



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 06:10 PM UTC

PDB ID : 9VKP / pdb\_00009vkp  
EMDB ID : EMD-65138  
Title : Cryo-EM structure of F-ATP synthase from Mycobacteroides abscessus (Rotational State 1)  
Authors : Fong, T.C.; Saw, W.-G.; Mathiyazakan, V.; Wong, C.F.; Grueber, G.  
Deposited on : 2025-06-23  
Resolution : 2.94 Å(reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

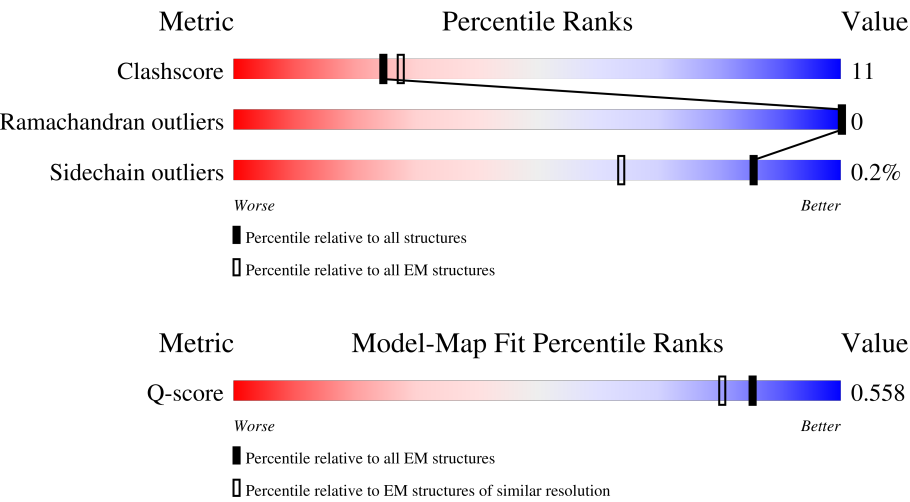
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.94 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.



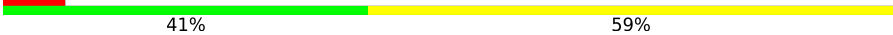
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13068 ( 2.44 - 3.44 )                                    |

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   | A     | 548    |                  |
| 1   | B     | 548    |                  |
| 1   | C     | 548    |                  |
| 2   | D     | 515    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 2   | E     | 515    | <br>72% 18% 10% |
| 2   | F     | 515    | <br>71% 20% 10% |
| 3   | G     | 308    | <br>73% 27% .   |
| 4   | H     | 121    | <br>7% 41% 59%  |
| 5   | b     | 177    | <br>27% 19% 55% |
| 6   | d     | 448    | <br>56% 29% 15% |

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 29467 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 ATP synthase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | B     | 523      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3959  | 2479 | 689 | 782 | 9 |         |       |
| 1   | C     | 520      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3938  | 2466 | 685 | 779 | 8 |         |       |
| 1   | A     | 531      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4021  | 2518 | 702 | 793 | 8 |         |       |

- Molecule 2 is a protein called ATP synthase subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | D     | 465      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3566  | 2251 | 610 | 692 | 13 |         |       |
| 2   | E     | 465      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3561  | 2247 | 609 | 692 | 13 |         |       |
| 2   | F     | 466      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3566  | 2250 | 610 | 693 | 13 |         |       |

There are 117 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 477     | GLY      | -      | expression tag | UNP B1MLW2 |
| D     | 478     | LEU      | -      | expression tag | UNP B1MLW2 |
| D     | 479     | SER      | -      | expression tag | UNP B1MLW2 |
| D     | 480     | GLY      | -      | expression tag | UNP B1MLW2 |
| D     | 481     | GLN      | -      | expression tag | UNP B1MLW2 |
| D     | 482     | PRO      | -      | expression tag | UNP B1MLW2 |
| D     | 483     | PRO      | -      | expression tag | UNP B1MLW2 |
| D     | 484     | ARG      | -      | expression tag | UNP B1MLW2 |
| D     | 485     | SER      | -      | expression tag | UNP B1MLW2 |
| D     | 486     | PRO      | -      | expression tag | UNP B1MLW2 |
| D     | 487     | SER      | -      | expression tag | UNP B1MLW2 |
| D     | 488     | SER      | -      | expression tag | UNP B1MLW2 |
| D     | 489     | GLY      | -      | expression tag | UNP B1MLW2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 490     | SER      | -      | expression tag | UNP B1MLW2 |
| D     | 491     | SER      | -      | expression tag | UNP B1MLW2 |
| D     | 492     | GLY      | -      | expression tag | UNP B1MLW2 |
| D     | 493     | GLY      | -      | expression tag | UNP B1MLW2 |
| D     | 494     | GLY      | -      | expression tag | UNP B1MLW2 |
| D     | 495     | GLY      | -      | expression tag | UNP B1MLW2 |
| D     | 496     | GLU      | -      | expression tag | UNP B1MLW2 |
| D     | 497     | ASN      | -      | expression tag | UNP B1MLW2 |
| D     | 498     | LEU      | -      | expression tag | UNP B1MLW2 |
| D     | 499     | TYR      | -      | expression tag | UNP B1MLW2 |
| D     | 500     | PHE      | -      | expression tag | UNP B1MLW2 |
| D     | 501     | GLN      | -      | expression tag | UNP B1MLW2 |
| D     | 502     | ASP      | -      | expression tag | UNP B1MLW2 |
| D     | 503     | TYR      | -      | expression tag | UNP B1MLW2 |
| D     | 504     | LYS      | -      | expression tag | UNP B1MLW2 |
| D     | 505     | ASP      | -      | expression tag | UNP B1MLW2 |
| D     | 506     | ASP      | -      | expression tag | UNP B1MLW2 |
| D     | 507     | ASP      | -      | expression tag | UNP B1MLW2 |
| D     | 508     | ASP      | -      | expression tag | UNP B1MLW2 |
| D     | 509     | LYS      | -      | expression tag | UNP B1MLW2 |
| D     | 510     | HIS      | -      | expression tag | UNP B1MLW2 |
| D     | 511     | HIS      | -      | expression tag | UNP B1MLW2 |
| D     | 512     | HIS      | -      | expression tag | UNP B1MLW2 |
| D     | 513     | HIS      | -      | expression tag | UNP B1MLW2 |
| D     | 514     | HIS      | -      | expression tag | UNP B1MLW2 |
| D     | 515     | HIS      | -      | expression tag | UNP B1MLW2 |
| E     | 477     | GLY      | -      | expression tag | UNP B1MLW2 |
| E     | 478     | LEU      | -      | expression tag | UNP B1MLW2 |
| E     | 479     | SER      | -      | expression tag | UNP B1MLW2 |
| E     | 480     | GLY      | -      | expression tag | UNP B1MLW2 |
| E     | 481     | GLN      | -      | expression tag | UNP B1MLW2 |
| E     | 482     | PRO      | -      | expression tag | UNP B1MLW2 |
| E     | 483     | PRO      | -      | expression tag | UNP B1MLW2 |
| E     | 484     | ARG      | -      | expression tag | UNP B1MLW2 |
| E     | 485     | SER      | -      | expression tag | UNP B1MLW2 |
| E     | 486     | PRO      | -      | expression tag | UNP B1MLW2 |
| E     | 487     | SER      | -      | expression tag | UNP B1MLW2 |
| E     | 488     | SER      | -      | expression tag | UNP B1MLW2 |
| E     | 489     | GLY      | -      | expression tag | UNP B1MLW2 |
| E     | 490     | SER      | -      | expression tag | UNP B1MLW2 |
| E     | 491     | SER      | -      | expression tag | UNP B1MLW2 |
| E     | 492     | GLY      | -      | expression tag | UNP B1MLW2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 493     | GLY      | -      | expression tag | UNP B1MLW2 |
| E     | 494     | GLY      | -      | expression tag | UNP B1MLW2 |
| E     | 495     | GLY      | -      | expression tag | UNP B1MLW2 |
| E     | 496     | GLU      | -      | expression tag | UNP B1MLW2 |
| E     | 497     | ASN      | -      | expression tag | UNP B1MLW2 |
| E     | 498     | LEU      | -      | expression tag | UNP B1MLW2 |
| E     | 499     | TYR      | -      | expression tag | UNP B1MLW2 |
| E     | 500     | PHE      | -      | expression tag | UNP B1MLW2 |
| E     | 501     | GLN      | -      | expression tag | UNP B1MLW2 |
| E     | 502     | ASP      | -      | expression tag | UNP B1MLW2 |
| E     | 503     | TYR      | -      | expression tag | UNP B1MLW2 |
| E     | 504     | LYS      | -      | expression tag | UNP B1MLW2 |
| E     | 505     | ASP      | -      | expression tag | UNP B1MLW2 |
| E     | 506     | ASP      | -      | expression tag | UNP B1MLW2 |
| E     | 507     | ASP      | -      | expression tag | UNP B1MLW2 |
| E     | 508     | ASP      | -      | expression tag | UNP B1MLW2 |
| E     | 509     | LYS      | -      | expression tag | UNP B1MLW2 |
| E     | 510     | HIS      | -      | expression tag | UNP B1MLW2 |
| E     | 511     | HIS      | -      | expression tag | UNP B1MLW2 |
| E     | 512     | HIS      | -      | expression tag | UNP B1MLW2 |
| E     | 513     | HIS      | -      | expression tag | UNP B1MLW2 |
| E     | 514     | HIS      | -      | expression tag | UNP B1MLW2 |
| E     | 515     | HIS      | -      | expression tag | UNP B1MLW2 |
| F     | 477     | GLY      | -      | expression tag | UNP B1MLW2 |
| F     | 478     | LEU      | -      | expression tag | UNP B1MLW2 |
| F     | 479     | SER      | -      | expression tag | UNP B1MLW2 |
| F     | 480     | GLY      | -      | expression tag | UNP B1MLW2 |
| F     | 481     | GLN      | -      | expression tag | UNP B1MLW2 |
| F     | 482     | PRO      | -      | expression tag | UNP B1MLW2 |
| F     | 483     | PRO      | -      | expression tag | UNP B1MLW2 |
| F     | 484     | ARG      | -      | expression tag | UNP B1MLW2 |
| F     | 485     | SER      | -      | expression tag | UNP B1MLW2 |
| F     | 486     | PRO      | -      | expression tag | UNP B1MLW2 |
| F     | 487     | SER      | -      | expression tag | UNP B1MLW2 |
| F     | 488     | SER      | -      | expression tag | UNP B1MLW2 |
| F     | 489     | GLY      | -      | expression tag | UNP B1MLW2 |
| F     | 490     | SER      | -      | expression tag | UNP B1MLW2 |
| F     | 491     | SER      | -      | expression tag | UNP B1MLW2 |
| F     | 492     | GLY      | -      | expression tag | UNP B1MLW2 |
| F     | 493     | GLY      | -      | expression tag | UNP B1MLW2 |
| F     | 494     | GLY      | -      | expression tag | UNP B1MLW2 |
| F     | 495     | GLY      | -      | expression tag | UNP B1MLW2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | 496     | GLU      | -      | expression tag | UNP B1MLW2 |
| F     | 497     | ASN      | -      | expression tag | UNP B1MLW2 |
| F     | 498     | LEU      | -      | expression tag | UNP B1MLW2 |
| F     | 499     | TYR      | -      | expression tag | UNP B1MLW2 |
| F     | 500     | PHE      | -      | expression tag | UNP B1MLW2 |
| F     | 501     | GLN      | -      | expression tag | UNP B1MLW2 |
| F     | 502     | ASP      | -      | expression tag | UNP B1MLW2 |
| F     | 503     | TYR      | -      | expression tag | UNP B1MLW2 |
| F     | 504     | LYS      | -      | expression tag | UNP B1MLW2 |
| F     | 505     | ASP      | -      | expression tag | UNP B1MLW2 |
| F     | 506     | ASP      | -      | expression tag | UNP B1MLW2 |
| F     | 507     | ASP      | -      | expression tag | UNP B1MLW2 |
| F     | 508     | ASP      | -      | expression tag | UNP B1MLW2 |
| F     | 509     | LYS      | -      | expression tag | UNP B1MLW2 |
| F     | 510     | HIS      | -      | expression tag | UNP B1MLW2 |
| F     | 511     | HIS      | -      | expression tag | UNP B1MLW2 |
| F     | 512     | HIS      | -      | expression tag | UNP B1MLW2 |
| F     | 513     | HIS      | -      | expression tag | UNP B1MLW2 |
| F     | 514     | HIS      | -      | expression tag | UNP B1MLW2 |
| F     | 515     | HIS      | -      | expression tag | UNP B1MLW2 |

- Molecule 3 is a protein called ATP synthase gamma chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | G     | 306      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2315  | 1451 | 412 | 448 | 4 |         |       |

- Molecule 4 is a protein called ATP synthase epsilon chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | H     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 920   | 573 | 161 | 185 | 1 |         |       |

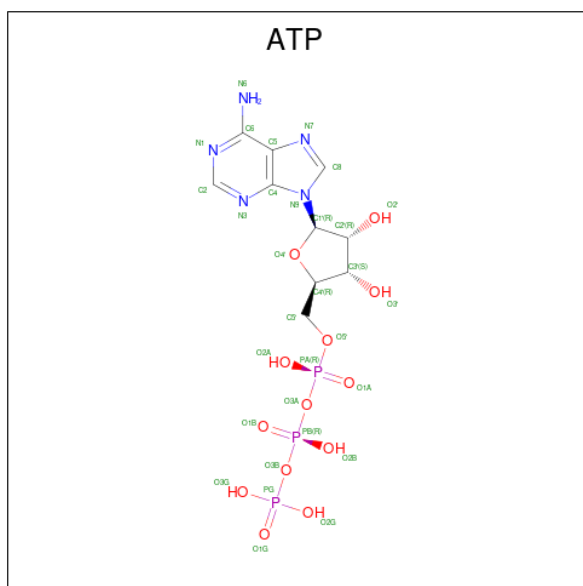
- Molecule 5 is a protein called ATP synthase subunit b.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | b     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 588   | 351 | 113 | 123 | 1 |         |       |

- Molecule 6 is a protein called ATP synthase subunit b-delta.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | d     | 382      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2850  | 1758 | 522 | 568 | 2 |         |       |

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 7   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 7   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 7   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 7   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 8   | B     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 8   | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 8   | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 8   | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

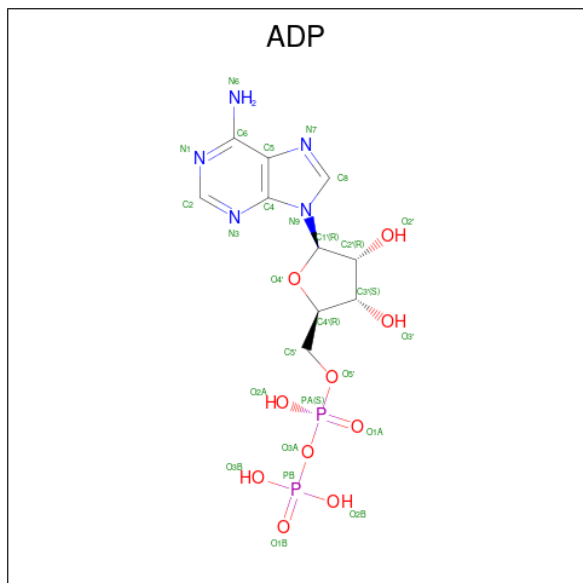
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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 8   | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

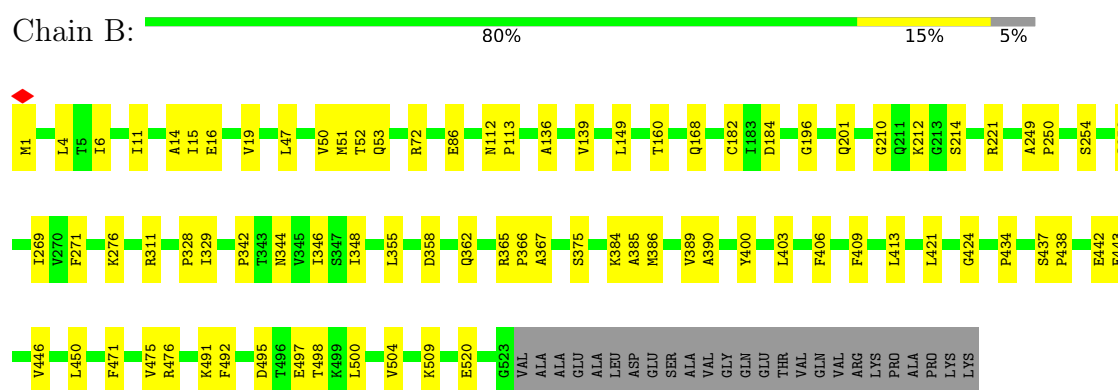


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 9   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 9   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

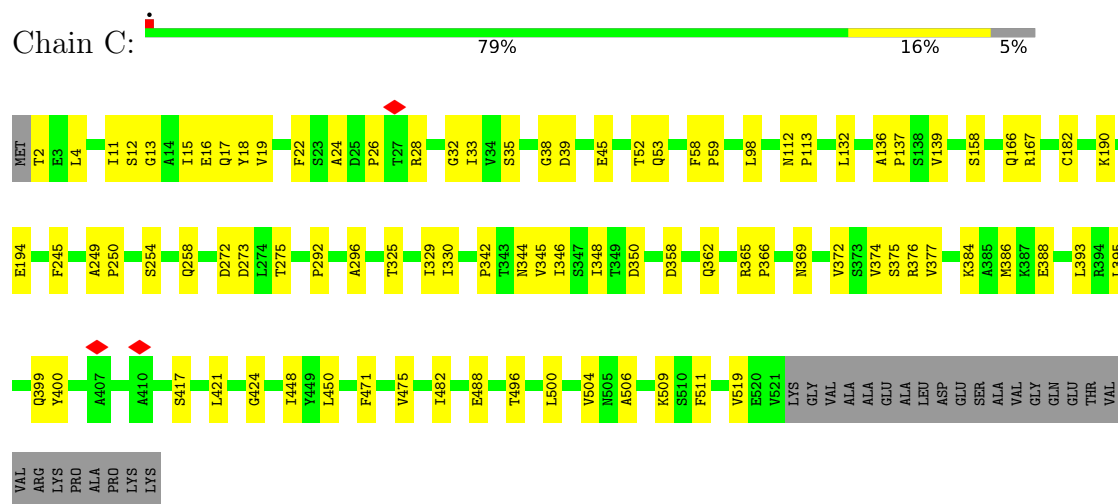
### 3 Residue-property plots

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

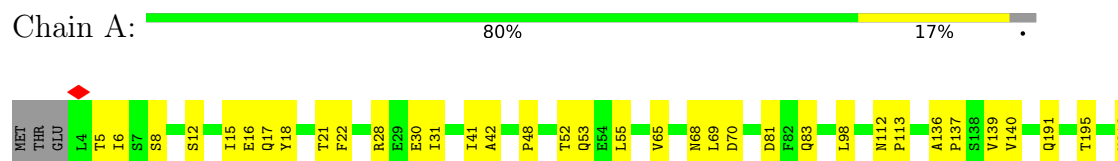
- Molecule 1: ATP synthase subunit alpha

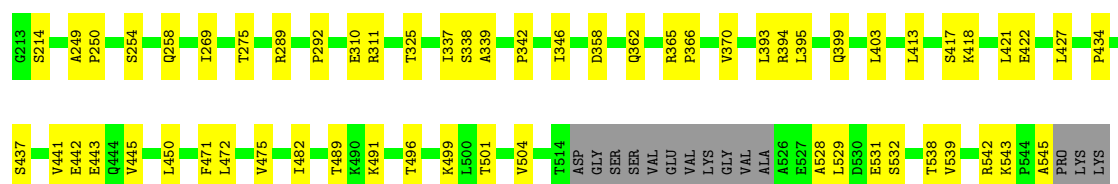


- Molecule 1: ATP synthase subunit alpha



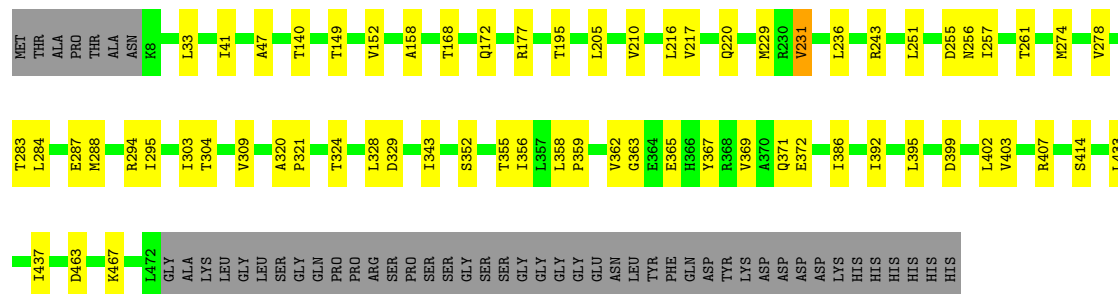
- Molecule 1: ATP synthase subunit alpha





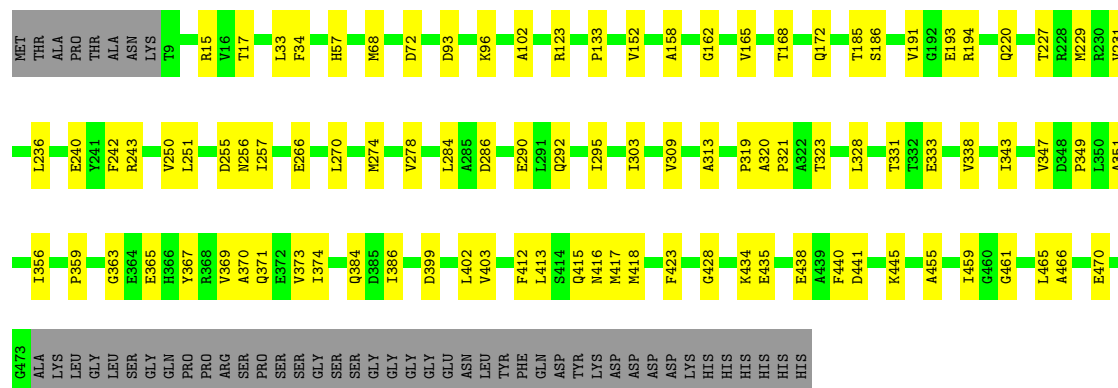
• Molecule 2: ATP synthase subunit beta

Chain D: 77% 13% 10%



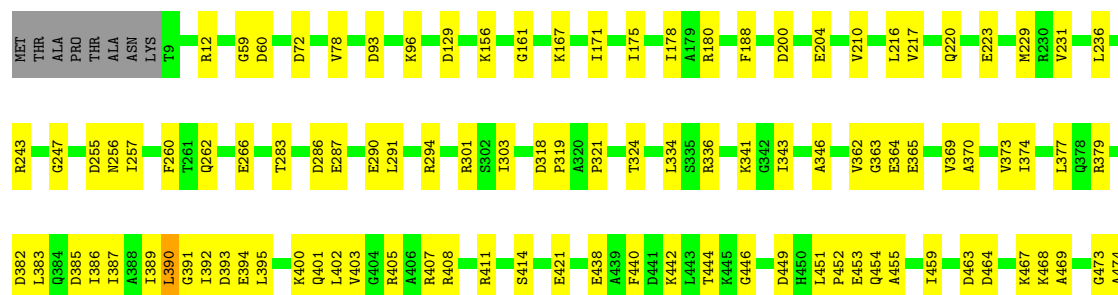
• Molecule 2: ATP synthase subunit beta

Chain E: 72% 18% 10%



• Molecule 2: ATP synthase subunit beta

Chain F: 71% 20% 10%



LYS  
LEU  
GLY  
LEU  
SER  
GLY  
GLN  
PRO  
PRO  
ARG  
SER  
PRO  
SER  
SER  
GLY  
SER  
SER  
GLY  
GLY  
GLY  
GLY  
GLY  
GLN  
ASN  
LEU  
TYR  
PHE  
GLN  
ASP  
TYR  
LYS  
ASP  
ASP  
ASP  
ASP  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 3: ATP synthase gamma chain

Chain G: 73% 27%

MET  
G2  
E7  
L8  
R9  
R10  
R11  
I12  
A17  
I18  
K19  
T22  
K23  
A24  
T28  
A29  
T30  
I33  
Q37  
V40  
Y46  
L63  
D64  
H65  
P66  
L67  
L68  
V69  
E70  
R71  
R76  
A77  
G78  
V79  
L80  
D85  
L97  
F98  
V99  
A100  
E101  
Y104  
A105  
L106  
V118  
V119  
G120  
A123  
L124  
N125  
Y126  
A137  
Y147  
A154  
V158  
L162  
A163  
G164  
D167  
P172  
G173  
L174  
I177  
G178  
V180  
D181  
L182  
H183  
H184  
I185  
M193  
L194  
A198  
R202  
I203  
A204  
P205  
M206  
E207  
V208  
E209  
V210  
V211  
G212  
E213  
A214  
A215  
G216  
T219  
Q220  
Y221  
S222  
L234  
L235  
P236  
R237  
Y238  
L239  
A240  
T241  
R242  
V243  
L248  
A256  
D270  
K274  
L278  
V299  
A306  
G307  
HIS

• Molecule 4: ATP synthase epsilon chain

Chain H: 7% 41% 59%

M1  
S2  
E3  
I4  
D5  
A10  
V11  
E12  
I15  
F22  
V23  
F24  
T25  
R26  
T27  
T28  
E31  
I34  
L35  
P36  
I39  
P40  
L41  
V42  
D48  
A49  
A50  
V51  
K52  
I53  
E54  
E56  
D60  
L61  
W62  
W63  
A64  
I65  
D66  
G67  
G68  
F69  
L70  
S71  
I72  
T73  
D74  
T75  
K76  
V77  
S78  
I79  
A84  
Q85  
A86  
R87  
I90  
D91  
E92  
A93  
K94  
A95  
K96  
T97  
D98  
S99  
G100  
S101  
E102  
D103  
V106  
A107  
G110  
R111  
A112  
R115  
A116  
L117  
G118  
Q119  
T120  
V121

• Molecule 5: ATP synthase subunit b

Chain b: 27% 19% 55%

MET  
GLY  
LEU  
LEU  
ALA  
HIS  
SER  
VAL  
ALA  
SER  
VAL  
ALA  
THR  
VAL  
VAL  
VAL  
VAL  
ALA  
ALA  
ALA  
ALA  
ALA  
GLU  
GLY  
GLY  
GLY  
LYS  
GLN  
ASN  
ASN  
PHE  
PHE  
LEU  
ILE  
PRO  
ASN  
GLY  
THR  
PHE  
ASP  
VAL  
VAL  
LEU  
ILE  
VAL  
ALA  
ALA  
VAL  
ILE  
THR  
GLY  
PHE  
PHE  
VAL  
VAL  
VAL  
PRO  
PRO  
ILE  
GLN  
VAL  
LEU  
LYS  
ALA  
ALA  
ALA  
ALA  
ALA  
GLU  
ALA  
ALA  
ASP  
Y89  
L93  
R97  
A107  
E110  
L115  
E116  
D117  
M118  
R119  
Q120  
R121  
A122  
N123  
A124  
E125  
A126  
T127  
A128  
V129  
T130  
E131  
T132  
A133  
L137  
A138  
R139  
Q140  
G141  
E142  
V143  
T144  
E147  
L148  
L155  
S156  
R157  
A160  
E161  
L164  
L168  
SER  
GLY  
PRO  
ALA  
ASN  
ALA  
ALA  
ARG  
GLY

• Molecule 6: ATP synthase subunit b-delta

Chain d: 56% 29% 15%

MET  
SER  
THR  
PHE  
ASP  
ILE  
GLY  
GLN  
LEU  
ILE  
ILE  
GLY  
PHE  
ALA  
VAL  
ILE  
VAL  
PHE  
LEU  
VAL  
VAL  
VAL  
LYS  
TYR  
VAL  
VAL  
VAL  
PRO  
PRO  
VAL  
VAL  
A91  
D92  
A93  
E94  
V95  
E96  
V100  
H101  
G102  
Q103  
V104  
Q105  
I106  
V107  
L108  
Q109  
R110  
T114  
A123  
V126  
R127  
R128  
A129  
L132  
V133  
V137  
A145  
ALA  
ILE  
GLU  
ALA  
R66  
A67  
D68  
Q71  
I72  
W73  
E74  
E75  
A76  
K77  
Q82  
I83  
S84  
K85  
Q86  
L87  
R88  
E89  
Q90  
A91  
D92  
A93  
E94  
V95  
E96  
V100  
H101  
G102  
Q103  
V104  
Q105  
I106  
V107  
L108  
Q109  
R110  
T114  
A123  
V126  
R127  
R128  
A129  
L132  
V133  
V137  
A145

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| V382 | K383 | A384 | A385 | A386 | P387 | I388 | R393 | T394 | R395 | L396 | V399 | T403 | Y404 | L412 | D413 | V414 | L418 | L419 | L422 | E430 | G433 | S434 | L435 | A442 | A443 | L446 | P447 | ASN  | V258 | R259 | V262 | E277 | Y278 | R281 | L282 | R287 | A288 | E289 | Q293 | I294 | V297 | E298 | D299 | Q300 | L314 | A315 | T316 | A325 | V329 | A330 | L331 | L332 | V335 | L336 | N341 | E342 | V343 | T344 | T345 | L348 | V352 | R353 | V358 | R359 | A360 | A363 | V364 | V367 | V372 |
| T146 | V147 | D148 | R149 | F150 | L151 | D152 | E153 | L154 | V161 | M175 | S179 | S182 | L183 | Q186 | V187 | S196 | L197 | L202 | S203 | E207 | L215 | L216 | V221 | K224 | H225 | L226 | S227 | E228 | P229 | V230 | D231 | E234 | K238 | L241 | V242 | L246 | K249 | I250 | G251 | A252 | P253 | A254 | L255 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 45839                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 1600                                    | Depositor |
| Magnification                        | 165000                                  | Depositor |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.802                                   | Depositor |
| Minimum map value                    | -0.337                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.020                                   | Depositor |
| Recommended contour level            | 0.072                                   | Depositor |
| Map size (Å)                         | 516.8, 516.8, 516.8                     | wwPDB     |
| Map dimensions                       | 680, 680, 680                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.76, 0.76, 0.76                        | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG

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     | 0.19         | 0/4083      | 0.32        | 0/5540      |
| 1   | B     | 0.16         | 0/4021      | 0.30        | 0/5455      |
| 1   | C     | 0.21         | 0/4000      | 0.30        | 0/5429      |
| 2   | D     | 0.13         | 0/3630      | 0.27        | 0/4926      |
| 2   | E     | 0.16         | 0/3625      | 0.31        | 0/4920      |
| 2   | F     | 0.21         | 0/3630      | 0.35        | 0/4927      |
| 3   | G     | 0.20         | 0/2347      | 0.35        | 0/3182      |
| 4   | H     | 0.44         | 0/933       | 0.64        | 0/1264      |
| 5   | b     | 0.35         | 0/588       | 0.54        | 0/792       |
| 6   | d     | 0.17         | 0/2874      | 0.33        | 0/3901      |
| All | All   | 0.20         | 0/29731     | 0.33        | 0/40336     |

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 [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     | 4021  | 0        | 4018     | 79      | 0            |
| 1   | B     | 3959  | 0        | 3956     | 57      | 0            |
| 1   | C     | 3938  | 0        | 3928     | 61      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | D     | 3566  | 0        | 3556     | 50      | 0            |
| 2   | E     | 3561  | 0        | 3546     | 72      | 0            |
| 2   | F     | 3566  | 0        | 3551     | 75      | 0            |
| 3   | G     | 2315  | 0        | 2346     | 80      | 0            |
| 4   | H     | 920   | 0        | 915      | 64      | 0            |
| 5   | b     | 588   | 0        | 589      | 39      | 0            |
| 6   | d     | 2850  | 0        | 2913     | 118     | 0            |
| 7   | A     | 31    | 0        | 12       | 0       | 0            |
| 7   | B     | 31    | 0        | 12       | 0       | 0            |
| 7   | C     | 31    | 0        | 12       | 0       | 0            |
| 7   | F     | 31    | 0        | 12       | 0       | 0            |
| 8   | A     | 1     | 0        | 0        | 0       | 0            |
| 8   | B     | 1     | 0        | 0        | 0       | 0            |
| 8   | C     | 1     | 0        | 0        | 0       | 0            |
| 8   | D     | 1     | 0        | 0        | 0       | 0            |
| 8   | E     | 1     | 0        | 0        | 0       | 0            |
| 9   | D     | 27    | 0        | 12       | 0       | 0            |
| 9   | E     | 27    | 0        | 12       | 2       | 0            |
| All | All   | 29467 | 0        | 29390    | 625     | 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 11.

All (625) 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) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:27:THR:HG22  | 4:H:28:THR:H     | 1.43                     | 0.84              |
| 4:H:103:ASP:HB3  | 4:H:106:VAL:HG12 | 1.63                     | 0.80              |
| 4:H:52:LYS:HG3   | 4:H:61:LEU:O     | 1.86                     | 0.76              |
| 3:G:214:ALA:HB2  | 1:A:542:ARG:HD2  | 1.71                     | 0.73              |
| 4:H:26:ARG:HD2   | 4:H:50:ALA:HB3   | 1.71                     | 0.73              |
| 3:G:202:ARG:HH21 | 3:G:205:PRO:HB2  | 1.53                     | 0.72              |
| 5:b:157:ARG:O    | 5:b:161:GLU:HG2  | 1.90                     | 0.72              |
| 5:b:107:ALA:O    | 5:b:110:GLU:HG3  | 1.89                     | 0.72              |
| 6:d:225:HIS:O    | 6:d:228:GLU:HG2  | 1.90                     | 0.70              |
| 2:D:288:MET:HA   | 2:D:288:MET:HE3  | 1.73                     | 0.69              |
| 3:G:105:ALA:HB3  | 1:A:528:ALA:HA   | 1.73                     | 0.69              |
| 1:B:409:PHE:CD2  | 3:G:28:ILE:HG13  | 2.27                     | 0.69              |
| 2:E:367:TYR:O    | 2:E:371:GLN:HG2  | 1.92                     | 0.69              |
| 1:B:450:LEU:HD11 | 1:B:471:PHE:CD2  | 2.28                     | 0.69              |
| 6:d:73:ALA:O     | 6:d:77:LYS:HG2   | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:434:PRO:HG2  | 1:B:437:SER:OG   | 1.92                     | 0.69              |
| 4:H:27:THR:HG22  | 4:H:28:THR:N     | 2.06                     | 0.69              |
| 6:d:161:VAL:HG11 | 1:A:28:ARG:HH12  | 1.57                     | 0.69              |
| 2:D:243:ARG:HD3  | 2:D:303:ILE:CD1  | 2.23                     | 0.68              |
| 2:E:102:ALA:HB2  | 2:E:231:VAL:HG22 | 1.75                     | 0.68              |
| 4:H:99:SER:HA    | 4:H:110:GLY:HA3  | 1.73                     | 0.68              |
| 4:H:4:ILE:HD12   | 4:H:4:ILE:H      | 1.57                     | 0.68              |
| 2:E:434:LYS:O    | 2:E:438:GLU:HG2  | 1.94                     | 0.68              |
| 2:F:236:LEU:HD21 | 2:F:294:ARG:HB2  | 1.75                     | 0.68              |
| 3:G:106:LEU:HA   | 1:A:528:ALA:HB1  | 1.75                     | 0.68              |
| 6:d:137:VAL:HG11 | 6:d:419:LEU:CD2  | 2.24                     | 0.68              |
| 4:H:96:LYS:HE2   | 4:H:121:VAL:HG13 | 1.76                     | 0.68              |
| 5:b:122:ALA:O    | 5:b:125:GLU:HG3  | 1.94                     | 0.68              |
| 2:D:236:LEU:HD21 | 2:D:294:ARG:HB2  | 1.75                     | 0.67              |
| 1:B:6:ILE:HD12   | 6:d:215:LEU:HD11 | 1.75                     | 0.67              |
| 1:A:254:SER:O    | 1:A:258:GLN:HG3  | 1.94                     | 0.67              |
| 2:F:161:GLY:HA3  | 2:F:167:LYS:HE3  | 1.76                     | 0.67              |
| 2:E:386:ILE:HD11 | 3:G:17:ALA:HB1   | 1.74                     | 0.67              |
| 2:E:417:MET:HE2  | 9:E:600:ADP:HN61 | 1.58                     | 0.67              |
| 6:d:92:ASP:O     | 6:d:95:VAL:HG22  | 1.94                     | 0.67              |
| 2:E:274:MET:HE3  | 3:G:299:VAL:HG22 | 1.77                     | 0.67              |
| 2:E:284:LEU:CD2  | 2:E:323:THR:HG21 | 2.25                     | 0.66              |
| 1:B:212:LYS:HE2  | 1:B:214:SER:HB2  | 1.78                     | 0.66              |
| 2:D:343:ILE:HG23 | 2:D:414:SER:HB3  | 1.78                     | 0.66              |
| 5:b:124:ALA:O    | 5:b:127:THR:HG22 | 1.96                     | 0.66              |
| 1:A:482:ILE:HG23 | 1:A:496:THR:HG23 | 1.77                     | 0.65              |
| 2:F:382:ASP:OD1  | 2:F:383:LEU:HG   | 1.95                     | 0.65              |
| 6:d:147:VAL:O    | 6:d:151:LEU:HD23 | 1.97                     | 0.65              |
| 2:E:243:ARG:HD3  | 2:E:303:ILE:CD1  | 2.27                     | 0.65              |
| 1:A:65:VAL:HG22  | 1:A:98:LEU:HD21  | 1.79                     | 0.65              |
| 2:F:243:ARG:HD3  | 2:F:303:ILE:HG13 | 1.77                     | 0.65              |
| 3:G:204:ALA:HB3  | 3:G:205:PRO:HD3  | 1.78                     | 0.65              |
| 2:E:15:ARG:HG2   | 1:A:70:ASP:HA    | 1.79                     | 0.64              |
| 5:b:89:TYR:CE1   | 5:b:93:LEU:HD22  | 2.32                     | 0.64              |
| 2:E:284:LEU:HD21 | 2:E:323:THR:HG21 | 1.77                     | 0.64              |
| 1:A:358:ASP:O    | 1:A:362:GLN:HG3  | 1.97                     | 0.64              |
| 1:C:18:TYR:CG    | 6:d:331:LEU:HD12 | 2.32                     | 0.64              |
| 2:F:391:GLY:HA3  | 2:F:394:GLU:HG3  | 1.77                     | 0.64              |
| 6:d:71:GLN:O     | 6:d:75:GLU:HG2   | 1.96                     | 0.64              |
| 2:F:379:ARG:HA   | 2:F:382:ASP:OD2  | 1.97                     | 0.64              |
| 3:G:167:ASP:HA   | 3:G:172:PRO:HA   | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:d:255:LEU:O    | 6:d:259:ARG:HG3  | 1.96                     | 0.64              |
| 6:d:336:LEU:HD11 | 6:d:348:LEU:HD12 | 1.79                     | 0.64              |
| 2:F:385:ASP:O    | 2:F:389:ILE:HG22 | 1.98                     | 0.64              |
| 1:C:292:PRO:HB2  | 1:C:296:ALA:HA   | 1.80                     | 0.64              |
| 4:H:41:LEU:O     | 4:H:71:SER:HA    | 1.98                     | 0.64              |
| 4:H:1:MET:O      | 4:H:36:PRO:HB3   | 1.97                     | 0.63              |
| 1:A:17:GLN:O     | 1:A:21:THR:HG22  | 1.99                     | 0.63              |
| 3:G:274:LYS:NZ   | 3:G:274:LYS:HB3  | 2.14                     | 0.63              |
| 1:B:409:PHE:HD2  | 3:G:28:ILE:HG13  | 1.62                     | 0.63              |
| 2:E:399:ASP:O    | 2:E:403:VAL:HG23 | 1.99                     | 0.63              |
| 2:D:152:VAL:HG22 | 2:D:356:ILE:HD13 | 1.80                     | 0.63              |
| 2:F:321:PRO:HA   | 2:F:324:THR:HG22 | 1.80                     | 0.63              |
| 5:b:148:LEU:HD11 | 1:A:12:SER:HB3   | 1.80                     | 0.62              |
| 1:A:413:LEU:HG   | 1:A:417:SER:HB2  | 1.80                     | 0.62              |
| 4:H:65:ILE:HG22  | 4:H:67:GLY:H     | 1.64                     | 0.62              |
| 4:H:92:GLU:O     | 4:H:96:LYS:HG2   | 2.00                     | 0.62              |
| 1:C:139:VAL:HG22 | 2:D:195:THR:HG23 | 1.82                     | 0.62              |
| 1:C:254:SER:O    | 1:C:258:GLN:HG3  | 1.99                     | 0.62              |
| 5:b:148:LEU:HD13 | 1:A:8:SER:HB3    | 1.80                     | 0.62              |
| 6:d:331:LEU:O    | 6:d:335:VAL:HG23 | 1.99                     | 0.62              |
| 2:F:459:ILE:HG13 | 2:F:464:ASP:HB3  | 1.80                     | 0.62              |
| 3:G:79:VAL:HG12  | 3:G:184:HIS:HB2  | 1.80                     | 0.62              |
| 6:d:82:GLN:O     | 6:d:86:GLN:HG3   | 2.00                     | 0.62              |
| 6:d:123:ALA:O    | 6:d:127:ARG:HG2  | 1.99                     | 0.61              |
| 5:b:133:ALA:HB1  | 6:d:106:ILE:HD11 | 1.81                     | 0.61              |
| 1:C:22:PHE:CZ    | 1:C:24:ALA:HB2   | 2.35                     | 0.61              |
| 2:D:33:LEU:HD12  | 2:D:33:LEU:H     | 1.66                     | 0.61              |
| 3:G:219:THR:OG1  | 4:H:40:PRO:HG2   | 1.99                     | 0.61              |
| 2:D:158:ALA:HB3  | 2:D:328:LEU:HD13 | 1.82                     | 0.61              |
| 2:D:392:ILE:HG13 | 2:D:392:ILE:O    | 2.00                     | 0.61              |
| 6:d:388:ILE:HD11 | 6:d:393:ARG:HG3  | 1.81                     | 0.61              |
| 6:d:288:ALA:HB2  | 6:d:343:VAL:HG11 | 1.83                     | 0.61              |
| 2:E:338:VAL:HG12 | 2:E:343:ILE:HB   | 1.82                     | 0.60              |
| 6:d:161:VAL:CG2  | 6:d:404:TYR:HA   | 2.31                     | 0.60              |
| 6:d:216:LEU:HD11 | 6:d:226:LEU:HD12 | 1.82                     | 0.60              |
| 1:A:489:THR:HG23 | 1:A:491:LYS:H    | 1.66                     | 0.60              |
| 1:A:501:THR:O    | 1:A:504:VAL:HG12 | 2.01                     | 0.60              |
| 2:F:401:GLN:O    | 2:F:405:ARG:HG3  | 2.01                     | 0.60              |
| 6:d:332:LEU:HD21 | 6:d:348:LEU:HB3  | 1.83                     | 0.60              |
| 6:d:442:ALA:HB2  | 1:A:22:PHE:CZ    | 2.36                     | 0.60              |
| 1:B:4:LEU:CD2    | 6:d:246:LEU:HD22 | 2.30                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:408:ARG:HG2  | 2:F:453:GLU:OE1  | 2.01                     | 0.60              |
| 1:B:358:ASP:O    | 1:B:362:GLN:HG3  | 2.02                     | 0.60              |
| 1:C:358:ASP:O    | 1:C:362:GLN:HG3  | 2.01                     | 0.60              |
| 5:b:126:ALA:O    | 5:b:130:THR:HG23 | 2.02                     | 0.60              |
| 6:d:363:ALA:O    | 6:d:367:VAL:HG23 | 2.01                     | 0.59              |
| 1:B:210:GLY:HA3  | 1:B:276:LYS:HD3  | 1.84                     | 0.59              |
| 1:C:16:GLU:HA    | 1:C:19:VAL:HG12  | 1.85                     | 0.59              |
| 4:H:39:ILE:HD12  | 4:H:40:PRO:HD2   | 1.84                     | 0.59              |
| 3:G:237:ARG:O    | 3:G:241:THR:HG23 | 2.01                     | 0.59              |
| 1:A:337:ILE:HD12 | 1:A:338:SER:N    | 2.17                     | 0.59              |
| 2:E:72:ASP:OD2   | 1:A:53:GLN:HG3   | 2.02                     | 0.59              |
| 4:H:115:ARG:HH22 | 4:H:120:THR:HG21 | 1.68                     | 0.59              |
| 6:d:137:VAL:HG11 | 6:d:419:LEU:HD21 | 1.82                     | 0.59              |
| 1:C:136:ALA:HB1  | 1:C:137:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:65:VAL:CG2   | 1:A:98:LEU:HD21  | 2.33                     | 0.59              |
| 4:H:27:THR:CG2   | 4:H:28:THR:H     | 2.12                     | 0.59              |
| 6:d:145:ALA:HB1  | 6:d:149:ARG:NH1  | 2.17                     | 0.59              |
| 6:d:325:ALA:O    | 6:d:329:VAL:HG23 | 2.03                     | 0.59              |
| 3:G:37:GLN:O     | 3:G:40:VAL:HG12  | 2.02                     | 0.59              |
| 2:F:262:GLN:O    | 2:F:266:GLU:HG3  | 2.03                     | 0.59              |
| 6:d:175:MET:HB3  | 6:d:179:SER:HB2  | 1.85                     | 0.59              |
| 6:d:446:LEU:HD23 | 1:A:18:TYR:CE2   | 2.38                     | 0.59              |
| 1:C:98:LEU:HG    | 1:C:132:LEU:HD12 | 1.84                     | 0.58              |
| 6:d:150:PHE:CE1  | 6:d:433:GLY:HA3  | 2.38                     | 0.58              |
| 1:A:342:PRO:O    | 1:A:346:ILE:HG13 | 2.02                     | 0.58              |
| 1:C:13:GLY:O     | 1:C:17:GLN:HG3   | 2.03                     | 0.58              |
| 4:H:93:ALA:O     | 4:H:97:THR:HG23  | 2.03                     | 0.58              |
| 1:B:471:PHE:O    | 1:B:475:VAL:HG23 | 2.03                     | 0.58              |
| 6:d:145:ALA:HB1  | 6:d:149:ARG:HH12 | 1.68                     | 0.58              |
| 2:E:266:GLU:O    | 2:E:270:LEU:HG   | 2.03                     | 0.58              |
| 5:b:141:GLY:HA2  | 5:b:144:THR:HG22 | 1.85                     | 0.58              |
| 6:d:103:GLN:O    | 6:d:106:ILE:HG22 | 2.02                     | 0.58              |
| 6:d:175:MET:HB3  | 6:d:179:SER:CB   | 2.34                     | 0.58              |
| 6:d:101:HIS:O    | 6:d:105:GLN:HG2  | 2.02                     | 0.58              |
| 1:C:330:ILE:HD11 | 1:C:345:VAL:HG21 | 1.85                     | 0.58              |
| 2:F:334:LEU:HA   | 2:F:346:ALA:O    | 2.04                     | 0.58              |
| 4:H:64:ALA:HB3   | 4:H:85:GLN:HB2   | 1.85                     | 0.58              |
| 2:E:365:GLU:O    | 2:E:369:VAL:HG23 | 2.04                     | 0.58              |
| 5:b:118:MET:HE3  | 6:d:91:ALA:HB1   | 1.85                     | 0.58              |
| 2:F:286:ASP:O    | 2:F:290:GLU:HG3  | 2.04                     | 0.58              |
| 2:E:386:ILE:HD11 | 3:G:17:ALA:CB    | 2.34                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:254:SER:O    | 1:B:258:GLN:HG3  | 2.04                     | 0.57              |
| 1:C:369:ASN:OD1  | 1:C:372:VAL:HG22 | 2.04                     | 0.57              |
| 1:B:384:LYS:HD3  | 1:B:491:LYS:NZ   | 2.18                     | 0.57              |
| 2:D:149:THR:HG21 | 2:D:352:SER:HB3  | 1.85                     | 0.57              |
| 3:G:209:GLU:HG2  | 1:A:539:VAL:O    | 2.03                     | 0.57              |
| 2:D:257:ILE:CG2  | 2:D:309:VAL:HG22 | 2.33                     | 0.57              |
| 6:d:238:LYS:O    | 6:d:242:VAL:HG23 | 2.04                     | 0.57              |
| 6:d:183:LEU:O    | 6:d:187:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:472:LEU:HA   | 1:A:475:VAL:HG12 | 1.87                     | 0.57              |
| 2:E:236:LEU:O    | 2:E:240:GLU:HG3  | 2.05                     | 0.57              |
| 2:F:362:VAL:HG23 | 2:F:363:GLY:H    | 1.69                     | 0.57              |
| 3:G:7:GLU:HG3    | 3:G:10:ARG:HH21  | 1.70                     | 0.57              |
| 1:B:47:LEU:HB3   | 1:B:50:VAL:CG2   | 2.34                     | 0.57              |
| 6:d:68:ASP:O     | 6:d:71:GLN:HG2   | 2.05                     | 0.57              |
| 6:d:298:GLU:CD   | 6:d:372:VAL:HG22 | 2.30                     | 0.56              |
| 4:H:79:ILE:N     | 4:H:79:ILE:HD12  | 2.20                     | 0.56              |
| 1:C:158:SER:HB3  | 1:C:386:MET:HE3  | 1.85                     | 0.56              |
| 2:D:367:TYR:O    | 2:D:371:GLN:HG2  | 2.05                     | 0.56              |
| 2:F:370:ALA:O    | 2:F:374:ILE:HG13 | 2.04                     | 0.56              |
| 3:G:66:PRO:O     | 3:G:69:VAL:HG12  | 2.05                     | 0.56              |
| 6:d:384:ALA:HB2  | 6:d:422:LEU:CD2  | 2.35                     | 0.56              |
| 2:F:343:ILE:HG23 | 2:F:414:SER:HB3  | 1.87                     | 0.56              |
| 3:G:29:ALA:O     | 3:G:33:ILE:HG13  | 2.06                     | 0.56              |
| 5:b:133:ALA:CB   | 6:d:106:ILE:HD11 | 2.36                     | 0.56              |
| 6:d:110:ARG:HG3  | 1:A:6:ILE:HD11   | 1.87                     | 0.56              |
| 2:D:217:VAL:HG12 | 2:D:231:VAL:HG23 | 1.88                     | 0.56              |
| 6:d:332:LEU:HD22 | 6:d:352:VAL:HG21 | 1.87                     | 0.56              |
| 2:D:220:GLN:HA   | 2:D:220:GLN:OE1  | 2.06                     | 0.56              |
| 2:F:283:THR:O    | 2:F:287:GLU:HG3  | 2.06                     | 0.55              |
| 5:b:125:GLU:O    | 5:b:129:VAL:HG23 | 2.06                     | 0.55              |
| 6:d:246:LEU:O    | 6:d:250:ILE:HG12 | 2.04                     | 0.55              |
| 1:C:500:LEU:O    | 1:C:504:VAL:HG23 | 2.07                     | 0.55              |
| 1:C:511:PHE:HD2  | 1:C:519:VAL:HG11 | 1.71                     | 0.55              |
| 1:B:47:LEU:O     | 1:B:50:VAL:HG23  | 2.06                     | 0.55              |
| 2:F:365:GLU:O    | 2:F:369:VAL:HG23 | 2.06                     | 0.55              |
| 3:G:213:GLU:OE1  | 1:A:543:LYS:HA   | 2.06                     | 0.55              |
| 2:E:338:VAL:CG1  | 2:E:343:ILE:HB   | 2.36                     | 0.55              |
| 6:d:293:GLN:O    | 6:d:297:VAL:HG23 | 2.07                     | 0.55              |
| 1:A:191:GLN:O    | 1:A:195:THR:HG23 | 2.06                     | 0.55              |
| 6:d:386:ALA:HB1  | 6:d:387:PRO:HD2  | 1.88                     | 0.55              |
| 3:G:183:LEU:HB2  | 3:G:204:ALA:HB2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:b:137:LEU:HD23 | 5:b:137:LEU:O    | 2.07                     | 0.55              |
| 2:D:243:ARG:HD3  | 2:D:303:ILE:HD12 | 1.89                     | 0.55              |
| 2:F:217:VAL:HG12 | 2:F:231:VAL:HG23 | 1.89                     | 0.55              |
| 1:C:58:PHE:HB3   | 1:C:59:PRO:HD2   | 1.88                     | 0.55              |
| 1:C:511:PHE:CD2  | 1:C:519:VAL:HG11 | 2.41                     | 0.55              |
| 4:H:62:TRP:HB3   | 4:H:116:ALA:O    | 2.07                     | 0.55              |
| 4:H:91:ASP:HB2   | 4:H:94:LYS:HB2   | 1.89                     | 0.55              |
| 1:A:370:VAL:HG13 | 1:A:394:ARG:HG3  | 1.88                     | 0.55              |
| 1:B:160:THR:HG23 | 1:B:375:SER:HB2  | 1.88                     | 0.54              |
| 1:A:212:LYS:HE3  | 1:A:214:SER:OG   | 2.06                     | 0.54              |
| 1:A:81:ASP:HB3   | 1:A:83:GLN:OE1   | 2.08                     | 0.54              |
| 4:H:103:ASP:CB   | 4:H:106:VAL:HG12 | 2.35                     | 0.54              |
| 6:d:446:LEU:HD23 | 1:A:18:TYR:HE2   | 1.72                     | 0.54              |
| 3:G:79:VAL:HG21  | 3:G:104:TYR:HE1  | 1.72                     | 0.54              |
| 1:A:393:LEU:HD11 | 1:A:427:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:418:LYS:O    | 1:A:422:GLU:HG2  | 2.07                     | 0.54              |
| 2:E:185:THR:HG21 | 2:E:242:PHE:CE2  | 2.43                     | 0.54              |
| 1:C:471:PHE:O    | 1:C:475:VAL:HG23 | 2.07                     | 0.54              |
| 3:G:210:TYR:HD1  | 1:A:543:LYS:O    | 1.91                     | 0.54              |
| 1:C:482:ILE:HG23 | 1:C:496:THR:HG23 | 1.88                     | 0.54              |
| 2:F:463:ASP:O    | 2:F:467:LYS:HD3  | 2.08                     | 0.54              |
| 5:b:137:LEU:HD11 | 6:d:110:ARG:HA   | 1.90                     | 0.54              |
| 6:d:316:THR:HG22 | 6:d:359:ARG:HH22 | 1.73                     | 0.54              |
| 3:G:124:LEU:HD21 | 3:G:137:ALA:HB2  | 1.89                     | 0.53              |
| 1:B:355:LEU:HA   | 1:B:367:ALA:O    | 2.09                     | 0.53              |
| 2:F:393:ASP:OD1  | 2:F:400:LYS:HA   | 2.08                     | 0.53              |
| 3:G:147:TYR:CE1  | 4:H:11:VAL:HG21  | 2.43                     | 0.53              |
| 6:d:126:VAL:HG11 | 6:d:443:ALA:HB2  | 1.89                     | 0.53              |
| 2:D:257:ILE:HG21 | 2:D:309:VAL:HG22 | 1.90                     | 0.53              |
| 2:D:274:MET:HE1  | 1:A:292:PRO:HD3  | 1.89                     | 0.53              |
| 2:E:370:ALA:O    | 2:E:374:ILE:HG13 | 2.09                     | 0.53              |
| 2:F:440:PHE:O    | 2:F:444:THR:HG23 | 2.08                     | 0.53              |
| 1:C:35:SER:OG    | 1:C:45:GLU:HG3   | 2.08                     | 0.53              |
| 2:D:365:GLU:O    | 2:D:369:VAL:HG23 | 2.07                     | 0.53              |
| 2:D:463:ASP:O    | 2:D:467:LYS:HG3  | 2.07                     | 0.53              |
| 3:G:214:ALA:HB2  | 1:A:542:ARG:CD   | 2.38                     | 0.53              |
| 3:G:238:TYR:O    | 3:G:242:ARG:HG2  | 2.08                     | 0.53              |
| 2:F:247:GLY:HA2  | 2:F:301:ARG:HG3  | 1.90                     | 0.53              |
| 6:d:336:LEU:HD11 | 6:d:348:LEU:CD1  | 2.39                     | 0.53              |
| 4:H:70:LEU:C     | 4:H:70:LEU:HD23  | 2.34                     | 0.53              |
| 2:E:466:ALA:O    | 2:E:470:GLU:HG2  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:8:LEU:O      | 3:G:12:ILE:HG13  | 2.09                     | 0.53              |
| 5:b:164:LEU:HD21 | 6:d:133:VAL:HG22 | 1.89                     | 0.53              |
| 1:B:184:ASP:OD1  | 1:B:438:PRO:HB3  | 2.09                     | 0.53              |
| 6:d:360:ALA:O    | 6:d:364:VAL:HG23 | 2.09                     | 0.53              |
| 2:E:191:VAL:HB   | 2:E:256:ASN:O    | 2.08                     | 0.53              |
| 4:H:48:ASP:HB3   | 4:H:112:ALA:HA   | 1.91                     | 0.53              |
| 3:G:33:ILE:HD11  | 3:G:256:ALA:HA   | 1.91                     | 0.52              |
| 2:F:401:GLN:HG2  | 2:F:405:ARG:HD2  | 1.91                     | 0.52              |
| 6:d:86:GLN:O     | 6:d:89:GLU:HG2   | 2.08                     | 0.52              |
| 1:C:350:ASP:O    | 1:C:376:ARG:HG3  | 2.09                     | 0.52              |
| 1:B:168:GLN:O    | 1:B:328:PRO:HD2  | 2.09                     | 0.52              |
| 1:C:342:PRO:O    | 1:C:346:ILE:HG13 | 2.10                     | 0.52              |
| 1:C:2:THR:HG22   | 1:C:4:LEU:H      | 1.73                     | 0.52              |
| 2:D:168:THR:O    | 2:D:172:GLN:HG3  | 2.08                     | 0.52              |
| 2:F:171:ILE:O    | 2:F:175:ILE:HG13 | 2.10                     | 0.52              |
| 2:F:451:LEU:H    | 2:F:451:LEU:HD12 | 1.74                     | 0.52              |
| 1:B:11:ILE:O     | 1:B:15:ILE:HG13  | 2.09                     | 0.52              |
| 3:G:97:LEU:HD13  | 3:G:126:TYR:CG   | 2.45                     | 0.52              |
| 6:d:395:ARG:O    | 6:d:399:VAL:HG22 | 2.10                     | 0.52              |
| 3:G:63:LEU:O     | 3:G:63:LEU:HD23  | 2.09                     | 0.52              |
| 6:d:68:ASP:O     | 6:d:72:ILE:HG13  | 2.10                     | 0.52              |
| 1:A:403:LEU:HG   | 1:A:421:LEU:HD21 | 1.92                     | 0.52              |
| 1:C:112:ASN:HB2  | 1:C:113:PRO:CD   | 2.40                     | 0.52              |
| 3:G:40:VAL:HA    | 3:G:248:LEU:HD23 | 1.91                     | 0.52              |
| 3:G:207:GLU:O    | 1:A:538:THR:HA   | 2.10                     | 0.52              |
| 1:C:417:SER:O    | 1:C:421:LEU:HD13 | 2.10                     | 0.52              |
| 3:G:221:TYR:HB3  | 4:H:42:VAL:HG22  | 1.92                     | 0.52              |
| 6:d:110:ARG:CG   | 1:A:6:ILE:HD11   | 2.40                     | 0.52              |
| 3:G:222:SER:HB3  | 4:H:41:LEU:HD23  | 1.91                     | 0.51              |
| 2:D:243:ARG:HB2  | 2:D:303:ILE:HD11 | 1.91                     | 0.51              |
| 2:F:12:ARG:HA    | 2:F:78:VAL:O     | 2.10                     | 0.51              |
| 3:G:278:LEU:HD13 | 3:G:278:LEU:C    | 2.36                     | 0.51              |
| 4:H:101:SER:HB2  | 4:H:106:VAL:HG13 | 1.93                     | 0.51              |
| 6:d:203:SER:O    | 6:d:207:GLU:HG3  | 2.10                     | 0.51              |
| 1:C:28:ARG:O     | 1:C:28:ARG:HG2   | 2.10                     | 0.51              |
| 2:E:359:PRO:HA   | 2:E:363:GLY:O    | 2.10                     | 0.51              |
| 3:G:46:TYR:HB2   | 4:H:10:ALA:O     | 2.10                     | 0.51              |
| 4:H:107:ALA:O    | 4:H:111:ARG:HG3  | 2.10                     | 0.51              |
| 6:d:258:VAL:O    | 6:d:262:VAL:HG22 | 2.11                     | 0.51              |
| 1:A:52:THR:HG22  | 1:A:53:GLN:HG2   | 1.93                     | 0.51              |
| 1:B:365:ARG:HA   | 1:B:366:PRO:C    | 2.36                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:329:ASP:O    | 2:D:355:THR:HG23 | 2.11                     | 0.51              |
| 2:F:390:LEU:HD22 | 3:G:30:THR:CG2   | 2.40                     | 0.51              |
| 4:H:94:LYS:HE2   | 4:H:94:LYS:N     | 2.25                     | 0.51              |
| 5:b:138:ALA:O    | 5:b:142:GLU:HG2  | 2.10                     | 0.51              |
| 1:B:14:ALA:HB1   | 6:d:241:LEU:CD1  | 2.41                     | 0.51              |
| 6:d:161:VAL:HG22 | 6:d:403:ILE:O    | 2.09                     | 0.51              |
| 6:d:182:SER:O    | 6:d:186:GLN:HG2  | 2.11                     | 0.51              |
| 2:E:369:VAL:O    | 2:E:373:VAL:HG23 | 2.11                     | 0.51              |
| 4:H:70:LEU:HD23  | 4:H:71:SER:N     | 2.26                     | 0.51              |
| 2:D:236:LEU:CD1  | 2:D:295:ILE:HG12 | 2.40                     | 0.51              |
| 2:E:93:ASP:OD1   | 2:E:96:LYS:HE2   | 2.10                     | 0.51              |
| 2:E:193:GLU:HG2  | 2:E:194:ARG:N    | 2.26                     | 0.51              |
| 2:F:459:ILE:HG13 | 2:F:464:ASP:CB   | 2.41                     | 0.50              |
| 1:C:22:PHE:CE2   | 1:C:24:ALA:HB2   | 2.47                     | 0.50              |
| 1:C:393:LEU:O    | 1:C:393:LEU:HD23 | 2.11                     | 0.50              |
| 6:d:149:ARG:O    | 6:d:153:GLU:HG3  | 2.10                     | 0.50              |
| 6:d:341:ASN:O    | 6:d:345:THR:HG23 | 2.10                     | 0.50              |
| 2:E:274:MET:HE3  | 3:G:299:VAL:CG2  | 2.40                     | 0.50              |
| 1:B:344:ASN:O    | 1:B:348:ILE:HG13 | 2.11                     | 0.50              |
| 1:B:403:LEU:CB   | 1:B:421:LEU:HD11 | 2.41                     | 0.50              |
| 2:E:402:LEU:O    | 2:E:402:LEU:HD23 | 2.11                     | 0.50              |
| 3:G:19:LYS:HD2   | 3:G:270:ASP:OD1  | 2.11                     | 0.50              |
| 2:F:175:ILE:O    | 2:F:178:ILE:HG22 | 2.11                     | 0.50              |
| 1:A:441:VAL:O    | 1:A:445:VAL:HG23 | 2.12                     | 0.50              |
| 2:E:68:MET:HA    | 2:E:68:MET:HE2   | 1.93                     | 0.50              |
| 2:F:373:VAL:O    | 2:F:377:LEU:HD13 | 2.12                     | 0.50              |
| 6:d:215:LEU:HD23 | 6:d:215:LEU:C    | 2.37                     | 0.50              |
| 2:E:152:VAL:HG22 | 2:E:356:ILE:HD13 | 1.92                     | 0.50              |
| 2:E:158:ALA:HB3  | 2:E:328:LEU:HD13 | 1.94                     | 0.50              |
| 5:b:164:LEU:CD2  | 6:d:133:VAL:HG22 | 2.41                     | 0.50              |
| 2:F:362:VAL:HG23 | 2:F:363:GLY:N    | 2.27                     | 0.50              |
| 4:H:15:ILE:HG13  | 4:H:84:ALA:HB3   | 1.94                     | 0.50              |
| 2:E:313:ALA:HB1  | 1:A:338:SER:HB2  | 1.94                     | 0.49              |
| 1:B:53:GLN:HG3   | 2:F:72:ASP:OD1   | 2.12                     | 0.49              |
| 4:H:35:LEU:HB2   | 4:H:36:PRO:HD2   | 1.94                     | 0.49              |
| 2:E:384:GLN:HA   | 2:E:384:GLN:OE1  | 2.12                     | 0.49              |
| 2:D:236:LEU:HD21 | 2:D:294:ARG:CB   | 2.43                     | 0.49              |
| 4:H:2:SER:O      | 4:H:4:ILE:HD12   | 2.12                     | 0.49              |
| 4:H:39:ILE:HD12  | 4:H:40:PRO:CD    | 2.42                     | 0.49              |
| 2:D:140:THR:O    | 2:D:177:ARG:HD3  | 2.13                     | 0.49              |
| 3:G:65:HIS:CD2   | 3:G:66:PRO:HD2   | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:d:150:PHE:CE2  | 6:d:154:LEU:HD11 | 2.47                     | 0.49              |
| 2:D:386:ILE:HD12 | 2:D:386:ILE:H    | 1.77                     | 0.49              |
| 3:G:164:GLY:HA3  | 3:G:180:VAL:O    | 2.13                     | 0.49              |
| 4:H:90:ILE:HB    | 4:H:117:LEU:HD11 | 1.95                     | 0.49              |
| 2:E:123:ARG:HD3  | 2:E:240:GLU:OE1  | 2.13                     | 0.48              |
| 2:E:284:LEU:C    | 2:E:284:LEU:HD23 | 2.39                     | 0.48              |
| 6:d:137:VAL:HG11 | 6:d:419:LEU:HD23 | 1.94                     | 0.48              |
| 6:d:419:LEU:O    | 6:d:435:LEU:HD12 | 2.14                     | 0.48              |
| 1:B:403:LEU:HB3  | 1:B:421:LEU:HD11 | 1.95                     | 0.48              |
| 1:C:182:CYS:SG   | 1:C:329:ILE:HD11 | 2.53                     | 0.48              |
| 3:G:105:ALA:CB   | 1:A:528:ALA:HA   | 2.41                     | 0.48              |
| 1:A:30:GLU:OE1   | 1:A:48:PRO:HD2   | 2.13                     | 0.48              |
| 6:d:137:VAL:O    | 6:d:137:VAL:HG22 | 2.14                     | 0.48              |
| 1:B:443:GLU:OE2  | 1:B:476:ARG:HD3  | 2.13                     | 0.48              |
| 2:D:386:ILE:HD12 | 2:D:386:ILE:N    | 2.28                     | 0.48              |
| 3:G:76:ARG:NH1   | 3:G:178:LEU:HD11 | 2.29                     | 0.48              |
| 3:G:80:LEU:HD23  | 3:G:185:ILE:HD13 | 1.95                     | 0.48              |
| 4:H:24:PHE:HE2   | 4:H:26:ARG:HE    | 1.62                     | 0.48              |
| 5:b:115:LEU:HD23 | 5:b:119:ARG:HG3  | 1.96                     | 0.48              |
| 6:d:278:TYR:CE2  | 6:d:282:LEU:HD11 | 2.49                     | 0.48              |
| 1:A:543:LYS:NZ   | 1:A:545:ALA:HB2  | 2.29                     | 0.48              |
| 4:H:15:ILE:HG13  | 4:H:84:ALA:CB    | 2.44                     | 0.48              |
| 4:H:52:LYS:HD2   | 4:H:62:TRP:CE2   | 2.48                     | 0.48              |
| 1:C:400:TYR:CG   | 1:C:424:GLY:HA3  | 2.49                     | 0.48              |
| 2:D:403:VAL:O    | 2:D:407:ARG:HG3  | 2.14                     | 0.48              |
| 3:G:274:LYS:HB3  | 3:G:274:LYS:HZ3  | 1.78                     | 0.48              |
| 3:G:24:ALA:O     | 3:G:28:ILE:HG12  | 2.13                     | 0.48              |
| 3:G:71:ARG:HH11  | 3:G:71:ARG:HA    | 1.79                     | 0.48              |
| 3:G:158:VAL:O    | 3:G:162:LEU:HG   | 2.14                     | 0.48              |
| 6:d:85:LYS:HA    | 6:d:88:ARG:HE    | 1.79                     | 0.48              |
| 6:d:331:LEU:C    | 6:d:331:LEU:HD23 | 2.38                     | 0.48              |
| 3:G:7:GLU:HG3    | 3:G:10:ARG:NH2   | 2.29                     | 0.48              |
| 3:G:172:PRO:HG2  | 3:G:177:ILE:C    | 2.38                     | 0.48              |
| 2:E:257:ILE:HG21 | 2:E:309:VAL:HG22 | 1.95                     | 0.48              |
| 6:d:221:VAL:O    | 6:d:224:LYS:HG2  | 2.14                     | 0.48              |
| 2:E:257:ILE:CG2  | 2:E:309:VAL:HG22 | 2.43                     | 0.47              |
| 2:E:455:ALA:O    | 2:E:465:LEU:HD12 | 2.14                     | 0.47              |
| 1:B:112:ASN:HB2  | 1:B:113:PRO:CD   | 2.44                     | 0.47              |
| 1:C:4:LEU:O      | 1:C:4:LEU:HG     | 2.14                     | 0.47              |
| 1:B:16:GLU:HA    | 1:B:19:VAL:HG12  | 1.95                     | 0.47              |
| 2:D:205:LEU:HD22 | 2:D:210:VAL:HG23 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:278:VAL:HG12 | 2:D:278:VAL:O    | 2.15                     | 0.47              |
| 2:F:255:ASP:HA   | 2:F:256:ASN:HA   | 1.62                     | 0.47              |
| 2:F:408:ARG:HH12 | 2:F:449:ASP:C    | 2.22                     | 0.47              |
| 3:G:18:ILE:O     | 3:G:22:THR:HG23  | 2.13                     | 0.47              |
| 3:G:33:ILE:CD1   | 3:G:256:ALA:HA   | 2.44                     | 0.47              |
| 3:G:106:LEU:HD13 | 1:A:529:LEU:O    | 2.14                     | 0.47              |
| 6:d:103:GLN:O    | 6:d:107:VAL:HG23 | 2.13                     | 0.47              |
| 1:B:495:ASP:O    | 1:B:498:THR:HG22 | 2.14                     | 0.47              |
| 6:d:242:VAL:HG21 | 6:d:262:VAL:HG21 | 1.95                     | 0.47              |
| 1:A:531:GLU:O    | 1:A:532:SER:HB3  | 2.13                     | 0.47              |
| 1:C:386:MET:HE1  | 1:C:448:ILE:HD12 | 1.96                     | 0.47              |
| 2:D:236:LEU:HD13 | 2:D:295:ILE:HG12 | 1.97                     | 0.47              |
| 2:D:243:ARG:HD3  | 2:D:303:ILE:HD11 | 1.94                     | 0.47              |
| 2:E:413:LEU:HD23 | 2:E:440:PHE:CZ   | 2.50                     | 0.47              |
| 2:F:210:VAL:HG12 | 2:F:210:VAL:O    | 2.15                     | 0.47              |
| 2:F:389:ILE:HG23 | 2:F:390:LEU:N    | 2.30                     | 0.47              |
| 2:F:390:LEU:HD22 | 3:G:30:THR:HG22  | 1.97                     | 0.47              |
| 3:G:65:HIS:CE1   | 3:G:67:LEU:HG    | 2.49                     | 0.47              |
| 5:b:89:TYR:HE1   | 5:b:93:LEU:HD22  | 1.79                     | 0.47              |
| 1:B:182:CYS:SG   | 1:B:329:ILE:HD11 | 2.55                     | 0.47              |
| 2:F:93:ASP:OD1   | 2:F:96:LYS:HE2   | 2.15                     | 0.47              |
| 4:H:62:TRP:HB2   | 4:H:87:ARG:NE    | 2.29                     | 0.47              |
| 6:d:114:ILE:CG1  | 1:A:6:ILE:HD12   | 2.44                     | 0.47              |
| 1:C:11:ILE:O     | 1:C:15:ILE:HG13  | 2.15                     | 0.47              |
| 2:D:216:LEU:N    | 2:D:216:LEU:HD12 | 2.30                     | 0.47              |
| 2:E:168:THR:O    | 2:E:172:GLN:HG3  | 2.14                     | 0.47              |
| 2:F:220:GLN:HB2  | 2:F:223:GLU:HG3  | 1.97                     | 0.47              |
| 4:H:25:THR:HG23  | 4:H:26:ARG:N     | 2.29                     | 0.47              |
| 1:B:386:MET:O    | 1:B:390:ALA:HB3  | 2.15                     | 0.47              |
| 1:B:500:LEU:O    | 1:B:504:VAL:HG23 | 2.16                     | 0.47              |
| 1:A:68:ASN:O     | 1:A:69:LEU:HD12  | 2.15                     | 0.47              |
| 1:B:384:LYS:HD3  | 1:B:491:LYS:HZ2  | 1.79                     | 0.46              |
| 1:C:166:GLN:HG2  | 1:C:167:ARG:N    | 2.29                     | 0.46              |
| 2:F:451:LEU:HD12 | 2:F:451:LEU:N    | 2.29                     | 0.46              |
| 6:d:161:VAL:HG21 | 6:d:404:TYR:HA   | 1.96                     | 0.46              |
| 2:E:243:ARG:HD3  | 2:E:303:ILE:HD11 | 1.95                     | 0.46              |
| 3:G:235:LEU:N    | 3:G:236:PRO:HD2  | 2.30                     | 0.46              |
| 6:d:396:LEU:HA   | 6:d:399:VAL:HG22 | 1.97                     | 0.46              |
| 1:C:12:SER:O     | 1:C:16:GLU:HG2   | 2.15                     | 0.46              |
| 1:A:21:THR:HG23  | 1:A:21:THR:O     | 2.14                     | 0.46              |
| 5:b:141:GLY:HA2  | 5:b:144:THR:CG2  | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:d:230:VAL:HB   | 6:d:234:GLU:OE1  | 2.14                     | 0.46              |
| 2:E:17:THR:HG23  | 2:E:17:THR:O     | 2.15                     | 0.46              |
| 2:D:402:LEU:C    | 2:D:402:LEU:HD23 | 2.41                     | 0.46              |
| 2:F:229:MET:O    | 2:F:229:MET:HG2  | 2.16                     | 0.46              |
| 3:G:99:VAL:HG21  | 3:G:198:ALA:HB3  | 1.96                     | 0.46              |
| 1:B:509:LYS:HA   | 1:B:520:GLU:OE2  | 2.15                     | 0.46              |
| 1:C:13:GLY:HA2   | 1:C:16:GLU:OE2   | 2.15                     | 0.46              |
| 2:D:283:THR:O    | 2:D:287:GLU:HG3  | 2.15                     | 0.46              |
| 2:F:438:GLU:O    | 2:F:442:LYS:HG3  | 2.16                     | 0.46              |
| 1:C:365:ARG:HA   | 1:C:366:PRO:C    | 2.41                     | 0.46              |
| 2:F:291:LEU:HD23 | 2:F:291:LEU:C    | 2.39                     | 0.46              |
| 2:F:394:GLU:OE1  | 2:F:394:GLU:HA   | 2.16                     | 0.46              |
| 2:F:454:GLN:O    | 2:F:454:GLN:HG3  | 2.15                     | 0.46              |
| 1:B:249:ALA:HB3  | 1:B:250:PRO:HD3  | 1.98                     | 0.46              |
| 5:b:119:ARG:HD3  | 6:d:94:GLU:OE1   | 2.16                     | 0.46              |
| 5:b:160:ALA:O    | 5:b:164:LEU:HD23 | 2.15                     | 0.46              |
| 1:C:112:ASN:HB2  | 1:C:113:PRO:HD2  | 1.98                     | 0.46              |
| 2:E:229:MET:HG2  | 2:E:229:MET:O    | 2.17                     | 0.46              |
| 3:G:79:VAL:HG21  | 3:G:104:TYR:CE1  | 2.49                     | 0.46              |
| 6:d:384:ALA:HB2  | 6:d:422:LEU:HD23 | 1.96                     | 0.45              |
| 1:A:482:ILE:HG12 | 1:A:499:LYS:HE3  | 1.98                     | 0.45              |
| 1:B:52:THR:HG22  | 1:B:53:GLN:HG2   | 1.98                     | 0.45              |
| 1:B:136:ALA:HB2  | 1:B:311:ARG:HG2  | 1.98                     | 0.45              |
| 2:D:358:LEU:O    | 2:D:362:VAL:HG22 | 2.16                     | 0.45              |
| 3:G:172:PRO:HG2  | 3:G:177:ILE:N    | 2.31                     | 0.45              |
| 3:G:202:ARG:HE   | 3:G:205:PRO:HG2  | 1.81                     | 0.45              |
| 2:E:415:GLN:HG2  | 2:E:416:ASN:N    | 2.32                     | 0.45              |
| 1:C:26:PRO:HG2   | 1:C:28:ARG:HB2   | 1.98                     | 0.45              |
| 3:G:118:VAL:O    | 3:G:137:ALA:HA   | 2.16                     | 0.45              |
| 3:G:124:LEU:HD21 | 3:G:137:ALA:CB   | 2.46                     | 0.45              |
| 4:H:5:ASP:HB3    | 4:H:76:LYS:HE3   | 1.99                     | 0.45              |
| 1:B:1:MET:HE1    | 1:B:4:LEU:HA     | 1.98                     | 0.45              |
| 2:D:261:THR:HG23 | 2:D:284:LEU:CD1  | 2.47                     | 0.45              |
| 2:D:395:LEU:HB3  | 2:D:399:ASP:HB2  | 1.98                     | 0.45              |
| 3:G:77:ALA:HB1   | 3:G:182:GLU:O    | 2.16                     | 0.45              |
| 3:G:221:TYR:CB   | 4:H:42:VAL:HG22  | 2.46                     | 0.45              |
| 6:d:289:GLU:HB2  | 6:d:294:ILE:HG13 | 1.98                     | 0.45              |
| 1:B:112:ASN:HB2  | 1:B:113:PRO:HD2  | 1.99                     | 0.45              |
| 2:F:318:ASP:OD1  | 2:F:319:PRO:HD2  | 2.16                     | 0.45              |
| 2:F:336:ARG:O    | 2:F:336:ARG:HD3  | 2.17                     | 0.45              |
| 4:H:26:ARG:HA    | 4:H:31:GLU:HA    | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:d:114:ILE:HD11 | 1:A:6:ILE:HD12   | 1.97                     | 0.45              |
| 1:A:249:ALA:HB3  | 1:A:250:PRO:HD3  | 1.98                     | 0.45              |
| 1:C:377:VAL:HG23 | 1:C:377:VAL:O    | 2.17                     | 0.45              |
| 4:H:72:ILE:HA    | 4:H:77:VAL:HA    | 1.98                     | 0.45              |
| 5:b:121:ARG:NH1  | 5:b:121:ARG:HB2  | 2.32                     | 0.45              |
| 2:F:389:ILE:HG23 | 2:F:390:LEU:H    | 1.81                     | 0.45              |
| 1:B:196:GLY:HA2  | 1:B:201:GLN:NE2  | 2.32                     | 0.45              |
| 2:E:320:ALA:HB3  | 2:E:321:PRO:HD3  | 1.99                     | 0.45              |
| 4:H:3:GLU:CD     | 4:H:56:GLU:HB3   | 2.42                     | 0.45              |
| 1:A:531:GLU:HG3  | 1:A:532:SER:H    | 1.81                     | 0.45              |
| 5:b:155:LEU:HD13 | 1:A:15:ILE:HG22  | 1.99                     | 0.44              |
| 1:C:16:GLU:HA    | 1:C:19:VAL:CG1   | 2.47                     | 0.44              |
| 2:E:96:LYS:HD3   | 2:E:185:THR:HG23 | 2.00                     | 0.44              |
| 2:F:161:GLY:CA   | 2:F:167:LYS:HE3  | 2.47                     | 0.44              |
| 2:F:386:ILE:HD11 | 2:F:395:LEU:HD13 | 1.98                     | 0.44              |
| 6:d:382:VAL:HG12 | 6:d:383:LYS:N    | 2.33                     | 0.44              |
| 1:A:112:ASN:HB2  | 1:A:113:PRO:CD   | 2.47                     | 0.44              |
| 1:C:4:LEU:HD22   | 6:d:300:GLN:HB3  | 1.99                     | 0.44              |
| 2:E:286:ASP:O    | 2:E:290:GLU:HG3  | 2.16                     | 0.44              |
| 2:F:200:ASP:O    | 2:F:204:GLU:HG3  | 2.18                     | 0.44              |
| 6:d:83:ILE:O     | 6:d:87:LEU:HD23  | 2.17                     | 0.44              |
| 3:G:101:GLU:OE1  | 3:G:101:GLU:HA   | 2.17                     | 0.44              |
| 1:B:406:PHE:HB3  | 1:B:413:LEU:HD11 | 2.00                     | 0.44              |
| 2:D:33:LEU:HD12  | 2:D:33:LEU:N     | 2.32                     | 0.44              |
| 2:E:292:GLN:HA   | 2:E:295:ILE:HD12 | 1.98                     | 0.44              |
| 2:F:459:ILE:CG1  | 2:F:464:ASP:HB3  | 2.46                     | 0.44              |
| 6:d:385:ALA:O    | 6:d:414:VAL:HG13 | 2.17                     | 0.44              |
| 1:A:136:ALA:HB1  | 1:A:137:PRO:HD2  | 1.99                     | 0.44              |
| 5:b:144:THR:HA   | 5:b:147:GLU:HB2  | 2.00                     | 0.44              |
| 6:d:129:ALA:O    | 6:d:133:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:365:ARG:HA   | 1:A:366:PRO:C    | 2.42                     | 0.44              |
| 1:A:472:LEU:O    | 1:A:475:VAL:HG12 | 2.18                     | 0.44              |
| 1:B:72:ARG:HD2   | 6:d:231:ASP:CG   | 2.43                     | 0.44              |
| 1:C:450:LEU:HD11 | 1:C:471:PHE:CD2  | 2.53                     | 0.44              |
| 2:D:359:PRO:HA   | 2:D:363:GLY:O    | 2.18                     | 0.44              |
| 2:E:185:THR:HG21 | 2:E:242:PHE:CD2  | 2.53                     | 0.44              |
| 3:G:97:LEU:HD13  | 3:G:126:TYR:CD2  | 2.52                     | 0.44              |
| 1:A:41:ILE:HG22  | 1:A:42:ALA:N     | 2.32                     | 0.44              |
| 1:C:249:ALA:HB3  | 1:C:250:PRO:HD3  | 1.99                     | 0.44              |
| 2:F:188:PHE:HB3  | 2:F:216:LEU:HD23 | 2.00                     | 0.44              |
| 2:F:408:ARG:NH1  | 2:F:449:ASP:HA   | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:85:ASP:OD1   | 3:G:120:GLY:HA2  | 2.18                     | 0.44              |
| 4:H:62:TRP:HB2   | 4:H:87:ARG:HE    | 1.82                     | 0.44              |
| 4:H:75:THR:HG23  | 4:H:76:LYS:NZ    | 2.33                     | 0.44              |
| 1:B:400:TYR:HB2  | 1:B:424:GLY:HA3  | 2.00                     | 0.43              |
| 2:E:227:THR:O    | 2:E:231:VAL:HG23 | 2.18                     | 0.43              |
| 3:G:202:ARG:NH2  | 3:G:205:PRO:HB2  | 2.25                     | 0.43              |
| 6:d:252:ALA:N    | 6:d:253:PRO:HD2  | 2.33                     | 0.43              |
| 1:B:269:ILE:HD13 | 1:B:271:PHE:CZ   | 2.52                     | 0.43              |
| 2:F:451:LEU:HB3  | 2:F:452:PRO:HD2  | 1.99                     | 0.43              |
| 2:E:319:PRO:O    | 2:E:323:THR:HG22 | 2.18                     | 0.43              |
| 6:d:314:LEU:HD11 | 6:d:331:LEU:CD2  | 2.48                     | 0.43              |
| 6:d:412:LEU:C    | 6:d:412:LEU:HD23 | 2.42                     | 0.43              |
| 2:F:421:GLU:O    | 2:F:421:GLU:HG2  | 2.19                     | 0.43              |
| 4:H:22:PHE:HD2   | 4:H:54:GLU:HG3   | 1.83                     | 0.43              |
| 1:B:86:GLU:HG3   | 2:E:57:HIS:HE1   | 1.84                     | 0.43              |
| 1:B:385:ALA:O    | 1:B:389:VAL:HG22 | 2.19                     | 0.43              |
| 2:D:255:ASP:HA   | 2:D:256:ASN:HA   | 1.56                     | 0.43              |
| 2:E:320:ALA:HB3  | 2:E:321:PRO:CD   | 2.48                     | 0.43              |
| 2:E:435:GLU:OE2  | 2:E:461:GLY:HA3  | 2.18                     | 0.43              |
| 2:F:390:LEU:HD13 | 3:G:30:THR:HG22  | 1.99                     | 0.43              |
| 3:G:183:LEU:HD12 | 3:G:204:ALA:HB2  | 2.00                     | 0.43              |
| 6:d:109:GLN:HA   | 6:d:109:GLN:OE1  | 2.18                     | 0.43              |
| 1:B:221:ARG:NH2  | 2:E:133:PRO:HD2  | 2.33                     | 0.43              |
| 3:G:193:MET:O    | 3:G:193:MET:HG3  | 2.18                     | 0.43              |
| 4:H:52:LYS:HZ1   | 4:H:60:ASP:CG    | 2.26                     | 0.43              |
| 2:D:41:ILE:O     | 2:D:47:ALA:HA    | 2.19                     | 0.43              |
| 5:b:137:LEU:HD23 | 5:b:137:LEU:C    | 2.44                     | 0.43              |
| 1:A:417:SER:O    | 1:A:421:LEU:HG   | 2.18                     | 0.43              |
| 1:C:395:LEU:O    | 1:C:399:GLN:HG3  | 2.19                     | 0.43              |
| 2:F:156:LYS:HD2  | 2:F:156:LYS:N    | 2.34                     | 0.43              |
| 2:F:387:ILE:O    | 2:F:392:ILE:HD13 | 2.18                     | 0.43              |
| 2:F:393:ASP:OD1  | 2:F:403:VAL:HG11 | 2.19                     | 0.43              |
| 3:G:194:LEU:O    | 3:G:194:LEU:HG   | 2.18                     | 0.43              |
| 5:b:118:MET:CE   | 6:d:91:ALA:HB1   | 2.48                     | 0.43              |
| 5:b:137:LEU:HD11 | 6:d:110:ARG:CA   | 2.48                     | 0.43              |
| 1:A:395:LEU:O    | 1:A:399:GLN:HG3  | 2.18                     | 0.43              |
| 1:A:442:GLU:HG2  | 1:A:443:GLU:N    | 2.33                     | 0.43              |
| 2:D:229:MET:O    | 2:D:229:MET:HG2  | 2.19                     | 0.43              |
| 2:E:278:VAL:HG12 | 2:E:278:VAL:O    | 2.18                     | 0.43              |
| 3:G:65:HIS:CG    | 3:G:66:PRO:HD2   | 2.54                     | 0.43              |
| 5:b:118:MET:HG2  | 6:d:95:VAL:CG1   | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:3:GLU:OE2    | 4:H:56:GLU:HB3   | 2.18                     | 0.43              |
| 1:C:38:GLY:O     | 1:C:39:ASP:HB2   | 2.19                     | 0.42              |
| 2:E:185:THR:HG22 | 2:E:186:SER:N    | 2.33                     | 0.42              |
| 5:b:115:LEU:HD23 | 5:b:115:LEU:C    | 2.44                     | 0.42              |
| 6:d:314:LEU:HD11 | 6:d:331:LEU:HD21 | 2.01                     | 0.42              |
| 1:C:386:MET:CE   | 1:C:448:ILE:HD12 | 2.49                     | 0.42              |
| 2:F:455:ALA:HA   | 2:F:468:LYS:HD3  | 2.00                     | 0.42              |
| 1:A:139:VAL:HG13 | 1:A:140:VAL:HG13 | 2.01                     | 0.42              |
| 1:C:52:THR:O     | 1:C:53:GLN:HB2   | 2.20                     | 0.42              |
| 1:C:506:ALA:O    | 1:C:509:LYS:HG2  | 2.19                     | 0.42              |
| 2:F:59:GLY:O     | 2:F:60:ASP:HB2   | 2.19                     | 0.42              |
| 6:d:314:LEU:CD1  | 6:d:331:LEU:HD21 | 2.50                     | 0.42              |
| 2:D:274:MET:SD   | 1:A:289:ARG:HA   | 2.59                     | 0.42              |
| 2:D:324:THR:HG22 | 2:D:324:THR:O    | 2.19                     | 0.42              |
| 2:E:220:GLN:OE1  | 2:E:220:GLN:HA   | 2.20                     | 0.42              |
| 5:b:155:LEU:HD21 | 1:A:16:GLU:OE1   | 2.19                     | 0.42              |
| 1:A:269:ILE:HG22 | 1:A:325:THR:O    | 2.18                     | 0.42              |
| 1:A:450:LEU:HD11 | 1:A:471:PHE:CD2  | 2.55                     | 0.42              |
| 1:B:442:GLU:O    | 1:B:446:VAL:HG23 | 2.19                     | 0.42              |
| 2:E:402:LEU:HD23 | 2:E:402:LEU:C    | 2.44                     | 0.42              |
| 2:F:341:LYS:HE3  | 2:F:341:LYS:HB2  | 1.87                     | 0.42              |
| 5:b:93:LEU:O     | 5:b:97:ARG:HG2   | 2.19                     | 0.42              |
| 6:d:203:SER:HB2  | 6:d:287:ARG:HH11 | 1.85                     | 0.42              |
| 1:A:55:LEU:HD21  | 1:A:98:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:275:THR:HG22 | 1:A:275:THR:O    | 2.19                     | 0.42              |
| 2:E:418:MET:SD   | 2:E:428:GLY:HA3  | 2.60                     | 0.42              |
| 4:H:52:LYS:HD2   | 4:H:62:TRP:CZ2   | 2.55                     | 0.42              |
| 6:d:399:VAL:O    | 6:d:403:ILE:HG13 | 2.19                     | 0.42              |
| 6:d:419:LEU:HD23 | 6:d:419:LEU:O    | 2.20                     | 0.42              |
| 1:A:212:LYS:HE2  | 1:A:212:LYS:HB3  | 1.78                     | 0.42              |
| 1:A:337:ILE:HD12 | 1:A:337:ILE:C    | 2.44                     | 0.42              |
| 3:G:221:TYR:OH   | 4:H:73:THR:HG23  | 2.19                     | 0.42              |
| 4:H:49:ALA:HB3   | 4:H:65:ILE:HB    | 2.01                     | 0.42              |
| 1:C:344:ASN:O    | 1:C:348:ILE:HG13 | 2.20                     | 0.42              |
| 2:E:328:LEU:HD13 | 2:E:331:THR:HG22 | 2.02                     | 0.42              |
| 2:F:451:LEU:HD23 | 2:F:469:ALA:HB2  | 2.02                     | 0.42              |
| 6:d:396:LEU:HA   | 6:d:399:VAL:CG2  | 2.50                     | 0.42              |
| 6:d:430:GLU:OE1  | 1:A:31:ILE:HD11  | 2.19                     | 0.42              |
| 1:A:258:GLN:OE1  | 1:A:311:ARG:HD3  | 2.19                     | 0.42              |
| 6:d:82:GLN:O     | 6:d:85:LYS:HG2   | 2.19                     | 0.42              |
| 6:d:132:LEU:O    | 6:d:132:LEU:HD23 | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:d:202:LEU:HD12 | 6:d:287:ARG:HB2  | 2.02                     | 0.42              |
| 1:B:50:VAL:HG12  | 1:B:51:MET:N     | 2.35                     | 0.41              |
| 4:H:96:LYS:CE    | 4:H:121:VAL:HG13 | 2.46                     | 0.41              |
| 1:B:492:PHE:CE2  | 1:B:497:GLU:HG2  | 2.55                     | 0.41              |
| 2:E:423:PHE:CE2  | 9:E:600:ADP:H3'  | 2.54                     | 0.41              |
| 2:F:407:ARG:O    | 2:F:411:ARG:HG2  | 2.19                     | 0.41              |
| 3:G:118:VAL:HG13 | 3:G:123:ALA:HB3  | 2.01                     | 0.41              |
| 4:H:35:LEU:N     | 4:H:35:LEU:HD23  | 2.35                     | 0.41              |
| 6:d:388:ILE:HD13 | 6:d:412:LEU:HD13 | 2.02                     | 0.41              |
| 1:C:400:TYR:CD1  | 1:C:424:GLY:HA3  | 2.55                     | 0.41              |
| 5:b:140:GLN:NE2  | 1:A:5:THR:HB     | 2.35                     | 0.41              |
| 5:b:141:GLY:CA   | 5:b:144:THR:HG22 | 2.49                     | 0.41              |
| 1:A:68:ASN:C     | 1:A:69:LEU:HD12  | 2.45                     | 0.41              |
| 1:C:16:GLU:CA    | 1:C:19:VAL:HG12  | 2.50                     | 0.41              |
| 1:C:166:GLN:O    | 1:C:325:THR:HG23 | 2.20                     | 0.41              |
| 1:C:273:ASP:CG   | 1:C:275:THR:HG22 | 2.46                     | 0.41              |
| 2:D:372:GLU:HA   | 2:D:372:GLU:OE1  | 2.20                     | 0.41              |
| 2:D:433:LEU:O    | 2:D:437:ILE:HG13 | 2.21                     | 0.41              |
| 2:E:412:PHE:CD1  | 2:E:459:ILE:HD11 | 2.55                     | 0.41              |
| 2:F:446:GLY:HA2  | 2:F:449:ASP:OD1  | 2.20                     | 0.41              |
| 4:H:23:VAL:HA    | 4:H:52:LYS:O     | 2.20                     | 0.41              |
| 1:A:339:ALA:HB3  | 1:A:342:PRO:HD2  | 2.01                     | 0.41              |
| 1:B:342:PRO:O    | 1:B:346:ILE:HG13 | 2.19                     | 0.41              |
| 2:D:320:ALA:HB3  | 2:D:321:PRO:CD   | 2.51                     | 0.41              |
| 6:d:418:LEU:HD22 | 6:d:434:SER:HB3  | 2.01                     | 0.41              |
| 1:B:221:ARG:HH21 | 2:E:133:PRO:HD2  | 1.86                     | 0.41              |
| 1:C:16:GLU:O     | 1:C:19:VAL:HG12  | 2.19                     | 0.41              |
| 2:E:33:LEU:O     | 2:E:34:PHE:HB2   | 2.20                     | 0.41              |
| 2:E:284:LEU:HD22 | 2:E:323:THR:HG21 | 2.02                     | 0.41              |
| 2:F:400:LYS:HA   | 2:F:403:VAL:HG12 | 2.02                     | 0.41              |
| 5:b:140:GLN:O    | 5:b:144:THR:HG22 | 2.21                     | 0.41              |
| 5:b:164:LEU:HD21 | 6:d:133:VAL:HG13 | 2.01                     | 0.41              |
| 1:B:139:VAL:O    | 1:B:139:VAL:HG22 | 2.21                     | 0.41              |
| 1:B:149:LEU:C    | 1:B:149:LEU:HD23 | 2.46                     | 0.41              |
| 2:D:158:ALA:HB3  | 2:D:328:LEU:CD1  | 2.48                     | 0.41              |
| 2:F:387:ILE:HG23 | 2:F:393:ASP:H    | 1.86                     | 0.41              |
| 2:E:162:GLY:H    | 2:E:165:VAL:HG21 | 1.85                     | 0.41              |
| 2:E:347:VAL:O    | 2:E:349:PRO:HD3  | 2.20                     | 0.41              |
| 2:F:473:GLY:O    | 2:F:474:ALA:HB2  | 2.21                     | 0.41              |
| 3:G:234:LEU:HD13 | 4:H:69:PHE:CE1   | 2.55                     | 0.41              |
| 3:G:239:LEU:O    | 3:G:243:VAL:HG23 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:11:VAL:HG13  | 4:H:12:GLU:HG3   | 2.02                     | 0.41              |
| 5:b:117:ASP:CG   | 5:b:121:ARG:HH12 | 2.29                     | 0.41              |
| 6:d:196:SER:O    | 6:d:197:LEU:HG   | 2.21                     | 0.41              |
| 6:d:358:VAL:HG12 | 6:d:359:ARG:N    | 2.35                     | 0.41              |
| 1:C:32:GLY:O     | 1:C:33:ILE:HD13  | 2.21                     | 0.41              |
| 1:C:190:LYS:HE3  | 1:C:194:GLU:OE2  | 2.20                     | 0.41              |
| 1:C:374:VAL:HG22 | 1:C:375:SER:N    | 2.36                     | 0.41              |
| 2:F:364:GLU:CD   | 2:F:364:GLU:H    | 2.29                     | 0.41              |
| 2:F:402:LEU:HD23 | 2:F:402:LEU:C    | 2.46                     | 0.41              |
| 4:H:23:VAL:HB    | 4:H:34:ILE:HG13  | 2.03                     | 0.41              |
| 4:H:53:ILE:HD13  | 4:H:63:TRP:HE1   | 1.86                     | 0.41              |
| 4:H:102:GLU:O    | 4:H:103:ASP:C    | 2.64                     | 0.41              |
| 6:d:353:ARG:O    | 6:d:353:ARG:HG2  | 2.20                     | 0.41              |
| 3:G:154:ALA:O    | 3:G:158:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:310:GLU:HG3  | 1:A:310:GLU:O    | 2.21                     | 0.41              |
| 6:d:96:GLU:O     | 6:d:100:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:434:PRO:HG2  | 1:A:437:SER:OG   | 2.21                     | 0.40              |
| 6:d:132:LEU:HD23 | 6:d:132:LEU:C    | 2.47                     | 0.40              |
| 1:C:384:LYS:O    | 1:C:388:GLU:HG3  | 2.21                     | 0.40              |
| 1:C:471:PHE:CZ   | 1:C:504:VAL:HG22 | 2.56                     | 0.40              |
| 2:D:251:LEU:HD23 | 2:D:304:THR:HB   | 2.02                     | 0.40              |
| 2:E:255:ASP:HA   | 2:E:256:ASN:HA   | 1.56                     | 0.40              |
| 2:E:441:ASP:O    | 2:E:445:LYS:HG2  | 2.20                     | 0.40              |
| 4:H:52:LYS:HE3   | 4:H:54:GLU:OE2   | 2.22                     | 0.40              |
| 6:d:277:GLU:O    | 6:d:281:ARG:HG3  | 2.21                     | 0.40              |
| 6:d:388:ILE:HD13 | 6:d:412:LEU:CD1  | 2.51                     | 0.40              |
| 1:B:4:LEU:HD11   | 6:d:249:LYS:HB3  | 2.03                     | 0.40              |
| 2:E:250:VAL:HG12 | 2:E:251:LEU:N    | 2.35                     | 0.40              |
| 2:F:400:LYS:O    | 2:F:403:VAL:HG12 | 2.21                     | 0.40              |
| 1:B:4:LEU:HD21   | 6:d:246:LEU:HD22 | 2.02                     | 0.40              |
| 1:B:471:PHE:CZ   | 1:B:504:VAL:HG22 | 2.57                     | 0.40              |
| 1:C:272:ASP:HA   | 1:C:273:ASP:HA   | 1.79                     | 0.40              |
| 2:E:333:GLU:OE1  | 2:E:351:ALA:HB1  | 2.22                     | 0.40              |
| 2:F:257:ILE:O    | 2:F:260:PHE:HB3  | 2.21                     | 0.40              |
| 5:b:128:ALA:O    | 5:b:132:THR:HG23 | 2.21                     | 0.40              |
| 1:A:531:GLU:HG3  | 1:A:532:SER:N    | 2.37                     | 0.40              |

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 527/548 (96%)   | 514 (98%)  | 13 (2%)  | 0        | 100         | 100 |
| 1   | B     | 521/548 (95%)   | 511 (98%)  | 10 (2%)  | 0        | 100         | 100 |
| 1   | C     | 518/548 (94%)   | 500 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 2   | D     | 463/515 (90%)   | 454 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 2   | E     | 463/515 (90%)   | 447 (96%)  | 16 (4%)  | 0        | 100         | 100 |
| 2   | F     | 464/515 (90%)   | 450 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 3   | G     | 304/308 (99%)   | 295 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 4   | H     | 119/121 (98%)   | 107 (90%)  | 12 (10%) | 0        | 100         | 100 |
| 5   | b     | 78/177 (44%)    | 77 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 6   | d     | 380/448 (85%)   | 372 (98%)  | 8 (2%)   | 0        | 100         | 100 |
| All | All   | 3837/4243 (90%) | 3727 (97%) | 110 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 426/440 (97%) | 426 (100%) | 0        | 100         | 100 |
| 1   | B     | 421/440 (96%) | 421 (100%) | 0        | 100         | 100 |
| 1   | C     | 419/440 (95%) | 417 (100%) | 2 (0%)   | 81          | 90  |
| 2   | D     | 383/422 (91%) | 382 (100%) | 1 (0%)   | 86          | 93  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 2   | E     | 382/422 (90%)   | 382 (100%)  | 0        | 100         | 100 |
| 2   | F     | 382/422 (90%)   | 379 (99%)   | 3 (1%)   | 73          | 84  |
| 3   | G     | 231/233 (99%)   | 231 (100%)  | 0        | 100         | 100 |
| 4   | H     | 96/96 (100%)    | 96 (100%)   | 0        | 100         | 100 |
| 5   | b     | 56/128 (44%)    | 56 (100%)   | 0        | 100         | 100 |
| 6   | d     | 298/350 (85%)   | 297 (100%)  | 1 (0%)   | 86          | 93  |
| All | All   | 3094/3393 (91%) | 3087 (100%) | 7 (0%)   | 85          | 95  |

All (7) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 245 | PHE  |
| 1   | C     | 488 | GLU  |
| 2   | D     | 231 | VAL  |
| 2   | F     | 129 | ASP  |
| 2   | F     | 180 | ARG  |
| 2   | F     | 390 | LEU  |
| 6   | d     | 106 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 68  | ASN  |
| 1   | C     | 141 | GLN  |
| 1   | C     | 335 | ASN  |
| 2   | D     | 327 | HIS  |
| 2   | D     | 415 | GLN  |
| 2   | E     | 105 | ASN  |
| 2   | F     | 248 | GLN  |
| 2   | F     | 381 | GLN  |
| 6   | d     | 176 | HIS  |
| 6   | d     | 313 | GLN  |
| 1   | A     | 433 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 7   | ATP  | B     | 600 | 8    | 32,33,33     | 0.54 | 0           | 48,52,52    | 0.58 | 0           |
| 7   | ATP  | F     | 600 | -    | 32,33,33     | 0.54 | 0           | 48,52,52    | 0.56 | 0           |
| 7   | ATP  | C     | 600 | 8    | 32,33,33     | 0.53 | 0           | 48,52,52    | 0.57 | 0           |
| 9   | ADP  | E     | 600 | 8    | 28,29,29     | 0.46 | 0           | 43,45,45    | 0.51 | 0           |
| 7   | ATP  | A     | 600 | 8    | 32,33,33     | 0.54 | 0           | 48,52,52    | 0.58 | 0           |
| 9   | ADP  | D     | 600 | 8    | 28,29,29     | 0.46 | 0           | 43,45,45    | 0.48 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 7   | ATP  | B     | 600 | 8    | -       | 0/22/38/38 | 0/3/3/3 |
| 7   | ATP  | F     | 600 | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 7   | ATP  | C     | 600 | 8    | -       | 1/22/38/38 | 0/3/3/3 |
| 9   | ADP  | E     | 600 | 8    | -       | 2/16/32/32 | 0/3/3/3 |
| 7   | ATP  | A     | 600 | 8    | -       | 1/22/38/38 | 0/3/3/3 |
| 9   | ADP  | D     | 600 | 8    | -       | 1/16/32/32 | 0/3/3/3 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

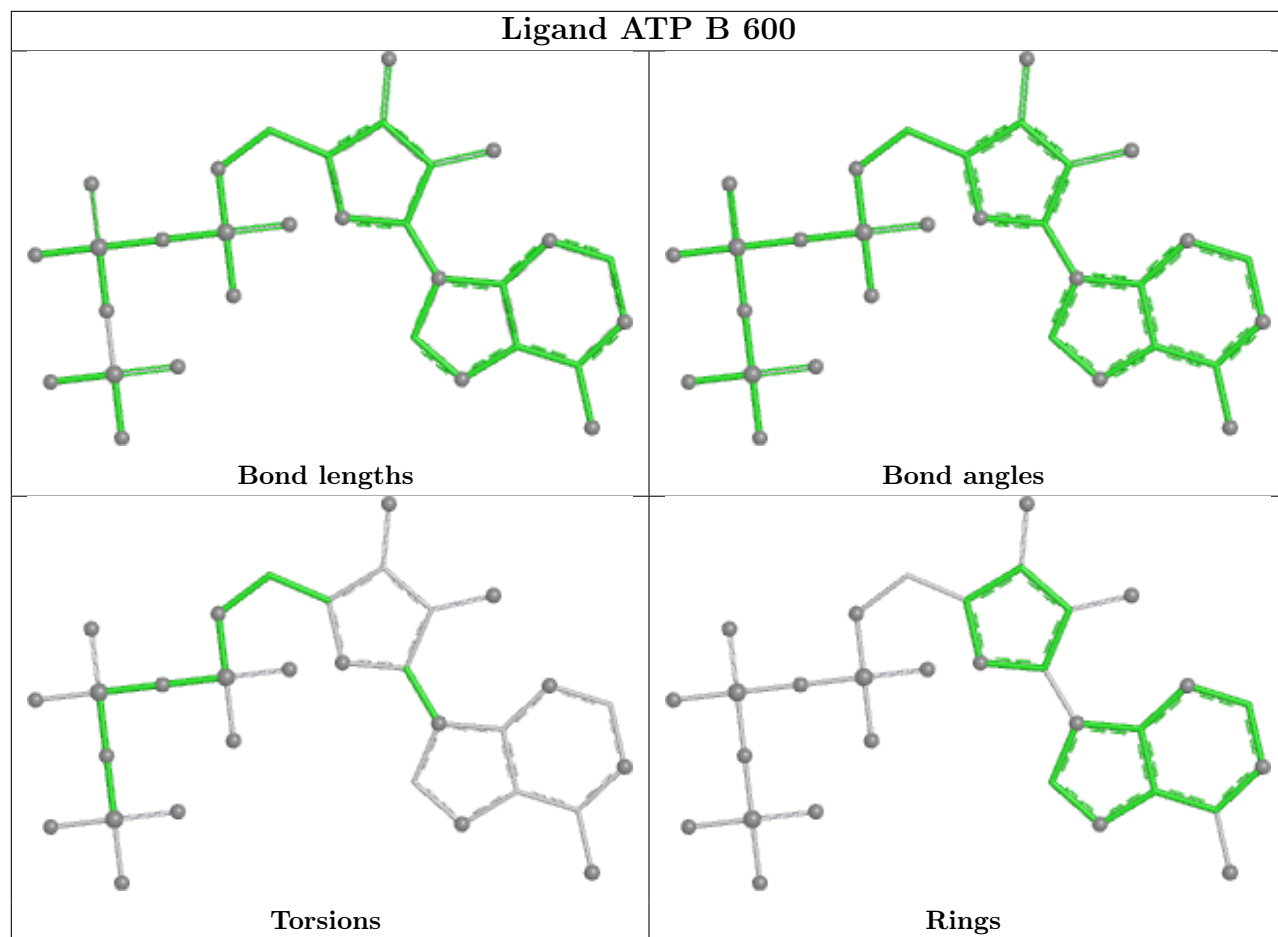
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | D     | 600 | ADP  | C5'-O5'-PA-O1A  |
| 9   | E     | 600 | ADP  | C5'-O5'-PA-O1A  |
| 7   | A     | 600 | ATP  | O4'-C4'-C5'-O5' |
| 7   | C     | 600 | ATP  | O4'-C4'-C5'-O5' |
| 9   | E     | 600 | ADP  | C2'-C1'-N9-C8   |
| 7   | F     | 600 | ATP  | O4'-C4'-C5'-O5' |

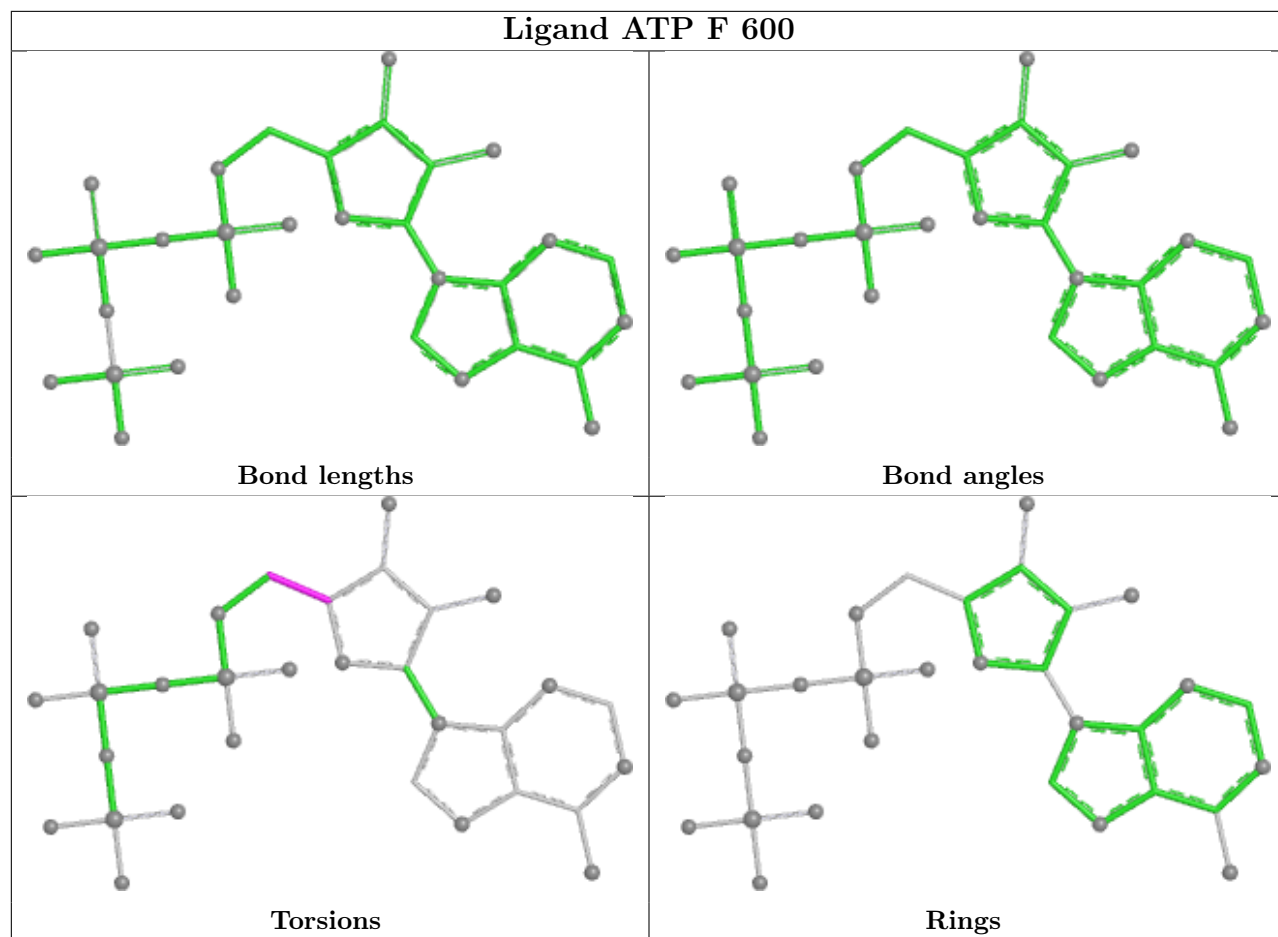
There are no ring outliers.

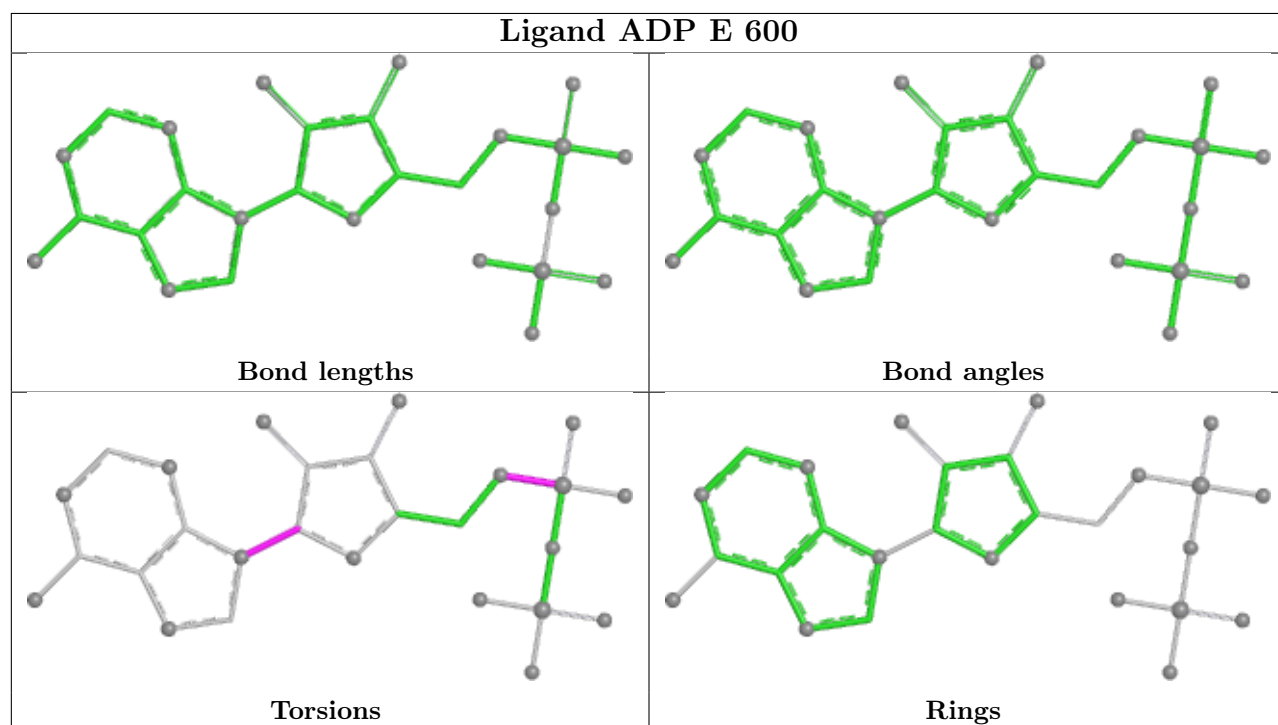
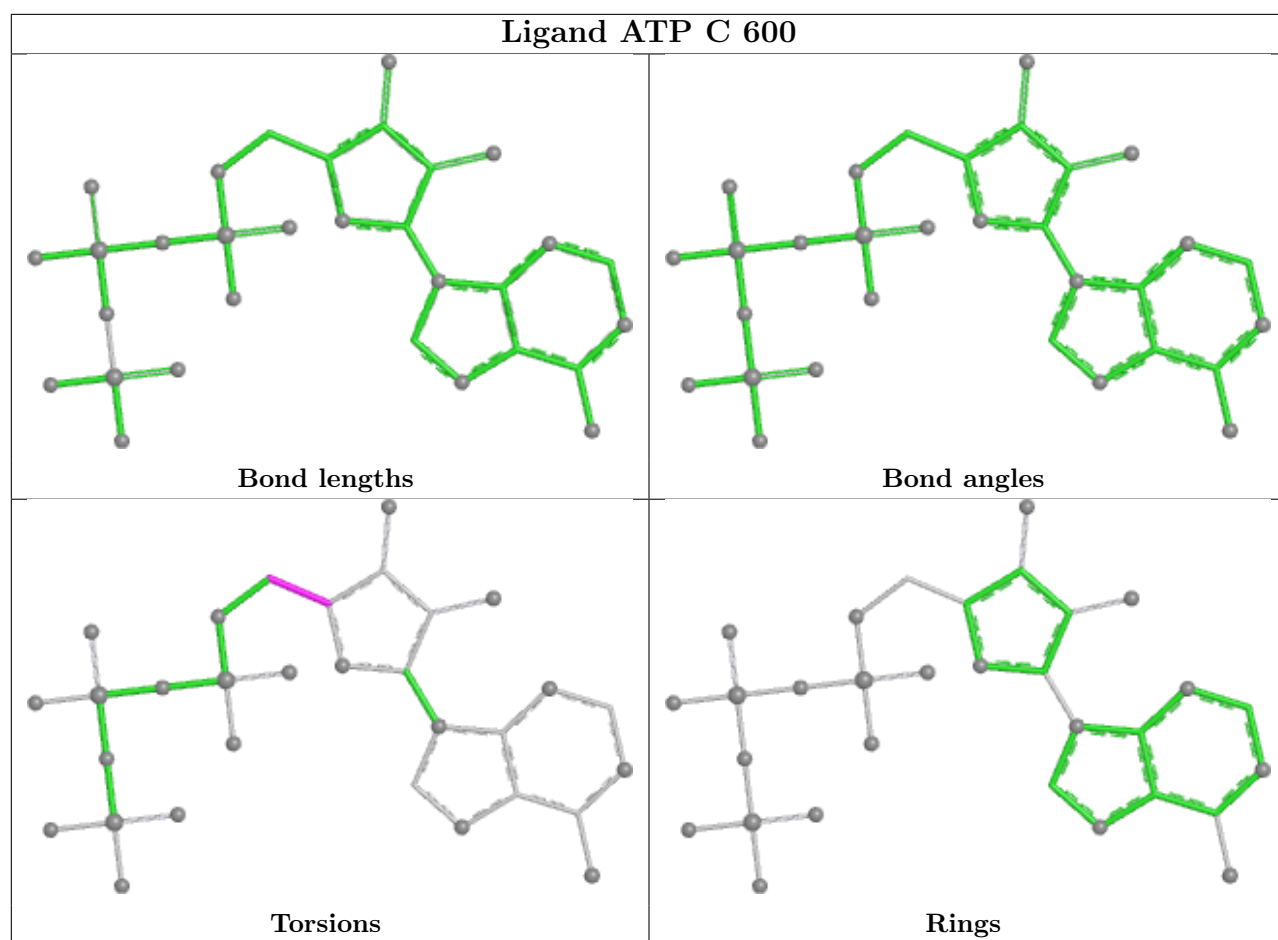
1 monomer is involved in 2 short contacts:

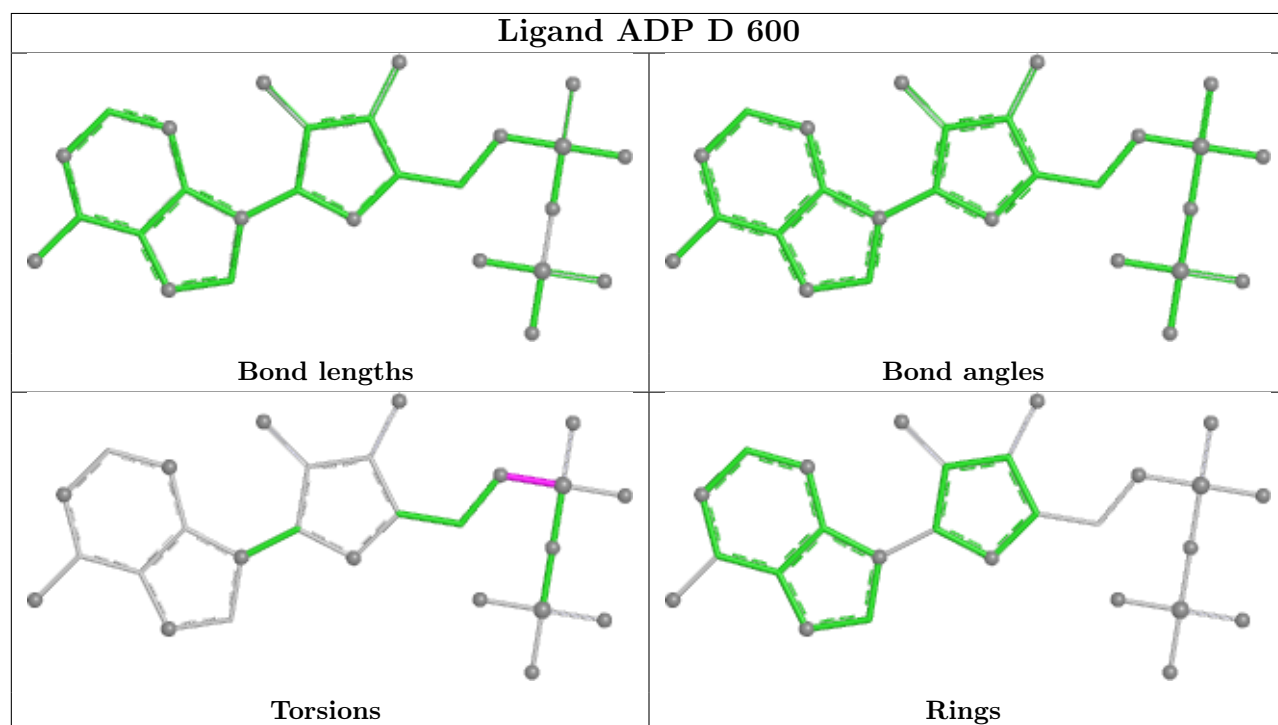
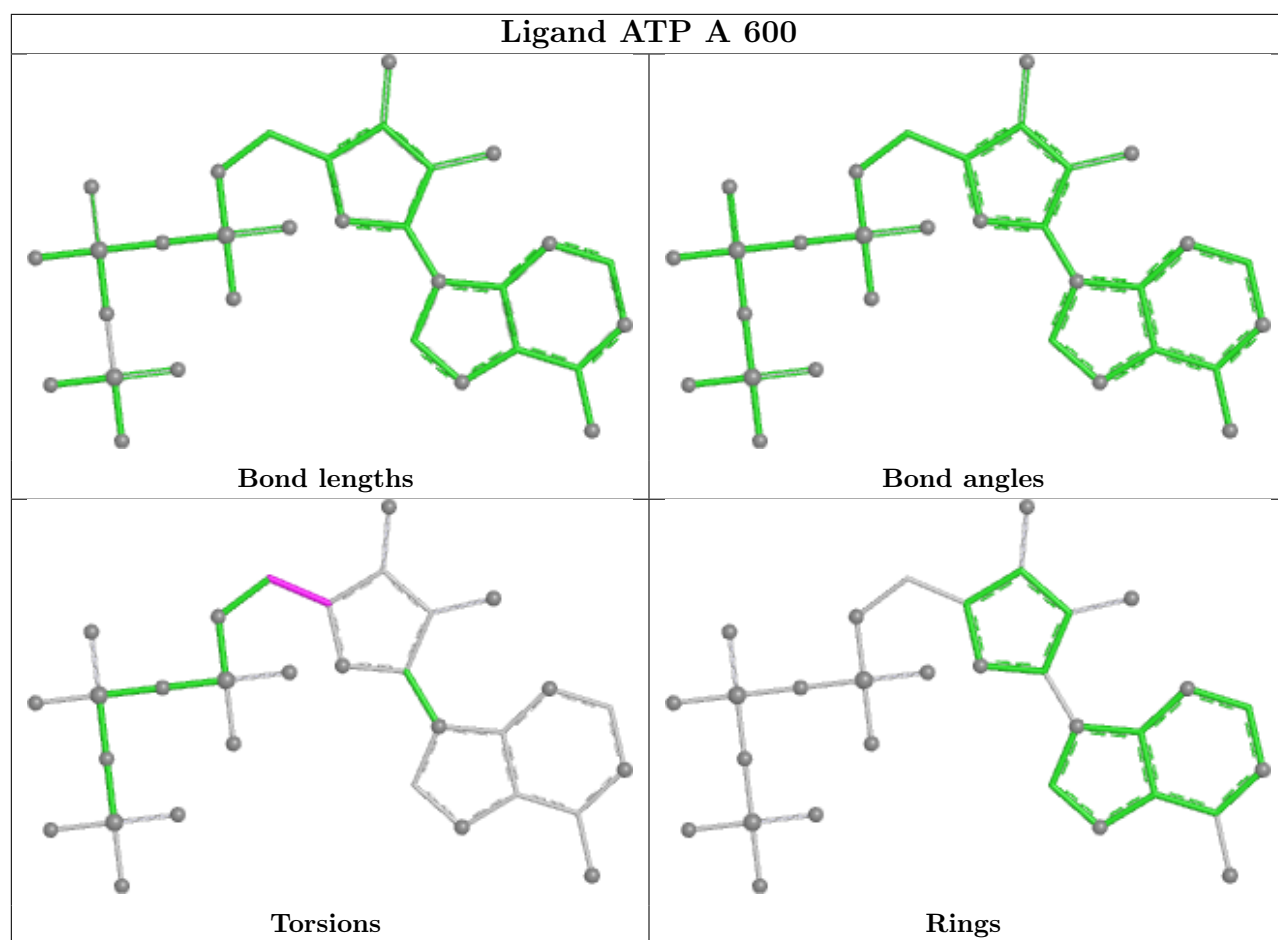
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | E     | 600 | ADP  | 2       | 0            |

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









## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



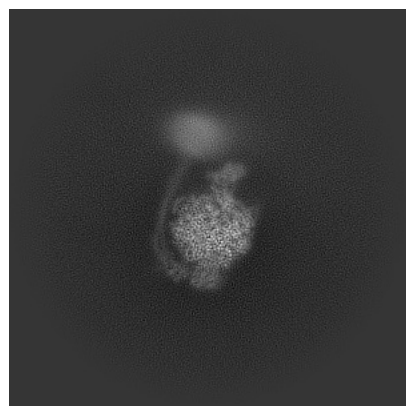
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65138. These allow visual inspection of the internal detail of the map and identification of artifacts.

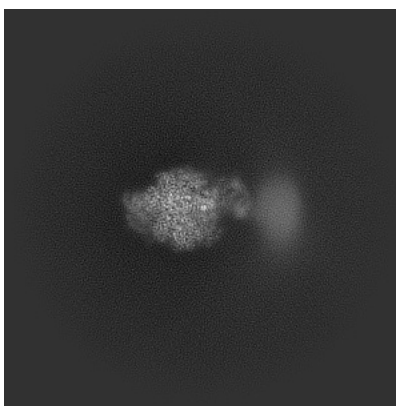
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

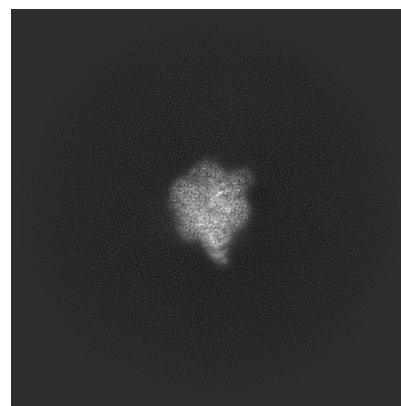
#### 6.1.1 Primary map



X

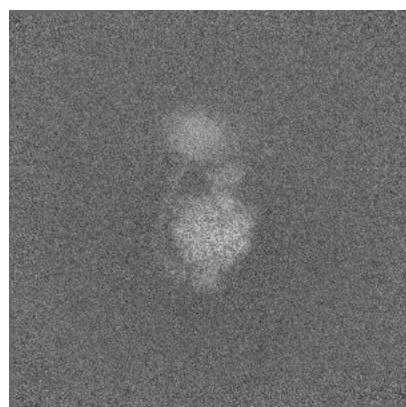


Y

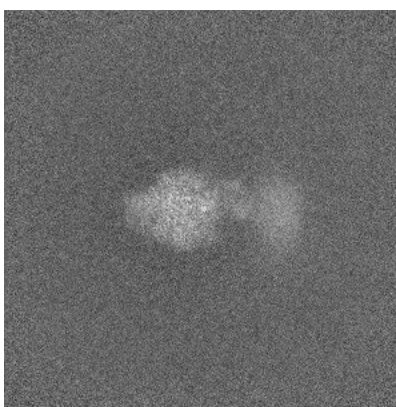


Z

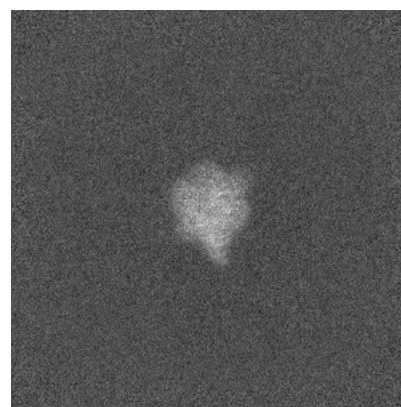
#### 6.1.2 Raw map



X



Y

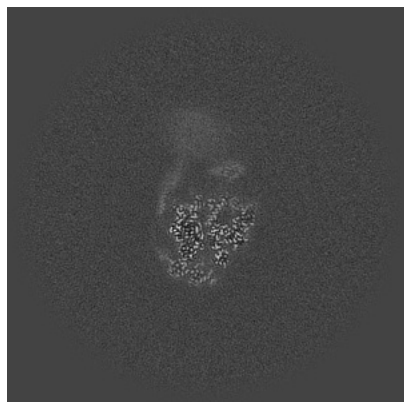


Z

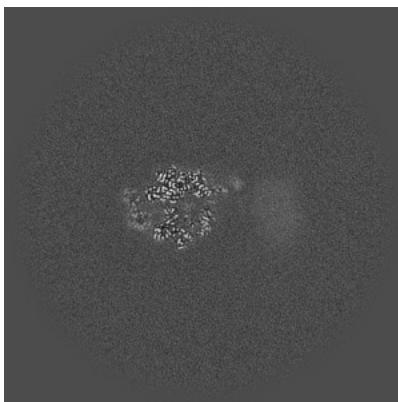
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

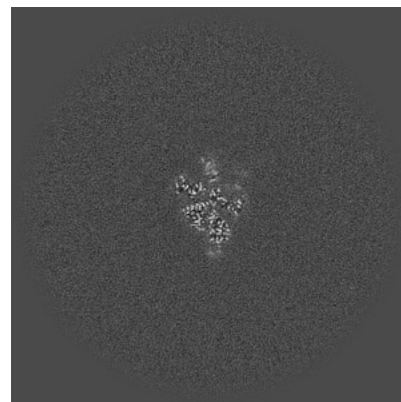
### 6.2.1 Primary map



X Index: 340

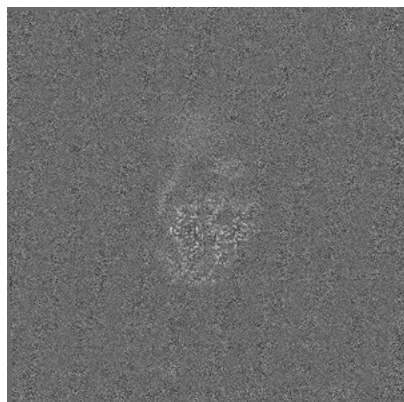


Y Index: 340

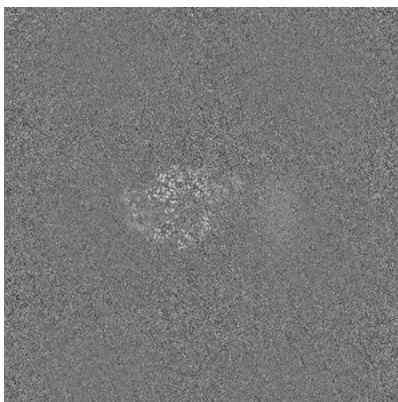


Z Index: 340

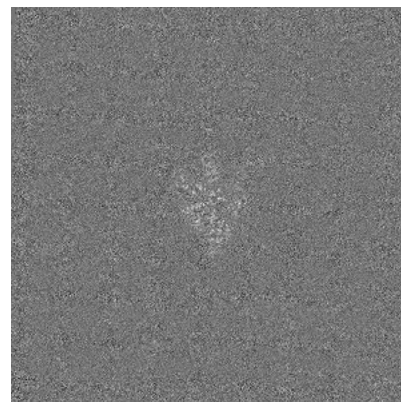
### 6.2.2 Raw map



X Index: 340



Y Index: 340

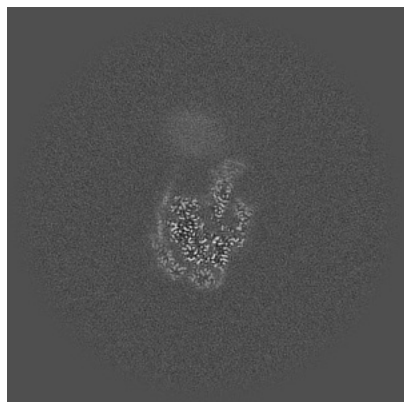


Z Index: 340

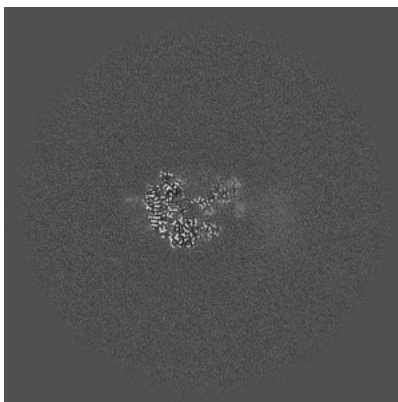
The images above show central slices of the map in three orthogonal directions.

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

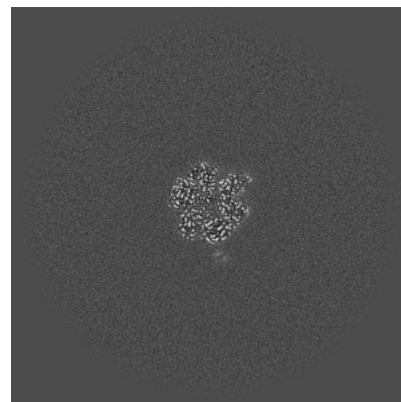
### 6.3.1 Primary map



X Index: 351

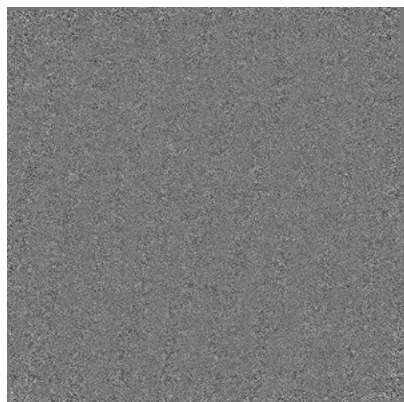


Y Index: 362

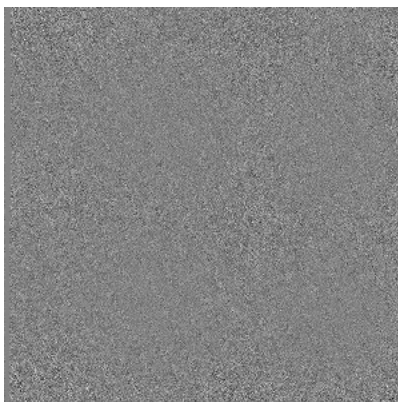


Z Index: 296

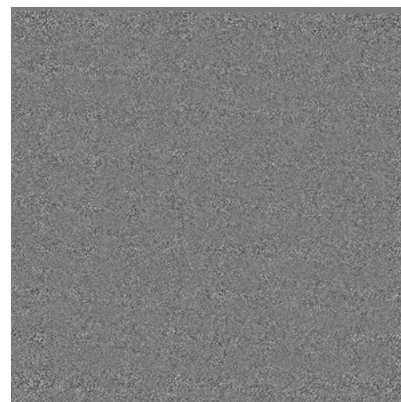
### 6.3.2 Raw map



X Index: 674



Y Index: 666



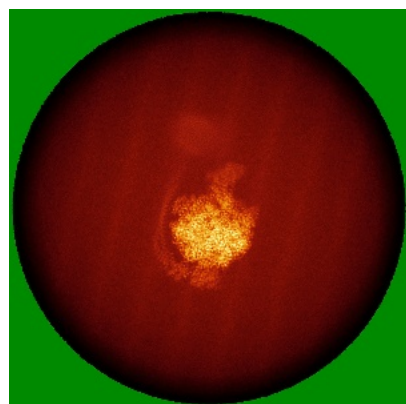
Z Index: 671

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

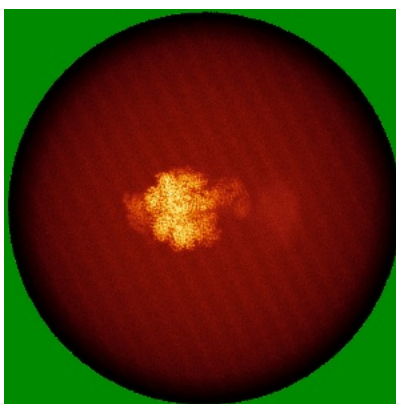


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

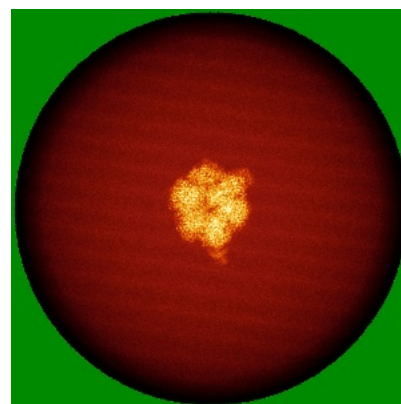
### 6.4.1 Primary map



X

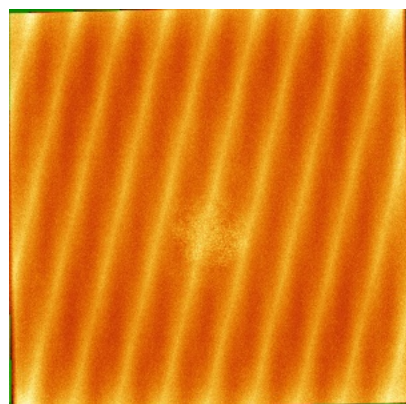


Y

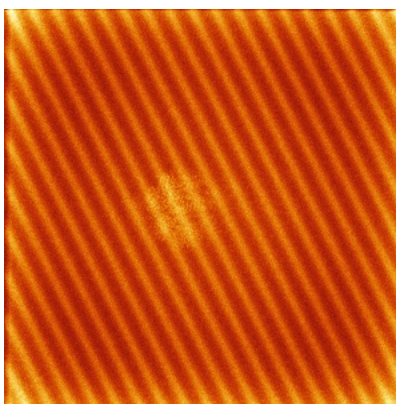


Z

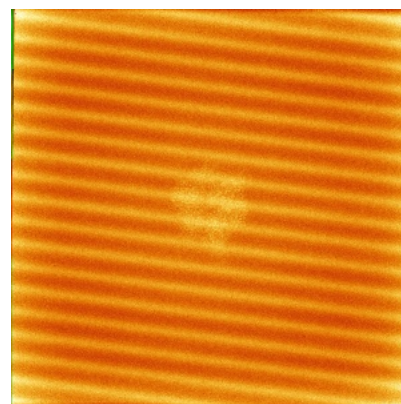
### 6.4.2 Raw map



X



Y



Z

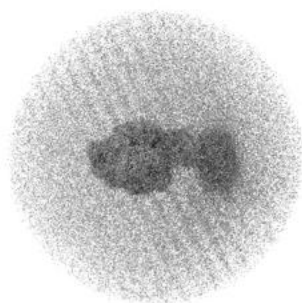
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

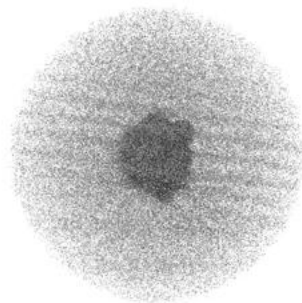
### 6.5.1 Primary map



X



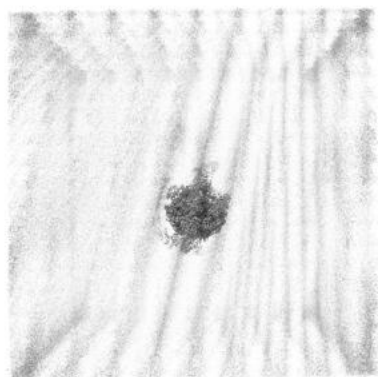
Y



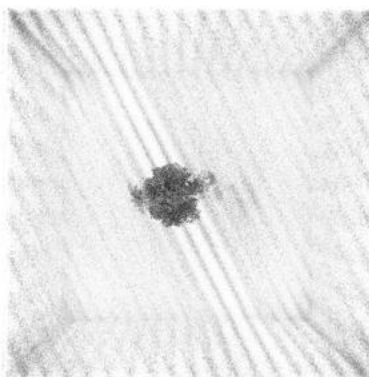
Z

The images above show the 3D surface view of the map at the recommended contour level 0.072. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

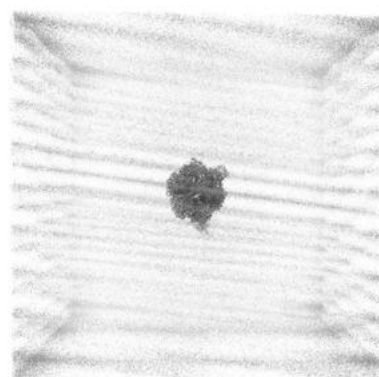
### 6.5.2 Raw map



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.

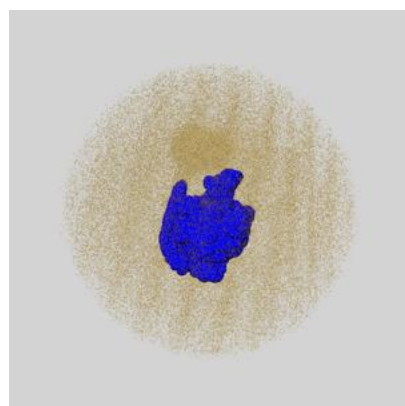
## 6.6 Mask visualisation [i](#)

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

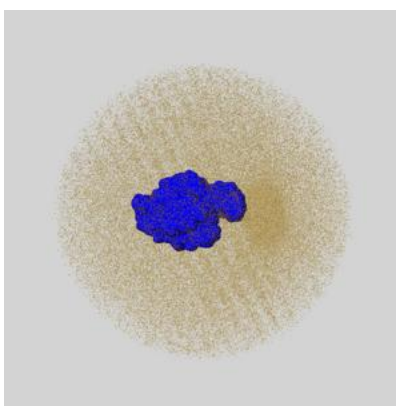
A mask typically either:

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

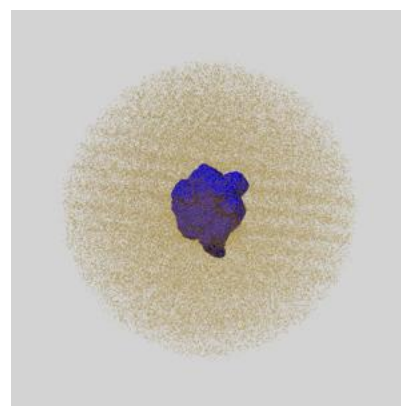
### 6.6.1 emd\_65138\_msk\_1.map [i](#)



X



Y

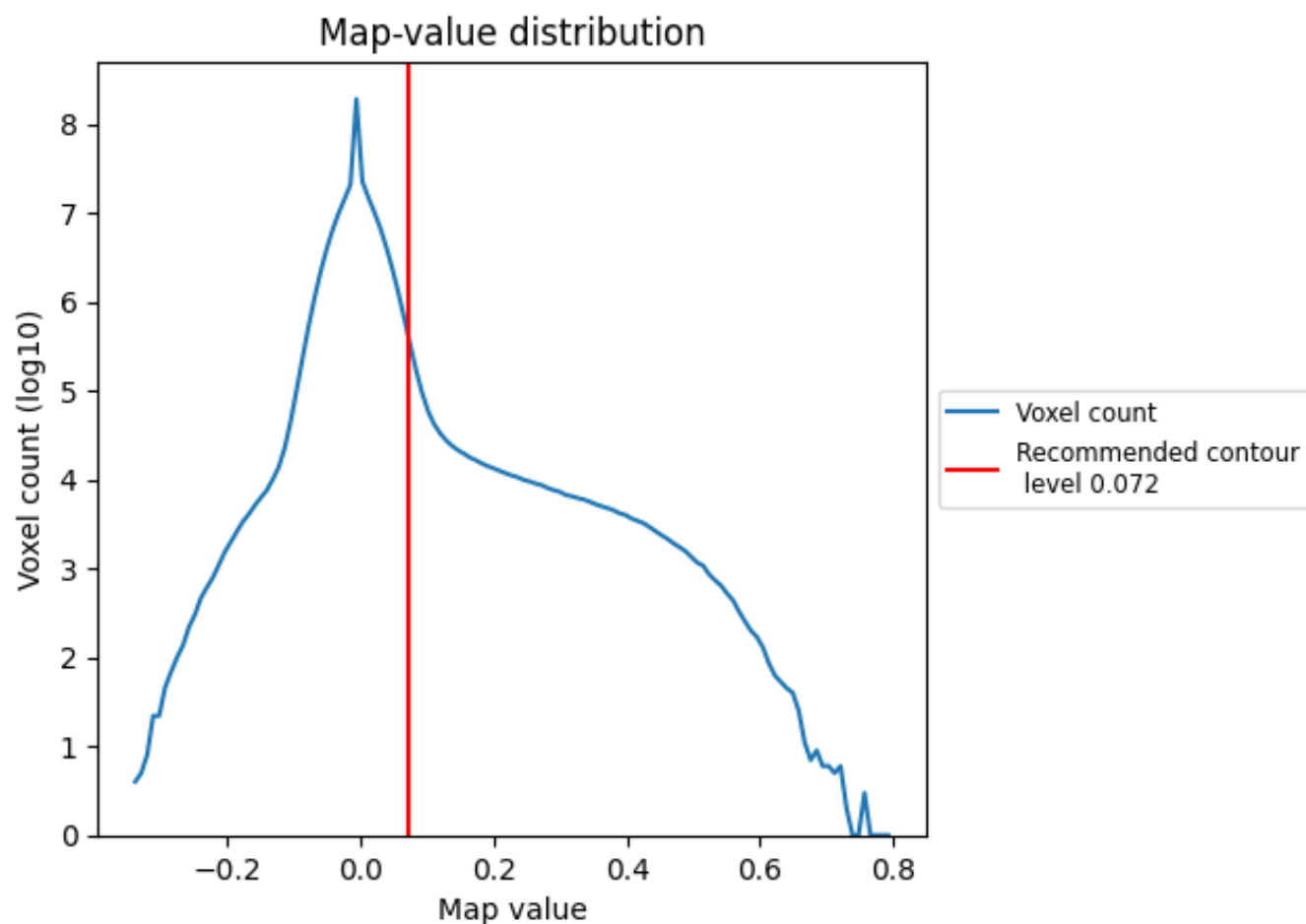


Z

## 7 Map analysis [i](#)

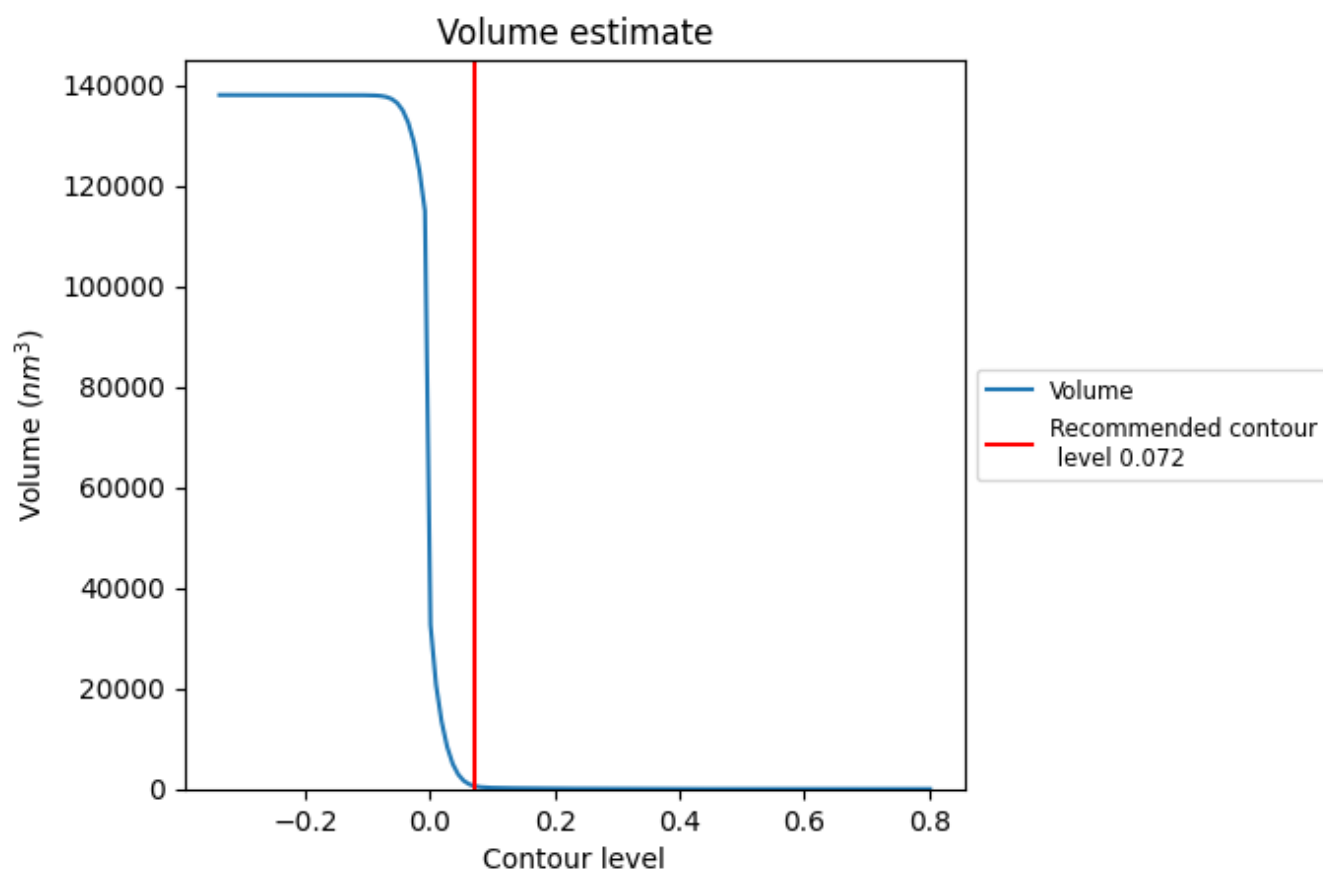
This section contains the results of statistical analysis of the map.

### 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](#)

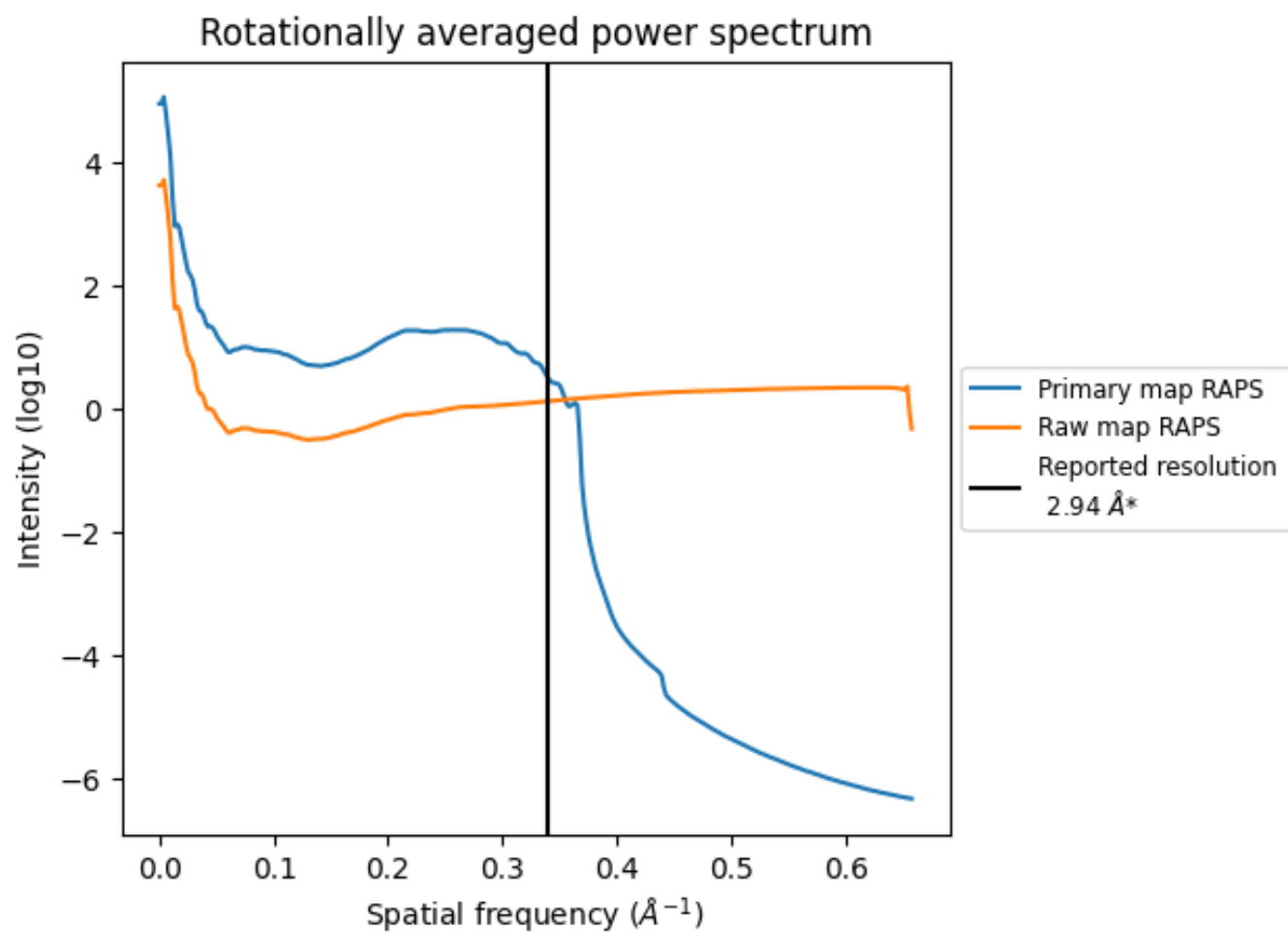


The volume at the recommended contour level is 560  $\text{nm}^3$ ; this corresponds to an approximate mass of 506 kDa.

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 ⓘ

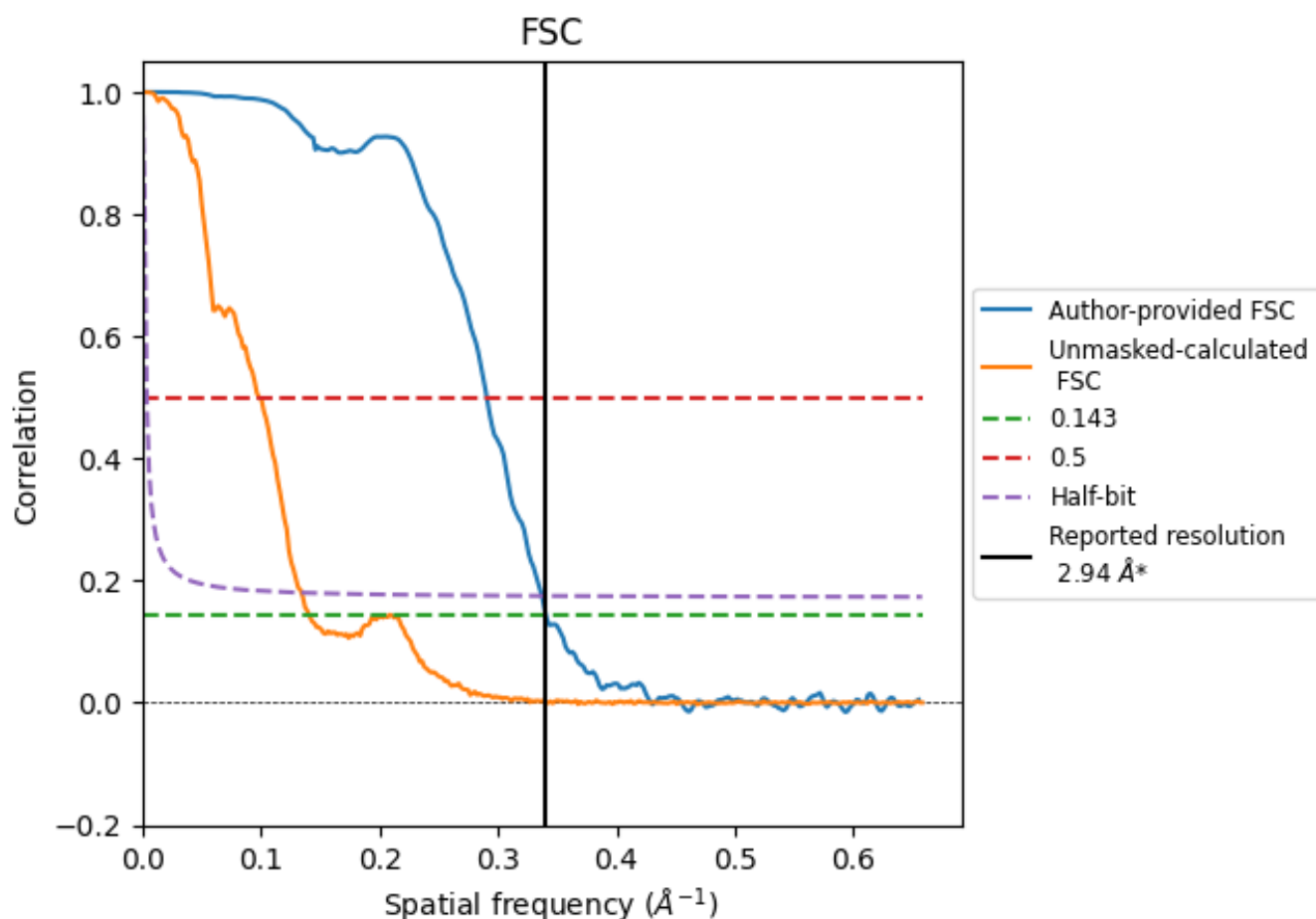


\*Reported resolution corresponds to spatial frequency of 0.340 Å<sup>-1</sup>

## 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 0.340 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

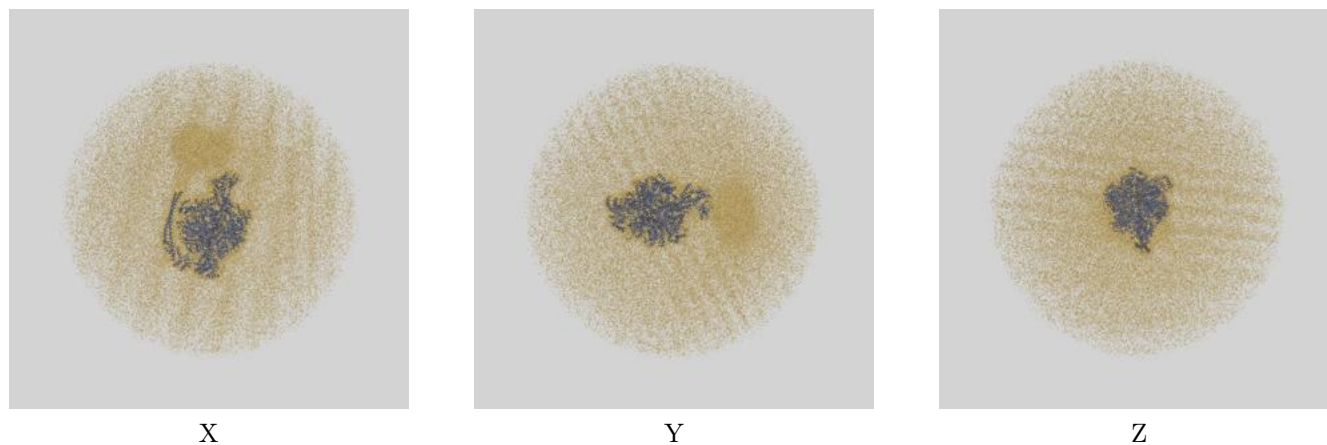
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 2.94                               | -     | -        |
| Author-provided FSC curve | 2.94                               | 3.44  | 2.97     |
| Unmasked-calculated*      | 7.10                               | 10.15 | 7.45     |

\*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 7.10 differs from the reported value 2.94 by more than 10 %

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

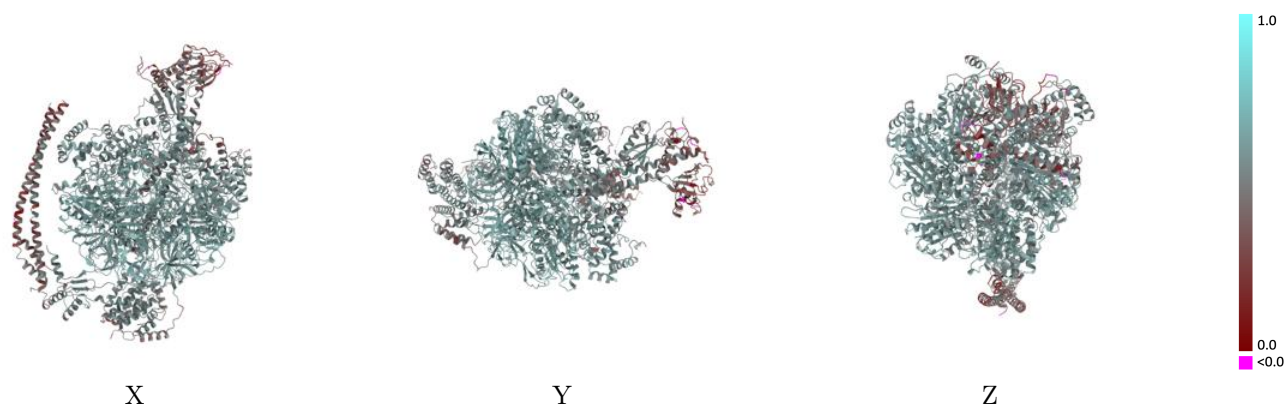
This section contains information regarding the fit between EMDB map EMD-65138 and PDB model 9VKP. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



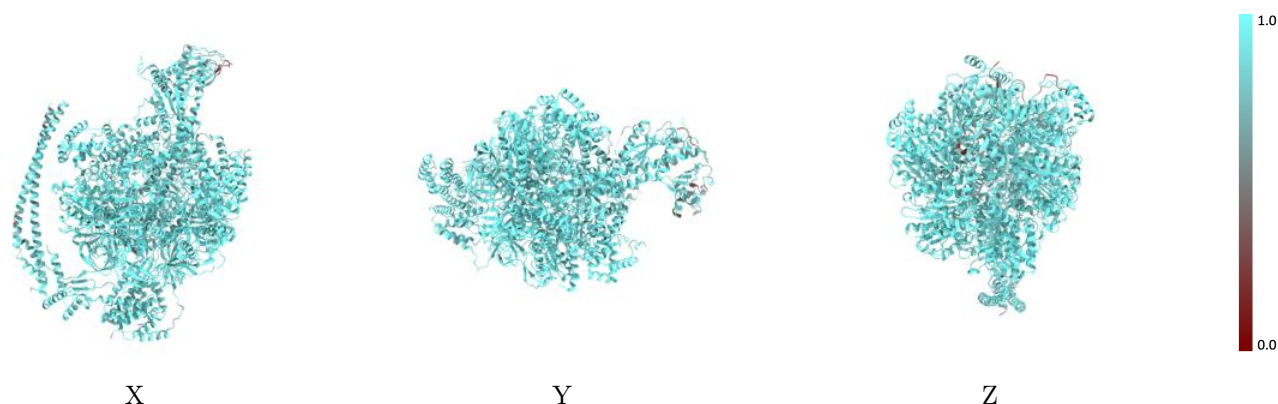
The images above show the 3D surface view of the map at the recommended contour level 0.072 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



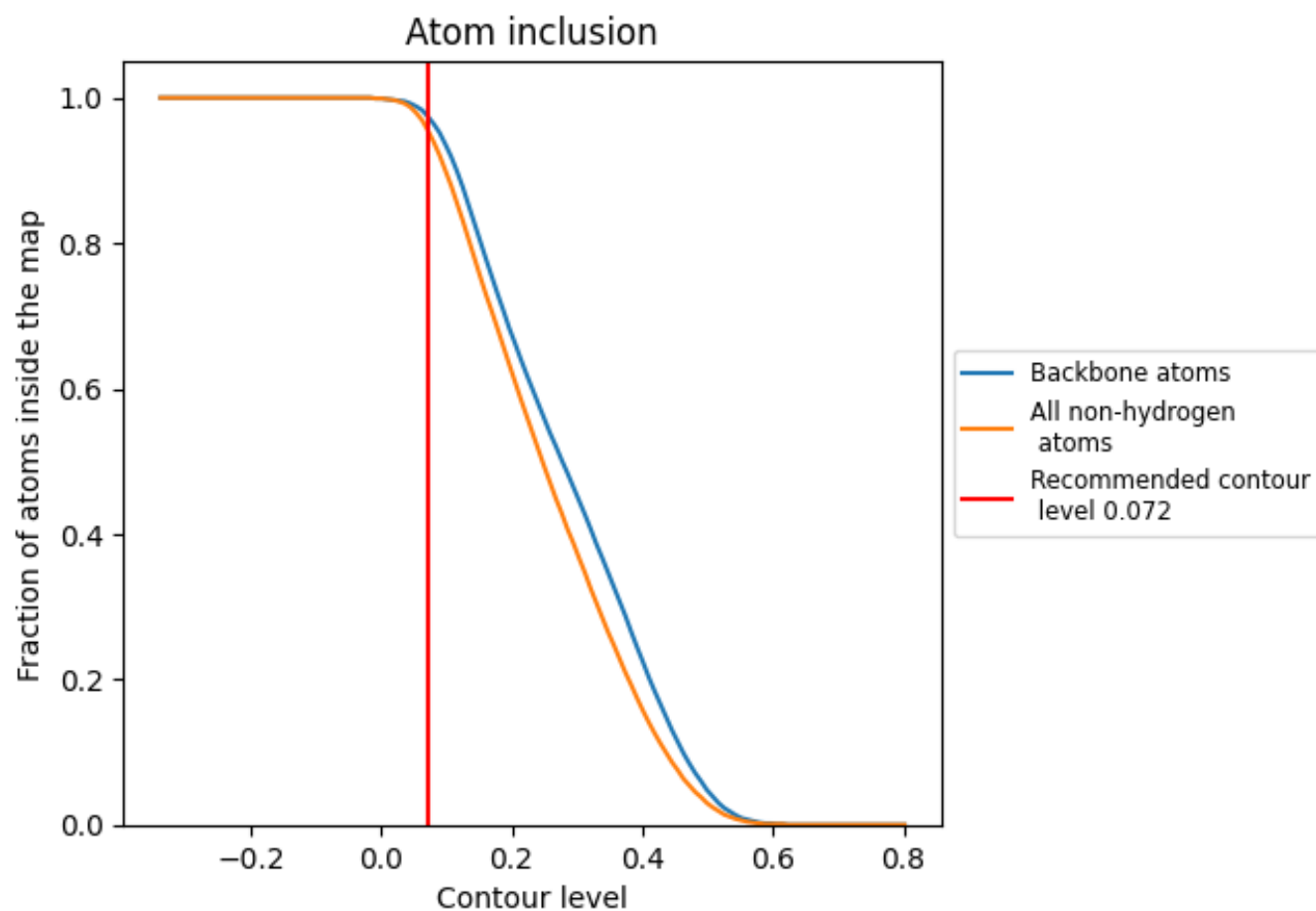
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.072).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.072) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9550 | <div></div> 0.5580 |
| A     | <div></div> 0.9690 | <div></div> 0.5820 |
| B     | <div></div> 0.9710 | <div></div> 0.5900 |
| C     | <div></div> 0.9680 | <div></div> 0.5840 |
| D     | <div></div> 0.9840 | <div></div> 0.6080 |
| E     | <div></div> 0.9790 | <div></div> 0.5910 |
| F     | <div></div> 0.9730 | <div></div> 0.5830 |
| G     | <div></div> 0.8970 | <div></div> 0.4740 |
| H     | <div></div> 0.7620 | <div></div> 0.3010 |
| b     | <div></div> 0.8330 | <div></div> 0.3720 |
| d     | <div></div> 0.9370 | <div></div> 0.5000 |

1.0

0.0

<0.0