



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:57 AM UTC

PDB ID : 1HB7 / pdb_00001hb7
EMDB ID : EMD-1013
Title : quasi-atomic resolution model of bacteriophage PRD1 sus1 mutant, obtained by combined cryo-EM and X-ray crystallography.
Authors : San Martin, C.; Burnett, R.M.; De Haas, F.; Heinkel, R.; Rutten, T.; Fuller, S.D.; Butcher, S.J.; Bamford, D.H.
Deposited on : 2001-04-12
Resolution : 14.00 Å(reported)
Based on initial model : 1HX6

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

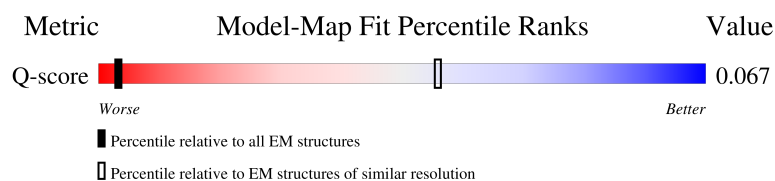
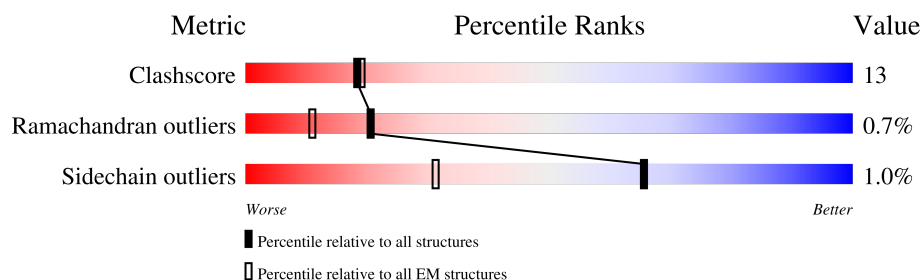
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 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	61 (13.50 - 14.50)

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	394	11% 77% 16% • 6%
1	B	394	10% 76% 16% • 5%
1	C	394	11% 79% 14% • 6%
1	D	394	10% 73% 20% • 6%

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Mol	Chain	Length	Quality of chain
1	E	394	
1	F	394	
1	G	394	
1	H	394	
1	I	394	
1	J	394	
1	K	394	
1	L	394	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34180 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.

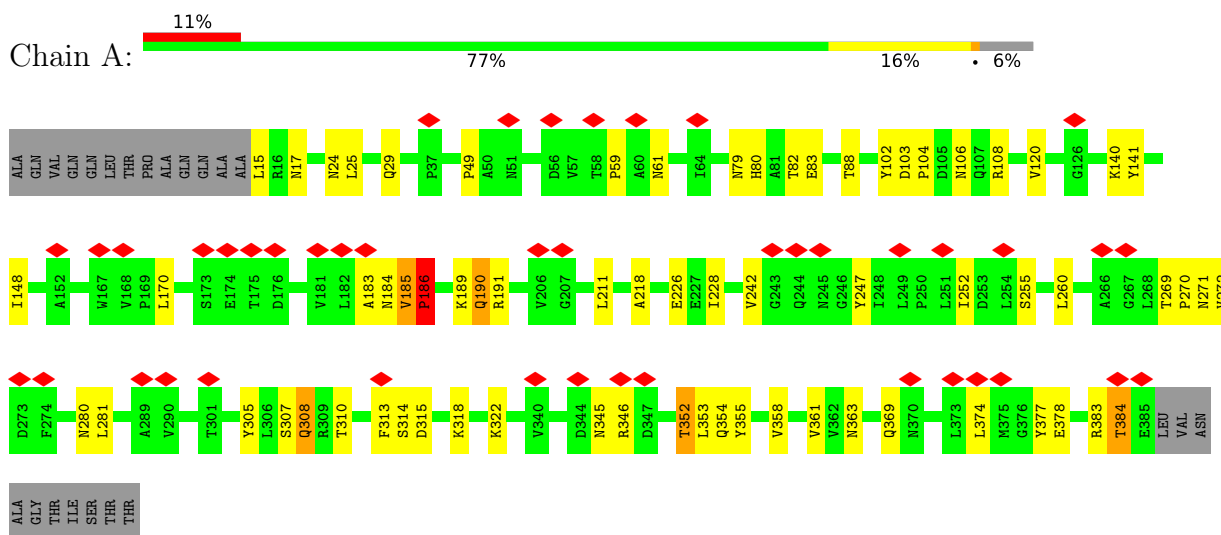
- Molecule 1 is a protein called BACTERIOPHAGE PRD1 SUS1 MUTANT CAPSID.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	B	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	C	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	D	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	E	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	F	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	G	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	H	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	I	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	J	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	K	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	L	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		

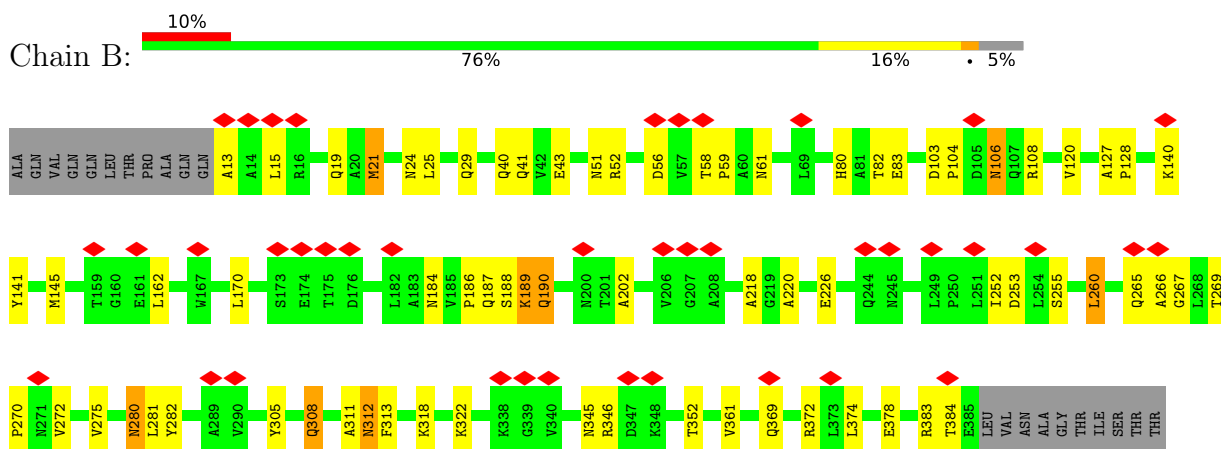
3 Residue-property plots

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.

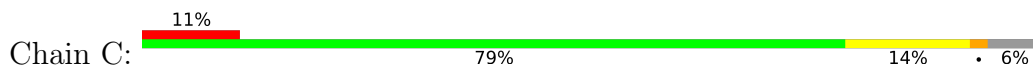
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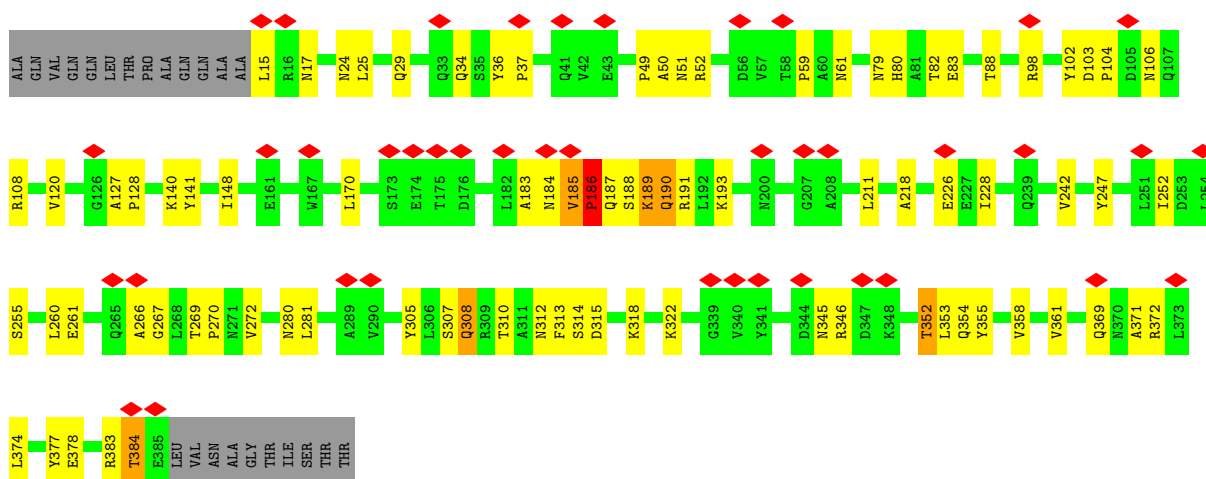
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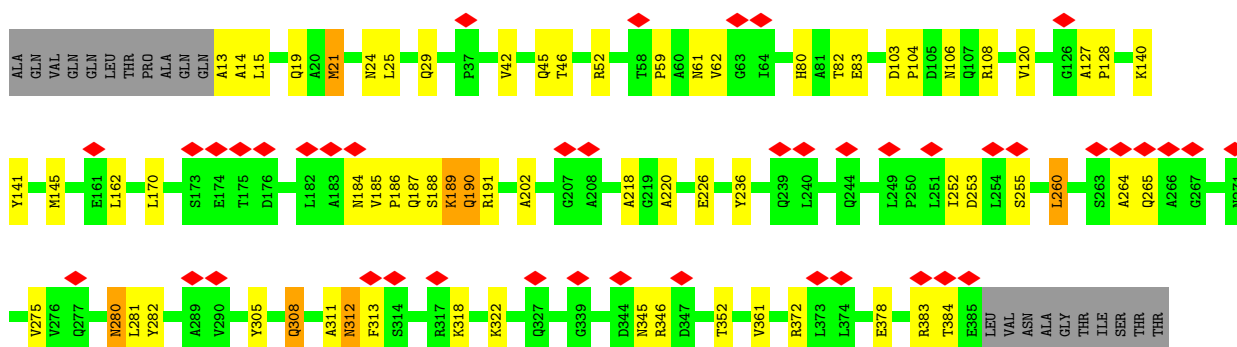
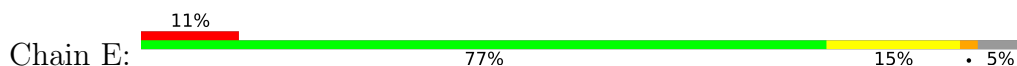
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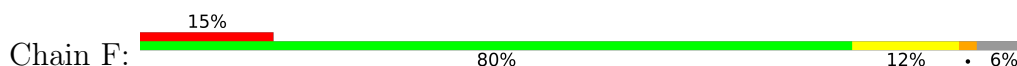
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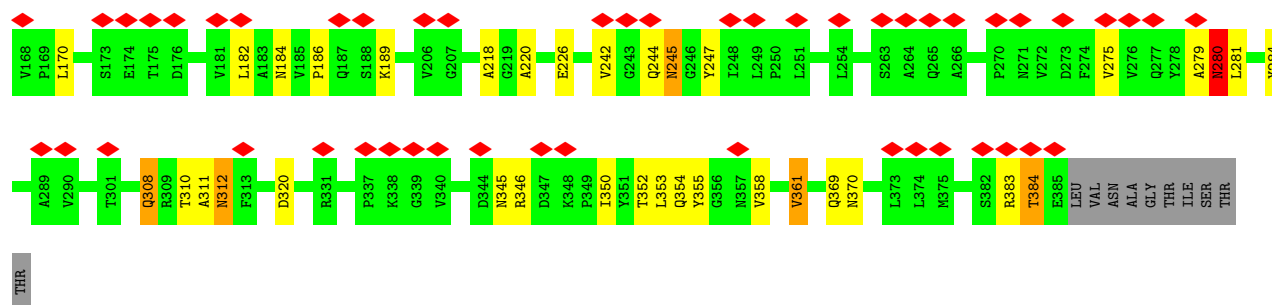


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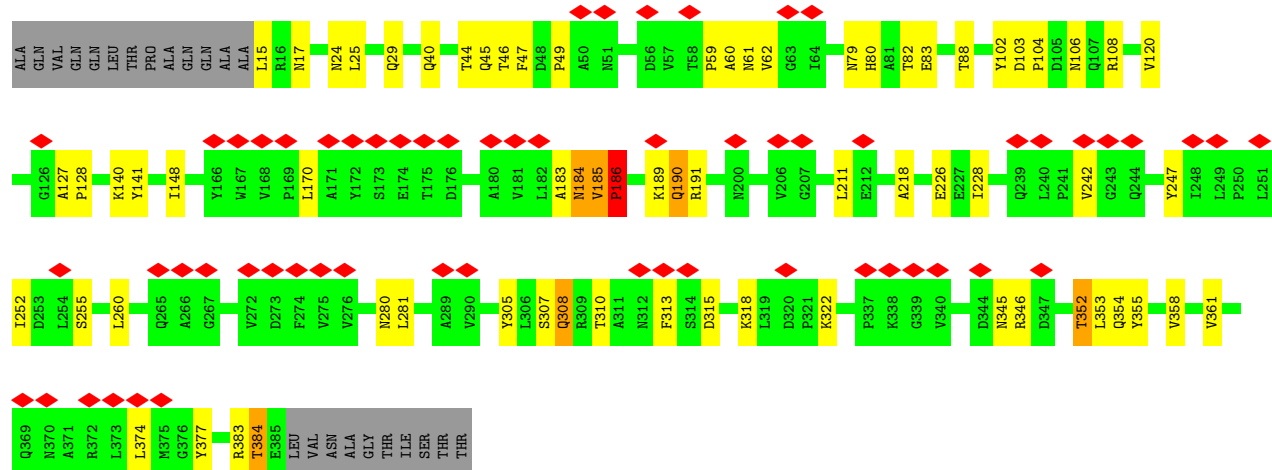
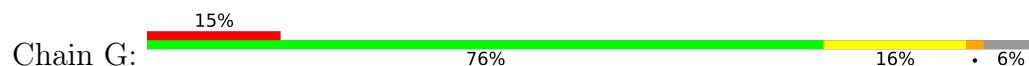


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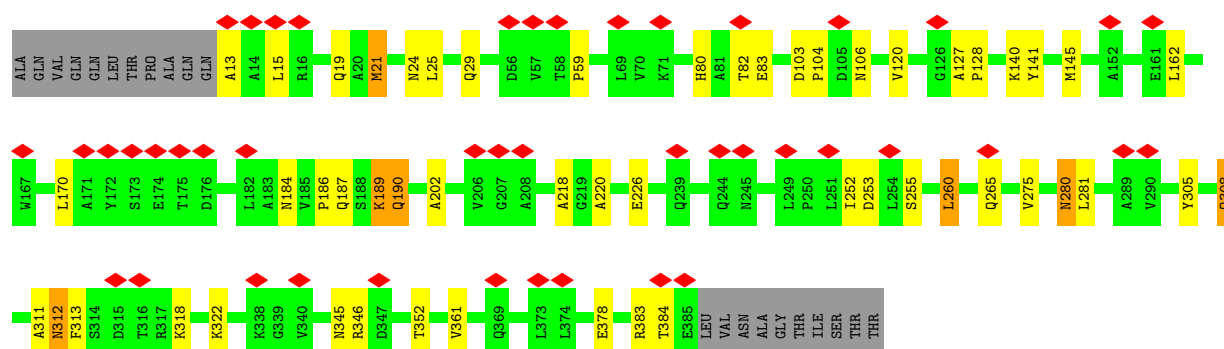
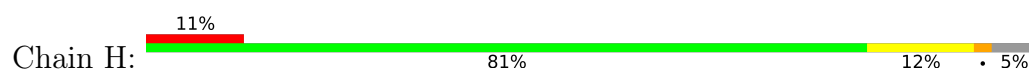




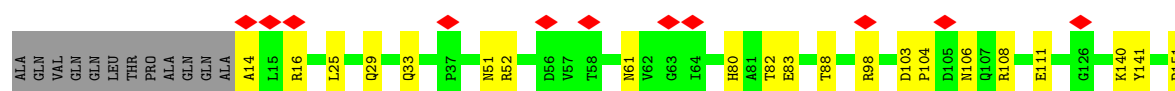
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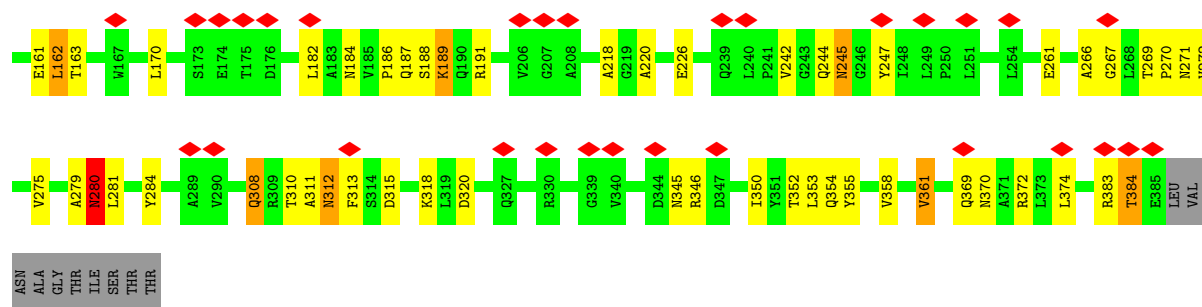


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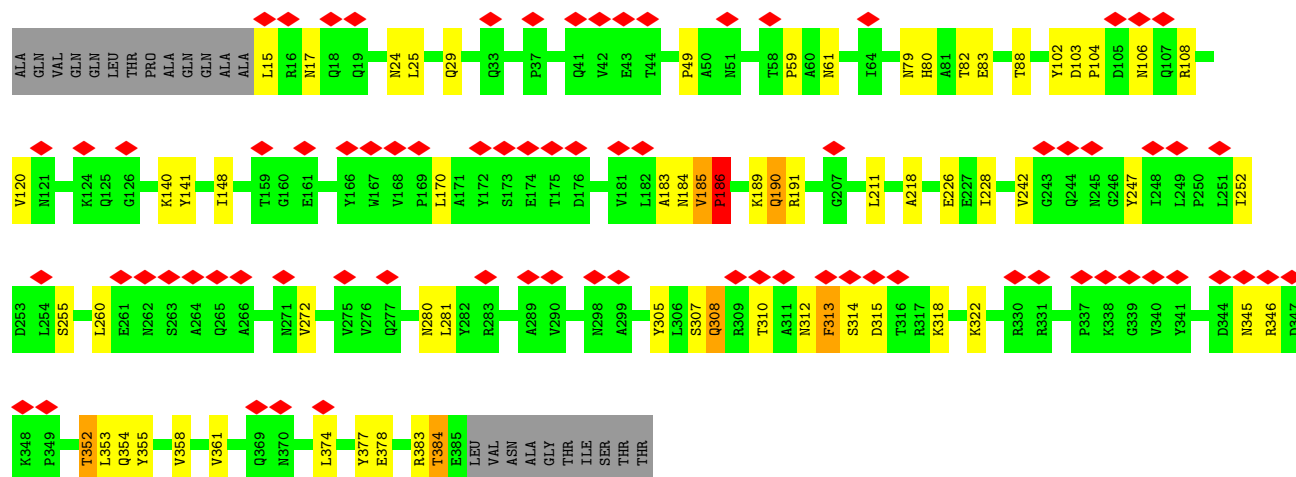
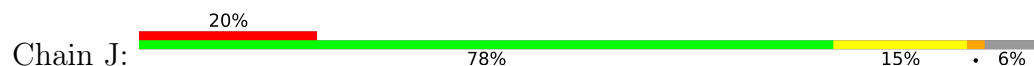


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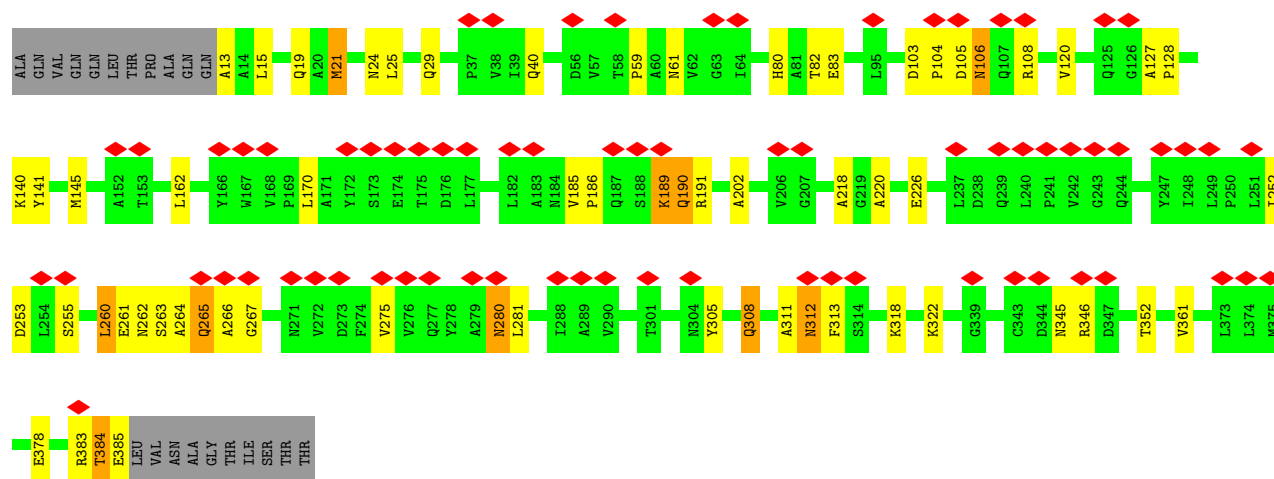
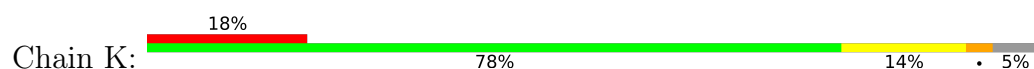




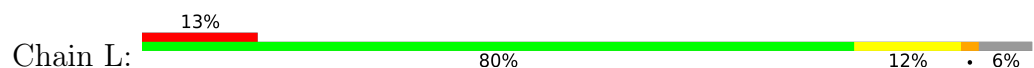
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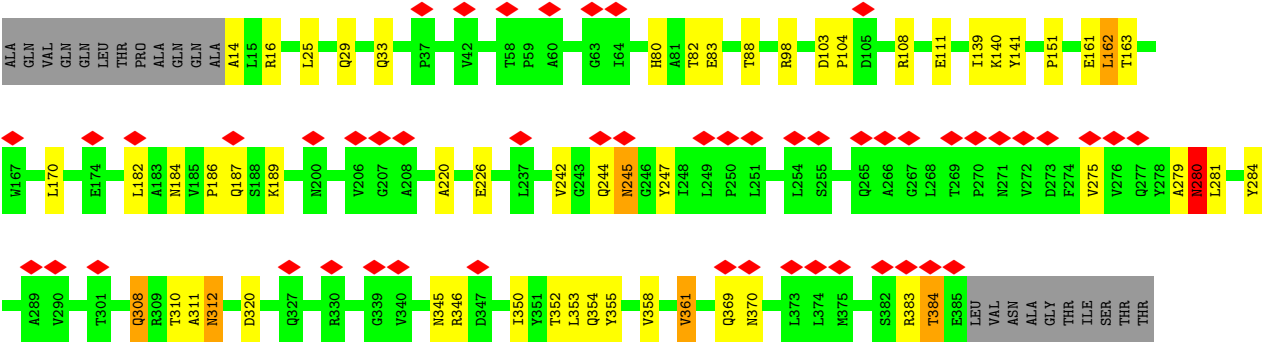


• Molecule 1: BACTERIOPHAGE PRD1 SUS1 MUTANT CAPSID



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1800	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	36000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	8.051	Depositor
Minimum map value	-4.790	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.3	Depositor
Map size ($\text{\AA}$)	880.64, 880.64, 880.64	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	3.44, 3.44, 3.44	Depositor

5 Model quality

5.1 Standard geometry

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	0.48	1/2902 (0.0%)	1.00	13/3971 (0.3%)
1	B	0.51	1/2910 (0.0%)	0.99	12/3982 (0.3%)
1	C	0.49	1/2926 (0.0%)	1.00	13/4003 (0.3%)
1	D	0.48	1/2902 (0.0%)	1.01	14/3971 (0.4%)
1	E	0.51	1/2910 (0.0%)	0.99	12/3982 (0.3%)
1	F	0.49	1/2926 (0.0%)	1.00	14/4003 (0.3%)
1	G	0.48	1/2902 (0.0%)	1.00	13/3971 (0.3%)
1	H	0.51	1/2910 (0.0%)	0.99	12/3982 (0.3%)
1	I	0.49	1/2926 (0.0%)	1.00	13/4003 (0.3%)
1	J	0.48	1/2902 (0.0%)	1.00	13/3971 (0.3%)
1	K	0.51	1/2910 (0.0%)	0.99	12/3982 (0.3%)
1	L	0.49	1/2926 (0.0%)	1.00	14/4003 (0.3%)
All	All	0.49	12/34952 (0.0%)	1.00	155/47824 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	384	THR	C-N	-7.16	1.23	1.33
1	A	384	THR	C-N	-7.14	1.23	1.33
1	I	384	THR	C-N	-7.13	1.23	1.33
1	E	384	THR	C-N	-7.11	1.23	1.33
1	K	384	THR	C-N	-7.11	1.23	1.33
1	L	384	THR	C-N	-7.07	1.23	1.33
1	D	384	THR	C-N	-7.06	1.23	1.33
1	G	384	THR	C-N	-7.04	1.23	1.33
1	F	384	THR	C-N	-7.03	1.23	1.33
1	H	384	THR	C-N	-7.01	1.23	1.33
1	B	384	THR	C-N	-7.00	1.23	1.33
1	C	384	THR	C-N	-7.00	1.23	1.33

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	170	LEU	N-CA-C	-10.86	97.56	112.12
1	D	170	LEU	N-CA-C	-10.84	97.59	112.12
1	G	170	LEU	N-CA-C	-10.82	97.62	112.12
1	A	170	LEU	N-CA-C	-10.81	97.64	112.12
1	F	170	LEU	N-CA-C	-10.56	97.97	112.12
1	C	170	LEU	N-CA-C	-10.56	97.97	112.12
1	I	170	LEU	N-CA-C	-10.46	98.10	112.12
1	L	170	LEU	N-CA-C	-10.46	98.10	112.12
1	E	170	LEU	N-CA-C	-9.78	99.01	112.12
1	B	170	LEU	N-CA-C	-9.55	99.05	112.13
1	K	170	LEU	N-CA-C	-9.55	99.04	112.13
1	H	170	LEU	N-CA-C	-9.54	99.07	112.13
1	G	184	ASN	N-CA-C	-9.01	101.55	112.54
1	J	184	ASN	N-CA-C	-9.01	101.55	112.54
1	A	184	ASN	N-CA-C	-8.94	101.64	112.54
1	D	184	ASN	N-CA-C	-8.93	101.65	112.54
1	C	141	TYR	N-CA-C	-8.05	100.15	110.53
1	I	141	TYR	N-CA-C	-8.04	100.15	110.53
1	L	141	TYR	N-CA-C	-7.99	100.22	110.53
1	F	141	TYR	N-CA-C	-7.95	100.27	110.53
1	F	226	GLU	N-CA-C	-7.78	103.40	113.12
1	G	226	GLU	N-CA-C	-7.75	102.16	111.69
1	A	226	GLU	N-CA-C	-7.74	102.17	111.69
1	I	226	GLU	N-CA-C	-7.72	103.47	113.12
1	C	226	GLU	N-CA-C	-7.71	103.48	113.12
1	L	226	GLU	N-CA-C	-7.68	103.52	113.12
1	J	226	GLU	N-CA-C	-7.68	102.25	111.69
1	J	141	TYR	N-CA-C	-7.63	101.02	110.41
1	D	226	GLU	N-CA-C	-7.63	102.31	111.69
1	G	141	TYR	N-CA-C	-7.62	101.04	110.41
1	B	226	GLU	N-CA-C	-7.61	102.33	111.69
1	H	226	GLU	N-CA-C	-7.60	102.34	111.69
1	K	226	GLU	N-CA-C	-7.60	102.34	111.69
1	A	141	TYR	N-CA-C	-7.59	101.08	110.41
1	D	141	TYR	N-CA-C	-7.57	101.10	110.41
1	E	226	GLU	N-CA-C	-7.56	102.39	111.69
1	C	140	LYS	N-CA-C	7.33	122.06	110.70
1	L	140	LYS	N-CA-C	7.32	122.05	110.70
1	B	190	GLN	N-CA-C	-7.32	99.98	110.59
1	I	140	LYS	N-CA-C	7.31	122.03	110.70
1	H	190	GLN	N-CA-C	-7.30	100.00	110.59
1	F	140	LYS	N-CA-C	7.30	122.02	110.70
1	B	141	TYR	N-CA-C	-7.28	101.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	190	GLN	N-CA-C	-7.28	100.03	110.59
1	E	190	GLN	N-CA-C	-7.27	100.05	110.59
1	H	141	TYR	N-CA-C	-7.25	101.17	110.53
1	K	141	TYR	N-CA-C	-7.23	101.20	110.53
1	E	141	TYR	N-CA-C	-7.22	101.22	110.53
1	D	352	THR	N-CA-C	6.88	118.58	111.14
1	G	352	THR	N-CA-C	6.85	118.54	111.14
1	J	352	THR	N-CA-C	6.84	118.53	111.14
1	A	352	THR	N-CA-C	6.84	118.52	111.14
1	F	354	GLN	N-CA-C	-6.64	105.72	113.88
1	C	354	GLN	N-CA-C	-6.62	105.73	113.88
1	L	354	GLN	N-CA-C	-6.62	105.74	113.88
1	I	354	GLN	N-CA-C	-6.61	105.75	113.88
1	J	361	VAL	N-CA-C	6.31	117.69	108.53
1	D	361	VAL	N-CA-C	6.31	117.68	108.53
1	G	361	VAL	N-CA-C	6.29	117.65	108.53
1	A	361	VAL	N-CA-C	6.29	117.65	108.53
1	L	361	VAL	N-CA-C	6.22	117.44	108.48
1	C	220	ALA	N-CA-C	6.20	118.56	111.11
1	L	220	ALA	N-CA-C	6.20	118.55	111.11
1	F	220	ALA	N-CA-C	6.20	118.55	111.11
1	I	361	VAL	N-CA-C	6.19	117.40	108.48
1	F	361	VAL	N-CA-C	6.19	117.39	108.48
1	B	361	VAL	N-CA-C	6.17	117.36	108.48
1	C	361	VAL	N-CA-C	6.16	117.35	108.48
1	E	220	ALA	N-CA-C	6.15	118.77	111.33
1	B	220	ALA	N-CA-C	6.13	118.75	111.33
1	H	361	VAL	N-CA-C	6.12	117.30	108.48
1	H	220	ALA	N-CA-C	6.12	118.74	111.33
1	I	220	ALA	N-CA-C	6.12	118.46	111.11
1	K	361	VAL	N-CA-C	6.12	117.29	108.48
1	K	220	ALA	N-CA-C	6.09	118.70	111.33
1	E	361	VAL	N-CA-C	6.08	117.23	108.48
1	C	308	GLN	N-CA-C	-6.00	99.12	108.90
1	F	308	GLN	N-CA-C	-5.93	99.24	108.90
1	I	308	GLN	N-CA-C	-5.93	99.24	108.90
1	L	308	GLN	N-CA-C	-5.92	99.25	108.90
1	E	140	LYS	N-CA-C	5.81	123.19	110.80
1	B	140	LYS	N-CA-C	5.78	123.11	110.80
1	K	140	LYS	N-CA-C	5.77	123.10	110.80
1	H	140	LYS	N-CA-C	5.77	123.09	110.80
1	A	189	LYS	N-CA-C	5.76	119.01	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	LYS	N-CA-C	5.74	118.97	110.48
1	D	189	LYS	N-CA-C	5.72	118.94	110.48
1	J	189	LYS	N-CA-C	5.70	118.91	110.48
1	E	202	ALA	N-CA-C	5.64	119.88	112.89
1	K	202	ALA	N-CA-C	5.61	119.84	112.89
1	H	202	ALA	N-CA-C	5.59	119.83	112.89
1	B	202	ALA	N-CA-C	5.57	119.80	112.89
1	C	346	ARG	N-CA-C	5.52	116.98	111.07
1	I	346	ARG	N-CA-C	5.52	116.97	111.07
1	I	280	ASN	N-CA-C	5.51	122.53	110.80
1	F	346	ARG	N-CA-C	5.50	116.96	111.07
1	L	346	ARG	N-CA-C	5.50	116.96	111.07
1	L	280	ASN	N-CA-C	5.48	122.47	110.80
1	C	280	ASN	N-CA-C	5.47	122.45	110.80
1	F	280	ASN	N-CA-C	5.46	122.43	110.80
1	D	308	GLN	N-CA-C	-5.40	99.63	108.76
1	G	308	GLN	N-CA-C	-5.40	99.63	108.76
1	A	308	GLN	N-CA-C	-5.40	99.64	108.76
1	J	308	GLN	N-CA-C	-5.39	99.65	108.76
1	B	275	VAL	N-CA-C	5.38	115.70	108.17
1	D	148	ILE	N-CA-C	-5.33	99.97	107.75
1	E	189	LYS	N-CA-C	5.33	118.37	110.48
1	J	148	ILE	N-CA-C	-5.32	99.98	107.75
1	E	275	VAL	N-CA-C	5.32	115.62	108.17
1	K	189	LYS	N-CA-C	5.31	118.34	110.48
1	H	275	VAL	N-CA-C	5.31	115.60	108.17
1	B	189	LYS	N-CA-C	5.31	118.33	110.48
1	H	189	LYS	N-CA-C	5.30	118.33	110.48
1	K	275	VAL	N-CA-C	5.29	115.58	108.17
1	G	148	ILE	N-CA-C	-5.28	100.03	107.75
1	G	140	LYS	N-CA-C	5.28	122.04	110.80
1	A	148	ILE	N-CA-C	-5.26	100.07	107.75
1	I	320	ASP	N-CA-C	-5.25	102.63	110.20
1	J	140	LYS	N-CA-C	5.24	121.97	110.80
1	D	140	LYS	N-CA-C	5.23	121.94	110.80
1	A	140	LYS	N-CA-C	5.23	121.93	110.80
1	C	320	ASP	N-CA-C	-5.22	102.68	110.20
1	H	308	GLN	N-CA-C	-5.20	99.98	108.76
1	F	189	LYS	N-CA-C	5.19	118.21	110.52
1	F	320	ASP	N-CA-C	-5.19	102.73	110.20
1	B	308	GLN	N-CA-C	-5.17	100.02	108.76
1	I	189	LYS	N-CA-C	5.17	118.17	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	320	ASP	N-CA-C	-5.16	102.76	110.20
1	A	88	THR	N-CA-C	-5.16	103.23	110.35
1	E	308	GLN	N-CA-C	-5.16	100.05	108.76
1	C	189	LYS	N-CA-C	5.15	118.14	110.52
1	L	189	LYS	N-CA-C	5.15	118.14	110.52
1	K	308	GLN	N-CA-C	-5.14	100.07	108.76
1	F	88	THR	N-CA-C	-5.13	103.27	110.35
1	L	88	THR	N-CA-C	-5.13	103.27	110.35
1	D	88	THR	N-CA-C	-5.12	103.28	110.35
1	C	88	THR	N-CA-C	-5.11	103.30	110.35
1	G	190	GLN	N-CA-C	-5.11	102.95	110.52
1	H	346	ARG	N-CA-C	5.11	116.85	111.28
1	J	88	THR	N-CA-C	-5.11	103.30	110.35
1	K	346	ARG	N-CA-C	5.11	116.84	111.28
1	G	88	THR	N-CA-C	-5.09	103.32	110.35
1	I	88	THR	N-CA-C	-5.09	103.33	110.35
1	A	190	GLN	N-CA-C	-5.07	103.02	110.52
1	B	346	ARG	N-CA-C	5.05	116.79	111.28
1	E	346	ARG	N-CA-C	5.05	116.78	111.28
1	J	190	GLN	N-CA-C	-5.05	103.05	110.52
1	D	34	GLN	N-CA-C	5.04	119.50	112.90
1	F	139	ILE	N-CA-C	-5.04	103.08	109.58
1	A	346	ARG	N-CA-C	5.04	116.77	111.28
1	J	346	ARG	N-CA-C	5.04	116.77	111.28
1	D	190	GLN	N-CA-C	-5.03	103.08	110.52
1	D	346	ARG	N-CA-C	5.02	116.76	111.28
1	G	346	ARG	N-CA-C	5.01	116.74	111.28
1	L	139	ILE	N-CA-C	-5.01	103.12	109.58

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	2837	0	2709	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2847	0	2723	209	0
1	C	2861	0	2751	94	0
1	D	2837	0	2705	170	0
1	E	2847	0	2723	169	0
1	F	2861	0	2752	36	0
1	G	2837	0	2710	86	0
1	H	2847	0	2729	35	0
1	I	2861	0	2742	207	0
1	J	2837	0	2710	70	0
1	K	2847	0	2729	132	0
1	L	2861	0	2752	34	0
All	All	34180	0	32735	876	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (876) 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:269:THR:CG2	1:K:263:SER:HB2	1.19	1.65
1:B:189:LYS:CG	1:E:61:ASN:HB2	1.19	1.62
1:A:269:THR:HG22	1:K:263:SER:CB	1.16	1.61
1:B:372:ARG:CD	1:D:269:THR:HG21	1.21	1.57
1:B:372:ARG:HD3	1:D:269:THR:CG2	1.12	1.56
1:B:269:THR:CB	1:I:372:ARG:HD3	1.13	1.55
1:D:372:ARG:NH1	1:I:272:VAL:CG2	1.68	1.52
1:C:186:PRO:CG	1:I:188:SER:C	1.77	1.47
1:B:52:ARG:CD	1:E:45:GLN:NE2	1.76	1.46
1:D:189:LYS:HE2	1:G:61:ASN:N	1.14	1.46
1:E:188:SER:N	1:K:186:PRO:CD	1.76	1.46
1:B:189:LYS:HG2	1:E:61:ASN:CB	1.43	1.45
1:B:372:ARG:NH1	1:D:272:VAL:HG23	1.29	1.45
1:E:372:ARG:CZ	1:J:272:VAL:CG2	1.97	1.42
1:E:372:ARG:CZ	1:J:272:VAL:HG21	1.48	1.41
1:B:61:ASN:OD1	1:E:186:PRO:CB	1.68	1.41
1:D:189:LYS:CE	1:G:61:ASN:H	1.34	1.41
1:C:186:PRO:CB	1:I:61:ASN:ND2	1.83	1.41
1:B:106:ASN:CG	1:E:62:VAL:HG11	1.42	1.39
1:B:269:THR:OG1	1:I:372:ARG:CD	1.72	1.38
1:B:108:ARG:CD	1:D:314:SER:HB2	1.55	1.37
1:A:269:THR:CG2	1:K:263:SER:CB	1.81	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:SER:C	1:K:186:PRO:HG3	1.48	1.35
1:B:269:THR:CB	1:I:372:ARG:CD	2.05	1.33
1:C:186:PRO:CG	1:I:188:SER:O	1.70	1.33
1:B:108:ARG:HD3	1:D:314:SER:CB	1.55	1.33
1:A:305:TYR:HE2	1:K:108:ARG:NH1	1.25	1.33
1:B:41:GLN:O	1:K:106:ASN:HB2	1.29	1.31
1:D:266:ALA:HB3	1:I:267:GLY:O	1.18	1.31
1:D:187:GLN:CB	1:G:186:PRO:HA	1.62	1.30
1:E:191:ARG:NH2	1:K:40:GLN:HE22	1.29	1.29
1:A:269:THR:HG21	1:K:263:SER:OG	1.24	1.29
1:D:372:ARG:CZ	1:I:272:VAL:HG23	1.61	1.29
1:B:269:THR:HG21	1:I:372:ARG:CB	1.64	1.28
1:A:305:TYR:CE2	1:K:108:ARG:NH1	2.03	1.27
1:B:51:ASN:O	1:E:46:THR:N	1.66	1.27
1:D:372:ARG:HD3	1:I:269:THR:OG1	1.16	1.25
1:D:52:ARG:HG3	1:G:44:THR:O	1.36	1.25
1:B:272:VAL:HG23	1:I:372:ARG:NH1	1.50	1.24
1:D:261:GLU:OE1	1:I:313:PHE:CB	1.85	1.24
1:D:51:ASN:OD1	1:G:47:PHE:HA	1.28	1.24
1:B:106:ASN:OD1	1:E:62:VAL:CG1	1.86	1.24
1:D:98:ARG:NH1	1:I:318:LYS:HZ2	1.35	1.24
1:C:186:PRO:HG3	1:I:188:SER:O	1.27	1.23
1:B:41:GLN:O	1:K:106:ASN:CB	1.87	1.23
1:E:189:LYS:CG	1:K:61:ASN:HB2	1.70	1.22
1:B:56:ASP:OD1	1:E:42:VAL:O	1.57	1.20
1:B:52:ARG:HD3	1:E:45:GLN:CD	1.66	1.20
1:C:186:PRO:HG3	1:I:188:SER:C	0.91	1.19
1:B:318:LYS:NZ	1:I:98:ARG:NH1	1.91	1.19
1:B:318:LYS:NZ	1:I:98:ARG:HH12	1.39	1.19
1:B:269:THR:CG2	1:I:372:ARG:HD3	1.73	1.18
1:B:372:ARG:NH1	1:D:272:VAL:CG2	2.06	1.18
1:D:98:ARG:NH1	1:I:318:LYS:NZ	1.90	1.18
1:B:52:ARG:HD3	1:E:45:GLN:NE2	0.84	1.17
1:D:50:ALA:O	1:G:46:THR:HB	1.44	1.16
1:D:372:ARG:CD	1:I:269:THR:OG1	1.91	1.16
1:D:372:ARG:HD3	1:I:269:THR:CB	1.74	1.16
1:B:189:LYS:HG3	1:E:61:ASN:HB2	1.24	1.15
1:C:45:GLN:HG3	1:I:52:ARG:HB2	1.19	1.14
1:E:372:ARG:HH11	1:J:272:VAL:CB	1.61	1.13
1:B:189:LYS:CG	1:E:61:ASN:CB	2.13	1.13
1:B:269:THR:OG1	1:I:372:ARG:HD2	1.48	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:ARG:NH1	1:J:272:VAL:CB	2.12	1.13
1:C:46:THR:O	1:I:51:ASN:HA	1.49	1.12
1:D:98:ARG:HH12	1:I:318:LYS:NZ	1.41	1.11
1:B:372:ARG:HD3	1:D:269:THR:CB	1.79	1.11
1:E:188:SER:N	1:K:186:PRO:HD3	1.04	1.11
1:B:272:VAL:CG2	1:I:372:ARG:NH1	2.13	1.11
1:C:186:PRO:HG3	1:I:189:LYS:N	1.64	1.10
1:B:269:THR:HB	1:I:372:ARG:HD3	1.14	1.10
1:C:61:ASN:HB2	1:I:189:LYS:HG2	1.19	1.10
1:C:186:PRO:HG2	1:I:188:SER:O	1.47	1.10
1:B:51:ASN:HA	1:E:46:THR:O	1.51	1.10
1:D:372:ARG:HD2	1:I:272:VAL:HG21	1.19	1.10
1:C:186:PRO:HB3	1:I:61:ASN:ND2	1.64	1.09
1:B:106:ASN:OD1	1:E:62:VAL:HG11	0.92	1.09
1:A:270:PRO:HD2	1:K:264:ALA:H	1.00	1.09
1:D:189:LYS:HG2	1:G:61:ASN:HB2	1.26	1.08
1:C:186:PRO:HB2	1:I:61:ASN:HD22	1.13	1.08
1:D:266:ALA:CB	1:I:267:GLY:O	2.00	1.08
1:D:189:LYS:NZ	1:G:60:ALA:HA	1.67	1.08
1:E:188:SER:H	1:K:186:PRO:CD	1.45	1.08
1:B:267:GLY:CA	1:I:266:ALA:HB3	1.82	1.08
1:B:269:THR:HG21	1:I:372:ARG:HB3	1.08	1.08
1:B:106:ASN:CG	1:E:62:VAL:CG1	2.25	1.07
1:B:51:ASN:CA	1:E:46:THR:O	2.02	1.06
1:C:186:PRO:HB2	1:I:61:ASN:ND2	1.66	1.06
1:E:282:TYR:OH	1:J:312:ASN:CB	2.02	1.06
1:C:186:PRO:HD2	1:I:187:GLN:N	1.61	1.06
1:A:314:SER:N	1:K:384:THR:HA	1.46	1.06
1:C:45:GLN:CG	1:I:52:ARG:HB2	1.85	1.05
1:D:372:ARG:NH1	1:I:272:VAL:HG23	0.73	1.05
1:E:188:SER:N	1:K:186:PRO:CG	2.21	1.04
1:E:191:ARG:HH22	1:K:40:GLN:NE2	1.55	1.04
1:D:372:ARG:NH1	1:I:270:PRO:O	1.90	1.02
1:C:186:PRO:CG	1:I:61:ASN:HD21	1.72	1.02
1:B:267:GLY:C	1:I:266:ALA:HB3	1.84	1.02
1:D:191:ARG:HD3	1:G:60:ALA:HB1	1.39	1.02
1:D:372:ARG:HB3	1:I:269:THR:HG21	1.42	1.02
1:B:61:ASN:OD1	1:E:186:PRO:HB3	0.84	1.01
1:B:269:THR:CG2	1:I:372:ARG:HB3	1.90	1.01
1:E:187:GLN:CB	1:K:185:VAL:HG22	1.91	1.01
1:D:193:LYS:HE3	1:G:40:GLN:NE2	1.76	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:HB3	1:E:45:GLN:HG2	1.35	1.01
1:B:58:THR:CG2	1:K:186:PRO:O	2.03	1.00
1:B:52:ARG:CD	1:E:45:GLN:HE21	1.49	1.00
1:B:318:LYS:HZ1	1:I:98:ARG:NH1	1.49	0.99
1:E:189:LYS:CD	1:K:61:ASN:HB2	1.93	0.99
1:B:318:LYS:HZ2	1:I:98:ARG:HH12	1.10	0.99
1:A:363:ASN:ND2	1:K:108:ARG:HH22	1.61	0.98
1:D:372:ARG:CD	1:I:272:VAL:HG21	1.93	0.98
1:B:372:ARG:CD	1:D:269:THR:CG2	2.02	0.97
1:C:186:PRO:CB	1:I:61:ASN:HD21	1.58	0.97
1:A:269:THR:CG2	1:K:263:SER:OG	1.94	0.97
1:E:108:ARG:HD3	1:J:314:SER:HB2	1.43	0.97
1:B:267:GLY:O	1:I:266:ALA:HB3	1.65	0.97
1:D:108:ARG:HH12	1:I:315:ASP:N	1.54	0.97
1:D:374:LEU:HD21	1:I:272:VAL:CG2	1.95	0.97
1:A:269:THR:HG21	1:K:263:SER:HG	1.19	0.96
1:B:188:SER:H	1:E:186:PRO:CD	1.78	0.96
1:E:188:SER:H	1:K:186:PRO:CG	1.77	0.96
1:B:189:LYS:HG2	1:E:61:ASN:CG	1.91	0.96
1:B:372:ARG:HH12	1:D:272:VAL:HG23	1.24	0.95
1:D:52:ARG:HB2	1:G:45:GLN:CG	1.96	0.95
1:C:186:PRO:CG	1:I:61:ASN:ND2	2.29	0.95
1:C:61:ASN:HB2	1:I:189:LYS:CG	1.95	0.94
1:B:52:ARG:CB	1:E:45:GLN:HG2	1.96	0.94
1:D:372:ARG:HH12	1:I:272:VAL:HG23	1.29	0.94
1:A:314:SER:H	1:K:384:THR:CA	1.74	0.94
1:B:106:ASN:HB2	1:E:62:VAL:HG13	1.48	0.93
1:B:269:THR:OG1	1:I:372:ARG:HD3	1.43	0.93
1:E:372:ARG:NH1	1:J:272:VAL:HG22	1.27	0.93
1:D:98:ARG:CZ	1:I:318:LYS:HZ2	1.81	0.93
1:E:61:ASN:OD1	1:K:186:PRO:CB	2.17	0.93
1:C:186:PRO:HD2	1:I:186:PRO:C	1.94	0.93
1:B:272:VAL:HG21	1:I:374:LEU:HD21	1.48	0.92
1:D:266:ALA:HB3	1:I:267:GLY:C	1.93	0.92
1:C:186:PRO:CD	1:I:187:GLN:N	2.18	0.92
1:D:189:LYS:HZ1	1:G:60:ALA:HA	1.34	0.91
1:B:61:ASN:CG	1:E:186:PRO:HB3	1.95	0.91
1:A:269:THR:CG2	1:K:265:GLN:HE22	1.83	0.91
1:B:43:GLU:OE2	1:K:189:LYS:HG2	1.71	0.91
1:E:108:ARG:CD	1:J:314:SER:HB2	2.00	0.91
1:A:305:TYR:HE2	1:K:108:ARG:HH11	1.13	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLN:OE1	1:D:369:GLN:NE2	2.04	0.90
1:D:108:ARG:NH1	1:I:315:ASP:H	1.59	0.90
1:C:46:THR:N	1:I:51:ASN:O	2.04	0.90
1:E:191:ARG:NH2	1:K:40:GLN:NE2	2.14	0.90
1:D:189:LYS:CG	1:G:61:ASN:HB2	2.01	0.90
1:B:43:GLU:HG3	1:K:189:LYS:HD3	1.51	0.90
1:E:187:GLN:CB	1:K:185:VAL:CG2	2.49	0.90
1:A:270:PRO:HD2	1:K:264:ALA:N	1.86	0.90
1:B:267:GLY:O	1:I:266:ALA:CB	2.20	0.89
1:D:189:LYS:CE	1:G:60:ALA:HA	2.02	0.89
1:D:372:ARG:HD2	1:I:272:VAL:CG2	2.03	0.89
1:E:185:VAL:O	1:K:186:PRO:HG2	1.72	0.89
1:C:45:GLN:HG3	1:I:52:ARG:CB	2.02	0.88
1:D:372:ARG:CZ	1:I:272:VAL:CG2	2.33	0.88
1:D:52:ARG:HD2	1:G:45:GLN:HB2	1.53	0.88
1:A:369:GLN:OE1	1:K:266:ALA:HB3	1.73	0.88
1:E:189:LYS:HD3	1:K:61:ASN:HB2	1.54	0.88
1:B:189:LYS:HD3	1:E:61:ASN:N	1.89	0.88
1:B:272:VAL:HG23	1:I:372:ARG:HH12	1.37	0.88
1:B:40:GLN:NE2	1:K:105:ASP:O	2.07	0.88
1:B:269:THR:OG1	1:I:372:ARG:NH1	2.07	0.88
1:B:58:THR:HG22	1:K:186:PRO:O	1.74	0.87
1:B:188:SER:H	1:E:186:PRO:CG	1.88	0.87
1:E:188:SER:O	1:K:186:PRO:HG3	1.74	0.87
1:B:372:ARG:CG	1:D:269:THR:HG21	2.05	0.86
1:B:269:THR:HG21	1:I:372:ARG:CD	2.06	0.86
1:C:62:VAL:HG11	1:I:106:ASN:CG	2.00	0.86
1:E:191:ARG:HH22	1:K:40:GLN:HE22	0.88	0.86
1:D:374:LEU:HD21	1:I:272:VAL:HG22	1.56	0.86
1:B:189:LYS:HD3	1:E:61:ASN:H	1.37	0.85
1:E:264:ALA:CB	1:J:272:VAL:CG1	2.53	0.85
1:B:318:LYS:HZ2	1:I:98:ARG:NH1	1.66	0.85
1:B:372:ARG:HH11	1:D:272:VAL:CG2	1.84	0.85
1:D:189:LYS:HE2	1:G:60:ALA:C	2.01	0.85
1:E:189:LYS:CG	1:K:61:ASN:CB	2.53	0.84
1:B:272:VAL:HG21	1:I:374:LEU:CD2	2.08	0.84
1:B:318:LYS:NZ	1:I:98:ARG:CZ	2.40	0.84
1:D:98:ARG:HH12	1:I:318:LYS:HZ2	0.87	0.84
1:E:188:SER:C	1:K:186:PRO:CG	2.44	0.84
1:B:372:ARG:NH1	1:D:270:PRO:O	2.10	0.84
1:D:51:ASN:O	1:G:45:GLN:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ARG:CZ	1:I:270:PRO:O	2.25	0.83
1:B:269:THR:HG21	1:I:372:ARG:CG	2.08	0.83
1:D:52:ARG:HB2	1:G:45:GLN:HG3	1.59	0.82
1:B:52:ARG:HD3	1:E:45:GLN:HE22	1.40	0.82
1:E:189:LYS:HG2	1:K:61:ASN:HB2	1.59	0.82
1:B:189:LYS:CD	1:E:61:ASN:H	1.92	0.82
1:D:51:ASN:OD1	1:G:47:PHE:CA	2.20	0.82
1:D:189:LYS:CE	1:G:61:ASN:N	2.10	0.81
1:B:188:SER:H	1:E:186:PRO:HG3	1.45	0.81
1:C:45:GLN:OE1	1:I:52:ARG:HD2	1.82	0.80
1:D:52:ARG:CG	1:G:44:THR:O	2.25	0.80
1:D:98:ARG:NH1	1:I:318:LYS:HZ1	1.79	0.80
1:E:372:ARG:NH1	1:J:272:VAL:CG2	0.66	0.80
1:E:189:LYS:HG3	1:K:61:ASN:HB2	1.64	0.80
1:A:363:ASN:HD22	1:K:108:ARG:HH22	1.29	0.80
1:D:98:ARG:CZ	1:I:318:LYS:NZ	2.45	0.79
1:D:80:HIS:CD2	1:D:83:GLU:H	2.01	0.79
1:B:267:GLY:C	1:I:266:ALA:CB	2.56	0.79
1:G:80:HIS:CD2	1:G:83:GLU:H	2.01	0.78
1:D:374:LEU:HD21	1:I:272:VAL:HG21	1.64	0.78
1:E:189:LYS:HG2	1:K:61:ASN:CB	2.11	0.78
1:B:106:ASN:CB	1:E:62:VAL:CG1	2.61	0.78
1:B:269:THR:CG2	1:I:372:ARG:CD	2.47	0.78
1:B:372:ARG:NE	1:D:269:THR:HG21	1.99	0.78
1:B:52:ARG:CG	1:E:45:GLN:HE21	1.96	0.78
1:J:80:HIS:CD2	1:J:83:GLU:H	2.01	0.78
1:D:193:LYS:HE3	1:G:40:GLN:HE21	1.47	0.78
1:B:189:LYS:HE3	1:B:190:GLN:O	1.84	0.78
1:D:372:ARG:HD3	1:I:269:THR:HB	1.65	0.78
1:H:189:LYS:HE3	1:H:190:GLN:O	1.84	0.78
1:A:80:HIS:CD2	1:A:83:GLU:H	2.01	0.77
1:D:106:ASN:ND2	1:D:191:ARG:HH22	1.83	0.77
1:J:106:ASN:ND2	1:J:191:ARG:HH22	1.83	0.77
1:A:106:ASN:ND2	1:A:191:ARG:HH22	1.83	0.77
1:E:189:LYS:HE3	1:E:190:GLN:O	1.84	0.77
1:B:372:ARG:HH11	1:D:272:VAL:HG23	1.41	0.76
1:E:108:ARG:NH2	1:J:313:PHE:H	1.81	0.76
1:G:106:ASN:ND2	1:G:191:ARG:HH22	1.83	0.76
1:D:108:ARG:HH12	1:I:315:ASP:H	0.82	0.76
1:D:191:ARG:HD3	1:G:60:ALA:CB	2.12	0.76
1:D:374:LEU:CD2	1:I:272:VAL:HG22	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ARG:CZ	1:K:40:GLN:HE22	1.98	0.76
1:C:45:GLN:CD	1:I:52:ARG:HB2	2.10	0.76
1:C:184:ASN:O	1:I:188:SER:CA	2.34	0.76
1:A:308:GLN:HE22	1:A:345:ASN:HD21	1.34	0.75
1:E:188:SER:H	1:K:186:PRO:HD3	0.96	0.75
1:G:308:GLN:HE22	1:G:345:ASN:HD21	1.34	0.75
1:K:189:LYS:HE3	1:K:190:GLN:O	1.84	0.75
1:C:184:ASN:O	1:I:188:SER:N	2.10	0.75
1:E:188:SER:CA	1:K:186:PRO:HG3	2.15	0.75
1:B:188:SER:N	1:E:186:PRO:CD	2.46	0.75
1:B:188:SER:H	1:E:186:PRO:HD3	1.46	0.74
1:A:269:THR:HG21	1:K:265:GLN:HE22	1.50	0.74
1:B:106:ASN:HB2	1:E:62:VAL:CG1	2.17	0.74
1:B:51:ASN:CB	1:E:46:THR:O	2.35	0.74
1:E:264:ALA:CB	1:J:272:VAL:HG13	2.15	0.74
1:J:308:GLN:HE22	1:J:345:ASN:HD21	1.34	0.74
1:B:43:GLU:CG	1:K:189:LYS:HD3	2.18	0.73
1:C:45:GLN:HG3	1:I:51:ASN:O	1.87	0.73
1:D:280:ASN:HD22	1:D:355:TYR:N	1.86	0.73
1:A:280:ASN:HD22	1:A:355:TYR:N	1.86	0.73
1:B:189:LYS:HG2	1:E:61:ASN:HB2	0.73	0.73
1:B:269:THR:HG1	1:I:372:ARG:HD2	1.51	0.73
1:E:372:ARG:HH12	1:J:272:VAL:HG22	1.06	0.73
1:D:189:LYS:NZ	1:G:59:PRO:O	2.21	0.73
1:B:108:ARG:HD3	1:D:314:SER:HB2	0.76	0.73
1:B:270:PRO:O	1:I:372:ARG:NH1	2.20	0.73
1:J:280:ASN:HD22	1:J:355:TYR:N	1.86	0.73
1:A:269:THR:CB	1:K:263:SER:HB2	2.16	0.73
1:B:267:GLY:CA	1:I:266:ALA:CB	2.63	0.73
1:B:188:SER:N	1:E:186:PRO:HD3	2.02	0.73
1:G:280:ASN:HD22	1:G:355:TYR:N	1.86	0.73
1:B:267:GLY:HA3	1:I:266:ALA:HB3	1.71	0.72
1:C:186:PRO:HG2	1:I:61:ASN:ND2	2.02	0.72
1:B:106:ASN:CB	1:E:62:VAL:HG11	2.20	0.72
1:D:308:GLN:HE22	1:D:345:ASN:HD21	1.34	0.72
1:I:29:GLN:O	1:I:33:GLN:HG3	1.90	0.72
1:D:193:LYS:CE	1:G:40:GLN:NE2	2.53	0.71
1:B:106:ASN:CB	1:E:62:VAL:HG13	2.21	0.71
1:C:186:PRO:HB3	1:I:61:ASN:HD21	1.34	0.71
1:D:372:ARG:HB3	1:I:269:THR:CG2	2.18	0.71
1:E:372:ARG:NE	1:J:272:VAL:HG21	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:PRO:CB	1:I:61:ASN:HD22	1.72	0.71
1:D:188:SER:HB2	1:G:184:ASN:O	1.90	0.71
1:B:52:ARG:HB3	1:E:45:GLN:CG	2.17	0.71
1:C:62:VAL:HG23	1:I:191:ARG:HE	1.56	0.71
1:B:318:LYS:HZ2	1:I:98:ARG:CZ	2.01	0.71
1:H:322:LYS:HD3	1:I:163:THR:HG21	1.73	0.71
1:A:280:ASN:O	1:A:281:LEU:HB3	1.91	0.71
1:C:44:THR:O	1:I:52:ARG:HG3	1.91	0.70
1:B:80:HIS:CD2	1:B:83:GLU:H	2.09	0.70
1:E:372:ARG:HH12	1:J:272:VAL:CG2	0.77	0.70
1:K:80:HIS:CD2	1:K:83:GLU:H	2.09	0.70
1:F:29:GLN:O	1:F:33:GLN:HG3	1.90	0.70
1:K:322:LYS:HD3	1:L:163:THR:HG21	1.73	0.70
1:L:29:GLN:O	1:L:33:GLN:HG3	1.90	0.70
1:E:322:LYS:HD3	1:F:163:THR:HG21	1.73	0.70
1:J:280:ASN:O	1:J:281:LEU:HB3	1.91	0.70
1:I:98:ARG:NH2	1:I:111:GLU:OE2	2.25	0.70
1:D:280:ASN:O	1:D:281:LEU:HB3	1.91	0.70
1:H:80:HIS:CD2	1:H:83:GLU:H	2.09	0.70
1:B:269:THR:HB	1:I:372:ARG:CD	1.97	0.70
1:C:45:GLN:CG	1:I:51:ASN:O	2.39	0.70
1:D:50:ALA:O	1:G:46:THR:CB	2.31	0.70
1:B:322:LYS:HD3	1:C:163:THR:HG21	1.73	0.69
1:E:80:HIS:CD2	1:E:83:GLU:H	2.09	0.69
1:C:29:GLN:O	1:C:33:GLN:HG3	1.90	0.69
1:C:80:HIS:CD2	1:C:83:GLU:H	2.10	0.69
1:E:264:ALA:HB1	1:J:272:VAL:HG11	1.72	0.69
1:F:80:HIS:CD2	1:F:83:GLU:H	2.10	0.69
1:L:98:ARG:NH2	1:L:111:GLU:OE2	2.25	0.69
1:B:369:GLN:OE1	1:I:369:GLN:OE1	1.97	0.69
1:B:52:ARG:HD3	1:E:45:GLN:HE21	0.87	0.69
1:D:310:THR:HG22	1:D:358:VAL:HG22	1.75	0.69
1:E:188:SER:N	1:K:186:PRO:HG3	2.01	0.69
1:G:280:ASN:O	1:G:281:LEU:HB3	1.91	0.69
1:D:80:HIS:HD2	1:D:83:GLU:H	1.39	0.69
1:D:261:GLU:CD	1:I:313:PHE:CB	2.65	0.69
1:G:310:THR:HG22	1:G:358:VAL:HG22	1.75	0.69
1:L:80:HIS:CD2	1:L:83:GLU:H	2.10	0.69
1:F:98:ARG:NH2	1:F:111:GLU:OE2	2.25	0.69
1:B:318:LYS:HZ2	1:I:98:ARG:NH2	1.90	0.68
1:A:269:THR:HG23	1:K:265:GLN:NE2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ARG:NH2	1:C:111:GLU:OE2	2.25	0.68
1:A:310:THR:HG22	1:A:358:VAL:HG22	1.75	0.68
1:B:41:GLN:O	1:K:106:ASN:CG	2.35	0.68
1:D:189:LYS:CE	1:G:60:ALA:CA	2.71	0.68
1:A:80:HIS:HD2	1:A:82:THR:H	1.42	0.68
1:I:80:HIS:CD2	1:I:83:GLU:H	2.11	0.68
1:A:269:THR:HG23	1:K:265:GLN:HE22	1.58	0.68
1:A:363:ASN:ND2	1:K:108:ARG:NH2	2.39	0.68
1:C:46:THR:O	1:I:51:ASN:CA	2.36	0.68
1:B:272:VAL:CG2	1:I:374:LEU:CD2	2.71	0.68
1:D:98:ARG:NH2	1:I:318:LYS:HZ2	1.92	0.67
1:E:264:ALA:HB1	1:J:272:VAL:CG1	2.24	0.67
1:B:372:ARG:NE	1:D:269:THR:CG2	2.56	0.67
1:J:80:HIS:HD2	1:J:82:THR:H	1.42	0.67
1:J:310:THR:HG22	1:J:358:VAL:HG22	1.75	0.67
1:J:80:HIS:HD2	1:J:83:GLU:H	1.39	0.67
1:J:106:ASN:HD22	1:J:191:ARG:HH22	1.42	0.67
1:C:62:VAL:HG13	1:I:106:ASN:HB2	1.77	0.67
1:E:61:ASN:OD1	1:K:186:PRO:HB3	1.95	0.67
1:D:80:HIS:HD2	1:D:82:THR:H	1.42	0.67
1:D:280:ASN:HD22	1:D:355:TYR:H	1.43	0.67
1:F:80:HIS:HD2	1:F:83:GLU:H	1.43	0.66
1:C:62:VAL:HG11	1:I:106:ASN:ND2	2.09	0.66
1:D:189:LYS:NZ	1:G:60:ALA:CA	2.53	0.66
1:A:314:SER:CA	1:K:383:ARG:O	2.44	0.66
1:D:372:ARG:NH1	1:I:272:VAL:CB	2.56	0.66
1:G:80:HIS:HD2	1:G:82:THR:H	1.42	0.66
1:H:308:GLN:HE22	1:H:345:ASN:HD21	1.43	0.66
1:A:80:HIS:HD2	1:A:83:GLU:H	1.39	0.66
1:E:61:ASN:OD1	1:K:186:PRO:CG	2.43	0.66
1:E:372:ARG:CD	1:J:272:VAL:HG21	2.25	0.66
1:E:308:GLN:HE22	1:E:345:ASN:HD21	1.43	0.66
1:G:280:ASN:HD22	1:G:355:TYR:H	1.43	0.66
1:L:80:HIS:HD2	1:L:83:GLU:H	1.43	0.66
1:L:308:GLN:HE22	1:L:345:ASN:HD21	1.44	0.66
1:G:106:ASN:HD22	1:G:191:ARG:HH22	1.42	0.65
1:A:106:ASN:HD22	1:A:191:ARG:HH22	1.42	0.65
1:B:272:VAL:HG23	1:I:372:ARG:CZ	2.25	0.65
1:D:106:ASN:HD22	1:D:191:ARG:HH22	1.42	0.65
1:B:308:GLN:HE22	1:B:345:ASN:HD21	1.43	0.65
1:B:318:LYS:NZ	1:I:98:ARG:NH2	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LYS:HZ2	1:I:98:ARG:HH22	1.44	0.65
1:C:80:HIS:HD2	1:C:83:GLU:H	1.43	0.65
1:C:308:GLN:HE22	1:C:345:ASN:HD21	1.44	0.65
1:G:80:HIS:HD2	1:G:83:GLU:H	1.39	0.65
1:H:184:ASN:O	1:H:186:PRO:HD3	1.97	0.65
1:F:308:GLN:HE22	1:F:345:ASN:HD21	1.44	0.65
1:B:184:ASN:O	1:B:186:PRO:HD3	1.97	0.65
1:A:269:THR:CG2	1:K:265:GLN:NE2	2.58	0.65
1:C:61:ASN:CB	1:I:189:LYS:HG2	2.12	0.65
1:C:80:HIS:HD2	1:C:82:THR:H	1.45	0.65
1:I:308:GLN:HE22	1:I:345:ASN:HD21	1.44	0.65
1:J:280:ASN:HD22	1:J:355:TYR:H	1.43	0.65
1:K:80:HIS:HD2	1:K:83:GLU:H	1.44	0.64
1:L:80:HIS:HD2	1:L:82:THR:H	1.45	0.64
1:B:52:ARG:NE	1:E:45:GLN:NE2	2.46	0.64
1:E:24:ASN:HD21	1:E:253:ASP:H	1.46	0.64
1:A:271:ASN:O	1:K:261:GLU:OE2	2.14	0.64
1:B:24:ASN:HD21	1:B:253:ASP:H	1.46	0.64
1:I:80:HIS:HD2	1:I:83:GLU:H	1.43	0.64
1:B:80:HIS:HD2	1:B:83:GLU:H	1.44	0.64
1:D:189:LYS:HG2	1:G:61:ASN:CB	2.16	0.64
1:E:80:HIS:HD2	1:E:83:GLU:H	1.44	0.64
1:I:80:HIS:HD2	1:I:82:THR:H	1.45	0.64
1:K:308:GLN:HE22	1:K:345:ASN:HD21	1.43	0.64
1:E:184:ASN:O	1:E:186:PRO:HD3	1.97	0.63
1:A:280:ASN:HD22	1:A:355:TYR:H	1.43	0.63
1:F:80:HIS:HD2	1:F:82:THR:H	1.45	0.63
1:H:80:HIS:HD2	1:H:83:GLU:H	1.44	0.63
1:B:61:ASN:OD1	1:E:186:PRO:CG	2.43	0.63
1:D:51:ASN:C	1:G:45:GLN:HG3	2.24	0.63
1:H:24:ASN:HD21	1:H:253:ASP:H	1.46	0.63
1:B:43:GLU:OE2	1:K:189:LYS:CG	2.46	0.62
1:A:106:ASN:HD22	1:A:191:ARG:NH2	1.98	0.62
1:B:188:SER:N	1:E:186:PRO:HG3	2.13	0.62
1:K:24:ASN:HD21	1:K:253:ASP:H	1.46	0.62
1:J:308:GLN:HE22	1:J:345:ASN:ND2	1.98	0.62
1:A:314:SER:H	1:K:384:THR:HA	0.83	0.62
1:D:51:ASN:OD1	1:G:46:THR:O	2.18	0.62
1:D:106:ASN:HD22	1:D:191:ARG:NH2	1.98	0.62
1:E:189:LYS:HD3	1:K:61:ASN:CB	2.29	0.62
1:J:106:ASN:HD22	1:J:191:ARG:NH2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:HE22	1:A:345:ASN:ND2	1.98	0.61
1:E:108:ARG:HD3	1:J:314:SER:CB	2.27	0.61
1:D:108:ARG:NH1	1:I:315:ASP:N	2.24	0.61
1:B:372:ARG:CD	1:D:269:THR:CB	2.64	0.61
1:D:52:ARG:HB2	1:G:45:GLN:CB	2.29	0.61
1:G:185:VAL:CB	1:G:186:PRO:CD	2.79	0.61
1:A:185:VAL:CB	1:A:186:PRO:CD	2.79	0.61
1:E:255:SER:HA	1:E:383:ARG:HD2	1.83	0.61
1:H:255:SER:HA	1:H:383:ARG:HD2	1.83	0.61
1:D:188:SER:CB	1:G:184:ASN:O	2.48	0.61
1:H:80:HIS:HD2	1:H:82:THR:H	1.49	0.61
1:B:313:PHE:CB	1:I:261:GLU:CD	2.75	0.60
1:G:106:ASN:HD22	1:G:191:ARG:NH2	1.98	0.60
1:E:372:ARG:HH12	1:J:272:VAL:HG23	0.57	0.60
1:G:308:GLN:HE22	1:G:345:ASN:ND2	1.97	0.60
1:K:80:HIS:HD2	1:K:82:THR:H	1.49	0.60
1:B:255:SER:HA	1:B:383:ARG:HD2	1.83	0.60
1:J:185:VAL:CB	1:J:186:PRO:CD	2.79	0.60
1:G:25:LEU:O	1:G:29:GLN:HG3	2.01	0.60
1:C:61:ASN:HB2	1:I:189:LYS:CD	2.31	0.60
1:B:40:GLN:HE21	1:K:105:ASP:C	2.09	0.60
1:D:185:VAL:CB	1:D:186:PRO:CD	2.79	0.60
1:K:255:SER:HA	1:K:383:ARG:HD2	1.83	0.60
1:B:59:PRO:HG2	1:B:190:GLN:HB2	1.84	0.60
1:J:25:LEU:O	1:J:29:GLN:HG3	2.01	0.60
1:D:371:ALA:O	1:I:269:THR:HG21	2.02	0.60
1:A:25:LEU:O	1:A:29:GLN:HG3	2.01	0.59
1:D:308:GLN:HE22	1:D:345:ASN:ND2	1.98	0.59
1:E:80:HIS:HD2	1:E:82:THR:H	1.49	0.59
1:B:372:ARG:NH1	1:D:272:VAL:HG21	2.15	0.59
1:A:305:TYR:OH	1:K:108:ARG:CZ	2.51	0.59
1:B:43:GLU:CD	1:K:189:LYS:HD3	2.27	0.59
1:B:51:ASN:C	1:E:46:THR:O	2.45	0.59
1:A:314:SER:N	1:K:384:THR:CA	2.42	0.59
1:B:267:GLY:O	1:I:266:ALA:HB2	2.00	0.59
1:E:61:ASN:OD1	1:K:186:PRO:HG2	2.03	0.59
1:D:25:LEU:O	1:D:29:GLN:HG3	2.01	0.59
1:D:52:ARG:HB2	1:G:45:GLN:CD	2.26	0.59
1:E:59:PRO:HG2	1:E:190:GLN:HB2	1.84	0.59
1:A:80:HIS:CD2	1:A:82:THR:H	2.21	0.58
1:A:305:TYR:CZ	1:K:108:ARG:NH1	2.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:59:PRO:HG2	1:K:190:GLN:HB2	1.84	0.58
1:E:108:ARG:NH2	1:J:313:PHE:N	2.51	0.58
1:K:25:LEU:O	1:K:29:GLN:HG3	2.04	0.58
1:B:267:GLY:HA2	1:I:266:ALA:CB	2.31	0.58
1:B:282:TYR:OH	1:D:312:ASN:CB	2.52	0.58
1:E:264:ALA:HB3	1:J:272:VAL:CG1	2.33	0.58
1:E:372:ARG:NH1	1:J:272:VAL:HG23	0.97	0.58
1:A:15:LEU:C	1:A:17:ASN:H	2.12	0.58
1:D:15:LEU:C	1:D:17:ASN:H	2.12	0.58
1:B:80:HIS:HD2	1:B:82:THR:H	1.49	0.58
1:E:25:LEU:O	1:E:29:GLN:HG3	2.04	0.58
1:H:59:PRO:HG2	1:H:190:GLN:HB2	1.84	0.58
1:L:103:ASP:HB2	1:L:104:PRO:CD	2.34	0.58
1:B:272:VAL:CG2	1:I:372:ARG:HH11	2.14	0.57
1:G:15:LEU:C	1:G:17:ASN:H	2.12	0.57
1:C:103:ASP:HB2	1:C:104:PRO:CD	2.34	0.57
1:C:279:ALA:O	1:C:280:ASN:O	2.22	0.57
1:F:279:ALA:O	1:F:280:ASN:O	2.22	0.57
1:A:369:GLN:CD	1:K:266:ALA:HB3	2.29	0.57
1:F:103:ASP:HB2	1:F:104:PRO:CD	2.34	0.57
1:E:372:ARG:CZ	1:J:272:VAL:HG23	1.98	0.57
1:H:25:LEU:O	1:H:29:GLN:HG3	2.04	0.57
1:I:279:ALA:O	1:I:280:ASN:O	2.22	0.57
1:B:266:ALA:HB3	1:D:267:GLY:O	2.05	0.57
1:C:62:VAL:CG2	1:I:191:ARG:HE	2.18	0.57
1:D:80:HIS:CD2	1:D:82:THR:H	2.21	0.57
1:I:103:ASP:HB2	1:I:104:PRO:CD	2.34	0.57
1:B:267:GLY:HA2	1:I:266:ALA:HB3	1.82	0.57
1:B:108:ARG:CD	1:D:314:SER:CB	2.42	0.57
1:L:279:ALA:O	1:L:280:ASN:O	2.22	0.57
1:B:25:LEU:O	1:B:29:GLN:HG3	2.04	0.56
1:G:80:HIS:CD2	1:G:82:THR:H	2.21	0.56
1:L:308:GLN:HE22	1:L:345:ASN:ND2	2.03	0.56
1:A:314:SER:HA	1:K:383:ARG:O	2.04	0.56
1:B:186:PRO:C	1:E:185:VAL:HA	1.91	0.56
1:L:383:ARG:HG2	1:L:384:THR:N	2.21	0.56
1:D:193:LYS:CE	1:G:40:GLN:HE21	2.16	0.56
1:E:61:ASN:OD1	1:K:186:PRO:HB2	2.04	0.56
1:F:308:GLN:HE22	1:F:345:ASN:ND2	2.03	0.56
1:D:372:ARG:CD	1:I:269:THR:CB	2.67	0.56
1:C:280:ASN:O	1:C:281:LEU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:308:GLN:HE22	1:I:345:ASN:ND2	2.03	0.56
1:J:15:LEU:C	1:J:17:ASN:H	2.12	0.56
1:J:80:HIS:CD2	1:J:82:THR:H	2.21	0.56
1:B:318:LYS:CE	1:I:98:ARG:HH12	2.19	0.56
1:E:188:SER:O	1:K:186:PRO:CG	2.49	0.56
1:C:383:ARG:HG2	1:C:384:THR:N	2.21	0.55
1:L:352:THR:O	1:L:353:LEU:HB2	2.06	0.55
1:I:280:ASN:O	1:I:281:LEU:HB2	2.06	0.55
1:D:185:VAL:CB	1:D:186:PRO:HD2	2.37	0.55
1:I:352:THR:O	1:I:353:LEU:HB2	2.06	0.55
1:J:185:VAL:CB	1:J:186:PRO:HD2	2.37	0.55
1:L:280:ASN:O	1:L:281:LEU:HB2	2.06	0.55
1:L:352:THR:O	1:L:353:LEU:CB	2.54	0.55
1:B:41:GLN:C	1:K:106:ASN:CG	2.66	0.55
1:B:272:VAL:CG2	1:I:372:ARG:CZ	2.83	0.55
1:F:352:THR:O	1:F:353:LEU:CB	2.54	0.55
1:A:270:PRO:O	1:K:262:ASN:O	2.25	0.55
1:F:280:ASN:O	1:F:281:LEU:HB2	2.06	0.55
1:C:61:ASN:ND2	1:I:189:LYS:HD3	2.21	0.55
1:C:308:GLN:HE22	1:C:345:ASN:ND2	2.03	0.55
1:C:352:THR:O	1:C:353:LEU:HB2	2.06	0.55
1:F:80:HIS:CD2	1:F:82:THR:H	2.25	0.55
1:F:383:ARG:HG2	1:F:384:THR:N	2.21	0.55
1:F:352:THR:O	1:F:353:LEU:HB2	2.06	0.55
1:I:383:ARG:HG2	1:I:384:THR:N	2.21	0.55
1:A:185:VAL:CB	1:A:186:PRO:HD2	2.37	0.55
1:B:41:GLN:O	1:K:106:ASN:HB3	2.00	0.54
1:C:352:THR:O	1:C:353:LEU:CB	2.55	0.54
1:E:187:GLN:C	1:K:186:PRO:N	2.31	0.54
1:B:51:ASN:HB3	1:E:46:THR:O	2.06	0.54
1:C:80:HIS:CD2	1:C:82:THR:H	2.25	0.54
1:D:372:ARG:CD	1:I:272:VAL:CG2	2.69	0.54
1:D:372:ARG:NH2	1:I:270:PRO:O	2.40	0.54
1:D:374:LEU:CD2	1:I:272:VAL:CG2	2.75	0.54
1:I:352:THR:O	1:I:353:LEU:CB	2.54	0.54
1:G:185:VAL:CB	1:G:186:PRO:HD2	2.36	0.54
1:I:25:LEU:O	1:I:29:GLN:HG3	2.08	0.54
1:F:25:LEU:O	1:F:29:GLN:HG3	2.08	0.54
1:L:80:HIS:CD2	1:L:82:THR:H	2.25	0.54
1:C:244:GLN:O	1:C:245:ASN:CB	2.56	0.54
1:L:25:LEU:O	1:L:29:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:244:GLN:O	1:L:245:ASN:CB	2.56	0.54
1:B:189:LYS:CG	1:E:61:ASN:H	2.21	0.53
1:H:80:HIS:CD2	1:H:82:THR:H	2.27	0.53
1:B:51:ASN:O	1:E:46:THR:CA	2.54	0.53
1:B:272:VAL:CG2	1:I:374:LEU:HD21	2.27	0.53
1:I:80:HIS:CD2	1:I:82:THR:H	2.25	0.53
1:K:80:HIS:CD2	1:K:82:THR:H	2.27	0.53
1:K:120:VAL:HG21	1:K:260:LEU:HD13	1.91	0.53
1:C:186:PRO:HA	1:I:189:LYS:HB3	1.91	0.53
1:D:372:ARG:NE	1:I:272:VAL:HG21	2.22	0.53
1:H:120:VAL:HG21	1:H:260:LEU:HD13	1.91	0.53
1:I:244:GLN:O	1:I:245:ASN:CB	2.56	0.53
1:F:244:GLN:O	1:F:245:ASN:CB	2.56	0.53
1:E:120:VAL:HG21	1:E:260:LEU:HD13	1.91	0.53
1:B:51:ASN:O	1:E:46:THR:O	2.28	0.52
1:D:52:ARG:HA	1:G:45:GLN:HA	1.91	0.52
1:E:264:ALA:HB2	1:J:272:VAL:HG13	1.92	0.52
1:D:98:ARG:NH2	1:I:318:LYS:NZ	2.55	0.52
1:C:25:LEU:O	1:C:29:GLN:HG3	2.08	0.52
1:A:305:TYR:CZ	1:A:318:LYS:HE3	2.45	0.52
1:B:318:LYS:NZ	1:I:98:ARG:HH22	2.05	0.52
1:B:374:LEU:HD21	1:D:272:VAL:HG21	1.92	0.52
1:E:189:LYS:N	1:K:186:PRO:HG3	2.16	0.52
1:G:305:TYR:CZ	1:G:318:LYS:HE3	2.45	0.52
1:B:272:VAL:HG22	1:I:374:LEU:HD22	1.91	0.52
1:H:308:GLN:HE22	1:H:345:ASN:ND2	2.08	0.52
1:K:308:GLN:HE22	1:K:345:ASN:ND2	2.08	0.52
1:B:80:HIS:CD2	1:B:82:THR:H	2.27	0.52
1:B:186:PRO:O	1:E:185:VAL:HA	2.10	0.52
1:D:372:ARG:NH1	1:I:272:VAL:N	2.58	0.52
1:D:372:ARG:NE	1:I:272:VAL:CG2	2.70	0.52
1:J:305:TYR:CZ	1:J:318:LYS:HE3	2.45	0.52
1:J:307:SER:OG	1:J:315:ASP:HB3	2.10	0.52
1:B:120:VAL:HG21	1:B:260:LEU:HD13	1.91	0.51
1:D:51:ASN:O	1:G:45:GLN:CG	2.54	0.51
1:D:305:TYR:CZ	1:D:318:LYS:HE3	2.45	0.51
1:E:80:HIS:CD2	1:E:82:THR:H	2.27	0.51
1:B:106:ASN:OD1	1:E:236:TYR:CE1	2.63	0.51
1:H:280:ASN:O	1:H:281:LEU:HB2	2.10	0.51
1:B:269:THR:OG1	1:I:372:ARG:CZ	2.58	0.51
1:B:51:ASN:HB3	1:E:52:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:HG22	1:K:263:SER:CA	2.22	0.51
1:B:189:LYS:HG3	1:E:61:ASN:CB	2.09	0.51
1:C:62:VAL:CG1	1:I:106:ASN:CG	2.80	0.51
1:D:307:SER:OG	1:D:315:ASP:HB3	2.10	0.51
1:G:307:SER:OG	1:G:315:ASP:HB3	2.10	0.51
1:B:280:ASN:O	1:B:281:LEU:HB2	2.10	0.51
1:B:308:GLN:HE22	1:B:345:ASN:ND2	2.08	0.51
1:K:280:ASN:O	1:K:281:LEU:HB2	2.10	0.51
1:B:41:GLN:NE2	1:K:106:ASN:HD21	2.09	0.51
1:C:184:ASN:O	1:I:188:SER:HB2	2.11	0.51
1:C:184:ASN:C	1:I:188:SER:HA	2.35	0.51
1:D:189:LYS:CD	1:G:61:ASN:HB2	2.41	0.51
1:E:280:ASN:O	1:E:281:LEU:HB2	2.10	0.51
1:D:188:SER:CA	1:G:184:ASN:O	2.58	0.50
1:D:255:SER:HA	1:D:383:ARG:HD2	1.94	0.50
1:D:372:ARG:HH12	1:I:272:VAL:N	2.10	0.50
1:A:307:SER:OG	1:A:315:ASP:HB3	2.10	0.50
1:E:13:ALA:C	1:E:15:LEU:H	2.20	0.50
1:C:61:ASN:CG	1:I:189:LYS:NZ	2.59	0.50
1:A:305:TYR:OH	1:K:108:ARG:NH2	2.45	0.50
1:A:314:SER:N	1:K:383:ARG:O	2.45	0.50
1:I:108:ARG:HD2	1:I:111:GLU:OE1	2.12	0.50
1:J:49:PRO:HG3	1:J:228:ILE:HD12	1.93	0.50
1:A:255:SER:HA	1:A:383:ARG:HD2	1.94	0.49
1:D:49:PRO:HG3	1:D:228:ILE:HD12	1.93	0.49
1:D:98:ARG:HH12	1:I:318:LYS:CE	2.20	0.49
1:J:308:GLN:NE2	1:J:345:ASN:HD21	2.07	0.49
1:K:322:LYS:CD	1:L:163:THR:HG21	2.42	0.49
1:A:49:PRO:HG3	1:A:228:ILE:HD12	1.93	0.49
1:B:272:VAL:CG2	1:I:374:LEU:HD22	2.42	0.49
1:E:308:GLN:HE22	1:E:345:ASN:ND2	2.08	0.49
1:F:108:ARG:HD2	1:F:111:GLU:OE1	2.12	0.49
1:G:280:ASN:ND2	1:G:355:TYR:HB2	2.27	0.49
1:J:255:SER:HA	1:J:383:ARG:HD2	1.94	0.49
1:J:280:ASN:ND2	1:J:355:TYR:HB2	2.27	0.49
1:D:308:GLN:NE2	1:D:345:ASN:HD21	2.07	0.49
1:G:49:PRO:HG3	1:G:228:ILE:HD12	1.93	0.49
1:L:108:ARG:HD2	1:L:111:GLU:OE1	2.12	0.49
1:A:280:ASN:ND2	1:A:355:TYR:HB2	2.27	0.49
1:E:15:LEU:O	1:E:19:GLN:HG3	2.13	0.49
1:G:103:ASP:HB2	1:G:104:PRO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ALA:C	1:B:15:LEU:H	2.20	0.49
1:B:40:GLN:NE2	1:K:105:ASP:C	2.69	0.49
1:B:106:ASN:ND2	1:E:62:VAL:HG21	2.27	0.49
1:K:13:ALA:C	1:K:15:LEU:H	2.20	0.49
1:E:322:LYS:CD	1:F:163:THR:HG21	2.42	0.49
1:C:108:ARG:HD2	1:C:111:GLU:OE1	2.12	0.49
1:A:272:VAL:HA	1:K:261:GLU:OE2	2.13	0.49
1:H:13:ALA:C	1:H:15:LEU:H	2.20	0.49
1:H:21:MET:HE2	1:H:21:MET:HA	1.95	0.49
1:K:21:MET:HA	1:K:21:MET:HE2	1.95	0.49
1:D:280:ASN:ND2	1:D:355:TYR:HB2	2.27	0.49
1:G:255:SER:HA	1:G:383:ARG:HD2	1.94	0.49
1:A:103:ASP:HB2	1:A:104:PRO:CD	2.43	0.48
1:A:310:THR:O	1:K:385:GLU:N	2.45	0.48
1:B:21:MET:HE2	1:B:21:MET:HA	1.95	0.48
1:H:15:LEU:O	1:H:19:GLN:HG3	2.13	0.48
1:J:103:ASP:HB2	1:J:104:PRO:CD	2.43	0.48
1:K:15:LEU:O	1:K:19:GLN:HG3	2.13	0.48
1:H:322:LYS:CD	1:I:163:THR:HG21	2.42	0.48
1:E:21:MET:HE2	1:E:21:MET:HA	1.95	0.48
1:J:120:VAL:HG21	1:J:260:LEU:HD13	1.96	0.48
1:B:272:VAL:CB	1:I:372:ARG:NH1	2.76	0.48
1:D:103:ASP:HB2	1:D:104:PRO:CD	2.43	0.48
1:E:103:ASP:HB2	1:E:104:PRO:CD	2.44	0.48
1:B:15:LEU:O	1:B:19:GLN:HG3	2.13	0.48
1:B:372:ARG:HD3	1:D:269:THR:HG21	0.54	0.48
1:C:308:GLN:NE2	1:C:345:ASN:HD21	2.11	0.48
1:A:120:VAL:HG21	1:A:260:LEU:HD13	1.96	0.48
1:H:103:ASP:HB2	1:H:104:PRO:CD	2.44	0.48
1:B:52:ARG:HB2	1:E:45:GLN:HG2	1.90	0.48
1:K:103:ASP:HB2	1:K:104:PRO:CD	2.44	0.48
1:B:103:ASP:HB2	1:B:104:PRO:CD	2.44	0.47
1:H:311:ALA:O	1:H:312:ASN:C	2.57	0.47
1:J:102:TYR:CE2	1:J:108:ARG:HG3	2.49	0.47
1:A:270:PRO:O	1:K:263:SER:HA	2.13	0.47
1:C:184:ASN:C	1:I:188:SER:CA	2.86	0.47
1:C:281:LEU:N	1:C:281:LEU:HD12	2.29	0.47
1:D:102:TYR:CE2	1:D:108:ARG:HG3	2.49	0.47
1:F:281:LEU:N	1:F:281:LEU:HD12	2.30	0.47
1:A:102:TYR:CE2	1:A:108:ARG:HG3	2.49	0.47
1:B:269:THR:OG1	1:I:372:ARG:NE	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PRO:HG2	1:K:264:ALA:HB3	1.96	0.47
1:L:281:LEU:HD12	1:L:281:LEU:N	2.29	0.47
1:D:120:VAL:HG21	1:D:260:LEU:HD13	1.96	0.47
1:G:120:VAL:HG21	1:G:260:LEU:HD13	1.96	0.47
1:G:352:THR:O	1:G:353:LEU:CB	2.63	0.47
1:J:352:THR:O	1:J:353:LEU:CB	2.63	0.47
1:B:311:ALA:O	1:B:312:ASN:C	2.57	0.47
1:C:45:GLN:HG3	1:I:51:ASN:C	2.39	0.47
1:C:184:ASN:O	1:I:188:SER:CB	2.63	0.47
1:C:185:VAL:HG13	1:I:187:GLN:N	2.24	0.47
1:D:352:THR:O	1:D:353:LEU:CB	2.63	0.47
1:G:102:TYR:CE2	1:G:108:ARG:HG3	2.49	0.47
1:D:188:SER:HA	1:G:184:ASN:O	2.15	0.47
1:E:372:ARG:HH11	1:J:272:VAL:CG2	0.81	0.47
1:G:308:GLN:NE2	1:G:345:ASN:HD21	2.07	0.47
1:B:372:ARG:HD2	1:D:272:VAL:HG21	1.97	0.47
1:D:106:ASN:ND2	1:G:62:VAL:HG21	2.30	0.47
1:E:311:ALA:O	1:E:312:ASN:C	2.57	0.47
1:F:308:GLN:NE2	1:F:345:ASN:HD21	2.11	0.47
1:I:308:GLN:NE2	1:I:345:ASN:HD21	2.11	0.47
1:I:14:ALA:C	1:I:16:ARG:H	2.23	0.46
1:K:311:ALA:O	1:K:312:ASN:C	2.57	0.46
1:A:308:GLN:NE2	1:A:345:ASN:HD21	2.07	0.46
1:A:352:THR:O	1:A:353:LEU:CB	2.62	0.46
1:B:188:SER:HA	1:E:184:ASN:HA	1.98	0.46
1:I:184:ASN:O	1:I:186:PRO:HD3	2.16	0.46
1:A:369:GLN:HE22	1:K:267:GLY:N	2.13	0.46
1:F:14:ALA:C	1:F:16:ARG:H	2.23	0.46
1:L:308:GLN:NE2	1:L:345:ASN:HD21	2.11	0.46
1:A:59:PRO:HD2	1:A:190:GLN:HB2	1.98	0.46
1:B:272:VAL:HG21	1:I:372:ARG:NH1	2.21	0.46
1:C:14:ALA:C	1:C:16:ARG:H	2.23	0.46
1:D:52:ARG:CD	1:G:45:GLN:HB2	2.36	0.46
1:I:281:LEU:HD12	1:I:281:LEU:N	2.30	0.46
1:E:108:ARG:CZ	1:J:313:PHE:H	2.28	0.46
1:J:59:PRO:HD2	1:J:190:GLN:HB2	1.98	0.46
1:E:187:GLN:CB	1:K:185:VAL:HG13	2.45	0.46
1:H:59:PRO:CG	1:H:190:GLN:HB2	2.46	0.46
1:E:24:ASN:HD22	1:E:252:ILE:H	1.64	0.46
1:B:21:MET:HE3	1:B:252:ILE:HD13	1.99	0.45
1:D:79:ASN:O	1:D:79:ASN:CG	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:PRO:O	1:E:187:GLN:CB	2.65	0.45
1:B:322:LYS:CD	1:C:163:THR:HG21	2.42	0.45
1:E:21:MET:HE3	1:E:252:ILE:HD13	1.98	0.45
1:E:83:GLU:HB3	1:E:218:ALA:HB3	1.98	0.45
1:H:83:GLU:HB3	1:H:218:ALA:HB3	1.99	0.45
1:I:311:ALA:O	1:I:312:ASN:CB	2.65	0.45
1:B:41:GLN:HE22	1:K:191:ARG:HH21	1.64	0.45
1:E:185:VAL:O	1:K:186:PRO:CG	2.55	0.45
1:G:59:PRO:HD2	1:G:190:GLN:HB2	1.98	0.45
1:G:79:ASN:CG	1:G:79:ASN:O	2.59	0.45
1:G:106:ASN:ND2	1:G:191:ARG:NH2	2.56	0.45
1:H:305:TYR:CZ	1:H:318:LYS:HE3	2.51	0.45
1:K:24:ASN:HD22	1:K:252:ILE:H	1.64	0.45
1:K:305:TYR:CZ	1:K:318:LYS:HE3	2.51	0.45
1:L:184:ASN:O	1:L:186:PRO:HD3	2.16	0.45
1:B:305:TYR:CZ	1:B:318:LYS:HE3	2.51	0.45
1:H:21:MET:HE3	1:H:252:ILE:HD13	1.98	0.45
1:L:14:ALA:C	1:L:16:ARG:H	2.23	0.45
1:D:59:PRO:HD2	1:D:190:GLN:HB2	1.98	0.45
1:J:79:ASN:CG	1:J:79:ASN:O	2.60	0.45
1:B:83:GLU:HB3	1:B:218:ALA:HB3	1.99	0.45
1:C:62:VAL:CG1	1:I:106:ASN:HB2	2.45	0.45
1:F:311:ALA:O	1:F:312:ASN:CB	2.65	0.45
1:H:186:PRO:O	1:H:187:GLN:CB	2.64	0.45
1:L:311:ALA:O	1:L:312:ASN:CB	2.65	0.45
1:D:36:TYR:HA	1:D:37:PRO:HD3	1.83	0.45
1:E:305:TYR:CZ	1:E:318:LYS:HE3	2.51	0.45
1:F:184:ASN:O	1:F:186:PRO:HD3	2.16	0.45
1:F:310:THR:HG22	1:F:358:VAL:HG22	1.99	0.45
1:J:83:GLU:HB3	1:J:218:ALA:HB3	1.99	0.45
1:L:310:THR:HG22	1:L:358:VAL:HG22	1.99	0.45
1:D:187:GLN:CB	1:G:186:PRO:CA	2.58	0.45
1:I:103:ASP:HB2	1:I:104:PRO:HD2	2.00	0.45
1:J:211:LEU:HD21	1:J:374:LEU:HD13	1.99	0.45
1:H:280:ASN:HA	1:H:352:THR:OG1	2.18	0.44
1:I:310:THR:HG22	1:I:358:VAL:HG22	1.99	0.44
1:K:59:PRO:CG	1:K:190:GLN:HB2	2.46	0.44
1:B:308:GLN:NE2	1:B:345:ASN:HD21	2.14	0.44
1:C:45:GLN:HG2	1:I:51:ASN:O	2.16	0.44
1:G:15:LEU:C	1:G:17:ASN:N	2.76	0.44
1:A:322:LYS:HE2	1:B:145:MET:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:CG	1:B:190:GLN:HB2	2.46	0.44
1:C:103:ASP:HB2	1:C:104:PRO:HD2	1.99	0.44
1:C:311:ALA:O	1:C:312:ASN:CB	2.65	0.44
1:K:83:GLU:HB3	1:K:218:ALA:HB3	1.99	0.44
1:E:59:PRO:CG	1:E:190:GLN:HB2	2.46	0.44
1:E:280:ASN:HA	1:E:352:THR:OG1	2.18	0.44
1:A:79:ASN:CG	1:A:79:ASN:O	2.60	0.44
1:A:307:SER:HB2	1:A:318:LYS:HA	2.00	0.44
1:D:98:ARG:HH22	1:I:318:LYS:HZ2	1.62	0.44
1:F:103:ASP:HB2	1:F:104:PRO:HD2	1.99	0.44
1:J:307:SER:HB2	1:J:318:LYS:HA	2.00	0.44
1:B:24:ASN:HD22	1:B:252:ILE:H	1.64	0.44
1:B:188:SER:N	1:E:186:PRO:N	2.62	0.44
1:C:62:VAL:HG21	1:I:106:ASN:OD1	2.18	0.44
1:G:83:GLU:HB3	1:G:218:ALA:HB3	1.99	0.44
1:J:322:LYS:HE2	1:K:145:MET:O	2.17	0.44
1:B:186:PRO:O	1:B:187:GLN:CB	2.65	0.44
1:D:61:ASN:HB3	1:D:183:ALA:O	2.18	0.44
1:K:21:MET:HE3	1:K:252:ILE:HD13	1.98	0.44
1:A:15:LEU:C	1:A:17:ASN:N	2.76	0.44
1:A:83:GLU:HB3	1:A:218:ALA:HB3	1.99	0.44
1:D:322:LYS:HE2	1:E:145:MET:O	2.18	0.44
1:C:45:GLN:HG3	1:I:52:ARG:CA	2.47	0.44
1:G:61:ASN:HB3	1:G:183:ALA:O	2.18	0.44
1:L:103:ASP:HB2	1:L:104:PRO:HD2	1.99	0.44
1:B:280:ASN:HA	1:B:352:THR:OG1	2.18	0.43
1:B:372:ARG:NE	1:D:269:THR:HG22	2.34	0.43
1:D:211:LEU:HD21	1:D:374:LEU:HD13	1.99	0.43
1:G:322:LYS:HE2	1:H:145:MET:O	2.18	0.43
1:J:15:LEU:C	1:J:17:ASN:N	2.76	0.43
1:A:211:LEU:HD21	1:A:374:LEU:HD13	1.99	0.43
1:B:24:ASN:ND2	1:B:252:ILE:H	2.16	0.43
1:B:313:PHE:CB	1:I:261:GLU:OE1	2.66	0.43
1:D:83:GLU:HB3	1:D:218:ALA:HB3	1.99	0.43
1:G:307:SER:HB2	1:G:318:LYS:HA	2.00	0.43
1:H:24:ASN:HD22	1:H:252:ILE:H	1.64	0.43
1:B:188:SER:N	1:E:186:PRO:CG	2.68	0.43
1:D:307:SER:HB2	1:D:318:LYS:HA	2.00	0.43
1:D:372:ARG:HH12	1:I:271:ASN:C	2.26	0.43
1:K:280:ASN:HA	1:K:352:THR:OG1	2.18	0.43
1:C:186:PRO:HG3	1:I:189:LYS:CA	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:TYR:HB2	1:J:191:ARG:HB2	2.01	0.43
1:A:102:TYR:HB2	1:A:191:ARG:HB2	2.01	0.43
1:I:151:PRO:HD2	1:I:162:LEU:HD22	2.01	0.43
1:A:260:LEU:HA	1:A:377:TYR:O	2.19	0.43
1:B:189:LYS:CG	1:E:61:ASN:CA	2.94	0.43
1:C:310:THR:HG22	1:C:358:VAL:HG22	1.99	0.43
1:D:102:TYR:HB2	1:D:191:ARG:HB2	2.01	0.43
1:D:372:ARG:HD2	1:I:269:THR:OG1	2.03	0.43
1:L:161:GLU:C	1:L:162:LEU:HD23	2.44	0.43
1:B:189:LYS:CG	1:E:61:ASN:N	2.82	0.43
1:C:182:LEU:HD11	1:C:184:ASN:ND2	2.34	0.43
1:A:269:THR:HG23	1:K:265:GLN:CD	2.43	0.43
1:C:151:PRO:HD2	1:C:162:LEU:HD22	2.00	0.43
1:D:15:LEU:C	1:D:17:ASN:N	2.76	0.43
1:G:211:LEU:HD21	1:G:374:LEU:HD13	1.99	0.43
1:H:260:LEU:HD22	1:H:378:GLU:HG3	2.01	0.43
1:J:61:ASN:HB3	1:J:183:ALA:O	2.18	0.43
1:K:260:LEU:HD22	1:K:378:GLU:HG3	2.01	0.43
1:L:151:PRO:HD2	1:L:162:LEU:HD22	2.01	0.43
1:A:61:ASN:HB3	1:A:183:ALA:O	2.18	0.43
1:D:266:ALA:HB3	1:I:267:GLY:CA	2.48	0.43
1:E:24:ASN:ND2	1:E:252:ILE:H	2.16	0.43
1:G:260:LEU:HA	1:G:377:TYR:O	2.19	0.43
1:L:182:LEU:HD11	1:L:184:ASN:ND2	2.34	0.43
1:B:52:ARG:CD	1:E:45:GLN:CD	2.57	0.43
1:B:189:LYS:HB3	1:K:186:PRO:HB2	2.00	0.43
1:B:260:LEU:HD22	1:B:378:GLU:HG3	2.01	0.42
1:I:284:TYR:HB2	1:I:350:ILE:HB	2.01	0.42
1:B:272:VAL:HB	1:I:372:ARG:HH11	1.84	0.42
1:E:260:LEU:HD22	1:E:378:GLU:HG3	2.01	0.42
1:E:372:ARG:HD2	1:J:272:VAL:HG21	1.98	0.42
1:I:161:GLU:C	1:I:162:LEU:HD23	2.44	0.42
1:B:127:ALA:O	1:B:128:PRO:C	2.63	0.42
1:C:284:TYR:HB2	1:C:350:ILE:HB	2.01	0.42
1:C:369:GLN:O	1:C:370:ASN:HB2	2.20	0.42
1:D:260:LEU:HA	1:D:377:TYR:O	2.19	0.42
1:H:311:ALA:O	1:H:313:PHE:N	2.52	0.42
1:K:24:ASN:ND2	1:K:252:ILE:H	2.16	0.42
1:A:242:VAL:HG22	1:A:247:TYR:CD2	2.55	0.42
1:B:108:ARG:HD3	1:D:314:SER:OG	2.09	0.42
1:B:311:ALA:O	1:B:313:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLU:C	1:C:162:LEU:HD23	2.43	0.42
1:F:161:GLU:C	1:F:162:LEU:HD23	2.44	0.42
1:F:284:TYR:HB2	1:F:350:ILE:HB	2.02	0.42
1:G:102:TYR:HB2	1:G:191:ARG:HB2	2.01	0.42
1:G:242:VAL:HG22	1:G:247:TYR:CD2	2.55	0.42
1:J:242:VAL:HG22	1:J:247:TYR:CD2	2.55	0.42
1:J:352:THR:C	1:J:354:GLN:H	2.28	0.42
1:K:127:ALA:O	1:K:128:PRO:C	2.62	0.42
1:A:314:SER:CB	1:K:383:ARG:O	2.68	0.42
1:F:151:PRO:HD2	1:F:162:LEU:HD22	2.00	0.42
1:F:182:LEU:HD11	1:F:184:ASN:ND2	2.34	0.42
1:G:352:THR:C	1:G:354:GLN:H	2.28	0.42
1:H:24:ASN:ND2	1:H:252:ILE:H	2.16	0.42
1:C:242:VAL:HG22	1:C:247:TYR:CD2	2.55	0.42
1:D:352:THR:C	1:D:354:GLN:H	2.28	0.42
1:D:242:VAL:HG22	1:D:247:TYR:CD2	2.55	0.42
1:E:308:GLN:NE2	1:E:345:ASN:HD21	2.14	0.42
1:F:242:VAL:HG22	1:F:247:TYR:CD2	2.55	0.42
1:F:369:GLN:O	1:F:370:ASN:HB2	2.20	0.42
1:A:318:LYS:NZ	1:K:108:ARG:HB2	2.34	0.42
1:E:191:ARG:CZ	1:K:40:GLN:NE2	2.72	0.42
1:K:311:ALA:C	1:K:313:PHE:N	2.77	0.42
1:L:369:GLN:O	1:L:370:ASN:HB2	2.20	0.42
1:A:106:ASN:ND2	1:A:191:ARG:NH2	2.56	0.42
1:I:182:LEU:HD11	1:I:184:ASN:ND2	2.34	0.42
1:I:275:VAL:HG22	1:I:361:VAL:HG22	2.02	0.42
1:A:24:ASN:CG	1:A:252:ILE:HB	2.45	0.41
1:C:275:VAL:HG22	1:C:361:VAL:HG22	2.02	0.41
1:J:24:ASN:CG	1:J:252:ILE:HB	2.45	0.41
1:J:260:LEU:HA	1:J:377:TYR:O	2.19	0.41
1:K:311:ALA:O	1:K:313:PHE:N	2.52	0.41
1:E:108:ARG:CZ	1:J:313:PHE:N	2.83	0.41
1:E:311:ALA:O	1:E:313:PHE:N	2.52	0.41
1:F:275:VAL:HG22	1:F:361:VAL:HG22	2.02	0.41
1:G:24:ASN:CG	1:G:252:ILE:HB	2.45	0.41
1:D:24:ASN:CG	1:D:252:ILE:HB	2.45	0.41
1:A:352:THR:C	1:A:354:GLN:H	2.28	0.41
1:B:51:ASN:HA	1:E:46:THR:C	2.38	0.41
1:I:242:VAL:HG22	1:I:247:TYR:CD2	2.55	0.41
1:E:127:ALA:O	1:E:128:PRO:C	2.63	0.41
1:E:189:LYS:HB3	1:K:186:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:260:LEU:HD22	1:J:378:GLU:HG2	2.03	0.41
1:L:275:VAL:HG22	1:L:361:VAL:HG22	2.02	0.41
1:C:98:ARG:HE	1:C:98:ARG:HB3	1.69	0.41
1:H:127:ALA:O	1:H:128:PRO:C	2.63	0.41
1:B:311:ALA:C	1:B:313:PHE:N	2.77	0.41
1:C:62:VAL:CG1	1:I:106:ASN:CB	2.99	0.41
1:D:266:ALA:CB	1:I:267:GLY:C	2.75	0.41
1:E:311:ALA:C	1:E:313:PHE:N	2.77	0.41
1:L:242:VAL:HG22	1:L:247:TYR:CD2	2.55	0.41
1:L:284:TYR:HB2	1:L:350:ILE:HB	2.01	0.41
1:B:103:ASP:HB2	1:B:104:PRO:HD2	2.03	0.41
1:B:312:ASN:O	1:B:313:PHE:C	2.64	0.41
1:C:238:ASP:CG	1:I:106:ASN:HD22	2.26	0.41
1:I:83:GLU:HB3	1:I:218:ALA:HB3	2.03	0.41
1:B:266:ALA:HB3	1:D:267:GLY:C	2.46	0.40
1:B:372:ARG:CZ	1:D:269:THR:HG22	2.51	0.40
1:F:83:GLU:HB3	1:F:218:ALA:HB3	2.03	0.40
1:I:162:LEU:HD23	1:I:162:LEU:N	2.36	0.40
1:H:312:ASN:O	1:H:313:PHE:C	2.64	0.40
1:A:260:LEU:HD22	1:A:378:GLU:HG2	2.03	0.40
1:B:188:SER:C	1:E:186:PRO:HG3	2.46	0.40
1:B:267:GLY:HA2	1:I:266:ALA:HB1	2.03	0.40
1:C:83:GLU:HB3	1:C:218:ALA:HB3	2.03	0.40
1:E:13:ALA:O	1:E:14:ALA:HB3	2.22	0.40
1:F:352:THR:O	1:F:353:LEU:HG	2.22	0.40
1:F:162:LEU:HD23	1:F:162:LEU:N	2.37	0.40
1:G:127:ALA:O	1:G:128:PRO:C	2.65	0.40
1:C:162:LEU:HD23	1:C:162:LEU:N	2.36	0.40
1:C:352:THR:O	1:C:353:LEU:HG	2.21	0.40
1:D:127:ALA:O	1:D:128:PRO:C	2.65	0.40
1:D:260:LEU:HD22	1:D:378:GLU:HG2	2.03	0.40
1:H:311:ALA:C	1:H:313:PHE:N	2.77	0.40
1:I:369:GLN:O	1:I:370:ASN:HB2	2.20	0.40
1:L:186:PRO:O	1:L:187:GLN:CB	2.69	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	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	11	46
1	B	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	36	72
1	C	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	16	54
1	D	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	11	46
1	E	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	36	72
1	F	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	16	54
1	G	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	11	46
1	H	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	36	72
1	I	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	16	54
1	J	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	11	46
1	K	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	36	72
1	L	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	16	54
All	All	4440/4728 (94%)	4184 (94%)	224 (5%)	32 (1%)	20	56

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	VAL
1	C	245	ASN
1	C	280	ASN
1	C	312	ASN
1	D	185	VAL
1	F	245	ASN
1	F	280	ASN
1	F	312	ASN
1	G	185	VAL
1	I	245	ASN
1	I	280	ASN
1	I	312	ASN

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Mol	Chain	Res	Type
1	J	185	VAL
1	L	245	ASN
1	L	280	ASN
1	L	312	ASN
1	A	186	PRO
1	A	313	PHE
1	D	186	PRO
1	D	313	PHE
1	G	186	PRO
1	G	313	PHE
1	J	186	PRO
1	J	313	PHE
1	B	312	ASN
1	E	312	ASN
1	H	312	ASN
1	K	312	ASN
1	A	384	THR
1	D	384	THR
1	G	384	THR
1	J	384	THR

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	292/325 (90%)	291 (100%)	1 (0%)	86	86
1	B	294/325 (90%)	288 (98%)	6 (2%)	48	66
1	C	298/325 (92%)	296 (99%)	2 (1%)	76	81
1	D	292/325 (90%)	291 (100%)	1 (0%)	86	86
1	E	294/325 (90%)	288 (98%)	6 (2%)	48	66
1	F	298/325 (92%)	296 (99%)	2 (1%)	76	81
1	G	292/325 (90%)	291 (100%)	1 (0%)	86	86
1	H	294/325 (90%)	288 (98%)	6 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	298/325 (92%)	296 (99%)	2 (1%)	76	81
1	J	292/325 (90%)	291 (100%)	1 (0%)	86	86
1	K	294/325 (90%)	288 (98%)	6 (2%)	48	66
1	L	298/325 (92%)	296 (99%)	2 (1%)	76	81
All	All	3536/3900 (91%)	3500 (99%)	36 (1%)	65	78

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	PRO
1	B	21	MET
1	B	106	ASN
1	B	162	LEU
1	B	260	LEU
1	B	265	GLN
1	B	280	ASN
1	C	162	LEU
1	C	355	TYR
1	D	186	PRO
1	E	21	MET
1	E	106	ASN
1	E	162	LEU
1	E	260	LEU
1	E	265	GLN
1	E	280	ASN
1	F	162	LEU
1	F	355	TYR
1	G	186	PRO
1	H	21	MET
1	H	106	ASN
1	H	162	LEU
1	H	260	LEU
1	H	265	GLN
1	H	280	ASN
1	I	162	LEU
1	I	355	TYR
1	J	186	PRO
1	K	21	MET
1	K	106	ASN
1	K	162	LEU
1	K	260	LEU

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Mol	Chain	Res	Type
1	K	265	GLN
1	K	280	ASN
1	L	162	LEU
1	L	355	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	41	GLN
1	A	45	GLN
1	A	61	ASN
1	A	79	ASN
1	A	80	HIS
1	A	106	ASN
1	A	200	ASN
1	A	280	ASN
1	A	308	GLN
1	B	24	ASN
1	B	33	GLN
1	B	41	GLN
1	B	80	HIS
1	B	107	GLN
1	B	146	ASN
1	B	190	GLN
1	B	200	ASN
1	B	271	ASN
1	B	304	ASN
1	B	308	GLN
1	B	357	ASN
1	C	41	GLN
1	C	61	ASN
1	C	79	ASN
1	C	80	HIS
1	C	146	ASN
1	C	190	GLN
1	C	304	ASN
1	C	308	GLN
1	C	354	GLN
1	D	19	GLN
1	D	41	GLN
1	D	45	GLN

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Mol	Chain	Res	Type
1	D	61	ASN
1	D	79	ASN
1	D	80	HIS
1	D	106	ASN
1	D	200	ASN
1	D	280	ASN
1	D	308	GLN
1	D	370	ASN
1	E	24	ASN
1	E	33	GLN
1	E	45	GLN
1	E	80	HIS
1	E	106	ASN
1	E	107	GLN
1	E	146	ASN
1	E	190	GLN
1	E	200	ASN
1	E	271	ASN
1	E	304	ASN
1	E	308	GLN
1	E	357	ASN
1	E	369	GLN
1	F	41	GLN
1	F	79	ASN
1	F	80	HIS
1	F	146	ASN
1	F	190	GLN
1	F	304	ASN
1	F	308	GLN
1	F	354	GLN
1	G	19	GLN
1	G	40	GLN
1	G	41	GLN
1	G	45	GLN
1	G	61	ASN
1	G	79	ASN
1	G	80	HIS
1	G	106	ASN
1	G	200	ASN
1	G	280	ASN
1	G	308	GLN
1	H	24	ASN

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Mol	Chain	Res	Type
1	H	33	GLN
1	H	41	GLN
1	H	61	ASN
1	H	80	HIS
1	H	106	ASN
1	H	107	GLN
1	H	146	ASN
1	H	190	GLN
1	H	200	ASN
1	H	271	ASN
1	H	304	ASN
1	H	308	GLN
1	H	357	ASN
1	I	41	GLN
1	I	61	ASN
1	I	79	ASN
1	I	80	HIS
1	I	146	ASN
1	I	190	GLN
1	I	304	ASN
1	I	308	GLN
1	I	354	GLN
1	J	19	GLN
1	J	41	GLN
1	J	45	GLN
1	J	61	ASN
1	J	79	ASN
1	J	80	HIS
1	J	106	ASN
1	J	200	ASN
1	J	280	ASN
1	J	308	GLN
1	K	24	ASN
1	K	33	GLN
1	K	40	GLN
1	K	41	GLN
1	K	80	HIS
1	K	107	GLN
1	K	146	ASN
1	K	190	GLN
1	K	200	ASN
1	K	265	GLN

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Mol	Chain	Res	Type
1	K	271	ASN
1	K	304	ASN
1	K	345	ASN
1	K	357	ASN
1	L	41	GLN
1	L	79	ASN
1	L	80	HIS
1	L	146	ASN
1	L	304	ASN
1	L	345	ASN
1	L	354	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.

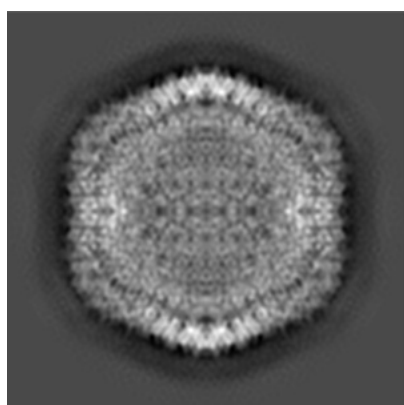
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1013. These allow visual inspection of the internal detail of the map and identification of artifacts.

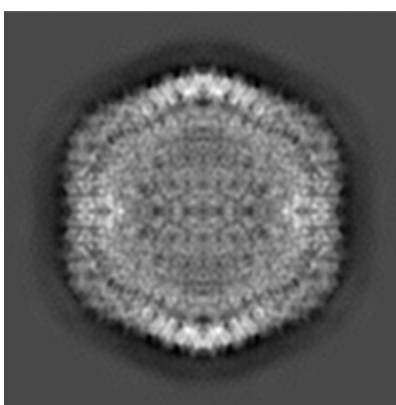
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

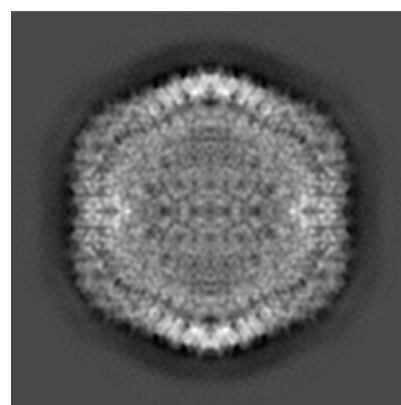
6.1.1 Primary map



X



Y

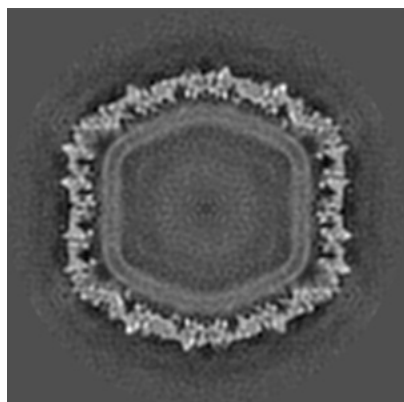


Z

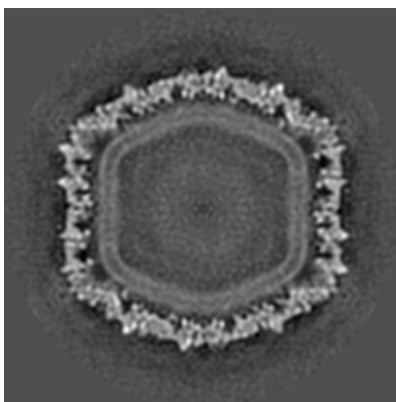
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

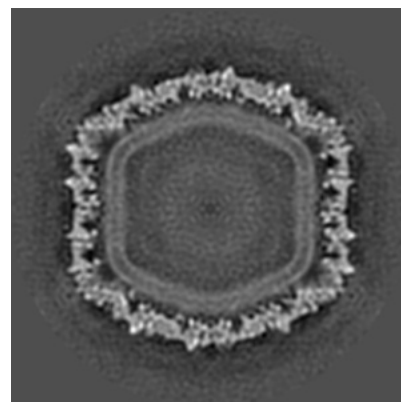
6.2.1 Primary map



X Index: 128



Y Index: 128

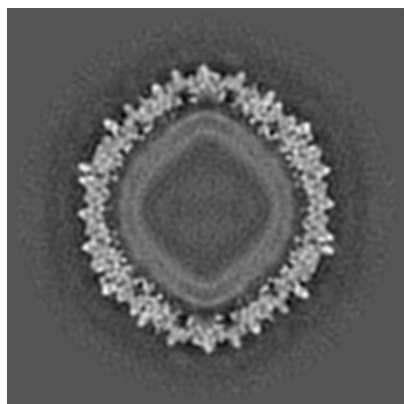


Z Index: 128

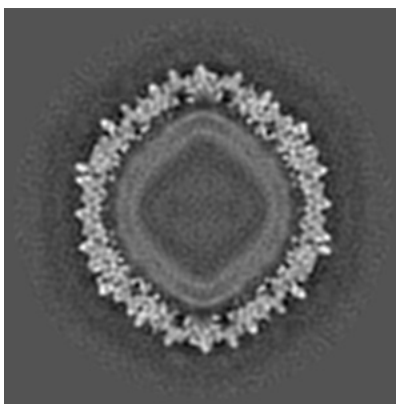
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

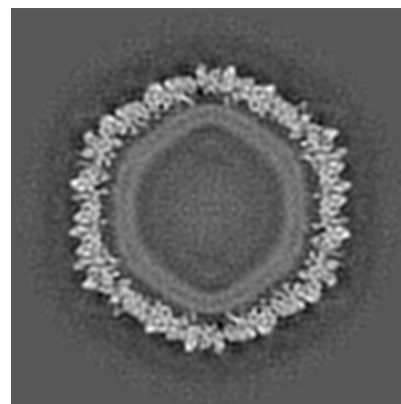
6.3.1 Primary map



X Index: 165



Y Index: 165

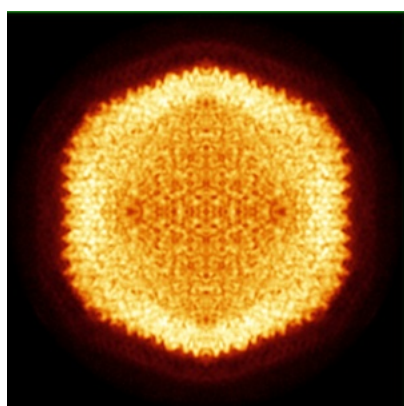


Z Index: 151

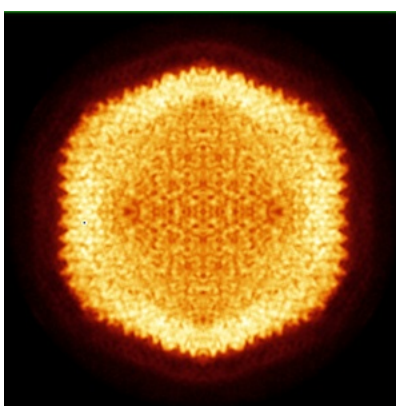
The images above show the largest variance slices of the map in three orthogonal directions.

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

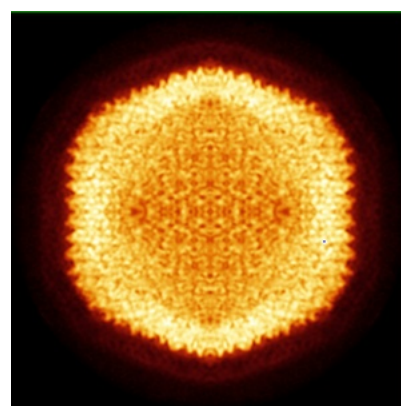
6.4.1 Primary map



X



Y

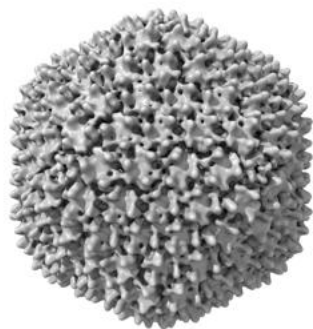


Z

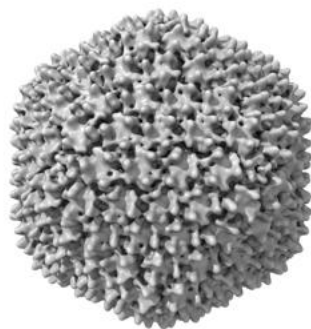
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

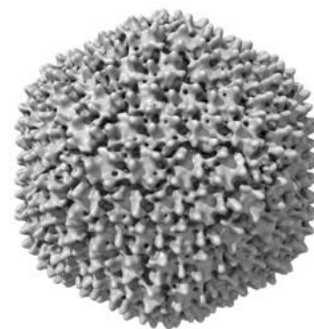
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

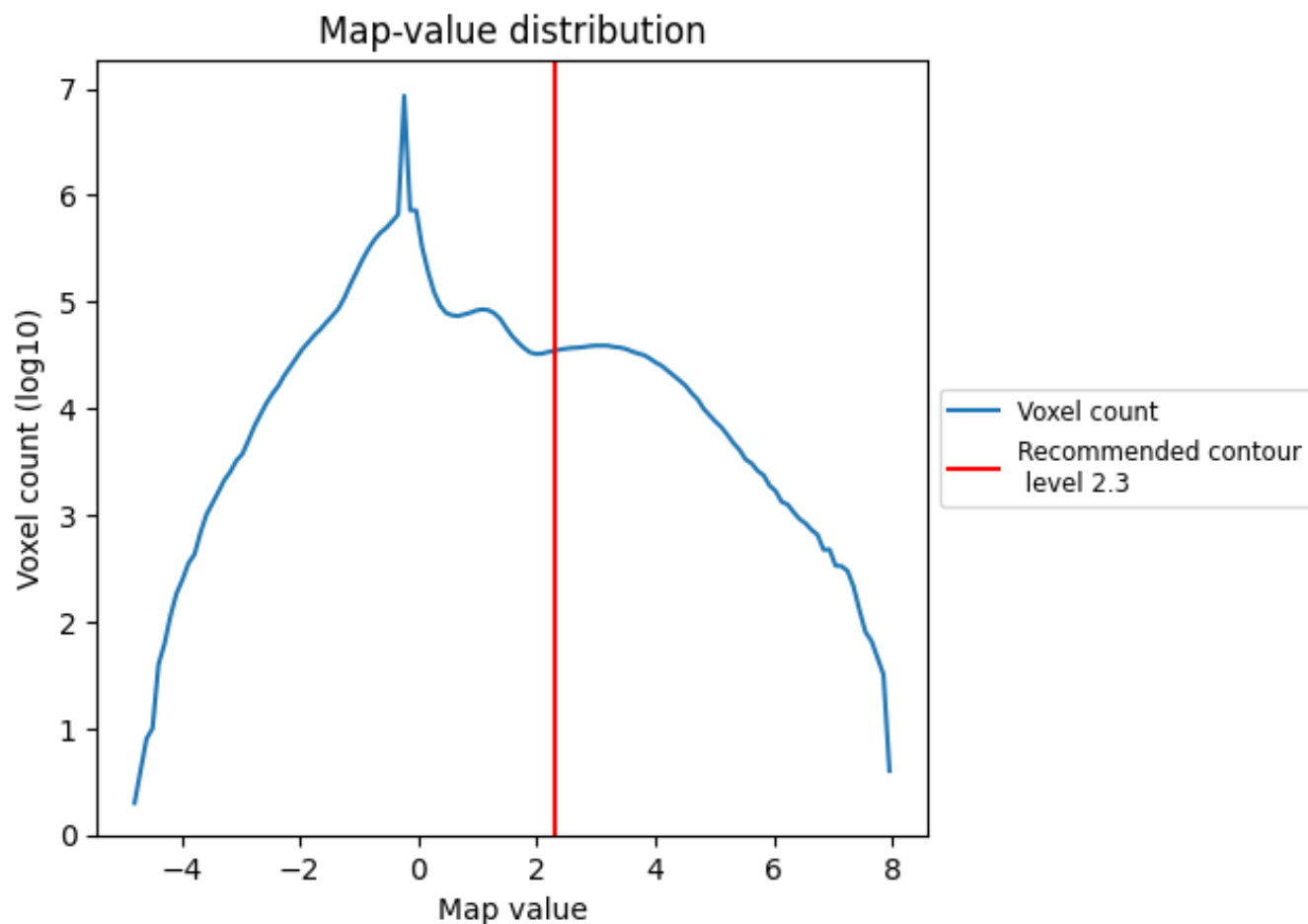
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

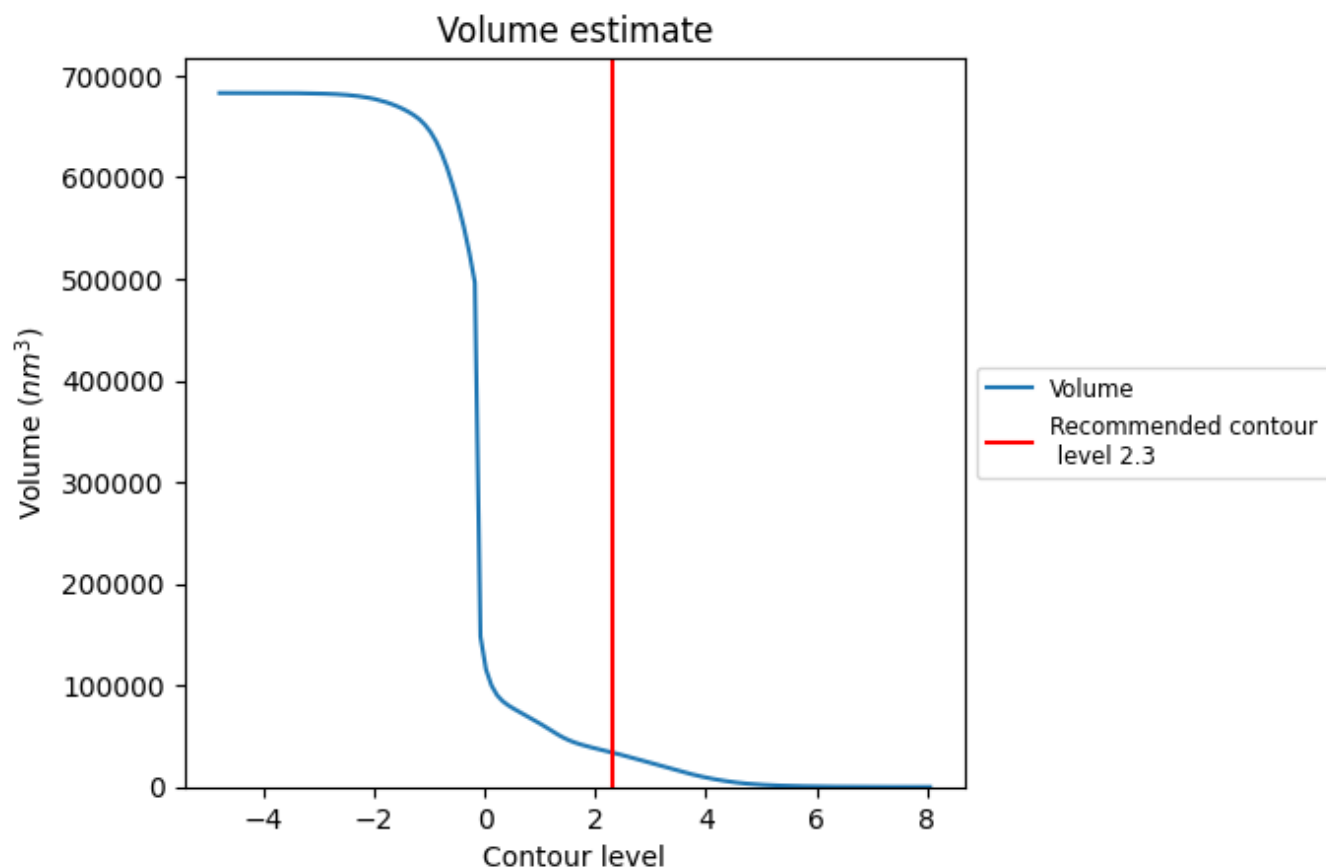
This section contains the results of statistical analysis of the map.

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.

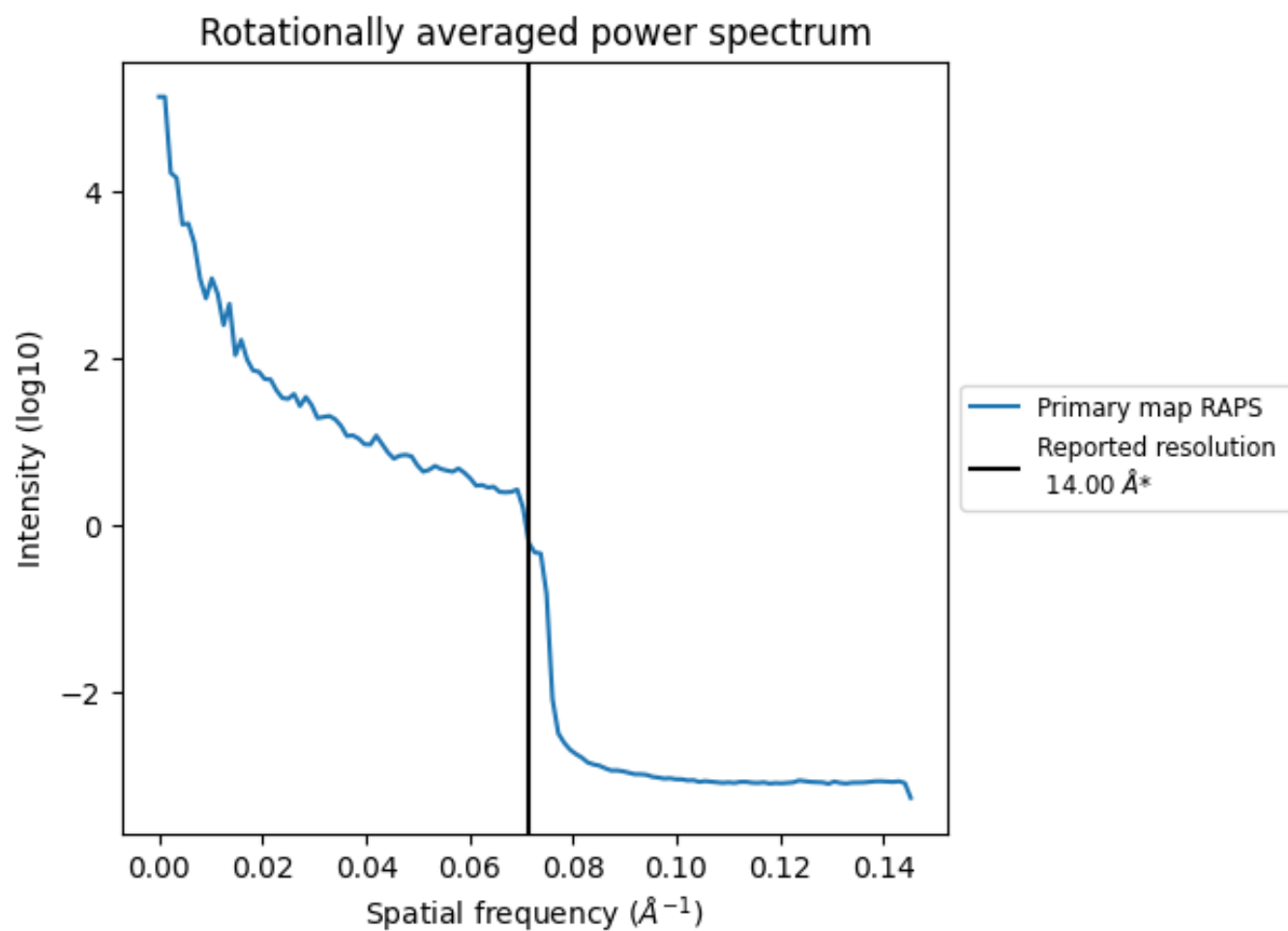
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34019 nm^3 ; this corresponds to an approximate mass of 30730 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 0.071 Å⁻¹

8 Fourier-Shell correlation

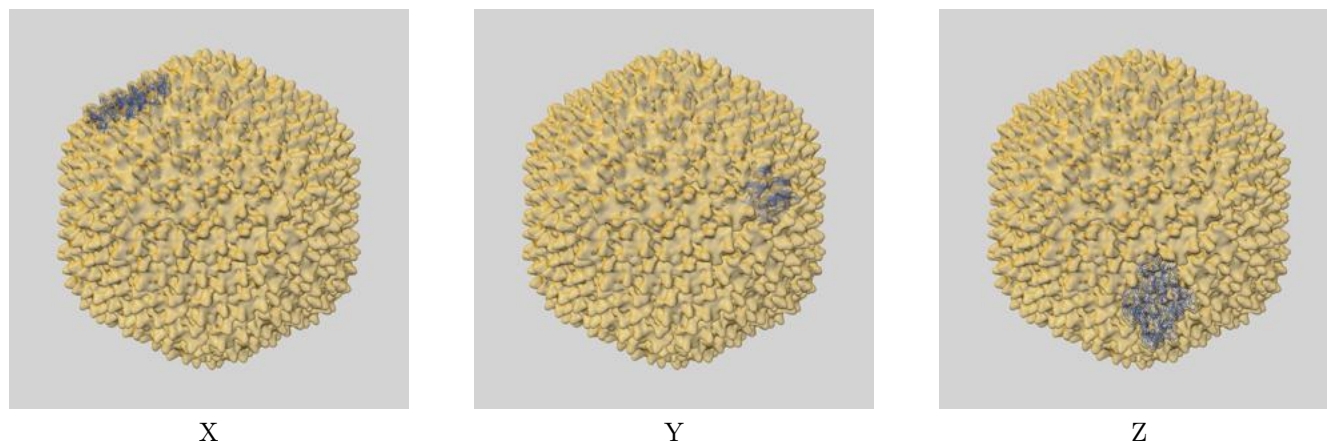
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

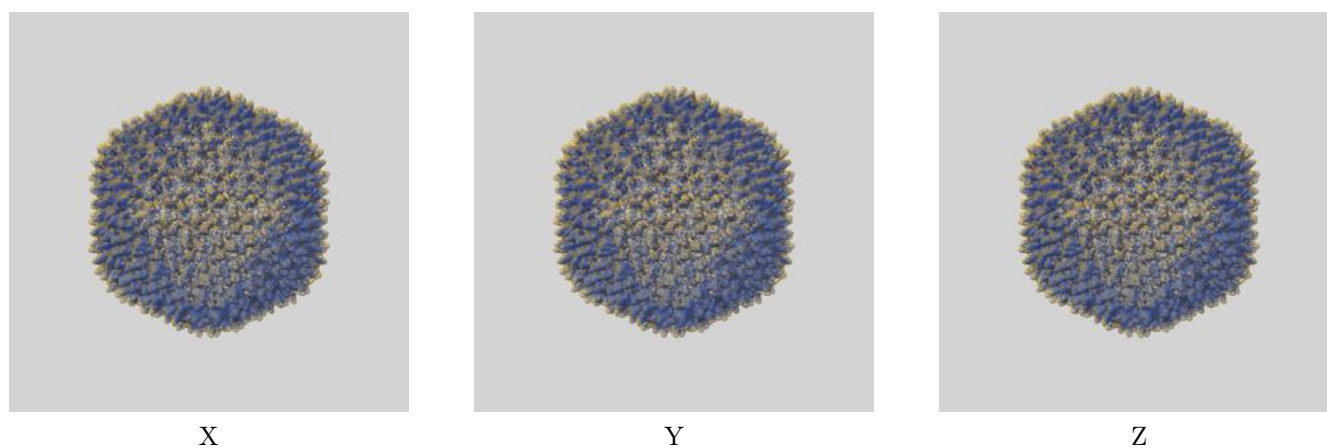
This section contains information regarding the fit between EMDB map EMD-1013 and PDB model 1HB7. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

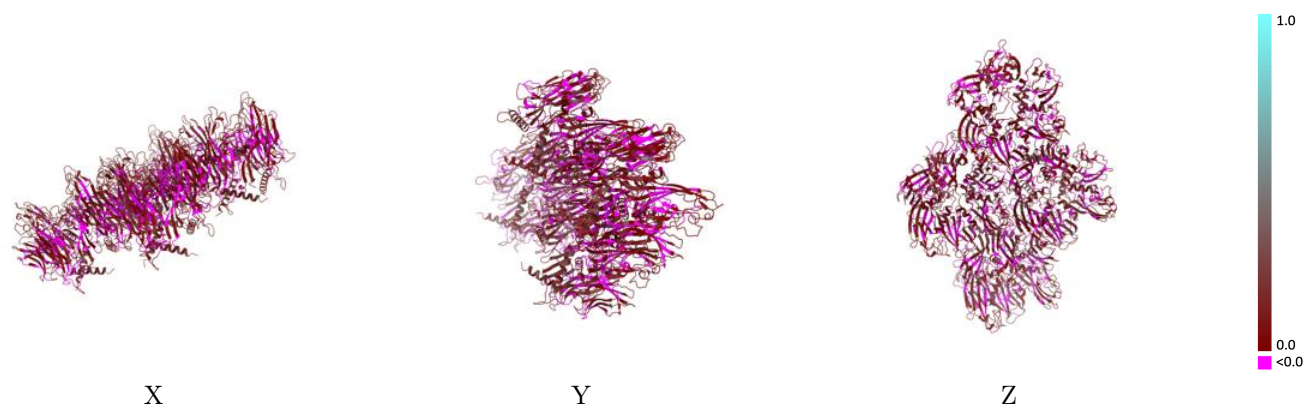


9.1.2 Map-model assembly overlay [i](#)



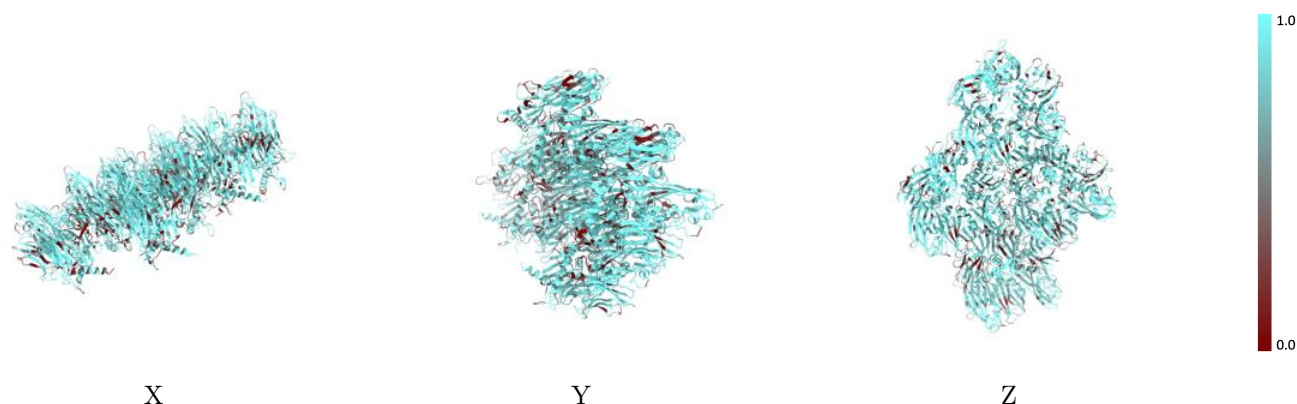
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



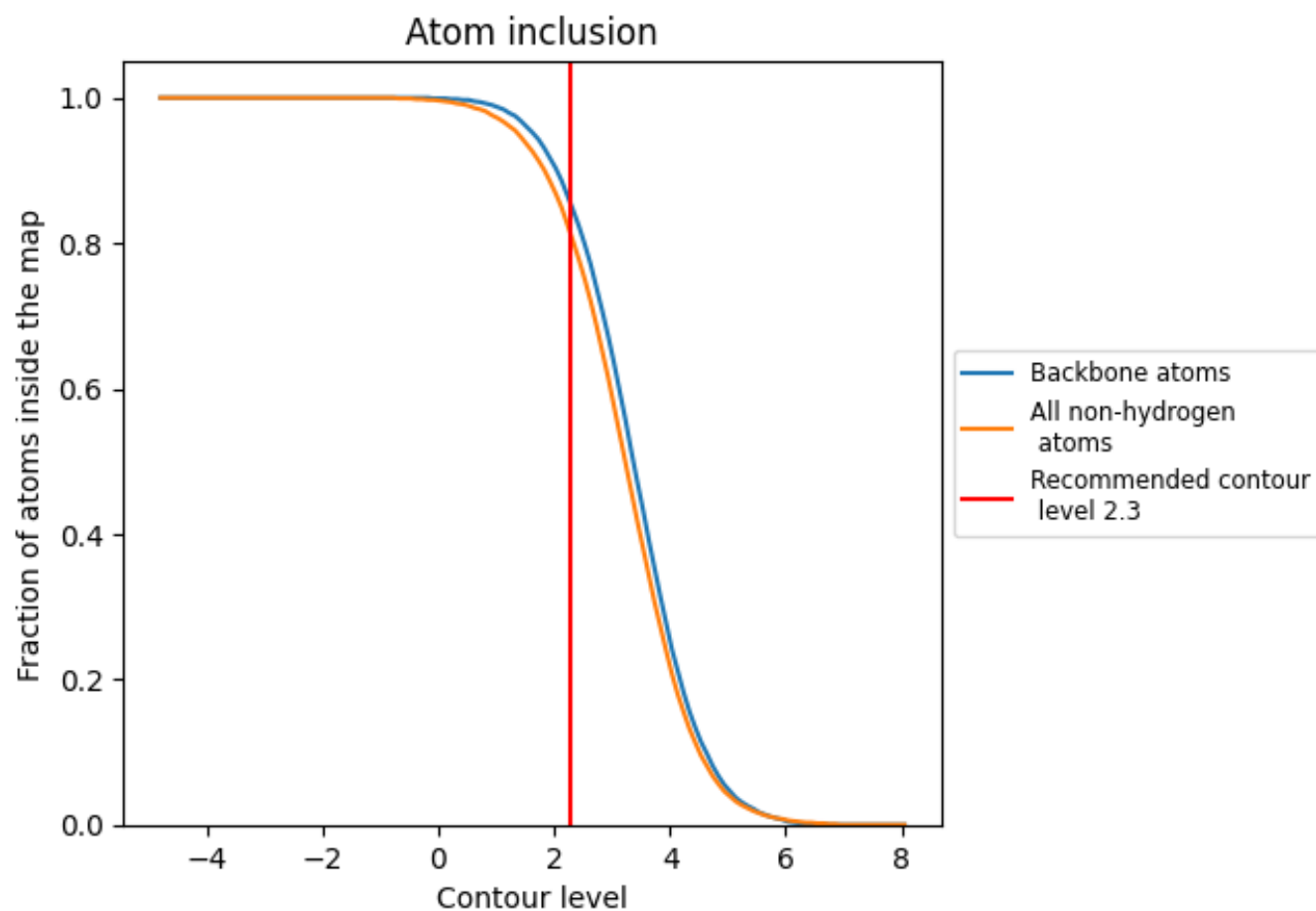
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (2.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8100	 0.0670
A	 0.8430	 0.0770
B	 0.8380	 0.0690
C	 0.8340	 0.0710
D	 0.8350	 0.0670
E	 0.8370	 0.0700
F	 0.7880	 0.0650
G	 0.7880	 0.0640
H	 0.8290	 0.0660
I	 0.8300	 0.0630
J	 0.7490	 0.0620
K	 0.7420	 0.0680
L	 0.8060	 0.0640

