



Full wwPDB EM Validation Report ⓘ

Apr 29, 2026 – 06:17 PM JST

PDB ID : 9VED / pdb_00009ved
EMDB ID : EMD-64998
Title : The cryo-EM structure of mouse Piezo1-MDFI complex
Authors : Zhang, Y.; Dai, F.; Zhou, Z.; Dai, F.; Cheng, D.; Ma, X.; Omidkhoda, S.F.;
Clarke, J.; Zhang, H.; Laden, M.; Guo, Y.; Li, J.V.; Liu, R.; Wong, E.S.;
Zhang, Y.; Cox, C.D.
Deposited on : 2025-06-09
Resolution : 3.63 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

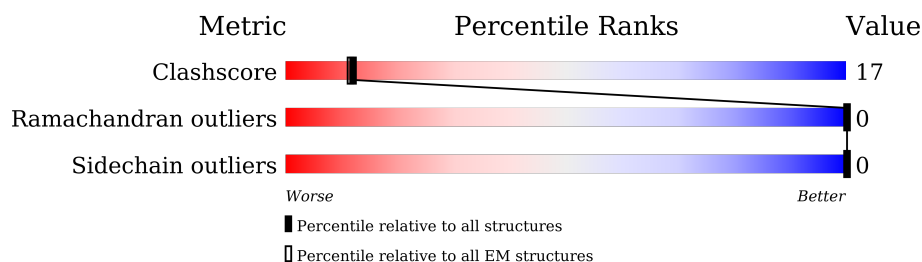
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.63 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2815	29% 14% 57%
1	B	2815	29% 14% 57%
1	C	2815	29% 14% 57%
2	D	269	6% . 92%
2	E	269	. . 92%
2	F	269	. . 92%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29400 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 Piezo-type mechanosensitive ion channel component 1, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1223	Total	C	N	O	S	0	0
			9652	6324	1626	1651	51		
1	C	1223	Total	C	N	O	S	0	0
			9652	6324	1626	1651	51		
1	B	1223	Total	C	N	O	S	0	0
			9652	6324	1626	1651	51		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2548	SER	-	linker	UNP E2JF22
A	2549	ASN	-	linker	UNP E2JF22
A	2550	SER	-	linker	UNP E2JF22
A	2551	LEU	-	linker	UNP E2JF22
A	2552	GLU	-	linker	UNP E2JF22
A	2553	VAL	-	linker	UNP E2JF22
A	2554	LEU	-	linker	UNP E2JF22
A	2555	PHE	-	linker	UNP E2JF22
A	2556	GLN	-	linker	UNP E2JF22
A	2557	GLY	-	linker	UNP E2JF22
A	2558	PRO	-	linker	UNP E2JF22
A	2559	THR	-	linker	UNP E2JF22
A	2560	ALA	-	linker	UNP E2JF22
A	2561	ALA	-	linker	UNP E2JF22
A	2562	ALA	-	linker	UNP E2JF22
A	2563	ALA	-	linker	UNP E2JF22
A	2564	VAL	-	linker	UNP E2JF22
A	2627	LEU	PHE	conflict	UNP P42212
A	2628	THR	SER	conflict	UNP P42212
A	2769	LYS	ALA	conflict	UNP P42212
A	2794	LEU	HIS	conflict	UNP P42212
A	2802	SER	-	expression tag	UNP P42212
A	2803	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2804	GLY	-	expression tag	UNP P42212
A	2805	GLY	-	expression tag	UNP P42212
A	2806	HIS	-	expression tag	UNP P42212
A	2807	HIS	-	expression tag	UNP P42212
A	2808	HIS	-	expression tag	UNP P42212
A	2809	HIS	-	expression tag	UNP P42212
A	2810	HIS	-	expression tag	UNP P42212
A	2811	HIS	-	expression tag	UNP P42212
A	2812	HIS	-	expression tag	UNP P42212
A	2813	HIS	-	expression tag	UNP P42212
A	2814	HIS	-	expression tag	UNP P42212
A	2815	HIS	-	expression tag	UNP P42212
C	2548	SER	-	linker	UNP E2JF22
C	2549	ASN	-	linker	UNP E2JF22
C	2550	SER	-	linker	UNP E2JF22
C	2551	LEU	-	linker	UNP E2JF22
C	2552	GLU	-	linker	UNP E2JF22
C	2553	VAL	-	linker	UNP E2JF22
C	2554	LEU	-	linker	UNP E2JF22
C	2555	PHE	-	linker	UNP E2JF22
C	2556	GLN	-	linker	UNP E2JF22
C	2557	GLY	-	linker	UNP E2JF22
C	2558	PRO	-	linker	UNP E2JF22
C	2559	THR	-	linker	UNP E2JF22
C	2560	ALA	-	linker	UNP E2JF22
C	2561	ALA	-	linker	UNP E2JF22
C	2562	ALA	-	linker	UNP E2JF22
C	2563	ALA	-	linker	UNP E2JF22
C	2564	VAL	-	linker	UNP E2JF22
C	2627	LEU	PHE	conflict	UNP P42212
C	2628	THR	SER	conflict	UNP P42212
C	2769	LYS	ALA	conflict	UNP P42212
C	2794	LEU	HIS	conflict	UNP P42212
C	2802	SER	-	expression tag	UNP P42212
C	2803	GLY	-	expression tag	UNP P42212
C	2804	GLY	-	expression tag	UNP P42212
C	2805	GLY	-	expression tag	UNP P42212
C	2806	HIS	-	expression tag	UNP P42212
C	2807	HIS	-	expression tag	UNP P42212
C	2808	HIS	-	expression tag	UNP P42212
C	2809	HIS	-	expression tag	UNP P42212
C	2810	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2811	HIS	-	expression tag	UNP P42212
C	2812	HIS	-	expression tag	UNP P42212
C	2813	HIS	-	expression tag	UNP P42212
C	2814	HIS	-	expression tag	UNP P42212
C	2815	HIS	-	expression tag	UNP P42212
B	2548	SER	-	linker	UNP E2JF22
B	2549	ASN	-	linker	UNP E2JF22
B	2550	SER	-	linker	UNP E2JF22
B	2551	LEU	-	linker	UNP E2JF22
B	2552	GLU	-	linker	UNP E2JF22
B	2553	VAL	-	linker	UNP E2JF22
B	2554	LEU	-	linker	UNP E2JF22
B	2555	PHE	-	linker	UNP E2JF22
B	2556	GLN	-	linker	UNP E2JF22
B	2557	GLY	-	linker	UNP E2JF22
B	2558	PRO	-	linker	UNP E2JF22
B	2559	THR	-	linker	UNP E2JF22
B	2560	ALA	-	linker	UNP E2JF22
B	2561	ALA	-	linker	UNP E2JF22
B	2562	ALA	-	linker	UNP E2JF22
B	2563	ALA	-	linker	UNP E2JF22
B	2564	VAL	-	linker	UNP E2JF22
B	2627	LEU	PHE	conflict	UNP P42212
B	2628	THR	SER	conflict	UNP P42212
B	2769	LYS	ALA	conflict	UNP P42212
B	2794	LEU	HIS	conflict	UNP P42212
B	2802	SER	-	expression tag	UNP P42212
B	2803	GLY	-	expression tag	UNP P42212
B	2804	GLY	-	expression tag	UNP P42212
B	2805	GLY	-	expression tag	UNP P42212
B	2806	HIS	-	expression tag	UNP P42212
B	2807	HIS	-	expression tag	UNP P42212
B	2808	HIS	-	expression tag	UNP P42212
B	2809	HIS	-	expression tag	UNP P42212
B	2810	HIS	-	expression tag	UNP P42212
B	2811	HIS	-	expression tag	UNP P42212
B	2812	HIS	-	expression tag	UNP P42212
B	2813	HIS	-	expression tag	UNP P42212
B	2814	HIS	-	expression tag	UNP P42212
B	2815	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called Isoform I-mfA of MyoD family inhibitor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	21	Total 148	C 86	N 21	O 33	S 8	0	0
2	D	21	Total 148	C 86	N 21	O 33	S 8	0	0
2	E	21	Total 148	C 86	N 21	O 33	S 8	0	0

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	MET	-	initiating methionine	UNP P70331
F	-21	ASP	-	expression tag	UNP P70331
F	-20	TYR	-	expression tag	UNP P70331
F	-19	LYS	-	expression tag	UNP P70331
F	-18	ASP	-	expression tag	UNP P70331
F	-17	ASP	-	expression tag	UNP P70331
F	-16	ASP	-	expression tag	UNP P70331
F	-15	ASP	-	expression tag	UNP P70331
F	-14	LYS	-	expression tag	UNP P70331
F	-13	GLY	-	expression tag	UNP P70331
F	-12	GLY	-	expression tag	UNP P70331
F	-11	GLY	-	expression tag	UNP P70331
F	-10	GLY	-	expression tag	UNP P70331
F	-9	SER	-	expression tag	UNP P70331
F	-8	SER	-	expression tag	UNP P70331
F	-7	THR	-	expression tag	UNP P70331
F	-6	THR	-	expression tag	UNP P70331
F	-5	ASN	-	expression tag	UNP P70331
F	-4	GLY	-	expression tag	UNP P70331
F	-3	SER	-	expression tag	UNP P70331
F	-2	SER	-	expression tag	UNP P70331
F	-1	ALA	-	expression tag	UNP P70331
F	0	THR	-	expression tag	UNP P70331
D	-22	MET	-	initiating methionine	UNP P70331
D	-21	ASP	-	expression tag	UNP P70331
D	-20	TYR	-	expression tag	UNP P70331
D	-19	LYS	-	expression tag	UNP P70331
D	-18	ASP	-	expression tag	UNP P70331
D	-17	ASP	-	expression tag	UNP P70331
D	-16	ASP	-	expression tag	UNP P70331
D	-15	ASP	-	expression tag	UNP P70331
D	-14	LYS	-	expression tag	UNP P70331
D	-13	GLY	-	expression tag	UNP P70331

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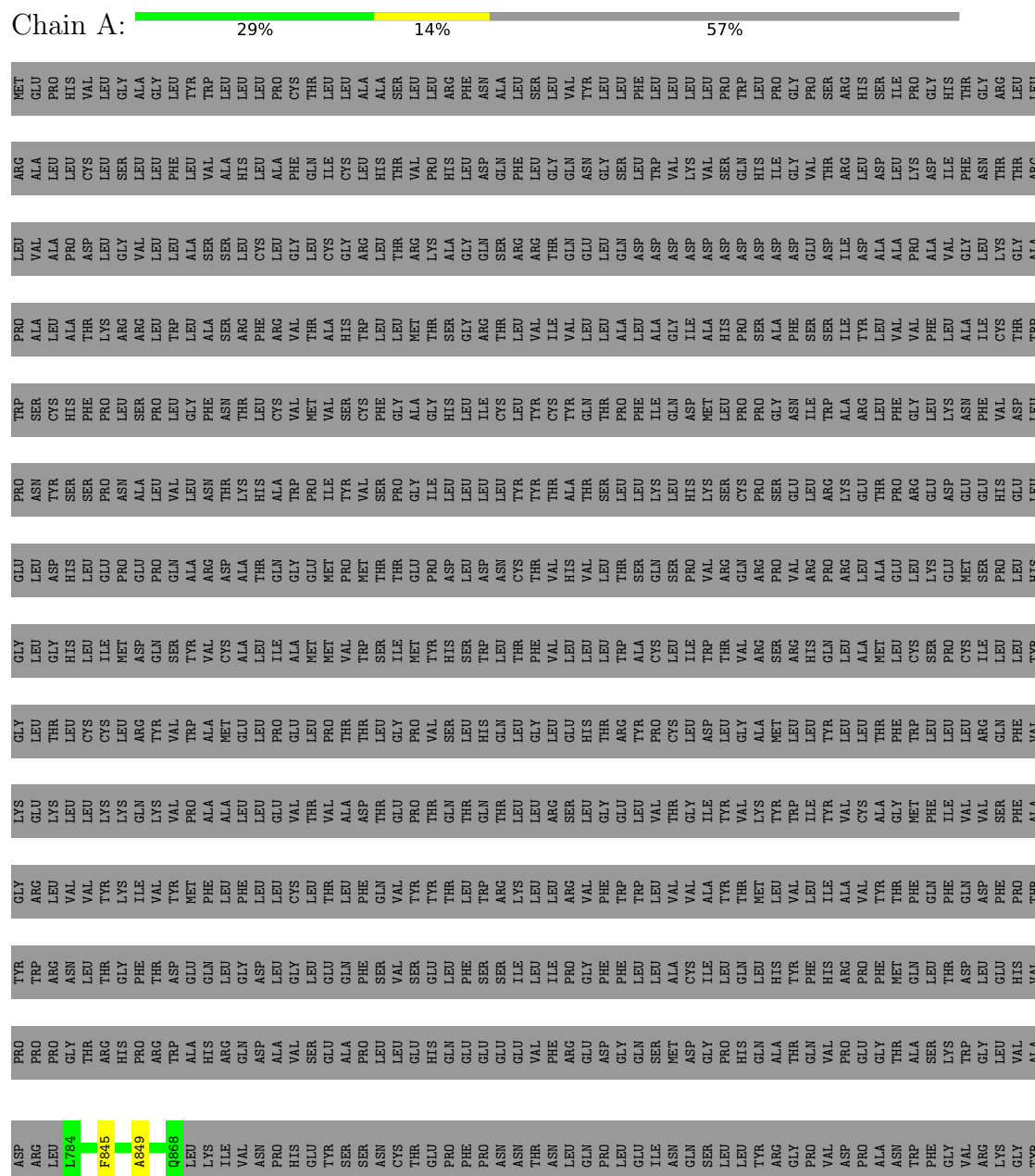
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	expression tag	UNP P70331
D	-11	GLY	-	expression tag	UNP P70331
D	-10	GLY	-	expression tag	UNP P70331
D	-9	SER	-	expression tag	UNP P70331
D	-8	SER	-	expression tag	UNP P70331
D	-7	THR	-	expression tag	UNP P70331
D	-6	THR	-	expression tag	UNP P70331
D	-5	ASN	-	expression tag	UNP P70331
D	-4	GLY	-	expression tag	UNP P70331
D	-3	SER	-	expression tag	UNP P70331
D	-2	SER	-	expression tag	UNP P70331
D	-1	ALA	-	expression tag	UNP P70331
D	0	THR	-	expression tag	UNP P70331
E	-22	MET	-	initiating methionine	UNP P70331
E	-21	ASP	-	expression tag	UNP P70331
E	-20	TYR	-	expression tag	UNP P70331
E	-19	LYS	-	expression tag	UNP P70331
E	-18	ASP	-	expression tag	UNP P70331
E	-17	ASP	-	expression tag	UNP P70331
E	-16	ASP	-	expression tag	UNP P70331
E	-15	ASP	-	expression tag	UNP P70331
E	-14	LYS	-	expression tag	UNP P70331
E	-13	GLY	-	expression tag	UNP P70331
E	-12	GLY	-	expression tag	UNP P70331
E	-11	GLY	-	expression tag	UNP P70331
E	-10	GLY	-	expression tag	UNP P70331
E	-9	SER	-	expression tag	UNP P70331
E	-8	SER	-	expression tag	UNP P70331
E	-7	THR	-	expression tag	UNP P70331
E	-6	THR	-	expression tag	UNP P70331
E	-5	ASN	-	expression tag	UNP P70331
E	-4	GLY	-	expression tag	UNP P70331
E	-3	SER	-	expression tag	UNP P70331
E	-2	SER	-	expression tag	UNP P70331
E	-1	ALA	-	expression tag	UNP P70331
E	0	THR	-	expression tag	UNP P70331

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. 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. 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: Piezo-type mechanosensitive ion channel component 1, Green fluorescent protein



PRO	ASN	E1027	D1097	F1189	CYS	GLY	ALA	ARG	GLY	SER	LYS	ASP	PRO	GLY	THR	GLY	ASP	GLY	THR	GLY	ASP	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR
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- Molecule 2: Isoform I-mfA of MyoD family inhibitor

92%

[illegible]

92%

[illegible]

92%

LEU	ASP	GLN	LEU	ALA	MET
ASP	CYS	GLN	LEU	ARG	ASP
CYS	GLY	GLU	PRO	SER	TYR
ILE	ASP	ASP	ASN	THR	LYS
VAL	ASP	CYS	SER	HIS	ASP
ASP	ASP	CYS	SER	PRO	ASP
ALA	ALA	CYS	SER	VAL	ASP
C226	C227	HIS	HIS	ALA	LYS
E230	E228	CYS	LEU	SER	GLY
S229	E228	ILE	SER	GLY	GLY
D231	E230	LEU	GLU	GLU	GLY
I235	D231	CYS	PRO	GLY	SER
E238	I235	PHE	SER	PHE	SER
C239	E238	LEU	GLY	PRO	THR
L242	C243	CYS	ALA	GLU	THR
F244	E243	GLY	GLY	GLU	ASN
S245	F244	THR	HIS	ALA	GLY
S246	S245	ILE	ALA	ALA	SER
	S246	LEU	LEU	PRO	SER
		LEU	GLY	THR	THR
		ASP	SER	GLY	THR
		CYS	LYS	LEU	GLY
		ALA	ALA	ASP	GLY
		THR	THR	ASP	VAL
		SER	THR	VAL	PRO
		SER	GLN	PRO	SER
		GLU	ALA	THR	ALA
		CYS	GLY	GLU	ALA
		CYS	ARG	ALA	LEU
		CYS	LYS	VAL	ASP
		GLY	SER	THR	PRO
		SER	ARG	CYS	ALA
		GLY	GLN	GLN	THR
		CYS	ALA	GLN	MET
		ASP	ARG	GLY	SER
		ASP	SER	ASN	LEU
		GLU	ALA	PRO	LEU
		THR	THR	GLN	PRO
		CYS	GLY	GLY	GLY
		ASP	LEU	CYS	LEU
		GLY	PRO	THR	VAL
		THR	LEU	PRO	VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	56377	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 ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/9876	0.59	0/13401
1	B	0.50	0/9876	0.59	0/13401
1	C	0.50	0/9876	0.59	0/13401
2	D	0.39	0/148	0.62	0/195
2	E	0.39	0/148	0.62	0/195
2	F	0.38	0/148	0.62	0/195
All	All	0.50	0/30072	0.59	0/40788

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	9652	0	9495	358	0
1	B	9652	0	9495	361	0
1	C	9652	0	9495	344	0
2	D	148	0	130	9	0
2	E	148	0	130	12	0
2	F	148	0	130	12	0
All	All	29400	0	28875	1005	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 17.

All (1005) 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:1029:ILE:HA	1:A:1033:TRP:CD1	1.98	0.98
1:B:1029:ILE:HA	1:B:1033:TRP:CD1	1.97	0.98
1:C:1029:ILE:HA	1:C:1033:TRP:CD1	1.98	0.98
1:B:1118:GLU:HB3	1:B:1120:GLN:HG3	1.48	0.95
1:A:1118:GLU:HB3	1:A:1120:GLN:HG3	1.49	0.94
1:C:1118:GLU:HB3	1:C:1120:GLN:HG3	1.49	0.94
1:C:1559:LEU:HG	1:C:1653:ARG:HD2	1.56	0.88
1:A:2490:HIS:HD1	1:B:2494:PHE:HD2	1.16	0.88
1:C:1412:TYR:OH	1:B:2537:GLU:OE2	1.92	0.86
1:A:1559:LEU:HG	1:A:1653:ARG:HD2	1.56	0.85
1:B:1142:ASN:O	1:B:1147:ARG:NH2	2.09	0.85
1:B:1559:LEU:HG	1:B:1653:ARG:HD2	1.56	0.85
1:C:1142:ASN:O	1:C:1147:ARG:NH2	2.08	0.85
1:A:1142:ASN:O	1:A:1147:ARG:NH2	2.09	0.85
1:A:1687:SER:OG	1:A:1796:HIS:ND1	2.12	0.81
1:B:1687:SER:OG	1:B:1796:HIS:ND1	2.12	0.81
1:B:1029:ILE:HA	1:B:1033:TRP:HD1	1.45	0.81
1:C:1687:SER:OG	1:C:1796:HIS:ND1	2.12	0.81
1:C:1326:ALA:HA	1:C:1649:LEU:HD11	1.63	0.80
1:B:1326:ALA:HA	1:B:1649:LEU:HD11	1.63	0.80
1:A:2133:GLU:HG3	1:C:2485:PHE:HD2	1.47	0.79
1:A:2191:MET:HE1	2:D:238:GLU:HB3	1.63	0.79
1:C:2046:LYS:NZ	1:C:2093:SER:OG	2.14	0.79
1:A:2467:VAL:HG13	1:B:1996:TRP:CH2	2.18	0.78
1:A:1326:ALA:HA	1:A:1649:LEU:HD11	1.63	0.78
1:A:2492:ILE:HD11	1:B:2530:ILE:HD12	1.66	0.78
1:B:1002:ILE:HD13	1:B:1010:VAL:HG22	1.66	0.78
1:A:2333:VAL:HG21	1:A:2382:PRO:HG3	1.66	0.78
1:C:1002:ILE:HD13	1:C:1010:VAL:HG22	1.66	0.77
1:C:2333:VAL:HG21	1:C:2382:PRO:HG3	1.66	0.77
1:A:1002:ILE:HD13	1:A:1010:VAL:HG22	1.66	0.77
1:A:2018:GLN:OE1	1:C:2211:SER:OG	2.02	0.77
1:A:1029:ILE:HA	1:A:1033:TRP:HD1	1.45	0.77
1:A:2182:LYS:NZ	1:B:2144:ASP:HA	1.98	0.77
1:B:2333:VAL:HG21	1:B:2382:PRO:HG3	1.66	0.77
1:C:1029:ILE:HA	1:C:1033:TRP:HD1	1.45	0.76
1:A:2537:GLU:OE2	1:B:1412:TYR:OH	2.02	0.76
1:C:2113:LYS:O	1:C:2118:ASN:ND2	2.20	0.75
1:B:2113:LYS:O	1:B:2118:ASN:ND2	2.20	0.75
1:A:2046:LYS:NZ	1:A:2093:SER:OG	2.14	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2046:LYS:NZ	1:B:2093:SER:OG	2.14	0.74
1:A:1684:ALA:O	1:A:1799:GLN:NE2	2.18	0.74
1:A:2113:LYS:O	1:A:2118:ASN:ND2	2.20	0.74
1:A:2211:SER:HB2	1:B:1995:PHE:HZ	1.51	0.74
1:A:2420:GLY:N	1:A:2425:ASP:OD2	2.21	0.74
1:B:2420:GLY:N	1:B:2425:ASP:OD2	2.20	0.74
1:C:2420:GLY:N	1:C:2425:ASP:OD2	2.21	0.74
1:B:2407:ARG:NH2	1:B:2428:GLU:OE2	2.21	0.73
1:C:2407:ARG:NH2	1:C:2428:GLU:OE2	2.21	0.73
1:A:2407:ARG:NH2	1:A:2428:GLU:OE2	2.21	0.72
1:B:2313:ALA:O	1:B:2351:ARG:NH2	2.23	0.72
1:A:2179:LYS:HE2	1:B:1406:VAL:HG21	1.72	0.72
1:C:2313:ALA:O	1:C:2351:ARG:NH2	2.23	0.72
1:B:1684:ALA:O	1:B:1799:GLN:NE2	2.18	0.71
1:C:1684:ALA:O	1:C:1799:GLN:NE2	2.18	0.71
1:A:2313:ALA:O	1:A:2351:ARG:NH2	2.23	0.71
1:A:2493:MET:HA	1:B:2534:ARG:HG3	1.73	0.70
1:C:2069:THR:HG22	1:C:2070:GLU:H	1.57	0.70
1:A:2133:GLU:HG3	1:C:2485:PHE:CD2	2.27	0.69
1:B:2069:THR:HG22	1:B:2070:GLU:H	1.57	0.69
1:C:2235:TYR:HD1	1:C:2304:MET:HG3	1.58	0.69
1:C:1246:ILE:HG13	1:C:1251:LEU:HB2	1.74	0.69
1:B:2191:MET:HE1	2:E:238:GLU:HB3	1.73	0.69
1:A:1246:ILE:HG13	1:A:1251:LEU:HB2	1.74	0.69
1:B:1550:GLU:HG3	1:B:1551:VAL:HG12	1.75	0.69
1:A:1550:GLU:HG3	1:A:1551:VAL:HG12	1.75	0.68
1:B:1246:ILE:HG13	1:B:1251:LEU:HB2	1.74	0.68
1:A:2211:SER:HB2	1:B:1995:PHE:CZ	2.28	0.68
1:A:2069:THR:HG22	1:A:2070:GLU:H	1.57	0.68
1:A:2318:ARG:HE	1:A:2339:LYS:HE3	1.59	0.68
1:C:1203:THR:O	1:C:1207:LEU:HB2	1.94	0.68
1:A:2283:THR:HG22	1:A:2447:VAL:HG22	1.76	0.68
1:B:1117:GLU:HG2	1:B:1118:GLU:HG2	1.76	0.68
1:A:2235:TYR:HD1	1:A:2304:MET:HG3	1.58	0.68
1:C:2283:THR:HG22	1:C:2447:VAL:HG22	1.76	0.68
1:B:1203:THR:O	1:B:1207:LEU:HB2	1.94	0.68
1:A:2108:ASN:HB3	1:A:2111:THR:HG22	1.76	0.68
1:B:2283:THR:HG22	1:B:2447:VAL:HG22	1.76	0.67
1:C:1550:GLU:HG3	1:C:1551:VAL:HG12	1.75	0.67
1:A:1117:GLU:HG2	1:A:1118:GLU:HG2	1.76	0.67
1:C:1731:MET:HE3	1:C:1806:TRP:HZ2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2235:TYR:HD1	1:B:2304:MET:HG3	1.58	0.67
1:A:1731:MET:HE3	1:A:1806:TRP:HZ2	1.58	0.67
1:B:1731:MET:HE3	1:B:1806:TRP:HZ2	1.58	0.67
1:A:1984:ASP:HB3	1:A:2031:MET:HE2	1.77	0.67
1:C:2318:ARG:HE	1:C:2339:LYS:HE3	1.59	0.67
1:B:2108:ASN:HB3	1:B:2111:THR:HG22	1.76	0.67
1:B:2304:MET:HE2	1:B:2358:LEU:HD22	1.76	0.67
1:C:1117:GLU:HG2	1:C:1118:GLU:HG2	1.76	0.67
1:B:2318:ARG:HE	1:B:2339:LYS:HE3	1.59	0.66
1:A:1203:THR:O	1:A:1207:LEU:HB2	1.94	0.66
1:A:1345:LEU:HD12	1:A:2104:ARG:HE	1.60	0.66
1:C:2021:LEU:HD11	1:B:2208:LEU:HA	1.77	0.66
1:C:2304:MET:HE2	1:C:2358:LEU:HD22	1.76	0.66
1:A:845:PHE:O	1:A:849:ALA:N	2.27	0.66
1:C:1724:ARG:NH2	1:C:1805:LEU:O	2.29	0.66
1:C:2105:ILE:HG13	1:C:2106:LEU:HD12	1.77	0.66
1:A:1724:ARG:NH2	1:A:1805:LEU:O	2.29	0.66
1:C:1032:LEU:HG	1:C:1036:TYR:HB2	1.77	0.66
1:C:1984:ASP:HB3	1:C:2031:MET:HE2	1.77	0.66
1:A:1994:GLY:HA3	1:A:2078:VAL:HG11	1.78	0.66
1:A:2105:ILE:HG13	1:A:2106:LEU:HD12	1.77	0.66
1:B:1994:GLY:HA3	1:B:2078:VAL:HG11	1.78	0.66
1:B:1032:LEU:HG	1:B:1036:TYR:HB2	1.77	0.66
1:B:1724:ARG:NH2	1:B:1805:LEU:O	2.29	0.66
1:C:2108:ASN:HB3	1:C:2111:THR:HG22	1.76	0.66
1:C:2108:ASN:OD1	1:C:2109:PHE:N	2.29	0.66
1:C:1345:LEU:HD12	1:C:2104:ARG:HE	1.60	0.66
1:C:1994:GLY:HA3	1:C:2078:VAL:HG11	1.78	0.65
1:A:1148:SER:OG	1:A:1151:ASP:OD2	2.13	0.65
1:A:2108:ASN:OD1	1:A:2109:PHE:N	2.29	0.65
1:C:2123:GLN:HG2	2:F:244:PHE:CD2	2.31	0.65
1:B:1345:LEU:HD12	1:B:2104:ARG:HE	1.60	0.65
1:A:1032:LEU:HG	1:A:1036:TYR:HB2	1.77	0.65
1:A:2128:VAL:HG11	1:A:2131:LEU:HD12	1.79	0.65
1:A:2235:TYR:CD1	1:A:2304:MET:HG3	2.32	0.65
1:A:2304:MET:HE2	1:A:2358:LEU:HD22	1.77	0.65
1:C:2530:ILE:HD12	1:B:2492:ILE:HD11	1.77	0.65
1:B:1984:ASP:HB3	1:B:2031:MET:HE2	1.77	0.65
1:B:2105:ILE:HG13	1:B:2106:LEU:HD12	1.77	0.65
1:B:2356:GLN:O	1:B:2364:GLN:NE2	2.29	0.65
1:B:2373:PRO:HB2	1:B:2376:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1996:TRP:CH2	1:B:2467:VAL:HG13	2.32	0.65
1:C:2356:GLN:O	1:C:2364:GLN:NE2	2.29	0.65
1:B:2108:ASN:OD1	1:B:2109:PHE:N	2.29	0.65
1:A:2373:PRO:HB2	1:A:2376:ILE:HD11	1.79	0.65
1:A:2191:MET:CE	2:D:238:GLU:HB3	2.27	0.65
1:C:1246:ILE:HA	1:C:1251:LEU:HD23	1.79	0.65
1:A:2356:GLN:O	1:A:2364:GLN:NE2	2.29	0.64
1:B:2235:TYR:CD1	1:B:2304:MET:HG3	2.32	0.64
1:C:2128:VAL:HG11	1:C:2131:LEU:HD12	1.79	0.64
1:C:2235:TYR:CD1	1:C:2304:MET:HG3	2.32	0.64
1:B:845:PHE:O	1:B:849:ALA:N	2.28	0.64
1:C:2373:PRO:HB2	1:C:2376:ILE:HD11	1.79	0.64
1:B:1246:ILE:HA	1:B:1251:LEU:HD23	1.80	0.64
1:A:2133:GLU:OE1	1:C:2482:ARG:NE	2.17	0.64
1:C:1020:ILE:HA	1:C:1033:TRP:HH2	1.62	0.64
1:B:1020:ILE:HA	1:B:1033:TRP:HH2	1.62	0.64
1:A:1020:ILE:HA	1:A:1033:TRP:HH2	1.62	0.64
1:B:2533:TYR:CE1	1:B:2539:MET:HE1	2.33	0.64
1:C:2533:TYR:CE1	1:C:2539:MET:HE1	2.33	0.64
1:B:1159:ARG:HG2	1:B:1160:TYR:CD1	2.34	0.63
1:C:1159:ARG:HG2	1:C:1160:TYR:CD1	2.34	0.63
1:C:2123:GLN:HG2	2:F:244:PHE:HD2	1.64	0.63
1:A:2533:TYR:CE1	1:A:2539:MET:HE1	2.33	0.63
1:B:2128:VAL:HG11	1:B:2131:LEU:HD12	1.79	0.63
1:A:1246:ILE:HA	1:A:1251:LEU:HD23	1.80	0.63
1:B:1661:GLU:OE1	1:B:1664:ARG:NH1	2.31	0.63
1:B:2198:PHE:CZ	1:B:2202:ILE:HD11	2.34	0.63
1:A:1661:GLU:OE1	1:A:1664:ARG:NH1	2.31	0.62
1:A:1159:ARG:HG2	1:A:1160:TYR:CD1	2.34	0.62
1:A:2123:GLN:HG2	2:D:244:PHE:HD2	1.64	0.62
1:C:2184:LYS:NZ	2:F:231:ASP:OD1	2.27	0.62
1:C:1661:GLU:OE1	1:C:1664:ARG:NH1	2.31	0.62
1:C:2198:PHE:CZ	1:C:2202:ILE:HD11	2.34	0.62
1:B:1148:SER:OG	1:B:1151:ASP:OD2	2.14	0.62
1:A:2182:LYS:HZ3	1:B:2144:ASP:HA	1.63	0.62
1:A:2198:PHE:CZ	1:A:2202:ILE:HD11	2.34	0.61
1:C:845:PHE:O	1:C:849:ALA:N	2.28	0.61
1:B:2377:ARG:NH1	1:B:2451:ASP:OD2	2.33	0.61
1:B:1722:ILE:HG23	1:B:1723:PRO:HD2	1.82	0.61
1:C:2191:MET:HE1	2:F:238:GLU:HB3	1.83	0.61
1:C:2377:ARG:NH1	1:C:2451:ASP:OD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2377:ARG:NH1	1:A:2451:ASP:OD2	2.33	0.61
1:A:2021:LEU:HD11	1:C:2208:LEU:HA	1.83	0.60
1:B:2041:LYS:HG3	1:B:2105:ILE:HD13	1.84	0.60
1:A:1722:ILE:HG23	1:A:1723:PRO:HD2	1.82	0.60
1:A:2030:THR:HG23	1:A:2049:PHE:HZ	1.66	0.60
1:A:2208:LEU:HA	1:B:2021:LEU:HD11	1.83	0.60
1:A:2271:GLN:O	1:A:2274:SER:OG	2.20	0.60
1:C:1995:PHE:HZ	1:B:2211:SER:HB2	1.66	0.60
1:C:1722:ILE:HG23	1:C:1723:PRO:HD2	1.82	0.60
1:C:2041:LYS:HG3	1:C:2105:ILE:HD13	1.84	0.60
1:A:2372:PHE:HD2	1:A:2434:LEU:HD21	1.67	0.59
1:C:2372:PHE:HD2	1:C:2434:LEU:HD21	1.67	0.59
1:C:2497:LEU:HD21	1:C:2539:MET:HE2	1.84	0.59
1:B:2497:LEU:HD21	1:B:2539:MET:HE2	1.84	0.59
1:A:1671:ARG:HG3	1:A:1672:THR:HG23	1.84	0.59
1:A:2182:LYS:HZ2	1:B:2144:ASP:HA	1.65	0.59
1:B:2030:THR:HG23	1:B:2049:PHE:HZ	1.66	0.59
1:C:1315:GLN:HE21	1:C:1537:GLU:HB2	1.67	0.59
1:C:2030:THR:HG23	1:C:2049:PHE:HZ	1.66	0.59
1:B:2191:MET:CE	2:E:238:GLU:HB3	2.33	0.59
1:A:1020:ILE:HD11	1:A:1040:LEU:HD12	1.85	0.59
1:A:1315:GLN:HE21	1:A:1537:GLU:HB2	1.67	0.59
1:A:1521:ARG:HE	1:A:1528:ARG:CZ	2.16	0.59
1:A:2301:ARG:NH2	1:A:2358:LEU:O	2.35	0.59
1:C:1134:ARG:HG3	1:C:1137:PRO:HG3	1.85	0.59
1:B:1671:ARG:HG3	1:B:1672:THR:HG23	1.84	0.59
1:B:1134:ARG:HG3	1:B:1137:PRO:HG3	1.85	0.59
1:B:1315:GLN:HE21	1:B:1537:GLU:HB2	1.68	0.59
1:B:1521:ARG:HE	1:B:1528:ARG:CZ	2.16	0.59
1:A:2497:LEU:HD21	1:A:2539:MET:HE2	1.84	0.59
1:C:1671:ARG:HG3	1:C:1672:THR:HG23	1.84	0.59
1:B:2372:PHE:HD2	1:B:2434:LEU:HD21	1.67	0.59
1:B:1020:ILE:HD11	1:B:1040:LEU:HD12	1.85	0.59
1:B:2301:ARG:NH2	1:B:2358:LEU:O	2.35	0.58
1:A:1141:PRO:HB2	1:A:1304:HIS:ND1	2.19	0.58
1:C:1521:ARG:HE	1:C:1528:ARG:CZ	2.16	0.58
1:C:2378:ALA:N	1:C:2449:PHE:O	2.36	0.58
1:A:2210:MET:HE3	1:A:2466:ILE:HG23	1.85	0.58
1:A:2485:PHE:CG	1:B:2153:MET:HE2	2.38	0.58
1:C:1020:ILE:HD11	1:C:1040:LEU:HD12	1.85	0.58
1:A:1134:ARG:HG3	1:A:1137:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:PRO:HB2	1:B:1304:HIS:ND1	2.19	0.58
1:B:2210:MET:HE3	1:B:2466:ILE:HG23	1.85	0.58
1:A:2041:LYS:HG3	1:A:2105:ILE:HD13	1.84	0.58
1:C:2410:VAL:HG12	1:C:2426:PHE:HA	1.86	0.58
1:A:2021:LEU:HD23	1:C:2204:TRP:HE1	1.67	0.58
1:B:2123:GLN:HG2	2:E:244:PHE:CD2	2.39	0.58
1:C:1141:PRO:HB2	1:C:1304:HIS:ND1	2.19	0.58
1:B:2271:GLN:O	1:B:2274:SER:OG	2.20	0.57
1:A:2390:LEU:HD11	1:A:2449:PHE:HE2	1.69	0.57
1:C:1109:GLN:O	1:C:1113:ALA:HB3	2.04	0.57
1:B:1143:PHE:CE1	1:B:1154:LYS:HD3	2.39	0.57
1:A:1702:THR:HB	1:A:1784:LYS:HD2	1.86	0.57
1:B:1025:ARG:O	1:B:1029:ILE:HG12	2.05	0.57
1:B:2123:GLN:HG2	2:E:244:PHE:HD2	1.69	0.57
1:A:2021:LEU:HD23	1:C:2204:TRP:NE1	2.20	0.57
1:C:2271:GLN:O	1:C:2274:SER:OG	2.20	0.57
1:C:2301:ARG:NH2	1:C:2358:LEU:O	2.35	0.57
1:A:1143:PHE:CE1	1:A:1154:LYS:HD3	2.39	0.57
1:B:2390:LEU:HD11	1:B:2449:PHE:HE2	1.70	0.57
1:C:2165:ILE:HD11	2:F:245:SER:OG	2.04	0.57
1:C:2390:LEU:HD11	1:C:2449:PHE:HE2	1.69	0.57
1:B:1318:ARG:NH2	1:B:1537:GLU:OE1	2.38	0.57
1:A:1109:GLN:O	1:A:1113:ALA:HB3	2.04	0.57
1:C:1025:ARG:O	1:C:1029:ILE:HG12	2.05	0.57
1:C:2210:MET:HE3	1:C:2466:ILE:HG23	1.85	0.57
1:B:1109:GLN:O	1:B:1113:ALA:HB3	2.04	0.57
1:A:1165:VAL:HG22	1:A:1289:PHE:HB3	1.87	0.56
1:C:1143:PHE:CE1	1:C:1154:LYS:HD3	2.39	0.56
1:B:2378:ALA:N	1:B:2449:PHE:O	2.36	0.56
1:A:1996:TRP:CH2	1:C:2467:VAL:HG13	2.40	0.56
1:C:1148:SER:OG	1:C:1151:ASP:OD2	2.13	0.56
1:C:1315:GLN:NE2	1:C:1537:GLU:HB2	2.21	0.56
1:C:1318:ARG:NH2	1:C:1537:GLU:OE1	2.38	0.56
1:B:1702:THR:HB	1:B:1784:LYS:HD2	1.86	0.56
1:B:2410:VAL:HG12	1:B:2426:PHE:HA	1.86	0.56
1:A:2407:ARG:HD3	1:A:2426:PHE:HE2	1.71	0.56
1:B:2407:ARG:HD3	1:B:2426:PHE:HE2	1.71	0.56
1:A:2378:ALA:N	1:A:2449:PHE:O	2.36	0.56
1:A:2402:ARG:N	1:A:2433:GLU:O	2.25	0.56
1:B:1555:VAL:HA	1:B:1558:GLN:CD	2.31	0.56
1:A:1008:PHE:HB3	1:A:1080:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:O	1:A:1029:ILE:HG12	2.05	0.56
1:A:1406:VAL:HG21	1:C:2179:LYS:HE2	1.87	0.56
1:A:1555:VAL:HA	1:A:1558:GLN:CD	2.31	0.56
1:B:1409:SER:O	1:B:1409:SER:OG	2.22	0.56
1:A:2410:VAL:HG12	1:A:2426:PHE:HA	1.86	0.56
1:C:1555:VAL:HA	1:C:1558:GLN:CD	2.31	0.56
1:B:1315:GLN:NE2	1:B:1537:GLU:HB2	2.21	0.56
1:C:1702:THR:HB	1:C:1784:LYS:HD2	1.86	0.56
1:C:2349:THR:HA	1:C:2352:ARG:HH22	1.71	0.56
1:A:2390:LEU:HD11	1:A:2449:PHE:CE2	2.42	0.55
1:C:1719:MET:O	1:C:1720:LEU:HD23	2.06	0.55
1:A:1318:ARG:NH2	1:A:1537:GLU:OE1	2.38	0.55
1:A:1719:MET:O	1:A:1720:LEU:HD23	2.06	0.55
1:C:1008:PHE:HB3	1:C:1080:LEU:HD13	1.87	0.55
1:C:2018:GLN:OE1	1:B:2211:SER:OG	2.24	0.55
1:C:2391:GLN:HB2	1:C:2397:ASP:HB2	1.88	0.55
1:A:1522:ALA:HA	1:A:1525:LYS:HD3	1.88	0.55
1:C:2390:LEU:HD11	1:C:2449:PHE:CE2	2.42	0.55
1:C:2407:ARG:HD3	1:C:2426:PHE:HE2	1.71	0.55
1:C:992:GLU:HG3	1:C:1291:LEU:CD2	2.36	0.55
1:B:1008:PHE:HB3	1:B:1080:LEU:HD13	1.88	0.55
1:C:1165:VAL:HG22	1:C:1289:PHE:HB3	1.87	0.55
1:C:2308:LEU:HD13	1:C:2354:LEU:HB3	1.89	0.55
1:A:992:GLU:HG3	1:A:1291:LEU:CD2	2.36	0.55
1:B:992:GLU:HG3	1:B:1291:LEU:CD2	2.36	0.55
1:B:1165:VAL:HG22	1:B:1289:PHE:HB3	1.87	0.55
1:A:1315:GLN:NE2	1:A:1537:GLU:HB2	2.21	0.55
1:B:1150:LEU:HD11	1:B:1154:LYS:HE3	1.88	0.55
1:B:1522:ALA:HA	1:B:1525:LYS:HD3	1.88	0.55
1:B:2390:LEU:HD11	1:B:2449:PHE:CE2	2.42	0.55
1:C:1522:ALA:HA	1:C:1525:LYS:HD3	1.89	0.55
1:C:1969:LYS:HD3	1:C:1970:TYR:N	2.22	0.54
1:B:1969:LYS:HD3	1:B:1970:TYR:N	2.22	0.54
1:B:2308:LEU:HD13	1:B:2354:LEU:HB3	1.89	0.54
1:A:2391:GLN:HB2	1:A:2397:ASP:HB2	1.88	0.54
1:C:1001:VAL:HG21	1:C:1013:HIS:ND1	2.22	0.54
1:C:1150:LEU:HD11	1:C:1154:LYS:HE3	1.89	0.54
1:A:1138:ASN:ND2	1:A:1141:PRO:HB3	2.22	0.54
1:A:1150:LEU:HD11	1:A:1154:LYS:HE3	1.89	0.54
1:A:2192:GLY:HA3	1:B:2141:VAL:HG21	1.88	0.54
1:A:2349:THR:HA	1:A:2352:ARG:HH22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1701:VAL:HG12	1:C:1784:LYS:HD3	1.89	0.54
1:A:2308:LEU:HD13	1:A:2354:LEU:HB3	1.89	0.54
1:C:1138:ASN:ND2	1:C:1141:PRO:HB3	2.22	0.54
1:B:1170:PHE:CD1	1:B:1787:LEU:HD13	2.43	0.54
1:A:2485:PHE:CD2	1:B:2153:MET:HE2	2.42	0.54
1:A:1170:PHE:CD1	1:A:1787:LEU:HD13	2.42	0.54
1:A:1969:LYS:HD3	1:A:1970:TYR:N	2.22	0.54
1:A:2523:GLU:OE2	1:C:2180:GLY:HA2	2.07	0.54
1:C:2494:PHE:HD2	1:B:2490:HIS:HD1	1.52	0.54
1:B:1551:VAL:HG22	1:B:1554:GLY:H	1.73	0.54
1:B:1701:VAL:HG12	1:B:1784:LYS:HD3	1.89	0.54
1:B:2349:THR:HA	1:B:2352:ARG:HH22	1.71	0.54
1:C:1170:PHE:CD1	1:C:1787:LEU:HD13	2.42	0.54
1:B:2368:ILE:HD12	1:B:2403:ILE:HD12	1.90	0.54
2:E:227:CYS:SG	2:E:228:GLU:N	2.81	0.54
1:B:1001:VAL:HG21	1:B:1013:HIS:ND1	2.22	0.54
1:A:2184:LYS:HB2	1:A:2187:VAL:HG12	1.89	0.54
1:A:2290:SER:O	1:A:2290:SER:OG	2.25	0.54
1:C:1141:PRO:O	1:C:1143:PHE:N	2.40	0.54
1:C:2184:LYS:HB2	1:C:2187:VAL:HG12	1.89	0.54
1:C:2402:ARG:N	1:C:2433:GLU:O	2.25	0.54
1:A:1001:VAL:HG21	1:A:1013:HIS:ND1	2.22	0.54
1:C:1044:LEU:HB3	1:C:1101:LEU:HD13	1.90	0.54
1:B:1719:MET:O	1:B:1720:LEU:HD23	2.06	0.54
1:A:2104:ARG:HD3	1:A:2515:GLU:OE1	2.08	0.53
1:C:1551:VAL:HG22	1:C:1554:GLY:H	1.73	0.53
1:C:2497:LEU:HD23	1:C:2543:THR:HG21	1.90	0.53
1:B:1008:PHE:HB2	1:B:1079:TRP:CH2	2.44	0.53
1:B:2391:GLN:HB2	1:B:2397:ASP:HB2	1.88	0.53
1:A:1141:PRO:O	1:A:1143:PHE:N	2.40	0.53
1:A:1551:VAL:HG22	1:A:1554:GLY:H	1.73	0.53
1:A:1701:VAL:HG12	1:A:1784:LYS:HD3	1.89	0.53
1:A:2204:TRP:CE2	1:B:2025:LEU:HD12	2.43	0.53
1:B:2497:LEU:HD23	1:B:2543:THR:HG21	1.90	0.53
2:F:227:CYS:SG	2:F:228:GLU:N	2.81	0.53
1:A:1008:PHE:HB2	1:A:1079:TRP:CH2	2.44	0.53
1:C:1029:ILE:CA	1:C:1033:TRP:HD1	2.19	0.53
1:B:1184:TYR:OH	1:B:1217:ASN:OD1	2.26	0.53
1:B:1771:PRO:O	1:B:1775:GLY:N	2.42	0.53
1:B:2184:LYS:HB2	1:B:2187:VAL:HG12	1.89	0.53
1:B:1007:ASN:HD21	1:B:1009:MET:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1670:GLY:HA2	1:B:1674:ARG:HG3	1.91	0.53
1:B:2104:ARG:HD3	1:B:2515:GLU:OE1	2.08	0.53
2:D:227:CYS:SG	2:D:228:GLU:N	2.81	0.53
1:C:1007:ASN:HD21	1:C:1009:MET:HB3	1.73	0.53
1:B:1699:HIS:NE2	1:B:2062:PHE:CE2	2.77	0.53
1:A:1044:LEU:HB3	1:A:1101:LEU:HD13	1.90	0.53
1:A:1184:TYR:OH	1:A:1217:ASN:OD1	2.26	0.53
1:A:2256:TYR:OH	1:A:2273:ILE:O	2.26	0.53
1:C:1020:ILE:HG23	1:C:1033:TRP:CZ3	2.44	0.53
1:C:1771:PRO:O	1:C:1775:GLY:N	2.42	0.53
1:C:2133:GLU:HG3	1:B:2485:PHE:HD2	1.74	0.53
1:B:1044:LEU:HB3	1:B:1101:LEU:HD13	1.90	0.53
1:B:1320:PHE:O	1:B:1324:ASN:ND2	2.42	0.53
1:B:2340:HIS:O	1:B:2340:HIS:ND1	2.42	0.53
1:A:1007:ASN:HD21	1:A:1009:MET:HB3	1.73	0.53
1:A:2040:ARG:NH2	1:A:2142:TRP:O	2.42	0.53
1:A:2544:ARG:NH1	1:B:1411:ASP:OD1	2.41	0.53
1:C:1008:PHE:HB2	1:C:1079:TRP:CH2	2.44	0.53
1:C:2340:HIS:O	1:C:2340:HIS:ND1	2.42	0.53
1:B:1138:ASN:ND2	1:B:1141:PRO:HB3	2.22	0.53
1:A:1699:HIS:NE2	1:A:2062:PHE:CE2	2.77	0.53
1:A:1771:PRO:O	1:A:1775:GLY:N	2.42	0.53
1:C:1320:PHE:O	1:C:1324:ASN:ND2	2.42	0.53
1:C:2368:ILE:HD12	1:C:2403:ILE:HD12	1.90	0.52
1:A:1320:PHE:O	1:A:1324:ASN:ND2	2.42	0.52
1:A:1403:HIS:HB2	1:C:2178:PRO:O	2.09	0.52
1:A:2368:ILE:HD12	1:A:2403:ILE:HD12	1.90	0.52
1:A:2497:LEU:HD23	1:A:2543:THR:HG21	1.90	0.52
1:C:1184:TYR:OH	1:C:1217:ASN:OD1	2.26	0.52
1:C:2040:ARG:NH2	1:C:2142:TRP:O	2.42	0.52
1:C:2464:TYR:HA	1:C:2467:VAL:HB	1.91	0.52
1:A:1142:ASN:HA	1:A:1304:HIS:CE1	2.45	0.52
1:A:1344:GLN:OE1	1:A:1347:ARG:NH2	2.35	0.52
1:B:2497:LEU:H	1:B:2497:LEU:HD12	1.74	0.52
1:B:2516:THR:O	1:B:2516:THR:HG22	2.10	0.52
1:B:1141:PRO:O	1:B:1143:PHE:N	2.40	0.52
1:B:2140:TRP:CD1	1:B:2145:THR:HG21	2.45	0.52
1:C:1409:SER:O	1:C:1409:SER:OG	2.22	0.52
1:C:1670:GLY:HA2	1:C:1674:ARG:HG3	1.91	0.52
1:C:2191:MET:CE	2:F:238:GLU:HB3	2.39	0.52
1:B:1533:VAL:O	1:B:1537:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1743:THR:HG22	1:B:1776:LEU:HD11	1.92	0.52
1:B:2464:TYR:HA	1:B:2467:VAL:HB	1.91	0.52
1:B:1020:ILE:HG23	1:B:1033:TRP:CZ3	2.44	0.52
1:B:2040:ARG:NH2	1:B:2142:TRP:O	2.42	0.52
1:A:1029:ILE:CA	1:A:1033:TRP:HD1	2.19	0.52
1:A:2231:LYS:NZ	1:B:2244:GLN:HE22	2.08	0.52
1:B:1029:ILE:CA	1:B:1033:TRP:HD1	2.18	0.52
1:B:1109:GLN:O	1:B:1113:ALA:CB	2.58	0.52
1:A:1020:ILE:HG23	1:A:1033:TRP:CZ3	2.44	0.52
1:C:1533:VAL:O	1:C:1537:GLU:HG3	2.10	0.52
1:C:1699:HIS:NE2	1:C:2062:PHE:CE2	2.77	0.52
1:C:2058:HIS:NE2	1:C:2083:TYR:OH	2.32	0.52
1:C:2104:ARG:HD3	1:C:2515:GLU:OE1	2.08	0.52
1:B:1724:ARG:HH22	1:B:1805:LEU:H	1.57	0.52
1:A:1670:GLY:HA2	1:A:1674:ARG:HG3	1.91	0.51
1:A:2140:TRP:CD1	1:A:2145:THR:HG21	2.45	0.51
1:A:2340:HIS:ND1	1:A:2340:HIS:O	2.42	0.51
1:A:2490:HIS:HA	1:B:2494:PHE:CE2	2.45	0.51
1:A:2497:LEU:HD12	1:A:2497:LEU:H	1.75	0.51
1:B:1035:ASN:O	1:B:1038:LEU:HB3	2.11	0.51
1:B:2290:SER:O	1:B:2290:SER:OG	2.25	0.51
1:C:1961:PHE:O	1:C:1965:ILE:HG13	2.11	0.51
1:C:2516:THR:HG22	1:C:2516:THR:O	2.09	0.51
1:B:1961:PHE:O	1:B:1965:ILE:HG13	2.11	0.51
1:B:2402:ARG:N	1:B:2433:GLU:O	2.25	0.51
1:C:1142:ASN:HA	1:C:1304:HIS:CE1	2.45	0.51
1:B:2256:TYR:OH	1:B:2273:ILE:O	2.26	0.51
1:A:1724:ARG:HH22	1:A:1805:LEU:H	1.57	0.51
1:A:2225:ASP:HB3	1:A:2324:GLN:HB3	1.92	0.51
1:C:984:PHE:HB3	1:C:987:TYR:HB3	1.93	0.51
1:A:984:PHE:HB3	1:A:987:TYR:HB3	1.93	0.51
1:A:2123:GLN:HG2	2:D:244:PHE:CD2	2.44	0.51
1:C:2497:LEU:HD12	1:C:2497:LEU:H	1.74	0.51
1:B:1142:ASN:HA	1:B:1304:HIS:CE1	2.45	0.51
1:A:2516:THR:HG22	1:A:2516:THR:O	2.09	0.51
1:C:1109:GLN:O	1:C:1113:ALA:CB	2.58	0.51
1:C:2140:TRP:CD1	1:C:2145:THR:HG21	2.45	0.51
1:C:2225:ASP:HB3	1:C:2324:GLN:HB3	1.92	0.51
1:A:1035:ASN:O	1:A:1038:LEU:HB3	2.11	0.51
1:A:1109:GLN:O	1:A:1113:ALA:CB	2.58	0.51
1:A:1533:VAL:O	1:A:1537:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:967:ARG:N	1:C:1120:GLN:HB3	2.26	0.51
1:C:973:ASP:O	1:C:976:SER:OG	2.22	0.51
1:A:1044:LEU:CB	1:A:1101:LEU:HD13	2.41	0.51
1:B:1736:PHE:CE2	1:B:1740:MET:HE2	2.46	0.51
1:A:1360:ARG:NH2	1:A:2524:GLU:OE2	2.44	0.51
1:A:1736:PHE:CE2	1:A:1740:MET:HE2	2.46	0.51
1:C:1736:PHE:CE2	1:C:1740:MET:HE2	2.46	0.51
1:B:967:ARG:N	1:B:1120:GLN:HB3	2.26	0.51
1:B:1360:ARG:NH2	1:B:2524:GLU:OE2	2.44	0.51
1:B:2148:SER:OG	1:B:2149:LEU:N	2.44	0.51
1:A:1743:THR:HG22	1:A:1776:LEU:HD11	1.92	0.51
1:C:1724:ARG:HH22	1:C:1805:LEU:H	1.57	0.51
1:C:2191:MET:HE1	2:F:239:CYS:N	2.26	0.51
1:B:984:PHE:HB3	1:B:987:TYR:HB3	1.93	0.51
1:B:2225:ASP:HB3	1:B:2324:GLN:HB3	1.92	0.51
1:A:1201:LYS:O	1:A:1206:GLN:NE2	2.44	0.50
1:A:1961:PHE:O	1:A:1965:ILE:HG13	2.10	0.50
1:A:2148:SER:OG	1:A:2149:LEU:N	2.44	0.50
1:C:1731:MET:HE3	1:C:1806:TRP:CZ2	2.43	0.50
1:B:1044:LEU:CB	1:B:1101:LEU:HD13	2.41	0.50
1:A:2464:TYR:HA	1:A:2467:VAL:HB	1.91	0.50
1:C:1360:ARG:NH2	1:C:2524:GLU:OE2	2.44	0.50
1:C:1743:THR:HG22	1:C:1776:LEU:HD11	1.92	0.50
1:B:1201:LYS:O	1:B:1206:GLN:NE2	2.44	0.50
1:A:967:ARG:N	1:A:1120:GLN:HB3	2.26	0.50
1:A:2490:HIS:ND1	1:B:2494:PHE:HD2	1.98	0.50
1:C:2227:THR:HB	1:C:2322:ASN:HB3	1.93	0.50
1:A:2235:TYR:HE1	1:A:2304:MET:HA	1.77	0.50
1:A:2409:GLN:NE2	1:A:2410:VAL:O	2.44	0.50
1:C:2256:TYR:OH	1:C:2273:ILE:O	2.26	0.50
1:A:2030:THR:HG23	1:A:2049:PHE:CZ	2.47	0.50
1:B:2235:TYR:HE1	1:B:2304:MET:HA	1.77	0.50
1:B:2373:PRO:HB3	1:B:2398:TYR:CE1	2.47	0.50
1:C:1035:ASN:O	1:C:1038:LEU:HB3	2.11	0.50
1:C:2235:TYR:HE1	1:C:2304:MET:HA	1.77	0.50
1:B:1651:ASP:O	1:B:1652:ARG:NH1	2.45	0.50
1:B:1731:MET:HE3	1:B:1806:TRP:CZ2	2.43	0.50
1:C:2409:GLN:NE2	1:C:2410:VAL:O	2.44	0.50
1:C:1044:LEU:CB	1:C:1101:LEU:HD13	2.41	0.49
1:B:1987:ASP:OD1	1:B:2082:TRP:NE1	2.45	0.49
1:A:1651:ASP:O	1:A:1652:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1987:ASP:OD1	1:A:2082:TRP:NE1	2.45	0.49
1:A:2244:GLN:HG2	1:A:2245:GLN:N	2.28	0.49
1:B:2244:GLN:HG2	1:B:2245:GLN:N	2.27	0.49
1:A:974:LEU:HG	1:A:975:LEU:HD12	1.94	0.49
1:C:2244:GLN:HG2	1:C:2245:GLN:N	2.28	0.49
1:C:2373:PRO:HB3	1:C:2398:TYR:CE1	2.47	0.49
1:B:2409:GLN:NE2	1:B:2410:VAL:O	2.44	0.49
1:C:2534:ARG:HG3	1:B:2493:MET:HA	1.93	0.49
1:A:2325:ARG:NH2	1:A:2379:PRO:O	2.46	0.49
1:A:2467:VAL:HG13	1:B:1996:TRP:CZ3	2.48	0.49
1:C:2030:THR:HG23	1:C:2049:PHE:CZ	2.47	0.49
1:B:2325:ARG:NH2	1:B:2379:PRO:O	2.46	0.49
1:A:1013:HIS:HE2	1:A:1047:GLN:NE2	2.10	0.49
1:A:1412:TYR:OH	1:C:2537:GLU:OE2	2.23	0.49
1:A:2227:THR:HB	1:A:2322:ASN:HB3	1.93	0.49
1:A:2373:PRO:HB3	1:A:2398:TYR:CE1	2.47	0.49
1:C:1651:ASP:O	1:C:1652:ARG:NH1	2.45	0.49
1:B:974:LEU:HG	1:B:975:LEU:HD12	1.94	0.49
1:B:1694:ILE:HG21	1:B:1789:GLN:HA	1.95	0.49
1:B:2227:THR:HB	1:B:2322:ASN:HB3	1.93	0.49
1:A:1074:SER:O	1:A:1077:ILE:HG22	2.13	0.49
1:C:1782:TYR:CE2	1:C:1783:ILE:HG23	2.48	0.49
1:C:2211:SER:O	1:C:2215:SER:OG	2.31	0.49
1:C:1016:TRP:CZ2	1:C:1043:PHE:HE2	2.31	0.49
1:C:1995:PHE:CZ	1:B:2211:SER:HB2	2.46	0.49
1:C:2325:ARG:NH2	1:C:2379:PRO:O	2.46	0.49
1:A:1016:TRP:CZ2	1:A:1043:PHE:HE2	2.31	0.48
1:C:974:LEU:HG	1:C:975:LEU:HD12	1.94	0.48
1:C:2133:GLU:OE1	1:B:2482:ARG:NE	2.29	0.48
1:C:2191:MET:HE1	2:F:238:GLU:C	2.38	0.48
1:B:1013:HIS:HE2	1:B:1047:GLN:NE2	2.10	0.48
1:B:1344:GLN:OE1	1:B:1347:ARG:NH2	2.35	0.48
1:B:2485:PHE:HE1	2:E:242:LEU:HD11	1.78	0.48
1:C:1013:HIS:HE2	1:C:1047:GLN:NE2	2.10	0.48
1:C:1026:ARG:O	1:C:1029:ILE:HB	2.13	0.48
1:C:1987:ASP:OD1	1:C:2082:TRP:NE1	2.46	0.48
1:C:2393:ASP:C	1:C:2395:GLU:H	2.21	0.48
1:B:1026:ARG:O	1:B:1029:ILE:HB	2.13	0.48
1:B:1074:SER:O	1:B:1077:ILE:HG22	2.13	0.48
1:B:2295:ARG:HD3	1:B:2295:ARG:HA	1.63	0.48
1:A:1782:TYR:CE2	1:A:1783:ILE:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2191:MET:HE1	2:D:238:GLU:C	2.38	0.48
1:C:1074:SER:O	1:C:1077:ILE:HG22	2.13	0.48
1:B:1521:ARG:HB3	1:B:1528:ARG:NH2	2.28	0.48
1:A:1031:ARG:HD2	1:A:1032:LEU:HB2	1.95	0.48
1:C:2130:PHE:HA	1:C:2133:GLU:OE2	2.13	0.48
1:B:1142:ASN:HA	1:B:1304:HIS:NE2	2.29	0.48
1:A:2130:PHE:HA	1:A:2133:GLU:OE2	2.14	0.48
1:C:1362:SER:O	1:C:1365:SER:OG	2.31	0.48
1:C:1406:VAL:HG21	1:B:2179:LYS:HE2	1.94	0.48
1:C:1521:ARG:HB3	1:C:1528:ARG:NH2	2.28	0.48
1:C:2148:SER:OG	1:C:2149:LEU:N	2.44	0.48
1:B:1362:SER:O	1:B:1365:SER:OG	2.31	0.48
1:B:1787:LEU:O	1:B:1791:MET:HG2	2.14	0.48
1:A:1694:ILE:HG21	1:A:1789:GLN:HA	1.95	0.48
1:A:2281:ILE:HD13	1:A:2449:PHE:CE1	2.49	0.48
1:C:1189:PHE:HZ	1:C:1741:VAL:HG11	1.79	0.48
1:C:1344:GLN:OE1	1:C:1347:ARG:NH2	2.35	0.48
1:B:1159:ARG:HG2	1:B:1160:TYR:HD1	1.77	0.48
1:B:1198:LEU:HD11	1:B:1209:LEU:HD23	1.96	0.48
1:A:1026:ARG:O	1:A:1029:ILE:HB	2.13	0.48
1:C:1142:ASN:HA	1:C:1304:HIS:NE2	2.29	0.48
1:C:1198:LEU:HD11	1:C:1209:LEU:HD23	1.96	0.48
1:C:1791:MET:HE3	1:C:1791:MET:HA	1.96	0.48
1:B:2244:GLN:HG2	1:B:2245:GLN:H	1.79	0.48
1:A:1521:ARG:HB3	1:A:1528:ARG:NH2	2.28	0.48
1:A:2295:ARG:HD3	1:A:2295:ARG:HA	1.63	0.48
1:C:1694:ILE:HG21	1:C:1789:GLN:HA	1.95	0.48
1:A:1142:ASN:HA	1:A:1304:HIS:NE2	2.29	0.48
1:B:1214:ILE:HG12	1:B:1290:LEU:HG	1.96	0.48
1:A:2261:GLN:HA	1:A:2264:ASP:OD1	2.14	0.47
1:B:1699:HIS:NE2	1:B:2062:PHE:HE2	2.12	0.47
1:B:1791:MET:HE3	1:B:1791:MET:HA	1.96	0.47
1:B:2130:PHE:HA	1:B:2133:GLU:OE2	2.13	0.47
1:B:2211:SER:O	1:B:2215:SER:OG	2.31	0.47
1:A:2352:ARG:NH1	1:A:2352:ARG:HB3	2.29	0.47
1:C:1787:LEU:O	1:C:1791:MET:HG2	2.14	0.47
1:C:2261:GLN:HA	1:C:2264:ASP:OD1	2.14	0.47
1:B:1143:PHE:HZ	1:B:1301:TYR:CD2	2.32	0.47
1:B:1189:PHE:HZ	1:B:1741:VAL:HG11	1.79	0.47
1:A:2393:ASP:C	1:A:2395:GLU:H	2.22	0.47
1:A:2467:VAL:HG22	1:B:1996:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1699:HIS:NE2	1:A:2062:PHE:HE2	2.13	0.47
1:A:2492:ILE:HD11	1:B:2530:ILE:CD1	2.42	0.47
1:C:2281:ILE:HD13	1:C:2449:PHE:CE1	2.49	0.47
1:B:1016:TRP:CZ2	1:B:1043:PHE:HE2	2.31	0.47
1:B:1179:ILE:HG23	1:B:1179:ILE:O	2.15	0.47
1:B:1329:LYS:HD3	1:B:1649:LEU:HD12	1.96	0.47
1:B:1782:TYR:CE2	1:B:1783:ILE:HG23	2.48	0.47
1:A:1143:PHE:HZ	1:A:1301:TYR:CD2	2.32	0.47
1:A:1170:PHE:HB2	1:A:1188:CYS:SG	2.55	0.47
1:A:1179:ILE:HG23	1:A:1179:ILE:O	2.14	0.47
1:A:1538:ARG:O	1:A:1542:THR:HG23	2.15	0.47
1:A:1787:LEU:O	1:A:1791:MET:HG2	2.14	0.47
1:A:1791:MET:HE3	1:A:1791:MET:HA	1.96	0.47
1:C:1031:ARG:HD2	1:C:1032:LEU:HB2	1.96	0.47
1:C:1170:PHE:HB2	1:C:1188:CYS:SG	2.55	0.47
1:C:2244:GLN:HG2	1:C:2245:GLN:H	1.79	0.47
1:C:2352:ARG:NH1	1:C:2352:ARG:HB3	2.29	0.47
1:B:2462:ALA:HA	1:B:2466:ILE:HG22	1.96	0.47
1:A:1159:ARG:HG2	1:A:1160:TYR:HD1	1.77	0.47
1:A:1198:LEU:HD11	1:A:1209:LEU:HD23	1.96	0.47
1:A:1329:LYS:HD3	1:A:1649:LEU:HD12	1.97	0.47
1:B:1031:ARG:HD2	1:B:1032:LEU:HB2	1.95	0.47
1:B:1744:LYS:HB2	1:B:1744:LYS:HE2	1.74	0.47
1:B:2030:THR:HG23	1:B:2049:PHE:CZ	2.47	0.47
1:B:2281:ILE:HD13	1:B:2449:PHE:CE1	2.49	0.47
1:A:1214:ILE:HG12	1:A:1290:LEU:HG	1.97	0.47
1:A:1731:MET:HE3	1:A:1806:TRP:CZ2	2.43	0.47
1:A:2131:LEU:HA	1:A:2131:LEU:HD23	1.69	0.47
1:C:987:TYR:OH	1:C:1119:TRP:HA	2.15	0.47
1:C:1179:ILE:O	1:C:1179:ILE:HG23	2.14	0.47
1:C:1200:GLN:HE22	1:C:1309:LEU:HB3	1.80	0.47
1:C:1329:LYS:HD3	1:C:1649:LEU:HD12	1.97	0.47
1:C:1699:HIS:NE2	1:C:2062:PHE:HE2	2.13	0.47
1:C:2410:VAL:H	1:C:2426:PHE:HB3	1.80	0.47
1:C:2462:ALA:HA	1:C:2466:ILE:HG22	1.96	0.47
1:B:1716:LEU:HA	1:B:1716:LEU:HD23	1.63	0.47
1:B:2131:LEU:O	1:B:2135:ARG:HB3	2.15	0.47
1:B:2187:VAL:HG23	2:E:235:ILE:HG12	1.97	0.47
1:B:2261:GLN:HA	1:B:2264:ASP:OD1	2.14	0.47
1:B:2352:ARG:HB3	1:B:2352:ARG:NH1	2.29	0.47
1:B:2410:VAL:H	1:B:2426:PHE:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:PHE:HZ	1:A:1741:VAL:HG11	1.79	0.47
1:A:2462:ALA:HA	1:A:2466:ILE:HG22	1.96	0.47
1:C:1200:GLN:NE2	1:C:1309:LEU:HB3	2.30	0.47
1:A:2211:SER:O	1:A:2215:SER:OG	2.31	0.47
1:B:1170:PHE:HB2	1:B:1188:CYS:SG	2.55	0.47
1:B:2393:ASP:C	1:B:2395:GLU:H	2.22	0.47
1:B:2440:ASP:OD1	1:B:2440:ASP:N	2.48	0.47
1:A:1200:GLN:NE2	1:A:1309:LEU:HB3	2.30	0.46
1:A:1362:SER:O	1:A:1365:SER:OG	2.31	0.46
1:C:1020:ILE:HA	1:C:1033:TRP:CH2	2.48	0.46
1:C:2502:ARG:HH21	1:C:2546:ARG:HD3	1.80	0.46
1:B:987:TYR:OH	1:B:1119:TRP:HA	2.15	0.46
1:B:1200:GLN:NE2	1:B:1309:LEU:HB3	2.30	0.46
1:A:2244:GLN:HG2	1:A:2245:GLN:H	1.79	0.46
1:C:1538:ARG:O	1:C:1542:THR:HG23	2.15	0.46
1:C:2133:GLU:HG3	1:B:2485:PHE:CD2	2.49	0.46
1:C:2485:PHE:HE1	2:F:242:LEU:HD11	1.80	0.46
1:B:1538:ARG:O	1:B:1542:THR:HG23	2.15	0.46
1:B:1699:HIS:ND1	1:B:1707:SER:O	2.48	0.46
1:A:1744:LYS:HB2	1:A:1744:LYS:HE2	1.73	0.46
1:A:2534:ARG:O	1:C:2540:ILE:HD11	2.15	0.46
1:C:2219:VAL:N	1:C:2453:VAL:O	2.47	0.46
1:A:973:ASP:O	1:A:976:SER:OG	2.22	0.46
1:A:2131:LEU:O	1:A:2135:ARG:HB3	2.15	0.46
1:A:2219:VAL:N	1:A:2453:VAL:O	2.47	0.46
1:A:2440:ASP:HB2	1:A:2443:LEU:HB2	1.98	0.46
1:C:1214:ILE:HG12	1:C:1290:LEU:HG	1.97	0.46
1:C:2440:ASP:HB2	1:C:2443:LEU:HB2	1.98	0.46
1:B:987:TYR:HA	1:B:1110:VAL:HG11	1.98	0.46
1:A:987:TYR:OH	1:A:1119:TRP:HA	2.15	0.46
1:A:2033:ILE:O	1:A:2037:LEU:HD23	2.16	0.46
1:C:1143:PHE:HZ	1:C:1301:TYR:CD2	2.32	0.46
1:B:2140:TRP:CE3	1:B:2149:LEU:HD13	2.51	0.46
1:A:1724:ARG:HH22	1:A:1805:LEU:N	2.14	0.46
1:A:2245:GLN:HB3	1:A:2246:PRO:CD	2.46	0.46
1:B:1724:ARG:HH22	1:B:1805:LEU:N	2.14	0.46
1:A:1524:THR:HG21	1:A:1682:CYS:HA	1.98	0.46
1:A:2410:VAL:H	1:A:2426:PHE:HB3	1.80	0.46
1:A:2425:ASP:HB3	1:A:2426:PHE:HD1	1.81	0.46
1:C:1159:ARG:HG2	1:C:1160:TYR:HD1	1.77	0.46
1:C:1201:LYS:O	1:C:1206:GLN:NE2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1699:HIS:ND1	1:C:1707:SER:O	2.48	0.46
1:C:2140:TRP:CE3	1:C:2149:LEU:HD13	2.51	0.46
1:C:2425:ASP:HB3	1:C:2426:PHE:HD1	1.81	0.46
1:C:2131:LEU:O	1:C:2135:ARG:HB3	2.15	0.46
1:A:1699:HIS:ND1	1:A:1707:SER:O	2.48	0.46
1:A:2224:ILE:HD13	1:A:2326:ASP:HB3	1.98	0.46
1:A:2490:HIS:ND1	1:B:2494:PHE:CD2	2.62	0.46
1:A:2516:THR:O	1:A:2518:GLU:N	2.49	0.46
1:C:2290:SER:O	1:C:2290:SER:OG	2.25	0.46
1:B:1984:ASP:HB3	1:B:2031:MET:CE	2.45	0.46
1:B:2149:LEU:HA	1:B:2149:LEU:HD12	1.69	0.46
1:B:2516:THR:O	1:B:2518:GLU:N	2.49	0.46
1:B:2516:THR:C	1:B:2518:GLU:H	2.24	0.46
1:A:2498:PRO:HD3	1:B:2534:ARG:NH2	2.31	0.45
1:C:1984:ASP:HB3	1:C:2031:MET:CE	2.45	0.45
1:C:2033:ILE:O	1:C:2037:LEU:HD23	2.16	0.45
1:C:2442:ASN:OD1	1:C:2442:ASN:N	2.49	0.45
1:B:1232:CYS:SG	1:B:1233:VAL:HG23	2.57	0.45
1:B:1524:THR:HG21	1:B:1682:CYS:HA	1.98	0.45
1:B:1670:GLY:O	1:B:1674:ARG:NH2	2.49	0.45
1:B:2502:ARG:HH21	1:B:2546:ARG:HD3	1.80	0.45
1:A:1191:LEU:HD23	1:A:1191:LEU:HA	1.79	0.45
1:C:1969:LYS:HD3	1:C:1970:TYR:C	2.42	0.45
1:B:1200:GLN:HE22	1:B:1309:LEU:HB3	1.80	0.45
1:B:1328:LEU:HD23	1:B:1328:LEU:HA	1.85	0.45
1:A:1008:PHE:HB2	1:A:1079:TRP:CZ3	2.51	0.45
1:A:2502:ARG:HH21	1:A:2546:ARG:HD3	1.80	0.45
1:C:998:ALA:O	1:C:1001:VAL:HG22	2.17	0.45
1:C:1217:ASN:O	1:C:1220:VAL:HG12	2.17	0.45
1:C:2516:THR:O	1:C:2518:GLU:N	2.49	0.45
1:B:2245:GLN:HB3	1:B:2246:PRO:CD	2.46	0.45
1:A:2516:THR:C	1:A:2518:GLU:H	2.24	0.45
1:C:1008:PHE:HB2	1:C:1079:TRP:CZ3	2.51	0.45
1:C:1189:PHE:CD1	1:C:1738:GLU:HG3	2.52	0.45
1:C:1724:ARG:HH22	1:C:1805:LEU:N	2.14	0.45
1:A:1189:PHE:CD1	1:A:1738:GLU:HG3	2.51	0.45
1:A:1670:GLY:O	1:A:1674:ARG:NH2	2.49	0.45
1:A:1969:LYS:HD3	1:A:1970:TYR:C	2.41	0.45
1:B:1969:LYS:HD3	1:B:1970:TYR:C	2.42	0.45
1:B:2207:LEU:HD12	1:B:2207:LEU:HA	1.77	0.45
1:B:2440:ASP:HB2	1:B:2443:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:LYS:HD3	1:A:988:LYS:HA	1.76	0.45
1:A:998:ALA:O	1:A:1001:VAL:HG22	2.17	0.45
1:A:1984:ASP:CB	1:A:2031:MET:HE2	2.46	0.45
1:A:2140:TRP:CE3	1:A:2149:LEU:HD13	2.51	0.45
1:A:2429:TRP:CE2	1:C:2297:SER:HB2	2.52	0.45
1:C:987:TYR:HA	1:C:1110:VAL:HG11	1.98	0.45
1:B:2425:ASP:HB3	1:B:2426:PHE:HD1	1.81	0.45
1:A:1227:LEU:HD23	1:A:1227:LEU:HA	1.80	0.45
1:C:1670:GLY:O	1:C:1674:ARG:NH2	2.50	0.45
1:B:1008:PHE:HB2	1:B:1079:TRP:CZ3	2.51	0.45
1:B:1189:PHE:CD1	1:B:1738:GLU:HG3	2.51	0.45
1:B:1217:ASN:O	1:B:1220:VAL:HG12	2.17	0.45
1:A:1027:GLU:HG2	1:A:1028:ALA:N	2.32	0.45
1:C:1232:CYS:SG	1:C:1233:VAL:HG23	2.57	0.45
1:C:2245:GLN:HB3	1:C:2246:PRO:CD	2.46	0.45
1:A:987:TYR:HA	1:A:1110:VAL:HG11	1.98	0.45
1:C:2191:MET:HG3	1:C:2195:ILE:HD12	1.99	0.45
1:C:2516:THR:C	1:C:2518:GLU:H	2.24	0.45
1:B:2224:ILE:HD13	1:B:2326:ASP:HB3	1.98	0.45
1:A:2434:LEU:HB2	1:A:2437:CYS:SG	2.57	0.45
1:C:1774:LEU:HD12	1:C:1774:LEU:HA	1.70	0.45
1:B:1349:MET:HE1	1:B:2516:THR:HB	1.99	0.45
1:B:2434:LEU:HB2	1:B:2437:CYS:SG	2.57	0.45
1:C:1170:PHE:CE1	1:C:1787:LEU:HB2	2.52	0.44
1:B:998:ALA:O	1:B:1002:ILE:HG12	2.17	0.44
1:B:1020:ILE:HA	1:B:1033:TRP:CH2	2.48	0.44
1:B:1191:LEU:HD23	1:B:1191:LEU:HA	1.79	0.44
1:B:2033:ILE:O	1:B:2037:LEU:HD23	2.16	0.44
1:B:2035:ARG:HH12	1:B:2109:PHE:HZ	1.65	0.44
2:F:228:GLU:HG2	2:F:229:SER:H	1.82	0.44
1:A:1349:MET:HE1	1:A:2516:THR:HB	1.99	0.44
1:A:2245:GLN:OE1	1:A:2245:GLN:HA	2.18	0.44
1:C:1007:ASN:HB2	1:C:1079:TRP:O	2.18	0.44
1:C:1349:MET:HE1	1:C:2516:THR:HB	1.99	0.44
1:B:2058:HIS:NE2	1:B:2083:TYR:OH	2.32	0.44
1:A:1200:GLN:HE22	1:A:1309:LEU:HB3	1.80	0.44
1:A:1411:ASP:HB3	1:A:1413:PHE:CD2	2.53	0.44
1:A:1984:ASP:HB3	1:A:2031:MET:CE	2.45	0.44
1:C:1282:TRP:HA	1:C:1285:ILE:HG22	1.99	0.44
1:C:2245:GLN:OE1	1:C:2245:GLN:HA	2.17	0.44
1:C:2443:LEU:HD23	1:C:2443:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2165:ILE:HD11	2:E:245:SER:OG	2.17	0.44
1:B:2184:LYS:NZ	2:E:231:ASP:OD1	2.31	0.44
1:A:1701:VAL:CG1	1:A:1784:LYS:HD3	2.48	0.44
1:C:1027:GLU:HG2	1:C:1028:ALA:N	2.32	0.44
1:C:1524:THR:HG21	1:C:1682:CYS:HA	1.98	0.44
1:C:2434:LEU:HB2	1:C:2437:CYS:SG	2.57	0.44
1:B:1217:ASN:HA	1:B:1220:VAL:HG12	1.99	0.44
1:B:1411:ASP:HB3	1:B:1413:PHE:CD2	2.53	0.44
1:A:1217:ASN:HA	1:A:1220:VAL:HG12	1.99	0.44
1:A:2442:ASN:OD1	1:A:2442:ASN:N	2.50	0.44
1:B:1027:GLU:HG2	1:B:1028:ALA:N	2.32	0.44
1:B:2388:LYS:HB3	1:B:2389:GLN:NE2	2.32	0.44
1:A:1232:CYS:SG	1:A:1233:VAL:HG23	2.57	0.44
1:A:1774:LEU:HD12	1:A:1774:LEU:HA	1.71	0.44
1:A:2191:MET:HG3	1:A:2195:ILE:HD12	1.99	0.44
1:B:1322:LEU:HD22	1:B:1530:MET:HG3	1.99	0.44
1:B:2108:ASN:HB3	1:B:2111:THR:CG2	2.47	0.44
1:B:2191:MET:HG3	1:B:2195:ILE:HD12	1.99	0.44
1:B:2219:VAL:N	1:B:2453:VAL:O	2.47	0.44
2:E:228:GLU:HG2	2:E:229:SER:H	1.82	0.44
1:A:2519:LEU:HD23	1:A:2519:LEU:HA	1.77	0.44
1:C:2224:ILE:HD13	1:C:2326:ASP:HB3	1.99	0.44
1:B:1080:LEU:HG	1:B:1082:LEU:HD23	2.00	0.44
1:A:1217:ASN:O	1:A:1220:VAL:HG12	2.17	0.44
1:A:1322:LEU:HD22	1:A:1530:MET:HG3	1.99	0.44
1:C:998:ALA:O	1:C:1002:ILE:HG12	2.18	0.44
1:C:2388:LYS:HB3	1:C:2389:GLN:NE2	2.33	0.44
2:D:228:GLU:HG2	2:D:229:SER:H	1.82	0.44
1:A:2035:ARG:HH12	1:A:2109:PHE:HZ	1.65	0.44
1:C:1217:ASN:HA	1:C:1220:VAL:HG12	1.99	0.44
1:C:1716:LEU:HD23	1:C:1716:LEU:HA	1.63	0.44
1:C:2436:ASP:OD1	1:C:2436:ASP:N	2.51	0.44
1:B:998:ALA:O	1:B:1001:VAL:HG22	2.17	0.44
1:B:1243:CYS:O	1:B:1246:ILE:HG22	2.18	0.44
1:B:1984:ASP:CB	1:B:2031:MET:HE2	2.46	0.44
1:A:998:ALA:O	1:A:1002:ILE:HG12	2.18	0.43
1:A:1007:ASN:HB2	1:A:1079:TRP:O	2.18	0.43
1:A:1080:LEU:HG	1:A:1082:LEU:HD23	2.00	0.43
1:A:1170:PHE:CE1	1:A:1787:LEU:HB2	2.52	0.43
1:A:1243:CYS:O	1:A:1246:ILE:HG22	2.18	0.43
1:A:1971:ARG:HD2	1:A:2098:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1411:ASP:HB3	1:C:1413:PHE:CD2	2.53	0.43
1:B:973:ASP:O	1:B:976:SER:OG	2.22	0.43
1:B:1701:VAL:CG1	1:B:1784:LYS:HD3	2.48	0.43
1:B:2228:VAL:HG21	1:B:2286:ILE:HD13	2.00	0.43
1:A:2137:VAL:O	1:A:2141:VAL:HG23	2.18	0.43
1:A:2541:LYS:O	1:A:2541:LYS:HG2	2.18	0.43
1:C:2352:ARG:HB3	1:C:2352:ARG:CZ	2.48	0.43
1:B:1170:PHE:CE1	1:B:1787:LEU:HB2	2.53	0.43
1:B:2436:ASP:OD1	1:B:2436:ASP:N	2.51	0.43
1:A:1552:ARG:HD3	1:A:1553:ARG:HH22	1.83	0.43
1:A:2062:PHE:O	1:A:2066:PRO:HG2	2.19	0.43
1:A:2276:TYR:CE1	1:A:2449:PHE:HB3	2.54	0.43
1:C:2228:VAL:HG21	1:C:2286:ILE:HD13	2.00	0.43
1:B:1007:ASN:HB2	1:B:1079:TRP:O	2.18	0.43
1:A:2228:VAL:HG21	1:A:2286:ILE:HD13	2.00	0.43
1:A:2238:LEU:HD23	1:A:2430:TRP:CD2	2.54	0.43
1:C:2276:TYR:CE1	1:C:2449:PHE:HB3	2.54	0.43
1:B:1282:TRP:HA	1:B:1285:ILE:HG22	1.99	0.43
1:B:2442:ASN:OD1	1:B:2442:ASN:N	2.49	0.43
1:A:1097:ASP:OD1	1:A:1098:PHE:N	2.52	0.43
1:A:2191:MET:HE1	2:D:238:GLU:CB	2.42	0.43
1:A:2529:LEU:HA	1:A:2529:LEU:HD12	1.81	0.43
1:C:1335:ARG:HH22	1:C:1971:ARG:H	1.67	0.43
1:B:1204:ARG:HA	1:B:1204:ARG:HD2	1.88	0.43
1:B:2062:PHE:O	1:B:2066:PRO:HG2	2.18	0.43
1:A:2371:LEU:N	1:A:2399:LEU:O	2.47	0.43
1:A:2388:LYS:HB3	1:A:2389:GLN:NE2	2.33	0.43
1:C:2153:MET:HE2	1:B:2485:PHE:CG	2.53	0.43
1:B:2238:LEU:HD23	1:B:2430:TRP:CD2	2.54	0.43
1:B:2245:GLN:HA	1:B:2245:GLN:OE1	2.17	0.43
1:B:2352:ARG:HB3	1:B:2352:ARG:CZ	2.48	0.43
1:A:2280:ASP:O	1:A:2450:SER:OG	2.37	0.43
1:C:1552:ARG:HD3	1:C:1553:ARG:HH22	1.83	0.43
1:B:1097:ASP:OD1	1:B:1098:PHE:N	2.52	0.43
1:B:1971:ARG:HD2	1:B:2098:ARG:O	2.19	0.43
1:B:2361:ARG:HH11	1:B:2364:GLN:CD	2.27	0.43
1:A:1744:LYS:NZ	1:A:1775:GLY:O	2.52	0.43
1:A:2343:GLU:O	1:A:2344:LEU:HD23	2.19	0.43
1:C:1243:CYS:O	1:C:1246:ILE:HG22	2.18	0.43
1:C:1971:ARG:HD2	1:C:2098:ARG:O	2.18	0.43
1:C:2244:GLN:N	1:C:2244:GLN:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2525:LEU:HA	1:B:2525:LEU:HD23	1.76	0.43
1:A:1020:ILE:HA	1:A:1033:TRP:CH2	2.48	0.43
1:A:2361:ARG:HH11	1:A:2364:GLN:CD	2.27	0.43
1:C:1331:ILE:HD13	1:C:1331:ILE:HA	1.89	0.43
1:C:1540:LEU:HA	1:C:1543:GLN:HG2	2.01	0.43
1:C:1985:ILE:HD13	1:C:1985:ILE:HA	1.92	0.43
1:C:2062:PHE:O	1:C:2066:PRO:HG2	2.19	0.43
1:C:2092:LEU:HD23	1:C:2092:LEU:HA	1.76	0.43
1:C:2380:ASN:OD1	1:C:2453:VAL:HG22	2.19	0.43
1:B:970:LEU:HD12	1:B:977:CYS:HA	2.01	0.43
1:A:1991:ILE:HD11	1:A:2082:TRP:HE1	1.83	0.43
1:A:2149:LEU:HD12	1:A:2149:LEU:HA	1.70	0.43
1:A:2179:LYS:HA	1:B:1402:ASP:O	2.19	0.43
1:A:2467:VAL:HG22	1:B:1996:TRP:CD2	2.54	0.43
1:C:1080:LEU:HG	1:C:1082:LEU:HD23	2.00	0.43
1:C:1701:VAL:CG1	1:C:1784:LYS:HD3	2.48	0.43
1:C:2238:LEU:HD23	1:C:2430:TRP:CE3	2.54	0.43
1:B:1774:LEU:HA	1:B:1774:LEU:HD12	1.70	0.43
1:B:2137:VAL:O	1:B:2141:VAL:HG23	2.19	0.43
1:B:2238:LEU:HD23	1:B:2430:TRP:CE3	2.54	0.43
1:B:2244:GLN:OE1	1:B:2244:GLN:N	2.52	0.43
1:B:2276:TYR:CE1	1:B:2449:PHE:HB3	2.53	0.43
1:A:2238:LEU:HD23	1:A:2430:TRP:CE3	2.54	0.42
1:A:2244:GLN:N	1:A:2244:GLN:OE1	2.52	0.42
1:C:1322:LEU:HD22	1:C:1530:MET:HG3	2.00	0.42
1:C:2187:VAL:HG23	2:F:235:ILE:HG12	2.01	0.42
1:C:2238:LEU:HD23	1:C:2430:TRP:CD2	2.54	0.42
1:C:2343:GLU:O	1:C:2344:LEU:HD23	2.19	0.42
1:A:1282:TRP:HA	1:A:1285:ILE:HG22	1.99	0.42
1:A:2352:ARG:HB3	1:A:2352:ARG:CZ	2.48	0.42
1:C:1991:ILE:HD11	1:C:2082:TRP:HE1	1.83	0.42
1:C:2035:ARG:HH12	1:C:2109:PHE:HZ	1.65	0.42
1:C:2070:GLU:OE1	1:C:2075:GLN:HB2	2.19	0.42
1:C:2137:VAL:O	1:C:2141:VAL:HG23	2.19	0.42
1:C:2286:ILE:HG13	1:C:2444:LEU:HB2	2.01	0.42
1:B:1077:ILE:HD11	1:B:1083:PRO:HA	2.01	0.42
1:B:1338:GLU:OE1	1:B:2103:THR:HG22	2.20	0.42
1:B:1552:ARG:HD3	1:B:1553:ARG:HH22	1.83	0.42
1:B:1991:ILE:HD11	1:B:2082:TRP:HE1	1.83	0.42
1:B:2131:LEU:HA	1:B:2131:LEU:HD23	1.69	0.42
1:A:1338:GLU:OE1	1:A:2103:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:ILE:HD13	1:A:1992:ILE:HA	1.89	0.42
1:C:1097:ASP:OD1	1:C:1098:PHE:N	2.52	0.42
1:C:1191:LEU:HA	1:C:1191:LEU:HD23	1.79	0.42
1:C:2338:GLU:CG	1:C:2339:LYS:H	2.32	0.42
1:B:1173:GLY:HA3	1:B:1184:TYR:HB2	2.01	0.42
1:A:1335:ARG:HH22	1:A:1971:ARG:H	1.67	0.42
1:A:2053:LEU:HA	1:A:2053:LEU:HD12	1.81	0.42
1:A:2058:HIS:NE2	1:A:2083:TYR:OH	2.32	0.42
1:A:2133:GLU:CG	1:C:2485:PHE:CD2	3.01	0.42
1:C:2016:VAL:HG12	1:C:2017:PRO:HD3	2.02	0.42
1:B:2070:GLU:OE1	1:B:2075:GLN:HB2	2.19	0.42
1:A:2286:ILE:HG13	1:A:2444:LEU:HB2	2.02	0.42
1:C:1077:ILE:HD11	1:C:1083:PRO:HA	2.01	0.42
1:C:1147:ARG:HD3	1:C:1147:ARG:H	1.84	0.42
1:B:1530:MET:O	1:B:1534:LEU:HD23	2.20	0.42
1:B:2541:LYS:O	1:B:2541:LYS:HG2	2.18	0.42
1:A:1147:ARG:H	1:A:1147:ARG:HD3	1.84	0.42
1:C:1530:MET:O	1:C:1534:LEU:HD23	2.20	0.42
1:B:1147:ARG:H	1:B:1147:ARG:HD3	1.84	0.42
1:B:1334:HIS:HA	1:B:1337:ILE:HG22	2.02	0.42
1:A:1717:TRP:CD1	1:A:1717:TRP:C	2.98	0.42
1:A:2338:GLU:CG	1:A:2339:LYS:H	2.32	0.42
1:A:2485:PHE:HE1	2:D:242:LEU:HD11	1.84	0.42
1:C:970:LEU:HD12	1:C:977:CYS:HA	2.01	0.42
1:C:1717:TRP:CD1	1:C:1717:TRP:C	2.98	0.42
1:C:2047:LEU:HA	1:C:2097:ILE:HD13	2.02	0.42
1:C:2541:LYS:O	1:C:2541:LYS:HG2	2.18	0.42
1:B:2128:VAL:CG1	1:B:2131:LEU:HD12	2.49	0.42
1:A:1020:ILE:HG23	1:A:1033:TRP:CH2	2.55	0.42
1:C:1020:ILE:HG23	1:C:1033:TRP:CH2	2.55	0.42
1:C:2121:LEU:HD23	1:C:2121:LEU:HA	1.77	0.42
1:B:1992:ILE:HD13	1:B:1992:ILE:HA	1.89	0.42
1:B:2380:ASN:OD1	1:B:2453:VAL:HG22	2.19	0.42
1:A:1540:LEU:HA	1:A:1543:GLN:HG2	2.01	0.42
1:A:2016:VAL:HG12	1:A:2017:PRO:HD3	2.02	0.42
1:A:2070:GLU:OE1	1:A:2075:GLN:HB2	2.19	0.42
1:A:2380:ASN:OD1	1:A:2453:VAL:HG22	2.19	0.42
1:C:1173:GLY:HA3	1:C:1184:TYR:HB2	2.01	0.42
1:C:1326:ALA:N	1:C:1649:LEU:HD21	2.35	0.42
1:C:1553:ARG:HH11	1:C:1556:LEU:HD11	1.85	0.42
1:C:2405:LEU:HD12	1:C:2430:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1335:ARG:HH22	1:B:1971:ARG:H	1.67	0.42
1:B:2343:GLU:O	1:B:2344:LEU:HD23	2.19	0.42
1:A:2492:ILE:HD13	1:A:2492:ILE:HG21	1.85	0.42
1:C:1996:TRP:CZ3	1:B:2467:VAL:HG13	2.55	0.42
1:C:2361:ARG:HH11	1:C:2364:GLN:CD	2.27	0.42
1:B:1200:GLN:H	1:B:1200:GLN:HG2	1.72	0.42
1:B:1694:ILE:HD13	1:B:1694:ILE:HA	1.88	0.42
1:B:2016:VAL:HG12	1:B:2017:PRO:HD3	2.02	0.42
1:A:970:LEU:HD12	1:A:977:CYS:HA	2.01	0.41
1:A:1081:TYR:O	1:A:1082:LEU:HD22	2.20	0.41
1:A:2221:ASN:HB2	1:A:2453:VAL:HG23	2.02	0.41
1:A:2485:PHE:CD1	1:B:2153:MET:HE2	2.54	0.41
1:C:988:LYS:HD3	1:C:988:LYS:HA	1.76	0.41
1:B:1020:ILE:HG23	1:B:1033:TRP:CH2	2.55	0.41
1:B:2047:LEU:HA	1:B:2097:ILE:HD13	2.02	0.41
1:B:2221:ASN:HB2	1:B:2453:VAL:HG23	2.02	0.41
1:A:1047:GLN:HA	1:A:1050:LEU:HB2	2.02	0.41
1:A:1077:ILE:HD11	1:A:1083:PRO:HA	2.01	0.41
1:C:1338:GLU:OE1	1:C:2103:THR:HG22	2.19	0.41
1:B:1090:ASN:OD1	1:B:1091:SER:N	2.54	0.41
1:B:1553:ARG:HH11	1:B:1556:LEU:HD11	1.85	0.41
1:A:1090:ASN:OD1	1:A:1091:SER:N	2.53	0.41
1:A:1204:ARG:HD2	1:A:1204:ARG:HA	1.88	0.41
1:A:2204:TRP:CZ2	1:B:2025:LEU:HD12	2.55	0.41
1:A:2207:LEU:HD12	1:A:2207:LEU:HA	1.78	0.41
1:A:2354:LEU:HD23	1:A:2354:LEU:HA	1.91	0.41
1:C:2089:TYR:CD2	1:C:2089:TYR:C	2.98	0.41
1:B:1540:LEU:HA	1:B:1543:GLN:HG2	2.01	0.41
1:B:2467:VAL:O	1:B:2471:VAL:HG12	2.20	0.41
1:A:1326:ALA:N	1:A:1649:LEU:HD21	2.35	0.41
1:A:2405:LEU:HD12	1:A:2430:TRP:CE2	2.55	0.41
1:A:2429:TRP:HZ2	1:C:2299:PRO:HG2	1.85	0.41
1:C:1207:LEU:HD13	1:C:1207:LEU:HA	1.91	0.41
1:B:1047:GLN:HA	1:B:1050:LEU:HB2	2.02	0.41
1:B:1326:ALA:N	1:B:1649:LEU:HD21	2.35	0.41
1:B:1783:ILE:HG13	1:B:1783:ILE:O	2.21	0.41
1:B:2089:TYR:CD2	1:B:2089:TYR:C	2.98	0.41
1:B:2349:THR:HA	1:B:2352:ARG:NH2	2.35	0.41
1:B:2443:LEU:HA	1:B:2443:LEU:HD23	1.82	0.41
1:B:2492:ILE:HG21	1:B:2492:ILE:HD13	1.85	0.41
1:A:1173:GLY:HA3	1:A:1184:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:LEU:HD23	1:A:1185:LEU:HA	1.73	0.41
1:A:1281:ILE:HG23	1:A:1282:TRP:N	2.36	0.41
1:C:1744:LYS:NZ	1:C:1775:GLY:O	2.52	0.41
1:C:1984:ASP:CB	1:C:2031:MET:HE2	2.46	0.41
1:B:1717:TRP:CD1	1:B:1717:TRP:C	2.98	0.41
1:B:2191:MET:HE1	2:E:239:CYS:N	2.35	0.41
1:B:2338:GLU:CG	1:B:2339:LYS:H	2.32	0.41
1:A:1149:TYR:HD1	1:A:1665:PHE:HZ	1.68	0.41
1:A:1334:HIS:HA	1:A:1337:ILE:HG22	2.02	0.41
1:A:1553:ARG:HH11	1:A:1556:LEU:HD11	1.85	0.41
1:A:2121:LEU:HD23	1:A:2121:LEU:HA	1.77	0.41
1:C:1515:GLY:O	1:C:1518:ARG:HG2	2.21	0.41
1:A:1985:ILE:HD13	1:A:1985:ILE:HA	1.92	0.41
1:A:2028:PHE:HB3	1:C:2200:ILE:HD13	2.03	0.41
1:C:1281:ILE:HG23	1:C:1282:TRP:N	2.36	0.41
1:B:1744:LYS:NZ	1:B:1775:GLY:O	2.52	0.41
1:B:2092:LEU:HD23	1:B:2092:LEU:HA	1.76	0.41
1:C:2207:LEU:HD12	1:C:2207:LEU:HA	1.77	0.41
1:C:2467:VAL:O	1:C:2471:VAL:HG12	2.20	0.41
1:C:2519:LEU:HA	1:C:2519:LEU:HD23	1.76	0.41
1:B:1281:ILE:HG23	1:B:1282:TRP:N	2.36	0.41
1:B:2405:LEU:HD12	1:B:2430:TRP:CE2	2.55	0.41
1:A:1530:MET:O	1:A:1534:LEU:HD23	2.20	0.41
1:A:1552:ARG:HG2	1:A:1553:ARG:NH1	2.36	0.41
1:A:2089:TYR:CD2	1:A:2089:TYR:C	2.98	0.41
1:A:2467:VAL:O	1:A:2471:VAL:HG12	2.20	0.41
1:C:1013:HIS:CD2	1:C:1047:GLN:HE22	2.39	0.41
1:C:1090:ASN:OD1	1:C:1091:SER:N	2.53	0.41
1:C:1773:ILE:HD13	1:C:1773:ILE:HA	1.88	0.41
1:C:1800:LEU:HD22	1:C:1806:TRP:CE3	2.56	0.41
1:C:2015:GLN:HB3	1:C:2016:VAL:H	1.71	0.41
1:C:2128:VAL:CG1	1:C:2131:LEU:HD12	2.49	0.41
1:C:2371:LEU:N	1:C:2399:LEU:O	2.47	0.41
1:B:1033:TRP:HA	1:B:1036:TYR:HB3	2.03	0.41
1:B:2165:ILE:HG23	1:B:2165:ILE:HD12	1.78	0.41
1:A:1189:PHE:CZ	1:A:1741:VAL:HG11	2.55	0.41
1:A:2188:LYS:HG2	1:B:2140:TRP:CZ2	2.56	0.41
1:C:1017:LEU:HA	1:C:1020:ILE:HD12	2.03	0.41
1:C:1081:TYR:O	1:C:1082:LEU:HD22	2.21	0.41
1:C:2041:LYS:CG	1:C:2105:ILE:HD13	2.51	0.41
1:B:2015:GLN:HB3	1:B:2016:VAL:H	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2059:ILE:HD13	1:B:2059:ILE:HA	1.90	0.41
1:A:1017:LEU:HA	1:A:1020:ILE:HD12	2.03	0.40
1:A:1024:ARG:HB2	1:A:1294:ARG:HH22	1.86	0.40
1:A:1200:GLN:H	1:A:1200:GLN:HG2	1.72	0.40
1:A:1701:VAL:HG12	1:A:1702:THR:N	2.36	0.40
1:A:2258:GLU:O	1:A:2261:GLN:HG2	2.21	0.40
1:C:1515:GLY:HA2	1:C:1518:ARG:HG2	2.03	0.40
1:C:1552:ARG:HG2	1:C:1553:ARG:NH1	2.36	0.40
1:C:2221:ASN:HB2	1:C:2453:VAL:HG23	2.02	0.40
1:C:2245:GLN:HG2	1:B:2339:LYS:NZ	2.36	0.40
1:C:2280:ASP:O	1:C:2450:SER:OG	2.37	0.40
1:C:2349:THR:HA	1:C:2352:ARG:NH2	2.35	0.40
1:B:1081:TYR:O	1:B:1082:LEU:HD22	2.20	0.40
1:B:1515:GLY:O	1:B:1518:ARG:HG2	2.21	0.40
1:B:2191:MET:HE1	2:E:238:GLU:C	2.46	0.40
1:B:2280:ASP:O	1:B:2450:SER:OG	2.37	0.40
1:B:2475:LEU:HD23	1:B:2475:LEU:HA	1.83	0.40
1:A:1800:LEU:HD22	1:A:1806:TRP:CE3	2.56	0.40
1:A:2092:LEU:HD23	1:A:2092:LEU:HA	1.76	0.40
1:C:1016:TRP:CE2	1:C:1043:PHE:HE2	2.39	0.40
1:C:1047:GLN:HA	1:C:1050:LEU:HB2	2.02	0.40
1:C:1358:LYS:HB2	1:C:1358:LYS:HE3	1.93	0.40
1:C:1701:VAL:HG12	1:C:1702:THR:N	2.36	0.40
1:C:2149:LEU:HA	1:C:2149:LEU:HD12	1.70	0.40
1:B:1115:ARG:O	1:B:1117:GLU:N	2.55	0.40
1:B:1552:ARG:HG2	1:B:1553:ARG:NH1	2.36	0.40
1:B:2258:GLU:O	1:B:2261:GLN:HG2	2.21	0.40
1:B:2286:ILE:HG13	1:B:2444:LEU:HB2	2.01	0.40
1:B:2422:LYS:HD3	1:B:2422:LYS:HA	1.93	0.40
1:A:2324:GLN:HB2	1:A:2335:TYR:HE2	1.86	0.40
1:A:2485:PHE:CG	1:B:2153:MET:CE	3.05	0.40
1:A:2525:LEU:HA	1:A:2525:LEU:HD23	1.76	0.40
1:C:1149:TYR:HD1	1:C:1665:PHE:HZ	1.68	0.40
1:C:1992:ILE:HD13	1:C:1992:ILE:HA	1.89	0.40
1:C:2308:LEU:HA	1:C:2351:ARG:HD3	2.03	0.40
1:B:1016:TRP:CE2	1:B:1043:PHE:HE2	2.39	0.40
1:B:1185:LEU:HA	1:B:1185:LEU:HD23	1.73	0.40
1:B:1701:VAL:HG12	1:B:1702:THR:N	2.36	0.40
1:B:1800:LEU:HD22	1:B:1806:TRP:CE3	2.56	0.40
1:B:2121:LEU:HD23	1:B:2121:LEU:HA	1.77	0.40
1:A:1016:TRP:CE2	1:A:1043:PHE:HE2	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:TRP:HA	1:A:1036:TYR:HB3	2.03	0.40
1:A:1515:GLY:O	1:A:1518:ARG:HG2	2.21	0.40
1:A:1528:ARG:O	1:A:1531:SER:OG	2.33	0.40
1:A:1716:LEU:HA	1:A:1716:LEU:HD23	1.63	0.40
1:A:2108:ASN:HB3	1:A:2111:THR:CG2	2.47	0.40
1:A:2323:PHE:CE1	1:A:2448:ILE:HG21	2.57	0.40
1:A:2376:ILE:HB	1:A:2448:ILE:HG22	2.04	0.40
1:C:1033:TRP:HA	1:C:1036:TYR:HB3	2.03	0.40
1:C:1328:LEU:HD23	1:C:1328:LEU:HA	1.85	0.40
1:C:1717:TRP:CD1	1:C:1717:TRP:O	2.75	0.40
1:C:1783:ILE:HG13	1:C:1783:ILE:O	2.21	0.40
1:C:2258:GLU:O	1:C:2261:GLN:HG2	2.21	0.40
1:C:2324:GLN:HB2	1:C:2335:TYR:HE2	1.86	0.40
1:B:1017:LEU:HA	1:B:1020:ILE:HD12	2.03	0.40
1:B:2308:LEU:HA	1:B:2351:ARG:HD3	2.04	0.40
1:A:1203:THR:HA	1:A:1206:GLN:NE2	2.37	0.40
1:A:2308:LEU:HA	1:A:2351:ARG:HD3	2.04	0.40
1:A:2372:PHE:CD2	1:A:2434:LEU:HD21	2.53	0.40
1:C:1334:HIS:HA	1:C:1337:ILE:HG22	2.02	0.40
1:C:2033:ILE:HD13	1:C:2033:ILE:HA	1.91	0.40
1:B:1717:TRP:CD1	1:B:1717:TRP:O	2.75	0.40
1:B:2371:LEU:N	1:B:2399:LEU:O	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1193/2815 (42%)	1098 (92%)	95 (8%)	0	100	100
1	B	1193/2815 (42%)	1097 (92%)	96 (8%)	0	100	100
1	C	1193/2815 (42%)	1098 (92%)	95 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	19/269 (7%)	18 (95%)	1 (5%)	0	100	100
2	E	19/269 (7%)	18 (95%)	1 (5%)	0	100	100
2	F	19/269 (7%)	18 (95%)	1 (5%)	0	100	100
All	All	3636/9252 (39%)	3347 (92%)	289 (8%)	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	983/2477 (40%)	983 (100%)	0	100	100
1	B	983/2477 (40%)	983 (100%)	0	100	100
1	C	983/2477 (40%)	983 (100%)	0	100	100
2	D	19/218 (9%)	19 (100%)	0	100	100
2	E	19/218 (9%)	19 (100%)	0	100	100
2	F	19/218 (9%)	19 (100%)	0	100	100
All	All	3006/8085 (37%)	3006 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1047	GLN
1	A	1225	ASN
1	A	1408	HIS
1	A	1526	HIS
1	A	1543	GLN
1	A	1698	ASN
1	A	1748	GLN
1	A	2389	GLN

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Mol	Chain	Res	Type
1	C	1047	GLN
1	C	1225	ASN
1	C	1408	HIS
1	C	1526	HIS
1	C	1543	GLN
1	C	1698	ASN
1	C	1748	GLN
1	C	2389	GLN
1	C	2490	HIS
1	B	1047	GLN
1	B	1225	ASN
1	B	1526	HIS
1	B	1543	GLN
1	B	1698	ASN
1	B	1748	GLN
1	B	2244	GLN
1	B	2389	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.