



## Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 02:35 PM EST

PDB ID : 8VLP  
EMDB ID : EMD-43341  
Title : Composite structure of human FASN with NADPH in State 3  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-11  
Resolution : 3.20 Å (reported)  
Based on initial model : 3HHD

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.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

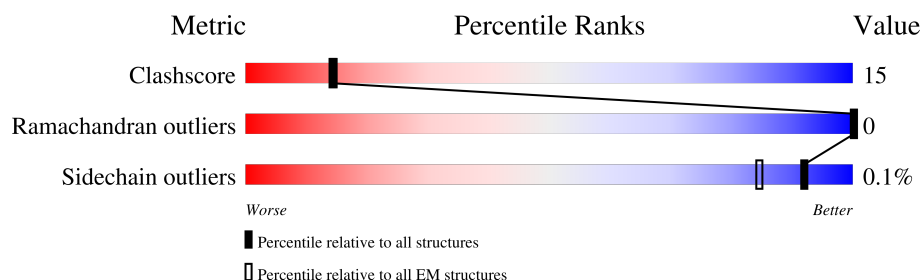
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2553	 60% 20% 19%
1	B	2553	 61% 20% 19%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50709 atoms, of which 18827 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2068	Total	C	H	N	O	S	0	0
			25176	10041	9343	2785	2934	73		
1	B	2071	Total	C	H	N	O	S	0	0
			25237	10054	9380	2789	2941	73		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	expression tag	UNP P49327
A	-30	SER	-	expression tag	UNP P49327
A	-29	TYR	-	expression tag	UNP P49327
A	-28	TYR	-	expression tag	UNP P49327
A	-27	ASP	-	expression tag	UNP P49327
A	-26	TYR	-	expression tag	UNP P49327
A	-25	LYS	-	expression tag	UNP P49327
A	-24	ASP	-	expression tag	UNP P49327
A	-23	ASP	-	expression tag	UNP P49327
A	-22	ASP	-	expression tag	UNP P49327
A	-21	ASP	-	expression tag	UNP P49327
A	-20	LYS	-	expression tag	UNP P49327
A	-19	ASP	-	expression tag	UNP P49327
A	-18	TYR	-	expression tag	UNP P49327
A	-17	ASP	-	expression tag	UNP P49327
A	-16	ILE	-	expression tag	UNP P49327
A	-15	PRO	-	expression tag	UNP P49327
A	-14	THR	-	expression tag	UNP P49327
A	-13	THR	-	expression tag	UNP P49327
A	-12	GLU	-	expression tag	UNP P49327
A	-11	ASN	-	expression tag	UNP P49327
A	-10	LEU	-	expression tag	UNP P49327
A	-9	TYR	-	expression tag	UNP P49327
A	-8	PHE	-	expression tag	UNP P49327
A	-7	GLN	-	expression tag	UNP P49327
A	-6	GLY	-	expression tag	UNP P49327

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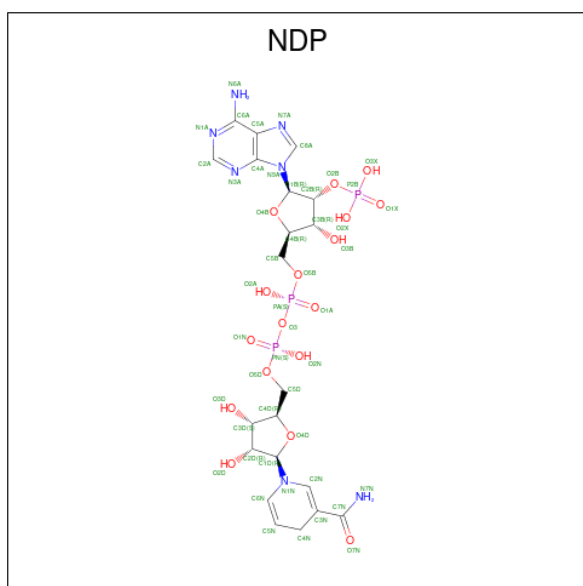
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
A	1151	THR	LYS	conflict	UNP P49327
A	2512	LEU	-	expression tag	UNP P49327
A	2513	GLU	-	expression tag	UNP P49327
A	2514	HIS	-	expression tag	UNP P49327
A	2515	HIS	-	expression tag	UNP P49327
A	2516	HIS	-	expression tag	UNP P49327
A	2517	HIS	-	expression tag	UNP P49327
A	2518	HIS	-	expression tag	UNP P49327
A	2519	HIS	-	expression tag	UNP P49327
A	2520	HIS	-	expression tag	UNP P49327
A	2521	HIS	-	expression tag	UNP P49327
B	-31	MET	-	expression tag	UNP P49327
B	-30	SER	-	expression tag	UNP P49327
B	-29	TYR	-	expression tag	UNP P49327
B	-28	TYR	-	expression tag	UNP P49327
B	-27	ASP	-	expression tag	UNP P49327
B	-26	TYR	-	expression tag	UNP P49327
B	-25	LYS	-	expression tag	UNP P49327
B	-24	ASP	-	expression tag	UNP P49327
B	-23	ASP	-	expression tag	UNP P49327
B	-22	ASP	-	expression tag	UNP P49327
B	-21	ASP	-	expression tag	UNP P49327
B	-20	LYS	-	expression tag	UNP P49327
B	-19	ASP	-	expression tag	UNP P49327
B	-18	TYR	-	expression tag	UNP P49327
B	-17	ASP	-	expression tag	UNP P49327
B	-16	ILE	-	expression tag	UNP P49327
B	-15	PRO	-	expression tag	UNP P49327
B	-14	THR	-	expression tag	UNP P49327
B	-13	THR	-	expression tag	UNP P49327
B	-12	GLU	-	expression tag	UNP P49327
B	-11	ASN	-	expression tag	UNP P49327
B	-10	LEU	-	expression tag	UNP P49327
B	-9	TYR	-	expression tag	UNP P49327
B	-8	PHE	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLN	-	expression tag	UNP P49327
B	-6	GLY	-	expression tag	UNP P49327
B	-5	ALA	-	expression tag	UNP P49327
B	-4	MET	-	expression tag	UNP P49327
B	-3	GLY	-	expression tag	UNP P49327
B	-2	SER	-	expression tag	UNP P49327
B	-1	GLY	-	expression tag	UNP P49327
B	0	ILE	-	expression tag	UNP P49327
B	1	PRO	-	expression tag	UNP P49327
B	1151	THR	LYS	conflict	UNP P49327
B	2512	LEU	-	expression tag	UNP P49327
B	2513	GLU	-	expression tag	UNP P49327
B	2514	HIS	-	expression tag	UNP P49327
B	2515	HIS	-	expression tag	UNP P49327
B	2516	HIS	-	expression tag	UNP P49327
B	2517	HIS	-	expression tag	UNP P49327
B	2518	HIS	-	expression tag	UNP P49327
B	2519	HIS	-	expression tag	UNP P49327
B	2520	HIS	-	expression tag	UNP P49327
B	2521	HIS	-	expression tag	UNP P49327

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).

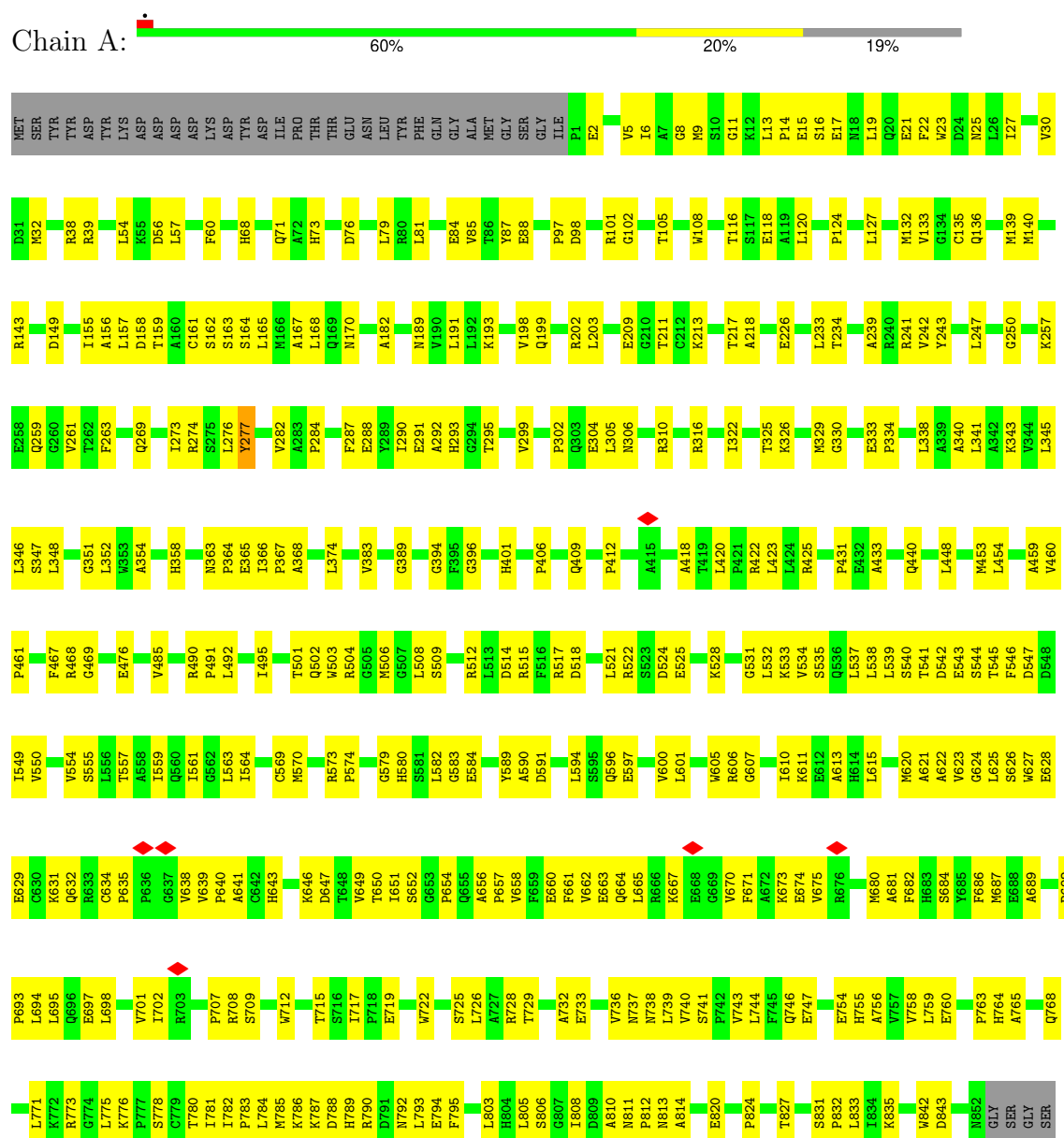


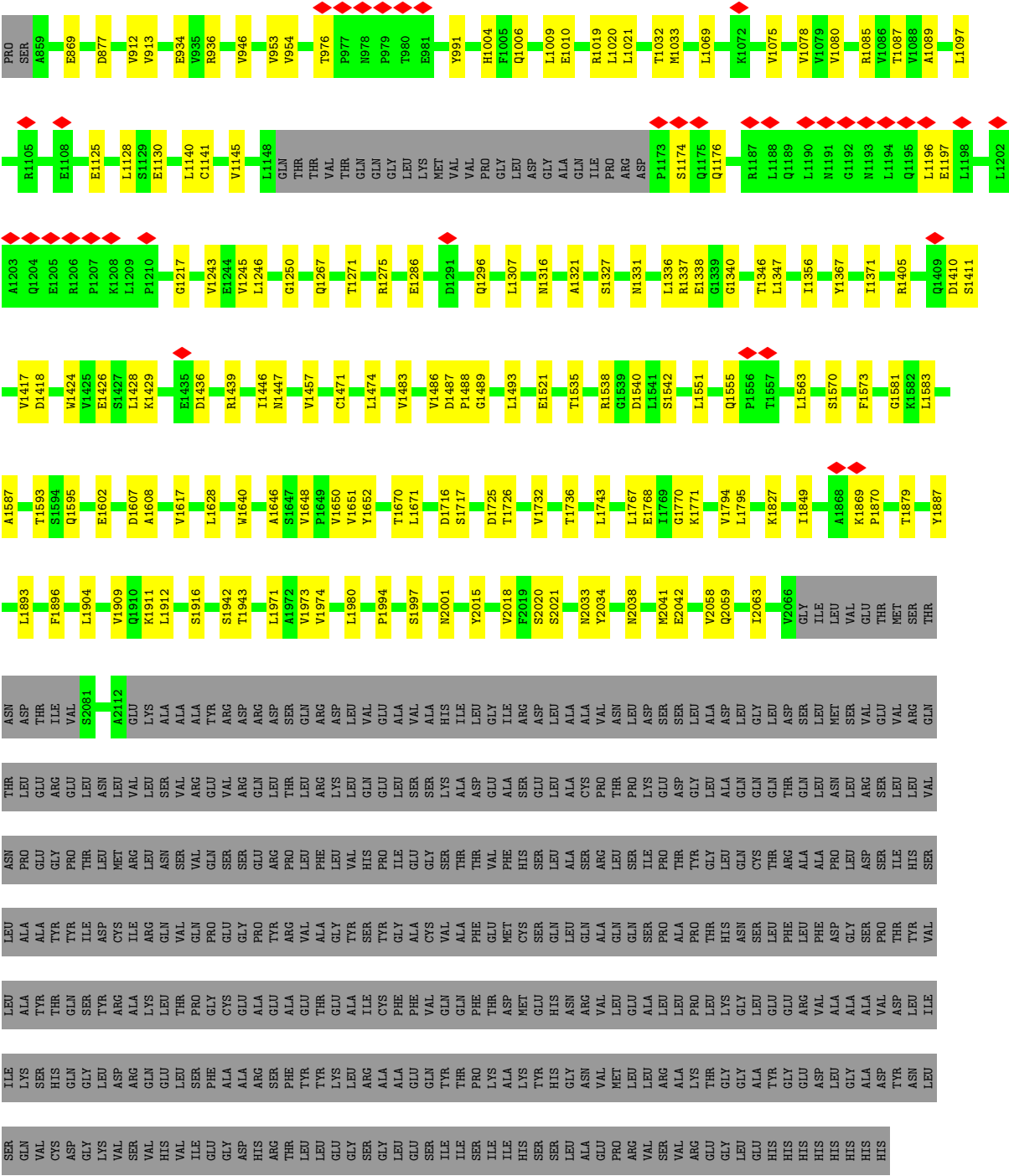
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 3 Residue-property plots

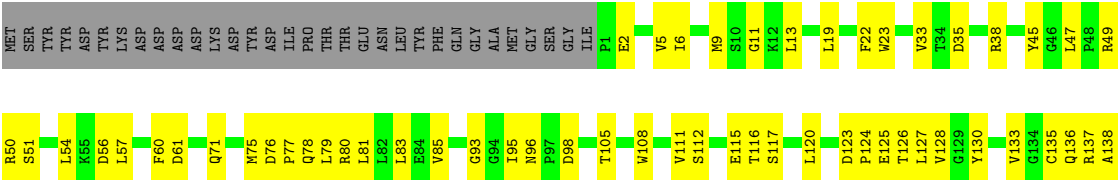
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Fatty acid synthase





● Molecule 1: Fatty acid synthase





LEU	VAL	THR	GLN	GLY	LEU	LYS	MET	VAL	PRO	SER	THR	LEU	LYS	GLN	GLY	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	GLY	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LEU	LYS	GLN	ILE	PRO	SER	THR	LE
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HIS	GLY	GLU	PHE	ARG	THR	ASP
HIS	GLU	ARG	LEU	ALA	GLN	SER
HIS	ASP	VAL	PHE	ALA	LEU	LEU
HIS	GLY	ALA	ASP	PRO	ASN	SER
HIS	GLY	ALA	GLY	LEU	ASN	SER
HIS	ALA	ALA	SER	ASP	ARG	VAL
HIS	ASP	VAL	PRO	SER	SER	GLU
	TYR	ASP	THR	ILE	LEU	VAL
	ASN	LEU	TYR	HIS	LEU	ARG
	LEU	ILE	VAL	SER	VAL	GLN
	SER	ILE	LEU	LEU	ASN	THR
	GLN	LYS	ALA	ALA	PRO	LEU
	VAL	SER	TYR	ALA	GLU	GLU
	CYS	HIS	THR	TYR	GLY	ARG
	ASP	HIS	GLN	TYR	PRO	GLN
	GLY	GLY	SER	ILE	THR	LEU
	LYS	LEU	TYR	ASP	LEU	ASN
	VAL	ASP	ARG	CYS	MET	LEU
	SER	ARG	ALA	ILE	ARG	VAL
	VAL	GLN	LYS	ILE	LEU	VAL
	HIS	GLU	LEU	GLN	ASN	SER
	GLY	LEU	THR	VAL	SER	VAL
	ILE	SER	PRO	GLN	VAL	ARG
	GLU	PHE	GLY	PRO	GLN	GLU
	GLY	ALA	CYS	PRO	GLN	GLU
	GLY	ALA	ALA	VAL	LEU	LEU
	LEU	ALA	PHE	GLY	ILE	LEU
	GLU	GLU	PHE	ALA	GLU	SER
	SER	GLN	VAL	CYS	GLY	SER
	ILE	TYR	GLN	VAL	SER	LYS
	ILE	THR	GLN	ALA	THR	ALA
	SER	PRO	PHE	PHE	THR	ASP
	ILE	LYS	THR	GLU	VAL	GLU
	ILE	ALA	ASP	MET	PHE	GLU
	HIS	LYS	ILE	CYS	HIS	SER
	SER	TYR	GLU	SER	LEU	LEU
	LEU	GLY	ASN	LEU	ALA	ALA
	ALA	ASN	ARG	GLN	SER	CYS
	GLU	VAL	VAL	ALA	ARG	PRO
	PRO	MET	LEU	ALA	LEU	THR
	ARG	LEU	GLU	GLN	SER	THR
	VAL	LEU	ALA	SER	ILE	LYS
	SER	ARG	LEU	PRO	PRO	GLY
	VAL	ALA	LEU	ALA	THR	ASP
	ARG	LYS	PRO	PRO	TYR	GLY
	GLU	THR	LEU	THR	GLY	GLN
	GLY	GLY	LYS	HIS	LEU	ALA
	LEU	GLY	GLY	ASN	GLN	GLN
	HIS	GLU	ALA	SER	CYS	GLN
	THR	THR	GLU	LEU	THR	GLN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131766	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 ( $e^-/\text{\AA}^2$ )	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.757	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.197	Depositor
Map size ( $\text{\AA}$ )	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.069, 1.069, 1.069	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.27	0/16198	0.47	0/22023
1	B	0.28	0/16222	0.48	0/22055
All	All	0.27	0/32420	0.48	0/44078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15833	9343	15809	504	0
1	B	15857	9380	15826	477	0
2	A	96	52	52	4	0
2	B	96	52	52	0	0
All	All	31882	18827	31739	966	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (966) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:LEU:HD11	1:A:629:GLU:HB2	1.34	1.08
1:B:9:MET:HE1	1:B:342:ALA:HA	1.38	1.04
1:A:628:GLU:HA	1:A:631:LYS:HE2	1.41	1.02
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.46	0.97
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.53	0.92
1:B:687:MET:HA	1:B:690:ILE:HD13	1.52	0.92
1:B:626:SER:HB2	1:B:629:GLU:HG3	1.51	0.91
1:B:771:LEU:HB3	1:B:781:ILE:CD1	2.00	0.91
1:B:782:ILE:HG22	1:B:782:ILE:O	1.70	0.90
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.51	0.89
1:B:640:PRO:HA	1:B:651:ILE:HD13	1.55	0.89
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.53	0.88
1:A:164:SER:HB2	1:A:338:LEU:CD1	2.04	0.86
1:B:440:GLN:HG3	1:B:833:LEU:HD22	1.54	0.86
1:B:325:THR:HB	1:B:343:LYS:HD3	1.56	0.86
1:A:621:ALA:HA	1:A:674:GLU:HA	1.58	0.85
1:A:725:SER:HA	1:A:728:ARG:HH12	1.42	0.85
1:B:757:VAL:HG13	1:B:782:ILE:HD12	1.58	0.84
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.60	0.83
1:B:158:ASP:O	1:B:163:SER:HB3	1.77	0.83
1:B:757:VAL:CG1	1:B:782:ILE:HD12	2.09	0.83
1:B:674:GLU:HG2	1:B:676:ARG:HH22	1.44	0.82
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.62	0.82
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.60	0.81
1:B:752:VAL:O	1:B:776:LYS:NZ	2.13	0.81
1:A:420:LEU:HD21	1:A:512:ARG:HB3	1.63	0.81
1:B:623:VAL:HG12	1:B:625:LEU:HG	1.61	0.81
1:A:503:TRP:H	1:A:506:MET:HE3	1.46	0.80
1:B:625:LEU:HD21	1:B:670:VAL:HG11	1.61	0.80
1:A:127:LEU:HD11	1:B:198:VAL:HG12	1.62	0.80
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.11	0.80
1:B:682:PHE:HA	1:B:687:MET:SD	2.21	0.80
1:A:502:GLN:HA	1:A:506:MET:HE1	1.61	0.80
1:B:771:LEU:HB3	1:B:781:ILE:HD12	1.64	0.80
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.63	0.79
1:B:585:VAL:HG12	1:B:599:ALA:HB1	1.65	0.79
1:B:1773:ASP:OD1	1:B:1778:HIS:ND1	2.16	0.79
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.65	0.79
1:B:1837:GLU:N	1:B:1837:GLU:OE1	2.17	0.78
1:B:468:ARG:HD2	1:B:485:VAL:HG21	1.65	0.78
1:A:623:VAL:HG12	1:A:625:LEU:H	1.48	0.78
1:B:596:GLN:O	1:B:600:VAL:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:MET:HG3	1:B:559:ILE:HD11	1.66	0.77
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.67	0.77
1:A:418:ALA:HA	1:A:422:ARG:HH21	1.50	0.77
1:A:628:GLU:OE1	1:A:628:GLU:N	2.18	0.77
1:B:1429:LYS:NZ	1:B:1981:GLU:O	2.17	0.77
1:A:189:ASN:HD22	1:A:334:PRO:HD2	1.48	0.77
1:A:625:LEU:HD11	1:A:629:GLU:CB	2.15	0.77
1:A:468:ARG:HD2	1:A:485:VAL:HG21	1.66	0.77
1:A:365:GLU:N	1:A:365:GLU:OE1	2.17	0.76
1:B:771:LEU:HB3	1:B:781:ILE:HD11	1.66	0.76
1:B:623:VAL:HG21	1:B:665:LEU:HD13	1.67	0.76
1:B:139:MET:HE3	1:B:139:MET:HA	1.66	0.76
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.67	0.76
1:B:626:SER:HB2	1:B:629:GLU:CG	2.15	0.76
1:A:540:SER:HB3	1:A:545:THR:HG21	1.66	0.76
1:B:621:ALA:O	1:B:651:ILE:N	2.16	0.75
1:A:732:ALA:O	1:A:736:VAL:HG23	1.85	0.75
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.50	0.75
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.69	0.75
1:B:1109:GLN:N	1:B:1109:GLN:OE1	2.19	0.74
1:B:216:ASP:OD1	1:B:217:THR:N	2.20	0.74
1:B:182:ALA:CB	1:B:234:THR:HG22	2.17	0.74
1:B:5:VAL:HB	1:B:242:VAL:HG13	1.69	0.74
1:A:502:GLN:HA	1:A:506:MET:CE	2.18	0.74
1:A:725:SER:HA	1:A:728:ARG:NH1	2.02	0.74
1:B:540:SER:OG	1:B:545:THR:HG21	1.87	0.74
1:A:622:ALA:N	1:A:673:LYS:O	2.20	0.73
1:B:290:ILE:HG23	1:B:322:ILE:HD12	1.68	0.73
1:A:209:GLU:OE1	1:A:209:GLU:N	2.21	0.73
1:A:274:ARG:HA	1:A:277:TYR:CE2	2.22	0.73
1:A:694:LEU:O	1:A:698:LEU:HG	1.88	0.73
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.53	0.73
1:B:164:SER:HB2	1:B:338:LEU:HG	1.70	0.73
1:B:511:MET:HE1	1:B:517:ARG:HG3	1.69	0.73
1:B:757:VAL:HG13	1:B:782:ILE:CD1	2.18	0.73
1:A:596:GLN:O	1:A:600:VAL:HG23	1.90	0.72
1:A:620:MET:HE1	1:A:682:PHE:HB2	1.70	0.72
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.70	0.72
1:A:506:MET:HG3	1:A:559:ILE:HD11	1.71	0.72
1:A:788:ASP:O	1:A:790:ARG:NH2	2.22	0.72
1:A:1010:GLU:OE2	1:A:1019:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.22	0.72
1:A:1716:ASP:OD1	1:A:1717:SER:N	2.22	0.72
1:B:591:ASP:OD2	1:B:712:TRP:HB2	1.89	0.72
1:B:639:VAL:HG13	1:B:640:PRO:HD2	1.72	0.72
1:A:661:PHE:O	1:A:665:LEU:HG	1.90	0.71
1:B:663:GLU:O	1:B:667:LYS:HG3	1.90	0.71
1:A:657:PRO:O	1:A:660:GLU:HG2	1.89	0.71
1:A:1327:SER:O	1:A:1331:ASN:ND2	2.23	0.71
1:A:563:LEU:HD11	1:A:785:MET:HE3	1.73	0.71
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.73	0.71
1:A:820:GLU:OE1	1:A:820:GLU:N	2.22	0.71
1:A:1337:ARG:NH1	1:A:1338:GLU:O	2.24	0.71
1:A:259:GLN:N	1:A:259:GLN:OE1	2.23	0.71
1:B:672:ALA:O	1:B:673:LYS:HD2	1.91	0.71
1:A:737:ASN:OD1	1:A:741:SER:OG	2.08	0.70
1:B:719:GLU:HA	1:B:722:TRP:NE1	2.06	0.70
1:A:409:GLN:HB3	1:A:824:PRO:HA	1.74	0.70
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.72	0.70
1:B:694:LEU:HD23	1:B:698:LEU:HG	1.71	0.70
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.73	0.70
1:B:191:LEU:N	1:B:226:GLU:OE2	2.15	0.70
1:B:628:GLU:OE1	1:B:628:GLU:N	2.20	0.70
1:B:292:ALA:HB2	1:B:322:ILE:HD11	1.73	0.69
1:B:622:ALA:HA	1:B:650:THR:HA	1.74	0.69
1:A:277:TYR:CE1	1:A:284:PRO:HG3	2.27	0.69
1:A:182:ALA:CB	1:A:234:THR:HG22	2.23	0.69
1:A:293:HIS:N	1:A:304:GLU:OE2	2.23	0.69
1:B:732:ALA:O	1:B:736:VAL:HG23	1.93	0.69
1:B:235:LYS:HE3	1:B:238:LEU:HD13	1.75	0.69
1:A:276:LEU:HD12	1:A:401:HIS:HB3	1.74	0.69
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.74	0.69
1:A:580:HIS:HD2	1:A:743:VAL:HG11	1.57	0.68
1:A:790:ARG:HA	1:A:790:ARG:NE	2.07	0.68
1:B:166:MET:HE3	1:B:251:THR:HG21	1.73	0.68
1:A:646:LYS:HG3	1:A:647:ASP:OD1	1.92	0.68
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.09	0.68
1:B:1206:ARG:NH2	1:B:1319:VAL:O	2.26	0.68
1:A:1607:ASP:OD1	1:A:1608:ALA:N	2.27	0.68
1:A:549:ILE:HD11	1:A:611:LYS:HG3	1.75	0.68
1:A:584:GLU:HG3	1:A:712:TRP:HZ2	1.59	0.68
1:A:627:TRP:HA	1:A:649:VAL:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ARG:NH1	1:B:464:ALA:O	2.26	0.68
1:B:503:TRP:H	1:B:506:MET:CE	2.06	0.68
1:A:628:GLU:HA	1:A:631:LYS:CE	2.21	0.67
1:B:704:GLU:HG2	1:B:704:GLU:O	1.95	0.67
1:A:625:LEU:HD12	1:A:626:SER:H	1.58	0.67
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.29	0.67
1:A:9:MET:HE1	1:A:345:LEU:HB3	1.77	0.67
1:A:503:TRP:CH2	1:A:506:MET:HA	2.29	0.67
1:B:549:ILE:HD11	1:B:553:PHE:CZ	2.30	0.67
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.77	0.67
1:B:325:THR:HB	1:B:343:LYS:CD	2.25	0.67
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.30	0.67
1:B:524:ASP:OD1	1:B:534:VAL:HB	1.95	0.67
1:B:697:GLU:O	1:B:701:VAL:HG23	1.95	0.67
1:A:158:ASP:O	1:B:138:ALA:HB2	1.95	0.66
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.75	0.66
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.28	0.66
1:B:687:MET:HE3	1:B:739:LEU:HG	1.75	0.66
1:B:698:LEU:HB2	1:B:732:ALA:HB1	1.78	0.66
1:A:1275:ARG:O	1:A:1296:GLN:NE2	2.28	0.66
1:B:1228:LEU:HD21	1:B:1256:ILE:HD12	1.76	0.66
1:A:504:ARG:HA	1:A:546:PHE:CE1	2.30	0.66
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.76	0.66
1:B:504:ARG:HD2	1:B:543:GLU:OE1	1.95	0.66
1:A:663:GLU:O	1:A:667:LYS:HG2	1.95	0.66
1:A:57:LEU:HD23	1:A:81:LEU:HD11	1.78	0.66
1:A:768:GLN:HG3	1:A:781:ILE:HG21	1.77	0.66
1:B:215:PHE:CE1	1:B:305:LEU:HD11	2.31	0.66
1:B:685:TYR:HA	1:B:688:GLU:HG3	1.77	0.66
1:B:506:MET:HG3	1:B:559:ILE:CD1	2.26	0.66
1:B:757:VAL:CG1	1:B:782:ILE:CD1	2.73	0.66
1:A:506:MET:HG3	1:A:559:ILE:CD1	2.26	0.65
1:A:639:VAL:HB	1:A:640:PRO:HD2	1.77	0.65
1:B:782:ILE:O	1:B:782:ILE:CG2	2.43	0.65
1:B:1487:ASP:N	1:B:1490:SER:OG	2.30	0.65
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.29	0.65
1:A:84:GLU:O	1:A:88:GLU:HG3	1.96	0.65
1:A:9:MET:HE2	1:A:345:LEU:HD13	1.78	0.65
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.23	0.65
1:A:640:PRO:HA	1:A:651:ILE:HG22	1.79	0.65
1:A:514:ASP:OD1	1:A:515:ARG:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ASP:OD2	1:B:450:PHE:HB2	1.96	0.65
1:B:537:LEU:HD11	1:B:551:HIS:ND1	2.12	0.65
1:B:1195:GLN:O	1:B:1199:ALA:N	2.29	0.65
1:A:694:LEU:O	1:A:694:LEU:HD12	1.98	0.65
1:B:182:ALA:HB2	1:B:234:THR:HG22	1.79	0.65
1:B:1327:SER:O	1:B:1331:ASN:ND2	2.29	0.64
1:A:21:GLU:O	1:A:25:ASN:ND2	2.30	0.64
1:A:189:ASN:ND2	1:A:333:GLU:OE1	2.28	0.64
1:A:625:LEU:CD1	1:A:629:GLU:HB2	2.22	0.64
1:A:1997:SER:O	1:A:2001:ASN:ND2	2.30	0.64
1:B:620:MET:HG2	1:B:677:THR:HG21	1.79	0.64
1:A:161:CYS:HA	1:A:333:GLU:O	1.97	0.64
1:A:502:GLN:OE1	1:A:502:GLN:N	2.30	0.64
1:A:550:VAL:O	1:A:554:VAL:HG23	1.96	0.64
1:B:549:ILE:HD11	1:B:553:PHE:CE2	2.32	0.64
1:B:71:GLN:O	1:B:71:GLN:NE2	2.28	0.64
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.30	0.64
1:B:477:ARG:HH22	1:B:790:ARG:HD2	1.63	0.64
1:B:460:VAL:HG13	1:B:461:PRO:HD2	1.79	0.64
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.29	0.63
1:B:766:LEU:HD23	1:B:766:LEU:O	1.98	0.63
1:A:610:ILE:HG22	1:A:680:MET:HE1	1.80	0.63
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.30	0.63
1:B:290:ILE:HG23	1:B:322:ILE:CD1	2.28	0.63
1:B:595:SER:N	1:B:598:GLU:OE1	2.19	0.63
1:B:501:THR:OG1	1:B:764:HIS:HB3	1.97	0.63
1:B:115:GLU:OE1	1:B:193:LYS:N	2.31	0.63
1:A:528:LYS:O	1:A:528:LYS:NZ	2.19	0.63
1:A:698:LEU:HB2	1:A:732:ALA:HB1	1.80	0.63
1:B:717:ILE:HD12	1:B:717:ILE:O	1.99	0.63
1:A:737:ASN:HA	1:A:740:VAL:HG22	1.81	0.63
1:B:662:VAL:O	1:B:666:ARG:HG2	1.98	0.63
1:B:659:PHE:O	1:B:663:GLU:HG3	1.98	0.63
1:A:274:ARG:HA	1:A:277:TYR:CD2	2.33	0.62
1:B:38:ARG:NH1	1:B:54:LEU:O	2.32	0.62
1:B:625:LEU:CD2	1:B:670:VAL:HG11	2.29	0.62
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.34	0.62
1:A:9:MET:HE2	1:A:345:LEU:CD1	2.29	0.62
1:B:674:GLU:HG2	1:B:676:ARG:NH2	2.12	0.62
1:B:721:GLN:OE1	1:B:721:GLN:N	2.33	0.62
1:A:120:LEU:HD12	1:A:135:CYS:SG	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:TRP:CA	1:A:649:VAL:HG21	2.29	0.62
1:B:120:LEU:HD12	1:B:135:CYS:SG	2.40	0.62
1:B:687:MET:CE	1:B:739:LEU:HG	2.29	0.62
1:A:504:ARG:HA	1:A:546:PHE:HE1	1.62	0.62
1:A:627:TRP:CZ3	1:A:643:HIS:HB2	2.35	0.62
1:B:291:GLU:OE2	1:B:325:THR:HG22	1.99	0.62
1:B:567:LEU:HA	1:B:570:MET:CE	2.29	0.62
1:B:607:GLY:HA2	1:B:610:ILE:HD12	1.81	0.62
1:A:540:SER:CB	1:A:545:THR:HG21	2.30	0.61
1:A:692:PRO:O	1:A:695:LEU:HG	2.00	0.61
1:A:247:LEU:HD23	1:A:282:VAL:HG21	1.83	0.61
1:B:504:ARG:HH21	1:B:541:THR:HB	1.65	0.61
1:B:1439:ARG:O	1:B:1468:ARG:NH1	2.34	0.61
1:A:211:THR:HG22	1:A:213:LYS:HG3	1.82	0.61
1:B:560:GLN:O	1:B:564:ILE:HG13	2.01	0.61
1:A:365:GLU:O	1:A:367:PRO:HD3	2.00	0.61
1:A:657:PRO:HA	1:A:660:GLU:HG2	1.82	0.61
1:B:469:GLY:HA2	1:B:805:LEU:HD21	1.82	0.61
1:A:431:PRO:HG3	1:A:467:PHE:CE2	2.36	0.61
1:B:111:VAL:HG13	1:B:137:ARG:HD2	1.82	0.61
1:A:628:GLU:CA	1:A:631:LYS:HE2	2.22	0.60
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.01	0.60
1:B:325:THR:HG21	1:B:340:ALA:HA	1.83	0.60
1:B:440:GLN:HG3	1:B:833:LEU:CD2	2.29	0.60
1:B:2033:ASN:OD1	1:B:2034:TYR:N	2.34	0.60
1:A:39:ARG:HD2	1:A:191:LEU:O	2.01	0.60
1:A:755:HIS:ND1	1:A:778:SER:HB2	2.16	0.60
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.82	0.60
1:B:767:LEU:O	1:B:771:LEU:HD23	2.01	0.60
1:B:664:GLN:HA	1:B:667:LYS:HD2	1.82	0.60
1:B:771:LEU:CB	1:B:781:ILE:HD12	2.32	0.60
1:B:1197:GLU:OE1	1:B:1197:GLU:N	2.33	0.60
1:A:495:ILE:HD12	1:A:771:LEU:HD21	1.84	0.60
1:A:629:GLU:OE1	1:A:629:GLU:N	2.27	0.60
1:A:831:SER:OG	1:A:832:PRO:HD3	2.01	0.60
1:B:139:MET:HE3	1:B:142:ASN:HB2	1.83	0.60
1:B:736:VAL:O	1:B:740:VAL:HG22	2.01	0.60
1:B:1122:HIS:ND1	1:B:1511:TRP:O	2.34	0.60
1:A:418:ALA:HB2	1:A:448:LEU:HD11	1.83	0.60
1:B:1025:ASN:OD1	1:B:1028:SER:OG	2.15	0.60
1:B:705:PRO:HB3	1:B:730:SER:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG12	1:B:127:LEU:HD11	1.83	0.59
1:A:420:LEU:HD21	1:A:512:ARG:CB	2.30	0.59
1:A:518:ASP:O	1:A:522:ARG:HG3	2.02	0.59
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.33	0.59
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.34	0.59
1:A:869:GLU:N	1:A:869:GLU:OE1	2.36	0.59
1:B:1205:GLU:O	1:B:1209:LEU:N	2.34	0.59
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.35	0.59
1:A:217:THR:HG22	1:A:364:PRO:HD3	1.84	0.59
1:A:597:GLU:HG2	1:A:601:LEU:HD11	1.84	0.59
1:A:628:GLU:O	1:A:631:LYS:HG2	2.02	0.59
1:B:76:ASP:OD1	1:B:77:PRO:HD2	2.02	0.59
1:B:621:ALA:HA	1:B:674:GLU:HA	1.85	0.59
1:B:548:ASP:HB3	1:B:551:HIS:HB2	1.85	0.59
1:A:508:LEU:HD11	1:A:538:LEU:O	2.03	0.59
1:B:182:ALA:HB1	1:B:234:THR:HG22	1.83	0.59
1:B:290:ILE:O	1:B:322:ILE:HD12	2.02	0.59
1:B:537:LEU:O	1:B:540:SER:OG	2.17	0.59
1:B:1250:GLY:O	1:B:1316:ASN:ND2	2.35	0.59
1:A:522:ARG:NH1	1:A:596:GLN:OE1	2.36	0.58
1:A:534:VAL:O	1:A:538:LEU:HG	2.03	0.58
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.85	0.58
1:A:124:PRO:HG3	1:B:195:ASN:OD1	2.04	0.58
1:A:157:LEU:HD21	1:A:170:ASN:ND2	2.18	0.58
1:A:641:ALA:H	1:A:651:ILE:HA	1.68	0.58
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.86	0.58
1:B:664:GLN:OE1	1:B:667:LYS:HD2	2.04	0.58
1:A:582:LEU:HD12	1:A:583:GLY:H	1.68	0.58
1:B:657:PRO:HA	1:B:660:GLU:OE1	2.03	0.58
1:A:654:PRO:HG3	1:A:686:PHE:HZ	1.69	0.58
1:A:6:ILE:HG12	1:A:233:LEU:HD21	1.86	0.58
1:A:159:THR:O	1:A:163:SER:HB3	2.04	0.58
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.38	0.58
1:A:717:ILE:HG22	1:A:722:TRP:HD1	1.68	0.58
1:A:1551:LEU:HD12	1:A:1563:LEU:HD11	1.86	0.58
1:B:768:GLN:NE2	1:B:783:PRO:HB3	2.19	0.58
1:A:1426:GLU:OE1	1:A:1429:LYS:NZ	2.23	0.58
1:B:1300:ALA:O	1:B:1331:ASN:ND2	2.37	0.58
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.39	0.58
1:A:514:ASP:OD1	1:A:515:ARG:HG2	2.04	0.58
1:B:273:ILE:O	1:B:277:TYR:CD2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ARG:HA	1:B:277:TYR:CE2	2.39	0.58
1:B:643:HIS:ND1	1:B:747:GLU:OE2	2.36	0.57
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.86	0.57
1:A:418:ALA:CA	1:A:422:ARG:HH21	2.17	0.57
1:A:626:SER:HB3	1:A:629:GLU:OE2	2.03	0.57
1:B:623:VAL:CG1	1:B:625:LEU:HG	2.33	0.57
1:B:1199:ALA:O	1:B:1203:ALA:N	2.35	0.57
1:A:626:SER:HB3	1:A:629:GLU:OE1	2.03	0.57
1:A:719:GLU:HA	1:A:722:TRP:CD1	2.38	0.57
1:B:527:VAL:HG11	1:B:532:LEU:HD11	1.85	0.57
1:A:433:ALA:HB2	1:A:835:LYS:HB2	1.86	0.57
1:A:658:VAL:O	1:A:662:VAL:HG23	2.05	0.57
1:A:733:GLU:OE1	1:A:733:GLU:N	2.27	0.57
1:A:737:ASN:HA	1:A:740:VAL:CG2	2.35	0.57
1:B:676:ARG:HG2	1:B:676:ARG:HH11	1.70	0.57
1:B:694:LEU:HD23	1:B:694:LEU:O	2.04	0.57
1:A:524:ASP:OD1	1:A:533:LYS:HA	2.04	0.57
1:B:622:ALA:N	1:B:673:LYS:O	2.23	0.57
1:B:673:LYS:HA	1:B:673:LYS:HE3	1.86	0.57
1:A:182:ALA:HB2	1:A:234:THR:HG22	1.86	0.57
1:A:460:VAL:HG13	1:A:461:PRO:HD2	1.87	0.57
1:B:166:MET:CE	1:B:251:THR:HG21	2.35	0.57
1:B:11:GLY:HA2	1:B:85:VAL:CG1	2.34	0.57
1:B:161:CYS:HB2	1:B:394:GLY:HA2	1.86	0.57
1:B:623:VAL:CG2	1:B:665:LEU:HD13	2.35	0.57
1:B:692:PRO:O	1:B:696:GLN:HG3	2.04	0.57
1:A:182:ALA:HB1	1:A:234:THR:HG22	1.86	0.56
1:A:684:SER:HG	1:A:686:PHE:HD2	1.53	0.56
1:B:316:ARG:NH1	1:B:320:LEU:HB2	2.19	0.56
1:B:674:GLU:N	1:B:674:GLU:OE1	2.38	0.56
1:B:737:ASN:HA	1:B:740:VAL:CG2	2.34	0.56
1:A:341:LEU:O	1:A:345:LEU:HG	2.05	0.56
1:B:508:LEU:CD2	1:B:539:LEU:HD23	2.35	0.56
1:B:1928:GLN:OE1	1:B:1931:ARG:NH2	2.37	0.56
1:B:620:MET:HE1	1:B:682:PHE:N	2.19	0.56
1:B:673:LYS:HA	1:B:673:LYS:CE	2.35	0.56
1:A:136:GLN:HB3	1:A:139:MET:HG2	1.87	0.56
1:A:13:LEU:HD13	1:A:329:MET:CE	2.34	0.56
1:B:761:ILE:HG12	1:B:784:LEU:HD11	1.88	0.56
1:A:524:ASP:HB2	1:A:534:VAL:HG22	1.87	0.56
1:B:105:THR:HG23	1:B:182:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ARG:O	1:B:521:LEU:HG	2.06	0.56
1:A:570:MET:CE	1:A:810:ALA:HB1	2.35	0.56
1:B:136:GLN:HB3	1:B:139:MET:HG2	1.87	0.56
1:A:776:LYS:H	1:A:776:LYS:HD2	1.71	0.56
1:B:771:LEU:O	1:B:775:LEU:HB2	2.04	0.56
1:A:626:SER:HB3	1:A:629:GLU:CD	2.26	0.56
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.41	0.56
1:A:503:TRP:HB3	1:A:787:LYS:HE3	1.88	0.55
1:B:689:ALA:O	1:B:692:PRO:HD2	2.05	0.55
1:A:1446:ILE:HG22	1:A:1474:LEU:HD12	1.88	0.55
1:B:225:SER:OG	1:B:330:GLY:HA3	2.06	0.55
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.06	0.55
1:A:412:PRO:HD3	1:A:824:PRO:HG2	1.88	0.55
1:B:508:LEU:HD21	1:B:539:LEU:HD23	1.88	0.55
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.41	0.55
1:B:761:ILE:HA	1:B:784:LEU:HD12	1.87	0.55
1:A:8:GLY:HA2	1:A:243:TYR:HE2	1.71	0.55
1:A:299:VAL:O	1:A:302:PRO:HD2	2.07	0.55
1:A:343:LYS:HE2	1:A:354:ALA:HB3	1.89	0.55
1:A:563:LEU:HD11	1:A:785:MET:CE	2.37	0.55
1:B:591:ASP:OD1	1:B:711:ARG:NH1	2.34	0.55
1:B:224:ARG:HG2	1:B:333:GLU:OE2	2.07	0.55
1:B:191:LEU:HG	1:B:226:GLU:CG	2.37	0.55
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.42	0.55
1:B:769:ALA:O	1:B:773:ARG:HG2	2.07	0.55
1:A:1243:VAL:HG23	1:A:1271:THR:HG23	1.88	0.55
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.39	0.55
1:B:761:ILE:HG12	1:B:784:LEU:CD1	2.36	0.55
1:B:782:ILE:HG21	1:B:803:LEU:HD13	1.89	0.55
1:A:132:MET:HE1	1:B:200:PHE:CE2	2.42	0.54
1:A:771:LEU:O	1:A:775:LEU:HB2	2.06	0.54
1:A:1428:LEU:HD22	1:A:1980:LEU:HD21	1.89	0.54
1:B:1445:ALA:O	1:B:1446:ILE:HD13	2.07	0.54
1:B:1545:ARG:HE	1:B:1876:ILE:HD11	1.70	0.54
1:A:976:THR:HG23	1:A:976:THR:O	2.07	0.54
1:B:502:GLN:HG2	1:B:506:MET:CE	2.37	0.54
1:B:656:ALA:O	1:B:660:GLU:HG3	2.07	0.54
1:B:157:LEU:O	1:B:157:LEU:HD12	2.06	0.54
1:A:420:LEU:HD11	1:A:512:ARG:HD2	1.89	0.54
1:A:652:SER:OG	1:A:681:ALA:HB1	2.08	0.54
1:B:319:PRO:HB3	1:B:372:GLY:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.41	0.54
1:A:293:HIS:CD2	1:A:295:THR:HG23	2.43	0.54
1:B:78:GLN:HB3	1:B:188:ILE:HD12	1.90	0.54
1:B:215:PHE:HE1	1:B:305:LEU:HD11	1.72	0.54
1:B:655:GLN:O	1:B:658:VAL:HG12	2.07	0.54
1:A:542:ASP:OD2	1:A:544:SER:OG	2.26	0.54
1:A:1446:ILE:HD12	1:A:1447:ASN:N	2.22	0.54
1:B:627:TRP:HB2	1:B:643:HIS:CD2	2.43	0.54
1:A:191:LEU:N	1:A:226:GLU:OE1	2.25	0.54
1:A:325:THR:HB	1:A:343:LYS:HD3	1.89	0.54
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.90	0.54
1:B:624:GLY:O	1:B:625:LEU:HD23	2.08	0.54
1:B:676:ARG:HA	1:B:676:ARG:NE	2.21	0.54
1:B:606:ARG:O	1:B:610:ILE:HG13	2.07	0.54
1:B:746:GLN:O	1:B:746:GLN:NE2	2.41	0.54
1:B:1228:LEU:HD21	1:B:1256:ILE:CD1	2.37	0.54
1:B:635:PRO:HD3	1:B:661:PHE:CE1	2.43	0.54
1:B:1879:THR:O	1:B:1907:ARG:NH1	2.41	0.54
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.39	0.53
1:A:418:ALA:HA	1:A:422:ARG:NH2	2.20	0.53
1:B:402:ILE:HD12	1:B:404:LEU:HD21	1.90	0.53
1:B:537:LEU:HD11	1:B:551:HIS:CG	2.43	0.53
1:A:288:GLU:HG2	1:A:288:GLU:O	2.08	0.53
1:A:629:GLU:CD	1:A:629:GLU:H	2.11	0.53
1:A:1446:ILE:HG22	1:A:1474:LEU:CD1	2.39	0.53
1:B:9:MET:HG3	1:B:19:LEU:CD1	2.37	0.53
1:B:191:LEU:C	1:B:192:LEU:HD12	2.29	0.53
1:B:790:ARG:HG3	1:B:791:ASP:N	2.24	0.53
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	1.90	0.53
1:B:203:LEU:HD13	1:B:205:MET:HE2	1.90	0.53
1:A:557:THR:O	1:A:561:ILE:HG13	2.08	0.53
1:B:553:PHE:CD1	1:B:582:LEU:HD22	2.43	0.53
1:B:694:LEU:O	1:B:698:LEU:HG	2.08	0.53
1:A:647:ASP:OD2	1:A:773:ARG:HD3	2.09	0.53
1:B:205:MET:O	1:B:221:GLY:HA3	2.08	0.53
1:B:290:ILE:HD12	1:B:389:GLY:O	2.09	0.53
1:B:1272:ALA:O	1:B:1295:GLY:N	2.42	0.53
1:A:509:SER:HB2	1:A:792:ASN:HB2	1.90	0.53
1:A:661:PHE:CE2	1:A:665:LEU:HD21	2.44	0.53
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.91	0.53
1:B:574:PRO:HG2	1:B:577:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:THR:OG1	1:A:763:PRO:HG2	2.09	0.53
1:B:534:VAL:O	1:B:538:LEU:HD13	2.09	0.53
1:B:1110:GLN:NE2	1:B:2085:PRO:O	2.41	0.53
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.89	0.53
1:B:235:LYS:HE3	1:B:238:LEU:CD1	2.38	0.53
1:A:660:GLU:HA	1:A:663:GLU:OE2	2.10	0.52
1:A:1794:VAL:O	1:A:1795:LEU:HD23	2.09	0.52
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.72	0.52
1:B:1555:GLN:N	1:B:1556:PRO:HD2	2.25	0.52
1:A:13:LEU:HD22	1:A:329:MET:HE1	1.91	0.52
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	1.90	0.52
1:B:207:SER:HB2	1:B:220:ASN:HB2	1.91	0.52
1:A:760:GLU:OE2	1:A:765:ALA:HA	2.10	0.52
1:B:23:TRP:HB2	1:B:346:LEU:HD13	1.90	0.52
1:B:83:LEU:HD12	1:B:144:LEU:HD21	1.92	0.52
1:A:9:MET:HG3	1:A:19:LEU:CD1	2.40	0.52
1:A:13:LEU:HD13	1:A:329:MET:HE3	1.91	0.52
1:A:76:ASP:HA	1:A:116:THR:HG21	1.91	0.52
1:A:504:ARG:HD2	1:A:541:THR:O	2.09	0.52
1:A:573:ARG:HD3	1:A:574:PRO:HD2	1.92	0.52
1:A:625:LEU:HD12	1:A:626:SER:N	2.23	0.52
1:B:1391:LEU:HD23	1:B:1392:LYS:N	2.25	0.52
1:A:610:ILE:CG2	1:A:680:MET:HE1	2.38	0.52
1:B:371:ASP:OD1	1:B:372:GLY:N	2.37	0.52
1:A:698:LEU:O	1:A:702:ILE:N	2.23	0.52
1:A:597:GLU:CG	1:A:601:LEU:HD11	2.40	0.52
1:A:1942:SER:O	1:A:1943:THR:OG1	2.17	0.52
1:A:292:ALA:HB2	1:A:322:ILE:HD11	1.92	0.52
1:A:605:TRP:CD1	1:A:701:VAL:HG21	2.45	0.52
1:A:657:PRO:HA	1:A:660:GLU:CD	2.31	0.52
1:B:502:GLN:HG2	1:B:506:MET:HE3	1.92	0.52
1:B:1190:LEU:O	1:B:1195:GLN:NE2	2.42	0.52
1:B:1602:GLU:HB3	1:B:1650:VAL:HG23	1.92	0.52
1:A:68:HIS:HB3	1:A:71:GLN:OE1	2.10	0.52
1:A:261:VAL:HG12	1:B:146:PHE:CD1	2.45	0.52
1:A:623:VAL:HG12	1:A:625:LEU:N	2.22	0.52
1:A:1535:THR:HG23	1:A:1535:THR:O	2.10	0.52
1:B:754:GLU:OE2	1:B:778:SER:HB3	2.09	0.52
1:A:620:MET:HG2	1:A:652:SER:HB2	1.92	0.51
1:B:1080:VAL:HG22	1:B:1087:THR:HG23	1.92	0.51
1:A:1573:PHE:HE1	2:A:2601:NDP:H61A	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:SER:H	1:B:356:ASN:ND2	2.09	0.51
1:B:687:MET:HE1	1:B:739:LEU:O	2.09	0.51
1:A:425:ARG:HD3	1:A:812:PRO:HD3	1.92	0.51
1:A:606:ARG:HH21	1:A:739:LEU:HD13	1.74	0.51
1:A:1555:GLN:N	1:A:1555:GLN:OE1	2.42	0.51
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.30	0.51
1:A:476:GLU:N	1:A:794:GLU:OE2	2.37	0.51
1:A:570:MET:HE2	1:A:810:ALA:HB1	1.93	0.51
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.10	0.51
1:B:1371:ILE:O	1:B:1372:LEU:HD12	2.10	0.51
1:A:780:THR:C	1:A:781:ILE:HD12	2.30	0.51
1:A:1367:TYR:CE2	1:A:1371:ILE:HD11	2.46	0.51
1:B:159:THR:HG22	1:B:159:THR:O	2.10	0.51
1:B:495:ILE:CD1	1:B:578:VAL:HB	2.40	0.51
1:B:555:SER:O	1:B:559:ILE:HG13	2.11	0.51
1:B:879:THR:C	1:B:880:LEU:HD12	2.32	0.51
1:A:202:ARG:NH1	1:B:127:LEU:O	2.43	0.51
1:A:580:HIS:CD2	1:A:743:VAL:HG11	2.42	0.51
1:A:786:LYS:HB3	1:A:789:HIS:HB2	1.93	0.51
1:B:737:ASN:HA	1:B:740:VAL:HG22	1.91	0.51
1:A:11:GLY:HA2	1:A:85:VAL:CG1	2.41	0.51
1:A:133:VAL:O	1:A:139:MET:HG3	2.11	0.51
1:B:33:VAL:HB	1:B:50:ARG:NH2	2.25	0.51
1:B:550:VAL:O	1:B:554:VAL:HG23	2.10	0.51
1:B:658:VAL:O	1:B:662:VAL:HG23	2.11	0.51
1:B:60:PHE:HB3	1:B:842:TRP:CD1	2.46	0.50
1:B:491:PRO:HG2	1:B:756:ALA:HA	1.92	0.50
1:B:576:GLY:C	1:B:577:ILE:HD12	2.31	0.50
1:B:1016:ASP:O	1:B:1080:VAL:N	2.40	0.50
1:A:13:LEU:HB3	1:A:329:MET:HE1	1.93	0.50
1:A:433:ALA:CB	1:A:835:LYS:HB2	2.42	0.50
1:A:694:LEU:HD12	1:A:698:LEU:HG	1.94	0.50
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.31	0.50
1:B:13:LEU:HD12	1:B:22:PHE:CG	2.46	0.50
1:B:203:LEU:HD13	1:B:205:MET:CE	2.41	0.50
1:B:708:ARG:HD2	1:B:734:TYR:CE2	2.46	0.50
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.11	0.50
1:A:579:GLY:O	1:A:715:THR:HG21	2.11	0.50
1:A:783:PRO:O	1:A:784:LEU:HB2	2.10	0.50
1:A:1457:VAL:HG11	1:A:1471:CYS:HB2	1.92	0.50
1:B:125:GLU:OE2	1:B:126:THR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HB	1:A:242:VAL:HG13	1.94	0.50
1:B:442:LEU:HD12	1:B:442:LEU:O	2.10	0.50
1:B:549:ILE:CG2	1:B:611:LYS:HG3	2.41	0.50
1:B:623:VAL:HG21	1:B:665:LEU:CD1	2.38	0.50
1:A:9:MET:CE	1:A:345:LEU:CD1	2.90	0.50
1:A:168:LEU:HD23	1:A:168:LEU:O	2.12	0.50
1:A:364:PRO:HG2	1:A:365:GLU:OE1	2.11	0.50
1:A:1141:CYS:O	1:A:1145:VAL:HG23	2.11	0.50
1:B:191:LEU:O	1:B:192:LEU:HD12	2.10	0.50
1:A:584:GLU:HB2	1:A:738:ASN:HD21	1.76	0.50
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.42	0.50
1:A:717:ILE:HD11	1:A:726:LEU:HB3	1.94	0.50
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.27	0.50
1:B:625:LEU:HB2	1:B:630:CYS:SG	2.51	0.50
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.94	0.50
1:A:657:PRO:HA	1:A:660:GLU:CG	2.42	0.50
1:B:139:MET:HA	1:B:139:MET:CE	2.38	0.50
1:B:759:LEU:HD23	1:B:782:ILE:HG22	1.94	0.50
1:A:293:HIS:O	1:A:326:LYS:HD2	2.11	0.49
1:A:351:GLY:C	1:A:352:LEU:HD12	2.33	0.49
1:B:1454:VAL:HG22	1:B:1503:MET:HE1	1.94	0.49
1:A:257:LYS:HE3	1:A:263:PHE:O	2.12	0.49
1:A:660:GLU:O	1:A:663:GLU:HG2	2.12	0.49
1:A:686:PHE:HB2	1:A:687:MET:HE3	1.92	0.49
1:B:655:GLN:HA	1:B:658:VAL:HG12	1.93	0.49
1:B:1602:GLU:OE2	1:B:1851:LYS:NZ	2.45	0.49
1:A:9:MET:HE3	1:A:243:TYR:CE1	2.47	0.49
1:A:2033:ASN:OD1	1:A:2034:TYR:N	2.45	0.49
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.45	0.49
1:B:617:PRO:HB2	1:B:655:GLN:OE1	2.11	0.49
1:A:217:THR:HG22	1:A:364:PRO:CD	2.43	0.49
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.25	0.49
1:A:641:ALA:N	1:A:650:THR:O	2.43	0.49
1:A:276:LEU:CD1	1:A:401:HIS:HB3	2.42	0.49
1:A:635:PRO:HD3	1:A:661:PHE:CE1	2.48	0.49
1:A:746:GLN:O	1:A:746:GLN:NE2	2.46	0.49
1:B:51:SER:HA	1:B:223:CYS:SG	2.53	0.49
1:B:499:MET:HE1	1:B:581:SER:HB3	1.94	0.49
1:B:685:TYR:HA	1:B:688:GLU:CG	2.42	0.49
1:A:1336:LEU:HD11	1:A:1340:GLY:HA3	1.95	0.49
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LEU:O	1:B:525:GLU:HG2	2.12	0.49
1:A:25:ASN:HA	1:A:30:VAL:HG12	1.95	0.49
1:B:1014:GLU:OE1	1:B:1014:GLU:N	2.44	0.49
1:A:877:ASP:OD2	1:A:1004:HIS:ND1	2.46	0.49
1:B:191:LEU:HD22	1:B:224:ARG:NH2	2.28	0.49
1:B:680:MET:HB2	1:B:682:PHE:CE2	2.47	0.49
1:B:1130:GLU:OE1	1:B:1130:GLU:N	2.40	0.49
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.43	0.49
1:A:412:PRO:HD3	1:A:824:PRO:CG	2.43	0.49
1:A:620:MET:HB2	1:A:675:VAL:CG1	2.43	0.49
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	2.13	0.49
1:B:207:SER:HB3	1:B:221:GLY:N	2.28	0.48
1:B:623:VAL:HG13	1:B:671:PHE:O	2.13	0.48
1:B:645:SER:HB3	1:B:648:THR:OG1	2.13	0.48
1:B:692:PRO:HD2	1:B:693:PRO:HD2	1.94	0.48
1:B:745:PHE:CE2	1:B:749:LEU:HD11	2.48	0.48
1:A:673:LYS:HE3	1:A:674:GLU:O	2.12	0.48
1:A:783:PRO:HB2	1:A:795:PHE:HE2	1.78	0.48
1:A:1130:GLU:OE1	1:A:1130:GLU:N	2.42	0.48
1:A:1570:SER:OG	1:A:1646:ALA:O	2.22	0.48
1:B:691:ALA:O	1:B:695:LEU:N	2.33	0.48
1:B:701:VAL:HB	1:B:702:ILE:HD12	1.95	0.48
1:A:570:MET:HG2	1:A:811:ASN:O	2.13	0.48
1:A:692:PRO:HD2	1:A:693:PRO:HD2	1.95	0.48
1:A:694:LEU:HD11	1:A:698:LEU:HD11	1.94	0.48
1:A:1538:ARG:NH2	1:A:1581:GLY:O	2.46	0.48
1:B:584:GLU:HG3	1:B:738:ASN:OD1	2.13	0.48
1:A:953:VAL:HG22	1:A:954:VAL:HG23	1.95	0.48
1:A:1243:VAL:HG21	1:A:1307:LEU:HD13	1.94	0.48
1:B:123:ASP:HB3	1:B:126:THR:OG1	2.13	0.48
1:A:189:ASN:O	1:A:226:GLU:HB2	2.13	0.48
1:A:597:GLU:O	1:A:601:LEU:HG	2.14	0.48
1:B:643:HIS:ND1	1:B:746:GLN:HB3	2.28	0.48
1:A:535:SER:O	1:A:539:LEU:HD22	2.13	0.48
1:B:553:PHE:HE2	1:B:610:ILE:CD1	2.27	0.48
1:A:11:GLY:HA2	1:A:85:VAL:HG13	1.96	0.48
1:A:124:PRO:HA	1:A:127:LEU:CD2	2.44	0.48
1:A:161:CYS:CB	1:A:394:GLY:HA2	2.38	0.48
1:A:460:VAL:CG1	1:A:461:PRO:HD2	2.43	0.48
1:A:597:GLU:HG2	1:A:601:LEU:CD1	2.44	0.48
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ASP:OD1	1:B:548:ASP:N	2.46	0.48
1:B:768:GLN:NE2	1:B:781:ILE:HG21	2.29	0.48
1:A:189:ASN:HD22	1:A:334:PRO:CD	2.22	0.48
1:A:665:LEU:O	1:A:670:VAL:HG22	2.14	0.48
1:A:1743:LEU:HD11	1:A:1767:LEU:HD11	1.96	0.48
1:B:124:PRO:HA	1:B:127:LEU:HD23	1.95	0.48
1:B:293:HIS:O	1:B:326:LYS:HD2	2.13	0.48
1:B:423:LEU:HD23	1:B:812:PRO:HB3	1.96	0.48
1:A:689:ALA:O	1:A:692:PRO:HD2	2.14	0.48
1:A:1909:VAL:HG11	1:A:1912:LEU:HD13	1.94	0.48
1:B:468:ARG:CD	1:B:485:VAL:HG21	2.39	0.48
1:A:302:PRO:HA	1:A:366:ILE:HD11	1.96	0.48
1:A:1196:LEU:HD12	1:A:1197:GLU:N	2.29	0.48
1:B:96:ASN:OD1	1:B:98:ASP:HB2	2.14	0.48
1:B:273:ILE:HG22	1:B:277:TYR:HE2	1.79	0.48
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.49	0.47
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	1.96	0.47
1:B:322:ILE:HG22	1:B:375:GLN:O	2.13	0.47
1:B:494:PHE:O	1:B:495:ILE:HD13	2.13	0.47
1:B:504:ARG:HD2	1:B:543:GLU:CD	2.34	0.47
1:B:606:ARG:NH1	1:B:739:LEU:HB2	2.29	0.47
1:B:691:ALA:HB1	1:B:736:VAL:HG11	1.96	0.47
1:B:693:PRO:HA	1:B:696:GLN:OE1	2.14	0.47
1:A:199:GLN:HG2	1:B:127:LEU:HD13	1.95	0.47
1:A:542:ASP:O	1:A:545:THR:HG23	2.14	0.47
1:A:1418:ASP:OD2	1:A:1446:ILE:N	2.44	0.47
1:B:617:PRO:HB2	1:B:655:GLN:CD	2.35	0.47
1:B:1750:GLU:N	1:B:1773:ASP:OD2	2.47	0.47
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.50	0.47
1:A:1078:VAL:HA	1:A:1089:ALA:HB2	1.96	0.47
1:B:191:LEU:HG	1:B:226:GLU:HG3	1.96	0.47
1:B:1612:ARG:NH2	1:B:1640:TRP:O	2.47	0.47
1:A:241:ARG:NH2	1:A:827:THR:O	2.47	0.47
1:A:1487:ASP:OD2	1:A:1489:GLY:N	2.45	0.47
1:B:56:ASP:OD1	1:B:57:LEU:N	2.48	0.47
1:B:212:CYS:SG	1:B:222:TYR:HA	2.55	0.47
1:B:1607:ASP:OD1	1:B:1608:ALA:N	2.46	0.47
1:A:56:ASP:OD1	1:A:57:LEU:N	2.48	0.47
1:A:490:ARG:HD3	1:A:806:SER:O	2.14	0.47
1:A:664:GLN:O	1:A:667:LYS:HB2	2.14	0.47
1:B:207:SER:HB3	1:B:221:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.38	0.47
1:B:585:VAL:HG12	1:B:599:ALA:CB	2.41	0.47
1:B:639:VAL:CG1	1:B:640:PRO:HD2	2.41	0.47
1:B:1366:GLN:O	1:B:1369:GLN:N	2.47	0.47
1:A:241:ARG:HD2	1:A:453:MET:CE	2.45	0.47
1:A:501:THR:HB	1:A:764:HIS:HB3	1.96	0.47
1:A:697:GLU:O	1:A:701:VAL:HG23	2.14	0.47
1:B:692:PRO:HB2	1:B:693:PRO:HD3	1.95	0.47
1:B:744:LEU:HB3	1:B:747:GLU:OE1	2.14	0.47
1:A:621:ALA:CA	1:A:674:GLU:HA	2.36	0.47
1:B:676:ARG:HG2	1:B:676:ARG:NH1	2.29	0.47
1:A:6:ILE:HG12	1:A:233:LEU:CD2	2.45	0.47
1:A:665:LEU:HB3	1:A:670:VAL:HG21	1.96	0.47
1:B:133:VAL:O	1:B:139:MET:HG3	2.14	0.47
1:B:409:GLN:OE1	1:B:409:GLN:HA	2.14	0.47
1:A:425:ARG:HH21	1:A:811:ASN:HD22	1.62	0.47
1:B:620:MET:HE1	1:B:682:PHE:O	2.15	0.47
1:B:759:LEU:CD2	1:B:782:ILE:HG22	2.45	0.47
1:A:105:THR:HG23	1:A:182:ALA:C	2.34	0.46
1:A:118:GLU:OE1	1:A:193:LYS:NZ	2.38	0.46
1:A:287:PHE:O	1:A:316:ARG:NH1	2.48	0.46
1:B:60:PHE:HB3	1:B:842:TRP:NE1	2.30	0.46
1:B:309:THR:O	1:B:313:CYS:HB2	2.15	0.46
1:B:543:GLU:OE1	1:B:543:GLU:HA	2.15	0.46
1:B:620:MET:CE	1:B:682:PHE:N	2.78	0.46
1:B:11:GLY:HA2	1:B:85:VAL:HG13	1.97	0.46
1:B:1652:TYR:CD1	1:B:1823:VAL:HG22	2.51	0.46
1:A:73:HIS:ND1	1:A:843:ASP:OD1	2.46	0.46
1:A:159:THR:HA	1:B:138:ALA:HB1	1.97	0.46
1:A:162:SER:OG	1:A:394:GLY:N	2.48	0.46
1:A:628:GLU:HG3	1:A:631:LYS:NZ	2.30	0.46
1:A:1346:THR:HG22	1:A:1347:LEU:N	2.30	0.46
1:B:425:ARG:NH1	1:B:810:ALA:O	2.48	0.46
1:B:1206:ARG:CZ	1:B:1209:LEU:HD13	2.45	0.46
1:A:491:PRO:HG2	1:A:756:ALA:HA	1.97	0.46
1:A:717:ILE:HG22	1:A:722:TRP:CD1	2.50	0.46
1:B:523:SER:O	1:B:527:VAL:HG23	2.16	0.46
1:A:9:MET:CE	1:A:345:LEU:HD13	2.45	0.46
1:B:1246:LEU:HD11	1:B:1299:PRO:HG3	1.97	0.46
1:A:6:ILE:HA	1:A:233:LEU:HD23	1.98	0.46
1:A:108:TRP:HB3	1:A:167:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:CG1	1:B:50:ARG:HB3	2.46	0.46
1:B:620:MET:HE2	1:B:682:PHE:HB2	1.96	0.46
1:B:664:GLN:HA	1:B:667:LYS:CD	2.45	0.46
1:B:745:PHE:O	1:B:749:LEU:HG	2.15	0.46
1:A:425:ARG:HH22	1:A:459:ALA:HB2	1.80	0.46
1:A:549:ILE:HD11	1:A:607:GLY:O	2.15	0.46
1:A:569:CYS:SG	1:A:814:ALA:HB1	2.55	0.46
1:A:613:ALA:HB1	1:A:615:LEU:HG	1.97	0.46
1:B:139:MET:HE3	1:B:139:MET:CA	2.43	0.46
1:B:511:MET:HE3	1:B:511:MET:O	2.16	0.46
1:A:728:ARG:HB2	1:A:728:ARG:CZ	2.46	0.46
1:B:606:ARG:NH1	1:B:739:LEU:HD13	2.31	0.46
1:B:620:MET:SD	1:B:652:SER:HB3	2.55	0.46
1:B:11:GLY:HA2	1:B:85:VAL:HG11	1.97	0.46
1:B:13:LEU:HD22	1:B:329:MET:CE	2.46	0.46
1:A:13:LEU:HD12	1:A:22:PHE:CG	2.51	0.46
1:A:155:ILE:HG22	1:A:156:ALA:N	2.31	0.46
1:A:1085:ARG:NH2	1:A:1097:LEU:O	2.49	0.46
1:B:9:MET:HG3	1:B:19:LEU:HD11	1.98	0.46
1:B:188:ILE:HG22	1:B:228:VAL:HG13	1.98	0.46
1:A:39:ARG:NH2	1:A:226:GLU:OE2	2.49	0.45
1:A:57:LEU:CD2	1:A:81:LEU:HD11	2.46	0.45
1:A:524:ASP:OD1	1:A:533:LYS:HG2	2.16	0.45
1:A:1033:MET:CE	1:A:1089:ALA:HB3	2.46	0.45
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.31	0.45
1:A:1768:GLU:OE2	1:A:1770:GLY:N	2.49	0.45
1:B:257:LYS:HE3	1:B:263:PHE:O	2.15	0.45
1:B:641:ALA:HB2	1:B:652:SER:HB3	1.98	0.45
1:B:791:ASP:OD2	1:B:794:GLU:HG3	2.16	0.45
1:A:213:LYS:HG2	1:A:358:HIS:HB3	1.98	0.45
1:A:627:TRP:HB2	1:A:643:HIS:CD2	2.51	0.45
1:B:668:GLU:HB2	1:B:670:VAL:HG23	1.99	0.45
1:A:347:SER:HB3	1:A:352:LEU:O	2.16	0.45
1:B:692:PRO:HB2	1:B:693:PRO:CD	2.45	0.45
1:A:707:PRO:HA	1:A:728:ARG:O	2.16	0.45
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.52	0.45
1:B:203:LEU:HD23	1:B:203:LEU:HA	1.82	0.45
1:B:574:PRO:CG	1:B:577:ILE:HD11	2.46	0.45
1:B:1213:PRO:O	1:B:1217:GLY:N	2.50	0.45
1:A:13:LEU:HB3	1:A:14:PRO:CD	2.47	0.45
1:A:638:VAL:HG11	1:A:651:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:SER:CB	1:B:334:PRO:HG3	2.45	0.45
1:B:1315:CYS:SG	1:B:1332:MET:SD	3.15	0.45
1:A:573:ARG:HA	1:A:573:ARG:NE	2.32	0.45
1:A:692:PRO:HB2	1:A:693:PRO:HD3	1.98	0.45
1:A:503:TRP:CD1	1:A:787:LYS:HG3	2.52	0.45
1:B:508:LEU:O	1:B:511:MET:HB2	2.17	0.45
1:B:534:VAL:CG2	1:B:554:VAL:HG12	2.47	0.45
1:B:620:MET:O	1:B:674:GLU:HA	2.17	0.45
1:B:677:THR:HB	1:B:682:PHE:HE2	1.81	0.45
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.52	0.45
1:B:1245:VAL:HB	1:B:1246:LEU:HD12	1.99	0.45
1:B:1451:SER:OG	1:B:1453:VAL:HG13	2.17	0.45
1:A:368:ALA:HB3	1:A:374:LEU:HD12	1.99	0.45
1:A:591:ASP:OD2	1:A:709:SER:HB3	2.16	0.45
1:A:5:VAL:HG21	1:A:239:ALA:HB2	1.97	0.45
1:A:5:VAL:HG21	1:A:239:ALA:CB	2.46	0.45
1:A:1128:LEU:HD21	1:A:1217:GLY:C	2.37	0.45
1:A:1971:LEU:N	1:A:1971:LEU:HD12	2.31	0.45
1:B:692:PRO:CD	1:B:693:PRO:HD2	2.47	0.45
1:A:15:GLU:OE2	1:A:38:ARG:NH2	2.49	0.45
1:A:420:LEU:HD23	1:A:793:LEU:CD2	2.47	0.45
1:B:499:MET:HA	1:B:556:LEU:CD2	2.47	0.45
1:B:627:TRP:NE1	1:B:631:LYS:HE2	2.31	0.45
1:A:105:THR:HG23	1:A:182:ALA:O	2.17	0.44
1:A:764:HIS:CG	1:A:787:LYS:HB2	2.52	0.44
1:B:1445:ALA:C	1:B:1446:ILE:HD13	2.37	0.44
1:B:527:VAL:HG12	1:B:527:VAL:O	2.17	0.44
1:B:556:LEU:HD12	1:B:763:PRO:HG3	1.99	0.44
1:B:687:MET:O	1:B:690:ILE:HB	2.17	0.44
1:A:702:ILE:N	1:A:702:ILE:HD12	2.32	0.44
1:A:736:VAL:O	1:A:740:VAL:HG22	2.16	0.44
1:A:1009:LEU:HD21	1:A:1021:LEU:HD21	2.00	0.44
1:A:363:ASN:HB3	1:A:366:ILE:HD13	1.98	0.44
1:A:646:LYS:HG3	1:A:647:ASP:N	2.32	0.44
1:A:692:PRO:HB2	1:A:693:PRO:CD	2.48	0.44
1:A:692:PRO:CD	1:A:693:PRO:HD2	2.47	0.44
1:A:1140:LEU:HD13	1:A:1174:SER:OG	2.18	0.44
1:B:47:LEU:HD22	1:B:197:SER:HB3	2.00	0.44
1:B:251:THR:HG22	1:B:252:ASN:N	2.32	0.44
1:B:644:ASN:HB2	1:B:648:THR:OG1	2.16	0.44
1:B:681:ALA:O	1:B:684:SER:OG	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLY:C	1:A:383:VAL:HG23	2.38	0.44
1:A:606:ARG:O	1:A:610:ILE:HG13	2.18	0.44
1:A:811:ASN:OD1	1:A:813:ASN:HB2	2.17	0.44
1:A:1540:ASP:OD1	1:A:1542:SER:N	2.44	0.44
1:B:75:MET:HE1	1:B:79:LEU:HG	1.99	0.44
1:B:128:VAL:HG21	1:B:130:TYR:CZ	2.53	0.44
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.80	0.44
1:A:299:VAL:C	1:A:302:PRO:HD2	2.38	0.44
1:A:570:MET:HE3	1:A:810:ALA:HB1	1.98	0.44
1:A:584:GLU:CB	1:A:738:ASN:HD21	2.30	0.44
1:A:708:ARG:N	1:A:728:ARG:O	2.43	0.44
1:B:511:MET:HE3	1:B:517:ARG:HB2	2.00	0.44
1:B:760:GLU:HB3	1:B:783:PRO:HA	1.99	0.44
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.99	0.44
1:A:468:ARG:CD	1:A:485:VAL:HG21	2.41	0.44
1:A:537:LEU:HA	1:A:540:SER:OG	2.17	0.44
1:B:447:ASP:HB3	1:B:450:PHE:HB3	2.00	0.44
1:B:1072:LYS:HD2	1:B:1072:LYS:N	2.33	0.44
1:B:1178:LEU:HD21	1:B:1215:LEU:HD11	1.99	0.44
1:A:8:GLY:HA2	1:A:243:TYR:CE2	2.50	0.44
1:A:17:GLU:HA	1:A:17:GLU:OE1	2.18	0.44
1:A:305:LEU:HD23	1:A:366:ILE:HG21	2.00	0.44
1:A:476:GLU:HG3	1:A:794:GLU:OE2	2.17	0.44
1:A:631:LYS:HG3	1:A:632:GLN:OE1	2.18	0.44
1:A:1411:SER:OG	1:A:1439:ARG:NH2	2.50	0.44
1:A:1887:TYR:HD1	1:A:1909:VAL:HG13	1.82	0.44
1:B:620:MET:O	1:B:674:GLU:HB2	2.18	0.44
1:B:1348:LEU:HD22	1:B:1374:GLN:HB3	1.99	0.44
1:A:760:GLU:CD	1:A:765:ALA:HA	2.39	0.43
1:A:934:GLU:OE1	1:A:936:ARG:NH2	2.51	0.43
1:A:1640:TRP:CZ3	1:A:1648:VAL:HG21	2.53	0.43
1:B:83:LEU:HD12	1:B:144:LEU:CD2	2.48	0.43
1:B:219:GLY:O	1:B:298:LYS:HG2	2.17	0.43
1:B:242:VAL:HG23	1:B:822:PRO:HB3	2.00	0.43
1:B:740:VAL:HG23	1:B:741:SER:H	1.83	0.43
1:B:836:TRP:HB2	1:B:838:HIS:NE2	2.33	0.43
1:B:1242:VAL:HA	1:B:1312:LEU:O	2.17	0.43
1:B:1714:GLN:OE1	1:B:1714:GLN:N	2.47	0.43
1:A:2021:SER:HA	2:A:2602:NDP:H5N	2.00	0.43
1:B:2097:LEU:O	1:B:2097:LEU:HD23	2.17	0.43
1:A:158:ASP:HB2	1:B:156:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LEU:N	1:A:532:LEU:HD22	2.33	0.43
1:A:790:ARG:HH11	1:A:790:ARG:HG2	1.82	0.43
1:A:1771:LYS:HE3	1:A:1795:LEU:HD22	2.00	0.43
1:B:81:LEU:O	1:B:85:VAL:HG23	2.18	0.43
1:B:332:PRO:O	1:B:336:SER:HB3	2.18	0.43
1:A:60:PHE:HB3	1:A:842:TRP:CD1	2.53	0.43
1:A:351:GLY:O	1:A:352:LEU:HD12	2.17	0.43
1:A:425:ARG:HD3	1:A:812:PRO:CD	2.48	0.43
1:A:503:TRP:CG	1:A:787:LYS:HG3	2.52	0.43
1:B:250:GLY:HA3	1:B:276:LEU:HD21	2.01	0.43
1:B:288:GLU:O	1:B:288:GLU:HG2	2.19	0.43
1:B:307:GLY:HA2	1:B:310:ARG:CZ	2.49	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.83	0.43
1:A:544:SER:O	1:A:547:ASP:HB3	2.19	0.43
1:A:634:CYS:HB3	1:A:638:VAL:O	2.17	0.43
1:A:686:PHE:HB2	1:A:687:MET:CE	2.49	0.43
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	2.00	0.43
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.53	0.43
1:B:1364:GLU:N	1:B:1365:PRO:HD2	2.34	0.43
1:A:306:ASN:HB3	1:A:310:ARG:HH12	1.83	0.43
1:A:1827:LYS:NZ	1:A:1849:ILE:O	2.44	0.43
1:B:117:SER:HB3	1:B:135:CYS:HB3	2.01	0.43
1:B:542:ASP:HB3	1:B:545:THR:OG1	2.17	0.43
1:A:495:ILE:HD12	1:A:758:VAL:HG11	2.00	0.43
1:A:620:MET:HB2	1:A:675:VAL:HG13	2.01	0.43
1:A:1275:ARG:NH2	1:A:1321:ALA:O	2.52	0.43
1:A:1483:VAL:O	1:A:1483:VAL:HG13	2.18	0.43
1:B:628:GLU:H	1:B:628:GLU:CD	2.16	0.43
1:B:768:GLN:HE22	1:B:781:ILE:CG2	2.32	0.43
1:A:261:VAL:HG12	1:B:146:PHE:CG	2.53	0.43
1:A:423:LEU:HD23	1:A:812:PRO:HB3	2.01	0.43
1:A:549:ILE:HD12	1:A:550:VAL:N	2.34	0.43
1:A:503:TRP:N	1:A:506:MET:HE3	2.26	0.43
1:A:542:ASP:OD1	1:A:543:GLU:N	2.52	0.43
1:A:754:GLU:HG3	1:A:778:SER:OG	2.18	0.43
1:A:1080:VAL:HG22	1:A:1087:THR:HG23	2.00	0.43
1:B:54:LEU:HD12	1:B:57:LEU:HD21	2.00	0.43
1:B:93:GLY:O	1:B:95:ILE:HD12	2.19	0.43
1:B:745:PHE:CE2	1:B:749:LEU:HD21	2.54	0.43
1:A:425:ARG:HH21	1:A:811:ASN:ND2	2.16	0.43
1:A:431:PRO:HG3	1:A:467:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLN:HG3	1:A:546:PHE:HB3	2.01	0.43
1:A:763:PRO:O	1:A:785:MET:HG2	2.19	0.43
1:B:9:MET:CE	1:B:342:ALA:HA	2.26	0.43
1:B:33:VAL:HG12	1:B:50:ARG:HB3	2.01	0.43
1:B:248:ASN:HB2	1:B:280:ALA:HB2	2.00	0.43
1:B:1845:GLN:OE1	1:B:1847:LYS:NZ	2.44	0.43
1:B:506:MET:HE2	1:B:506:MET:HB3	1.62	0.42
1:B:1349:ARG:HA	1:B:1371:ILE:HD11	2.01	0.42
1:A:584:GLU:CB	1:A:738:ASN:ND2	2.82	0.42
1:A:765:ALA:HB2	1:A:783:PRO:HB3	2.02	0.42
1:B:2:GLU:OE1	1:B:2:GLU:HA	2.19	0.42
1:B:6:ILE:HG23	1:B:231:VAL:CG1	2.49	0.42
1:B:76:ASP:HA	1:B:116:THR:HG21	2.00	0.42
1:B:368:ALA:HB1	1:B:374:LEU:HB2	2.01	0.42
1:A:492:LEU:HD11	1:A:759:LEU:CD1	2.49	0.42
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.92	0.42
1:A:946:VAL:O	1:A:953:VAL:HG12	2.19	0.42
1:A:1879:THR:HG23	1:A:2015:TYR:OH	2.18	0.42
1:B:569:CYS:SG	1:B:814:ALA:HB1	2.59	0.42
1:B:852:ASN:OD1	1:B:901:ARG:NH1	2.52	0.42
1:B:2022:VAL:HG13	1:B:2060:TRP:O	2.20	0.42
1:A:124:PRO:HG2	1:B:45:TYR:CZ	2.55	0.42
1:A:759:LEU:HD21	1:A:803:LEU:HD13	2.01	0.42
1:B:124:PRO:HA	1:B:127:LEU:CD2	2.50	0.42
1:A:517:ARG:O	1:A:521:LEU:HD23	2.19	0.42
1:A:555:SER:O	1:A:559:ILE:HG13	2.19	0.42
1:A:1336:LEU:O	1:A:1405:ARG:NE	2.53	0.42
1:B:79:LEU:O	1:B:83:LEU:HD13	2.19	0.42
1:B:646:LYS:HA	1:B:646:LYS:HD2	1.78	0.42
1:B:702:ILE:HD12	1:B:702:ILE:N	2.34	0.42
1:A:81:LEU:O	1:A:85:VAL:HG23	2.19	0.42
1:A:654:PRO:O	1:A:658:VAL:HG23	2.20	0.42
1:A:692:PRO:N	1:A:693:PRO:HD2	2.35	0.42
1:B:765:ALA:HB1	1:B:768:GLN:HE21	1.83	0.42
1:B:1253:TYR:OH	1:B:1283:ALA:HB1	2.19	0.42
1:A:776:LYS:HD2	1:A:776:LYS:N	2.34	0.42
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.47	0.42
1:B:231:VAL:HG12	1:B:233:LEU:HD12	2.00	0.42
1:A:155:ILE:N	1:A:155:ILE:HD12	2.34	0.42
1:A:290:ILE:HD12	1:A:389:GLY:O	2.19	0.42
1:A:418:ALA:N	1:A:422:ARG:HH21	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:PRO:HA	1:A:729:THR:HA	2.00	0.42
1:A:717:ILE:O	1:A:722:TRP:NE1	2.50	0.42
1:A:1033:MET:HE3	1:A:1089:ALA:HB3	2.01	0.42
1:A:1794:VAL:C	1:A:1795:LEU:HD23	2.40	0.42
1:A:9:MET:CE	1:A:243:TYR:CD1	3.02	0.42
1:A:785:MET:HG3	1:A:792:ASN:OD1	2.19	0.42
1:B:76:ASP:OD1	1:B:116:THR:OG1	2.34	0.42
1:B:326:LYS:NZ	1:B:336:SER:HB2	2.34	0.42
1:A:13:LEU:HB2	1:A:16:SER:OG	2.20	0.42
1:A:27:ILE:HD12	1:A:27:ILE:HA	1.88	0.42
1:B:35:ASP:OD1	1:B:49:ARG:HB3	2.20	0.42
1:B:61:ASP:OD2	1:B:837:ASP:HB3	2.20	0.42
1:B:504:ARG:HH21	1:B:541:THR:CB	2.31	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.93	0.41
1:A:624:GLY:N	1:A:671:PHE:O	2.38	0.41
1:A:1245:VAL:HG23	1:A:1246:LEU:HD12	2.01	0.41
1:B:409:GLN:HB3	1:B:824:PRO:HA	2.02	0.41
1:B:754:GLU:O	1:B:755:HIS:HB2	2.19	0.41
1:B:1571:LEU:CD2	1:B:1622:LEU:HD11	2.49	0.41
1:A:13:LEU:HD22	1:A:329:MET:CE	2.50	0.41
1:A:1593:THR:HG22	1:A:1595:GLN:H	1.85	0.41
1:B:108:TRP:HB3	1:B:167:ALA:HB1	2.02	0.41
1:B:212:CYS:SG	1:B:223:CYS:N	2.89	0.41
1:B:698:LEU:HB2	1:B:732:ALA:CB	2.48	0.41
1:A:506:MET:HE2	1:A:763:PRO:HB2	2.03	0.41
1:A:1069:LEU:HD11	1:A:1075:VAL:HG11	2.02	0.41
1:A:2020:SER:N	1:A:2058:VAL:O	2.47	0.41
1:B:848:GLU:H	1:B:848:GLU:CD	2.23	0.41
1:A:79:LEU:HB2	1:A:140:MET:SD	2.61	0.41
1:A:594:LEU:HD23	1:A:594:LEU:HA	1.93	0.41
1:A:1436:ASP:OD1	1:A:1436:ASP:N	2.52	0.41
1:A:2020:SER:OG	1:A:2021:SER:N	2.54	0.41
1:B:75:MET:HE3	1:B:79:LEU:HD23	2.01	0.41
1:B:1246:LEU:HD12	1:B:1246:LEU:N	2.35	0.41
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.20	0.41
1:A:2063:ILE:HG12	2:A:2602:NDP:C7N	2.50	0.41
1:B:664:GLN:O	1:B:667:LYS:HB2	2.20	0.41
1:A:525:GLU:OE1	1:A:525:GLU:HA	2.20	0.41
1:A:1732:VAL:O	1:A:1736:THR:OG1	2.23	0.41
1:B:326:LYS:HE3	1:B:331:HIS:CD2	2.55	0.41
1:B:499:MET:CE	1:B:581:SER:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1763:HIS:N	1:B:1788:ASN:O	2.53	0.41
1:A:54:LEU:HD12	1:A:57:LEU:HD21	2.01	0.41
1:A:79:LEU:CD2	1:A:143:ARG:HG3	2.46	0.41
1:A:310:ARG:NH1	1:A:310:ARG:HG3	2.35	0.41
1:A:694:LEU:HD12	1:A:694:LEU:C	2.40	0.41
1:B:615:LEU:HB2	1:B:616:PRO:HD2	2.02	0.41
1:B:740:VAL:HG23	1:B:741:SER:N	2.36	0.41
1:B:981:GLU:N	1:B:982:PRO:HD3	2.35	0.41
1:B:1366:GLN:O	1:B:1370:GLY:N	2.52	0.41
1:B:1594:SER:OG	1:B:1596:ASP:OD1	2.39	0.41
1:A:269:GLN:O	1:A:273:ILE:HG13	2.20	0.41
1:A:754:GLU:O	1:A:755:HIS:HB2	2.21	0.41
1:A:1973:VAL:H	2:A:2602:NDP:H52A	1.84	0.41
1:B:654:PRO:HB2	1:B:657:PRO:CG	2.50	0.41
1:B:654:PRO:C	1:B:657:PRO:HD2	2.41	0.41
1:B:707:PRO:HA	1:B:729:THR:HA	2.02	0.41
1:B:726:LEU:HD23	1:B:727:ALA:N	2.35	0.41
1:B:1606:ARG:HE	1:B:1612:ARG:HG3	1.85	0.41
1:B:2020:SER:OG	1:B:2021:SER:N	2.52	0.41
1:A:22:PHE:HD1	1:A:32:MET:CE	2.34	0.41
1:A:23:TRP:HB2	1:A:346:LEU:HD13	2.03	0.41
1:A:87:TYR:CE1	1:A:97:PRO:HG2	2.55	0.41
1:A:348:LEU:HD13	1:A:406:PRO:CB	2.47	0.41
1:A:620:MET:O	1:A:675:VAL:HG12	2.21	0.41
1:A:687:MET:CE	1:A:687:MET:N	2.84	0.41
1:A:912:VAL:HG22	1:A:913:VAL:N	2.35	0.41
1:B:267:ASP:O	1:B:271:GLN:HG3	2.21	0.41
1:B:524:ASP:O	1:B:528:LYS:N	2.54	0.41
1:B:528:LYS:HB3	1:B:528:LYS:HE2	1.87	0.41
1:A:241:ARG:HD2	1:A:453:MET:HE3	2.02	0.41
1:A:492:LEU:HD13	1:A:808:ILE:CD1	2.51	0.41
1:A:641:ALA:HB2	1:A:652:SER:N	2.36	0.41
1:B:549:ILE:HG23	1:B:550:VAL:N	2.36	0.41
1:B:605:TRP:HD1	1:B:701:VAL:HG21	1.86	0.41
1:A:326:LYS:HA	1:A:330:GLY:O	2.21	0.40
1:A:606:ARG:NH2	1:A:739:LEU:HA	2.36	0.40
1:A:643:HIS:ND1	1:A:747:GLU:OE2	2.54	0.40
1:A:1869:LYS:NZ	1:A:1870:PRO:O	2.53	0.40
1:B:1125:GLU:OE1	1:B:1125:GLU:N	2.54	0.40
1:A:98:ASP:HA	1:A:101:ARG:HG3	2.03	0.40
1:A:102:GLY:N	1:A:149:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LYS:HE2	1:A:218:ALA:O	2.20	0.40
1:A:1521:GLU:OE1	1:A:1521:GLU:N	2.52	0.40
1:B:597:GLU:H	1:B:597:GLU:CD	2.25	0.40
1:B:912:VAL:HG22	1:B:913:VAL:N	2.36	0.40
1:B:924:ILE:HD12	1:B:924:ILE:N	2.37	0.40
1:B:1052:VAL:HG11	1:B:1055:ILE:HD11	2.03	0.40
1:B:1450:THR:HG1	1:B:1996:TYR:HH	1.65	0.40
1:A:531:GLY:C	1:A:532:LEU:HD22	2.42	0.40
1:A:1583:LEU:HD11	1:A:1587:ALA:HB3	2.03	0.40
1:B:351:GLY:O	1:B:352:LEU:HD12	2.22	0.40
1:A:396:GLY:CA	1:B:142:ASN:HD22	2.25	0.40
1:B:685:TYR:CA	1:B:688:GLU:HG3	2.50	0.40
1:B:1209:LEU:N	1:B:1210:PRO:HD2	2.37	0.40
1:B:1228:LEU:HD23	1:B:1260:LEU:HD21	2.04	0.40
1:B:1654:THR:HG21	1:B:1680:VAL:HG22	2.04	0.40
1:B:2022:VAL:O	1:B:2026:ARG:N	2.52	0.40
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.21	0.40
1:A:9:MET:HE2	1:A:345:LEU:HD12	2.03	0.40
1:A:290:ILE:HG23	1:A:290:ILE:O	2.22	0.40
1:A:694:LEU:CD1	1:A:698:LEU:HD11	2.52	0.40
1:A:744:LEU:HB3	1:A:747:GLU:CG	2.51	0.40
1:A:1417:VAL:HG23	1:A:1424:TRP:CD2	2.57	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	2060/2553 (81%)	2021 (98%)	39 (2%)	0	100	100
1	B	2063/2553 (81%)	2026 (98%)	37 (2%)	0	100	100
All	All	4123/5106 (81%)	4047 (98%)	76 (2%)	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	1705/2117 (80%)	1703 (100%)	2 (0%)	92	98
1	B	1708/2117 (81%)	1708 (100%)	0	100	100
All	All	3413/4234 (81%)	3411 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	TYR
1	A	1896	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	580	HIS
1	B	142	ASN
1	B	768	GLN
1	B	1331	ASN
1	B	1345	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NDP	A	2601	-	47,52,52	0.65	0	61,80,80	0.87	2 (3%)
2	NDP	A	2602	-	47,52,52	0.66	0	61,80,80	0.80	2 (3%)
2	NDP	B	2601	-	47,52,52	0.68	0	61,80,80	0.77	2 (3%)
2	NDP	B	2602	-	47,52,52	0.65	0	61,80,80	0.88	3 (4%)

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
2	NDP	A	2601	-	-	12/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	8/30/77/77	0/5/5/5
2	NDP	B	2601	-	-	11/30/77/77	0/5/5/5
2	NDP	B	2602	-	-	10/30/77/77	0/5/5/5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2602	NDP	P2B-O2B-C2B	-3.97	112.82	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.90	113.01	123.43
2	A	2601	NDP	C4B-O4B-C1B	-2.81	107.36	109.92
2	B	2601	NDP	P2B-O2B-C2B	-2.66	116.32	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2602	NDP	C3N-C2N-N1N	-2.57	119.44	123.20
2	B	2601	NDP	C5A-C6A-N6A	2.40	123.96	120.31
2	A	2602	NDP	C5A-C6A-N6A	2.29	123.80	120.31
2	A	2601	NDP	C5A-C6A-N6A	2.25	123.74	120.31
2	B	2602	NDP	C5A-C6A-N6A	2.09	123.50	120.31

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5D-O5D-PN-O3
2	A	2601	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C5B-O5B-PA-O2A
2	A	2602	NDP	C5B-O5B-PA-O3
2	A	2602	NDP	O4B-C4B-C5B-O5B
2	A	2602	NDP	C5D-O5D-PN-O3
2	A	2602	NDP	C5D-O5D-PN-O2N
2	B	2601	NDP	C5D-O5D-PN-O1N
2	B	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	C5B-O5B-PA-O1A
2	B	2602	NDP	C5B-O5B-PA-O2A
2	B	2602	NDP	O4D-C1D-N1N-C6N
2	B	2601	NDP	O4D-C1D-N1N-C2N
2	A	2602	NDP	C3B-C4B-C5B-O5B
2	B	2601	NDP	O4B-C4B-C5B-O5B
2	B	2601	NDP	C3B-C4B-C5B-O5B
2	A	2601	NDP	C3B-C2B-O2B-P2B
2	A	2602	NDP	O4D-C1D-N1N-C6N
2	A	2601	NDP	C1B-C2B-O2B-P2B
2	B	2602	NDP	C4B-C5B-O5B-PA
2	B	2602	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	C2N-C3N-C7N-O7N
2	A	2601	NDP	C5D-O5D-PN-O2N
2	B	2601	NDP	C5D-O5D-PN-O3
2	B	2601	NDP	C5D-O5D-PN-O2N
2	B	2602	NDP	C5B-O5B-PA-O3
2	B	2602	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	C4D-C5D-O5D-PN

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
2	B	2601	NDP	C3B-C2B-O2B-P2B
2	A	2601	NDP	C3B-C4B-C5B-O5B
2	A	2601	NDP	C2B-O2B-P2B-O1X
2	A	2602	NDP	C4B-C5B-O5B-PA
2	A	2601	NDP	C2B-O2B-P2B-O2X
2	B	2601	NDP	C2B-O2B-P2B-O3X
2	B	2602	NDP	C3B-C4B-C5B-O5B
2	B	2601	NDP	C1B-C2B-O2B-P2B
2	B	2601	NDP	PA-O3-PN-O1N

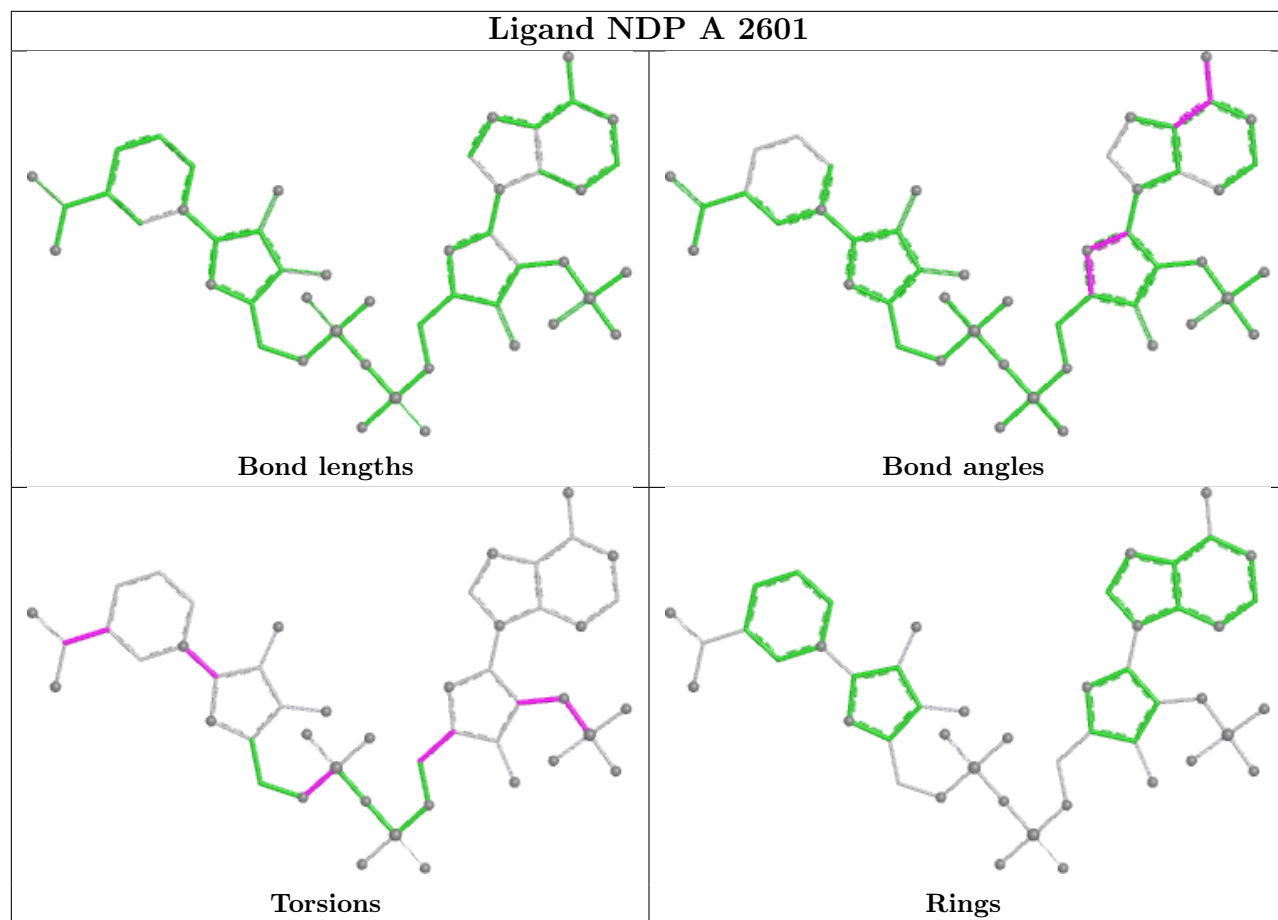
There are no ring outliers.

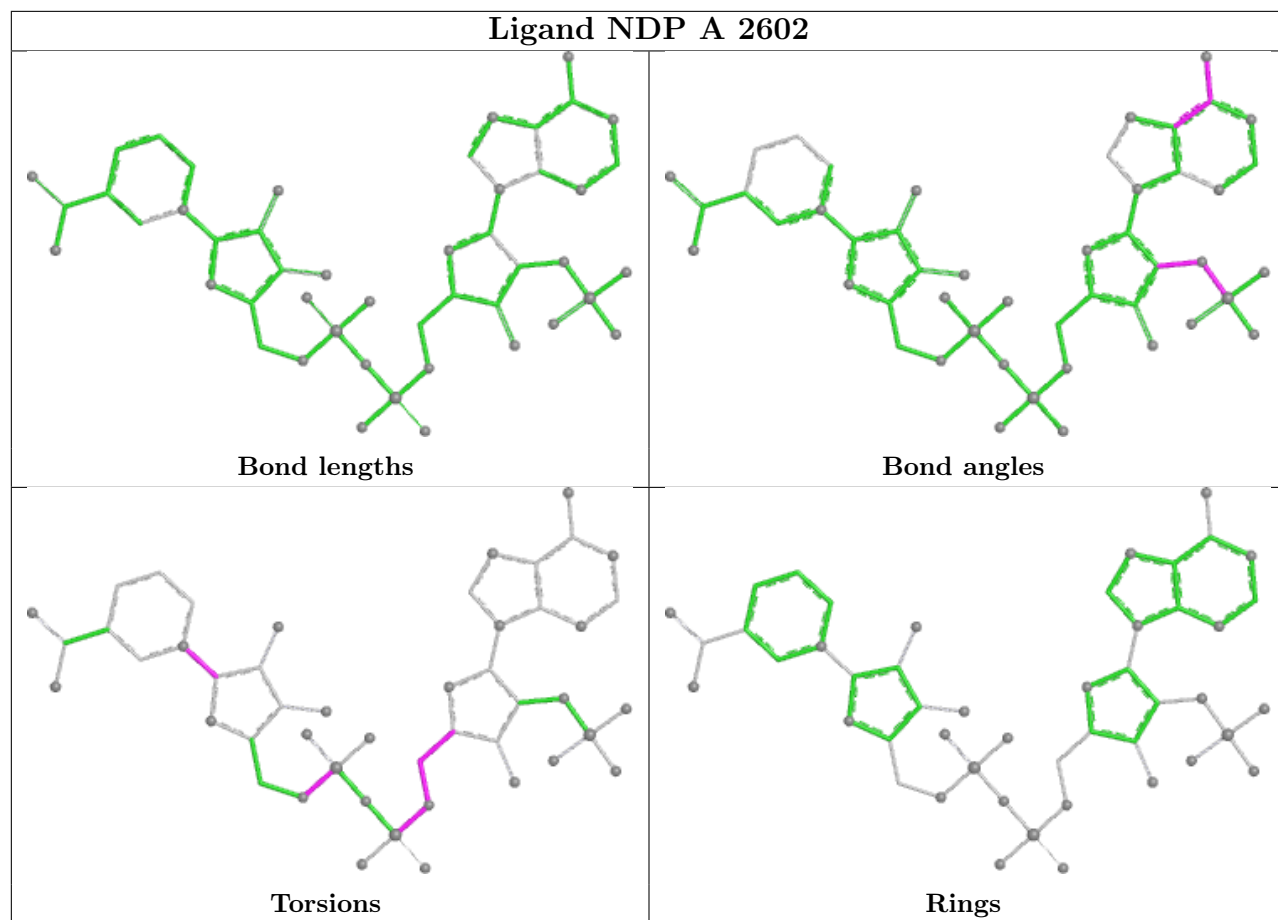
2 monomers are involved in 4 short contacts:

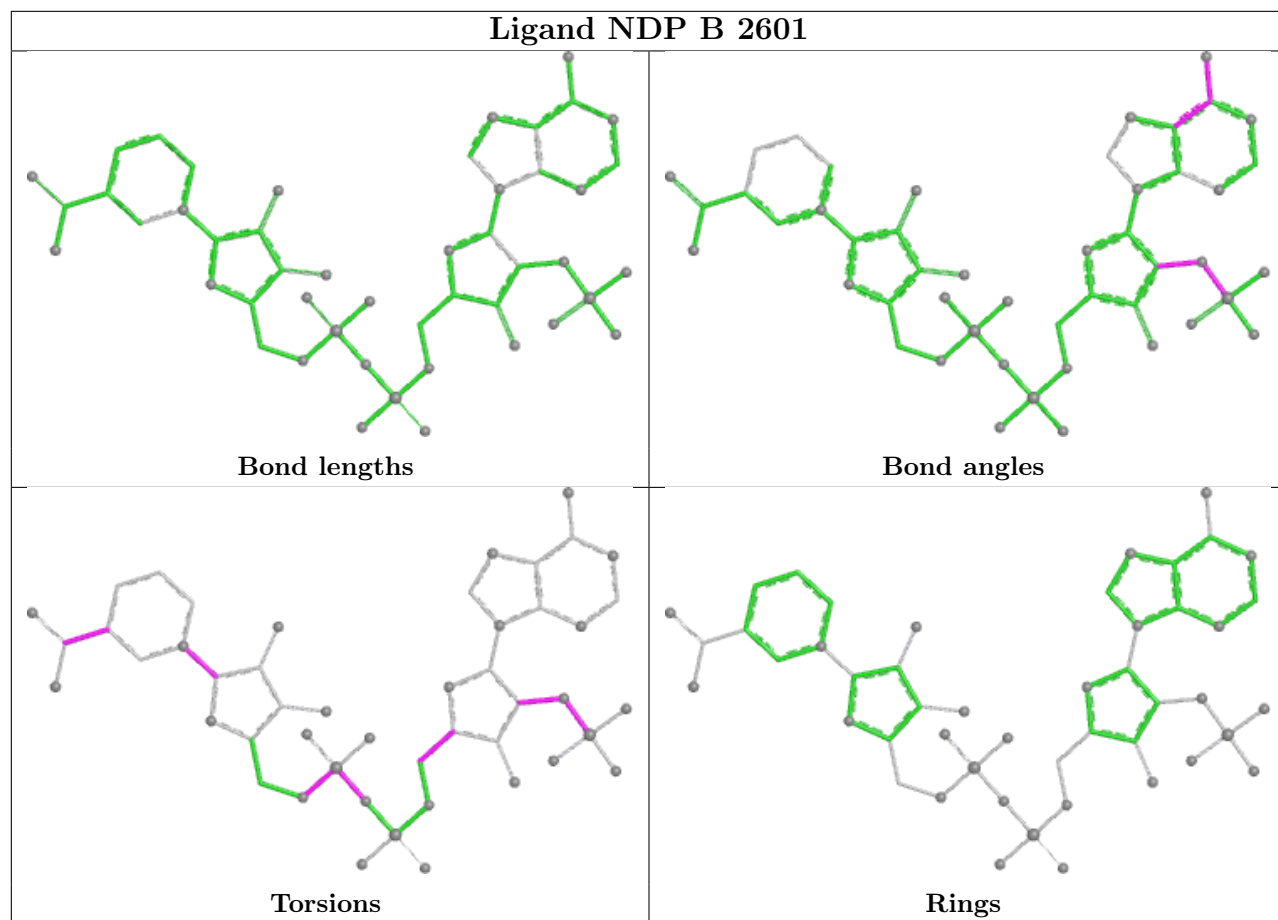
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	NDP	1	0
2	A	2602	NDP	3	0

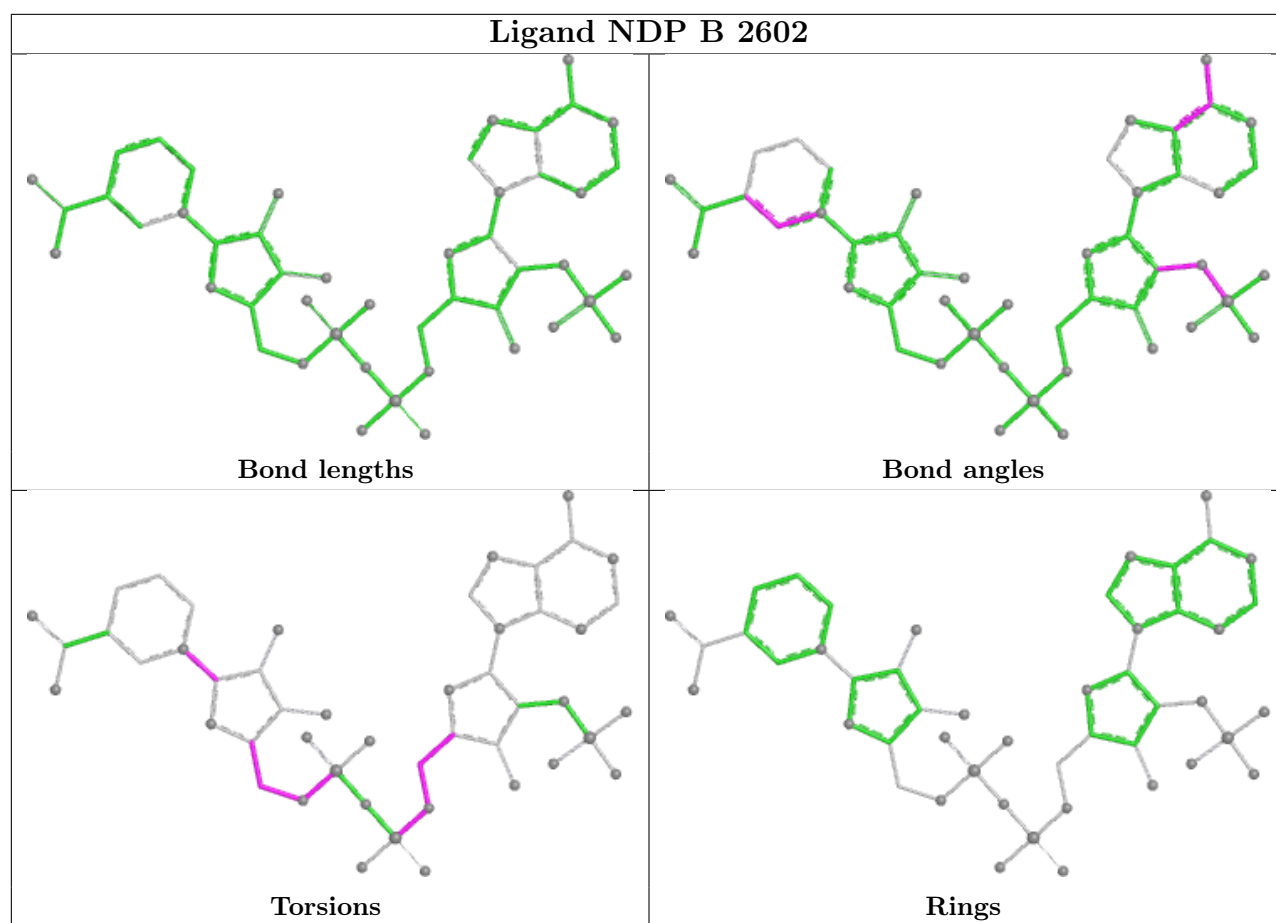
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

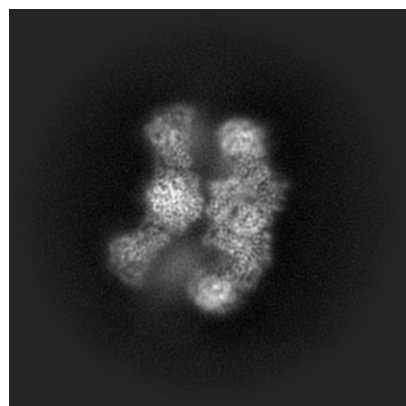
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43341. These allow visual inspection of the internal detail of the map and identification of artifacts.

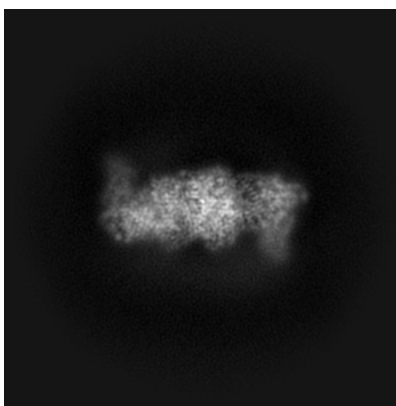
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

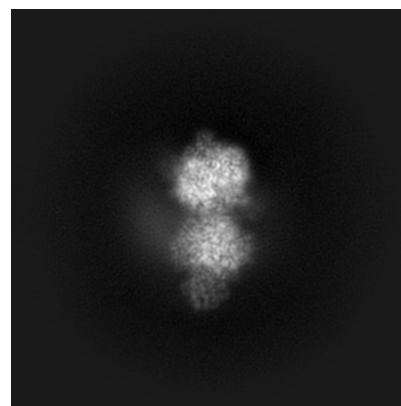
#### 6.1.1 Primary map



X

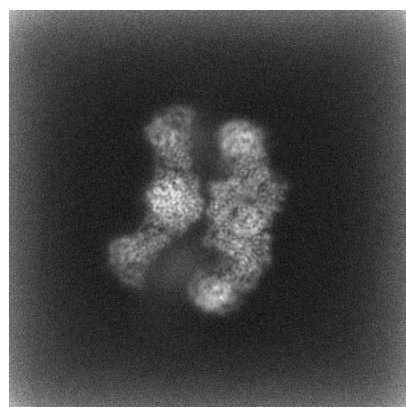


Y

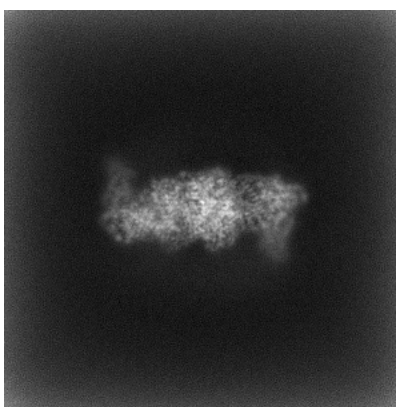


Z

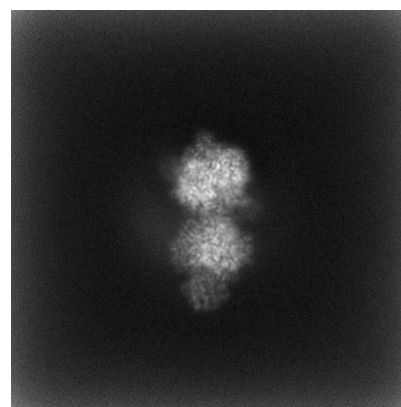
#### 6.1.2 Raw map



X



Y

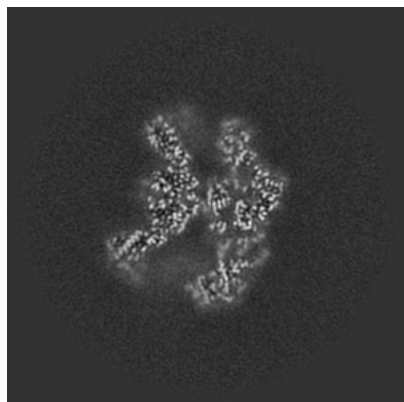


Z

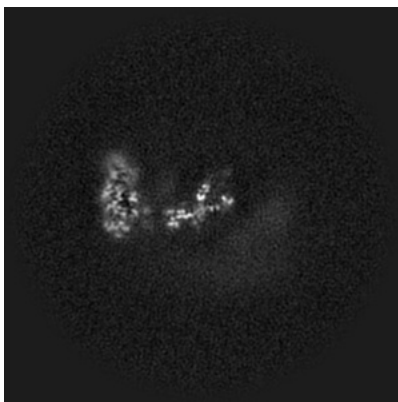
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

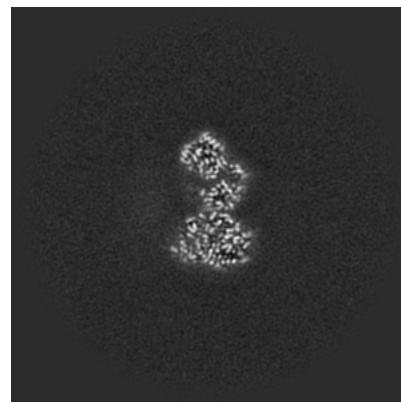
### 6.2.1 Primary map



X Index: 180

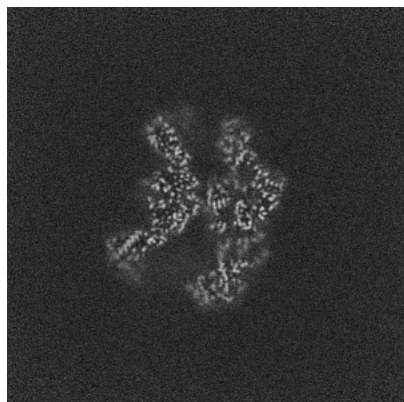


Y Index: 180



Z Index: 180

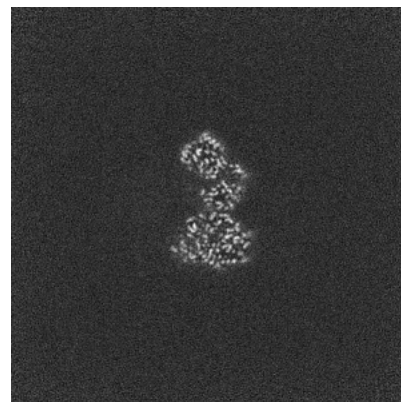
### 6.2.2 Raw map



X Index: 180



Y Index: 180

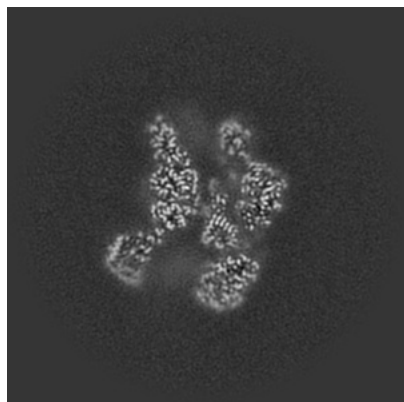


Z Index: 180

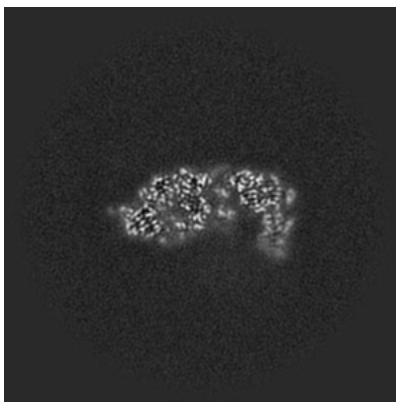
The images above show central slices of the map in three orthogonal directions.

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

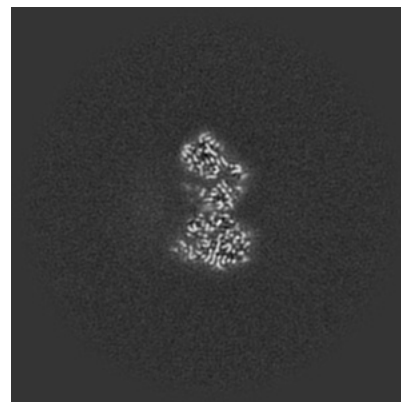
### 6.3.1 Primary map



X Index: 175

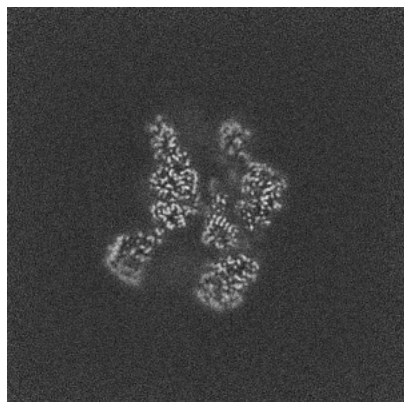


Y Index: 212

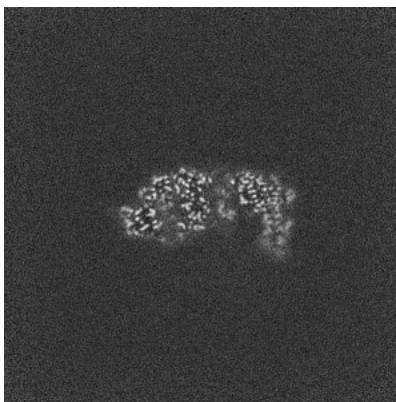


Z Index: 179

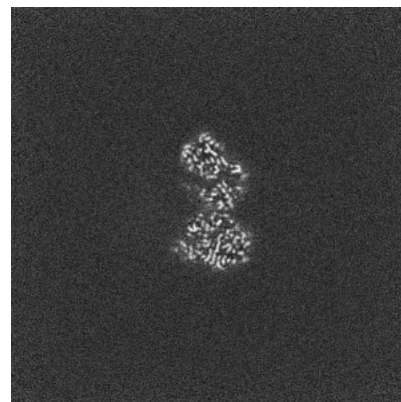
### 6.3.2 Raw map



X Index: 175



Y Index: 213



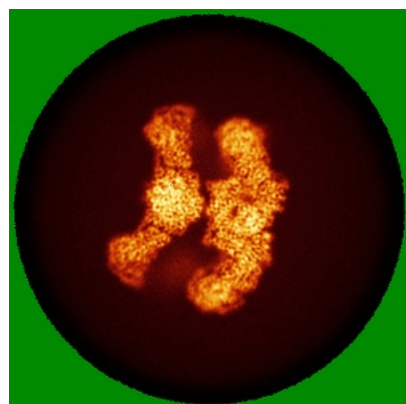
Z Index: 179

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

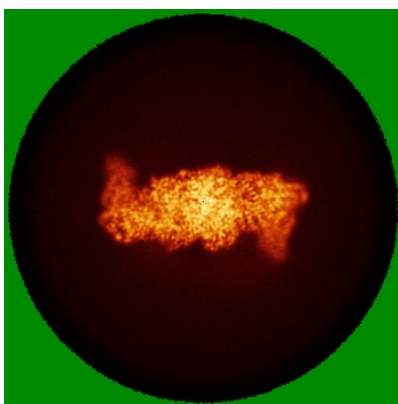


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

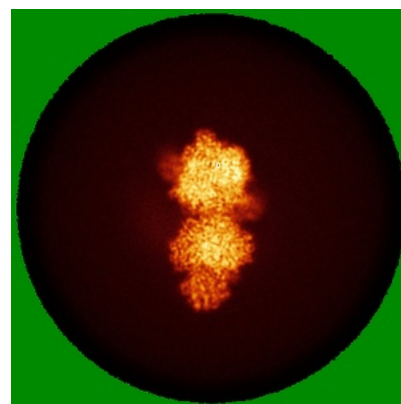
### 6.4.1 Primary map



X

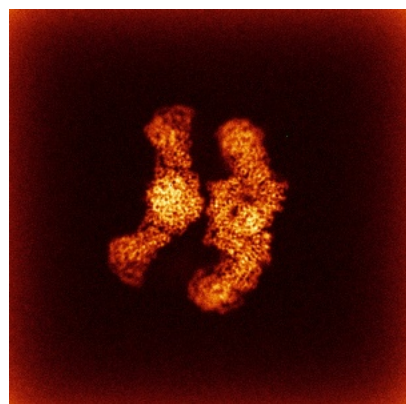


Y

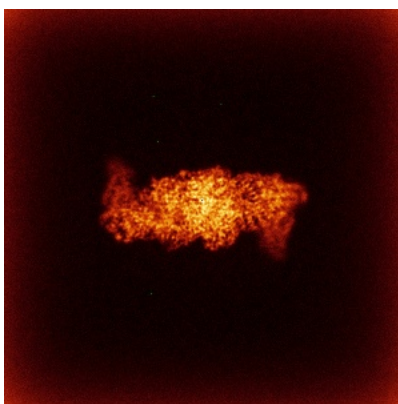


Z

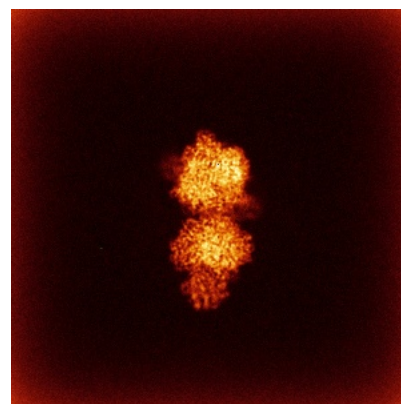
### 6.4.2 Raw map



X



Y



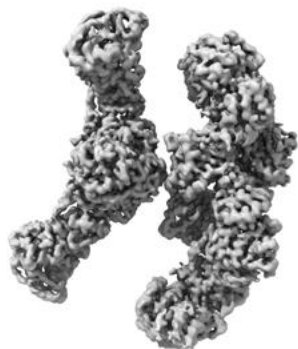
Z

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.

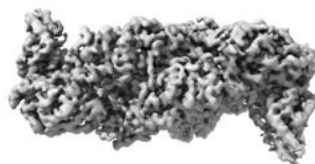


## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.197. 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.

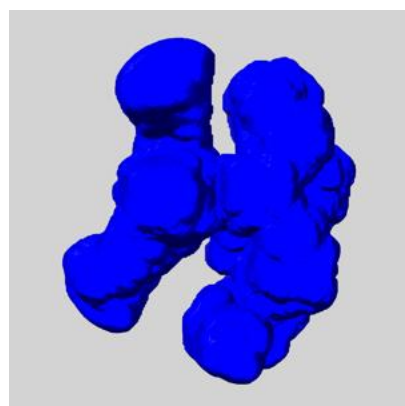
## 6.6 Mask visualisation [i](#)

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

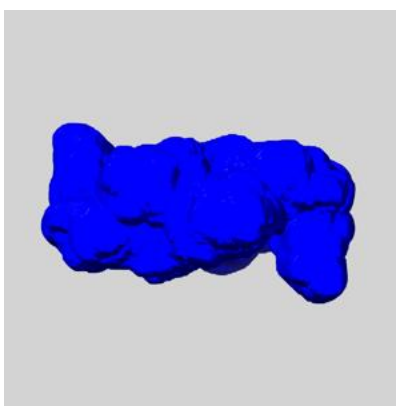
A mask typically either:

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

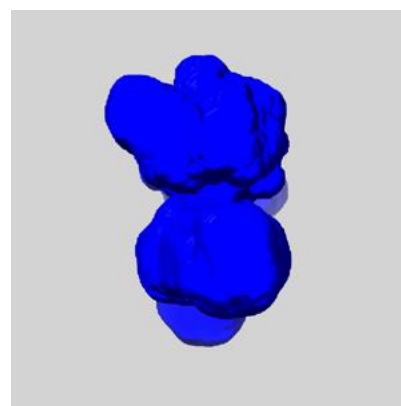
### 6.6.1 emd\_43341\_msk\_1.map [i](#)



X



Y

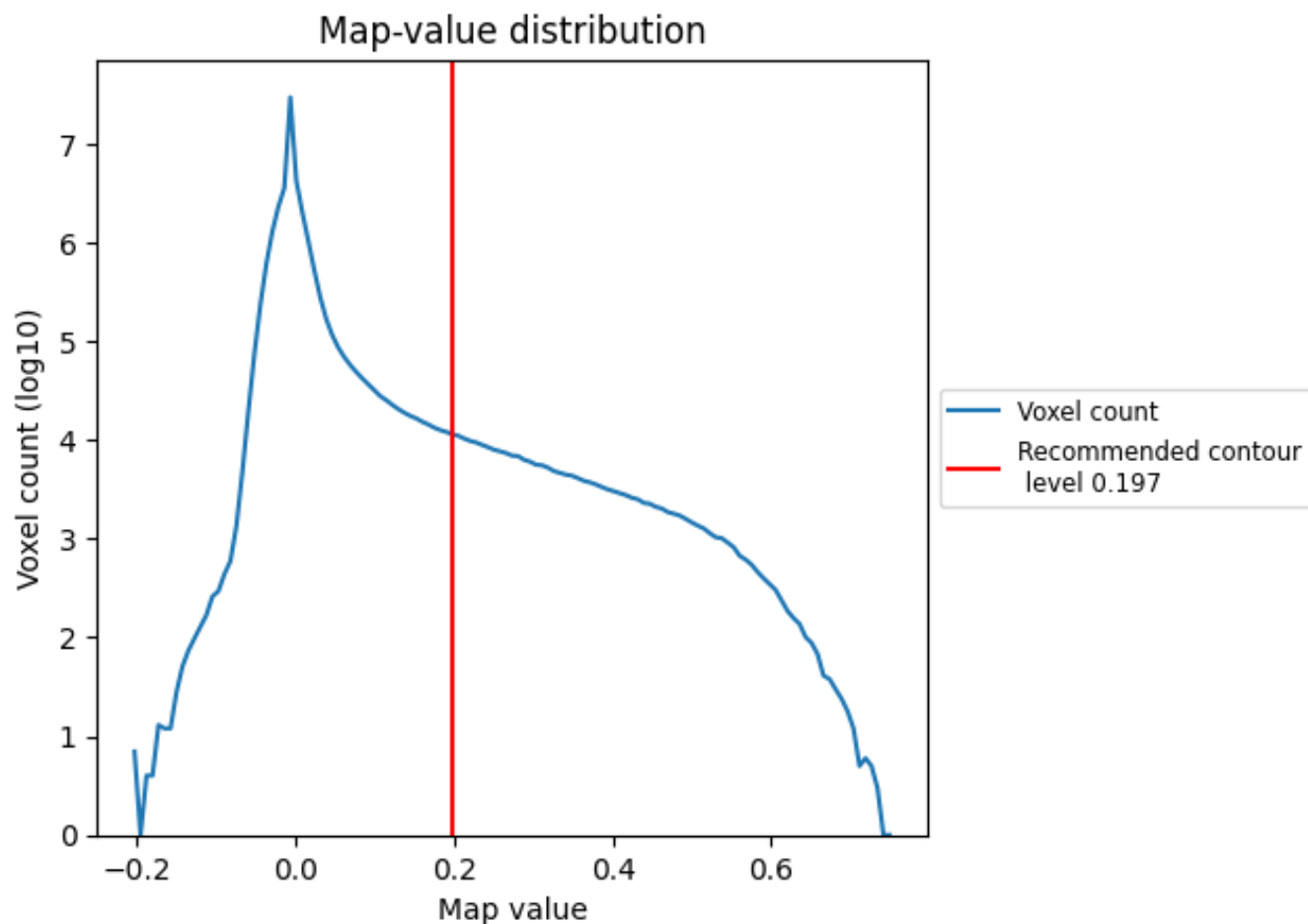


Z

## 7 Map analysis [i](#)

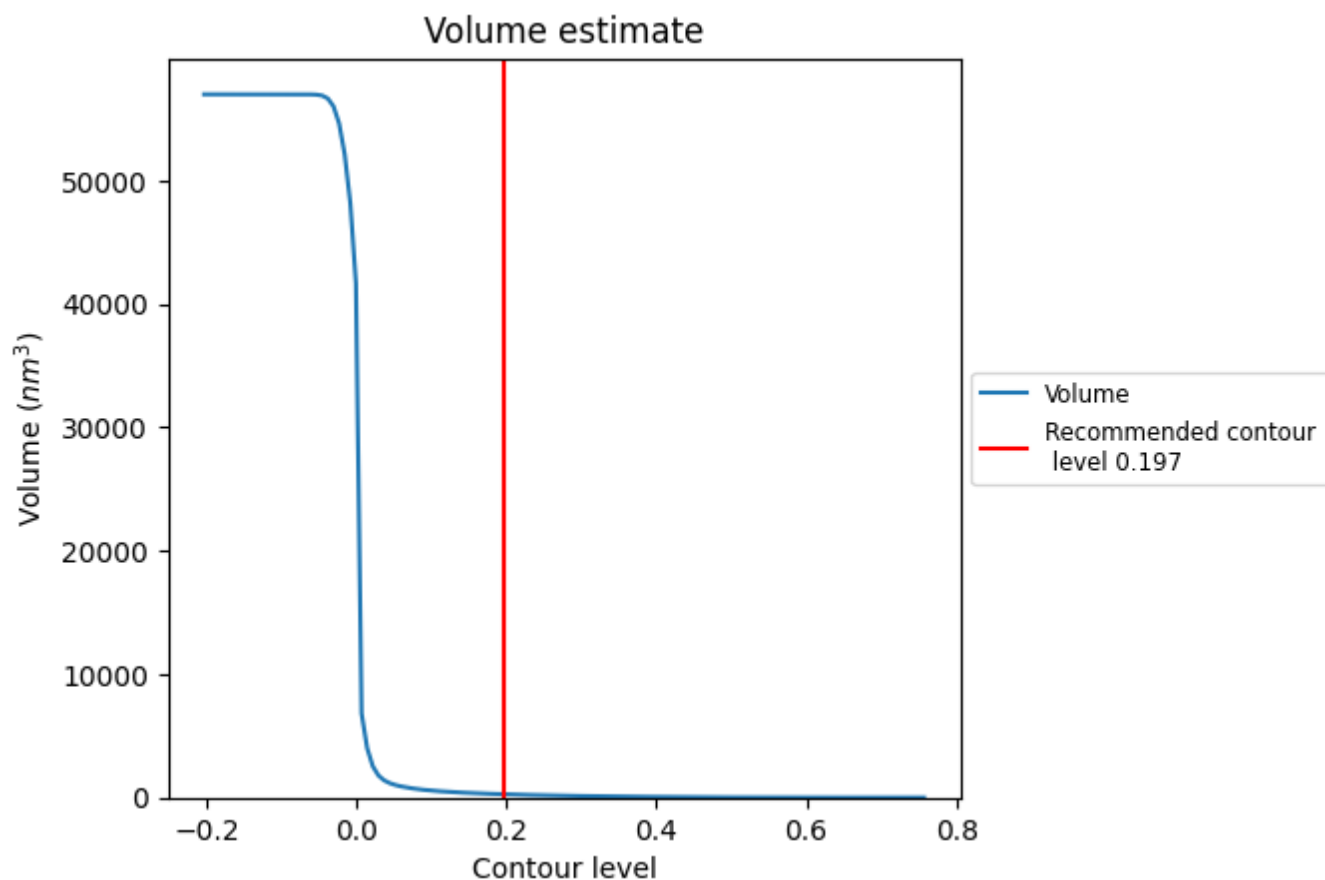
This section contains the results of statistical analysis of the map.

### 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.

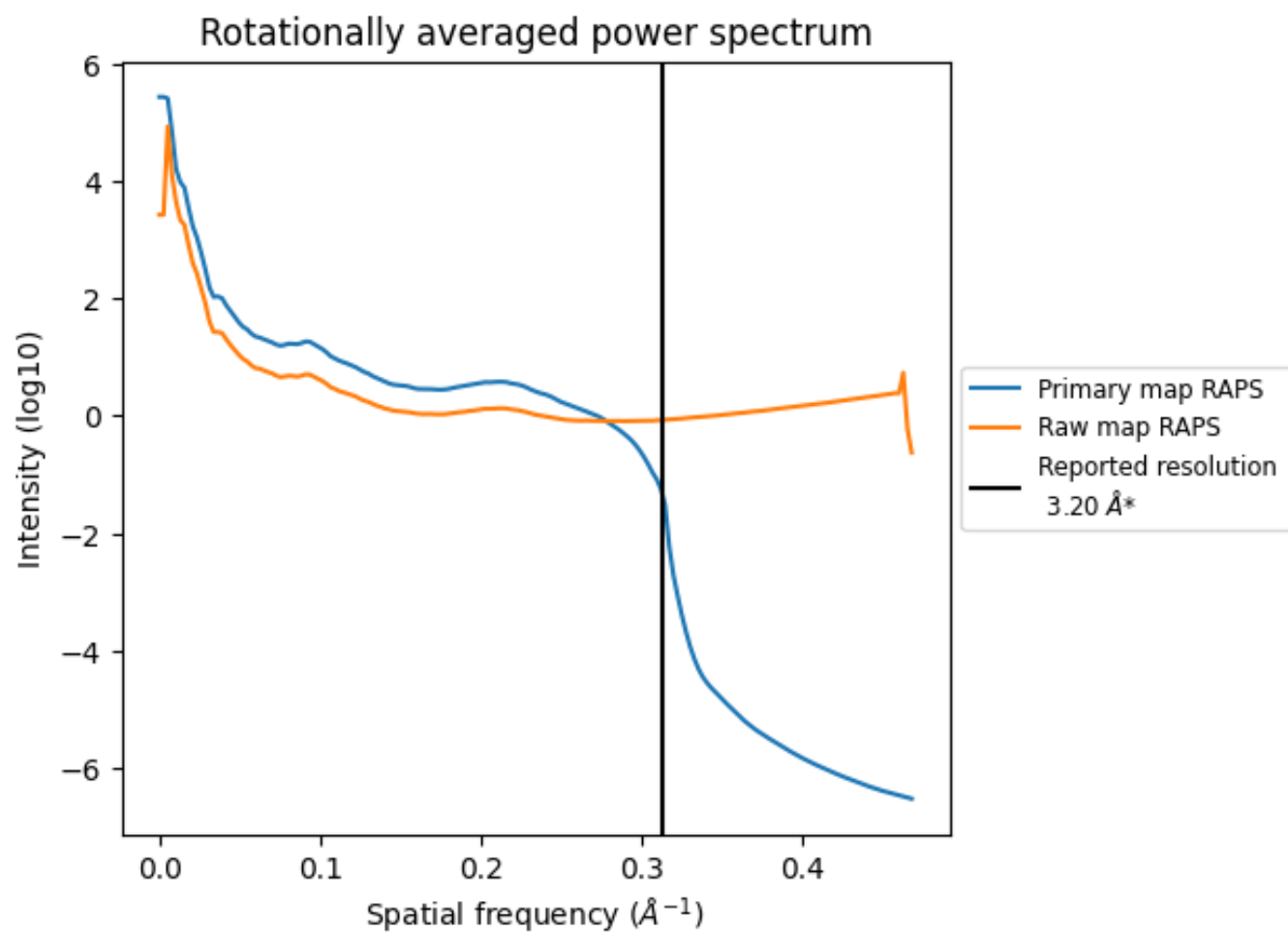
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 267 nm<sup>3</sup>; this corresponds to an approximate mass of 241 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 ⓘ

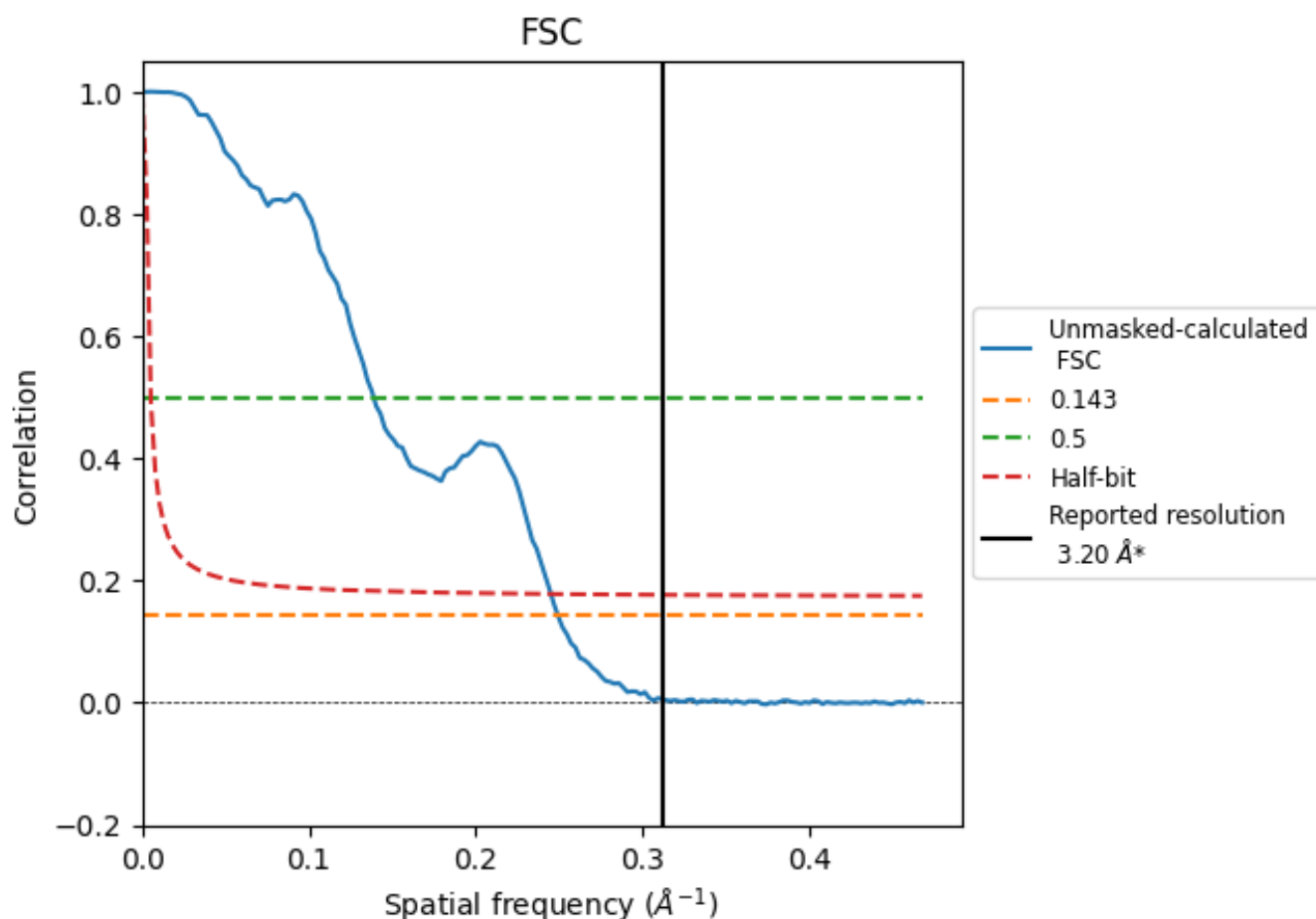


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

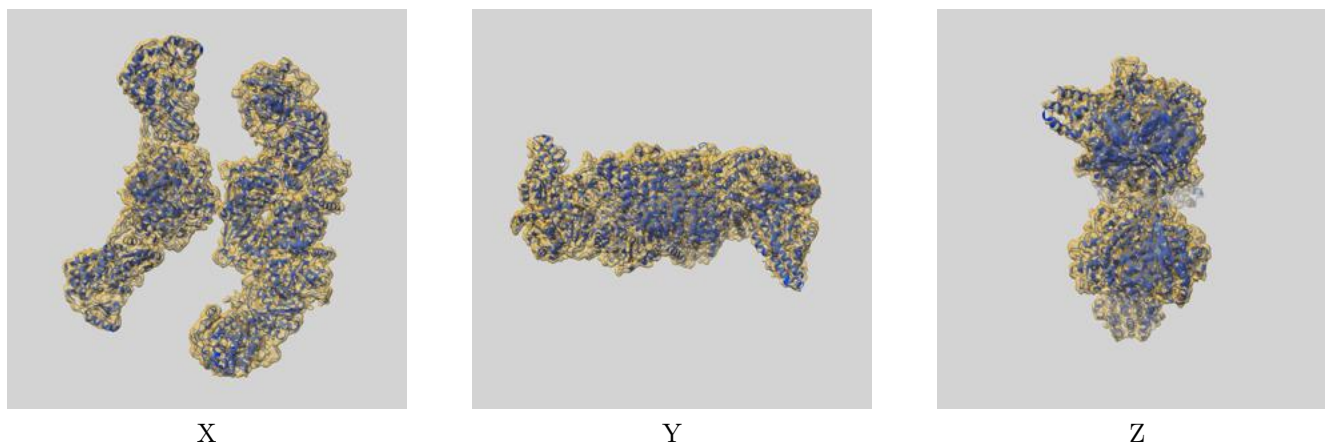
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.20	4.08

\*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 4.01 differs from the reported value 3.2 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-43341 and PDB model 8VLP. Per-residue inclusion information can be found in section 3 on page 7.

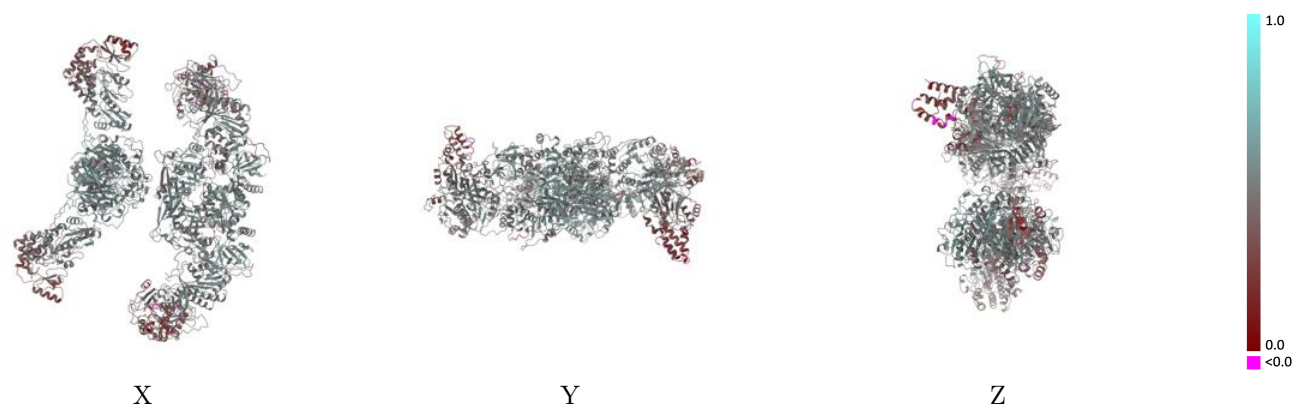
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.197 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.

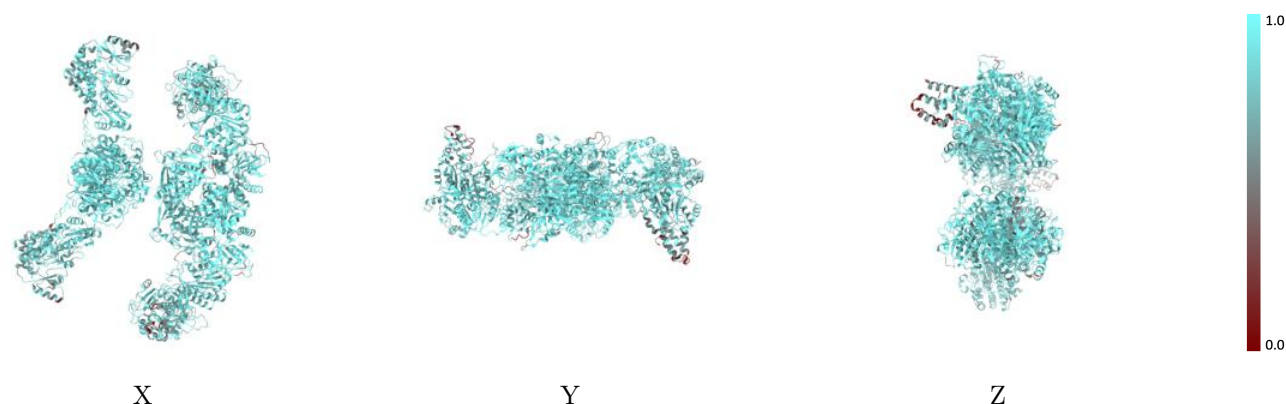


## 9.2 Q-score mapped to coordinate model [i](#)



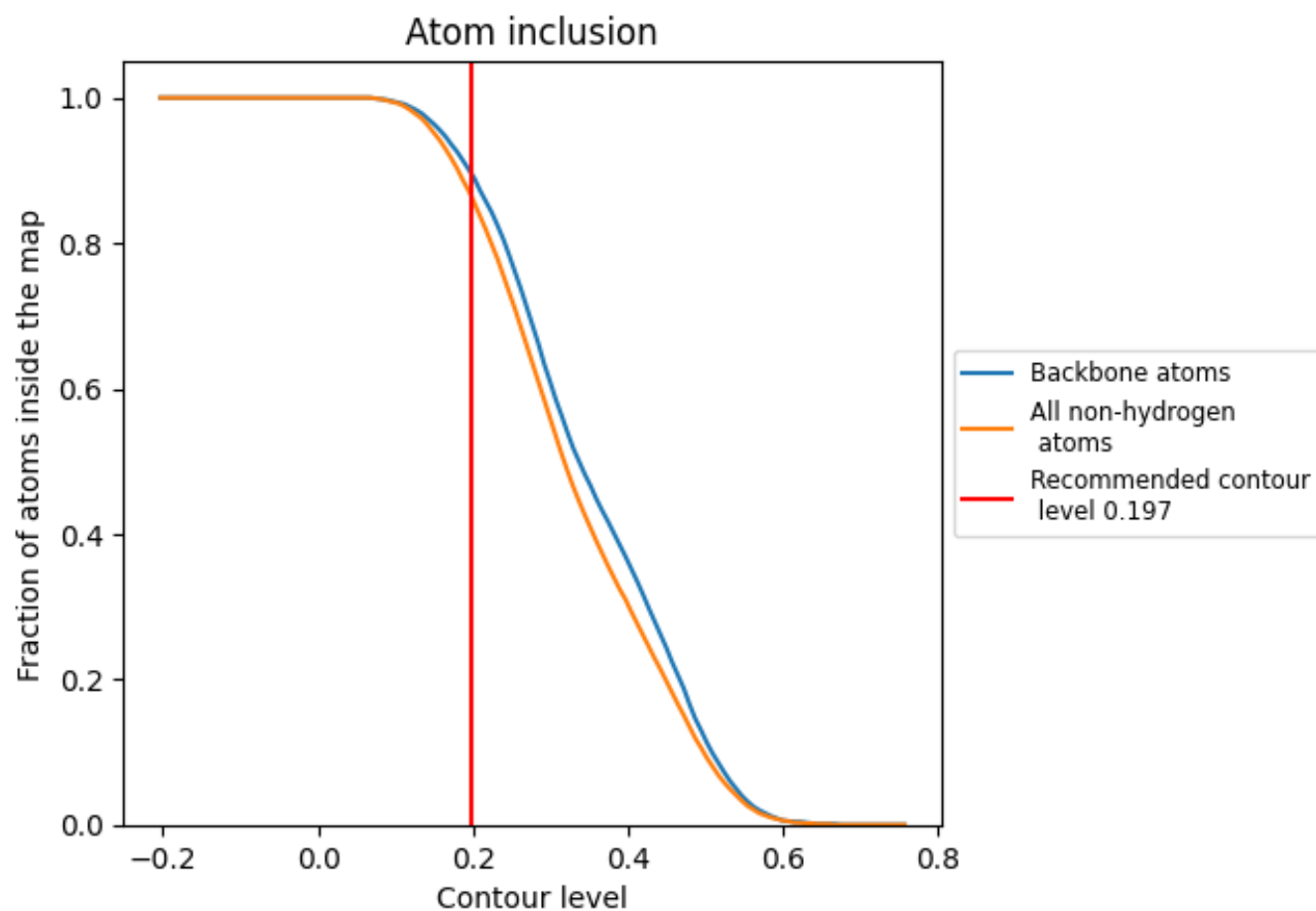
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.197).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8670	<div></div> 0.4740
A	<div></div> 0.8690	<div></div> 0.4750
B	<div></div> 0.8650	<div></div> 0.4730

