



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:58 PM UTC

PDB ID : 8TV0 / pdb_00008tv0
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

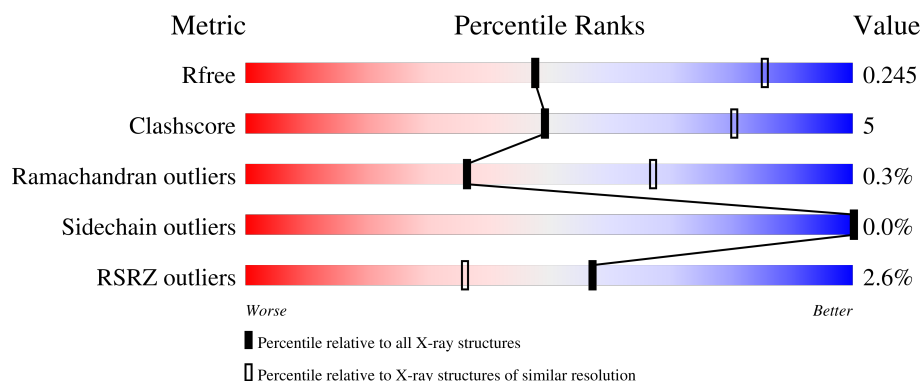
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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	2% 86% 14%
1	B	2537	4% 87% 13%
1	C	2537	3% 85% 14%
1	D	2537	3% 86% 13%
1	E	2537	% 87% 12%

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
1	A	2537	Total 20007	C 12625	N 3415	O 3894	S 12	Se 61	0	0	0
1	B	2537	Total 20007	C 12625	N 3415	O 3894	S 12	Se 61	0	0	0
1	C	2537	Total 20007	C 12625	N 3415	O 3894	S 12	Se 61	0	0	0
1	D	2537	Total 20007	C 12625	N 3415	O 3894	S 12	Se 61	0	0	0
1	E	2537	Total 20007	C 12625	N 3415	O 3894	S 12	Se 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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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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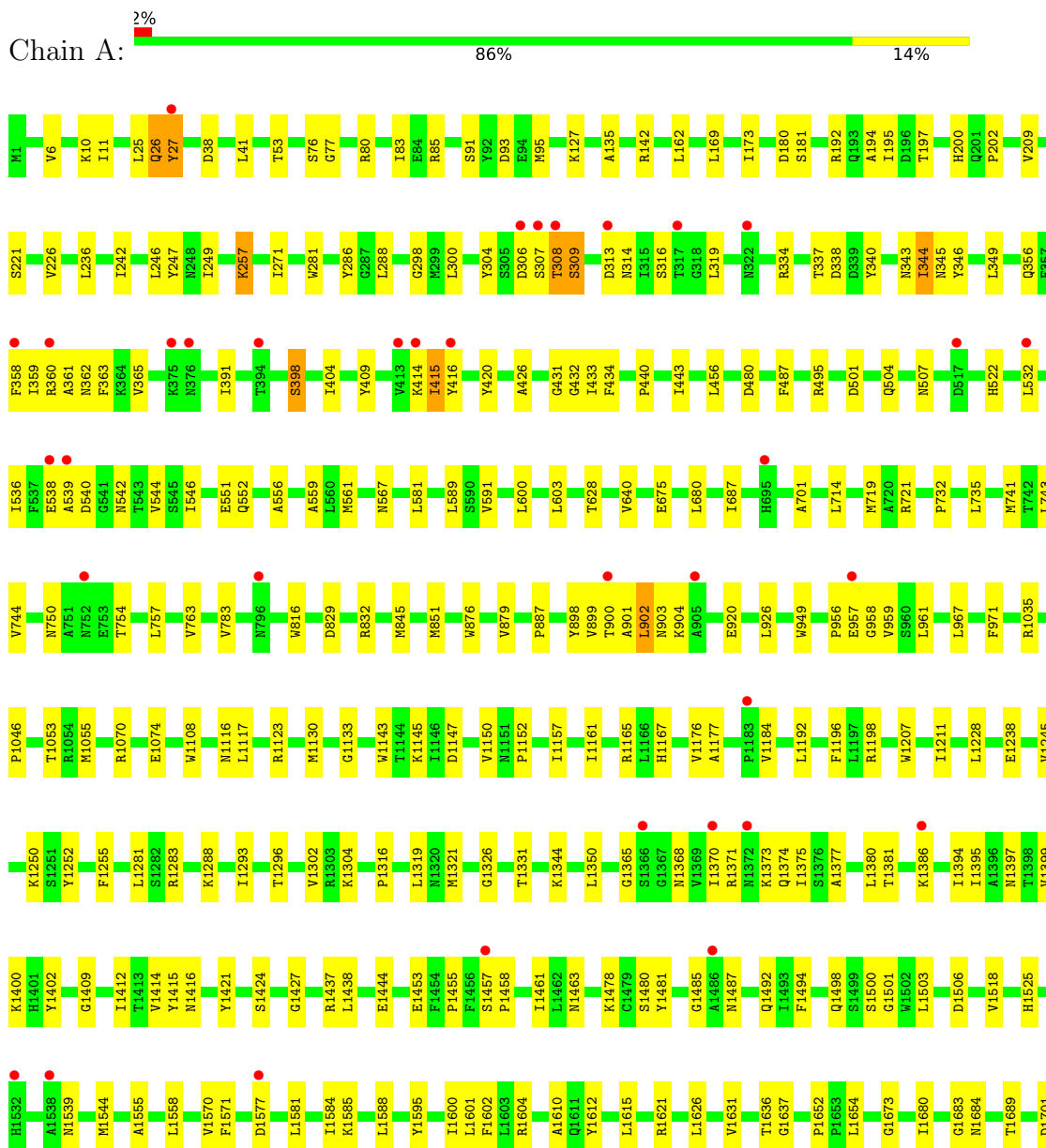
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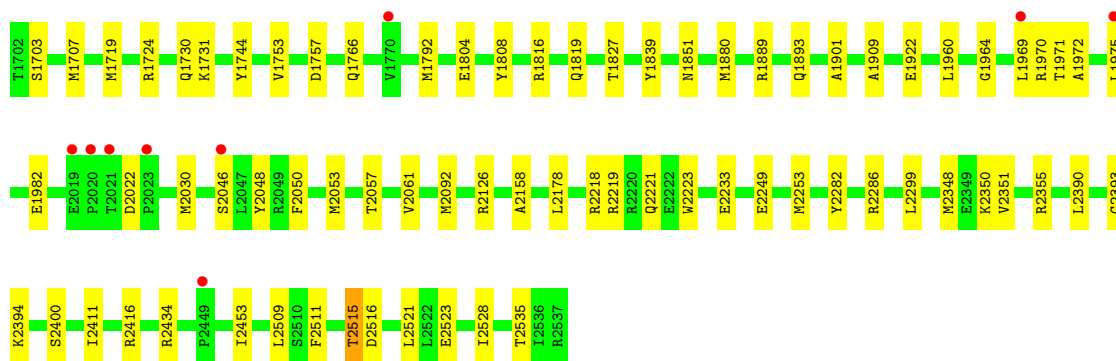
Chain	Residue	Modelled	Actual	Comment	Reference
E	1920	THR	ALA	conflict	UNP N1NRW3
E	1943	GLY	VAL	conflict	UNP N1NRW3
E	1947	GLN	HIS	conflict	UNP N1NRW3
E	1959	MSE	ALA	conflict	UNP N1NRW3
E	1961	GLY	ASP	conflict	UNP N1NRW3
E	1962	ARG	ASN	conflict	UNP N1NRW3
E	1964	GLY	GLU	conflict	UNP N1NRW3
E	1966	SER	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

3 Residue-property plots [i](#)

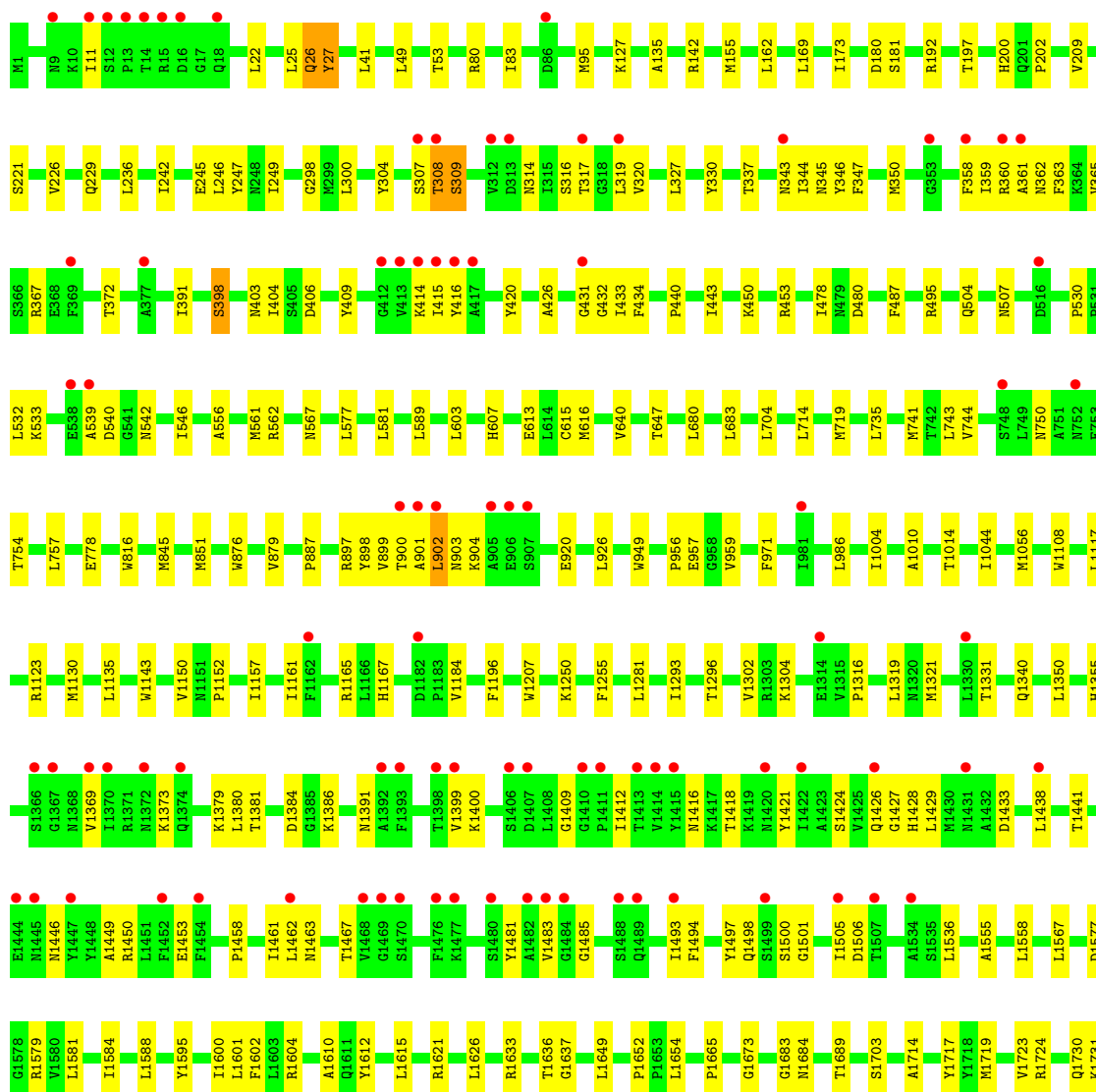
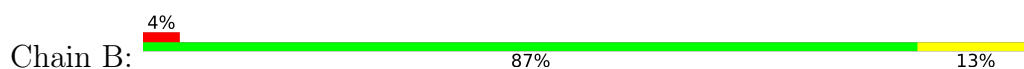
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

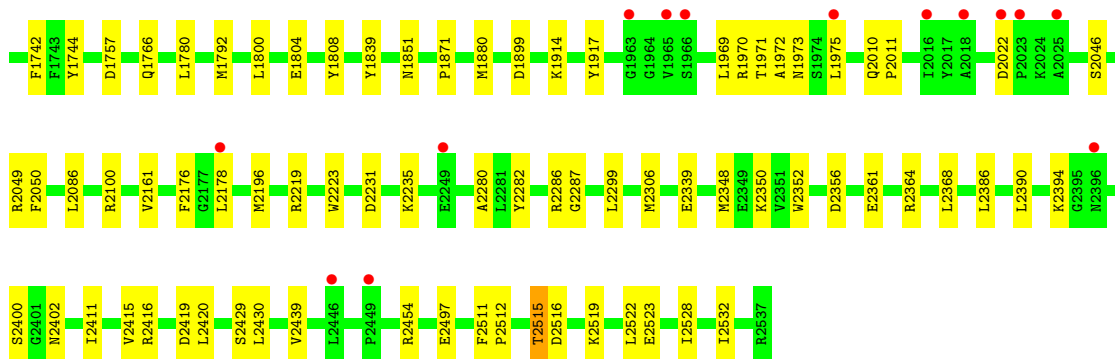
• Molecule 1: XptA2



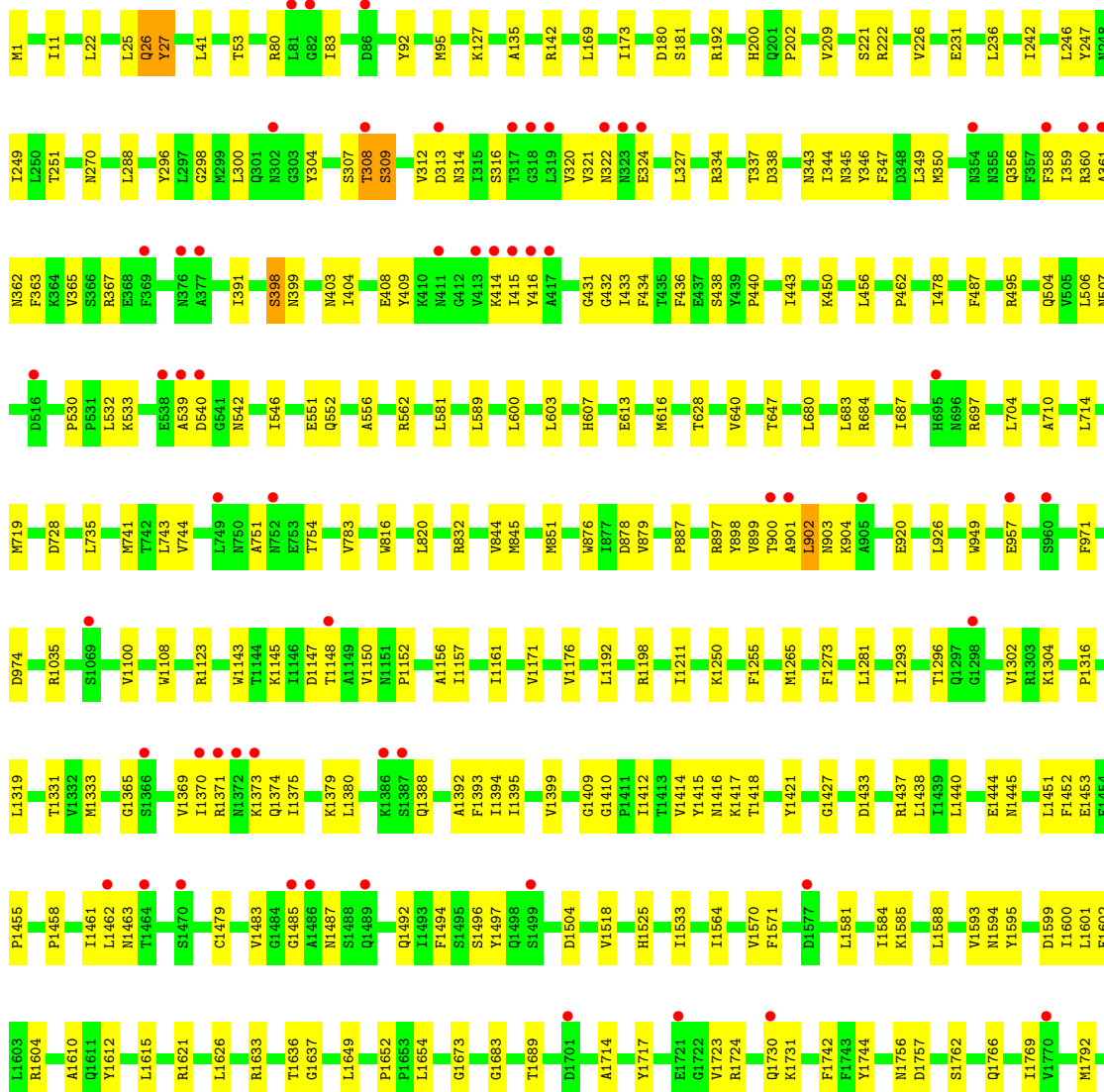
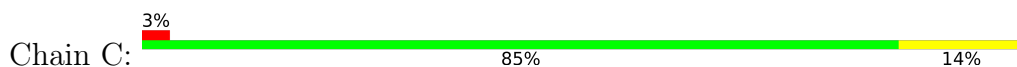


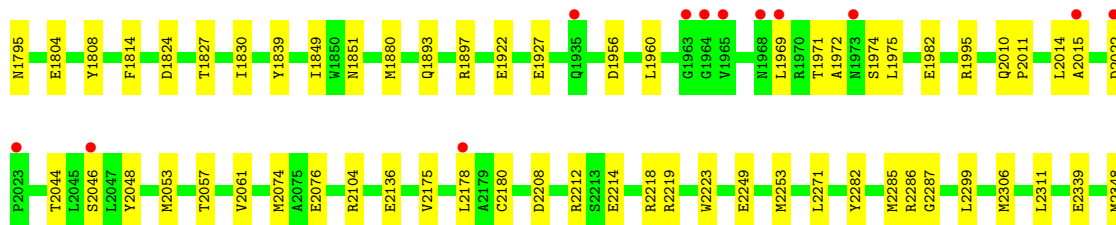
• Molecule 1: XptA2



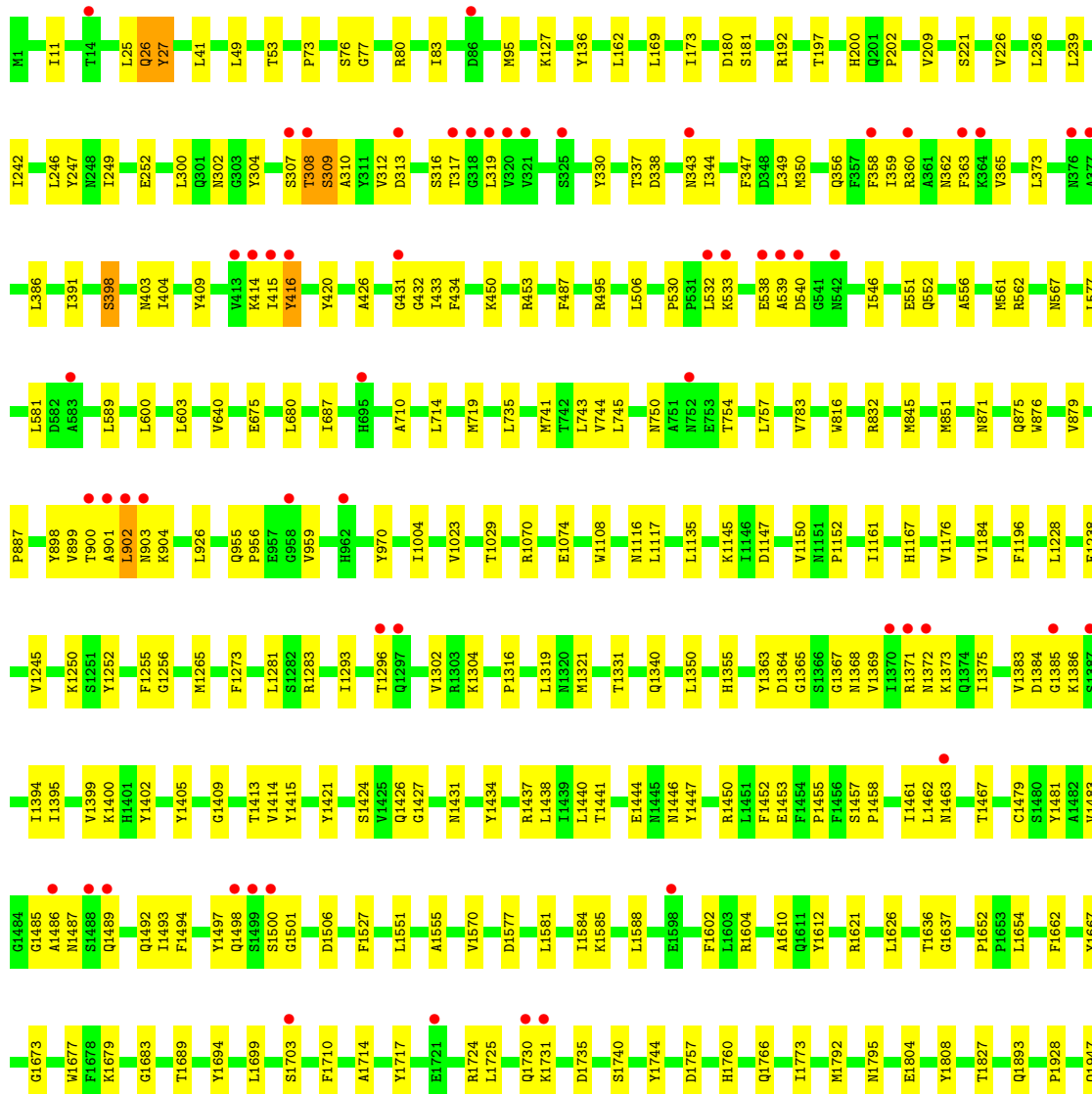
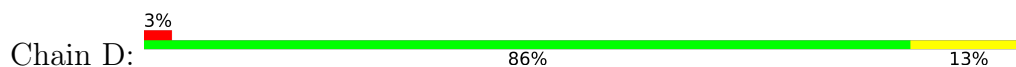


• Molecule 1: XptA2



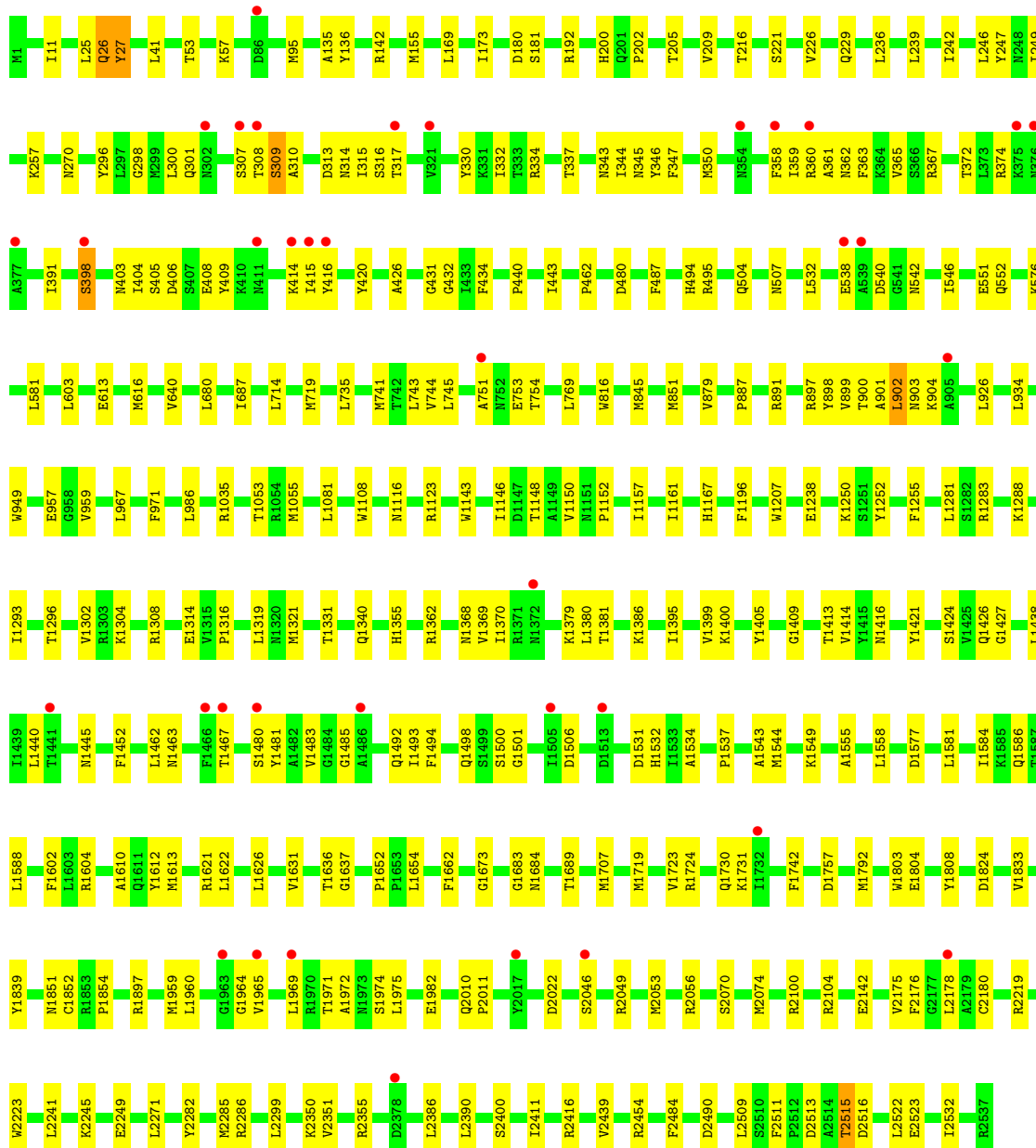
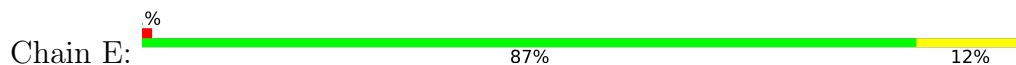


• Molecule 1: XptA2





• Molecule 1: XptA2



4 Data and refinement statistics

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 48.73 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.73-3.10) 90.3 (48.73-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.194 , 0.247 0.193 , 0.245	Depositor DCC
R_{free} test set	2001 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.10	0/20353	0.32	6/27534 (0.0%)
1	B	0.10	0/20353	0.31	4/27534 (0.0%)
1	C	0.10	0/20353	0.32	4/27534 (0.0%)
1	D	0.11	0/20353	0.32	4/27534 (0.0%)
1	E	0.10	0/20353	0.31	4/27534 (0.0%)
All	All	0.10	0/101765	0.32	22/137670 (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 (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	GLN	CA-C-N	9.00	137.90	121.70
1	D	26	GLN	C-N-CA	9.00	137.90	121.70
1	A	26	GLN	CA-C-N	8.78	137.51	121.70
1	A	26	GLN	C-N-CA	8.78	137.51	121.70
1	B	26	GLN	CA-C-N	8.72	137.41	121.70
1	B	26	GLN	C-N-CA	8.72	137.41	121.70
1	C	26	GLN	CA-C-N	8.64	137.25	121.70
1	C	26	GLN	C-N-CA	8.64	137.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2515	THR	CA-C-N	8.61	137.19	121.70
1	D	2515	THR	C-N-CA	8.61	137.19	121.70
1	B	2515	THR	CA-C-N	8.59	137.17	121.70
1	B	2515	THR	C-N-CA	8.59	137.17	121.70
1	E	26	GLN	CA-C-N	8.57	137.12	121.70
1	E	26	GLN	C-N-CA	8.57	137.12	121.70
1	A	2515	THR	CA-C-N	8.52	137.04	121.70
1	A	2515	THR	C-N-CA	8.52	137.04	121.70
1	E	2515	THR	CA-C-N	8.45	136.90	121.70
1	E	2515	THR	C-N-CA	8.45	136.90	121.70
1	C	2515	THR	CA-C-N	8.20	136.45	121.70
1	C	2515	THR	C-N-CA	8.20	136.45	121.70
1	A	415	ILE	CA-C-N	5.22	131.51	121.54
1	A	415	ILE	C-N-CA	5.22	131.51	121.54

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 ⓘ

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	233	0
1	B	20007	0	19597	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	20007	0	19597	239	0
1	D	20007	0	19597	228	0
1	E	20007	0	19597	206	0
All	All	100035	0	97985	1076	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 (1076) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1500:SER:OG	1:D:1501:GLY:N	2.25	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:D:95:MSE:O	1:D:1971:THR:OG1	2.16	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
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:A:901:ALA:O	1:A:902:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:MSE:O	1:E:1971:THR:OG1	2.18	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:920:GLU:OE1	1:D:533:LYS:NZ	2.37	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: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: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:A:1145:LYS:NZ	1:A:1147:ASP:OD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:901:ALA:O	1:D:902:LEU:HB2	2.03	0.56
1:A:680:LEU:HD11	1:A:757:LEU:HD21	1.88	0.56
1:E:901:ALA:O	1:E:902:LEU:HB2	2.04	0.56
1:C:433:ILE:HD11	1:C:539:ALA:HB2	1.87	0.56
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:C:901:ALA:O	1:C:902:LEU:HB2	2.04	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:B:1914:LYS:NZ	1:C:974:ASP:OD2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:337:THR:HG22	1:D:338:ASP:CG	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:1694:TYR:OH	1:D:1710:PHE:O	2.24	0.52
1:A:958:GLY:O	1:A:1400:LYS:NZ	2.38	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:E:899:VAL:O	1:E:900:THR:OG1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1480:SER:OG	1:A:1481:TYR:N	2.43	0.51
1:B:95:MSE:O	1:B:1971:THR:OG1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:398:SER:OG	1:C:398:SER:O	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:902:LEU:C	1:E:904:LYS:H	2.20	0.48
1:E:2386:LEU:HD21	1:E:2522:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:902:LEU:C	1:D:904:LYS:H	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:902:LEU:C	1:C:904:LYS:H	2.22	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:902:LEU:C	1:A:904:LYS:H	2.22	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:538:GLU:CD	1:A:591:VAL:HG13	2.40	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
1:B:372:THR:HA	1:B:416:TYR:O	2.15	0.47
1:B:902:LEU:C	1:B:904:LYS:H	2.21	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: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:D:1444:GLU:C	1:D:1446:ASN:H	2.23	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:306:ASP:OD2	1:E:1974:SER:OG	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:337:THR:HG22	1:A:338:ASP:CG	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:403:ASN:O	1:C:404:ILE:HG13	2.17	0.45
1:C:1417:LYS:NZ	1:C:1504:ASP:OD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:309:SER:OG	1:E:310:ALA:N	2.50	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:B:1899:ASP:OD1	1:B:1917:TYR:OH	2.30	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:403:ASN:C	1:E:404:ILE:HG13	2.42	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:538:GLU:C	1:E:540:ASP:H	2.26	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
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: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:538:GLU:C	1:A:540:ASP:H	2.27	0.42
1:A:750:ASN:HB3	1:A:754:THR:HG22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:A:1368:ASN:N	2.52	0.42
1:C:345:ASN:HB2	1:C:361:ALA:HB3	2.01	0.42
1:D:538:GLU:C	1:D:540:ASP:H	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:ASP:O	1:A:1585:LYS:NZ	2.42	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
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:B:25:LEU:C	1:B:27:TYR:HB3	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1023:VAL:O	1:D:1029:THR:OG1	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:1384:ASP:OD1	1:B:1384:ASP:N	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	36	67
1	B	2535/2537 (100%)	2412 (95%)	115 (4%)	8 (0%)	36	67
1	C	2535/2537 (100%)	2410 (95%)	116 (5%)	9 (0%)	30	61
1	D	2535/2537 (100%)	2404 (95%)	124 (5%)	7 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	2535/2537 (100%)	2406 (95%)	121 (5%)	8 (0%)	36	67
All	All	12675/12685 (100%)	12043 (95%)	593 (5%)	39 (0%)	36	67

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
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

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Mol	Chain	Res	Type
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%)	2171 (100%)	1 (0%)	100	100
1	B	2172/2111 (103%)	2172 (100%)	0	100	100
1	C	2172/2111 (103%)	2172 (100%)	0	100	100
1	D	2172/2111 (103%)	2170 (100%)	2 (0%)	88	90
1	E	2172/2111 (103%)	2172 (100%)	0	100	100
All	All	10860/10555 (103%)	10857 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LYS
1	D	416	TYR
1	D	1740	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	ASN
1	A	504	GLN
1	A	507	ASN
1	A	512	ASN
1	A	695	HIS
1	A	772	GLN
1	A	921	ASN
1	A	932	GLN

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Mol	Chain	Res	Type
1	A	1103	ASN
1	A	1340	GLN
1	A	1355	HIS
1	A	1356	ASN
1	A	1446	ASN
1	A	1471	ASN
1	A	1532	HIS
1	A	1563	ASN
1	A	1596	ASN
1	A	1661	ASN
1	A	1692	GLN
1	A	1720	HIS
1	A	1950	GLN
1	A	2010	GLN
1	A	2103	GLN
1	A	2125	ASN
1	A	2258	GLN
1	A	2262	GLN
1	A	2373	GLN
1	A	2388	GLN
1	A	2435	GLN
1	B	60	ASN
1	B	172	HIS
1	B	301	GLN
1	B	449	ASN
1	B	494	HIS
1	B	504	GLN
1	B	513	GLN
1	B	542	ASN
1	B	585	ASN
1	B	762	HIS
1	B	772	GLN
1	B	833	GLN
1	B	868	GLN
1	B	875	GLN
1	B	884	HIS
1	B	921	ASN
1	B	955	GLN
1	B	975	ASN
1	B	1103	ASN
1	B	1199	HIS
1	B	1355	HIS

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Mol	Chain	Res	Type
1	B	1539	ASN
1	B	1562	ASN
1	B	1563	ASN
1	B	1614	GLN
1	B	1661	ASN
1	B	1684	ASN
1	B	1692	GLN
1	B	1720	HIS
1	B	1851	ASN
1	B	1877	ASN
1	B	1954	GLN
1	B	2010	GLN
1	B	2125	ASN
1	B	2273	GLN
1	B	2396	ASN
1	B	2410	GLN
1	B	2435	GLN
1	B	2458	ASN
1	C	60	ASN
1	C	504	GLN
1	C	507	ASN
1	C	512	ASN
1	C	552	GLN
1	C	585	ASN
1	C	772	GLN
1	C	868	GLN
1	C	884	HIS
1	C	921	ASN
1	C	929	GLN
1	C	1103	ASN
1	C	1199	HIS
1	C	1356	ASN
1	C	1388	GLN
1	C	1391	ASN
1	C	1416	ASN
1	C	1498	GLN
1	C	1563	ASN
1	C	1692	GLN
1	C	1934	GLN
1	C	1954	GLN
1	C	1973	ASN
1	C	2103	GLN

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Mol	Chain	Res	Type
1	C	2240	GLN
1	C	2258	GLN
1	C	2483	GLN
1	D	294	GLN
1	D	411	ASN
1	D	449	ASN
1	D	507	ASN
1	D	512	ASN
1	D	585	ASN
1	D	695	HIS
1	D	696	ASN
1	D	833	GLN
1	D	903	ASN
1	D	921	ASN
1	D	955	GLN
1	D	1199	HIS
1	D	1335	ASN
1	D	1355	HIS
1	D	1471	ASN
1	D	1487	ASN
1	D	1498	GLN
1	D	1562	ASN
1	D	1692	GLN
1	D	1720	HIS
1	D	2240	GLN
1	D	2258	GLN
1	D	2266	GLN
1	D	2268	GLN
1	D	2435	GLN
1	D	2458	ASN
1	E	26	GLN
1	E	56	GLN
1	E	60	ASN
1	E	172	HIS
1	E	449	ASN
1	E	507	ASN
1	E	671	ASN
1	E	713	HIS
1	E	955	GLN
1	E	1103	ASN
1	E	1199	HIS
1	E	1340	GLN

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Mol	Chain	Res	Type
1	E	1372	ASN
1	E	1420	ASN
1	E	1498	GLN
1	E	1562	ASN
1	E	1563	ASN
1	E	1692	GLN
1	E	1877	ASN
1	E	1954	GLN
1	E	1973	ASN
1	E	2010	GLN
1	E	2258	GLN
1	E	2388	GLN
1	E	2410	GLN
1	E	2531	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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%)	-0.09	44 (1%) 67 47	26, 47, 80, 160	0
1	B	2476/2537 (97%)	0.02	103 (4%) 40 22	25, 47, 109, 166	0
1	C	2476/2537 (97%)	-0.07	73 (2%) 53 32	24, 44, 82, 165	0
1	D	2476/2537 (97%)	-0.09	67 (2%) 56 35	22, 43, 76, 173	0
1	E	2476/2537 (97%)	-0.10	37 (1%) 72 52	24, 45, 83, 161	0
All	All	12380/12685 (97%)	-0.07	324 (2%) 57 36	22, 45, 85, 173	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	414	LYS	6.8
1	A	414	LYS	6.5
1	B	1468	VAL	6.4
1	E	414	LYS	6.2
1	B	1454	PHE	5.1
1	A	1486	ALA	5.1
1	B	13	PRO	5.1
1	B	901	ALA	5.1
1	B	414	LYS	5.1
1	C	1486	ALA	5.0
1	A	416	TYR	5.0
1	B	14	THR	4.9
1	C	538	GLU	4.8
1	D	539	ALA	4.8
1	D	414	LYS	4.8
1	B	358	PHE	4.6
1	D	358	PHE	4.6
1	D	86	ASP	4.5
1	D	1372	ASN	4.5
1	B	1399	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	538	GLU	4.4
1	C	1372	ASN	4.3
1	A	905	ALA	4.2
1	A	317	THR	4.2
1	C	376	ASN	4.2
1	E	1372	ASN	4.1
1	B	16	ASP	4.1
1	C	901	ALA	4.0
1	C	322	ASN	4.0
1	D	317	THR	4.0
1	B	538	GLU	3.9
1	A	313	ASP	3.9
1	C	317	THR	3.8
1	E	317	THR	3.8
1	C	539	ALA	3.8
1	C	2391	ARG	3.8
1	D	377	ALA	3.8
1	B	1445	ASN	3.8
1	B	2396	ASN	3.8
1	B	317	THR	3.8
1	A	752	ASN	3.7
1	B	1369	VAL	3.7
1	D	903	ASN	3.7
1	B	313	ASP	3.6
1	C	360	ARG	3.6
1	C	358	PHE	3.6
1	C	540	ASP	3.6
1	B	1505	ILE	3.6
1	D	901	ALA	3.6
1	D	307	SER	3.6
1	C	1770	VAL	3.5
1	D	321	VAL	3.5
1	E	411	ASN	3.5
1	D	1486	ALA	3.5
1	A	539	ALA	3.5
1	B	539	ALA	3.5
1	B	1965	VAL	3.4
1	C	377	ALA	3.4
1	B	308	THR	3.4
1	D	1385	GLY	3.3
1	A	360	ARG	3.3
1	C	81	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1370	ILE	3.3
1	B	1182	ASP	3.3
1	B	1393	PHE	3.3
1	B	906	GLU	3.3
1	C	752	ASN	3.2
1	B	2025	ALA	3.2
1	B	1411	PRO	3.2
1	B	1398	THR	3.2
1	A	1975	LEU	3.2
1	C	1973	ASN	3.2
1	C	900	THR	3.2
1	D	320	VAL	3.1
1	C	354	ASN	3.1
1	B	377	ALA	3.1
1	C	2023	PRO	3.1
1	D	416	TYR	3.1
1	B	353	GLY	3.1
1	B	1406	SER	3.1
1	D	1499	SER	3.1
1	A	358	PHE	3.0
1	C	411	ASN	3.0
1	C	2046	SER	3.0
1	B	1367	GLY	3.0
1	B	1374	GLN	3.0
1	B	1480	SER	3.0
1	C	1499	SER	3.0
1	A	2020	PRO	3.0
1	D	752	ASN	3.0
1	C	413	VAL	2.9
1	D	1370	ILE	2.9
1	A	1969	LEU	2.9
1	C	1148	THR	2.9
1	B	307	SER	2.9
1	B	1476	PHE	2.9
1	D	540	ASP	2.9
1	B	1507	THR	2.9
1	E	1965	VAL	2.9
1	A	306	ASP	2.9
1	C	1963	GLY	2.9
1	C	415	ILE	2.9
1	A	538	GLU	2.9
1	A	1538	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	431	GLY	2.8
1	A	1457	SER	2.8
1	C	905	ALA	2.8
1	A	308	THR	2.8
1	B	1484	GLY	2.8
1	B	1415	TYR	2.8
1	B	1470	SER	2.8
1	C	417	ALA	2.8
1	B	1483	VAL	2.8
1	C	1386	LYS	2.8
1	E	1467	THR	2.8
1	B	1438	LEU	2.8
1	D	415	ILE	2.8
1	E	416	TYR	2.8
1	B	18	GLN	2.8
1	C	86	ASP	2.8
1	C	313	ASP	2.8
1	C	1965	VAL	2.8
1	E	354	ASN	2.7
1	A	2046	SER	2.7
1	E	538	GLU	2.7
1	D	360	ARG	2.7
1	D	902	LEU	2.7
1	C	957	GLU	2.7
1	B	516	ASP	2.7
1	A	376	ASN	2.7
1	A	2023	PRO	2.7
1	B	1963	GLY	2.7
1	E	1486	ALA	2.7
1	E	358	PHE	2.7
1	C	82	GLY	2.7
1	A	394	THR	2.7
1	D	1296	THR	2.7
1	A	1577	ASP	2.7
1	D	1598	GLU	2.6
1	B	1975	LEU	2.6
1	E	307	SER	2.6
1	C	2022	ASP	2.6
1	E	415	ILE	2.6
1	B	1431	ASN	2.6
1	D	318	GLY	2.6
1	B	1444	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1721	GLU	2.6
1	B	902	LEU	2.6
1	B	1534	ALA	2.6
1	D	2015	ALA	2.6
1	B	12	SER	2.6
1	B	2446	LEU	2.6
1	C	1462	LEU	2.6
1	E	1969	LEU	2.6
1	B	15	ARG	2.6
1	D	1489	GLN	2.6
1	B	1469	GLY	2.6
1	C	2178	LEU	2.6
1	E	375	LYS	2.6
1	B	2016	ILE	2.6
1	C	1730	GLN	2.6
1	B	1452	PHE	2.5
1	C	416	TYR	2.5
1	D	958	GLY	2.5
1	C	319	LEU	2.5
1	C	1373	LYS	2.5
1	D	1730	GLN	2.5
1	D	1731	LYS	2.5
1	E	2378	ASP	2.5
1	D	2018	ALA	2.5
1	A	796	ASN	2.5
1	D	1463	ASN	2.5
1	B	360	ARG	2.5
1	E	2017	TYR	2.5
1	B	1482	ALA	2.5
1	B	1499	SER	2.5
1	E	398	SER	2.5
1	E	905	ALA	2.5
1	B	11	ILE	2.5
1	D	900	THR	2.5
1	E	308	THR	2.5
1	C	324	GLU	2.4
1	A	375	LYS	2.4
1	D	376	ASN	2.4
1	C	1969	LEU	2.4
1	D	308	THR	2.4
1	E	1441	THR	2.4
1	D	1387	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	1480	SER	2.4
1	E	360	ARG	2.4
1	B	1407	ASP	2.4
1	D	413	VAL	2.4
1	E	321	VAL	2.4
1	B	1426	GLN	2.4
1	B	1366	SER	2.4
1	B	9	ASN	2.4
1	D	962	HIS	2.4
1	D	2016	ILE	2.4
1	C	1489	GLN	2.4
1	B	2449	PRO	2.4
1	B	343	ASN	2.3
1	B	416	TYR	2.3
1	B	905	ALA	2.3
1	C	516	ASP	2.3
1	D	363	PHE	2.3
1	A	1770	VAL	2.3
1	C	960	SER	2.3
1	A	1370	ILE	2.3
1	A	2021	THR	2.3
1	D	14	THR	2.3
1	D	431	GLY	2.3
1	C	1577	ASP	2.3
1	B	369	PHE	2.3
1	B	2178	LEU	2.3
1	C	1935	GLN	2.3
1	A	957	GLU	2.3
1	C	1721	GLU	2.3
1	B	1488	SER	2.3
1	C	323	ASN	2.3
1	C	1968	ASN	2.3
1	D	1969	LEU	2.3
1	B	1422	ILE	2.3
1	D	1488	SER	2.3
1	D	1703	SER	2.3
1	E	2046	SER	2.3
1	E	2178	LEU	2.3
1	C	302	ASN	2.3
1	D	343	ASN	2.3
1	D	542	ASN	2.3
1	D	1297	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	86	ASP	2.3
1	B	1477	LYS	2.3
1	D	1371	ARG	2.3
1	A	1183	PRO	2.3
1	A	2449	PRO	2.3
1	B	981	ILE	2.3
1	C	361	ALA	2.3
1	C	1298	GLY	2.3
1	B	1462	LEU	2.3
1	A	1366	SER	2.3
1	A	1372	ASN	2.3
1	B	752	ASN	2.3
1	E	302	ASN	2.3
1	A	517	ASP	2.3
1	D	2378	ASP	2.3
1	E	1513	ASP	2.3
1	A	532	LEU	2.2
1	C	695	HIS	2.2
1	B	1489	GLN	2.2
1	D	313	ASP	2.2
1	B	900	THR	2.2
1	B	1447	TYR	2.2
1	A	307	SER	2.2
1	B	1966	SER	2.2
1	D	325	SER	2.2
1	B	312	VAL	2.2
1	B	415	ILE	2.2
1	E	377	ALA	2.2
1	C	369	PHE	2.2
1	C	308	THR	2.2
1	C	1464	THR	2.2
1	A	27	TYR	2.2
1	A	413	VAL	2.2
1	C	2377	SER	2.2
1	B	1330	LEU	2.2
1	C	749	LEU	2.2
1	B	1392	ALA	2.2
1	B	1410	GLY	2.2
1	C	318	GLY	2.2
1	E	1963	GLY	2.2
1	E	376	ASN	2.2
1	B	413	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1414	VAL	2.1
1	B	319	LEU	2.1
1	A	1386	LYS	2.1
1	C	1485	GLY	2.1
1	E	1466	PHE	2.1
1	B	86	ASP	2.1
1	C	1370	ILE	2.1
1	D	2017	TYR	2.1
1	C	1371	ARG	2.1
1	D	583	ALA	2.1
1	C	1366	SER	2.1
1	D	1976	VAL	2.1
1	B	1493	ILE	2.1
1	D	1975	LEU	2.1
1	B	2018	ALA	2.1
1	B	1314	GLU	2.1
1	B	748	SER	2.1
1	A	322	ASN	2.1
1	A	695	HIS	2.1
1	C	1701	ASP	2.1
1	E	1505	ILE	2.1
1	A	900	THR	2.1
1	B	361	ALA	2.1
1	E	751	ALA	2.1
1	C	1964	GLY	2.1
1	B	2249	GLU	2.1
1	C	1387	SER	2.1
1	D	1500	SER	2.1
1	D	364	LYS	2.1
1	D	532	LEU	2.1
1	B	2022	ASP	2.1
1	D	2515	THR	2.1
1	E	539	ALA	2.1
1	D	1977	GLY	2.1
1	B	1162	PHE	2.1
1	C	1069	SER	2.0
1	E	1732	ILE	2.0
1	B	1413	THR	2.0
1	B	907	SER	2.0
1	C	1470	SER	2.0
1	B	1372	ASN	2.0
1	B	1420	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1532	HIS	2.0
1	D	695	HIS	2.0
1	B	417	ALA	2.0
1	C	2015	ALA	2.0
1	B	412	GLY	2.0
1	B	2023	PRO	2.0
1	D	533	LYS	2.0
1	D	1498	GLN	2.0
1	A	2019	GLU	2.0
1	D	319	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.