2:Z:36:ILE:HD11	2:Z:48:LYS:HB2	1.99	0.43
2:Z:108:ALA:HB2	2:a:88:MET:SD	2.59	0.43
2:b:177:ASP:OD1	2:b:177:ASP:N	2.51	0.43
2:f:23:LEU:HD12	2:f:24:LEU:HG	2.00	0.43
2:g:23:LEU:HD12	2:g:24:LEU:HG	2.00	0.43
1:L:298:THR:HG21	1:M:242:GLN:NE2	2.34	0.43
1:R:202:ARG:NH1	2:p:192:ASP:O	2.52	0.43
2:i:36:ILE:HD11	2:i:48:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:23:LEU:HD12	2:k:24:LEU:HG	2.00	0.43
2:p:36:ILE:HD11	2:p:48:LYS:HB2	2.00	0.43
1:T:247:ARG:HG2	1:T:247:ARG:NH1	2.33	0.43
2:g:177:ASP:OD1	2:g:177:ASP:N	2.51	0.43
2:n:177:ASP:OD1	2:n:177:ASP:N	2.51	0.43
2:v:36:ILE:HD11	2:v:48:LYS:HB2	2.00	0.43
2:s:23:LEU:HD12	2:s:24:LEU:HG	2.00	0.42
2:t:177:ASP:OD1	2:t:177:ASP:N	2.51	0.42
2:u:37:ALA:HB2	2:v:69:VAL:HG12	2.01	0.42
1:Q:247:ARG:HG2	1:Q:247:ARG:NH1	2.33	0.42
1:V:215:ASP:CB	2:t:202:VAL:HG13	2.47	0.42
2:j:23:LEU:HD12	2:j:24:LEU:HG	2.00	0.42
2:k:36:ILE:HD11	2:k:48:LYS:HB2	2.00	0.42
2:o:36:ILE:HD11	2:o:48:LYS:HB2	2.00	0.42
2:t:112:ARG:HG2	2:u:129:HIS:HE1	1.84	0.42
1:S:178:GLY:HA3	2:q:196:GLN:OE1	2.19	0.42
1:S:247:ARG:HG2	1:S:247:ARG:NH1	2.33	0.42
1:U:247:ARG:HG2	1:U:247:ARG:NH1	2.33	0.42
2:b:112:ARG:HG2	2:c:129:HIS:HE1	1.83	0.42
2:q:23:LEU:HD12	2:q:24:LEU:HG	2.00	0.42
2:q:36:ILE:HD11	2:q:48:LYS:HB2	2.00	0.42
2:r:23:LEU:HD12	2:r:24:LEU:HG	2.00	0.42
2:r:36:ILE:HD11	2:r:48:LYS:HB2	2.00	0.42
1:L:298:THR:HG21	1:M:242:GLN:HE22	1.84	0.42
2:h:177:ASP:OD1	2:h:177:ASP:N	2.51	0.42
1:U:338:ARG:HH12	1:V:358:ALA:HB1	1.84	0.42
2:d:111:GLN:HB3	2:e:83:VAL:HG11	2.01	0.42
2:m:36:ILE:HD11	2:m:48:LYS:HB2	1.99	0.42
2:q:124:LEU:HD22	2:r:75:TYR:CE1	2.54	0.42
2:t:36:ILE:HD11	2:t:48:LYS:HB2	2.00	0.42
2:v:33:ASN:OD1	2:v:48:LYS:NZ	2.50	0.42
1:O:247:ARG:HG2	1:O:247:ARG:NH1	2.33	0.42
1:Q:202:ARG:CZ	2:o:192:ASP:O	2.66	0.42
1:O:298:THR:HG21	1:P:242:GLN:HE22	1.84	0.42
1:R:343:VAL:HG11	2:o:162:HIS:CE1	2.55	0.42
2:e:29:GLN:NE2	2:f:25:LYS:H	2.18	0.42
1:E:181:LYS:HE2	1:F:219:ASN:HD21	1.84	0.42
1:N:247:ARG:HG2	1:N:247:ARG:NH1	2.33	0.42
1:V:247:ARG:HG2	1:V:247:ARG:NH1	2.33	0.42
2:i:177:ASP:N	2:i:177:ASP:OD1	2.51	0.42
2:j:177:ASP:OD1	2:j:177:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:177:ASP:OD1	2:m:177:ASP:N	2.51	0.42
1:K:298:THR:HG21	1:L:242:GLN:NE2	2.35	0.42
2:c:124:LEU:HD22	2:d:75:TYR:CE1	2.55	0.42
2:e:112:ARG:HG2	2:f:129:HIS:HE1	1.85	0.42
1:E:182:GLU:OE2	1:F:221:ARG:CD	2.68	0.41
1:M:202:ARG:NH1	2:k:192:ASP:O	2.52	0.41
1:T:213:ARG:HH21	2:r:64:ASP:CG	2.27	0.41
1:D:340:ARG:CZ	2:a:166:ASP:OD2	2.68	0.41
1:H:338:ARG:HH12	1:I:358:ALA:HB1	1.85	0.41
1:I:343:VAL:HG11	2:f:162:HIS:NE2	2.34	0.41
2:Z:33:ASN:OD1	2:Z:48:LYS:NZ	2.50	0.41
2:l:177:ASP:OD1	2:l:177:ASP:N	2.51	0.41
2:t:123:VAL:HG22	2:t:154:TYR:HE1	1.86	0.41
2:u:123:VAL:HG22	2:u:154:TYR:HE1	1.86	0.41
1:A:343:VAL:HG11	2:v:162:HIS:NE2	2.36	0.41
1:G:209:GLN:OE1	2:d:195:LEU:HD22	2.21	0.41
1:M:202:ARG:HH21	2:k:41:MET:HG3	1.86	0.41
2:b:33:ASN:OD1	2:b:48:LYS:NZ	2.50	0.41
2:k:123:VAL:HG22	2:k:154:TYR:HE1	1.86	0.41
2:k:177:ASP:N	2:k:177:ASP:OD1	2.51	0.41
2:l:123:VAL:HG22	2:l:154:TYR:HE1	1.86	0.41
2:s:123:VAL:HG22	2:s:154:TYR:HE1	1.86	0.41
1:F:206:TRP:CE2	2:d:43:ASN:ND2	2.88	0.41
2:c:123:VAL:HG22	2:c:154:TYR:HE1	1.86	0.41
2:d:112:ARG:HH11	2:e:84:GLU:HG2	1.79	0.41
2:e:123:VAL:HG22	2:e:154:TYR:HE1	1.86	0.41
2:h:123:VAL:HG22	2:h:154:TYR:HE1	1.86	0.41
1:A:219:ASN:HD21	1:X:181:LYS:HE2	1.85	0.41
1:M:247:ARG:HG2	1:M:247:ARG:NH1	2.33	0.41
1:Q:332:ASP:OD2	1:R:360:GLU:CD	2.62	0.41
1:W:247:ARG:HG2	1:W:247:ARG:NH1	2.33	0.41
2:a:123:VAL:HG22	2:a:154:TYR:HE1	1.86	0.41
2:d:123:VAL:HG22	2:d:154:TYR:HE1	1.86	0.41
2:f:123:VAL:HG22	2:f:154:TYR:HE1	1.86	0.41
2:i:123:VAL:HG22	2:i:154:TYR:HE1	1.86	0.41
2:j:123:VAL:HG22	2:j:154:TYR:HE1	1.86	0.41
2:m:123:VAL:HG22	2:m:154:TYR:HE1	1.85	0.41
2:t:109:ILE:HD11	2:u:132:TYR:HD2	1.83	0.41
2:v:123:VAL:HG22	2:v:154:TYR:HE1	1.86	0.41
1:C:205:LEU:HD11	2:Z:190:ARG:NH2	2.35	0.41
1:X:209:GLN:OE1	2:u:195:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:123:VAL:HG22	2:b:154:TYR:HE1	1.86	0.41
2:l:37:ALA:HB2	2:m:69:VAL:HG12	2.03	0.41
1:L:247:ARG:HG2	1:L:247:ARG:NH1	2.33	0.41
1:R:333:ASP:HB3	2:p:164:ILE:HD11	2.03	0.41
1:X:202:ARG:NH1	2:v:192:ASP:O	2.54	0.41
2:Y:110:GLU:OE2	2:v:112:ARG:NE	2.52	0.41
2:Y:123:VAL:HG22	2:Y:154:TYR:HE1	1.86	0.41
2:Y:170:PHE:HZ	2:Z:129:HIS:CD2	2.39	0.41
2:f:173:ASN:HB2	2:g:147:HIS:HB3	2.02	0.41
2:g:123:VAL:HG22	2:g:154:TYR:HE1	1.86	0.41
2:l:173:ASN:HB2	2:m:147:HIS:HB3	2.02	0.41
2:o:33:ASN:OD1	2:o:48:LYS:NZ	2.50	0.41
2:r:123:VAL:HG22	2:r:154:TYR:HE1	1.86	0.41
2:u:33:ASN:OD1	2:u:48:LYS:NZ	2.50	0.41
2:Z:123:VAL:HG22	2:Z:154:TYR:HE1	1.86	0.41
2:j:29:GLN:NE2	2:k:25:LYS:H	2.19	0.41
2:m:112:ARG:NH1	2:n:84:GLU:HG2	2.35	0.41
2:q:123:VAL:HG22	2:q:154:TYR:HE1	1.86	0.41
1:P:334:VAL:HG22	2:n:164:ILE:HG21	2.03	0.40
1:R:202:ARG:NH2	2:p:41:MET:HG3	2.35	0.40
1:X:202:ARG:HH21	2:v:41:MET:HG3	1.86	0.40
2:d:33:ASN:OD1	2:d:48:LYS:NZ	2.50	0.40
2:f:37:ALA:HB2	2:g:69:VAL:HG12	2.03	0.40
2:p:123:VAL:HG22	2:p:154:TYR:HE1	1.86	0.40
1:R:206:TRP:CE3	2:p:43:ASN:HB2	2.56	0.40
1:S:252:GLU:HA	1:S:253:PRO:HD3	1.91	0.40
1:X:247:ARG:HG2	1:X:247:ARG:NH1	2.33	0.40
1:E:247:ARG:HG2	1:E:247:ARG:NH1	2.33	0.40
1:K:338:ARG:NH1	1:L:358:ALA:CB	2.84	0.40
2:Y:25:LYS:H	2:v:29:GLN:NE2	2.19	0.40
2:c:33:ASN:OD1	2:c:48:LYS:NZ	2.50	0.40
2:s:29:GLN:NE2	2:t:25:LYS:H	2.19	0.40
1:A:247:ARG:HG2	1:A:247:ARG:NH1	2.33	0.40
1:D:247:ARG:HG2	1:D:247:ARG:NH1	2.33	0.40
1:E:252:GLU:HA	1:E:253:PRO:HD3	1.91	0.40
1:G:247:ARG:HG2	1:G:247:ARG:NH1	2.33	0.40
1:H:247:ARG:HG2	1:H:247:ARG:NH1	2.33	0.40
1:I:247:ARG:HG2	1:I:247:ARG:NH1	2.33	0.40
2:n:29:GLN:NE2	2:o:25:LYS:H	2.19	0.40
2:n:123:VAL:HG22	2:n:154:TYR:HE1	1.86	0.40
1:F:247:ARG:HG2	1:F:247:ARG:NH1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:247:ARG:HG2	1:J:247:ARG:NH1	2.33	0.40
1:X:205:LEU:HD11	2:u:190:ARG:NH2	2.37	0.40
2:b:173:ASN:HB2	2:c:147:HIS:HB3	2.03	0.40
2:r:29:GLN:NE2	2:s:25:LYS:H	2.19	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	A	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	B	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	C	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	D	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	E	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	F	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	G	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	H	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	I	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	J	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	K	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	L	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	M	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	N	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	O	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	P	192/392 (49%)	187 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	R	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	S	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	T	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	U	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	V	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	W	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
1	X	192/392 (49%)	187 (97%)	5 (3%)	0	100	100
2	Y	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	Z	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
2	a	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
2	b	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	c	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	d	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
2	e	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
2	f	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	g	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	h	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
2	i	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
2	j	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	k	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
2	l	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	m	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	n	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	o	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
2	p	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	q	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	r	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
2	s	182/252 (72%)	175 (96%)	7 (4%)	0	100	100
2	t	182/252 (72%)	176 (97%)	6 (3%)	0	100	100
2	u	182/252 (72%)	175 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	v	182/252 (72%)	174 (96%)	8 (4%)	0	100	100
All	All	8976/15456 (58%)	8689 (97%)	287 (3%)	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	A	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	B	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	C	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	D	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	E	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	F	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	G	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	H	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	I	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	J	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	K	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	L	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	M	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	N	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	O	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	P	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	Q	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	R	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	S	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	T	167/337 (50%)	161 (96%)	6 (4%)	31	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	V	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	W	167/337 (50%)	161 (96%)	6 (4%)	31	56
1	X	167/337 (50%)	161 (96%)	6 (4%)	31	56
2	Y	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	Z	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	a	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	b	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	c	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	d	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	e	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	f	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	g	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	h	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	i	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	j	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	k	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	l	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	m	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	n	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	o	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	p	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	q	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	r	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	s	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	t	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	u	155/215 (72%)	147 (95%)	8 (5%)	21	48
2	v	155/215 (72%)	147 (95%)	8 (5%)	21	48
All	All	7728/13248 (58%)	7392 (96%)	336 (4%)	27	52

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLU
1	A	217	ASP
1	A	247	ARG
1	A	271	GLU
1	A	295	ASP
1	A	333	ASP
1	B	182	GLU
1	B	217	ASP
1	B	247	ARG
1	B	271	GLU
1	B	295	ASP
1	B	333	ASP
1	C	182	GLU
1	C	217	ASP
1	C	247	ARG
1	C	271	GLU
1	C	295	ASP
1	C	333	ASP
1	D	182	GLU
1	D	217	ASP
1	D	247	ARG
1	D	271	GLU
1	D	295	ASP
1	D	333	ASP
1	E	182	GLU
1	E	217	ASP
1	E	247	ARG
1	E	271	GLU
1	E	295	ASP
1	E	333	ASP
1	F	182	GLU
1	F	217	ASP
1	F	247	ARG
1	F	271	GLU
1	F	295	ASP
1	F	333	ASP
1	G	182	GLU
1	G	217	ASP
1	G	247	ARG
1	G	271	GLU
1	G	295	ASP
1	G	333	ASP
1	H	182	GLU

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Mol	Chain	Res	Type
1	H	217	ASP
1	H	247	ARG
1	H	271	GLU
1	H	295	ASP
1	H	333	ASP
1	I	182	GLU
1	I	217	ASP
1	I	247	ARG
1	I	271	GLU
1	I	295	ASP
1	I	333	ASP
1	J	182	GLU
1	J	217	ASP
1	J	247	ARG
1	J	271	GLU
1	J	295	ASP
1	J	333	ASP
1	K	182	GLU
1	K	217	ASP
1	K	247	ARG
1	K	271	GLU
1	K	295	ASP
1	K	333	ASP
1	L	182	GLU
1	L	217	ASP
1	L	247	ARG
1	L	271	GLU
1	L	295	ASP
1	L	333	ASP
1	M	182	GLU
1	M	217	ASP
1	M	247	ARG
1	M	271	GLU
1	M	295	ASP
1	M	333	ASP
1	N	182	GLU
1	N	217	ASP
1	N	247	ARG
1	N	271	GLU
1	N	295	ASP
1	N	333	ASP
1	O	182	GLU

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Mol	Chain	Res	Type
1	O	217	ASP
1	O	247	ARG
1	O	271	GLU
1	O	295	ASP
1	O	333	ASP
1	P	182	GLU
1	P	217	ASP
1	P	247	ARG
1	P	271	GLU
1	P	295	ASP
1	P	333	ASP
1	Q	182	GLU
1	Q	217	ASP
1	Q	247	ARG
1	Q	271	GLU
1	Q	295	ASP
1	Q	333	ASP
1	R	182	GLU
1	R	217	ASP
1	R	247	ARG
1	R	271	GLU
1	R	295	ASP
1	R	333	ASP
1	S	182	GLU
1	S	217	ASP
1	S	247	ARG
1	S	271	GLU
1	S	295	ASP
1	S	333	ASP
1	T	182	GLU
1	T	217	ASP
1	T	247	ARG
1	T	271	GLU
1	T	295	ASP
1	T	333	ASP
1	U	182	GLU
1	U	217	ASP
1	U	247	ARG
1	U	271	GLU
1	U	295	ASP
1	U	333	ASP
1	V	182	GLU

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Mol	Chain	Res	Type
1	V	217	ASP
1	V	247	ARG
1	V	271	GLU
1	V	295	ASP
1	V	333	ASP
1	W	182	GLU
1	W	217	ASP
1	W	247	ARG
1	W	271	GLU
1	W	295	ASP
1	W	333	ASP
1	X	182	GLU
1	X	217	ASP
1	X	247	ARG
1	X	271	GLU
1	X	295	ASP
1	X	333	ASP
2	Y	30	GLU
2	Y	51	SER
2	Y	62	GLU
2	Y	121	GLU
2	Y	135	ASP
2	Y	163	GLN
2	Y	192	ASP
2	Y	202	VAL
2	Z	30	GLU
2	Z	51	SER
2	Z	62	GLU
2	Z	121	GLU
2	Z	135	ASP
2	Z	163	GLN
2	Z	192	ASP
2	Z	202	VAL
2	a	30	GLU
2	a	51	SER
2	a	62	GLU
2	a	121	GLU
2	a	135	ASP
2	a	163	GLN
2	a	192	ASP
2	a	202	VAL
2	b	30	GLU

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Mol	Chain	Res	Type
2	b	51	SER
2	b	62	GLU
2	b	121	GLU
2	b	135	ASP
2	b	163	GLN
2	b	192	ASP
2	b	202	VAL
2	c	30	GLU
2	c	51	SER
2	c	62	GLU
2	c	121	GLU
2	c	135	ASP
2	c	163	GLN
2	c	192	ASP
2	c	202	VAL
2	d	30	GLU
2	d	51	SER
2	d	62	GLU
2	d	121	GLU
2	d	135	ASP
2	d	163	GLN
2	d	192	ASP
2	d	202	VAL
2	e	30	GLU
2	e	51	SER
2	e	62	GLU
2	e	121	GLU
2	e	135	ASP
2	e	163	GLN
2	e	192	ASP
2	e	202	VAL
2	f	30	GLU
2	f	51	SER
2	f	62	GLU
2	f	121	GLU
2	f	135	ASP
2	f	163	GLN
2	f	192	ASP
2	f	202	VAL
2	g	30	GLU
2	g	51	SER
2	g	62	GLU

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Mol	Chain	Res	Type
2	g	121	GLU
2	g	135	ASP
2	g	163	GLN
2	g	192	ASP
2	g	202	VAL
2	h	30	GLU
2	h	51	SER
2	h	62	GLU
2	h	121	GLU
2	h	135	ASP
2	h	163	GLN
2	h	192	ASP
2	h	202	VAL
2	i	30	GLU
2	i	51	SER
2	i	62	GLU
2	i	121	GLU
2	i	135	ASP
2	i	163	GLN
2	i	192	ASP
2	i	202	VAL
2	j	30	GLU
2	j	51	SER
2	j	62	GLU
2	j	121	GLU
2	j	135	ASP
2	j	163	GLN
2	j	192	ASP
2	j	202	VAL
2	k	30	GLU
2	k	51	SER
2	k	62	GLU
2	k	121	GLU
2	k	135	ASP
2	k	163	GLN
2	k	192	ASP
2	k	202	VAL
2	l	30	GLU
2	l	51	SER
2	l	62	GLU
2	l	121	GLU
2	l	135	ASP

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Mol	Chain	Res	Type
2	l	163	GLN
2	l	192	ASP
2	l	202	VAL
2	m	30	GLU
2	m	51	SER
2	m	62	GLU
2	m	121	GLU
2	m	135	ASP
2	m	163	GLN
2	m	192	ASP
2	m	202	VAL
2	n	30	GLU
2	n	51	SER
2	n	62	GLU
2	n	121	GLU
2	n	135	ASP
2	n	163	GLN
2	n	192	ASP
2	n	202	VAL
2	o	30	GLU
2	o	51	SER
2	o	62	GLU
2	o	121	GLU
2	o	135	ASP
2	o	163	GLN
2	o	192	ASP
2	o	202	VAL
2	p	30	GLU
2	p	51	SER
2	p	62	GLU
2	p	121	GLU
2	p	135	ASP
2	p	163	GLN
2	p	192	ASP
2	p	202	VAL
2	q	30	GLU
2	q	51	SER
2	q	62	GLU
2	q	121	GLU
2	q	135	ASP
2	q	163	GLN
2	q	192	ASP

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Mol	Chain	Res	Type
2	q	202	VAL
2	r	30	GLU
2	r	51	SER
2	r	62	GLU
2	r	121	GLU
2	r	135	ASP
2	r	163	GLN
2	r	192	ASP
2	r	202	VAL
2	s	30	GLU
2	s	51	SER
2	s	62	GLU
2	s	121	GLU
2	s	135	ASP
2	s	163	GLN
2	s	192	ASP
2	s	202	VAL
2	t	30	GLU
2	t	51	SER
2	t	62	GLU
2	t	121	GLU
2	t	135	ASP
2	t	163	GLN
2	t	192	ASP
2	t	202	VAL
2	u	30	GLU
2	u	51	SER
2	u	62	GLU
2	u	121	GLU
2	u	135	ASP
2	u	163	GLN
2	u	192	ASP
2	u	202	VAL
2	v	30	GLU
2	v	51	SER
2	v	62	GLU
2	v	121	GLU
2	v	135	ASP
2	v	163	GLN
2	v	192	ASP
2	v	202	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	318	ASN
1	A	356	GLN
1	B	310	GLN
1	B	318	ASN
1	C	242	GLN
1	C	318	ASN
1	C	356	GLN
1	D	310	GLN
1	D	318	ASN
1	E	310	GLN
1	E	318	ASN
1	E	356	GLN
1	F	219	ASN
1	F	242	GLN
1	F	310	GLN
1	F	318	ASN
1	F	356	GLN
1	G	310	GLN
1	G	318	ASN
1	G	356	GLN
1	H	310	GLN
1	H	318	ASN
1	H	356	GLN
1	I	310	GLN
1	I	318	ASN
1	I	356	GLN
1	J	318	ASN
1	J	356	GLN
1	K	310	GLN
1	K	318	ASN
1	L	219	ASN
1	L	242	GLN
1	L	310	GLN
1	L	318	ASN
1	L	356	GLN
1	M	310	GLN
1	M	318	ASN
1	M	356	GLN
1	N	310	GLN
1	N	318	ASN
1	N	356	GLN

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Mol	Chain	Res	Type
1	O	219	ASN
1	O	318	ASN
1	O	356	GLN
1	P	310	GLN
1	P	318	ASN
1	Q	310	GLN
1	Q	318	ASN
1	Q	356	GLN
1	R	219	ASN
1	R	242	GLN
1	R	310	GLN
1	R	318	ASN
1	R	356	GLN
1	S	310	GLN
1	S	318	ASN
1	S	356	GLN
1	T	219	ASN
1	T	310	GLN
1	T	318	ASN
1	T	356	GLN
1	U	310	GLN
1	U	318	ASN
1	U	356	GLN
1	V	310	GLN
1	V	318	ASN
1	V	356	GLN
1	W	310	GLN
1	W	318	ASN
1	W	356	GLN
1	X	310	GLN
1	X	318	ASN
1	X	356	GLN
2	Z	111	GLN
2	a	29	GLN
2	a	173	ASN
2	b	129	HIS
2	c	111	GLN
2	d	43	ASN
2	e	29	GLN
2	h	162	HIS
2	j	29	GLN
2	k	129	HIS

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Mol	Chain	Res	Type
2	n	162	HIS
2	o	162	HIS
2	p	129	HIS
2	q	29	GLN
2	r	29	GLN
2	r	129	HIS
2	s	129	HIS
2	s	162	HIS
2	t	162	HIS
2	u	29	GLN
2	u	162	HIS
2	v	29	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](#)

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.

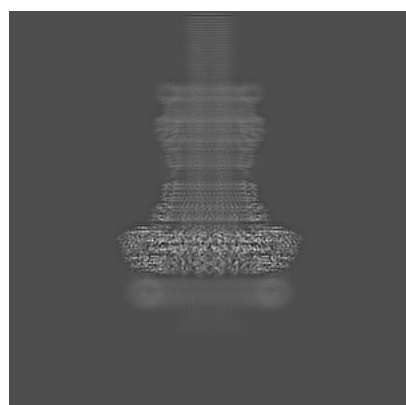
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8913. These allow visual inspection of the internal detail of the map and identification of artifacts.

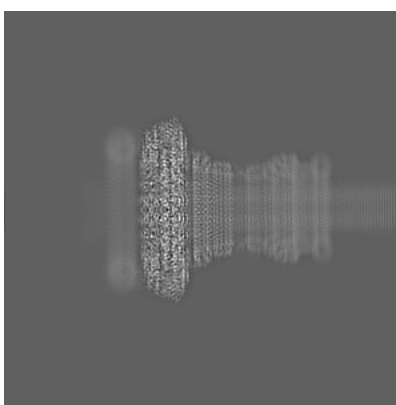
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

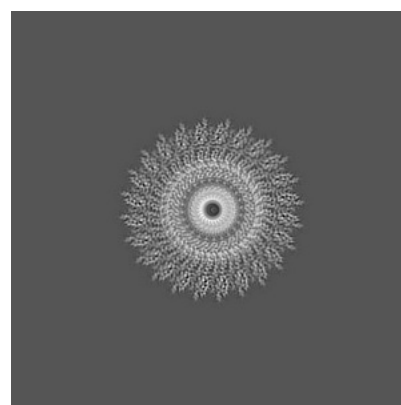
6.1.1 Primary map



X



Y

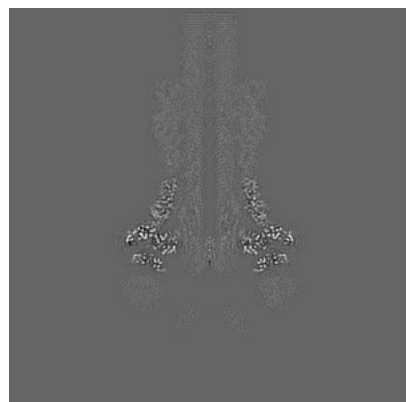


Z

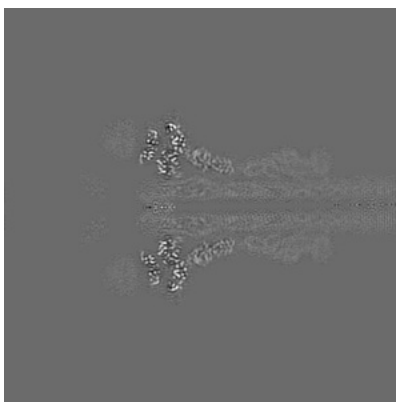
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

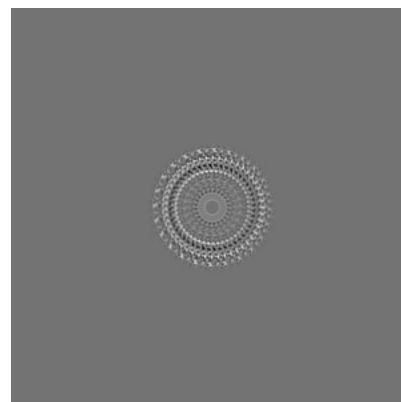
6.2.1 Primary map



X Index: 150



Y Index: 150

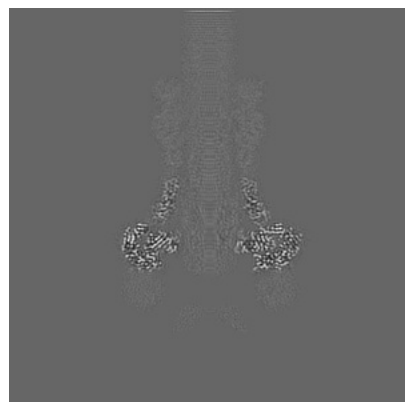


Z Index: 150

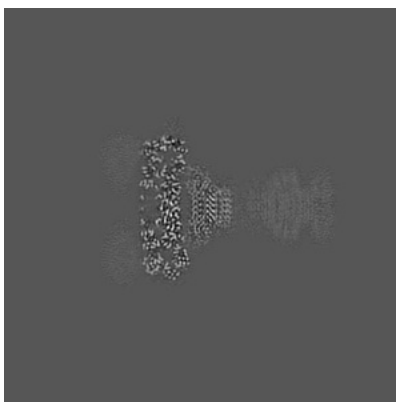
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

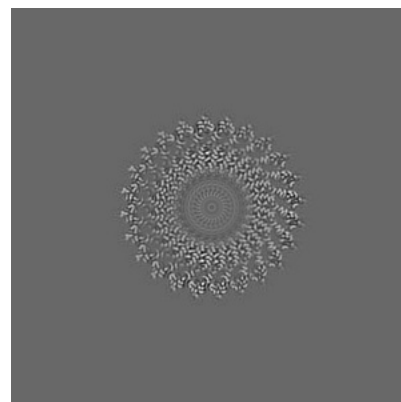
6.3.1 Primary map



X Index: 143



Y Index: 117

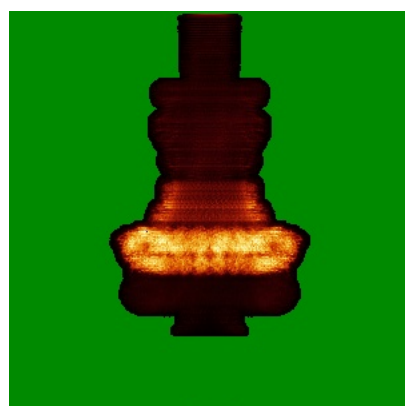


Z Index: 126

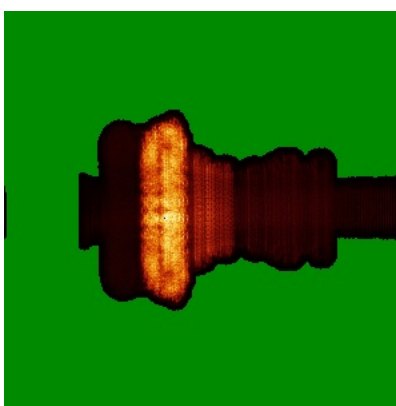
The images above show the largest variance slices of the map in three orthogonal directions.

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

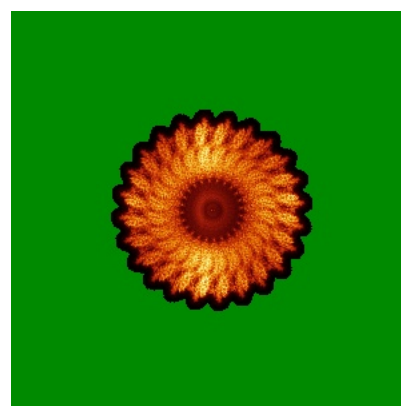
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

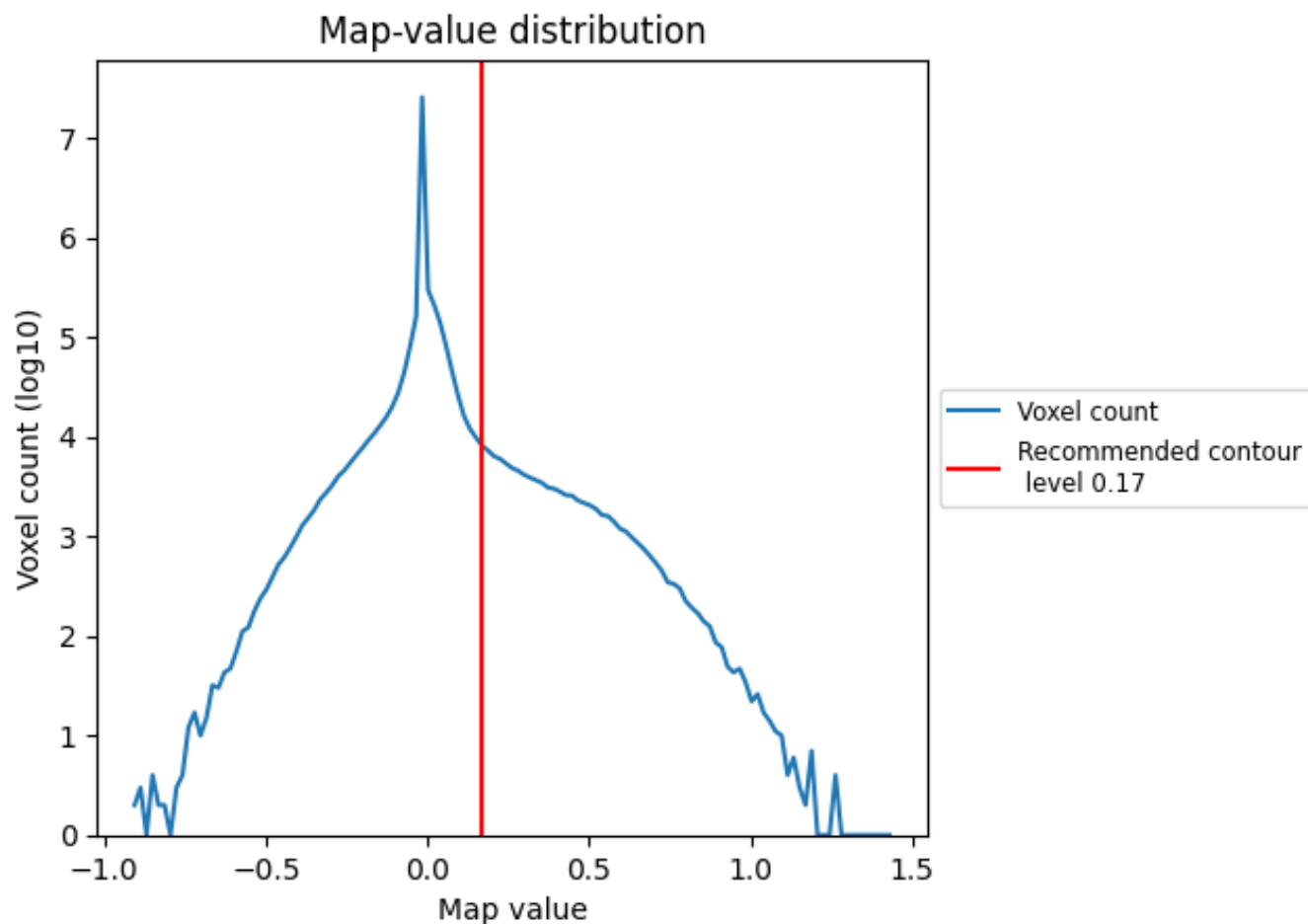
6.6 Mask visualisation

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

7 Map analysis [i](#)

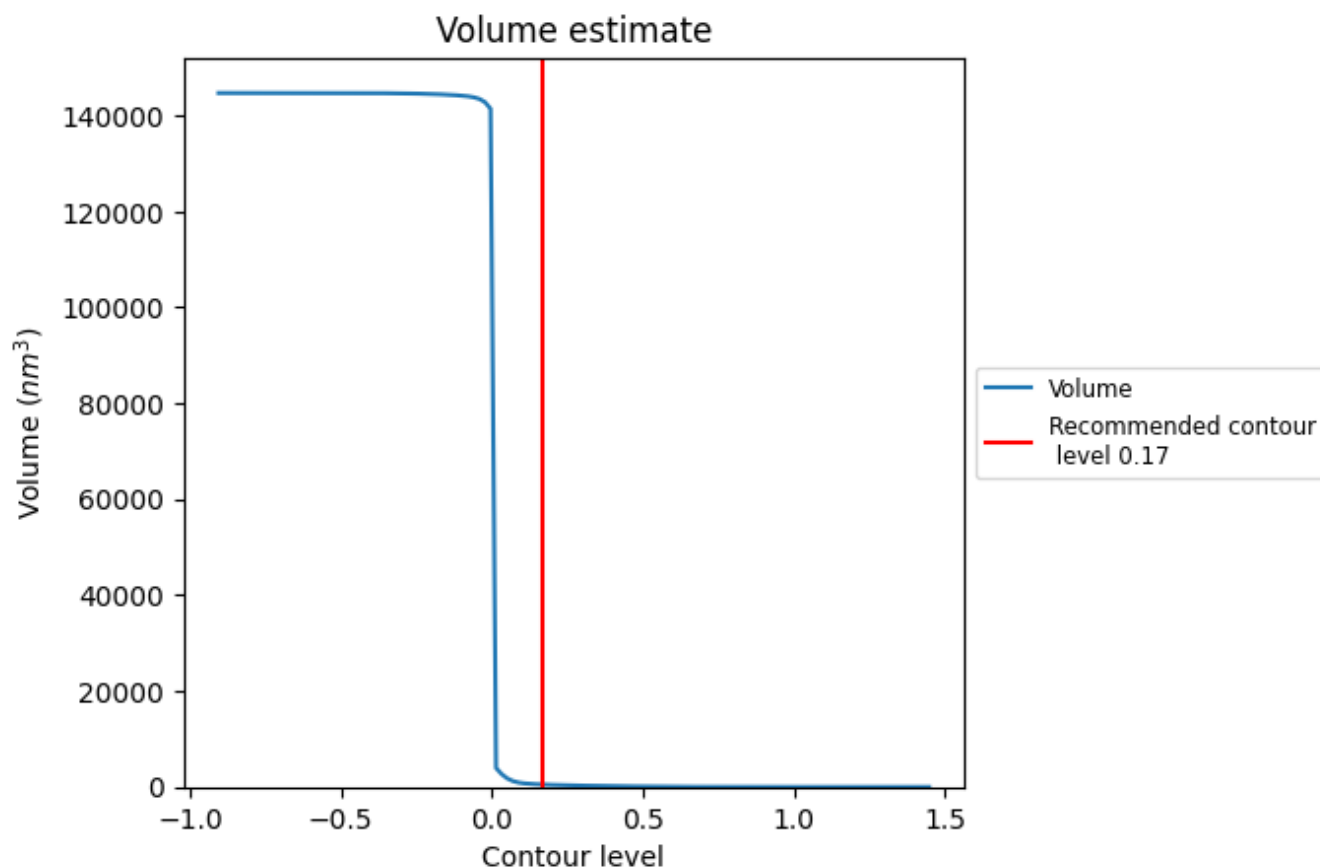
This section contains the results of statistical analysis of the map.

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.

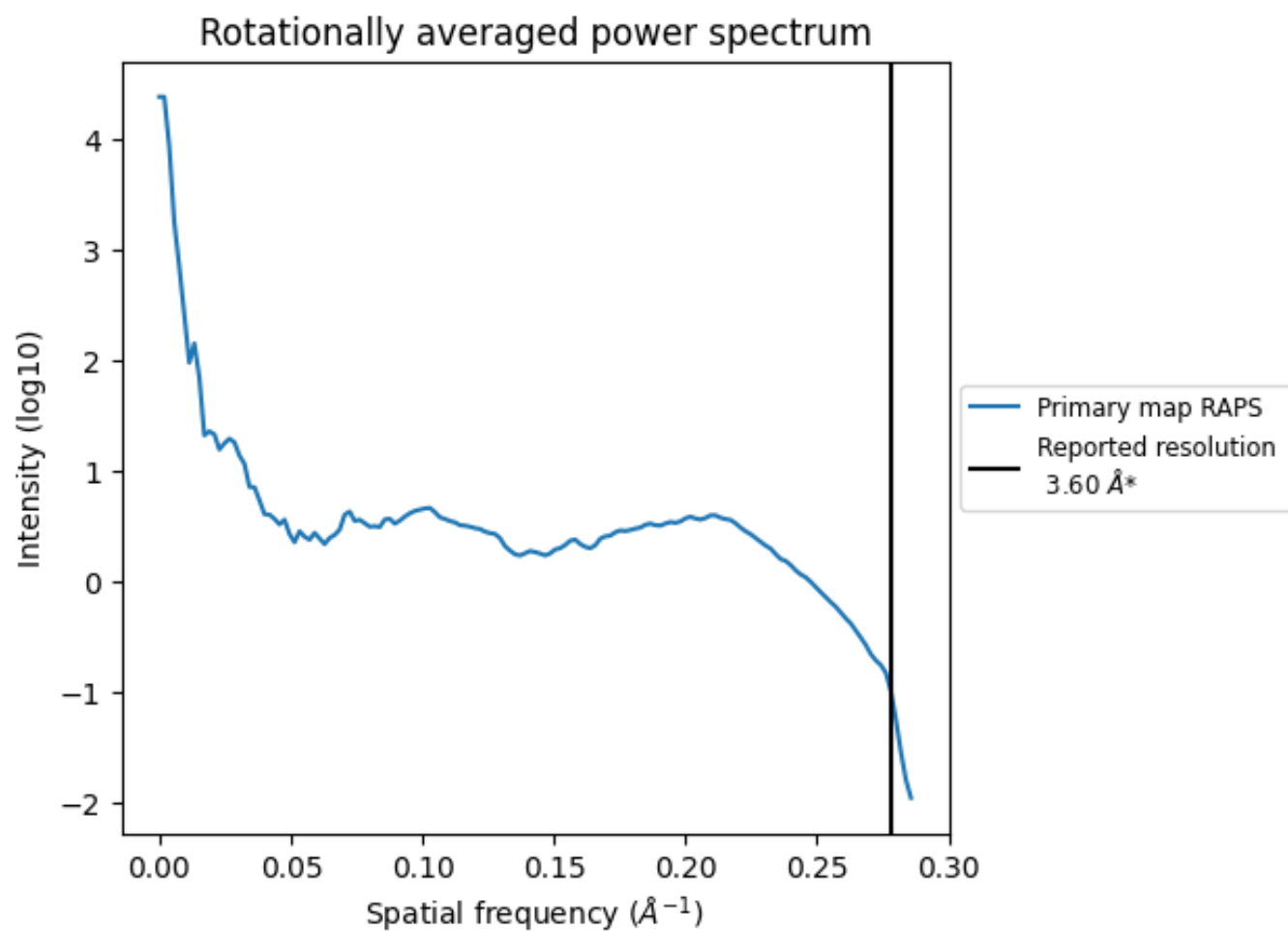
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 502 nm³; this corresponds to an approximate mass of 454 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 0.278 Å⁻¹

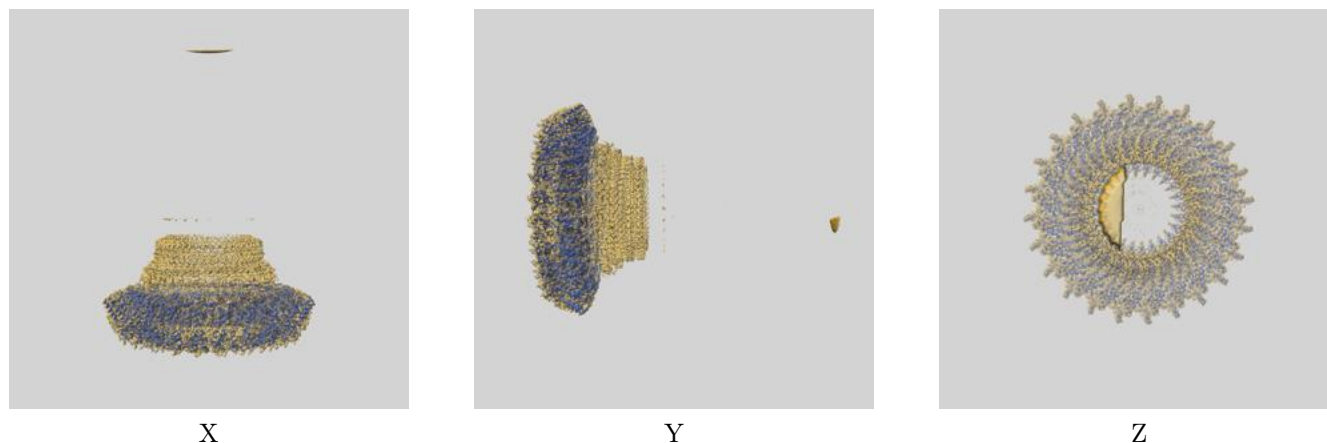
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

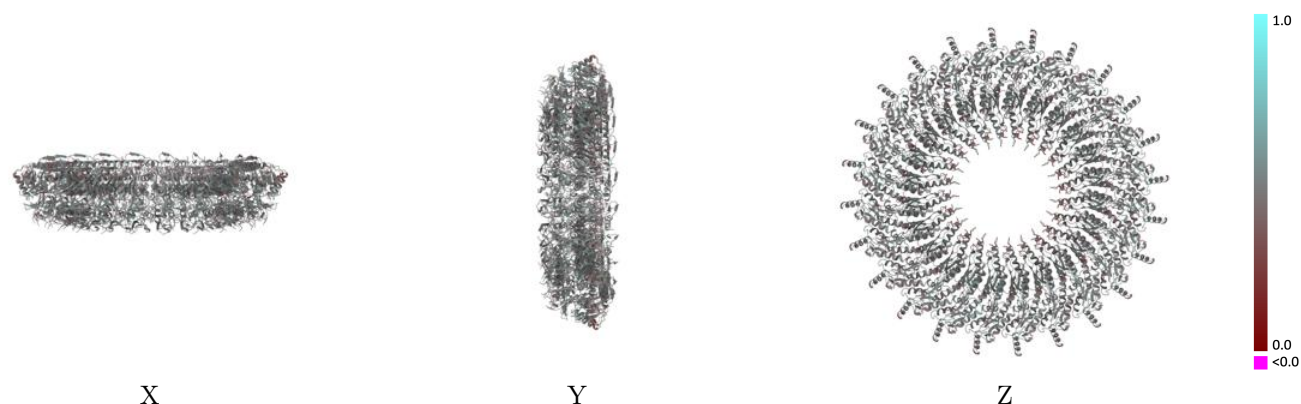
This section contains information regarding the fit between EMDB map EMD-8913 and PDB model 6DUZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



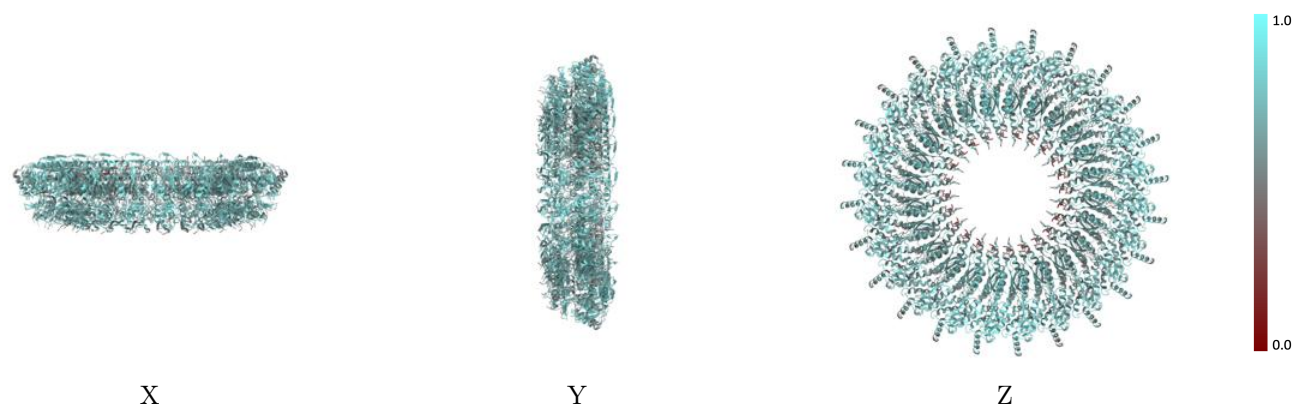
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



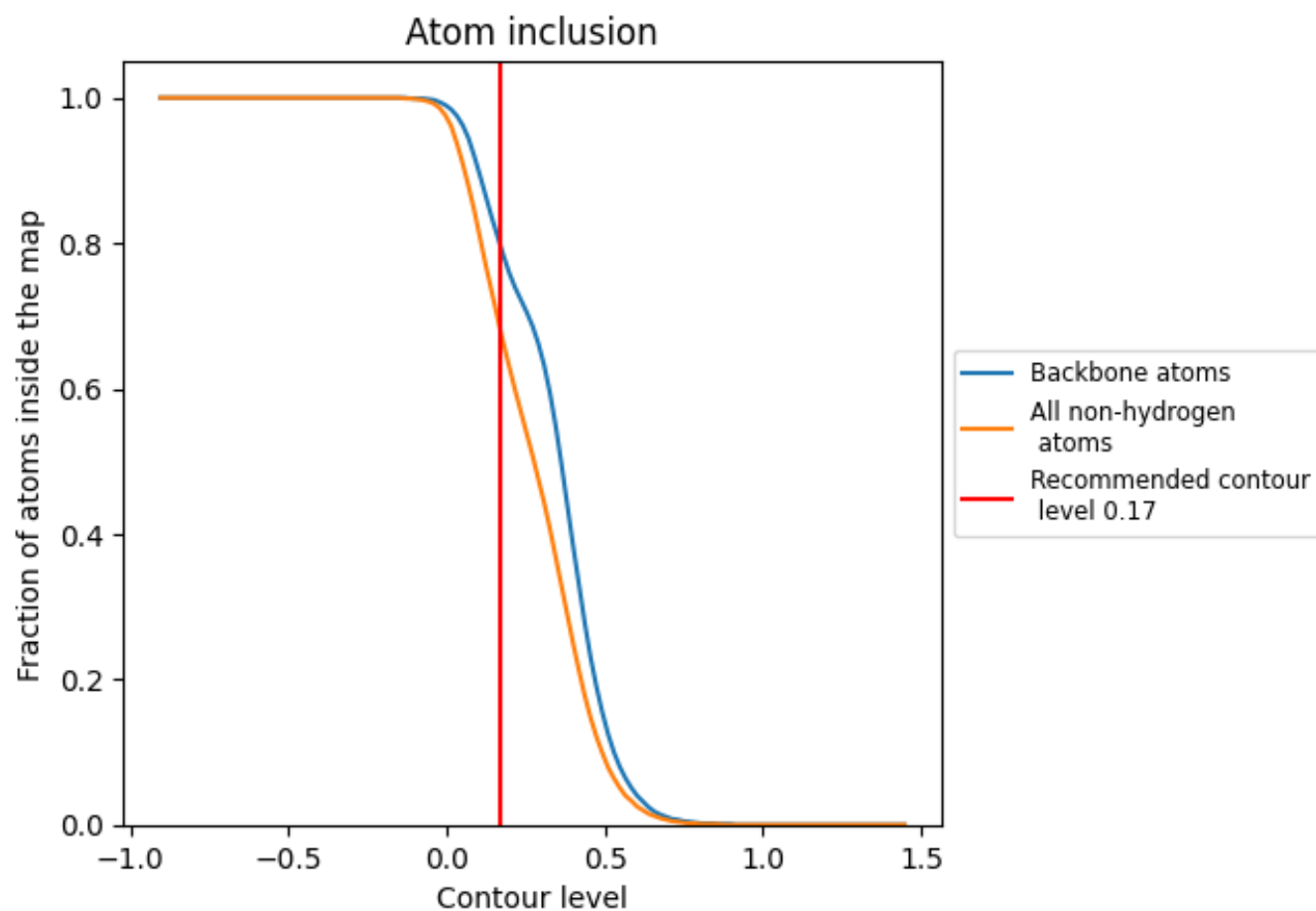
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6800	 0.4730
A	 0.6710	 0.4680
B	 0.6500	 0.4770
C	 0.6820	 0.4780
D	 0.7210	 0.4800
E	 0.7410	 0.4850
F	 0.6930	 0.4700
G	 0.6580	 0.4760
H	 0.6630	 0.4740
I	 0.6950	 0.4760
J	 0.7030	 0.4770
K	 0.6980	 0.4760
L	 0.6620	 0.4680
M	 0.6580	 0.4680
N	 0.6860	 0.4750
O	 0.7330	 0.4850
P	 0.7480	 0.4640
Q	 0.7420	 0.4780
R	 0.6780	 0.4710
S	 0.6670	 0.4790
T	 0.6730	 0.4700
U	 0.7000	 0.4790
V	 0.7180	 0.4790
W	 0.7370	 0.4830
X	 0.7100	 0.4840
Y	 0.6440	 0.4760
Z	 0.6510	 0.4560
a	 0.6800	 0.4560
b	 0.7160	 0.4790
c	 0.7040	 0.4670
d	 0.6760	 0.4720
e	 0.6610	 0.4710
f	 0.6530	 0.4690
g	 0.6540	 0.4740
h	 0.6500	 0.4770



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Chain	Atom inclusion	Q-score
i	 0.6490	 0.4700
j	 0.6410	 0.4710
k	 0.6470	 0.4680
l	 0.6780	 0.4780
m	 0.7030	 0.4840
n	 0.7110	 0.4760
o	 0.6720	 0.4750
p	 0.6340	 0.4620
q	 0.6140	 0.4620
r	 0.6290	 0.4620
s	 0.6440	 0.4710
t	 0.6640	 0.4650
u	 0.6630	 0.4580
v	 0.6530	 0.4750