



## Full wwPDB EM Validation Report ⓘ

May 23, 2024 – 09:45 AM EDT

PDB ID : 3EPC  
EMDB ID : EMD-1570  
Title : CryoEM structure of poliovirus receptor bound to poliovirus type 1  
Authors : Zhang, P.; Mueller, S.; Morais, M.C.; Bator, C.M.; Bowman, V.D.; Hafenstein, S.; Wimmer, E.; Rossmann, M.G.  
Deposited on : 2008-09-29  
Resolution : 8.00 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

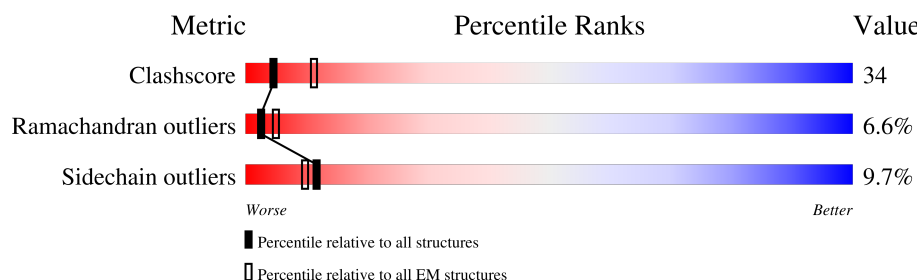
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	R	213	<div> <div>18%</div> <div>38%</div> <div>41%</div> <div>17%</div> <div>.</div> </div>
2	1	283	<div> <div>55%</div> <div>35%</div> <div>9%</div> <div>.</div> </div>
3	2	268	<div> <div>56%</div> <div>34%</div> <div>8%</div> <div>.</div> </div>
4	4	68	<div> <div>40%</div> <div>40%</div> <div>13%</div> <div>7%</div> </div>
5	3	235	<div> <div>51%</div> <div>38%</div> <div>9%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SPH	1	0	X	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8292 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 Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	213	Total	C	N	O	S	0	0
			1638	1038	281	310	9		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	105	ASP	ASN	engineered mutation	UNP P15151
R	120	SER	ASN	engineered mutation	UNP P15151
R	188	GLN	ASN	engineered mutation	UNP P15151
R	218	GLN	ASN	engineered mutation	UNP P15151
R	237	SER	ASN	engineered mutation	UNP P15151

- Molecule 2 is a protein called Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	283	Total	C	N	O	S	0	0
			2222	1416	378	423	5		

- Molecule 3 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	268	Total	C	N	O	S	0	0
			2085	1317	358	396	14		

- Molecule 4 is a protein called Protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	63	Total	C	N	O	S	0	1
			477	293	82	101	1		

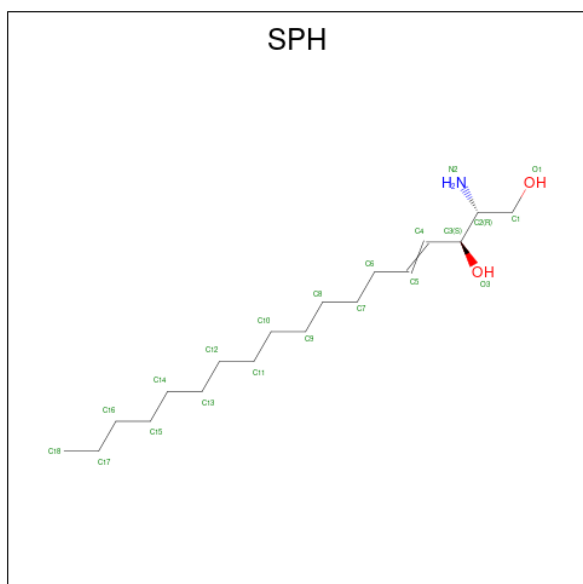
- Molecule 5 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	235	Total	C	N	O	S	0	0
			1834	1169	299	349	17		

There is a discrepancy between the modelled and reference sequences:

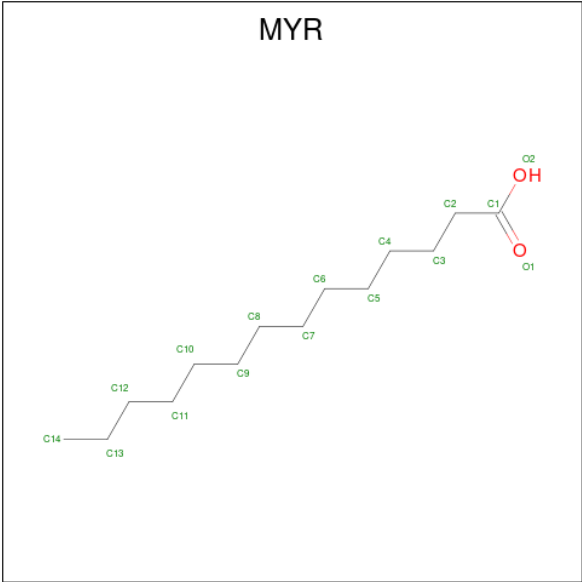
Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	SEE REMARK 999	UNP P03300

- Molecule 6 is SPHINGOSINE (three-letter code: SPH) (formula:  $C_{18}H_{37}NO_2$ ).



Mol	Chain	Residues	Atoms				AltConf
6	1	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).

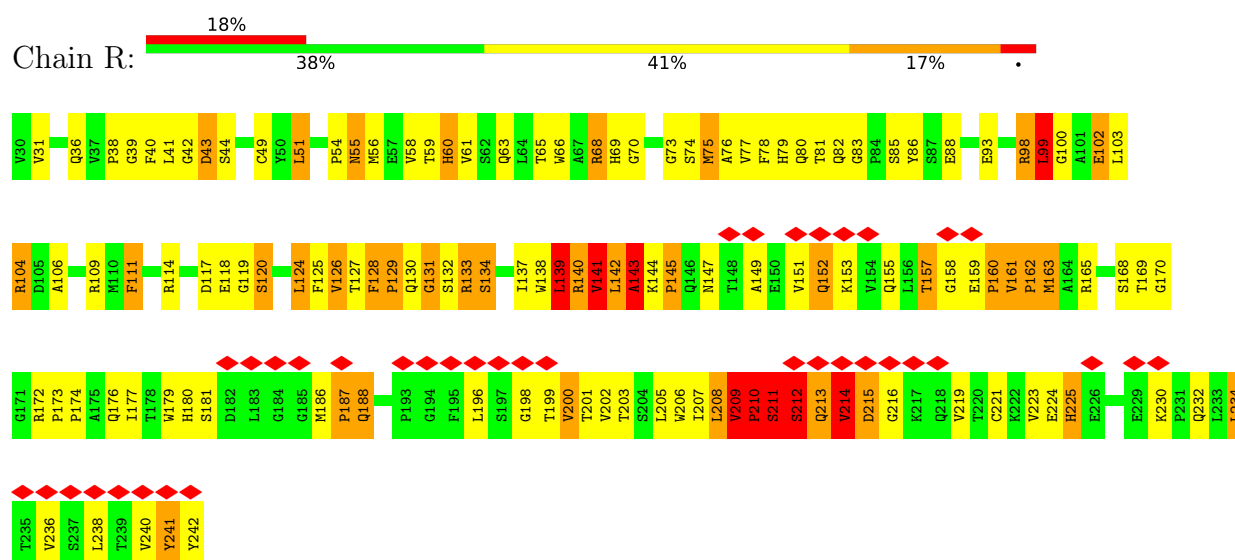


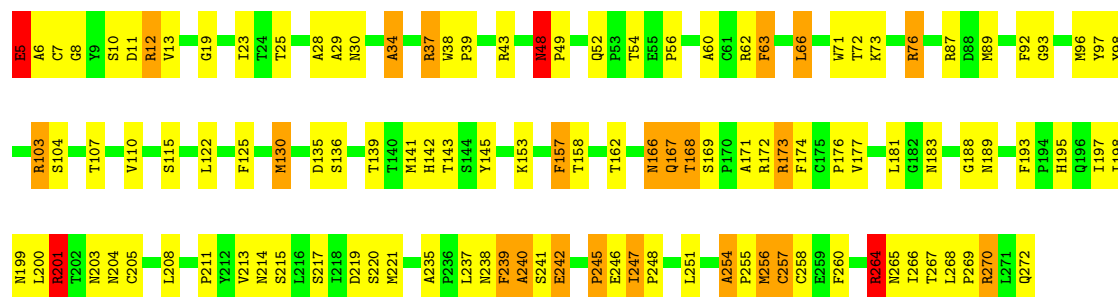
Mol	Chain	Residues	Atoms			AltConf
7	4	1	Total	C	O	0
			15	14	1	

### 3 Residue-property plots

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

#### • Molecule 1: Poliovirus receptor

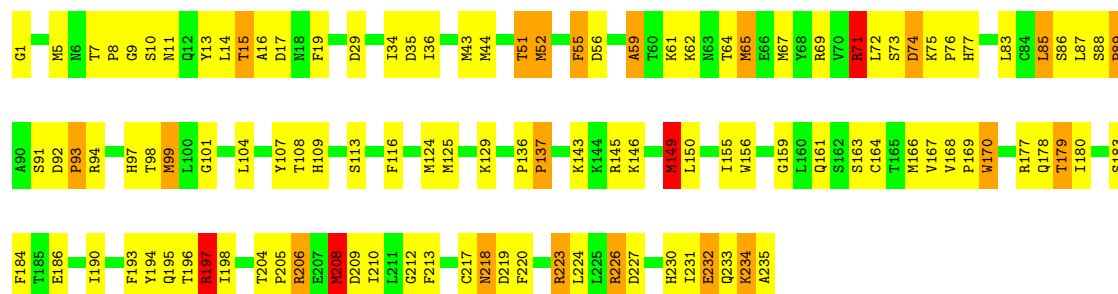




• Molecule 4: Protein VP4



• Molecule 5: Protein VP3





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	857	Depositor
Maximum defocus (nm)	2126	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	32.252	Depositor
Minimum map value	-6.836	Depositor
Average map value	1.633	Depositor
Map value standard deviation	5.404	Depositor
Recommended contour level	7.03	Depositor
Map size ( $\text{\AA}$ )	575.05005, 575.05005, 575.05005	wwPDB
Map dimensions	217, 217, 217	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.65, 2.65, 2.65	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	R	0.41	0/1678	0.77	4/2289 (0.2%)
2	1	1.92	2/2285 (0.1%)	2.09	33/3124 (1.1%)
3	2	1.95	8/2142 (0.4%)	2.10	38/2928 (1.3%)
4	4	1.95	5/484 (1.0%)	2.11	11/653 (1.7%)
5	3	1.92	5/1881 (0.3%)	2.07	33/2562 (1.3%)
All	All	1.74	20/8470 (0.2%)	1.90	119/11556 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	R	1	6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	1	GLY	N-CA	9.08	1.59	1.46
2	1	20	ALA	N-CA	7.91	1.62	1.46
4	4	23	SER	N-CA	7.73	1.61	1.46
4	4	14	GLU	CD-OE2	6.59	1.32	1.25
3	2	5	GLU	N-CA	5.85	1.58	1.46
4	4	47	SER	C-N	-5.46	1.21	1.34
4	4	11	GLY	N-CA	5.35	1.54	1.46
3	2	19	GLY	N-CA	5.33	1.54	1.46
3	2	245	PRO	C-N	-5.27	1.22	1.34
2	1	93	ASP	C-N	-5.21	1.22	1.34
4	4	14	GLU	N-CA	5.21	1.56	1.46
5	3	159	GLY	N-CA	5.18	1.53	1.46
3	2	93	GLY	N-CA	5.16	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	30	ASN	C-N	-5.14	1.22	1.34
5	3	101	GLY	N-CA	5.14	1.53	1.46
3	2	19	GLY	CA-C	5.09	1.59	1.51
3	2	188	GLY	N-CA	5.08	1.53	1.46
5	3	9	GLY	N-CA	5.07	1.53	1.46
3	2	235	ALA	C-N	-5.03	1.24	1.34
5	3	9	GLY	CA-C	5.03	1.59	1.51

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	211	SER	O-C-N	-8.58	108.97	122.70
5	3	197	ARG	NE-CZ-NH2	7.74	124.17	120.30
5	3	69	ARG	NE-CZ-NH2	7.63	124.11	120.30
5	3	223	ARG	NE-CZ-NH2	7.63	124.11	120.30
3	2	264	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	1	267	ARG	NE-CZ-NH2	7.57	124.08	120.30
2	1	275	ARG	NE-CZ-NH2	7.54	124.07	120.30
3	2	43	ARG	NE-CZ-NH2	7.52	124.06	120.30
2	1	64	ARG	NE-CZ-NH2	7.50	124.05	120.30
5	3	226	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	1	193	ARG	NE-CZ-NH2	7.49	124.05	120.30
3	2	201	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	1	129	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	1	243	ARG	NE-CZ-NH2	7.47	124.04	120.30
3	2	176	PRO	CA-N-CD	-7.45	101.07	111.50
2	1	120	ARG	NE-CZ-NH2	7.44	124.02	120.30
4	4	34	ARG	NE-CZ-NH2	7.44	124.02	120.30
3	2	103	ARG	NE-CZ-NH2	7.43	124.01	120.30
2	1	258	ARG	NE-CZ-NH2	7.41	124.01	120.30
5	3	206	ARG	NE-CZ-NH2	7.41	124.01	120.30
3	2	172	ARG	NE-CZ-NH2	7.41	124.00	120.30
5	3	177	ARG	NE-CZ-NH2	7.41	124.00	120.30
3	2	37	ARG	NE-CZ-NH2	7.40	124.00	120.30
2	1	24	ARG	NE-CZ-NH2	7.40	124.00	120.30
5	3	145	ARG	NE-CZ-NH2	7.40	124.00	120.30
2	1	72	ARG	NE-CZ-NH2	7.39	124.00	120.30
3	2	62	ARG	NE-CZ-NH2	7.39	123.99	120.30
2	1	272	ARG	NE-CZ-NH2	7.37	123.98	120.30
3	2	76	ARG	NE-CZ-NH2	7.35	123.98	120.30
3	2	270	ARG	NE-CZ-NH2	7.35	123.97	120.30
2	1	70	ARG	NE-CZ-NH2	7.34	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	12	ARG	NE-CZ-NH2	7.34	123.97	120.30
5	3	71	ARG	NE-CZ-NH2	7.33	123.96	120.30
2	1	119	ARG	NE-CZ-NH2	7.32	123.96	120.30
3	2	87	ARG	NE-CZ-NH2	7.30	123.95	120.30
5	3	94	ARG	NE-CZ-NH2	7.29	123.94	120.30
3	2	173	ARG	NE-CZ-NH2	7.28	123.94	120.30
2	1	83	ARG	NE-CZ-NH2	7.18	123.89	120.30
2	1	146	ASN	CB-CA-C	-6.77	96.86	110.40
2	1	130	PHE	N-CA-C	6.60	128.81	111.00
3	2	193	PHE	CB-CA-C	-6.58	97.24	110.40
3	2	174	PHE	CB-CA-C	-6.35	97.71	110.40
5	3	166	MET	CG-SD-CE	6.31	110.29	100.20
3	2	125	PHE	N-CA-C	6.27	127.93	111.00
3	2	204	ASN	CB-CA-C	-6.25	97.89	110.40
5	3	44	MET	CG-SD-CE	6.25	110.20	100.20
5	3	65	MET	CG-SD-CE	6.25	110.19	100.20
1	R	99	LEU	CA-CB-CG	6.24	129.65	115.30
3	2	89	MET	CG-SD-CE	6.21	110.14	100.20
5	3	193	PHE	CB-CA-C	-6.21	97.99	110.40
5	3	125	MET	CG-SD-CE	6.19	110.10	100.20
5	3	67	MET	CG-SD-CE	6.18	110.08	100.20
5	3	19	PHE	CB-CA-C	-6.17	98.05	110.40
5	3	124	MET	CG-SD-CE	6.16	110.05	100.20
4	4	8	GLN	O-C-N	6.15	132.54	122.70
3	2	96	MET	CG-SD-CE	6.14	110.03	100.20
2	1	158	MET	CG-SD-CE	6.14	110.02	100.20
3	2	130	MET	CG-SD-CE	6.13	110.01	100.20
2	1	90	MET	CG-SD-CE	6.12	110.00	100.20
5	3	208	MET	CG-SD-CE	6.11	109.98	100.20
5	3	99	MET	CG-SD-CE	6.11	109.98	100.20
5	3	149	MET	CG-SD-CE	6.10	109.97	100.20
3	2	221	MET	CG-SD-CE	6.10	109.95	100.20
3	2	256	MET	CG-SD-CE	6.10	109.95	100.20
5	3	43	MET	CG-SD-CE	6.10	109.95	100.20
5	3	52	MET	CG-SD-CE	6.08	109.93	100.20
3	2	141	MET	CG-SD-CE	6.08	109.93	100.20
5	3	5	MET	CG-SD-CE	6.08	109.92	100.20
3	2	260	PHE	N-CA-C	6.07	127.39	111.00
2	1	136	PHE	N-CA-C	6.02	127.25	111.00
3	2	63	PHE	N-CA-C	6.02	127.25	111.00
4	4	67	MET	CG-SD-CE	6.00	109.80	100.20
2	1	132	MET	CG-SD-CE	5.99	109.79	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	211	SER	CA-C-N	5.89	130.16	117.20
2	1	237	PHE	N-CA-C	5.89	126.90	111.00
3	2	125	PHE	CB-CA-C	-5.86	98.68	110.40
4	4	25	ILE	O-C-N	5.77	131.93	122.70
2	1	130	PHE	CB-CA-C	-5.75	98.91	110.40
3	2	203	ASN	N-CA-C	5.60	126.13	111.00
5	3	213	PHE	CB-CA-C	-5.57	99.27	110.40
2	1	212	PHE	CB-CA-C	-5.53	99.33	110.40
2	1	141	ASN	O-C-N	5.52	131.53	122.70
5	3	232	GLU	O-C-N	5.50	131.50	122.70
4	4	46	PHE	N-CA-C	5.50	125.84	111.00
2	1	125	PHE	CB-CA-C	-5.46	99.49	110.40
2	1	124	PHE	CA-C-N	-5.42	105.27	117.20
4	4	46	PHE	CB-CA-C	-5.41	99.57	110.40
4	4	53	PHE	CB-CA-C	-5.41	99.58	110.40
4	4	47	SER	O-C-N	5.39	131.33	122.70
5	3	220	PHE	CB-CA-C	-5.39	99.63	110.40
5	3	55	PHE	N-CA-C	5.38	125.53	111.00
3	2	174	PHE	N-CA-C	5.32	125.37	111.00
3	2	247	ILE	O-C-N	5.29	131.15	121.10
3	2	157	PHE	CB-CA-C	-5.28	99.84	110.40
2	1	272	ARG	O-C-N	5.28	131.13	121.10
1	R	209	VAL	N-CA-C	5.28	125.25	111.00
5	3	220	PHE	N-CA-C	5.27	125.22	111.00
2	1	208	PHE	CB-CA-C	-5.26	99.87	110.40
3	2	239	PHE	N-CA-C	5.26	125.19	111.00
5	3	19	PHE	N-CA-C	5.25	125.19	111.00
5	3	55	PHE	CB-CA-C	-5.23	99.94	110.40
4	4	40	ALA	O-C-N	5.23	131.06	122.70
3	2	183	ASN	N-CA-C	5.21	125.07	111.00
3	2	63	PHE	CB-CA-C	-5.18	100.04	110.40
3	2	246	GLU	O-C-N	5.18	130.99	122.70
2	1	218	LYS	CB-CA-C	-5.15	100.09	110.40
5	3	193	PHE	N-CA-C	5.14	124.89	111.00
5	3	116	PHE	CB-CA-C	-5.13	100.14	110.40
5	3	184	PHE	CB-CA-C	-5.11	100.19	110.40
3	2	260	PHE	CB-CA-C	-5.09	100.21	110.40
2	1	180	ASN	CB-CA-C	-5.09	100.22	110.40
2	1	243	ARG	O-C-N	5.09	130.84	122.70
2	1	237	PHE	CB-CA-C	-5.08	100.23	110.40
3	2	92	PHE	CB-CA-C	-5.08	100.25	110.40
3	2	254	ALA	O-C-N	5.07	130.74	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	81	PHE	CB-CA-C	-5.04	100.31	110.40
4	4	39	ASN	CB-CA-C	-5.04	100.33	110.40
3	2	193	PHE	O-C-N	5.03	130.66	121.10
4	4	44	GLN	O-C-N	5.02	130.73	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	R	141	VAL	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	140	ARG	Peptide
1	R	143	ALA	Peptide
1	R	210	PRO	Peptide
1	R	211	SER	Peptide
1	R	212	SER	Mainchain
1	R	213	GLN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1638	0	1617	246	0
2	1	2222	0	2173	190	0
3	2	2085	0	2000	97	0
4	4	477	0	457	33	0
5	3	1834	0	1815	131	0
6	1	21	0	36	23	0
7	4	15	0	27	1	0
All	All	8292	0	8125	564	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 34.

All (564) 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:R:130:GLN:NE2	2:1:105:PHE:CE1	1.75	1.52
1:R:128:PHE:HE2	2:1:108:TRP:NE1	1.18	1.40
1:R:130:GLN:CG	2:1:105:PHE:O	1.70	1.37
1:R:130:GLN:NE2	2:1:105:PHE:CZ	1.97	1.32
3:2:5:GLU:CG	3:2:7:CYS:HB3	1.58	1.32
1:R:132:SER:OG	2:1:107:VAL:HG11	1.37	1.22
2:1:132:MET:CE	6:1:0:SPH:H81	1.69	1.22
1:R:128:PHE:CE2	2:1:108:TRP:NE1	2.05	1.22
1:R:73:GLY:HA3	5:3:97:HIS:CD2	1.77	1.19
2:1:177:THR:HG21	2:1:182:SER:OG	1.40	1.19
2:1:182:SER:H	5:3:15:THR:CG2	1.58	1.16
3:2:5:GLU:HG2	3:2:7:CYS:HB3	1.19	1.15
1:R:114:ARG:HH12	5:3:59:ALA:HB1	1.03	1.14
1:R:132:SER:OG	2:1:107:VAL:CG1	1.94	1.14
3:2:48:ASN:HB3	3:2:49:PRO:HD3	1.18	1.14
1:R:75:MET:CE	5:3:92:ASP:HA	1.73	1.14
1:R:75:MET:HE2	5:3:92:ASP:HA	1.27	1.14
2:1:182:SER:H	5:3:15:THR:HG21	1.10	1.14
2:1:237:PHE:CE2	6:1:0:SPH:H71	1.82	1.14
3:2:5:GLU:CG	3:2:7:CYS:CB	2.25	1.13
1:R:161:VAL:HB	1:R:163:MET:HB2	1.21	1.13
1:R:43:ASP:HB2	1:R:44:SER:CA	1.79	1.12
1:R:75:MET:HE2	5:3:92:ASP:CA	1.80	1.11
1:R:83:GLY:HA3	2:1:226:ASP:O	1.50	1.11
1:R:114:ARG:NH1	5:3:59:ALA:CB	2.13	1.11
1:R:130:GLN:HB2	2:1:106:ALA:HA	1.34	1.08
1:R:162:PRO:HD2	1:R:163:MET:HA	1.30	1.08
1:R:130:GLN:HA	2:1:107:VAL:HB	1.29	1.07
3:2:48:ASN:HB3	3:2:49:PRO:CD	1.86	1.06
1:R:43:ASP:CB	1:R:44:SER:HA	1.85	1.06
1:R:128:PHE:CE1	2:1:114:ASP:OD1	1.76	1.05
1:R:98:ARG:HD3	1:R:104:ARG:HH21	1.21	1.04
2:1:132:MET:HE1	6:1:0:SPH:C8	1.88	1.04
1:R:130:GLN:HG3	2:1:105:PHE:C	1.76	1.04
5:3:167:VAL:O	5:3:169:PRO:HD3	1.57	1.03
3:2:5:GLU:HG3	3:2:7:CYS:HB3	1.41	1.02
3:2:5:GLU:HG3	3:2:7:CYS:CB	1.90	1.01
1:R:98:ARG:HD3	1:R:104:ARG:NH2	1.75	1.01
1:R:114:ARG:HH12	5:3:59:ALA:CB	1.71	1.00
1:R:54:PRO:HA	1:R:55:ASN:HB2	1.44	1.00
1:R:128:PHE:CE2	2:1:108:TRP:CD1	2.50	1.00
1:R:130:GLN:HG3	2:1:105:PHE:O	0.82	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:37:ARG:O	3:2:211:PRO:HG3	1.64	0.98
1:R:82:GLN:HB2	2:1:228:LEU:H	1.28	0.98
1:R:177:ILE:HD12	1:R:205:LEU:HB2	1.45	0.98
1:R:114:ARG:NH1	5:3:59:ALA:HB1	1.75	0.98
1:R:75:MET:CE	5:3:92:ASP:CG	2.33	0.96
2:1:22:THR:HG22	2:1:24:ARG:H	1.32	0.94
3:2:5:GLU:HG3	3:2:7:CYS:CA	1.99	0.93
1:R:75:MET:HE2	5:3:92:ASP:CB	1.97	0.93
1:R:141:VAL:HG23	1:R:141:VAL:O	1.68	0.93
3:2:5:GLU:OE2	3:2:7:CYS:HB2	1.66	0.93
1:R:132:SER:HB2	2:1:166:VAL:HG11	1.49	0.93
2:1:132:MET:HE1	6:1:0:SPH:H81	0.94	0.92
1:R:129:PRO:O	2:1:107:VAL:O	1.87	0.92
1:R:142:LEU:HD23	1:R:172:ARG:HB3	1.52	0.92
1:R:68:ARG:HD2	1:R:76:ALA:HB3	1.52	0.92
1:R:130:GLN:HE21	2:1:105:PHE:HE1	1.04	0.92
1:R:99:LEU:HD23	3:2:142:HIS:NE2	1.85	0.91
3:2:5:GLU:CD	3:2:7:CYS:H	1.72	0.91
5:3:83:LEU:HD12	5:3:83:LEU:O	1.69	0.91
1:R:75:MET:CE	5:3:92:ASP:CA	2.33	0.91
2:1:56:VAL:HB	2:1:57:PRO:HD2	1.52	0.90
1:R:128:PHE:CD2	2:1:108:TRP:CD1	2.60	0.89
1:R:162:PRO:CD	1:R:163:MET:HA	2.03	0.89
1:R:142:LEU:CD2	1:R:172:ARG:HB3	2.03	0.88
1:R:43:ASP:HB2	1:R:44:SER:HA	0.91	0.87
5:3:71:ARG:NH1	5:3:209:ASP:OD2	2.07	0.87
3:2:267:THR:O	3:2:269:PRO:HD3	1.75	0.87
2:1:112:TYR:HE2	6:1:0:SPH:HO3	0.90	0.86
3:2:168:THR:CG2	3:2:169:SER:N	2.35	0.86
2:1:144:GLU:C	2:1:146:ASN:H	1.79	0.86
2:1:144:GLU:O	2:1:146:ASN:N	2.09	0.86
3:2:168:THR:HG22	3:2:169:SER:N	1.90	0.85
3:2:270:ARG:O	3:2:270:ARG:HG2	1.73	0.85
2:1:182:SER:N	5:3:15:THR:CG2	2.40	0.84
2:1:237:PHE:CE2	6:1:0:SPH:C7	2.61	0.84
3:2:5:GLU:HG3	3:2:7:CYS:N	1.93	0.83
5:3:149:MET:HE2	5:3:150:LEU:HD23	1.59	0.83
1:R:128:PHE:HE2	2:1:108:TRP:CD1	1.93	0.83
1:R:132:SER:CB	2:1:166:VAL:HG11	2.06	0.83
1:R:73:GLY:HA3	5:3:97:HIS:NE2	1.92	0.83
1:R:132:SER:HB2	2:1:166:VAL:CG1	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:128:PHE:HE1	2:1:114:ASP:OD1	1.52	0.82
3:2:34:ALA:HB3	3:2:211:PRO:HD2	1.61	0.82
1:R:130:GLN:HA	2:1:107:VAL:CB	2.10	0.82
2:1:193:ARG:NH1	5:3:8:PRO:HG2	1.94	0.82
1:R:82:GLN:CB	2:1:228:LEU:H	1.92	0.82
5:3:232:GLU:OE1	5:3:234:LYS:HG2	1.78	0.81
2:1:182:SER:N	5:3:15:THR:HG21	1.94	0.81
1:R:54:PRO:CA	1:R:55:ASN:HB2	2.11	0.81
3:2:166:ASN:O	3:2:166:ASN:OD1	1.97	0.80
1:R:130:GLN:HG2	2:1:107:VAL:HG23	1.63	0.79
1:R:82:GLN:CB	2:1:228:LEU:N	2.46	0.79
4:4:14:GLU:HG2	4:4:16:SER:HB2	1.63	0.79
2:1:158:MET:SD	2:1:177:THR:HG23	2.22	0.79
1:R:75:MET:CG	5:3:91:SER:O	2.30	0.79
1:R:141:VAL:O	1:R:141:VAL:CG2	2.30	0.79
1:R:130:GLN:CB	2:1:106:ALA:HA	2.14	0.78
1:R:75:MET:HE2	5:3:92:ASP:CG	2.02	0.78
1:R:83:GLY:HA3	2:1:226:ASP:C	2.04	0.78
2:1:219:ASP:O	2:1:219:ASP:OD2	2.01	0.78
1:R:75:MET:HG3	5:3:91:SER:O	1.83	0.78
1:R:215:ASP:O	1:R:238:LEU:HB3	1.85	0.77
2:1:237:PHE:CZ	6:1:0:SPH:H71	2.20	0.77
1:R:130:GLN:CD	2:1:105:PHE:CE1	2.57	0.77
1:R:143:ALA:O	1:R:225:HIS:NE2	2.17	0.77
2:1:27:LEU:HB3	2:1:28:PRO:HD2	1.66	0.77
1:R:128:PHE:HD2	2:1:108:TRP:HD1	1.33	0.76
1:R:128:PHE:CD2	2:1:108:TRP:HD1	2.01	0.76
1:R:130:GLN:CA	2:1:107:VAL:H	2.00	0.75
5:3:7:THR:HB	5:3:8:PRO:HD2	1.67	0.75
1:R:63:GLN:HG2	1:R:81:THR:HA	1.69	0.75
1:R:99:LEU:HG	2:1:226:ASP:OD1	1.87	0.75
5:3:149:MET:CE	5:3:150:LEU:CD2	2.65	0.74
3:2:242:GLU:OE2	3:2:242:GLU:N	2.19	0.74
1:R:140:ARG:O	1:R:141:VAL:HB	1.87	0.74
1:R:173:PRO:HG2	1:R:225:HIS:HE1	1.52	0.74
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.71	0.73
4:4:14:GLU:HG2	4:4:16:SER:H	1.50	0.73
4:4:14:GLU:HG2	4:4:16:SER:N	2.03	0.73
4:4:14:GLU:CG	4:4:16:SER:HB2	2.19	0.73
1:R:142:LEU:O	1:R:143:ALA:HB2	1.86	0.73
3:2:5:GLU:HG2	3:2:7:CYS:CB	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:182:SER:H	5:3:15:THR:HG22	1.52	0.72
5:3:71:ARG:HB2	5:3:71:ARG:CZ	2.19	0.72
5:3:74:ASP:HA	5:3:198:ILE:O	1.89	0.72
1:R:80:GLN:HG2	1:R:98:ARG:HG2	1.71	0.72
1:R:40:PHE:CZ	1:R:144:LYS:HB3	2.24	0.72
3:2:5:GLU:OE1	3:2:5:GLU:CA	2.38	0.72
4:4:14:GLU:C	4:4:16:SER:H	1.94	0.71
3:2:168:THR:HG22	3:2:169:SER:H	1.54	0.71
1:R:73:GLY:CA	5:3:97:HIS:NE2	2.52	0.71
5:3:210:ILE:O	5:3:210:ILE:HG13	1.89	0.71
3:2:5:GLU:CG	3:2:7:CYS:H	2.02	0.71
3:2:38:TRP:CD1	3:2:39:PRO:HD2	2.26	0.71
1:R:128:PHE:O	2:1:108:TRP:HA	1.90	0.71
2:1:22:THR:HG22	2:1:24:ARG:N	2.03	0.71
1:R:128:PHE:HB3	1:R:129:PRO:HD3	1.70	0.71
3:2:5:GLU:OE1	3:2:5:GLU:HA	1.91	0.70
4:4:10:VAL:CG2	4:4:25:ILE:HD12	2.22	0.70
1:R:124:LEU:HA	1:R:134:SER:HB2	1.74	0.70
1:R:41:LEU:CB	1:R:142:LEU:O	2.40	0.70
1:R:104:ARG:HD2	1:R:106:ALA:HB2	1.74	0.70
5:3:232:GLU:OE1	5:3:234:LYS:CG	2.39	0.69
1:R:73:GLY:CA	5:3:97:HIS:CD2	2.69	0.69
3:2:34:ALA:HB3	3:2:211:PRO:CD	2.22	0.69
4:4:10:VAL:HG12	4:4:13:HIS:CE1	2.27	0.69
1:R:68:ARG:HD2	1:R:76:ALA:CB	2.21	0.69
1:R:165:ARG:HG3	1:R:206:TRP:HB3	1.73	0.69
5:3:71:ARG:HH12	5:3:209:ASP:CG	1.95	0.69
5:3:195:GLN:OE1	5:3:195:GLN:HA	1.92	0.69
5:3:234:LYS:O	5:3:235:ALA:HB3	1.91	0.69
1:R:132:SER:CB	2:1:107:VAL:HG11	2.23	0.69
4:4:42:SER:OG	4:4:44:GLN:HB2	1.92	0.69
4:4:65:ALA:HB1	4:4:66:PRO:HD2	1.73	0.69
5:3:196:THR:O	5:3:197:ARG:HB3	1.93	0.68
1:R:75:MET:O	5:3:93:PRO:HG3	1.93	0.68
5:3:97:HIS:CE1	5:3:230:HIS:ND1	2.60	0.68
2:1:103:LYS:HD3	2:1:170:TRP:CD2	2.27	0.68
3:2:12:ARG:HA	3:2:28:ALA:O	1.93	0.68
2:1:112:TYR:HE2	6:1:0:SPH:O3	1.71	0.68
4:4:61:LEU:O	4:4:61:LEU:HG	1.93	0.68
3:2:5:GLU:OE1	3:2:6:ALA:N	2.27	0.68
5:3:149:MET:CE	5:3:150:LEU:HD23	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:149:MET:HE2	5:3:150:LEU:CD2	2.22	0.68
1:R:75:MET:CG	5:3:92:ASP:HA	2.24	0.67
1:R:99:LEU:O	3:2:142:HIS:CD2	2.47	0.67
5:3:234:LYS:O	5:3:235:ALA:CB	2.40	0.67
1:R:130:GLN:CB	2:1:107:VAL:H	2.08	0.67
5:3:97:HIS:CE1	5:3:230:HIS:CE1	2.83	0.67
2:1:132:MET:CE	6:1:0:SPH:C8	2.58	0.67
1:R:98:ARG:HG3	1:R:99:LEU:H	1.60	0.67
1:R:40:PHE:CE1	1:R:143:ALA:HB1	2.31	0.66
3:2:5:GLU:CG	3:2:7:CYS:N	2.58	0.66
1:R:173:PRO:HG2	1:R:225:HIS:CE1	2.30	0.66
2:1:90:MET:HE1	2:1:240:LEU:O	1.96	0.66
4:4:14:GLU:CD	4:4:16:SER:HB2	2.15	0.66
1:R:130:GLN:HA	2:1:107:VAL:N	2.11	0.65
1:R:59:THR:HG23	1:R:127:THR:HG23	1.77	0.65
1:R:142:LEU:O	1:R:143:ALA:CB	2.44	0.65
3:2:110:VAL:HG22	3:2:251:LEU:HD12	1.77	0.65
2:1:177:THR:CG2	2:1:182:SER:OG	2.33	0.65
1:R:240:VAL:O	1:R:241:TYR:HD2	1.79	0.65
2:1:22:THR:HB	2:1:25:ASP:OD1	1.97	0.64
3:2:264:ARG:HD3	5:3:136:PRO:O	1.98	0.64
3:2:38:TRP:CG	3:2:39:PRO:HD2	2.32	0.64
1:R:157:THR:OG1	1:R:158:GLY:HA2	1.97	0.64
2:1:90:MET:CE	2:1:240:LEU:O	2.46	0.64
2:1:176:GLN:HE22	5:3:233:GLN:NE2	1.95	0.64
1:R:159:GLU:N	1:R:160:PRO:HD3	2.13	0.64
2:1:182:SER:N	5:3:15:THR:HG22	2.11	0.64
1:R:215:ASP:O	1:R:238:LEU:CB	2.45	0.64
1:R:83:GLY:H	2:1:227:SER:HA	1.62	0.63
2:1:159:TYR:HB2	6:1:0:SPH:H162	1.79	0.63
2:1:159:TYR:O	2:1:161:PRO:HD3	1.98	0.63
1:R:130:GLN:CA	2:1:107:VAL:HB	2.17	0.63
2:1:237:PHE:CZ	6:1:0:SPH:H4	2.33	0.63
3:2:143:THR:HG23	3:2:173:ARG:HA	1.79	0.63
1:R:40:PHE:HZ	1:R:144:LYS:HB3	1.64	0.62
4:4:60:VAL:HG12	4:4:60:VAL:O	1.98	0.62
4:4:57:ILE:HD11	4:4:61:LEU:HB3	1.81	0.62
5:3:85:LEU:CD2	5:3:86:SER:N	2.62	0.62
1:R:75:MET:HE1	5:3:92:ASP:CG	2.20	0.62
1:R:215:ASP:HB3	1:R:216:GLY:CA	2.30	0.62
5:3:77:HIS:HE1	5:3:194:TYR:O	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:85:LEU:HD22	5:3:86:SER:N	2.13	0.62
1:R:149:ALA:HB2	1:R:234:LEU:HD12	1.81	0.62
2:1:103:LYS:HD3	2:1:170:TRP:CG	2.34	0.61
2:1:213:SER:O	5:3:183:SER:HB3	2.00	0.61
2:1:237:PHE:CE2	6:1:0:SPH:C4	2.83	0.61
1:R:66:TRP:HB2	1:R:78:PHE:HB3	1.81	0.61
2:1:128:SER:HB3	2:1:207:HIS:CE1	2.35	0.61
3:2:63:PHE:CD1	3:2:254:ALA:HB2	2.36	0.61
1:R:114:ARG:NH1	5:3:59:ALA:HB3	2.10	0.61
1:R:131:GLY:H	2:1:107:VAL:HB	1.66	0.61
1:R:139:LEU:HD22	1:R:140:ARG:HG3	1.80	0.61
2:1:218:LYS:O	2:1:220:GLN:N	2.34	0.61
4:4:55:GLU:N	4:4:56:PRO:HD3	2.15	0.60
5:3:75:LYS:HB2	5:3:76:PRO:HD2	1.81	0.60
2:1:92:VAL:HG12	2:1:106:ALA:H	1.66	0.60
1:R:82:GLN:HB3	2:1:228:LEU:N	2.15	0.60
1:R:85:SER:HB2	2:1:214:LYS:NZ	2.17	0.60
1:R:151:VAL:HA	1:R:163:MET:O	2.01	0.60
3:2:267:THR:HG22	3:2:269:PRO:HD3	1.84	0.60
5:3:208:MET:HE2	5:3:208:MET:H	1.66	0.60
3:2:5:GLU:CD	3:2:7:CYS:HB2	2.22	0.60
1:R:86:TYR:CE1	2:1:224:LEU:CD1	2.85	0.59
1:R:162:PRO:HD3	1:R:209:VAL:O	2.01	0.59
2:1:133:GLU:O	2:1:133:GLU:HG2	2.01	0.59
1:R:181:SER:HB3	1:R:219:VAL:HG23	1.85	0.59
4:4:10:VAL:HG21	4:4:25:ILE:HD12	1.82	0.59
1:R:130:GLN:HA	2:1:107:VAL:H	1.63	0.59
2:1:249:ASN:CG	2:1:250:PRO:HD2	2.22	0.59
1:R:132:SER:H	2:1:107:VAL:HG11	1.66	0.59
3:2:239:PHE:CD2	3:2:240:ALA:N	2.71	0.59
1:R:162:PRO:HD3	1:R:208:LEU:H	1.67	0.59
1:R:83:GLY:N	2:1:227:SER:HA	2.18	0.59
3:2:264:ARG:NH1	5:3:137:PRO:O	2.35	0.59
5:3:83:LEU:HD12	5:3:83:LEU:C	2.23	0.58
1:R:215:ASP:HB3	1:R:216:GLY:HA2	1.85	0.58
1:R:143:ALA:O	1:R:225:HIS:CE1	2.56	0.58
1:R:41:LEU:HB2	1:R:142:LEU:O	2.03	0.58
1:R:188:GLN:HB3	1:R:208:LEU:O	2.04	0.58
2:1:104:LEU:O	2:1:104:LEU:HG	2.02	0.58
5:3:87:LEU:HD13	5:3:190:ILE:HD11	1.86	0.58
5:3:88:SER:HB3	5:3:91:SER:OG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:5:GLU:CD	3:2:7:CYS:CB	2.71	0.58
1:R:68:ARG:HG2	1:R:70:GLY:HA3	1.85	0.58
1:R:128:PHE:HE2	2:1:108:TRP:HE1	0.62	0.58
1:R:214:VAL:HG22	1:R:215:ASP:H	1.67	0.58
5:3:77:HIS:CE1	5:3:194:TYR:O	2.57	0.58
2:1:176:GLN:HE22	5:3:233:GLN:HE21	1.50	0.57
1:R:75:MET:CE	5:3:92:ASP:CB	2.70	0.57
4:4:10:VAL:CG1	4:4:13:HIS:CE1	2.87	0.57
1:R:99:LEU:CG	2:1:226:ASP:OD1	2.53	0.57
1:R:130:GLN:CB	2:1:107:VAL:N	2.68	0.57
3:2:5:GLU:C	3:2:7:CYS:N	2.57	0.57
2:1:144:GLU:C	2:1:146:ASN:N	2.50	0.57
3:2:25:THR:HG23	3:2:25:THR:O	2.04	0.57
1:R:40:PHE:HZ	1:R:144:LYS:HD3	1.70	0.57
1:R:65:THR:HB	1:R:124:LEU:HG	1.86	0.56
1:R:151:VAL:HG21	1:R:238:LEU:HA	1.86	0.56
2:1:176:GLN:NE2	5:3:233:GLN:NE2	2.53	0.56
5:3:149:MET:O	5:3:149:MET:HG2	2.02	0.56
1:R:75:MET:HG2	5:3:91:SER:O	2.06	0.56
1:R:75:MET:HG2	5:3:92:ASP:HA	1.87	0.56
1:R:130:GLN:HA	2:1:107:VAL:CA	2.35	0.56
3:2:195:HIS:HA	3:2:208:LEU:HD21	1.87	0.56
2:1:218:LYS:C	2:1:220:GLN:H	2.08	0.56
1:R:82:GLN:HB2	2:1:228:LEU:N	2.04	0.56
1:R:131:GLY:HA2	1:R:133:ARG:HD3	1.86	0.56
1:R:117:ASP:HB2	1:R:141:VAL:CG1	2.36	0.56
2:1:45:THR:OG1	2:1:46:ALA:N	2.38	0.56
1:R:130:GLN:HG2	2:1:107:VAL:N	2.21	0.56
5:3:34:ILE:O	5:3:36:ILE:N	2.39	0.56
2:1:216:PRO:HG2	3:2:145:TYR:CD1	2.41	0.56
4:4:42:SER:C	4:4:44:GLN:H	2.07	0.56
5:3:218:ASN:HD22	5:3:219:ASP:N	2.03	0.56
1:R:130:GLN:CB	2:1:105:PHE:O	2.52	0.55
1:R:41:LEU:HB3	1:R:142:LEU:O	2.05	0.55
1:R:130:GLN:CA	2:1:107:VAL:N	2.69	0.55
1:R:85:SER:HB2	2:1:214:LYS:HZ3	1.71	0.55
1:R:172:ARG:HA	1:R:201:THR:H	1.70	0.55
1:R:130:GLN:HE21	2:1:107:VAL:HG23	1.71	0.55
1:R:42:GLY:N	1:R:43:ASP:HA	2.22	0.55
5:3:204:THR:CG2	5:3:205:PRO:HD2	2.36	0.54
1:R:120:SER:HB3	1:R:138:TRP:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:166:ASN:OD1	3:2:168:THR:HG22	2.06	0.54
5:3:73:SER:HA	5:3:208:MET:CE	2.38	0.54
1:R:99:LEU:CD2	3:2:142:HIS:NE2	2.66	0.54
1:R:41:LEU:HB2	1:R:141:VAL:O	2.07	0.54
2:1:237:PHE:CD2	6:1:0:SPH:C7	2.91	0.54
1:R:41:LEU:HD22	1:R:42:GLY:H	1.72	0.54
1:R:147:ASN:ND2	1:R:223:VAL:HG21	2.22	0.54
3:2:5:GLU:CG	3:2:7:CYS:HB2	2.34	0.54
3:2:60:ALA:O	3:2:255:PRO:HG2	2.08	0.54
1:R:80:GLN:CG	1:R:98:ARG:HG2	2.38	0.53
1:R:152:GLN:O	1:R:163:MET:HB3	2.08	0.53
3:2:256:MET:O	3:2:258:CYS:N	2.42	0.53
4:4:10:VAL:HG11	4:4:13:HIS:ND1	2.23	0.53
5:3:55:PHE:HE1	5:3:212:GLY:HA3	1.73	0.53
4:4:42:SER:HG	4:4:44:GLN:HB2	1.73	0.53
5:3:83:LEU:O	5:3:83:LEU:CD1	2.50	0.53
5:3:104:LEU:O	5:3:179:THR:HG21	2.08	0.53
1:R:36:GLN:NE2	1:R:137:ILE:HG13	2.23	0.53
1:R:44:SER:HG	1:R:111:PHE:HD1	1.56	0.53
3:2:110:VAL:HG22	3:2:251:LEU:CD1	2.39	0.53
5:3:107:TYR:O	5:3:179:THR:HG21	2.08	0.53
2:1:193:ARG:CZ	5:3:8:PRO:HG2	2.38	0.53
1:R:49:CYS:HB2	1:R:66:TRP:HZ2	1.73	0.53
1:R:117:ASP:CB	1:R:141:VAL:HG13	2.38	0.53
1:R:161:VAL:HB	1:R:163:MET:CB	2.14	0.53
2:1:280:TYR:HB3	2:1:285:ASP:O	2.09	0.53
1:R:40:PHE:CZ	1:R:144:LYS:CB	2.92	0.52
4:4:14:GLU:HG2	4:4:16:SER:CB	2.37	0.52
2:1:112:TYR:CD2	6:1:0:SPH:H5	2.43	0.52
1:R:127:THR:HG22	1:R:129:PRO:HD2	1.91	0.52
2:1:38:SER:OG	2:1:39:LYS:N	2.41	0.52
2:1:105:PHE:O	2:1:105:PHE:CD1	2.62	0.52
5:3:149:MET:HE1	5:3:150:LEU:CD2	2.40	0.52
2:1:183:ILE:HD11	2:1:194:ILE:HG12	1.91	0.52
2:1:218:LYS:HD3	3:2:268:LEU:HB3	1.91	0.52
3:2:98:TYR:CE1	3:2:266:ILE:HD12	2.45	0.52
3:2:122:LEU:HB2	3:2:198:ILE:HB	1.90	0.52
1:R:80:GLN:O	1:R:98:ARG:NH2	2.42	0.52
1:R:130:GLN:CD	2:1:105:PHE:O	2.45	0.52
1:R:73:GLY:N	1:R:74:SER:HA	2.25	0.51
1:R:98:ARG:C	1:R:100:GLY:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:134:SER:O	2:1:168:GLU:HG2	2.10	0.51
3:2:136:SER:OG	3:2:139:THR:HG22	2.10	0.51
1:R:117:ASP:CB	1:R:141:VAL:CG1	2.88	0.51
5:3:178:GLN:C	5:3:180:ILE:H	2.14	0.51
2:1:209:TYR:O	2:1:230:GLY:HA2	2.10	0.51
4:4:13:HIS:CD2	4:4:13:HIS:H	2.27	0.51
2:1:112:TYR:HD2	6:1:0:SPH:H5	1.76	0.51
1:R:41:LEU:N	1:R:142:LEU:O	2.43	0.51
2:1:95:PRO:HD2	2:1:103:LYS:HG3	1.93	0.51
2:1:158:MET:SD	2:1:177:THR:CG2	2.96	0.51
5:3:89:PRO:HB2	5:3:104:LEU:CD2	2.41	0.51
3:2:13:VAL:HA	3:2:25:THR:O	2.10	0.51
1:R:98:ARG:CG	1:R:99:LEU:H	2.24	0.51
4:4:10:VAL:CG1	4:4:13:HIS:ND1	2.74	0.50
1:R:187:PRO:O	1:R:188:GLN:HG3	2.11	0.50
3:2:198:ILE:HG22	3:2:198:ILE:O	2.11	0.50
4:4:55:GLU:N	4:4:56:PRO:CD	2.74	0.50
2:1:22:THR:CG2	2:1:24:ARG:H	2.16	0.50
5:3:14:LEU:O	5:3:16:ALA:N	2.44	0.50
5:3:129:LYS:O	5:3:195:GLN:HB3	2.12	0.50
1:R:169:THR:HA	1:R:202:VAL:HG23	1.93	0.50
2:1:237:PHE:CD2	6:1:0:SPH:H71	2.40	0.50
2:1:218:LYS:C	2:1:220:GLN:N	2.65	0.50
4:4:10:VAL:HG22	4:4:25:ILE:HD12	1.93	0.50
4:4:24:THR:HG23	4:4:24:THR:O	2.10	0.50
1:R:93:GLU:HB3	1:R:109:ARG:HB3	1.92	0.50
3:2:5:GLU:CD	3:2:7:CYS:N	2.53	0.50
2:1:261:LEU:C	2:1:261:LEU:HD23	2.31	0.49
1:R:130:GLN:CG	2:1:105:PHE:CD1	2.95	0.49
2:1:48:GLU:HA	3:2:197:ILE:HB	1.94	0.49
1:R:158:GLY:HA3	1:R:159:GLU:HB3	1.94	0.49
2:1:159:TYR:CB	6:1:0:SPH:H162	2.42	0.49
1:R:85:SER:CB	2:1:214:LYS:NZ	2.75	0.49
5:3:87:LEU:HD13	5:3:190:ILE:CD1	2.43	0.49
1:R:102:GLU:HG3	1:R:104:ARG:NH1	2.28	0.49
1:R:145:PRO:HA	1:R:170:GLY:O	2.12	0.49
5:3:89:PRO:HB2	5:3:104:LEU:HD23	1.95	0.49
1:R:155:GLN:NE2	1:R:212:SER:H	2.10	0.48
2:1:30:THR:HB	2:1:66:VAL:HB	1.95	0.48
5:3:155:ILE:HG22	5:3:155:ILE:O	2.13	0.48
5:3:183:SER:O	5:3:186:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:86:TYR:CE1	2:1:224:LEU:HD12	2.47	0.48
3:2:213:VAL:O	3:2:214:ASN:HB2	2.12	0.48
1:R:54:PRO:CA	1:R:55:ASN:CB	2.87	0.48
3:2:110:VAL:O	3:2:205:CYS:HB2	2.13	0.48
1:R:60:HIS:O	1:R:128:PHE:N	2.26	0.48
2:1:169:LYS:O	2:1:171:ASP:N	2.46	0.48
3:2:267:THR:C	3:2:269:PRO:HD3	2.33	0.48
2:1:130:PHE:O	2:1:130:PHE:CD1	2.66	0.48
3:2:66:LEU:N	3:2:66:LEU:HD23	2.29	0.48
1:R:129:PRO:C	2:1:107:VAL:O	2.52	0.48
1:R:130:GLN:HB2	2:1:107:VAL:H	1.78	0.48
5:3:85:LEU:CD2	5:3:85:LEU:C	2.82	0.48
1:R:128:PHE:HB3	1:R:129:PRO:CD	2.43	0.47
5:3:109:HIS:HB2	5:3:223:ARG:HG2	1.95	0.47
5:3:156:TRP:CD1	5:3:164:CYS:HB2	2.49	0.47
1:R:86:TYR:CE1	2:1:224:LEU:HD11	2.48	0.47
2:1:78:GLU:OE1	2:1:265:HIS:N	2.47	0.47
2:1:237:PHE:CZ	6:1:0:SPH:C4	2.96	0.47
4:4:14:GLU:C	4:4:16:SER:N	2.64	0.47
2:1:105:PHE:O	2:1:105:PHE:CG	2.68	0.47
1:R:180:HIS:HA	1:R:186:MET:HG3	1.96	0.47
2:1:103:LYS:NZ	2:1:246:ASN:O	2.47	0.47
3:2:76:ARG:HB2	3:2:157:PHE:O	2.14	0.47
1:R:98:ARG:CD	1:R:104:ARG:NH2	2.64	0.47
2:1:237:PHE:HE2	6:1:0:SPH:C4	2.26	0.47
1:R:75:MET:CE	5:3:92:ASP:OD2	2.63	0.47
2:1:90:MET:CE	2:1:242:VAL:HG23	2.45	0.47
3:2:48:ASN:CB	3:2:49:PRO:CD	2.65	0.47
5:3:13:TYR:C	5:3:13:TYR:CD2	2.86	0.47
5:3:14:LEU:O	5:3:14:LEU:HG	2.13	0.47
5:3:233:GLN:O	5:3:235:ALA:N	2.47	0.47
1:R:98:ARG:O	1:R:99:LEU:HD22	2.15	0.47
1:R:179:TRP:CZ3	1:R:219:VAL:HG22	2.49	0.47
2:1:233:SER:O	2:1:235:ASN:N	2.48	0.47
1:R:99:LEU:O	3:2:142:HIS:HD2	1.94	0.47
1:R:186:MET:O	1:R:188:GLN:N	2.48	0.47
2:1:291:LEU:C	2:1:293:PRO:HD3	2.35	0.47
3:2:97:TYR:CE1	3:2:269:PRO:HG3	2.50	0.47
5:3:56:ASP:OD1	5:3:61:LYS:HE3	2.14	0.47
1:R:161:VAL:HG12	1:R:208:LEU:HB2	1.97	0.47
1:R:224:GLU:O	1:R:225:HIS:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:38:PRO:HA	1:R:39:GLY:HA3	1.66	0.46
4:4:14:GLU:O	4:4:16:SER:N	2.48	0.46
1:R:152:GLN:HB2	1:R:153:LYS:HA	1.97	0.46
2:1:124:PHE:CE1	2:1:274:PRO:HG3	2.50	0.46
2:1:184:PHE:HB2	5:3:13:TYR:HB3	1.97	0.46
3:2:219:ASP:CG	3:2:220:SER:H	2.15	0.46
2:1:169:LYS:C	2:1:171:ASP:H	2.19	0.46
3:2:214:ASN:OD1	3:2:215:SER:N	2.48	0.46
5:3:85:LEU:HD22	5:3:85:LEU:C	2.36	0.46
1:R:170:GLY:HA2	1:R:200:VAL:HG13	1.96	0.46
3:2:54:THR:O	3:2:56:PRO:HD3	2.16	0.46
3:2:71:TRP:CD1	3:2:71:TRP:C	2.88	0.46
5:3:149:MET:CE	5:3:150:LEU:HG	2.46	0.46
1:R:75:MET:SD	5:3:92:ASP:HA	2.52	0.46
1:R:130:GLN:CG	2:1:106:ALA:HA	2.45	0.46
1:R:132:SER:HB2	2:1:166:VAL:HG13	1.97	0.46
3:2:71:TRP:CD1	3:2:72:THR:N	2.84	0.46
5:3:85:LEU:HD23	5:3:86:SER:N	2.31	0.46
1:R:117:ASP:HB2	1:R:141:VAL:HG13	1.96	0.46
7:4:1:MYR:H71	7:4:1:MYR:H101	1.66	0.46
1:R:40:PHE:CZ	1:R:144:LYS:HD3	2.50	0.46
1:R:132:SER:N	2:1:107:VAL:HG11	2.31	0.46
1:R:133:ARG:HB2	2:1:167:PRO:O	2.16	0.46
5:3:73:SER:C	5:3:75:LYS:H	2.19	0.46
1:R:117:ASP:HB3	1:R:141:VAL:HG13	1.98	0.46
1:R:133:ARG:HG3	2:1:168:GLU:HA	1.97	0.46
1:R:157:THR:OG1	1:R:158:GLY:CA	2.64	0.46
2:1:169:LYS:C	2:1:171:ASP:N	2.69	0.46
5:3:231:ILE:HG13	5:3:232:GLU:N	2.30	0.46
1:R:130:GLN:CG	2:1:107:VAL:N	2.79	0.45
1:R:188:GLN:O	1:R:207:ILE:HG22	2.16	0.45
1:R:240:VAL:O	1:R:241:TYR:CD2	2.64	0.45
3:2:256:MET:O	3:2:257:CYS:C	2.55	0.45
5:3:156:TRP:CD1	5:3:156:TRP:C	2.89	0.45
1:R:241:TYR:HA	1:R:242:TYR:C	2.37	0.45
2:1:159:TYR:CG	6:1:0:SPH:H142	2.51	0.45
4:4:49:ASP:OD1	4:4:51:SER:HB2	2.17	0.45
3:2:239:PHE:O	3:2:240:ALA:C	2.55	0.45
5:3:87:LEU:HG	5:3:87:LEU:O	2.17	0.45
1:R:99:LEU:HD23	3:2:142:HIS:CE1	2.49	0.45
2:1:128:SER:HB3	2:1:207:HIS:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:130:GLN:HG3	2:1:105:PHE:CD1	2.52	0.45
1:R:131:GLY:N	2:1:107:VAL:HB	2.28	0.45
1:R:172:ARG:O	1:R:174:PRO:HD3	2.17	0.44
2:1:27:LEU:HB3	2:1:28:PRO:CD	2.40	0.44
3:2:5:GLU:C	3:2:7:CYS:H	2.18	0.44
5:3:62:LYS:O	5:3:64:THR:HG23	2.17	0.44
5:3:149:MET:HE1	5:3:150:LEU:HG	2.00	0.44
2:1:233:SER:C	2:1:235:ASN:N	2.69	0.44
2:1:237:PHE:HZ	6:1:0:SPH:H4	1.77	0.44
3:2:5:GLU:OE1	3:2:5:GLU:C	2.55	0.44
1:R:142:LEU:HB3	1:R:143:ALA:H	1.49	0.44
3:2:219:ASP:OD1	3:2:220:SER:N	2.37	0.44
5:3:204:THR:HG23	5:3:205:PRO:HD2	2.00	0.44
1:R:104:ARG:HD3	1:R:104:ARG:HA	1.57	0.44
1:R:130:GLN:HE22	1:R:133:ARG:HD2	1.82	0.44
2:1:53:ASN:C	2:1:55:LEU:H	2.22	0.44
2:1:107:VAL:O	2:1:107:VAL:HG12	2.16	0.44
2:1:161:PRO:HG2	5:3:226:ARG:HB2	1.98	0.43
3:2:29:ALA:HA	4:4:68:LEU:HD21	2.00	0.43
1:R:31:VAL:HG12	1:R:51:LEU:HD11	1.98	0.43
1:R:41:LEU:H	1:R:143:ALA:HB2	1.83	0.43
3:2:256:MET:C	3:2:258:CYS:N	2.71	0.43
1:R:82:GLN:O	1:R:98:ARG:HG3	2.18	0.43
1:R:162:PRO:HB2	1:R:238:LEU:HG	2.00	0.43
3:2:158:THR:O	3:2:177:VAL:HA	2.18	0.43
4:4:42:SER:C	4:4:44:GLN:N	2.72	0.43
5:3:195:GLN:OE1	5:3:195:GLN:CA	2.64	0.43
1:R:85:SER:CB	2:1:214:LYS:HZ3	2.31	0.43
5:3:51:THR:HG21	5:3:99:MET:H	1.82	0.43
5:3:218:ASN:HD22	5:3:219:ASP:H	1.67	0.43
1:R:65:THR:HA	1:R:78:PHE:O	2.18	0.43
1:R:69:HIS:N	1:R:70:GLY:HA3	2.33	0.43
2:1:56:VAL:HB	2:1:57:PRO:CD	2.36	0.43
2:1:234:LEU:HD23	2:1:234:LEU:HA	1.87	0.43
5:3:10:SER:O	5:3:11:ASN:HB2	2.19	0.43
3:2:166:ASN:O	3:2:168:THR:N	2.51	0.43
5:3:190:ILE:O	5:3:190:ILE:HG22	2.18	0.43
1:R:207:ILE:HA	1:R:208:LEU:HB3	2.00	0.43
3:2:5:GLU:HG3	3:2:8:GLY:N	2.34	0.43
1:R:31:VAL:HG11	1:R:134:SER:HA	2.01	0.43
2:1:38:SER:HG	2:1:40:GLU:H	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:176:GLN:NE2	5:3:233:GLN:HE21	2.15	0.43
3:2:107:THR:O	3:2:107:THR:HG22	2.16	0.43
3:2:135:ASP:OD2	3:2:171:ALA:HB3	2.19	0.43
5:3:74:ASP:CG	5:3:206:ARG:HE	2.22	0.43
1:R:168:SER:HB3	1:R:203:THR:HG23	2.01	0.42
1:R:177:ILE:HG22	1:R:223:VAL:HG22	2.00	0.42
2:1:81:PHE:O	2:1:83:ARG:N	2.34	0.42
2:1:105:PHE:C	2:1:105:PHE:CD1	2.91	0.42
2:1:273:PRO:HB3	3:2:189:ASN:HB2	2.01	0.42
3:2:168:THR:HG23	3:2:169:SER:N	2.26	0.42
1:R:114:ARG:HH11	5:3:59:ALA:CB	2.18	0.42
2:1:78:GLU:O	2:1:82:ALA:N	2.52	0.42
5:3:113:SER:O	5:3:217:CYS:HB2	2.19	0.42
5:3:170:TRP:O	5:3:170:TRP:CG	2.71	0.42
1:R:144:LYS:HA	1:R:145:PRO:HD3	1.89	0.42
5:3:233:GLN:O	5:3:233:GLN:HG2	2.19	0.42
5:3:73:SER:HA	5:3:208:MET:HE1	2.01	0.42
1:R:114:ARG:NH1	5:3:59:ALA:HB2	2.24	0.42
1:R:142:LEU:HD21	1:R:172:ARG:HB3	1.97	0.42
2:1:177:THR:HG22	2:1:180:ASN:HB2	2.01	0.42
3:2:5:GLU:O	3:2:7:CYS:N	2.53	0.42
5:3:196:THR:O	5:3:197:ARG:CB	2.63	0.42
4:4:61:LEU:O	4:4:61:LEU:CG	2.62	0.42
1:R:159:GLU:H	1:R:160:PRO:HD3	1.82	0.42
2:1:37:HIS:CD2	2:1:37:HIS:O	2.73	0.42
2:1:93:ASP:C	2:1:93:ASP:OD2	2.58	0.42
1:R:79:HIS:CD2	2:1:234:LEU:HD12	2.54	0.42
1:R:133:ARG:HB2	2:1:168:GLU:HA	2.02	0.42
1:R:221:CYS:HB3	1:R:234:LEU:HG	2.02	0.42
5:3:14:LEU:HB3	5:3:17:ASP:HB3	2.02	0.42
1:R:75:MET:HG2	5:3:91:SER:C	2.41	0.42
3:2:198:ILE:HD13	3:2:205:CYS:HA	2.01	0.42
2:1:24:ARG:O	2:1:24:ARG:HG3	2.20	0.41
2:1:155:TYR:N	2:1:155:TYR:CD2	2.86	0.41
3:2:71:TRP:CE2	3:2:237:LEU:HB2	2.55	0.41
2:1:132:MET:CE	6:1:0:SPH:C10	2.98	0.41
2:1:237:PHE:CG	6:1:0:SPH:H92	2.55	0.41
3:2:199:ASN:O	3:2:201:ARG:N	2.52	0.41
5:3:233:GLN:O	5:3:234:LYS:C	2.59	0.41
1:R:142:LEU:HD23	1:R:173:PRO:HD3	2.03	0.41
3:2:264:ARG:HB2	3:2:265:ASN:H	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:65:ALA:HB1	4:4:66:PRO:CD	2.45	0.41
5:3:108:THR:HB	5:3:224:LEU:HB3	2.02	0.41
1:R:157:THR:CB	1:R:158:GLY:HA2	2.50	0.41
2:1:212:PHE:CD1	2:1:212:PHE:N	2.87	0.41
5:3:149:MET:CE	5:3:150:LEU:CG	2.98	0.41
1:R:76:ALA:H	1:R:77:VAL:HG23	1.85	0.41
2:1:178:SER:OG	5:3:227:ASP:OD2	2.28	0.41
2:1:257:ILE:HD12	2:1:257:ILE:N	2.36	0.41
5:3:136:PRO:O	5:3:137:PRO:O	2.39	0.41
1:R:126:VAL:HA	1:R:132:SER:HA	2.03	0.41
2:1:22:THR:HB	2:1:25:ASP:CG	2.41	0.41
4:4:4:GLN:O	4:4:4:GLN:HG3	2.21	0.41
5:3:98:THR:O	5:3:99:MET:C	2.59	0.41
1:R:210:PRO:HB2	1:R:211:SER:H	1.68	0.41
2:1:123:GLU:C	2:1:125:PHE:H	2.22	0.41
3:2:23:ILE:HD12	3:2:63:PHE:CZ	2.56	0.41
3:2:247:ILE:HA	3:2:248:PRO:HD3	1.92	0.41
5:3:136:PRO:HA	5:3:137:PRO:HD3	1.95	0.41
1:R:186:MET:N	1:R:187:PRO:CD	2.84	0.40
1:R:125:PHE:CD1	1:R:125:PHE:N	2.89	0.40
1:R:40:PHE:HZ	1:R:144:LYS:CB	2.29	0.40
1:R:118:GLU:HA	1:R:119:GLY:HA3	1.89	0.40
2:1:57:PRO:O	2:1:61:VAL:HG22	2.22	0.40
2:1:182:SER:O	5:3:15:THR:HG22	2.22	0.40
3:2:181:LEU:HG	3:2:181:LEU:O	2.21	0.40
1:R:69:HIS:CD2	1:R:120:SER:OG	2.75	0.40
2:1:217:LEU:O	2:1:218:LYS:C	2.59	0.40
3:2:242:GLU:O	3:2:245:PRO:HD3	2.21	0.40
5:3:71:ARG:HG3	5:3:72:LEU:N	2.36	0.40
3:2:104:SER:HB2	3:2:258:CYS:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	211/213 (99%)	136 (64%)	50 (24%)	25 (12%)	0	6
2	1	281/283 (99%)	222 (79%)	43 (15%)	16 (6%)	1	18
3	2	266/268 (99%)	222 (84%)	36 (14%)	8 (3%)	4	28
4	4	59/68 (87%)	47 (80%)	7 (12%)	5 (8%)	1	12
5	3	233/235 (99%)	180 (77%)	38 (16%)	15 (6%)	1	16
All	All	1050/1067 (98%)	807 (77%)	174 (17%)	69 (7%)	2	16

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	55	ASN
1	R	99	LEU
1	R	143	ALA
1	R	188	GLN
1	R	210	PRO
1	R	212	SER
2	1	82	ALA
2	1	145	THR
2	1	219	ASP
3	2	200	LEU
3	2	257	CYS
5	3	15	THR
5	3	29	ASP
5	3	35	ASP
5	3	137	PRO
5	3	197	ARG
1	R	139	LEU
1	R	141	VAL
1	R	198	GLY
2	1	146	ASN
2	1	170	TRP
2	1	234	LEU
2	1	236	ASP
3	2	130	MET
3	2	167	GLN
4	4	15	ASN
5	3	170	TRP
5	3	179	THR

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Mol	Chain	Res	Type
5	3	234	LYS
1	R	56	MET
1	R	88	GLU
1	R	131	GLY
1	R	134	SER
1	R	160	PRO
1	R	161	VAL
1	R	187	PRO
1	R	215	ASP
2	1	210	ASP
2	1	232	ALA
3	2	240	ALA
5	3	168	VAL
1	R	142	LEU
1	R	225	HIS
1	R	232	GLN
2	1	54	PRO
2	1	57	PRO
2	1	165	PRO
2	1	218	LYS
2	1	275	ARG
3	2	48	ASN
3	2	166	ASN
4	4	60	VAL
5	3	65	MET
2	1	216	PRO
3	2	34	ALA
4	4	9	LYS
5	3	59	ALA
5	3	74	ASP
5	3	89	PRO
5	3	161	GLN
4	4	56	PRO
1	R	162	PRO
1	R	209	VAL
2	1	250	PRO
1	R	145	PRO
5	3	93	PRO
1	R	129	PRO
1	R	214	VAL
4	4	11	GLY

### 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	R	185/185 (100%)	150 (81%)	35 (19%)	1	8
2	1	245/245 (100%)	230 (94%)	15 (6%)	18	44
3	2	228/228 (100%)	208 (91%)	20 (9%)	10	31
4	4	54/57 (95%)	46 (85%)	8 (15%)	3	15
5	3	210/210 (100%)	199 (95%)	11 (5%)	23	48
All	All	922/925 (100%)	833 (90%)	89 (10%)	12	27

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	43	ASP
1	R	51	LEU
1	R	58	VAL
1	R	60	HIS
1	R	61	VAL
1	R	68	ARG
1	R	75	MET
1	R	98	ARG
1	R	99	LEU
1	R	102	GLU
1	R	103	LEU
1	R	104	ARG
1	R	111	PHE
1	R	120	SER
1	R	124	LEU
1	R	126	VAL
1	R	128	PHE
1	R	133	ARG
1	R	139	LEU
1	R	141	VAL
1	R	152	GLN
1	R	157	THR
1	R	163	MET

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Mol	Chain	Res	Type
1	R	176	GLN
1	R	196	LEU
1	R	199	THR
1	R	200	VAL
1	R	208	LEU
1	R	212	SER
1	R	213	GLN
1	R	214	VAL
1	R	230	LYS
1	R	234	LEU
1	R	236	VAL
1	R	241	TYR
2	1	38	SER
2	1	83	ARG
2	1	97	SER
2	1	100	ASN
2	1	129	ARG
2	1	143	THR
2	1	146	ASN
2	1	147	ASN
2	1	149	HIS
2	1	177	THR
2	1	220	GLN
2	1	221	SER
2	1	224	LEU
2	1	255	SER
2	1	287	LYS
3	2	5	GLU
3	2	10	SER
3	2	11	ASP
3	2	48	ASN
3	2	52	GLN
3	2	66	LEU
3	2	73	LYS
3	2	103	ARG
3	2	115	SER
3	2	153	LYS
3	2	162	THR
3	2	167	GLN
3	2	168	THR
3	2	201	ARG
3	2	217	SER

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Mol	Chain	Res	Type
3	2	238	ASN
3	2	241	SER
3	2	242	GLU
3	2	264	ARG
3	2	272	GLN
4	4	6	SER
4	4	7	SER
4	4	36	SER
4	4	42	SER
4	4	49	ASP
4	4	52	LYS
4	4	61	LEU
4	4	64	THR
5	3	51	THR
5	3	52	MET
5	3	71	ARG
5	3	85	LEU
5	3	143	LYS
5	3	146	LYS
5	3	149	MET
5	3	163	SER
5	3	197	ARG
5	3	208	MET
5	3	218	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	36	GLN
1	R	55	ASN
1	R	69	HIS
1	R	80	GLN
1	R	130	GLN
1	R	147	ASN
1	R	152	GLN
1	R	155	GLN
1	R	232	GLN
2	1	37	HIS
2	1	117	GLN
3	2	48	ASN
3	2	119	GLN
3	2	165	ASN

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Mol	Chain	Res	Type
4	4	13	HIS
4	4	31	ASN
5	3	218	ASN
5	3	233	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	MYR	4	1	4	14,14,15	0.99	1 (7%)	13,13,15	0.92	0
6	SPH	1	0	-	19,20,20	1.38	2 (10%)	18,21,21	1.65	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MYR	4	1	4	-	7/12/12/13	-
6	SPH	1	0	-	2/2/2/4	12/21/21/21	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	0	SPH	C4-C5	5.12	1.53	1.31
7	4	1	MYR	O2-C1	-3.34	1.24	1.42
6	1	0	SPH	C3-C4	2.03	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	0	SPH	C3-C4-C5	-5.50	112.52	124.79
6	1	0	SPH	C6-C5-C4	-2.69	113.38	125.39

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	1	0	SPH	C3
6	1	0	SPH	C2

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	0	SPH	O1-C1-C2-N2
6	1	0	SPH	O1-C1-C2-C3
6	1	0	SPH	C1-C2-C3-O3
6	1	0	SPH	C1-C2-C3-C4
6	1	0	SPH	N2-C2-C3-C4
6	1	0	SPH	C2-C3-C4-C5
6	1	0	SPH	O3-C3-C4-C5
7	4	1	MYR	C7-C8-C9-C10
7	4	1	MYR	C10-C11-C12-C13
7	4	1	MYR	C5-C6-C7-C8
7	4	1	MYR	C6-C7-C8-C9
6	1	0	SPH	C11-C12-C13-C14
7	4	1	MYR	C11-C12-C13-C14
6	1	0	SPH	C4-C5-C6-C7
7	4	1	MYR	C9-C10-C11-C12
6	1	0	SPH	C7-C8-C9-C10
7	4	1	MYR	C1-C2-C3-C4

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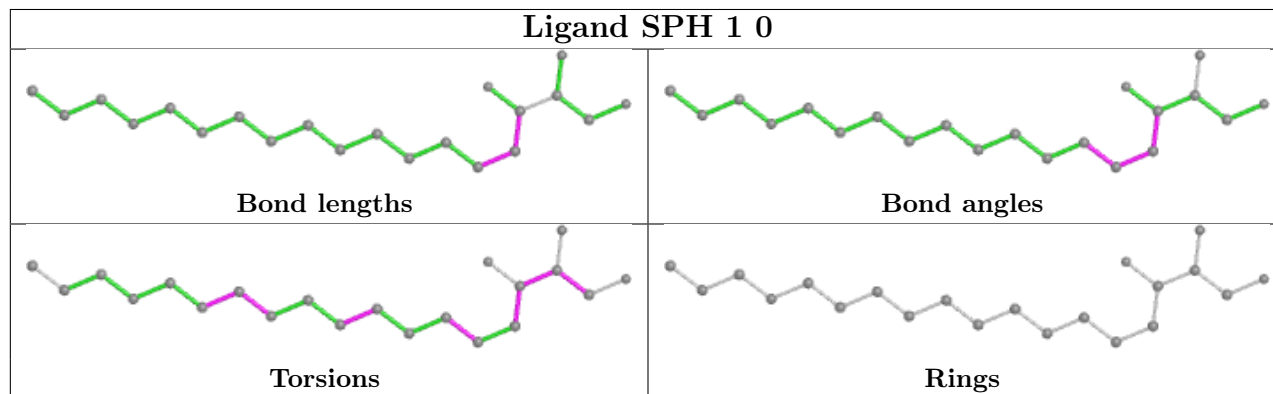
Mol	Chain	Res	Type	Atoms
6	1	0	SPH	C10-C11-C12-C13
6	1	0	SPH	N2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	4	1	MYR	1	0
6	1	0	SPH	23	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

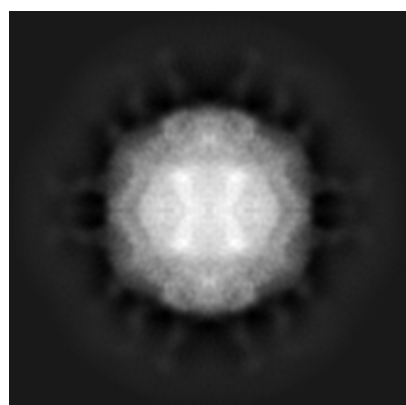
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1570. These allow visual inspection of the internal detail of the map and identification of artifacts.

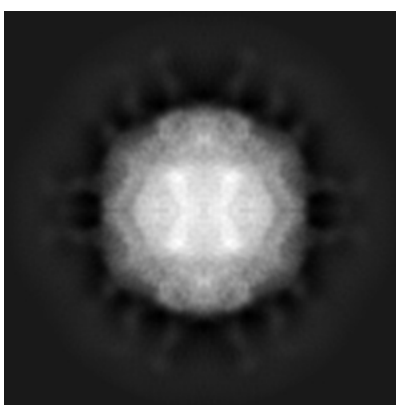
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

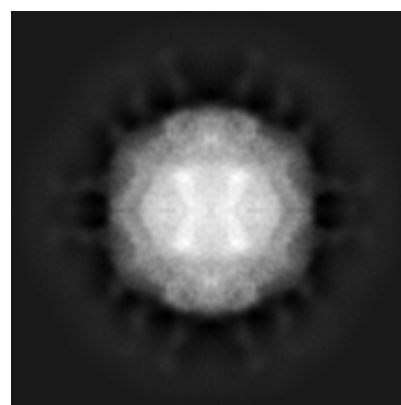
#### 6.1.1 Primary map



X



Y

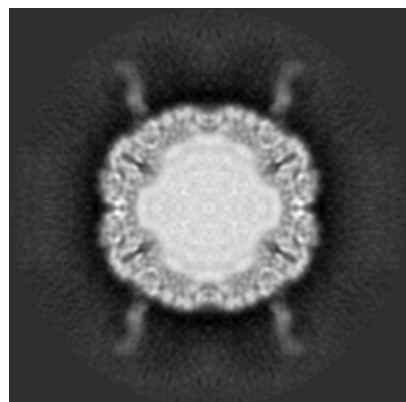


Z

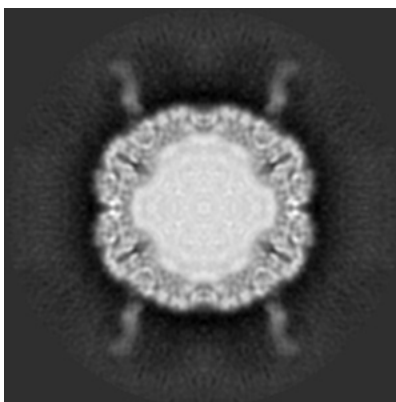
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

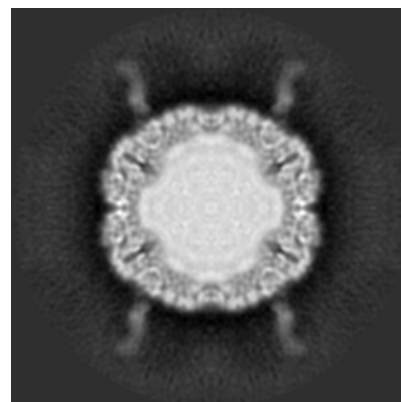
#### 6.2.1 Primary map



X Index: 108



Y Index: 108

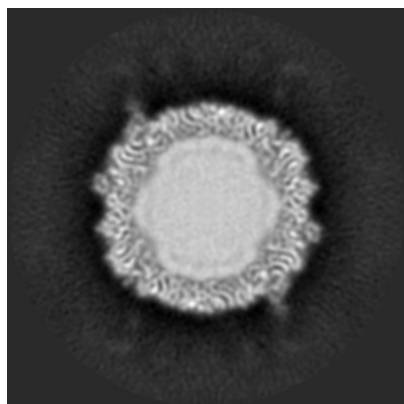


Z Index: 108

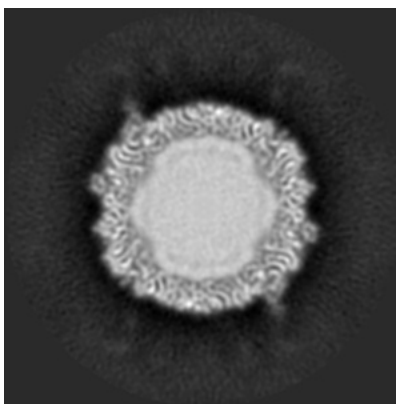
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

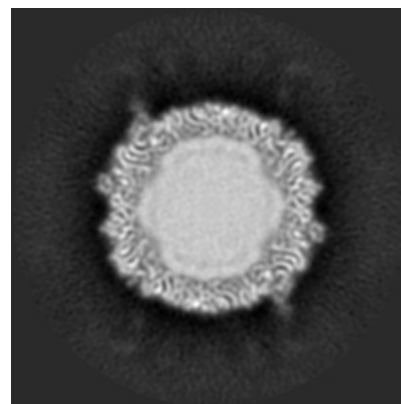
### 6.3.1 Primary map



X Index: 114



Y Index: 114

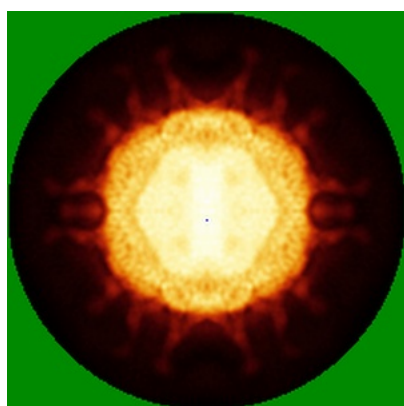


Z Index: 114

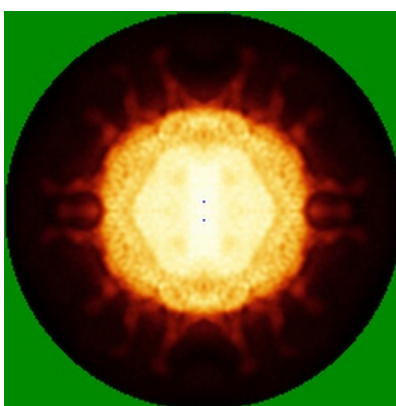
The images above show the largest variance slices of the map in three orthogonal directions.

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

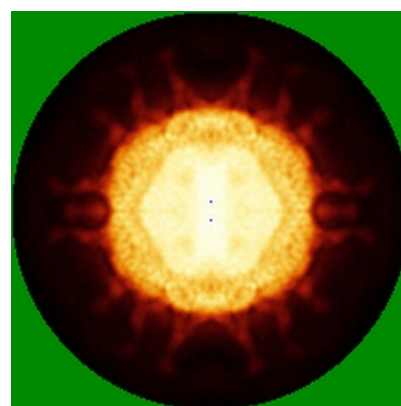
### 6.4.1 Primary map



X



Y

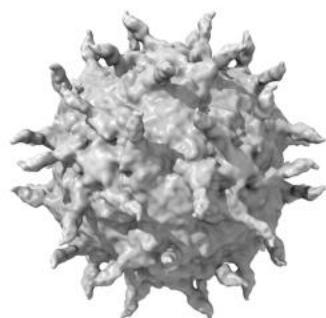


Z

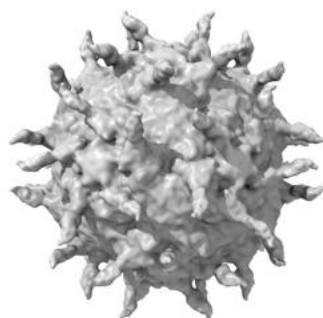
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

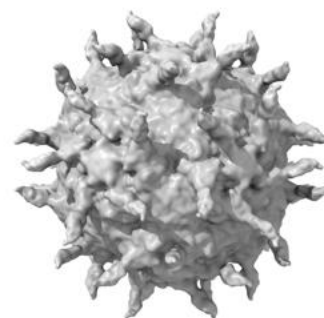
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

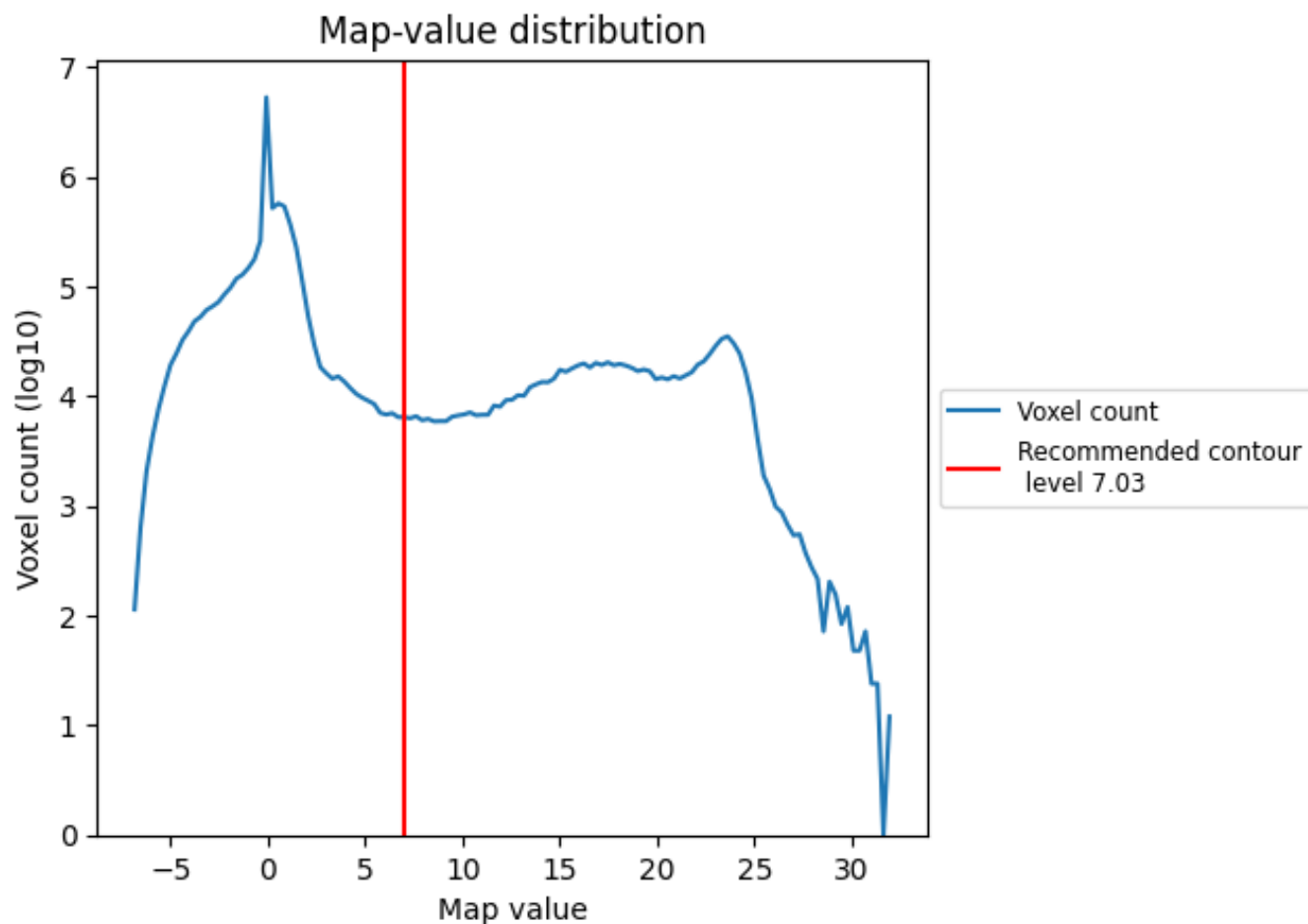
## 6.6 Mask visualisation [i](#)

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.

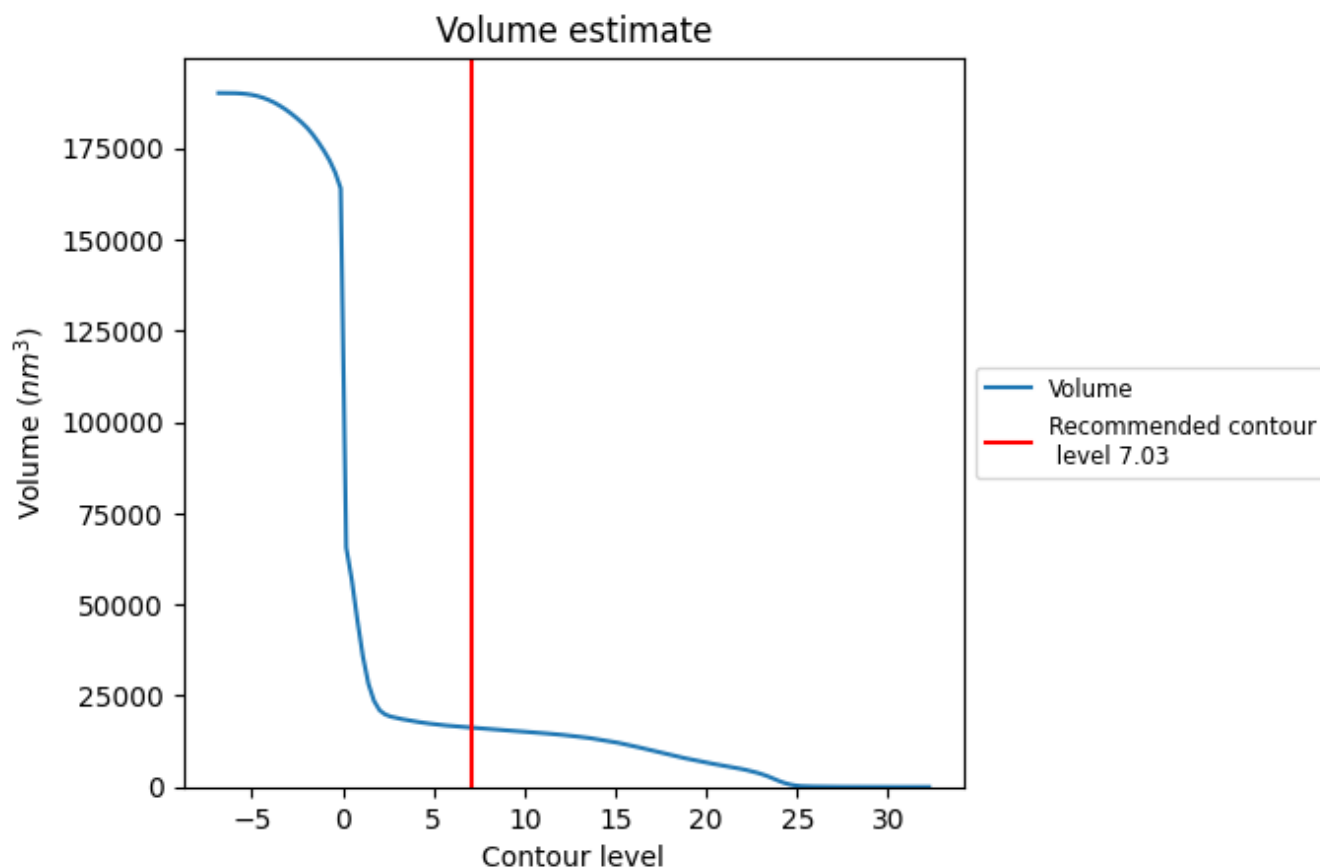
### 7.1 Map-value distribution [i](#)



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.



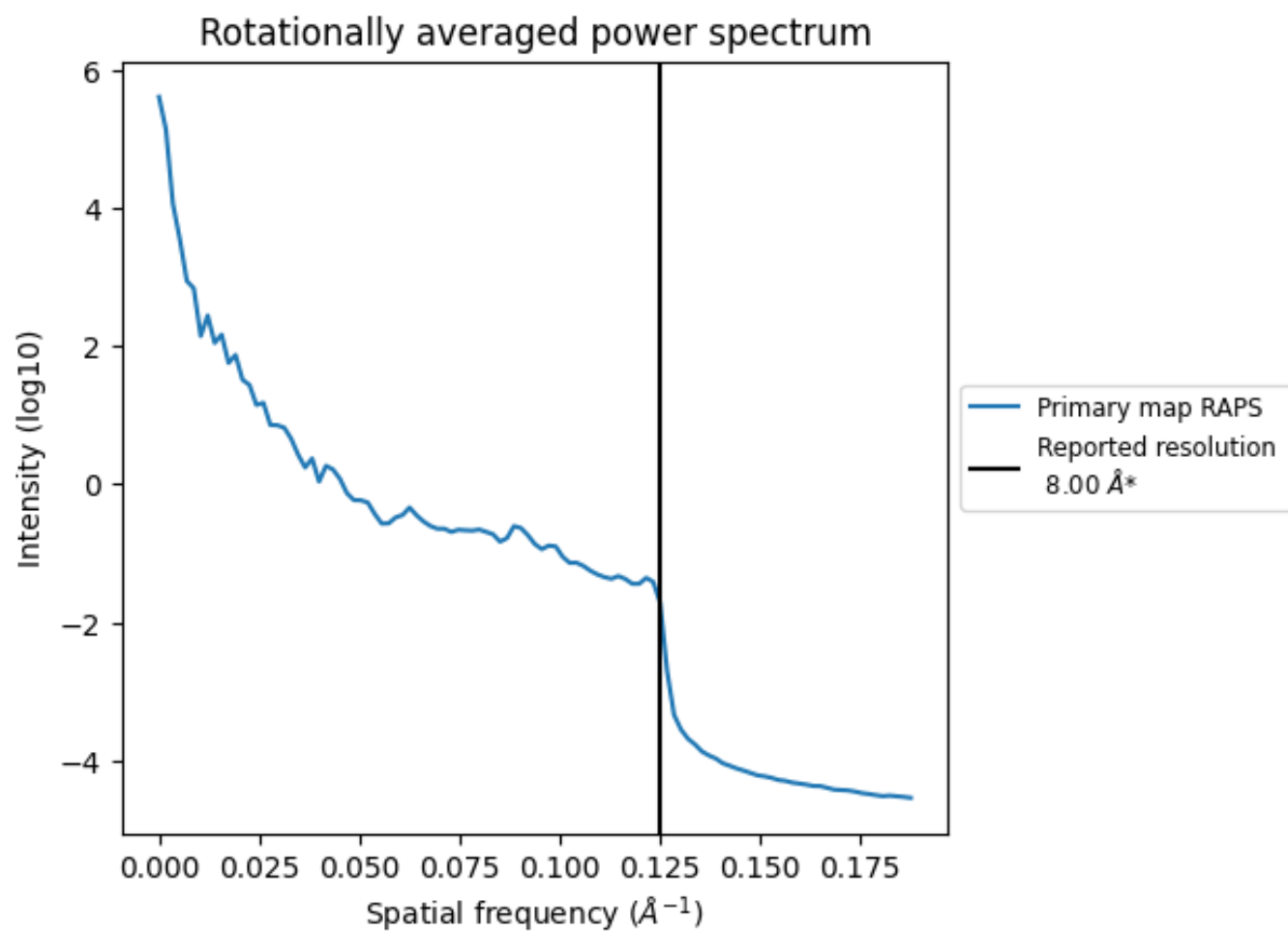
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 16285  $\text{nm}^3$ ; this corresponds to an approximate mass of 14711 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 0.125 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

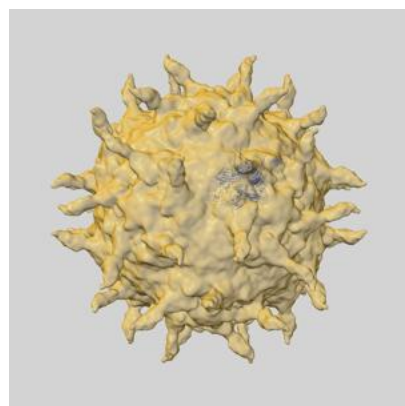
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

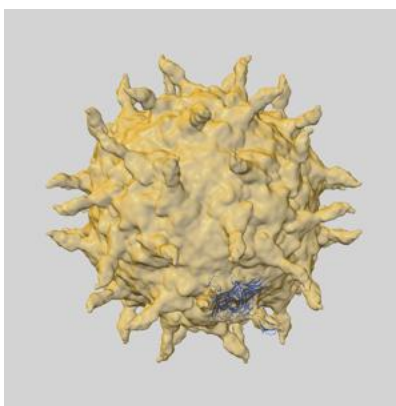
This section contains information regarding the fit between EMDB map EMD-1570 and PDB model 3EPC. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlays

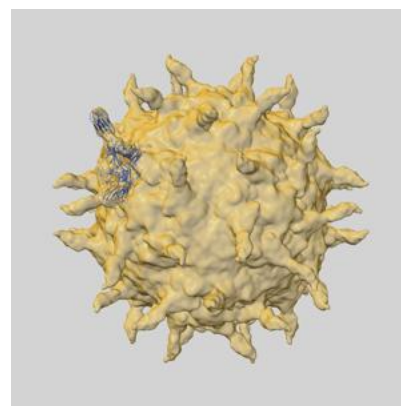
#### 9.1.1 Map-model overlay [i](#)



X

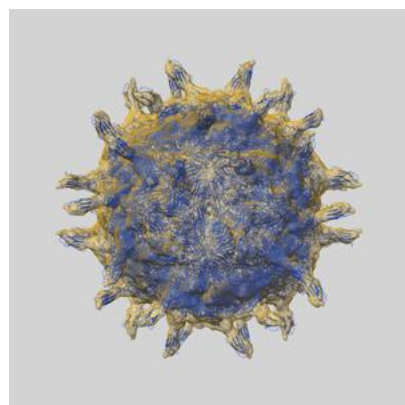


Y

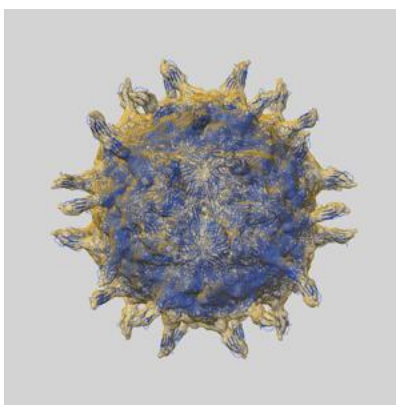


Z

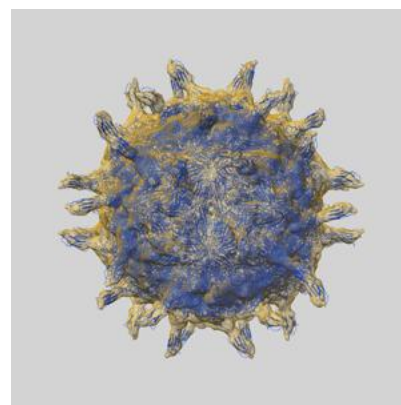
#### 9.1.2 Map-model assembly overlay [i](#)



X



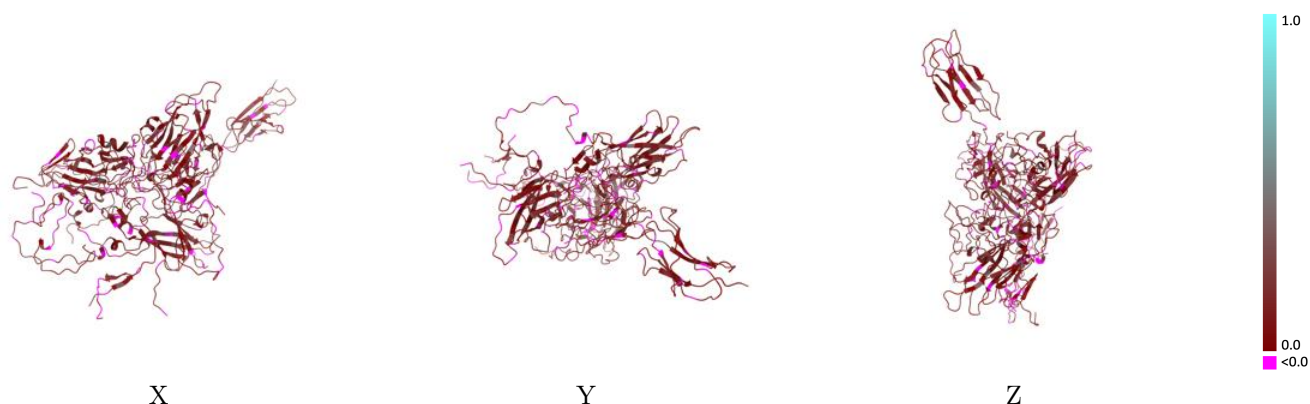
Y



Z

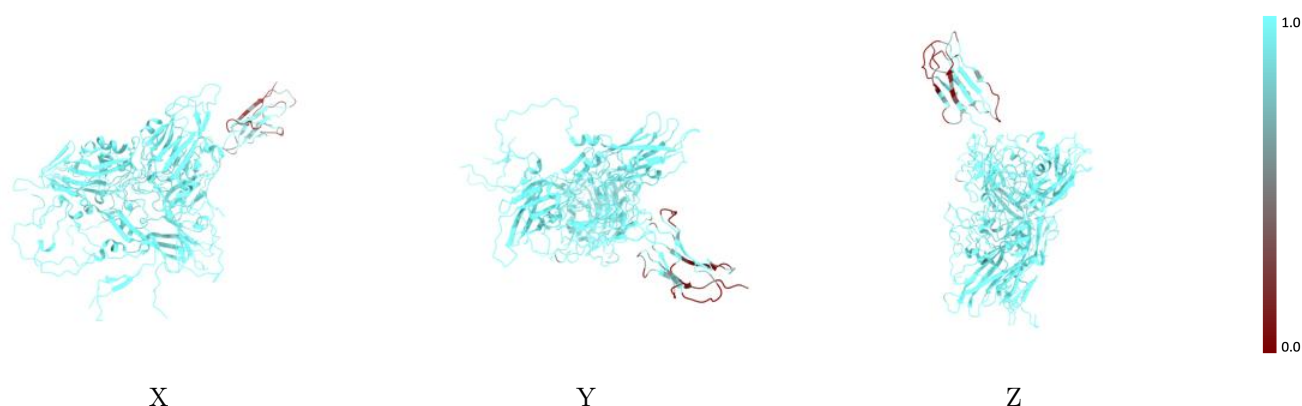
The images above show the 3D surface view of the map at the recommended contour level 7.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



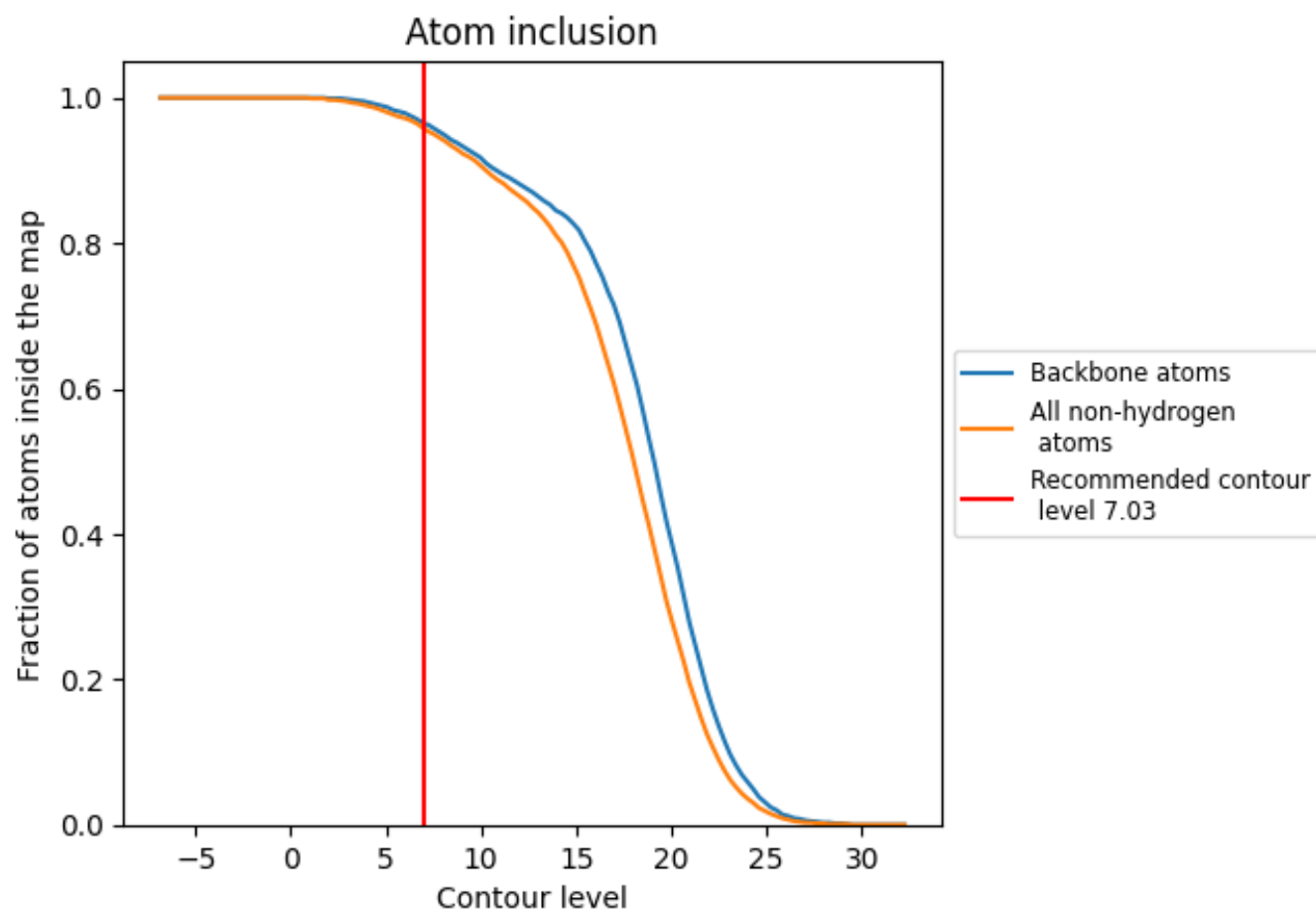
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (7.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9570	<div></div> 0.1070
1	<div></div> 1.0000	<div></div> 0.1020
2	<div></div> 0.9970	<div></div> 0.1100
3	<div></div> 1.0000	<div></div> 0.1130
4	<div></div> 0.9940	<div></div> 0.0580
R	<div></div> 0.7890	<div></div> 0.1170

