



Full wwPDB EM Validation Report ⓘ

Apr 29, 2026 – 06:17 PM JST

PDB ID : 9VEE / pdb_00009vee
EMDB ID : EMD-65005
Title : The cryo-EM structure of human Piezo2-MDFIC2 complex (composite map)
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 : 3.36 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

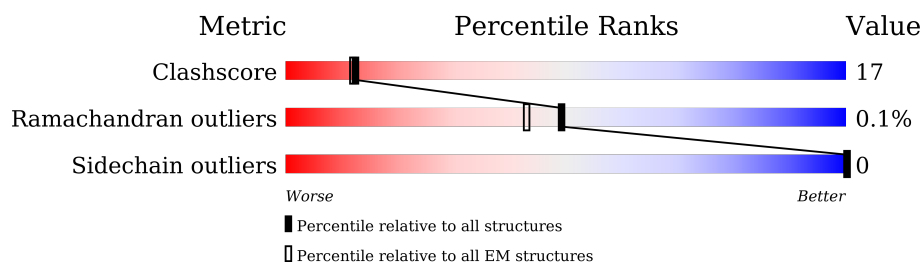
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	3020	29% 17% 54%
1	B	3020	29% 17% 54%
1	C	3020	29% 17% 54%
2	D	211	7% . 90%
2	E	211	6% . 90%
2	F	211	6% . 90%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34893 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 2, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1396	Total	C	N	O	S	0	0
			11465	7568	1851	1969	77		
1	B	1396	Total	C	N	O	S	0	0
			11465	7568	1851	1969	77		
1	C	1396	Total	C	N	O	S	0	0
			11465	7568	1851	1969	77		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2753	SER	-	linker	UNP Q9H5I5
A	2754	ASN	-	linker	UNP Q9H5I5
A	2755	SER	-	linker	UNP Q9H5I5
A	2756	LEU	-	linker	UNP Q9H5I5
A	2757	GLU	-	linker	UNP Q9H5I5
A	2758	VAL	-	linker	UNP Q9H5I5
A	2759	LEU	-	linker	UNP Q9H5I5
A	2760	PHE	-	linker	UNP Q9H5I5
A	2761	GLN	-	linker	UNP Q9H5I5
A	2762	GLY	-	linker	UNP Q9H5I5
A	2763	PRO	-	linker	UNP Q9H5I5
A	2764	THR	-	linker	UNP Q9H5I5
A	2765	ALA	-	linker	UNP Q9H5I5
A	2766	ALA	-	linker	UNP Q9H5I5
A	2767	ALA	-	linker	UNP Q9H5I5
A	2768	ALA	-	linker	UNP Q9H5I5
A	2769	VAL	-	linker	UNP Q9H5I5
A	2832	LEU	PHE	conflict	UNP P42212
A	2833	THR	SER	conflict	UNP P42212
A	2974	LYS	ALA	conflict	UNP P42212
A	2999	LEU	HIS	conflict	UNP P42212
A	3007	SER	-	expression tag	UNP P42212
A	3008	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3009	GLY	-	expression tag	UNP P42212
A	3010	GLY	-	expression tag	UNP P42212
A	3011	HIS	-	expression tag	UNP P42212
A	3012	HIS	-	expression tag	UNP P42212
A	3013	HIS	-	expression tag	UNP P42212
A	3014	HIS	-	expression tag	UNP P42212
A	3015	HIS	-	expression tag	UNP P42212
A	3016	HIS	-	expression tag	UNP P42212
A	3017	HIS	-	expression tag	UNP P42212
A	3018	HIS	-	expression tag	UNP P42212
A	3019	HIS	-	expression tag	UNP P42212
A	3020	HIS	-	expression tag	UNP P42212
B	2753	SER	-	linker	UNP Q9H5I5
B	2754	ASN	-	linker	UNP Q9H5I5
B	2755	SER	-	linker	UNP Q9H5I5
B	2756	LEU	-	linker	UNP Q9H5I5
B	2757	GLU	-	linker	UNP Q9H5I5
B	2758	VAL	-	linker	UNP Q9H5I5
B	2759	LEU	-	linker	UNP Q9H5I5
B	2760	PHE	-	linker	UNP Q9H5I5
B	2761	GLN	-	linker	UNP Q9H5I5
B	2762	GLY	-	linker	UNP Q9H5I5
B	2763	PRO	-	linker	UNP Q9H5I5
B	2764	THR	-	linker	UNP Q9H5I5
B	2765	ALA	-	linker	UNP Q9H5I5
B	2766	ALA	-	linker	UNP Q9H5I5
B	2767	ALA	-	linker	UNP Q9H5I5
B	2768	ALA	-	linker	UNP Q9H5I5
B	2769	VAL	-	linker	UNP Q9H5I5
B	2832	LEU	PHE	conflict	UNP P42212
B	2833	THR	SER	conflict	UNP P42212
B	2974	LYS	ALA	conflict	UNP P42212
B	2999	LEU	HIS	conflict	UNP P42212
B	3007	SER	-	expression tag	UNP P42212
B	3008	GLY	-	expression tag	UNP P42212
B	3009	GLY	-	expression tag	UNP P42212
B	3010	GLY	-	expression tag	UNP P42212
B	3011	HIS	-	expression tag	UNP P42212
B	3012	HIS	-	expression tag	UNP P42212
B	3013	HIS	-	expression tag	UNP P42212
B	3014	HIS	-	expression tag	UNP P42212
B	3015	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3016	HIS	-	expression tag	UNP P42212
B	3017	HIS	-	expression tag	UNP P42212
B	3018	HIS	-	expression tag	UNP P42212
B	3019	HIS	-	expression tag	UNP P42212
B	3020	HIS	-	expression tag	UNP P42212
C	2753	SER	-	linker	UNP Q9H5I5
C	2754	ASN	-	linker	UNP Q9H5I5
C	2755	SER	-	linker	UNP Q9H5I5
C	2756	LEU	-	linker	UNP Q9H5I5
C	2757	GLU	-	linker	UNP Q9H5I5
C	2758	VAL	-	linker	UNP Q9H5I5
C	2759	LEU	-	linker	UNP Q9H5I5
C	2760	PHE	-	linker	UNP Q9H5I5
C	2761	GLN	-	linker	UNP Q9H5I5
C	2762	GLY	-	linker	UNP Q9H5I5
C	2763	PRO	-	linker	UNP Q9H5I5
C	2764	THR	-	linker	UNP Q9H5I5
C	2765	ALA	-	linker	UNP Q9H5I5
C	2766	ALA	-	linker	UNP Q9H5I5
C	2767	ALA	-	linker	UNP Q9H5I5
C	2768	ALA	-	linker	UNP Q9H5I5
C	2769	VAL	-	linker	UNP Q9H5I5
C	2832	LEU	PHE	conflict	UNP P42212
C	2833	THR	SER	conflict	UNP P42212
C	2974	LYS	ALA	conflict	UNP P42212
C	2999	LEU	HIS	conflict	UNP P42212
C	3007	SER	-	expression tag	UNP P42212
C	3008	GLY	-	expression tag	UNP P42212
C	3009	GLY	-	expression tag	UNP P42212
C	3010	GLY	-	expression tag	UNP P42212
C	3011	HIS	-	expression tag	UNP P42212
C	3012	HIS	-	expression tag	UNP P42212
C	3013	HIS	-	expression tag	UNP P42212
C	3014	HIS	-	expression tag	UNP P42212
C	3015	HIS	-	expression tag	UNP P42212
C	3016	HIS	-	expression tag	UNP P42212
C	3017	HIS	-	expression tag	UNP P42212
C	3018	HIS	-	expression tag	UNP P42212
C	3019	HIS	-	expression tag	UNP P42212
C	3020	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called MyoD family inhibitor domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	21	Total 166	C 100	N 26	O 36	S 4	0	0
2	D	21	Total 166	C 100	N 26	O 36	S 4	0	0
2	E	21	Total 166	C 100	N 26	O 36	S 4	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	MET	-	initiating methionine	UNP A0A1B0GVS7
F	-20	ASP	-	expression tag	UNP A0A1B0GVS7
F	-19	TYR	-	expression tag	UNP A0A1B0GVS7
F	-18	LYS	-	expression tag	UNP A0A1B0GVS7
F	-17	ASP	-	expression tag	UNP A0A1B0GVS7
F	-16	ASP	-	expression tag	UNP A0A1B0GVS7
F	-15	ASP	-	expression tag	UNP A0A1B0GVS7
F	-14	ASP	-	expression tag	UNP A0A1B0GVS7
F	-13	LYS	-	expression tag	UNP A0A1B0GVS7
F	-12	GLY	-	expression tag	UNP A0A1B0GVS7
F	-11	LEU	-	expression tag	UNP A0A1B0GVS7
F	-10	GLU	-	expression tag	UNP A0A1B0GVS7
F	-9	VAL	-	expression tag	UNP A0A1B0GVS7
F	-8	LEU	-	expression tag	UNP A0A1B0GVS7
F	-7	PHE	-	expression tag	UNP A0A1B0GVS7
F	-6	GLN	-	expression tag	UNP A0A1B0GVS7
F	-5	GLY	-	expression tag	UNP A0A1B0GVS7
F	-4	PRO	-	expression tag	UNP A0A1B0GVS7
F	-3	GLY	-	expression tag	UNP A0A1B0GVS7
F	-2	SER	-	expression tag	UNP A0A1B0GVS7
F	-1	SER	-	expression tag	UNP A0A1B0GVS7
F	0	THR	-	expression tag	UNP A0A1B0GVS7
D	-21	MET	-	initiating methionine	UNP A0A1B0GVS7
D	-20	ASP	-	expression tag	UNP A0A1B0GVS7
D	-19	TYR	-	expression tag	UNP A0A1B0GVS7
D	-18	LYS	-	expression tag	UNP A0A1B0GVS7
D	-17	ASP	-	expression tag	UNP A0A1B0GVS7
D	-16	ASP	-	expression tag	UNP A0A1B0GVS7
D	-15	ASP	-	expression tag	UNP A0A1B0GVS7
D	-14	ASP	-	expression tag	UNP A0A1B0GVS7
D	-13	LYS	-	expression tag	UNP A0A1B0GVS7
D	-12	GLY	-	expression tag	UNP A0A1B0GVS7
D	-11	LEU	-	expression tag	UNP A0A1B0GVS7

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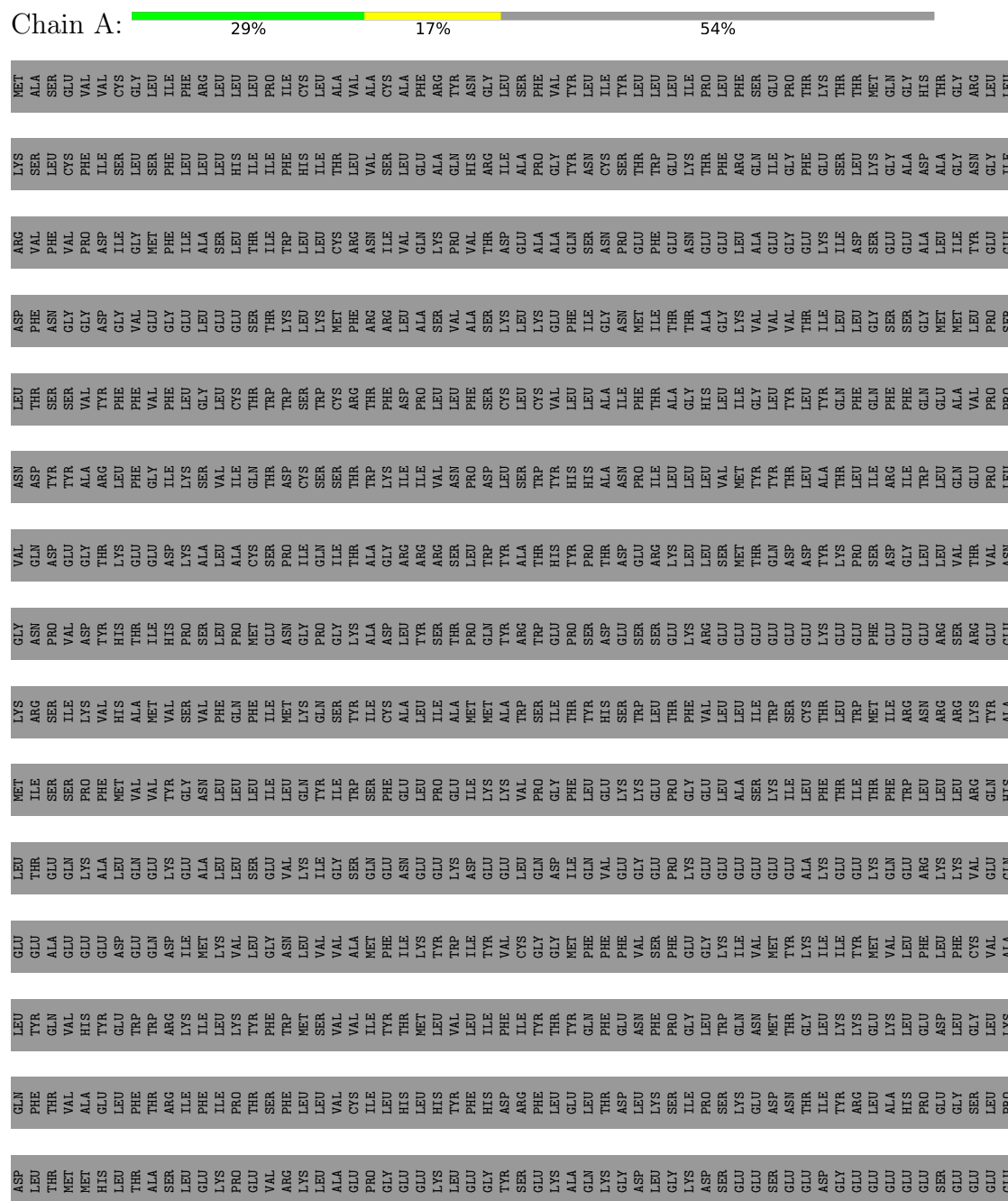
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	GLU	-	expression tag	UNP A0A1B0GVS7
D	-9	VAL	-	expression tag	UNP A0A1B0GVS7
D	-8	LEU	-	expression tag	UNP A0A1B0GVS7
D	-7	PHE	-	expression tag	UNP A0A1B0GVS7
D	-6	GLN	-	expression tag	UNP A0A1B0GVS7
D	-5	GLY	-	expression tag	UNP A0A1B0GVS7
D	-4	PRO	-	expression tag	UNP A0A1B0GVS7
D	-3	GLY	-	expression tag	UNP A0A1B0GVS7
D	-2	SER	-	expression tag	UNP A0A1B0GVS7
D	-1	SER	-	expression tag	UNP A0A1B0GVS7
D	0	THR	-	expression tag	UNP A0A1B0GVS7
E	-21	MET	-	initiating methionine	UNP A0A1B0GVS7
E	-20	ASP	-	expression tag	UNP A0A1B0GVS7
E	-19	TYR	-	expression tag	UNP A0A1B0GVS7
E	-18	LYS	-	expression tag	UNP A0A1B0GVS7
E	-17	ASP	-	expression tag	UNP A0A1B0GVS7
E	-16	ASP	-	expression tag	UNP A0A1B0GVS7
E	-15	ASP	-	expression tag	UNP A0A1B0GVS7
E	-14	ASP	-	expression tag	UNP A0A1B0GVS7
E	-13	LYS	-	expression tag	UNP A0A1B0GVS7
E	-12	GLY	-	expression tag	UNP A0A1B0GVS7
E	-11	LEU	-	expression tag	UNP A0A1B0GVS7
E	-10	GLU	-	expression tag	UNP A0A1B0GVS7
E	-9	VAL	-	expression tag	UNP A0A1B0GVS7
E	-8	LEU	-	expression tag	UNP A0A1B0GVS7
E	-7	PHE	-	expression tag	UNP A0A1B0GVS7
E	-6	GLN	-	expression tag	UNP A0A1B0GVS7
E	-5	GLY	-	expression tag	UNP A0A1B0GVS7
E	-4	PRO	-	expression tag	UNP A0A1B0GVS7
E	-3	GLY	-	expression tag	UNP A0A1B0GVS7
E	-2	SER	-	expression tag	UNP A0A1B0GVS7
E	-1	SER	-	expression tag	UNP A0A1B0GVS7
E	0	THR	-	expression tag	UNP A0A1B0GVS7

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 2, Green fluorescent protein



K2482	M2404	S2306	D2197	SER	ALA	L1948	ARG	GLU	ALA	ALA	ASN	ILE	THR	GLU	R1193
M2483	V2410	C2312	I2202	PHE	ARG	I1949	MET	ALA	THR	THR	ILE	THR	ASP	GLU	D1194
F2485	L2411	V2318	G2207	SER	VAL	F1950	ALA	VAL	GLY	GLY	LEU	ASP	ASP	ASP	Y1196
L2486	L2412	L2319	R1962	ASN	SER	R1962	SER	PRO	THR	TYR	W1666	THR	GLU	GLU	P1196
N2488	I2413	L2319	R1962	ARG	ASP	R1962	ASP	VAL	VAL	VAL	W1666	THR	ARG	ARG	W1197
Y2489	I2415	S2326	I1969	SER	ASP	I1969	ASP	ASP	GLY	GLY	I1670	ALA	GLU	GLU	F1199
E2490	V2416	S2326	V1970	GLN	GLU	V1970	ASP	ASP	ASP	ASP	I1670	LEU	ALA	ALA	F1204
K2491	W2417	L2339	I1971	GLN	LEU	I1971	SER	SER	SER	ALA	E1673	ARG	ASP	ASP	N1205
V2496	W2417	V2330	T1972	GLY	SER	T1972	THR	THR	GLY	GLY	E1673	ARG	GLN	GLN	D1206
F2498	F2418	N2331	E1973	THR	GLY	E1973	ASP	ASP	ALA	ALA	I1677	HIS	LYS	LYS	N1207
L2499	L2426	L2332	Y1980	THR	HIS	Y1980	LYS	LYS	GLU	GLU	S1678	LYS	ALA	ALA	I1208
E2500	LYS	F2333	F1981	THR	GLY	F1981	LEU	LEU	GLU	GLU	T1679	GLY	LYS	LYS	I1209
G2501	SER	ARG	F1982	THR	ARG	F1982	GLY	GLY	ALA	ALA	V1680	LYS	GLY	GLY	K1210
N2504	VAL	ILE	F1988	THR	ASN	F1988	SER	SER	LEU	LEU	R1682	ARG	LYS	LYS	D1216
S2505	A2430	SER	TRP	SER	ASN	TRP	ILE	THR	THR	THR	R1682	SER	LYS	LYS	F1217
L2506	N2434	GLN	ASN	GLN	SER	ASN	LEU	PRO	PRO	GLU	F1684	ALA	GLN	GLN	I1218
W2507	F2343	LYS	LYS	LYS	ASP	LYS	PRO	GLU	GLU	THR	R1685	ARG	TRP	TRP	V1219
T2508	L2437	GLY	ASP	GLY	SER	ASP	P1873	GLU	GLU	GLU	C1686	GLY	ARG	ARG	P1223
D2438	T2345	SER	VAL	SER	LEU	VAL	L1874	LEU	LEU	LEU	M1687	GLY	PRO	PRO	K1360
T2509	E2346	ASP	GLU	LYS	LYS	GLU	T1875	GLU	GLU	GLU	L1688	ARG	GLY	GLY	M1361
S2510	L2347	SER	VAL	VAL	SER	VAL	L1878	GLN	GLN	GLN	T1689	LYS	ARG	ARG	L1226
P2511	S2440	GLN	ASN	ILE	ASN	ASN	T1879	PHE	PHE	THR	R1690	ARG	GLY	GLY	F1230
P2512	W2441	SER	LYS	SER	ASN	LYS	T1879	THR	THR	THR	E1691	ARG	ALA	ALA	R1240
S2513	T2442	ILE	ASP	LEU	LEU	ASP	A1880	SER	SER	SER	I1692	ARG	GLY	GLY	I1240
K2514	L2443	GLN	LYS	ALA	ALA	LYS	S1881	THR	THR	THR	P1698	GLY	GLY	GLY	M1254
K2515	T2444	LYS	TYR	SER	ALA	TYR	E1882	LEU	LEU	GLN	T1699	SER	GLY	GLY	G1256
K2516	W2354	LYS	VAL	SER	SER	VAL	K1887	GLY	GLY	GLY	R1700	LYS	GLY	GLY	D1257
S2517	W2355	LYS	VAL	GLY	VAL	VAL	M1888	ASP	ASP	THR	E1701	GLY	GLY	GLY	I1371
P2517	W2355	LYS	VAL	LYS	GLU	GLU	P2003	ASP	VAL	THR	S1702	GLY	GLY	GLY	V1375
L2522	P2460	GLY	GLY	ARG	SER	SER	P2004	VAL	VAL	THR	S1702	GLY	GLY	GLY	M1263
D2523	T2461	GLU	GLU	ARG	SER	VAL	F1889	GLU	GLU	GLU	I1703	PRO	GLU	GLU	A1268
F2524	L2452	LEU	THR	THR	HIS	VAL	D1891	ALA	ALA	THR	M1705	VAL	GLU	GLU	A1387
N2525	T2453	MET	T2243	MET	THR	VAL	E1892	PRO	PRO	ILE	M1706	THR	THR	THR	A1388
M2454	M2454	GLU	V2244	GLU	PHE	PHE	L1894	SER	SER	GLU	Y1707	GLU	GLU	GLU	C1389
S2455	S2455	LYS	V2245	LYS	LYS	PRO	E1895	TYR	TYR	VAL	Q1708	ASP	GLU	GLU	N1274
A2456	A2456	LYS	V2246	LEU	GLN	GLN	E1896	SER	SER	SER	M1709	ARG	LEU	LEU	F1275
Q2457	Q2457	ARG	K2254	GLN	ALA	ALA	S1897	LYS	LYS	ALA	H1710	GLY	LEU	LEU	V1276
V2463	M2464	LEU	K2254	GLU	THR	THR	E1898	VAL	VAL	GLN	I1711	ASP	LYS	LYS	K1392
M2464	D2465	LEU	K2259	LEU	ALA	ALA	K1899	SER	SER	GLU	M1713	GLU	GLU	GLU	I1280
Q2466	Q2466	ILE	K2259	ILE	VAL	VAL	V1902	PHE	PHE	GLU	S1718	LEU	ASP	ASP	H1281
Q2467	Q2467	LYS	L2286	LYS	ARG	ARG	V1929	GLU	GLU	GLU	S1718	GLY	GLU	GLU	C1282
S2468	S2468	ALA	W2273	ALA	ALA	ARG	I1930	HIS	HIS	GLY	S1718	LEU	PRO	PRO	R1283
F2469	F2469	LYS	W2273	LYS	LYS	LYS	I1930	LEU	LEU	THR	S1718	GLY	PRO	PRO	D1287
N2470	N2470	ALA	R2284	ALA	ARG	ARG	M1933	SER	SER	THR	S1718	GLY	ARG	ARG	K1290
K2471	K2471	PHE	K2285	PHE	SER	SER	H1934	PHE	PHE	THR	S1718	GLY	ARG	ARG	K1290
F2472	F2472	THR	F2286	THR	GLY	GLY	H1934	GLY	GLY	ALA	S1718	GLY	SER	SER	F1294
I2473	I2473	ILE	F2287	ILE	SER	SER	M1936	SER	SER	PRO	S1718	GLY	ALA	ALA	F1294
Q2474	Q2474	LYS	Q2288	LYS	SER	SER	V1936	GLN	GLN	GLU	S1718	GLY	GLY	GLY	E1409
A2475	A2475	LYS	N2289	LYS	SER	SER	S1937	ASP	ASP	PRO	S1937	GLY	GLN	GLN	F1298
F2476	F2476	GLY	T2164	GLY	GLU	GLU	A1938	ASP	ASP	GLU	A1938	ILE	VAL	VAL	V1301
S2477	S2477	LYS	K2185	LYS	PRO	PRO	S1939	SER	SER	ALA	A1939	GLY	GLN	GLN	I1412
K2478	K2478	GLY	K2185	GLY	SER	SER	M1940	ALA	ALA	ALA	A1940	GLY	LYS	LYS	I1304
D2479	D2479	GLN	V2189	GLN	GLN	GLN	T1941	LYS	LYS	GLY	A1941	ARG	ALA	ALA	I1305
T2480	T2480	ARG	V2189	ARG	ARG	ARG	T1942	GLY	GLY	GLU	A1942	ILE	ILE	ILE	F1306
G2481	G2481	SER	L2305	SER	SER	SER		ASN	ASN	TYR		GLY	TRP	TRP	

ASP	CYS	ARG	HIS	ALA	MET
CYS	ASP	ASP	ARG	ASP	TYR
ASP	MET	THR	THR	LYS	LYS
ASP	ASP	GLU	GLU	PRO	ASP
CYS	GLU	GLU	GLU	ILE	ASP
SER	LEU	CYS	CYS	ASN	ASP
LEU	LEU	ALA	ALA	ILE	ASP
PHE	PHE	ALA	ALA	ILE	GLY
GLU	GLU	SER	SER	VAL	LYS
S169	S169	LEU	LEU	ILE	LEU
E172	E172	ILE	ILE	ASN	GLU
T173	T173	LEU	LEU	VAL	GLU
A180	A180	ALA	ALA	VAL	VAL
M181	M181	CYS	CYS	SER	PHE
E182	E182	LEU	LEU	ASP	GLN
I183	I183	PHE	PHE	ASN	GLY
S184	S184	GLN	GLN	ASN	PRO
E185	E185	THR	THR	THR	SER
		ASP	ASP	GLY	THR
		CYS	CYS	PRO	MET
R189	R189	LEU	LEU	ALA	SER
		LEU	LEU	LYS	GLU
		MET	MET	GLU	THR
		LEU	LEU	ASN	GLU
		PRO	PRO	PRO	LEU
		GLY	GLY	ASN	GLU
		THR	THR	GLU	LYS
		CYS	CYS	LYS	ILE
		VAL	VAL	LEU	VAL
		ARG	ARG	SER	ARG
		THR	THR	GLU	THR
		LYS	LYS	SER	ALA
		MET	MET	THR	HIS
		CYS	CYS	SER	LEU
		CYS	CYS	LEU	GLU
		PRO	PRO	SER	ASN
		SER	SER	SER	ASP
		ARG	ARG	LEU	LYS
		THR	THR	GLU	ASN
		TYR	TYR	GLU	ASN
		HIS	HIS	CYS	ILE
		THR	THR	GLN	SER
		SER	SER	THR	THR
		ASP	ASP	PHE	LEU
		GLU	GLU	THR	LYS
		ASN	ASN	TYR	ASP
		HIS	HIS	LEU	THR
		SER	SER	GLN	GLN
		ARG	ARG	THR	LEU
		ASN	ASN	ASP	THR
		ASP	ASP	THR	ASN
		CYS	CYS	ALA	ALA
		SER	SER	VAL	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203045	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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	1/11775 (0.0%)	0.52	4/15965 (0.0%)
1	B	0.40	1/11775 (0.0%)	0.52	4/15965 (0.0%)
1	C	0.40	1/11775 (0.0%)	0.52	4/15965 (0.0%)
2	D	0.32	0/167	0.74	0/223
2	E	0.32	0/167	0.74	0/223
2	F	0.32	0/167	0.74	0/223
All	All	0.40	3/35826 (0.0%)	0.53	12/48564 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2509	ILE	C-N	-6.48	1.24	1.33
1	C	2509	ILE	C-N	-6.44	1.24	1.33
1	A	2509	ILE	C-N	-6.43	1.24	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2509	ILE	CA-C-N	8.51	133.61	120.68
1	C	2509	ILE	C-N-CA	8.51	133.61	120.68
1	A	2509	ILE	CA-C-N	8.48	133.56	120.68
1	A	2509	ILE	C-N-CA	8.48	133.56	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2509	ILE	CA-C-N	8.47	133.56	120.68
1	B	2509	ILE	C-N-CA	8.47	133.56	120.68
1	A	2696	ILE	N-CA-C	-6.20	105.00	111.58
1	B	2696	ILE	N-CA-C	-6.19	105.02	111.58
1	C	2696	ILE	N-CA-C	-6.18	105.03	111.58
1	B	2003	PRO	N-CA-C	5.11	116.94	110.70
1	C	2003	PRO	N-CA-C	5.09	116.91	110.70
1	A	2003	PRO	N-CA-C	5.09	116.91	110.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2630	TRP	Peptide
1	A	2642	ASN	Peptide
1	B	2630	TRP	Peptide
1	B	2642	ASN	Peptide
1	C	2630	TRP	Peptide
1	C	2642	ASN	Peptide

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	11465	0	11592	424	0
1	B	11465	0	11592	415	0
1	C	11465	0	11592	411	0
2	D	166	0	153	14	0
2	E	166	0	153	16	0
2	F	166	0	153	14	0
All	All	34893	0	35235	1185	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 (1185) 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:2630:TRP:HZ2	1:B:2512:PRO:HD2	1.34	0.93
1:A:2630:TRP:CZ2	1:B:2512:PRO:HD2	2.08	0.88
1:A:2003:PRO:HD2	1:A:2004:PRO:HD2	1.55	0.88
1:C:1204:PHE:HB3	1:C:1209:ILE:HD11	1.56	0.88
1:C:2003:PRO:HD2	1:C:2004:PRO:HD2	1.55	0.88
1:C:2381:TRP:HH2	2:E:184:SER:HB3	1.38	0.88
1:B:2003:PRO:HD2	1:B:2004:PRO:HD2	1.55	0.87
1:A:1204:PHE:HB3	1:A:1209:ILE:HD11	1.56	0.87
1:B:1204:PHE:HB3	1:B:1209:ILE:HD11	1.56	0.86
1:B:976:ALA:HB2	1:B:979:ARG:HH21	1.43	0.84
1:A:976:ALA:HB2	1:A:979:ARG:HH21	1.43	0.83
1:A:2362:LEU:N	2:D:182:GLU:OE2	2.12	0.83
1:C:976:ALA:HB2	1:C:979:ARG:HH21	1.43	0.82
1:B:2381:TRP:HH2	2:D:184:SER:HB3	1.44	0.82
1:A:2512:PRO:HD2	1:C:2630:TRP:HZ2	1.45	0.81
1:B:1177:ILE:HG13	1:B:1226:LEU:HD11	1.64	0.80
1:A:1177:ILE:HG13	1:A:1226:LEU:HD11	1.64	0.79
1:C:1308:THR:HG1	1:C:1418:CYS:HG	1.28	0.78
1:C:2381:TRP:CH2	2:E:184:SER:HB3	2.18	0.78
1:B:1308:THR:HG1	1:B:1418:CYS:HG	1.24	0.78
1:A:2347:LEU:HD21	1:B:2412:LEU:HD13	1.66	0.78
1:B:2457:GLN:OE1	1:C:2516:LYS:NZ	2.15	0.78
1:C:1177:ILE:HG13	1:C:1226:LEU:HD11	1.64	0.77
1:A:2345:THR:OG1	1:B:2686:ARG:NH1	2.17	0.77
1:C:2469:PHE:O	1:C:2474:GLN:NE2	2.15	0.77
1:A:1263:MET:HE1	1:A:1343:LEU:HD12	1.67	0.77
1:A:2469:PHE:O	1:A:2474:GLN:NE2	2.14	0.77
1:C:2544:ALA:HA	1:C:2657:VAL:HG21	1.68	0.76
1:C:1263:MET:HE1	1:C:1343:LEU:HD12	1.67	0.76
1:A:1706:TYR:O	1:A:1710:HIS:ND1	2.19	0.75
1:B:1263:MET:HE1	1:B:1343:LEU:HD12	1.67	0.75
1:B:1706:TYR:O	1:B:1710:HIS:ND1	2.19	0.75
1:B:2381:TRP:CZ3	2:D:181:MET:HG3	2.22	0.75
1:C:2359:THR:HG23	1:C:2723:LEU:HD23	1.69	0.74
1:B:2544:ALA:HA	1:B:2657:VAL:HG21	1.68	0.74
1:A:1099:THR:HG21	1:A:1254:MET:HE3	1.69	0.74
1:A:2544:ALA:HA	1:A:2657:VAL:HG21	1.68	0.74
1:B:2558:LYS:HD2	1:B:2559:ASN:H	1.53	0.74
1:C:2558:LYS:HD2	1:C:2559:ASN:H	1.53	0.73
1:A:2359:THR:HG23	1:A:2723:LEU:HD23	1.69	0.73
1:B:2469:PHE:O	1:B:2474:GLN:NE2	2.14	0.73
1:C:1099:THR:HG21	1:C:1254:MET:HE3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2529:SER:HA	1:C:2556:PRO:HA	1.71	0.73
1:A:1542:HIS:CE1	1:B:2389:PRO:HB2	2.23	0.73
1:C:2451:ILE:HB	1:C:2631:TRP:CD1	2.24	0.73
1:A:2451:ILE:HB	1:A:2631:TRP:CD1	2.24	0.73
1:A:2496:VAL:HG22	1:A:2651:VAL:HG22	1.71	0.73
1:B:2359:THR:HG23	1:B:2723:LEU:HD23	1.69	0.73
1:C:1706:TYR:O	1:C:1710:HIS:ND1	2.19	0.73
1:B:2496:VAL:HG22	1:B:2651:VAL:HG22	1.71	0.72
1:A:2558:LYS:HD2	1:A:2559:ASN:H	1.53	0.72
1:B:2451:ILE:HB	1:B:2631:TRP:CD1	2.24	0.72
1:A:2529:SER:HA	1:A:2556:PRO:HA	1.71	0.72
1:A:1308:THR:HG1	1:A:1418:CYS:HG	1.30	0.72
1:B:1099:THR:HG21	1:B:1254:MET:HE3	1.69	0.72
1:B:1180:GLN:HG2	1:B:1226:LEU:HD13	1.72	0.72
1:B:2529:SER:HA	1:B:2556:PRO:HA	1.71	0.72
1:A:1180:GLN:HG2	1:A:1226:LEU:HD13	1.72	0.71
1:B:1700:ARG:HG2	1:B:1704:HIS:CE1	2.25	0.71
1:C:2496:VAL:HG22	1:C:2651:VAL:HG22	1.71	0.71
1:C:2381:TRP:CZ3	2:E:181:MET:HG3	2.25	0.71
1:B:2537:GLN:NE2	1:B:2547:GLU:OE2	2.24	0.71
1:B:959:SER:OG	1:B:962:ASN:OD1	2.09	0.71
1:A:1700:ARG:HG2	1:A:1704:HIS:CE1	2.26	0.71
1:C:2717:VAL:HG11	1:C:2725:LEU:HB2	1.73	0.70
1:A:2537:GLN:NE2	1:A:2547:GLU:OE2	2.24	0.70
1:C:2537:GLN:NE2	1:C:2547:GLU:OE2	2.24	0.70
1:A:1388:ALA:HB2	1:A:1406:PRO:HG2	1.74	0.70
1:B:1388:ALA:HB2	1:B:1406:PRO:HG2	1.74	0.70
1:B:2381:TRP:CH2	2:D:184:SER:HB3	2.25	0.70
1:C:2232:PRO:HB2	1:C:2236:MET:HE2	1.73	0.70
1:C:1180:GLN:HG2	1:C:1226:LEU:HD13	1.72	0.70
1:B:2381:TRP:HZ3	2:D:181:MET:HG3	1.55	0.70
1:C:2606:LEU:HD21	1:C:2611:PHE:HA	1.74	0.70
1:B:1144:MET:HE1	1:B:1361:ASN:HB3	1.74	0.70
1:A:2353:TRP:HH2	1:B:2404:MET:HE3	1.56	0.70
1:C:959:SER:OG	1:C:962:ASN:OD1	2.09	0.69
1:C:1144:MET:HE1	1:C:1361:ASN:HB3	1.74	0.69
1:A:959:SER:OG	1:A:962:ASN:OD1	2.09	0.69
1:C:1700:ARG:HG2	1:C:1704:HIS:CE1	2.26	0.69
1:B:2232:PRO:HB2	1:B:2236:MET:HE2	1.73	0.69
1:A:2232:PRO:HB2	1:A:2236:MET:HE2	1.72	0.69
1:A:2717:VAL:HG11	1:A:2725:LEU:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2606:LEU:HD21	1:B:2611:PHE:HA	1.74	0.69
1:A:1144:MET:HE1	1:A:1361:ASN:HB3	1.74	0.69
1:C:1554:PHE:HE2	1:C:2735:PHE:HD2	1.41	0.69
1:C:1388:ALA:HB2	1:C:1406:PRO:HG2	1.74	0.69
1:A:2333:PHE:HE1	2:F:184:SER:HB2	1.58	0.69
1:A:2442:THR:OG1	1:A:2533:SER:OG	2.11	0.69
1:B:2442:THR:OG1	1:B:2533:SER:OG	2.11	0.69
1:A:2606:LEU:HD21	1:A:2611:PHE:HA	1.74	0.68
1:A:1039:ILE:HD13	1:A:1189:PRO:HB2	1.76	0.68
1:B:1554:PHE:HE2	1:B:2735:PHE:HD2	1.41	0.68
1:A:2630:TRP:CH2	1:B:2510:SER:HB3	2.27	0.68
1:B:2717:VAL:HG11	1:B:2725:LEU:HB2	1.73	0.68
1:A:1554:PHE:HE2	1:A:2735:PHE:HD2	1.41	0.68
1:A:2392:ARG:NH2	1:C:2724:GLU:O	2.26	0.68
1:B:1039:ILE:HD13	1:B:1189:PRO:HB2	1.76	0.68
2:F:182:GLU:OE2	1:C:2362:LEU:N	2.27	0.68
1:B:2414:CYS:HA	1:B:2418:PHE:HD2	1.59	0.68
1:C:1687:MET:HE1	1:C:1889:PHE:HB3	1.76	0.68
1:C:1039:ILE:HD13	1:C:1189:PRO:HB2	1.76	0.67
1:C:2414:CYS:HA	1:C:2418:PHE:HD2	1.59	0.67
1:A:2347:LEU:HB3	1:A:2351:MET:HE2	1.77	0.67
1:B:1687:MET:HE1	1:B:1889:PHE:HB3	1.75	0.67
1:A:1687:MET:HE1	1:A:1889:PHE:HB3	1.76	0.67
1:A:2414:CYS:HA	1:A:2418:PHE:HD2	1.59	0.67
1:B:2347:LEU:HB3	1:B:2351:MET:HE2	1.77	0.67
1:C:2480:THR:HA	1:C:2483:MET:HB2	1.77	0.67
1:C:2585:LYS:HB3	1:C:2611:PHE:HB3	1.77	0.67
1:B:2480:THR:HA	1:B:2483:MET:HB2	1.77	0.67
1:A:2466:GLN:O	1:A:2491:LYS:NZ	2.29	0.66
1:C:2347:LEU:HB3	1:C:2351:MET:HE2	1.77	0.66
1:B:2466:GLN:O	1:B:2491:LYS:NZ	2.29	0.66
1:B:2585:LYS:HB3	1:B:2611:PHE:HB3	1.77	0.66
1:C:2466:GLN:O	1:C:2491:LYS:NZ	2.29	0.66
1:A:2381:TRP:HH2	2:F:184:SER:HB3	1.60	0.66
1:A:2585:LYS:HB3	1:A:2611:PHE:HB3	1.77	0.66
1:A:2480:THR:HA	1:A:2483:MET:HB2	1.77	0.65
1:C:2616:ILE:HG22	1:C:2633:LEU:HG	1.78	0.65
1:A:1692:ILE:HD13	1:A:1698:PRO:HD3	1.79	0.65
1:B:1692:ILE:HD13	1:B:1698:PRO:HD3	1.79	0.65
1:C:1308:THR:OG1	1:C:1418:CYS:SG	2.47	0.65
1:B:2504:ASN:OD1	1:B:2505:SER:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2381:TRP:HZ3	2:E:181:MET:HG3	1.60	0.65
1:A:2616:ILE:HG22	1:A:2633:LEU:HG	1.78	0.65
1:C:2236:MET:SD	1:C:2273:TRP:NE1	2.69	0.65
1:B:2362:LEU:N	2:E:182:GLU:OE2	2.30	0.64
1:A:1452:ALA:HB2	1:A:2037:GLY:HA3	1.80	0.64
1:A:2381:TRP:HZ3	2:F:181:MET:HG3	1.61	0.64
1:C:1692:ILE:HD13	1:C:1698:PRO:HD3	1.79	0.64
1:A:2259:LYS:NZ	1:A:2306:SER:OG	2.25	0.64
1:B:2616:ILE:HG22	1:B:2633:LEU:HG	1.78	0.64
1:A:2504:ASN:OD1	1:A:2505:SER:N	2.30	0.64
1:C:976:ALA:HA	1:C:979:ARG:HE	1.63	0.64
1:B:1094:ILE:HG21	1:B:1115:ILE:HG22	1.80	0.63
1:A:976:ALA:HA	1:A:979:ARG:HE	1.63	0.63
1:A:1094:ILE:HG21	1:A:1115:ILE:HG22	1.80	0.63
1:B:1452:ALA:HB2	1:B:2037:GLY:HA3	1.80	0.63
1:C:1094:ILE:HG21	1:C:1115:ILE:HG22	1.80	0.63
1:C:2473:ILE:HG12	1:C:2486:LEU:HD21	1.80	0.63
1:C:2504:ASN:OD1	1:C:2505:SER:N	2.30	0.63
1:B:2723:LEU:HD22	1:C:2395:LYS:NZ	2.13	0.63
1:A:2565:ILE:HG13	1:A:2581:VAL:HG11	1.81	0.63
1:B:2473:ILE:HG12	1:B:2486:LEU:HD21	1.81	0.63
1:A:2236:MET:SD	1:A:2273:TRP:NE1	2.69	0.63
1:B:1095:PHE:HB2	1:B:1097:ASP:CG	2.24	0.63
1:C:1452:ALA:HB2	1:C:2037:GLY:HA3	1.80	0.62
1:C:2565:ILE:HG13	1:C:2581:VAL:HG11	1.81	0.62
1:A:2396:LYS:HB2	1:A:2401:LYS:HD2	1.82	0.62
1:B:976:ALA:HA	1:B:979:ARG:HE	1.63	0.62
1:A:1095:PHE:HB2	1:A:1097:ASP:CG	2.24	0.62
1:A:2473:ILE:HG12	1:A:2486:LEU:HD21	1.81	0.62
1:B:2630:TRP:HZ2	1:C:2512:PRO:HD2	1.63	0.62
1:C:1095:PHE:HB2	1:C:1097:ASP:CG	2.24	0.62
1:C:1282:CYS:HA	1:C:1287:ASP:OD2	2.00	0.62
1:A:1282:CYS:HA	1:A:1287:ASP:OD2	2.00	0.62
1:A:2404:MET:HE1	2:F:182:GLU:CD	2.25	0.62
1:A:2463:VAL:HG13	1:A:2464:MET:H	1.64	0.62
1:B:1541:ASP:O	1:C:2392:ARG:HB2	2.00	0.62
1:B:2259:LYS:NZ	1:B:2306:SER:OG	2.25	0.62
1:A:2512:PRO:HD2	1:C:2630:TRP:CZ2	2.30	0.61
1:B:1390:THR:HG21	1:B:1409:GLU:HA	1.82	0.61
1:C:2463:VAL:HG13	1:C:2464:MET:H	1.64	0.61
1:B:1282:CYS:HA	1:B:1287:ASP:OD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2538:ARG:NH1	1:B:2594:PRO:O	2.33	0.61
1:C:2396:LYS:HB2	1:C:2401:LYS:HD2	1.82	0.61
1:C:2442:THR:OG1	1:C:2533:SER:OG	2.11	0.61
1:C:2003:PRO:CD	1:C:2004:PRO:HD2	2.29	0.61
1:A:950:ILE:HG21	1:A:969:TRP:CD1	2.36	0.61
1:A:2395:LYS:NZ	1:C:2723:LEU:HD22	2.15	0.61
1:B:2396:LYS:HB2	1:B:2401:LYS:HD2	1.82	0.61
1:B:2463:VAL:HG13	1:B:2464:MET:H	1.64	0.61
1:C:1390:THR:HG21	1:C:1409:GLU:HA	1.82	0.61
1:A:2504:ASN:HA	1:B:2513:SER:OG	1.99	0.61
1:B:1492:LYS:NZ	1:B:2728:ASP:OD2	2.27	0.61
1:B:2565:ILE:HG13	1:B:2581:VAL:HG11	1.81	0.61
1:A:2538:ARG:NH1	1:A:2594:PRO:O	2.33	0.61
1:B:1318:MET:HE3	1:B:1318:MET:HA	1.83	0.61
1:B:1962:ARG:HB2	1:B:2042:ASP:HB3	1.83	0.61
1:A:1318:MET:HE3	1:A:1318:MET:HA	1.83	0.61
1:C:1941:ILE:O	1:C:1971:TYR:OH	2.19	0.61
1:C:2538:ARG:NH1	1:C:2594:PRO:O	2.33	0.61
1:A:2482:ALA:C	1:A:2483:MET:HE2	2.26	0.61
1:A:2454:MET:HE3	1:A:2499:LEU:HD12	1.83	0.60
1:C:2482:ALA:C	1:C:2483:MET:HE2	2.26	0.60
1:C:950:ILE:HG21	1:C:969:TRP:CD1	2.36	0.60
1:A:1391:VAL:HB	1:A:1394:TYR:HB2	1.83	0.60
1:B:2482:ALA:C	1:B:2483:MET:HE2	2.26	0.60
1:C:1391:VAL:HB	1:C:1394:TYR:HB2	1.84	0.60
1:A:1390:THR:HG21	1:A:1409:GLU:HA	1.82	0.60
1:B:2454:MET:HE3	1:B:2499:LEU:HD12	1.83	0.60
1:B:2587:TYR:HB3	1:B:2612:MET:HB2	1.84	0.60
1:C:2556:PRO:O	1:C:2557:LEU:HG	2.02	0.60
1:B:2336:GLN:NE2	2:D:184:SER:OG	2.32	0.60
1:C:1318:MET:HA	1:C:1318:MET:HE3	1.83	0.60
1:B:950:ILE:HG21	1:B:969:TRP:CD1	2.36	0.60
1:B:1391:VAL:HB	1:B:1394:TYR:HB2	1.83	0.60
1:A:1350:ILE:HD11	1:A:1422:LEU:HB3	1.84	0.60
1:A:2558:LYS:HD2	1:A:2559:ASN:N	2.16	0.59
1:A:2621:ASP:HB2	1:A:2628:SER:HB2	1.85	0.59
1:B:2236:MET:SD	1:B:2273:TRP:NE1	2.69	0.59
1:B:2602:ILE:HG21	1:B:2605:LEU:HD13	1.84	0.59
1:C:1040:ASP:HB2	1:C:1043:GLU:HG2	1.84	0.59
1:C:2587:TYR:HB3	1:C:2612:MET:HB2	1.84	0.59
1:A:2003:PRO:CD	1:A:2004:PRO:HD2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2602:ILE:HG21	1:A:2605:LEU:HD13	1.84	0.59
1:A:2615:THR:OG1	1:A:2634:ASN:ND2	2.36	0.59
1:B:2558:LYS:HD2	1:B:2559:ASN:N	2.16	0.59
1:C:2440:SER:OG	1:C:2535:SER:HB3	2.03	0.59
1:A:2347:LEU:HD21	1:B:2412:LEU:CD1	2.32	0.59
1:A:2556:PRO:O	1:A:2557:LEU:HG	2.02	0.59
1:C:1962:ARG:HB2	1:C:2042:ASP:HB3	1.83	0.59
1:C:2454:MET:HE3	1:C:2499:LEU:HD12	1.83	0.59
1:A:1454:LEU:HD21	1:A:1880:ALA:HB2	1.85	0.59
1:B:2440:SER:OG	1:B:2535:SER:HB3	2.03	0.59
1:B:1350:ILE:HD11	1:B:1422:LEU:HB3	1.84	0.59
1:B:1454:LEU:HD21	1:B:1880:ALA:HB2	1.85	0.59
1:B:2415:ILE:HG13	1:B:2416:VAL:HG23	1.85	0.59
1:A:1962:ARG:HB2	1:A:2042:ASP:HB3	1.82	0.59
1:A:2440:SER:OG	1:A:2535:SER:HB3	2.03	0.59
1:A:2480:THR:HB	1:A:2484:GLN:HE21	1.67	0.59
1:B:2639:ARG:HB2	1:B:2649:GLU:OE2	2.03	0.59
1:C:2480:THR:HB	1:C:2484:GLN:HE21	1.67	0.59
1:A:2392:ARG:NH1	1:C:2727:GLU:OE1	2.36	0.59
1:C:2639:ARG:HB2	1:C:2649:GLU:OE2	2.03	0.59
1:A:1040:ASP:HB2	1:A:1043:GLU:HG2	1.84	0.58
1:B:2556:PRO:O	1:B:2557:LEU:HG	2.02	0.58
1:C:1454:LEU:HD21	1:C:1880:ALA:HB2	1.85	0.58
1:C:2621:ASP:HB2	1:C:2628:SER:HB2	1.85	0.58
1:B:1281:HIS:O	1:B:1283:ARG:NH1	2.37	0.58
1:C:2558:LYS:HD2	1:C:2559:ASN:N	2.17	0.58
1:C:2602:ILE:HG21	1:C:2605:LEU:HD13	1.84	0.58
1:A:2587:TYR:HB3	1:A:2612:MET:HB2	1.84	0.58
1:A:2377:ILE:HG21	2:F:188:TYR:CD1	2.39	0.58
1:B:2003:PRO:CD	1:B:2004:PRO:HD2	2.29	0.58
1:C:1350:ILE:HD11	1:C:1422:LEU:HB3	1.84	0.58
1:C:1403:CYS:SG	1:C:1404:THR:N	2.76	0.58
1:B:1040:ASP:HB2	1:B:1043:GLU:HG2	1.84	0.58
1:B:2621:ASP:HB2	1:B:2628:SER:HB2	1.85	0.58
1:C:1700:ARG:HG2	1:C:1704:HIS:HE1	1.69	0.58
1:B:2615:THR:OG1	1:B:2634:ASN:ND2	2.35	0.58
1:C:1690:ARG:NH2	1:C:1893:GLU:OE1	2.36	0.58
1:C:2615:THR:OG1	1:C:2634:ASN:ND2	2.35	0.58
1:A:1690:ARG:NH2	1:A:1893:GLU:OE1	2.37	0.58
1:B:2336:GLN:HE21	2:D:184:SER:HG	1.52	0.58
1:C:1205:ASN:O	1:C:1209:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2415:ILE:HG13	1:C:2416:VAL:HG23	1.85	0.58
1:A:2468:SER:O	1:A:2473:ILE:N	2.30	0.58
1:A:2697:MET:HE3	1:A:2740:PRO:HB3	1.86	0.58
1:B:965:PHE:CE1	1:B:1063:MET:HE1	2.39	0.58
1:C:2336:GLN:NE2	2:E:184:SER:OG	2.31	0.58
1:C:2697:MET:HE3	1:C:2740:PRO:HB3	1.86	0.58
1:A:965:PHE:CE1	1:A:1063:MET:HE1	2.39	0.58
1:B:2697:MET:HE3	1:B:2740:PRO:HB3	1.86	0.58
1:C:965:PHE:CE1	1:C:1063:MET:HE1	2.39	0.58
1:A:2510:SER:HB3	1:C:2630:TRP:CH2	2.39	0.58
1:B:2480:THR:HB	1:B:2484:GLN:HE21	1.67	0.58
1:C:1679:THR:O	1:C:1683:ILE:HG12	2.04	0.58
1:C:2404:MET:HE1	2:E:182:GLU:CD	2.29	0.58
1:A:1281:HIS:O	1:A:1283:ARG:NH1	2.37	0.57
1:A:2412:LEU:HD13	1:C:2347:LEU:HD21	1.85	0.57
1:A:2737:TYR:HE2	1:B:2693:SER:HG	1.52	0.57
1:B:1044:TRP:CE3	1:B:1188:PRO:HG3	2.39	0.57
1:B:1403:CYS:SG	1:B:1404:THR:N	2.76	0.57
1:B:1263:MET:HB3	1:B:1340:LYS:HG2	1.86	0.57
1:B:1700:ARG:HG2	1:B:1704:HIS:HE1	1.69	0.57
1:B:2639:ARG:O	1:B:2642:ASN:ND2	2.30	0.57
1:A:1205:ASN:O	1:A:1209:ILE:HG12	2.04	0.57
1:A:1403:CYS:SG	1:A:1404:THR:N	2.76	0.57
1:A:2415:ILE:HG13	1:A:2416:VAL:HG23	1.85	0.57
1:A:1263:MET:HB3	1:A:1340:LYS:HG2	1.86	0.57
1:B:1712:MET:HA	1:B:1712:MET:HE3	1.87	0.57
1:C:1281:HIS:O	1:C:1283:ARG:NH1	2.37	0.57
1:B:1679:THR:O	1:B:1683:ILE:HG12	2.04	0.57
1:B:1690:ARG:NH2	1:B:1893:GLU:OE1	2.37	0.57
1:C:1480:GLN:O	1:C:1484:ILE:HD12	2.04	0.57
1:C:1044:TRP:CE3	1:C:1188:PRO:HG3	2.39	0.57
1:A:2395:LYS:HZ3	1:C:2723:LEU:HD22	1.69	0.57
1:A:2639:ARG:HB2	1:A:2649:GLU:OE2	2.03	0.57
1:A:1679:THR:O	1:A:1683:ILE:HG12	2.04	0.57
1:A:1044:TRP:CE3	1:A:1188:PRO:HG3	2.39	0.56
1:C:1263:MET:HB3	1:C:1340:LYS:HG2	1.86	0.56
1:A:1480:GLN:O	1:A:1484:ILE:HD12	2.04	0.56
1:A:1700:ARG:HG2	1:A:1704:HIS:HE1	1.69	0.56
1:A:1941:ILE:O	1:A:1971:TYR:OH	2.19	0.56
1:A:2381:TRP:CZ3	2:F:181:MET:HG3	2.40	0.56
1:A:2467:GLN:HA	1:A:2470:ASN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2639:ARG:O	1:A:2642:ASN:ND2	2.30	0.56
1:B:1480:GLN:O	1:B:1484:ILE:HD12	2.04	0.56
1:C:1268:ALA:HB2	1:C:1442:LYS:HE3	1.88	0.56
1:C:2404:MET:HE1	2:E:182:GLU:OE1	2.04	0.56
1:C:2467:GLN:HA	1:C:2470:ASN:HB2	1.87	0.56
1:B:1205:ASN:O	1:B:1209:ILE:HG12	2.04	0.56
1:B:2467:GLN:HA	1:B:2470:ASN:HB2	1.87	0.56
1:A:1887:LYS:HD3	1:A:1888:MET:H	1.71	0.56
1:C:1492:LYS:NZ	1:C:2728:ASP:OD2	2.27	0.56
1:A:1712:MET:HE3	1:A:1712:MET:HA	1.87	0.56
1:A:1031:LYS:NZ	1:A:1218:ILE:O	2.39	0.55
1:A:2724:GLU:O	1:B:2392:ARG:NH2	2.39	0.55
1:B:1268:ALA:HB2	1:B:1442:LYS:HE3	1.88	0.55
1:B:1709:ASN:OD1	1:B:1713:ASN:ND2	2.39	0.55
1:C:2259:LYS:NZ	1:C:2306:SER:OG	2.25	0.55
1:C:2468:SER:O	1:C:2473:ILE:N	2.30	0.55
1:A:1492:LYS:NZ	1:A:2728:ASP:OD2	2.27	0.55
1:A:2686:ARG:NH2	1:C:2339:ARG:O	2.39	0.55
1:B:1044:TRP:NE1	1:B:1186:GLY:O	2.39	0.55
1:C:1709:ASN:OD1	1:C:1713:ASN:ND2	2.39	0.55
1:C:1210:LYS:NZ	1:C:1393:GLY:O	2.40	0.55
1:A:1709:ASN:OD1	1:A:1713:ASN:ND2	2.39	0.55
1:A:2737:TYR:HE2	1:B:2693:SER:OG	1.88	0.55
1:B:1887:LYS:HD3	1:B:1888:MET:H	1.70	0.55
1:C:1712:MET:HE3	1:C:1712:MET:HA	1.87	0.55
1:C:1887:LYS:HD3	1:C:1888:MET:H	1.70	0.55
1:B:1121:LYS:NZ	1:B:1257:ASP:O	2.40	0.55
1:B:2468:SER:O	1:B:2473:ILE:N	2.30	0.55
1:B:2630:TRP:CZ2	1:C:2512:PRO:HD2	2.41	0.55
1:C:2489:TYR:CE1	1:C:2654:ASN:HA	2.42	0.55
1:C:2284:ARG:HH21	1:C:2288:GLN:HB3	1.72	0.55
1:A:1196:PRO:HA	1:A:1199:PHE:HD2	1.72	0.55
1:A:1268:ALA:HB2	1:A:1442:LYS:HE3	1.87	0.55
1:A:2450:PRO:HB2	1:A:2453:THR:HG23	1.90	0.55
1:B:1210:LYS:NZ	1:B:1393:GLY:O	2.40	0.55
1:B:2511:PRO:HB2	1:B:2512:PRO:HD3	1.89	0.55
1:A:941:HIS:O	1:A:945:ILE:HD12	2.07	0.54
1:A:1210:LYS:NZ	1:A:1393:GLY:O	2.40	0.54
1:A:2703:ASN:OD1	1:A:2749:GLU:HA	2.07	0.54
1:B:2450:PRO:HB2	1:B:2453:THR:HG23	1.89	0.54
1:B:2489:TYR:CE1	1:B:2654:ASN:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2517:MET:HE2	1:B:2569:ILE:HD13	1.88	0.54
1:C:2703:ASN:OD1	1:C:2749:GLU:HA	2.07	0.54
1:A:2284:ARG:HH21	1:A:2288:GLN:HB3	1.72	0.54
1:C:1031:LYS:NZ	1:C:1218:ILE:O	2.39	0.54
1:A:2511:PRO:HB2	1:A:2512:PRO:HD3	1.89	0.54
1:B:1031:LYS:NZ	1:B:1218:ILE:O	2.39	0.54
1:B:2703:ASN:OD1	1:B:2749:GLU:HA	2.07	0.54
1:C:1444:SER:OG	1:C:1685:ARG:NH1	2.40	0.54
1:A:1044:TRP:NE1	1:A:1186:GLY:O	2.39	0.54
1:A:2189:VAL:HG11	1:A:2305:LEU:HD22	1.90	0.54
1:B:941:HIS:O	1:B:945:ILE:HD12	2.07	0.54
1:B:1894:LEU:O	1:B:1897:SER:OG	2.21	0.54
1:C:2592:LYS:HB2	1:C:2600:LYS:H	1.73	0.54
1:A:1121:LYS:NZ	1:A:1257:ASP:O	2.40	0.54
1:B:2630:TRP:CH2	1:C:2510:SER:HB3	2.42	0.54
1:C:1196:PRO:HA	1:C:1199:PHE:HD2	1.72	0.54
1:C:1121:LYS:NZ	1:C:1257:ASP:O	2.40	0.54
1:C:1950:PHE:HZ	1:C:2300:CYS:HG	1.55	0.54
1:A:2517:MET:HE2	1:A:2569:ILE:HD13	1.88	0.54
1:B:2189:VAL:HG11	1:B:2305:LEU:HD22	1.90	0.54
1:B:2284:ARG:HH21	1:B:2288:GLN:HB3	1.72	0.54
1:C:941:HIS:O	1:C:945:ILE:HD12	2.07	0.54
1:A:957:GLU:HB3	1:A:962:ASN:HD21	1.73	0.54
1:A:1444:SER:OG	1:A:1685:ARG:NH1	2.40	0.54
1:A:2489:TYR:CE1	1:A:2654:ASN:HA	2.42	0.54
1:A:2526:SER:O	1:A:2562:ARG:NH2	2.36	0.54
1:A:2724:GLU:OE2	1:B:2392:ARG:NE	2.41	0.54
1:B:1196:PRO:HA	1:B:1199:PHE:HD2	1.73	0.54
1:C:2511:PRO:HB2	1:C:2512:PRO:HD3	1.89	0.54
1:A:2457:GLN:NE2	1:B:2520:GLU:OE1	2.41	0.54
1:C:2469:PHE:HA	1:C:2473:ILE:HB	1.90	0.54
1:B:1444:SER:OG	1:B:1685:ARG:NH1	2.40	0.53
1:B:2592:LYS:HB2	1:B:2600:LYS:H	1.73	0.53
1:B:2723:LEU:HD22	1:C:2395:LYS:HZ3	1.72	0.53
1:C:1044:TRP:CZ3	1:C:1188:PRO:HG3	2.43	0.53
1:C:2450:PRO:HB2	1:C:2453:THR:HG23	1.89	0.53
1:B:1044:TRP:CZ3	1:B:1188:PRO:HG3	2.43	0.53
1:B:1076:HIS:HA	1:B:1079:TYR:CE1	2.43	0.53
1:C:2189:VAL:HG11	1:C:2305:LEU:HD22	1.90	0.53
1:B:2643:PRO:HD2	1:B:2646:GLN:NE2	2.24	0.53
1:C:957:GLU:HB3	1:C:962:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:TRP:NE1	1:C:1186:GLY:O	2.39	0.53
1:A:1076:HIS:HA	1:A:1079:TYR:CE1	2.43	0.53
1:C:920:PHE:HA	1:C:923:PHE:CE1	2.44	0.53
1:A:951:ILE:HD12	1:A:966:LEU:HD13	1.91	0.53
1:B:920:PHE:HA	1:B:923:PHE:CE1	2.44	0.53
1:C:2692:ILE:HG21	2:E:189:ARG:HH22	1.74	0.53
1:A:2592:LYS:HB2	1:A:2600:LYS:H	1.73	0.53
1:B:957:GLU:HB3	1:B:962:ASN:HD21	1.73	0.53
1:B:2404:MET:HE1	2:D:182:GLU:OE1	2.08	0.53
1:C:2517:MET:HE2	1:C:2569:ILE:HD13	1.89	0.53
1:B:2353:TRP:CZ2	1:C:2401:LYS:HG2	2.44	0.53
1:B:2469:PHE:HA	1:B:2473:ILE:HB	1.91	0.53
1:C:1076:HIS:HA	1:C:1079:TYR:CE1	2.43	0.53
1:A:1044:TRP:CZ3	1:A:1188:PRO:HG3	2.43	0.53
1:A:2402:TYR:OH	1:C:2355:TRP:NE1	2.37	0.53
1:C:951:ILE:HD12	1:C:966:LEU:HD13	1.91	0.53
1:C:2643:PRO:HD2	1:C:2646:GLN:NE2	2.24	0.53
1:A:920:PHE:HA	1:A:923:PHE:CE1	2.44	0.53
1:C:1029:LEU:HD23	1:C:1035:TYR:HD2	1.74	0.53
1:B:1298:PHE:CA	1:B:1425:GLN:HE22	2.23	0.52
1:B:1950:PHE:HZ	1:B:2300:CYS:HG	1.56	0.52
1:A:2479:ASP:O	1:A:2483:MET:HG2	2.10	0.52
1:A:2627:ASN:OD1	1:A:2628:SER:N	2.39	0.52
1:A:2686:ARG:NH1	1:C:2345:THR:OG1	2.43	0.52
1:B:1114:PHE:O	1:B:1118:PHE:N	2.42	0.52
1:B:2526:SER:O	1:B:2562:ARG:NH2	2.36	0.52
1:C:954:SER:O	1:C:1181:TYR:OH	2.18	0.52
1:C:1298:PHE:CA	1:C:1425:GLN:HE22	2.23	0.52
1:A:2469:PHE:HA	1:A:2473:ILE:HB	1.91	0.52
1:A:1298:PHE:CA	1:A:1425:GLN:HE22	2.22	0.52
1:A:1894:LEU:O	1:A:1897:SER:OG	2.21	0.52
1:B:2410:VAL:HA	1:B:2413:ILE:HG22	1.92	0.52
1:C:2336:GLN:HE21	2:E:184:SER:HG	1.56	0.52
1:C:2479:ASP:O	1:C:2483:MET:HG2	2.10	0.52
1:A:1029:LEU:HD23	1:A:1035:TYR:HD2	1.74	0.52
1:A:2211:PHE:CE2	1:A:2236:MET:HE3	2.45	0.52
1:B:2232:PRO:HA	1:B:2235:VAL:HG22	1.91	0.52
1:C:2211:PHE:CE2	1:C:2236:MET:HE3	2.45	0.52
1:A:1294:PHE:CE2	1:A:1433:TYR:HB2	2.45	0.52
1:A:2232:PRO:HA	1:A:2235:VAL:HG22	1.91	0.52
1:A:2410:VAL:HA	1:A:2413:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2643:PRO:HD2	1:A:2646:GLN:NE2	2.24	0.52
1:B:1294:PHE:CE2	1:B:1433:TYR:HB2	2.45	0.52
1:B:2211:PHE:CE2	1:B:2236:MET:HE3	2.44	0.52
1:C:1114:PHE:O	1:C:1118:PHE:N	2.43	0.52
1:C:2639:ARG:O	1:C:2642:ASN:ND2	2.30	0.52
1:A:1114:PHE:O	1:A:1118:PHE:N	2.42	0.52
1:B:2404:MET:HE1	2:D:182:GLU:CD	2.35	0.52
1:C:2410:VAL:HA	1:C:2413:ILE:HG22	1.92	0.52
1:A:2339:ARG:O	1:B:2686:ARG:NH2	2.43	0.52
1:B:2479:ASP:O	1:B:2483:MET:HG2	2.10	0.52
1:B:2692:ILE:HG21	2:D:189:ARG:HH22	1.75	0.52
1:C:1294:PHE:CE2	1:C:1433:TYR:HB2	2.45	0.52
1:C:2526:SER:O	1:C:2562:ARG:NH2	2.36	0.52
1:B:1316:PHE:O	1:B:1352:TYR:OH	2.28	0.51
1:C:1316:PHE:O	1:C:1352:TYR:OH	2.28	0.51
1:C:2232:PRO:HA	1:C:2235:VAL:HG22	1.91	0.51
1:A:1933:ASN:ND2	1:A:2022:GLN:OE1	2.43	0.51
1:C:1138:ARG:HH22	1:C:1180:GLN:CD	2.18	0.51
1:A:1138:ARG:HH22	1:A:1180:GLN:CD	2.18	0.51
1:C:1456:GLN:O	1:C:1459:ILE:HG22	2.11	0.51
1:A:1950:PHE:HZ	1:A:2300:CYS:HG	1.56	0.51
1:C:2468:SER:HA	1:C:2472:PHE:HB3	1.93	0.51
1:A:2394:GLN:O	1:C:2359:THR:HG22	2.10	0.51
1:B:1138:ARG:HH22	1:B:1180:GLN:CD	2.18	0.51
1:A:2463:VAL:HG13	1:A:2464:MET:N	2.26	0.51
1:B:2015:TYR:CD2	1:B:2016:VAL:HG13	2.46	0.51
1:A:1219:VAL:HB	1:A:1395:GLN:HE21	1.76	0.51
1:B:1029:LEU:HD23	1:B:1035:TYR:HD2	1.74	0.51
1:C:2015:TYR:CD2	1:C:2016:VAL:HG13	2.46	0.51
1:C:2627:ASN:OD1	1:C:2628:SER:N	2.39	0.51
1:B:951:ILE:HD12	1:B:966:LEU:HD13	1.91	0.51
1:B:1456:GLN:O	1:B:1459:ILE:HG22	2.11	0.51
1:A:1134:VAL:HG11	1:A:1146:HIS:CD2	2.46	0.51
1:A:1456:GLN:O	1:A:1459:ILE:HG22	2.11	0.51
1:B:2551:ASP:OD1	1:B:2552:LYS:N	2.44	0.51
1:A:1488:GLN:HG3	1:A:2725:LEU:HD22	1.93	0.50
1:A:2015:TYR:CD2	1:A:2016:VAL:HG13	2.46	0.50
1:B:1488:GLN:HG3	1:B:2725:LEU:HD22	1.93	0.50
1:B:1705:MET:N	1:B:1705:MET:HE2	2.26	0.50
1:C:1488:GLN:HG3	1:C:2725:LEU:HD22	1.93	0.50
1:C:1933:ASN:ND2	1:C:2022:GLN:OE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2404:MET:HE3	1:C:2353:TRP:HH2	1.76	0.50
1:A:2559:ASN:HB3	1:A:2560:ILE:HD12	1.94	0.50
1:B:2345:THR:OG1	1:C:2686:ARG:NH1	2.44	0.50
1:A:2522:LEU:HA	1:A:2563:LYS:NZ	2.27	0.50
1:B:1134:VAL:HG11	1:B:1146:HIS:CD2	2.46	0.50
1:C:997:LYS:NZ	1:C:1047:LEU:HD13	2.27	0.50
1:C:1934:HIS:ND1	1:C:1942:THR:O	2.44	0.50
1:A:1934:HIS:ND1	1:A:1942:THR:O	2.45	0.50
1:C:1894:LEU:O	1:C:1897:SER:OG	2.21	0.50
1:C:2559:ASN:HB3	1:C:2560:ILE:HD12	1.94	0.50
1:C:2702:PRO:HG2	1:C:2747:THR:O	2.12	0.50
1:C:1134:VAL:HG11	1:C:1146:HIS:CD2	2.46	0.50
1:B:2343:PHE:O	1:B:2347:LEU:HD23	2.12	0.50
1:C:2463:VAL:HG13	1:C:2464:MET:N	2.26	0.50
1:A:997:LYS:NZ	1:A:1047:LEU:HD13	2.27	0.50
1:A:2442:THR:HB	1:A:2453:THR:HG22	1.94	0.50
1:A:2468:SER:HA	1:A:2472:PHE:HB3	1.93	0.50
1:B:1081:ARG:HH12	1:B:1088:ALA:HB3	1.77	0.50
1:C:1705:MET:HE2	1:C:1705:MET:N	2.26	0.50
1:C:2343:PHE:O	1:C:2347:LEU:HD23	2.12	0.50
1:C:2378:LEU:HB3	1:C:2704:VAL:HG21	1.93	0.50
1:A:2343:PHE:O	1:A:2347:LEU:HD23	2.12	0.50
1:A:2547:GLU:HG3	1:A:2548:ILE:HG13	1.93	0.50
1:B:1131:SER:OG	1:B:1150:LEU:HD13	2.12	0.50
1:C:2547:GLU:HG3	1:C:2548:ILE:HG13	1.93	0.50
1:A:1699:THR:O	1:A:1702:SER:OG	2.24	0.49
1:A:1705:MET:HE2	1:A:1705:MET:N	2.26	0.49
1:B:1542:HIS:CE1	1:C:2390:GLN:C	2.90	0.49
1:A:2646:GLN:HG3	1:A:2647:ALA:N	2.27	0.49
1:B:997:LYS:NZ	1:B:1047:LEU:HD13	2.27	0.49
1:B:1545:MET:HE3	1:C:2392:ARG:NH2	2.28	0.49
1:B:2442:THR:HB	1:B:2453:THR:HG22	1.94	0.49
1:B:2468:SER:HA	1:B:2472:PHE:HB3	1.93	0.49
1:C:1280:ILE:HD13	1:C:1440:ASP:HB2	1.93	0.49
1:C:1349:LEU:HG	1:C:1422:LEU:HD21	1.94	0.49
1:A:1280:ILE:HD13	1:A:1440:ASP:HB2	1.93	0.49
1:A:1305:ILE:HD11	1:A:1422:LEU:HD11	1.95	0.49
1:A:2400:VAL:HG12	1:A:2404:MET:HE2	1.94	0.49
2:F:172:GLU:CD	2:F:173:THR:H	2.21	0.49
1:B:1219:VAL:HB	1:B:1395:GLN:HE21	1.76	0.49
1:B:1934:HIS:ND1	1:B:1942:THR:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2400:VAL:HG12	1:B:2404:MET:HE2	1.94	0.49
1:B:2463:VAL:HG13	1:B:2464:MET:N	2.26	0.49
1:B:2559:ASN:HB3	1:B:2560:ILE:HD12	1.94	0.49
1:B:2646:GLN:HG3	1:B:2647:ALA:N	2.27	0.49
2:E:172:GLU:CD	2:E:173:THR:H	2.21	0.49
1:A:2507:TRP:CZ3	1:A:2514:LYS:HE2	2.48	0.49
1:A:2702:PRO:HG2	1:A:2747:THR:O	2.12	0.49
1:B:2507:TRP:CZ3	1:B:2514:LYS:HE2	2.48	0.49
1:C:1450:ARG:O	1:C:1453:GLU:HG2	2.13	0.49
1:A:1349:LEU:HG	1:A:1422:LEU:HD21	1.94	0.49
1:A:2353:TRP:CH2	1:B:2404:MET:HE3	2.44	0.49
1:A:2378:LEU:HB3	1:A:2704:VAL:HG21	1.93	0.49
1:A:2440:SER:HG	1:A:2535:SER:HB3	1.77	0.49
1:B:1280:ILE:HD13	1:B:1440:ASP:HB2	1.93	0.49
1:B:2702:PRO:HG2	1:B:2747:THR:O	2.12	0.49
1:C:2522:LEU:HA	1:C:2563:LYS:NZ	2.27	0.49
1:B:2378:LEU:HB3	1:B:2704:VAL:HG21	1.93	0.49
1:B:2547:GLU:HG3	1:B:2548:ILE:HG13	1.93	0.49
1:C:2442:THR:HB	1:C:2453:THR:HG22	1.94	0.49
1:A:1450:ARG:O	1:A:1453:GLU:HG2	2.13	0.49
1:C:1001:GLN:HG3	1:C:1051:SER:HB3	1.95	0.49
1:B:960:LEU:HB2	1:B:1185:ILE:HD11	1.95	0.49
1:B:1450:ARG:O	1:B:1453:GLU:HG2	2.13	0.49
1:B:1933:ASN:ND2	1:B:2022:GLN:OE1	2.43	0.49
1:A:1081:ARG:HH12	1:A:1088:ALA:HB3	1.77	0.49
1:A:1131:SER:OG	1:A:1150:LEU:HD13	2.12	0.49
1:B:954:SER:O	1:B:1181:TYR:OH	2.18	0.49
1:B:2489:TYR:CZ	1:B:2654:ASN:HA	2.48	0.49
1:B:2742:THR:HG22	1:B:2745:LYS:HE2	1.95	0.49
1:A:1179:PHE:CE2	1:A:1183:ILE:HD11	2.48	0.49
1:B:1179:PHE:CE2	1:B:1183:ILE:HD11	2.48	0.49
1:C:1131:SER:OG	1:C:1150:LEU:HD13	2.12	0.49
1:C:1219:VAL:HB	1:C:1395:GLN:HE21	1.76	0.49
1:B:2454:MET:SD	1:B:2500:GLU:HB3	2.53	0.48
1:C:1305:ILE:HD11	1:C:1422:LEU:HD11	1.95	0.48
1:C:2329:TYR:OH	1:C:2384:SER:OG	2.24	0.48
1:A:1001:GLN:HG3	1:A:1051:SER:HB3	1.95	0.48
1:B:1542:HIS:ND1	1:C:2390:GLN:O	2.46	0.48
1:B:2372:TYR:HB2	1:B:2711:CYS:SG	2.53	0.48
2:D:172:GLU:CD	2:D:173:THR:H	2.21	0.48
1:A:1123:GLY:O	1:A:1126:THR:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:GLN:HG3	1:B:1051:SER:HB3	1.95	0.48
1:B:1936:VAL:HG11	1:B:2018:TYR:CE2	2.49	0.48
1:B:2522:LEU:HA	1:B:2563:LYS:NZ	2.27	0.48
1:B:1543:ALA:HB2	1:C:2391:PRO:O	2.13	0.48
1:B:1699:THR:O	1:B:1702:SER:OG	2.24	0.48
1:B:2375:ILE:HG23	1:B:2704:VAL:HB	1.95	0.48
1:C:934:MET:N	1:C:934:MET:HE2	2.29	0.48
1:A:1154:LEU:O	1:A:1157:ARG:HD2	2.13	0.48
1:C:2372:TYR:HB2	1:C:2711:CYS:SG	2.53	0.48
1:C:2507:TRP:CZ3	1:C:2514:LYS:HE2	2.48	0.48
1:A:1706:TYR:C	1:A:1710:HIS:HD1	2.18	0.48
1:A:2489:TYR:CZ	1:A:2654:ASN:HA	2.48	0.48
1:A:2551:ASP:OD1	1:A:2552:LYS:N	2.44	0.48
1:A:2630:TRP:HZ2	1:B:2512:PRO:CD	2.17	0.48
1:B:1666:TRP:CZ2	1:B:1670:ILE:HD11	2.49	0.48
1:C:974:PRO:O	1:C:1240:ARG:NH2	2.47	0.48
1:C:2400:VAL:HG12	1:C:2404:MET:HE2	1.94	0.48
1:A:974:PRO:O	1:A:1240:ARG:NH2	2.47	0.48
1:B:974:PRO:HB2	1:B:975:TYR:CD1	2.49	0.48
1:B:1349:LEU:HG	1:B:1422:LEU:HD21	1.94	0.48
1:C:2616:ILE:HD12	1:C:2631:TRP:CZ3	2.49	0.48
1:A:954:SER:O	1:A:1181:TYR:OH	2.18	0.48
1:B:950:ILE:HD13	1:B:969:TRP:CD1	2.49	0.48
1:B:1962:ARG:N	1:B:2042:ASP:OD2	2.47	0.48
1:C:1081:ARG:HH12	1:C:1088:ALA:HB3	1.77	0.48
1:C:1205:ASN:O	1:C:1208:ILE:HG22	2.14	0.48
1:A:1666:TRP:CZ2	1:A:1670:ILE:HD11	2.49	0.48
1:B:1305:ILE:HD11	1:B:1422:LEU:HD11	1.95	0.48
1:B:1941:ILE:O	1:B:1971:TYR:OH	2.19	0.48
1:B:2592:LYS:HA	1:B:2654:ASN:OD1	2.14	0.48
1:C:1154:LEU:O	1:C:1157:ARG:HD2	2.13	0.48
1:C:1179:PHE:CE2	1:C:1183:ILE:HD11	2.48	0.48
1:C:1706:TYR:C	1:C:1710:HIS:HD1	2.18	0.48
1:C:2646:GLN:HG3	1:C:2647:ALA:N	2.27	0.48
1:C:2744:ILE:O	1:C:2748:ARG:HG3	2.14	0.48
1:A:2372:TYR:HB2	1:A:2711:CYS:SG	2.53	0.48
1:A:2616:ILE:HD12	1:A:2631:TRP:CZ3	2.49	0.48
1:B:1205:ASN:O	1:B:1208:ILE:HG22	2.13	0.48
1:B:2744:ILE:O	1:B:2748:ARG:HG3	2.14	0.48
1:A:1962:ARG:N	1:A:2042:ASP:OD2	2.47	0.47
1:C:974:PRO:HB2	1:C:975:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1274:ASN:OD1	1:C:1276:VAL:HG22	2.14	0.47
1:C:1962:ARG:N	1:C:2042:ASP:OD2	2.47	0.47
1:C:2551:ASP:OD1	1:C:2552:LYS:N	2.44	0.47
1:A:974:PRO:HB2	1:A:975:TYR:CD1	2.49	0.47
1:A:1274:ASN:OD1	1:A:1276:VAL:HG22	2.14	0.47
1:B:934:MET:HE2	1:B:934:MET:N	2.29	0.47
1:B:1197:TRP:HE1	1:B:1216:ASP:HB2	1.79	0.47
1:C:1666:TRP:CZ2	1:C:1670:ILE:HD11	2.49	0.47
1:C:1936:VAL:HG11	1:C:2018:TYR:CE2	2.49	0.47
1:A:960:LEU:HB2	1:A:1185:ILE:HD11	1.95	0.47
1:A:1205:ASN:O	1:A:1208:ILE:HG22	2.13	0.47
1:B:974:PRO:O	1:B:1240:ARG:NH2	2.47	0.47
1:C:1112:LYS:O	1:C:1116:ASN:ND2	2.48	0.47
1:C:1899:LYS:HA	1:C:1902:VAL:HG22	1.96	0.47
1:C:1948:LEU:HD12	1:C:1948:LEU:HA	1.56	0.47
1:C:2489:TYR:CZ	1:C:2654:ASN:HA	2.48	0.47
1:A:1144:MET:HE1	1:A:1361:ASN:CB	2.43	0.47
1:A:2454:MET:SD	1:A:2500:GLU:HB3	2.53	0.47
1:A:2574:THR:O	1:A:2578:LYS:HG2	2.14	0.47
1:C:1123:GLY:O	1:C:1126:THR:N	2.45	0.47
1:C:1197:TRP:HE1	1:C:1216:ASP:HB2	1.80	0.47
1:A:934:MET:N	1:A:934:MET:HE2	2.29	0.47
1:A:1061:LEU:HD22	1:A:1064:LEU:HD12	1.96	0.47
1:A:2353:TRP:HH2	1:B:2404:MET:CE	2.27	0.47
1:A:2381:TRP:CH2	2:F:184:SER:HB3	2.46	0.47
1:A:2417:TRP:CZ2	1:C:2234:LEU:HG	2.50	0.47
1:B:2574:THR:O	1:B:2578:LYS:HG2	2.14	0.47
1:C:1029:LEU:HD23	1:C:1035:TYR:CD2	2.50	0.47
1:C:1982:PHE:HD2	1:C:2009:VAL:HG21	1.79	0.47
1:C:2454:MET:SD	1:C:2500:GLU:HB3	2.53	0.47
1:C:2574:THR:O	1:C:2578:LYS:HG2	2.14	0.47
1:A:950:ILE:HD13	1:A:969:TRP:CD1	2.49	0.47
1:A:1306:PHE:CD1	1:A:2020:LEU:HD13	2.50	0.47
1:A:1936:VAL:HG11	1:A:2018:TYR:CE2	2.49	0.47
1:B:1481:MET:HE3	1:B:1481:MET:HB3	1.68	0.47
1:C:950:ILE:HD13	1:C:969:TRP:CD1	2.49	0.47
1:C:960:LEU:HB2	1:C:1185:ILE:HD11	1.95	0.47
1:A:1290:LYS:O	1:A:1294:PHE:HD1	1.98	0.47
1:A:1666:TRP:CE2	1:A:1670:ILE:HD11	2.50	0.47
1:A:2592:LYS:HA	1:A:2654:ASN:OD1	2.14	0.47
1:A:2742:THR:HG22	1:A:2745:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2744:ILE:O	1:A:2748:ARG:HG3	2.14	0.47
1:B:1061:LEU:HD22	1:B:1064:LEU:HD12	1.96	0.47
1:B:1154:LEU:O	1:B:1157:ARG:HD2	2.13	0.47
1:B:1306:PHE:CD1	1:B:2020:LEU:HD13	2.50	0.47
1:B:1365:ILE:O	1:B:1369:GLY:N	2.48	0.47
1:B:1899:LYS:HA	1:B:1902:VAL:HG22	1.96	0.47
1:B:2616:ILE:HD12	1:B:2631:TRP:CZ3	2.49	0.47
1:C:2440:SER:HG	1:C:2535:SER:HB3	1.79	0.47
1:A:2375:ILE:HG23	1:A:2704:VAL:HB	1.95	0.47
1:B:1290:LYS:O	1:B:1294:PHE:HD1	1.98	0.47
1:C:1306:PHE:CD1	1:C:2020:LEU:HD13	2.50	0.47
1:A:1197:TRP:HE1	1:A:1216:ASP:HB2	1.79	0.47
1:B:1192:CYS:SG	1:B:1193:ARG:N	2.86	0.47
1:B:1301:VAL:HG22	1:B:1421:PHE:HB3	1.97	0.47
1:C:1290:LYS:O	1:C:1294:PHE:HD1	1.98	0.47
1:C:2592:LYS:HD2	1:C:2654:ASN:CG	2.40	0.47
1:A:1365:ILE:O	1:A:1369:GLY:N	2.48	0.47
1:A:1899:LYS:HA	1:A:1902:VAL:HG22	1.96	0.47
1:B:1982:PHE:HD2	1:B:2009:VAL:HG21	1.79	0.47
1:B:2467:GLN:CB	1:B:2470:ASN:HB2	2.45	0.47
1:C:2592:LYS:HA	1:C:2654:ASN:OD1	2.14	0.47
1:A:1982:PHE:HD2	1:A:2009:VAL:HG21	1.80	0.46
1:B:1112:LYS:O	1:B:1116:ASN:ND2	2.47	0.46
1:B:2528:PHE:HB3	1:B:2557:LEU:HD12	1.97	0.46
1:C:966:LEU:HD23	1:C:1181:TYR:CG	2.50	0.46
1:C:2375:ILE:HG23	1:C:2704:VAL:HB	1.95	0.46
1:A:1542:HIS:ND1	1:B:2389:PRO:HB2	2.30	0.46
1:A:1948:LEU:HD12	1:A:1948:LEU:HA	1.56	0.46
1:A:2326:SER:OG	1:A:2331:ASN:OD1	2.26	0.46
1:A:2444:THR:HA	1:A:2450:PRO:HA	1.97	0.46
1:B:1123:GLY:O	1:B:1126:THR:N	2.45	0.46
1:B:1274:ASN:OD1	1:B:1276:VAL:HG22	2.14	0.46
1:C:2742:THR:HG22	1:C:2745:LYS:HE2	1.96	0.46
1:A:966:LEU:HD23	1:A:1181:TYR:CG	2.50	0.46
1:A:1887:LYS:HD3	1:A:1888:MET:N	2.30	0.46
1:A:1889:PHE:CE1	1:A:1891:ASP:HB3	2.51	0.46
1:A:2343:PHE:HB3	1:B:2412:LEU:HD11	1.97	0.46
1:A:2396:LYS:HA	1:A:2396:LYS:HD2	1.74	0.46
1:A:2592:LYS:HD2	1:A:2654:ASN:CG	2.40	0.46
1:B:1144:MET:HE1	1:B:1361:ASN:CB	2.43	0.46
1:B:2444:THR:HA	1:B:2450:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2606:LEU:HD11	1:B:2612:MET:HE3	1.98	0.46
1:B:2630:TRP:O	1:B:2631:TRP:CD1	2.68	0.46
1:C:1041:PRO:O	1:C:1045:VAL:HG22	2.15	0.46
1:C:1365:ILE:O	1:C:1369:GLY:N	2.48	0.46
1:C:1673:GLU:O	1:C:1677:ILE:HG13	2.15	0.46
1:C:1936:VAL:HG11	1:C:2018:TYR:HE2	1.81	0.46
1:C:2630:TRP:O	1:C:2631:TRP:CD1	2.68	0.46
1:A:1112:LYS:O	1:A:1116:ASN:ND2	2.48	0.46
1:A:2367:CYS:SG	1:B:2696:ILE:HD11	2.55	0.46
1:B:1666:TRP:CE2	1:B:1670:ILE:HD11	2.50	0.46
1:B:1938:ALA:HB2	1:B:2286:PHE:HD2	1.81	0.46
1:B:2627:ASN:OD1	1:B:2628:SER:N	2.39	0.46
1:C:1666:TRP:CE2	1:C:1670:ILE:HD11	2.50	0.46
1:C:1889:PHE:CE1	1:C:1891:ASP:HB3	2.51	0.46
1:C:2692:ILE:HG21	2:E:189:ARG:NH2	2.30	0.46
1:A:1304:ILE:HG22	1:A:1418:CYS:SG	2.56	0.46
1:A:1308:THR:OG1	1:A:1418:CYS:SG	2.47	0.46
1:A:1687:MET:O	1:A:1691:GLU:HG2	2.16	0.46
1:B:1673:GLU:O	1:B:1677:ILE:HG13	2.15	0.46
1:B:2468:SER:OG	1:B:2469:PHE:N	2.49	0.46
1:C:1304:ILE:HG22	1:C:1418:CYS:SG	2.56	0.46
1:A:1029:LEU:HD23	1:A:1035:TYR:CD2	2.50	0.46
1:A:1940:MET:HB3	1:A:2007:ILE:HD12	1.98	0.46
1:A:2468:SER:OG	1:A:2469:PHE:N	2.48	0.46
1:A:2552:LYS:O	1:A:2553:LEU:HD23	2.16	0.46
1:B:1024:ILE:HG23	1:B:1028:GLU:HB2	1.98	0.46
1:B:2558:LYS:HE2	1:B:2584:GLU:OE2	2.16	0.46
1:A:2630:TRP:O	1:A:2631:TRP:CD1	2.68	0.46
1:B:1048:ARG:H	1:B:1048:ARG:HD3	1.81	0.46
1:B:1940:MET:HB3	1:B:2007:ILE:HD12	1.98	0.46
1:C:938:LEU:O	1:C:942:ILE:HB	2.16	0.46
1:C:1061:LEU:HD22	1:C:1064:LEU:HD12	1.96	0.46
1:C:1940:MET:HB3	1:C:2007:ILE:HD12	1.98	0.46
1:A:1689:THR:HA	1:A:1692:ILE:HG22	1.98	0.46
1:A:2333:PHE:CE1	2:F:184:SER:HB2	2.44	0.46
1:A:2359:THR:HG22	1:B:2394:GLN:O	2.16	0.46
1:B:1687:MET:O	1:B:1691:GLU:HG2	2.16	0.46
1:C:2558:LYS:HE2	1:C:2584:GLU:OE2	2.16	0.46
1:C:2568:MET:SD	1:C:2618:LEU:N	2.87	0.46
1:A:1301:VAL:HG22	1:A:1421:PHE:HB3	1.97	0.46
1:B:1887:LYS:HD3	1:B:1888:MET:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2568:MET:SD	1:B:2618:LEU:N	2.87	0.46
1:C:1301:VAL:HG22	1:C:1421:PHE:HB3	1.97	0.46
1:C:2438:ASP:OD1	1:C:2456:ALA:HB3	2.16	0.46
1:C:2463:VAL:CG1	1:C:2464:MET:H	2.29	0.46
1:A:1938:ALA:HB2	1:A:2286:PHE:HD2	1.81	0.46
1:C:1029:LEU:O	1:C:1036:SER:OG	2.30	0.46
1:C:1887:LYS:HD3	1:C:1888:MET:N	2.30	0.46
1:C:2440:SER:HA	1:C:2455:SER:O	2.16	0.46
1:C:2467:GLN:CB	1:C:2470:ASN:HB2	2.45	0.46
1:A:938:LEU:O	1:A:942:ILE:HB	2.16	0.45
1:A:1477:LEU:HD21	1:A:2720:THR:HG22	1.98	0.45
1:A:1895:GLU:HB3	1:A:1899:LYS:HZ3	1.80	0.45
1:A:2438:ASP:OD1	1:A:2456:ALA:HB3	2.16	0.45
1:A:2467:GLN:CB	1:A:2470:ASN:HB2	2.45	0.45
1:B:1029:LEU:HD23	1:B:1035:TYR:CD2	2.50	0.45
1:B:1889:PHE:CE1	1:B:1891:ASP:HB3	2.51	0.45
1:B:2440:SER:HA	1:B:2455:SER:O	2.16	0.45
1:B:2643:PRO:HG2	1:B:2646:GLN:CD	2.42	0.45
1:C:1048:ARG:H	1:C:1048:ARG:HD3	1.80	0.45
1:C:1938:ALA:HB2	1:C:2286:PHE:HD2	1.81	0.45
1:C:2552:LYS:O	1:C:2553:LEU:HD23	2.16	0.45
1:C:2621:ASP:HB2	1:C:2628:SER:CB	2.46	0.45
1:A:1098:ILE:HG23	1:A:1102:HIS:HB3	1.99	0.45
1:A:1673:GLU:O	1:A:1677:ILE:HG13	2.15	0.45
1:B:1304:ILE:HG22	1:B:1418:CYS:SG	2.56	0.45
1:B:1477:LEU:HD21	1:B:2720:THR:HG22	1.98	0.45
1:B:1936:VAL:HG11	1:B:2018:TYR:HE2	1.81	0.45
1:B:2592:LYS:HD2	1:B:2654:ASN:CG	2.40	0.45
1:B:2621:ASP:HB2	1:B:2628:SER:CB	2.46	0.45
1:C:1144:MET:HE1	1:C:1361:ASN:CB	2.43	0.45
1:C:1687:MET:O	1:C:1691:GLU:HG2	2.16	0.45
1:C:1878:LEU:HG	1:C:1882:GLU:HB2	1.99	0.45
1:C:2444:THR:HA	1:C:2450:PRO:HA	1.96	0.45
1:A:1100:ARG:HB2	1:A:1256:GLY:H	1.82	0.45
1:A:2346:GLU:OE2	1:B:2686:ARG:HA	2.16	0.45
1:A:2486:LEU:HG	1:A:2487:GLU:H	1.82	0.45
1:A:2558:LYS:HE2	1:A:2584:GLU:OE2	2.16	0.45
1:A:2643:PRO:HG2	1:A:2646:GLN:CD	2.42	0.45
1:B:1108:ILE:O	1:B:1112:LYS:HG3	2.16	0.45
1:B:1555:GLU:O	1:B:1557:ASP:N	2.48	0.45
1:C:1317:CYS:HB2	1:C:1980:TYR:OH	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1878:LEU:HG	1:A:1882:GLU:HB2	1.99	0.45
1:B:966:LEU:HD23	1:B:1181:TYR:CG	2.50	0.45
1:B:1041:PRO:O	1:B:1045:VAL:HG22	2.15	0.45
1:B:1098:ILE:HG23	1:B:1102:HIS:HB3	1.98	0.45
1:B:1100:ARG:HB2	1:B:1256:GLY:H	1.82	0.45
1:C:2643:PRO:HG2	1:C:2646:GLN:CD	2.42	0.45
1:A:1108:ILE:O	1:A:1112:LYS:HG3	2.16	0.45
1:A:1317:CYS:HB2	1:A:1980:TYR:OH	2.16	0.45
1:A:2592:LYS:HD2	1:A:2654:ASN:OD1	2.17	0.45
1:A:2727:GLU:OE1	1:B:2392:ARG:NH1	2.49	0.45
1:B:1706:TYR:C	1:B:1710:HIS:HD1	2.18	0.45
1:B:1878:LEU:HG	1:B:1882:GLU:HB2	1.99	0.45
1:B:2391:PRO:HB2	1:B:2394:GLN:HG2	1.99	0.45
1:B:2463:VAL:CG1	1:B:2464:MET:H	2.29	0.45
1:C:2468:SER:OG	1:C:2469:PHE:N	2.48	0.45
1:C:2606:LEU:HD11	1:C:2612:MET:HE3	1.98	0.45
1:A:2528:PHE:HB3	1:A:2557:LEU:HD12	1.97	0.45
1:B:985:VAL:HA	1:B:988:VAL:HG22	1.99	0.45
1:B:1317:CYS:HB2	1:B:1980:TYR:OH	2.16	0.45
1:C:1100:ARG:HB2	1:C:1256:GLY:H	1.82	0.45
1:C:1192:CYS:SG	1:C:1193:ARG:N	2.86	0.45
1:C:1477:LEU:HD21	1:C:2720:THR:HG22	1.99	0.45
1:C:2003:PRO:HD2	1:C:2004:PRO:CD	2.37	0.45
1:A:1041:PRO:O	1:A:1045:VAL:HG22	2.15	0.45
1:A:1936:VAL:HG11	1:A:2018:TYR:HE2	1.81	0.45
1:B:1360:LYS:HD3	1:B:1410:ALA:HB1	1.99	0.45
1:B:1689:THR:HA	1:B:1692:ILE:HG22	1.98	0.45
1:B:2486:LEU:HG	1:B:2487:GLU:H	1.82	0.45
1:C:1108:ILE:O	1:C:1112:LYS:HG3	2.16	0.45
1:C:2391:PRO:HB2	1:C:2394:GLN:HG2	1.99	0.45
1:A:1048:ARG:H	1:A:1048:ARG:HD3	1.81	0.45
1:B:2266:LEU:HD12	1:B:2266:LEU:HA	1.80	0.45
1:B:2727:GLU:OE1	1:C:2392:ARG:NH1	2.49	0.45
1:C:1098:ILE:HG23	1:C:1102:HIS:HB3	1.98	0.45
1:C:2528:PHE:HB3	1:C:2557:LEU:HD12	1.97	0.45
1:A:1024:ILE:HG23	1:A:1028:GLU:HB2	1.98	0.45
1:A:1125:GLU:OE1	1:A:1125:GLU:N	2.47	0.45
1:A:1895:GLU:HB3	1:A:1899:LYS:NZ	2.32	0.45
1:A:2378:LEU:O	1:A:2382:ARG:HG2	2.17	0.45
1:A:2404:MET:HE1	2:F:182:GLU:OE1	2.16	0.45
1:A:2440:SER:HA	1:A:2455:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1447:LEU:HB3	1:A:1681:LEU:HD22	1.99	0.45
1:B:938:LEU:O	1:B:942:ILE:HB	2.16	0.45
1:B:2552:LYS:O	1:B:2553:LEU:HD23	2.16	0.45
1:C:1699:THR:O	1:C:1702:SER:OG	2.24	0.45
1:C:2404:MET:SD	2:E:182:GLU:HB3	2.57	0.45
1:C:2619:SER:O	1:C:2630:TRP:HB2	2.17	0.45
1:A:2448:TYR:OH	1:A:2516:LYS:HD2	2.17	0.44
1:B:956:LYS:HD2	1:B:956:LYS:HA	1.77	0.44
1:B:2511:PRO:O	1:B:2514:LYS:HB3	2.17	0.44
1:C:1360:LYS:HD3	1:C:1410:ALA:HB1	1.99	0.44
1:C:2037:GLY:O	1:C:2038:LEU:HG	2.18	0.44
1:C:2486:LEU:HG	1:C:2487:GLU:H	1.82	0.44
1:C:2500:GLU:HG2	1:C:2501:GLY:N	2.32	0.44
1:C:2734:ILE:HD13	1:C:2734:ILE:HA	1.83	0.44
1:B:963:TYR:O	1:B:967:ILE:HG12	2.17	0.44
1:B:1027:ASN:ND2	1:B:1030:ASN:OD1	2.51	0.44
1:B:2404:MET:SD	2:D:182:GLU:HB3	2.57	0.44
1:B:2500:GLU:HG2	1:B:2501:GLY:N	2.32	0.44
1:B:2619:SER:O	1:B:2630:TRP:HB2	2.17	0.44
1:C:1024:ILE:HG23	1:C:1028:GLU:HB2	1.98	0.44
1:C:1341:SER:O	1:C:1345:TYR:HD1	2.00	0.44
1:C:1689:THR:HA	1:C:1692:ILE:HG22	1.98	0.44
1:C:2254:LYS:HD3	1:C:2318:VAL:HG22	2.00	0.44
1:C:2448:TYR:OH	1:C:2516:LYS:HD2	2.17	0.44
1:A:1360:LYS:HD3	1:A:1410:ALA:HB1	1.98	0.44
1:A:1979:LYS:NZ	1:A:2019:ASP:OD2	2.37	0.44
1:A:2621:ASP:HB2	1:A:2628:SER:CB	2.46	0.44
1:B:2254:LYS:HD3	1:B:2318:VAL:HG22	2.00	0.44
1:C:2378:LEU:O	1:C:2382:ARG:HG2	2.17	0.44
1:C:2511:PRO:O	1:C:2514:LYS:HB3	2.17	0.44
1:C:2592:LYS:HD2	1:C:2654:ASN:OD1	2.17	0.44
1:C:2688:PHE:CD1	2:E:189:ARG:HG3	2.53	0.44
1:A:1494:GLY:HA2	1:A:1497:ARG:NE	2.33	0.44
1:A:2606:LEU:HD11	1:A:2612:MET:HE3	1.98	0.44
1:B:973:LEU:HD23	1:B:973:LEU:HA	1.84	0.44
1:B:2015:TYR:HD2	1:B:2016:VAL:HG13	1.82	0.44
1:B:2037:GLY:O	1:B:2038:LEU:HG	2.18	0.44
1:C:1494:GLY:HA2	1:C:1497:ARG:NE	2.33	0.44
1:C:2534:TRP:CZ2	1:C:2551:ASP:HB3	2.52	0.44
1:A:1341:SER:O	1:A:1345:TYR:HD1	2.00	0.44
1:A:2500:GLU:HG2	1:A:2501:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2734:ILE:HD13	1:A:2734:ILE:HA	1.83	0.44
1:B:947:SER:O	1:B:951:ILE:HG12	2.18	0.44
1:B:1895:GLU:HB3	1:B:1899:LYS:NZ	2.32	0.44
1:A:1027:ASN:ND2	1:A:1030:ASN:OD1	2.51	0.44
1:A:1895:GLU:N	1:A:1895:GLU:OE2	2.51	0.44
1:A:1929:VAL:HG11	1:A:2022:GLN:HA	1.99	0.44
1:A:2254:LYS:HD3	1:A:2318:VAL:HG22	1.99	0.44
1:A:2619:SER:O	1:A:2630:TRP:HB2	2.17	0.44
1:B:1341:SER:O	1:B:1345:TYR:HD1	2.00	0.44
1:B:1929:VAL:HG11	1:B:2022:GLN:HA	1.99	0.44
1:B:1969:ILE:O	1:B:1973:GLU:HG3	2.17	0.44
1:B:2378:LEU:O	1:B:2382:ARG:HG2	2.17	0.44
1:C:1418:CYS:O	1:C:1422:LEU:HD13	2.18	0.44
1:C:1447:LEU:HB3	1:C:1681:LEU:HD22	1.99	0.44
1:C:1895:GLU:HB3	1:C:1899:LYS:NZ	2.32	0.44
1:A:956:LYS:HA	1:A:956:LYS:HD2	1.77	0.44
1:A:1875:THR:HA	1:A:1878:LEU:HB2	2.00	0.44
1:A:2534:TRP:CZ2	1:A:2551:ASP:HB3	2.52	0.44
1:B:1895:GLU:OE2	1:B:1895:GLU:N	2.51	0.44
1:B:2340:LEU:HD23	1:B:2340:LEU:HA	1.88	0.44
1:B:2448:TYR:OH	1:B:2516:LYS:HD2	2.17	0.44
1:B:2592:LYS:HD2	1:B:2654:ASN:OD1	2.17	0.44
1:B:2716:LEU:O	1:B:2720:THR:HG23	2.18	0.44
1:C:2243:THR:HA	1:C:2246:VAL:HG12	2.00	0.44
1:C:2716:LEU:O	1:C:2720:THR:HG23	2.18	0.44
1:A:963:TYR:O	1:A:967:ILE:HG12	2.17	0.44
1:A:2391:PRO:HB2	1:A:2394:GLN:HG2	1.99	0.44
1:A:2516:LYS:NZ	1:C:2457:GLN:OE1	2.40	0.44
1:A:2568:MET:SD	1:A:2618:LEU:N	2.87	0.44
1:B:1418:CYS:O	1:B:1422:LEU:HD13	2.18	0.44
1:B:2289:ASN:HB3	1:B:2292:ALA:HB3	2.00	0.44
1:B:2347:LEU:HD21	1:C:2412:LEU:HD13	2.00	0.44
1:B:2438:ASP:OD1	1:B:2456:ALA:HB3	2.16	0.44
1:B:2534:TRP:CZ2	1:B:2551:ASP:HB3	2.52	0.44
1:A:1969:ILE:O	1:A:1973:GLU:HG3	2.18	0.44
1:A:2401:LYS:HG2	1:C:2353:TRP:CZ2	2.53	0.44
1:A:2452:PHE:CD2	1:A:2633:LEU:HD13	2.53	0.44
1:A:2511:PRO:O	1:A:2514:LYS:HB3	2.17	0.44
1:A:2577:SER:O	1:A:2617:ILE:HD11	2.18	0.44
1:A:2723:LEU:HD22	1:B:2395:LYS:HZ3	1.81	0.44
1:B:1321:LEU:HD23	1:B:1321:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1681:LEU:HD23	1:B:1681:LEU:HA	1.80	0.44
1:B:2003:PRO:HD2	1:B:2004:PRO:CD	2.38	0.44
1:C:963:TYR:O	1:C:967:ILE:HG12	2.17	0.44
1:C:1387:LEU:HD23	1:C:1387:LEU:HA	1.81	0.44
1:C:1969:ILE:O	1:C:1973:GLU:HG3	2.18	0.44
1:A:1339:ILE:HG22	1:A:1343:LEU:HG	2.00	0.43
1:A:2037:GLY:O	1:A:2038:LEU:HG	2.18	0.43
1:A:2185:ALA:O	1:A:2312:CYS:HB3	2.18	0.43
1:C:994:ILE:HG12	1:C:1061:LEU:HD11	2.00	0.43
1:C:1555:GLU:O	1:C:1557:ASP:N	2.47	0.43
1:C:2185:ALA:O	1:C:2312:CYS:HB3	2.18	0.43
1:A:1194:ASP:OD1	1:A:1195:TYR:N	2.48	0.43
1:A:1220:ARG:HA	1:A:1220:ARG:HD2	1.72	0.43
1:A:2015:TYR:HD2	1:A:2016:VAL:HG13	1.82	0.43
1:B:2577:SER:O	1:B:2617:ILE:HD11	2.18	0.43
1:C:1187:ILE:HG23	1:C:1188:PRO:HD2	2.00	0.43
1:A:1418:CYS:O	1:A:1422:LEU:HD13	2.18	0.43
1:A:2630:TRP:CZ2	1:B:2511:PRO:HD2	2.53	0.43
1:B:1205:ASN:OD1	1:B:1206:ASP:N	2.48	0.43
1:B:1945:LEU:HD12	1:B:1945:LEU:HA	1.72	0.43
1:B:2396:LYS:HD2	1:B:2396:LYS:HA	1.75	0.43
1:C:1950:PHE:HZ	1:C:2300:CYS:SG	2.42	0.43
1:A:985:VAL:HA	1:A:988:VAL:HG22	1.99	0.43
1:A:1941:ILE:HD12	1:A:2008:GLY:O	2.19	0.43
1:A:2243:THR:HA	1:A:2246:VAL:HG12	2.00	0.43
1:B:1290:LYS:HD3	1:B:1290:LYS:HA	1.81	0.43
1:B:1339:ILE:HG22	1:B:1343:LEU:HG	2.00	0.43
1:B:1447:LEU:HB3	1:B:1681:LEU:HD22	1.99	0.43
1:B:2467:GLN:OE1	1:B:2467:GLN:N	2.51	0.43
1:C:947:SER:O	1:C:951:ILE:HG12	2.18	0.43
1:C:1097:ASP:O	1:C:1099:THR:HG23	2.19	0.43
1:C:1895:GLU:OE2	1:C:1895:GLU:N	2.51	0.43
1:A:947:SER:O	1:A:951:ILE:HG12	2.18	0.43
1:A:2463:VAL:CG1	1:A:2464:MET:H	2.29	0.43
1:A:2738:ARG:HG2	1:B:2697:MET:HA	2.01	0.43
1:C:1047:LEU:HD23	1:C:1047:LEU:H	1.83	0.43
1:C:1099:THR:H	1:C:1102:HIS:HB2	1.84	0.43
1:C:1941:ILE:HD12	1:C:2008:GLY:O	2.18	0.43
1:A:1290:LYS:HD2	1:A:1294:PHE:HE1	1.84	0.43
1:A:1950:PHE:HZ	1:A:2300:CYS:SG	2.41	0.43
1:A:2355:TRP:NE1	1:B:2402:TYR:OH	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2437:LEU:HD12	1:A:2438:ASP:HB2	2.01	0.43
1:A:2537:GLN:HE22	1:A:2547:GLU:CD	2.27	0.43
1:A:2716:LEU:O	1:A:2720:THR:HG23	2.18	0.43
1:B:2185:ALA:O	1:B:2312:CYS:HB3	2.18	0.43
1:C:978:LEU:HD22	1:C:981:LEU:HD21	2.00	0.43
1:C:1188:PRO:HA	1:C:1189:PRO:HD3	1.90	0.43
1:C:1875:THR:HA	1:C:1878:LEU:HB2	2.00	0.43
1:C:1929:VAL:HG11	1:C:2022:GLN:HA	1.99	0.43
1:C:2396:LYS:HD2	1:C:2396:LYS:HA	1.75	0.43
1:A:1099:THR:H	1:A:1102:HIS:HB2	1.84	0.43
1:A:2530:VAL:HG23	1:A:2556:PRO:O	2.19	0.43
1:B:2452:PHE:CD2	1:B:2633:LEU:HD13	2.53	0.43
1:B:2688:PHE:CD1	2:D:189:ARG:HG3	2.53	0.43
1:C:985:VAL:HA	1:C:988:VAL:HG22	1.99	0.43
1:C:1027:ASN:ND2	1:C:1030:ASN:OD1	2.51	0.43
1:C:1343:LEU:HD23	1:C:1343:LEU:HA	1.70	0.43
1:C:1447:LEU:HD13	1:C:1447:LEU:HA	1.79	0.43
1:A:1187:ILE:HG23	1:A:1188:PRO:HD2	2.00	0.43
1:A:2451:ILE:HB	1:A:2631:TRP:CG	2.53	0.43
2:F:182:GLU:O	2:F:185:GLU:HB2	2.19	0.43
1:B:1494:GLY:HA2	1:B:1497:ARG:NE	2.33	0.43
1:B:1875:THR:HA	1:B:1878:LEU:HB2	2.00	0.43
1:C:1290:LYS:HD2	1:C:1294:PHE:HE1	1.84	0.43
1:C:2577:SER:O	1:C:2617:ILE:HD11	2.18	0.43
1:A:2266:LEU:HD12	1:A:2266:LEU:HA	1.80	0.43
1:A:2412:LEU:HD11	1:C:2343:PHE:HB3	2.01	0.43
1:A:2709:LYS:HE3	1:A:2709:LYS:HB3	1.94	0.43
1:B:1097:ASP:O	1:B:1099:THR:HG23	2.19	0.43
1:C:1263:MET:HE3	1:C:1263:MET:HA	2.00	0.43
1:C:1321:LEU:HD23	1:C:1321:LEU:HA	1.81	0.43
1:C:2467:GLN:OE1	1:C:2467:GLN:N	2.52	0.43
1:A:924:LEU:HA	1:A:927:PHE:CD1	2.54	0.43
1:A:994:ILE:HG12	1:A:1061:LEU:HD11	2.00	0.43
1:A:1047:LEU:H	1:A:1047:LEU:HD23	1.83	0.43
1:A:1879:THR:OG1	1:A:1882:GLU:HG2	2.19	0.43
1:B:1930:ILE:HD12	1:B:1949:ILE:HD11	2.01	0.43
1:B:2240:GLN:O	1:B:2244:MET:HG3	2.19	0.43
1:B:2437:LEU:HD12	1:B:2438:ASP:HB2	2.01	0.43
2:D:182:GLU:O	2:D:185:GLU:HB2	2.19	0.43
1:C:994:ILE:O	1:C:998:MET:HG2	2.19	0.43
1:C:1205:ASN:OD1	1:C:1206:ASP:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2015:TYR:HD2	1:C:2016:VAL:HG13	1.81	0.43
1:C:2451:ILE:HB	1:C:2631:TRP:CG	2.53	0.43
1:C:2593:ALA:H	1:C:2654:ASN:HB2	1.84	0.43
1:A:1396:MET:SD	1:A:1397:PRO:HD2	2.59	0.42
1:B:994:ILE:O	1:B:998:MET:HG2	2.19	0.42
1:B:1941:ILE:HD12	1:B:2008:GLY:O	2.19	0.42
1:C:2530:VAL:HG23	1:C:2556:PRO:O	2.19	0.42
1:C:2635:LEU:HB3	1:C:2639:ARG:NH1	2.34	0.42
2:E:182:GLU:O	2:E:185:GLU:HB2	2.19	0.42
1:A:1205:ASN:OD1	1:A:1206:ASP:N	2.48	0.42
1:A:2635:LEU:HB3	1:A:2639:ARG:NH1	2.35	0.42
1:B:994:ILE:HG12	1:B:1061:LEU:HD11	2.00	0.42
1:B:1047:LEU:HD23	1:B:1047:LEU:H	1.83	0.42
1:C:1412:ILE:HA	1:C:1415:ASP:HB3	2.00	0.42
1:C:2437:LEU:HD12	1:C:2438:ASP:HB2	2.01	0.42
1:C:2491:LYS:HE2	1:C:2491:LYS:HB2	1.83	0.42
1:A:1144:MET:HA	1:A:1144:MET:HE2	2.01	0.42
1:A:1263:MET:HE3	1:A:1263:MET:HA	2.01	0.42
1:A:2593:ALA:H	1:A:2654:ASN:HB2	1.84	0.42
1:B:1197:TRP:HB3	1:B:1204:PHE:HD2	1.84	0.42
1:B:1263:MET:HE3	1:B:1263:MET:HA	2.01	0.42
1:B:1290:LYS:HD2	1:B:1294:PHE:HE1	1.84	0.42
1:B:1708:GLN:O	1:B:1711:ILE:HG22	2.19	0.42
1:B:2243:THR:HA	1:B:2246:VAL:HG12	2.00	0.42
1:C:2240:GLN:O	1:C:2244:MET:HG3	2.19	0.42
1:C:2289:ASN:HB3	1:C:2292:ALA:HB3	2.00	0.42
1:A:1097:ASP:O	1:A:1099:THR:HG23	2.19	0.42
1:A:2240:GLN:O	1:A:2244:MET:HG3	2.19	0.42
1:A:2289:ASN:HB3	1:A:2292:ALA:HB3	2.00	0.42
1:A:2395:LYS:HZ1	1:C:2723:LEU:HD13	1.85	0.42
1:A:2467:GLN:OE1	1:A:2467:GLN:N	2.51	0.42
1:A:2668:TYR:CG	1:A:2669:GLY:N	2.88	0.42
1:B:978:LEU:HD22	1:B:981:LEU:HD21	2.00	0.42
1:B:1484:ILE:HG12	1:B:2713:ASP:OD1	2.20	0.42
1:B:2270:ILE:HD13	1:B:2270:ILE:HA	1.91	0.42
1:C:1125:GLU:OE1	1:C:1125:GLU:N	2.47	0.42
1:C:1144:MET:HE2	1:C:1144:MET:HA	2.01	0.42
1:C:1895:GLU:HB3	1:C:1899:LYS:HZ3	1.84	0.42
1:C:2339:ARG:HG3	1:C:2345:THR:HG21	2.02	0.42
1:C:2452:PHE:CD2	1:C:2633:LEU:HD13	2.53	0.42
1:A:978:LEU:HD22	1:A:981:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:NH1	1:A:1103:LEU:HD23	2.35	0.42
1:A:1412:ILE:HA	1:A:1415:ASP:HB3	2.01	0.42
1:A:2384:SER:OG	2:F:181:MET:SD	2.72	0.42
1:B:1100:ARG:NH1	1:B:1103:LEU:HD23	2.35	0.42
1:B:2668:TYR:CG	1:B:2669:GLY:N	2.88	0.42
1:C:924:LEU:HA	1:C:927:PHE:CD1	2.54	0.42
1:C:2668:TYR:CG	1:C:2669:GLY:N	2.88	0.42
1:A:994:ILE:O	1:A:998:MET:HG2	2.19	0.42
1:A:1197:TRP:HB3	1:A:1204:PHE:HD2	1.84	0.42
1:A:1484:ILE:HG12	1:A:2713:ASP:OD1	2.20	0.42
1:A:1930:ILE:HD12	1:A:1949:ILE:HD11	2.01	0.42
1:A:2339:ARG:HG3	1:A:2345:THR:HG21	2.02	0.42
1:A:2387:ARG:C	1:A:2389:PRO:HD3	2.44	0.42
1:B:924:LEU:HA	1:B:927:PHE:CD1	2.54	0.42
1:B:1371:ILE:O	1:B:1375:VAL:HG23	2.20	0.42
1:B:2353:TRP:CD1	1:B:2358:THR:HG21	2.55	0.42
1:B:2530:VAL:HG23	1:B:2556:PRO:O	2.19	0.42
1:C:1350:ILE:CD1	1:C:1422:LEU:HB3	2.49	0.42
1:C:1396:MET:SD	1:C:1397:PRO:HD2	2.59	0.42
1:C:1708:GLN:O	1:C:1711:ILE:HG22	2.19	0.42
1:C:1939:SER:HB2	1:C:2008:GLY:H	1.85	0.42
1:C:2353:TRP:CD1	1:C:2358:THR:HG21	2.55	0.42
1:A:1371:ILE:O	1:A:1375:VAL:HG23	2.20	0.42
1:B:1144:MET:HE2	1:B:1144:MET:HA	2.02	0.42
1:B:1350:ILE:CD1	1:B:1422:LEU:HB3	2.49	0.42
1:B:1412:ILE:HA	1:B:1415:ASP:HB3	2.00	0.42
1:C:1339:ILE:HG22	1:C:1343:LEU:HG	2.00	0.42
1:C:2471:LYS:O	1:C:2475:ALA:N	2.53	0.42
1:A:1173:LEU:HD23	1:A:1173:LEU:HA	1.79	0.42
1:A:2471:LYS:O	1:A:2475:ALA:N	2.53	0.42
1:B:2387:ARG:C	1:B:2389:PRO:HD3	2.44	0.42
1:B:2514:LYS:HE3	1:B:2514:LYS:HB2	1.84	0.42
1:C:1100:ARG:NH1	1:C:1103:LEU:HD23	2.35	0.42
1:A:1184:CYS:SG	1:A:1223:PRO:HB3	2.60	0.42
1:B:1099:THR:H	1:B:1102:HIS:HB2	1.84	0.42
1:B:1187:ILE:HG23	1:B:1188:PRO:HD2	2.00	0.42
1:B:1950:PHE:HZ	1:B:2300:CYS:SG	2.41	0.42
1:B:2464:MET:HA	1:B:2464:MET:HE3	2.02	0.42
1:B:2523:ASP:N	1:B:2523:ASP:OD1	2.53	0.42
1:C:2464:MET:HE3	1:C:2464:MET:HA	2.02	0.42
1:B:1184:CYS:SG	1:B:1223:PRO:HB3	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1939:SER:HB2	1:B:2008:GLY:H	1.85	0.42
1:B:2339:ARG:HG3	1:B:2345:THR:HG21	2.02	0.42
1:B:2486:LEU:C	1:B:2488:ASN:H	2.28	0.42
1:C:2434:ASN:HB2	1:C:2657:VAL:CG1	2.50	0.42
1:A:1350:ILE:CD1	1:A:1422:LEU:HB3	2.49	0.41
1:B:1879:THR:OG1	1:B:1882:GLU:HG2	2.19	0.41
1:B:2398:LYS:HE3	1:B:2398:LYS:HB2	1.89	0.41
1:B:2477:SER:C	1:B:2479:ASP:H	2.28	0.41
1:C:1364:SER:HA	1:C:1367:ALA:HB3	2.02	0.41
1:C:2326:SER:OG	1:C:2331:ASN:OD1	2.25	0.41
1:C:2477:SER:C	1:C:2479:ASP:H	2.28	0.41
1:C:2704:VAL:O	1:C:2704:VAL:HG23	2.20	0.41
1:A:1157:ARG:NE	1:A:1157:ARG:HA	2.36	0.41
1:A:2391:PRO:O	1:C:1543:ALA:HB2	2.20	0.41
1:A:2444:THR:HG22	1:A:2446:GLY:O	2.20	0.41
1:A:2445:LEU:HD12	1:A:2530:VAL:HG22	2.02	0.41
1:B:2434:ASN:HB2	1:B:2657:VAL:CG1	2.50	0.41
1:B:2444:THR:HG22	1:B:2446:GLY:O	2.20	0.41
1:B:2451:ILE:HB	1:B:2631:TRP:CG	2.53	0.41
1:B:2635:LEU:HB3	1:B:2639:ARG:NH1	2.34	0.41
1:B:2698:PHE:HD2	1:C:2694:HIS:HD1	1.62	0.41
1:C:1194:ASP:OD1	1:C:1195:TYR:N	2.48	0.41
1:C:1197:TRP:HB3	1:C:1204:PHE:HD2	1.84	0.41
1:C:1339:ILE:HD11	1:C:1435:LEU:HD11	2.02	0.41
1:C:1681:LEU:HD23	1:C:1681:LEU:HA	1.80	0.41
1:C:2523:ASP:OD1	1:C:2523:ASP:N	2.53	0.41
1:C:2679:LEU:HD23	1:C:2679:LEU:HA	1.80	0.41
1:A:948:SER:HA	1:A:1230:PHE:CE2	2.55	0.41
1:A:1708:GLN:O	1:A:1711:ILE:HG22	2.19	0.41
1:A:2417:TRP:CE2	1:C:2234:LEU:HG	2.55	0.41
1:A:2698:PHE:CD2	1:B:2694:HIS:ND1	2.75	0.41
1:B:948:SER:HA	1:B:1230:PHE:CE2	2.55	0.41
1:B:1220:ARG:HD2	1:B:1220:ARG:HA	1.72	0.41
1:B:1339:ILE:HD11	1:B:1435:LEU:HD11	2.02	0.41
1:C:1184:CYS:SG	1:C:1223:PRO:HB3	2.60	0.41
1:A:2464:MET:HE3	1:A:2464:MET:HA	2.02	0.41
1:A:2635:LEU:HA	1:A:2635:LEU:HD12	1.76	0.41
1:B:936:TRP:HE3	1:B:1077:GLN:HE22	1.69	0.41
1:B:997:LYS:HZ1	1:B:1047:LEU:HD13	1.84	0.41
1:B:1364:SER:HA	1:B:1367:ALA:HB3	2.02	0.41
1:B:1396:MET:SD	1:B:1397:PRO:HD2	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2026:LEU:HA	1:B:2026:LEU:HD23	1.87	0.41
1:C:1371:ILE:O	1:C:1375:VAL:HG23	2.20	0.41
1:C:1879:THR:OG1	1:C:1882:GLU:HG2	2.19	0.41
1:C:2197:ASP:OD2	1:C:2244:MET:HG2	2.20	0.41
1:C:2387:ARG:C	1:C:2389:PRO:HD3	2.44	0.41
1:C:2537:GLN:HE22	1:C:2547:GLU:CD	2.27	0.41
1:C:2635:LEU:HD12	1:C:2635:LEU:HA	1.76	0.41
1:A:1192:CYS:SG	1:A:1193:ARG:N	2.86	0.41
1:A:1481:MET:HE3	1:A:1481:MET:HB3	1.68	0.41
1:A:1691:GLU:HG3	1:A:1706:TYR:HE2	1.86	0.41
1:A:2627:ASN:HB3	1:C:2626:TYR:CE1	2.56	0.41
1:A:2688:PHE:CD1	2:F:189:ARG:HG3	2.55	0.41
1:B:1157:ARG:NE	1:B:1157:ARG:HA	2.35	0.41
1:B:2299:LYS:HD3	1:B:2299:LYS:HA	1.79	0.41
1:B:2326:SER:OG	1:B:2331:ASN:OD1	2.26	0.41
1:B:2679:LEU:HD23	1:B:2679:LEU:HA	1.80	0.41
1:C:948:SER:HA	1:C:1230:PHE:CE2	2.55	0.41
1:C:1103:LEU:HD13	1:C:1113:TYR:CD2	2.56	0.41
1:A:1103:LEU:HD13	1:A:1113:TYR:CD2	2.56	0.41
1:A:2197:ASP:OD2	1:A:2244:MET:HG2	2.21	0.41
1:A:2523:ASP:HA	1:A:2524:PRO:HD3	1.94	0.41
1:C:1691:GLU:HG3	1:C:1706:TYR:HE2	1.86	0.41
1:C:2318:VAL:O	1:C:2318:VAL:HG23	2.20	0.41
1:C:2410:VAL:O	1:C:2413:ILE:HG22	2.21	0.41
1:C:2486:LEU:C	1:C:2488:ASN:H	2.28	0.41
1:A:921:LEU:HD23	1:A:921:LEU:HA	1.91	0.41
1:A:2410:VAL:O	1:A:2413:ILE:HG22	2.21	0.41
1:A:2477:SER:C	1:A:2479:ASP:H	2.28	0.41
1:A:2523:ASP:N	1:A:2523:ASP:OD1	2.53	0.41
1:A:2704:VAL:O	1:A:2704:VAL:HG23	2.21	0.41
1:B:2318:VAL:HG23	1:B:2318:VAL:O	2.21	0.41
1:B:2659:PRO:HA	1:B:2660:PRO:HD3	1.96	0.41
1:C:1135:ILE:HG22	1:C:1361:ASN:HD22	1.86	0.41
1:C:1484:ILE:HG12	1:C:2713:ASP:OD1	2.20	0.41
1:A:936:TRP:HE3	1:A:1077:GLN:HE22	1.69	0.41
1:A:2318:VAL:HG23	1:A:2318:VAL:O	2.21	0.41
1:A:2445:LEU:HG	1:A:2528:PHE:HE2	1.86	0.41
1:A:2486:LEU:C	1:A:2488:ASN:H	2.28	0.41
1:B:1135:ILE:HG22	1:B:1361:ASN:HD22	1.86	0.41
1:B:1343:LEU:HD23	1:B:1343:LEU:HA	1.70	0.41
1:B:2197:ASP:OD2	1:B:2244:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2471:LYS:O	1:B:2475:ALA:N	2.53	0.41
1:B:2558:LYS:NZ	1:B:2560:ILE:HB	2.35	0.41
1:B:2704:VAL:HG23	1:B:2704:VAL:O	2.21	0.41
1:C:1367:ALA:HB2	1:C:1387:LEU:HB3	2.03	0.41
1:C:2333:PHE:CZ	2:E:180:ALA:HB1	2.56	0.41
1:C:2558:LYS:NZ	1:C:2560:ILE:HB	2.35	0.41
1:A:1339:ILE:HD11	1:A:1435:LEU:HD11	2.02	0.41
1:A:2003:PRO:HD2	1:A:2004:PRO:CD	2.37	0.41
1:A:2212:GLY:HA2	1:A:2232:PRO:HG2	2.03	0.41
1:A:2353:TRP:CD1	1:A:2358:THR:HG21	2.55	0.41
1:A:2514:LYS:HB2	1:A:2514:LYS:HE3	1.84	0.41
1:A:2619:SER:HB3	1:A:2630:TRP:CD1	2.56	0.41
1:A:2630:TRP:CH2	1:B:2512:PRO:HD2	2.53	0.41
1:B:1103:LEU:HD13	1:B:1113:TYR:CD2	2.56	0.41
1:B:1547:ARG:O	1:B:1547:ARG:HG3	2.21	0.41
1:B:1946:PRO:HB2	1:B:2271:HIS:HE1	1.86	0.41
1:B:2410:VAL:O	1:B:2413:ILE:HG22	2.21	0.41
1:C:1930:ILE:HD12	1:C:1949:ILE:HD11	2.01	0.41
1:C:2523:ASP:HA	1:C:2524:PRO:HD3	1.94	0.41
1:A:1364:SER:HA	1:A:1367:ALA:HB3	2.02	0.41
1:A:1946:PRO:HB2	1:A:2271:HIS:HE1	1.86	0.41
1:A:2457:GLN:OE1	1:B:2516:LYS:NZ	2.32	0.41
1:A:2558:LYS:NZ	1:A:2560:ILE:HB	2.35	0.41
1:A:2583:ILE:HB	1:A:2614:ILE:HG22	2.03	0.41
1:A:2738:ARG:HH21	1:B:2701:LEU:HD23	1.85	0.41
1:B:2504:ASN:HA	1:C:2513:SER:OG	2.21	0.41
1:C:924:LEU:HA	1:C:927:PHE:CE1	2.56	0.41
1:C:1157:ARG:NE	1:C:1157:ARG:HA	2.35	0.41
1:C:2266:LEU:HD12	1:C:2266:LEU:HA	1.80	0.41
1:C:2619:SER:HB3	1:C:2630:TRP:CD1	2.56	0.41
1:A:1135:ILE:HG22	1:A:1361:ASN:HD22	1.86	0.40
1:A:1939:SER:HB2	1:A:2008:GLY:H	1.85	0.40
1:B:2445:LEU:HD12	1:B:2530:VAL:HG22	2.02	0.40
1:B:2583:ILE:HB	1:B:2614:ILE:HG22	2.03	0.40
1:C:936:TRP:HE3	1:C:1077:GLN:HE22	1.69	0.40
1:C:1190:ALA:HB3	1:C:1191:PRO:HD3	2.03	0.40
1:C:2013:GLU:OE1	1:C:2013:GLU:N	2.52	0.40
1:C:2212:GLY:HA2	1:C:2232:PRO:HG2	2.03	0.40
1:C:2584:GLU:O	1:C:2585:LYS:C	2.64	0.40
1:A:1188:PRO:HA	1:A:1189:PRO:HD3	1.90	0.40
1:A:1190:ALA:HB3	1:A:1191:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:LEU:HD23	1:A:1321:LEU:HA	1.81	0.40
1:A:2259:LYS:HD2	1:A:2259:LYS:HA	1.94	0.40
1:A:2549:ALA:HB1	1:A:2599:SER:HB2	2.03	0.40
1:B:2593:ALA:H	1:B:2654:ASN:HB2	1.84	0.40
1:C:2207:GLY:O	1:C:2211:PHE:HB2	2.22	0.40
1:C:2549:ALA:HB1	1:C:2599:SER:HB2	2.03	0.40
1:A:1033:LEU:O	1:A:1039:ILE:HD11	2.22	0.40
1:A:1343:LEU:HA	1:A:1343:LEU:HD23	1.70	0.40
1:A:1547:ARG:O	1:A:1547:ARG:HG3	2.21	0.40
1:A:2421:LEU:HB2	1:C:2234:LEU:HD21	2.02	0.40
1:A:2643:PRO:HG2	1:A:2646:GLN:OE1	2.22	0.40
1:A:2718:ARG:HB2	1:A:2726:GLU:OE1	2.22	0.40
1:B:921:LEU:HD23	1:B:921:LEU:HA	1.91	0.40
1:B:1691:GLU:HG3	1:B:1706:TYR:HE2	1.86	0.40
1:B:2378:LEU:HD23	1:B:2704:VAL:HG11	2.03	0.40
1:B:2718:ARG:HB2	1:B:2726:GLU:OE1	2.22	0.40
1:C:2467:GLN:CA	1:C:2470:ASN:HB2	2.51	0.40
1:A:2434:ASN:HB2	1:A:2657:VAL:CG1	2.51	0.40
1:A:2679:LEU:HA	1:A:2679:LEU:HD23	1.80	0.40
1:B:1002:LEU:HD12	1:B:1002:LEU:HA	1.97	0.40
1:B:1544:SER:O	1:B:1544:SER:OG	2.38	0.40
1:B:2207:GLY:O	1:B:2211:PHE:HB2	2.22	0.40
1:C:1033:LEU:O	1:C:1039:ILE:HD11	2.21	0.40
1:C:1547:ARG:HG3	1:C:1547:ARG:O	2.21	0.40
1:C:2378:LEU:HD23	1:C:2704:VAL:HG11	2.03	0.40
1:C:2718:ARG:HB2	1:C:2726:GLU:OE1	2.21	0.40
1:A:2195:LEU:HD23	1:A:2195:LEU:HA	1.97	0.40
1:A:2398:LYS:HE3	1:A:2398:LYS:HB2	1.89	0.40
1:A:2558:LYS:HZ2	1:A:2560:ILE:CD1	2.35	0.40
1:B:1934:HIS:NE2	1:B:2275:PHE:CE2	2.87	0.40
1:B:2445:LEU:HG	1:B:2528:PHE:HE2	1.86	0.40
1:B:2584:GLU:O	1:B:2585:LYS:C	2.64	0.40
1:B:2635:LEU:HD12	1:B:2635:LEU:HA	1.76	0.40
1:C:957:GLU:HB3	1:C:962:ASN:ND2	2.36	0.40
1:C:2202:ILE:HD13	1:C:2202:ILE:HA	1.91	0.40
1:C:2319:LEU:HD23	1:C:2319:LEU:HA	1.96	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	1378/3020 (46%)	1254 (91%)	122 (9%)	2 (0%)	48	76
1	B	1378/3020 (46%)	1255 (91%)	121 (9%)	2 (0%)	48	76
1	C	1378/3020 (46%)	1255 (91%)	121 (9%)	2 (0%)	48	76
2	D	19/211 (9%)	18 (95%)	1 (5%)	0	100	100
2	E	19/211 (9%)	18 (95%)	1 (5%)	0	100	100
2	F	19/211 (9%)	18 (95%)	1 (5%)	0	100	100
All	All	4191/9693 (43%)	3818 (91%)	367 (9%)	6 (0%)	49	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2556	PRO
1	B	2556	PRO
1	C	2556	PRO
1	A	1025	PRO
1	B	1025	PRO
1	C	1025	PRO

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	1268/2707 (47%)	1268 (100%)	0	100	100
1	B	1268/2707 (47%)	1268 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1268/2707 (47%)	1268 (100%)	0	100	100
2	D	20/198 (10%)	20 (100%)	0	100	100
2	E	20/198 (10%)	20 (100%)	0	100	100
2	F	20/198 (10%)	20 (100%)	0	100	100
All	All	3864/8715 (44%)	3864 (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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	931	GLN
1	A	1027	ASN
1	A	1059	ASN
1	A	1084	ASN
1	A	1425	GLN
1	A	1696	ASN
1	A	1713	ASN
1	A	2484	GLN
1	A	2537	GLN
1	A	2598	ASN
1	B	931	GLN
1	B	1027	ASN
1	B	1084	ASN
1	B	1425	GLN
1	B	1542	HIS
1	B	1696	ASN
1	B	1713	ASN
1	B	2484	GLN
1	B	2537	GLN
1	B	2598	ASN
1	C	931	GLN
1	C	1027	ASN
1	C	1084	ASN
1	C	1696	ASN
1	C	1713	ASN
1	C	2484	GLN
1	C	2537	GLN
1	C	2598	ASN

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 [i](#)

There are no chain breaks in this entry.