



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 08:33 PM UTC

PDB ID : 8TQE / pdb_00008tqe
EMDB ID : EMD-41503
Title : XptA2 wild type
Authors : Martin, C.L.; Binshtein, E.M.; Aller, S.G.
Deposited on : 2023-08-07
Resolution : 3.10 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

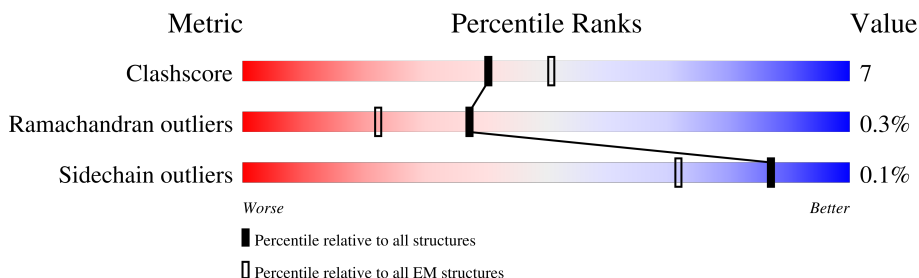
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

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

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 100035 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called XptA2.

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

There are 320 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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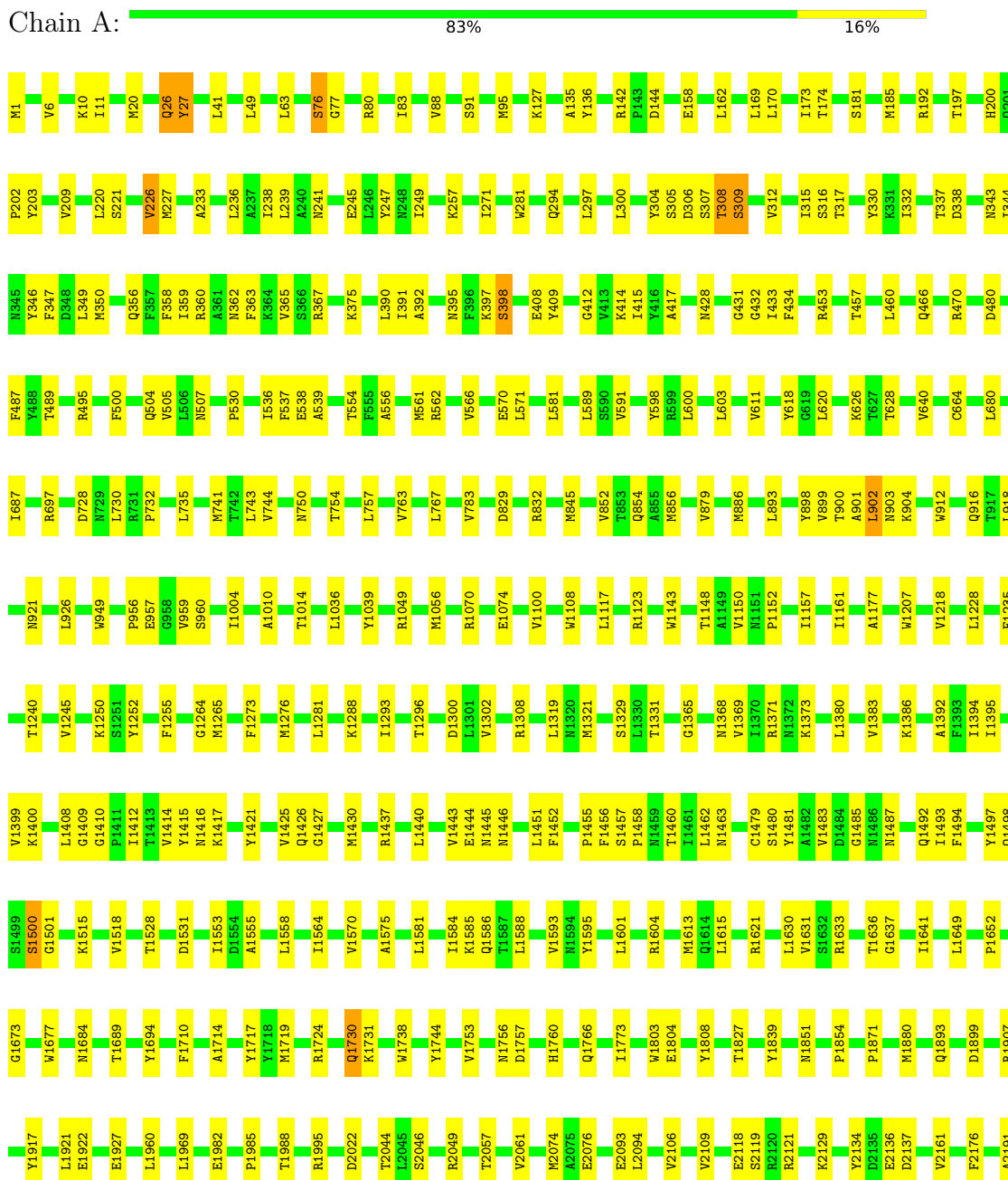
Continued from previous page...

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

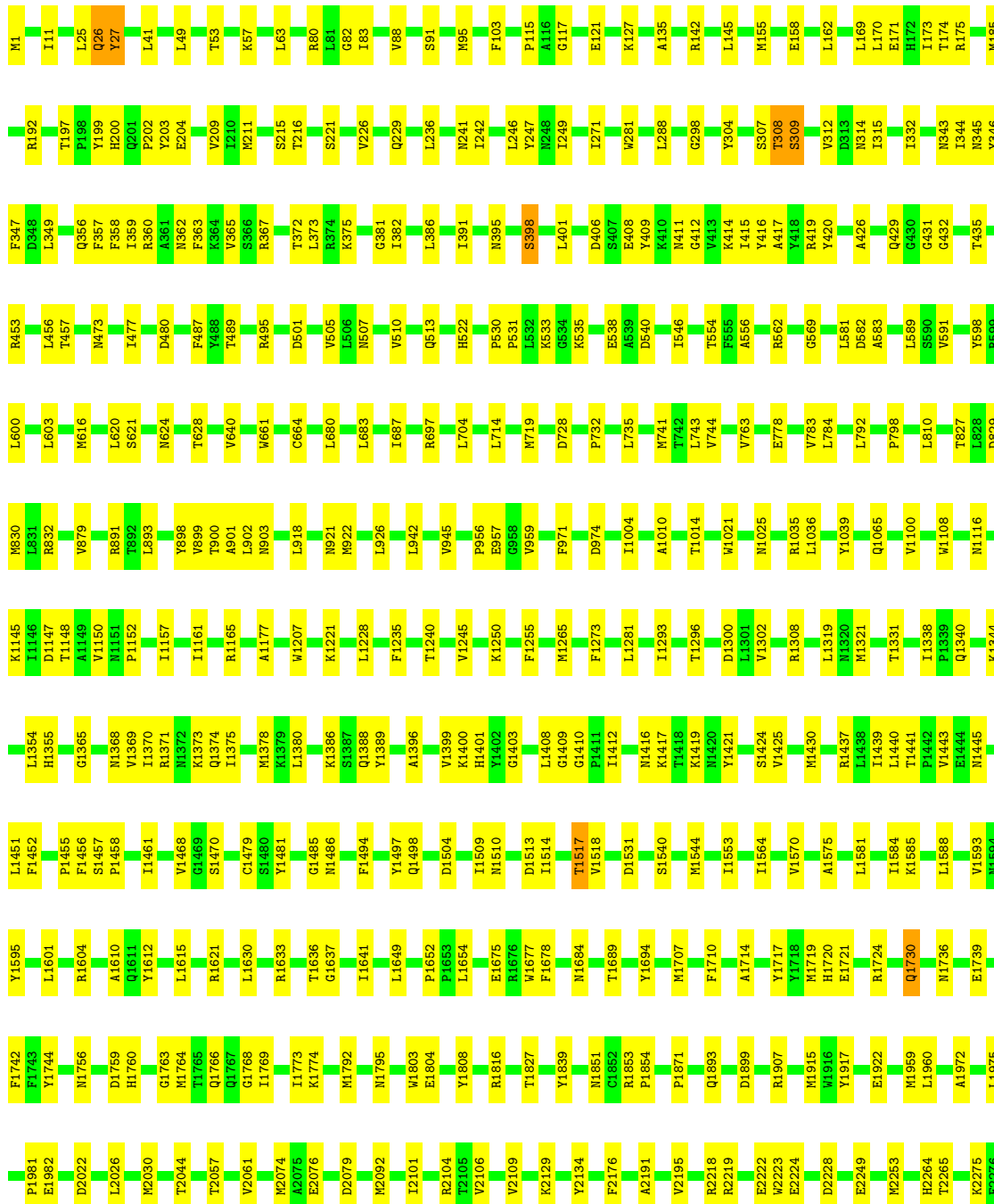
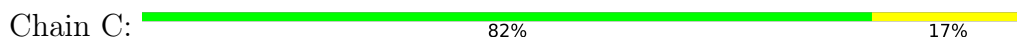
3 Residue-property plots

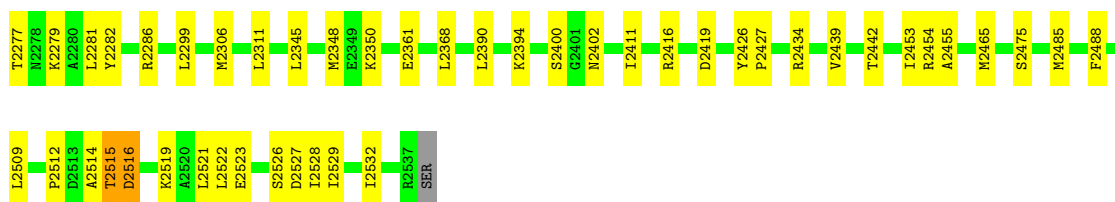
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

• Molecule 1: XptA2



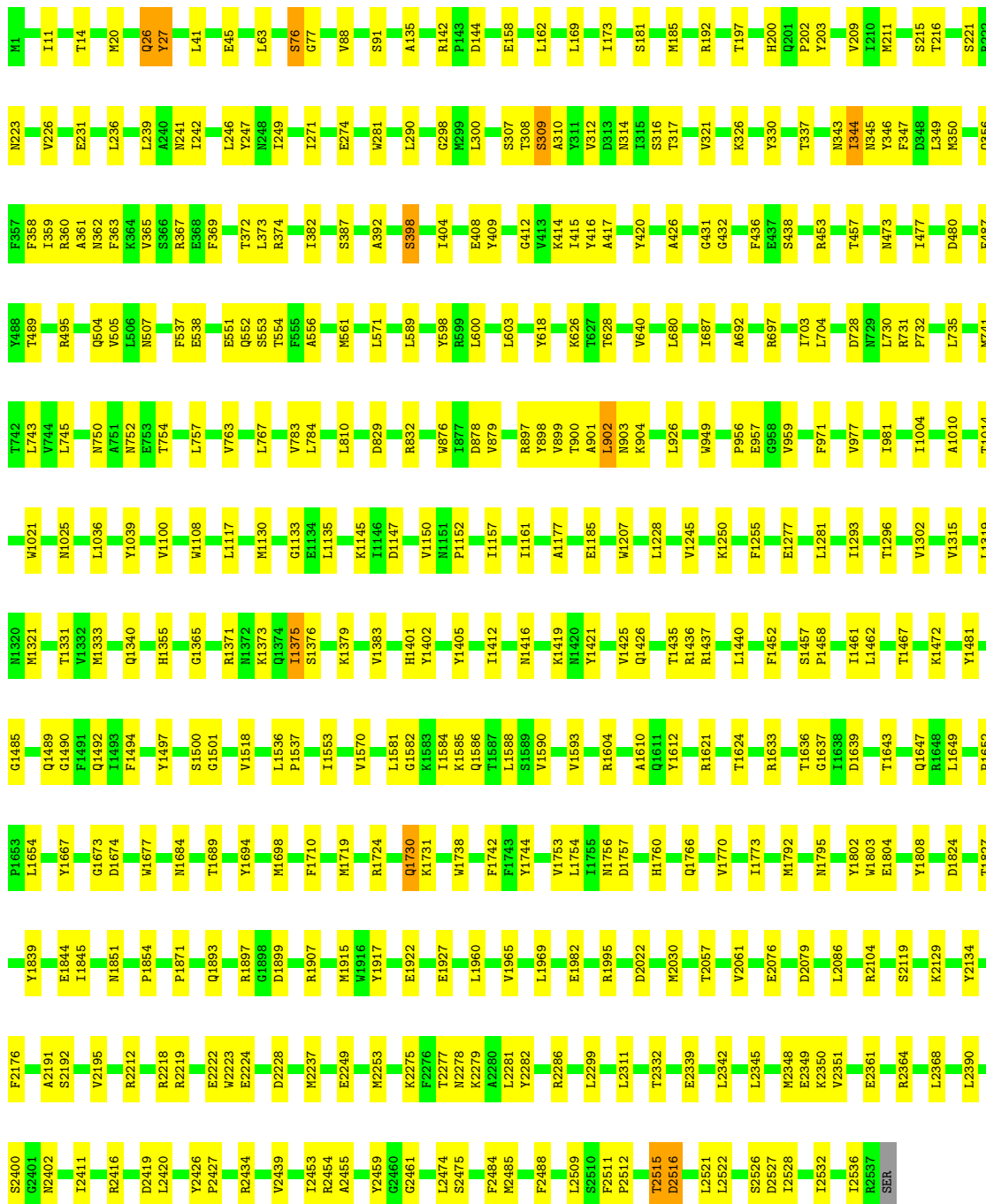
- Molecule 1: XptA2





• Molecule 1: XptA2

Chain D: 84% 15%



• Molecule 1: XptA2

Chain E:



R2218	R2434	L1960	R1724	I1514	I1412	F1255	P956	D690	D501	V365	L236	M1
R2219		L1969	R1730	T1517	M1416	M1265	E957	M691	Q504	S366	L239	I11
W2223	V2439	L1969	Q1730	V1518	K1417	F1273	Q958	D728	Q504	S367	L239	I11
E2224		L1972	K1731	L1536	T1418	F1273	W959	W729	V505	E368	A240	T14
D2228	T2442	A1972		P1537	K1419		L961	L730	N607	F369	N241	T14
T2453		L1975	F1742	I1553	N1420	L1281	L967	R731	G508	L373	L246	Q18
M2237		E1982	Y1744	I1553	Y1421	K1288	L967	P732	S509	R374	Y247	Q26
E2249					S1424		F971	I737	V510	I382	N248	Y27
					V1426	T1296			Q513		L249	
W2253	W2465	L1994	V1753	V1570	Q1426		T1004	V744	P530	S387	N270	L41
L2271	L2474	D2008	D1757	L1581	G1427	D1300	A1010	A751	P531	I391	L282	L49
	S2475	G2009	H1760	L1584	L1428	V1315		N752				Y50
		Q2010		K1585	M1430		T1014	E753	K535	N395	L283	
K2275	F2484	D2022	Q1766	Q1586	R1437	L1319	L1036	V763	F537	S398		I54
F2276	W2485			T1587	N1320	N1320			E538	N399	L297	I83
T2277		L2026	I1773	L1588	L1440	M1321	Y1039	L767	A539		G298	
K2278	F2488	M2030	D1793	V1593	M1445	T1331	V1100	V783	N403	I404	M299	S91
A2280	L2509		S1796	R1604		M1333		L784	G541		L300	
L2281		M2053			F1452		W1108		N542			K127
Y2282	A2514					Q1340		I804	T554	E408	Y304	
T2515	T2515	R2056	W1803	Y1612	P1455		M1116		F555	Y409	A135	
D2516	D2516	T2057	E1804	R1621	F1456	S1343	L1117	L810	A556	S307		
K2519			Y1808	R1633	S1457		D1126	D829	G412	T308	T308	R142
		V2061	T1827		P1458	H1355			V413	P143	S309	P143
L2311	L2822	A2062		T1636	I1461	N1368	I1127	R632	M561	K414	V312	
R2312	E2523	Q2063	Y1839	G1637	L1462	V1369	S1128		R562	I415	D313	E158
S2526		F2067			N1463	L1370	M1130	D839	V566	A417	N314	
D2527			N1851	L1649		R1371			Y418	Y418	L315	L162
M2348		E2076			T1467		L1135	I849	E570	R419	S316	
V2351	L2529		P1854	P1652		K1373			L571	Y420	V320	L169
E2354		D2079	P1871	P1653	K1478	Q1374	I1146	M856	L589	A426	V320	
R2364		E2093		L1654	C1479	I1375	D1147	N862	S590	Q929	L327	I173
K2385		I2101	M1880	G1673	Y1481	M1378	T1148		V591	L332	L332	S181
			M1881	W1677	L1482	K1379	A1149	V879	Y598	G430		D182
		R2104	Y1852		V1483	L1380	N1151		R599	G431	T337	M185
		S2119	Q1893	H1681	D1484		P1152	L893	L600	I433		
K2394			D1899	N1684	N1487	V1383	I1157	Y898	L603	F436	N343	R192
V2397		K2129	R1907	T1689	Q1492	Q1388	I1161	V899	L603	B453	N345	T197
S2400		Y2134	Y1917	G1690	I1493	D1384	A1177	T300	V606	Y345	T345	T197
L2406		F2176	L1921	R1691	F1494	A1396	T628	A801	L902	F347	D948	H200
T2411		A2191	E1922	Y1694	Y1497	A1396	E1185	N903	N903	T457	L349	Y203
				Q1498	Q1498	K1400	V640	K904	I641	D480	Q356	Q208
		V2195	Q1934	F1710	S1499	K1400	F1235	L318	W642	F357	F357	V209
R2416			S1946		S1500		T1240	L926	V646	F487	F358	L220
L2420		S2211		A1714	G1501	D1407		Y937	I676	R495	I359	S221
				Y1717	I1509	L1408	K1250				A361	
				Y1718	I1509	G1409	S1251			L498	N362	V226
		E2214	T1948	Y1718	M1510	G1410	Y1252	W849	L680	S499	F363	M227

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	198591	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	0.19	0/20413	0.41	10/27714 (0.0%)
1	B	0.19	0/20413	0.40	7/27714 (0.0%)
1	C	0.19	0/20413	0.41	8/27714 (0.0%)
1	D	0.19	0/20413	0.41	8/27714 (0.0%)
1	E	0.18	0/20413	0.40	6/27714 (0.0%)
All	All	0.19	0/102065	0.41	39/138570 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
All	All	0	7

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2515	THR	CA-C-N	15.35	149.34	121.70
1	D	2515	THR	C-N-CA	15.35	149.34	121.70
1	D	26	GLN	CA-C-N	14.95	148.61	121.70
1	D	26	GLN	C-N-CA	14.95	148.61	121.70
1	B	26	GLN	CA-C-N	14.73	148.22	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

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

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	19592	287	0
1	B	20007	0	19592	314	0
1	C	20007	0	19592	299	0
1	D	20007	0	19592	266	0
1	E	20007	0	19592	290	0
All	All	100035	0	97960	1376	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1376 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2515:THR:H	1:D:2516:ASP:HB2	1.36	0.90
1:A:2515:THR:H	1:A:2516:ASP:HB2	1.37	0.90
1:B:2515:THR:H	1:B:2516:ASP:HB2	1.36	0.89
1:E:2515:THR:H	1:E:2516:ASP:HB2	1.39	0.88
1:C:2515:THR:H	1:C:2516:ASP:HB2	1.40	0.87

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2535/2538 (100%)	2415 (95%)	112 (4%)	8 (0%)	36	67
1	B	2535/2538 (100%)	2420 (96%)	107 (4%)	8 (0%)	36	67
1	C	2535/2538 (100%)	2417 (95%)	111 (4%)	7 (0%)	36	67
1	D	2535/2538 (100%)	2426 (96%)	101 (4%)	8 (0%)	36	67
1	E	2535/2538 (100%)	2417 (95%)	110 (4%)	8 (0%)	36	67
All	All	12675/12690 (100%)	12095 (95%)	541 (4%)	39 (0%)	37	67

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2022	ASP
1	B	2516	ASP
1	D	2022	ASP
1	D	2516	ASP
1	E	27	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2108/2175 (97%)	2104 (100%)	4 (0%)	87	89
1	B	2172/2175 (100%)	2171 (100%)	1 (0%)	100	100
1	C	2172/2175 (100%)	2166 (100%)	6 (0%)	86	87
1	D	2172/2175 (100%)	2169 (100%)	3 (0%)	88	90
1	E	2172/2175 (100%)	2171 (100%)	1 (0%)	100	100
All	All	10796/10875 (99%)	10781 (100%)	15 (0%)	87	90

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1915	MET
1	D	1915	MET
1	C	2044	THR
1	E	961	LEU
1	D	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1684	ASN
1	D	507	ASN
1	E	1815	GLN
1	C	1692	GLN
1	C	2435	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 Map visualisation

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

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.