



## Full wwPDB EM Validation Report ⓘ

Sep 14, 2026 – 06:35 PM JST

PDB ID : 9U43 / pdb\_00009u43  
EMDB ID : EMD-63832  
Title : Cryo-EM structure of D-peptide-GPCR-Gq complex  
Authors : Liu, S.H.; Zhang, Y.J.; Hua, T.; Liu, Z.J.  
Deposited on : 2025-03-19  
Resolution : 3.02 Å(reported)

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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.dev133  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

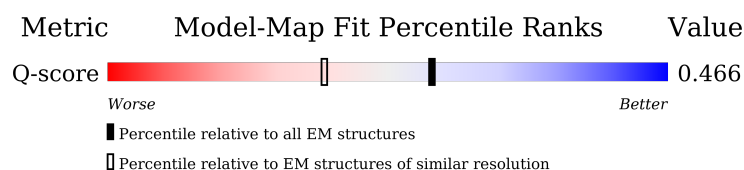
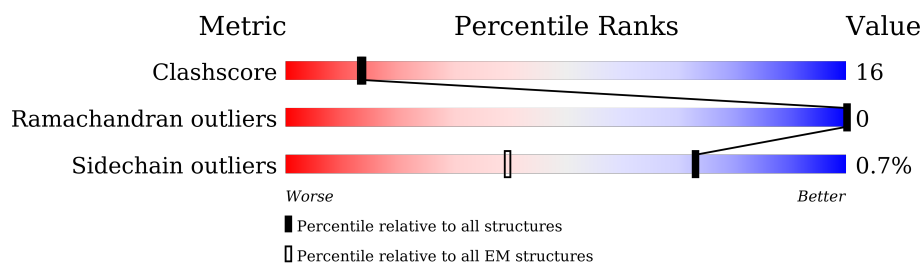
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.02 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13913 ( 2.52 - 3.52 )                                    |

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     | 855    |                  |
| 2   | P     | 10     |                  |
| 3   | A     | 246    |                  |
| 4   | B     | 377    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 5   | G     | 71     |  |
| 6   | N     | 157    |  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8211 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 exo-alpha-sialidase, Vasopressin V1a receptor.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | R     | 290      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2326  | 1529 | 394 | 380 | 23 |         |       |

There are 47 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| R     | -458    | MET      | -      | initiating methionine | UNP Q59310 |
| R     | -457    | LYS      | -      | expression tag        | UNP Q59310 |
| R     | -456    | THR      | -      | expression tag        | UNP Q59310 |
| R     | -455    | ILE      | -      | expression tag        | UNP Q59310 |
| R     | -454    | ILE      | -      | expression tag        | UNP Q59310 |
| R     | -453    | ALA      | -      | expression tag        | UNP Q59310 |
| R     | -452    | LEU      | -      | expression tag        | UNP Q59310 |
| R     | -451    | SER      | -      | expression tag        | UNP Q59310 |
| R     | -450    | TYR      | -      | expression tag        | UNP Q59310 |
| R     | -449    | ILE      | -      | expression tag        | UNP Q59310 |
| R     | -448    | PHE      | -      | expression tag        | UNP Q59310 |
| R     | -447    | CYS      | -      | expression tag        | UNP Q59310 |
| R     | -446    | LEU      | -      | expression tag        | UNP Q59310 |
| R     | -445    | VAL      | -      | expression tag        | UNP Q59310 |
| R     | -444    | PHE      | -      | expression tag        | UNP Q59310 |
| R     | -443    | ALA      | -      | expression tag        | UNP Q59310 |
| R     | -442    | ASP      | -      | expression tag        | UNP Q59310 |
| R     | -441    | TYR      | -      | expression tag        | UNP Q59310 |
| R     | -440    | LYS      | -      | expression tag        | UNP Q59310 |
| R     | -439    | ASP      | -      | expression tag        | UNP Q59310 |
| R     | -438    | ASP      | -      | expression tag        | UNP Q59310 |
| R     | -437    | ASP      | -      | expression tag        | UNP Q59310 |
| R     | -436    | ASP      | -      | expression tag        | UNP Q59310 |
| R     | -435    | ALA      | -      | expression tag        | UNP Q59310 |
| R     | -434    | GLY      | -      | expression tag        | UNP Q59310 |
| R     | -433    | ARG      | -      | expression tag        | UNP Q59310 |
| R     | -432    | ALA      | -      | expression tag        | UNP Q59310 |
| R     | -281    | SER      | GLY    | conflict              | UNP Q59310 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| R     | 112     | LYS      | ASP    | engineered mutation | UNP P37288 |
| R     | 379     | LEU      | -      | expression tag      | UNP P37288 |
| R     | 380     | GLU      | -      | expression tag      | UNP P37288 |
| R     | 381     | VAL      | -      | expression tag      | UNP P37288 |
| R     | 382     | LEU      | -      | expression tag      | UNP P37288 |
| R     | 383     | PHE      | -      | expression tag      | UNP P37288 |
| R     | 384     | GLN      | -      | expression tag      | UNP P37288 |
| R     | 385     | GLY      | -      | expression tag      | UNP P37288 |
| R     | 386     | PRO      | -      | expression tag      | UNP P37288 |
| R     | 387     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 388     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 389     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 390     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 391     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 392     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 393     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 394     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 395     | HIS      | -      | expression tag      | UNP P37288 |
| R     | 396     | HIS      | -      | expression tag      | UNP P37288 |

- Molecule 2 is a protein called Arg-vasopressin.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 2   | P     | 10       | Total | C  | N  | O  | S | 0       | 1     |
|     |       |          | 75    | 46 | 15 | 12 | 2 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| P     | 8       | DAR      | ARG    | engineered mutation | UNP P01185 |
| P     | 10      | NH2      | -      | amidation           | UNP P01185 |

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(q) subunit alpha-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | A     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1813  | 1144 | 322 | 340 | 7 |         |       |

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | B     | 338      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2600  | 1604 | 467 | 508 | 21 |         |       |

There are 38 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | -5      | MET      | -      | initiating methionine | UNP P62873 |
| B     | -4      | HIS      | -      | expression tag        | UNP P62873 |
| B     | -3      | HIS      | -      | expression tag        | UNP P62873 |
| B     | -2      | HIS      | -      | expression tag        | UNP P62873 |
| B     | -1      | HIS      | -      | expression tag        | UNP P62873 |
| B     | 0       | HIS      | -      | expression tag        | UNP P62873 |
| B     | 1       | HIS      | -      | expression tag        | UNP P62873 |
| B     | 2       | GLY      | -      | expression tag        | UNP P62873 |
| B     | 3       | SER      | -      | expression tag        | UNP P62873 |
| B     | 4       | LEU      | -      | expression tag        | UNP P62873 |
| B     | 5       | LEU      | -      | expression tag        | UNP P62873 |
| B     | 6       | GLN      | -      | expression tag        | UNP P62873 |
| B     | 346     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 347     | SER      | -      | expression tag        | UNP P62873 |
| B     | 348     | SER      | -      | expression tag        | UNP P62873 |
| B     | 349     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 350     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 351     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 352     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 353     | SER      | -      | expression tag        | UNP P62873 |
| B     | 354     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 355     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 356     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 357     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 358     | SER      | -      | expression tag        | UNP P62873 |
| B     | 359     | SER      | -      | expression tag        | UNP P62873 |
| B     | 360     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 361     | VAL      | -      | expression tag        | UNP P62873 |
| B     | 362     | SER      | -      | expression tag        | UNP P62873 |
| B     | 363     | GLY      | -      | expression tag        | UNP P62873 |
| B     | 364     | TRP      | -      | expression tag        | UNP P62873 |
| B     | 365     | ARG      | -      | expression tag        | UNP P62873 |
| B     | 366     | LEU      | -      | expression tag        | UNP P62873 |
| B     | 367     | PHE      | -      | expression tag        | UNP P62873 |
| B     | 368     | LYS      | -      | expression tag        | UNP P62873 |
| B     | 369     | LYS      | -      | expression tag        | UNP P62873 |
| B     | 370     | ILE      | -      | expression tag        | UNP P62873 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 371     | SER      | -      | expression tag | UNP P62873 |

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | G     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 436   | 273 | 77 | 83 | 3 |         |       |

- Molecule 6 is a protein called Nanobody 35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | N     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 961   | 599 | 168 | 188 | 6 |         |       |



ASP  
THR  
LEU  
GLU  
VAL  
LEU  
PHE  
GLN  
GLY  
PRO  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 2: Arg-vasopressin

Chain P: 

G1  
Y2  
N5  
C6  
P7  
R8  
G9  
9H210

• Molecule 3: Guanine nucleotide-binding protein G(q) subunit alpha-1

Chain A: 

MET  
GLY  
SER  
THR  
VAL  
SER  
ALA  
E8  
D9  
K10  
A11  
K17  
L23  
G27  
E28  
K29  
R32  
L38  
G45  
K46  
S47  
T48  
I49  
V50  
LYS  
GLN  
MET  
ARG  
ILE  
LEU  
HIS  
GLY  
SER  
GLY  
GLY  
SER  
GLY  
THR  
GLY  
I182  
D190  
V199  
Q202  
R207  
K208  
W209  
I210

T220  
S225  
Y228  
W230  
E233  
A234  
L235  
F238  
W242  
N243  
N244  
L247  
V252  
F255  
L262  
K265  
S271  
K272  
I273  
E274  
D275  
Y276  
F277  
E287  
D288  
T290  
P291  
E295  
T300  
K303  
Y304  
K308  
I313  
S314  
S317  
G318  
D319  
G320

R338  
F341  
N342  
D343  
C344  
K345  
D346  
I347  
I348  
N351  
K352  
L353  
R354  
E355  
N356  
N357  
L358  
V359

• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 

MET  
HIS  
HIS  
HIS  
HIS  
HIS  
GLY  
SER  
LEU  
LEU  
GLN  
SER  
E8  
L9  
D10  
Q11  
L12  
R13  
Q14  
E15  
A16  
E17  
Q18  
L19  
Q22  
R27  
A31  
D32  
S36  
T39  
W47  
I48  
Q49  
T52  
R53  
R54  
T55  
L56  
L60  
T63  
N66  
V76  
S77  
A78  
G82  
K83  
L84

T92  
I98  
P99  
L100  
V105  
M106  
T107  
C108  
A109  
V117  
A119  
L122  
D123  
N124  
I128  
Y129  
N130  
L131  
K132  
T133  
R134  
E135  
G136  
N137  
V140  
S141  
R142  
H147  
Y150  
C153  
L157  
D158  
D159  
V163  
T164  
G165  
S166  
G167  
D168  
T169  
I170  
C171  
A172  
L173  
W174  
D175  
I176

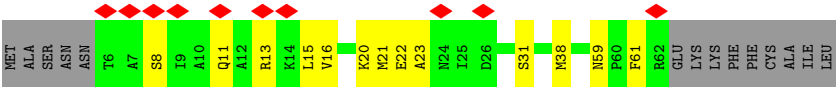
F185  
G190  
D191  
V192  
L195  
S196  
S206  
G207  
A208  
C209  
D210  
K214  
L215  
W216  
D217  
V218  
V219  
E220  
G221  
R224  
Q225  
H230  
E231  
I237  
C238  
F239  
F240  
F241  
N242  
T246  
G249  
S250  
D251  
A253  
T254  
C255  
R256  
L257  
F258  
D259  
Q264  
S265  
L266  
G267  
T268  
I274  
T275  
C276

T279  
S280  
V281  
S282  
F283  
S284  
R288  
L289  
L290  
L291  
D295  
D303  
A304  
L305  
K306  
R319  
V320  
S321  
C322  
L323  
K330  
A331  
V332  
A333  
T334  
G335  
S336  
W337  
I343  
K344  
N345  
GLY  
SER  
SER  
GLY  
GLY  
GLY  
GLY  
SER  
GLY  
GLY  
GLY  
SER  
SER  
GLY  
VAL  
SER  
GLY  
TRP  
ARG  
LEU  
PHE  
LYS

LYS  
ILE  
SER

• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G: 



• Molecule 6: Nanobody 35



## 4 Experimental information

| Property                             | Value                              | Source    |
|--------------------------------------|------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                    | Depositor |
| Imposed symmetry                     | POINT, Not provided                |           |
| Number of particles used             | 310743                             | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                  | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY                | Depositor |
| Microscope                           | FEI TALOS ARCTICA                  | Depositor |
| Voltage (kV)                         | 300                                | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                 | Depositor |
| Minimum defocus (nm)                 | 800                                | Depositor |
| Maximum defocus (nm)                 | 1800                               | Depositor |
| Magnification                        | Not provided                       |           |
| Image detector                       | GATAN K3 (6k x 4k)                 | Depositor |
| Maximum map value                    | 2.256                              | Depositor |
| Minimum map value                    | -0.002                             | Depositor |
| Average map value                    | 0.001                              | Depositor |
| Map value standard deviation         | 0.022                              | Depositor |
| Recommended contour level            | 0.1                                | Depositor |
| Map size ( $\text{\AA}$ )            | 266.24, 266.24, 266.24             | wwPDB     |
| Map dimensions                       | 320, 320, 320                      | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                   | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.83199996, 0.83199996, 0.83199996 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAR, NH2

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     | 0.16         | 0/2395      | 0.32        | 0/3267      |
| 2   | P     | 0.17         | 0/64        | 0.28        | 0/84        |
| 3   | A     | 0.17         | 0/1846      | 0.30        | 0/2486      |
| 4   | B     | 0.17         | 0/2647      | 0.34        | 0/3589      |
| 5   | G     | 0.12         | 0/442       | 0.26        | 0/597       |
| 6   | N     | 0.16         | 0/981       | 0.30        | 0/1329      |
| All | All   | 0.16         | 0/8375      | 0.32        | 0/11352     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | R     | 2326  | 0        | 2359     | 84      | 0            |
| 2   | P     | 75    | 0        | 64       | 5       | 0            |
| 3   | A     | 1813  | 0        | 1791     | 63      | 0            |
| 4   | B     | 2600  | 0        | 2505     | 99      | 0            |
| 5   | G     | 436   | 0        | 448      | 12      | 0            |
| 6   | N     | 961   | 0        | 928      | 34      | 0            |
| All | All   | 8211  | 0        | 8095     | 259     | 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 16.

All (259) 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:160:LEU:HD11 | 3:A:348:ILE:HD13 | 1.49                     | 0.92              |
| 1:R:285:ALA:HB2  | 3:A:359:VAL:HA   | 1.56                     | 0.86              |
| 1:R:288:ARG:NH2  | 3:A:357:ASN:ND2  | 2.28                     | 0.81              |
| 3:A:355:GLU:OE1  | 3:A:355:GLU:C    | 2.23                     | 0.80              |
| 4:B:39:THR:HB    | 4:B:305:LEU:HD13 | 1.65                     | 0.77              |
| 4:B:36:SER:HB3   | 4:B:267:MET:HE2  | 1.67                     | 0.76              |
| 1:R:160:LEU:HD11 | 3:A:348:ILE:CD1  | 2.16                     | 0.75              |
| 3:A:357:ASN:ND2  | 3:A:357:ASN:O    | 2.20                     | 0.74              |
| 3:A:347:ILE:HG22 | 3:A:351:MET:HE3  | 1.70                     | 0.74              |
| 4:B:158:ASP:OD1  | 4:B:159:ASP:N    | 2.19                     | 0.73              |
| 6:N:61:THR:CG2   | 6:N:64:VAL:HG22  | 2.19                     | 0.73              |
| 4:B:128:ILE:HD13 | 4:B:176:ILE:HD12 | 1.72                     | 0.71              |
| 4:B:52:THR:HG23  | 4:B:52:THR:O     | 1.90                     | 0.71              |
| 6:N:12:VAL:HG11  | 6:N:18:LEU:HD11  | 1.72                     | 0.71              |
| 4:B:16:ALA:HB2   | 5:G:16:VAL:HG22  | 1.72                     | 0.70              |
| 3:A:207:ARG:HH11 | 6:N:100:PRO:HB3  | 1.56                     | 0.70              |
| 1:R:192:ILE:HG22 | 1:R:193:GLU:N    | 2.06                     | 0.70              |
| 1:R:93:LEU:HD22  | 1:R:145:MET:HE1  | 1.73                     | 0.69              |
| 4:B:27:ARG:O     | 4:B:264:GLN:NE2  | 2.26                     | 0.69              |
| 1:R:162:GLN:CG   | 3:A:28:GLU:OE2   | 2.42                     | 0.68              |
| 3:A:230:ARG:NH1  | 3:A:233:GLU:OE2  | 2.26                     | 0.68              |
| 4:B:276:CYS:HB2  | 4:B:295:ASP:HB3  | 1.73                     | 0.68              |
| 6:N:2:VAL:HG23   | 6:N:27:PHE:HD2   | 1.58                     | 0.68              |
| 4:B:295:ASP:OD1  | 4:B:295:ASP:O    | 2.12                     | 0.68              |
| 6:N:61:THR:HG23  | 6:N:64:VAL:HG22  | 1.76                     | 0.67              |
| 3:A:355:GLU:C    | 3:A:355:GLU:CD   | 2.62                     | 0.67              |
| 4:B:142:ARG:HB3  | 4:B:142:ARG:NH1  | 2.10                     | 0.67              |
| 4:B:259:ASP:HB2  | 4:B:266:LEU:HD22 | 1.76                     | 0.66              |
| 4:B:230:HIS:NE2  | 4:B:248:THR:OG1  | 2.24                     | 0.66              |
| 1:R:185:GLN:HA   | 1:R:188:VAL:HG12 | 1.78                     | 0.65              |
| 1:R:288:ARG:NH2  | 3:A:357:ASN:HD22 | 1.95                     | 0.64              |
| 1:R:162:GLN:HG3  | 3:A:28:GLU:OE2   | 1.96                     | 0.64              |
| 3:A:190:ASP:OD2  | 3:A:338:ARG:NH1  | 2.28                     | 0.63              |
| 3:A:342:ASN:O    | 3:A:345:LYS:HB3  | 1.99                     | 0.63              |
| 1:R:214:ARG:HH12 | 1:R:316:TRP:HA   | 1.63                     | 0.63              |
| 6:N:34:MET:HE2   | 6:N:98:ARG:HA    | 1.80                     | 0.63              |
| 1:R:111:TRP:CH2  | 1:R:203:CYS:HB3  | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:54:GLU:OE1   | 1:R:112:LYS:HD2  | 2.00                     | 0.62              |
| 3:A:355:GLU:CD   | 3:A:355:GLU:O    | 2.43                     | 0.62              |
| 4:B:291:LEU:HD22 | 4:B:332:VAL:HG21 | 1.81                     | 0.62              |
| 1:R:166:ARG:O    | 1:R:170:MET:HG2  | 2.00                     | 0.61              |
| 6:N:38:ARG:NH1   | 6:N:90:ASP:OD1   | 2.32                     | 0.61              |
| 6:N:34:MET:HE1   | 6:N:98:ARG:HB2   | 1.82                     | 0.61              |
| 1:R:144:VAL:HG13 | 1:R:170:MET:HE2  | 1.82                     | 0.61              |
| 1:R:118:ARG:HD3  | 1:R:118:ARG:H    | 1.66                     | 0.61              |
| 4:B:253:ALA:HB1  | 4:B:274:ILE:HG22 | 1.82                     | 0.60              |
| 4:B:19:LEU:HD21  | 5:G:23:ALA:HB2   | 1.84                     | 0.60              |
| 4:B:254:THR:OG1  | 4:B:256:ARG:NH1  | 2.34                     | 0.60              |
| 6:N:32:TYR:O     | 6:N:72:ARG:NH2   | 2.29                     | 0.60              |
| 3:A:244:ASN:ND2  | 6:N:106:ASP:OD2  | 2.34                     | 0.60              |
| 1:R:349:MET:HE2  | 1:R:356:LEU:HD12 | 1.83                     | 0.60              |
| 1:R:100:VAL:HG12 | 1:R:134:GLY:C    | 2.28                     | 0.59              |
| 1:R:104:GLN:HA   | 1:R:131:GLN:HG2  | 1.85                     | 0.59              |
| 1:R:192:ILE:CG2  | 1:R:193:GLU:N    | 2.66                     | 0.58              |
| 4:B:56:LEU:HD23  | 4:B:92:THR:HG23  | 1.83                     | 0.58              |
| 6:N:63:SER:O     | 6:N:67:ARG:NH2   | 2.35                     | 0.58              |
| 6:N:94:TYR:O     | 6:N:121:GLY:HA2  | 2.02                     | 0.58              |
| 1:R:288:ARG:HH21 | 3:A:357:ASN:HD22 | 1.50                     | 0.58              |
| 1:R:46:ARG:HD3   | 1:R:115:TYR:CG   | 2.38                     | 0.58              |
| 3:A:210:ILE:HG12 | 3:A:247:LEU:HD11 | 1.86                     | 0.58              |
| 6:N:2:VAL:HG21   | 6:N:98:ARG:HH21  | 1.68                     | 0.58              |
| 6:N:37:VAL:HG12  | 6:N:47:TRP:HA    | 1.86                     | 0.58              |
| 1:R:208:ILE:HG13 | 1:R:210:PRO:HD2  | 1.86                     | 0.57              |
| 3:A:314:SER:O    | 3:A:317:SER:OG   | 2.22                     | 0.57              |
| 1:R:247:VAL:HG22 | 1:R:282:ILE:HG23 | 1.85                     | 0.57              |
| 1:R:97:ASP:O     | 1:R:100:VAL:HG22 | 2.05                     | 0.57              |
| 1:R:204:TRP:HZ3  | 2:P:8:DAR:HH11   | 1.53                     | 0.57              |
| 6:N:29:PHE:HE2   | 6:N:72:ARG:HB2   | 1.70                     | 0.56              |
| 5:G:15:LEU:C     | 5:G:15:LEU:HD23  | 2.30                     | 0.56              |
| 1:R:244:TRP:HB2  | 1:R:286:LYS:HE3  | 1.87                     | 0.56              |
| 1:R:285:ALA:HA   | 3:A:358:LEU:O    | 2.06                     | 0.56              |
| 1:R:107:PRO:HB2  | 1:R:131:GLN:HE21 | 1.71                     | 0.56              |
| 4:B:230:HIS:ND1  | 4:B:250:SER:OG   | 2.35                     | 0.56              |
| 3:A:319:ASP:OD1  | 3:A:319:ASP:N    | 2.39                     | 0.56              |
| 1:R:85:ARG:NH1   | 3:A:356:TYR:OH   | 2.38                     | 0.56              |
| 1:R:93:LEU:HD21  | 1:R:344:ASN:HB3  | 1.88                     | 0.56              |
| 1:R:86:MET:HE1   | 1:R:352:SER:HB3  | 1.88                     | 0.56              |
| 4:B:39:THR:CB    | 4:B:305:LEU:HD13 | 2.35                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:84:LEU:HB3   | 4:B:98:ILE:HB    | 1.87                     | 0.55              |
| 1:R:153:VAL:HG11 | 1:R:239:ILE:HG23 | 1.89                     | 0.55              |
| 3:A:355:GLU:OE1  | 3:A:355:GLU:O    | 2.25                     | 0.55              |
| 4:B:231:GLU:O    | 6:N:98:ARG:NH2   | 2.40                     | 0.55              |
| 3:A:265:LYS:HE2  | 3:A:271:SER:HB3  | 1.89                     | 0.54              |
| 1:R:159:THR:O    | 1:R:163:PRO:HG3  | 2.08                     | 0.54              |
| 3:A:353:LEU:HB3  | 3:A:359:VAL:HG23 | 1.88                     | 0.54              |
| 4:B:196:SER:HB2  | 4:B:237:ILE:HG23 | 1.90                     | 0.54              |
| 1:R:285:ALA:CB   | 3:A:359:VAL:HA   | 2.31                     | 0.54              |
| 4:B:100:LEU:HD13 | 4:B:105:VAL:HG21 | 1.89                     | 0.54              |
| 1:R:307:PHE:O    | 1:R:311:GLN:HG2  | 2.07                     | 0.54              |
| 6:N:94:TYR:O     | 6:N:121:GLY:CA   | 2.56                     | 0.54              |
| 3:A:182:ILE:HG12 | 3:A:199:VAL:HG22 | 1.90                     | 0.53              |
| 1:R:288:ARG:NH2  | 3:A:357:ASN:HD21 | 2.04                     | 0.52              |
| 4:B:206:SER:OG   | 4:B:216:TRP:NE1  | 2.35                     | 0.52              |
| 4:B:237:ILE:HG13 | 4:B:248:THR:HG22 | 1.91                     | 0.52              |
| 6:N:33:LYS:HD3   | 6:N:52:SER:HA    | 1.92                     | 0.52              |
| 1:R:44:ASP:OD1   | 1:R:198:THR:HG21 | 2.10                     | 0.52              |
| 1:R:331:THR:HG22 | 2:P:7:PRO:HB2    | 1.91                     | 0.51              |
| 4:B:167:GLY:HA2  | 4:B:191:ASP:OD1  | 2.10                     | 0.51              |
| 1:R:116:ARG:NH2  | 1:R:194:VAL:HG21 | 2.24                     | 0.51              |
| 1:R:108:GLN:HG2  | 1:R:131:GLN:HE22 | 1.75                     | 0.51              |
| 4:B:52:THR:O     | 4:B:52:THR:CG2   | 2.59                     | 0.51              |
| 3:A:272:LYS:O    | 3:A:274:GLU:N    | 2.38                     | 0.51              |
| 4:B:14:GLN:O     | 4:B:17:GLU:HG3   | 2.11                     | 0.51              |
| 4:B:19:LEU:O     | 4:B:22:GLN:HG3   | 2.10                     | 0.51              |
| 3:A:228:TYR:CE2  | 3:A:265:LYS:HD3  | 2.45                     | 0.51              |
| 1:R:162:GLN:HA   | 3:A:28:GLU:OE2   | 2.11                     | 0.50              |
| 3:A:225:SER:HB2  | 3:A:262:LEU:HD22 | 1.93                     | 0.50              |
| 4:B:165:SER:HB3  | 4:B:195:LEU:HD12 | 1.93                     | 0.50              |
| 1:R:284:ARG:HA   | 1:R:287:ILE:HG12 | 1.93                     | 0.50              |
| 1:R:222:GLY:HA2  | 1:R:226:VAL:HB   | 1.94                     | 0.50              |
| 3:A:8:GLU:HG3    | 3:A:10:LYS:H     | 1.77                     | 0.50              |
| 1:R:100:VAL:HG21 | 1:R:341:SER:OG   | 2.12                     | 0.50              |
| 1:R:162:GLN:HB3  | 1:R:165:ARG:HG2  | 1.94                     | 0.49              |
| 1:R:292:MET:HA   | 1:R:351:PHE:CZ   | 2.47                     | 0.49              |
| 1:R:125:ARG:HB3  | 1:R:186:TYR:HD1  | 1.78                     | 0.49              |
| 1:R:76:LEU:HD13  | 1:R:91:ARG:HB2   | 1.95                     | 0.49              |
| 1:R:162:GLN:HG2  | 3:A:28:GLU:OE2   | 2.12                     | 0.49              |
| 1:R:292:MET:HG3  | 1:R:351:PHE:CE2  | 2.47                     | 0.49              |
| 3:A:289:ALA:HB1  | 3:A:304:TYR:HE2  | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:10:ASP:OD1   | 4:B:10:ASP:N     | 2.46                     | 0.49              |
| 1:R:111:TRP:HZ3  | 1:R:128:LYS:HE2  | 1.77                     | 0.48              |
| 1:R:226:VAL:O    | 1:R:230:VAL:HG23 | 2.12                     | 0.48              |
| 6:N:61:THR:HG22  | 6:N:64:VAL:HG22  | 1.92                     | 0.48              |
| 3:A:182:ILE:HD11 | 4:B:122:LEU:HB3  | 1.94                     | 0.48              |
| 4:B:217:ASP:OD2  | 4:B:224:ARG:NH1  | 2.46                     | 0.48              |
| 3:A:38:LEU:HD11  | 3:A:46:LYS:HB3   | 1.93                     | 0.48              |
| 4:B:76:VAL:HG21  | 4:B:117:VAL:HG11 | 1.96                     | 0.48              |
| 1:R:336:LEU:HD22 | 1:R:339:LEU:CD1  | 2.44                     | 0.48              |
| 4:B:250:SER:OG   | 4:B:252:ASP:OD1  | 2.22                     | 0.48              |
| 3:A:220:ILE:HG23 | 3:A:255:PHE:CD2  | 2.48                     | 0.48              |
| 4:B:78:ALA:HB1   | 4:B:105:VAL:HG11 | 1.96                     | 0.48              |
| 4:B:284:SER:HB2  | 4:B:289:LEU:HD12 | 1.96                     | 0.48              |
| 1:R:112:LYS:HE3  | 1:R:335:LEU:HD21 | 1.96                     | 0.48              |
| 4:B:336:SER:OG   | 4:B:337:TRP:N    | 2.47                     | 0.47              |
| 3:A:23:LEU:HD11  | 4:B:83:LYS:HG3   | 1.96                     | 0.47              |
| 3:A:275:ASP:OD1  | 3:A:275:ASP:N    | 2.44                     | 0.47              |
| 4:B:217:ASP:HB3  | 4:B:220:GLU:OE2  | 2.14                     | 0.47              |
| 4:B:323:LEU:HD12 | 4:B:334:THR:OG1  | 2.15                     | 0.47              |
| 4:B:214:LYS:HD3  | 4:B:216:TRP:CZ2  | 2.49                     | 0.47              |
| 4:B:330:MET:HB3  | 5:G:61:PHE:HE1   | 1.79                     | 0.47              |
| 1:R:156:PRO:O    | 1:R:159:THR:HB   | 2.15                     | 0.47              |
| 4:B:282:SER:HB3  | 4:B:323:LEU:HD23 | 1.96                     | 0.47              |
| 4:B:66:MET:HE1   | 4:B:333:ALA:HB3  | 1.96                     | 0.47              |
| 4:B:279:THR:OG1  | 4:B:320:VAL:O    | 2.27                     | 0.47              |
| 6:N:109:ASP:OD2  | 6:N:115:TYR:CD1  | 2.68                     | 0.47              |
| 3:A:45:GLY:O     | 3:A:48:THR:OG1   | 2.33                     | 0.47              |
| 6:N:32:TYR:CD2   | 6:N:98:ARG:HD2   | 2.50                     | 0.47              |
| 4:B:117:VAL:HG23 | 4:B:131:LEU:HD11 | 1.97                     | 0.47              |
| 3:A:220:ILE:HG23 | 3:A:255:PHE:HD2  | 1.78                     | 0.46              |
| 1:R:98:LEU:HD22  | 1:R:102:PHE:HE2  | 1.81                     | 0.46              |
| 4:B:345:ASN:ND2  | 5:G:59:ASN:OD1   | 2.48                     | 0.46              |
| 1:R:288:ARG:CZ   | 3:A:357:ASN:HD21 | 2.29                     | 0.46              |
| 3:A:209:TRP:HB2  | 4:B:122:LEU:HD21 | 1.96                     | 0.46              |
| 4:B:163:VAL:HG12 | 4:B:195:LEU:HD11 | 1.97                     | 0.46              |
| 1:R:103:PHE:CG   | 1:R:130:LEU:HD23 | 2.50                     | 0.46              |
| 4:B:147:HIS:CD2  | 4:B:174:TRP:HZ2  | 2.33                     | 0.46              |
| 6:N:67:ARG:NH1   | 6:N:90:ASP:OD2   | 2.45                     | 0.46              |
| 1:R:103:PHE:HB3  | 1:R:130:LEU:HB3  | 1.98                     | 0.46              |
| 4:B:164:THR:OG1  | 4:B:174:TRP:NE1  | 2.41                     | 0.46              |
| 4:B:129:TYR:CE2  | 4:B:140:VAL:HG22 | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:34:MET:HB3   | 6:N:79:LEU:HD22  | 1.98                     | 0.46              |
| 4:B:142:ARG:HD3  | 4:B:176:ILE:O    | 2.15                     | 0.46              |
| 4:B:267:MET:HG2  | 4:B:268:THR:N    | 2.31                     | 0.46              |
| 1:R:192:ILE:CG2  | 1:R:193:GLU:H    | 2.28                     | 0.46              |
| 3:A:320:GLY:O    | 3:A:354:ARG:NH1  | 2.49                     | 0.46              |
| 4:B:12:LEU:O     | 5:G:13:ARG:NH2   | 2.48                     | 0.46              |
| 1:R:98:LEU:HD22  | 1:R:102:PHE:CE2  | 2.50                     | 0.46              |
| 4:B:32:ASP:OD1   | 5:G:31:SER:OG    | 2.30                     | 0.45              |
| 1:R:97:ASP:HA    | 1:R:100:VAL:HG22 | 1.97                     | 0.45              |
| 4:B:39:THR:HG21  | 4:B:305:LEU:HB2  | 1.99                     | 0.45              |
| 5:G:8:SER:O      | 5:G:11:GLN:HG3   | 2.15                     | 0.45              |
| 6:N:109:ASP:O    | 6:N:115:TYR:CZ   | 2.69                     | 0.45              |
| 4:B:63:ILE:O     | 4:B:321:SER:OG   | 2.29                     | 0.45              |
| 3:A:273:ILE:O    | 3:A:277:PHE:N    | 2.38                     | 0.44              |
| 4:B:303:ASP:HB3  | 4:B:306:LYS:HB2  | 1.99                     | 0.44              |
| 5:G:13:ARG:HH21  | 5:G:16:VAL:HG21  | 1.82                     | 0.44              |
| 3:A:27:GLY:HA3   | 4:B:60:LEU:HD13  | 1.98                     | 0.44              |
| 1:R:162:GLN:HG3  | 3:A:28:GLU:CD    | 2.41                     | 0.44              |
| 1:R:84:SER:OG    | 3:A:355:GLU:OE2  | 2.31                     | 0.44              |
| 4:B:36:SER:HA    | 4:B:267:MET:HE1  | 1.99                     | 0.44              |
| 4:B:176:ILE:HD13 | 4:B:176:ILE:HA   | 1.86                     | 0.44              |
| 4:B:266:LEU:HD12 | 4:B:266:LEU:HA   | 1.72                     | 0.44              |
| 4:B:66:MET:HB2   | 4:B:66:MET:HE2   | 1.75                     | 0.44              |
| 4:B:230:HIS:NE2  | 4:B:256:ARG:HB2  | 2.32                     | 0.44              |
| 4:B:281:VAL:HG13 | 4:B:290:LEU:HD11 | 2.00                     | 0.44              |
| 1:R:143:VAL:HG13 | 1:R:231:ILE:HG21 | 1.99                     | 0.44              |
| 4:B:169:THR:HG22 | 4:B:190:GLY:O    | 2.18                     | 0.44              |
| 4:B:240:PHE:HD2  | 4:B:242:ASN:H    | 1.66                     | 0.44              |
| 1:R:224:ILE:O    | 1:R:228:PRO:HG2  | 2.18                     | 0.44              |
| 3:A:235:LEU:HD22 | 3:A:313:ILE:HD12 | 1.99                     | 0.44              |
| 3:A:202:GLN:OE1  | 4:B:150:TYR:N    | 2.51                     | 0.43              |
| 1:R:128:LYS:HG3  | 1:R:189:PHE:CG   | 2.53                     | 0.43              |
| 6:N:70:ILE:HG22  | 6:N:81:LEU:HD13  | 1.98                     | 0.43              |
| 6:N:83:MET:HE1   | 6:N:124:VAL:HG11 | 2.00                     | 0.43              |
| 4:B:288:ARG:HA   | 4:B:288:ARG:HD2  | 1.77                     | 0.43              |
| 1:R:292:MET:HB2  | 1:R:292:MET:HE3  | 1.83                     | 0.43              |
| 3:A:295:GLU:OE2  | 3:A:303:LYS:NZ   | 2.38                     | 0.43              |
| 3:A:338:ARG:O    | 3:A:341:PHE:HB3  | 2.18                     | 0.43              |
| 3:A:347:ILE:HG22 | 3:A:351:MET:CE   | 2.45                     | 0.43              |
| 4:B:107:THR:OG1  | 4:B:153:CYS:HA   | 2.18                     | 0.43              |
| 4:B:128:ILE:HG13 | 4:B:141:SER:HB3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:142:ARG:HB3  | 4:B:142:ARG:HH11 | 1.80                     | 0.43              |
| 4:B:191:ASP:HB3  | 4:B:209:CYS:SG   | 2.59                     | 0.43              |
| 1:R:43:ARG:H     | 1:R:43:ARG:HD3   | 1.83                     | 0.43              |
| 3:A:308:LYS:HE2  | 3:A:308:LYS:HB2  | 1.85                     | 0.43              |
| 4:B:82:GLY:HA2   | 4:B:100:LEU:HD12 | 2.01                     | 0.43              |
| 4:B:163:VAL:HG22 | 4:B:173:LEU:HD13 | 2.01                     | 0.43              |
| 4:B:242:ASN:OD1  | 4:B:242:ASN:C    | 2.62                     | 0.43              |
| 6:N:104:THR:OG1  | 6:N:106:ASP:OD1  | 2.37                     | 0.43              |
| 4:B:9:LEU:HD12   | 4:B:12:LEU:HB2   | 2.01                     | 0.43              |
| 1:R:287:ILE:HA   | 1:R:290:VAL:HG12 | 2.01                     | 0.42              |
| 3:A:291:PRO:HB3  | 3:A:300:THR:HG21 | 2.00                     | 0.42              |
| 4:B:129:TYR:HE2  | 4:B:140:VAL:HG22 | 1.84                     | 0.42              |
| 6:N:64:VAL:HG11  | 6:N:68:PHE:CE2   | 2.54                     | 0.42              |
| 1:R:116:ARG:HB3  | 1:R:201:ARG:O    | 2.20                     | 0.42              |
| 1:R:220:MET:HB3  | 1:R:220:MET:HE3  | 1.77                     | 0.42              |
| 1:R:335:LEU:O    | 2:P:2:TYR:OH     | 2.23                     | 0.42              |
| 3:A:29:LYS:HG3   | 3:A:32:ARG:HH21  | 1.83                     | 0.42              |
| 4:B:157:LEU:HD23 | 4:B:157:LEU:HA   | 1.89                     | 0.42              |
| 6:N:27:PHE:CZ    | 6:N:98:ARG:HD3   | 2.55                     | 0.42              |
| 6:N:35:ASN:OD1   | 6:N:35:ASN:N     | 2.53                     | 0.42              |
| 4:B:83:LYS:HA    | 4:B:83:LYS:HD3   | 1.74                     | 0.42              |
| 1:R:128:LYS:HD3  | 1:R:128:LYS:HA   | 1.74                     | 0.42              |
| 6:N:51:ILE:HB    | 6:N:70:ILE:HD11  | 2.02                     | 0.42              |
| 6:N:4:LEU:HB3    | 6:N:22:CYS:SG    | 2.60                     | 0.42              |
| 4:B:257:LEU:O    | 4:B:266:LEU:N    | 2.51                     | 0.42              |
| 1:R:62:PHE:O     | 1:R:66:VAL:HG22  | 2.20                     | 0.41              |
| 4:B:54:ARG:HB2   | 4:B:343:ILE:HD12 | 2.02                     | 0.41              |
| 6:N:34:MET:CE    | 6:N:98:ARG:HA    | 2.49                     | 0.41              |
| 3:A:202:GLN:NE2  | 4:B:124:ASN:OD1  | 2.53                     | 0.41              |
| 4:B:39:THR:HB    | 4:B:305:LEU:CD1  | 2.43                     | 0.41              |
| 5:G:20:LYS:HG3   | 5:G:21:MET:N     | 2.35                     | 0.41              |
| 3:A:46:LYS:HB2   | 3:A:46:LYS:HE3   | 1.78                     | 0.41              |
| 1:R:106:LEU:HB3  | 1:R:107:PRO:HD3  | 2.03                     | 0.41              |
| 4:B:185:PHE:CE1  | 4:B:221:GLY:HA2  | 2.56                     | 0.41              |
| 3:A:238:PHE:HE1  | 3:A:252:VAL:HG11 | 1.86                     | 0.41              |
| 4:B:192:VAL:HA   | 4:B:208:ALA:HA   | 2.02                     | 0.41              |
| 4:B:252:ASP:OD1  | 4:B:252:ASP:N    | 2.50                     | 0.41              |
| 4:B:66:MET:CE    | 4:B:333:ALA:HB3  | 2.51                     | 0.41              |
| 4:B:109:ALA:HB3  | 4:B:118:ALA:HB3  | 2.02                     | 0.41              |
| 4:B:133:THR:HG21 | 4:B:137:ASN:O    | 2.20                     | 0.41              |
| 4:B:295:ASP:OD1  | 4:B:319:ARG:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:70:SER:O     | 1:R:74:LEU:HG    | 2.21                     | 0.41              |
| 1:R:322:TRP:NE1  | 2:P:5:ASN:O      | 2.40                     | 0.41              |
| 1:R:331:THR:HA   | 2:P:7:PRO:HG2    | 2.03                     | 0.41              |
| 1:R:158:LYS:HZ3  | 1:R:158:LYS:HB2  | 1.84                     | 0.41              |
| 5:G:38:MET:HE3   | 5:G:38:MET:HB3   | 1.81                     | 0.41              |
| 6:N:74:ASN:OD1   | 6:N:74:ASN:N     | 2.53                     | 0.41              |
| 1:R:224:ILE:C    | 1:R:228:PRO:HG2  | 2.46                     | 0.40              |
| 4:B:305:LEU:HD12 | 4:B:305:LEU:C    | 2.46                     | 0.40              |
| 1:R:282:ILE:HD12 | 1:R:282:ILE:HA   | 1.96                     | 0.40              |
| 3:A:344:CYS:O    | 3:A:348:ILE:HG13 | 2.20                     | 0.40              |
| 4:B:9:LEU:HA     | 4:B:12:LEU:HB2   | 2.03                     | 0.40              |
| 4:B:171:CYS:SG   | 4:B:192:VAL:HG11 | 2.61                     | 0.40              |
| 4:B:305:LEU:HD12 | 4:B:305:LEU:O    | 2.21                     | 0.40              |
| 4:B:225:GLN:HA   | 5:G:22:GLU:OE1   | 2.21                     | 0.40              |
| 1:R:239:ILE:HG22 | 1:R:289:THR:HG21 | 2.03                     | 0.40              |
| 3:A:242:TRP:NE1  | 3:A:314:SER:O    | 2.54                     | 0.40              |
| 4:B:133:THR:HG23 | 4:B:136:GLY:H    | 1.86                     | 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     | 286/855 (34%)   | 275 (96%) | 11 (4%) | 0        | 100         | 100 |
| 2   | P     | 7/10 (70%)      | 6 (86%)   | 1 (14%) | 0        | 100         | 100 |
| 3   | A     | 217/246 (88%)   | 203 (94%) | 14 (6%) | 0        | 100         | 100 |
| 4   | B     | 336/377 (89%)   | 325 (97%) | 11 (3%) | 0        | 100         | 100 |
| 5   | G     | 55/71 (78%)     | 55 (100%) | 0       | 0        | 100         | 100 |
| 6   | N     | 124/157 (79%)   | 122 (98%) | 2 (2%)  | 0        | 100         | 100 |
| All | All   | 1025/1716 (60%) | 986 (96%) | 39 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | R     | 253/734 (34%)  | 253 (100%) | 0        | 100         | 100 |
| 2   | P     | 7/7 (100%)     | 6 (86%)    | 1 (14%)  | 3           | 15  |
| 3   | A     | 197/213 (92%)  | 196 (100%) | 1 (0%)   | 81          | 88  |
| 4   | B     | 281/308 (91%)  | 279 (99%)  | 2 (1%)   | 76          | 85  |
| 5   | G     | 46/58 (79%)    | 46 (100%)  | 0        | 100         | 100 |
| 6   | N     | 104/127 (82%)  | 102 (98%)  | 2 (2%)   | 50          | 75  |
| All | All   | 888/1447 (61%) | 882 (99%)  | 6 (1%)   | 73          | 85  |

All (6) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 6   | CYS  |
| 3   | A     | 50  | VAL  |
| 4   | B     | 176 | ILE  |
| 4   | B     | 239 | PHE  |
| 6   | N     | 35  | ASN  |
| 6   | N     | 96  | CYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 185 | GLN  |
| 1   | R     | 242 | ASN  |
| 3   | A     | 232 | GLN  |
| 3   | A     | 236 | ASN  |
| 3   | A     | 244 | ASN  |
| 3   | A     | 357 | ASN  |
| 4   | B     | 37  | GLN  |
| 4   | B     | 345 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | N     | 3   | 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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63832. These allow visual inspection of the internal detail of the map and identification of artifacts.

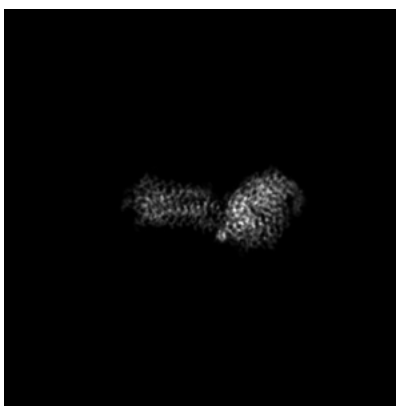
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

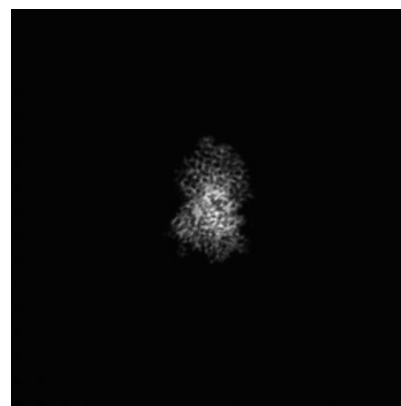
#### 6.1.1 Primary map



X

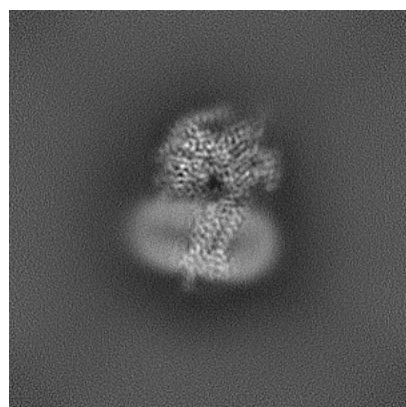


Y

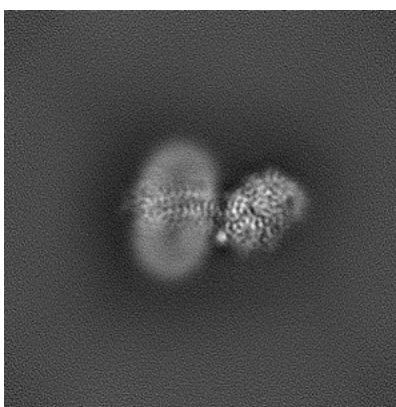


Z

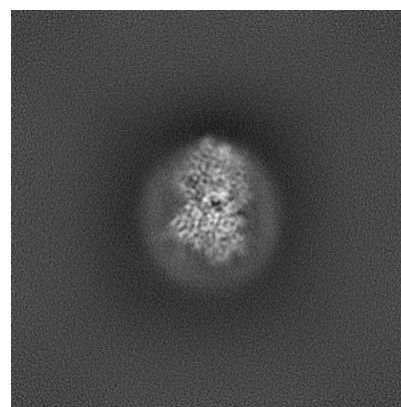
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

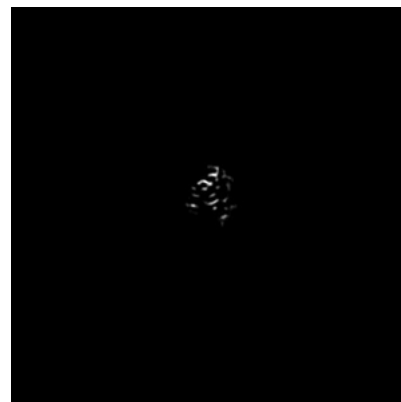
### 6.2.1 Primary map



X Index: 160

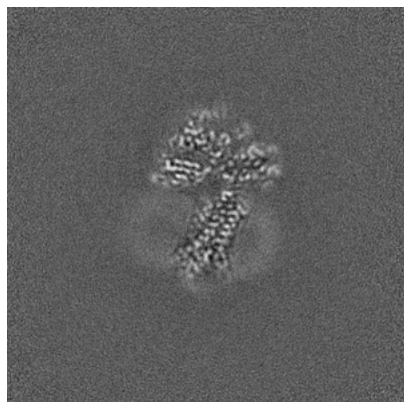


Y Index: 160

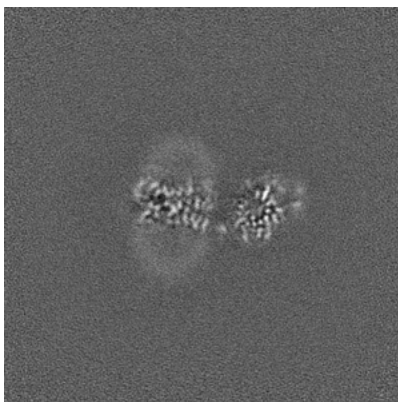


Z Index: 160

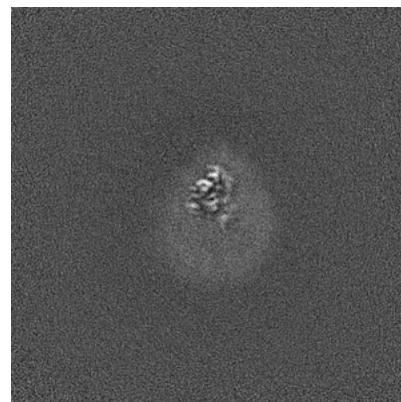
### 6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 158

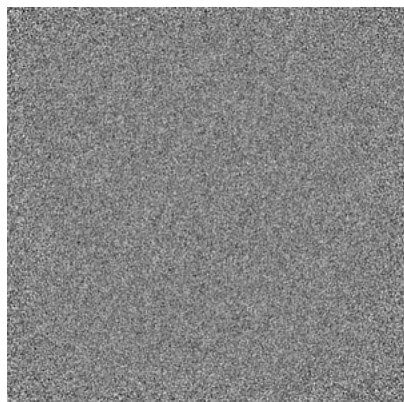


Y Index: 146

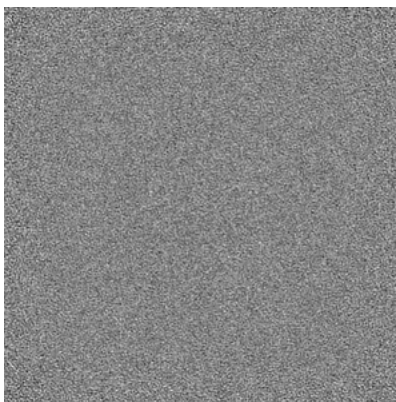


Z Index: 190

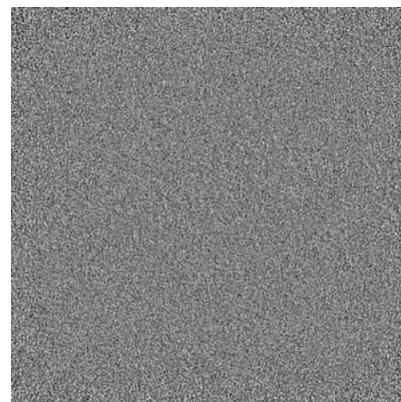
### 6.3.2 Raw map



X Index: 0



Y Index: 0

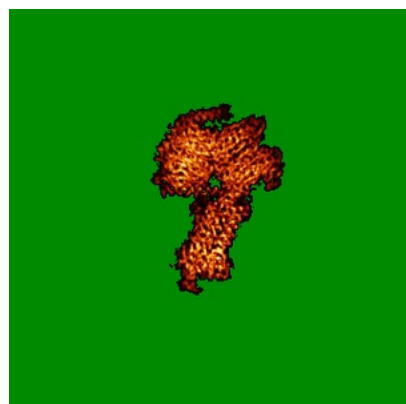


Z Index: 0

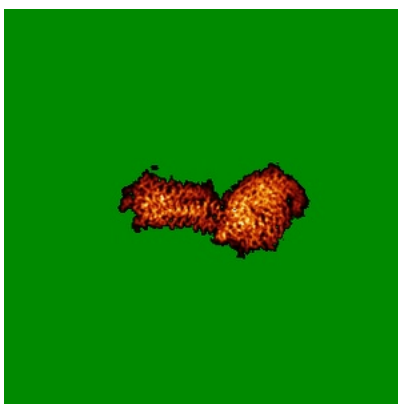
The images above show the largest variance slices of the map in three orthogonal directions.

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

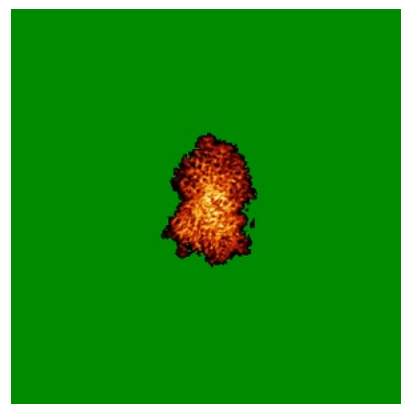
### 6.4.1 Primary map



X

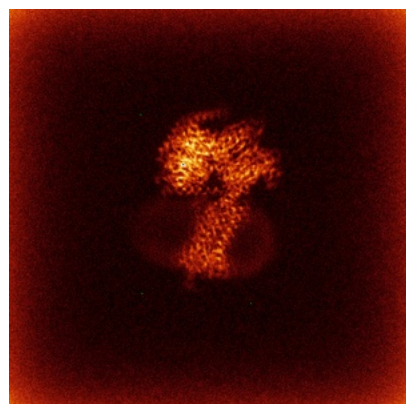


Y

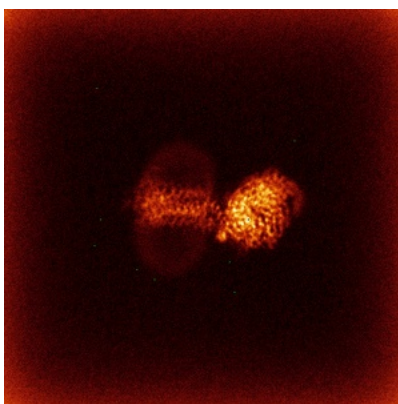


Z

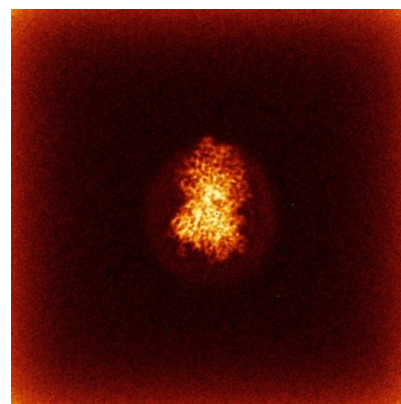
### 6.4.2 Raw map



X



Y

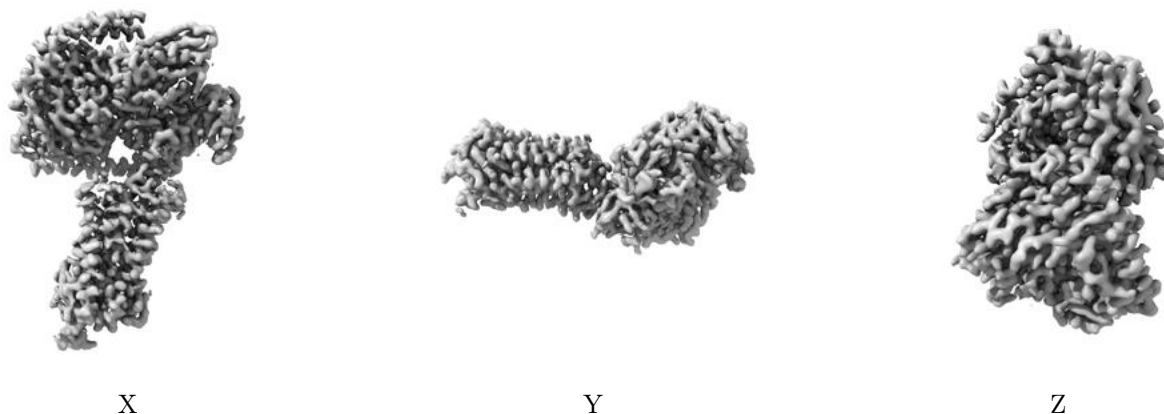


Z

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

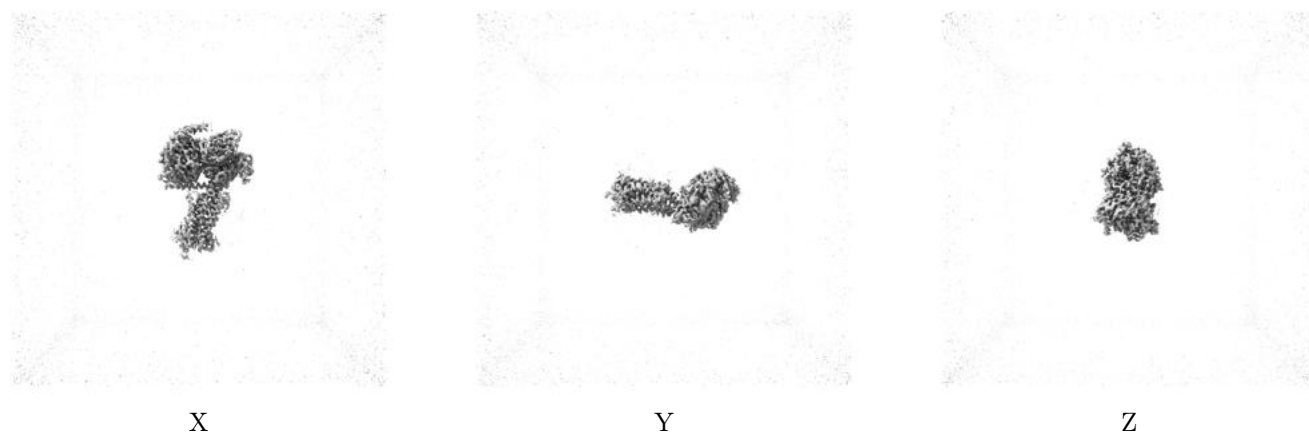
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

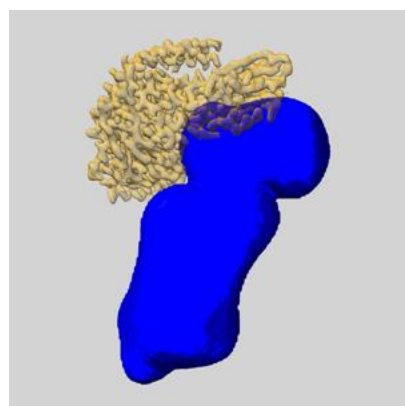
## 6.6 Mask visualisation [i](#)

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

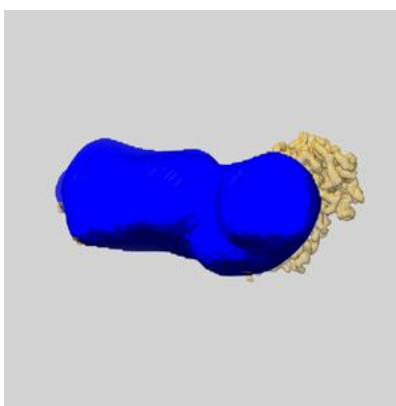
A mask typically either:

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

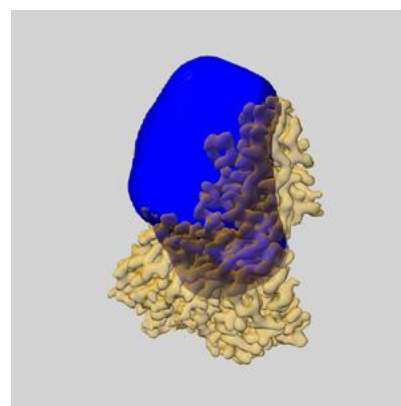
### 6.6.1 emd\_63832\_msk\_1.map [i](#)



X



Y

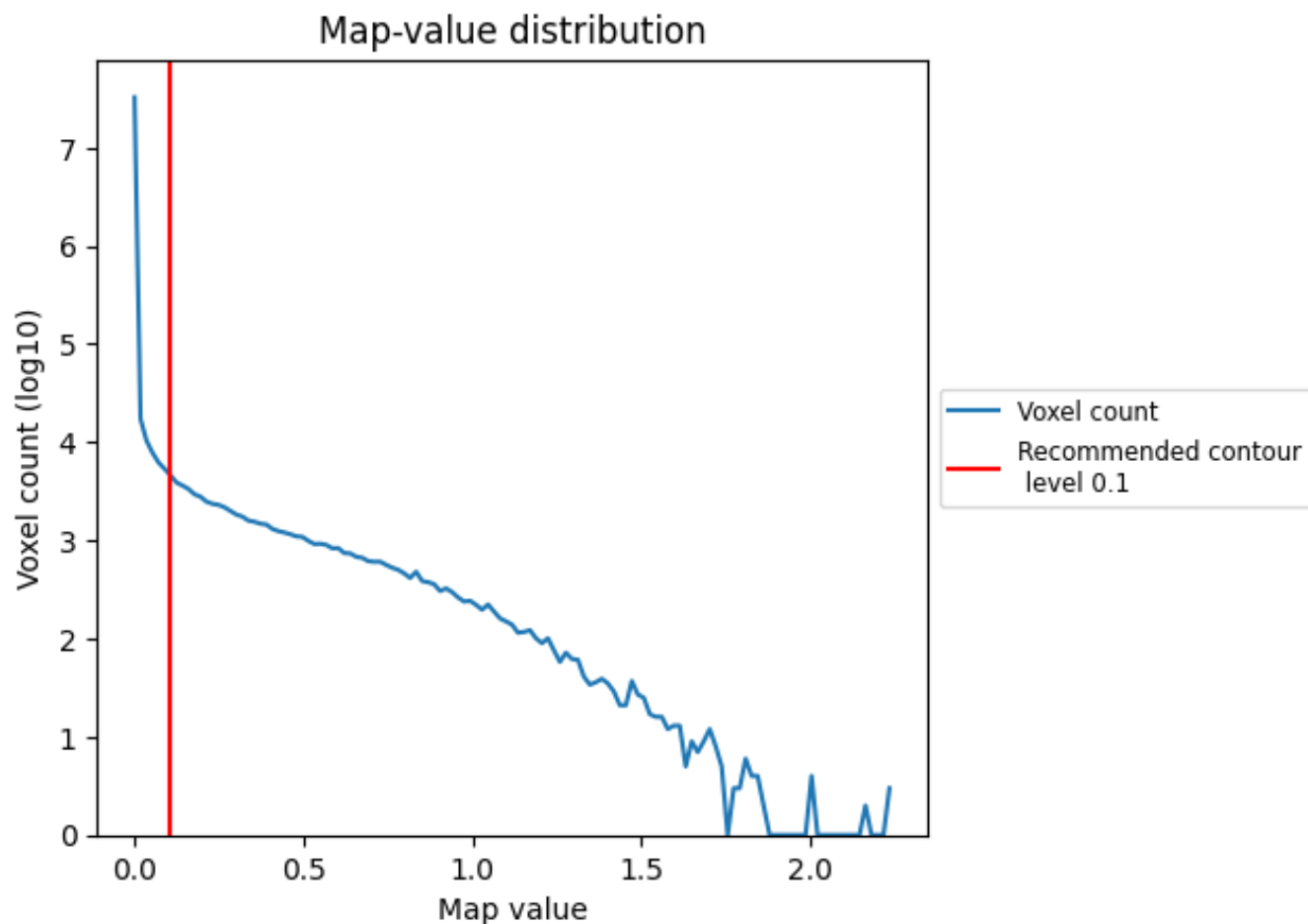


Z

## 7 Map analysis [i](#)

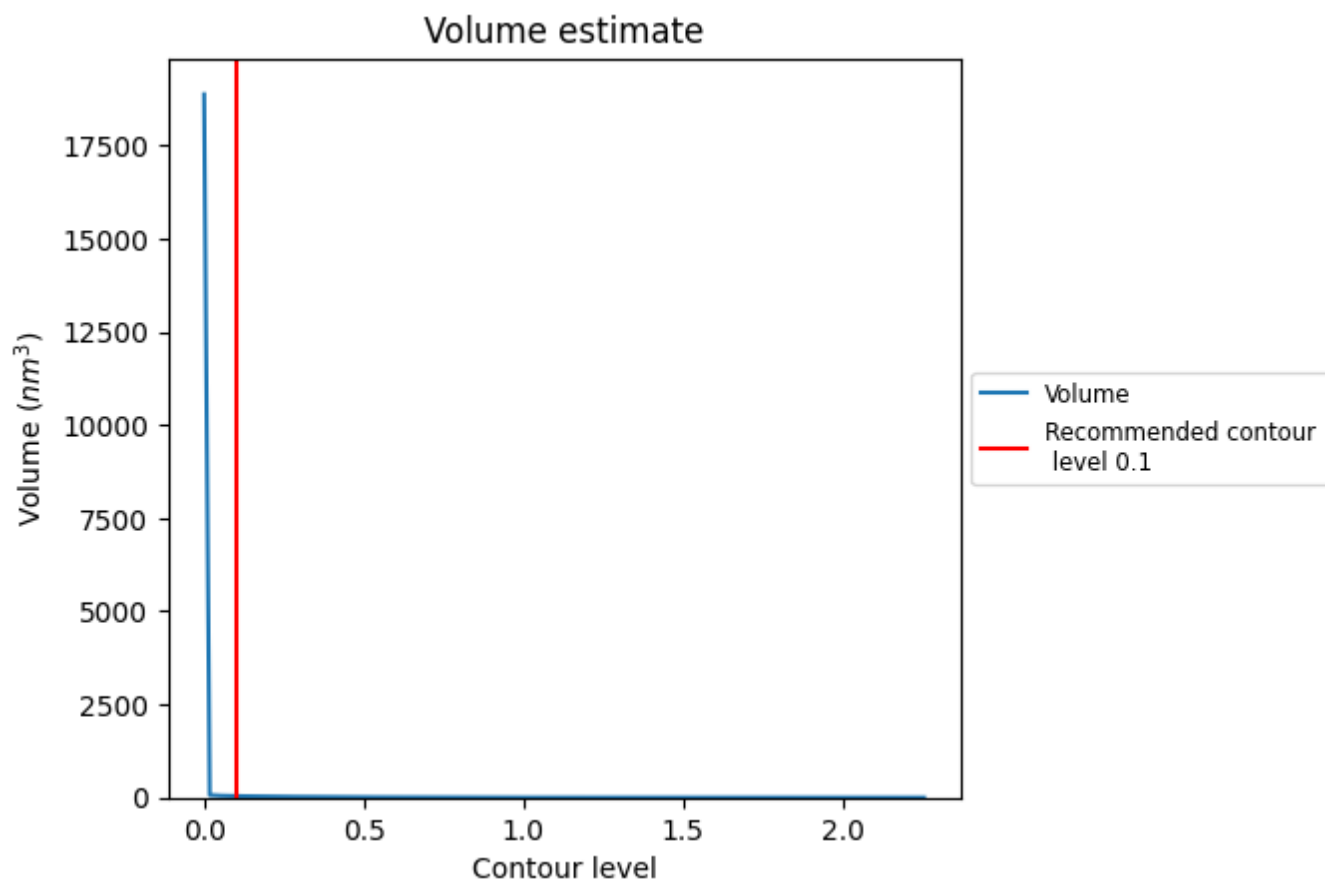
This section contains the results of statistical analysis of the map.

### 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.

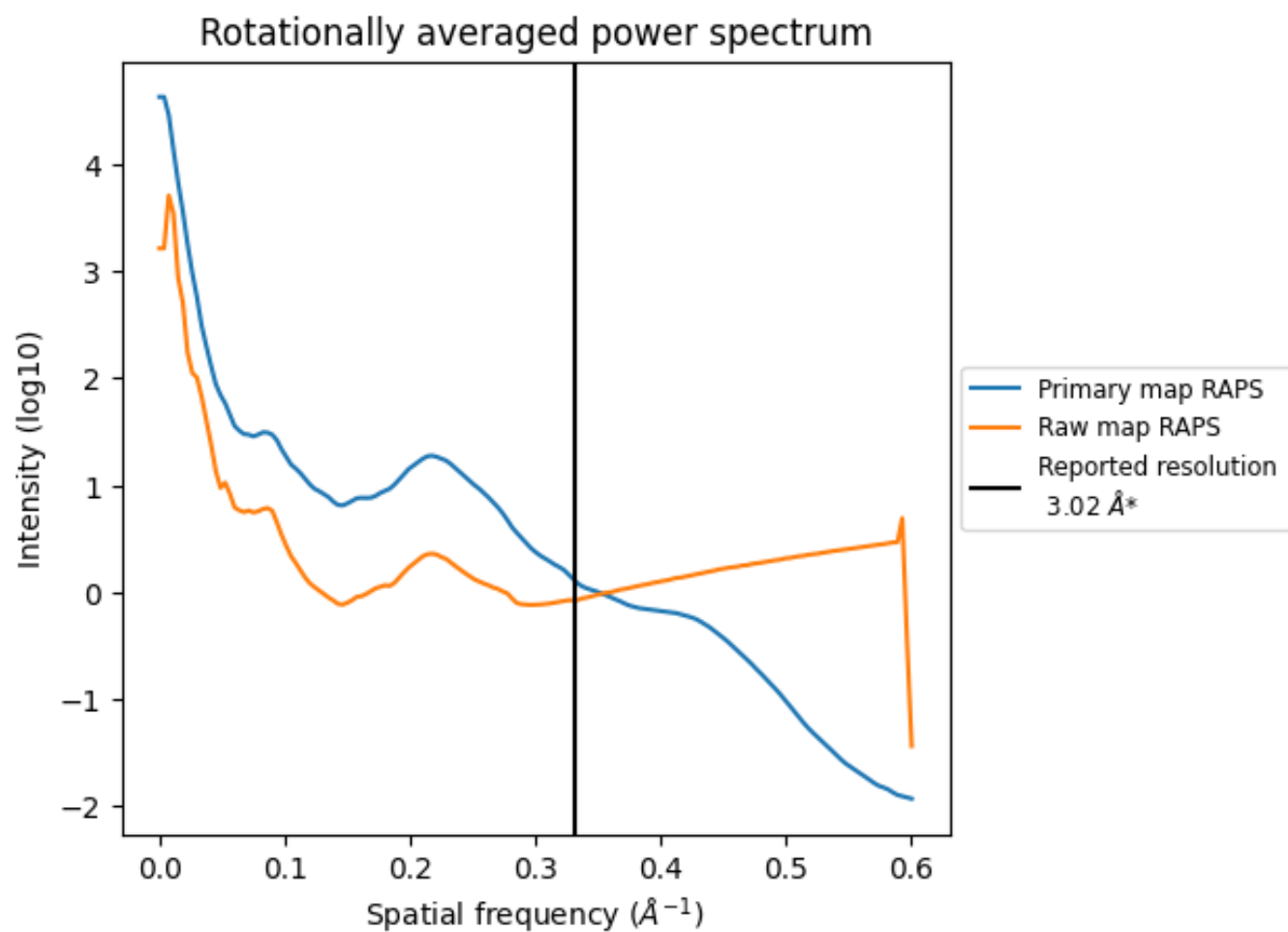
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40  $\text{nm}^3$ ; this corresponds to an approximate mass of 36 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 ⓘ

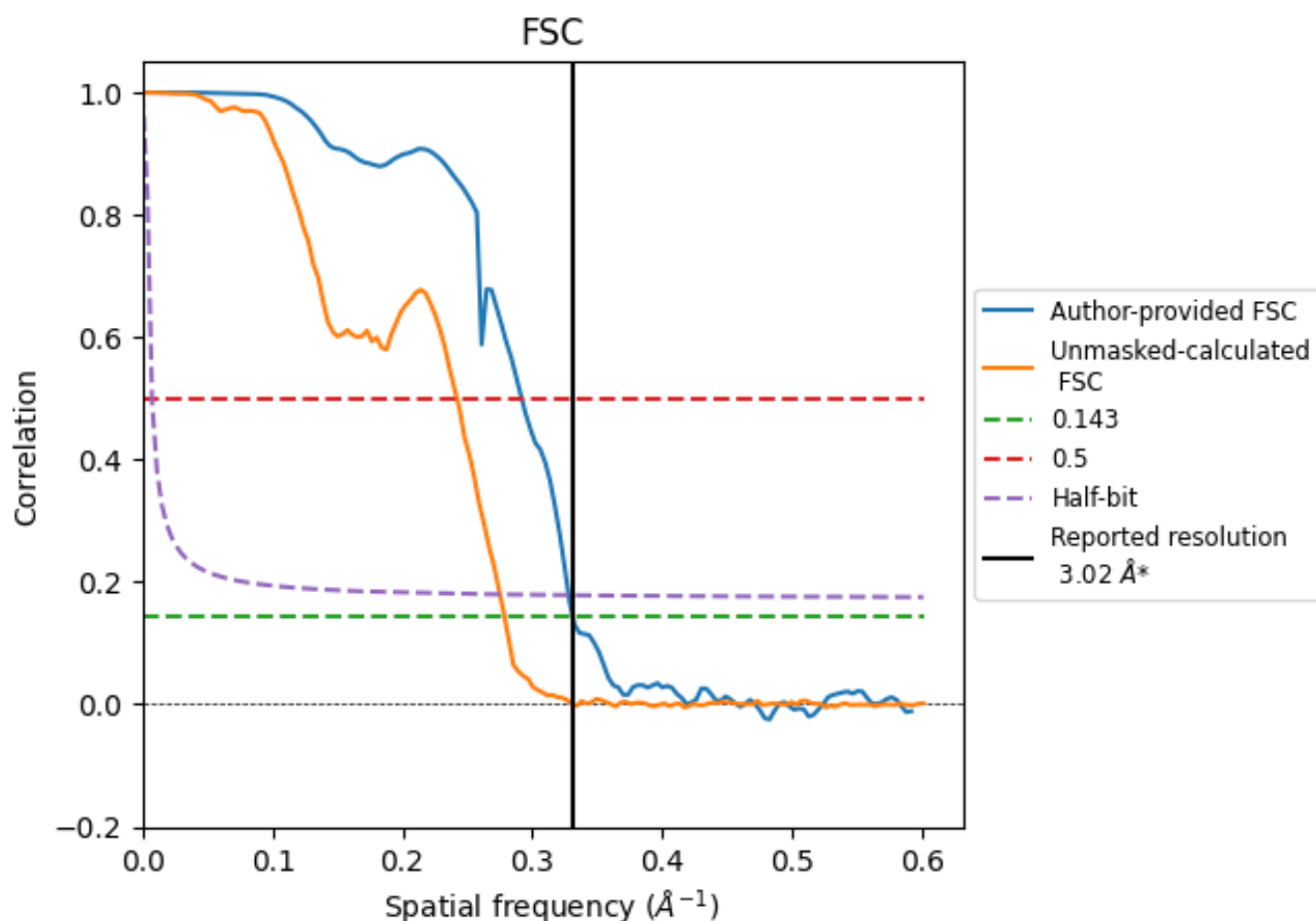


\*Reported resolution corresponds to spatial frequency of 0.331 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.331  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

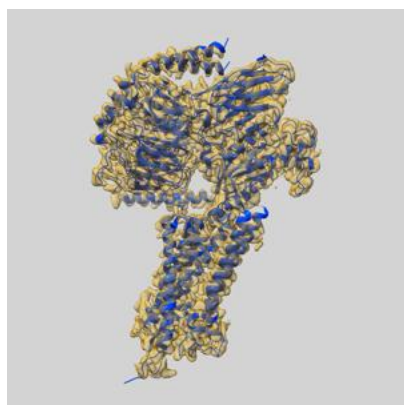
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.02                               | -    | -        |
| Author-provided FSC curve | 3.02                               | 3.43 | 3.05     |
| Unmasked-calculated*      | 3.59                               | 4.13 | 3.64     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 3.02 by more than 10 %

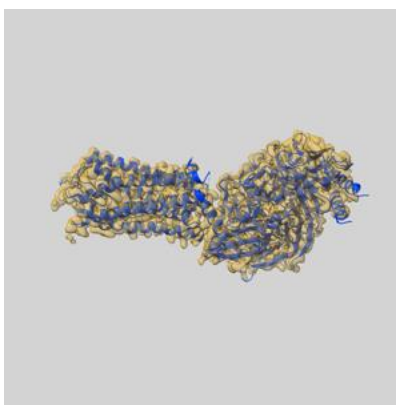
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63832 and PDB model 9U43. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

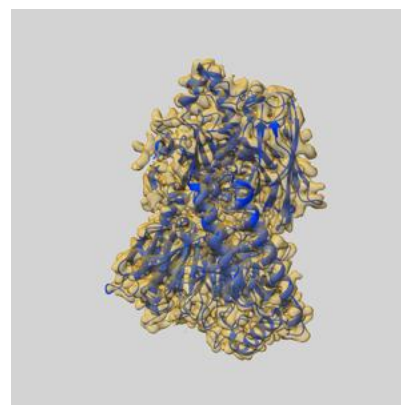
### 9.1 Map-model overlay [i](#)



X



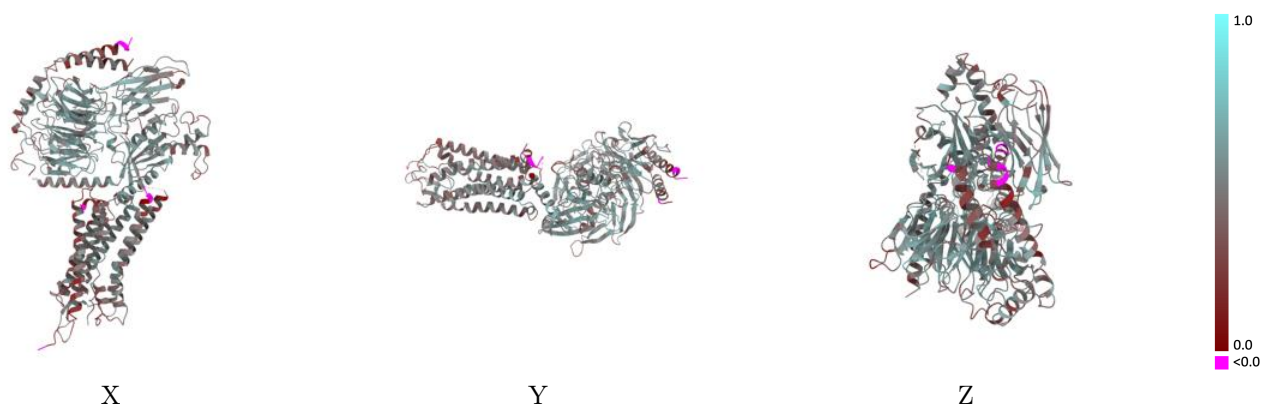
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)



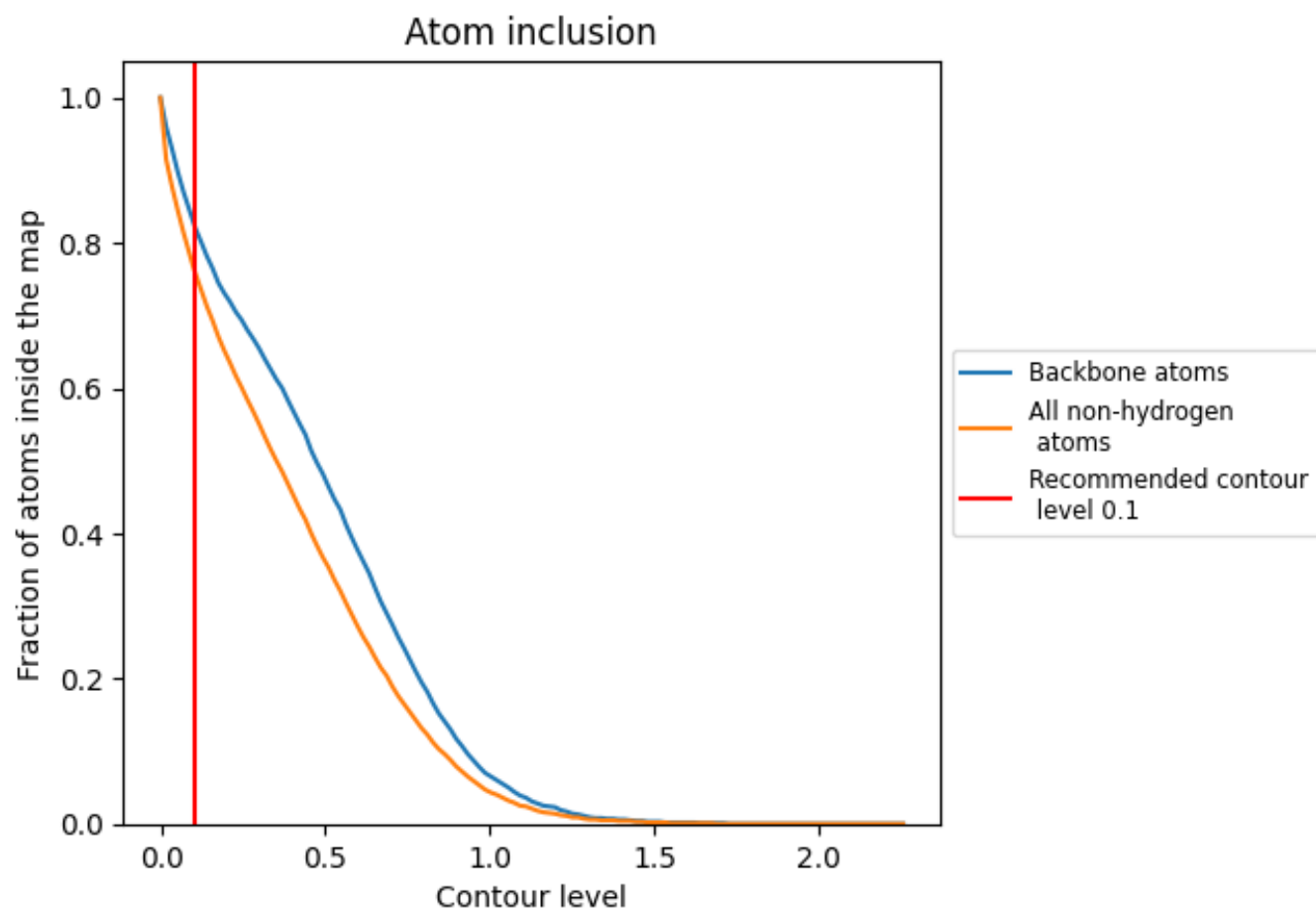
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.7640</div> | <div><div></div>0.4660</div> |
| A     | <div><div></div>0.7820</div> | <div><div></div>0.4940</div> |
| B     | <div><div></div>0.8030</div> | <div><div></div>0.5070</div> |
| G     | <div><div></div>0.6200</div> | <div><div></div>0.3710</div> |
| N     | <div><div></div>0.7920</div> | <div><div></div>0.4890</div> |
| P     | <div><div></div>0.9310</div> | <div><div></div>0.4750</div> |
| R     | <div><div></div>0.7180</div> | <div><div></div>0.4040</div> |

1.0

0.0

<0.0