



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:47 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 wwPDB X-ray Structure Validation Summary 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

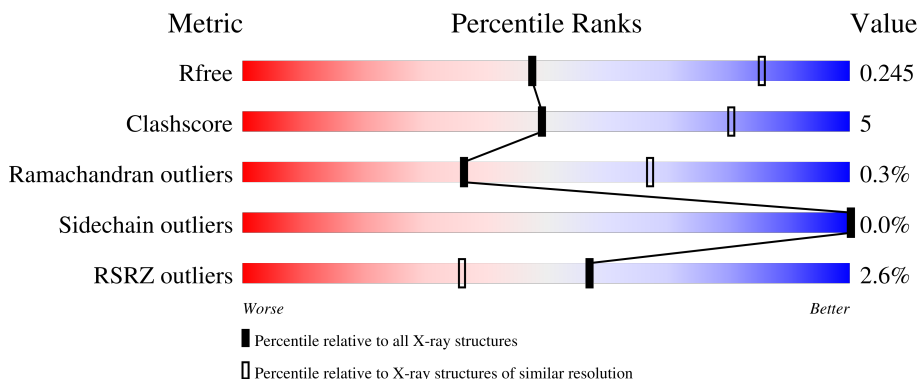
1 Overall quality at a glance

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	C	N	O	S	Se	0	0	0
			20007	12625	3415	3894	12	61			
1	B	2537	Total	C	N	O	S	Se	0	0	0
			20007	12625	3415	3894	12	61			
1	C	2537	Total	C	N	O	S	Se	0	0	0
			20007	12625	3415	3894	12	61			
1	D	2537	Total	C	N	O	S	Se	0	0	0
			20007	12625	3415	3894	12	61			
1	E	2537	Total	C	N	O	S	Se	0	0	0
			20007	12625	3415	3894	12	61			

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

Continued on next page...

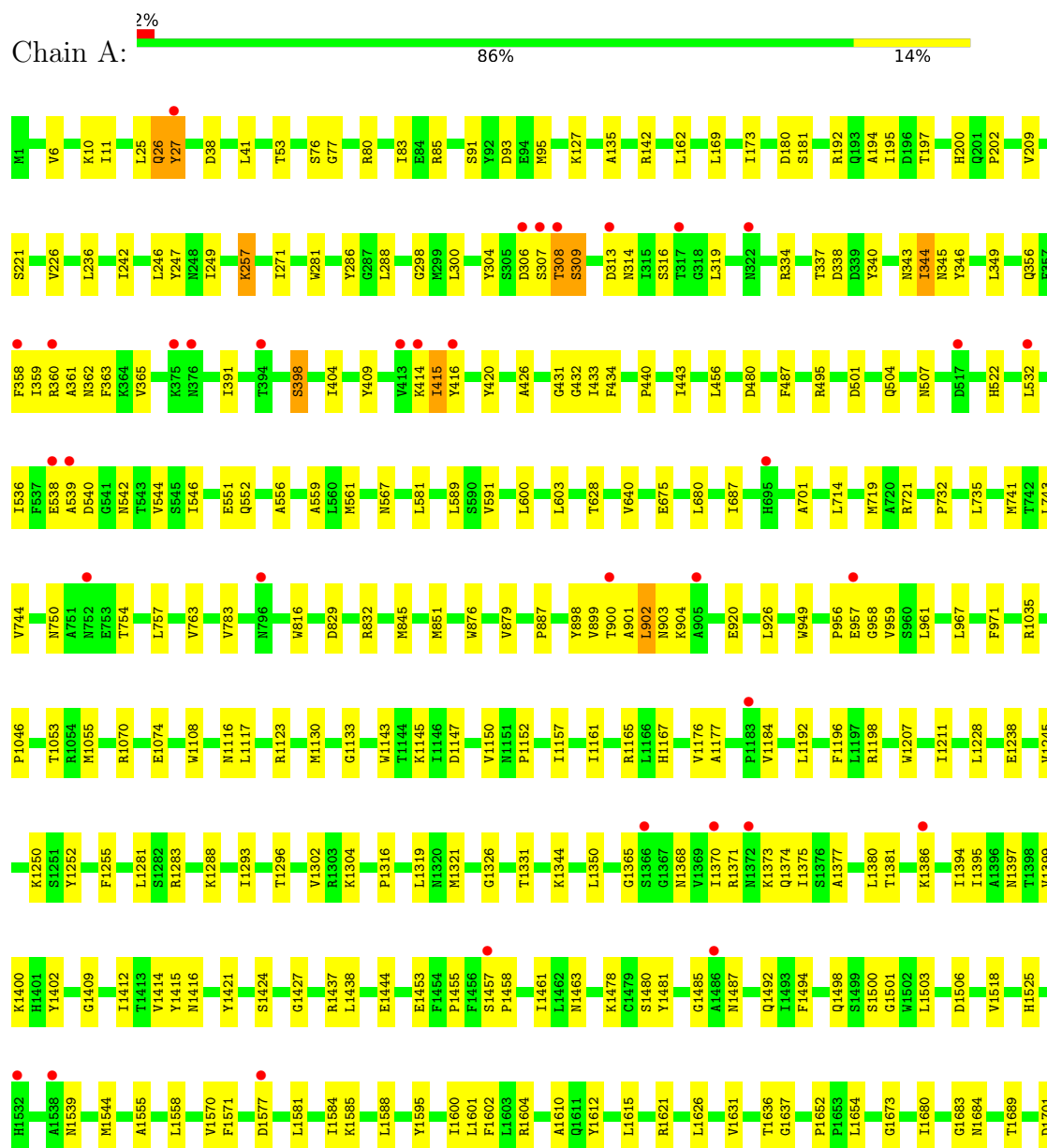
Continued from previous page...

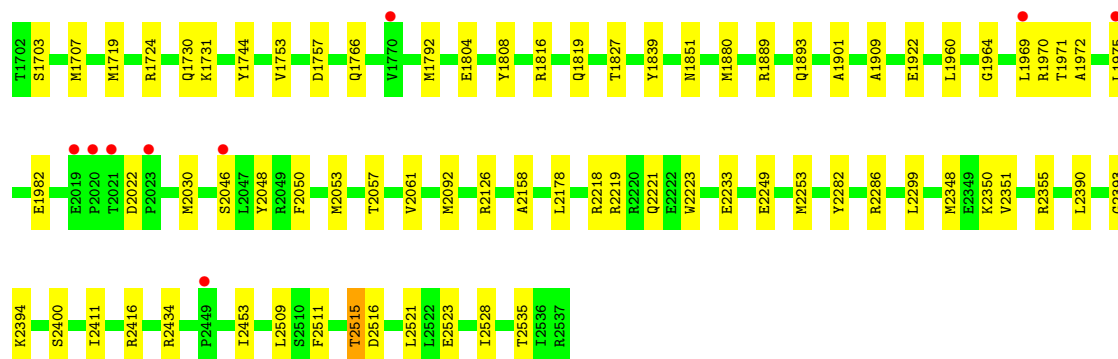
Chain	Residue	Modelled	Actual	Comment	Reference
E	1920	THR	ALA	conflict	UNP N1NRW3
E	1943	GLY	VAL	conflict	UNP N1NRW3
E	1947	GLN	HIS	conflict	UNP N1NRW3
E	1959	MSE	ALA	conflict	UNP N1NRW3
E	1961	GLY	ASP	conflict	UNP N1NRW3
E	1962	ARG	ASN	conflict	UNP N1NRW3
E	1964	GLY	GLU	conflict	UNP N1NRW3
E	1966	SER	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](#)

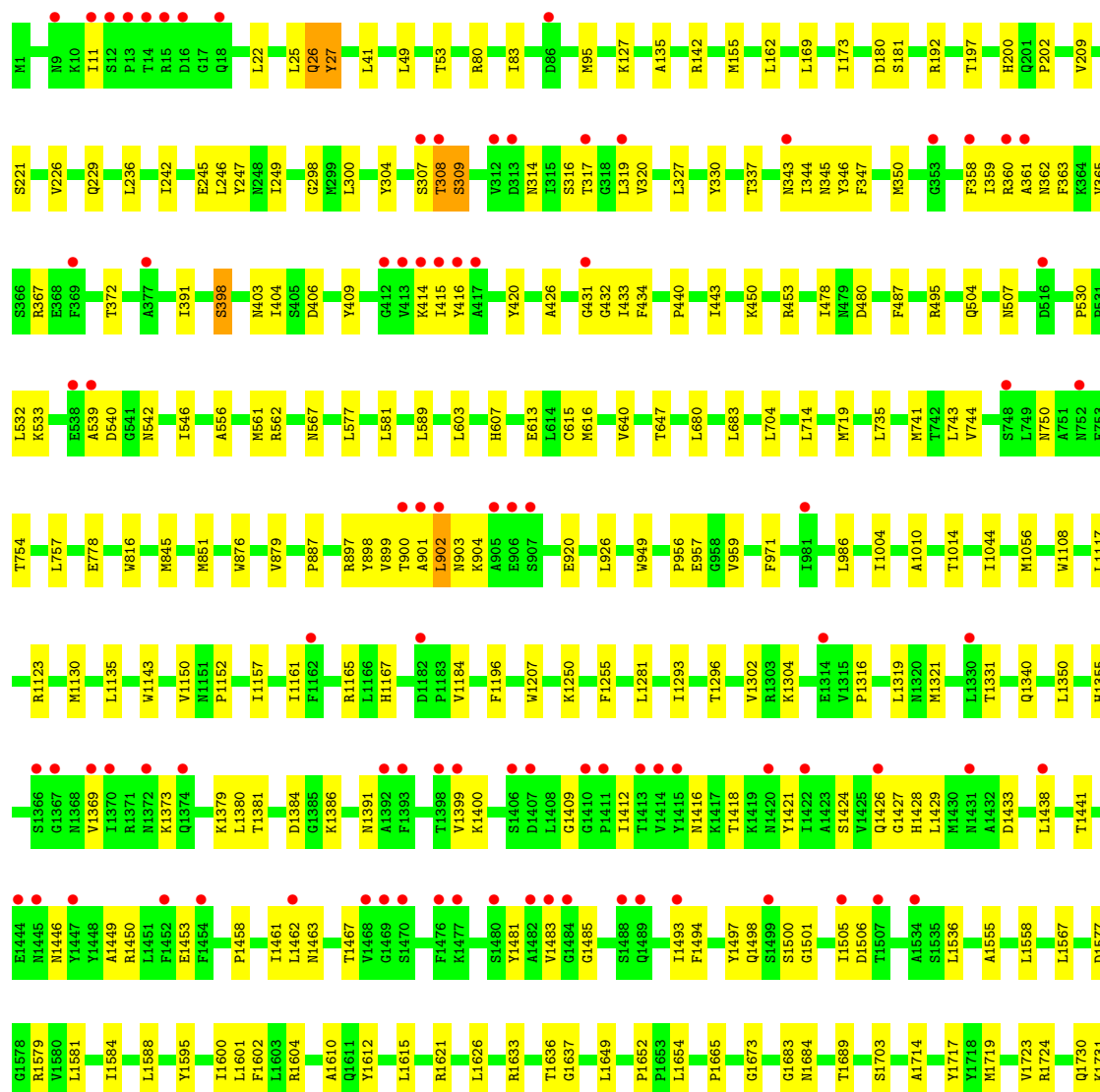
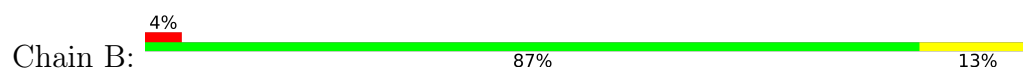
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

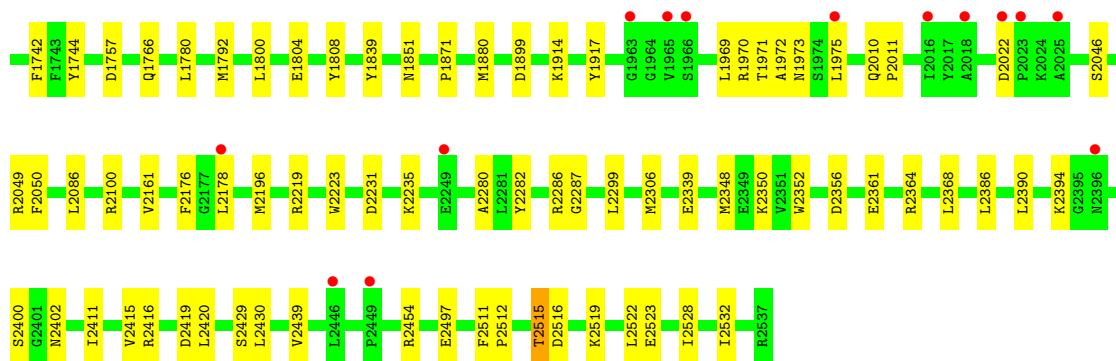
• Molecule 1: XptA2



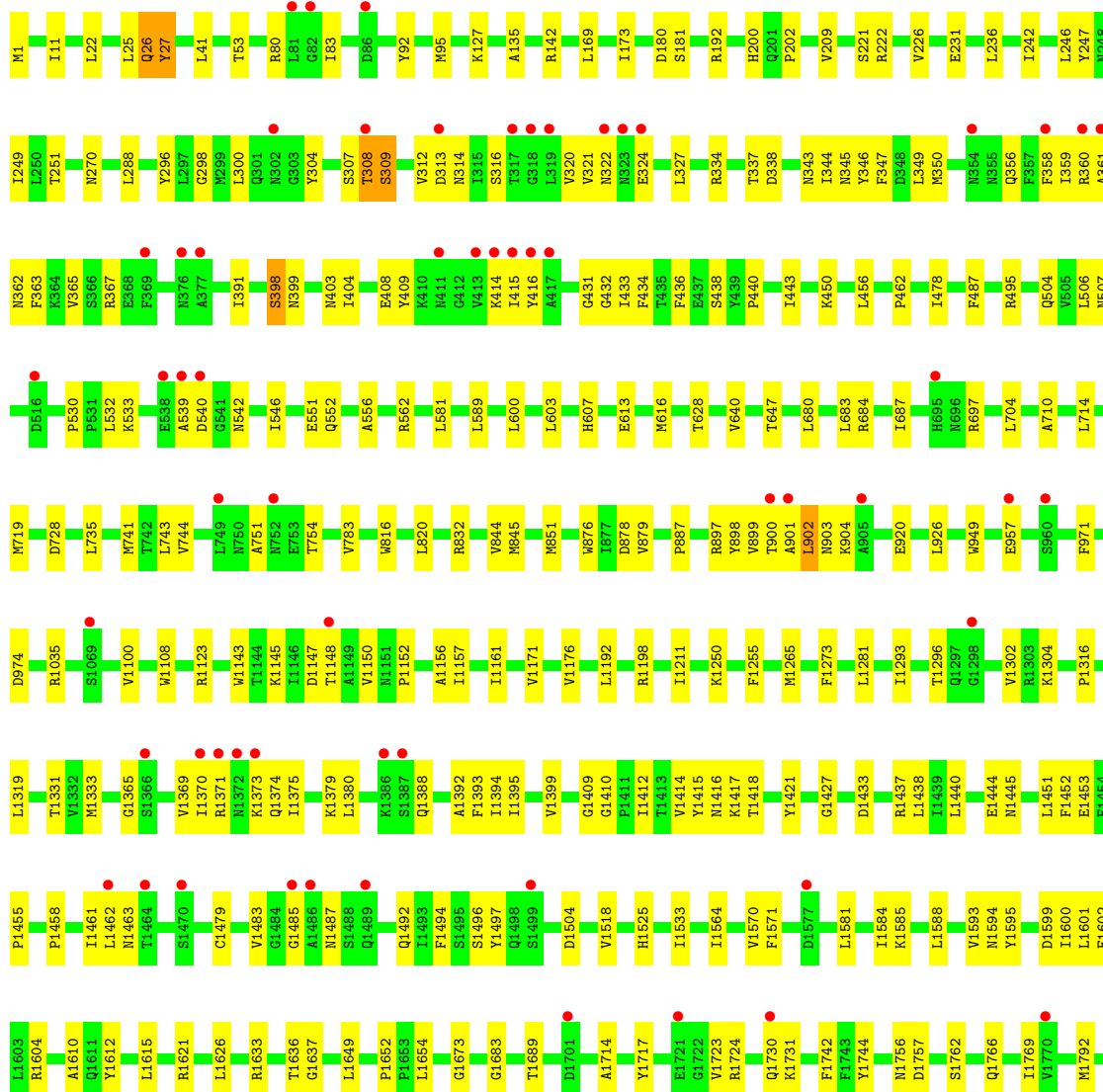
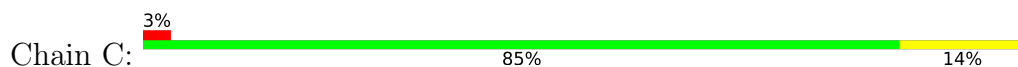


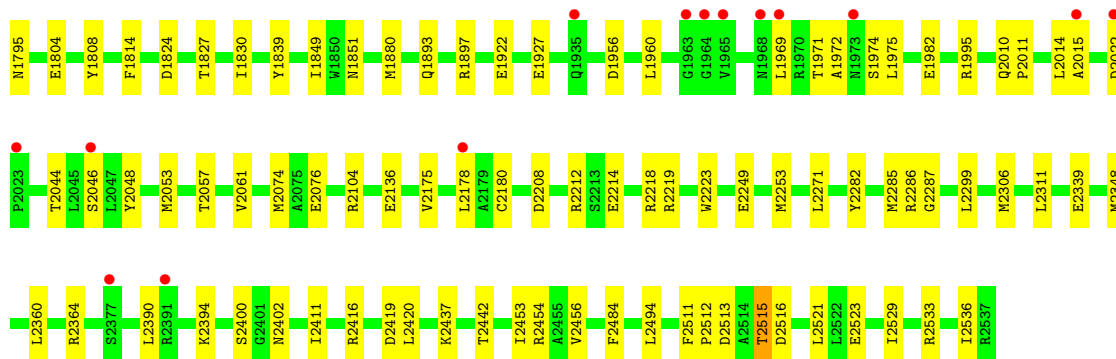
• Molecule 1: XptA2



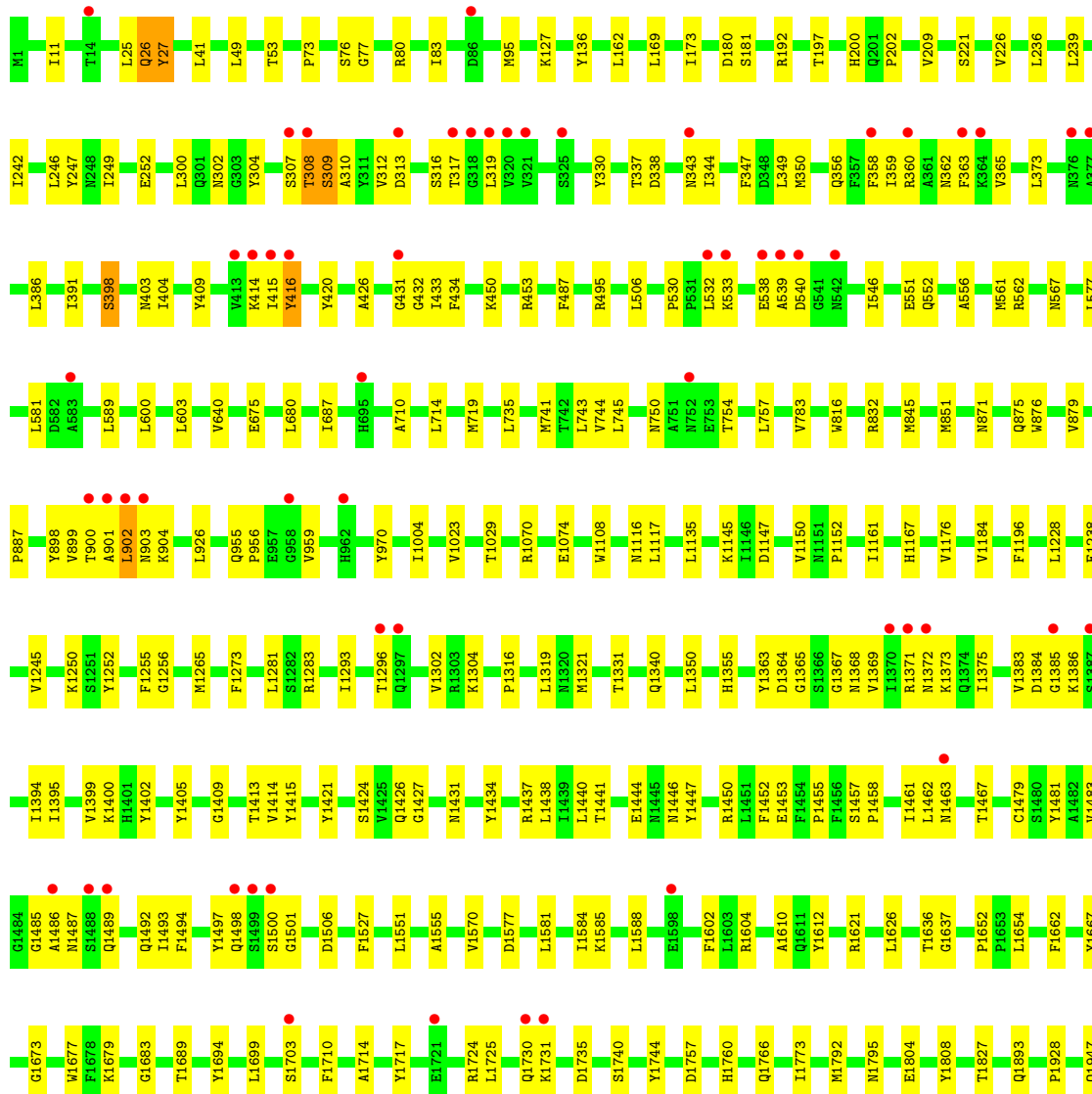
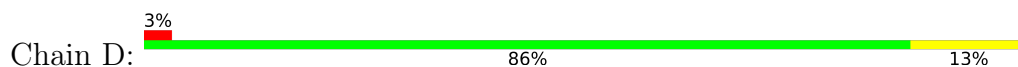


• Molecule 1: XptA2



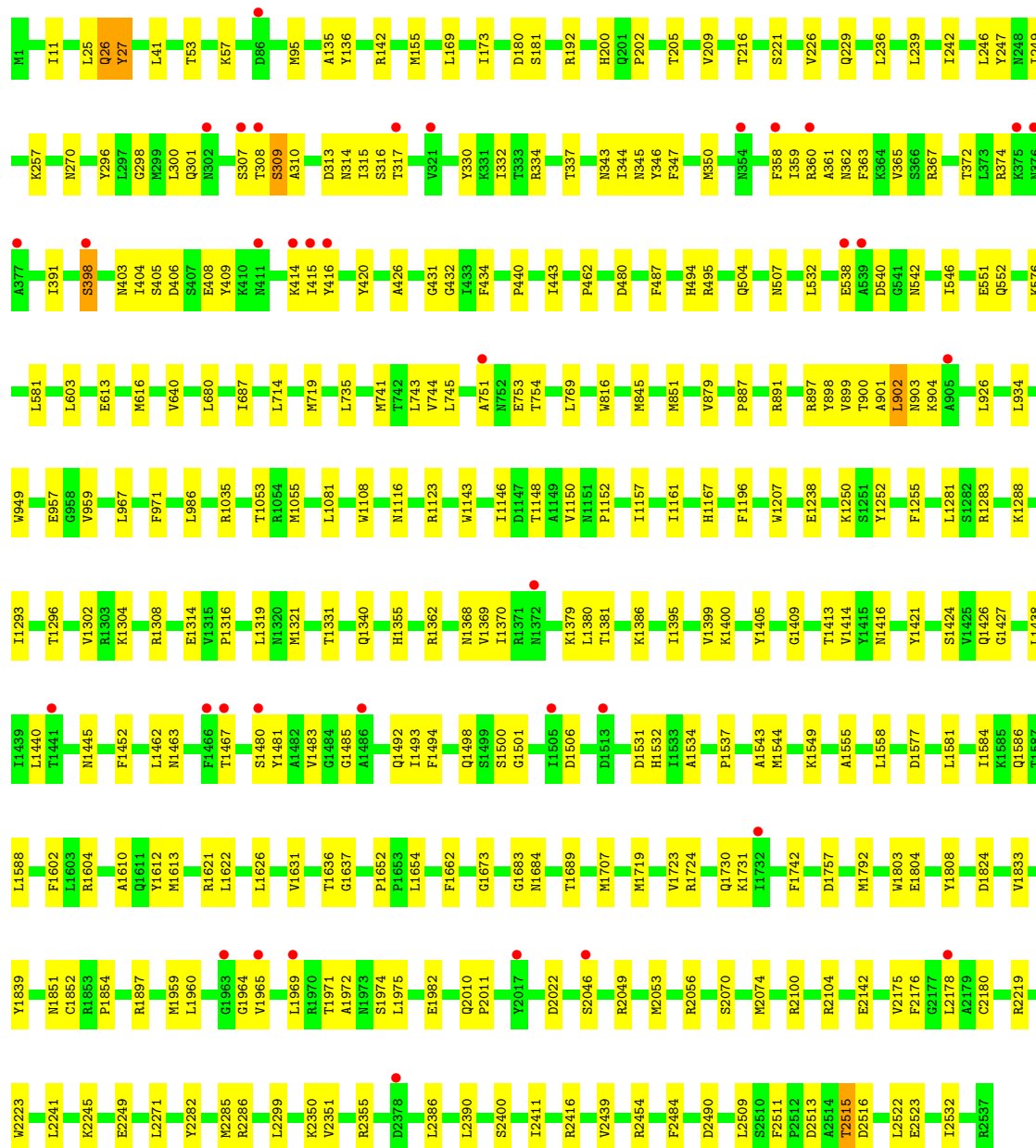
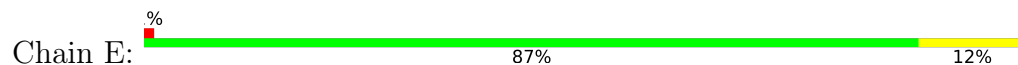


• Molecule 1: XptA2





• 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 [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	0.10	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.

The worst 5 of 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

There are no chirality outliers.

5 of 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

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
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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
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

5 of 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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1720	HIS
1	E	2010	GLN
1	D	2268	GLN
1	E	955	GLN
1	B	1199	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

The worst 5 of 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

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.