



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 03:42 AM EST

PDB ID : 8TV0
Title : XptA2 wild type
Authors : Martin, C.L.; Aller, S.G.
Deposited on : 2023-08-17
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

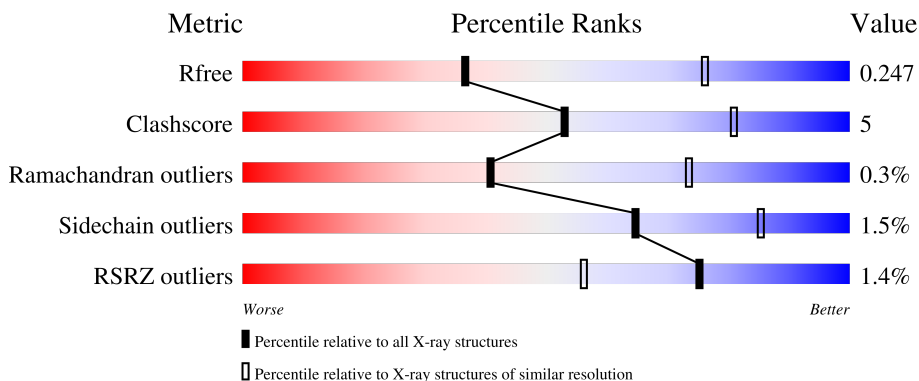
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	2537	 85% 15%
1	B	2537	 86% 13%
1	C	2537	 84% 15%
1	D	2537	 86% 14%
1	E	2537	 87% 13%

2 Entry composition

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 ZeroOcc column contains the number of atoms modelled with zero occupancy, 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						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	2537	20007	12625	3415	3894	12	61	0	0	0
1	B	2537	20007	12625	3415	3894	12	61	0	0	0
1	C	2537	20007	12625	3415	3894	12	61	0	0	0
1	D	2537	20007	12625	3415	3894	12	61	0	0	0
1	E	2537	20007	12625	3415	3894	12	61	0	0	0

There are 330 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	686	SER	ARG	conflict	UNP N1NRW3
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	1484	GLY	ASP	conflict	UNP N1NRW3
A	1486	ALA	ASN	conflict	UNP N1NRW3
A	1514	ILE	VAL	conflict	UNP N1NRW3
A	1519	MSE	VAL	conflict	UNP N1NRW3
A	1877	ASN	TYR	conflict	UNP N1NRW3
A	1880	MSE	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	MSE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2149	LEU	PHE	conflict	UNP N1NRW3
A	2161	VAL	ALA	conflict	UNP N1NRW3
A	2164	ILE	VAL	conflict	UNP N1NRW3
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1126	ASP	ASN	conflict	UNP N1NRW3
B	1250	LYS	VAL	conflict	UNP N1NRW3
B	1253	SER	PRO	conflict	UNP N1NRW3
B	1257	GLY	ASP	conflict	UNP N1NRW3
B	1258	SER	ASN	conflict	UNP N1NRW3
B	1484	GLY	ASP	conflict	UNP N1NRW3
B	1486	ALA	ASN	conflict	UNP N1NRW3
B	1514	ILE	VAL	conflict	UNP N1NRW3
B	1519	MSE	VAL	conflict	UNP N1NRW3
B	1877	ASN	TYR	conflict	UNP N1NRW3
B	1880	MSE	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	MSE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1484	GLY	ASP	conflict	UNP N1NRW3
C	1486	ALA	ASN	conflict	UNP N1NRW3
C	1514	ILE	VAL	conflict	UNP N1NRW3
C	1519	MSE	VAL	conflict	UNP N1NRW3
C	1877	ASN	TYR	conflict	UNP N1NRW3
C	1880	MSE	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	MSE	ALA	conflict	UNP N1NRW3
C	1961	GLY	ASP	conflict	UNP N1NRW3
C	1962	ARG	ASN	conflict	UNP N1NRW3

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	1484	GLY	ASP	conflict	UNP N1NRW3
D	1486	ALA	ASN	conflict	UNP N1NRW3
D	1514	ILE	VAL	conflict	UNP N1NRW3
D	1519	MSE	VAL	conflict	UNP N1NRW3
D	1877	ASN	TYR	conflict	UNP N1NRW3
D	1880	MSE	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	MSE	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

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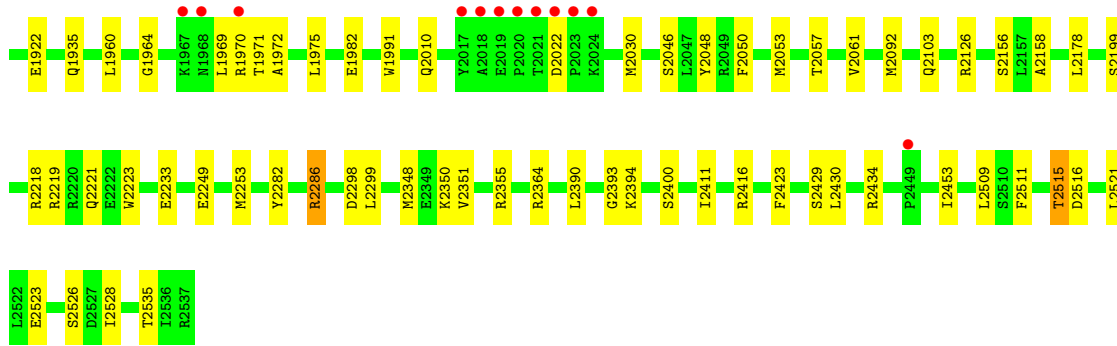
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Chain	Residue	Modelled	Actual	Comment	Reference
E	391	ILE	VAL	conflict	UNP N1NRW3
E	407	SER	ASN	conflict	UNP N1NRW3
E	410	LYS	ARG	conflict	UNP N1NRW3
E	566	VAL	ILE	conflict	UNP N1NRW3
E	583	ALA	THR	conflict	UNP N1NRW3
E	586	THR	ILE	conflict	UNP N1NRW3
E	587	ILE	LEU	conflict	UNP N1NRW3
E	592	PHE	PRO	conflict	UNP N1NRW3
E	606	VAL	ALA	conflict	UNP N1NRW3
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	1484	GLY	ASP	conflict	UNP N1NRW3
E	1486	ALA	ASN	conflict	UNP N1NRW3
E	1514	ILE	VAL	conflict	UNP N1NRW3
E	1519	MSE	VAL	conflict	UNP N1NRW3
E	1877	ASN	TYR	conflict	UNP N1NRW3
E	1880	MSE	THR	conflict	UNP N1NRW3
E	1884	ILE	VAL	conflict	UNP N1NRW3

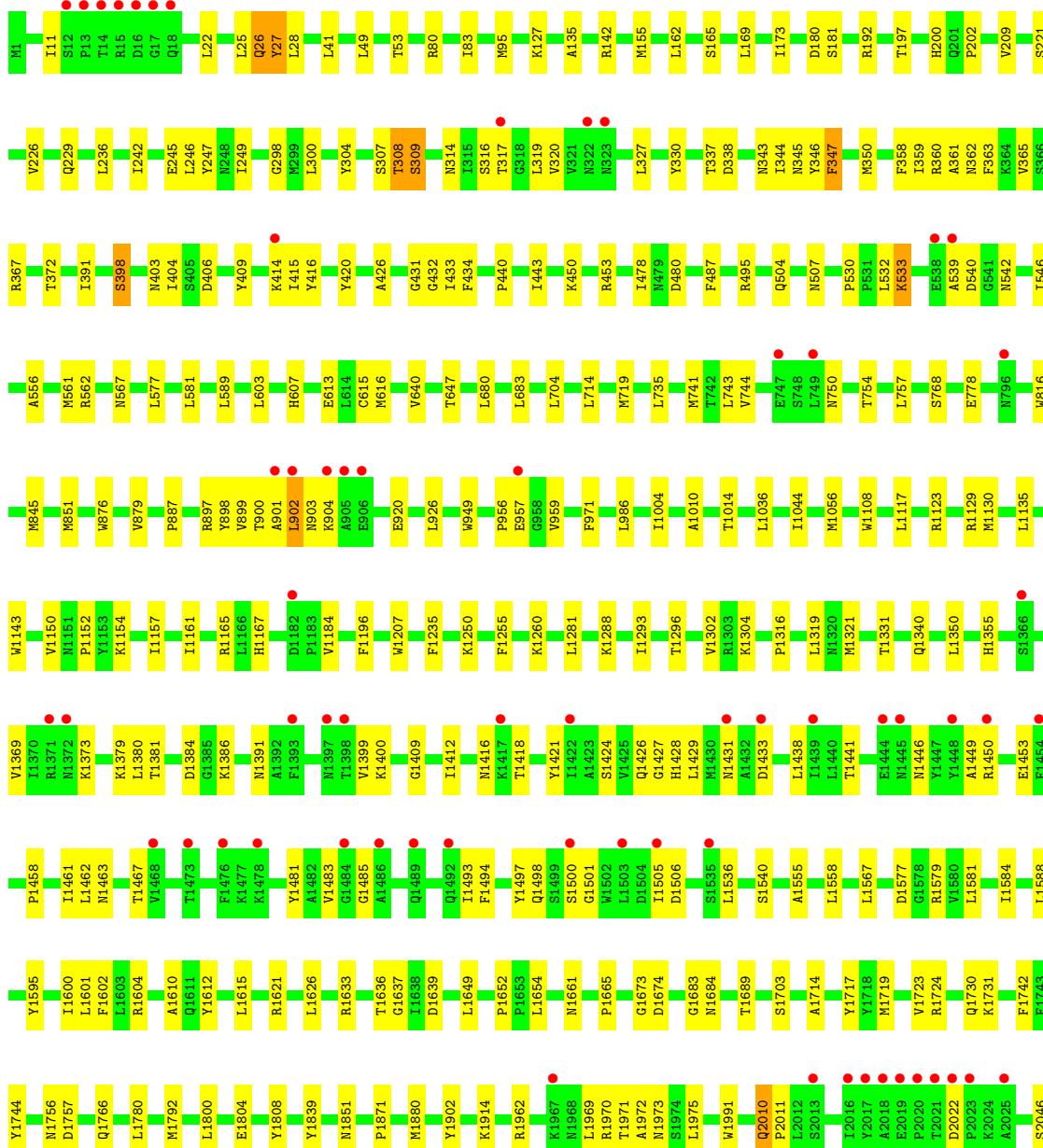
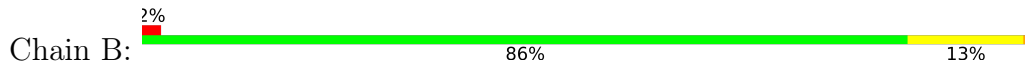
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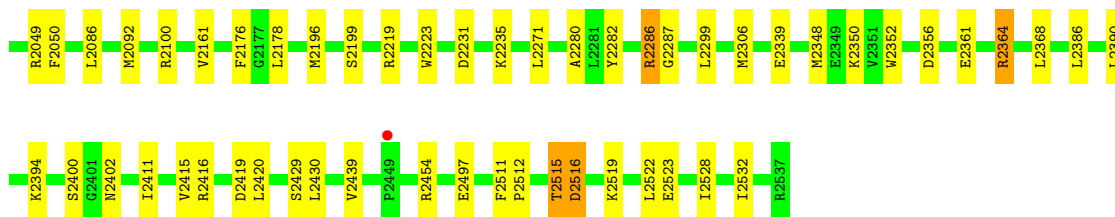
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Chain	Residue	Modelled	Actual	Comment	Reference
E	1920	THR	ALA	conflict	UNP N1NRW3
E	1943	GLY	VAL	conflict	UNP N1NRW3
E	1947	GLN	HIS	conflict	UNP N1NRW3
E	1959	MSE	ALA	conflict	UNP N1NRW3
E	1961	GLY	ASP	conflict	UNP N1NRW3
E	1962	ARG	ASN	conflict	UNP 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
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

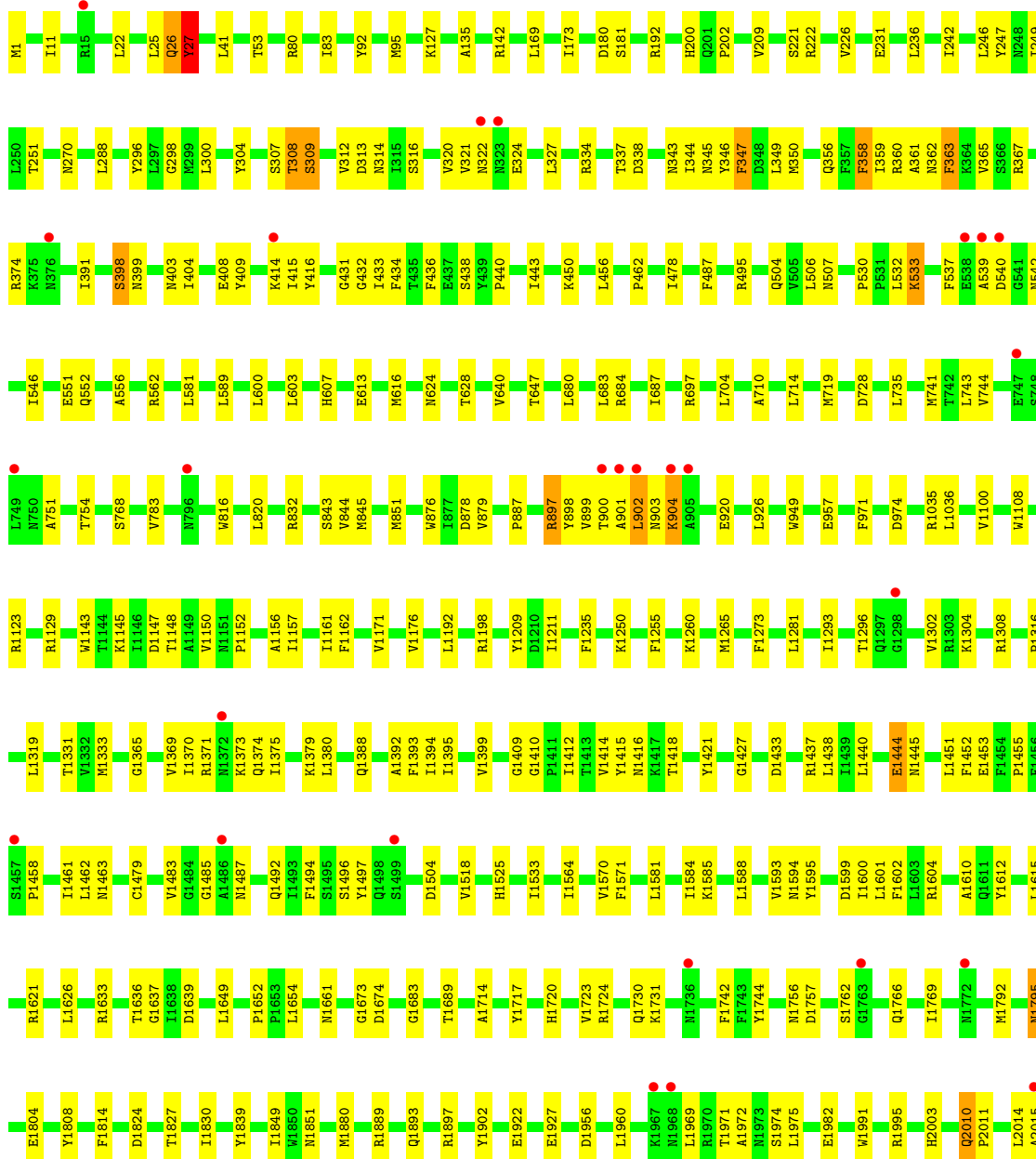
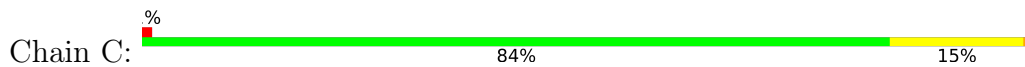


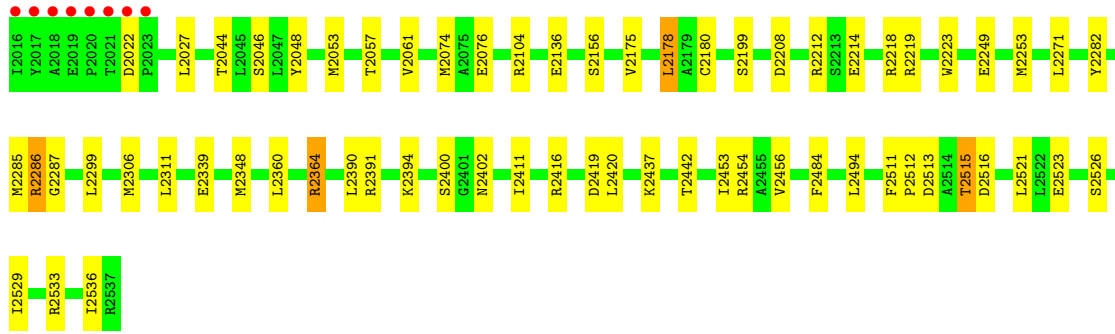
• Molecule 1: XptA2



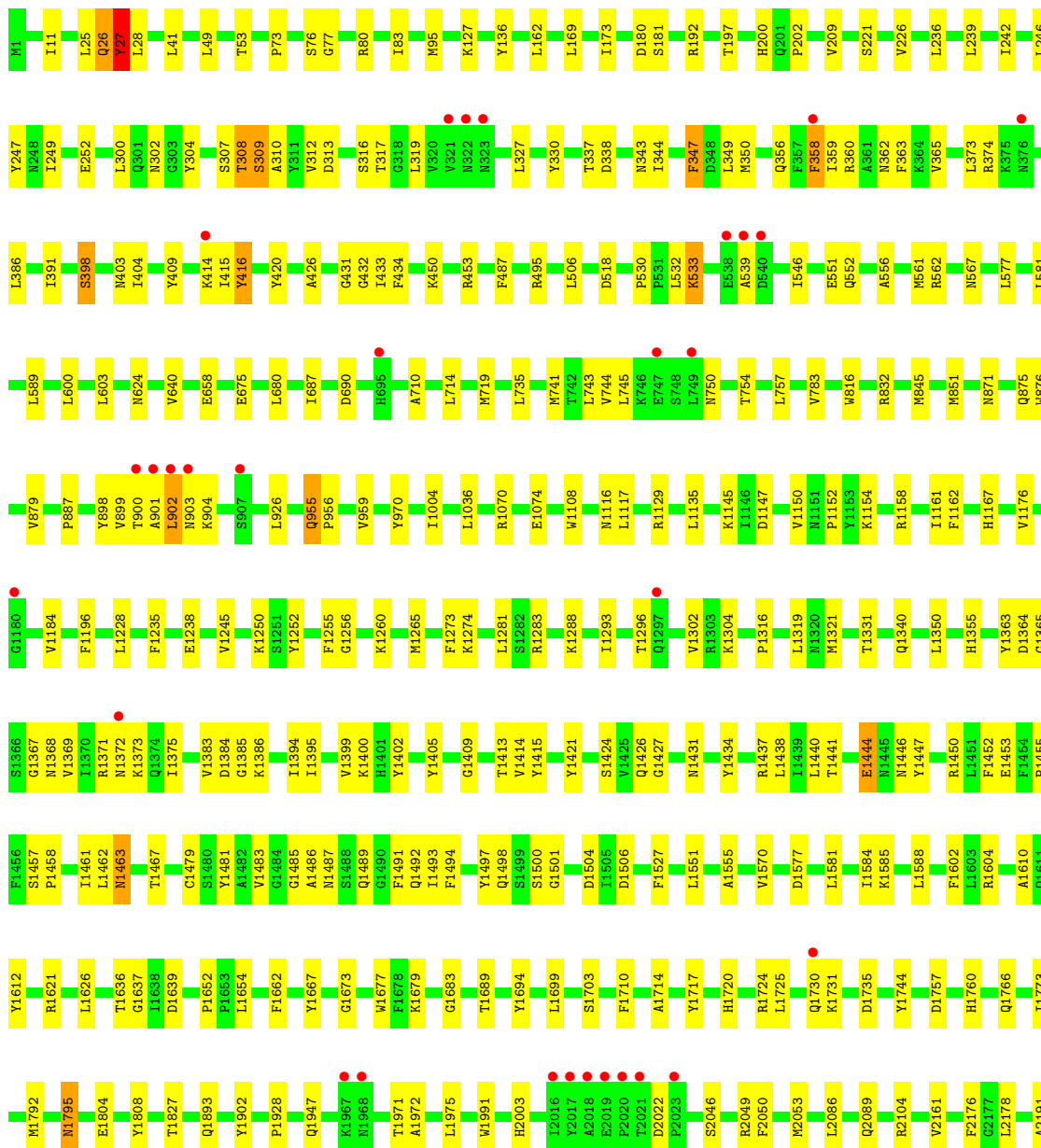
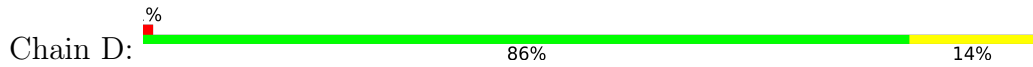


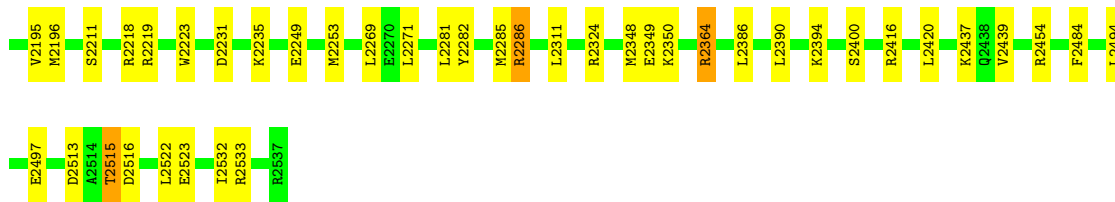
• Molecule 1: XptA2



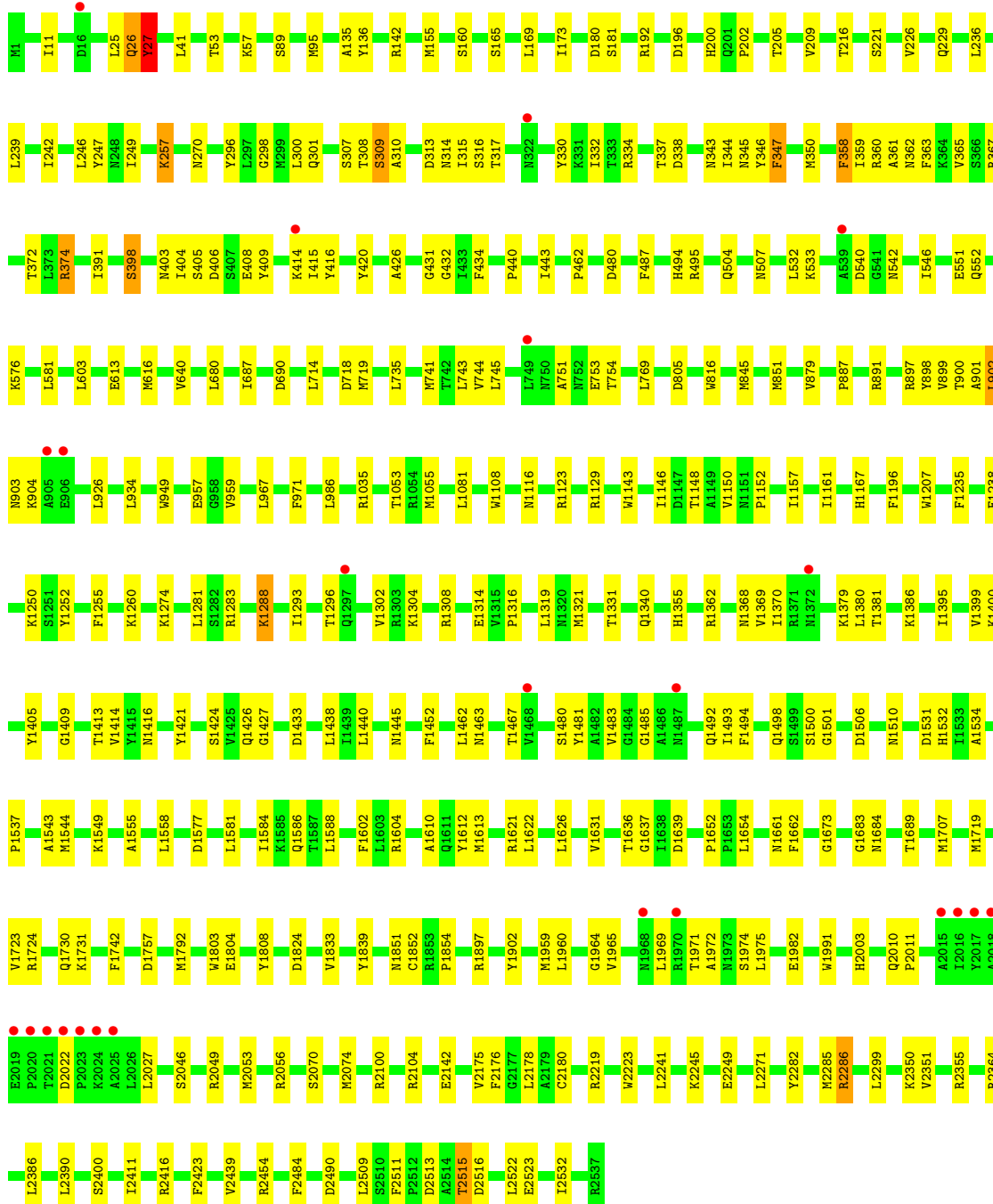
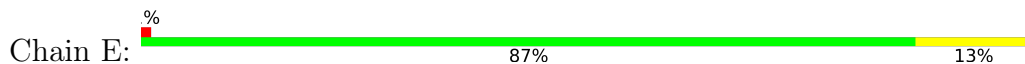


● Molecule 1: XptA2





• Molecule 1: XptA2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	175.13Å 176.93Å 509.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 3.10 49.59 – 2.94	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.73-3.10) 83.0 (49.59-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.96Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.194 , 0.247 0.193 , 0.247	Depositor DCC
R_{free} test set	1947 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtrriage
Anisotropy	0.330	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.014 for k,h,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	100035	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.24	0/20353	0.48	2/27534 (0.0%)
1	B	0.24	0/20353	0.48	2/27534 (0.0%)
1	C	0.24	0/20353	0.48	2/27534 (0.0%)
1	D	0.24	0/20353	0.48	2/27534 (0.0%)
1	E	0.24	0/20353	0.48	2/27534 (0.0%)
All	All	0.24	0/101765	0.48	10/137670 (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	3
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	11

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	GLN	C-N-CA	6.48	137.90	121.70
1	A	26	GLN	C-N-CA	6.32	137.51	121.70
1	B	26	GLN	C-N-CA	6.28	137.41	121.70
1	C	26	GLN	C-N-CA	6.22	137.25	121.70
1	D	2515	THR	C-N-CA	6.20	137.19	121.70
1	B	2515	THR	C-N-CA	6.19	137.17	121.70
1	E	26	GLN	C-N-CA	6.17	137.12	121.70
1	A	2515	THR	C-N-CA	6.14	137.04	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2515	THR	C-N-CA	6.08	136.90	121.70
1	C	2515	THR	C-N-CA	5.90	136.45	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1457	SER	Peptide
1	A	398	SER	Peptide
1	A	532	LEU	Peptide
1	B	398	SER	Peptide
1	B	532	LEU	Peptide
1	C	398	SER	Peptide
1	C	532	LEU	Peptide
1	D	398	SER	Peptide
1	D	532	LEU	Peptide
1	E	398	SER	Peptide
1	E	532	LEU	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	19597	232	0
1	B	20007	0	19597	222	0
1	C	20007	0	19597	237	0
1	D	20007	0	19597	226	0
1	E	20007	0	19597	204	0
All	All	100035	0	97985	1068	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 5.

All (1068) 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:E:415:ILE:O	1:E:416:TYR:HD1	1.50	0.95
1:A:2515:THR:H	1:A:2516:ASP:HB2	1.39	0.87
1:B:404:ILE:HD13	1:B:414:LYS:HD2	1.59	0.83
1:E:2515:THR:H	1:E:2516:ASP:HB2	1.43	0.82
1:E:1531:ASP:OD2	1:E:1532:HIS:ND1	2.13	0.82
1:B:2100:ARG:HB3	1:C:2253:MSE:HE1	1.62	0.82
1:B:2515:THR:H	1:B:2516:ASP:HB2	1.45	0.80
1:D:2515:THR:H	1:D:2516:ASP:HB2	1.45	0.80
1:D:404:ILE:HD13	1:D:414:LYS:HD2	1.63	0.80
1:D:1506:ASP:HB3	1:D:1577:ASP:HB2	1.64	0.80
1:D:1744:TYR:HB2	1:D:1766:GLN:HG2	1.63	0.80
1:A:1035:ARG:NH2	1:A:1982:GLU:OE2	2.15	0.79
1:C:350:MSE:HE3	1:C:359:ILE:HD12	1.63	0.79
1:C:404:ILE:HD13	1:C:414:LYS:HD2	1.64	0.78
1:E:1684:ASN:HB3	1:E:1719:MSE:HB2	1.66	0.78
1:C:135:ALA:HB2	1:C:957:GLU:HB2	1.66	0.77
1:E:350:MSE:HE3	1:E:359:ILE:HD12	1.67	0.77
1:C:1150:VAL:HG12	1:C:1152:PRO:HD3	1.67	0.76
1:B:1150:VAL:HG12	1:B:1152:PRO:HD3	1.66	0.76
1:C:1485:GLY:HA3	1:C:1494:PHE:H	1.49	0.75
1:B:1612:TYR:HB3	1:B:1654:LEU:HD22	1.68	0.75
1:C:360:ARG:NH2	1:C:362:ASN:OD1	2.19	0.75
1:E:1409:GLY:HA3	1:E:1427:GLY:H	1.52	0.74
1:E:1485:GLY:HA3	1:E:1494:PHE:H	1.52	0.74
1:C:1370:ILE:HA	1:C:1374:GLN:HG3	1.67	0.74
1:C:2515:THR:H	1:C:2516:ASP:HB2	1.52	0.74
1:E:1500:SER:OG	1:E:1501:GLY:N	2.20	0.74
1:E:404:ILE:HD13	1:E:414:LYS:HD2	1.69	0.74
1:E:135:ALA:HB2	1:E:957:GLU:HB2	1.70	0.73
1:D:1150:VAL:HG12	1:D:1152:PRO:HD3	1.69	0.73
1:C:1612:TYR:HB3	1:C:1654:LEU:HD22	1.71	0.73
1:A:1150:VAL:HG12	1:A:1152:PRO:HD3	1.71	0.73
1:E:360:ARG:NH2	1:E:362:ASN:OD1	2.21	0.73
1:A:1500:SER:OG	1:A:1501:GLY:N	2.22	0.72
1:A:415:ILE:O	1:A:416:TYR:HD1	1.73	0.72
1:C:1370:ILE:HG12	1:C:1374:GLN:HE21	1.54	0.72
1:A:1744:TYR:HB2	1:A:1766:GLN:HG2	1.72	0.71
1:D:1612:TYR:HB3	1:D:1654:LEU:HD22	1.71	0.71
1:B:1409:GLY:HA3	1:B:1427:GLY:H	1.54	0.71
1:D:415:ILE:HD13	1:D:434:PHE:HE2	1.55	0.71
1:D:551:GLU:HG2	1:D:552:GLN:HG2	1.73	0.71
1:D:433:ILE:HD11	1:D:539:ALA:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:VAL:HG23	1:C:391:ILE:HA	1.73	0.70
1:D:360:ARG:NH2	1:D:362:ASN:OD1	2.23	0.70
1:C:1319:LEU:HD22	1:C:1588:LEU:HD13	1.72	0.70
1:E:415:ILE:O	1:E:416:TYR:CD1	2.40	0.70
1:E:1150:VAL:HG12	1:E:1152:PRO:HD3	1.71	0.70
1:E:1440:LEU:HB2	1:E:1452:PHE:HB2	1.73	0.70
1:C:1333:MSE:HE2	1:C:1584:ILE:HD12	1.72	0.70
1:D:1437:ARG:HB2	1:D:1486:ALA:HB1	1.72	0.70
1:A:1319:LEU:HD22	1:A:1588:LEU:HD13	1.71	0.70
1:D:1500:SER:OG	1:D:1501:GLY:N	2.25	0.69
1:B:1804:GLU:HA	1:B:1808:TYR:HB2	1.74	0.69
1:A:1255:PHE:HB3	1:A:1281:LEU:HG	1.73	0.69
1:A:2515:THR:N	1:A:2516:ASP:HB2	2.08	0.69
1:A:714:LEU:HD22	1:A:719:MSE:HG2	1.75	0.69
1:A:135:ALA:HB2	1:A:957:GLU:HB2	1.73	0.68
1:A:1689:THR:O	1:A:1724:ARG:NH2	2.25	0.68
1:B:415:ILE:O	1:B:416:TYR:HD1	1.75	0.68
1:D:1485:GLY:HA2	1:D:1494:PHE:H	1.58	0.68
1:B:504:GLN:O	1:B:507:ASN:ND2	2.27	0.67
1:B:1744:TYR:HB2	1:B:1766:GLN:HG2	1.75	0.67
1:E:1612:TYR:HB3	1:E:1654:LEU:HD22	1.76	0.67
1:A:2046:SER:HB2	1:A:2053:MSE:HE3	1.77	0.67
1:E:1621:ARG:NH2	1:E:1652:PRO:O	2.27	0.67
1:C:714:LEU:HD22	1:C:719:MSE:HG2	1.76	0.67
1:B:1621:ARG:NH2	1:B:1652:PRO:O	2.28	0.67
1:A:1485:GLY:HA3	1:A:1494:PHE:H	1.60	0.66
1:C:1683:GLY:HA3	1:C:1724:ARG:HB2	1.77	0.66
1:E:687:ILE:HD11	1:E:741:MSE:HG2	1.77	0.66
1:B:1331:THR:HG21	1:B:1581:LEU:HD22	1.76	0.66
1:D:1319:LEU:HD22	1:D:1588:LEU:HD13	1.77	0.66
1:A:83:ILE:HG12	1:A:1880:MSE:HE1	1.78	0.66
1:B:192:ARG:HG2	1:B:249:ILE:HD11	1.77	0.66
1:E:1426:GLN:HB3	1:E:1462:LEU:HD22	1.77	0.66
1:B:1626:LEU:HD13	1:B:1792:MSE:HE1	1.76	0.66
1:A:1130:MSE:HE3	1:A:1133:GLY:HA2	1.77	0.66
1:B:242:ILE:HA	1:B:246:LEU:HD23	1.78	0.66
1:B:1683:GLY:HA3	1:B:1724:ARG:HB2	1.76	0.66
1:E:1506:ASP:HB3	1:E:1577:ASP:HB2	1.78	0.66
1:A:1373:LYS:HD3	1:A:1412:ILE:HG13	1.79	0.65
1:A:360:ARG:NH2	1:A:362:ASN:OD1	2.29	0.65
1:A:343:ASN:HA	1:A:363:PHE:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ILE:HG12	1:E:431:GLY:HA3	1.76	0.65
1:B:229:GLN:O	1:B:897:ARG:NH2	2.30	0.65
1:C:540:ASP:OD2	1:C:542:ASN:HB2	1.97	0.65
1:D:603:LEU:HD11	1:D:640:VAL:HG22	1.77	0.65
1:D:1795:ASN:O	1:D:1795:ASN:ND2	2.29	0.65
1:A:1684:ASN:HB3	1:A:1719:MSE:HB2	1.78	0.65
1:B:360:ARG:NH2	1:B:362:ASN:OD1	2.30	0.65
1:B:2515:THR:N	1:B:2516:ASP:HB2	2.12	0.65
1:E:343:ASN:HA	1:E:363:PHE:HB2	1.79	0.65
1:A:1804:GLU:HA	1:A:1808:TYR:HB2	1.79	0.65
1:D:1458:PRO:HD2	1:D:1461:ILE:HG21	1.79	0.64
1:E:1319:LEU:HD22	1:E:1588:LEU:HD13	1.79	0.64
1:B:2400:SER:O	1:B:2416:ARG:NH2	2.31	0.64
1:B:346:TYR:HE1	1:B:359:ILE:HG22	1.62	0.64
1:A:1506:ASP:HB3	1:A:1577:ASP:HB2	1.80	0.64
1:C:603:LEU:HD11	1:C:640:VAL:HG22	1.80	0.64
1:D:1304:LYS:HG2	1:D:1602:PHE:HB3	1.79	0.64
1:D:1440:LEU:HB2	1:D:1452:PHE:HB2	1.80	0.64
1:D:2515:THR:N	1:D:2516:ASP:HB2	2.13	0.64
1:D:1689:THR:O	1:D:1724:ARG:NH2	2.31	0.64
1:A:415:ILE:HD13	1:A:434:PHE:HE2	1.63	0.63
1:E:2515:THR:N	1:E:2516:ASP:HB2	2.11	0.63
1:D:221:SER:OG	1:D:495:ARG:NH2	2.32	0.63
1:D:1238:GLU:OE2	1:D:1283:ARG:NH2	2.24	0.63
1:A:603:LEU:HD11	1:A:640:VAL:HG22	1.79	0.63
1:A:1683:GLY:HA3	1:A:1724:ARG:HB2	1.80	0.63
1:D:1365:GLY:H	1:D:1371:ARG:HD3	1.63	0.63
1:A:365:VAL:HG23	1:A:391:ILE:HA	1.80	0.63
1:B:1689:THR:O	1:B:1724:ARG:NH2	2.31	0.63
1:C:2046:SER:HB2	1:C:2053:MSE:HE3	1.81	0.63
1:E:346:TYR:HE1	1:E:359:ILE:HG22	1.63	0.63
1:E:1304:LYS:HG2	1:E:1602:PHE:HB3	1.81	0.63
1:B:2050:PHE:HE1	1:B:2348:MSE:HE3	1.64	0.63
1:B:135:ALA:HB2	1:B:957:GLU:HB2	1.81	0.63
1:C:1035:ARG:NH2	1:C:1982:GLU:OE2	2.31	0.63
1:D:1683:GLY:HA3	1:D:1724:ARG:HB2	1.79	0.63
1:B:1304:LYS:HG2	1:B:1602:PHE:HB3	1.81	0.62
1:C:343:ASN:HA	1:C:363:PHE:HB2	1.81	0.62
1:C:2515:THR:HB	1:C:2516:ASP:HB2	1.80	0.62
1:A:242:ILE:HA	1:A:246:LEU:HD23	1.81	0.62
1:A:540:ASP:OD2	1:A:542:ASN:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ILE:HG12	1:A:431:GLY:HA3	1.82	0.62
1:A:1304:LYS:HG2	1:A:1602:PHE:HB3	1.82	0.62
1:B:415:ILE:HG12	1:B:431:GLY:HA3	1.82	0.62
1:D:1437:ARG:HG3	1:D:1455:PRO:HA	1.81	0.62
1:A:85:ARG:NH1	1:A:93:ASP:OD2	2.28	0.62
1:B:603:LEU:HD11	1:B:640:VAL:HG22	1.80	0.62
1:B:1426:GLN:HB3	1:B:1462:LEU:HD22	1.80	0.62
1:E:1626:LEU:HD13	1:E:1792:MSE:HE1	1.82	0.62
1:B:1373:LYS:HB3	1:B:1412:ILE:HG21	1.82	0.61
1:D:1405:TYR:OH	1:D:1492:GLN:OE1	2.18	0.61
1:E:221:SER:OG	1:E:495:ARG:NH2	2.32	0.61
1:C:687:ILE:HD11	1:C:741:MSE:HG2	1.83	0.61
1:D:1610:ALA:HB2	1:D:1652:PRO:HG2	1.82	0.61
1:D:2390:LEU:HD12	1:D:2523:GLU:HG2	1.82	0.61
1:C:1744:TYR:HB2	1:C:1766:GLN:HG2	1.82	0.61
1:D:192:ARG:HG2	1:D:249:ILE:HD11	1.83	0.61
1:D:2400:SER:O	1:D:2416:ARG:NH2	2.34	0.61
1:E:11:ILE:HD11	1:E:41:LEU:HD11	1.83	0.61
1:B:530:PRO:O	1:B:562:ARG:NH2	2.25	0.61
1:B:1970:ARG:NH1	1:C:1433:ASP:OD1	2.33	0.61
1:D:365:VAL:HG23	1:D:391:ILE:HA	1.80	0.60
1:A:433:ILE:HD11	1:A:539:ALA:HB2	1.83	0.60
1:B:540:ASP:OD2	1:B:542:ASN:HB2	2.01	0.60
1:B:2178:LEU:HD21	1:C:2178:LEU:HD22	1.82	0.60
1:C:2400:SER:O	1:C:2416:ARG:NH2	2.35	0.60
1:B:343:ASN:HA	1:B:363:PHE:HB2	1.83	0.60
1:C:2136:GLU:OE2	1:D:2218:ARG:NH1	2.34	0.60
1:D:95:MSE:O	1:D:1971:THR:OG1	2.16	0.60
1:A:901:ALA:O	1:A:902:LEU:HB2	2.02	0.60
1:B:1319:LEU:HD22	1:B:1588:LEU:HD13	1.83	0.60
1:B:1673:GLY:HA3	1:B:1731:LYS:HE2	1.84	0.60
1:D:226:VAL:HG21	1:D:879:VAL:HG11	1.83	0.60
1:B:226:VAL:HG21	1:B:879:VAL:HG11	1.83	0.60
1:B:1555:ALA:HB1	1:B:1558:LEU:HD11	1.84	0.60
1:C:95:MSE:O	1:C:1971:THR:OG1	2.19	0.60
1:E:365:VAL:HG23	1:E:391:ILE:HA	1.82	0.60
1:A:680:LEU:HD22	1:A:744:VAL:HG22	1.84	0.60
1:D:2104:ARG:NH1	1:E:2249:GLU:OE2	2.35	0.60
1:C:226:VAL:HG21	1:C:879:VAL:HG11	1.84	0.60
1:B:2390:LEU:HD12	1:B:2523:GLU:HG2	1.84	0.59
1:D:955:GLN:NE2	1:D:1498:GLN:OE1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1409:GLY:HA3	1:C:1427:GLY:H	1.67	0.59
1:C:2453:ILE:HG12	1:C:2521:LEU:HD21	1.85	0.59
1:E:95:MSE:O	1:E:1971:THR:OG1	2.18	0.59
1:C:415:ILE:O	1:C:416:TYR:HD1	1.85	0.59
1:C:247:TYR:CZ	1:C:898:TYR:HB3	2.38	0.59
1:E:2390:LEU:HD12	1:E:2523:GLU:HG2	1.85	0.59
1:A:1365:GLY:H	1:A:1371:ARG:HD3	1.68	0.59
1:B:365:VAL:HG23	1:B:391:ILE:HA	1.84	0.59
1:C:2390:LEU:HD12	1:C:2523:GLU:HG2	1.84	0.59
1:A:1970:ARG:NH1	1:B:1433:ASP:OD1	2.35	0.59
1:C:2515:THR:N	1:C:2516:ASP:HB2	2.18	0.59
1:E:1369:VAL:HG11	1:E:1399:VAL:HB	1.85	0.59
1:B:2515:THR:H	1:B:2516:ASP:CB	2.15	0.59
1:B:901:ALA:O	1:B:902:LEU:HB2	2.03	0.59
1:B:95:MSE:O	1:B:1971:THR:OG1	2.18	0.58
1:B:1500:SER:OG	1:B:1501:GLY:N	2.36	0.58
1:D:1369:VAL:HG11	1:D:1399:VAL:HB	1.85	0.58
1:B:1302:VAL:HG12	1:B:1604:ARG:HG2	1.85	0.58
1:E:229:GLN:O	1:E:897:ARG:NH2	2.36	0.58
1:E:236:LEU:HB2	1:E:487:PHE:HB2	1.85	0.58
1:E:1804:GLU:HA	1:E:1808:TYR:HB2	1.85	0.58
1:A:2253:MSE:HE1	1:E:2100:ARG:HB3	1.85	0.58
1:C:1804:GLU:HA	1:C:1808:TYR:HB2	1.84	0.58
1:E:1689:THR:O	1:E:1724:ARG:NH2	2.37	0.58
1:B:2515:THR:HB	1:B:2516:ASP:HB2	1.85	0.58
1:E:1255:PHE:HB3	1:E:1281:LEU:HG	1.85	0.58
1:D:350:MSE:HE2	1:D:359:ILE:HD12	1.84	0.58
1:D:2515:THR:H	1:D:2516:ASP:CB	2.17	0.58
1:D:2515:THR:HB	1:D:2516:ASP:HB2	1.85	0.58
1:E:242:ILE:HA	1:E:246:LEU:HD23	1.85	0.58
1:A:1409:GLY:HA3	1:A:1427:GLY:H	1.69	0.58
1:B:1321:MSE:HB3	1:B:1584:ILE:HG21	1.85	0.58
1:A:346:TYR:HE1	1:A:359:ILE:HG22	1.69	0.58
1:E:1972:ALA:O	1:E:1975:LEU:N	2.34	0.58
1:C:2044:THR:HB	1:C:2306:MSE:HE3	1.86	0.58
1:C:415:ILE:HG12	1:C:431:GLY:HA3	1.85	0.58
1:A:2299:LEU:HD22	1:E:2350:LYS:HD2	1.86	0.57
1:B:1483:VAL:HG13	1:B:1493:ILE:HG23	1.86	0.57
1:D:343:ASN:HA	1:D:363:PHE:HB2	1.86	0.57
1:A:1250:LYS:HD3	1:A:1296:THR:HG22	1.86	0.57
1:B:956:PRO:HG2	1:B:959:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2350:LYS:HD2	1:C:2299:LEU:HD22	1.85	0.57
1:E:307:SER:O	1:E:309:SER:N	2.38	0.57
1:A:956:PRO:HG2	1:A:959:VAL:HB	1.86	0.57
1:C:2411:ILE:HG22	1:C:2511:PHE:HB2	1.86	0.57
1:D:1145:LYS:NZ	1:D:1147:ASP:OD1	2.37	0.57
1:D:2350:LYS:HD2	1:E:2299:LEU:HD22	1.85	0.57
1:E:735:LEU:HD11	1:E:743:LEU:HD12	1.86	0.57
1:C:851:MSE:HE3	1:C:887:PRO:HD3	1.86	0.57
1:B:209:VAL:HG22	1:B:926:LEU:HD11	1.86	0.57
1:B:680:LEU:HD11	1:B:757:LEU:HD21	1.87	0.57
1:B:1441:THR:HB	1:B:1450:ARG:HA	1.86	0.57
1:E:136:TYR:OH	1:E:1400:LYS:NZ	2.34	0.57
1:E:1302:VAL:HG12	1:E:1604:ARG:HG2	1.86	0.57
1:A:2249:GLU:O	1:A:2253:MSE:HG3	2.04	0.57
1:B:11:ILE:HD11	1:B:41:LEU:HD11	1.85	0.57
1:B:1703:SER:HB3	1:C:1379:LYS:HE2	1.85	0.57
1:E:2515:THR:HB	1:E:2516:ASP:HB2	1.87	0.57
1:C:1626:LEU:HD13	1:C:1792:MSE:HE1	1.86	0.57
1:D:1457:SER:HB2	1:D:1458:PRO:HD3	1.86	0.57
1:D:901:ALA:O	1:D:902:LEU:HB2	2.03	0.57
1:A:95:MSE:O	1:A:1971:THR:OG1	2.21	0.56
1:D:680:LEU:HD11	1:D:757:LEU:HD21	1.86	0.56
1:E:209:VAL:HG22	1:E:926:LEU:HD11	1.87	0.56
1:E:714:LEU:HD22	1:E:719:MSE:HG2	1.86	0.56
1:E:1683:GLY:HA3	1:E:1724:ARG:HB2	1.87	0.56
1:B:83:ILE:HG12	1:B:1880:MSE:HE1	1.87	0.56
1:C:313:ASP:OD1	1:C:334:ARG:NH2	2.37	0.56
1:C:920:GLU:OE1	1:D:533:LYS:NZ	2.37	0.56
1:D:26:GLN:N	1:D:27:TYR:HB3	2.20	0.56
1:C:95:MSE:HE3	1:C:1956:ASP:HB3	1.87	0.56
1:E:901:ALA:O	1:E:902:LEU:HB2	2.04	0.56
1:A:1145:LYS:NZ	1:A:1147:ASP:OD1	2.35	0.56
1:B:307:SER:O	1:B:309:SER:N	2.38	0.56
1:B:1340:GLN:HB2	1:B:1355:HIS:HB2	1.87	0.56
1:B:358:PHE:HB2	1:B:398:SER:HB3	1.87	0.56
1:C:901:ALA:O	1:C:902:LEU:HB2	2.04	0.56
1:D:1413:THR:HG21	1:D:1440:LEU:HD11	1.87	0.56
1:E:2515:THR:H	1:E:2516:ASP:CB	2.17	0.56
1:C:307:SER:O	1:C:309:SER:N	2.39	0.56
1:A:680:LEU:HD11	1:A:757:LEU:HD21	1.88	0.56
1:C:433:ILE:HD11	1:C:539:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2282:TYR:O	1:D:2286:ARG:HG2	2.06	0.56
1:E:546:ILE:HD11	1:E:581:LEU:HD21	1.86	0.56
1:D:358:PHE:HB2	1:D:398:SER:HB3	1.88	0.56
1:D:1621:ARG:NH2	1:D:1652:PRO:O	2.39	0.56
1:D:180:ASP:OD1	1:D:181:SER:N	2.39	0.56
1:D:242:ILE:HA	1:D:246:LEU:HD23	1.87	0.56
1:D:714:LEU:HD22	1:D:719:MSE:HG2	1.88	0.56
1:E:347:PHE:CZ	1:E:360:ARG:HD2	2.39	0.56
1:C:1621:ARG:NH2	1:C:1652:PRO:O	2.38	0.55
1:D:1636:THR:HG22	1:D:1637:GLY:H	1.72	0.55
1:C:1293:ILE:HG13	1:C:1302:VAL:HG23	1.88	0.55
1:C:1972:ALA:O	1:C:1975:LEU:N	2.36	0.55
1:C:2249:GLU:O	1:C:2253:MSE:HG3	2.05	0.55
1:D:687:ILE:HG23	1:D:745:LEU:HD21	1.88	0.55
1:D:2437:LYS:HE2	1:D:2494:LEU:HD12	1.88	0.55
1:E:409:TYR:CE1	1:E:414:LYS:HD3	2.42	0.55
1:E:415:ILE:HG12	1:E:431:GLY:CA	2.36	0.55
1:A:735:LEU:HD11	1:A:743:LEU:HD12	1.88	0.55
1:A:1636:THR:HG22	1:A:1637:GLY:H	1.71	0.55
1:A:2390:LEU:HD12	1:A:2523:GLU:HG2	1.86	0.55
1:B:1255:PHE:HB3	1:B:1281:LEU:HG	1.87	0.55
1:C:735:LEU:HD11	1:C:743:LEU:HD12	1.88	0.55
1:B:1438:LEU:O	1:B:1453:GLU:HA	2.06	0.55
1:D:1394:ILE:HG23	1:D:1415:TYR:HB3	1.89	0.55
1:A:2400:SER:O	1:A:2416:ARG:NH2	2.39	0.55
1:C:530:PRO:O	1:C:562:ARG:NH2	2.29	0.55
1:C:1636:THR:HG22	1:C:1637:GLY:H	1.72	0.55
1:E:226:VAL:HG21	1:E:879:VAL:HG11	1.89	0.55
1:B:1293:ILE:HG13	1:B:1302:VAL:HG23	1.88	0.55
1:A:337:THR:HG22	1:A:338:ASP:OD2	2.07	0.55
1:C:346:TYR:HE1	1:C:359:ILE:HG22	1.72	0.55
1:D:1626:LEU:HD13	1:D:1792:MSE:HE1	1.89	0.55
1:D:209:VAL:HG22	1:D:926:LEU:HD11	1.88	0.55
1:C:192:ARG:HG2	1:C:249:ILE:HD11	1.88	0.55
1:E:2049:ARG:NH1	1:E:2490:ASP:O	2.39	0.55
1:C:11:ILE:HD11	1:C:41:LEU:HD11	1.88	0.54
1:D:1228:LEU:HD11	1:D:1245:VAL:HG13	1.89	0.54
1:A:561:MSE:HE3	1:A:567:ASN:HA	1.89	0.54
1:C:409:TYR:CE1	1:C:414:LYS:HD3	2.42	0.54
1:E:1238:GLU:OE2	1:E:1283:ARG:NH2	2.30	0.54
1:B:26:GLN:N	1:B:27:TYR:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ILE:HG21	1:B:432:GLY:N	2.22	0.54
1:C:1304:LYS:HG2	1:C:1602:PHE:HB3	1.89	0.54
1:D:200:HIS:CE1	1:D:202:PRO:HG2	2.42	0.54
1:C:1762:SER:HB2	1:C:1769:ILE:HD11	1.90	0.54
1:E:1662:PHE:HB2	1:E:1707:MSE:HE2	1.88	0.54
1:A:200:HIS:CE1	1:A:202:PRO:HG2	2.43	0.54
1:B:221:SER:OG	1:B:495:ARG:NH2	2.40	0.54
1:B:1130:MSE:HG3	1:B:1135:LEU:HD13	1.90	0.54
1:D:1673:GLY:HA3	1:D:1731:LYS:HE2	1.89	0.54
1:E:1250:LYS:HD3	1:E:1296:THR:HG22	1.90	0.54
1:A:1238:GLU:OE2	1:A:1283:ARG:NH2	2.25	0.54
1:B:556:ALA:HB1	1:B:589:LEU:HD11	1.90	0.54
1:B:1636:THR:HG22	1:B:1637:GLY:H	1.73	0.54
1:B:750:ASN:HB3	1:B:754:THR:HG22	1.89	0.54
1:E:200:HIS:CE1	1:E:202:PRO:HG2	2.43	0.54
1:C:221:SER:OG	1:C:495:ARG:NH2	2.41	0.54
1:A:226:VAL:HG21	1:A:879:VAL:HG11	1.90	0.53
1:A:247:TYR:CZ	1:A:898:TYR:HB3	2.43	0.53
1:B:247:TYR:OH	1:B:480:ASP:OD1	2.18	0.53
1:D:1399:VAL:HG12	1:D:1497:TYR:HD2	1.73	0.53
1:B:180:ASP:OD1	1:B:181:SER:N	2.41	0.53
1:B:2282:TYR:O	1:B:2286:ARG:HG2	2.07	0.53
1:C:1:MSE:HE3	1:C:1564:ILE:HG23	1.90	0.53
1:C:2515:THR:H	1:C:2516:ASP:CB	2.18	0.53
1:D:1409:GLY:HA3	1:D:1427:GLY:H	1.72	0.53
1:E:345:ASN:HB2	1:E:361:ALA:HB3	1.89	0.53
1:C:1601:LEU:HD23	1:C:1615:LEU:HB2	1.91	0.53
1:D:304:TYR:HB3	1:D:308:THR:HG21	1.90	0.53
1:E:2046:SER:HB2	1:E:2053:MSE:HE3	1.89	0.53
1:A:2030:MSE:HE1	1:B:2280:ALA:H	1.73	0.53
1:B:613:GLU:HA	1:B:616:MSE:HE3	1.91	0.53
1:D:1424:SER:O	1:D:1463:ASN:HA	2.09	0.53
1:E:315:ILE:HG22	1:E:332:ILE:HB	1.89	0.53
1:E:1413:THR:HG21	1:E:1440:LEU:HD11	1.90	0.53
1:B:433:ILE:HD11	1:B:539:ALA:HB2	1.91	0.53
1:B:714:LEU:HD22	1:B:719:MSE:HG2	1.91	0.53
1:E:1293:ILE:HG13	1:E:1302:VAL:HG23	1.90	0.53
1:E:247:TYR:OH	1:E:480:ASP:OD1	2.23	0.53
1:C:1673:GLY:HA3	1:C:1731:LYS:HE2	1.90	0.53
1:D:337:THR:HG22	1:D:338:ASP:OD2	2.09	0.53
1:D:409:TYR:CE1	1:D:414:LYS:HD3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:680:LEU:HD22	1:E:744:VAL:HG22	1.91	0.53
1:A:1293:ILE:HG13	1:A:1302:VAL:HG23	1.91	0.52
1:A:80:ARG:HA	1:A:83:ILE:HD12	1.91	0.52
1:B:247:TYR:CZ	1:B:898:TYR:HB3	2.44	0.52
1:B:347:PHE:CZ	1:B:360:ARG:HD2	2.44	0.52
1:B:2178:LEU:HD11	1:C:2178:LEU:HD13	1.90	0.52
1:C:1458:PRO:HD2	1:C:1461:ILE:HG21	1.91	0.52
1:B:1972:ALA:O	1:B:1975:LEU:N	2.39	0.52
1:E:1368:ASN:HD21	1:E:1370:ILE:HB	1.74	0.52
1:B:406:ASP:HA	1:B:409:TYR:HD2	1.75	0.52
1:A:1394:ILE:HG23	1:A:1415:TYR:HB3	1.91	0.52
1:A:1555:ALA:HB1	1:A:1558:LEU:HD11	1.91	0.52
1:D:1972:ALA:O	1:D:1975:LEU:N	2.35	0.52
1:E:298:GLY:HA3	1:E:314:ASN:HB2	1.91	0.52
1:A:1252:TYR:O	1:A:1288:LYS:NZ	2.35	0.52
1:B:1485:GLY:CA	1:B:1494:PHE:H	2.23	0.52
1:A:1485:GLY:HA2	1:A:1494:PHE:CD2	2.45	0.52
1:B:409:TYR:CE1	1:B:414:LYS:HD3	2.44	0.52
1:B:1316:PRO:HG2	1:B:1588:LEU:HD11	1.92	0.52
1:C:242:ILE:HA	1:C:246:LEU:HD23	1.92	0.52
1:C:415:ILE:HG21	1:C:432:GLY:N	2.24	0.52
1:E:603:LEU:HD11	1:E:640:VAL:HG22	1.91	0.52
1:A:958:GLY:O	1:A:1400:LYS:NZ	2.38	0.52
1:A:1610:ALA:HB2	1:A:1652:PRO:HG2	1.91	0.52
1:C:1440:LEU:HB2	1:C:1452:PHE:HB2	1.92	0.52
1:D:1804:GLU:HA	1:D:1808:TYR:HB2	1.91	0.52
1:E:851:MSE:HE3	1:E:887:PRO:HD3	1.92	0.52
1:A:1321:MSE:HB3	1:A:1584:ILE:HG21	1.90	0.52
1:A:1487:ASN:HB2	1:A:1492:GLN:HB2	1.91	0.52
1:C:83:ILE:HG12	1:C:1880:MSE:HE1	1.92	0.52
1:D:1438:LEU:O	1:D:1453:GLU:HA	2.10	0.52
1:C:200:HIS:CE1	1:C:202:PRO:HG2	2.45	0.52
1:D:1293:ILE:HG13	1:D:1302:VAL:HG23	1.91	0.52
1:D:1340:GLN:HB2	1:D:1355:HIS:HB2	1.92	0.52
1:E:1321:MSE:HB3	1:E:1584:ILE:HG21	1.91	0.52
1:E:1368:ASN:ND2	1:E:1370:ILE:HB	2.24	0.52
1:A:11:ILE:HD11	1:A:41:LEU:HD11	1.92	0.51
1:B:2086:LEU:HD22	1:C:2271:LEU:HD13	1.91	0.51
1:C:546:ILE:HD11	1:C:581:LEU:HD21	1.91	0.51
1:D:1384:ASP:OD1	1:D:1385:GLY:N	2.44	0.51
1:D:1489:GLN:OE1	1:D:1489:GLN:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1480:SER:OG	1:A:1481:TYR:N	2.43	0.51
1:C:288:LEU:HD21	1:C:456:LEU:HD21	1.92	0.51
1:C:2048:TYR:HB2	1:C:2053:MSE:HE2	1.91	0.51
1:A:1972:ALA:O	1:A:1975:LEU:N	2.38	0.51
1:A:2351:VAL:HG22	1:A:2355:ARG:HD3	1.93	0.51
1:B:2411:ILE:HG22	1:B:2511:PHE:HB2	1.92	0.51
1:A:345:ASN:HB2	1:A:361:ALA:HB3	1.92	0.51
1:B:169:LEU:O	1:B:173:ILE:HG12	2.11	0.51
1:B:2402:ASN:ND2	1:B:2419:ASP:OD2	2.42	0.51
1:A:26:GLN:N	1:A:27:TYR:HB3	2.25	0.51
1:A:1621:ARG:HB2	1:A:1654:LEU:HD11	1.92	0.51
1:A:1703:SER:HB3	1:B:1379:LYS:HE2	1.93	0.51
1:C:169:LEU:O	1:C:173:ILE:HG12	2.11	0.51
1:C:697:ARG:NH1	1:C:728:ASP:OD2	2.35	0.51
1:C:1265:MSE:HE3	1:C:1273:PHE:CD2	2.46	0.51
1:E:1636:THR:HG22	1:E:1637:GLY:H	1.75	0.51
1:B:1684:ASN:HB3	1:B:1719:MSE:HB2	1.92	0.51
1:A:1370:ILE:HA	1:A:1374:GLN:HG3	1.92	0.51
1:A:2515:THR:HB	1:A:2516:ASP:HB2	1.92	0.51
1:C:1487:ASN:HB2	1:C:1492:GLN:HB2	1.92	0.51
1:D:899:VAL:O	1:D:900:THR:OG1	2.25	0.51
1:E:192:ARG:HG2	1:E:249:ILE:HD11	1.93	0.51
1:B:899:VAL:O	1:B:900:THR:OG1	2.28	0.51
1:C:1409:GLY:HA3	1:C:1427:GLY:N	2.26	0.51
1:D:2178:LEU:HD11	1:E:2178:LEU:HD13	1.92	0.51
1:E:374:ARG:NH2	1:E:403:ASN:O	2.40	0.51
1:E:1673:GLY:HA3	1:E:1731:LYS:HE2	1.92	0.51
1:C:899:VAL:O	1:C:900:THR:OG1	2.27	0.51
1:D:347:PHE:CZ	1:D:360:ARG:HD2	2.46	0.51
1:D:1321:MSE:HB3	1:D:1584:ILE:HG21	1.92	0.51
1:E:1381:THR:HB	1:E:1386:LYS:HA	1.93	0.51
1:E:1483:VAL:HG13	1:E:1493:ILE:HG23	1.93	0.51
1:E:180:ASP:OD1	1:E:181:SER:N	2.43	0.50
1:A:1621:ARG:NH2	1:A:1652:PRO:O	2.45	0.50
1:C:1333:MSE:HE1	1:C:1571:PHE:CB	2.42	0.50
1:D:735:LEU:HD11	1:D:743:LEU:HD12	1.93	0.50
1:E:247:TYR:CZ	1:E:898:TYR:HB3	2.47	0.50
1:E:613:GLU:HA	1:E:616:MSE:HE3	1.92	0.50
1:A:307:SER:O	1:A:309:SER:N	2.44	0.50
1:B:1409:GLY:HA3	1:B:1427:GLY:N	2.24	0.50
1:B:1485:GLY:HA3	1:B:1494:PHE:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ILE:HD13	1:C:434:PHE:HE2	1.75	0.50
1:C:680:LEU:HD22	1:C:744:VAL:HG22	1.93	0.50
1:B:80:ARG:HA	1:B:83:ILE:HD12	1.93	0.50
1:C:415:ILE:HG12	1:C:431:GLY:CA	2.41	0.50
1:C:556:ALA:HB1	1:C:589:LEU:HD11	1.94	0.50
1:D:1426:GLN:HB3	1:D:1462:LEU:HB3	1.93	0.50
1:B:415:ILE:HG12	1:B:431:GLY:CA	2.40	0.50
1:D:80:ARG:HA	1:D:83:ILE:HD12	1.94	0.50
1:D:680:LEU:HD22	1:D:744:VAL:HG22	1.94	0.50
1:D:1108:TRP:CE2	1:D:1161:ILE:HD11	2.47	0.50
1:E:2282:TYR:O	1:E:2286:ARG:HG2	2.12	0.50
1:A:344:ILE:HG12	1:A:360:ARG:HH21	1.77	0.50
1:A:1395:ILE:HG22	1:A:1414:VAL:HG22	1.94	0.50
1:A:1816:ARG:NH1	1:A:1819:GLN:OE1	2.44	0.50
1:D:415:ILE:O	1:D:416:TYR:HD1	1.95	0.50
1:D:1331:THR:HG21	1:D:1581:LEU:HD22	1.92	0.50
1:E:751:ALA:HB3	1:E:753:GLU:HG3	1.92	0.50
1:A:1612:TYR:HB3	1:A:1654:LEU:HG	1.94	0.50
1:C:270:ASN:O	1:C:1445:ASN:ND2	2.45	0.50
1:C:358:PHE:HB2	1:C:398:SER:OG	2.11	0.50
1:E:25:LEU:O	1:E:53:THR:HG21	2.12	0.50
1:E:751:ALA:O	1:E:754:THR:HG23	2.12	0.50
1:A:851:MSE:HE3	1:A:887:PRO:HD3	1.94	0.50
1:B:1429:LEU:HD23	1:B:1429:LEU:H	1.76	0.50
1:D:1424:SER:HB2	1:D:1438:LEU:HD11	1.94	0.50
1:E:26:GLN:N	1:E:27:TYR:HB3	2.26	0.50
1:B:735:LEU:HD11	1:B:743:LEU:HD12	1.93	0.49
1:D:956:PRO:HG2	1:D:959:VAL:HB	1.94	0.49
1:D:1255:PHE:HB3	1:D:1281:LEU:HG	1.92	0.49
1:D:2249:GLU:O	1:D:2253:MSE:HG3	2.11	0.49
1:E:540:ASP:OD2	1:E:542:ASN:HB2	2.12	0.49
1:D:337:THR:HG22	1:D:338:ASP:CG	2.32	0.49
1:C:26:GLN:N	1:C:27:TYR:HB3	2.27	0.49
1:C:1795:ASN:O	1:C:1795:ASN:ND2	2.39	0.49
1:A:816:TRP:HE1	1:A:845:MSE:SE	2.46	0.49
1:C:320:VAL:HA	1:C:327:LEU:HA	1.94	0.49
1:D:307:SER:O	1:D:309:SER:N	2.45	0.49
1:E:551:GLU:HG3	1:E:552:GLN:HG2	1.93	0.49
1:E:816:TRP:HE1	1:E:845:MSE:SE	2.44	0.49
1:A:1673:GLY:HA3	1:A:1731:LYS:HE2	1.94	0.49
1:A:1827:THR:OG1	1:A:1893:GLN:NE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:GLU:HA	1:C:616:MSE:HE3	1.94	0.49
1:C:1437:ARG:HB3	1:C:1455:PRO:HA	1.94	0.49
1:E:1340:GLN:HB2	1:E:1355:HIS:HB2	1.95	0.49
1:C:1849:ILE:HD11	1:D:1367:GLY:HA3	1.93	0.49
1:D:1409:GLY:HA3	1:D:1427:GLY:N	2.27	0.49
1:D:2386:LEU:HD21	1:D:2522:LEU:HB3	1.94	0.49
1:D:675:GLU:OE2	1:D:675:GLU:N	2.45	0.49
1:D:2050:PHE:HE1	1:D:2348:MSE:HE3	1.76	0.49
1:E:2411:ILE:HG22	1:E:2511:PHE:HB2	1.95	0.49
1:C:1250:LYS:HD3	1:C:1296:THR:HG22	1.94	0.49
1:C:1689:THR:O	1:C:1724:ARG:NH2	2.44	0.49
1:E:169:LEU:O	1:E:173:ILE:HG12	2.13	0.49
1:E:300:LEU:HA	1:E:316:SER:O	2.12	0.49
1:D:2390:LEU:HD11	1:D:2522:LEU:HB2	1.95	0.49
1:E:415:ILE:HG21	1:E:432:GLY:N	2.28	0.49
1:A:180:ASP:OD1	1:A:181:SER:N	2.46	0.49
1:A:1631:VAL:HG11	1:B:1165:ARG:HB3	1.94	0.49
1:A:2515:THR:H	1:A:2516:ASP:CB	2.16	0.49
1:B:25:LEU:O	1:B:53:THR:HG21	2.13	0.49
1:D:360:ARG:HD3	1:D:386:LEU:HD11	1.94	0.49
1:A:169:LEU:O	1:A:173:ILE:HG12	2.12	0.48
1:B:420:TYR:CD1	1:B:426:ALA:HB2	2.48	0.48
1:D:415:ILE:HG21	1:D:432:GLY:N	2.28	0.48
1:E:2386:LEU:HD21	1:E:2522:LEU:HB3	1.94	0.48
1:A:501:ASP:HB3	1:A:522:HIS:ND1	2.28	0.48
1:A:2282:TYR:O	1:A:2286:ARG:HG2	2.12	0.48
1:B:1426:GLN:NE2	1:B:1428:HIS:O	2.42	0.48
1:C:222:ARG:NH1	1:C:878:ASP:OD2	2.46	0.48
1:D:2281:LEU:HG	1:D:2285:MSE:HE2	1.95	0.48
1:E:1308:ARG:HD2	1:E:1314:GLU:OE2	2.13	0.48
1:C:1108:TRP:CE2	1:C:1161:ILE:HD11	2.49	0.48
1:E:2439:VAL:HG22	1:E:2532:ILE:HG22	1.94	0.48
1:C:1610:ALA:HB2	1:C:1652:PRO:HG2	1.95	0.48
1:E:1555:ALA:HB1	1:E:1558:LEU:HD11	1.96	0.48
1:A:304:TYR:HB3	1:A:308:THR:HG21	1.95	0.48
1:A:1438:LEU:O	1:A:1453:GLU:HA	2.12	0.48
1:B:337:THR:N	1:B:431:GLY:O	2.44	0.48
1:C:1375:ILE:HG22	1:C:1379:LYS:HD2	1.96	0.48
1:D:317:THR:HG22	1:D:330:TYR:CE2	2.49	0.48
1:D:2349:GLU:OE1	1:E:2056:ARG:NH1	2.46	0.48
1:A:1150:VAL:HG11	1:A:1157:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1302:VAL:HG12	1:C:1604:ARG:HG2	1.95	0.48
1:C:1633:ARG:HH12	1:C:1649:LEU:HD21	1.78	0.48
1:B:1167:HIS:CD2	1:B:1196:PHE:HB3	2.49	0.48
1:C:1145:LYS:NZ	1:C:1147:ASP:OD1	2.47	0.48
1:D:247:TYR:CZ	1:D:898:TYR:HB3	2.48	0.48
1:E:1960:LEU:HD12	1:E:1964:GLY:HA2	1.96	0.48
1:C:304:TYR:HB3	1:C:308:THR:HG21	1.94	0.48
1:C:684:ARG:NH1	1:C:744:VAL:O	2.46	0.48
1:D:1302:VAL:HG12	1:D:1604:ARG:HG2	1.95	0.48
1:D:1487:ASN:HD22	1:D:1492:GLN:HG3	1.79	0.48
1:A:415:ILE:HG21	1:A:432:GLY:N	2.29	0.48
1:C:1365:GLY:H	1:C:1371:ARG:HD3	1.79	0.48
1:E:1399:VAL:HG13	1:E:1498:GLN:O	2.14	0.48
1:A:1409:GLY:HA3	1:A:1427:GLY:N	2.28	0.47
1:C:80:ARG:HA	1:C:83:ILE:HD12	1.96	0.47
1:C:751:ALA:O	1:C:754:THR:HG23	2.15	0.47
1:A:1444:GLU:HB2	1:A:1481:TYR:CG	2.49	0.47
1:B:320:VAL:HA	1:B:327:LEU:HA	1.96	0.47
1:B:851:MSE:HE3	1:B:887:PRO:HD3	1.96	0.47
1:B:1384:ASP:OD1	1:B:1384:ASP:N	2.43	0.47
1:B:2231:ASP:OD2	1:B:2235:LYS:HE2	2.15	0.47
1:B:192:ARG:HD2	1:B:245:GLU:OE2	2.14	0.47
1:C:440:PRO:HG2	1:C:443:ILE:HD12	1.96	0.47
1:C:450:LYS:HB3	1:C:478:ILE:HD12	1.96	0.47
1:C:1399:VAL:HG12	1:C:1497:TYR:HD2	1.78	0.47
1:C:1714:ALA:HB3	1:C:1717:TYR:HB2	1.96	0.47
1:C:173:ILE:HD12	1:C:949:TRP:CE3	2.50	0.47
1:C:2360:LEU:HB2	1:C:2536:ILE:HB	1.96	0.47
1:D:1316:PRO:HG2	1:D:1588:LEU:HD11	1.96	0.47
1:E:406:ASP:HA	1:E:409:TYR:HD2	1.80	0.47
1:E:2454:ARG:HH22	1:E:2513:ASP:HB2	1.79	0.47
1:A:1184:VAL:HG21	1:C:2178:LEU:O	2.14	0.47
1:B:1056:MSE:HG3	1:B:1804:GLU:OE2	2.15	0.47
1:D:2196:MSE:HE2	1:D:2196:MSE:HA	1.95	0.47
1:B:1108:TRP:CE2	1:B:1161:ILE:HD11	2.50	0.47
1:C:337:THR:HG22	1:C:338:ASP:OD1	2.15	0.47
1:C:2178:LEU:HD11	1:D:2178:LEU:HD12	1.96	0.47
1:E:1252:TYR:O	1:E:1288:LYS:NZ	2.41	0.47
1:A:415:ILE:O	1:A:416:TYR:CD1	2.62	0.47
1:A:1070:ARG:O	1:A:1074:GLU:HG2	2.13	0.47
1:A:1108:TRP:CE2	1:A:1161:ILE:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:THR:HA	1:B:416:TYR:O	2.15	0.47
1:B:2386:LEU:HD21	1:B:2522:LEU:HB3	1.97	0.47
1:C:231:GLU:HG3	1:C:897:ARG:HB3	1.96	0.47
1:C:1483:VAL:HG22	1:C:1496:SER:HB3	1.96	0.47
1:D:1694:TYR:OH	1:D:1710:PHE:O	2.24	0.47
1:E:1416:ASN:HB3	1:E:1421:TYR:HB2	1.97	0.47
1:E:2074:MSE:SE	1:E:2285:MSE:HE3	2.65	0.47
1:C:1570:VAL:HG22	1:C:1585:LYS:HG2	1.96	0.47
1:D:415:ILE:HG12	1:D:431:GLY:HA3	1.96	0.47
1:E:1108:TRP:CE2	1:E:1161:ILE:HD11	2.49	0.47
1:E:1824:ASP:OD1	1:E:1897:ARG:NH2	2.48	0.47
1:E:1839:TYR:CE1	1:E:1851:ASN:HB2	2.50	0.47
1:A:1458:PRO:HD2	1:A:1461:ILE:HG21	1.97	0.47
1:A:1518:VAL:HG22	1:A:1525:HIS:HB2	1.97	0.47
1:C:1827:THR:OG1	1:C:1893:GLN:NE2	2.38	0.47
1:E:1534:ALA:HA	1:E:1549:LYS:HE3	1.97	0.47
1:B:1506:ASP:HB3	1:B:1577:ASP:HB2	1.97	0.47
1:C:1150:VAL:HG11	1:C:1157:ILE:HD12	1.96	0.47
1:E:2351:VAL:HG22	1:E:2355:ARG:HD3	1.97	0.47
1:A:1626:LEU:HD13	1:A:1792:MSE:HE1	1.97	0.46
1:C:2442:THR:HB	1:C:2529:ILE:HB	1.96	0.46
1:A:1399:VAL:HG13	1:A:1498:GLN:O	2.16	0.46
1:B:345:ASN:HB2	1:B:361:ALA:HB3	1.97	0.46
1:C:360:ARG:NH1	1:C:362:ASN:HD21	2.13	0.46
1:D:1250:LYS:HD3	1:D:1296:THR:HG22	1.98	0.46
1:D:1363:TYR:O	1:D:1371:ARG:NH1	2.48	0.46
1:E:142:ARG:HD2	1:E:971:PHE:O	2.15	0.46
1:A:2158:ALA:HB3	1:B:2196:MSE:HE2	1.96	0.46
1:C:1380:LEU:HD21	1:C:1463:ASN:HB3	1.98	0.46
1:A:142:ARG:HD2	1:A:971:PHE:O	2.15	0.46
1:B:1595:TYR:HA	1:B:1600:ILE:HD11	1.97	0.46
1:C:414:LYS:HB2	1:C:434:PHE:CD2	2.51	0.46
1:C:2282:TYR:O	1:C:2286:ARG:HG2	2.15	0.46
1:D:2219:ARG:HD3	1:D:2223:TRP:CH2	2.50	0.46
1:E:414:LYS:HB2	1:E:434:PHE:CD2	2.50	0.46
1:E:2400:SER:O	1:E:2416:ARG:NH2	2.48	0.46
1:A:313:ASP:OD1	1:A:334:ARG:NH2	2.44	0.46
1:C:209:VAL:HG22	1:C:926:LEU:HD11	1.97	0.46
1:C:551:GLU:HG3	1:C:552:GLN:HG2	1.97	0.46
1:C:1395:ILE:HG22	1:C:1414:VAL:HG22	1.97	0.46
1:C:1518:VAL:HG22	1:C:1525:HIS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1594:ASN:ND2	1:C:1599:ASP:OD2	2.39	0.46
1:E:173:ILE:HD12	1:E:949:TRP:CE3	2.50	0.46
1:B:2394:LYS:HE2	1:B:2394:LYS:HB2	1.75	0.46
1:C:1839:TYR:CE1	1:C:1851:ASN:HB2	2.50	0.46
1:D:750:ASN:HB3	1:D:754:THR:HG22	1.97	0.46
1:D:902:LEU:O	1:D:903:ASN:HB2	2.16	0.46
1:A:76:SER:N	1:A:77:GLY:HA3	2.29	0.46
1:A:1424:SER:O	1:A:1463:ASN:HA	2.16	0.46
1:A:1539:ASN:HA	1:A:1544:MSE:HE3	1.98	0.46
1:B:561:MSE:HE3	1:B:567:ASN:HA	1.98	0.46
1:D:415:ILE:HD13	1:D:434:PHE:CE2	2.44	0.46
1:D:1399:VAL:HG13	1:D:1498:GLN:O	2.16	0.46
1:D:2089:GLN:HG3	1:D:2269:LEU:HD11	1.98	0.46
1:A:556:ALA:HB1	1:A:589:LEU:HD11	1.98	0.46
1:A:2218:ARG:HH11	1:A:2221:GLN:HE22	1.64	0.46
1:B:816:TRP:HE1	1:B:845:MSE:SE	2.48	0.46
1:B:1123:ARG:HD2	1:B:1143:TRP:CE2	2.51	0.46
1:B:1250:LYS:HD3	1:B:1296:THR:HG22	1.98	0.46
1:B:1424:SER:O	1:B:1463:ASN:HA	2.16	0.46
1:C:349:LEU:HD11	1:C:356:GLN:HB3	1.98	0.46
1:C:1123:ARG:HD2	1:C:1143:TRP:CE2	2.51	0.46
1:C:1331:THR:HG21	1:C:1581:LEU:HD22	1.98	0.46
1:D:1483:VAL:HG13	1:D:1493:ILE:HG23	1.97	0.46
1:A:298:GLY:HA3	1:A:314:ASN:HB2	1.96	0.46
1:B:440:PRO:HG2	1:B:443:ILE:HD12	1.97	0.46
1:A:247:TYR:OH	1:A:480:ASP:OD1	2.31	0.46
1:B:1399:VAL:HG13	1:B:1498:GLN:O	2.15	0.46
1:C:298:GLY:HA3	1:C:314:ASN:HB2	1.97	0.46
1:D:1440:LEU:HB3	1:D:1479:CYS:SG	2.56	0.46
1:D:1760:HIS:HB2	1:D:1773:ILE:HB	1.97	0.46
1:D:2049:ARG:NH2	1:D:2497:GLU:OE2	2.49	0.46
1:E:1405:TYR:OH	1:E:1492:GLN:OE1	2.27	0.46
1:A:546:ILE:HD11	1:A:581:LEU:HD21	1.98	0.45
1:A:961:LEU:HD13	1:A:967:LEU:HD13	1.98	0.45
1:B:1380:LEU:HD11	1:B:1463:ASN:HB3	1.97	0.45
1:D:1252:TYR:HE2	1:D:1293:ILE:HG22	1.81	0.45
1:B:2430:LEU:HD11	1:C:2456:VAL:HG21	1.98	0.45
1:D:169:LEU:O	1:D:173:ILE:HG12	2.17	0.45
1:D:816:TRP:HE1	1:D:845:MSE:SE	2.49	0.45
1:E:1537:PRO:HG2	1:E:1544:MSE:HE2	1.99	0.45
1:A:358:PHE:HB2	1:A:398:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ILE:HG12	1:A:431:GLY:CA	2.45	0.45
1:A:1165:ARG:HB3	1:E:1631:VAL:HG11	1.97	0.45
1:A:1595:TYR:HA	1:A:1600:ILE:HD11	1.96	0.45
1:B:1416:ASN:HB3	1:B:1421:TYR:HB2	1.99	0.45
1:C:1922:GLU:HB3	1:D:1004:ILE:HD13	1.97	0.45
1:D:1256:GLY:HA2	1:D:1281:LEU:HD23	1.98	0.45
1:D:1265:MSE:HE3	1:D:1273:PHE:CD2	2.52	0.45
1:E:1757:ASP:OD1	1:E:1757:ASP:N	2.47	0.45
1:A:209:VAL:HG22	1:A:926:LEU:HD11	1.99	0.45
1:A:1123:ARG:HD2	1:A:1143:TRP:CE2	2.51	0.45
1:A:1601:LEU:HD23	1:A:1615:LEU:HB2	1.97	0.45
1:C:2014:LEU:HD23	1:C:2015:ALA:O	2.16	0.45
1:C:2219:ARG:HD3	1:C:2223:TRP:CH2	2.50	0.45
1:A:2048:TYR:HB2	1:A:2053:MSE:HE2	1.98	0.45
1:B:1381:THR:HB	1:B:1386:LYS:HA	1.98	0.45
1:C:2339:GLU:OE1	1:C:2339:GLU:N	2.45	0.45
1:E:2142:GLU:OE1	1:E:2219:ARG:NH2	2.50	0.45
1:A:25:LEU:O	1:A:53:THR:HG21	2.16	0.45
1:A:675:GLU:H	1:A:675:GLU:HG2	1.58	0.45
1:A:2178:LEU:HD11	1:B:2178:LEU:HD13	1.98	0.45
1:B:1446:ASN:HB3	1:B:1449:ALA:HB3	1.98	0.45
1:B:2368:LEU:HD23	1:B:2368:LEU:HA	1.79	0.45
1:D:403:ASN:O	1:D:404:ILE:HG13	2.16	0.45
1:D:2046:SER:HB2	1:D:2053:MSE:HE3	1.98	0.45
1:A:300:LEU:HA	1:A:316:SER:O	2.16	0.45
1:A:1177:ALA:HB3	1:B:2176:PHE:HB2	1.98	0.45
1:A:1731:LYS:N	1:A:1731:LYS:HD3	2.32	0.45
1:B:450:LYS:HB3	1:B:478:ILE:HD12	1.98	0.45
1:B:1601:LEU:HD23	1:B:1615:LEU:HB2	1.99	0.45
1:C:337:THR:N	1:C:431:GLY:O	2.43	0.45
1:D:11:ILE:HD11	1:D:41:LEU:HD11	1.98	0.45
1:D:197:THR:O	1:D:453:ARG:NH1	2.50	0.45
1:D:2394:LYS:HB2	1:D:2394:LYS:HE2	1.86	0.45
1:E:309:SER:OG	1:E:310:ALA:N	2.50	0.45
1:C:1255:PHE:HB3	1:C:1281:LEU:HG	1.98	0.45
1:D:1372:ASN:HB2	1:D:1373:LYS:HD2	1.99	0.45
1:A:91:SER:HB3	1:A:1960:LEU:HD11	1.99	0.45
1:A:1207:TRP:CD1	1:E:1116:ASN:HB2	2.52	0.45
1:B:1731:LYS:HD3	1:B:1731:LYS:N	2.31	0.45
1:C:92:TYR:HA	1:C:1960:LEU:HD21	1.99	0.45
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ASN:O	1:C:404:ILE:HG13	2.17	0.45
1:C:2402:ASN:ND2	1:C:2419:ASP:OD2	2.45	0.45
1:D:76:SER:N	1:D:77:GLY:HA3	2.30	0.45
1:D:546:ILE:HD11	1:D:581:LEU:HD21	1.99	0.45
1:E:2219:ARG:HD3	1:E:2223:TRP:CZ2	2.52	0.45
1:A:551:GLU:HG3	1:A:552:GLN:HG2	1.98	0.45
1:B:680:LEU:HD22	1:B:744:VAL:HG22	1.99	0.45
1:B:1117:LEU:HD12	1:B:1117:LEU:HA	1.90	0.45
1:C:1333:MSE:HE1	1:C:1571:PHE:HB3	1.98	0.45
1:D:603:LEU:HD12	1:D:603:LEU:HA	1.84	0.45
1:D:1364:ASP:OD2	1:D:1371:ARG:NE	2.50	0.45
1:D:1570:VAL:HG22	1:D:1585:LYS:HG2	1.99	0.45
1:E:576:LYS:HG2	1:E:581:LEU:HD12	1.99	0.45
1:E:687:ILE:HG23	1:E:745:LEU:HD21	1.99	0.45
1:E:1380:LEU:HD21	1:E:1463:ASN:HB3	1.99	0.45
1:A:1397:ASN:HB2	1:A:1503:LEU:HD13	1.98	0.44
1:B:319:LEU:HD12	1:B:319:LEU:HA	1.84	0.44
1:C:236:LEU:HB2	1:C:487:PHE:HB2	1.98	0.44
1:C:1410:GLY:HA3	1:C:1497:TYR:CE1	2.52	0.44
1:D:309:SER:OG	1:D:310:ALA:N	2.50	0.44
1:A:414:LYS:HE3	1:A:414:LYS:HB3	1.84	0.44
1:A:899:VAL:O	1:A:900:THR:OG1	2.29	0.44
1:A:1198:ARG:HH22	1:B:2161:VAL:HG21	1.81	0.44
1:C:300:LEU:HA	1:C:316:SER:O	2.17	0.44
1:C:1416:ASN:HB3	1:C:1421:TYR:HB2	1.98	0.44
1:D:530:PRO:O	1:D:562:ARG:NH2	2.31	0.44
1:D:687:ILE:HD11	1:D:741:MSE:HG2	1.99	0.44
1:D:1135:LEU:HD12	1:D:1135:LEU:HA	1.85	0.44
1:D:1395:ILE:HG22	1:D:1414:VAL:HG22	1.99	0.44
1:A:192:ARG:HG2	1:A:249:ILE:HD11	1.99	0.44
1:A:1960:LEU:HD12	1:A:1964:GLY:HA2	1.98	0.44
1:D:561:MSE:HE3	1:D:567:ASN:HA	2.00	0.44
1:E:135:ALA:HB3	1:E:959:VAL:HG23	2.00	0.44
1:C:1824:ASP:OD1	1:C:1897:ARG:NH2	2.50	0.44
1:D:49:LEU:HD12	1:D:49:LEU:HA	1.80	0.44
1:D:226:VAL:HG12	1:D:876:TRP:CE2	2.52	0.44
1:D:247:TYR:HE2	1:D:900:THR:H	1.64	0.44
1:E:216:THR:HG22	1:E:494:HIS:HD2	1.82	0.44
1:E:1035:ARG:NH2	1:E:1982:GLU:OE2	2.46	0.44
1:A:504:GLN:O	1:A:507:ASN:ND2	2.51	0.44
1:A:1402:TYR:HB2	1:A:1498:GLN:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2350:LYS:HD2	1:B:2299:LEU:HD22	1.99	0.44
1:C:820:LEU:HD22	1:C:844:VAL:HG12	1.99	0.44
1:D:1385:GLY:HA2	1:D:1386:LYS:HA	1.70	0.44
1:D:1431:ASN:HB3	1:D:1434:TYR:CD2	2.52	0.44
1:E:1146:ILE:HG22	1:E:1148:THR:HG22	2.00	0.44
1:A:1302:VAL:HG12	1:A:1604:ARG:HG2	2.00	0.44
1:C:415:ILE:HG21	1:C:432:GLY:H	1.83	0.44
1:C:1192:LEU:HB2	1:C:1211:ILE:HD13	2.00	0.44
1:D:783:VAL:HG13	1:D:832:ARG:HG3	2.00	0.44
1:E:367:ARG:HE	1:E:367:ARG:HB2	1.66	0.44
1:E:902:LEU:C	1:E:904:LYS:H	2.20	0.44
1:E:1319:LEU:HD11	1:E:1586:GLN:HG2	2.00	0.44
1:E:1409:GLY:HA3	1:E:1427:GLY:N	2.25	0.44
1:E:1959:MSE:SE	1:E:1965:VAL:HB	2.67	0.44
1:E:2070:SER:O	1:E:2074:MSE:HG3	2.18	0.44
1:A:349:LEU:HD11	1:A:356:GLN:HB3	1.99	0.44
1:A:409:TYR:CE1	1:A:414:LYS:HD3	2.53	0.44
1:A:1331:THR:HG21	1:A:1581:LEU:HA	2.00	0.44
1:A:2394:LYS:HB2	1:A:2394:LYS:HE2	1.77	0.44
1:B:1505:ILE:HG22	1:B:1579:ARG:HD3	1.98	0.44
1:C:1148:THR:HG23	1:C:1150:VAL:HG23	2.00	0.44
1:D:902:LEU:C	1:D:904:LYS:H	2.20	0.44
1:D:1167:HIS:CD2	1:D:1196:PHE:HB3	2.52	0.44
1:E:420:TYR:CD1	1:E:426:ALA:HB2	2.53	0.44
1:A:306:ASP:OD2	1:E:1974:SER:OG	2.27	0.44
1:A:420:TYR:CD1	1:A:426:ALA:HB2	2.53	0.44
1:B:304:TYR:HB3	1:B:308:THR:HG21	1.98	0.44
1:C:367:ARG:HE	1:C:367:ARG:HB2	1.70	0.44
1:C:404:ILE:HG23	1:C:408:GLU:HG3	2.00	0.44
1:C:1394:ILE:HG23	1:C:1415:TYR:HB3	2.00	0.44
1:E:405:SER:OG	1:E:408:GLU:HG2	2.17	0.44
1:A:1680:ILE:CD1	1:A:1707:MSE:HE1	2.47	0.44
1:A:2411:ILE:HG22	1:A:2511:PHE:HB2	1.98	0.44
1:B:546:ILE:HD11	1:B:581:LEU:HD21	1.99	0.44
1:B:577:LEU:HD12	1:B:615:CYS:SG	2.58	0.44
1:B:2454:ARG:O	1:B:2512:PRO:HD2	2.18	0.44
1:C:1462:LEU:HB2	1:C:1463:ASN:ND2	2.33	0.44
1:D:1447:TYR:O	1:D:1450:ARG:HD3	2.18	0.44
1:A:257:LYS:N	1:A:257:LYS:HD2	2.33	0.43
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.75	0.43
1:B:2439:VAL:HG22	1:B:2532:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1100:VAL:HB	1:C:1593:VAL:HG22	2.00	0.43
1:D:1441:THR:O	1:D:1481:TYR:HB2	2.18	0.43
1:E:899:VAL:O	1:E:900:THR:OG1	2.27	0.43
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.86	0.43
1:B:197:THR:O	1:B:453:ARG:NH1	2.51	0.43
1:B:415:ILE:O	1:B:416:TYR:CD1	2.63	0.43
1:B:1458:PRO:HD2	1:B:1461:ILE:HG21	2.00	0.43
1:B:2287:GLY:HA3	1:C:710:ALA:HB2	2.00	0.43
1:D:414:LYS:HE3	1:D:414:LYS:HB3	1.83	0.43
1:D:420:TYR:CD1	1:D:426:ALA:HB2	2.53	0.43
1:D:1714:ALA:HB3	1:D:1717:TYR:HB2	1.99	0.43
1:D:2231:ASP:OD2	1:D:2235:LYS:HE2	2.18	0.43
1:D:2454:ARG:HH22	1:D:2513:ASP:HB2	1.83	0.43
1:E:967:LEU:HD23	1:E:967:LEU:HA	1.82	0.43
1:A:1116:ASN:HB2	1:B:1207:TRP:CD1	2.53	0.43
1:A:2092:MSE:HE2	1:A:2092:MSE:HB3	1.97	0.43
1:B:226:VAL:HG12	1:B:876:TRP:CE2	2.53	0.43
1:B:415:ILE:HG21	1:B:432:GLY:H	1.84	0.43
1:B:1485:GLY:HA2	1:B:1494:PHE:CG	2.52	0.43
1:B:2515:THR:CA	1:B:2516:ASP:HB2	2.48	0.43
1:C:1388:GLN:HG2	1:C:1393:PHE:HZ	1.84	0.43
1:E:1167:HIS:CD2	1:E:1196:PHE:HB3	2.54	0.43
1:B:750:ASN:HB3	1:B:754:THR:CG2	2.49	0.43
1:B:1044:ILE:HD13	1:B:1871:PRO:HB2	2.00	0.43
1:C:347:PHE:CZ	1:C:360:ARG:HD2	2.53	0.43
1:C:1369:VAL:HG11	1:C:1399:VAL:HB	2.00	0.43
1:E:1424:SER:O	1:E:1463:ASN:HA	2.18	0.43
1:A:536:ILE:HD12	1:A:559:ALA:HB3	2.01	0.43
1:A:600:LEU:HD21	1:A:628:THR:HG21	2.00	0.43
1:A:1744:TYR:CE1	1:A:1753:VAL:HB	2.53	0.43
1:B:317:THR:HG22	1:B:330:TYR:CE2	2.53	0.43
1:B:347:PHE:CD1	1:B:415:ILE:HD11	2.53	0.43
1:B:1914:LYS:NZ	1:C:974:ASP:OD2	2.37	0.43
1:C:414:LYS:HB2	1:C:434:PHE:HD2	1.84	0.43
1:C:1438:LEU:O	1:C:1453:GLU:HA	2.17	0.43
1:C:2394:LYS:HB2	1:C:2394:LYS:HE2	1.71	0.43
1:D:136:TYR:OH	1:D:1400:LYS:HE2	2.18	0.43
1:D:300:LEU:HA	1:D:316:SER:O	2.17	0.43
1:E:26:GLN:NE2	1:E:57:LYS:HG3	2.33	0.43
1:A:195:ILE:HD13	1:A:286:TYR:HD1	1.84	0.43
1:A:1839:TYR:CE1	1:A:1851:ASN:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1481:TYR:HA	1:B:1497:TYR:O	2.19	0.43
1:D:1827:THR:OG1	1:D:1893:GLN:NE2	2.49	0.43
1:E:317:THR:HG22	1:E:330:TYR:CE2	2.53	0.43
1:E:360:ARG:NH1	1:E:362:ASN:HD21	2.17	0.43
1:E:1331:THR:HG21	1:E:1581:LEU:HD22	1.99	0.43
1:A:404:ILE:HD13	1:A:414:LYS:NZ	2.33	0.43
1:A:1167:HIS:CE1	1:A:1196:PHE:HB3	2.54	0.43
1:A:1570:VAL:HG22	1:A:1585:LYS:HG2	2.00	0.43
1:B:1391:ASN:HB3	1:B:1418:THR:OG1	2.17	0.43
1:B:2046:SER:HB3	1:B:2306:MSE:HE2	2.00	0.43
1:E:2219:ARG:HD3	1:E:2223:TRP:CH2	2.54	0.43
1:A:783:VAL:HG13	1:A:832:ARG:HG3	2.01	0.43
1:A:1192:LEU:HB2	1:A:1211:ILE:HD13	2.00	0.43
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.88	0.43
1:B:1633:ARG:HH12	1:B:1649:LEU:HD21	1.83	0.43
1:C:1595:TYR:HA	1:C:1600:ILE:HD11	1.99	0.43
1:C:1621:ARG:HB2	1:C:1654:LEU:HD21	2.00	0.43
1:C:2533:ARG:HB3	1:D:2484:PHE:CE1	2.54	0.43
1:D:506:LEU:HD12	1:D:506:LEU:HA	1.88	0.43
1:D:1731:LYS:HD3	1:D:1731:LYS:N	2.33	0.43
1:E:851:MSE:HE2	1:E:851:MSE:HB3	1.96	0.43
1:E:902:LEU:O	1:E:903:ASN:HB2	2.19	0.43
1:E:1395:ILE:HG22	1:E:1414:VAL:HG22	2.00	0.43
1:A:1701:ASP:OD1	1:A:1701:ASP:N	2.52	0.43
1:A:1922:GLU:HB3	1:B:1004:ILE:HD13	2.00	0.43
1:B:902:LEU:C	1:B:904:LYS:H	2.21	0.43
1:B:2352:TRP:O	1:B:2356:ASP:HB2	2.17	0.43
1:B:2361:GLU:OE1	1:C:2484:PHE:N	2.40	0.43
1:E:296:TYR:CZ	1:E:462:PRO:HG3	2.54	0.43
1:E:1485:GLY:HA2	1:E:1494:PHE:CD2	2.53	0.43
1:A:135:ALA:HB3	1:A:959:VAL:HG23	2.00	0.43
1:A:221:SER:OG	1:A:495:ARG:NH2	2.50	0.43
1:A:1331:THR:HG21	1:A:1581:LEU:HD22	2.00	0.43
1:A:2515:THR:CA	1:A:2516:ASP:HB2	2.49	0.43
1:B:403:ASN:O	1:B:404:ILE:HG13	2.19	0.43
1:B:1350:LEU:HB3	1:B:1555:ALA:O	2.19	0.43
1:B:2368:LEU:HD21	1:B:2415:VAL:HG21	2.01	0.43
1:C:1156:ALA:HB3	1:C:1171:VAL:HG22	2.00	0.43
1:D:1117:LEU:HD12	1:D:1117:LEU:HA	1.85	0.43
1:E:313:ASP:OD1	1:E:334:ARG:NH2	2.47	0.43
1:E:603:LEU:HD12	1:E:603:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:VAL:HG11	1:A:556:ALA:HB3	2.01	0.42
1:A:687:ILE:HD11	1:A:741:MSE:HG2	2.01	0.42
1:B:1714:ALA:HB3	1:B:1717:TYR:HB2	2.01	0.42
1:C:180:ASP:OD1	1:C:181:SER:N	2.50	0.42
1:C:816:TRP:HE1	1:C:845:MSE:SE	2.52	0.42
1:C:902:LEU:C	1:C:904:LYS:H	2.22	0.42
1:D:871:ASN:O	1:D:875:GLN:HG3	2.20	0.42
1:D:1383:VAL:HG11	1:D:1467:THR:HB	2.01	0.42
1:E:581:LEU:HD23	1:E:581:LEU:HA	1.81	0.42
1:E:1362:ARG:HD3	1:E:1543:ALA:HB2	2.01	0.42
1:E:1969:LEU:H	1:E:1969:LEU:HD12	1.84	0.42
1:E:2515:THR:CA	1:E:2516:ASP:HB2	2.49	0.42
1:A:10:LYS:HE3	1:A:10:LYS:HB3	1.78	0.42
1:A:750:ASN:HB3	1:A:754:THR:HG22	2.01	0.42
1:A:902:LEU:C	1:A:904:LYS:H	2.22	0.42
1:A:1117:LEU:HD12	1:A:1117:LEU:HA	1.86	0.42
1:A:1326:GLY:HA3	1:A:1331:THR:HG23	2.01	0.42
1:A:1416:ASN:HB3	1:A:1421:TYR:HB2	1.99	0.42
1:B:2049:ARG:NH2	1:B:2497:GLU:OE2	2.52	0.42
1:C:2454:ARG:HH22	1:C:2513:ASP:HB2	1.84	0.42
1:C:2515:THR:CA	1:C:2516:ASP:HB2	2.49	0.42
1:E:1480:SER:OG	1:E:1481:TYR:N	2.51	0.42
1:E:2454:ARG:NH2	1:E:2513:ASP:HB2	2.35	0.42
1:A:1368:ASN:N	1:A:1368:ASN:OD1	2.52	0.42
1:C:345:ASN:HB2	1:C:361:ALA:HB3	2.01	0.42
1:E:205:THR:HG23	1:E:934:LEU:HD21	2.02	0.42
1:E:2241:LEU:O	1:E:2245:LYS:HG2	2.19	0.42
1:B:607:HIS:HB3	1:B:647:THR:HG21	2.02	0.42
1:B:1567:LEU:HB3	1:B:1588:LEU:HB3	2.00	0.42
1:B:1839:TYR:CE1	1:B:1851:ASN:HB2	2.55	0.42
1:B:1969:LEU:HD12	1:B:1969:LEU:H	1.84	0.42
1:B:2364:ARG:NH2	1:B:2420:LEU:O	2.53	0.42
1:C:2010:GLN:HG3	1:C:2011:PRO:HD2	2.00	0.42
1:C:2287:GLY:HA3	1:D:710:ALA:HB2	2.01	0.42
1:D:1365:GLY:N	1:D:1371:ARG:HD3	2.33	0.42
1:D:1368:ASN:N	1:D:1368:ASN:OD1	2.51	0.42
1:D:1667:TYR:HA	1:D:1699:LEU:HD23	2.00	0.42
1:E:270:ASN:O	1:E:1445:ASN:ND2	2.51	0.42
1:B:920:GLU:OE1	1:C:533:LYS:NZ	2.51	0.42
1:D:127:LYS:HB3	1:D:127:LYS:HE2	1.77	0.42
1:E:1053:THR:HG21	1:E:1055:MSE:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2104:ARG:HA	1:E:2104:ARG:HD3	1.83	0.42
1:B:298:GLY:HA3	1:B:314:ASN:HB2	2.01	0.42
1:E:1613:MSE:HB2	1:E:1622:LEU:HD11	2.02	0.42
1:A:1368:ASN:ND2	1:A:1370:ILE:HB	2.35	0.42
1:B:1757:ASP:OD1	1:B:1757:ASP:N	2.50	0.42
1:C:607:HIS:HB3	1:C:647:THR:HG21	2.01	0.42
1:C:1533:ILE:HD12	1:C:1533:ILE:HA	1.92	0.42
1:D:1383:VAL:HG12	1:D:1421:TYR:CZ	2.55	0.42
1:D:2515:THR:CA	1:D:2516:ASP:HB2	2.49	0.42
1:E:1610:ALA:HB2	1:E:1652:PRO:HG2	2.02	0.42
1:E:2010:GLN:HG3	1:E:2011:PRO:HD2	2.01	0.42
1:A:6:VAL:O	1:A:10:LYS:HG3	2.19	0.42
1:A:701:ALA:HB1	1:A:721:ARG:HG3	2.01	0.42
1:A:902:LEU:O	1:A:903:ASN:HB2	2.20	0.42
1:A:1228:LEU:HD11	1:A:1245:VAL:HG13	2.02	0.42
1:A:1437:ARG:HB3	1:A:1455:PRO:HA	2.00	0.42
1:A:1901:ALA:O	1:A:1909:ALA:HB1	2.19	0.42
1:B:1536:LEU:HD23	1:B:1536:LEU:HA	1.94	0.42
1:B:2368:LEU:HD12	1:B:2528:ILE:HB	2.02	0.42
1:C:142:ARG:HD2	1:C:971:PHE:O	2.20	0.42
1:C:321:VAL:O	1:C:321:VAL:HG13	2.20	0.42
1:C:2076:GLU:OE2	1:D:2282:TYR:OH	2.34	0.42
1:C:2437:LYS:HE2	1:C:2494:LEU:HD12	2.02	0.42
1:D:1176:VAL:HG13	1:E:2176:PHE:CZ	2.55	0.42
1:A:340:TYR:OH	1:A:346:TYR:HA	2.20	0.42
1:B:155:MSE:HB2	1:B:986:LEU:HD12	2.02	0.42
1:C:25:LEU:O	1:C:53:THR:HG21	2.20	0.42
1:E:337:THR:N	1:E:431:GLY:O	2.46	0.42
1:E:1081:LEU:HD23	1:E:1081:LEU:HA	1.93	0.42
1:A:226:VAL:HG12	1:A:876:TRP:CE2	2.55	0.42
1:A:920:GLU:OE1	1:B:533:LYS:NZ	2.52	0.42
1:B:683:LEU:HD21	1:B:704:LEU:HD22	2.02	0.42
1:C:251:THR:HB	1:C:900:THR:HG22	2.02	0.42
1:C:1756:ASN:OD1	1:C:1756:ASN:N	2.53	0.42
1:D:349:LEU:HD11	1:D:356:GLN:HB3	2.02	0.42
1:D:1116:ASN:HB2	1:E:1207:TRP:CD1	2.55	0.42
1:A:2219:ARG:HD3	1:A:2223:TRP:CH2	2.55	0.41
1:A:2434:ARG:HA	1:A:2535:THR:O	2.20	0.41
1:C:1373:LYS:HD3	1:C:1412:ILE:HG13	2.02	0.41
1:D:25:LEU:O	1:D:53:THR:HG21	2.19	0.41
1:D:959:VAL:HG21	1:D:970:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1723:VAL:O	1:E:1742:PHE:HA	2.20	0.41
1:B:350:MSE:HE2	1:B:359:ILE:HD12	2.01	0.41
1:B:1756:ASN:N	1:B:1756:ASN:OD1	2.54	0.41
1:C:2104:ARG:HD3	1:C:2104:ARG:HA	1.91	0.41
1:C:2515:THR:CB	1:C:2516:ASP:HB2	2.48	0.41
1:D:414:LYS:HB2	1:D:434:PHE:CD2	2.55	0.41
1:D:1444:GLU:C	1:D:1446:ASN:H	2.23	0.41
1:A:236:LEU:HB2	1:A:487:PHE:HB2	2.01	0.41
1:A:1046:PRO:HD3	1:A:1889:ARG:NH2	2.35	0.41
1:A:2050:PHE:HE1	1:A:2348:MSE:HE3	1.84	0.41
1:B:2010:GLN:HG3	1:B:2011:PRO:HD2	2.02	0.41
1:C:2175:VAL:HG23	1:C:2180:CYS:HA	2.02	0.41
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.84	0.41
1:D:851:MSE:HE3	1:D:887:PRO:HD3	2.02	0.41
1:D:1677:TRP:CZ3	1:D:1679:LYS:HG3	2.55	0.41
1:D:2439:VAL:HG22	1:D:2532:ILE:HG22	2.03	0.41
1:E:414:LYS:HE3	1:E:414:LYS:HB3	1.86	0.41
1:A:538:GLU:CD	1:A:591:VAL:HG13	2.40	0.41
1:A:1707:MSE:HE3	1:A:1707:MSE:HB2	1.89	0.41
1:A:2249:GLU:OE2	1:E:2104:ARG:NH1	2.53	0.41
1:B:300:LEU:HA	1:B:316:SER:O	2.20	0.41
1:B:1800:LEU:O	1:B:1804:GLU:HG3	2.20	0.41
1:C:683:LEU:HD11	1:C:704:LEU:HD23	2.03	0.41
1:E:1123:ARG:HD2	1:E:1143:TRP:CE2	2.55	0.41
1:E:1731:LYS:HD3	1:E:1731:LYS:N	2.36	0.41
1:E:1803:TRP:CZ2	1:E:1854:PRO:HB2	2.56	0.41
1:E:2175:VAL:HG23	1:E:2180:CYS:HA	2.02	0.41
1:B:902:LEU:O	1:B:903:ASN:HB2	2.21	0.41
1:B:2515:THR:O	1:B:2519:LYS:HD2	2.20	0.41
1:C:902:LEU:O	1:C:903:ASN:HB2	2.19	0.41
1:C:1198:ARG:HH22	1:D:2161:VAL:HG21	1.85	0.41
1:C:2074:MSE:SE	1:C:2285:MSE:HE3	2.71	0.41
1:C:2208:ASP:O	1:C:2212:ARG:HG3	2.21	0.41
1:D:249:ILE:O	1:D:450:LYS:HE2	2.21	0.41
1:D:577:LEU:HD23	1:D:600:LEU:HD13	2.03	0.41
1:E:239:LEU:HD23	1:E:239:LEU:HA	1.96	0.41
1:E:1148:THR:HG23	1:E:1150:VAL:HG23	2.01	0.41
1:A:194:ALA:HB3	1:A:197:THR:OG1	2.20	0.41
1:A:1350:LEU:HB3	1:A:1555:ALA:O	2.21	0.41
1:A:2126:ARG:NH2	1:A:2233:GLU:OE1	2.38	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1369:VAL:HG11	1:B:1399:VAL:HB	2.02	0.41
1:B:1610:ALA:HB2	1:B:1652:PRO:HG2	2.02	0.41
1:B:1723:VAL:O	1:B:1742:PHE:HA	2.20	0.41
1:C:506:LEU:HD12	1:C:506:LEU:HA	1.90	0.41
1:D:312:VAL:N	1:D:313:ASP:HA	2.36	0.41
1:D:415:ILE:HG12	1:D:431:GLY:CA	2.49	0.41
1:D:1662:PHE:HZ	1:D:1725:LEU:HD22	1.86	0.41
1:D:1703:SER:HB3	1:E:1379:LYS:HE2	2.01	0.41
1:A:173:ILE:HD12	1:A:949:TRP:CE3	2.55	0.41
1:A:2429:SER:O	1:A:2430:LEU:HB2	2.21	0.41
1:B:719:MSE:HE3	1:B:778:GLU:HA	2.02	0.41
1:C:1814:PHE:CD1	1:C:1830:ILE:HB	2.55	0.41
1:D:252:GLU:O	1:D:450:LYS:NZ	2.37	0.41
1:D:373:LEU:O	1:D:416:TYR:HB2	2.19	0.41
1:D:1485:GLY:CA	1:D:1494:PHE:H	2.31	0.41
1:E:229:GLN:NE2	1:E:891:ARG:HH22	2.18	0.41
1:A:1053:THR:HG21	1:A:1055:MSE:HE3	2.03	0.41
1:B:127:LYS:HB3	1:B:127:LYS:HE2	1.71	0.41
1:B:2429:SER:O	1:B:2430:LEU:HB2	2.20	0.41
1:C:226:VAL:HG12	1:C:876:TRP:CE2	2.55	0.41
1:C:312:VAL:N	1:C:313:ASP:HA	2.35	0.41
1:C:1176:VAL:HG13	1:D:2176:PHE:CE1	2.56	0.41
1:C:1316:PRO:HG2	1:C:1588:LEU:HD11	2.02	0.41
1:C:1392:ALA:H	1:C:1418:THR:HG23	1.85	0.41
1:C:1731:LYS:HD3	1:C:1731:LYS:N	2.35	0.41
1:D:1402:TYR:CE2	1:D:1481:TYR:HE1	2.39	0.41
1:D:1757:ASP:OD1	1:D:1757:ASP:N	2.51	0.41
1:D:2311:LEU:HD22	1:D:2348:MSE:HG2	2.02	0.41
1:A:1377:ALA:HA	1:A:1380:LEU:HD12	2.02	0.41
1:A:1381:THR:HG22	1:A:1386:LYS:HA	2.03	0.41
1:A:2393:GLY:O	1:A:2394:LYS:HD3	2.20	0.41
1:B:173:ILE:HD12	1:B:949:TRP:CE3	2.56	0.41
1:B:360:ARG:NH1	1:B:362:ASN:HD21	2.18	0.41
1:B:1150:VAL:HG11	1:B:1157:ILE:HD12	2.03	0.41
1:B:1400:LYS:O	1:B:1498:GLN:N	2.54	0.41
1:B:1421:TYR:CE1	1:B:1467:THR:HG22	2.56	0.41
1:B:2339:GLU:OE1	1:B:2339:GLU:N	2.48	0.41
1:C:296:TYR:CZ	1:C:462:PRO:HG3	2.56	0.41
1:C:1757:ASP:OD1	1:C:1757:ASP:N	2.46	0.41
1:C:2454:ARG:O	1:C:2512:PRO:HD2	2.21	0.41
1:D:27:TYR:CE1	1:D:1947:GLN:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.96	0.41
1:D:1371:ARG:HA	1:D:1375:ILE:HD13	2.03	0.41
1:D:2364:ARG:NH2	1:D:2420:LEU:O	2.54	0.41
1:D:2533:ARG:HB3	1:E:2484:PHE:CZ	2.56	0.41
1:E:155:MSE:HB2	1:E:986:LEU:HD12	2.03	0.41
1:E:257:LYS:HD2	1:E:257:LYS:N	2.35	0.41
1:E:358:PHE:HB2	1:E:398:SER:HB3	2.02	0.41
1:E:504:GLN:O	1:E:507:ASN:ND2	2.53	0.41
1:E:1316:PRO:HG2	1:E:1588:LEU:HD11	2.03	0.41
1:A:732:PRO:HB3	1:A:763:VAL:HG21	2.03	0.41
1:A:1316:PRO:HG2	1:A:1588:LEU:HD11	2.03	0.41
1:A:1970:ARG:H	1:A:1970:ARG:HG2	1.53	0.41
1:C:2057:THR:O	1:C:2061:VAL:HG23	2.21	0.41
1:C:2214:GLU:O	1:C:2218:ARG:HG2	2.21	0.41
1:C:2311:LEU:HD22	1:C:2348:MSE:HG2	2.03	0.41
1:D:302:ASN:HB3	1:D:1434:TYR:CE1	2.56	0.41
1:E:1150:VAL:HG11	1:E:1157:ILE:HD12	2.03	0.41
1:E:1424:SER:HB2	1:E:1438:LEU:HD11	2.02	0.41
1:E:1833:VAL:HG23	1:E:1852:CYS:HB2	2.03	0.41
1:A:440:PRO:HG2	1:A:443:ILE:HD12	2.03	0.40
1:A:2057:THR:O	1:A:2061:VAL:HG23	2.21	0.40
1:A:2453:ILE:HG12	1:A:2521:LEU:HD21	2.03	0.40
1:B:26:GLN:N	1:B:27:TYR:CB	2.84	0.40
1:D:236:LEU:HB2	1:D:487:PHE:HB2	2.03	0.40
1:D:1350:LEU:HB3	1:D:1555:ALA:O	2.21	0.40
1:D:2086:LEU:HD22	1:E:2271:LEU:HD13	2.02	0.40
1:D:2191:ALA:O	1:D:2195:VAL:HG13	2.21	0.40
1:E:2509:LEU:HD22	1:E:2511:PHE:CE1	2.56	0.40
1:A:337:THR:HG22	1:A:338:ASP:CG	2.42	0.40
1:A:1176:VAL:HG13	1:B:2176:PHE:CZ	2.57	0.40
1:A:1478:LYS:HB3	1:A:1478:LYS:HE2	1.86	0.40
1:A:1719:MSE:HE3	1:A:1719:MSE:HB3	2.02	0.40
1:A:1757:ASP:OD1	1:A:1757:ASP:N	2.48	0.40
1:C:347:PHE:CD1	1:C:415:ILE:HD11	2.56	0.40
1:C:600:LEU:HD21	1:C:628:THR:HG21	2.03	0.40
1:D:556:ALA:HB1	1:D:589:LEU:HD11	2.02	0.40
1:D:1724:ARG:NH1	1:D:1735:ASP:OD2	2.54	0.40
1:E:301:GLN:HB2	1:E:317:THR:HB	2.02	0.40
1:A:829:ASP:OD1	1:A:832:ARG:NH2	2.43	0.40
1:A:1321:MSE:HG3	1:A:1571:PHE:CE2	2.57	0.40
1:A:1344:LYS:HE3	1:A:1344:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:LEU:HD12	1:A:1969:LEU:H	1.86	0.40
1:A:2509:LEU:HD23	1:A:2528:ILE:HD13	2.04	0.40
1:B:200:HIS:CE1	1:B:202:PRO:HG2	2.56	0.40
1:B:704:LEU:HG	1:B:741:MSE:HE3	2.04	0.40
1:B:1010:ALA:O	1:B:1014:THR:HG23	2.21	0.40
1:B:1665:PRO:HG3	1:B:1780:LEU:HD13	2.04	0.40
1:C:247:TYR:CE1	1:C:898:TYR:HB3	2.56	0.40
1:C:603:LEU:HD12	1:C:603:LEU:HA	1.85	0.40
1:C:783:VAL:HG13	1:C:832:ARG:HG3	2.03	0.40
1:C:1723:VAL:O	1:C:1742:PHE:HA	2.22	0.40
1:C:2454:ARG:NH2	1:C:2513:ASP:HB2	2.36	0.40
1:D:247:TYR:CE1	1:D:898:TYR:HB3	2.56	0.40
1:E:372:THR:HA	1:E:416:TYR:O	2.21	0.40
1:E:769:LEU:HD12	1:E:769:LEU:HA	1.95	0.40
1:A:288:LEU:HD21	1:A:456:LEU:HD21	2.03	0.40
1:A:1371:ARG:HA	1:A:1375:ILE:HD12	2.03	0.40
1:A:2178:LEU:O	1:D:1184:VAL:HG21	2.20	0.40
1:B:142:ARG:HD2	1:B:971:PHE:O	2.22	0.40
1:B:367:ARG:HE	1:B:367:ARG:HB2	1.76	0.40
1:B:2219:ARG:HD3	1:B:2223:TRP:CZ2	2.57	0.40
1:C:322:ASN:HA	1:C:324:GLU:O	2.21	0.40
1:C:436:PHE:CZ	1:C:438:SER:HB2	2.57	0.40
1:C:504:GLN:O	1:C:507:ASN:ND2	2.55	0.40
1:C:1972:ALA:O	1:C:1974:SER:N	2.54	0.40
1:C:2364:ARG:NH2	1:C:2420:LEU:O	2.55	0.40
1:D:73:PRO:HB2	1:D:1928:PRO:HG3	2.03	0.40
1:D:300:LEU:HD12	1:D:317:THR:HA	2.02	0.40
1:D:319:LEU:HD12	1:D:319:LEU:HA	1.82	0.40
1:D:1070:ARG:O	1:D:1074:GLU:HG2	2.20	0.40
1:D:1527:PHE:CG	1:D:1551:LEU:HD22	2.57	0.40
1:A:127:LYS:HE2	1:A:127:LYS:HB3	1.72	0.40
1:A:271:ILE:HD13	1:A:281:TRP:HZ2	1.87	0.40
1:B:22:LEU:HD12	1:B:22:LEU:HA	1.94	0.40
1:B:236:LEU:HB2	1:B:487:PHE:HB2	2.03	0.40
1:B:414:LYS:HB2	1:B:434:PHE:CD2	2.57	0.40
1:B:1135:LEU:HD12	1:B:1135:LEU:HA	1.85	0.40
1:B:1184:VAL:HG21	1:D:2178:LEU:O	2.21	0.40
1:C:22:LEU:HD12	1:C:22:LEU:HA	1.87	0.40
1:C:1451:LEU:HB2	1:C:1479:CYS:SG	2.61	0.40
1:C:1927:GLU:OE2	1:C:1995:ARG:NH1	2.53	0.40
1:C:1969:LEU:HD12	1:C:1969:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:PRO:HG2	1:E:443:ILE:HD12	2.02	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 X-ray entries followed by that with respect to entries of similar resolution.

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	2535/2537 (100%)	2411 (95%)	117 (5%)	7 (0%)	41	73
1	B	2535/2537 (100%)	2412 (95%)	115 (4%)	8 (0%)	41	73
1	C	2535/2537 (100%)	2410 (95%)	116 (5%)	9 (0%)	34	69
1	D	2535/2537 (100%)	2404 (95%)	124 (5%)	7 (0%)	41	73
1	E	2535/2537 (100%)	2406 (95%)	121 (5%)	8 (0%)	41	73
All	All	12675/12685 (100%)	12043 (95%)	593 (5%)	39 (0%)	41	73

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	2022	ASP
1	B	27	TYR
1	B	2022	ASP
1	C	27	TYR
1	C	2022	ASP
1	D	27	TYR
1	D	2022	ASP
1	E	27	TYR
1	E	309	SER
1	E	2022	ASP
1	A	309	SER
1	A	1730	GLN

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Mol	Chain	Res	Type
1	B	309	SER
1	B	1730	GLN
1	C	309	SER
1	C	1444	GLU
1	C	1730	GLN
1	D	309	SER
1	E	308	THR
1	E	1730	GLN
1	B	308	THR
1	C	308	THR
1	D	1730	GLN
1	E	1467	THR
1	A	308	THR
1	A	902	LEU
1	D	902	LEU
1	A	344	ILE
1	B	344	ILE
1	B	1973	ASN
1	C	344	ILE
1	D	308	THR
1	D	344	ILE
1	E	344	ILE
1	B	902	LEU
1	C	399	ASN
1	C	902	LEU
1	E	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 X-ray entries followed by that with respect to entries of similar resolution.

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	2172/2111 (103%)	2139 (98%)	33 (2%)	65 85
1	B	2172/2111 (103%)	2145 (99%)	27 (1%)	71 88
1	C	2172/2111 (103%)	2133 (98%)	39 (2%)	59 82
1	D	2172/2111 (103%)	2135 (98%)	37 (2%)	60 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	2172/2111 (103%)	2142 (99%)	30 (1%)	67 86
All	All	10860/10555 (103%)	10694 (98%)	166 (2%)	65 85

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	A	257	LYS
1	A	327	LEU
1	A	347	PHE
1	A	358	PHE
1	A	374	ARG
1	A	398	SER
1	A	533	LYS
1	A	690	ASP
1	A	768	SER
1	A	822	ASN
1	A	965	ASP
1	A	1129	ARG
1	A	1158	ARG
1	A	1235	PHE
1	A	1260	LYS
1	A	1288	LYS
1	A	1436	ARG
1	A	1639	ASP
1	A	1890	LEU
1	A	1902	TYR
1	A	1908	ASP
1	A	1935	GLN
1	A	1991	TRP
1	A	2010	GLN
1	A	2103	GLN
1	A	2156	SER
1	A	2199	SER
1	A	2286	ARG
1	A	2298	ASP
1	A	2364	ARG
1	A	2423	PHE
1	A	2526	SER
1	B	28	LEU
1	B	165	SER
1	B	338	ASP

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Mol	Chain	Res	Type
1	B	347	PHE
1	B	533	LYS
1	B	768	SER
1	B	1036	LEU
1	B	1129	ARG
1	B	1154	LYS
1	B	1235	PHE
1	B	1260	LYS
1	B	1288	LYS
1	B	1431	ASN
1	B	1540	SER
1	B	1639	ASP
1	B	1661	ASN
1	B	1674	ASP
1	B	1902	TYR
1	B	1962	ARG
1	B	1991	TRP
1	B	2010	GLN
1	B	2092	MSE
1	B	2199	SER
1	B	2271	LEU
1	B	2286	ARG
1	B	2364	ARG
1	B	2516	ASP
1	C	27	TYR
1	C	347	PHE
1	C	358	PHE
1	C	363	PHE
1	C	374	ARG
1	C	533	LYS
1	C	537	PHE
1	C	624	ASN
1	C	768	SER
1	C	843	SER
1	C	897	ARG
1	C	904	LYS
1	C	1036	LEU
1	C	1129	ARG
1	C	1162	PHE
1	C	1209	TYR
1	C	1235	PHE
1	C	1260	LYS

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Mol	Chain	Res	Type
1	C	1308	ARG
1	C	1444	GLU
1	C	1504	ASP
1	C	1639	ASP
1	C	1661	ASN
1	C	1674	ASP
1	C	1720	HIS
1	C	1795	ASN
1	C	1889	ARG
1	C	1902	TYR
1	C	1991	TRP
1	C	2003	HIS
1	C	2010	GLN
1	C	2027	LEU
1	C	2156	SER
1	C	2178	LEU
1	C	2199	SER
1	C	2286	ARG
1	C	2364	ARG
1	C	2391	ARG
1	C	2526	SER
1	D	27	TYR
1	D	28	LEU
1	D	327	LEU
1	D	347	PHE
1	D	358	PHE
1	D	374	ARG
1	D	416	TYR
1	D	518	ASP
1	D	533	LYS
1	D	624	ASN
1	D	658	GLU
1	D	690	ASP
1	D	955	GLN
1	D	1036	LEU
1	D	1129	ARG
1	D	1154	LYS
1	D	1158	ARG
1	D	1162	PHE
1	D	1235	PHE
1	D	1260	LYS
1	D	1274	LYS

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Mol	Chain	Res	Type
1	D	1288	LYS
1	D	1444	GLU
1	D	1463	ASN
1	D	1491	PHE
1	D	1504	ASP
1	D	1639	ASP
1	D	1720	HIS
1	D	1795	ASN
1	D	1902	TYR
1	D	1991	TRP
1	D	2003	HIS
1	D	2211	SER
1	D	2271	LEU
1	D	2286	ARG
1	D	2324	ARG
1	D	2364	ARG
1	E	27	TYR
1	E	89	SER
1	E	160	SER
1	E	165	SER
1	E	196	ASP
1	E	257	LYS
1	E	338	ASP
1	E	347	PHE
1	E	358	PHE
1	E	374	ARG
1	E	533	LYS
1	E	690	ASP
1	E	718	ASP
1	E	805	ASP
1	E	1129	ARG
1	E	1235	PHE
1	E	1260	LYS
1	E	1274	LYS
1	E	1288	LYS
1	E	1433	ASP
1	E	1510	ASN
1	E	1639	ASP
1	E	1661	ASN
1	E	1902	TYR
1	E	1991	TRP
1	E	2003	HIS

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Mol	Chain	Res	Type
1	E	2027	LEU
1	E	2286	ARG
1	E	2364	ARG
1	E	2423	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1374	GLN
1	D	955	GLN
1	D	1498	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2476/2537 (97%)	-0.44	27 (1%) 80 64	26, 47, 80, 160	0
1	B	2476/2537 (97%)	-0.32	63 (2%) 57 34	25, 47, 109, 166	0
1	C	2476/2537 (97%)	-0.42	35 (1%) 75 56	24, 44, 82, 165	0
1	D	2476/2537 (97%)	-0.43	30 (1%) 79 61	22, 43, 76, 173	0
1	E	2476/2537 (97%)	-0.43	24 (0%) 82 67	24, 45, 83, 161	0
All	All	12380/12685 (97%)	-0.41	179 (1%) 75 56	22, 45, 85, 173	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	ASN	8.0
1	D	2017	TYR	7.8
1	E	2017	TYR	7.8
1	B	15	ARG	7.3
1	B	2017	TYR	7.0
1	A	322	ASN	7.0
1	B	1445	ASN	6.9
1	D	2018	ALA	6.7
1	D	322	ASN	6.0
1	C	539	ALA	5.8
1	A	1968	ASN	5.8
1	A	2020	PRO	5.3
1	B	2022	ASP	5.2
1	E	2018	ALA	5.2
1	B	16	ASP	5.2
1	A	2017	TYR	5.1
1	D	901	ALA	5.0
1	A	414	LYS	4.9
1	D	2020	PRO	4.9
1	A	2022	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	2017	TYR	4.8
1	C	901	ALA	4.7
1	D	539	ALA	4.7
1	B	2020	PRO	4.6
1	D	903	ASN	4.5
1	E	2020	PRO	4.4
1	C	2018	ALA	4.3
1	D	1372	ASN	4.3
1	A	539	ALA	4.2
1	A	749	LEU	4.2
1	B	539	ALA	4.1
1	B	901	ALA	4.0
1	E	2015	ALA	4.0
1	C	414	LYS	4.0
1	E	1372	ASN	3.9
1	A	905	ALA	3.8
1	E	905	ALA	3.8
1	E	2023	PRO	3.8
1	B	1500	SER	3.8
1	B	2023	PRO	3.8
1	C	2023	PRO	3.7
1	E	414	LYS	3.7
1	C	1968	ASN	3.6
1	C	905	ALA	3.6
1	C	2016	ILE	3.6
1	A	2018	ALA	3.6
1	B	323	ASN	3.6
1	B	1468	VAL	3.6
1	C	1372	ASN	3.5
1	C	323	ASN	3.5
1	B	1492	GLN	3.4
1	A	376	ASN	3.4
1	A	2019	GLU	3.4
1	B	1489	GLN	3.4
1	D	902	LEU	3.4
1	C	1486	ALA	3.4
1	A	1372	ASN	3.3
1	B	14	THR	3.3
1	D	414	LYS	3.3
1	B	2018	ALA	3.3
1	B	322	ASN	3.3
1	D	2019	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	902	LEU	3.2
1	B	2016	ILE	3.2
1	C	747	GLU	3.2
1	B	13	PRO	3.1
1	D	1968	ASN	3.1
1	C	900	THR	3.1
1	B	1535	SER	3.1
1	E	2019	GLU	3.1
1	C	796	ASN	3.1
1	B	1486	ALA	3.1
1	A	957	GLU	3.1
1	D	907	SER	3.1
1	B	2021	THR	3.1
1	C	749	LEU	3.1
1	A	1967	LYS	3.0
1	E	322	ASN	3.0
1	A	15	ARG	3.0
1	A	2023	PRO	3.0
1	B	1484	GLY	3.0
1	B	1417	LYS	3.0
1	C	2015	ALA	3.0
1	D	323	ASN	3.0
1	B	2025	ALA	2.9
1	D	2021	THR	2.9
1	D	2016	ILE	2.9
1	C	376	ASN	2.9
1	C	538	GLU	2.9
1	B	1450	ARG	2.9
1	B	2019	GLU	2.8
1	B	747	GLU	2.8
1	B	1505	ILE	2.8
1	D	540	ASP	2.8
1	B	1398	THR	2.8
1	B	414	LYS	2.8
1	B	1372	ASN	2.8
1	C	2022	ASP	2.8
1	B	1366	SER	2.7
1	B	905	ALA	2.7
1	A	747	GLU	2.7
1	E	906	GLU	2.7
1	C	2019	GLU	2.7
1	E	1297	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	1180	GLY	2.7
1	A	538	GLU	2.6
1	D	376	ASN	2.6
1	B	1476	PHE	2.6
1	B	1439	ILE	2.6
1	D	695	HIS	2.6
1	C	902	LEU	2.6
1	B	538	GLU	2.6
1	E	2016	ILE	2.5
1	C	540	ASP	2.5
1	B	17	GLY	2.5
1	B	317	THR	2.5
1	B	904	LYS	2.5
1	A	2449	PRO	2.5
1	B	1967	LYS	2.5
1	B	906	GLU	2.5
1	B	1454	PHE	2.4
1	C	1457	SER	2.4
1	C	904	LYS	2.4
1	E	2025	ALA	2.4
1	B	1422	ILE	2.4
1	C	2020	PRO	2.4
1	A	2024	LYS	2.4
1	D	538	GLU	2.4
1	C	2021	THR	2.3
1	E	1970	ARG	2.3
1	E	2021	THR	2.3
1	B	1431	ASN	2.3
1	B	1444	GLU	2.3
1	C	15	ARG	2.3
1	E	2024	LYS	2.3
1	C	1736	ASN	2.3
1	E	1468	VAL	2.3
1	B	18	GLN	2.3
1	B	1433	ASP	2.2
1	D	900	THR	2.2
1	B	2449	PRO	2.2
1	E	1487	ASN	2.2
1	E	16	ASP	2.2
1	E	2022	ASP	2.2
1	D	1297	GLN	2.2
1	C	1967	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	749	LEU	2.2
1	A	2021	THR	2.2
1	B	1397	ASN	2.2
1	A	902	LEU	2.2
1	B	1393	PHE	2.2
1	B	1478	LYS	2.2
1	B	12	SER	2.1
1	C	1772	ASN	2.1
1	B	2013	SER	2.1
1	D	1730	GLN	2.1
1	D	747	GLU	2.1
1	B	796	ASN	2.1
1	A	1970	ARG	2.1
1	B	1473	THR	2.1
1	E	1968	ASN	2.1
1	D	2023	PRO	2.1
1	A	900	THR	2.1
1	B	1371	ARG	2.1
1	C	1298	GLY	2.1
1	D	358	PHE	2.1
1	A	317	THR	2.1
1	B	957	GLU	2.1
1	B	1448	TYR	2.1
1	E	539	ALA	2.1
1	C	1499	SER	2.1
1	A	323	ASN	2.0
1	D	321	VAL	2.0
1	B	1503	LEU	2.0
1	B	749	LEU	2.0
1	C	1763	GLY	2.0
1	D	1967	LYS	2.0
1	B	1182	ASP	2.0
1	D	749	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.