Full wwPDB EM Validation Report ⓘ

Oct 6, 2023 – 12:56 AM EDT

PDB ID	:	8TQE
EMDB ID	:	EMD-41503
Title	:	XptA2 wild type
Authors	:	Martin, C.L.; Binshtein, E.M.; Aller, S.G.
Deposited on	:	2023-08-07
Resolution	:	3.10 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:

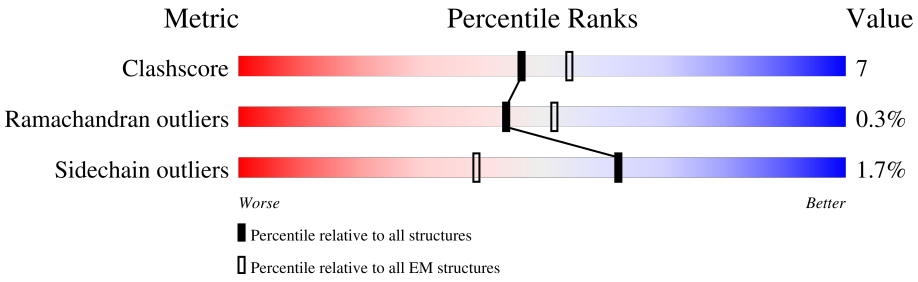
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2538	83% 16%
1	B	2538	81% 18%
1	C	2538	82% 17%
1	D	2538	84% 15%
1	E	2538	83% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 100035 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 XptA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2537	Total	C	N	O	S	0	0
			20007	12625	3415	3894	73		
1	B	2537	Total	C	N	O	S	0	0
			20007	12625	3415	3894	73		
1	C	2537	Total	C	N	O	S	0	0
			20007	12625	3415	3894	73		
1	D	2537	Total	C	N	O	S	0	0
			20007	12625	3415	3894	73		
1	E	2537	Total	C	N	O	S	0	0
			20007	12625	3415	3894	73		

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	HIS	PRO	conflict	UNP N1NRW3
A	343	ASN	HIS	conflict	UNP N1NRW3
A	344	ILE	VAL	conflict	UNP N1NRW3
A	360	ARG	CYS	conflict	UNP N1NRW3
A	365	VAL	ILE	conflict	UNP N1NRW3
A	377	ALA	SER	conflict	UNP N1NRW3
A	379	PRO	THR	conflict	UNP N1NRW3
A	391	ILE	VAL	conflict	UNP N1NRW3
A	407	SER	ASN	conflict	UNP N1NRW3
A	410	LYS	ARG	conflict	UNP N1NRW3
A	566	VAL	ILE	conflict	UNP N1NRW3
A	583	ALA	THR	conflict	UNP N1NRW3
A	586	THR	ILE	conflict	UNP N1NRW3
A	587	ILE	LEU	conflict	UNP N1NRW3
A	592	PHE	PRO	conflict	UNP N1NRW3
A	606	VAL	ALA	conflict	UNP N1NRW3
A	620	LEU	PHE	conflict	UNP N1NRW3
A	637	PRO	SER	conflict	UNP N1NRW3
A	682	ASN	THR	conflict	UNP N1NRW3
A	686	SER	ARG	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	695	HIS	SER	conflict	UNP N1NRW3
A	696	ASN	ASP	conflict	UNP N1NRW3
A	736	ASP	ASN	conflict	UNP N1NRW3
A	742	THR	MET	conflict	UNP N1NRW3
A	748	SER	THR	conflict	UNP N1NRW3
A	750	ASN	SER	conflict	UNP N1NRW3
A	751	ALA	ASP	conflict	UNP N1NRW3
A	752	ASN	GLU	conflict	UNP N1NRW3
A	788	GLY	ASP	conflict	UNP N1NRW3
A	790	ALA	VAL	conflict	UNP N1NRW3
A	795	LYS	ARG	conflict	UNP N1NRW3
A	796	ASN	SER	conflict	UNP N1NRW3
A	911	SER	ALA	conflict	UNP N1NRW3
A	914	GLU	LYS	conflict	UNP N1NRW3
A	923	GLU	ALA	conflict	UNP N1NRW3
A	1067	LYS	GLN	conflict	UNP N1NRW3
A	1075	ASP	GLU	conflict	UNP N1NRW3
A	1126	ASP	ASN	conflict	UNP N1NRW3
A	1250	LYS	VAL	conflict	UNP N1NRW3
A	1253	SER	PRO	conflict	UNP N1NRW3
A	1257	GLY	ASP	conflict	UNP N1NRW3
A	1258	SER	ASN	conflict	UNP N1NRW3
A	1514	ILE	VAL	conflict	UNP N1NRW3
A	1519	MET	VAL	conflict	UNP N1NRW3
A	1877	ASN	TYR	conflict	UNP N1NRW3
A	1880	MET	THR	conflict	UNP N1NRW3
A	1884	ILE	VAL	conflict	UNP N1NRW3
A	1920	THR	ALA	conflict	UNP N1NRW3
A	1943	GLY	VAL	conflict	UNP N1NRW3
A	1947	GLN	HIS	conflict	UNP N1NRW3
A	1959	MET	ALA	conflict	UNP N1NRW3
A	1961	GLY	ASP	conflict	UNP N1NRW3
A	1962	ARG	ASN	conflict	UNP N1NRW3
A	1964	GLY	GLU	conflict	UNP N1NRW3
A	1966	SER	ALA	conflict	UNP N1NRW3
A	1967	LYS	THR	conflict	UNP N1NRW3
A	1968	ASN	GLN	conflict	UNP N1NRW3
A	1969	LEU	PRO	conflict	UNP N1NRW3
A	2057	THR	ALA	conflict	UNP N1NRW3
A	2149	LEU	PHE	conflict	UNP N1NRW3
A	2161	VAL	ALA	conflict	UNP N1NRW3
A	2164	ILE	VAL	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2178	LEU	PHE	conflict	UNP N1NRW3
A	2430	LEU	PHE	conflict	UNP N1NRW3
B	172	HIS	PRO	conflict	UNP N1NRW3
B	343	ASN	HIS	conflict	UNP N1NRW3
B	344	ILE	VAL	conflict	UNP N1NRW3
B	360	ARG	CYS	conflict	UNP N1NRW3
B	365	VAL	ILE	conflict	UNP N1NRW3
B	377	ALA	SER	conflict	UNP N1NRW3
B	379	PRO	THR	conflict	UNP N1NRW3
B	391	ILE	VAL	conflict	UNP N1NRW3
B	407	SER	ASN	conflict	UNP N1NRW3
B	410	LYS	ARG	conflict	UNP N1NRW3
B	566	VAL	ILE	conflict	UNP N1NRW3
B	583	ALA	THR	conflict	UNP N1NRW3
B	586	THR	ILE	conflict	UNP N1NRW3
B	587	ILE	LEU	conflict	UNP N1NRW3
B	592	PHE	PRO	conflict	UNP N1NRW3
B	606	VAL	ALA	conflict	UNP N1NRW3
B	620	LEU	PHE	conflict	UNP N1NRW3
B	637	PRO	SER	conflict	UNP N1NRW3
B	682	ASN	THR	conflict	UNP N1NRW3
B	686	SER	ARG	conflict	UNP N1NRW3
B	695	HIS	SER	conflict	UNP N1NRW3
B	696	ASN	ASP	conflict	UNP N1NRW3
B	736	ASP	ASN	conflict	UNP N1NRW3
B	742	THR	MET	conflict	UNP N1NRW3
B	748	SER	THR	conflict	UNP N1NRW3
B	750	ASN	SER	conflict	UNP N1NRW3
B	751	ALA	ASP	conflict	UNP N1NRW3
B	752	ASN	GLU	conflict	UNP N1NRW3
B	788	GLY	ASP	conflict	UNP N1NRW3
B	790	ALA	VAL	conflict	UNP N1NRW3
B	795	LYS	ARG	conflict	UNP N1NRW3
B	796	ASN	SER	conflict	UNP N1NRW3
B	911	SER	ALA	conflict	UNP N1NRW3
B	914	GLU	LYS	conflict	UNP N1NRW3
B	923	GLU	ALA	conflict	UNP N1NRW3
B	1067	LYS	GLN	conflict	UNP N1NRW3
B	1075	ASP	GLU	conflict	UNP N1NRW3
B	1126	ASP	ASN	conflict	UNP N1NRW3
B	1250	LYS	VAL	conflict	UNP N1NRW3
B	1253	SER	PRO	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1257	GLY	ASP	conflict	UNP N1NRW3
B	1258	SER	ASN	conflict	UNP N1NRW3
B	1514	ILE	VAL	conflict	UNP N1NRW3
B	1519	MET	VAL	conflict	UNP N1NRW3
B	1877	ASN	TYR	conflict	UNP N1NRW3
B	1880	MET	THR	conflict	UNP N1NRW3
B	1884	ILE	VAL	conflict	UNP N1NRW3
B	1920	THR	ALA	conflict	UNP N1NRW3
B	1943	GLY	VAL	conflict	UNP N1NRW3
B	1947	GLN	HIS	conflict	UNP N1NRW3
B	1959	MET	ALA	conflict	UNP N1NRW3
B	1961	GLY	ASP	conflict	UNP N1NRW3
B	1962	ARG	ASN	conflict	UNP N1NRW3
B	1964	GLY	GLU	conflict	UNP N1NRW3
B	1966	SER	ALA	conflict	UNP N1NRW3
B	1967	LYS	THR	conflict	UNP N1NRW3
B	1968	ASN	GLN	conflict	UNP N1NRW3
B	1969	LEU	PRO	conflict	UNP N1NRW3
B	2057	THR	ALA	conflict	UNP N1NRW3
B	2149	LEU	PHE	conflict	UNP N1NRW3
B	2161	VAL	ALA	conflict	UNP N1NRW3
B	2164	ILE	VAL	conflict	UNP N1NRW3
B	2178	LEU	PHE	conflict	UNP N1NRW3
B	2430	LEU	PHE	conflict	UNP N1NRW3
C	172	HIS	PRO	conflict	UNP N1NRW3
C	343	ASN	HIS	conflict	UNP N1NRW3
C	344	ILE	VAL	conflict	UNP N1NRW3
C	360	ARG	CYS	conflict	UNP N1NRW3
C	365	VAL	ILE	conflict	UNP N1NRW3
C	377	ALA	SER	conflict	UNP N1NRW3
C	379	PRO	THR	conflict	UNP N1NRW3
C	391	ILE	VAL	conflict	UNP N1NRW3
C	407	SER	ASN	conflict	UNP N1NRW3
C	410	LYS	ARG	conflict	UNP N1NRW3
C	566	VAL	ILE	conflict	UNP N1NRW3
C	583	ALA	THR	conflict	UNP N1NRW3
C	586	THR	ILE	conflict	UNP N1NRW3
C	587	ILE	LEU	conflict	UNP N1NRW3
C	592	PHE	PRO	conflict	UNP N1NRW3
C	606	VAL	ALA	conflict	UNP N1NRW3
C	620	LEU	PHE	conflict	UNP N1NRW3
C	637	PRO	SER	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	682	ASN	THR	conflict	UNP N1NRW3
C	686	SER	ARG	conflict	UNP N1NRW3
C	695	HIS	SER	conflict	UNP N1NRW3
C	696	ASN	ASP	conflict	UNP N1NRW3
C	736	ASP	ASN	conflict	UNP N1NRW3
C	742	THR	MET	conflict	UNP N1NRW3
C	748	SER	THR	conflict	UNP N1NRW3
C	750	ASN	SER	conflict	UNP N1NRW3
C	751	ALA	ASP	conflict	UNP N1NRW3
C	752	ASN	GLU	conflict	UNP N1NRW3
C	788	GLY	ASP	conflict	UNP N1NRW3
C	790	ALA	VAL	conflict	UNP N1NRW3
C	795	LYS	ARG	conflict	UNP N1NRW3
C	796	ASN	SER	conflict	UNP N1NRW3
C	911	SER	ALA	conflict	UNP N1NRW3
C	914	GLU	LYS	conflict	UNP N1NRW3
C	923	GLU	ALA	conflict	UNP N1NRW3
C	1067	LYS	GLN	conflict	UNP N1NRW3
C	1075	ASP	GLU	conflict	UNP N1NRW3
C	1126	ASP	ASN	conflict	UNP N1NRW3
C	1250	LYS	VAL	conflict	UNP N1NRW3
C	1253	SER	PRO	conflict	UNP N1NRW3
C	1257	GLY	ASP	conflict	UNP N1NRW3
C	1258	SER	ASN	conflict	UNP N1NRW3
C	1514	ILE	VAL	conflict	UNP N1NRW3
C	1519	MET	VAL	conflict	UNP N1NRW3
C	1877	ASN	TYR	conflict	UNP N1NRW3
C	1880	MET	THR	conflict	UNP N1NRW3
C	1884	ILE	VAL	conflict	UNP N1NRW3
C	1920	THR	ALA	conflict	UNP N1NRW3
C	1943	GLY	VAL	conflict	UNP N1NRW3
C	1947	GLN	HIS	conflict	UNP N1NRW3
C	1959	MET	ALA	conflict	UNP N1NRW3
C	1961	GLY	ASP	conflict	UNP N1NRW3
C	1962	ARG	ASN	conflict	UNP N1NRW3
C	1964	GLY	GLU	conflict	UNP N1NRW3
C	1966	SER	ALA	conflict	UNP N1NRW3
C	1967	LYS	THR	conflict	UNP N1NRW3
C	1968	ASN	GLN	conflict	UNP N1NRW3
C	1969	LEU	PRO	conflict	UNP N1NRW3
C	2057	THR	ALA	conflict	UNP N1NRW3
C	2149	LEU	PHE	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2161	VAL	ALA	conflict	UNP N1NRW3
C	2164	ILE	VAL	conflict	UNP N1NRW3
C	2178	LEU	PHE	conflict	UNP N1NRW3
C	2430	LEU	PHE	conflict	UNP N1NRW3
D	172	HIS	PRO	conflict	UNP N1NRW3
D	343	ASN	HIS	conflict	UNP N1NRW3
D	344	ILE	VAL	conflict	UNP N1NRW3
D	360	ARG	CYS	conflict	UNP N1NRW3
D	365	VAL	ILE	conflict	UNP N1NRW3
D	377	ALA	SER	conflict	UNP N1NRW3
D	379	PRO	THR	conflict	UNP N1NRW3
D	391	ILE	VAL	conflict	UNP N1NRW3
D	407	SER	ASN	conflict	UNP N1NRW3
D	410	LYS	ARG	conflict	UNP N1NRW3
D	566	VAL	ILE	conflict	UNP N1NRW3
D	583	ALA	THR	conflict	UNP N1NRW3
D	586	THR	ILE	conflict	UNP N1NRW3
D	587	ILE	LEU	conflict	UNP N1NRW3
D	592	PHE	PRO	conflict	UNP N1NRW3
D	606	VAL	ALA	conflict	UNP N1NRW3
D	620	LEU	PHE	conflict	UNP N1NRW3
D	637	PRO	SER	conflict	UNP N1NRW3
D	682	ASN	THR	conflict	UNP N1NRW3
D	686	SER	ARG	conflict	UNP N1NRW3
D	695	HIS	SER	conflict	UNP N1NRW3
D	696	ASN	ASP	conflict	UNP N1NRW3
D	736	ASP	ASN	conflict	UNP N1NRW3
D	742	THR	MET	conflict	UNP N1NRW3
D	748	SER	THR	conflict	UNP N1NRW3
D	750	ASN	SER	conflict	UNP N1NRW3
D	751	ALA	ASP	conflict	UNP N1NRW3
D	752	ASN	GLU	conflict	UNP N1NRW3
D	788	GLY	ASP	conflict	UNP N1NRW3
D	790	ALA	VAL	conflict	UNP N1NRW3
D	795	LYS	ARG	conflict	UNP N1NRW3
D	796	ASN	SER	conflict	UNP N1NRW3
D	911	SER	ALA	conflict	UNP N1NRW3
D	914	GLU	LYS	conflict	UNP N1NRW3
D	923	GLU	ALA	conflict	UNP N1NRW3
D	1067	LYS	GLN	conflict	UNP N1NRW3
D	1075	ASP	GLU	conflict	UNP N1NRW3
D	1126	ASP	ASN	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1250	LYS	VAL	conflict	UNP N1NRW3
D	1253	SER	PRO	conflict	UNP N1NRW3
D	1257	GLY	ASP	conflict	UNP N1NRW3
D	1258	SER	ASN	conflict	UNP N1NRW3
D	1514	ILE	VAL	conflict	UNP N1NRW3
D	1519	MET	VAL	conflict	UNP N1NRW3
D	1877	ASN	TYR	conflict	UNP N1NRW3
D	1880	MET	THR	conflict	UNP N1NRW3
D	1884	ILE	VAL	conflict	UNP N1NRW3
D	1920	THR	ALA	conflict	UNP N1NRW3
D	1943	GLY	VAL	conflict	UNP N1NRW3
D	1947	GLN	HIS	conflict	UNP N1NRW3
D	1959	MET	ALA	conflict	UNP N1NRW3
D	1961	GLY	ASP	conflict	UNP N1NRW3
D	1962	ARG	ASN	conflict	UNP N1NRW3
D	1964	GLY	GLU	conflict	UNP N1NRW3
D	1966	SER	ALA	conflict	UNP N1NRW3
D	1967	LYS	THR	conflict	UNP N1NRW3
D	1968	ASN	GLN	conflict	UNP N1NRW3
D	1969	LEU	PRO	conflict	UNP N1NRW3
D	2057	THR	ALA	conflict	UNP N1NRW3
D	2149	LEU	PHE	conflict	UNP N1NRW3
D	2161	VAL	ALA	conflict	UNP N1NRW3
D	2164	ILE	VAL	conflict	UNP N1NRW3
D	2178	LEU	PHE	conflict	UNP N1NRW3
D	2430	LEU	PHE	conflict	UNP N1NRW3
E	172	HIS	PRO	conflict	UNP N1NRW3
E	343	ASN	HIS	conflict	UNP N1NRW3
E	344	ILE	VAL	conflict	UNP N1NRW3
E	360	ARG	CYS	conflict	UNP N1NRW3
E	365	VAL	ILE	conflict	UNP N1NRW3
E	377	ALA	SER	conflict	UNP N1NRW3
E	379	PRO	THR	conflict	UNP N1NRW3
E	391	ILE	VAL	conflict	UNP N1NRW3
E	407	SER	ASN	conflict	UNP N1NRW3
E	410	LYS	ARG	conflict	UNP N1NRW3
E	566	VAL	ILE	conflict	UNP N1NRW3
E	583	ALA	THR	conflict	UNP N1NRW3
E	586	THR	ILE	conflict	UNP N1NRW3
E	587	ILE	LEU	conflict	UNP N1NRW3
E	592	PHE	PRO	conflict	UNP N1NRW3
E	606	VAL	ALA	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	620	LEU	PHE	conflict	UNP N1NRW3
E	637	PRO	SER	conflict	UNP N1NRW3
E	682	ASN	THR	conflict	UNP N1NRW3
E	686	SER	ARG	conflict	UNP N1NRW3
E	695	HIS	SER	conflict	UNP N1NRW3
E	696	ASN	ASP	conflict	UNP N1NRW3
E	736	ASP	ASN	conflict	UNP N1NRW3
E	742	THR	MET	conflict	UNP N1NRW3
E	748	SER	THR	conflict	UNP N1NRW3
E	750	ASN	SER	conflict	UNP N1NRW3
E	751	ALA	ASP	conflict	UNP N1NRW3
E	752	ASN	GLU	conflict	UNP N1NRW3
E	788	GLY	ASP	conflict	UNP N1NRW3
E	790	ALA	VAL	conflict	UNP N1NRW3
E	795	LYS	ARG	conflict	UNP N1NRW3
E	796	ASN	SER	conflict	UNP N1NRW3
E	911	SER	ALA	conflict	UNP N1NRW3
E	914	GLU	LYS	conflict	UNP N1NRW3
E	923	GLU	ALA	conflict	UNP N1NRW3
E	1067	LYS	GLN	conflict	UNP N1NRW3
E	1075	ASP	GLU	conflict	UNP N1NRW3
E	1126	ASP	ASN	conflict	UNP N1NRW3
E	1250	LYS	VAL	conflict	UNP N1NRW3
E	1253	SER	PRO	conflict	UNP N1NRW3
E	1257	GLY	ASP	conflict	UNP N1NRW3
E	1258	SER	ASN	conflict	UNP N1NRW3
E	1514	ILE	VAL	conflict	UNP N1NRW3
E	1519	MET	VAL	conflict	UNP N1NRW3
E	1877	ASN	TYR	conflict	UNP N1NRW3
E	1880	MET	THR	conflict	UNP N1NRW3
E	1884	ILE	VAL	conflict	UNP N1NRW3
E	1920	THR	ALA	conflict	UNP N1NRW3
E	1943	GLY	VAL	conflict	UNP N1NRW3
E	1947	GLN	HIS	conflict	UNP N1NRW3
E	1959	MET	ALA	conflict	UNP N1NRW3
E	1961	GLY	ASP	conflict	UNP N1NRW3
E	1962	ARG	ASN	conflict	UNP N1NRW3
E	1964	GLY	GLU	conflict	UNP N1NRW3
E	1966	SER	ALA	conflict	UNP N1NRW3
E	1967	LYS	THR	conflict	UNP N1NRW3
E	1968	ASN	GLN	conflict	UNP N1NRW3
E	1969	LEU	PRO	conflict	UNP N1NRW3

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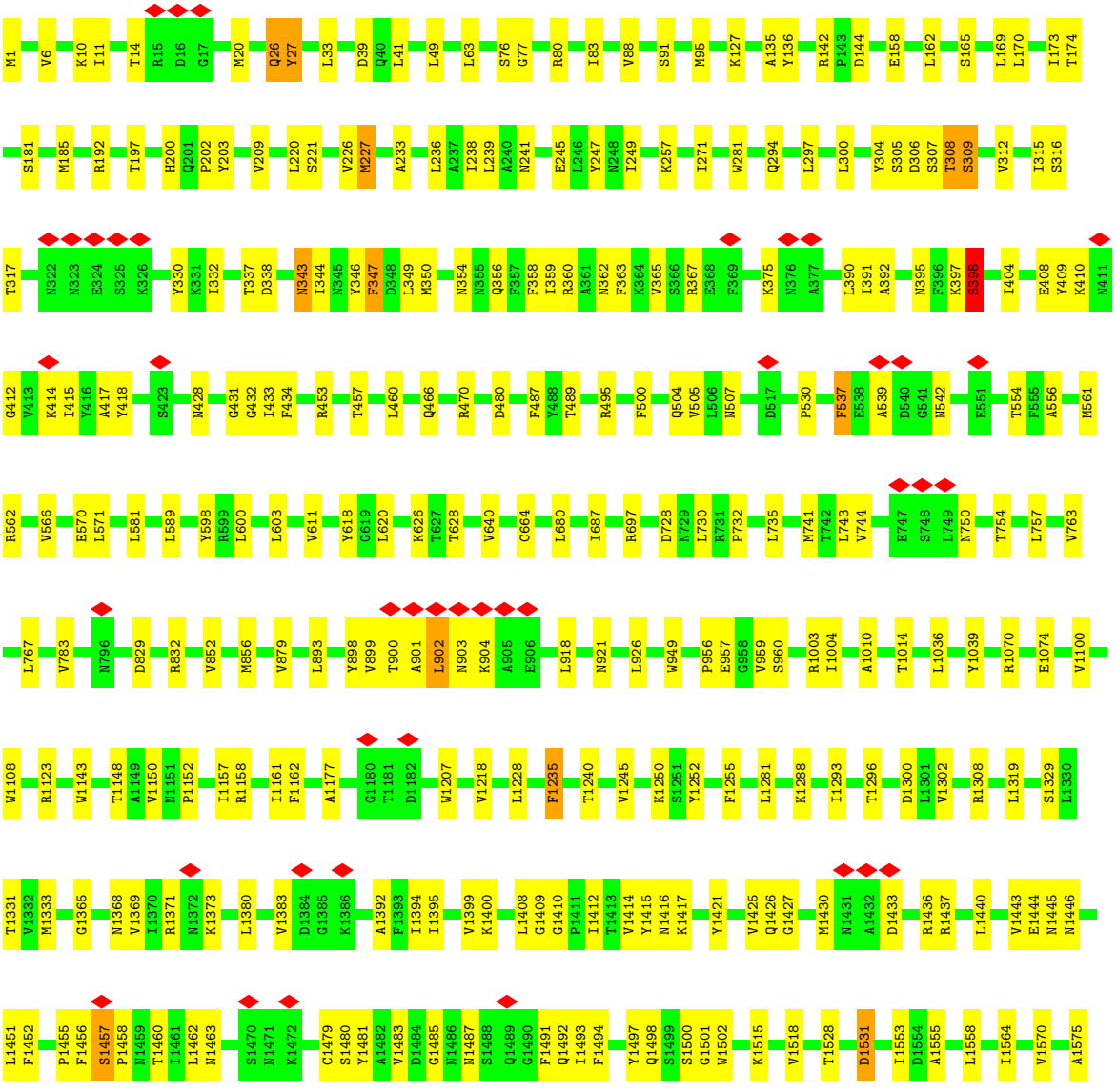
Chain	Residue	Modelled	Actual	Comment	Reference
E	2057	THR	ALA	conflict	UNP N1NRW3
E	2149	LEU	PHE	conflict	UNP N1NRW3
E	2161	VAL	ALA	conflict	UNP N1NRW3
E	2164	ILE	VAL	conflict	UNP N1NRW3
E	2178	LEU	PHE	conflict	UNP N1NRW3
E	2430	LEU	PHE	conflict	UNP N1NRW3

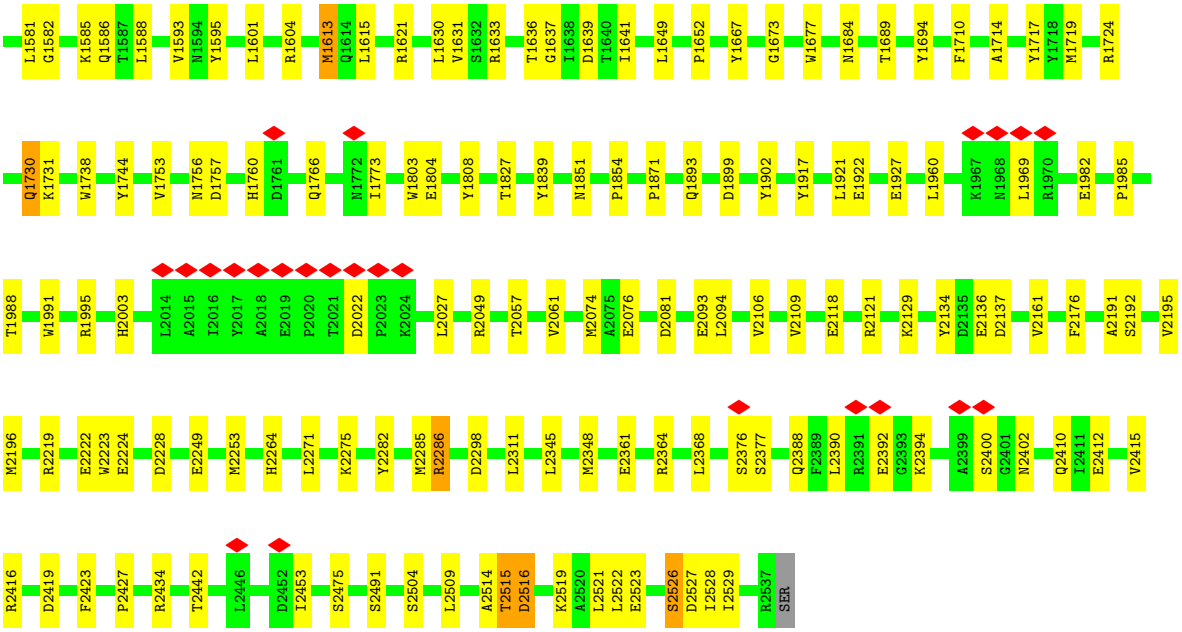
3 Residue-property plots (i)

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

- Molecule 1: XptA2

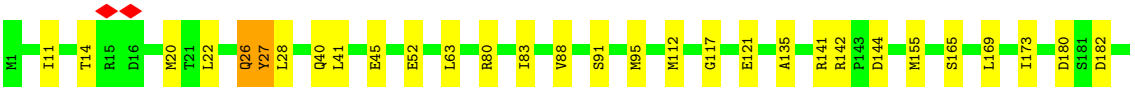
Chain A:

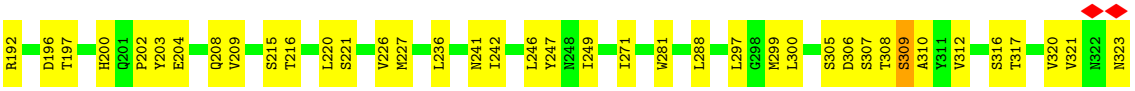


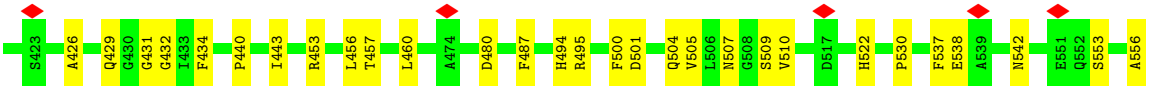


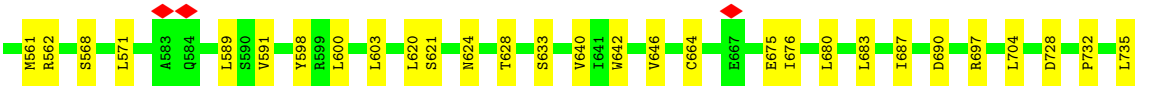
• Molecule 1: XptA2

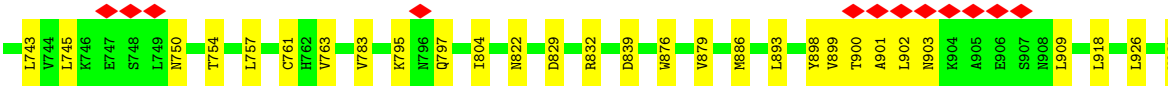
Chain B:

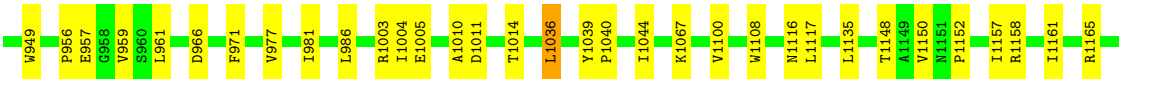


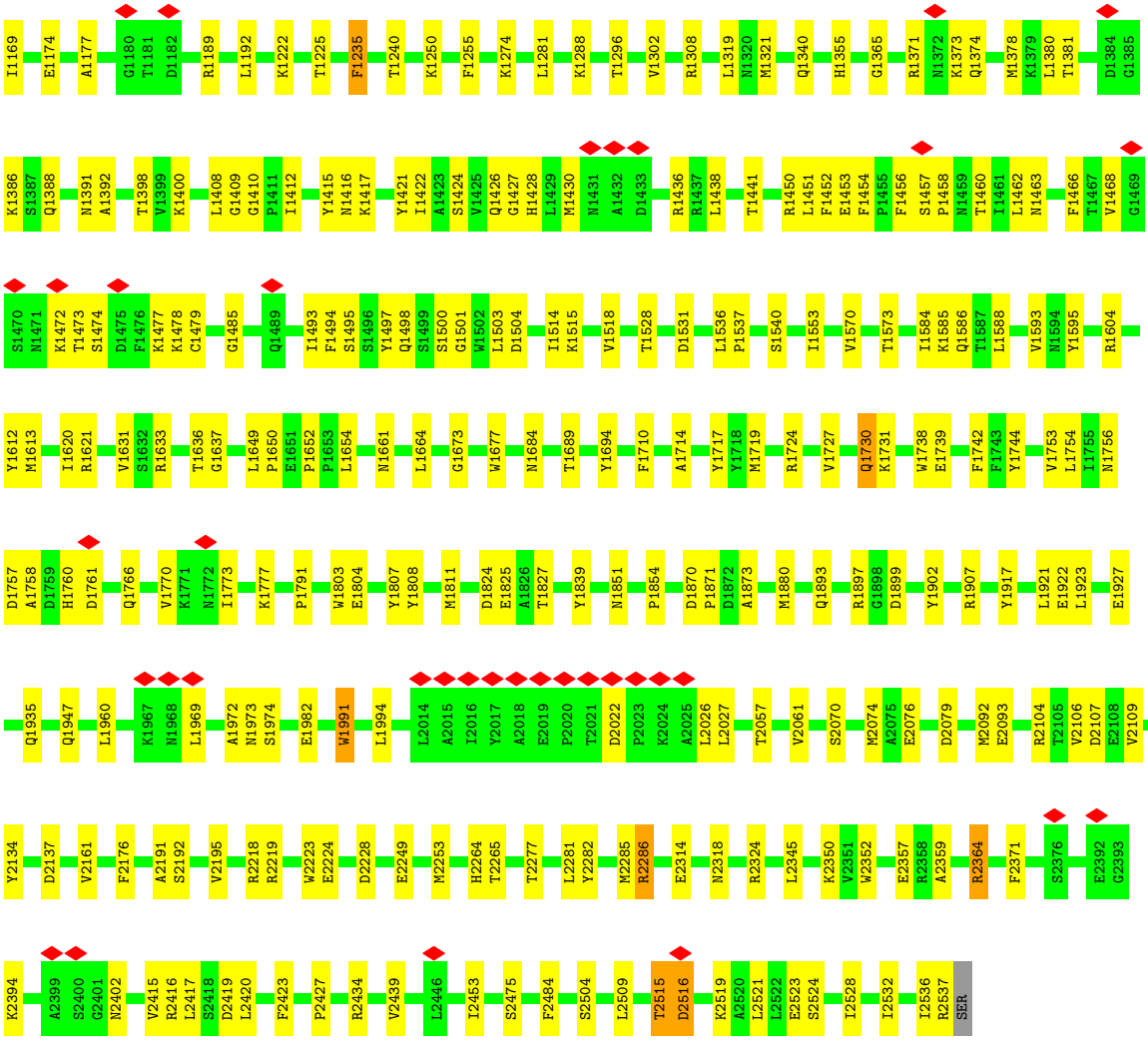






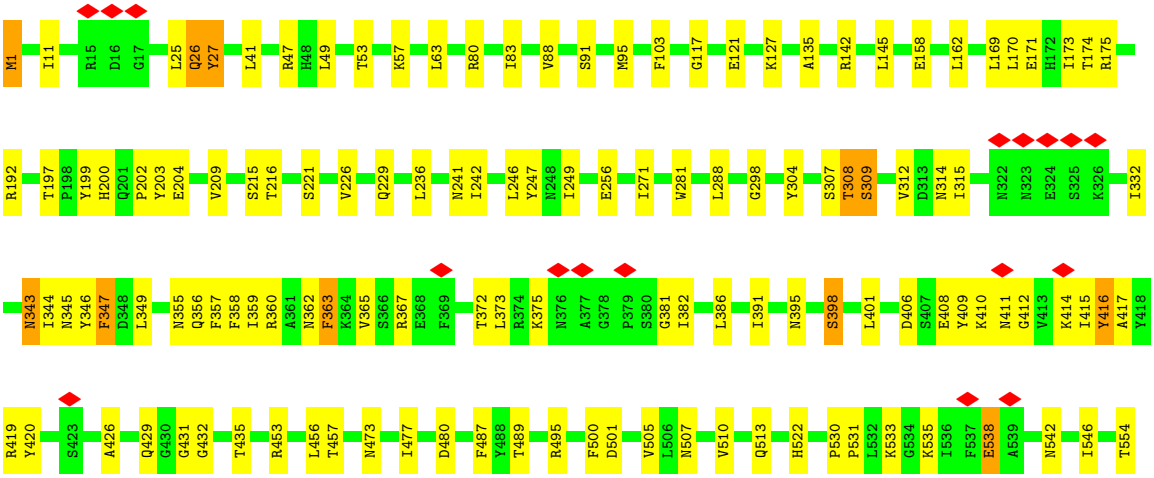


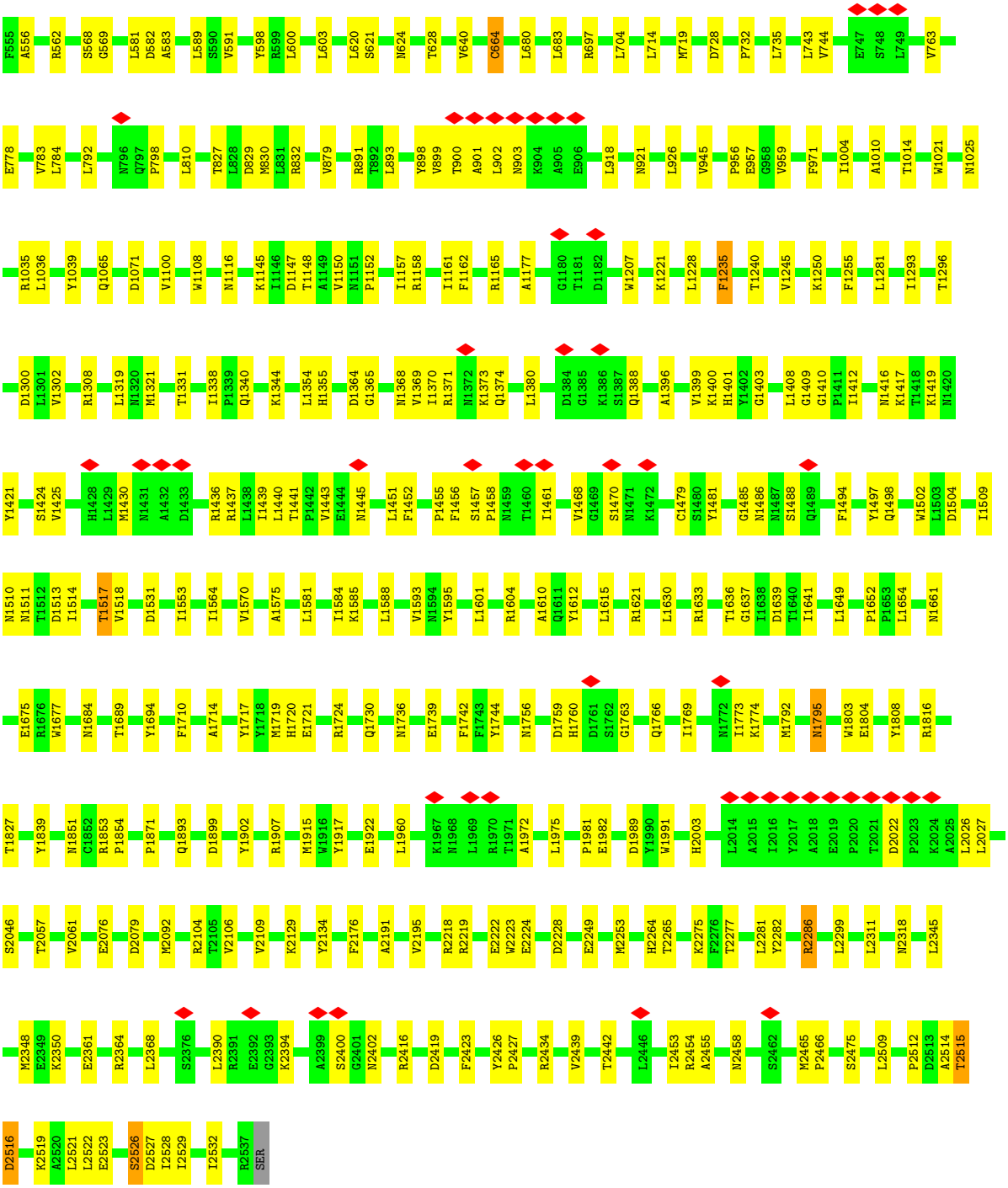




- Molecule 1: XptA2

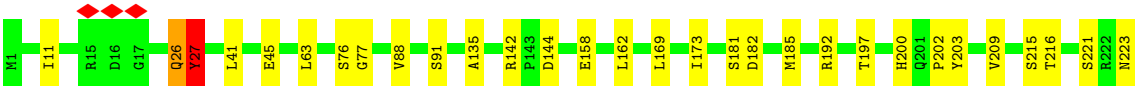
Chain C:

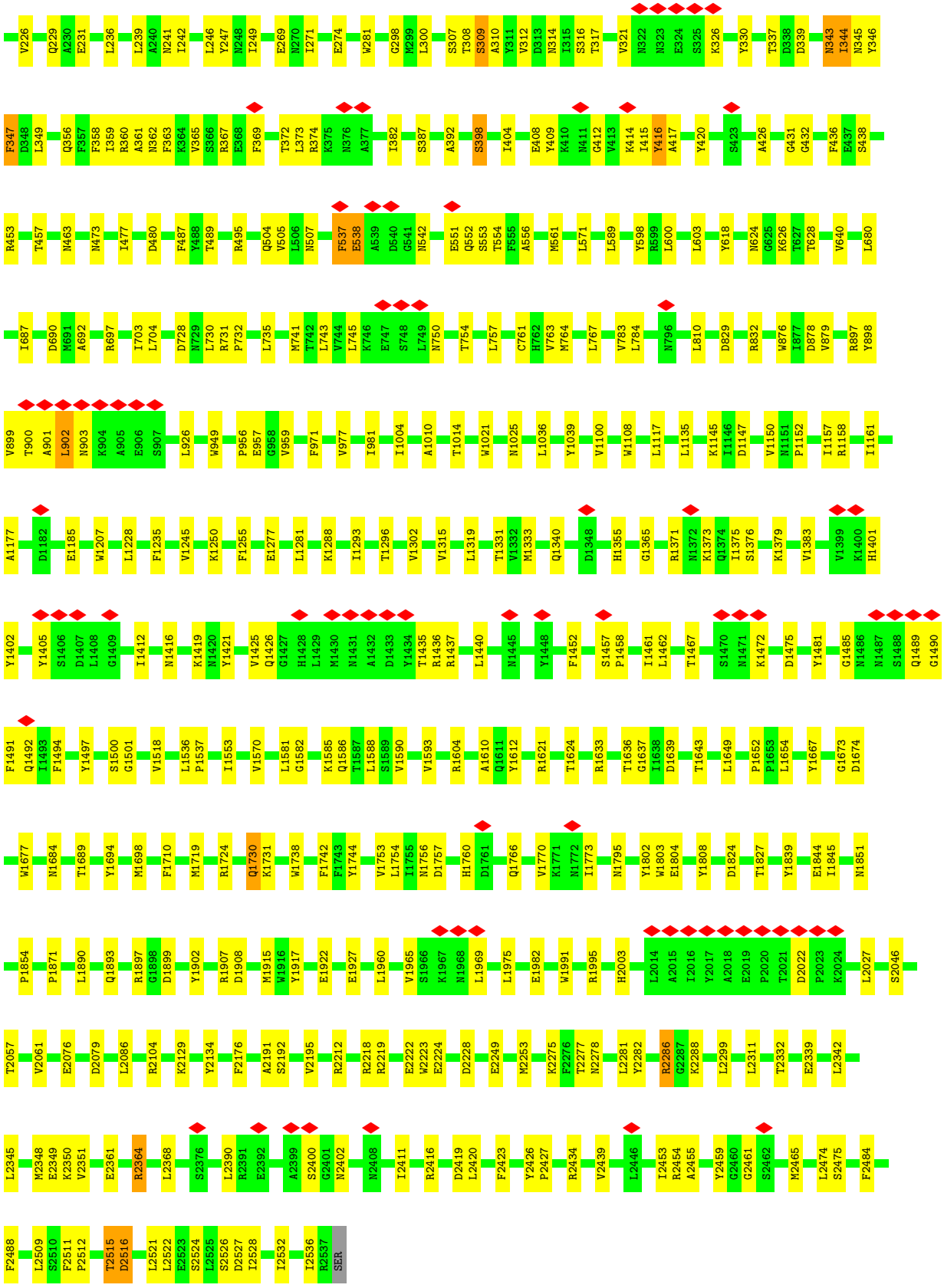




- Molecule 1: XptA2

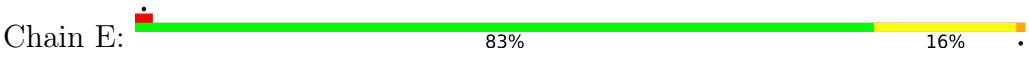
Chain D:

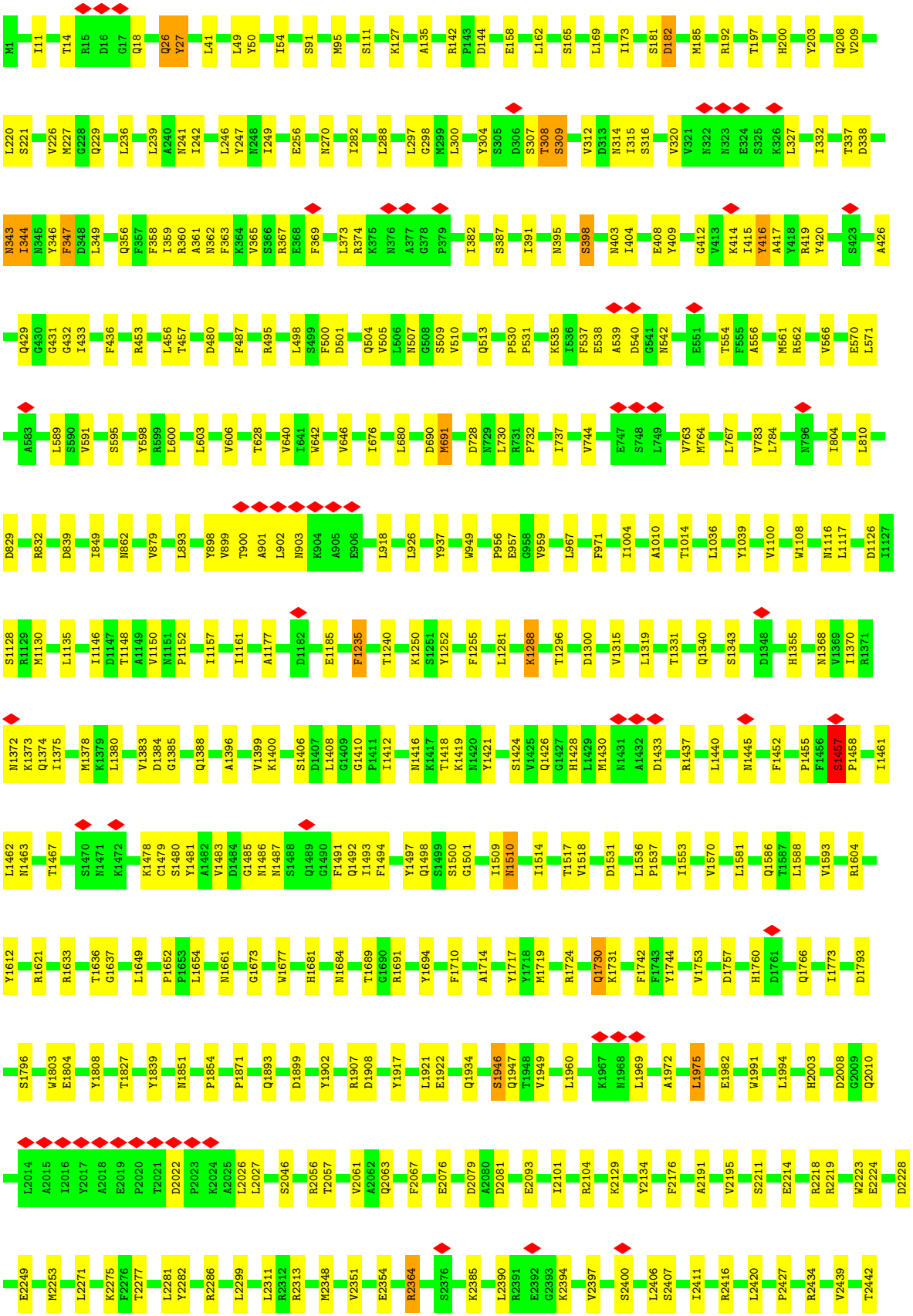


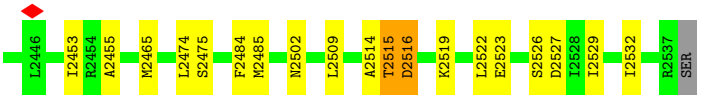


- Molecule 1: XptA2

Chain E:


83%
16%


M1 I11 T14 R15 D16 G17 Q18 Q26 Y27 L41 L49 Y50 I54 S91 M95 S111 K127 A135 R142 P143 D144 E158 L162 S165 L169 I173 S181 D182 M185 R192 T197 H200 Y203 Q208 V209
L220 S221 V226 M227 G228 Q229 L236 L239 A240 N241 I242 L246 Y247 N248 I249 E256 N270 I282 L288 L297 G298 M299 L300 Y304 S305 D306 S307 T308 S309 V312 D313 N314 I315 S316 V320 V321 N322 N323 E324 S325 K326 L327 I332 T337 D338
N343 I344 N345 Y346 F347 D348 L349 Q356 F357 F358 I359 R360 A361 N362 F363 K364 V365 S366 R367 E368 F369 L373 R374 K375 N376 A377 G378 P379 I382 S387 I391 N395 S398 N403 I404 E408 Y409 G412 V413 K414 I415 Y416 A417 Y418 R419 Y420 S423 A426
Q429 G430 G431 G432 I433 F436 R453 L456 T457 D480 F487 R495 L498 S499 F500 D501 Q504 V505 L506 N507 G508 S509 V510 Q513 P530 P531 K535 I536 F537 E538 A539 D540 G541 N542 E551 T554 F555 A556 M561 R562 V566 E570 L571
A583 L589 S590 V591 S595 Y598 R599 L600 L603 V606 T628 V640 I641 W642 V646 I676 L680 D690 M691 D728 N729 L730 R731 P732 I737 V744 E747 S748 L749 V763 M764 L767 V783 L784 N796 I804 L810
D829 R832 D839 I849 N862 V879 L893 Y898 V899 T900 A901 L902 N903 K904 A905 E906 L918 L926 Y937 W949 P956 E957 G958 V959 L967 F971 I1004 A1010 T1014 L1036 Y1039 V1100 W1108 N1116 L1117 D1126 I1127
S1128 R1129 M1130 L1135 I1146 D1147 T1148 A1149 V1150 N1151 P1152 I1157 I1161 A1177 D1182 E1185 F1235 T1240 K1250 S1251 Y1252 F1255 L1281 K1288 T1296 D1300 V1315 L1319 T1331 Q1340 S1343 D1348 H1355 N1368 V1369 I1370 R1371
N1372 K1373 Q1374 I1375 M1378 K1379 L1380 V1383 D1384 G1385 Q1388 A1396 V1399 K1400 S1406 D1407 L1408 G1409 G1410 P1411 I1412 N1416 K1417 T1418 K1419 N1420 Y1421 S1424 V1425 Q1426 G1427 H1428 L1429 M1430 N1431 A1432 D1433 R1437 L1440 N1445 F1452 P1455 F1456 S1457 P1458 I1461
L1462 N1463 T1467 S1470 N1471 K1472 K1478 C1479 S1480 Y1481 A1482 V1483 D1484 G1485 N1486 N1487 S1488 Q1489 G1490 F1491 Q1492 I1493 F1494 Y1497 Q1498 S1499 S1500 G1501 I1509 N1510 I1514 T1517 V1518 D1531 L1536 P1537 I1553 V1570 L1581 Q1586 T1587 L1588 V1593 R1604
Y1612 R1621 R1633 T1636 G1637 L1649 P1652 P1653 L1654 N1661 G1673 W1677 H1681 N1684 T1689 G1690 R1691 Y1694 F1710 A1714 Y1717 Y1718 M1719 R1724 Q1730 K1731 F1742 F1743 Y1744 V1753 D1757 H1760 D1761 Q1766 I1773 D1793
S1796 W1803 E1804 Y1808 T1827 Y1839 N1851 P1854 P1871 Q1893 D1899 Y1902 R1907 D1908 Y1917 L1921 E1922 Q1934 S1946 Q1947 T1948 V1949 L1960 K1967 N1968 L1969 A1972 L1975 E1982 W1991 L1994 H2003 D2008 G2009 Q2010
L2014 A2015 I2016 Y2017 A2018 E2019 P2020 T2021 D2022 P2023 K2024 A2025 L2026 L2027 S2046 R2056 T2057 V2061 A2062 Q2063 F2067 E2076 D2079 A2080 D2081 E2093 I2101 R2104 K2129 Y2134 F2176 A2191 V2195 S2211 E2214 R2218 R2219 W2223 E2224 D2228
E2249 M2253 L2271 K2275 F2276 T2277 L2281 Y2282 R2286 L2299 L2311 R2312 R2313 M2348 V2351 E2354 R2364 S2376 K2385 L2390 R2391 E2392 G2393 K2394 V2397 S2400 L2406 S2407 I2411 R2416 L2420 P2427 R2434 V2439 T2442


L2446
I2453
R2454
A2455
M2465
L2474
S2475
F2484
M2485
N2502
L2509
A2514
T2515
D2516
K2519
L2522
E2523
S2526
D2527
I2528
I2529
I2532
R2537
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	198591	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.099	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	448.872, 448.872, 448.872	wwPDB
Map dimensions	354, 354, 354	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	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	0.29	0/20413	0.51	3/27714 (0.0%)
1	B	0.29	0/20413	0.51	3/27714 (0.0%)
1	C	0.29	0/20413	0.51	5/27714 (0.0%)
1	D	0.29	0/20413	0.51	5/27714 (0.0%)
1	E	0.29	0/20413	0.51	4/27714 (0.0%)
All	All	0.29	0/102065	0.51	20/138570 (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	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
All	All	0	7

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	2515	THR	C-N-CA	11.05	149.34	121.70
1	D	26	GLN	C-N-CA	10.76	148.61	121.70
1	B	26	GLN	C-N-CA	10.61	148.22	121.70
1	E	26	GLN	C-N-CA	10.59	148.18	121.70
1	C	26	GLN	C-N-CA	10.53	148.03	121.70
1	A	26	GLN	C-N-CA	10.52	148.00	121.70
1	B	2515	THR	C-N-CA	10.38	147.65	121.70
1	C	2515	THR	C-N-CA	10.26	147.36	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2515	THR	C-N-CA	10.17	147.13	121.70
1	E	2515	THR	C-N-CA	10.13	147.03	121.70
1	C	798	PRO	N-CD-CG	-7.93	91.30	103.20
1	D	312	VAL	C-N-CA	7.29	139.93	121.70
1	E	1975	LEU	CA-CB-CG	7.17	131.78	115.30
1	B	312	VAL	C-N-CA	7.05	139.32	121.70
1	A	312	VAL	C-N-CA	7.02	139.26	121.70
1	C	312	VAL	C-N-CA	7.01	139.24	121.70
1	E	312	VAL	C-N-CA	6.85	138.83	121.70
1	D	1975	LEU	CA-CB-CG	6.45	130.13	115.30
1	C	1989	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	339	ASP	CB-CG-OD1	5.30	123.07	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	B	1457	SER	Peptide
1	B	398	SER	Peptide
1	C	398	SER	Peptide
1	D	398	SER	Peptide
1	E	1457	SER	Peptide
1	E	398	SER	Peptide

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	20007	0	19592	267	0
1	B	20007	0	19591	290	0
1	C	20007	0	19592	270	0
1	D	20007	0	19590	252	0
1	E	20007	0	19591	275	0
All	All	100035	0	97956	1288	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 7.

All (1288) 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:D:2515:THR:H	1:D:2516:ASP:HB2	1.36	0.90
1:A:2515:THR:H	1:A:2516:ASP:HB2	1.37	0.90
1:B:2515:THR:H	1:B:2516:ASP:HB2	1.36	0.89
1:E:2515:THR:H	1:E:2516:ASP:HB2	1.39	0.88
1:C:2515:THR:H	1:C:2516:ASP:HB2	1.40	0.87
1:B:1391:ASN:HD22	1:B:1416:ASN:HD21	1.21	0.85
1:E:1684:ASN:HB3	1:E:1719:MET:HB2	1.58	0.83
1:A:1440:LEU:HB2	1:A:1452:PHE:HB2	1.60	0.83
1:E:415:ILE:HG21	1:E:432:GLY:H	1.44	0.81
1:B:1684:ASN:HB3	1:B:1719:MET:HB2	1.60	0.81
1:A:338:ASP:OD2	1:A:428:ASN:ND2	2.15	0.80
1:E:1440:LEU:HB2	1:E:1452:PHE:HB2	1.64	0.80
1:D:1383:VAL:HG11	1:D:1467:THR:HB	1.64	0.80
1:C:415:ILE:HG12	1:C:431:GLY:HA3	1.64	0.79
1:E:1485:GLY:HA2	1:E:1494:PHE:HD2	1.47	0.79
1:C:1621:ARG:NH2	1:C:1652:PRO:O	2.16	0.78
1:B:1416:ASN:HB3	1:B:1421:TYR:HB2	1.65	0.78
1:B:1150:VAL:HG12	1:B:1152:PRO:HD3	1.66	0.77
1:C:513:GLN:HE22	1:C:538:GLU:HG2	1.49	0.77
1:D:1150:VAL:HG12	1:D:1152:PRO:HD3	1.66	0.77
1:E:1150:VAL:HG12	1:E:1152:PRO:HD3	1.67	0.77
1:A:1621:ARG:NH2	1:A:1652:PRO:O	2.18	0.77
1:C:1380:LEU:O	1:C:1388:GLN:NE2	2.19	0.76
1:B:1621:ARG:NH2	1:B:1652:PRO:O	2.18	0.76
1:B:135:ALA:HB2	1:B:957:GLU:HB2	1.68	0.76
1:D:1621:ARG:NH2	1:D:1652:PRO:O	2.19	0.75
1:E:1621:ARG:NH2	1:E:1652:PRO:O	2.20	0.75
1:B:415:ILE:HG12	1:B:431:GLY:HA3	1.69	0.75
1:A:1150:VAL:HG12	1:A:1152:PRO:HD3	1.69	0.74
1:E:1946:SER:HB3	1:E:1949:VAL:HG12	1.69	0.74
1:A:365:VAL:HG22	1:A:392:ALA:H	1.53	0.73
1:C:1150:VAL:HG12	1:C:1152:PRO:HD3	1.71	0.73
1:C:1684:ASN:HB3	1:C:1719:MET:HB2	1.69	0.73
1:D:274:GLU:HG2	1:D:1490:GLY:HA2	1.69	0.73
1:C:1612:TYR:HB3	1:C:1654:LEU:HD22	1.71	0.73
1:E:415:ILE:HG21	1:E:432:GLY:N	2.03	0.73
1:E:1485:GLY:HA3	1:E:1493:ILE:HA	1.70	0.72
1:A:1689:THR:O	1:A:1724:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1689:THR:O	1:B:1724:ARG:NH2	2.22	0.72
1:D:135:ALA:HB2	1:D:957:GLU:HB2	1.72	0.72
1:E:135:ALA:HB2	1:E:957:GLU:HB2	1.71	0.72
1:A:135:ALA:HB2	1:A:957:GLU:HB2	1.72	0.71
1:B:226:VAL:HG21	1:B:879:VAL:HG11	1.72	0.71
1:C:415:ILE:HG21	1:C:432:GLY:H	1.55	0.71
1:C:135:ALA:HB2	1:C:957:GLU:HB2	1.72	0.71
1:E:1689:THR:O	1:E:1724:ARG:NH2	2.23	0.71
1:C:2311:LEU:HD22	1:C:2348:MET:HG2	1.73	0.71
1:E:374:ARG:NH2	1:E:403:ASN:OD1	2.23	0.71
1:E:1500:SER:OG	1:E:1501:GLY:N	2.22	0.71
1:C:2402:ASN:ND2	1:C:2419:ASP:OD2	2.24	0.70
1:E:1373:LYS:HG3	1:E:1412:ILE:HG13	1.72	0.70
1:D:415:ILE:HG12	1:D:431:GLY:HA3	1.73	0.70
1:B:1612:TYR:HB3	1:B:1654:LEU:HD22	1.74	0.70
1:D:1440:LEU:HB2	1:D:1452:PHE:HB2	1.73	0.69
1:A:226:VAL:HG21	1:A:879:VAL:HG11	1.75	0.69
1:C:1255:PHE:HB3	1:C:1281:LEU:HG	1.75	0.69
1:A:1383:VAL:H	1:A:1421:TYR:HE1	1.41	0.69
1:C:554:THR:HG22	1:C:556:ALA:H	1.58	0.69
1:D:554:THR:HG22	1:D:556:ALA:H	1.57	0.69
1:B:404:ILE:HD13	1:B:414:LYS:HD2	1.76	0.68
1:E:1457:SER:HB3	1:E:1458:PRO:HD2	1.75	0.68
1:A:1039:TYR:OH	1:A:1982:GLU:O	2.12	0.68
1:B:1408:LEU:HD12	1:B:1495:SER:HB2	1.74	0.68
1:D:415:ILE:HG21	1:D:432:GLY:N	2.09	0.68
1:B:1039:TYR:OH	1:B:1982:GLU:O	2.11	0.67
1:B:1373:LYS:HG3	1:B:1412:ILE:HG21	1.77	0.67
1:C:1321:MET:HB3	1:C:1584:ILE:HG21	1.75	0.67
1:B:1907:ARG:NH1	1:C:158:GLU:OE1	2.28	0.67
1:D:226:VAL:HG21	1:D:879:VAL:HG11	1.76	0.67
1:A:750:ASN:HB3	1:A:754:THR:HG22	1.77	0.67
1:A:1827:THR:OG1	1:A:1893:GLN:NE2	2.27	0.66
1:C:346:TYR:HE1	1:C:359:ILE:HG22	1.60	0.66
1:E:343:ASN:HA	1:E:363:PHE:HB2	1.75	0.66
1:C:778:GLU:OE2	1:C:778:GLU:N	2.27	0.66
1:B:220:LEU:HG	1:B:227:MET:HG3	1.78	0.66
1:B:1485:GLY:HA2	1:B:1494:PHE:HD1	1.61	0.66
1:C:343:ASN:HA	1:C:363:PHE:HB2	1.76	0.66
1:C:226:VAL:HG21	1:C:879:VAL:HG11	1.78	0.66
1:D:977:VAL:HB	1:D:981:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:LEU:HD11	1:A:640:VAL:HG22	1.78	0.66
1:C:1689:THR:O	1:C:1724:ARG:NH2	2.29	0.66
1:C:204:GLU:OE2	1:C:241:ASN:ND2	2.24	0.66
1:C:1485:GLY:HA3	1:C:1494:PHE:H	1.61	0.65
1:B:1633:ARG:HH22	1:B:1649:LEU:HD21	1.61	0.65
1:E:1612:TYR:HB3	1:E:1654:LEU:HD22	1.79	0.65
1:A:415:ILE:HG21	1:A:432:GLY:N	2.11	0.65
1:C:2390:LEU:HD11	1:C:2522:LEU:HB3	1.78	0.65
1:B:373:LEU:HB2	1:B:416:TYR:HB3	1.79	0.65
1:E:1039:TYR:OH	1:E:1982:GLU:O	2.14	0.65
1:D:2400:SER:O	1:D:2416:ARG:NH2	2.30	0.65
1:A:1684:ASN:HB3	1:A:1719:MET:HB2	1.78	0.65
1:A:346:TYR:HE1	1:A:359:ILE:HG22	1.60	0.64
1:D:956:PRO:HG2	1:D:959:VAL:HB	1.80	0.64
1:D:26:GLN:N	1:D:27:TYR:HB3	2.13	0.64
1:C:221:SER:OG	1:C:495:ARG:NH2	2.29	0.64
1:D:343:ASN:HA	1:D:363:PHE:HB2	1.80	0.64
1:D:1331:THR:HG21	1:D:1581:LEU:HD13	1.78	0.64
1:E:2400:SER:O	1:E:2416:ARG:NH2	2.30	0.64
1:A:2400:SER:O	1:A:2416:ARG:NH2	2.31	0.64
1:E:226:VAL:HG21	1:E:879:VAL:HG11	1.79	0.64
1:E:1380:LEU:O	1:E:1388:GLN:NE2	2.31	0.64
1:B:2515:THR:N	1:B:2516:ASP:HB2	2.11	0.64
1:D:1684:ASN:HB3	1:D:1719:MET:HB2	1.79	0.64
1:A:1380:LEU:HD21	1:A:1463:ASN:HB3	1.80	0.63
1:A:1500:SER:OG	1:A:1501:GLY:N	2.30	0.63
1:E:346:TYR:HE1	1:E:359:ILE:HG22	1.63	0.63
1:B:956:PRO:HG2	1:B:959:VAL:HB	1.81	0.63
1:C:1373:LYS:NZ	1:C:1409:GLY:O	2.30	0.63
1:D:1612:TYR:HB3	1:D:1654:LEU:HD22	1.81	0.63
1:E:360:ARG:HH12	1:E:417:ALA:HB1	1.63	0.63
1:B:343:ASN:HA	1:B:363:PHE:HB2	1.78	0.63
1:E:600:LEU:HD21	1:E:628:THR:HG21	1.79	0.63
1:C:956:PRO:HG2	1:C:959:VAL:HB	1.80	0.63
1:E:1426:GLN:HB3	1:E:1462:LEU:HD22	1.80	0.63
1:C:489:THR:OG1	1:C:507:ASN:ND2	2.32	0.63
1:D:192:ARG:HG2	1:D:249:ILE:HD11	1.81	0.63
1:C:360:ARG:NH1	1:C:362:ASN:OD1	2.32	0.62
1:E:1416:ASN:HB3	1:E:1421:TYR:HB2	1.81	0.62
1:A:209:VAL:HG22	1:A:926:LEU:HD11	1.81	0.62
1:E:554:THR:HG22	1:E:556:ALA:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:TYR:HE1	1:B:359:ILE:HG22	1.65	0.62
1:A:1744:TYR:HB2	1:A:1766:GLN:HG2	1.81	0.62
1:B:1474:SER:O	1:B:1478:LYS:NZ	2.23	0.62
1:C:415:ILE:HG21	1:C:432:GLY:N	2.14	0.62
1:A:170:LEU:O	1:A:174:THR:HG23	2.00	0.62
1:B:600:LEU:HD21	1:B:628:THR:HG21	1.81	0.62
1:D:373:LEU:HB2	1:D:416:TYR:HB3	1.82	0.62
1:A:360:ARG:HH21	1:A:390:LEU:HD13	1.65	0.62
1:C:2519:LYS:O	1:C:2523:GLU:HG3	2.00	0.62
1:D:1228:LEU:HD11	1:D:1245:VAL:HG13	1.82	0.62
1:A:2515:THR:N	1:A:2516:ASP:HB2	2.12	0.61
1:E:1437:ARG:HB2	1:E:1455:PRO:HA	1.81	0.61
1:C:531:PRO:HG3	1:C:535:LYS:HE3	1.80	0.61
1:E:1430:MET:HG3	1:E:1494:PHE:HD1	1.66	0.61
1:B:1388:GLN:HE21	1:B:1416:ASN:HD22	1.48	0.61
1:D:1500:SER:OG	1:D:1501:GLY:N	2.30	0.61
1:D:2104:ARG:NH1	1:E:2249:GLU:OE1	2.33	0.61
1:A:221:SER:OG	1:A:495:ARG:NH2	2.34	0.61
1:C:1:MET:HB3	1:C:1564:ILE:HG23	1.82	0.61
1:C:1440:LEU:HB2	1:C:1452:PHE:HB2	1.81	0.61
1:C:1517:THR:HG23	1:C:1570:VAL:HB	1.83	0.61
1:D:1185:GLU:OE1	1:D:1185:GLU:N	2.33	0.61
1:E:1804:GLU:HA	1:E:1808:TYR:HB2	1.82	0.61
1:A:1531:ASP:OD1	1:A:1531:ASP:N	2.34	0.61
1:D:2411:ILE:HG22	1:D:2511:PHE:HB2	1.83	0.61
1:A:956:PRO:HG2	1:A:959:VAL:HB	1.82	0.61
1:D:346:TYR:HE1	1:D:359:ILE:HG22	1.66	0.61
1:E:2515:THR:N	1:E:2516:ASP:HB2	2.14	0.61
1:B:1899:ASP:OD1	1:B:1917:TYR:OH	2.16	0.61
1:B:353:GLY:O	1:B:354:ASN:ND2	2.33	0.61
1:E:181:SER:O	1:E:185:MET:HG2	2.01	0.61
1:E:1633:ARG:HH22	1:E:1649:LEU:HD21	1.64	0.60
1:B:1739:GLU:HG2	1:B:1777:LYS:HE3	1.81	0.60
1:C:600:LEU:HD21	1:C:628:THR:HG21	1.82	0.60
1:D:1412:ILE:HB	1:D:1425:VAL:HG12	1.83	0.60
1:C:192:ARG:HG2	1:C:249:ILE:HD11	1.84	0.60
1:B:1744:TYR:HB2	1:B:1766:GLN:HG2	1.83	0.60
1:B:415:ILE:HG21	1:B:432:GLY:N	2.16	0.60
1:E:415:ILE:HG12	1:E:431:GLY:HA3	1.83	0.60
1:E:504:GLN:HA	1:E:507:ASN:HD22	1.66	0.60
1:B:241:ASN:O	1:B:457:THR:OG1	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:ALA:HB3	1:C:2176:PHE:HB2	1.84	0.60
1:B:2104:ARG:NH1	1:C:2249:GLU:OE2	2.34	0.60
1:C:1370:ILE:HA	1:C:1374:GLN:HG3	1.82	0.60
1:C:2515:THR:N	1:C:2516:ASP:HB2	2.13	0.60
1:C:1827:THR:HG1	1:C:1893:GLN:HE22	1.50	0.60
1:E:307:SER:O	1:E:309:SER:N	2.35	0.60
1:A:220:LEU:HG	1:A:227:MET:HG3	1.82	0.60
1:A:415:ILE:HG12	1:A:431:GLY:HA3	1.82	0.60
1:C:375:LYS:HE3	1:C:381:GLY:HA2	1.83	0.59
1:D:404:ILE:HD13	1:D:414:LYS:HD2	1.82	0.59
1:C:2439:VAL:HG22	1:C:2532:ILE:HG23	1.84	0.59
1:D:1689:THR:O	1:D:1724:ARG:NH2	2.36	0.59
1:D:1744:TYR:HB2	1:D:1766:GLN:HG2	1.84	0.59
1:A:11:ILE:HD11	1:A:41:LEU:HG	1.85	0.59
1:B:374:ARG:NH1	1:B:403:ASN:O	2.35	0.59
1:E:2455:ALA:HB3	1:E:2474:LEU:HB2	1.83	0.59
1:A:489:THR:OG1	1:A:507:ASN:ND2	2.36	0.59
1:D:603:LEU:HD21	1:D:640:VAL:HG22	1.83	0.59
1:D:1340:GLN:HB2	1:D:1355:HIS:HB2	1.85	0.59
1:A:901:ALA:O	1:A:902:LEU:HB2	2.03	0.59
1:A:247:TYR:CZ	1:A:898:TYR:HB3	2.38	0.59
1:A:1319:LEU:HD22	1:A:1588:LEU:HD13	1.85	0.59
1:D:2515:THR:HB	1:D:2516:ASP:OD2	2.03	0.59
1:E:1185:GLU:N	1:E:1185:GLU:OE1	2.35	0.59
1:A:1633:ARG:HH22	1:A:1649:LEU:HD21	1.68	0.59
1:D:169:LEU:O	1:D:173:ILE:HG12	2.03	0.59
1:B:1250:LYS:HD3	1:B:1296:THR:HG22	1.84	0.58
1:C:1443:VAL:HG13	1:C:1445:ASN:H	1.66	0.58
1:D:1899:ASP:OD1	1:D:1917:TYR:OH	2.21	0.58
1:E:1250:LYS:HD3	1:E:1296:THR:HG22	1.84	0.58
1:B:408:GLU:O	1:B:412:GLY:HA3	2.03	0.58
1:C:209:VAL:HG22	1:C:926:LEU:HD11	1.84	0.58
1:E:1636:THR:HG22	1:E:1637:GLY:H	1.67	0.58
1:A:1487:ASN:HB2	1:A:1492:GLN:HB2	1.83	0.58
1:C:732:PRO:HB3	1:C:763:VAL:HG21	1.85	0.58
1:C:2249:GLU:O	1:C:2253:MET:HG3	2.03	0.58
1:D:1795:ASN:O	1:D:1795:ASN:ND2	2.36	0.58
1:D:2402:ASN:ND2	1:D:2419:ASP:OD2	2.37	0.58
1:E:11:ILE:HD11	1:E:41:LEU:HG	1.85	0.58
1:B:83:ILE:HG23	1:B:1880:MET:HE1	1.86	0.58
1:E:142:ARG:NH2	1:E:144:ASP:OD2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:O	1:A:173:ILE:HG12	2.04	0.58
1:B:360:ARG:HH12	1:B:417:ALA:HB1	1.69	0.58
1:B:1500:SER:OG	1:B:1501:GLY:N	2.37	0.58
1:C:1039:TYR:OH	1:C:1982:GLU:O	2.14	0.58
1:D:1333:MET:HE3	1:D:1582:GLY:HA3	1.86	0.58
1:A:1177:ALA:HB3	1:B:2176:PHE:HB2	1.87	0.57
1:D:358:PHE:HB2	1:D:398:SER:HB3	1.86	0.57
1:D:901:ALA:O	1:D:902:LEU:HB2	2.04	0.57
1:C:408:GLU:O	1:C:412:GLY:HA3	2.05	0.57
1:C:603:LEU:HD21	1:C:640:VAL:HG22	1.85	0.57
1:E:956:PRO:HG2	1:E:959:VAL:HB	1.85	0.57
1:A:1255:PHE:HB3	1:A:1281:LEU:HG	1.87	0.57
1:D:317:THR:HG22	1:D:330:TYR:CE2	2.39	0.57
1:D:337:THR:HG23	1:D:432:GLY:HA2	1.87	0.57
1:D:1039:TYR:OH	1:D:1982:GLU:O	2.15	0.57
1:B:209:VAL:HG22	1:B:926:LEU:HD11	1.85	0.57
1:B:1222:LYS:HB3	1:B:1225:THR:HG22	1.86	0.57
1:C:241:ASN:O	1:C:457:THR:OG1	2.22	0.57
1:C:373:LEU:O	1:C:416:TYR:HB2	2.04	0.57
1:A:2249:GLU:O	1:A:2253:MET:HG3	2.04	0.57
1:D:489:THR:OG1	1:D:507:ASN:ND2	2.37	0.57
1:E:2351:VAL:HA	1:E:2354:GLU:HG2	1.86	0.57
1:A:1899:ASP:OD1	1:A:1917:TYR:OH	2.22	0.57
1:B:2076:GLU:OE2	1:C:2282:TYR:OH	2.23	0.57
1:B:2509:LEU:HD23	1:B:2528:ILE:HD13	1.86	0.57
1:C:1250:LYS:HD3	1:C:1296:THR:HG22	1.85	0.57
1:C:2400:SER:O	1:C:2416:ARG:NH2	2.38	0.57
1:D:1760:HIS:HB2	1:D:1773:ILE:HB	1.86	0.57
1:E:297:LEU:O	1:E:316:SER:OG	2.19	0.57
1:C:513:GLN:NE2	1:C:538:GLU:HG2	2.19	0.57
1:D:1315:VAL:HG22	1:D:1590:VAL:HG22	1.85	0.57
1:A:1485:GLY:HA3	1:A:1494:PHE:H	1.69	0.56
1:B:2357:GLU:HB3	1:B:2537:ARG:HD2	1.87	0.56
1:E:2439:VAL:HG22	1:E:2532:ILE:HG22	1.86	0.56
1:A:343:ASN:HA	1:A:363:PHE:HB2	1.85	0.56
1:A:600:LEU:HD21	1:A:628:THR:HG21	1.87	0.56
1:C:1145:LYS:NZ	1:C:1147:ASP:OD1	2.35	0.56
1:C:1148:THR:HG23	1:C:1150:VAL:HG23	1.87	0.56
1:D:2427:PRO:O	1:D:2434:ARG:NH2	2.38	0.56
1:E:530:PRO:O	1:E:562:ARG:NH2	2.31	0.56
1:E:1681:HIS:CD2	1:E:1691:ARG:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1760:HIS:HB2	1:E:1773:ILE:HB	1.87	0.56
1:D:829:ASP:OD1	1:D:832:ARG:NH2	2.37	0.56
1:E:901:ALA:O	1:E:902:LEU:HB2	2.06	0.56
1:B:1570:VAL:HG22	1:B:1585:LYS:HG2	1.88	0.56
1:D:1255:PHE:HB3	1:D:1281:LEU:HG	1.87	0.56
1:E:1694:TYR:OH	1:E:1710:PHE:O	2.18	0.56
1:B:1417:LYS:NZ	1:B:1504:ASP:OD1	2.35	0.56
1:B:1426:GLN:HB3	1:B:1462:LEU:HD22	1.87	0.56
1:D:750:ASN:HB3	1:D:754:THR:HG22	1.87	0.56
1:E:1331:THR:HG21	1:E:1581:LEU:HD22	1.86	0.56
1:A:530:PRO:O	1:A:562:ARG:NH2	2.32	0.56
1:A:2249:GLU:OE1	1:E:2104:ARG:NH1	2.39	0.56
1:B:155:MET:HG3	1:B:986:LEU:HD12	1.86	0.56
1:C:697:ARG:NH1	1:C:728:ASP:OD2	2.35	0.56
1:D:1100:VAL:HB	1:D:1593:VAL:HG22	1.88	0.56
1:D:1827:THR:OG1	1:D:1893:GLN:NE2	2.30	0.56
1:E:1255:PHE:HB3	1:E:1281:LEU:HG	1.87	0.56
1:C:347:PHE:CE2	1:C:415:ILE:HD11	2.41	0.56
1:C:373:LEU:HG	1:C:382:ILE:HD13	1.88	0.56
1:C:1319:LEU:HD22	1:C:1588:LEU:HD13	1.86	0.56
1:E:1485:GLY:HA2	1:E:1494:PHE:CD2	2.37	0.56
1:B:2093:GLU:OE1	1:C:2264:HIS:NE2	2.34	0.56
1:C:169:LEU:O	1:C:173:ILE:HG12	2.04	0.56
1:C:1804:GLU:HA	1:C:1808:TYR:HB2	1.88	0.56
1:E:209:VAL:HG22	1:E:926:LEU:HD11	1.88	0.56
1:A:561:MET:HG3	1:A:571:LEU:HD22	1.87	0.56
1:B:221:SER:OG	1:B:495:ARG:NH2	2.37	0.56
1:B:898:TYR:HE1	1:B:909:LEU:HD11	1.70	0.56
1:B:1424:SER:O	1:B:1463:ASN:HA	2.06	0.56
1:D:1416:ASN:HB3	1:D:1421:TYR:HB2	1.88	0.56
1:D:1927:GLU:OE2	1:D:1995:ARG:NH1	2.31	0.56
1:E:1319:LEU:HD11	1:E:1586:GLN:HG2	1.88	0.56
1:E:1408:LEU:HD23	1:E:1428:HIS:HB2	1.88	0.56
1:E:236:LEU:HB2	1:E:487:PHE:HB2	1.87	0.55
1:E:1406:SER:OG	1:E:1430:MET:SD	2.63	0.55
1:A:1408:LEU:HD21	1:A:1430:MET:HG3	1.88	0.55
1:B:409:TYR:CE1	1:B:414:LYS:HD3	2.41	0.55
1:B:1485:GLY:HA2	1:B:1494:PHE:CD1	2.41	0.55
1:C:247:TYR:CZ	1:C:898:TYR:HB3	2.41	0.55
1:C:901:ALA:O	1:C:902:LEU:HB2	2.06	0.55
1:C:1694:TYR:OH	1:C:1710:PHE:O	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HA	1:A:83:ILE:HD12	1.88	0.55
1:B:1319:LEU:HD22	1:B:1588:LEU:HD13	1.88	0.55
1:D:1319:LEU:HD22	1:D:1588:LEU:HD13	1.88	0.55
1:D:2509:LEU:HD23	1:D:2528:ILE:HD13	1.87	0.55
1:A:1416:ASN:HB3	1:A:1421:TYR:HB2	1.87	0.55
1:A:2402:ASN:ND2	1:A:2419:ASP:OD2	2.35	0.55
1:D:223:ASN:ND2	1:D:878:ASP:OD2	2.39	0.55
1:E:1517:THR:HG23	1:E:1570:VAL:HB	1.87	0.55
1:C:1369:VAL:HG21	1:C:1399:VAL:HB	1.88	0.55
1:D:209:VAL:HG22	1:D:926:LEU:HD11	1.89	0.55
1:D:735:LEU:HD11	1:D:743:LEU:HD12	1.88	0.55
1:B:2219:ARG:HD3	1:B:2223:TRP:CH2	2.42	0.55
1:E:2406:LEU:HG	1:E:2411:ILE:HG12	1.87	0.55
1:B:2249:GLU:O	1:B:2253:MET:HG3	2.06	0.55
1:D:1177:ALA:HB3	1:E:2176:PHE:HB2	1.89	0.55
1:E:1340:GLN:HB3	1:E:1355:HIS:HB2	1.89	0.55
1:E:1518:VAL:HG21	1:E:1553:ILE:HG12	1.88	0.55
1:A:1483:VAL:HG13	1:A:1493:ILE:HG23	1.88	0.55
1:A:1804:GLU:HA	1:A:1808:TYR:HB2	1.88	0.55
1:B:236:LEU:HB2	1:B:487:PHE:HB2	1.89	0.55
1:B:2104:ARG:NH2	1:B:2107:ASP:OD2	2.35	0.55
1:D:1536:LEU:HD23	1:D:1537:PRO:HD2	1.88	0.55
1:D:2219:ARG:HD3	1:D:2223:TRP:CH2	2.42	0.55
1:A:1443:VAL:HG13	1:A:1445:ASN:H	1.72	0.55
1:A:2129:LYS:NZ	1:B:2228:ASP:OD2	2.40	0.55
1:B:169:LEU:O	1:B:173:ILE:HG12	2.07	0.55
1:B:1738:TRP:HZ2	1:B:1770:VAL:HG11	1.72	0.55
1:A:315:ILE:HG22	1:A:332:ILE:HB	1.89	0.54
1:D:11:ILE:HD11	1:D:41:LEU:HG	1.88	0.54
1:E:2390:LEU:HD11	1:E:2522:LEU:HB3	1.88	0.54
1:B:80:ARG:HA	1:B:83:ILE:HG12	1.89	0.54
1:B:142:ARG:NH2	1:B:144:ASP:OD2	2.32	0.54
1:E:642:TRP:HZ2	1:E:804:ILE:HG21	1.72	0.54
1:A:732:PRO:HB3	1:A:763:VAL:HG21	1.88	0.54
1:A:2282:TYR:OH	1:E:2076:GLU:OE2	2.23	0.54
1:B:1255:PHE:HB3	1:B:1281:LEU:HG	1.90	0.54
1:C:80:ARG:HA	1:C:83:ILE:HG12	1.89	0.54
1:C:307:SER:O	1:C:309:SER:N	2.40	0.54
1:A:1100:VAL:HB	1:A:1593:VAL:HG22	1.89	0.54
1:A:1601:LEU:HD23	1:A:1615:LEU:HB2	1.88	0.54
1:A:2093:GLU:OE1	1:B:2264:HIS:NE2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:SER:O	1:D:185:MET:HG2	2.07	0.54
1:D:1150:VAL:HG11	1:D:1157:ILE:HD12	1.88	0.54
1:E:347:PHE:CZ	1:E:415:ILE:HD11	2.43	0.54
1:B:192:ARG:HG2	1:B:249:ILE:HD11	1.90	0.54
1:A:236:LEU:HB2	1:A:487:PHE:HB2	1.90	0.54
1:B:91:SER:HB3	1:B:1960:LEU:HD11	1.88	0.54
1:B:2453:ILE:HG23	1:B:2521:LEU:HD21	1.90	0.54
1:C:1408:LEU:HD21	1:C:1430:MET:HG2	1.89	0.54
1:A:697:ARG:NH1	1:A:728:ASP:OD2	2.36	0.54
1:B:307:SER:O	1:B:309:SER:N	2.41	0.54
1:E:1100:VAL:HB	1:E:1593:VAL:HG22	1.89	0.54
1:A:504:GLN:HA	1:A:507:ASN:ND2	2.23	0.54
1:B:901:ALA:O	1:B:902:LEU:HB2	2.07	0.54
1:C:1633:ARG:HH22	1:C:1649:LEU:HD21	1.71	0.54
1:D:2076:GLU:OE2	1:E:2282:TYR:OH	2.26	0.54
1:E:1509:ILE:HG12	1:E:1514:ILE:HD11	1.90	0.54
1:A:1369:VAL:HG11	1:A:1399:VAL:HB	1.90	0.54
1:C:1235:PHE:HB3	1:C:1240:THR:HG22	1.88	0.54
1:C:2427:PRO:O	1:C:2434:ARG:NH2	2.40	0.54
1:B:1807:TYR:O	1:B:1811:MET:HG2	2.08	0.53
1:B:2519:LYS:O	1:B:2523:GLU:HG3	2.08	0.53
1:D:1738:TRP:HE3	1:D:1756:ASN:HD22	1.54	0.53
1:D:2057:THR:O	1:D:2061:VAL:HG23	2.08	0.53
1:E:1319:LEU:HD22	1:E:1588:LEU:HD13	1.90	0.53
1:B:621:SER:O	1:B:624:ASN:ND2	2.41	0.53
1:D:551:GLU:HG2	1:D:552:GLN:HG2	1.90	0.53
1:D:1405:TYR:OH	1:D:1492:GLN:OE1	2.15	0.53
1:D:2453:ILE:HG23	1:D:2521:LEU:HD21	1.90	0.53
1:E:365:VAL:HG13	1:E:367:ARG:HH21	1.73	0.53
1:E:404:ILE:HD13	1:E:414:LYS:HD2	1.90	0.53
1:E:732:PRO:HB3	1:E:763:VAL:HG21	1.90	0.53
1:C:1714:ALA:HB3	1:C:1717:TYR:HB2	1.90	0.53
1:A:554:THR:HG22	1:A:556:ALA:H	1.72	0.53
1:C:315:ILE:HG22	1:C:332:ILE:HB	1.89	0.53
1:B:1374:GLN:O	1:B:1378:MET:HG3	2.08	0.53
1:C:1401:HIS:NE2	1:C:1403:GLY:O	2.41	0.53
1:D:221:SER:OG	1:D:495:ARG:NH2	2.39	0.53
1:E:501:ASP:O	1:E:505:VAL:HG23	2.09	0.53
1:A:307:SER:O	1:A:309:SER:N	2.42	0.53
1:C:735:LEU:HD11	1:C:743:LEU:HD12	1.90	0.53
1:D:1436:ARG:HG2	1:D:1494:PHE:HE2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:THR:HA	1:C:416:TYR:O	2.08	0.53
1:E:690:ASP:OD2	1:E:691:MET:N	2.41	0.53
1:A:829:ASP:OD1	1:A:832:ARG:NH2	2.39	0.53
1:A:2076:GLU:OE2	1:B:2282:TYR:OH	2.26	0.53
1:C:360:ARG:HD2	1:C:386:LEU:HD13	1.91	0.53
1:A:192:ARG:HG2	1:A:249:ILE:HD11	1.90	0.53
1:C:11:ILE:HD11	1:C:41:LEU:HG	1.90	0.53
1:C:347:PHE:CE1	1:C:360:ARG:HG3	2.44	0.53
1:D:2249:GLU:O	1:D:2253:MET:HG3	2.10	0.53
1:E:247:TYR:CZ	1:E:898:TYR:HB3	2.44	0.53
1:B:1664:LEU:HD21	1:B:1727:VAL:HG21	1.91	0.52
1:B:2282:TYR:O	1:B:2286:ARG:HG2	2.08	0.52
1:D:1319:LEU:HD11	1:D:1586:GLN:HG2	1.90	0.52
1:A:2427:PRO:O	1:A:2434:ARG:NH2	2.41	0.52
1:D:600:LEU:HD21	1:D:628:THR:HG21	1.90	0.52
1:D:2129:LYS:NZ	1:E:2228:ASP:OD2	2.43	0.52
1:E:408:GLU:O	1:E:412:GLY:HA3	2.10	0.52
1:E:603:LEU:HD21	1:E:640:VAL:HG22	1.92	0.52
1:E:1510:ASN:O	1:E:1514:ILE:HD12	2.10	0.52
1:A:317:THR:HG22	1:A:330:TYR:CE2	2.45	0.52
1:A:404:ILE:HD13	1:A:414:LYS:HZ2	1.75	0.52
1:B:1804:GLU:HA	1:B:1808:TYR:HB2	1.91	0.52
1:C:2219:ARG:HD3	1:C:2223:TRP:CH2	2.45	0.52
1:E:1803:TRP:CZ2	1:E:1854:PRO:HB2	2.44	0.52
1:A:1437:ARG:HB3	1:A:1455:PRO:HA	1.92	0.52
1:B:1921:LEU:HD13	1:B:1994:LEU:HD13	1.92	0.52
1:C:236:LEU:HB2	1:C:487:PHE:HB2	1.91	0.52
1:B:11:ILE:HD11	1:B:41:LEU:HG	1.92	0.52
1:B:697:ARG:NH1	1:B:728:ASP:OD2	2.41	0.52
1:B:2129:LYS:NZ	1:C:2228:ASP:OD2	2.43	0.52
1:D:236:LEU:HB2	1:D:487:PHE:HB2	1.91	0.52
1:D:347:PHE:HE2	1:D:417:ALA:HB2	1.75	0.52
1:D:697:ARG:NH1	1:D:728:ASP:OD2	2.36	0.52
1:B:2074:MET:SD	1:B:2285:MET:HE3	2.50	0.52
1:B:2137:ASP:O	1:C:2218:ARG:NH2	2.42	0.52
1:C:117:GLY:O	1:C:121:GLU:HG2	2.10	0.52
1:D:1373:LYS:HB3	1:D:1412:ILE:HG13	1.91	0.52
1:E:169:LEU:O	1:E:173:ILE:HG12	2.09	0.52
1:E:349:LEU:HD11	1:E:356:GLN:HB3	1.91	0.52
1:B:22:LEU:HD21	1:B:52:GLU:HB3	1.91	0.52
1:B:63:LEU:HD11	1:B:88:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:CE1	1:B:415:ILE:HD11	2.45	0.52
1:B:360:ARG:HE	1:B:362:ASN:CG	2.13	0.52
1:B:561:MET:HG3	1:B:571:LEU:HD22	1.91	0.52
1:B:2277:THR:HA	1:B:2281:LEU:HD23	1.90	0.52
1:D:365:VAL:HG22	1:D:392:ALA:H	1.75	0.52
1:B:247:TYR:CZ	1:B:898:TYR:HB3	2.45	0.52
1:B:1531:ASP:OD1	1:B:1531:ASP:N	2.42	0.52
1:B:1922:GLU:HB3	1:C:1004:ILE:HD13	1.92	0.52
1:C:1485:GLY:CA	1:C:1494:PHE:H	2.23	0.52
1:C:1744:TYR:HB2	1:C:1766:GLN:HG2	1.92	0.52
1:E:1400:LYS:H	1:E:1498:GLN:HG2	1.75	0.52
1:A:1252:TYR:O	1:A:1288:LYS:NZ	2.37	0.52
1:A:1319:LEU:HD11	1:A:1586:GLN:HG2	1.92	0.52
1:B:1036:LEU:HD11	1:B:1871:PRO:HD3	1.92	0.52
1:C:473:ASN:ND2	1:C:477:ILE:HG12	2.25	0.52
1:C:2509:LEU:HD23	1:C:2528:ILE:HD13	1.92	0.52
1:D:373:LEU:HD22	1:D:382:ILE:HD13	1.92	0.52
1:D:504:GLN:HA	1:D:507:ASN:ND2	2.25	0.52
1:E:221:SER:OG	1:E:495:ARG:NH2	2.39	0.52
1:A:346:TYR:OH	1:A:395:ASN:OD1	2.20	0.51
1:A:893:LEU:HD23	1:A:918:LEU:HD21	1.93	0.51
1:A:2134:TYR:CE1	1:A:2224:GLU:HB2	2.44	0.51
1:A:2410:GLN:NE2	1:A:2412:GLU:OE2	2.42	0.51
1:B:732:PRO:HB3	1:B:763:VAL:HG21	1.91	0.51
1:B:1477:LYS:HB2	1:B:1478:LYS:HZ2	1.74	0.51
1:C:2076:GLU:OE2	1:D:2282:TYR:OH	2.27	0.51
1:D:556:ALA:HB1	1:D:589:LEU:HD11	1.92	0.51
1:E:538:GLU:HG3	1:E:591:VAL:HG22	1.91	0.51
1:A:1300:ASP:OD2	1:A:1604:ARG:NH2	2.35	0.51
1:A:2074:MET:HE1	1:A:2285:MET:HB3	1.91	0.51
1:B:415:ILE:HG12	1:B:431:GLY:CA	2.38	0.51
1:B:556:ALA:HB1	1:B:589:LEU:HD11	1.92	0.51
1:B:1673:GLY:HA3	1:B:1731:LYS:HE2	1.92	0.51
1:B:1827:THR:HG1	1:B:1893:GLN:HE22	1.54	0.51
1:B:2350:LYS:HD2	1:C:2299:LEU:HD22	1.91	0.51
1:C:582:ASP:OD2	1:C:583:ALA:N	2.41	0.51
1:E:373:LEU:HG	1:E:382:ILE:HD13	1.92	0.51
1:D:1677:TRP:CZ2	1:D:1730:GLN:HB2	2.46	0.51
1:A:505:VAL:HG11	1:A:598:TYR:HD2	1.76	0.51
1:B:1694:TYR:OH	1:B:1710:PHE:O	2.22	0.51
1:B:2314:GLU:OE2	1:B:2352:TRP:NE1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:THR:HG22	1:A:1637:GLY:H	1.75	0.51
1:B:620:LEU:HD22	1:B:664:CYS:HB3	1.93	0.51
1:C:1899:ASP:OD1	1:C:1917:TYR:OH	2.24	0.51
1:D:732:PRO:HB3	1:D:763:VAL:HG21	1.91	0.51
1:C:1827:THR:OG1	1:C:1893:GLN:NE2	2.28	0.51
1:A:1738:TRP:HE3	1:A:1756:ASN:HD22	1.57	0.51
1:B:1636:THR:HG22	1:B:1637:GLY:H	1.76	0.51
1:C:358:PHE:HB2	1:C:398:SER:OG	2.11	0.51
1:D:1435:THR:HG22	1:D:1437:ARG:HD3	1.92	0.51
1:E:373:LEU:HB2	1:E:416:TYR:HB3	1.92	0.51
1:E:1744:TYR:HB2	1:E:1766:GLN:OE1	2.11	0.51
1:A:1004:ILE:HD13	1:E:1922:GLU:HB3	1.92	0.51
1:A:2057:THR:O	1:A:2061:VAL:HG23	2.10	0.51
1:B:1803:TRP:CZ2	1:B:1854:PRO:HB2	2.46	0.51
1:C:170:LEU:O	1:C:174:THR:HG23	2.10	0.51
1:C:1108:TRP:CE2	1:C:1161:ILE:HD11	2.46	0.51
1:E:220:LEU:HG	1:E:227:MET:HG3	1.93	0.51
1:E:1458:PRO:HB2	1:E:1461:ILE:HB	1.92	0.51
1:A:241:ASN:O	1:A:457:THR:OG1	2.28	0.51
1:A:271:ILE:HD13	1:A:281:TRP:HZ2	1.75	0.51
1:A:2509:LEU:HD23	1:A:2528:ILE:HD13	1.93	0.51
1:C:1440:LEU:HB3	1:C:1479:CYS:HB3	1.92	0.51
1:E:2411:ILE:HD12	1:E:2522:LEU:HD23	1.93	0.51
1:A:257:LYS:HD3	1:A:257:LYS:N	2.25	0.51
1:A:408:GLU:O	1:A:412:GLY:HA3	2.10	0.51
1:B:216:THR:HG22	1:B:494:HIS:HB3	1.91	0.51
1:B:1340:GLN:HB2	1:B:1355:HIS:HB2	1.93	0.51
1:D:307:SER:O	1:D:309:SER:N	2.44	0.51
1:D:680:LEU:HD11	1:D:757:LEU:HD21	1.93	0.51
1:D:2218:ARG:O	1:D:2222:GLU:HG2	2.11	0.51
1:D:2311:LEU:HD22	1:D:2348:MET:HG2	1.93	0.51
1:E:241:ASN:O	1:E:457:THR:OG1	2.29	0.51
1:E:2249:GLU:O	1:E:2253:MET:HG3	2.11	0.51
1:A:349:LEU:HD11	1:A:356:GLN:HB3	1.91	0.50
1:C:367:ARG:HD2	1:C:367:ARG:N	2.26	0.50
1:E:315:ILE:HG22	1:E:332:ILE:HB	1.93	0.50
1:E:1235:PHE:HB3	1:E:1240:THR:HG22	1.93	0.50
1:B:510:VAL:HB	1:B:591:VAL:HG12	1.93	0.50
1:B:750:ASN:HB3	1:B:754:THR:HG22	1.94	0.50
1:C:200:HIS:HB3	1:C:203:TYR:HB3	1.93	0.50
1:C:1340:GLN:HB2	1:C:1355:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PHE:HB2	1:B:398:SER:HB3	1.93	0.50
1:B:1235:PHE:HB3	1:B:1240:THR:HG23	1.93	0.50
1:C:893:LEU:HD23	1:C:918:LEU:HD21	1.92	0.50
1:E:26:GLN:N	1:E:27:TYR:HB3	2.26	0.50
1:B:1870:ASP:HB3	1:B:1873:ALA:HB3	1.93	0.50
1:C:2057:THR:O	1:C:2061:VAL:HG23	2.11	0.50
1:D:142:ARG:NH2	1:D:144:ASP:OD2	2.36	0.50
1:D:241:ASN:O	1:D:457:THR:OG1	2.28	0.50
1:E:347:PHE:CE2	1:E:415:ILE:HD11	2.45	0.50
1:A:80:ARG:HD3	1:A:83:ILE:HD12	1.93	0.50
1:A:735:LEU:HD11	1:A:743:LEU:HD12	1.94	0.50
1:C:1416:ASN:HB3	1:C:1421:TYR:HB2	1.92	0.50
1:B:1319:LEU:HD11	1:B:1586:GLN:HG2	1.93	0.50
1:B:1415:TYR:CE2	1:B:1473:THR:HG22	2.47	0.50
1:D:2342:LEU:HD13	1:E:2063:GLN:NE2	2.27	0.50
1:A:1457:SER:HB3	1:A:1458:PRO:CD	2.41	0.50
1:A:1677:TRP:CZ2	1:A:1730:GLN:HB2	2.46	0.50
1:B:735:LEU:HD11	1:B:743:LEU:HD12	1.94	0.50
1:C:899:VAL:O	1:C:899:VAL:HG12	2.12	0.50
1:D:197:THR:O	1:D:453:ARG:NH1	2.45	0.50
1:B:1408:LEU:HD21	1:B:1430:MET:HG2	1.94	0.50
1:B:2439:VAL:HG22	1:B:2532:ILE:HG22	1.93	0.50
1:D:63:LEU:HD11	1:D:88:VAL:HG21	1.94	0.50
1:D:271:ILE:HD13	1:D:281:TRP:HZ2	1.77	0.50
1:D:1383:VAL:HG12	1:D:1421:TYR:CE2	2.47	0.50
1:A:1760:HIS:HB2	1:A:1773:ILE:HB	1.93	0.50
1:A:2219:ARG:HD3	1:A:2223:TRP:CH2	2.47	0.50
1:D:1419:LYS:HB3	1:D:1421:TYR:CE1	2.47	0.50
1:E:1412:ILE:O	1:E:1424:SER:HA	2.12	0.50
1:A:1293:ILE:HG13	1:A:1302:VAL:HG23	1.94	0.49
1:C:1228:LEU:HD11	1:C:1245:VAL:HG13	1.93	0.49
1:C:1400:LYS:H	1:C:1498:GLN:HG2	1.77	0.49
1:E:893:LEU:HD23	1:E:918:LEU:HD21	1.94	0.49
1:C:347:PHE:CD2	1:C:415:ILE:HD11	2.47	0.49
1:A:783:VAL:HG13	1:A:832:ARG:HG3	1.95	0.49
1:E:531:PRO:HG3	1:E:535:LYS:NZ	2.27	0.49
1:B:505:VAL:HG11	1:B:598:TYR:HD2	1.76	0.49
1:C:26:GLN:N	1:C:27:TYR:HB3	2.26	0.49
1:C:530:PRO:O	1:C:562:ARG:NH2	2.25	0.49
1:D:1458:PRO:HD2	1:D:1461:ILE:HG21	1.93	0.49
1:D:1636:THR:HG22	1:D:1637:GLY:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1694:TYR:OH	1:D:1710:PHE:O	2.24	0.49
1:E:2427:PRO:O	1:E:2434:ARG:NH2	2.44	0.49
1:A:1010:ALA:O	1:A:1014:THR:HG23	2.13	0.49
1:B:1677:TRP:CZ2	1:B:1730:GLN:HB2	2.48	0.49
1:C:1150:VAL:HG11	1:C:1157:ILE:HD12	1.94	0.49
1:E:1150:VAL:HG11	1:E:1157:ILE:HD12	1.94	0.49
1:E:2057:THR:O	1:E:2061:VAL:HG23	2.12	0.49
1:A:1480:SER:OG	1:A:1481:TYR:N	2.45	0.49
1:B:899:VAL:O	1:B:900:THR:OG1	2.26	0.49
1:D:2275:LYS:O	1:D:2278:ASN:ND2	2.45	0.49
1:E:1375:ILE:HA	1:E:1378:MET:HE2	1.95	0.49
1:E:1673:GLY:HA3	1:E:1731:LYS:HE2	1.94	0.49
1:E:2313:ARG:NH2	1:E:2465:MET:HE2	2.27	0.49
1:A:1235:PHE:HB3	1:A:1240:THR:HG22	1.94	0.49
1:A:1302:VAL:HG12	1:A:1604:ARG:HG2	1.94	0.49
1:B:323:ASN:HD21	1:B:354:ASN:HD21	1.60	0.49
1:B:1116:ASN:HB2	1:C:1207:TRP:CD1	2.48	0.49
1:B:1441:THR:HB	1:B:1450:ARG:HA	1.94	0.49
1:B:1135:LEU:HD12	1:B:1620:ILE:HD13	1.94	0.49
1:C:63:LEU:HD11	1:C:88:VAL:HG21	1.94	0.49
1:D:2368:LEU:HD12	1:D:2528:ILE:HB	1.93	0.49
1:E:1126:ASP:OD1	1:E:1128:SER:OG	2.21	0.49
1:B:415:ILE:HG21	1:B:432:GLY:H	1.77	0.49
1:C:1518:VAL:HG21	1:C:1553:ILE:HG12	1.95	0.49
1:C:1636:THR:HG22	1:C:1637:GLY:H	1.78	0.49
1:E:1408:LEU:HD21	1:E:1430:MET:HG2	1.95	0.49
1:E:2134:TYR:CE1	1:E:2224:GLU:HB2	2.48	0.49
1:A:91:SER:HB3	1:A:1960:LEU:HD11	1.95	0.49
1:B:1150:VAL:HG11	1:B:1157:ILE:HD12	1.95	0.49
1:C:349:LEU:HD11	1:C:356:GLN:HB3	1.95	0.49
1:D:1302:VAL:HG12	1:D:1604:ARG:HG2	1.94	0.49
1:E:1372:ASN:C	1:E:1373:LYS:HD3	2.32	0.49
1:B:337:THR:HA	1:B:537:PHE:CE2	2.48	0.48
1:B:603:LEU:HD21	1:B:640:VAL:HG22	1.95	0.48
1:B:829:ASP:OD1	1:B:832:ARG:NH2	2.45	0.48
1:B:1409:GLY:HA3	1:B:1427:GLY:H	1.77	0.48
1:B:2057:THR:O	1:B:2061:VAL:HG23	2.13	0.48
1:C:1302:VAL:HG12	1:C:1604:ARG:HG2	1.95	0.48
1:A:367:ARG:N	1:A:367:ARG:HD2	2.27	0.48
1:A:556:ALA:HB1	1:A:589:LEU:HD11	1.94	0.48
1:A:1460:THR:HG23	1:A:1460:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1972:ALA:O	1:B:1974:SER:N	2.45	0.48
1:C:420:TYR:CD2	1:C:426:ALA:HB2	2.49	0.48
1:E:200:HIS:HB3	1:E:203:TYR:HB3	1.95	0.48
1:A:1570:VAL:HG22	1:A:1585:LYS:HG2	1.94	0.48
1:B:530:PRO:O	1:B:562:ARG:NH2	2.34	0.48
1:B:1010:ALA:O	1:B:1014:THR:HG23	2.13	0.48
1:C:556:ALA:HB1	1:C:589:LEU:HD11	1.95	0.48
1:D:704:LEU:HD11	1:D:741:MET:HG3	1.94	0.48
1:D:902:LEU:O	1:D:903:ASN:HB2	2.12	0.48
1:E:337:THR:HA	1:E:537:PHE:CE2	2.48	0.48
1:E:1383:VAL:H	1:E:1421:TYR:HE2	1.61	0.48
1:E:1899:ASP:OD1	1:E:1917:TYR:OH	2.22	0.48
1:C:2453:ILE:O	1:C:2475:SER:HA	2.12	0.48
1:D:409:TYR:CE1	1:D:414:LYS:HD3	2.48	0.48
1:E:1036:LEU:HD11	1:E:1871:PRO:HD3	1.95	0.48
1:B:2416:ARG:NH1	1:B:2504:SER:O	2.46	0.48
1:C:411:ASN:H	1:C:435:THR:HG23	1.78	0.48
1:C:1065:GLN:O	1:C:1816:ARG:NH2	2.47	0.48
1:D:1436:ARG:HG2	1:D:1494:PHE:CE2	2.48	0.48
1:D:2212:ARG:NH1	1:E:2211:SER:OG	2.46	0.48
1:E:1827:THR:OG1	1:E:1893:GLN:NE2	2.29	0.48
1:A:1331:THR:HG21	1:A:1581:LEU:HD13	1.96	0.48
1:D:200:HIS:HB3	1:D:203:TYR:HB3	1.96	0.48
1:D:1485:GLY:HA2	1:D:1494:PHE:H	1.78	0.48
1:E:862:ASN:OD1	1:E:862:ASN:N	2.43	0.48
1:E:902:LEU:O	1:E:903:ASN:HB2	2.14	0.48
1:A:680:LEU:HD11	1:A:757:LEU:HD21	1.95	0.48
1:B:795:LYS:O	1:B:797:GLN:HG2	2.13	0.48
1:B:1426:GLN:NE2	1:B:1428:HIS:O	2.44	0.48
1:C:827:THR:HA	1:C:830:MET:HE2	1.96	0.48
1:C:1510:ASN:O	1:C:1514:ILE:HD12	2.13	0.48
1:E:1921:LEU:HD13	1:E:1994:LEU:HD13	1.96	0.48
1:A:200:HIS:HB3	1:A:203:TYR:HB3	1.95	0.48
1:A:337:THR:HA	1:A:537:PHE:CE2	2.48	0.48
1:C:1036:LEU:HD11	1:C:1871:PRO:HD3	1.94	0.48
1:E:513:GLN:NE2	1:E:538:GLU:OE1	2.41	0.48
1:E:829:ASP:OD1	1:E:832:ARG:NH2	2.46	0.48
1:E:1744:TYR:CE1	1:E:1753:VAL:HB	2.49	0.48
1:A:2253:MET:HE3	1:E:2101:ILE:HG12	1.96	0.48
1:B:1738:TRP:HE3	1:B:1756:ASN:HD22	1.61	0.48
1:C:2515:THR:H	1:C:2516:ASP:CB	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1293:ILE:HG13	1:D:1302:VAL:HG23	1.96	0.48
1:E:1478:LYS:HA	1:E:1478:LYS:HD3	1.77	0.48
1:E:1793:ASP:HB3	1:E:1796:SER:HB3	1.94	0.48
1:A:409:TYR:CE1	1:A:414:LYS:HD3	2.49	0.48
1:A:620:LEU:HD22	1:A:664:CYS:HB3	1.96	0.48
1:B:117:GLY:O	1:B:121:GLU:HG2	2.14	0.48
1:C:1010:ALA:O	1:C:1014:THR:HG23	2.14	0.48
1:C:1792:MET:O	1:C:1853:ARG:NH1	2.36	0.48
1:D:899:VAL:O	1:D:900:THR:OG1	2.25	0.48
1:D:1633:ARG:HH22	1:D:1649:LEU:HD21	1.79	0.48
1:D:2455:ALA:HB3	1:D:2474:LEU:HB2	1.95	0.48
1:A:1601:LEU:HD22	1:A:1613:MET:SD	2.53	0.47
1:C:2277:THR:HA	1:C:2281:LEU:HD23	1.96	0.47
1:C:2519:LYS:NZ	1:C:2523:GLU:OE1	2.46	0.47
1:E:510:VAL:HB	1:E:591:VAL:HG12	1.95	0.47
1:E:1252:TYR:O	1:E:1288:LYS:NZ	2.35	0.47
1:E:2455:ALA:HB1	1:E:2509:LEU:HD11	1.95	0.47
1:A:365:VAL:HG13	1:A:391:ILE:HA	1.95	0.47
1:B:26:GLN:N	1:B:27:TYR:HB3	2.29	0.47
1:C:2104:ARG:HD3	1:C:2104:ARG:HA	1.65	0.47
1:B:360:ARG:HD2	1:B:386:LEU:HD13	1.96	0.47
1:B:2191:ALA:O	1:B:2195:VAL:HG13	2.14	0.47
1:C:510:VAL:HB	1:C:591:VAL:HG12	1.96	0.47
1:E:1972:ALA:O	1:E:1975:LEU:N	2.42	0.47
1:A:852:VAL:O	1:A:856:MET:HG3	2.14	0.47
1:B:1308:ARG:O	1:B:1595:TYR:OH	2.30	0.47
1:B:1514:ILE:HG12	1:B:1573:THR:HG23	1.96	0.47
1:C:1293:ILE:HG13	1:C:1302:VAL:HG23	1.96	0.47
1:C:1457:SER:OG	1:C:1458:PRO:HD3	2.14	0.47
1:C:1972:ALA:O	1:C:1975:LEU:HG	2.14	0.47
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.78	0.47
1:D:349:LEU:HD11	1:D:356:GLN:HB3	1.95	0.47
1:E:2219:ARG:HD3	1:E:2223:TRP:CH2	2.49	0.47
1:A:1443:VAL:HG11	1:A:1446:ASN:HB3	1.96	0.47
1:B:1515:LYS:HB3	1:B:1528:THR:HG22	1.97	0.47
1:B:1724:ARG:HG2	1:B:1742:PHE:CZ	2.49	0.47
1:C:2465:MET:HE3	1:C:2466:PRO:HD2	1.97	0.47
1:D:692:ALA:HA	1:D:741:MET:HE3	1.95	0.47
1:E:347:PHE:HE2	1:E:417:ALA:HB2	1.79	0.47
1:E:538:GLU:OE2	1:E:538:GLU:N	2.45	0.47
1:E:540:ASP:HB3	1:E:542:ASN:OD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1300:ASP:OD2	1:E:1604:ARG:NH2	2.36	0.47
1:A:337:THR:N	1:A:431:GLY:O	2.37	0.47
1:A:960:SER:HB3	1:A:1400:LYS:HD2	1.96	0.47
1:A:1250:LYS:HD3	1:A:1296:THR:HG22	1.96	0.47
1:B:2134:TYR:CE1	1:B:2224:GLU:HB2	2.50	0.47
1:C:473:ASN:HD21	1:C:477:ILE:H	1.61	0.47
1:A:375:LYS:HA	1:A:375:LYS:HD3	1.62	0.47
1:A:2519:LYS:O	1:A:2523:GLU:HG3	2.14	0.47
1:B:977:VAL:HB	1:B:981:ILE:HD11	1.96	0.47
1:B:1503:LEU:HD12	1:B:1504:ASP:H	1.80	0.47
1:B:1536:LEU:HD13	1:B:1537:PRO:HD2	1.97	0.47
1:C:215:SER:O	1:C:216:THR:OG1	2.27	0.47
1:C:1720:HIS:O	1:C:1721:GLU:HB2	2.14	0.47
1:C:2453:ILE:HG12	1:C:2521:LEU:HD21	1.96	0.47
1:D:1010:ALA:O	1:D:1014:THR:HG23	2.15	0.47
1:D:1489:GLN:OE1	1:D:1489:GLN:N	2.45	0.47
1:B:320:VAL:HA	1:B:327:LEU:HA	1.97	0.47
1:C:1177:ALA:HB3	1:D:2176:PHE:HB2	1.97	0.47
1:D:408:GLU:O	1:D:412:GLY:HA3	2.15	0.47
1:D:1518:VAL:HG21	1:D:1553:ILE:HG12	1.96	0.47
1:D:1673:GLY:HA3	1:D:1731:LYS:HE2	1.97	0.47
1:B:961:LEU:HB2	1:B:966:ASP:HB3	1.96	0.47
1:B:2402:ASN:ND2	1:B:2419:ASP:OD2	2.48	0.47
1:C:357:PHE:HA	1:C:401:LEU:HG	1.97	0.47
1:C:902:LEU:O	1:C:903:ASN:HB2	2.14	0.47
1:D:1757:ASP:OD1	1:D:1757:ASP:N	2.47	0.47
1:E:1483:VAL:HG13	1:E:1493:ILE:HG23	1.97	0.47
1:A:2311:LEU:HD22	1:A:2348:MET:HG2	1.96	0.47
1:D:414:LYS:HE3	1:D:414:LYS:HB3	1.78	0.47
1:D:687:ILE:HG23	1:D:745:LEU:HD21	1.97	0.47
1:D:2191:ALA:O	1:D:2195:VAL:HG13	2.14	0.47
1:E:2442:THR:HB	1:E:2529:ILE:HB	1.97	0.47
1:A:1631:VAL:HG11	1:B:1165:ARG:HB3	1.95	0.46
1:A:2515:THR:H	1:A:2516:ASP:CB	2.20	0.46
1:C:1116:ASN:HB2	1:D:1207:TRP:CD1	2.50	0.46
1:E:182:ASP:OD2	1:E:182:ASP:N	2.48	0.46
1:E:1418:THR:HG23	1:E:1419:LYS:HG3	1.97	0.46
1:E:1487:ASN:HB2	1:E:1492:GLN:HB3	1.97	0.46
1:A:127:LYS:HE2	1:A:127:LYS:HB3	1.63	0.46
1:A:1714:ALA:HB3	1:A:1717:TYR:HB2	1.97	0.46
1:A:2191:ALA:O	1:A:2195:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:HA	1:B:316:SER:O	2.15	0.46
1:B:1460:THR:O	1:B:1460:THR:HG23	2.14	0.46
1:C:1439:ILE:HD11	1:C:1486:ASN:HA	1.96	0.46
1:C:1570:VAL:HG22	1:C:1585:LYS:HG2	1.97	0.46
1:D:2350:LYS:HD2	1:E:2299:LEU:HD22	1.97	0.46
1:E:358:PHE:HB2	1:E:398:SER:HB3	1.96	0.46
1:A:1392:ALA:HB1	1:A:1417:LYS:NZ	2.31	0.46
1:C:304:TYR:HB3	1:C:308:THR:HG21	1.96	0.46
1:D:743:LEU:HD23	1:D:743:LEU:HA	1.82	0.46
1:A:26:GLN:N	1:A:27:TYR:HB3	2.30	0.46
1:A:899:VAL:O	1:A:900:THR:OG1	2.25	0.46
1:A:1070:ARG:O	1:A:1074:GLU:HG3	2.15	0.46
1:A:1444:GLU:HB2	1:A:1481:TYR:CG	2.50	0.46
1:C:1531:ASP:OD1	1:C:1531:ASP:N	2.43	0.46
1:D:1610:ALA:HB2	1:D:1652:PRO:HG2	1.97	0.46
1:D:1738:TRP:HZ2	1:D:1770:VAL:HG11	1.80	0.46
1:A:6:VAL:O	1:A:10:LYS:HG3	2.14	0.46
1:A:618:TYR:OH	1:A:626:LYS:O	2.19	0.46
1:A:1451:LEU:HB2	1:A:1479:CYS:SG	2.56	0.46
1:A:1694:TYR:OH	1:A:1710:PHE:O	2.24	0.46
1:A:1969:LEU:HD12	1:A:1969:LEU:H	1.80	0.46
1:B:1409:GLY:HA3	1:B:1427:GLY:N	2.31	0.46
1:D:300:LEU:HA	1:D:316:SER:O	2.15	0.46
1:D:1738:TRP:CZ2	1:D:1770:VAL:HG11	2.50	0.46
1:D:2086:LEU:HD22	1:E:2271:LEU:HD13	1.97	0.46
1:E:360:ARG:HE	1:E:362:ASN:CG	2.19	0.46
1:B:200:HIS:HB3	1:B:203:TYR:HB3	1.98	0.46
1:B:2427:PRO:O	1:B:2434:ARG:NH2	2.46	0.46
1:D:360:ARG:NH1	1:D:362:ASN:HD21	2.13	0.46
1:D:554:THR:HG22	1:D:556:ALA:N	2.29	0.46
1:D:1907:ARG:NH1	1:E:158:GLU:OE1	2.46	0.46
1:B:83:ILE:HD12	1:B:1880:MET:HE3	1.97	0.46
1:B:360:ARG:HE	1:B:362:ASN:ND2	2.14	0.46
1:C:1399:VAL:HG12	1:C:1497:TYR:HD2	1.80	0.46
1:C:2191:ALA:O	1:C:2195:VAL:HG13	2.16	0.46
1:C:2394:LYS:HB2	1:C:2394:LYS:HE2	1.76	0.46
1:E:414:LYS:HB3	1:E:414:LYS:HE3	1.77	0.46
1:E:1410:GLY:HA3	1:E:1497:TYR:CE1	2.51	0.46
1:A:300:LEU:HA	1:A:316:SER:O	2.15	0.46
1:A:902:LEU:O	1:A:903:ASN:HB2	2.15	0.46
1:A:1373:LYS:HD3	1:A:1412:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2275:LYS:HD3	1:E:2079:ASP:HB3	1.98	0.46
1:D:2079:ASP:OD2	1:E:2277:THR:OG1	2.26	0.46
1:D:2134:TYR:CE1	1:D:2224:GLU:HB2	2.50	0.46
1:D:2277:THR:HA	1:D:2281:LEU:HD23	1.97	0.46
1:E:300:LEU:HA	1:E:316:SER:O	2.15	0.46
1:E:346:TYR:OH	1:E:395:ASN:OD1	2.26	0.46
1:B:1758:ALA:O	1:B:1760:HIS:ND1	2.49	0.46
1:C:1575:ALA:HB2	1:C:1581:LEU:HD21	1.98	0.46
1:C:1760:HIS:HB2	1:C:1773:ILE:HB	1.98	0.46
1:D:1021:TRP:CE2	1:D:1025:ASN:HB3	2.51	0.46
1:D:2515:THR:N	1:D:2516:ASP:HB2	2.18	0.46
1:A:1803:TRP:CZ2	1:A:1854:PRO:HB2	2.50	0.46
1:A:2264:HIS:NE2	1:E:2093:GLU:OE1	2.37	0.46
1:A:2394:LYS:HB2	1:A:2394:LYS:HE2	1.74	0.46
1:B:1174:GLU:OE2	1:B:1189:ARG:NH2	2.39	0.46
1:B:1760:HIS:HB2	1:B:1773:ILE:HB	1.98	0.46
1:C:1338:ILE:HG21	1:C:1354:LEU:HB3	1.98	0.46
1:C:1509:ILE:HG12	1:C:1514:ILE:HD11	1.98	0.46
1:D:91:SER:HB3	1:D:1960:LEU:HD11	1.98	0.46
1:E:369:PHE:HD2	1:E:387:SER:HA	1.81	0.46
1:E:561:MET:HG3	1:E:571:LEU:HD22	1.97	0.46
1:E:2394:LYS:HB2	1:E:2394:LYS:HE2	1.72	0.46
1:A:730:LEU:HD12	1:A:767:LEU:HD11	1.98	0.45
1:A:1148:THR:HG23	1:A:1150:VAL:HG23	1.98	0.45
1:A:1395:ILE:HG22	1:A:1414:VAL:HG22	1.96	0.45
1:C:2219:ARG:O	1:C:2222:GLU:HG2	2.16	0.45
1:D:783:VAL:HG13	1:D:832:ARG:HG3	1.98	0.45
1:E:1108:TRP:CE2	1:E:1161:ILE:HD11	2.51	0.45
1:C:346:TYR:OH	1:C:395:ASN:OD1	2.25	0.45
1:C:829:ASP:OD1	1:C:832:ARG:NH2	2.47	0.45
1:D:2390:LEU:HD11	1:D:2522:LEU:HB2	1.97	0.45
1:D:2488:PHE:HB2	1:E:2485:MET:HE3	1.99	0.45
1:E:409:TYR:CE1	1:E:414:LYS:HD3	2.51	0.45
1:E:1440:LEU:HB3	1:E:1479:CYS:HB3	1.98	0.45
1:A:415:ILE:HD13	1:A:434:PHE:HE2	1.81	0.45
1:A:2253:MET:HE1	1:E:2104:ARG:HG3	1.99	0.45
1:B:197:THR:O	1:B:453:ARG:NH1	2.48	0.45
1:B:1454:PHE:CZ	1:B:1468:VAL:HG22	2.51	0.45
1:C:345:ASN:ND2	1:C:362:ASN:O	2.49	0.45
1:D:1803:TRP:CZ2	1:D:1854:PRO:HB2	2.51	0.45
1:D:215:SER:O	1:D:216:THR:OG1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:GLY:HA3	1:E:314:ASN:HB2	1.98	0.45
1:E:433:ILE:HD11	1:E:539:ALA:HB2	1.99	0.45
1:A:20:MET:HE2	1:A:20:MET:HB2	1.77	0.45
1:A:1365:GLY:H	1:A:1371:ARG:HD3	1.81	0.45
1:B:2079:ASP:HB3	1:C:2275:LYS:HD3	1.98	0.45
1:C:505:VAL:HG11	1:C:598:TYR:HD2	1.80	0.45
1:C:1601:LEU:HD23	1:C:1615:LEU:HB2	1.99	0.45
1:D:1108:TRP:CE2	1:D:1161:ILE:HD11	2.51	0.45
1:D:2439:VAL:HG22	1:D:2532:ILE:HG23	1.97	0.45
1:E:27:TYR:CD1	1:E:1947:GLN:HG3	2.52	0.45
1:E:1384:ASP:OD2	1:E:1385:GLY:N	2.47	0.45
1:E:1921:LEU:HD12	1:E:1921:LEU:HA	1.85	0.45
1:E:2219:ARG:HD3	1:E:2223:TRP:CZ2	2.52	0.45
1:B:347:PHE:CD1	1:B:415:ILE:HD11	2.52	0.45
1:C:2134:TYR:CE1	1:C:2224:GLU:HB2	2.51	0.45
1:D:247:TYR:CZ	1:D:898:TYR:HB3	2.52	0.45
1:D:1402:TYR:CE2	1:D:1481:TYR:HE1	2.35	0.45
1:A:566:VAL:HB	1:A:570:GLU:HB3	1.99	0.45
1:A:1308:ARG:O	1:A:1595:TYR:OH	2.34	0.45
1:B:200:HIS:CE1	1:B:202:PRO:HG2	2.52	0.45
1:B:1485:GLY:HA3	1:B:1493:ILE:HA	1.99	0.45
1:C:899:VAL:O	1:C:900:THR:OG1	2.27	0.45
1:C:1308:ARG:O	1:C:1595:TYR:OH	2.32	0.45
1:C:1675:GLU:OE1	1:C:1677:TRP:NE1	2.37	0.45
1:D:415:ILE:HG12	1:D:431:GLY:CA	2.45	0.45
1:D:2079:ASP:HB3	1:E:2275:LYS:HD3	1.98	0.45
1:E:332:ILE:HG12	1:E:436:PHE:HD1	1.82	0.45
1:E:1724:ARG:HG2	1:E:1742:PHE:CZ	2.52	0.45
1:C:229:GLN:OE1	1:C:891:ARG:NH2	2.41	0.45
1:E:192:ARG:HG2	1:E:249:ILE:HD11	1.98	0.45
1:E:344:ILE:HA	1:E:361:ALA:O	2.17	0.45
1:A:197:THR:O	1:A:453:ARG:NH1	2.50	0.45
1:A:921:ASN:ND2	1:B:553:SER:OG	2.42	0.45
1:A:1108:TRP:CE2	1:A:1161:ILE:HD11	2.52	0.45
1:C:2129:LYS:NZ	1:D:2228:ASP:OD2	2.48	0.45
1:D:226:VAL:HG12	1:D:876:TRP:CE2	2.52	0.45
1:A:358:PHE:HB2	1:A:398:SER:HB3	1.98	0.45
1:A:1927:GLU:OE2	1:A:1995:ARG:NH1	2.39	0.45
1:B:83:ILE:HD12	1:B:1880:MET:CE	2.47	0.45
1:B:743:LEU:HD13	1:B:757:LEU:HB2	1.99	0.45
1:B:1108:TRP:CE2	1:B:1161:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1839:TYR:CE1	1:C:1851:ASN:HB2	2.52	0.45
1:C:2454:ARG:O	1:C:2512:PRO:HD2	2.16	0.45
1:C:2455:ALA:HB1	1:C:2509:LEU:HD11	1.99	0.45
1:D:1036:LEU:HD11	1:D:1871:PRO:HD3	1.98	0.45
1:D:2453:ILE:O	1:D:2475:SER:HA	2.17	0.45
1:E:11:ILE:HD13	1:E:11:ILE:HA	1.83	0.45
1:A:142:ARG:NH2	1:A:144:ASP:OD2	2.42	0.44
1:A:1443:VAL:HG13	1:A:1446:ASN:H	1.82	0.44
1:A:1633:ARG:NH2	1:A:1649:LEU:HD21	2.32	0.44
1:A:1673:GLY:HA3	1:A:1731:LYS:HE2	1.99	0.44
1:B:504:GLN:HG2	1:B:509:SER:HB2	1.99	0.44
1:C:1331:THR:HG21	1:C:1581:LEU:HD13	1.99	0.44
1:D:173:ILE:HD12	1:D:949:TRP:CE3	2.51	0.44
1:D:298:GLY:HA3	1:D:314:ASN:HB2	1.97	0.44
1:D:1426:GLN:HB3	1:D:1462:LEU:HB3	1.98	0.44
1:E:1010:ALA:O	1:E:1014:THR:HG23	2.17	0.44
1:E:1399:VAL:HG12	1:E:1497:TYR:HD2	1.83	0.44
1:E:2453:ILE:O	1:E:2475:SER:HA	2.17	0.44
1:B:344:ILE:HA	1:B:361:ALA:O	2.16	0.44
1:B:902:LEU:O	1:B:903:ASN:HB2	2.15	0.44
1:B:1415:TYR:HD1	1:B:1422:ILE:HD12	1.82	0.44
1:C:554:THR:HG22	1:C:556:ALA:N	2.28	0.44
1:D:1145:LYS:NZ	1:D:1147:ASP:OD1	2.50	0.44
1:E:2311:LEU:HD22	1:E:2348:MET:HG2	1.99	0.44
1:A:2161:VAL:HG23	1:D:1117:LEU:HD11	1.98	0.44
1:A:2390:LEU:HD12	1:A:2523:GLU:HG2	1.99	0.44
1:A:2453:ILE:O	1:A:2475:SER:HA	2.17	0.44
1:B:893:LEU:HD23	1:B:918:LEU:HD21	1.99	0.44
1:B:1365:GLY:H	1:B:1371:ARG:HD3	1.81	0.44
1:B:1381:THR:HB	1:B:1386:LYS:HA	1.99	0.44
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.60	0.44
1:C:1756:ASN:HB3	1:C:1773:ILE:HG23	1.99	0.44
1:D:1250:LYS:HD3	1:D:1296:THR:HG22	1.99	0.44
1:D:1724:ARG:HG2	1:D:1742:PHE:CZ	2.52	0.44
1:E:111:SER:OG	1:E:1982:GLU:OE1	2.28	0.44
1:E:1757:ASP:OD1	1:E:1757:ASP:N	2.46	0.44
1:E:2191:ALA:O	1:E:2195:VAL:HG13	2.17	0.44
1:A:899:VAL:O	1:A:899:VAL:HG12	2.17	0.44
1:A:1399:VAL:HG12	1:A:1497:TYR:HD2	1.83	0.44
1:A:2388:GLN:O	1:A:2392:GLU:HG2	2.18	0.44
1:C:1724:ARG:HG2	1:C:1742:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:GLN:HG2	1:E:509:SER:HB2	1.99	0.44
1:E:1485:GLY:CA	1:E:1494:PHE:H	2.30	0.44
1:E:1677:TRP:CH2	1:E:1730:GLN:HB2	2.52	0.44
1:A:1150:VAL:HG11	1:A:1157:ILE:HD12	2.00	0.44
1:B:369:PHE:HD2	1:B:388:GLY:H	1.64	0.44
1:B:743:LEU:HD23	1:B:743:LEU:HA	1.81	0.44
1:B:1714:ALA:HB3	1:B:1717:TYR:HB2	2.00	0.44
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.74	0.44
1:D:473:ASN:ND2	1:D:477:ILE:H	2.15	0.44
1:D:1804:GLU:HA	1:D:1808:TYR:HB2	2.00	0.44
1:D:2282:TYR:O	1:D:2286:ARG:HG2	2.17	0.44
1:D:2364:ARG:NH2	1:D:2420:LEU:O	2.50	0.44
1:E:899:VAL:O	1:E:900:THR:OG1	2.33	0.44
1:E:967:LEU:HD23	1:E:967:LEU:HA	1.84	0.44
1:E:2008:ASP:OD2	1:E:2010:GLN:HG2	2.16	0.44
1:A:297:LEU:O	1:A:316:SER:OG	2.26	0.44
1:A:1518:VAL:HG21	1:A:1553:ILE:HG12	1.98	0.44
1:A:2390:LEU:HD11	1:A:2522:LEU:HB3	2.00	0.44
1:C:1412:ILE:O	1:C:1424:SER:HA	2.18	0.44
1:C:2345:LEU:HA	1:C:2348:MET:HE3	1.99	0.44
1:D:337:THR:HA	1:D:537:PHE:CE2	2.53	0.44
1:E:591:VAL:O	1:E:595:SER:OG	2.32	0.44
1:E:783:VAL:HG13	1:E:832:ARG:HG3	1.99	0.44
1:A:1839:TYR:CE1	1:A:1851:ASN:HB2	2.53	0.44
1:B:27:TYR:HD2	1:B:28:LEU:HD22	1.83	0.44
1:B:288:LEU:HD21	1:B:456:LEU:HD21	2.00	0.44
1:C:103:PHE:CE2	1:C:1981:PRO:HB2	2.53	0.44
1:C:714:LEU:HD22	1:C:719:MET:HG2	1.99	0.44
1:C:921:ASN:ND2	1:D:553:SER:OG	2.47	0.44
1:C:1736:ASN:HB2	1:C:1739:GLU:CD	2.38	0.44
1:C:2079:ASP:HB3	1:D:2275:LYS:HD3	1.99	0.44
1:D:321:VAL:HG12	1:D:326:LYS:O	2.18	0.44
1:D:505:VAL:HG11	1:D:598:TYR:HD2	1.83	0.44
1:D:1922:GLU:HB3	1:E:1004:ILE:HD13	1.99	0.44
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.88	0.44
1:A:1426:GLN:HB3	1:A:1462:LEU:HD22	1.99	0.44
1:B:375:LYS:HA	1:B:375:LYS:HD3	1.70	0.44
1:C:621:SER:O	1:C:624:ASN:ND2	2.51	0.44
1:C:1907:ARG:HH22	1:D:158:GLU:CD	2.20	0.44
1:E:142:ARG:HD2	1:E:971:PHE:O	2.17	0.44
1:E:288:LEU:HD21	1:E:456:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD11	1:A:88:VAL:HG21	1.99	0.44
1:A:200:HIS:CE1	1:A:202:PRO:HG2	2.53	0.44
1:A:337:THR:HG23	1:A:432:GLY:HA2	1.99	0.44
1:A:360:ARG:CZ	1:A:362:ASN:HD21	2.31	0.44
1:C:142:ARG:HD2	1:C:971:PHE:O	2.18	0.44
1:C:171:GLU:OE2	1:C:175:ARG:NH2	2.51	0.44
1:C:409:TYR:CE1	1:C:414:LYS:HD3	2.53	0.44
1:C:533:LYS:HD2	1:C:533:LYS:N	2.33	0.44
1:D:1674:ASP:HB2	1:D:1965:VAL:HG22	2.00	0.44
1:E:1374:GLN:NE2	1:E:1396:ALA:O	2.51	0.44
1:A:2453:ILE:HG23	1:A:2521:LEU:HD21	2.00	0.43
1:B:204:GLU:OE1	1:B:241:ASN:ND2	2.41	0.43
1:B:589:LEU:HD23	1:B:589:LEU:HA	1.86	0.43
1:B:1422:ILE:HG22	1:B:1466:PHE:HD2	1.83	0.43
1:B:1621:ARG:HB2	1:B:1654:LEU:HD21	1.99	0.43
1:D:2361:GLU:HG2	1:E:2484:PHE:CE2	2.53	0.43
1:E:419:ARG:HB3	1:E:429:GLN:HG3	1.99	0.43
1:A:505:VAL:HG11	1:A:598:TYR:CD2	2.53	0.43
1:A:1394:ILE:HB	1:A:1415:TYR:HB3	2.00	0.43
1:A:2049:ARG:HG3	1:A:2491:SER:O	2.18	0.43
1:B:1485:GLY:HA3	1:B:1494:PHE:H	1.84	0.43
1:B:2106:VAL:O	1:B:2109:VAL:HG22	2.18	0.43
1:D:373:LEU:HB2	1:D:416:TYR:CB	2.47	0.43
1:E:730:LEU:HD12	1:E:767:LEU:HD11	1.99	0.43
1:E:2514:ALA:HB1	1:E:2522:LEU:HD22	1.99	0.43
1:A:2442:THR:HB	1:A:2529:ILE:HB	2.01	0.43
1:B:1438:LEU:O	1:B:1453:GLU:HA	2.18	0.43
1:B:1757:ASP:OD1	1:B:1757:ASP:N	2.46	0.43
1:C:620:LEU:HD22	1:C:664:CYS:HB3	2.01	0.43
1:C:1373:LYS:HG3	1:C:1412:ILE:HG13	1.99	0.43
1:C:2092:MET:HG2	1:C:2265:THR:HG22	2.00	0.43
1:D:344:ILE:HA	1:D:361:ALA:O	2.18	0.43
1:E:197:THR:O	1:E:453:ARG:NH1	2.52	0.43
1:E:270:ASN:O	1:E:1445:ASN:ND2	2.52	0.43
1:E:1368:ASN:ND2	1:E:1370:ILE:HB	2.33	0.43
1:E:2364:ARG:NH2	1:E:2420:LEU:O	2.52	0.43
1:A:1036:LEU:HD11	1:A:1871:PRO:HD3	2.01	0.43
1:B:1824:ASP:OD1	1:B:1897:ARG:NH2	2.51	0.43
1:C:1035:ARG:NH2	1:C:1982:GLU:OE2	2.44	0.43
1:C:1100:VAL:HB	1:C:1593:VAL:HG22	1.99	0.43
1:C:2106:VAL:O	1:C:2109:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1365:GLY:H	1:D:1371:ARG:HD3	1.83	0.43
1:E:1457:SER:HB3	1:E:1458:PRO:CD	2.46	0.43
1:B:317:THR:HG22	1:B:330:TYR:CE2	2.54	0.43
1:B:2364:ARG:NH2	1:B:2420:LEU:O	2.51	0.43
1:D:247:TYR:OH	1:D:900:THR:N	2.51	0.43
1:D:1844:GLU:HG3	1:D:1845:ILE:N	2.34	0.43
1:E:320:VAL:HA	1:E:327:LEU:HA	2.00	0.43
1:A:136:TYR:CZ	1:A:959:VAL:HG22	2.53	0.43
1:C:2026:LEU:HD12	1:C:2026:LEU:HA	1.88	0.43
1:D:76:SER:N	1:D:77:GLY:HA3	2.34	0.43
1:D:420:TYR:CD2	1:D:426:ALA:HB2	2.54	0.43
1:D:810:LEU:HD12	1:D:810:LEU:HA	1.84	0.43
1:E:1677:TRP:CZ2	1:E:1730:GLN:HB2	2.53	0.43
1:B:142:ARG:HD2	1:B:971:PHE:O	2.18	0.43
1:B:620:LEU:HB3	1:B:804:ILE:HG13	2.01	0.43
1:B:1631:VAL:HG11	1:C:1165:ARG:HB3	2.01	0.43
1:B:1744:TYR:CE1	1:B:1753:VAL:HB	2.53	0.43
1:C:365:VAL:HG22	1:C:391:ILE:HA	2.00	0.43
1:C:680:LEU:HD22	1:C:744:VAL:HG22	1.99	0.43
1:C:1412:ILE:HB	1:C:1425:VAL:HG12	2.00	0.43
1:D:1839:TYR:CE1	1:D:1851:ASN:HB2	2.53	0.43
1:A:350:MET:HG3	1:A:359:ILE:HG13	2.01	0.43
1:A:687:ILE:HD11	1:A:741:MET:HG2	1.99	0.43
1:B:680:LEU:HD11	1:B:757:LEU:HD21	2.00	0.43
1:B:1100:VAL:HB	1:B:1593:VAL:HG22	2.00	0.43
1:B:1169:ILE:HD11	1:B:1192:LEU:HD11	2.01	0.43
1:B:1969:LEU:HD12	1:B:1969:LEU:H	1.84	0.43
1:C:415:ILE:HG12	1:C:431:GLY:CA	2.41	0.43
1:C:473:ASN:ND2	1:C:477:ILE:H	2.17	0.43
1:C:1922:GLU:HB3	1:D:1004:ILE:HD13	2.01	0.43
1:D:1744:TYR:CE1	1:D:1753:VAL:HB	2.54	0.43
1:E:242:ILE:HA	1:E:246:LEU:HD23	2.01	0.43
1:E:247:TYR:OH	1:E:900:THR:N	2.51	0.43
1:E:676:ILE:O	1:E:680:LEU:HG	2.19	0.43
1:E:680:LEU:HD22	1:E:744:VAL:HG22	2.01	0.43
1:E:1480:SER:OG	1:E:1481:TYR:N	2.52	0.43
1:E:2313:ARG:HH22	1:E:2465:MET:HE2	1.84	0.43
1:A:1515:LYS:HB3	1:A:1528:THR:HG22	2.01	0.43
1:B:321:VAL:HG12	1:B:326:LYS:O	2.19	0.43
1:B:2394:LYS:HE2	1:B:2394:LYS:HB2	1.78	0.43
1:C:2350:LYS:HD2	1:D:2299:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:PHE:HD1	1:E:500:PHE:HA	1.72	0.43
1:A:570:GLU:HG2	1:A:611:VAL:HB	2.01	0.43
1:A:1744:TYR:CE1	1:A:1753:VAL:HB	2.54	0.43
1:A:2176:PHE:HB2	1:E:1177:ALA:HB3	2.00	0.43
1:A:2282:TYR:O	1:A:2286:ARG:HG2	2.19	0.43
1:B:1302:VAL:HG23	1:B:1604:ARG:HG2	2.00	0.43
1:C:2514:ALA:HB1	1:C:2522:LEU:HD22	2.00	0.43
1:E:554:THR:HG22	1:E:556:ALA:N	2.31	0.43
1:A:238:ILE:HD13	1:A:238:ILE:HA	1.94	0.42
1:A:294:GLN:OE1	1:E:1934:GLN:NE2	2.43	0.42
1:A:414:LYS:HE3	1:A:414:LYS:HB3	1.88	0.42
1:A:1218:VAL:HG21	1:A:1245:VAL:HG12	2.01	0.42
1:A:1333:MET:HE3	1:A:1582:GLY:HA3	2.00	0.42
1:C:49:LEU:HD12	1:C:49:LEU:HA	1.87	0.42
1:C:2442:THR:HB	1:C:2529:ILE:HB	2.00	0.42
1:D:473:ASN:ND2	1:D:477:ILE:HG12	2.33	0.42
1:D:730:LEU:HD12	1:D:767:LEU:HD11	2.00	0.42
1:E:1437:ARG:HG2	1:E:1486:ASN:CB	2.48	0.42
1:A:1757:ASP:OD1	1:A:1757:ASP:N	2.44	0.42
1:A:2219:ARG:HD3	1:A:2223:TRP:CZ2	2.54	0.42
1:A:2219:ARG:O	1:A:2222:GLU:HG2	2.19	0.42
1:B:242:ILE:HA	1:B:246:LEU:HD23	2.01	0.42
1:B:305:SER:OG	1:B:306:ASP:N	2.52	0.42
1:B:419:ARG:HB3	1:B:429:GLN:HG3	2.02	0.42
1:B:1452:PHE:HZ	1:B:1472:LYS:HB3	1.84	0.42
1:A:581:LEU:HD23	1:A:581:LEU:HA	1.86	0.42
1:A:1456:PHE:HB3	1:A:1458:PRO:O	2.19	0.42
1:A:2361:GLU:HG2	1:B:2484:PHE:CE2	2.54	0.42
1:B:14:THR:HB	1:B:20:MET:HB2	2.00	0.42
1:B:1148:THR:HG23	1:B:1150:VAL:HG23	2.01	0.42
1:B:1518:VAL:HG21	1:B:1553:ILE:HG12	2.01	0.42
1:C:199:TYR:CD1	1:C:945:VAL:HG21	2.54	0.42
1:C:683:LEU:HD21	1:C:704:LEU:HD22	2.01	0.42
1:D:200:HIS:CE1	1:D:202:PRO:HG2	2.53	0.42
1:D:247:TYR:OH	1:D:480:ASP:OD1	2.25	0.42
1:D:561:MET:HG3	1:D:571:LEU:HD22	2.01	0.42
1:D:1457:SER:HB2	1:D:1458:PRO:HD3	2.00	0.42
1:E:415:ILE:HG12	1:E:431:GLY:CA	2.48	0.42
1:E:2385:LYS:HE3	1:E:2397:VAL:HG21	2.00	0.42
1:A:1:MET:HB2	1:A:1564:ILE:HG23	2.01	0.42
1:A:158:GLU:CD	1:E:1907:ARG:HH12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:TRP:CD1	1:E:1116:ASN:HB2	2.54	0.42
1:A:1368:ASN:N	1:A:1368:ASN:OD1	2.51	0.42
1:A:1555:ALA:HB1	1:A:1558:LEU:HD11	2.01	0.42
1:A:2106:VAL:O	1:A:2109:VAL:HG22	2.18	0.42
1:B:886:MET:CE	1:C:569:GLY:H	2.32	0.42
1:B:1456:PHE:HB3	1:B:1458:PRO:O	2.19	0.42
1:C:347:PHE:HE2	1:C:417:ALA:HB2	1.85	0.42
1:C:2361:GLU:HG2	1:D:2484:PHE:CE2	2.55	0.42
1:D:1570:VAL:HG22	1:D:1585:LYS:HG2	2.01	0.42
1:E:91:SER:HB3	1:E:1960:LEU:HD11	2.01	0.42
1:E:1536:LEU:HD13	1:E:1537:PRO:HD2	2.01	0.42
1:A:2228:ASP:OD2	1:E:2129:LYS:NZ	2.52	0.42
1:B:675:GLU:HG3	1:B:676:ILE:N	2.35	0.42
1:B:1478:LYS:N	1:B:1478:LYS:HD3	2.34	0.42
1:C:197:THR:O	1:C:453:ARG:NH1	2.53	0.42
1:C:271:ILE:HD13	1:C:281:TRP:HZ2	1.85	0.42
1:C:546:ILE:HD11	1:C:581:LEU:HD21	2.01	0.42
1:C:783:VAL:HG13	1:C:832:ARG:HG3	2.01	0.42
1:C:1630:LEU:HD22	1:C:1641:ILE:HG23	2.02	0.42
1:C:1795:ASN:O	1:C:1795:ASN:ND2	2.48	0.42
1:C:2426:TYR:HB2	1:C:2434:ARG:HH12	1.85	0.42
1:D:309:SER:OG	1:D:310:ALA:N	2.53	0.42
1:D:2057:THR:HG22	1:D:2345:LEU:HD11	2.02	0.42
1:D:2192:SER:O	1:D:2195:VAL:HG22	2.19	0.42
1:E:365:VAL:HG22	1:E:391:ILE:HA	2.01	0.42
1:E:1380:LEU:HD21	1:E:1463:ASN:HB3	2.01	0.42
1:A:415:ILE:HG12	1:A:431:GLY:CA	2.49	0.42
1:B:1436:ARG:HG2	1:B:1456:PHE:CD2	2.55	0.42
1:B:2070:SER:O	1:B:2074:MET:HG3	2.20	0.42
1:B:2359:ALA:HB2	1:B:2537:ARG:HH11	1.85	0.42
1:C:1803:TRP:CZ2	1:C:1854:PRO:HB2	2.54	0.42
1:D:1401:HIS:HB2	1:D:1497:TYR:CZ	2.55	0.42
1:D:1624:THR:HG1	1:D:1802:TYR:HH	1.36	0.42
1:E:360:ARG:HE	1:E:362:ASN:ND2	2.18	0.42
1:A:347:PHE:HE2	1:A:417:ALA:HB2	1.83	0.42
1:A:680:LEU:HD22	1:A:744:VAL:HG22	2.00	0.42
1:A:1443:VAL:CG1	1:A:1446:ASN:H	2.32	0.42
1:A:2192:SER:O	1:A:2195:VAL:HG22	2.20	0.42
1:A:2192:SER:O	1:A:2196:MET:HG2	2.19	0.42
1:B:2057:THR:HG22	1:B:2345:LEU:HD11	2.00	0.42
1:C:200:HIS:CE1	1:C:202:PRO:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1437:ARG:HB3	1:C:1455:PRO:HA	2.01	0.42
1:C:1907:ARG:NH1	1:D:158:GLU:OE1	2.50	0.42
1:C:2526:SER:OG	1:C:2527:ASP:N	2.53	0.42
1:D:374:ARG:HE	1:D:374:ARG:HB3	1.64	0.42
1:D:1639:ASP:O	1:D:1643:THR:HG23	2.20	0.42
1:E:531:PRO:HG3	1:E:535:LYS:HZ3	1.84	0.42
1:E:556:ALA:HB1	1:E:589:LEU:HD11	2.01	0.42
1:A:2136:GLU:OE2	1:B:2218:ARG:NH1	2.51	0.42
1:B:173:ILE:HD12	1:B:949:TRP:CE3	2.55	0.42
1:B:226:VAL:HG12	1:B:876:TRP:CE2	2.54	0.42
1:B:271:ILE:HD13	1:B:281:TRP:HZ2	1.85	0.42
1:B:1410:GLY:HA3	1:B:1497:TYR:CE1	2.54	0.42
1:C:1344:LYS:HB3	1:C:1344:LYS:HE3	1.81	0.42
1:D:231:GLU:HG3	1:D:897:ARG:HB3	2.02	0.42
1:D:372:THR:HA	1:D:416:TYR:O	2.20	0.42
1:D:436:PHE:CZ	1:D:438:SER:HB2	2.54	0.42
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.73	0.42
1:A:181:SER:O	1:A:185:MET:HG2	2.20	0.42
1:A:1667:TYR:OH	1:A:1673:GLY:O	2.25	0.42
1:A:2057:THR:HG22	1:A:2345:LEU:HD11	2.02	0.42
1:B:247:TYR:OH	1:B:480:ASP:OD1	2.23	0.42
1:B:420:TYR:CD1	1:B:426:ALA:HB2	2.55	0.42
1:B:1825:GLU:OE1	1:B:1825:GLU:N	2.45	0.42
1:C:1510:ASN:HB2	1:C:1513:ASP:HB2	2.01	0.42
1:D:142:ARG:HD2	1:D:971:PHE:O	2.20	0.42
1:D:1731:LYS:HD3	1:D:1731:LYS:N	2.35	0.42
1:E:2364:ARG:HB3	1:E:2532:ILE:HG13	2.02	0.42
1:A:76:SER:N	1:A:77:GLY:HA3	2.35	0.42
1:A:1228:LEU:HD11	1:A:1245:VAL:HG13	2.02	0.42
1:A:1922:GLU:HB3	1:B:1004:ILE:HD13	2.01	0.42
1:A:2137:ASP:O	1:B:2218:ARG:NH2	2.53	0.42
1:B:642:TRP:CZ2	1:B:646:VAL:HG21	2.55	0.42
1:B:902:LEU:HD23	1:B:902:LEU:HA	1.92	0.42
1:B:1400:LYS:HG2	1:B:1498:GLN:HB2	2.01	0.42
1:C:406:ASP:HA	1:C:409:TYR:HD2	1.84	0.42
1:C:1368:ASN:OD1	1:C:1368:ASN:N	2.53	0.42
1:C:1374:GLN:HE22	1:C:1396:ALA:H	1.67	0.42
1:C:1419:LYS:HB3	1:C:1421:TYR:CE1	2.55	0.42
1:C:1468:VAL:HG12	1:C:1470:SER:H	1.84	0.42
1:C:2368:LEU:HD23	1:C:2368:LEU:HA	1.84	0.42
1:D:367:ARG:HA	1:D:367:ARG:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1315:VAL:HG11	1:E:1343:SER:HB2	2.00	0.42
1:E:1731:LYS:HD3	1:E:1731:LYS:N	2.35	0.42
1:A:173:ILE:HD12	1:A:949:TRP:CE3	2.54	0.41
1:A:1123:ARG:HD2	1:A:1143:TRP:CE2	2.55	0.41
1:A:1575:ALA:HB2	1:A:1581:LEU:HD21	2.01	0.41
1:A:2376:SER:OG	1:A:2377:SER:N	2.53	0.41
1:B:414:LYS:HE3	1:B:414:LYS:HB3	1.81	0.41
1:B:683:LEU:HD21	1:B:704:LEU:HD22	2.02	0.41
1:B:687:ILE:HG23	1:B:745:LEU:HD21	2.02	0.41
1:B:1960:LEU:HD12	1:B:1960:LEU:HA	1.87	0.41
1:B:2434:ARG:HG2	1:B:2536:ILE:HG23	2.02	0.41
1:C:288:LEU:HD21	1:C:456:LEU:HD21	2.01	0.41
1:C:414:LYS:HB3	1:C:414:LYS:HE3	1.74	0.41
1:C:1388:GLN:HG3	1:C:1416:ASN:ND2	2.35	0.41
1:D:345:ASN:HB2	1:D:361:ALA:HB3	2.02	0.41
1:D:1824:ASP:OD1	1:D:1897:ARG:NH2	2.53	0.41
1:E:162:LEU:HD23	1:E:162:LEU:HA	1.77	0.41
1:E:1146:ILE:HG22	1:E:1148:THR:HG22	2.02	0.41
1:E:1399:VAL:HG13	1:E:1498:GLN:O	2.20	0.41
1:A:1329:SER:O	1:A:1329:SER:OG	2.30	0.41
1:B:247:TYR:OH	1:B:900:THR:N	2.52	0.41
1:B:1380:LEU:HD21	1:B:1463:ASN:HB3	2.02	0.41
1:B:2371:PHE:CE2	1:B:2415:VAL:HG13	2.55	0.41
1:C:298:GLY:HA3	1:C:314:ASN:HB2	2.01	0.41
1:C:415:ILE:HG13	1:C:416:TYR:N	2.34	0.41
1:D:1135:LEU:HD12	1:D:1135:LEU:HA	1.91	0.41
1:D:1371:ARG:NH1	1:D:1375:ILE:HG21	2.35	0.41
1:D:2339:GLU:HG3	1:E:2067:PHE:CE1	2.55	0.41
1:E:127:LYS:HB3	1:E:127:LYS:HE2	1.69	0.41
1:E:566:VAL:HB	1:E:570:GLU:HB2	2.02	0.41
1:A:433:ILE:HD11	1:A:539:ALA:HB2	2.03	0.41
1:A:1425:VAL:HG13	1:A:1463:ASN:OD1	2.19	0.41
1:A:2118:GLU:CD	1:A:2121:ARG:HH21	2.24	0.41
1:B:783:VAL:HG13	1:B:832:ARG:HG3	2.03	0.41
1:B:2417:LEU:HD23	1:B:2417:LEU:HA	1.93	0.41
1:C:501:ASP:HB3	1:C:522:HIS:ND1	2.35	0.41
1:A:554:THR:HG22	1:A:556:ALA:N	2.34	0.41
1:A:899:VAL:O	1:A:899:VAL:CG1	2.69	0.41
1:A:1731:LYS:N	1:A:1731:LYS:HD3	2.35	0.41
1:B:365:VAL:HG22	1:B:391:ILE:HA	2.02	0.41
1:B:1650:PRO:HA	1:B:1791:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:TYR:OH	1:C:480:ASP:OD1	2.25	0.41
1:C:1417:LYS:NZ	1:C:1504:ASP:OD2	2.30	0.41
1:C:1610:ALA:HB2	1:C:1652:PRO:HG2	2.01	0.41
1:C:1763:GLY:O	1:C:1769:ILE:HA	2.20	0.41
1:D:473:ASN:OD1	1:D:473:ASN:N	2.54	0.41
1:E:208:GLN:HG3	1:E:937:TYR:CD2	2.55	0.41
1:E:784:LEU:HD13	1:E:810:LEU:HD11	2.01	0.41
1:E:2214:GLU:O	1:E:2218:ARG:HG2	2.20	0.41
1:A:305:SER:OG	1:A:306:ASP:N	2.54	0.41
1:B:309:SER:OG	1:B:310:ALA:N	2.53	0.41
1:C:419:ARG:HB3	1:C:429:GLN:HG3	2.02	0.41
1:C:792:LEU:HD22	1:C:810:LEU:HD13	2.03	0.41
1:C:1759:ASP:OD1	1:C:1774:LYS:HA	2.20	0.41
1:D:242:ILE:HA	1:D:246:LEU:HD23	2.02	0.41
1:D:784:LEU:HD13	1:D:810:LEU:HD11	2.01	0.41
1:D:1742:PHE:O	1:D:1754:LEU:HD12	2.20	0.41
1:D:2426:TYR:HB2	1:D:2434:ARG:HH12	1.85	0.41
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.81	0.41
1:E:642:TRP:CZ2	1:E:646:VAL:HG21	2.55	0.41
1:E:2026:LEU:HD12	1:E:2026:LEU:HA	1.86	0.41
1:E:2519:LYS:O	1:E:2523:GLU:HG3	2.20	0.41
1:A:1410:GLY:HA3	1:A:1497:TYR:CE1	2.56	0.41
1:A:2094:LEU:HD23	1:A:2094:LEU:HA	1.91	0.41
1:C:1451:LEU:HB2	1:C:1479:CYS:SG	2.60	0.41
1:D:41:LEU:HD22	1:D:45:GLU:HB3	2.03	0.41
1:D:1969:LEU:HD12	1:D:1969:LEU:H	1.86	0.41
1:E:247:TYR:OH	1:E:480:ASP:OD1	2.23	0.41
1:E:1148:THR:HG23	1:E:1150:VAL:HG23	2.02	0.41
1:E:2526:SER:OG	1:E:2527:ASP:N	2.54	0.41
1:A:192:ARG:NH1	1:A:245:GLU:OE2	2.51	0.41
1:A:1921:LEU:HD12	1:A:1921:LEU:HA	1.92	0.41
1:B:1398:THR:O	1:B:1500:SER:OG	2.38	0.41
1:B:1731:LYS:HD3	1:B:1731:LYS:N	2.36	0.41
1:B:1742:PHE:O	1:B:1754:LEU:HD12	2.20	0.41
1:B:2092:MET:SD	1:B:2265:THR:HG22	2.60	0.41
1:C:1441:THR:O	1:C:1481:TYR:HB2	2.21	0.41
1:D:2368:LEU:HD23	1:D:2368:LEU:HA	1.74	0.41
1:D:2434:ARG:HG2	1:D:2536:ILE:HG23	2.02	0.41
1:D:2526:SER:OG	1:D:2527:ASP:N	2.53	0.41
1:E:304:TYR:HB3	1:E:308:THR:HG21	2.03	0.41
1:E:728:ASP:HB2	1:E:737:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:839:ASP:HA	1:E:849:ILE:HD13	2.02	0.41
1:E:1839:TYR:CE1	1:E:1851:ASN:HB2	2.56	0.41
1:A:466:GLN:O	1:A:470:ARG:HG3	2.20	0.41
1:A:504:GLN:HA	1:A:507:ASN:HD21	1.86	0.41
1:B:27:TYR:CD1	1:B:1947:GLN:HG3	2.55	0.41
1:B:299:MET:HE1	1:B:310:ALA:HA	2.03	0.41
1:B:1365:GLY:HA3	1:B:1371:ARG:HB2	2.01	0.41
1:C:26:GLN:NE2	1:C:57:LYS:HG3	2.36	0.41
1:C:505:VAL:HG11	1:C:598:TYR:CD2	2.55	0.41
1:C:1021:TRP:CE2	1:C:1025:ASN:HB3	2.56	0.41
1:D:2332:THR:HA	1:E:2281:LEU:HD12	2.03	0.41
1:E:173:ILE:HD12	1:E:949:TRP:CE3	2.56	0.41
1:E:1633:ARG:NH2	1:E:1649:LEU:HD21	2.34	0.41
1:A:460:LEU:HD23	1:A:500:PHE:HD1	1.86	0.41
1:A:1630:LEU:HD22	1:A:1641:ILE:HG23	2.02	0.41
1:B:41:LEU:HD22	1:B:45:GLU:HB3	2.03	0.41
1:B:208:GLN:HG3	1:B:937:TYR:CD2	2.56	0.41
1:B:297:LEU:O	1:B:316:SER:OG	2.31	0.41
1:B:403:ASN:O	1:B:404:ILE:HG13	2.21	0.41
1:B:440:PRO:HG2	1:B:443:ILE:HD12	2.02	0.41
1:B:1117:LEU:HD12	1:B:1117:LEU:HA	1.95	0.41
1:B:1274:LYS:HE3	1:B:1274:LYS:HB2	1.92	0.41
1:B:1392:ALA:HB3	1:B:1417:LYS:HG2	2.03	0.41
1:B:1923:LEU:HD23	1:B:1923:LEU:HA	1.94	0.41
1:B:2192:SER:O	1:B:2195:VAL:HG22	2.21	0.41
1:C:242:ILE:HA	1:C:246:LEU:HD23	2.03	0.41
1:C:1365:GLY:HA3	1:C:1371:ARG:HB2	2.03	0.41
1:C:2282:TYR:O	1:C:2286:ARG:HG2	2.20	0.41
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.93	0.41
1:D:347:PHE:CD2	1:D:415:ILE:HD11	2.56	0.41
1:D:369:PHE:CD2	1:D:387:SER:HA	2.56	0.41
1:D:538:GLU:H	1:D:538:GLU:HG3	1.58	0.41
1:D:1624:THR:OG1	1:D:1802:TYR:OH	2.14	0.41
1:D:1667:TYR:OH	1:D:1673:GLY:O	2.24	0.41
1:E:50:TYR:O	1:E:54:ILE:HG12	2.21	0.41
1:E:498:LEU:HD11	1:E:606:VAL:HG11	2.03	0.41
1:E:535:LYS:HA	1:E:535:LYS:HD3	1.96	0.41
1:C:1456:PHE:HB3	1:C:1458:PRO:O	2.21	0.41
1:C:1485:GLY:HA2	1:C:1494:PHE:CD1	2.56	0.41
1:D:1452:PHE:CZ	1:D:1472:LYS:HD3	2.55	0.41
1:A:304:TYR:HB3	1:A:308:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:CE1	1:A:415:ILE:HD11	2.55	0.40
1:A:1412:ILE:HB	1:A:1425:VAL:HB	2.02	0.40
1:A:2526:SER:OG	1:A:2527:ASP:N	2.53	0.40
1:B:215:SER:O	1:B:216:THR:OG1	2.34	0.40
1:B:415:ILE:HD13	1:B:434:PHE:HE2	1.86	0.40
1:B:1927:GLU:HB2	1:B:1991:TRP:CD2	2.56	0.40
1:C:91:SER:HB3	1:C:1960:LEU:HD11	2.03	0.40
1:C:1221:LYS:HE2	1:C:1221:LYS:HB2	1.87	0.40
1:C:1300:ASP:OD2	1:C:1604:ARG:NH2	2.42	0.40
1:D:1277:GLU:O	1:D:1281:LEU:HB2	2.21	0.40
1:D:1677:TRP:HA	1:D:1698:MET:HA	2.04	0.40
1:E:239:LEU:HD23	1:E:239:LEU:HA	1.91	0.40
1:E:1130:MET:HG3	1:E:1135:LEU:HD13	2.03	0.40
1:E:1969:LEU:H	1:E:1969:LEU:HD12	1.84	0.40
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.87	0.40
1:A:2368:LEU:HD21	1:A:2415:VAL:HG21	2.03	0.40
1:B:141:ARG:NH2	1:B:1005:GLU:OE2	2.41	0.40
1:B:365:VAL:HG22	1:B:392:ALA:H	1.85	0.40
1:B:1011:ASP:OD1	1:B:1011:ASP:N	2.47	0.40
1:B:1040:PRO:O	1:B:1044:ILE:HG12	2.21	0.40
1:B:2026:LEU:HD12	1:B:2026:LEU:HA	1.94	0.40
1:B:2104:ARG:HG3	1:C:2253:MET:HE1	2.03	0.40
1:B:2161:VAL:HG23	1:E:1117:LEU:HD11	2.02	0.40
1:C:784:LEU:HD13	1:C:810:LEU:HD11	2.03	0.40
1:C:1458:PRO:HD2	1:C:1461:ILE:HG21	2.02	0.40
1:D:618:TYR:OH	1:D:626:LYS:O	2.21	0.40
1:D:728:ASP:O	1:D:731:ARG:HG2	2.21	0.40
1:E:14:THR:HG22	1:E:18:GLN:O	2.21	0.40
1:E:504:GLN:O	1:E:507:ASN:ND2	2.53	0.40
1:E:505:VAL:HG11	1:E:598:TYR:HD2	1.87	0.40
1:A:247:TYR:OH	1:A:480:ASP:OD1	2.25	0.40
1:A:1399:VAL:HG13	1:A:1498:GLN:O	2.22	0.40
1:A:2514:ALA:HB1	1:A:2522:LEU:HD22	2.02	0.40
1:B:460:LEU:HD23	1:B:460:LEU:HA	1.90	0.40
1:B:507:ASN:OD1	1:B:507:ASN:C	2.60	0.40
1:B:1839:TYR:CE1	1:B:1851:ASN:HB2	2.56	0.40
1:C:145:LEU:HD23	1:C:145:LEU:HA	1.92	0.40
1:D:1633:ARG:NH2	1:D:1649:LEU:HD21	2.36	0.40
1:D:2349:GLU:OE2	1:E:2056:ARG:NH1	2.51	0.40
1:E:1730:GLN:O	1:E:1731:LYS:HB2	2.22	0.40
1:A:233:ALA:HB3	1:A:898:TYR:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LYS:HB3	1:A:397:LYS:HE3	1.89	0.40
1:A:1985:PRO:HA	1:A:1988:THR:OG1	2.22	0.40
1:B:501:ASP:HB3	1:B:522:HIS:ND1	2.36	0.40
1:B:1451:LEU:HB2	1:B:1479:CYS:SG	2.61	0.40
1:B:2453:ILE:O	1:B:2475:SER:HA	2.20	0.40
1:D:703:ILE:HD13	1:D:703:ILE:HA	1.95	0.40
1:D:2348:MET:O	1:D:2351:VAL:HG12	2.22	0.40
1:D:2454:ARG:O	1:D:2512:PRO:HD2	2.22	0.40
1:D:2459:TYR:CZ	1:D:2461:GLY:HA3	2.56	0.40
1:E:282:ILE:HD12	1:E:297:LEU:HD11	2.03	0.40
1:E:420:TYR:CD1	1:E:426:ALA:HB2	2.57	0.40
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.91	0.40
1:A:1409:GLY:HA3	1:A:1427:GLY:N	2.37	0.40
1:A:2368:LEU:HD23	1:A:2368:LEU:HA	1.77	0.40
1:B:1321:MET:HB3	1:B:1584:ILE:HG21	2.02	0.40
1:C:25:LEU:O	1:C:53:THR:HG21	2.22	0.40
1:C:1410:GLY:HA3	1:C:1497:TYR:CE1	2.57	0.40
1:D:1376:SER:HA	1:D:1379:LYS:HB2	2.04	0.40
1:E:1430:MET:HG3	1:E:1494:PHE:CD1	2.52	0.40
1:E:1714:ALA:HB3	1:E:1717:TYR:HB2	2.04	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	2535/2538 (100%)	2415 (95%)	112 (4%)	8 (0%)	41	73
1	B	2535/2538 (100%)	2420 (96%)	107 (4%)	8 (0%)	41	73
1	C	2535/2538 (100%)	2417 (95%)	111 (4%)	7 (0%)	41	73
1	D	2535/2538 (100%)	2426 (96%)	101 (4%)	8 (0%)	41	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	2535/2538 (100%)	2417 (95%)	110 (4%)	8 (0%)	41 73
All	All	12675/12690 (100%)	12095 (95%)	541 (4%)	39 (0%)	44 73

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2022	ASP
1	B	2516	ASP
1	D	2022	ASP
1	D	2516	ASP
1	E	27	TYR
1	A	27	TYR
1	A	2516	ASP
1	B	27	TYR
1	B	309	SER
1	C	27	TYR
1	C	309	SER
1	C	2022	ASP
1	C	2516	ASP
1	D	27	TYR
1	E	1730	GLN
1	E	2516	ASP
1	A	309	SER
1	A	1730	GLN
1	B	308	THR
1	B	1730	GLN
1	B	1973	ASN
1	B	2022	ASP
1	C	1730	GLN
1	D	309	SER
1	D	1730	GLN
1	E	308	THR
1	E	309	SER
1	E	2022	ASP
1	A	902	LEU
1	C	308	THR
1	E	1467	THR
1	A	344	ILE
1	B	344	ILE
1	C	344	ILE
1	D	308	THR
1	D	344	ILE

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Mol	Chain	Res	Type
1	E	344	ILE
1	A	308	THR
1	D	902	LEU

5.3.2 Protein sidechains (i)

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	2172/2175 (100%)	2133 (98%)	39 (2%)	59	82
1	B	2172/2175 (100%)	2130 (98%)	42 (2%)	57	81
1	C	2172/2175 (100%)	2132 (98%)	40 (2%)	59	82
1	D	2172/2175 (100%)	2138 (98%)	34 (2%)	62	84
1	E	2172/2175 (100%)	2141 (99%)	31 (1%)	67	86
All	All	10860/10875 (100%)	10674 (98%)	186 (2%)	62	83

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	33	LEU
1	A	39	ASP
1	A	95	MET
1	A	165	SER
1	A	227	MET
1	A	343	ASN
1	A	347	PHE
1	A	354	ASN
1	A	398	SER
1	A	410	LYS
1	A	418	TYR
1	A	537	PHE
1	A	542	ASN
1	A	904	LYS
1	A	1003	ARG

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Mol	Chain	Res	Type
1	A	1158	ARG
1	A	1162	PHE
1	A	1235	PHE
1	A	1433	ASP
1	A	1436	ARG
1	A	1457	SER
1	A	1491	PHE
1	A	1502	TRP
1	A	1531	ASP
1	A	1613	MET
1	A	1639	ASP
1	A	1902	TYR
1	A	1991	TRP
1	A	2003	HIS
1	A	2027	LEU
1	A	2081	ASP
1	A	2271	LEU
1	A	2286	ARG
1	A	2298	ASP
1	A	2364	ARG
1	A	2423	PHE
1	A	2504	SER
1	A	2526	SER
1	B	40	GLN
1	B	95	MET
1	B	112	MET
1	B	165	SER
1	B	180	ASP
1	B	182	ASP
1	B	196	ASP
1	B	343	ASN
1	B	347	PHE
1	B	358	PHE
1	B	363	PHE
1	B	364	LYS
1	B	416	TYR
1	B	500	PHE
1	B	538	GLU
1	B	542	ASN
1	B	568	SER
1	B	633	SER
1	B	690	ASP

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Mol	Chain	Res	Type
1	B	761	CYS
1	B	822	ASN
1	B	839	ASP
1	B	1003	ARG
1	B	1036	LEU
1	B	1067	LYS
1	B	1158	ARG
1	B	1235	PHE
1	B	1288	LYS
1	B	1540	SER
1	B	1613	MET
1	B	1661	ASN
1	B	1761	ASP
1	B	1902	TYR
1	B	1935	GLN
1	B	1991	TRP
1	B	2027	LEU
1	B	2286	ARG
1	B	2318	ASN
1	B	2324	ARG
1	B	2364	ARG
1	B	2423	PHE
1	B	2524	SER
1	C	1	MET
1	C	47	ARG
1	C	95	MET
1	C	256	GLU
1	C	343	ASN
1	C	347	PHE
1	C	355	ASN
1	C	363	PHE
1	C	410	LYS
1	C	416	TYR
1	C	500	PHE
1	C	538	GLU
1	C	542	ASN
1	C	568	SER
1	C	664	CYS
1	C	1071	ASP
1	C	1158	ARG
1	C	1162	PHE
1	C	1235	PHE

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Mol	Chain	Res	Type
1	C	1364	ASP
1	C	1436	ARG
1	C	1488	SER
1	C	1502	TRP
1	C	1511	ASN
1	C	1517	THR
1	C	1639	ASP
1	C	1661	ASN
1	C	1795	ASN
1	C	1902	TYR
1	C	1915	MET
1	C	1991	TRP
1	C	2003	HIS
1	C	2027	LEU
1	C	2046	SER
1	C	2286	ARG
1	C	2318	ASN
1	C	2364	ARG
1	C	2423	PHE
1	C	2458	ASN
1	C	2526	SER
1	D	27	TYR
1	D	182	ASP
1	D	229	GLN
1	D	269	GLU
1	D	343	ASN
1	D	347	PHE
1	D	416	TYR
1	D	463	ASN
1	D	537	PHE
1	D	538	GLU
1	D	542	ASN
1	D	624	ASN
1	D	690	ASP
1	D	761	CYS
1	D	764	MET
1	D	1158	ARG
1	D	1235	PHE
1	D	1288	LYS
1	D	1475	ASP
1	D	1491	PHE
1	D	1890	LEU

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Mol	Chain	Res	Type
1	D	1902	TYR
1	D	1908	ASP
1	D	1915	MET
1	D	1991	TRP
1	D	2003	HIS
1	D	2027	LEU
1	D	2046	SER
1	D	2286	ARG
1	D	2288	LYS
1	D	2364	ARG
1	D	2423	PHE
1	D	2465	MET
1	D	2524	SER
1	E	95	MET
1	E	165	SER
1	E	182	ASP
1	E	229	GLN
1	E	256	GLU
1	E	338	ASP
1	E	343	ASN
1	E	347	PHE
1	E	416	TYR
1	E	691	MET
1	E	764	MET
1	E	1235	PHE
1	E	1288	LYS
1	E	1433	ASP
1	E	1457	SER
1	E	1491	PHE
1	E	1510	ASN
1	E	1531	ASP
1	E	1661	ASN
1	E	1902	TYR
1	E	1908	ASP
1	E	1946	SER
1	E	1991	TRP
1	E	2003	HIS
1	E	2027	LEU
1	E	2046	SER
1	E	2081	ASP
1	E	2286	ARG
1	E	2364	ARG

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Mol	Chain	Res	Type
1	E	2407	SER
1	E	2502	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	ASN
1	B	323	ASN
1	B	354	ASN
1	B	1416	ASN
1	C	513	GLN
1	D	507	ASN
1	E	507	ASN
1	E	1815	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

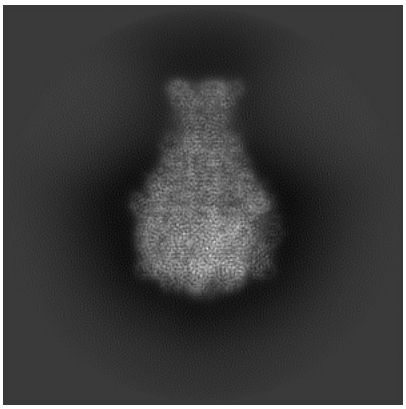
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41503. These allow visual inspection of the internal detail of the map and identification of artifacts.

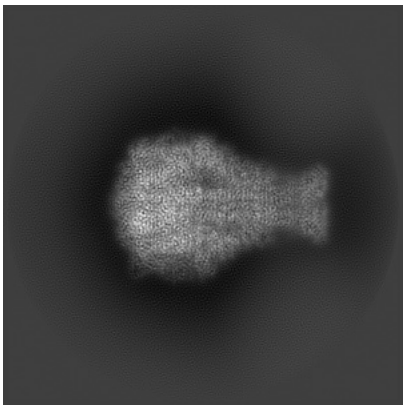
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

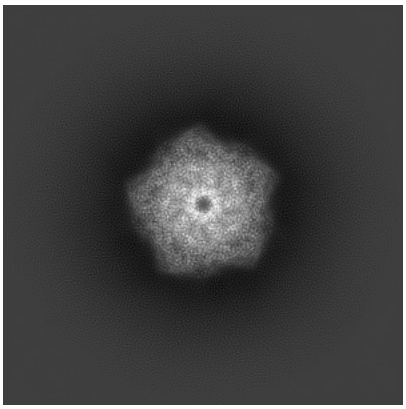
6.1.1 Primary map



X

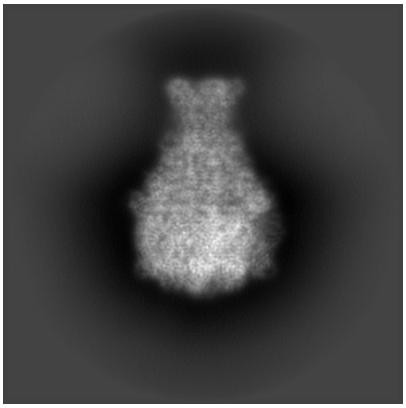


Y

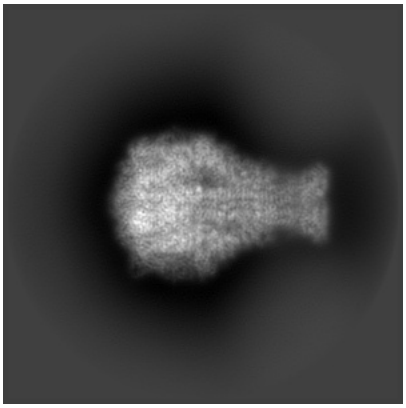


Z

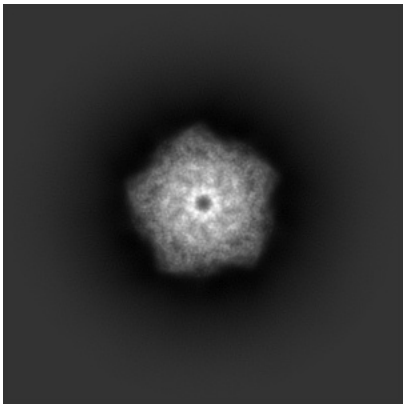
6.1.2 Raw map



X



Y

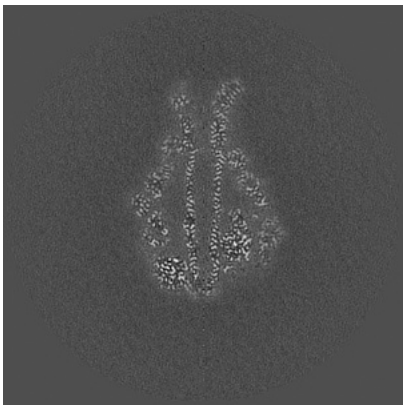


Z

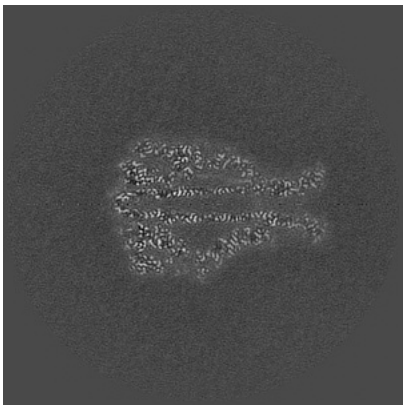
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

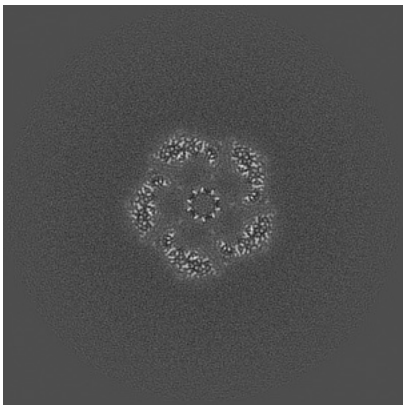
6.2.1 Primary map



X Index: 177

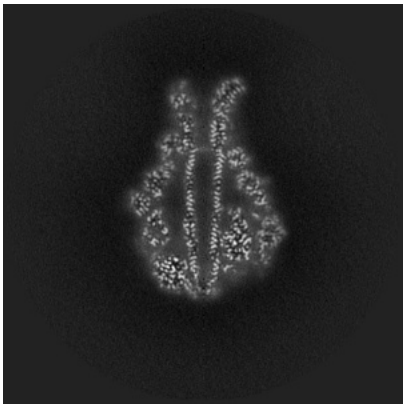


Y Index: 177

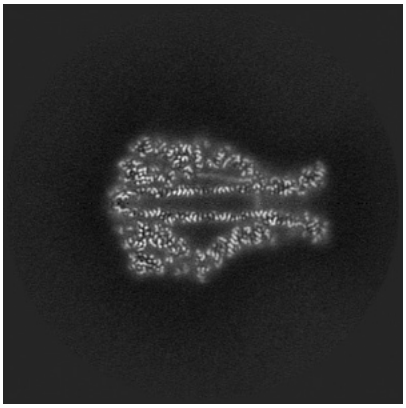


Z Index: 177

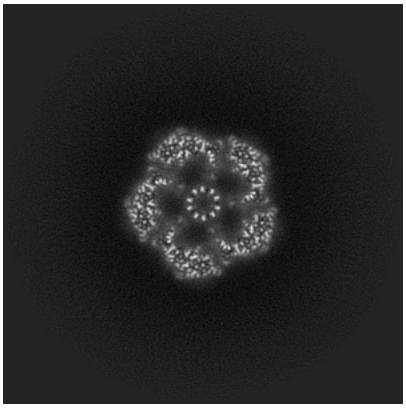
6.2.2 Raw map



X Index: 177



Y Index: 177

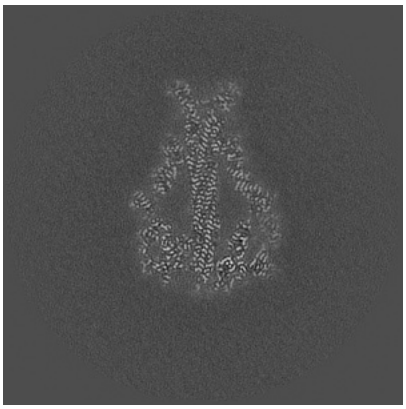


Z Index: 177

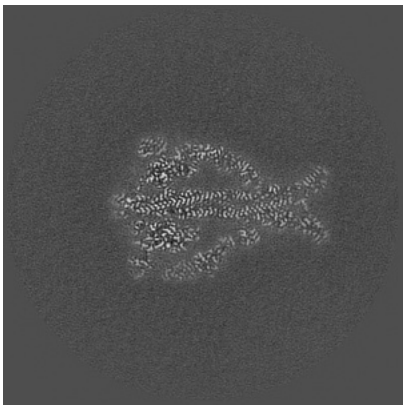
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

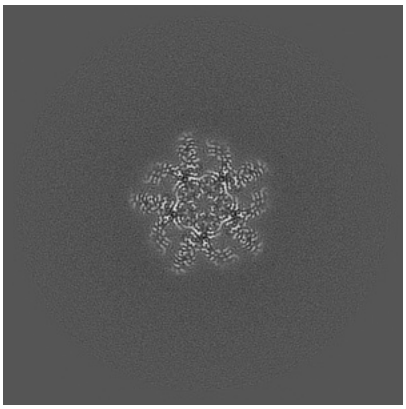
6.3.1 Primary map



X Index: 167

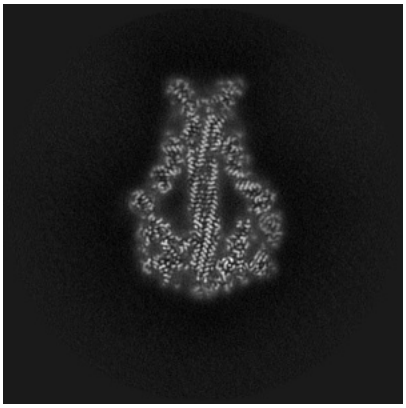


Y Index: 186

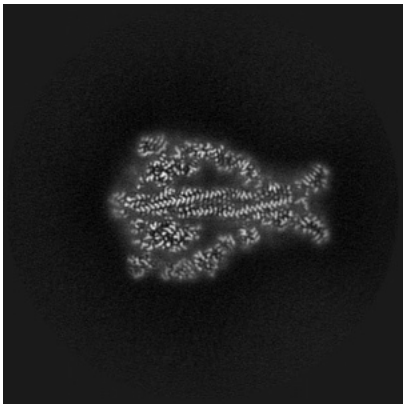


Z Index: 122

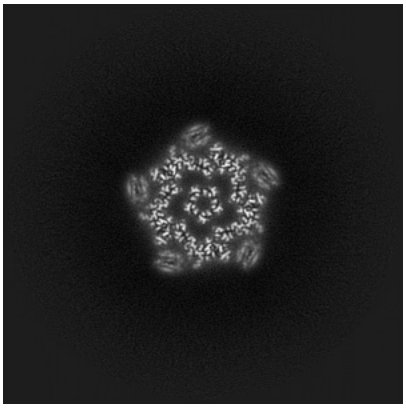
6.3.2 Raw map



X Index: 168



Y Index: 186

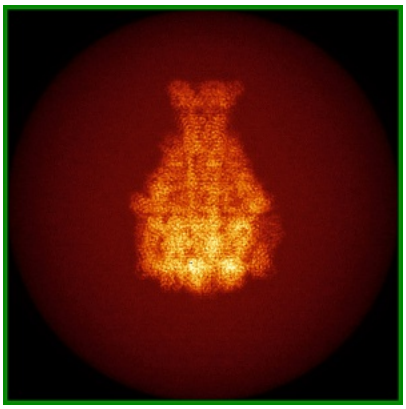


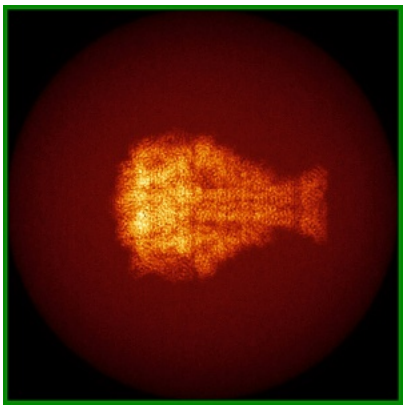
Z Index: 158

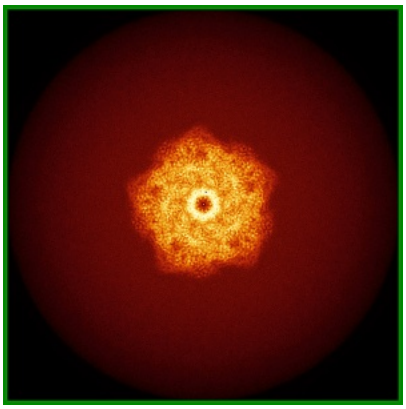
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

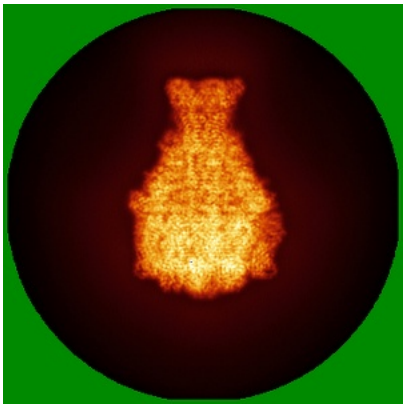
6.4.1 Primary map

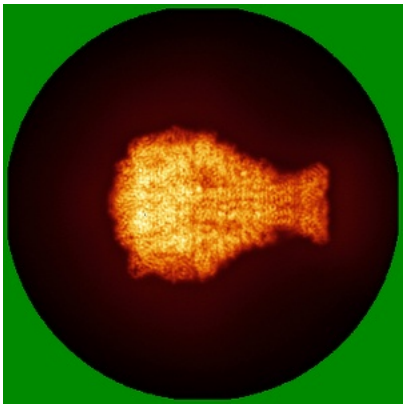

X

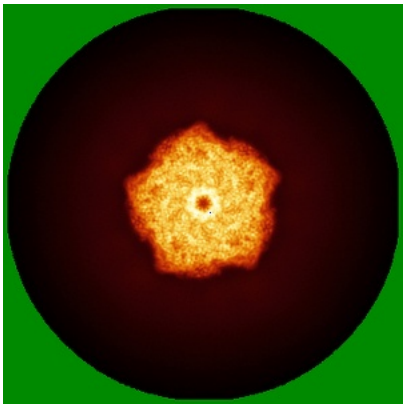

Y


Z

6.4.2 Raw map


X

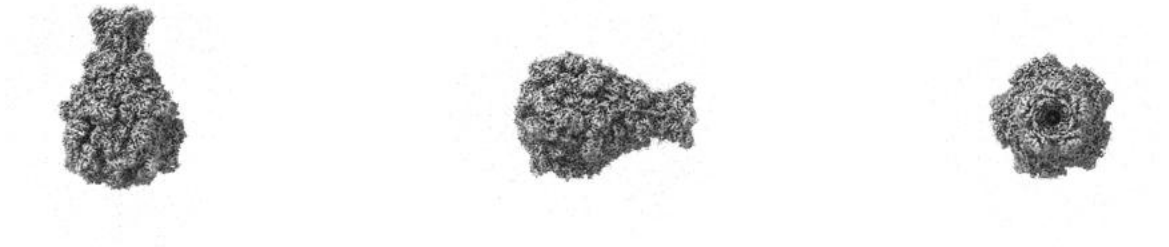

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

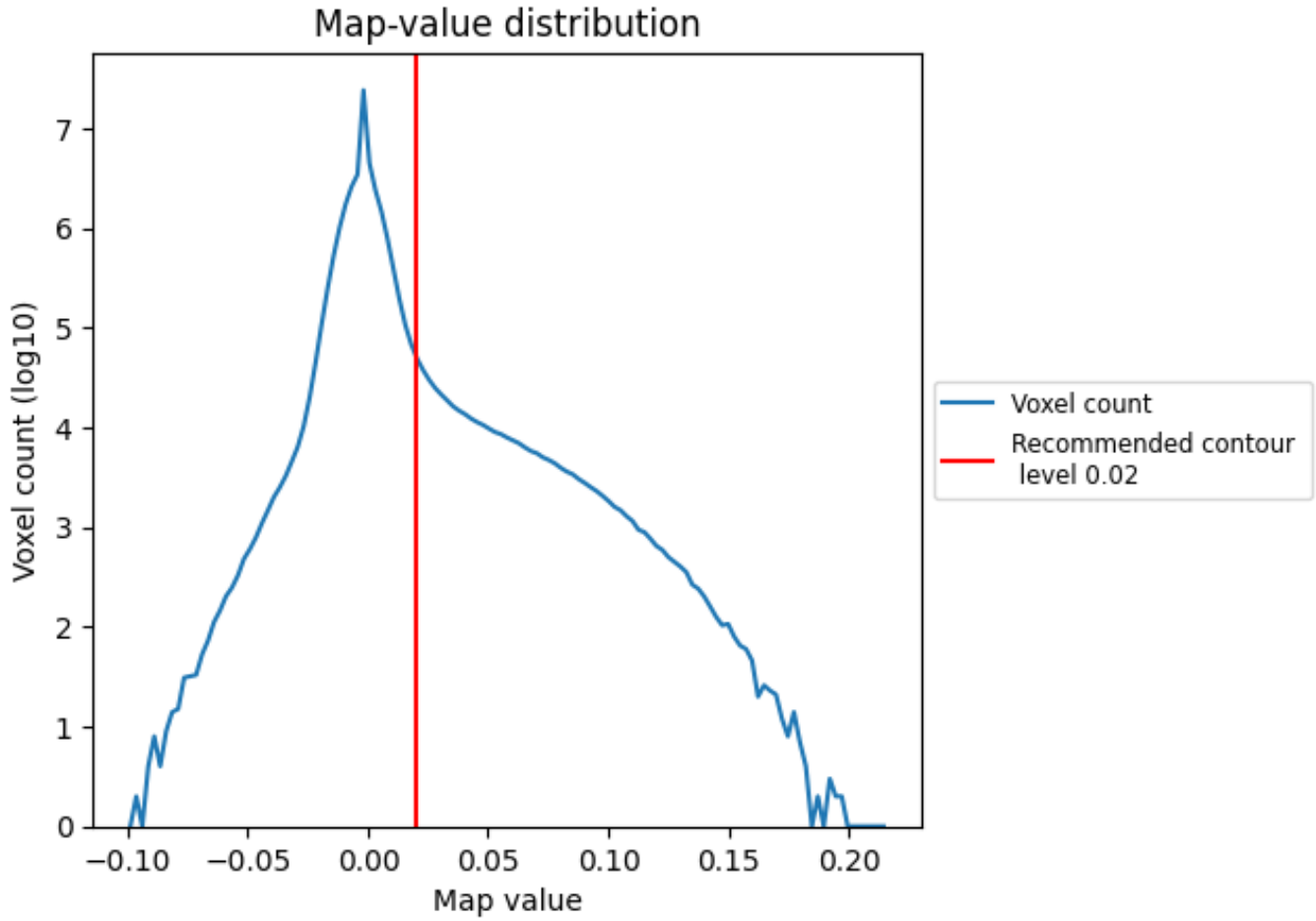
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

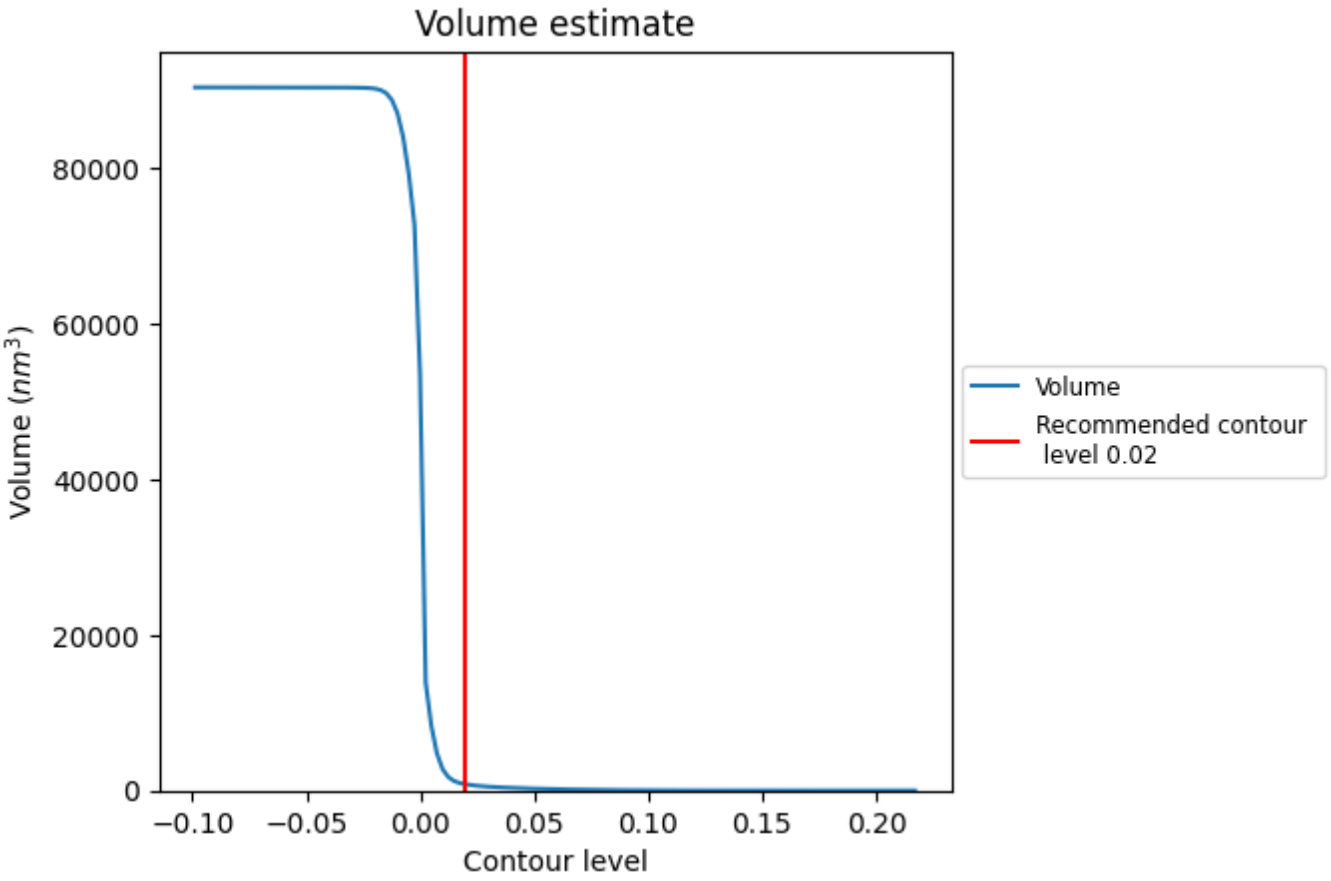
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

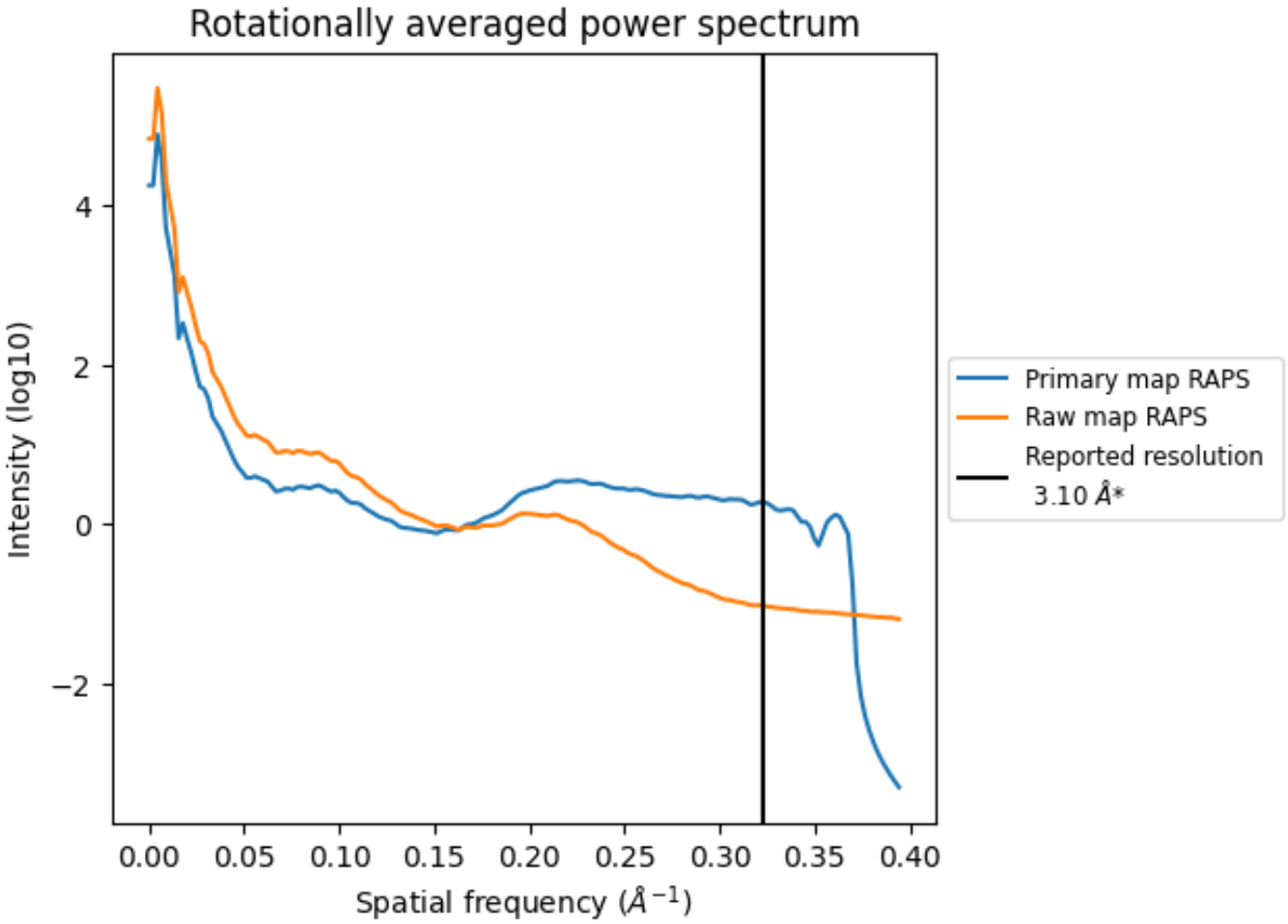
7.2 Volume estimate



The volume at the recommended contour level is 805 nm^3; this corresponds to an approximate mass of 727 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

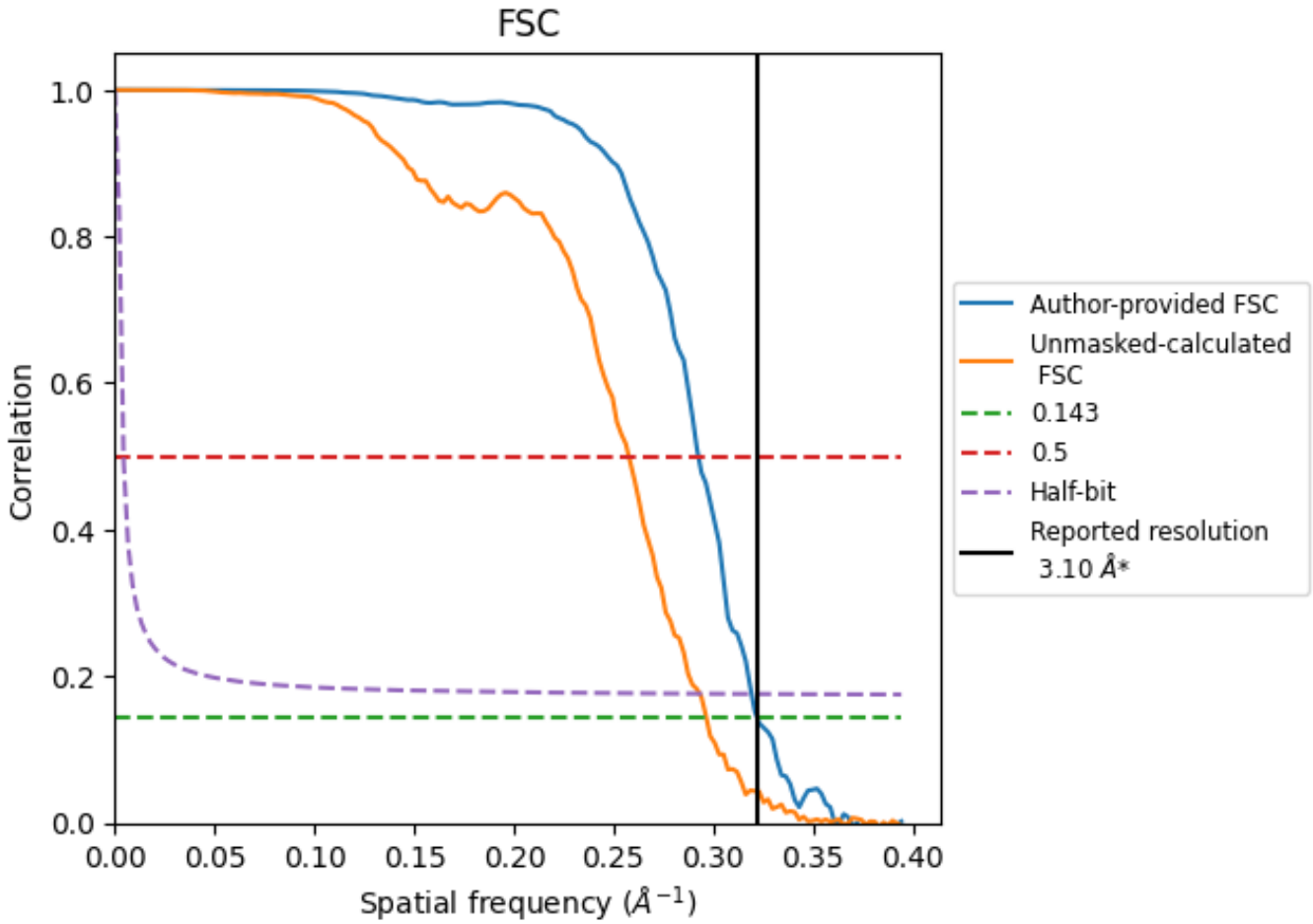


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.42	3.13
Unmasked-calculated*	3.37	3.88	3.41

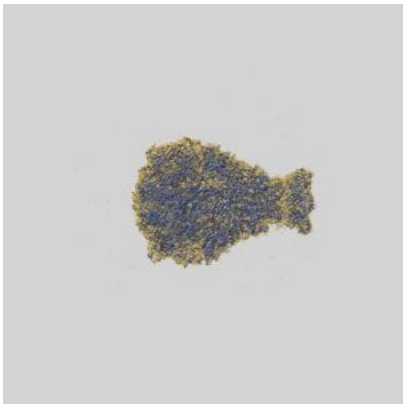
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

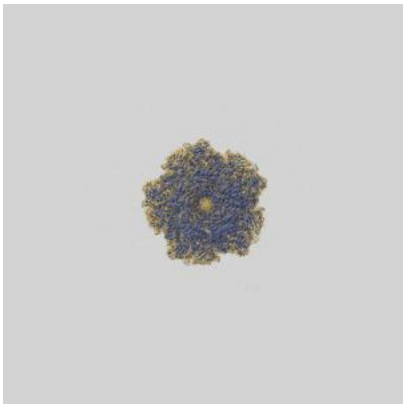
This section contains information regarding the fit between EMDB map EMD-41503 and PDB model 8TQE. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay

X



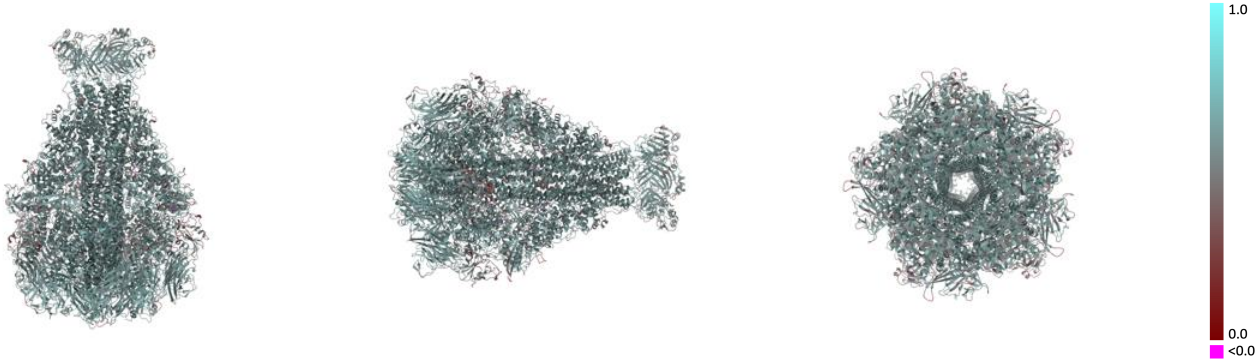
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

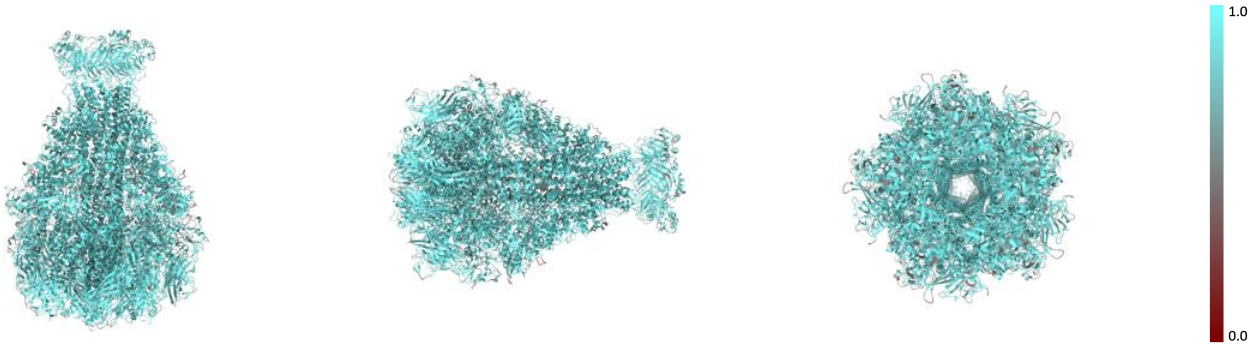
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

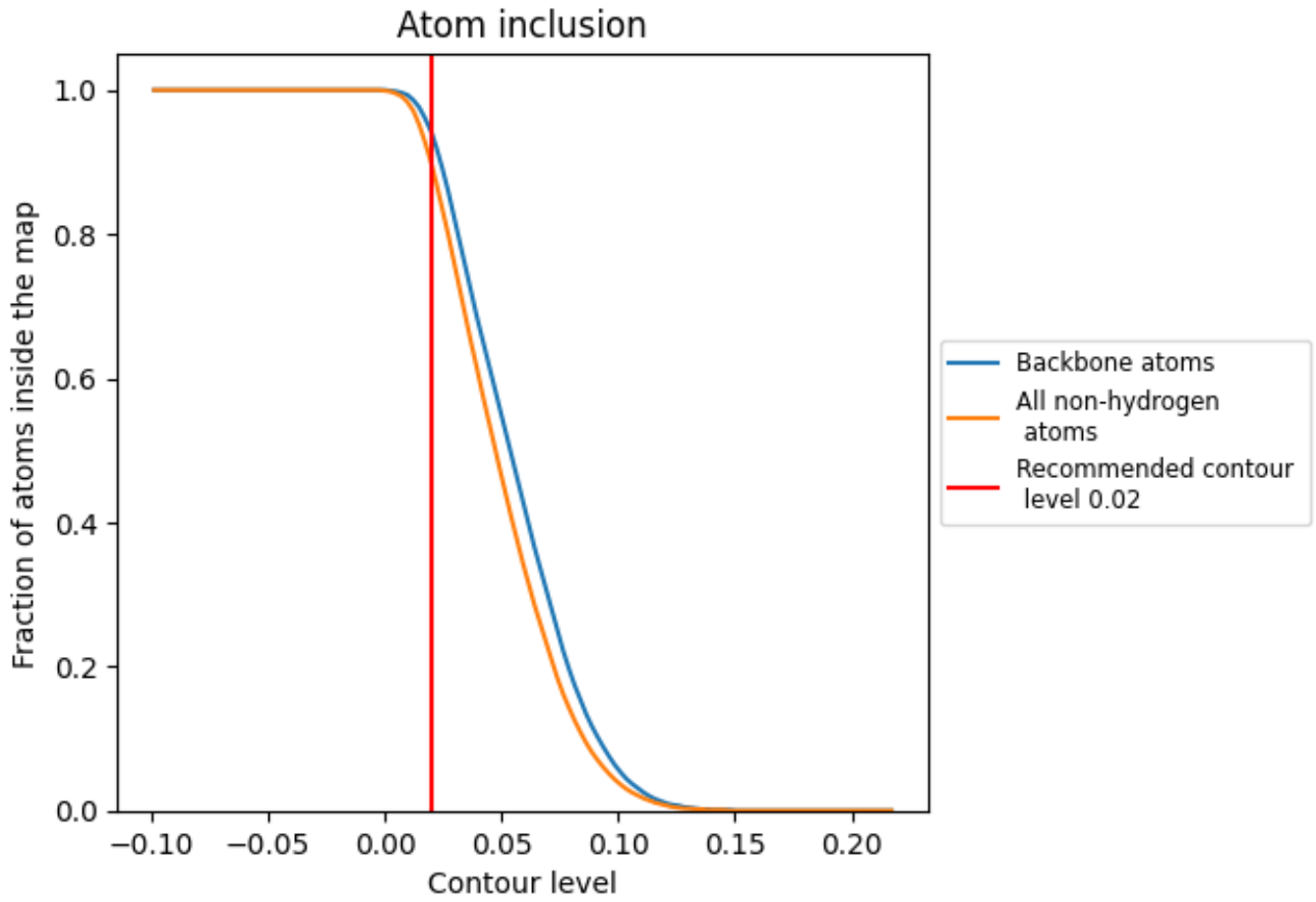
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.5620
A	0.8970	0.5620
B	0.8960	0.5620
C	0.8980	0.5630
D	0.8940	0.5600
E	0.8990	0.5630