Full wwPDB EM Validation Report ⓘ

Jan 6, 2025 – 05:16 PM EST

PDB ID	:	9D82
EMDB ID	:	EMD-46626
Title	:	Shigella flexneri bacteriophage B2 Icosahedral Reconstruction
Authors	:	Subramanian, S.; Bergland Drarvik, S.M.; Parent, K.N.
Deposited on	:	2024-08-18
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

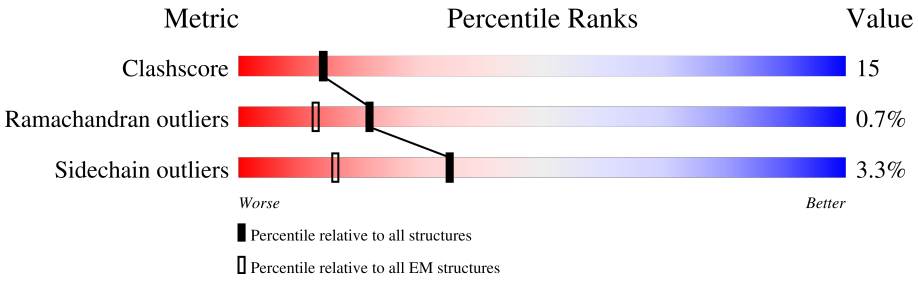
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	389	23% 69% 26%
1	B	389	23% 69% 28%
1	C	389	21% 68% 30%
1	D	389	22% 66% 30%
1	E	389	18% 62% 27% 10%
1	F	389	25% 68% 31%
1	G	389	23% 66% 29% 5%
1	H	389	22% 70% 26%

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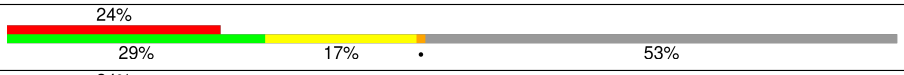
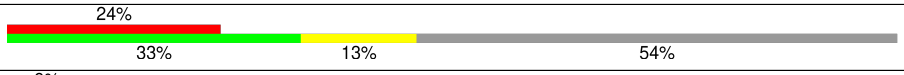
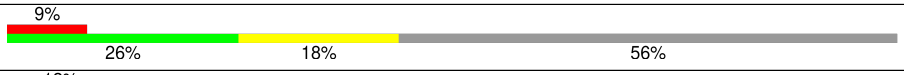
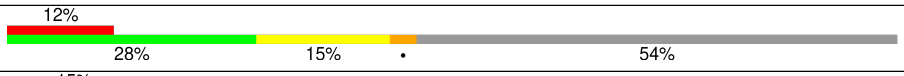
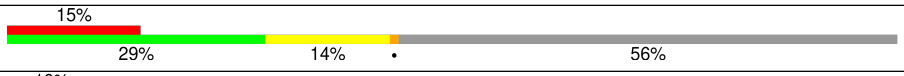
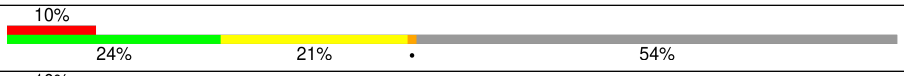
Mol	Chain	Length	Quality of chain
1	I	389	
2	J	99	
2	K	99	
2	L	99	
2	M	99	
2	N	99	
2	O	99	
2	P	99	
2	Q	99	
2	R	99	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28188 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 B2 Capsid.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	372	Total 2787	C 1784	N 457	O 535	S 11	0	0
1	B	384	Total 2887	C 1842	N 475	O 560	S 10	0	0
1	C	387	Total 2898	C 1852	N 478	O 559	S 9	0	0
1	D	384	Total 2929	C 1868	N 481	O 568	S 12	0	0
1	E	352	Total 2681	C 1718	N 439	O 512	S 12	0	0
1	F	388	Total 2922	C 1863	N 482	O 566	S 11	0	0
1	G	370	Total 2780	C 1770	N 455	O 544	S 11	0	0
1	H	379	Total 2837	C 1815	N 469	O 542	S 11	0	0
1	I	356	Total 2659	C 1707	N 438	O 505	S 9	0	0

- Molecule 2 is a protein called B2 Dec Gp45.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	47	Total 323	C 203	N 54	O 66	0	0
2	K	46	Total 318	C 200	N 53	O 65	0	0
2	L	46	Total 309	C 194	N 50	O 65	0	0
2	M	44	Total 295	C 185	N 50	O 60	0	0
2	N	46	Total 318	C 200	N 53	O 65	0	0
2	O	44	Total 300	C 188	N 51	O 61	0	0

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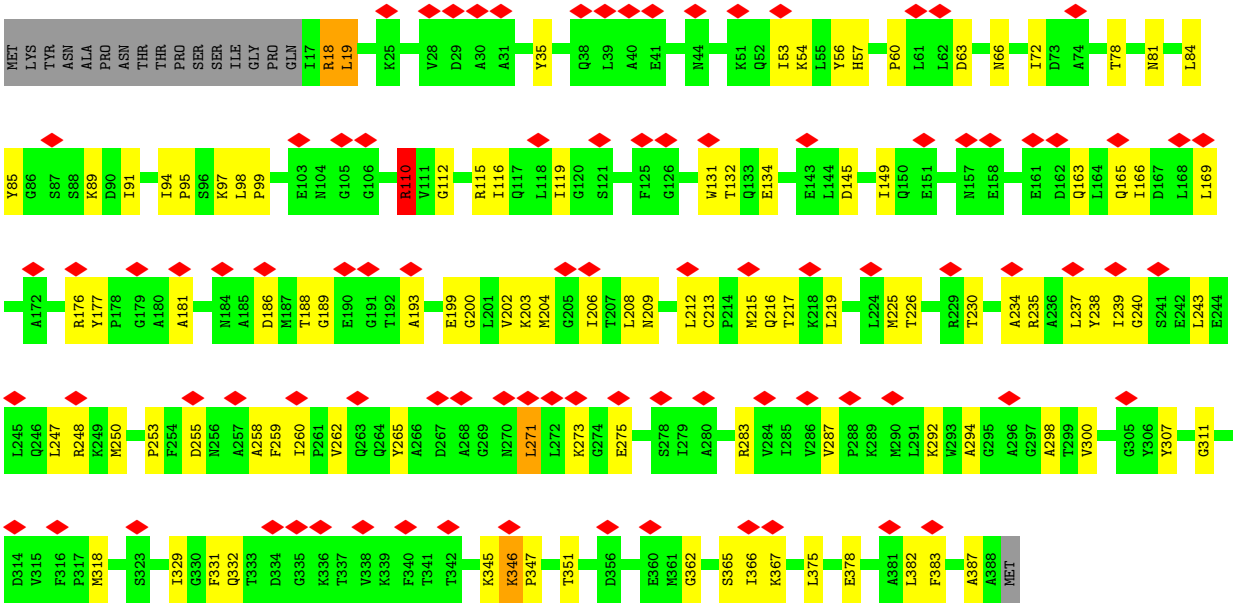
Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	46	Total	C	N	O	0	0
			313	197	51	65		
2	Q	46	Total	C	N	O	0	0
			318	200	53	65		
2	R	46	Total	C	N	O	0	0
			314	197	52	65		

3 Residue-property plots (i)

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.

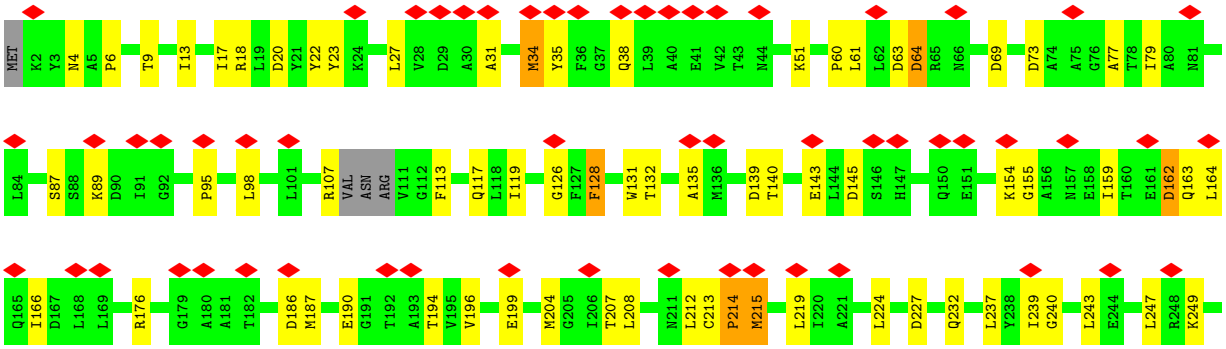
- Molecule 1: B2 Capsid

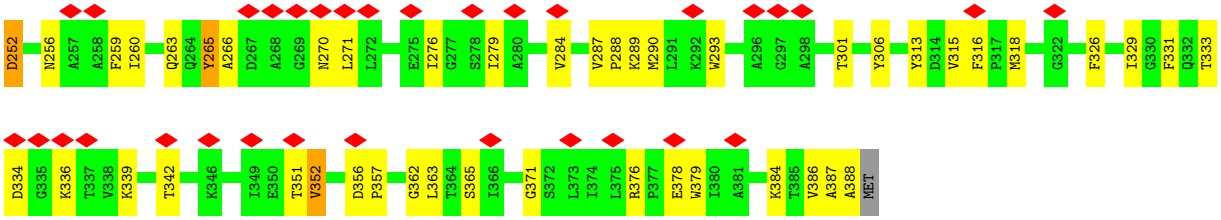
Chain A:



- Molecule 1: B2 Capsid

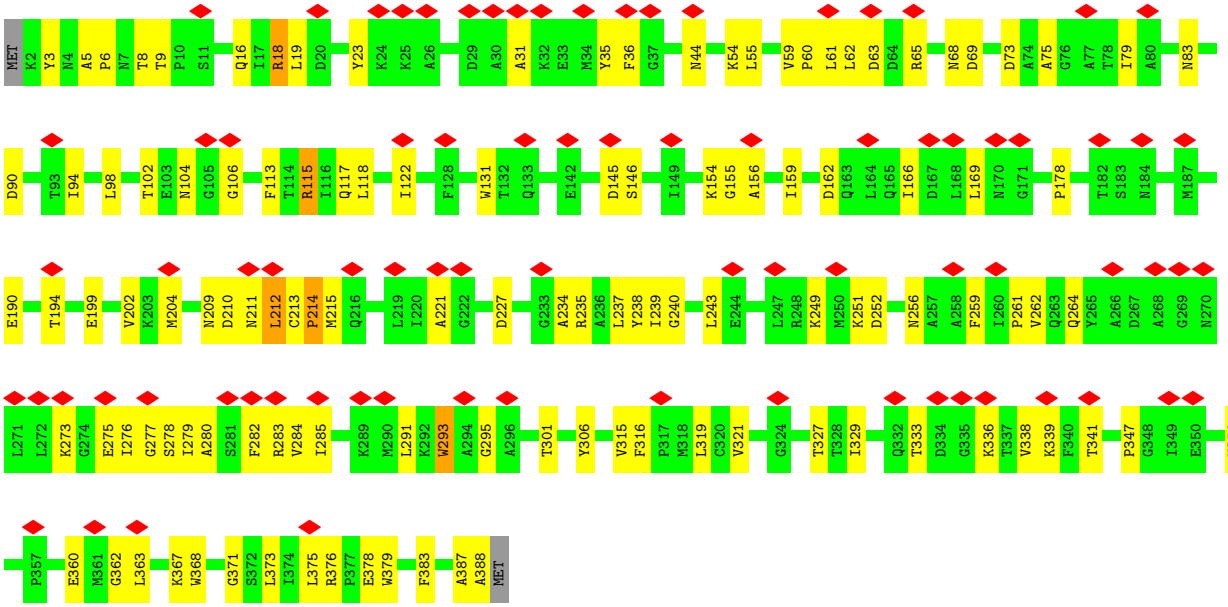
Chain B:





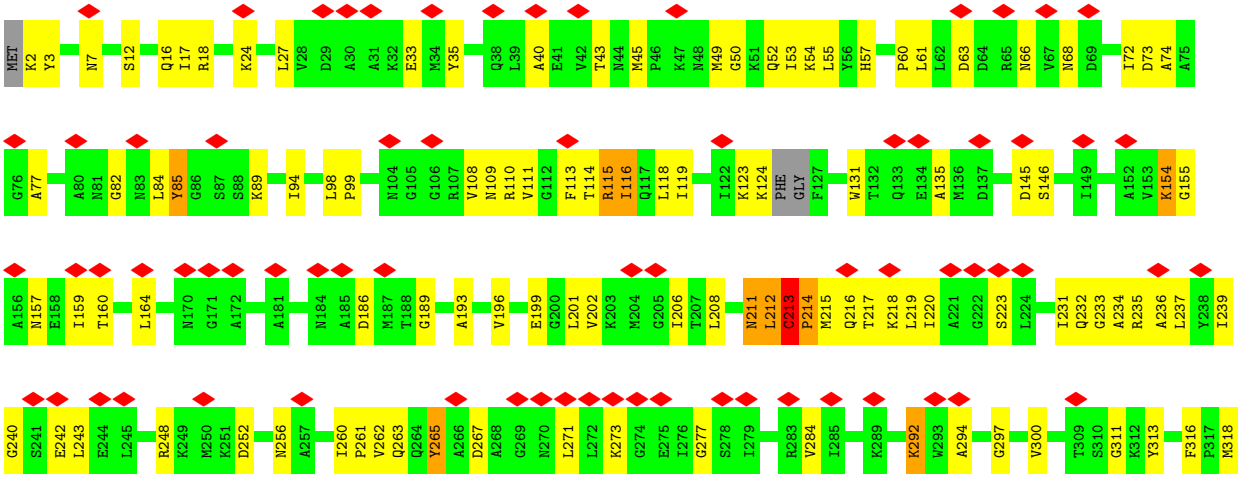
• Molecule 1: B2 Capsid

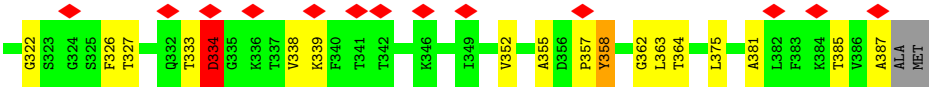
Chain C:



• Molecule 1: B2 Capsid

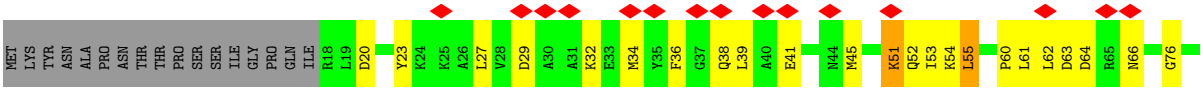
Chain D:

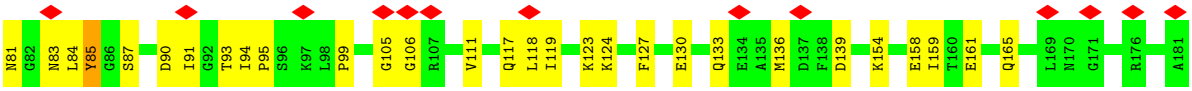


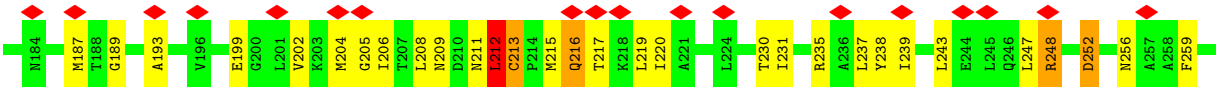


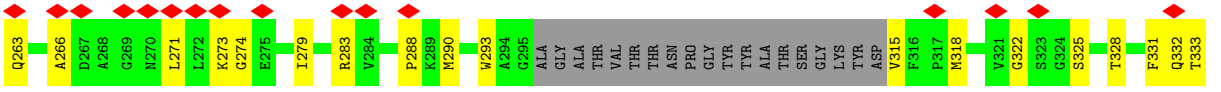
• Molecule 1: B2 Capsid

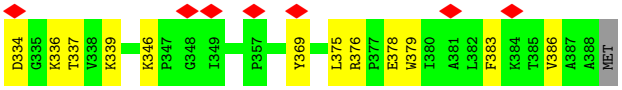
Chain E:





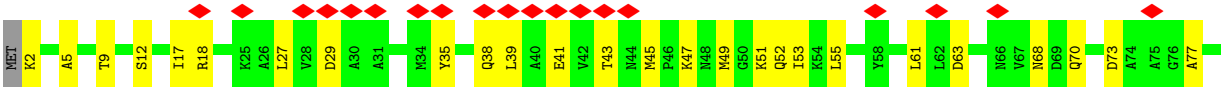


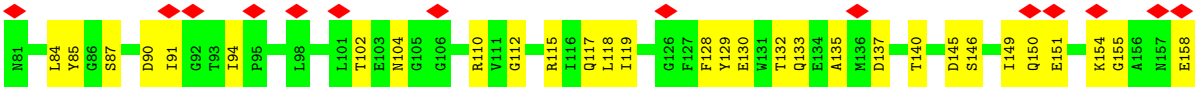


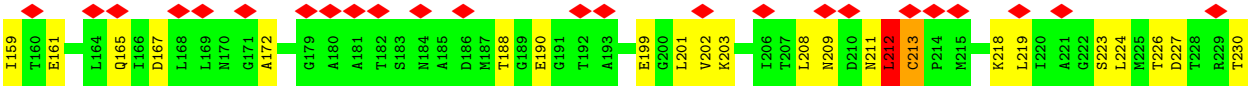


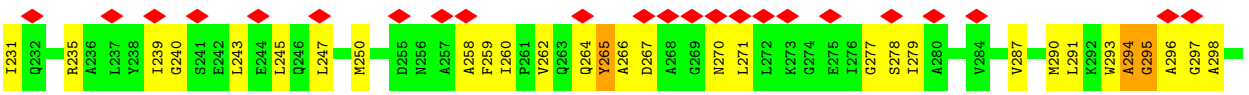
• Molecule 1: B2 Capsid

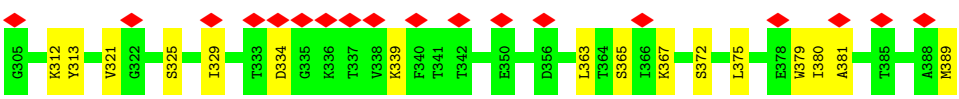
Chain F:





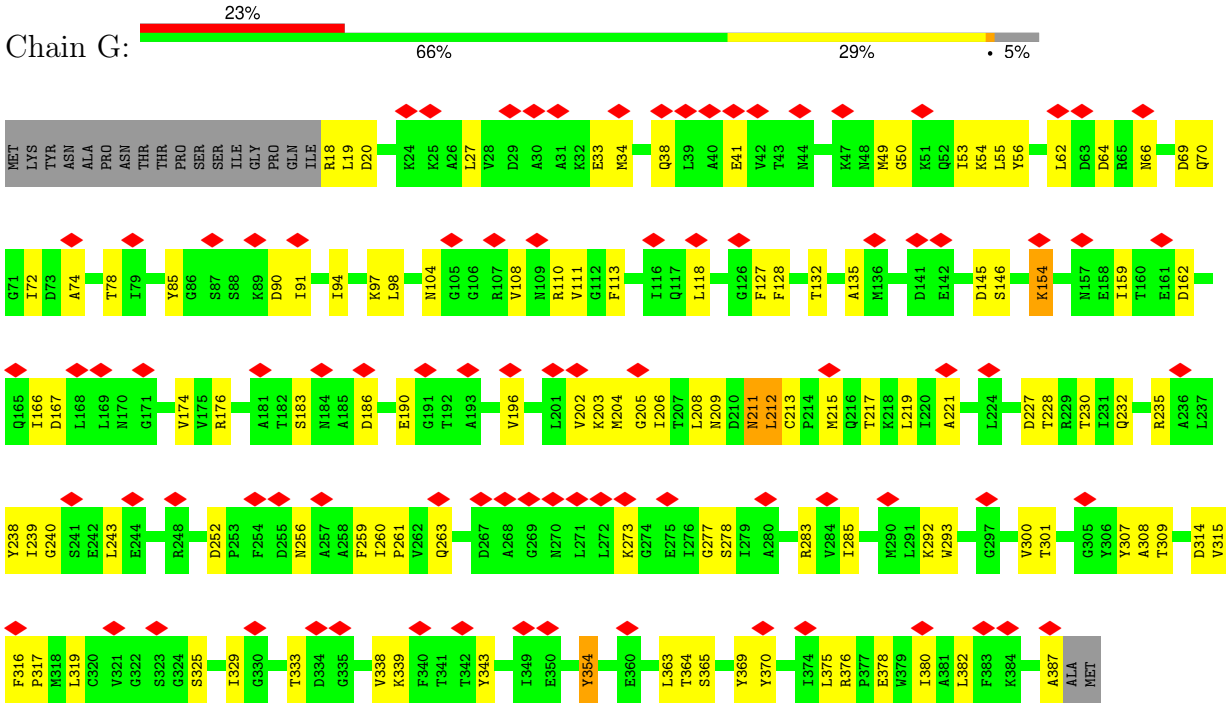






• Molecule 1: B2 Capsid

Chain G:

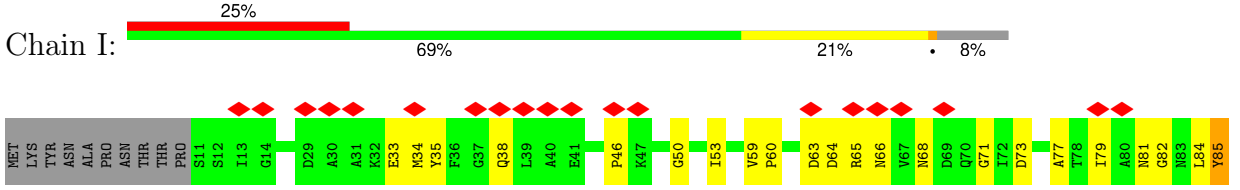


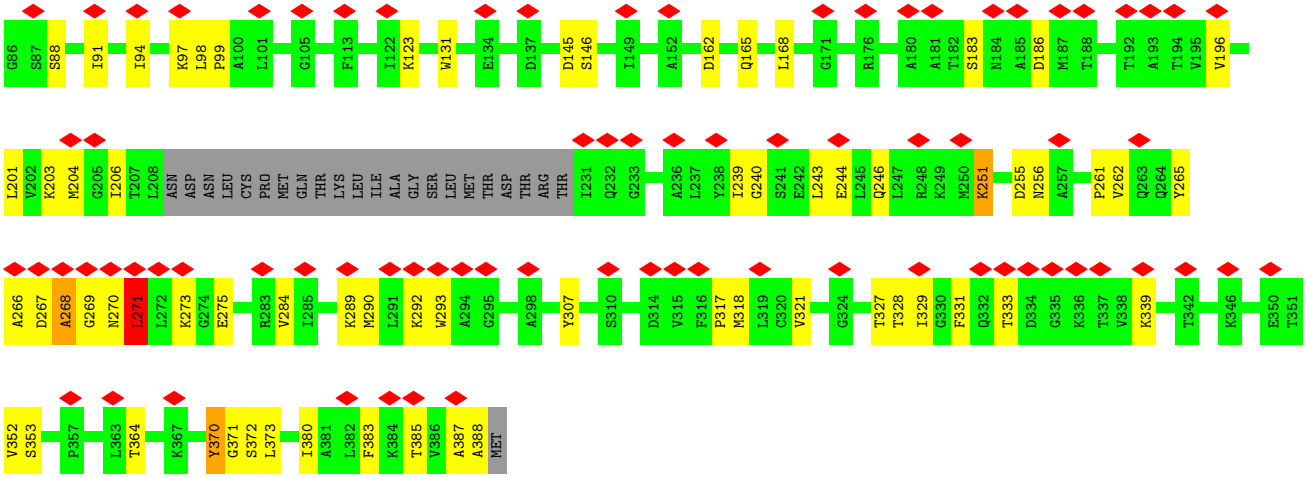
• Molecule 1: B2 Capsid

Chain H:

• Molecule 1: B2 Capsid

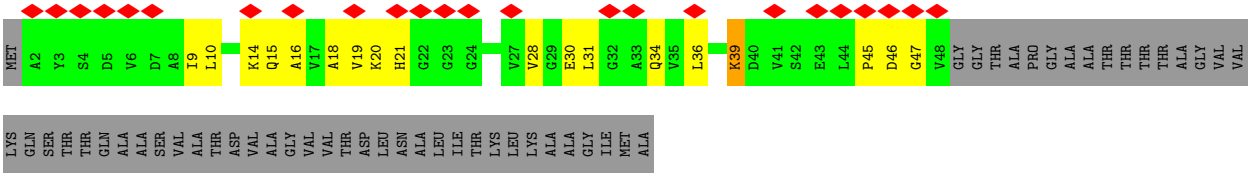
Chain I:





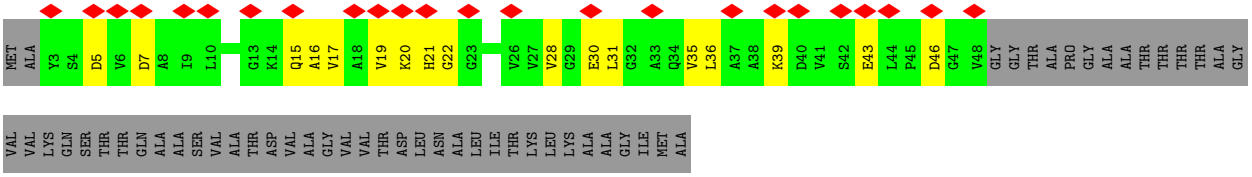
- Molecule 2: B2 Dec Gp45

Chain J:



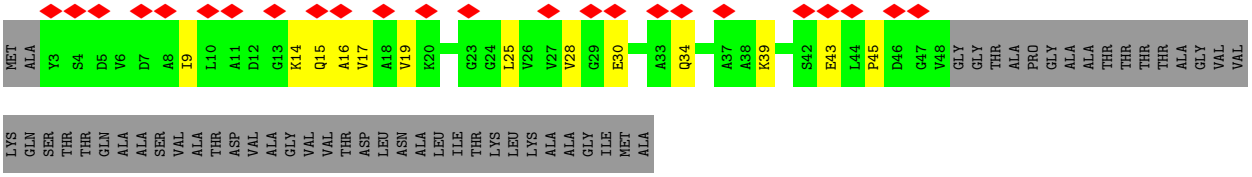
- Molecule 2: B2 Dec Gp45

Chain K:



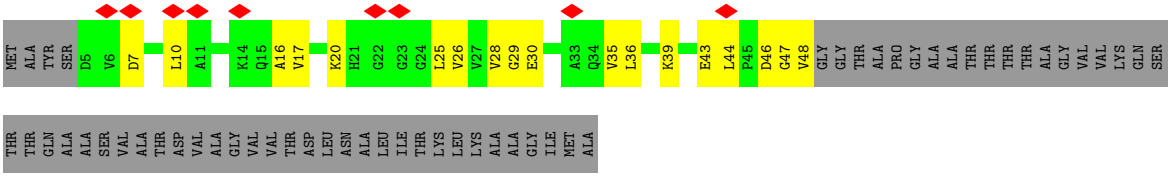
- Molecule 2: B2 Dec Gp45

Chain L:



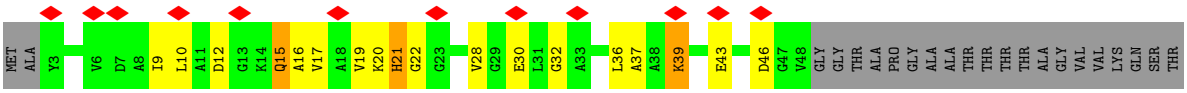
- Molecule 2: B2 Dec Gp45

Chain M:



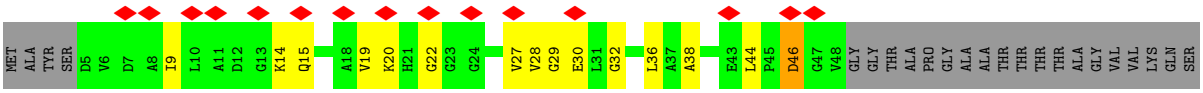
• Molecule 2: B2 Dec Gp45

Chain N:



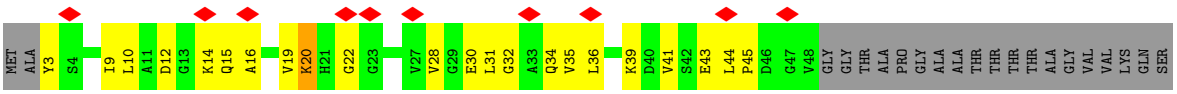
• Molecule 2: B2 Dec Gp45

Chain O:



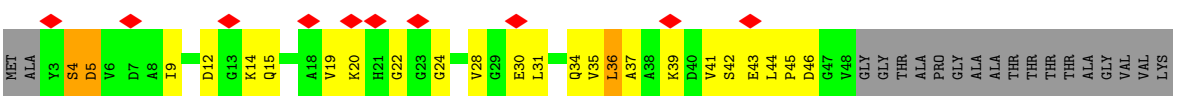
• Molecule 2: B2 Dec Gp45

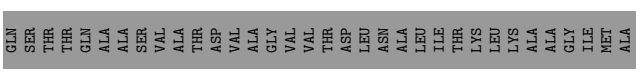
Chain P:



• Molecule 2: B2 Dec Gp45

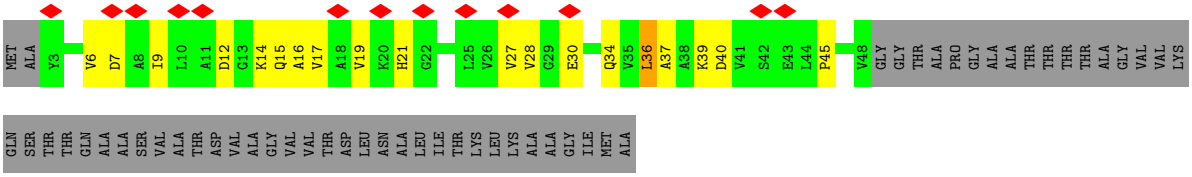
Chain Q:





• Molecule 2: B2 Dec Gp45

Chain R:


MET ALA Y3 V6 D7 A8 I9 L10 A11 D12 G13 K14 Q15 A16 V17 A18 V19 K20 H21 G22 L25 V26 V27 V28 G29 E30 Q34 V35 L36 A37 A38 K39 D40 V41 S42 E43 L44 P45 V48 GLY GLY THR ALA PRO GLY ALA ALA THR THR THR ALA GLY VAL VAL LYS
GLN SER THR THR GLN ALA ALA SER VAL ALA THR ASP VAL ALA GLY VAL VAL THR ASP LEU ASN ALA LEU ILE THR LYS LEU LYS ALA ALA GLY ILE MET ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	135384	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	1334.4, 1334.4, 1334.4	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.668, 1.668, 1.668	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	0.30	0/2844	0.51	0/3870
1	B	0.31	0/2946	0.53	0/4004
1	C	0.30	0/2959	0.53	0/4030
1	D	0.29	0/2988	0.51	1/4057 (0.0%)
1	E	0.30	0/2733	0.52	0/3706
1	F	0.29	0/2981	0.52	0/4054
1	G	0.28	0/2834	0.51	0/3851
1	H	0.28	0/2894	0.50	0/3935
1	I	0.30	0/2714	0.52	2/3689 (0.1%)
2	J	0.31	0/325	0.49	0/441
2	K	0.30	0/320	0.56	0/434
2	L	0.29	0/310	0.61	0/422
2	M	0.28	0/296	0.52	0/401
2	N	0.32	0/320	0.52	0/434
2	O	0.28	0/301	0.54	0/408
2	P	0.29	0/314	0.60	0/426
2	Q	0.29	0/320	0.56	1/434 (0.2%)
2	R	0.29	0/316	0.62	1/430 (0.2%)
All	All	0.29	0/28715	0.52	5/39026 (0.0%)

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	A	0	3
1	B	0	3
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	13

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	46	PRO	N-CD-CG	-6.67	93.19	103.20
2	R	36	LEU	CA-CB-CG	6.29	129.78	115.30
1	I	46	PRO	CA-N-CD	-6.07	103.00	111.50
2	Q	36	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	334	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	212	LEU	Peptide
1	B	107	ARG	Sidechain
1	B	212	LEU	Peptide
1	B	351	THR	Peptide
1	C	210	ASP	Mainchain
1	C	293	TRP	Peptide
1	D	213	CYS	Peptide
1	E	212	LEU	Peptide
1	F	212	LEU	Peptide
1	F	294	ALA	Peptide
1	I	268	ALA	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	A	2787	0	2707	76	0
1	B	2887	0	2811	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2898	0	2814	96	0
1	D	2929	0	2889	114	0
1	E	2681	0	2652	111	0
1	F	2922	0	2866	109	0
1	G	2780	0	2694	87	0
1	H	2837	0	2781	83	0
1	I	2659	0	2586	61	0
2	J	323	0	327	22	0
2	K	318	0	322	21	0
2	L	309	0	306	16	0
2	M	295	0	301	17	0
2	N	318	0	322	21	0
2	O	300	0	308	21	0
2	P	313	0	317	26	0
2	Q	318	0	322	31	0
2	R	314	0	311	18	0
All	All	28188	0	27636	864	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 15.

All (864) 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:F:295:GLY:HA2	1:F:312:LYS:HB2	1.49	0.94
1:G:212:LEU:HD12	1:G:378:GLU:HB2	1.54	0.90
1:D:115:ARG:NH2	1:E:139:ASP:OD2	2.05	0.89
1:F:287:VAL:HB	1:F:290:MET:HG3	1.58	0.82
1:C:239:ILE:HD11	1:C:243:LEU:HB2	1.63	0.80
1:F:212:LEU:HD21	1:F:379:TRP:HA	1.62	0.80
1:I:239:ILE:HD11	1:I:243:LEU:HD12	1.64	0.78
2:N:36:LEU:HD21	2:O:28:VAL:HG23	1.64	0.78
1:B:287:VAL:HB	1:B:290:MET:HE2	1.65	0.77
1:I:123:LYS:H	1:I:370:TYR:HB3	1.51	0.76
1:C:306:TYR:HA	1:C:388:ALA:HA	1.68	0.76
1:D:261:PRO:HB2	1:D:263:GLN:HG2	1.67	0.76
1:D:199:GLU:OE2	1:D:199:GLU:N	2.18	0.76
1:A:35:TYR:HD2	1:A:287:VAL:HG23	1.51	0.75
1:F:208:LEU:HD13	1:F:212:LEU:HG	1.68	0.75
1:C:3:TYR:CE1	1:C:6:PRO:HD3	2.22	0.75
2:N:30:GLU:OE1	2:N:30:GLU:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ILE:HG22	1:G:110:ARG:HB2	1.68	0.74
2:O:15:GLN:HG2	2:O:28:VAL:HG13	1.68	0.74
1:H:208:LEU:HD13	1:H:212:LEU:CD2	2.18	0.73
2:P:12:ASP:O	2:R:39:LYS:NZ	2.18	0.73
2:J:30:GLU:N	2:J:30:GLU:OE1	2.22	0.73
1:E:54:LYS:HB3	1:E:117:GLN:HE21	1.53	0.73
1:A:72:ILE:HD12	1:A:110:ARG:HD3	1.70	0.73
1:F:208:LEU:CD1	1:F:212:LEU:HG	2.19	0.73
1:H:212:LEU:HD12	1:H:213:CYS:N	2.04	0.72
1:E:208:LEU:HD11	1:E:212:LEU:HG	1.72	0.72
1:E:217:THR:HG21	1:E:283:ARG:HD2	1.70	0.72
1:E:333:THR:HA	1:E:339:LYS:HE3	1.73	0.71
1:I:328:THR:HG23	1:I:371:GLY:HA3	1.73	0.71
1:E:239:ILE:HD11	1:E:243:LEU:HB2	1.70	0.71
1:C:333:THR:HA	1:C:339:LYS:HD3	1.73	0.70
1:F:262:VAL:HB	1:F:277:GLY:H	1.56	0.70
1:I:251:LYS:HD2	1:I:255:ASP:HA	1.73	0.70
2:R:34:GLN:HB2	2:R:45:PRO:HG3	1.72	0.70
1:C:243:LEU:HD23	1:C:387:ALA:HB2	1.73	0.70
1:B:13:ILE:HG13	1:C:115:ARG:HD2	1.72	0.70
1:F:295:GLY:HA2	1:F:312:LYS:CB	2.22	0.70
1:F:291:LEU:HB3	1:G:91:ILE:HG12	1.73	0.70
1:G:49:MET:SD	1:G:50:GLY:N	2.65	0.70
2:Q:30:GLU:N	2:Q:30:GLU:OE1	2.24	0.70
1:F:218:LYS:HD3	1:F:219:LEU:N	2.07	0.69
1:D:89:LYS:NZ	1:E:288:PRO:O	2.25	0.69
2:P:39:LYS:NZ	2:Q:12:ASP:OD1	2.23	0.69
1:H:212:LEU:HD13	1:H:379:TRP:HB3	1.73	0.69
1:C:54:LYS:HG2	1:C:117:GLN:HE21	1.58	0.69
1:G:72:ILE:HA	1:G:78:THR:HA	1.75	0.69
2:P:14:LYS:NZ	2:R:37:ALA:O	2.24	0.68
1:A:209:ASN:HA	1:A:235:ARG:HH22	1.58	0.68
1:E:212:LEU:HD21	1:E:322:GLY:HA3	1.74	0.68
1:F:375:LEU:HB3	1:H:27:LEU:HD11	1.74	0.68
2:K:36:LEU:HD22	2:L:28:VAL:HG23	1.75	0.68
1:B:239:ILE:HD11	1:B:243:LEU:HG	1.76	0.68
1:A:345:LYS:NZ	1:D:352:VAL:O	2.22	0.68
1:H:53:ILE:HG21	1:H:329:ILE:HG21	1.76	0.68
1:E:60:PRO:HG2	1:E:63:ASP:HB2	1.73	0.67
2:J:15:GLN:NE2	2:K:21:HIS:O	2.27	0.67
1:D:68:ASN:HB2	1:D:82:GLY:HA3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:MET:HE1	1:E:383:PHE:HB2	1.76	0.67
1:D:115:ARG:NH2	1:E:139:ASP:CG	2.47	0.67
1:E:328:THR:HG21	1:E:337:THR:HG23	1.76	0.67
2:J:20:LYS:O	2:L:15:GLN:NE2	2.27	0.67
2:Q:39:LYS:NZ	2:R:12:ASP:O	2.27	0.67
1:E:45:MET:HB3	1:E:331:PHE:HA	1.77	0.67
2:P:32:GLY:O	2:P:36:LEU:HB2	1.95	0.67
1:E:165:GLN:HE22	1:E:290:MET:HA	1.59	0.67
1:D:355:ALA:HB1	2:Q:20:LYS:HG2	1.77	0.67
1:A:199:GLU:OE1	1:A:199:GLU:N	2.18	0.66
1:C:237:LEU:HB2	1:C:282:PHE:HB3	1.77	0.66
1:H:212:LEU:HA	1:H:379:TRP:CD1	2.29	0.66
1:D:375:LEU:HB3	1:E:27:LEU:HD11	1.76	0.66
1:A:81:ASN:ND2	1:A:84:LEU:O	2.27	0.66
1:D:49:MET:SD	1:D:50:GLY:N	2.66	0.66
1:B:73:ASP:HB2	1:B:79:ILE:HG12	1.77	0.66
1:E:212:LEU:HD12	1:E:235:ARG:HD3	1.78	0.65
1:E:266:ALA:HA	1:E:271:LEU:HD11	1.77	0.65
1:F:115:ARG:NH2	1:H:139:ASP:OD1	2.30	0.65
1:G:239:ILE:HD11	1:G:243:LEU:HD12	1.77	0.65
1:B:237:LEU:HD21	1:B:318:MET:HB3	1.78	0.65
1:D:2:LYS:N	1:D:12:SER:HG	1.94	0.65
1:F:227:ASP:HB3	1:G:230:THR:HG23	1.77	0.65
1:H:208:LEU:HD13	1:H:212:LEU:HD23	1.78	0.65
1:G:217:THR:HG21	1:G:283:ARG:HH11	1.61	0.65
1:C:211:ASN:O	1:C:213:CYS:N	2.29	0.65
1:F:38:GLN:OE1	1:F:38:GLN:N	2.22	0.65
2:R:15:GLN:OE1	2:R:16:ALA:N	2.25	0.65
1:C:6:PRO:HG3	1:C:19:LEU:HD22	1.79	0.64
1:E:212:LEU:HD23	1:E:379:TRP:CG	2.33	0.64
1:F:212:LEU:HD22	1:F:379:TRP:CD1	2.32	0.64
1:G:41:GLU:N	1:G:41:GLU:OE1	2.30	0.64
1:E:208:LEU:CD1	1:E:212:LEU:HB2	2.28	0.64
1:F:53:ILE:HD11	1:H:23:TYR:HB2	1.78	0.64
1:A:53:ILE:HD11	1:B:23:TYR:HB2	1.80	0.64
1:D:243:LEU:HD22	1:D:316:PHE:HB2	1.80	0.64
1:B:252:ASP:OD1	1:B:256:ASN:N	2.30	0.64
1:E:136:MET:SD	1:E:136:MET:N	2.70	0.64
1:F:102:THR:OG1	1:F:104:ASN:OD1	2.15	0.64
1:E:36:PHE:N	1:E:161:GLU:OE2	2.29	0.63
1:G:70:GLN:HB3	1:G:110:ARG:HE	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:MET:SD	1:H:50:GLY:N	2.71	0.63
1:I:204:MET:HE1	1:I:383:PHE:HB2	1.80	0.63
2:N:36:LEU:HD22	2:O:28:VAL:HA	1.79	0.63
1:A:367:LYS:HE2	1:D:358:TYR:HB3	1.80	0.63
1:F:203:LYS:HZ2	1:H:245:LEU:HD21	1.63	0.63
2:M:17:VAL:HG12	2:N:19:VAL:HA	1.81	0.63
2:Q:9:ILE:HD12	2:Q:9:ILE:H	1.64	0.63
1:A:204:MET:HE1	1:A:383:PHE:HB2	1.81	0.62
1:H:63:ASP:OD2	1:H:65:ARG:NH2	2.32	0.62
1:D:115:ARG:NH2	1:E:139:ASP:OD1	2.32	0.62
1:D:252:ASP:OD1	1:D:256:ASN:N	2.32	0.62
1:D:219:LEU:HD12	1:E:263:GLN:HB3	1.81	0.62
1:F:212:LEU:CD2	1:F:379:TRP:HA	2.30	0.62
2:L:9:ILE:HG21	2:L:16:ALA:HB2	1.82	0.62
1:G:252:ASP:OD1	1:G:256:ASN:N	2.32	0.62
1:E:238:TYR:HB3	1:E:290:MET:HE1	1.82	0.62
1:D:72:ILE:HG13	1:D:110:ARG:HD2	1.82	0.61
2:P:36:LEU:HG	2:Q:36:LEU:HD12	1.81	0.61
1:E:208:LEU:HD12	1:E:212:LEU:HB2	1.81	0.61
1:E:237:LEU:HD21	1:E:318:MET:HB3	1.81	0.61
1:B:199:GLU:OE1	1:B:199:GLU:N	2.24	0.61
1:E:209:ASN:HA	1:E:235:ARG:HH22	1.66	0.61
2:N:46:ASP:OD2	2:N:46:ASP:N	2.32	0.61
1:I:318:MET:HG3	1:I:383:PHE:HB3	1.82	0.61
2:Q:36:LEU:HD23	2:R:28:VAL:HA	1.82	0.61
1:A:35:TYR:CD2	1:A:287:VAL:HG23	2.35	0.61
1:H:237:LEU:HB2	1:H:282:PHE:HB3	1.81	0.61
2:N:43:GLU:N	2:N:43:GLU:OE2	2.33	0.61
1:E:187:MET:HE3	1:E:386:VAL:HG23	1.83	0.61
1:D:2:LYS:HZ1	1:H:103:GLU:HB2	1.65	0.60
2:M:29:GLY:HA3	2:O:38:ALA:H	1.66	0.60
1:A:60:PRO:HG2	1:A:63:ASP:HB2	1.82	0.60
1:F:208:LEU:HD21	1:F:381:ALA:HB2	1.83	0.60
1:F:230:THR:HG23	1:H:227:ASP:HB3	1.83	0.60
2:O:46:ASP:OD1	2:O:46:ASP:N	2.32	0.60
1:H:212:LEU:HD13	1:H:379:TRP:CB	2.32	0.60
1:D:55:LEU:HB2	1:D:118:LEU:HB2	1.82	0.60
1:E:64:ASP:N	1:E:87:SER:OG	2.34	0.60
1:F:27:LEU:HD11	1:G:375:LEU:HD12	1.84	0.60
1:B:145:ASP:OD2	1:B:145:ASP:N	2.34	0.60
1:C:209:ASN:HA	1:C:235:ARG:HH22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASP:OD1	1:C:256:ASN:N	2.31	0.60
1:C:259:PHE:HZ	1:C:276:ILE:HG12	1.66	0.60
1:D:110:ARG:NH2	1:E:130:GLU:OE2	2.34	0.60
1:D:186:ASP:OD1	1:D:186:ASP:N	2.35	0.60
1:B:176:ARG:HH12	1:B:207:THR:HG21	1.67	0.59
2:K:15:GLN:HB3	2:K:28:VAL:HG12	1.84	0.59
1:G:85:TYR:HB3	1:G:97:LYS:HB2	1.84	0.59
2:P:22:GLY:O	2:R:15:GLN:NE2	2.34	0.59
1:F:35:TYR:N	1:F:161:GLU:OE2	2.35	0.59
1:F:91:ILE:HD11	1:H:293:TRP:CE2	2.38	0.59
1:A:329:ILE:HD12	1:A:329:ILE:H	1.67	0.59
1:H:199:GLU:N	1:H:199:GLU:OE1	2.35	0.59
2:M:44:LEU:H	2:M:44:LEU:HD23	1.68	0.59
1:I:79:ILE:HD12	1:I:79:ILE:H	1.68	0.59
1:H:145:ASP:OD2	1:H:146:SER:N	2.36	0.59
1:I:84:LEU:HG	1:I:85:TYR:H	1.68	0.58
2:Q:36:LEU:HG	2:R:36:LEU:HD12	1.84	0.58
1:H:138:PHE:HB3	1:I:50:GLY:HA2	1.85	0.58
1:A:346:LYS:HA	1:A:346:LYS:HE2	1.85	0.58
1:G:206:ILE:HD13	1:G:209:ASN:HD22	1.68	0.58
2:J:39:LYS:HA	2:K:30:GLU:OE2	2.03	0.58
1:C:375:LEU:HB3	1:D:27:LEU:HD11	1.86	0.58
1:I:329:ILE:HG12	1:I:371:GLY:HA2	1.86	0.58
1:H:245:LEU:HG	1:H:249:LYS:HZ1	1.67	0.58
1:E:212:LEU:HD22	1:E:213:CYS:CB	2.34	0.58
1:I:328:THR:HA	1:I:372:SER:H	1.69	0.58
1:A:234:ALA:HB3	1:A:283:ARG:HG3	1.84	0.57
1:C:62:LEU:HD21	1:D:159:ILE:HD11	1.84	0.57
1:C:212:LEU:O	1:C:213:CYS:C	2.43	0.57
1:H:300:VAL:HA	1:H:311:GLY:HA2	1.85	0.57
1:B:239:ILE:HD13	1:B:318:MET:HG2	1.86	0.57
2:L:43:GLU:OE2	2:L:43:GLU:N	2.36	0.57
1:C:239:ILE:HG22	1:C:285:ILE:O	2.04	0.57
1:H:232:GLN:HE21	1:H:281:SER:HB3	1.69	0.57
1:A:57:HIS:HB3	1:A:116:ILE:HG22	1.85	0.57
1:E:199:GLU:HA	1:E:202:VAL:HG22	1.86	0.57
1:H:215:MET:O	1:H:216:GLN:C	2.43	0.57
2:P:39:LYS:NZ	2:Q:12:ASP:O	2.33	0.57
2:Q:15:GLN:HB3	2:Q:28:VAL:HG13	1.87	0.57
1:E:61:LEU:HB3	1:E:62:LEU:HD12	1.86	0.57
1:F:132:THR:HG23	1:F:135:ALA:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:THR:HB	1:F:298:ALA:HB3	1.87	0.57
1:C:251:LYS:HD3	1:H:254:PHE:HD1	1.70	0.57
1:B:60:PRO:HG2	1:B:63:ASP:HB2	1.86	0.57
1:F:208:LEU:HD13	1:F:212:LEU:CG	2.35	0.57
1:G:190:GLU:OE1	1:G:301:THR:OG1	2.18	0.56
1:G:243:LEU:HD11	1:G:316:PHE:HB2	1.87	0.56
1:H:85:TYR:HA	1:H:97:LYS:HE3	1.88	0.56
2:M:36:LEU:HD11	2:N:28:VAL:HG23	1.86	0.56
2:P:15:GLN:HB3	2:P:28:VAL:HG13	1.87	0.56
1:F:39:LEU:HD23	1:F:321:VAL:HG11	1.87	0.56
2:P:19:VAL:HA	2:R:17:VAL:HG12	1.86	0.56
1:H:189:GLY:HA2	1:H:193:ALA:HA	1.87	0.56
1:I:327:THR:O	1:I:373:LEU:N	2.36	0.56
1:G:53:ILE:HG21	1:G:329:ILE:HG21	1.86	0.56
1:I:53:ILE:HG21	1:I:329:ILE:HG21	1.86	0.56
1:C:106:GLY:HA3	2:R:21:HIS:NE2	2.21	0.56
1:I:59:VAL:HG21	1:I:65:ARG:HB2	1.88	0.56
1:I:352:VAL:HG23	1:I:353:SER:H	1.71	0.56
1:D:189:GLY:HA2	1:D:193:ALA:HA	1.87	0.56
1:H:160:THR:HG21	1:H:338:VAL:HG11	1.86	0.56
1:I:168:LEU:HD13	1:I:321:VAL:HG11	1.88	0.56
2:Q:34:GLN:HG2	2:Q:45:PRO:HG3	1.89	0.55
1:I:123:LYS:HG2	1:I:370:TYR:CD2	2.40	0.55
1:D:115:ARG:HH22	1:E:139:ASP:CG	2.09	0.55
2:P:15:GLN:NE2	2:P:16:ALA:H	2.04	0.55
1:B:34:MET:O	1:B:38:GLN:NE2	2.29	0.55
1:D:145:ASP:OD1	1:D:146:SER:N	2.40	0.55
1:C:6:PRO:CG	1:C:19:LEU:HD22	2.37	0.55
1:C:190:GLU:OE2	1:C:301:THR:N	2.39	0.55
1:D:211:ASN:O	1:D:213:CYS:N	2.40	0.55
1:E:212:LEU:HD23	1:E:379:TRP:CB	2.37	0.55
1:B:17:ILE:HG22	1:C:54:LYS:HD3	1.89	0.55
1:G:209:ASN:HA	1:G:235:ARG:HH22	1.72	0.55
2:J:20:LYS:HD3	2:J:21:HIS:H	1.72	0.55
2:P:43:GLU:OE1	2:P:43:GLU:N	2.39	0.55
1:I:307:TYR:HB2	1:I:387:ALA:HB3	1.88	0.55
2:M:30:GLU:OE2	2:M:30:GLU:N	2.36	0.55
2:P:15:GLN:HG3	2:Q:19:VAL:HG11	1.87	0.55
2:Q:19:VAL:HB	2:Q:24:GLY:HA2	1.87	0.55
1:E:62:LEU:HD23	1:E:85:TYR:CE1	2.42	0.55
2:O:30:GLU:OE2	2:O:30:GLU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:LEU:O	1:G:213:CYS:C	2.45	0.54
1:B:162:ASP:N	1:B:162:ASP:OD1	2.37	0.54
1:C:60:PRO:HG2	1:C:63:ASP:HB2	1.90	0.54
1:A:115:ARG:NH2	1:D:16:GLN:OE1	2.40	0.54
1:G:293:TRP:HZ3	1:G:317:PRO:HB3	1.71	0.54
1:H:318:MET:HE3	1:H:383:PHE:HB3	1.89	0.54
2:K:20:LYS:HG3	2:K:21:HIS:ND1	2.22	0.54
1:E:54:LYS:HD2	1:E:117:GLN:NE2	2.22	0.54
1:F:130:GLU:OE2	1:G:110:ARG:NH1	2.40	0.54
1:G:145:ASP:OD2	1:G:146:SER:N	2.40	0.54
1:A:95:PRO:HG3	1:B:166:ILE:HD13	1.90	0.54
1:B:266:ALA:HA	1:B:271:LEU:HD11	1.89	0.54
1:C:261:PRO:HD2	1:C:264:GLN:HG3	1.90	0.54
1:E:199:GLU:OE2	1:E:199:GLU:N	2.37	0.54
1:E:219:LEU:HD21	1:G:263:GLN:HA	1.88	0.54
1:F:334:ASP:HB2	1:F:339:LYS:HB2	1.90	0.54
1:G:308:ALA:HB1	1:G:314:ASP:H	1.72	0.54
1:D:60:PRO:HB2	1:D:63:ASP:HB2	1.88	0.54
1:A:253:PRO:HB3	1:B:249:LYS:NZ	2.23	0.54
1:D:160:THR:HG21	1:D:338:VAL:HG11	1.89	0.54
1:E:220:ILE:HD12	1:E:231:ILE:HD11	1.89	0.54
2:J:46:ASP:OD2	2:J:47:GLY:N	2.41	0.54
1:I:270:ASN:O	1:I:271:LEU:C	2.46	0.54
2:Q:31:LEU:O	2:Q:35:VAL:HG23	2.08	0.54
1:I:73:ASP:HB3	1:I:79:ILE:HD11	1.90	0.54
2:N:15:GLN:OE1	2:N:28:VAL:HG13	2.08	0.54
1:C:237:LEU:N	1:C:283:ARG:O	2.40	0.53
1:B:117:GLN:HE22	1:B:119:ILE:HB	1.73	0.53
1:B:249:LYS:HE3	1:B:249:LYS:HA	1.90	0.53
1:D:262:VAL:HA	1:D:265:TYR:CD2	2.43	0.53
1:G:208:LEU:HD12	1:G:213:CYS:CB	2.38	0.53
1:C:155:GLY:HA3	1:H:61:LEU:HD21	1.90	0.53
1:A:145:ASP:OD2	1:A:145:ASP:N	2.42	0.53
1:C:234:ALA:HB3	1:C:283:ARG:HG2	1.90	0.53
1:D:123:LYS:HE3	1:D:123:LYS:HA	1.90	0.53
1:H:208:LEU:HD21	1:H:381:ALA:HB2	1.91	0.53
2:L:30:GLU:H	2:L:30:GLU:CD	2.10	0.53
1:B:31:ALA:HB2	1:B:154:LYS:HD2	1.90	0.53
1:B:155:GLY:O	1:B:159:ILE:HG12	2.09	0.53
1:C:221:ALA:HB1	1:D:267:ASP:HB2	1.91	0.53
1:E:76:GLY:HA3	2:M:25:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:LYS:HE3	1:E:123:LYS:HA	1.91	0.53
1:E:209:ASN:OD1	1:E:235:ARG:NH2	2.42	0.53
1:F:85:TYR:HE2	1:H:159:ILE:HD13	1.72	0.53
1:I:333:THR:HG22	1:I:339:LYS:H	1.74	0.53
1:E:189:GLY:HA2	1:E:193:ALA:HA	1.89	0.53
1:F:250:MET:HG2	1:F:258:ALA:HB3	1.91	0.53
1:F:226:THR:OG1	1:G:228:THR:O	2.27	0.53
1:F:231:ILE:HD11	1:F:265:TYR:CG	2.43	0.53
1:H:60:PRO:HG2	1:H:63:ASP:HB2	1.90	0.53
2:K:7:ASP:N	2:K:7:ASP:OD1	2.41	0.53
2:P:30:GLU:OE2	2:P:30:GLU:N	2.36	0.53
1:E:212:LEU:HD23	1:E:379:TRP:HB3	1.91	0.53
1:F:35:TYR:HD2	1:F:287:VAL:HG13	1.73	0.53
1:G:132:THR:HG23	1:G:135:ALA:H	1.73	0.52
1:H:293:TRP:HB3	1:H:296:ALA:HB3	1.91	0.52
1:C:347:PRO:HD3	1:C:362:GLY:HA2	1.91	0.52
1:D:333:THR:HA	1:D:339:LYS:HE3	1.91	0.52
1:F:208:LEU:O	1:F:212:LEU:HB2	2.09	0.52
1:G:333:THR:HA	1:G:339:LYS:HD3	1.91	0.52
1:H:297:GLY:HA3	1:H:313:TYR:N	2.24	0.52
2:K:15:GLN:HG3	2:L:19:VAL:HG11	1.89	0.52
2:N:39:LYS:HD2	2:O:14:LYS:HD3	1.92	0.52
1:C:122:ILE:HD12	1:C:371:GLY:HA3	1.91	0.52
1:D:33:GLU:N	1:D:33:GLU:OE1	2.40	0.52
1:G:55:LEU:HB2	1:G:118:LEU:HB2	1.92	0.52
1:H:39:LEU:HD22	1:H:321:VAL:HG11	1.91	0.52
1:I:33:GLU:HG2	1:I:273:LYS:NZ	2.24	0.52
1:B:128:PHE:HB2	1:B:365:SER:HA	1.91	0.52
1:C:102:THR:OG1	1:C:104:ASN:OD1	2.24	0.52
1:D:277:GLY:H	1:D:284:VAL:HG12	1.74	0.52
1:G:183:SER:N	1:G:186:ASP:OD2	2.37	0.52
1:C:5:ALA:O	1:C:6:PRO:C	2.47	0.52
1:F:35:TYR:CD2	1:F:287:VAL:HG22	2.45	0.52
1:I:91:ILE:HA	1:I:94:ILE:HD12	1.92	0.52
2:K:15:GLN:OE1	2:K:16:ALA:N	2.37	0.52
2:Q:43:GLU:N	2:Q:43:GLU:OE2	2.43	0.52
1:C:336:LYS:HE3	1:C:336:LYS:HA	1.91	0.52
1:D:216:GLN:HE21	1:D:322:GLY:HA2	1.75	0.52
2:K:39:LYS:HD2	2:L:30:GLU:OE2	2.10	0.52
2:K:43:GLU:HG2	2:K:43:GLU:O	2.09	0.52
1:C:276:ILE:HG23	1:C:284:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:MET:HE2	1:G:203:LYS:HE3	1.91	0.52
1:H:212:LEU:HA	1:H:379:TRP:NE1	2.24	0.52
2:Q:46:ASP:N	2:Q:46:ASP:OD2	2.42	0.52
1:E:106:GLY:HA3	2:N:21:HIS:HE2	1.75	0.52
1:I:145:ASP:OD2	1:I:146:SER:N	2.42	0.52
2:M:28:VAL:HA	2:O:36:LEU:HD23	1.92	0.52
2:M:28:VAL:HA	2:O:36:LEU:CD2	2.41	0.51
1:F:239:ILE:HD11	1:F:243:LEU:HD22	1.92	0.51
1:G:167:ASP:OD2	1:G:370:TYR:OH	2.28	0.51
1:F:133:GLN:NE2	1:F:137:ASP:OD1	2.44	0.51
1:H:273:LYS:HA	1:H:273:LYS:HE2	1.92	0.51
2:Q:41:VAL:HA	2:Q:44:LEU:HD13	1.91	0.51
1:C:204:MET:SD	1:C:383:PHE:HB2	2.51	0.51
1:F:260:ILE:HG23	1:F:265:TYR:OH	2.10	0.51
1:F:63:ASP:HA	1:F:87:SER:HB3	1.91	0.51
2:R:16:ALA:HB2	2:R:27:VAL:HG23	1.93	0.51
1:F:2:LYS:N	1:F:12:SER:HG	2.09	0.51
2:J:21:HIS:HD2	2:L:16:ALA:HB3	1.75	0.51
1:A:365:SER:HB3	1:D:357:PRO:HB2	1.92	0.51
1:F:223:SER:HB3	1:F:224:LEU:HD22	1.92	0.51
1:I:33:GLU:HG2	1:I:273:LYS:HZ3	1.75	0.51
1:I:266:ALA:O	1:I:268:ALA:N	2.43	0.51
2:L:39:LYS:HB2	2:L:43:GLU:OE1	2.10	0.51
2:Q:15:GLN:HB3	2:Q:28:VAL:CG1	2.40	0.51
1:B:356:ASP:HA	1:H:106:GLY:HA2	1.91	0.51
1:D:109:ASN:HB2	1:E:127:PHE:HA	1.91	0.51
1:F:128:PHE:CZ	1:G:110:ARG:HG2	2.46	0.51
2:O:14:LYS:HE3	2:O:29:GLY:HA2	1.93	0.51
1:A:292:LYS:HE2	1:A:294:ALA:HB2	1.93	0.51
1:D:60:PRO:HG3	1:E:29:ASP:OD1	2.11	0.51
1:G:300:VAL:HG11	1:G:309:THR:HG23	1.92	0.51
1:I:370:TYR:CD1	1:I:371:GLY:N	2.74	0.51
2:J:10:LEU:HD11	2:K:22:GLY:HA3	1.93	0.51
2:P:31:LEU:O	2:P:35:VAL:HG23	2.11	0.51
1:A:177:TYR:HB3	1:A:181:ALA:HB3	1.93	0.51
1:B:135:ALA:HA	1:D:3:TYR:HB2	1.93	0.51
1:D:243:LEU:HD13	1:D:387:ALA:HB2	1.92	0.51
1:F:188:THR:HB	1:F:298:ALA:CB	2.40	0.51
1:D:57:HIS:HB3	1:D:116:ILE:HG22	1.93	0.50
2:K:30:GLU:OE2	2:K:30:GLU:N	2.43	0.50
2:K:31:LEU:O	2:K:35:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:PHE:HZ	1:B:276:ILE:HG22	1.74	0.50
1:D:297:GLY:HA3	1:D:313:TYR:HB2	1.94	0.50
1:F:17:ILE:HG13	1:F:18:ARG:H	1.77	0.50
2:K:46:ASP:N	2:K:46:ASP:OD1	2.42	0.50
1:D:237:LEU:HD11	1:D:318:MET:HB3	1.92	0.50
1:D:260:ILE:HG23	1:D:265:TYR:OH	2.11	0.50
1:F:293:TRP:CE2	1:G:91:ILE:HD12	2.46	0.50
1:G:69:ASP:OD2	1:G:70:GLN:N	2.45	0.50
1:G:260:ILE:HD12	1:G:261:PRO:HD2	1.93	0.50
1:H:95:PRO:HA	1:H:98:LEU:HD12	1.93	0.50
1:H:136:MET:SD	1:H:136:MET:N	2.83	0.50
1:H:209:ASN:HA	1:H:235:ARG:HH22	1.76	0.50
1:C:102:THR:O	1:D:124:LYS:NZ	2.43	0.50
1:D:208:LEU:HD21	1:D:381:ALA:HB2	1.94	0.50
1:E:378:GLU:OE2	1:E:378:GLU:N	2.38	0.50
2:P:34:GLN:OE1	2:P:45:PRO:HG3	2.12	0.50
1:B:259:PHE:HD1	1:B:279:ILE:HD11	1.76	0.50
1:C:31:ALA:HB2	1:C:154:LYS:HD3	1.93	0.50
1:H:297:GLY:HA3	1:H:313:TYR:H	1.76	0.50
1:C:178:PRO:HG2	1:C:194:THR:HB	1.92	0.50
1:D:43:THR:HG23	1:D:327:THR:HG21	1.92	0.50
1:B:128:PHE:CD2	1:B:363:LEU:HD11	2.47	0.50
1:B:140:THR:HG21	1:D:18:ARG:H	1.76	0.50
1:B:131:TRP:O	1:B:362:GLY:N	2.39	0.50
1:B:333:THR:HA	1:B:339:LYS:HE3	1.92	0.50
1:A:131:TRP:HE1	1:A:346:LYS:HZ1	1.59	0.50
1:D:292:LYS:HZ2	1:D:294:ALA:HB2	1.77	0.50
1:E:20:ASP:OD1	1:E:20:ASP:N	2.45	0.49
1:E:212:LEU:HB3	1:E:235:ARG:NH1	2.27	0.49
1:F:239:ILE:HD11	1:F:243:LEU:HB2	1.94	0.49
1:G:196:VAL:HG22	1:G:382:LEU:HD21	1.93	0.49
1:H:212:LEU:HD12	1:H:213:CYS:H	1.76	0.49
1:I:165:GLN:HE22	1:I:290:MET:HA	1.77	0.49
1:A:225:MET:HG3	1:A:226:THR:H	1.77	0.49
1:D:85:TYR:CZ	1:D:94:ILE:HG23	2.47	0.49
1:E:52:GLN:HB3	1:E:119:ILE:HD11	1.94	0.49
2:K:39:LYS:HG2	2:L:14:LYS:HZ3	1.77	0.49
1:I:275:GLU:HA	1:I:284:VAL:O	2.12	0.49
2:R:15:GLN:O	2:R:28:VAL:N	2.35	0.49
1:B:259:PHE:HE1	1:B:284:VAL:HG21	1.78	0.49
1:C:35:TYR:CE1	1:C:273:LYS:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LEU:HD23	1:C:118:LEU:HD12	1.95	0.49
1:A:199:GLU:HA	1:A:202:VAL:HG22	1.94	0.49
1:A:208:LEU:HD12	1:A:208:LEU:O	2.11	0.49
1:B:17:ILE:HG13	1:B:18:ARG:H	1.77	0.49
1:D:94:ILE:O	1:D:98:LEU:N	2.46	0.49
1:H:212:LEU:HD13	1:H:379:TRP:CG	2.47	0.49
1:H:287:VAL:HB	1:H:290:MET:HG2	1.93	0.49
1:G:176:ARG:HB2	1:G:382:LEU:HD12	1.95	0.49
1:I:289:LYS:HA	1:I:289:LYS:HE2	1.95	0.49
1:I:321:VAL:HG12	1:I:380:ILE:HD12	1.94	0.49
1:B:6:PRO:O	1:B:9:THR:N	2.45	0.49
1:B:18:ARG:NH2	1:D:18:ARG:HE	2.11	0.49
1:B:334:ASP:O	1:B:336:LYS:NZ	2.46	0.49
1:C:18:ARG:HD3	1:C:18:ARG:H	1.78	0.49
1:E:124:LYS:HD2	1:E:369:TYR:HB3	1.95	0.49
1:E:208:LEU:HG	1:E:235:ARG:NH1	2.28	0.49
1:F:70:GLN:HA	1:F:110:ARG:HH21	1.78	0.49
1:H:252:ASP:OD1	1:H:256:ASN:N	2.43	0.49
1:E:91:ILE:HG22	1:G:166:ILE:HG12	1.94	0.49
1:C:293:TRP:HE3	1:C:315:VAL:HG12	1.78	0.48
1:D:196:VAL:HG23	1:D:385:THR:HB	1.93	0.48
1:F:165:GLN:HE22	1:F:290:MET:HA	1.78	0.48
1:I:239:ILE:HD12	1:I:240:GLY:H	1.78	0.48
2:M:10:LEU:HD21	2:N:22:GLY:HA2	1.95	0.48
1:E:84:LEU:HD11	1:E:99:PRO:HG3	1.95	0.48
1:E:215:MET:O	1:E:216:GLN:C	2.50	0.48
1:I:60:PRO:HG2	1:I:63:ASP:HB2	1.95	0.48
1:I:262:VAL:HA	1:I:265:TYR:CE2	2.47	0.48
1:A:262:VAL:HG22	1:A:271:LEU:HD23	1.95	0.48
1:E:66:ASN:HB3	1:E:83:ASN:HB3	1.95	0.48
1:G:18:ARG:O	1:G:19:LEU:HD23	2.13	0.48
1:G:90:ASP:O	1:G:94:ILE:HG12	2.13	0.48
2:K:17:VAL:HG12	2:L:19:VAL:HG13	1.95	0.48
1:A:165:GLN:O	1:A:169:LEU:HD23	2.13	0.48
1:B:143:GLU:OE1	1:B:143:GLU:N	2.38	0.48
1:C:16:GLN:OE1	1:C:18:ARG:NH1	2.47	0.48
1:D:60:PRO:O	1:D:66:ASN:ND2	2.46	0.48
1:E:375:LEU:HB3	1:G:27:LEU:HD11	1.94	0.48
1:B:159:ILE:O	1:B:163:GLN:HG3	2.14	0.48
1:E:41:GLU:OE1	1:E:41:GLU:N	2.43	0.48
1:B:378:GLU:HG2	1:B:379:TRP:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:TYR:CD2	1:H:55:LEU:HD21	2.49	0.48
1:E:94:ILE:HG12	1:E:95:PRO:HD3	1.96	0.48
1:F:68:ASN:HD22	1:F:112:GLY:HA3	1.77	0.48
1:G:293:TRP:HB2	1:G:315:VAL:HB	1.94	0.48
2:M:35:VAL:HG22	2:M:48:VAL:HG11	1.93	0.48
1:A:186:ASP:OD1	1:A:186:ASP:N	2.40	0.48
1:D:74:ALA:HA	1:D:108:VAL:HG13	1.94	0.48
2:M:16:ALA:HB3	2:N:21:HIS:HB2	1.96	0.48
1:A:54:LYS:NZ	1:B:20:ASP:OD2	2.36	0.48
1:D:55:LEU:HD21	1:E:23:TYR:HD2	1.79	0.48
1:F:199:GLU:N	1:F:199:GLU:OE2	2.47	0.48
1:G:259:PHE:CE2	1:G:277:GLY:HA3	2.49	0.48
1:H:217:THR:HG22	1:H:234:ALA:O	2.14	0.48
1:I:251:LYS:NZ	1:I:256:ASN:O	2.45	0.48
1:H:244:GLU:O	1:H:248:ARG:HG3	2.13	0.48
1:B:4:ASN:HB3	1:D:135:ALA:HA	1.95	0.48
1:E:39:LEU:HD12	1:E:39:LEU:O	2.14	0.48
1:F:375:LEU:HD12	1:F:375:LEU:H	1.78	0.48
1:H:231:ILE:HD13	1:H:265:TYR:CE1	2.49	0.48
1:I:269:GLY:O	1:I:270:ASN:C	2.51	0.48
1:F:208:LEU:HD13	1:F:212:LEU:CD2	2.44	0.47
2:P:44:LEU:HD11	2:Q:31:LEU:HD23	1.95	0.47
1:F:5:ALA:H	1:F:9:THR:HG1	1.61	0.47
1:G:70:GLN:HA	1:G:110:ARG:HH21	1.79	0.47
1:G:127:PHE:O	1:G:365:SER:OG	2.22	0.47
1:A:216:GLN:HB2	1:A:235:ARG:HA	1.96	0.47
1:D:53:ILE:HD11	1:E:23:TYR:HB2	1.97	0.47
1:I:265:TYR:CG	1:I:266:ALA:N	2.81	0.47
1:F:190:GLU:HG2	1:F:313:TYR:CE2	2.49	0.47
1:E:90:ASP:O	1:E:94:ILE:HG23	2.14	0.47
1:G:325:SER:HA	1:G:375:LEU:O	2.15	0.47
1:A:94:ILE:O	1:A:98:LEU:N	2.48	0.47
1:A:237:LEU:HD11	1:A:318:MET:HG2	1.96	0.47
1:B:329:ILE:N	1:B:371:GLY:O	2.42	0.47
1:B:357:PRO:HG3	1:C:363:LEU:HD11	1.97	0.47
1:D:61:LEU:HD13	1:D:113:PHE:CE1	2.49	0.47
1:E:273:LYS:HD3	1:E:274:GLY:N	2.29	0.47
1:F:55:LEU:HB2	1:F:118:LEU:HB2	1.95	0.47
1:D:239:ILE:HD11	1:D:243:LEU:HD23	1.96	0.47
1:F:129:TYR:HB3	1:G:111:VAL:HG23	1.95	0.47
2:O:15:GLN:HG2	2:O:28:VAL:CG1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:LEU:N	1:H:151:GLU:OE1	2.47	0.47
1:C:35:TYR:HE1	1:C:273:LYS:HG2	1.80	0.47
1:H:239:ILE:HD11	1:H:243:LEU:HB2	1.97	0.47
2:O:9:ILE:O	2:O:14:LYS:HB2	2.15	0.47
1:A:176:ARG:HB2	1:A:204:MET:HE2	1.96	0.47
1:B:196:VAL:HG11	1:B:318:MET:SD	2.55	0.47
1:D:52:GLN:HB3	1:D:119:ILE:HD11	1.97	0.47
1:F:259:PHE:HA	1:F:279:ILE:HG12	1.97	0.47
1:F:291:LEU:HD11	1:G:94:ILE:HG13	1.96	0.47
1:A:188:THR:HB	1:A:298:ALA:HB3	1.97	0.46
1:C:23:TYR:HD2	1:H:55:LEU:HD21	1.80	0.46
1:C:131:TRP:O	1:C:362:GLY:N	2.48	0.46
1:E:212:LEU:HA	1:E:379:TRP:CD1	2.50	0.46
1:F:145:ASP:OD1	1:F:146:SER:N	2.48	0.46
1:F:325:SER:HB3	1:F:379:TRP:HB2	1.97	0.46
1:A:253:PRO:HB3	1:B:249:LYS:HZ2	1.79	0.46
1:C:259:PHE:CZ	1:C:276:ILE:HG12	2.49	0.46
1:C:378:GLU:HG2	1:C:379:TRP:HD1	1.80	0.46
1:E:252:ASP:OD2	1:E:256:ASN:N	2.32	0.46
1:F:27:LEU:HD22	1:G:376:ARG:HH12	1.80	0.46
2:N:37:ALA:HB2	2:O:27:VAL:HG13	1.96	0.46
2:P:15:GLN:NE2	2:Q:22:GLY:H	2.13	0.46
1:A:345:LYS:HD2	1:A:351:THR:HG22	1.97	0.46
1:C:243:LEU:HD11	1:C:316:PHE:HB3	1.96	0.46
1:E:293:TRP:HB2	1:E:315:VAL:HB	1.96	0.46
1:F:155:GLY:O	1:F:159:ILE:HG12	2.14	0.46
1:F:365:SER:OG	1:F:367:LYS:HE3	2.14	0.46
2:M:20:LYS:HA	2:M:20:LYS:HD3	1.74	0.46
2:O:32:GLY:O	2:O:36:LEU:N	2.39	0.46
1:C:329:ILE:N	1:C:371:GLY:O	2.38	0.46
1:A:91:ILE:HD11	1:B:293:TRP:CE2	2.51	0.46
1:C:199:GLU:OE1	1:C:199:GLU:N	2.27	0.46
1:D:201:LEU:HD23	1:D:201:LEU:HA	1.80	0.46
1:E:84:LEU:HD22	1:E:111:VAL:HG11	1.97	0.46
1:B:35:TYR:CD1	1:B:287:VAL:HG22	2.51	0.46
1:C:131:TRP:CE2	1:C:362:GLY:HA3	2.51	0.46
1:C:249:LYS:HE3	1:C:249:LYS:HA	1.98	0.46
1:H:135:ALA:O	1:H:139:ASP:HB2	2.15	0.46
1:B:51:LYS:HB2	1:B:51:LYS:HE3	1.69	0.46
1:B:64:ASP:N	1:B:87:SER:OG	2.46	0.46
1:C:278:SER:C	1:C:279:ILE:HD13	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LYS:HD2	1:D:316:PHE:CE2	2.51	0.46
1:H:137:ASP:HB3	1:I:331:PHE:HZ	1.80	0.46
2:K:5:ASP:HB3	2:K:7:ASP:OD1	2.15	0.46
2:P:39:LYS:O	2:Q:31:LEU:HB2	2.16	0.46
2:Q:9:ILE:HG23	2:Q:14:LYS:HB2	1.96	0.46
1:G:354:TYR:CE2	2:O:20:LYS:HG3	2.51	0.46
1:H:223:SER:HB3	1:H:268:ALA:HB2	1.97	0.46
2:J:34:GLN:HB3	2:J:45:PRO:HG3	1.98	0.46
1:C:94:ILE:HG22	1:C:98:LEU:HG	1.98	0.46
1:F:209:ASN:OD1	1:F:235:ARG:NH2	2.49	0.46
2:J:9:ILE:HD12	2:J:9:ILE:H	1.81	0.46
2:J:39:LYS:HB3	2:J:39:LYS:HE3	1.61	0.46
1:C:104:ASN:OD1	1:C:104:ASN:N	2.45	0.45
1:C:169:LEU:HD12	1:C:293:TRP:CZ2	2.52	0.45
1:D:239:ILE:HD11	1:D:243:LEU:HB3	1.99	0.45
1:E:212:LEU:CB	1:E:235:ARG:NH1	2.79	0.45
1:A:163:GLN:O	1:A:166:ILE:HG22	2.16	0.45
1:A:239:ILE:CD1	1:A:318:MET:HG3	2.46	0.45
1:C:9:THR:O	1:C:9:THR:OG1	2.30	0.45
1:F:45:MET:H	1:F:329:ILE:HG22	1.81	0.45
1:A:346:LYS:CE	1:A:347:PRO:HD2	2.46	0.45
1:D:49:MET:CE	1:D:50:GLY:H	2.30	0.45
1:D:85:TYR:OH	1:D:98:LEU:HD12	2.16	0.45
1:C:341:THR:HB	1:C:367:LYS:HG2	1.99	0.45
1:D:55:LEU:HD21	1:E:23:TYR:HB3	1.99	0.45
1:I:79:ILE:HG22	1:I:81:ASN:H	1.81	0.45
1:D:260:ILE:HD12	1:D:261:PRO:HD2	1.98	0.45
1:E:105:GLY:O	2:N:21:HIS:NE2	2.50	0.45
1:A:89:LYS:NZ	1:B:288:PRO:O	2.49	0.45
1:F:91:ILE:HG23	1:H:291:LEU:HB3	1.97	0.45
1:F:190:GLU:HG2	1:F:313:TYR:HE2	1.81	0.45
1:B:135:ALA:O	1:B:139:ASP:HB2	2.17	0.45
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.86	0.45
1:C:73:ASP:OD2	1:C:75:ALA:N	2.48	0.45
1:H:318:MET:O	1:H:382:LEU:HA	2.17	0.45
2:R:6:VAL:HA	2:R:9:ILE:HG12	1.99	0.45
1:A:230:THR:HG23	1:B:227:ASP:HB3	1.97	0.45
1:B:95:PRO:HA	1:B:98:LEU:HD12	1.97	0.45
1:C:275:GLU:HA	1:C:285:ILE:HD13	1.99	0.45
1:E:62:LEU:HD21	1:G:159:ILE:HG12	1.99	0.45
1:F:47:LYS:O	1:F:49:MET:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:GLN:HG2	1:F:119:ILE:HD11	1.98	0.45
1:F:55:LEU:HD11	1:H:23:TYR:HD2	1.82	0.45
1:G:27:LEU:HD23	1:G:27:LEU:HA	1.83	0.45
2:R:15:GLN:HB3	2:R:28:VAL:HG12	1.98	0.45
1:B:140:THR:HG22	1:D:18:ARG:HB2	1.98	0.45
1:C:73:ASP:HB3	1:C:79:ILE:HG13	1.99	0.45
1:D:35:TYR:CE1	1:D:273:LYS:HG2	2.52	0.45
1:D:231:ILE:HD11	1:D:265:TYR:CD2	2.52	0.45
1:F:266:ALA:HB2	1:G:219:LEU:HD11	1.99	0.45
1:H:234:ALA:HB3	1:H:283:ARG:HG2	1.99	0.45
2:Q:37:ALA:O	2:R:14:LYS:NZ	2.39	0.45
1:A:176:ARG:HH21	1:A:203:LYS:HB3	1.82	0.44
1:B:190:GLU:HG2	1:B:313:TYR:HE2	1.82	0.44
1:D:363:LEU:HD12	1:D:364:THR:H	1.83	0.44
1:E:54:LYS:HD2	1:E:117:GLN:HE22	1.82	0.44
1:E:62:LEU:HD23	1:E:85:TYR:HE1	1.82	0.44
1:E:205:GLY:O	1:E:209:ASN:ND2	2.51	0.44
1:F:208:LEU:HD12	1:F:212:LEU:HG	1.95	0.44
1:H:239:ILE:HG22	1:H:285:ILE:O	2.17	0.44
1:I:203:LYS:HA	1:I:206:ILE:HD12	1.99	0.44
1:D:55:LEU:HD23	1:D:55:LEU:HA	1.78	0.44
1:E:220:ILE:HB	1:E:231:ILE:HG13	1.99	0.44
1:G:128:PHE:HD1	1:G:363:LEU:HD11	1.82	0.44
2:J:9:ILE:HG23	2:J:14:LYS:HB2	1.99	0.44
2:P:3:TYR:HD1	2:P:9:ILE:HG23	1.83	0.44
2:P:34:GLN:OE1	2:P:35:VAL:N	2.51	0.44
1:A:99:PRO:HB2	1:B:126:GLY:O	2.17	0.44
1:C:131:TRP:CD2	1:C:362:GLY:HA3	2.52	0.44
1:D:232:GLN:OE1	1:E:248:ARG:NH2	2.51	0.44
1:E:54:LYS:CD	1:E:117:GLN:NE2	2.81	0.44
1:H:212:LEU:HD11	1:H:322:GLY:HA3	1.98	0.44
2:O:15:GLN:OE1	2:O:15:GLN:N	2.39	0.44
1:C:61:LEU:HD13	1:C:113:PHE:HD1	1.82	0.44
1:C:249:LYS:NZ	1:H:253:PRO:HB3	2.32	0.44
1:D:208:LEU:HD12	1:D:213:CYS:CB	2.47	0.44
1:D:218:LYS:HD2	1:D:218:LYS:N	2.32	0.44
1:E:325:SER:O	1:E:375:LEU:N	2.51	0.44
1:C:237:LEU:HD12	1:C:237:LEU:HA	1.92	0.44
1:G:33:GLU:OE1	1:G:33:GLU:N	2.33	0.44
2:N:9:ILE:HD12	2:N:16:ALA:HB2	2.00	0.44
1:A:378:GLU:OE1	1:A:378:GLU:N	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LYS:HG3	1:E:20:ASP:HB2	1.98	0.44
2:Q:9:ILE:CG2	2:Q:14:LYS:HB2	2.48	0.44
1:A:250:MET:O	1:A:258:ALA:N	2.43	0.44
1:G:66:ASN:HD21	1:G:113:PHE:HA	1.83	0.44
2:N:36:LEU:O	2:O:32:GLY:HA3	2.18	0.44
1:A:66:ASN:ND2	1:A:112:GLY:O	2.50	0.44
1:A:217:THR:HG22	1:A:234:ALA:O	2.18	0.44
1:B:239:ILE:N	1:B:290:MET:HE1	2.33	0.44
1:C:90:ASP:O	1:C:94:ILE:HD12	2.17	0.44
1:D:84:LEU:HD23	1:D:99:PRO:HD3	2.00	0.44
1:D:155:GLY:O	1:D:159:ILE:HG12	2.18	0.44
1:E:54:LYS:HG3	1:G:20:ASP:OD2	2.17	0.44
1:E:334:ASP:OD2	1:E:334:ASP:N	2.50	0.44
1:F:239:ILE:HD12	1:F:240:GLY:H	1.81	0.44
1:H:325:SER:O	1:H:375:LEU:N	2.51	0.44
2:J:19:VAL:HA	2:L:17:VAL:HG23	2.00	0.44
2:P:10:LEU:HD23	2:P:10:LEU:HA	1.87	0.44
1:B:287:VAL:HG12	1:B:289:LYS:H	1.83	0.44
1:G:285:ILE:HD13	1:G:285:ILE:HA	1.87	0.44
1:I:71:GLY:HA3	1:I:82:GLY:HA2	2.00	0.44
1:C:5:ALA:HB3	1:C:9:THR:OG1	2.18	0.43
1:E:133:GLN:O	1:E:133:GLN:NE2	2.51	0.43
1:F:128:PHE:HD2	1:F:363:LEU:HD11	1.82	0.43
1:F:208:LEU:HB3	1:F:235:ARG:NH1	2.33	0.43
2:L:16:ALA:HB1	2:L:25:LEU:HD21	2.00	0.43
1:C:327:THR:HG23	1:C:373:LEU:HB3	2.00	0.43
1:F:90:ASP:O	1:F:94:ILE:HG13	2.18	0.43
1:G:260:ILE:HG22	1:G:278:SER:O	2.18	0.43
1:I:66:ASN:OD1	1:I:68:ASN:ND2	2.51	0.43
2:L:34:GLN:OE1	2:L:34:GLN:N	2.51	0.43
1:A:243:LEU:HD23	1:A:387:ALA:HB2	2.00	0.43
1:A:262:VAL:HA	1:A:265:TYR:CE1	2.53	0.43
1:B:164:LEU:HD11	1:B:326:PHE:HE2	1.84	0.43
1:C:68:ASN:OD1	1:C:69:ASP:N	2.51	0.43
1:I:293:TRP:CZ3	1:I:317:PRO:HB3	2.52	0.43
2:L:34:GLN:HB3	2:L:45:PRO:HD3	2.00	0.43
1:B:132:THR:HG21	1:D:2:LYS:NZ	2.32	0.43
1:B:352:VAL:HA	1:B:356:ASP:O	2.18	0.43
1:D:211:ASN:O	1:D:212:LEU:C	2.56	0.43
1:I:94:ILE:O	1:I:98:LEU:HG	2.18	0.43
2:O:14:LYS:CE	2:O:29:GLY:HA2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:LEU:HD11	1:G:263:GLN:HB3	2.00	0.43
2:Q:39:LYS:HA	2:R:30:GLU:HB3	1.99	0.43
1:B:260:ILE:HB	1:B:265:TYR:OH	2.18	0.43
1:G:54:LYS:O	1:G:55:LEU:HD23	2.19	0.43
2:K:15:GLN:HB3	2:K:28:VAL:CG1	2.49	0.43
2:N:17:VAL:HG22	2:O:19:VAL:HG22	2.00	0.43
1:C:280:ALA:C	1:C:282:PHE:H	2.22	0.43
1:G:213:CYS:O	1:G:235:ARG:NH1	2.52	0.43
1:H:336:LYS:HA	1:H:336:LYS:HD3	1.91	0.43
1:I:183:SER:N	1:I:186:ASP:OD2	2.48	0.43
1:I:201:LEU:HD23	1:I:201:LEU:HA	1.84	0.43
1:C:262:VAL:HG23	1:C:276:ILE:C	2.38	0.43
1:G:238:TYR:N	1:G:319:LEU:O	2.46	0.43
2:J:15:GLN:O	2:J:28:VAL:N	2.30	0.43
1:A:219:LEU:HD11	1:B:263:GLN:HB3	2.00	0.43
1:B:61:LEU:HD12	1:B:113:PHE:CE1	2.54	0.43
1:B:204:MET:O	1:B:208:LEU:N	2.48	0.43
1:C:59:VAL:HG21	1:C:65:ARG:HB2	2.00	0.43
1:C:239:ILE:HD12	1:C:240:GLY:H	1.83	0.43
1:C:319:LEU:HD21	1:C:321:VAL:HB	2.00	0.43
1:D:232:GLN:O	1:D:232:GLN:HG3	2.18	0.43
1:F:199:GLU:HA	1:F:202:VAL:HG22	1.99	0.43
1:G:69:ASP:OD2	1:G:70:GLN:HG3	2.19	0.43
1:G:174:VAL:HB	1:G:380:ILE:HA	2.01	0.43
1:G:338:VAL:HG23	1:G:369:TYR:O	2.19	0.43
1:I:239:ILE:CD1	1:I:243:LEU:HD12	2.43	0.43
2:P:19:VAL:HG11	2:R:15:GLN:HG3	2.01	0.43
1:E:259:PHE:HD2	1:E:279:ILE:HD11	1.83	0.43
1:F:151:GLU:HA	1:F:154:LYS:HD3	2.01	0.43
1:G:343:TYR:O	1:G:364:THR:HA	2.19	0.43
1:D:202:VAL:O	1:D:206:ILE:HG12	2.19	0.42
1:D:217:THR:H	1:D:234:ALA:HB3	1.84	0.42
1:E:34:MET:O	1:E:38:GLN:NE2	2.46	0.42
1:F:41:GLU:OE1	1:F:41:GLU:N	2.52	0.42
1:H:55:LEU:HD23	1:H:55:LEU:HA	1.72	0.42
1:I:261:PRO:O	1:I:265:TYR:HD2	2.02	0.42
2:J:15:GLN:NE2	2:J:16:ALA:H	2.16	0.42
2:J:18:ALA:HB2	2:K:20:LYS:HB3	2.01	0.42
2:M:36:LEU:O	2:N:32:GLY:HA3	2.19	0.42
1:A:260:ILE:HD11	1:A:265:TYR:HE2	1.84	0.42
1:A:318:MET:O	1:A:382:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASP:OD1	1:C:146:SER:N	2.49	0.42
1:C:259:PHE:CE1	1:C:277:GLY:HA3	2.55	0.42
1:D:300:VAL:HG23	1:D:311:GLY:O	2.20	0.42
1:E:376:ARG:HB3	1:E:378:GLU:OE1	2.19	0.42
1:F:53:ILE:HD13	1:H:21:TYR:HD2	1.84	0.42
1:F:73:ASP:OD1	1:F:77:ALA:N	2.51	0.42
1:F:84:LEU:HD23	1:F:84:LEU:HA	1.88	0.42
1:F:140:THR:OG1	1:G:56:TYR:HE2	2.02	0.42
1:I:123:LYS:HE2	1:I:123:LYS:HB3	1.79	0.42
2:J:15:GLN:HG3	2:K:19:VAL:HG11	2.00	0.42
1:A:132:THR:OG1	1:A:134:GLU:HG2	2.20	0.42
1:A:200:GLY:HA2	1:A:203:LYS:HE2	2.00	0.42
1:A:204:MET:HE3	1:A:383:PHE:HD2	1.84	0.42
1:B:22:TYR:CD1	1:D:17:ILE:HD11	2.54	0.42
1:B:293:TRP:HB2	1:B:315:VAL:HB	2.01	0.42
1:E:81:ASN:ND2	1:E:83:ASN:O	2.48	0.42
1:E:208:LEU:HD12	1:E:208:LEU:O	2.20	0.42
1:I:85:TYR:HA	1:I:97:LYS:HE3	2.01	0.42
1:I:244:GLU:OE1	1:I:244:GLU:N	2.33	0.42
1:B:243:LEU:HD13	1:B:387:ALA:HB2	2.01	0.42
1:C:338:VAL:HG22	1:C:368:TRP:HB2	2.02	0.42
1:D:214:PRO:O	1:D:235:ARG:NE	2.50	0.42
1:F:29:ASP:O	1:F:154:LYS:NZ	2.51	0.42
1:B:73:ASP:HB3	1:B:77:ALA:O	2.19	0.42
1:D:73:ASP:N	1:D:77:ALA:O	2.42	0.42
1:D:196:VAL:HG21	1:D:318:MET:CE	2.49	0.42
1:D:300:VAL:HG22	1:D:313:TYR:CD1	2.54	0.42
1:E:34:MET:HG3	1:E:38:GLN:NE2	2.34	0.42
1:B:306:TYR:HA	1:B:388:ALA:HA	2.01	0.42
1:C:360:GLU:N	1:C:360:GLU:OE1	2.53	0.42
1:D:300:VAL:HG22	1:D:313:TYR:CE1	2.54	0.42
1:E:216:GLN:NE2	1:E:235:ARG:HB3	2.34	0.42
1:F:271:LEU:HA	1:F:271:LEU:HD23	1.78	0.42
1:A:189:GLY:HA2	1:A:193:ALA:HA	2.02	0.42
1:A:331:PHE:CD2	1:A:332:GLN:HG2	2.54	0.42
1:B:187:MET:SD	1:B:194:THR:OG1	2.69	0.42
1:C:94:ILE:O	1:C:98:LEU:N	2.53	0.42
1:C:162:ASP:O	1:C:166:ILE:HG22	2.20	0.42
1:E:91:ILE:HA	1:E:94:ILE:HG12	2.01	0.42
1:E:208:LEU:HG	1:E:235:ARG:HH11	1.84	0.42
1:F:167:ASP:OD2	1:F:372:SER:OG	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:LEU:HB3	1:F:213:CYS:CB	2.49	0.42
1:G:363:LEU:HD12	1:G:363:LEU:HA	1.86	0.42
1:H:304:PRO:HD2	1:H:306:TYR:HD2	1.84	0.42
1:A:375:LEU:HB3	1:B:27:LEU:HD11	2.02	0.42
1:B:342:THR:HA	1:B:365:SER:O	2.19	0.42
1:E:61:LEU:H	1:G:154:LYS:NZ	2.18	0.42
1:F:239:ILE:HD12	1:F:240:GLY:N	2.34	0.42
1:I:293:TRP:HZ3	1:I:317:PRO:HB3	1.85	0.42
2:N:20:LYS:HA	2:N:20:LYS:HD3	1.83	0.42
2:P:39:LYS:HA	2:Q:30:GLU:OE1	2.20	0.42
2:P:41:VAL:HA	2:P:44:LEU:HD13	2.02	0.42
1:A:54:LYS:HD3	1:A:119:ILE:HG13	2.02	0.42
1:A:145:ASP:O	1:A:149:ILE:HG22	2.20	0.42
1:B:243:LEU:O	1:B:247:LEU:HG	2.20	0.42
1:B:376:ARG:HD3	1:B:379:TRP:CE2	2.53	0.42
1:C:156:ALA:HA	1:C:159:ILE:HG22	2.02	0.42
1:D:131:TRP:O	1:D:362:GLY:N	2.49	0.42
1:F:245:LEU:HD13	1:G:202:VAL:HG21	2.02	0.42
1:H:102:THR:HG23	1:H:105:GLY:H	1.85	0.42
1:H:204:MET:SD	1:H:383:PHE:HB2	2.60	0.42
1:A:78:THR:O	1:A:78:THR:OG1	2.38	0.42
1:A:203:LYS:O	1:A:206:ILE:HG13	2.20	0.42
1:A:239:ILE:HG22	1:A:240:GLY:O	2.20	0.42
1:B:187:MET:CE	1:B:386:VAL:HG23	2.50	0.42
1:C:5:ALA:HA	1:C:6:PRO:HD2	1.82	0.42
1:D:35:TYR:HE1	1:D:273:LYS:HG2	1.84	0.42
1:D:216:GLN:OE1	1:D:236:ALA:N	2.35	0.42
1:E:55:LEU:N	1:E:118:LEU:O	2.42	0.42
1:E:90:ASP:HA	1:G:292:LYS:O	2.20	0.42
1:A:237:LEU:HG	1:A:239:ILE:HD11	2.01	0.41
1:C:234:ALA:CB	1:C:283:ARG:HG2	2.50	0.41
1:F:223:SER:HA	1:H:225:MET:HA	2.02	0.41
1:H:156:ALA:HA	1:H:159:ILE:HG22	2.01	0.41
1:H:337:THR:HG23	1:H:338:VAL:HG12	2.01	0.41
1:I:239:ILE:HD12	1:I:240:GLY:N	2.35	0.41
2:M:26:VAL:HG11	2:O:28:VAL:HG21	2.01	0.41
1:C:243:LEU:CD2	1:C:387:ALA:HB2	2.47	0.41
1:D:55:LEU:HD21	1:E:23:TYR:CD2	2.55	0.41
1:D:214:PRO:HB2	1:D:215:MET:H	1.61	0.41
1:D:262:VAL:HB	1:D:271:LEU:HD23	2.02	0.41
1:F:43:THR:OG1	1:F:329:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:LEU:HD12	1:F:363:LEU:HA	1.80	0.41
1:G:208:LEU:HB3	1:G:235:ARG:NH1	2.35	0.41
1:H:248:ARG:HH21	1:H:276:ILE:HD11	1.85	0.41
1:I:73:ASP:OD1	1:I:77:ALA:N	2.53	0.41
1:E:230:THR:HG23	1:G:227:ASP:HB3	2.01	0.41
1:E:336:LYS:N	1:E:336:LYS:HD2	2.34	0.41
1:F:262:VAL:HG23	1:F:271:LEU:HD21	2.02	0.41
1:G:375:LEU:H	1:G:375:LEU:HD23	1.85	0.41
2:N:10:LEU:HD21	2:O:22:GLY:HA3	2.02	0.41
2:P:15:GLN:OE1	2:Q:22:GLY:HA3	2.20	0.41
1:D:24:LYS:HB3	1:D:24:LYS:HE3	1.67	0.41
1:D:55:LEU:CD2	1:E:23:TYR:HB3	2.49	0.41
1:E:32:LYS:HG3	1:E:158:GLU:OE2	2.20	0.41
1:F:172:ALA:HA	1:F:380:ILE:HB	2.02	0.41
1:F:262:VAL:HA	1:F:265:TYR:CE2	2.56	0.41
2:M:39:LYS:HB2	2:M:43:GLU:OE1	2.21	0.41
1:A:248:ARG:HA	1:A:259:PHE:HD2	1.85	0.41
1:B:213:CYS:O	1:B:214:PRO:C	2.58	0.41
1:C:227:ASP:HB3	1:H:230:THR:HG23	2.02	0.41
1:D:40:ALA:HB2	1:D:326:PHE:CE2	2.56	0.41
1:F:128:PHE:CD2	1:F:363:LEU:HD11	2.54	0.41
1:F:389:MET:CE	1:G:203:LYS:HE3	2.50	0.41
2:P:20:LYS:HE3	2:P:20:LYS:HB3	1.94	0.41
2:Q:4:SER:OG	2:Q:5:ASP:N	2.54	0.41
1:A:243:LEU:O	1:A:247:LEU:HG	2.20	0.41
1:A:347:PRO:HG3	1:A:362:GLY:N	2.36	0.41
1:C:83:ASN:OD1	1:C:83:ASN:N	2.50	0.41
1:C:376:ARG:HD3	1:C:379:TRP:CD2	2.55	0.41
1:D:239:ILE:HG13	1:D:240:GLY:O	2.21	0.41
1:E:331:PHE:CE1	1:E:332:GLN:HG2	2.56	0.41
1:F:243:LEU:O	1:F:247:LEU:HG	2.20	0.41
2:Q:15:GLN:HG3	2:R:19:VAL:HG11	2.03	0.41
1:C:259:PHE:CD2	1:C:279:ILE:HD11	2.55	0.41
1:G:33:GLU:HG3	1:G:273:LYS:HZ1	1.85	0.41
1:G:98:LEU:HD23	1:G:98:LEU:HA	1.93	0.41
1:H:58:TYR:CD1	1:H:115:ARG:HB3	2.55	0.41
1:I:84:LEU:HD11	1:I:99:PRO:HD3	2.03	0.41
2:J:10:LEU:HD13	2:J:10:LEU:HA	1.88	0.41
2:J:16:ALA:HB3	2:K:21:HIS:HB2	2.02	0.41
2:L:15:GLN:HB3	2:L:28:VAL:HG13	2.02	0.41
1:B:186:ASP:OD1	1:B:186:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HD13	1:D:208:LEU:HA	1.93	0.41
1:D:219:LEU:HD13	1:D:233:GLY:H	1.86	0.41
1:E:202:VAL:O	1:E:206:ILE:HG12	2.21	0.41
1:F:145:ASP:O	1:F:149:ILE:HG22	2.21	0.41
1:H:214:PRO:O	1:H:216:GLN:N	2.54	0.41
1:I:33:GLU:HB2	1:I:35:TYR:CE2	2.56	0.41
1:I:131:TRP:HZ3	1:I:364:THR:OG1	2.04	0.41
1:I:251:LYS:HD2	1:I:255:ASP:CA	2.47	0.41
1:B:219:LEU:HD13	1:B:232:GLN:HA	2.02	0.41
1:B:224:LEU:HA	1:B:224:LEU:HD23	1.83	0.41
1:G:159:ILE:HD13	1:G:159:ILE:HA	1.93	0.41
1:G:239:ILE:HD12	1:G:240:GLY:H	1.86	0.41
1:I:246:GLN:HE22	1:I:388:ALA:HB2	1.85	0.41
2:M:46:ASP:OD1	2:M:47:GLY:N	2.53	0.41
2:Q:42:SER:OG	2:Q:43:GLU:OE2	2.23	0.41
1:A:97:LYS:HB3	1:A:97:LYS:HE2	1.87	0.41
1:B:239:ILE:HD12	1:B:240:GLY:H	1.86	0.41
1:C:199:GLU:HA	1:C:202:VAL:HG22	2.03	0.41
1:D:164:LEU:HD11	1:D:326:PHE:HE2	1.85	0.41
1:E:90:ASP:OD2	1:E:93:THR:HG23	2.20	0.41
1:E:247:LEU:O	1:E:259:PHE:HB2	2.21	0.41
1:F:212:LEU:HD13	1:F:213:CYS:CB	2.51	0.41
1:H:35:TYR:CD2	1:H:287:VAL:HG22	2.56	0.41
2:J:15:GLN:HB3	2:J:28:VAL:HB	2.02	0.41
1:A:91:ILE:HG22	1:B:166:ILE:HG12	2.02	0.40
1:A:238:TYR:O	1:A:239:ILE:HD13	2.20	0.40
1:B:18:ARG:HH21	1:D:18:ARG:HE	1.69	0.40
1:C:291:LEU:HA	1:C:291:LEU:HD13	1.78	0.40
1:D:61:LEU:HD11	1:D:111:VAL:HG21	2.03	0.40
1:D:154:LYS:HA	1:D:157:ASN:ND2	2.36	0.40
1:G:307:TYR:H	1:G:387:ALA:C	2.23	0.40
1:H:42:VAL:HG21	1:H:335:GLY:O	2.21	0.40
1:I:34:MET:O	1:I:38:GLN:HG2	2.21	0.40
2:M:7:ASP:N	2:M:7:ASP:OD2	2.53	0.40
1:A:85:TYR:CD2	1:A:94:ILE:HG23	2.56	0.40
1:B:316:PHE:O	1:B:384:LYS:HA	2.22	0.40
1:C:36:PHE:HE2	1:C:238:TYR:HD2	1.69	0.40
1:C:94:ILE:HD12	1:C:94:ILE:H	1.86	0.40
1:D:66:ASN:OD1	1:D:114:THR:HG23	2.20	0.40
1:D:220:ILE:HG13	1:D:231:ILE:HD12	2.02	0.40
1:D:334:ASP:C	1:D:334:ASP:OD1	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ILE:HD12	1:E:159:ILE:HA	1.77	0.40
1:H:333:THR:HA	1:H:339:LYS:HZ3	1.85	0.40
2:Q:20:LYS:HA	2:Q:20:LYS:HD2	1.86	0.40
1:A:365:SER:O	1:A:366:ILE:HD13	2.21	0.40
1:E:206:ILE:HG12	1:E:206:ILE:H	1.69	0.40
1:F:154:LYS:O	1:F:158:GLU:HG3	2.22	0.40
1:G:205:GLY:O	1:G:209:ASN:N	2.54	0.40
1:H:251:LYS:HD2	1:H:251:LYS:HA	1.76	0.40
1:H:363:LEU:HD12	1:H:364:THR:H	1.86	0.40
1:I:196:VAL:HG23	1:I:385:THR:HB	2.03	0.40
2:J:31:LEU:HD23	2:J:31:LEU:HA	1.81	0.40
2:N:10:LEU:HD23	2:N:10:LEU:HA	1.92	0.40
1:A:275:GLU:OE2	1:A:283:ARG:NE	2.54	0.40
1:A:300:VAL:HG22	1:A:311:GLY:HA2	2.04	0.40
1:B:190:GLU:OE1	1:B:301:THR:OG1	2.38	0.40
1:D:108:VAL:HG12	1:D:109:ASN:CG	2.42	0.40
1:E:51:LYS:HB3	1:E:51:LYS:HE2	1.70	0.40
1:F:159:ILE:HD13	1:G:62:LEU:HD11	2.03	0.40
1:F:227:ASP:O	1:F:264:GLN:HG2	2.21	0.40
1:G:74:ALA:HA	1:G:108:VAL:HA	2.03	0.40
2:J:36:LEU:HD12	2:J:36:LEU:HA	1.77	0.40
1:B:214:PRO:O	1:B:215:MET:C	2.60	0.40
1:D:231:ILE:HD11	1:D:265:TYR:CG	2.56	0.40
1:E:85:TYR:CD2	1:E:94:ILE:HB	2.56	0.40
1:F:201:LEU:HA	1:F:201:LEU:HD23	1.87	0.40
1:F:267:ASP:HB2	1:G:221:ALA:HB1	2.03	0.40
1:F:287:VAL:HB	1:F:290:MET:CG	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/389 (95%)	344 (93%)	24 (6%)	2 (0%)	25	56
1	B	380/389 (98%)	335 (88%)	42 (11%)	3 (1%)	16	46
1	C	385/389 (99%)	341 (89%)	39 (10%)	5 (1%)	10	36
1	D	380/389 (98%)	343 (90%)	34 (9%)	3 (1%)	16	46
1	E	348/389 (90%)	325 (93%)	21 (6%)	2 (1%)	22	53
1	F	386/389 (99%)	351 (91%)	30 (8%)	5 (1%)	10	36
1	G	368/389 (95%)	339 (92%)	28 (8%)	1 (0%)	37	66
1	H	375/389 (96%)	327 (87%)	45 (12%)	3 (1%)	16	46
1	I	352/389 (90%)	313 (89%)	37 (10%)	2 (1%)	22	53
2	J	45/99 (46%)	41 (91%)	4 (9%)	0	100	100
2	K	44/99 (44%)	43 (98%)	1 (2%)	0	100	100
2	L	44/99 (44%)	42 (96%)	2 (4%)	0	100	100
2	M	42/99 (42%)	40 (95%)	2 (5%)	0	100	100
2	N	44/99 (44%)	42 (96%)	2 (4%)	0	100	100
2	O	42/99 (42%)	38 (90%)	4 (10%)	0	100	100
2	P	44/99 (44%)	40 (91%)	4 (9%)	0	100	100
2	Q	44/99 (44%)	43 (98%)	1 (2%)	0	100	100
2	R	44/99 (44%)	42 (96%)	2 (4%)	0	100	100
All	All	3737/4392 (85%)	3389 (91%)	322 (9%)	26 (1%)	21	50

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	VAL
1	C	212	LEU
1	D	212	LEU
1	D	213	CYS
1	D	214	PRO
1	E	213	CYS
1	F	213	CYS
1	H	216	GLN
1	I	267	ASP
1	B	215	MET
1	E	216	GLN
1	F	295	GLY
1	F	296	ALA
1	H	215	MET

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Mol	Chain	Res	Type
1	A	19	LEU
1	C	215	MET
1	F	294	ALA
1	I	271	LEU
1	B	214	PRO
1	C	214	PRO
1	G	211	ASN
1	C	8	THR
1	H	213	CYS
1	C	295	GLY
1	F	297	GLY
1	A	213	CYS

5.3.2 Protein sidechains (i)

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	280/316 (89%)	270 (96%)	10 (4%)	30 57
1	B	294/316 (93%)	284 (97%)	10 (3%)	32 59
1	C	293/316 (93%)	288 (98%)	5 (2%)	56 74
1	D	306/316 (97%)	292 (95%)	14 (5%)	23 52
1	E	277/316 (88%)	267 (96%)	10 (4%)	30 57
1	F	300/316 (95%)	292 (97%)	8 (3%)	40 65
1	G	282/316 (89%)	270 (96%)	12 (4%)	25 53
1	H	288/316 (91%)	283 (98%)	5 (2%)	56 74
1	I	264/316 (84%)	256 (97%)	8 (3%)	36 62
2	J	32/66 (48%)	31 (97%)	1 (3%)	35 61
2	K	32/66 (48%)	32 (100%)	0	100 100
2	L	30/66 (46%)	30 (100%)	0	100 100
2	M	29/66 (44%)	29 (100%)	0	100 100
2	N	32/66 (48%)	28 (88%)	4 (12%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	O	30/66 (46%)	28 (93%)	2 (7%)	13 39
2	P	31/66 (47%)	30 (97%)	1 (3%)	34 61
2	Q	32/66 (48%)	30 (94%)	2 (6%)	15 41
2	R	31/66 (47%)	29 (94%)	2 (6%)	14 40
All	All	2863/3438 (83%)	2769 (97%)	94 (3%)	35 60

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	19	LEU
1	A	56	TYR
1	A	110	ARG
1	A	215	MET
1	A	255	ASP
1	A	271	LEU
1	A	273	LYS
1	A	307	TYR
1	A	346	LYS
1	B	34	MET
1	B	64	ASP
1	B	69	ASP
1	B	89	LYS
1	B	128	PHE
1	B	162	ASP
1	B	252	ASP
1	B	265	TYR
1	B	270	ASN
1	B	331	PHE
1	C	18	ARG
1	C	44	ASN
1	C	115	ARG
1	C	214	PRO
1	C	354	TYR
1	D	7	ASN
1	D	45	MET
1	D	85	TYR
1	D	115	ARG
1	D	116	ILE
1	D	154	LYS
1	D	211	ASN

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Mol	Chain	Res	Type
1	D	223	SER
1	D	242	GLU
1	D	248	ARG
1	D	265	TYR
1	D	292	LYS
1	D	334	ASP
1	D	358	TYR
1	E	51	LYS
1	E	53	ILE
1	E	55	LEU
1	E	85	TYR
1	E	154	LYS
1	E	211	ASN
1	E	212	LEU
1	E	248	ARG
1	E	252	ASP
1	E	346	LYS
1	F	51	LYS
1	F	117	GLN
1	F	150	GLN
1	F	211	ASN
1	F	212	LEU
1	F	265	TYR
1	F	270	ASN
1	F	278	SER
1	G	34	MET
1	G	38	GLN
1	G	64	ASP
1	G	104	ASN
1	G	154	LYS
1	G	162	ASP
1	G	204	MET
1	G	211	ASN
1	G	212	LEU
1	G	215	MET
1	G	232	GLN
1	G	354	TYR
1	H	39	LEU
1	H	154	LYS
1	H	211	ASN
1	H	270	ASN
1	H	339	LYS

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Mol	Chain	Res	Type
1	I	64	ASP
1	I	85	TYR
1	I	88	SER
1	I	162	ASP
1	I	251	LYS
1	I	271	LEU
1	I	292	LYS
1	I	370	TYR
2	J	39	LYS
2	N	12	ASP
2	N	15	GLN
2	N	21	HIS
2	N	39	LYS
2	O	44	LEU
2	O	46	ASP
2	P	20	LYS
2	Q	4	SER
2	Q	5	ASP
2	R	7	ASP
2	R	40	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	B	117	GLN
1	C	117	GLN
1	E	66	ASN
1	E	117	GLN
1	E	165	GLN
1	H	232	GLN
1	I	66	ASN
1	I	68	ASN
2	J	15	GLN
2	J	21	HIS
2	P	15	GLN

5.3.3 RNA

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.

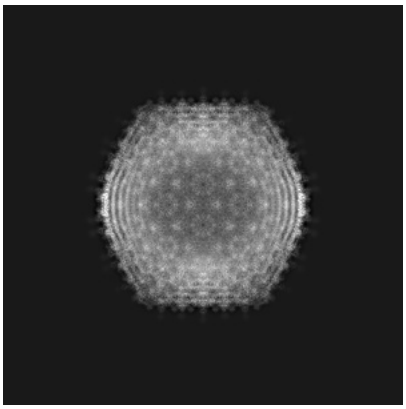
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46626. These allow visual inspection of the internal detail of the map and identification of artifacts.

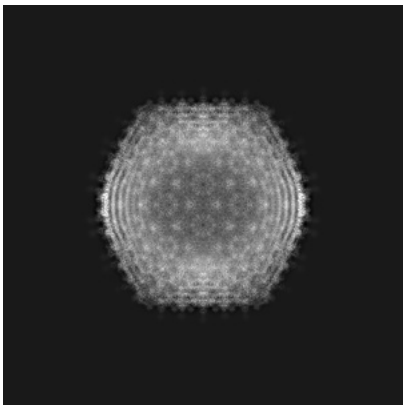
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

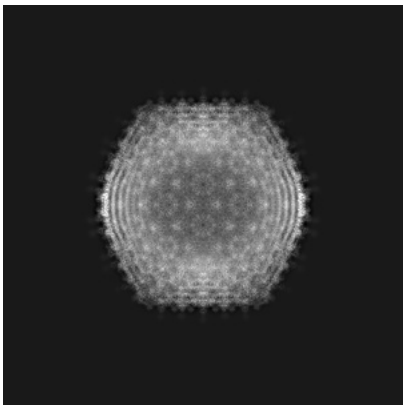
6.1.1 Primary map



X

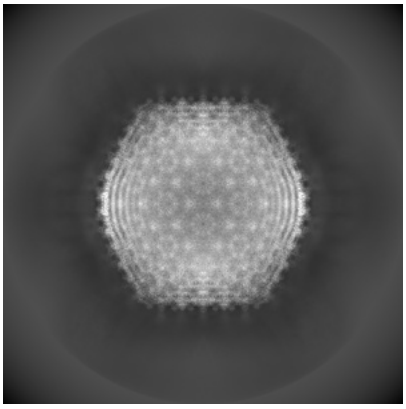


Y

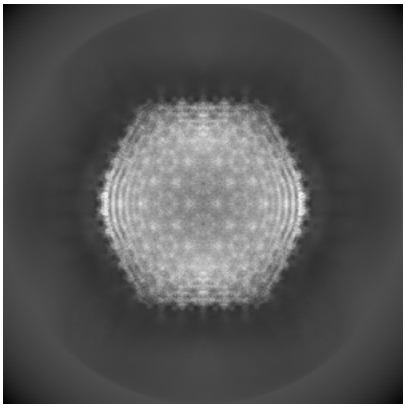


Z

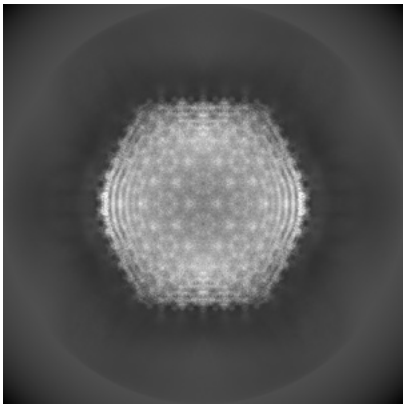
6.1.2 Raw map



X



Y

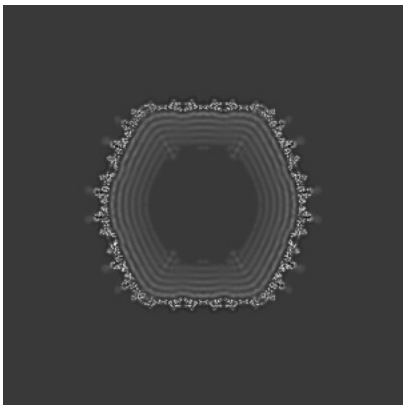


Z

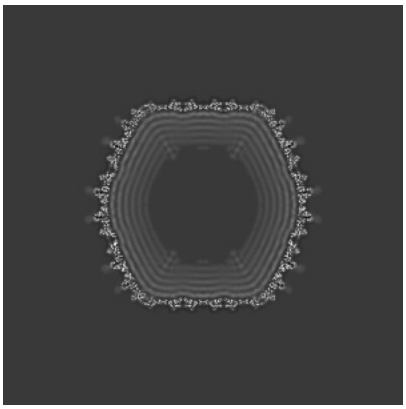
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

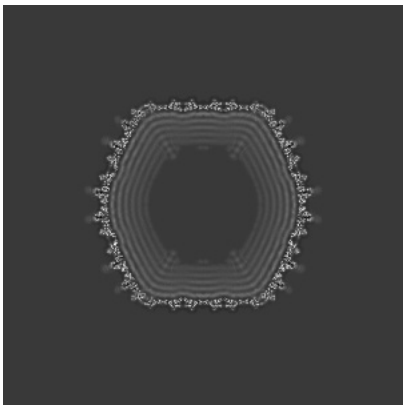
6.2.1 Primary map



X Index: 400

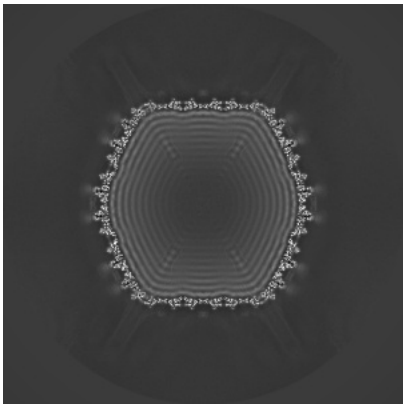


Y Index: 400

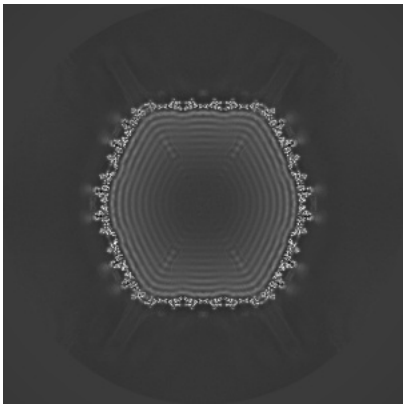


Z Index: 400

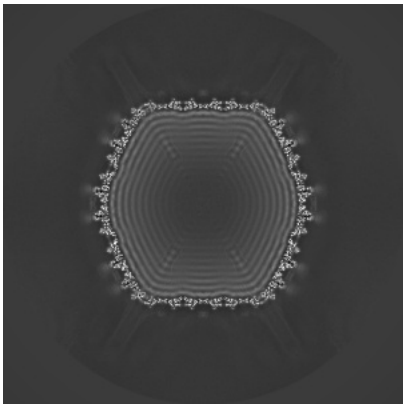
6.2.2 Raw map



X Index: 400



Y Index: 400

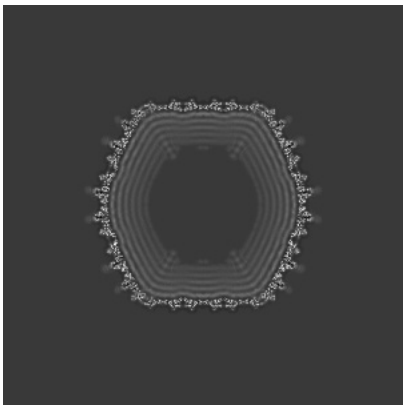


Z Index: 400

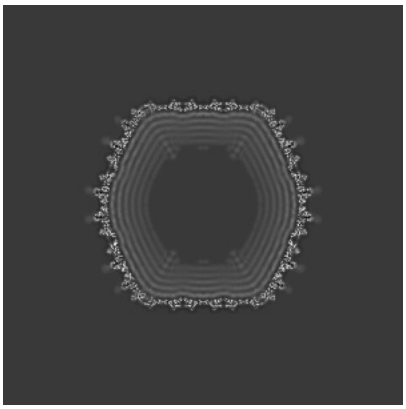
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

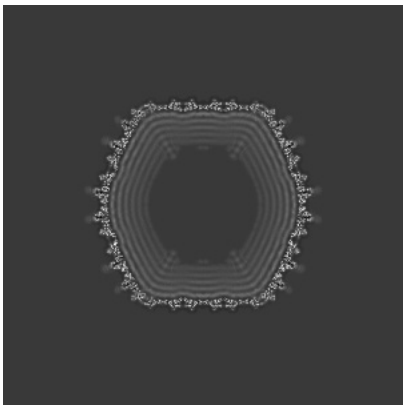
6.3.1 Primary map



X Index: 400

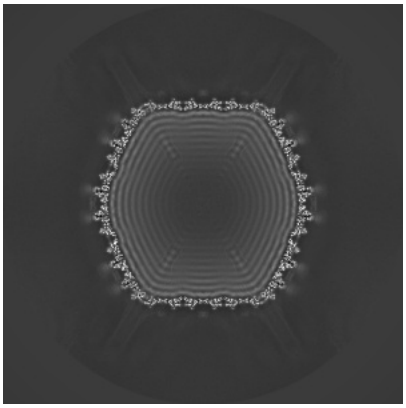


Y Index: 400

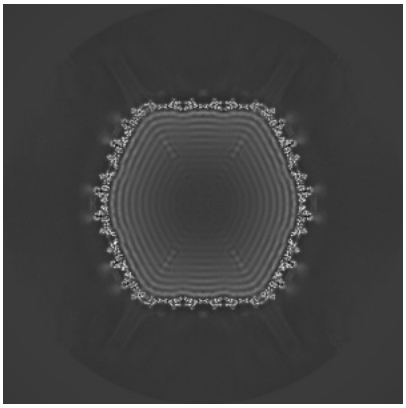


Z Index: 400

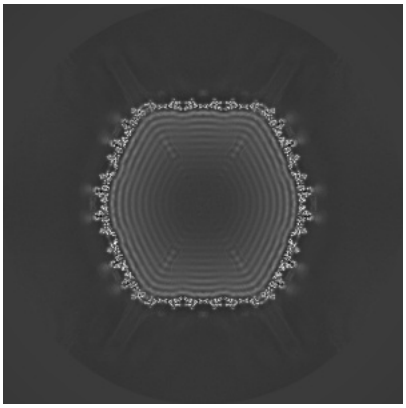
6.3.2 Raw map



X Index: 400



Y Index: 400

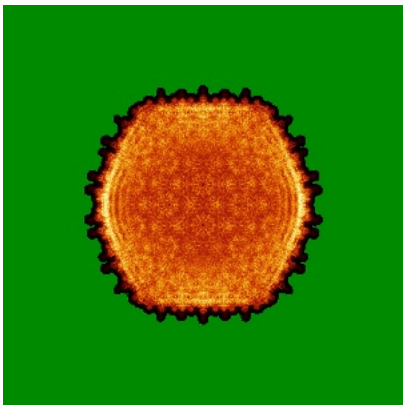


Z Index: 400

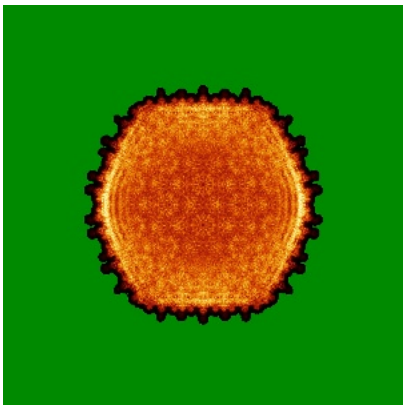
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

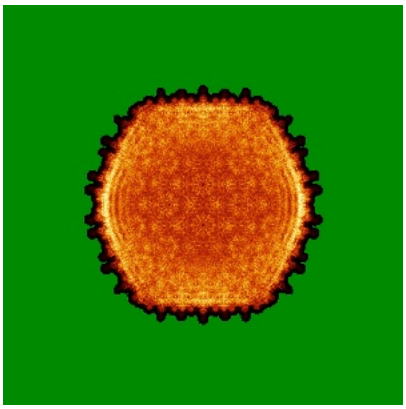
6.4.1 Primary map



X

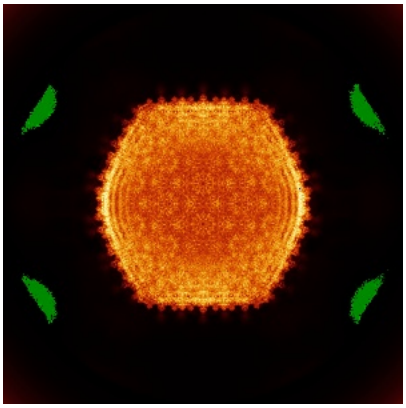


Y

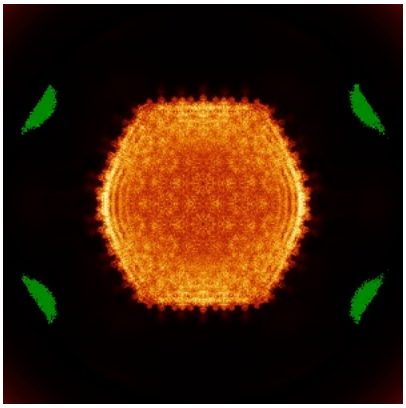


Z

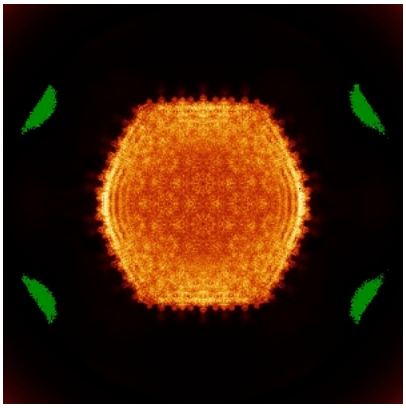
6.4.2 Raw map



X



Y

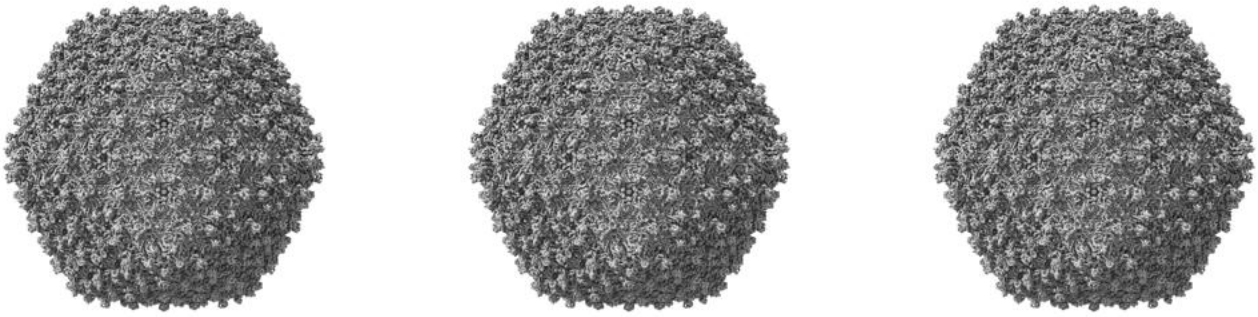


Z

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

6.5 Orthogonal surface views (i)

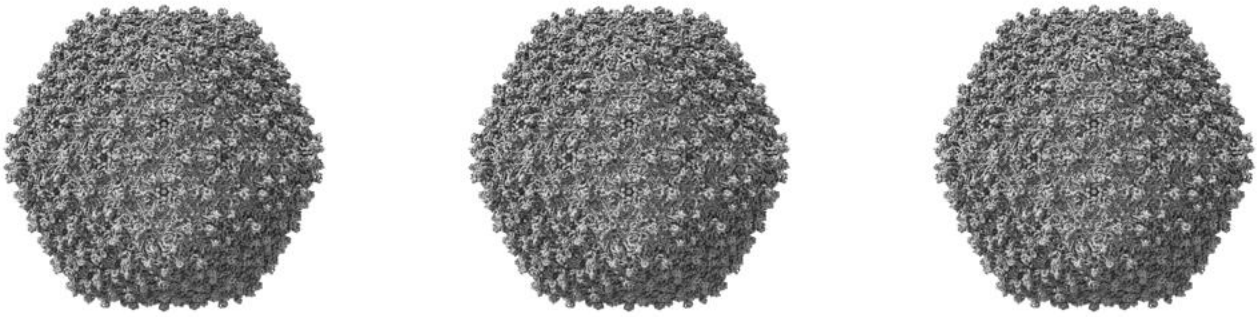
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

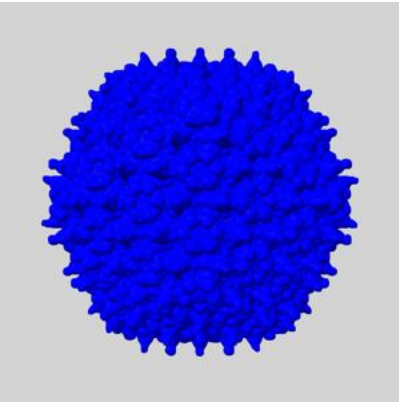
6.6 Mask visualisation (i)

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

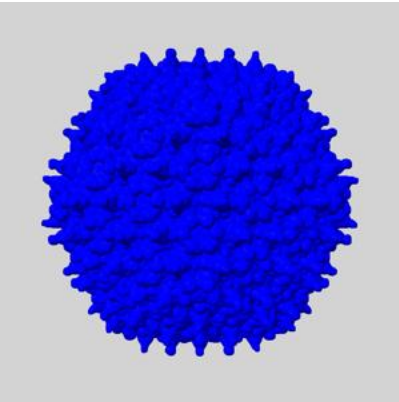
A mask typically either:

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

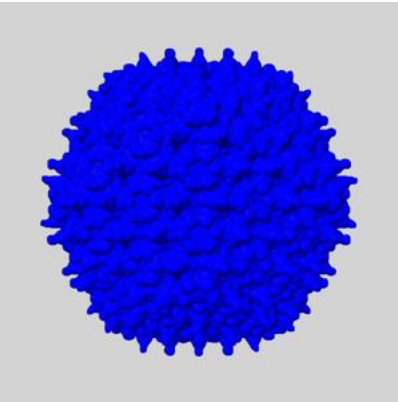
6.6.1 emd_46626_msk_1.map (i)



X



Y

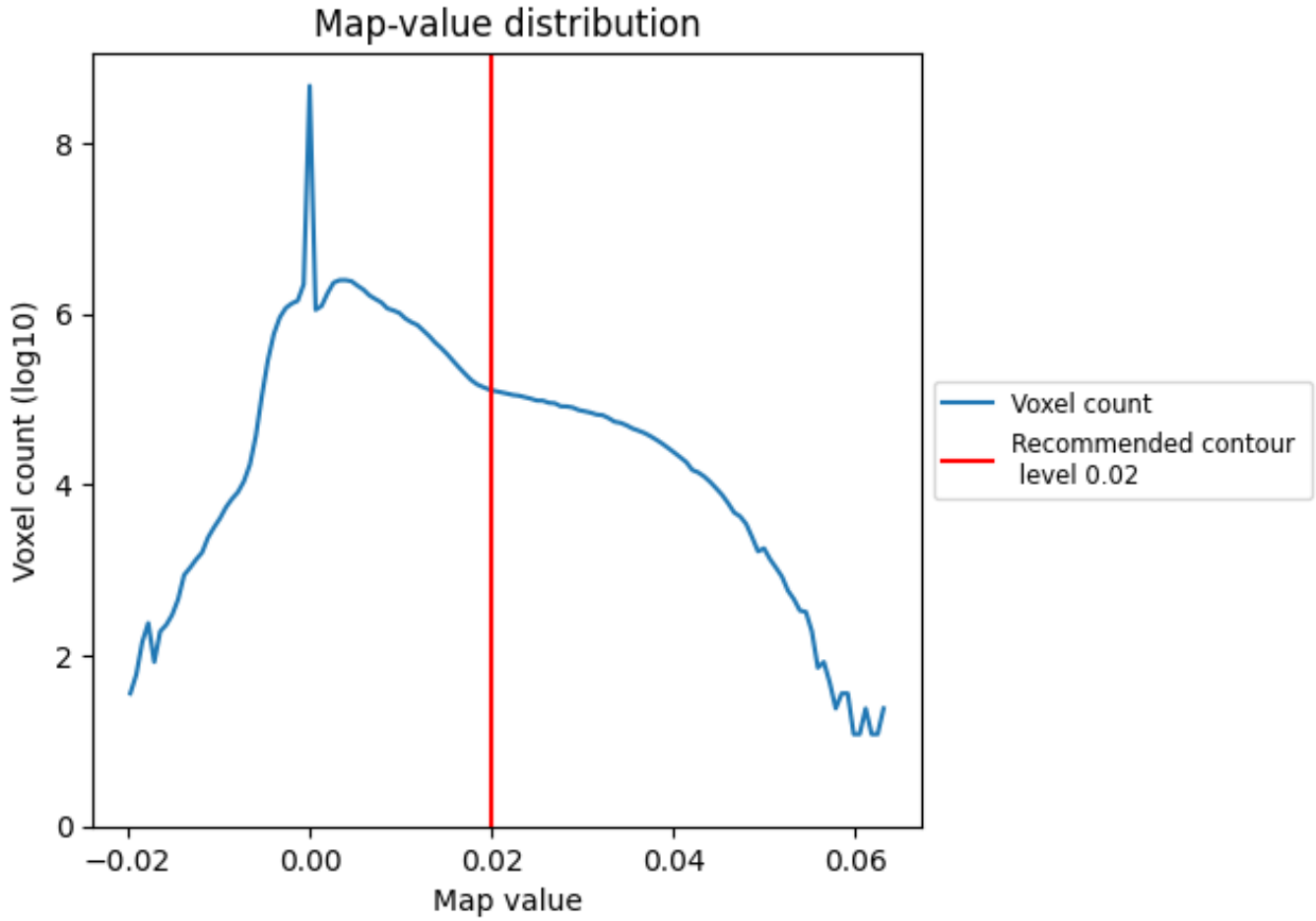


Z

7 Map analysis

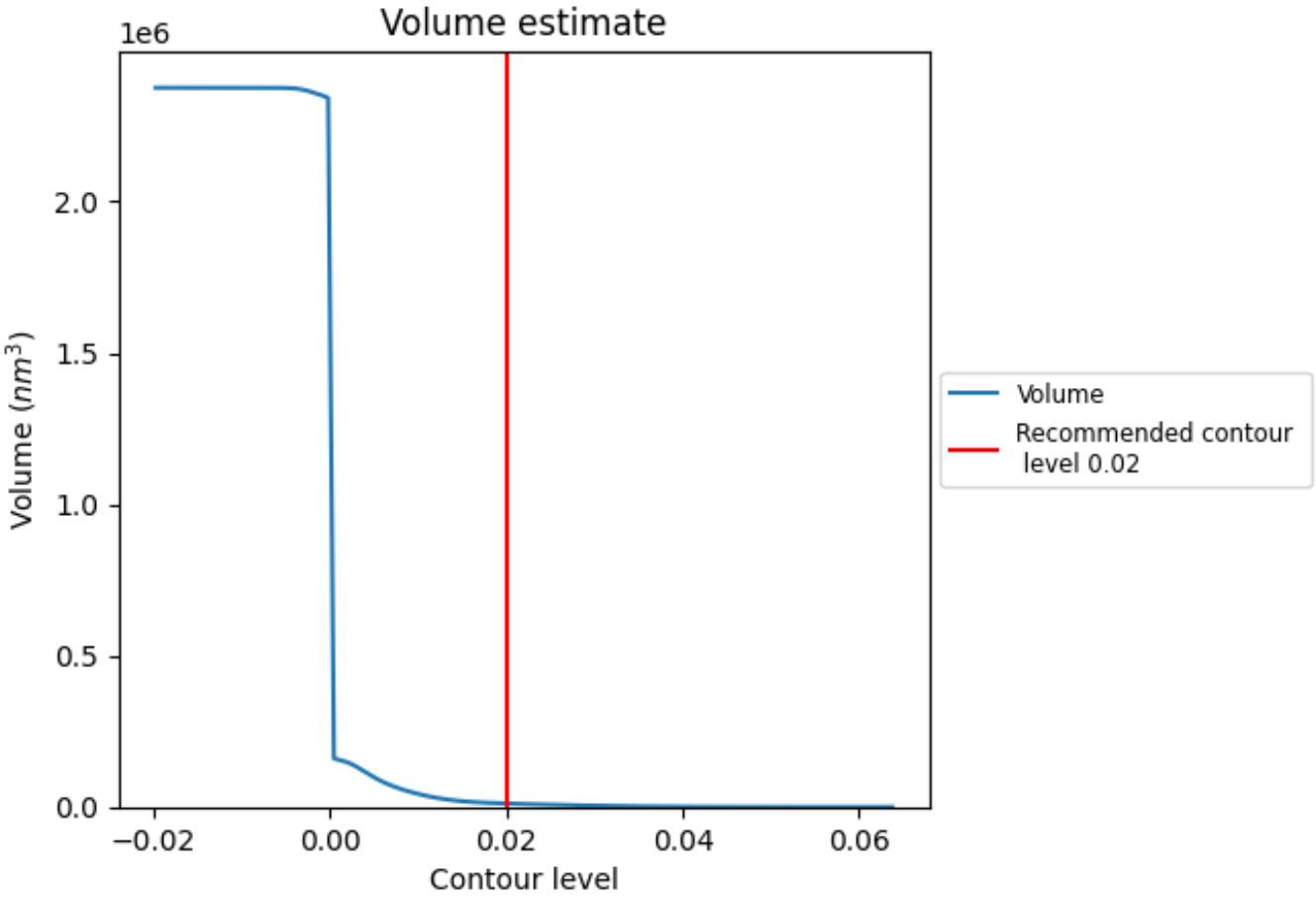
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

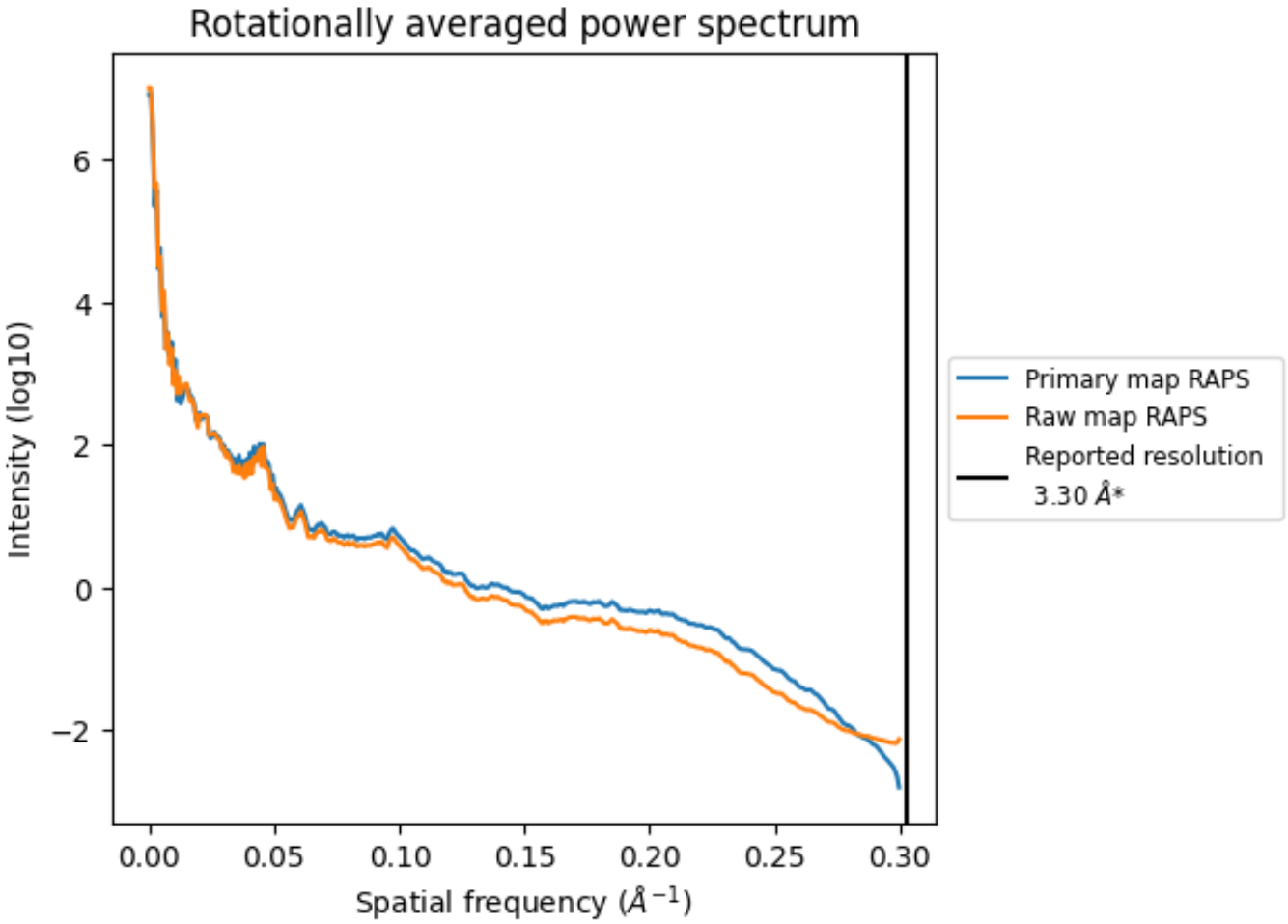
7.2 Volume estimate (i)



The volume at the recommended contour level is 11463 nm^3; this corresponds to an approximate mass of 10355 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 (i)

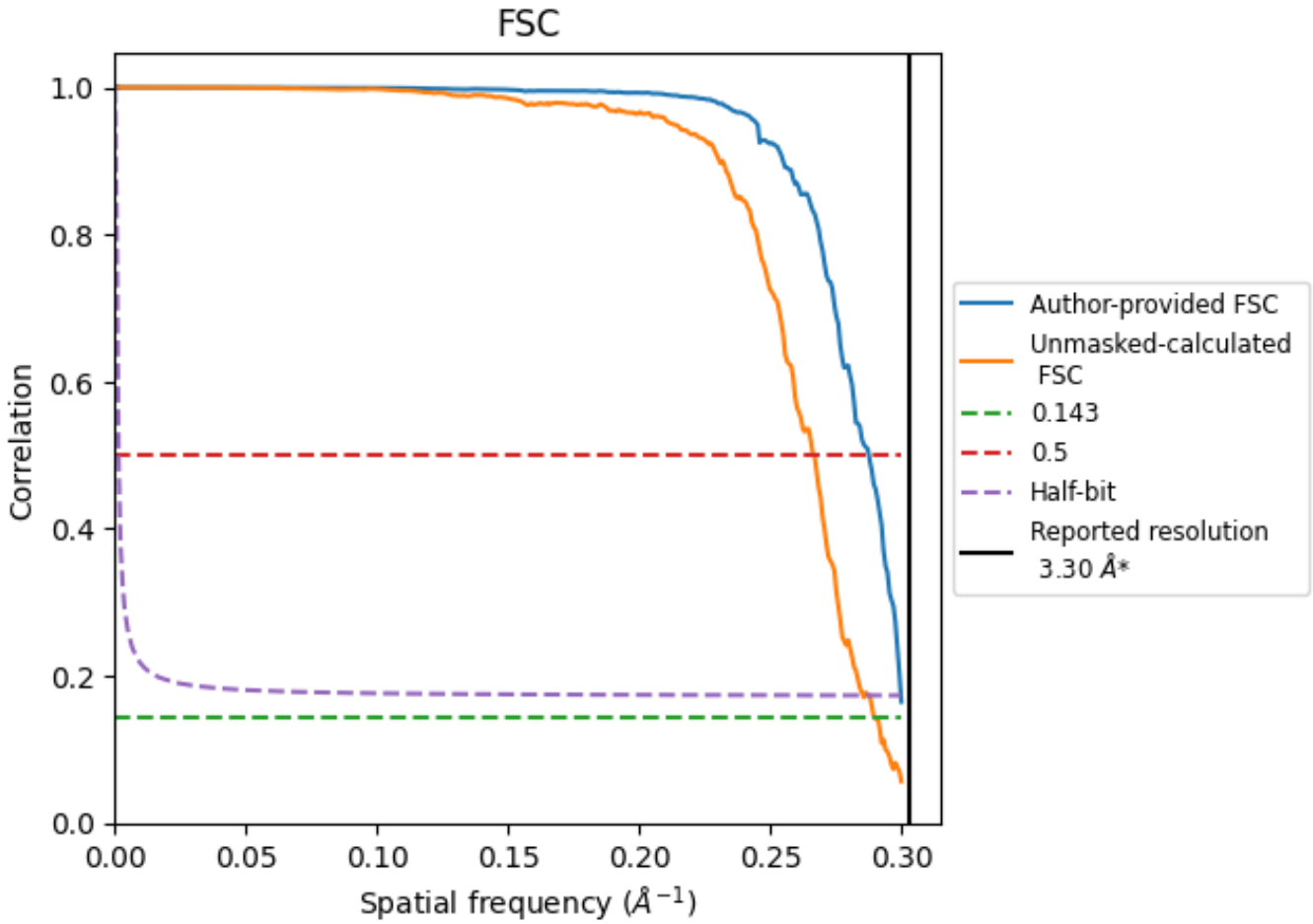


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	3.48	3.34
Unmasked-calculated*	3.45	3.75	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

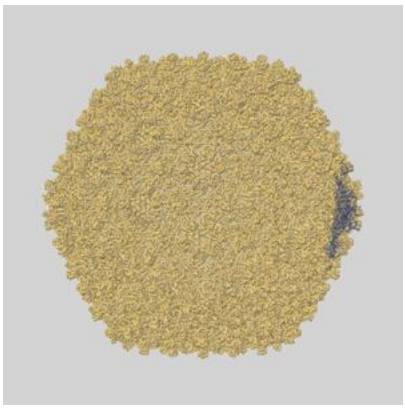
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46626 and PDB model 9D82. Per-residue inclusion information can be found in section 3 on page 6.

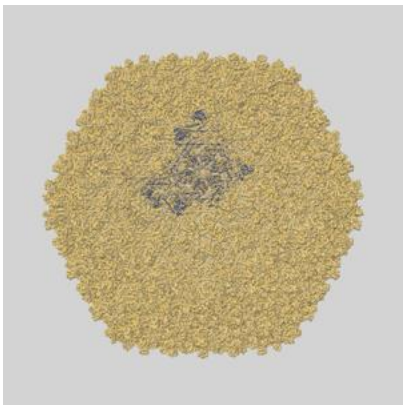
9.1 Map-model overlays

9.1.1 Map-model overlay

X

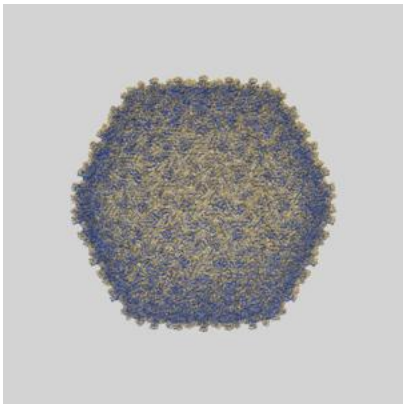


Y

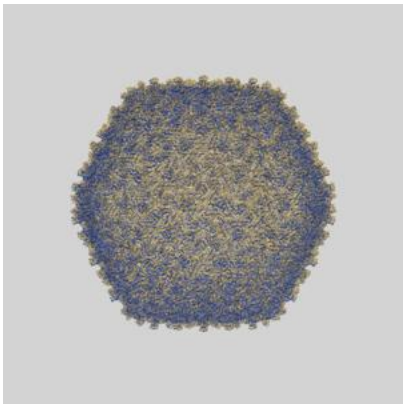


Z

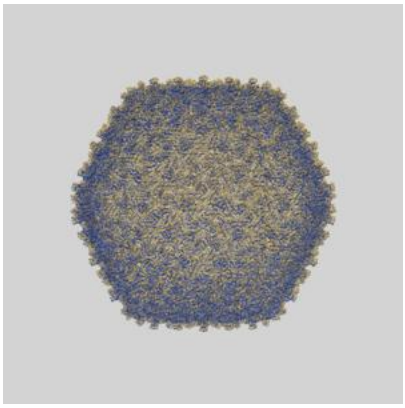
9.1.2 Map-model assembly overlay



X



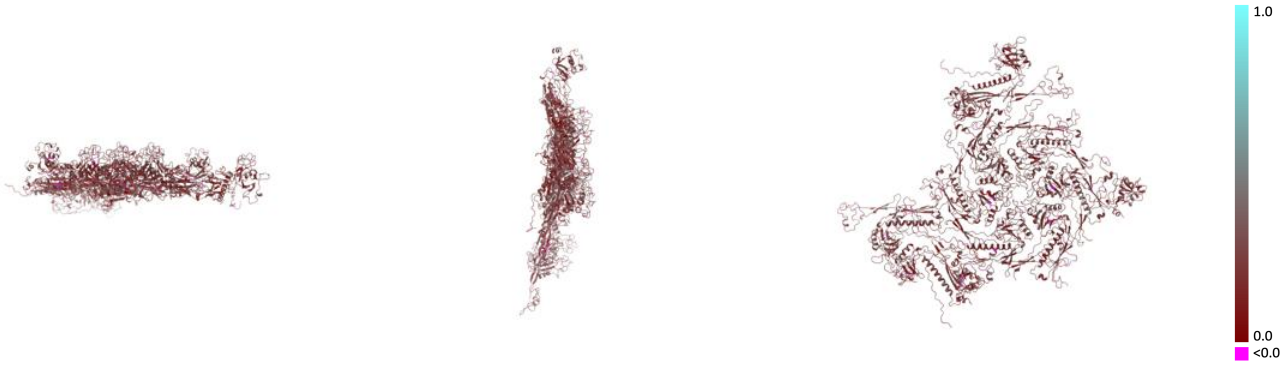
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

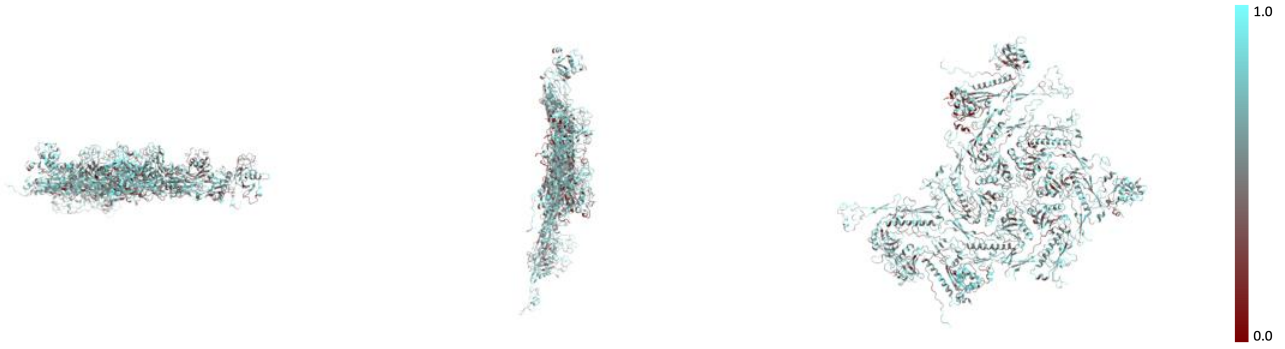
9.2 Q-score mapped to coordinate model



X Y Z

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

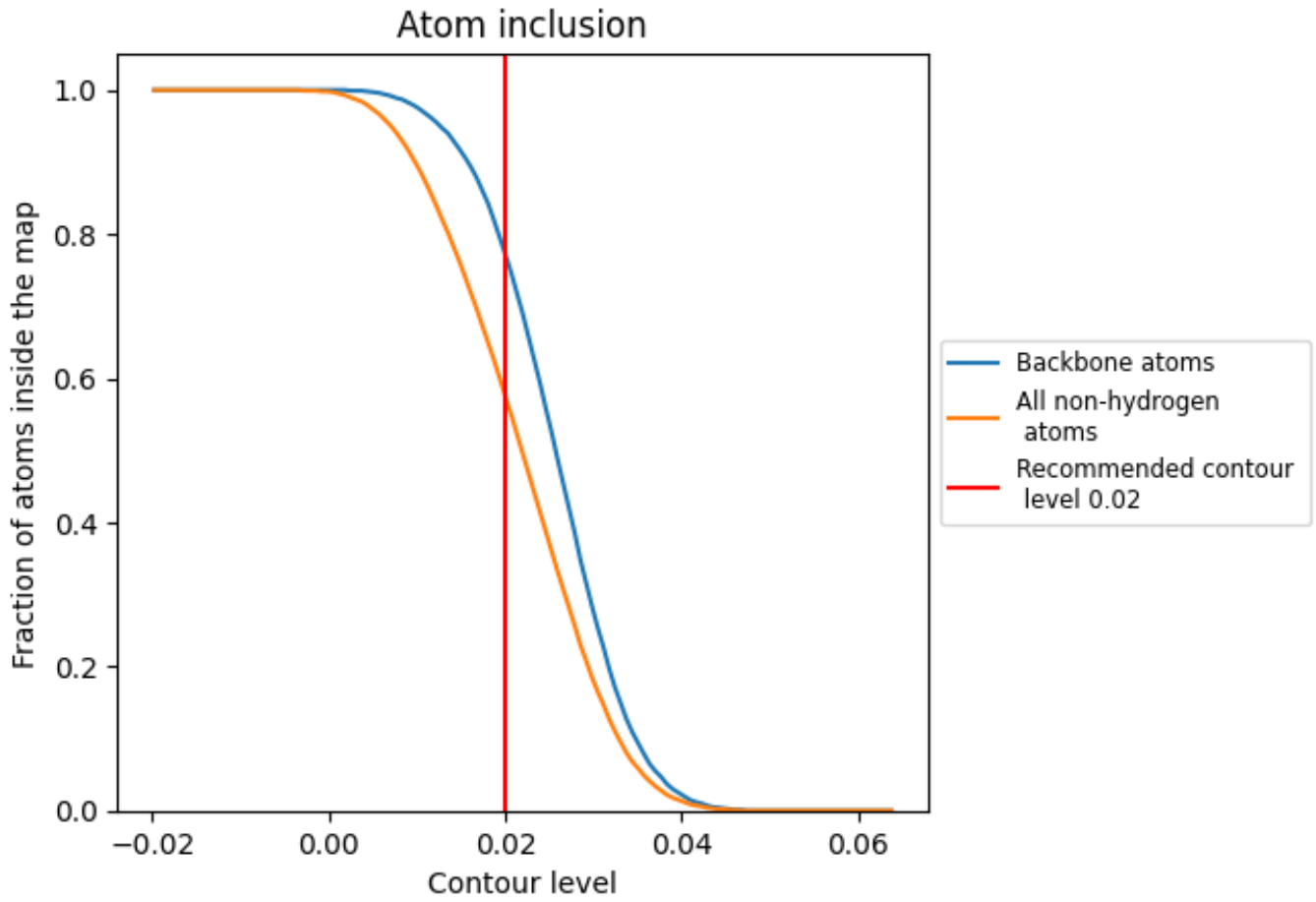
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5760	0.2480
A	0.5850	0.2340
B	0.5840	0.2480
C	0.5900	0.2470
D	0.5950	0.2510
E	0.5910	0.2520
F	0.5700	0.2540
G	0.5720	0.2450
H	0.5970	0.2560
I	0.5630	0.2490
J	0.4010	0.2340
K	0.4100	0.2200
L	0.3570	0.2490
M	0.6000	0.2500
N	0.5740	0.2750
O	0.5200	0.2300
P	0.6030	0.2250
Q	0.5680	0.2370
R	0.5530	0.2350