



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2025 – 08:28 AM JST

PDB ID : 9K1P / pdb_00009k1p
Title : crystal structure of Rtk- C2221
Authors : Xu, M.; Ran, T.; Wang, W.
Deposited on : 2024-10-16
Resolution : 2.89 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

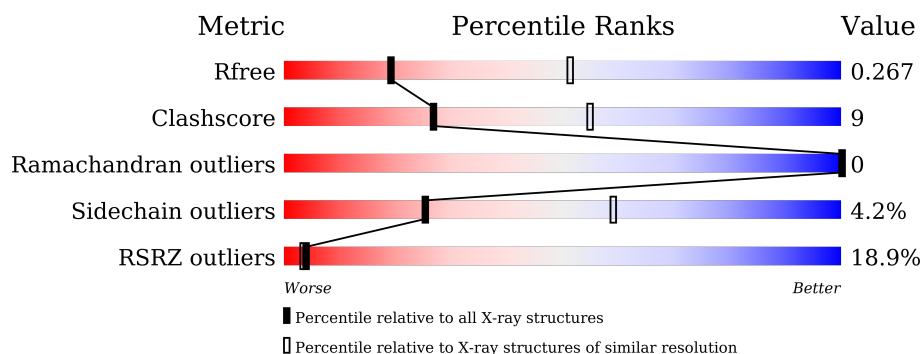
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	227	<div> <div>20%</div> <div>74%</div> <div>15%</div> <div>10%</div> </div>
1	B	227	<div> <div>15%</div> <div>79%</div> <div>11%</div> <div>9%</div> </div>
1	C	227	<div> <div>21%</div> <div>63%</div> <div>27%</div> <div>8%</div> </div>
1	D	227	<div> <div>20%</div> <div>74%</div> <div>18%</div> <div>7%</div> </div>
1	E	227	<div> <div>19%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>
1	F	227	<div> <div>19%</div> <div>73%</div> <div>16%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	227	<div><div></div><div>8%</div><div>69%</div><div>22%</div><div>8%</div></div>
1	H	227	<div><div></div><div>17%</div><div>62%</div><div>28%</div><div>10%</div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12491 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 Type VI secretion system-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	1	0
			1542	978	269	291	4			
1	B	207	Total	C	N	O	S	0	0	0
			1549	983	270	292	4			
1	C	209	Total	C	N	O	S	0	0	0
			1570	998	274	294	4			
1	D	210	Total	C	N	O	S	0	0	0
			1579	1004	276	295	4			
1	E	209	Total	C	N	O	S	0	0	0
			1570	998	274	294	4			
1	F	206	Total	C	N	O	S	0	0	0
			1542	978	269	291	4			
1	G	208	Total	C	N	O	S	0	0	0
			1562	992	273	293	4			
1	H	205	Total	C	N	O	S	0	0	0
			1537	975	268	290	4			

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP A0A2V4GN18
A	-11	PHE	-	expression tag	UNP A0A2V4GN18
A	-10	ALA	-	expression tag	UNP A0A2V4GN18
A	-9	LYS	-	expression tag	UNP A0A2V4GN18
A	-8	ILE	-	expression tag	UNP A0A2V4GN18
A	-7	GLU	-	expression tag	UNP A0A2V4GN18
A	-6	GLU	-	expression tag	UNP A0A2V4GN18
A	-5	GLY	-	expression tag	UNP A0A2V4GN18
A	-4	LYS	-	expression tag	UNP A0A2V4GN18
A	-3	LEU	-	expression tag	UNP A0A2V4GN18
A	-2	VAL	-	expression tag	UNP A0A2V4GN18
A	-1	ILE	-	expression tag	UNP A0A2V4GN18
A	0	HIS	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	ILE	conflict	UNP A0A2V4GN18
A	14	SER	THR	conflict	UNP A0A2V4GN18
A	40	SER	ALA	conflict	UNP A0A2V4GN18
A	87	VAL	ILE	conflict	UNP A0A2V4GN18
A	105	ILE	VAL	conflict	UNP A0A2V4GN18
A	120	THR	SER	conflict	UNP A0A2V4GN18
A	124	GLN	LYS	conflict	UNP A0A2V4GN18
A	147	THR	ASN	conflict	UNP A0A2V4GN18
A	153	VAL	LEU	conflict	UNP A0A2V4GN18
A	199	LEU	-	expression tag	UNP A0A2V4GN18
A	200	GLU	-	expression tag	UNP A0A2V4GN18
A	201	GLY	-	expression tag	UNP A0A2V4GN18
A	202	SER	-	expression tag	UNP A0A2V4GN18
A	203	GLU	-	expression tag	UNP A0A2V4GN18
A	204	PHE	-	expression tag	UNP A0A2V4GN18
A	205	LYS	-	expression tag	UNP A0A2V4GN18
A	206	LEU	-	expression tag	UNP A0A2V4GN18
A	207	VAL	-	expression tag	UNP A0A2V4GN18
A	208	ASP	-	expression tag	UNP A0A2V4GN18
A	209	HIS	-	expression tag	UNP A0A2V4GN18
A	210	HIS	-	expression tag	UNP A0A2V4GN18
A	211	HIS	-	expression tag	UNP A0A2V4GN18
A	212	HIS	-	expression tag	UNP A0A2V4GN18
A	213	HIS	-	expression tag	UNP A0A2V4GN18
A	214	HIS	-	expression tag	UNP A0A2V4GN18
B	-12	ALA	-	expression tag	UNP A0A2V4GN18
B	-11	PHE	-	expression tag	UNP A0A2V4GN18
B	-10	ALA	-	expression tag	UNP A0A2V4GN18
B	-9	LYS	-	expression tag	UNP A0A2V4GN18
B	-8	ILE	-	expression tag	UNP A0A2V4GN18
B	-7	GLU	-	expression tag	UNP A0A2V4GN18
B	-6	GLU	-	expression tag	UNP A0A2V4GN18
B	-5	GLY	-	expression tag	UNP A0A2V4GN18
B	-4	LYS	-	expression tag	UNP A0A2V4GN18
B	-3	LEU	-	expression tag	UNP A0A2V4GN18
B	-2	VAL	-	expression tag	UNP A0A2V4GN18
B	-1	ILE	-	expression tag	UNP A0A2V4GN18
B	0	HIS	-	expression tag	UNP A0A2V4GN18
B	1	MET	ILE	conflict	UNP A0A2V4GN18
B	14	SER	THR	conflict	UNP A0A2V4GN18
B	40	SER	ALA	conflict	UNP A0A2V4GN18
B	87	VAL	ILE	conflict	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
B	105	ILE	VAL	conflict	UNP A0A2V4GN18
B	120	THR	SER	conflict	UNP A0A2V4GN18
B	124	GLN	LYS	conflict	UNP A0A2V4GN18
B	147	THR	ASN	conflict	UNP A0A2V4GN18
B	153	VAL	LEU	conflict	UNP A0A2V4GN18
B	199	LEU	-	expression tag	UNP A0A2V4GN18
B	200	GLU	-	expression tag	UNP A0A2V4GN18
B	201	GLY	-	expression tag	UNP A0A2V4GN18
B	202	SER	-	expression tag	UNP A0A2V4GN18
B	203	GLU	-	expression tag	UNP A0A2V4GN18
B	204	PHE	-	expression tag	UNP A0A2V4GN18
B	205	LYS	-	expression tag	UNP A0A2V4GN18
B	206	LEU	-	expression tag	UNP A0A2V4GN18
B	207	VAL	-	expression tag	UNP A0A2V4GN18
B	208	ASP	-	expression tag	UNP A0A2V4GN18
B	209	HIS	-	expression tag	UNP A0A2V4GN18
B	210	HIS	-	expression tag	UNP A0A2V4GN18
B	211	HIS	-	expression tag	UNP A0A2V4GN18
B	212	HIS	-	expression tag	UNP A0A2V4GN18
B	213	HIS	-	expression tag	UNP A0A2V4GN18
B	214	HIS	-	expression tag	UNP A0A2V4GN18
C	-12	ALA	-	expression tag	UNP A0A2V4GN18
C	-11	PHE	-	expression tag	UNP A0A2V4GN18
C	-10	ALA	-	expression tag	UNP A0A2V4GN18
C	-9	LYS	-	expression tag	UNP A0A2V4GN18
C	-8	ILE	-	expression tag	UNP A0A2V4GN18
C	-7	GLU	-	expression tag	UNP A0A2V4GN18
C	-6	GLU	-	expression tag	UNP A0A2V4GN18
C	-5	GLY	-	expression tag	UNP A0A2V4GN18
C	-4	LYS	-	expression tag	UNP A0A2V4GN18
C	-3	LEU	-	expression tag	UNP A0A2V4GN18
C	-2	VAL	-	expression tag	UNP A0A2V4GN18
C	-1	ILE	-	expression tag	UNP A0A2V4GN18
C	0	HIS	-	expression tag	UNP A0A2V4GN18
C	1	MET	ILE	conflict	UNP A0A2V4GN18
C	14	SER	THR	conflict	UNP A0A2V4GN18
C	40	SER	ALA	conflict	UNP A0A2V4GN18
C	87	VAL	ILE	conflict	UNP A0A2V4GN18
C	105	ILE	VAL	conflict	UNP A0A2V4GN18
C	120	THR	SER	conflict	UNP A0A2V4GN18
C	124	GLN	LYS	conflict	UNP A0A2V4GN18
C	147	THR	ASN	conflict	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	153	VAL	LEU	conflict	UNP A0A2V4GN18
C	199	LEU	-	expression tag	UNP A0A2V4GN18
C	200	GLU	-	expression tag	UNP A0A2V4GN18
C	201	GLY	-	expression tag	UNP A0A2V4GN18
C	202	SER	-	expression tag	UNP A0A2V4GN18
C	203	GLU	-	expression tag	UNP A0A2V4GN18
C	204	PHE	-	expression tag	UNP A0A2V4GN18
C	205	LYS	-	expression tag	UNP A0A2V4GN18
C	206	LEU	-	expression tag	UNP A0A2V4GN18
C	207	VAL	-	expression tag	UNP A0A2V4GN18
C	208	ASP	-	expression tag	UNP A0A2V4GN18
C	209	HIS	-	expression tag	UNP A0A2V4GN18
C	210	HIS	-	expression tag	UNP A0A2V4GN18
C	211	HIS	-	expression tag	UNP A0A2V4GN18
C	212	HIS	-	expression tag	UNP A0A2V4GN18
C	213	HIS	-	expression tag	UNP A0A2V4GN18
C	214	HIS	-	expression tag	UNP A0A2V4GN18
D	-12	ALA	-	expression tag	UNP A0A2V4GN18
D	-11	PHE	-	expression tag	UNP A0A2V4GN18
D	-10	ALA	-	expression tag	UNP A0A2V4GN18
D	-9	LYS	-	expression tag	UNP A0A2V4GN18
D	-8	ILE	-	expression tag	UNP A0A2V4GN18
D	-7	GLU	-	expression tag	UNP A0A2V4GN18
D	-6	GLU	-	expression tag	UNP A0A2V4GN18
D	-5	GLY	-	expression tag	UNP A0A2V4GN18
D	-4	LYS	-	expression tag	UNP A0A2V4GN18
D	-3	LEU	-	expression tag	UNP A0A2V4GN18
D	-2	VAL	-	expression tag	UNP A0A2V4GN18
D	-1	ILE	-	expression tag	UNP A0A2V4GN18
D	0	HIS	-	expression tag	UNP A0A2V4GN18
D	1	MET	ILE	conflict	UNP A0A2V4GN18
D	14	SER	THR	conflict	UNP A0A2V4GN18
D	40	SER	ALA	conflict	UNP A0A2V4GN18
D	87	VAL	ILE	conflict	UNP A0A2V4GN18
D	105	ILE	VAL	conflict	UNP A0A2V4GN18
D	120	THR	SER	conflict	UNP A0A2V4GN18
D	124	GLN	LYS	conflict	UNP A0A2V4GN18
D	147	THR	ASN	conflict	UNP A0A2V4GN18
D	153	VAL	LEU	conflict	UNP A0A2V4GN18
D	199	LEU	-	expression tag	UNP A0A2V4GN18
D	200	GLU	-	expression tag	UNP A0A2V4GN18
D	201	GLY	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
D	202	SER	-	expression tag	UNP A0A2V4GN18
D	203	GLU	-	expression tag	UNP A0A2V4GN18
D	204	PHE	-	expression tag	UNP A0A2V4GN18
D	205	LYS	-	expression tag	UNP A0A2V4GN18
D	206	LEU	-	expression tag	UNP A0A2V4GN18
D	207	VAL	-	expression tag	UNP A0A2V4GN18
D	208	ASP	-	expression tag	UNP A0A2V4GN18
D	209	HIS	-	expression tag	UNP A0A2V4GN18
D	210	HIS	-	expression tag	UNP A0A2V4GN18
D	211	HIS	-	expression tag	UNP A0A2V4GN18
D	212	HIS	-	expression tag	UNP A0A2V4GN18
D	213	HIS	-	expression tag	UNP A0A2V4GN18
D	214	HIS	-	expression tag	UNP A0A2V4GN18
E	-12	ALA	-	expression tag	UNP A0A2V4GN18
E	-11	PHE	-	expression tag	UNP A0A2V4GN18
E	-10	ALA	-	expression tag	UNP A0A2V4GN18
E	-9	LYS	-	expression tag	UNP A0A2V4GN18
E	-8	ILE	-	expression tag	UNP A0A2V4GN18
E	-7	GLU	-	expression tag	UNP A0A2V4GN18
E	-6	GLU	-	expression tag	UNP A0A2V4GN18
E	-5	GLY	-	expression tag	UNP A0A2V4GN18
E	-4	LYS	-	expression tag	UNP A0A2V4GN18
E	-3	LEU	-	expression tag	UNP A0A2V4GN18
E	-2	VAL	-	expression tag	UNP A0A2V4GN18
E	-1	ILE	-	expression tag	UNP A0A2V4GN18
E	0	HIS	-	expression tag	UNP A0A2V4GN18
E	1	MET	ILE	conflict	UNP A0A2V4GN18
E	14	SER	THR	conflict	UNP A0A2V4GN18
E	40	SER	ALA	conflict	UNP A0A2V4GN18
E	87	VAL	ILE	conflict	UNP A0A2V4GN18
E	105	ILE	VAL	conflict	UNP A0A2V4GN18
E	120	THR	SER	conflict	UNP A0A2V4GN18
E	124	GLN	LYS	conflict	UNP A0A2V4GN18
E	147	THR	ASN	conflict	UNP A0A2V4GN18
E	153	VAL	LEU	conflict	UNP A0A2V4GN18
E	199	LEU	-	expression tag	UNP A0A2V4GN18
E	200	GLU	-	expression tag	UNP A0A2V4GN18
E	201	GLY	-	expression tag	UNP A0A2V4GN18
E	202	SER	-	expression tag	UNP A0A2V4GN18
E	203	GLU	-	expression tag	UNP A0A2V4GN18
E	204	PHE	-	expression tag	UNP A0A2V4GN18
E	205	LYS	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
E	206	LEU	-	expression tag	UNP A0A2V4GN18
E	207	VAL	-	expression tag	UNP A0A2V4GN18
E	208	ASP	-	expression tag	UNP A0A2V4GN18
E	209	HIS	-	expression tag	UNP A0A2V4GN18
E	210	HIS	-	expression tag	UNP A0A2V4GN18
E	211	HIS	-	expression tag	UNP A0A2V4GN18
E	212	HIS	-	expression tag	UNP A0A2V4GN18
E	213	HIS	-	expression tag	UNP A0A2V4GN18
E	214	HIS	-	expression tag	UNP A0A2V4GN18
F	-12	ALA	-	expression tag	UNP A0A2V4GN18
F	-11	PHE	-	expression tag	UNP A0A2V4GN18
F	-10	ALA	-	expression tag	UNP A0A2V4GN18
F	-9	LYS	-	expression tag	UNP A0A2V4GN18
F	-8	ILE	-	expression tag	UNP A0A2V4GN18
F	-7	GLU	-	expression tag	UNP A0A2V4GN18
F	-6	GLU	-	expression tag	UNP A0A2V4GN18
F	-5	GLY	-	expression tag	UNP A0A2V4GN18
F	-4	LYS	-	expression tag	UNP A0A2V4GN18
F	-3	LEU	-	expression tag	UNP A0A2V4GN18
F	-2	VAL	-	expression tag	UNP A0A2V4GN18
F	-1	ILE	-	expression tag	UNP A0A2V4GN18
F	0	HIS	-	expression tag	UNP A0A2V4GN18
F	1	MET	ILE	conflict	UNP A0A2V4GN18
F	14	SER	THR	conflict	UNP A0A2V4GN18
F	40	SER	ALA	conflict	UNP A0A2V4GN18
F	87	VAL	ILE	conflict	UNP A0A2V4GN18
F	105	ILE	VAL	conflict	UNP A0A2V4GN18
F	120	THR	SER	conflict	UNP A0A2V4GN18
F	124	GLN	LYS	conflict	UNP A0A2V4GN18
F	147	THR	ASN	conflict	UNP A0A2V4GN18
F	153	VAL	LEU	conflict	UNP A0A2V4GN18
F	199	LEU	-	expression tag	UNP A0A2V4GN18
F	200	GLU	-	expression tag	UNP A0A2V4GN18
F	201	GLY	-	expression tag	UNP A0A2V4GN18
F	202	SER	-	expression tag	UNP A0A2V4GN18
F	203	GLU	-	expression tag	UNP A0A2V4GN18
F	204	PHE	-	expression tag	UNP A0A2V4GN18
F	205	LYS	-	expression tag	UNP A0A2V4GN18
F	206	LEU	-	expression tag	UNP A0A2V4GN18
F	207	VAL	-	expression tag	UNP A0A2V4GN18
F	208	ASP	-	expression tag	UNP A0A2V4GN18
F	209	HIS	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
F	210	HIS	-	expression tag	UNP A0A2V4GN18
F	211	HIS	-	expression tag	UNP A0A2V4GN18
F	212	HIS	-	expression tag	UNP A0A2V4GN18
F	213	HIS	-	expression tag	UNP A0A2V4GN18
F	214	HIS	-	expression tag	UNP A0A2V4GN18
G	-12	ALA	-	expression tag	UNP A0A2V4GN18
G	-11	PHE	-	expression tag	UNP A0A2V4GN18
G	-10	ALA	-	expression tag	UNP A0A2V4GN18
G	-9	LYS	-	expression tag	UNP A0A2V4GN18
G	-8	ILE	-	expression tag	UNP A0A2V4GN18
G	-7	GLU	-	expression tag	UNP A0A2V4GN18
G	-6	GLU	-	expression tag	UNP A0A2V4GN18
G	-5	GLY	-	expression tag	UNP A0A2V4GN18
G	-4	LYS	-	expression tag	UNP A0A2V4GN18
G	-3	LEU	-	expression tag	UNP A0A2V4GN18
G	-2	VAL	-	expression tag	UNP A0A2V4GN18
G	-1	ILE	-	expression tag	UNP A0A2V4GN18
G	0	HIS	-	expression tag	UNP A0A2V4GN18
G	1	MET	ILE	conflict	UNP A0A2V4GN18
G	14	SER	THR	conflict	UNP A0A2V4GN18
G	40	SER	ALA	conflict	UNP A0A2V4GN18
G	87	VAL	ILE	conflict	UNP A0A2V4GN18
G	105	ILE	VAL	conflict	UNP A0A2V4GN18
G	120	THR	SER	conflict	UNP A0A2V4GN18
G	124	GLN	LYS	conflict	UNP A0A2V4GN18
G	147	THR	ASN	conflict	UNP A0A2V4GN18
G	153	VAL	LEU	conflict	UNP A0A2V4GN18
G	199	LEU	-	expression tag	UNP A0A2V4GN18
G	200	GLU	-	expression tag	UNP A0A2V4GN18
G	201	GLY	-	expression tag	UNP A0A2V4GN18
G	202	SER	-	expression tag	UNP A0A2V4GN18
G	203	GLU	-	expression tag	UNP A0A2V4GN18
G	204	PHE	-	expression tag	UNP A0A2V4GN18
G	205	LYS	-	expression tag	UNP A0A2V4GN18
G	206	LEU	-	expression tag	UNP A0A2V4GN18
G	207	VAL	-	expression tag	UNP A0A2V4GN18
G	208	ASP	-	expression tag	UNP A0A2V4GN18
G	209	HIS	-	expression tag	UNP A0A2V4GN18
G	210	HIS	-	expression tag	UNP A0A2V4GN18
G	211	HIS	-	expression tag	UNP A0A2V4GN18
G	212	HIS	-	expression tag	UNP A0A2V4GN18
G	213	HIS	-	expression tag	UNP A0A2V4GN18

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Chain	Residue	Modelled	Actual	Comment	Reference
G	214	HIS	-	expression tag	UNP A0A2V4GN18
H	-12	ALA	-	expression tag	UNP A0A2V4GN18
H	-11	PHE	-	expression tag	UNP A0A2V4GN18
H	-10	ALA	-	expression tag	UNP A0A2V4GN18
H	-9	LYS	-	expression tag	UNP A0A2V4GN18
H	-8	ILE	-	expression tag	UNP A0A2V4GN18
H	-7	GLU	-	expression tag	UNP A0A2V4GN18
H	-6	GLU	-	expression tag	UNP A0A2V4GN18
H	-5	GLY	-	expression tag	UNP A0A2V4GN18
H	-4	LYS	-	expression tag	UNP A0A2V4GN18
H	-3	LEU	-	expression tag	UNP A0A2V4GN18
H	-2	VAL	-	expression tag	UNP A0A2V4GN18
H	-1	ILE	-	expression tag	UNP A0A2V4GN18
H	0	HIS	-	expression tag	UNP A0A2V4GN18
H	1	MET	ILE	conflict	UNP A0A2V4GN18
H	14	SER	THR	conflict	UNP A0A2V4GN18
H	40	SER	ALA	conflict	UNP A0A2V4GN18
H	87	VAL	ILE	conflict	UNP A0A2V4GN18
H	105	ILE	VAL	conflict	UNP A0A2V4GN18
H	120	THR	SER	conflict	UNP A0A2V4GN18
H	124	GLN	LYS	conflict	UNP A0A2V4GN18
H	147	THR	ASN	conflict	UNP A0A2V4GN18
H	153	VAL	LEU	conflict	UNP A0A2V4GN18
H	199	LEU	-	expression tag	UNP A0A2V4GN18
H	200	GLU	-	expression tag	UNP A0A2V4GN18
H	201	GLY	-	expression tag	UNP A0A2V4GN18
H	202	SER	-	expression tag	UNP A0A2V4GN18
H	203	GLU	-	expression tag	UNP A0A2V4GN18
H	204	PHE	-	expression tag	UNP A0A2V4GN18
H	205	LYS	-	expression tag	UNP A0A2V4GN18
H	206	LEU	-	expression tag	UNP A0A2V4GN18
H	207	VAL	-	expression tag	UNP A0A2V4GN18
H	208	ASP	-	expression tag	UNP A0A2V4GN18
H	209	HIS	-	expression tag	UNP A0A2V4GN18
H	210	HIS	-	expression tag	UNP A0A2V4GN18
H	211	HIS	-	expression tag	UNP A0A2V4GN18
H	212	HIS	-	expression tag	UNP A0A2V4GN18
H	213	HIS	-	expression tag	UNP A0A2V4GN18
H	214	HIS	-	expression tag	UNP A0A2V4GN18

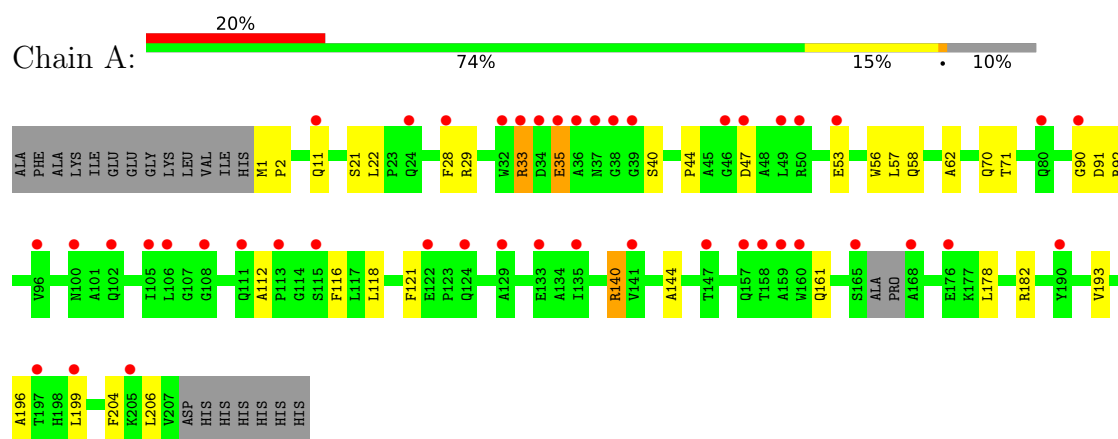
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	11	Total O 11 11	0	0
2	C	4	Total O 4 4	0	0
2	D	4	Total O 4 4	0	0
2	F	5	Total O 5 5	0	0
2	G	3	Total O 3 3	0	0
2	H	4	Total O 4 4	0	0

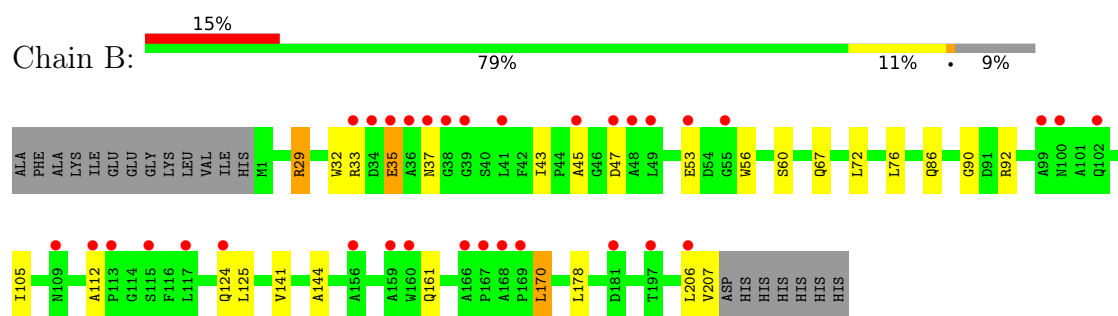
3 Residue-property plots [i](#)

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.

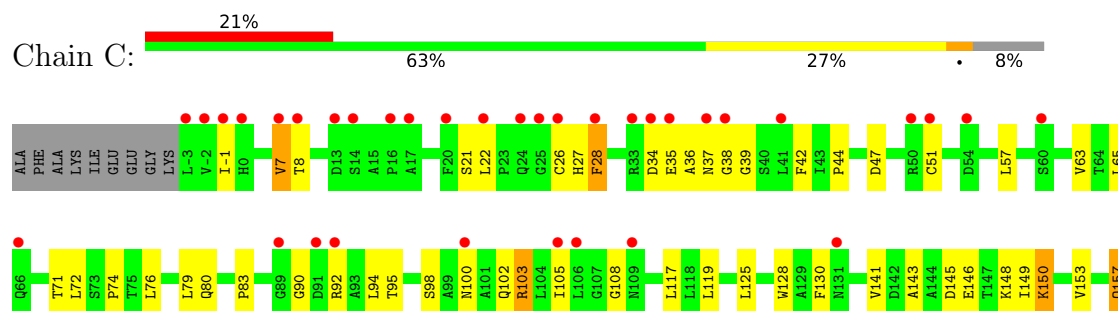
- Molecule 1: Type VI secretion system-associated protein



- Molecule 1: Type VI secretion system-associated protein

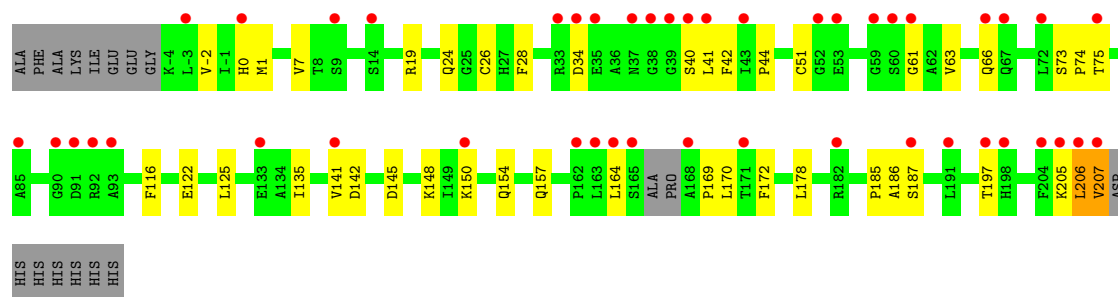
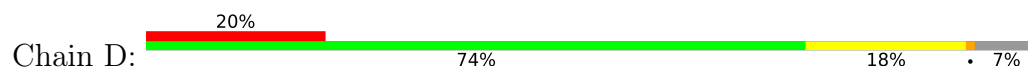


- Molecule 1: Type VI secretion system-associated protein

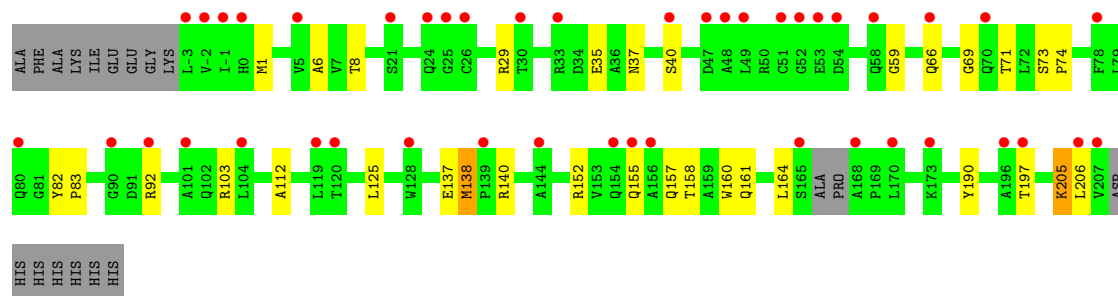
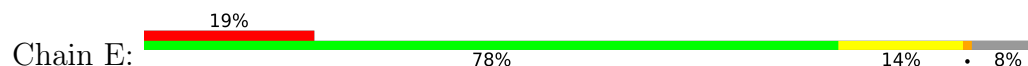




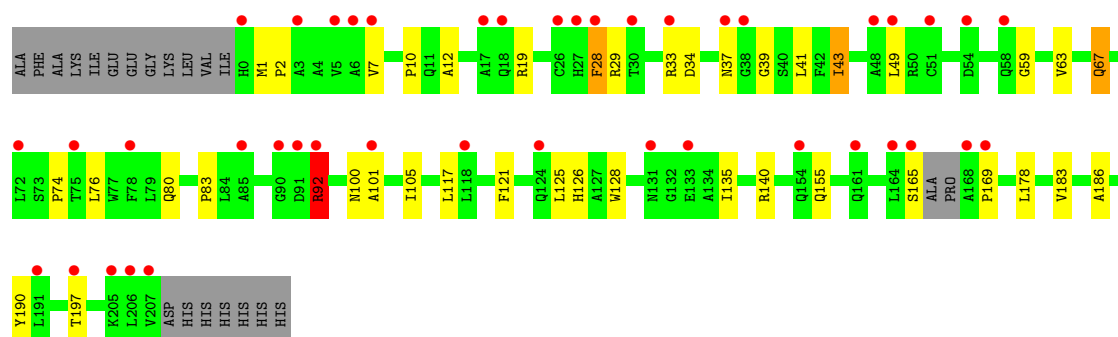
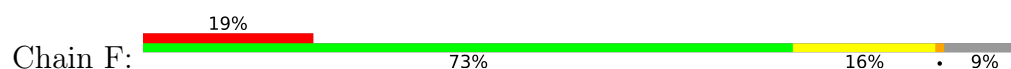
- Molecule 1: Type VI secretion system-associated protein



- Molecule 1: Type VI secretion system-associated protein

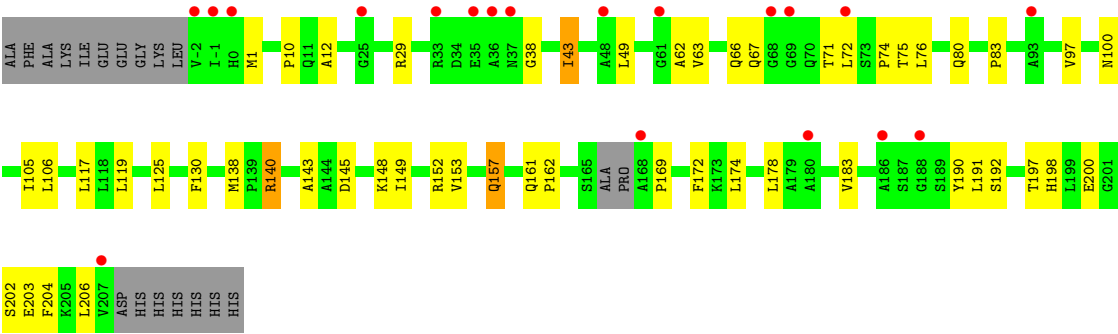


- Molecule 1: Type VI secretion system-associated protein

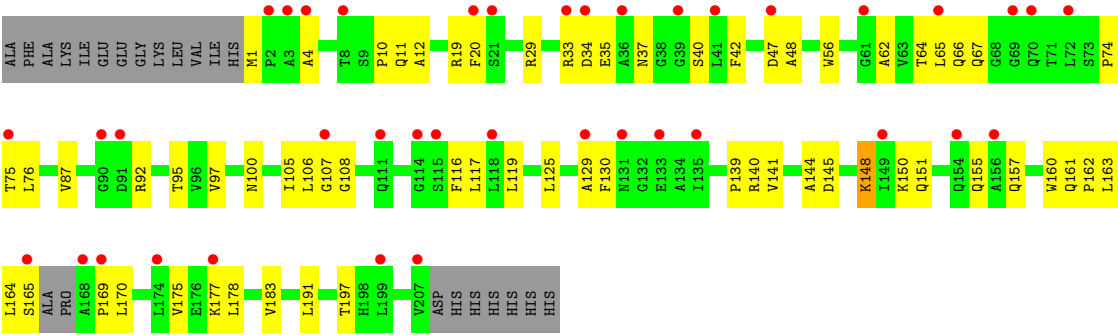


- Molecule 1: Type VI secretion system-associated protein





● Molecule 1: Type VI secretion system-associated protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	153.72Å 228.33Å 151.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.06 – 2.89 38.06 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.06-2.89) 88.6 (38.06-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.226 , 0.272 0.246 , 0.267	Depositor DCC
R_{free} test set	1991 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12491	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4717e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.93	0/1579	1.02	7/2154 (0.3%)
1	B	0.94	1/1588 (0.1%)	0.99	10/2168 (0.5%)
1	C	0.84	0/1608	1.17	4/2193 (0.2%)
1	D	0.69	0/1617	0.92	1/2204 (0.0%)
1	E	0.98	0/1608	1.03	11/2193 (0.5%)
1	F	0.83	0/1579	1.04	2/2153 (0.1%)
1	G	0.61	1/1600 (0.1%)	0.81	2/2182 (0.1%)
1	H	0.65	0/1574	0.85	3/2146 (0.1%)
All	All	0.82	2/12753 (0.0%)	0.98	40/17393 (0.2%)

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	C	0	2
1	F	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	43	ILE	CA-C	7.64	1.59	1.53
1	B	43	ILE	CA-C	6.25	1.58	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	GLY	N-CA-C	8.07	122.87	112.54
1	E	37	ASN	N-CA-C	-7.64	102.89	111.14
1	E	35	GLU	N-CA-C	-7.38	101.35	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	GLY	N-CA-C	6.91	120.85	112.49
1	A	90	GLY	N-CA-C	6.80	121.13	112.83
1	F	155	GLN	N-CA-C	-6.78	103.13	111.40
1	G	43	ILE	O-C-N	6.72	125.60	121.37
1	A	112	ALA	CA-C-N	-6.66	113.78	120.31
1	A	112	ALA	C-N-CA	-6.66	113.78	120.31
1	G	38	GLY	N-CA-C	-6.40	101.36	114.16
1	A	21	SER	N-CA-C	6.04	118.49	109.25
1	H	144	ALA	N-CA-C	-6.02	104.06	111.40
1	B	43	ILE	O-C-N	5.95	125.12	121.37
1	E	155	GLN	N-CA-C	-5.88	104.22	111.40
1	B	112	ALA	CA-C-N	-5.86	113.94	119.85
1	B	112	ALA	C-N-CA	-5.86	113.94	119.85
1	E	73	SER	CA-C-N	-5.83	113.96	120.14
1	E	73	SER	C-N-CA	-5.83	113.96	120.14
1	C	28	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	161	GLN	CA-C-N	-5.68	114.25	119.82
1	B	161	GLN	C-N-CA	-5.68	114.25	119.82
1	F	59	GLY	N-CA-C	5.67	118.65	111.85
1	B	125	LEU	N-CA-C	-5.64	106.39	113.72
1	E	103	ARG	N-CA-C	5.61	117.60	109.07
1	B	144	ALA	N-CA-C	-5.60	104.80	111.69
1	B	35	GLU	N-CA-C	-5.53	105.35	111.71
1	D	154	GLN	N-CA-C	-5.48	105.32	112.23
1	H	155	GLN	N-CA-C	-5.48	104.72	111.40
1	C	90	GLY	N-CA-C	5.43	119.45	112.83
1	C	35	GLU	N-CA-C	-5.35	105.92	113.20
1	E	205	LYS	CB-CG-CD	-5.35	98.99	111.30
1	A	28	PHE	N-CA-C	-5.30	101.12	109.50
1	A	144	ALA	N-CA-C	-5.29	105.59	111.36
1	H	35	GLU	N-CA-C	-5.25	105.58	112.72
1	B	86	GLN	N-CA-C	5.23	119.24	112.86
1	E	59	GLY	N-CA-C	5.22	118.36	111.52
1	A	161	GLN	N-CA-C	5.08	121.04	109.81
1	E	69	GLY	N-CA-C	-5.08	108.27	115.43
1	E	112	ALA	CA-C-N	-5.04	114.75	119.85
1	E	112	ALA	C-N-CA	-5.04	114.75	119.85

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Sidechain
1	C	103	ARG	Sidechain
1	C	182	ARG	Sidechain
1	F	92	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1542	0	1503	28	0
1	B	1549	0	1512	20	0
1	C	1570	0	1537	48	0
1	D	1579	0	1550	29	0
1	E	1570	0	1537	14	0
1	F	1542	0	1501	35	0
1	G	1562	0	1526	34	0
1	H	1537	0	1499	37	0
2	A	9	0	0	0	0
2	B	11	0	0	2	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	F	5	0	0	2	0
2	G	3	0	0	1	0
2	H	4	0	0	0	0
All	All	12491	0	12165	224	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 9.

All (224) 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:A:206:LEU:HD23	1:D:34:ASP:HB2	1.47	0.93
1:C:92:ARG:HD2	1:C:94:LEU:HD21	1.50	0.92
1:C:22:LEU:HD22	1:C:57:LEU:HD13	1.56	0.88
1:G:169:PRO:HG3	1:G:197:THR:HG23	1.54	0.87
1:B:33:ARG:HG3	2:B:302:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:PRO:HG2	1:C:76:LEU:HD11	1.57	0.82
1:A:70:GLN:HG2	1:A:71:THR:N	1.96	0.81
1:B:37:ASN:O	1:B:37:ASN:ND2	2.11	0.81
1:D:74:PRO:HG3	1:D:125:LEU:HD22	1.62	0.81
1:F:63:VAL:HG21	1:F:76:LEU:HD12	1.62	0.81
1:D:40:SER:HB2	1:D:66:GLN:HB2	1.61	0.81
1:A:33:ARG:NH2	1:A:121:PHE:CE2	2.49	0.80
1:C:22:LEU:CD2	1:C:57:LEU:HD13	2.11	0.79
1:G:138:MET:HE3	1:G:174:LEU:HD13	1.62	0.79
1:A:70:GLN:HG2	1:A:71:THR:H	1.48	0.78
1:C:92:ARG:CD	1:C:94:LEU:HD21	2.14	0.78
1:A:11:GLN:HA	1:A:182:ARG:HA	1.70	0.74
1:F:28:PHE:HZ	1:F:41:LEU:HD23	1.54	0.72
1:C:153:VAL:HG21	2:F:301:HOH:O	1.90	0.72
1:C:105:ILE:HG21	1:C:178:LEU:HD21	1.71	0.71
1:C:179:ALA:HB3	1:C:185:PRO:HA	1.75	0.69
1:F:28:PHE:HZ	1:F:41:LEU:CD2	2.05	0.68
1:B:32:TRP:HB3	1:C:206:LEU:HD22	1.76	0.68
1:C:79:LEU:HG	1:C:80:GLN:HG2	1.76	0.67
1:F:135:ILE:HD12	1:F:186:ALA:HB2	1.76	0.67
1:H:74:PRO:HG3	1:H:125:LEU:HD22	1.74	0.67
1:A:33:ARG:NH2	1:A:121:PHE:CD2	2.63	0.67
1:A:22:LEU:CD1	1:A:57:LEU:HD13	2.25	0.66
1:C:72:LEU:N	1:C:72:LEU:HD12	2.12	0.64
1:B:72:LEU:HD11	1:B:124:GLN:NE2	2.12	0.64
1:D:7:VAL:HG23	1:D:187:SER:HB3	1.80	0.64
1:A:22:LEU:HD12	1:A:57:LEU:HD13	1.79	0.63
1:B:33:ARG:HG2	2:B:311:HOH:O	1.98	0.63
1:D:157:GLN:HG2	1:D:172:PHE:HZ	1.63	0.63
1:F:29:ARG:O	1:F:83:PRO:HD3	1.99	0.63
1:F:28:PHE:CZ	1:F:41:LEU:CD2	2.82	0.62
1:H:1:MET:HE2	1:H:141:VAL:HA	1.81	0.62
1:F:33:ARG:HH12	1:F:101:ALA:HB1	1.65	0.61
1:H:117:LEU:HD22	1:H:130:PHE:CE1	2.35	0.61
1:F:169:PRO:HG3	1:F:197:THR:HG23	1.82	0.61
1:H:62:ALA:HB2	1:H:75:THR:HG22	1.83	0.60
1:H:95:THR:HG22	1:H:107:GLY:C	2.27	0.59
1:H:160:TRP:O	1:H:164:LEU:HG	2.02	0.59
1:H:4:ALA:HB2	1:H:140:ARG:NH1	2.16	0.59
1:G:145:ASP:HB3	1:G:148:LYS:HD2	1.85	0.58
1:C:153:VAL:CG2	2:F:301:HOH:O	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:CD2	1:D:34:ASP:HB2	2.30	0.57
1:F:34:ASP:HA	1:F:37:ASN:HD21	1.69	0.57
1:G:63:VAL:HB	1:G:76:LEU:CD1	2.34	0.57
1:C:71:THR:C	1:C:72:LEU:HD12	2.28	0.57
1:C:21:SER:HG	1:C:27:HIS:CD2	2.22	0.57
1:D:206:LEU:O	1:D:207:VAL:C	2.48	0.57
1:G:80:GLN:NE2	2:G:301:HOH:O	2.36	0.57
1:C:21:SER:OG	1:C:27:HIS:NE2	2.37	0.56
1:C:179:ALA:O	1:C:185:PRO:HA	2.06	0.56
1:F:28:PHE:CZ	1:F:41:LEU:HD23	2.40	0.56
1:A:199:LEU:CD1	1:G:203:GLU:HB2	2.36	0.56
1:C:72:LEU:N	1:C:72:LEU:CD1	2.69	0.55
1:D:61:GLY:C	1:D:75:THR:HG23	2.31	0.55
1:C:92:ARG:HD2	1:C:94:LEU:CD2	2.32	0.55
1:C:95:THR:HG23	1:C:108:GLY:HA3	1.89	0.55
1:H:95:THR:HG22	1:H:108:GLY:N	2.21	0.55
1:B:72:LEU:HD12	1:B:124:GLN:HG2	1.89	0.55
1:G:204:PHE:CD2	1:H:20:PHE:HD2	2.24	0.55
1:D:157:GLN:HG2	1:D:172:PHE:CZ	2.42	0.54
1:C:7:VAL:HG12	1:C:187:SER:HB3	1.88	0.54
1:D:19:ARG:HG2	1:G:191:LEU:HD11	1.88	0.54
1:C:83:PRO:HD2	1:C:128:TRP:HZ3	1.73	0.54
1:F:29:ARG:HD3	1:F:80:GLN:O	2.08	0.53
1:C:63:VAL:HB	1:C:76:LEU:HD13	1.89	0.53
1:F:74:PRO:HG3	1:F:125:LEU:HD22	1.90	0.53
1:G:74:PRO:HG3	1:G:125:LEU:HD22	1.91	0.53
1:H:175:VAL:HG22	1:H:177:LYS:H	1.74	0.53
1:F:2:PRO:HB2	1:F:140:ARG:HG2	1.90	0.53
1:B:206:LEU:HD23	1:C:34:ASP:HB2	1.91	0.52
1:F:63:VAL:HG22	1:F:76:LEU:HG	1.92	0.52
1:F:63:VAL:O	1:F:74:PRO:HD2	2.09	0.52
1:F:63:VAL:HG21	1:F:76:LEU:CD1	2.35	0.51
1:G:161:GLN:HG3	1:G:162:PRO:HD3	1.93	0.51
1:B:72:LEU:CD1	1:B:124:GLN:HG2	2.40	0.51
1:G:153:VAL:HG13	1:G:172:PHE:CG	2.46	0.51
1:G:157:GLN:O	1:G:161:GLN:HG2	2.11	0.51
1:F:28:PHE:CZ	1:F:41:LEU:HD21	2.46	0.51
1:A:47:ASP:HB2	1:B:47:ASP:C	2.36	0.50
1:D:116:PHE:CD1	1:D:178:LEU:HD22	2.47	0.50
1:F:37:ASN:HB2	1:F:67:GLN:HG3	1.93	0.50
1:C:42:PHE:O	1:C:44:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASN:OD1	1:C:38:GLY:N	2.45	0.49
1:G:62:ALA:HA	1:G:75:THR:HA	1.94	0.49
1:H:29:ARG:HD2	1:H:56:TRP:CZ3	2.48	0.49
1:D:1:MET:HE2	1:D:141:VAL:HA	1.92	0.49
1:C:21:SER:OG	1:C:27:HIS:CD2	2.65	0.49
1:F:7:VAL:HG23	1:F:7:VAL:O	2.12	0.49
1:H:40:SER:O	1:H:65:LEU:HA	2.13	0.49
1:C:157:GLN:HG2	1:C:172:PHE:HZ	1.78	0.49
1:D:24:GLN:CD	1:D:24:GLN:H	2.21	0.48
1:A:11:GLN:OE1	1:A:11:GLN:N	2.43	0.48
1:C:203:GLU:HB3	1:E:197:THR:HG23	1.94	0.48
1:C:98:SER:HB3	1:C:105:ILE:HD12	1.96	0.48
1:F:12:ALA:HB1	1:F:100:ASN:ND2	2.29	0.48
1:G:117:LEU:HD22	1:G:130:PHE:CE1	2.49	0.48
1:D:135:ILE:HG21	1:D:178:LEU:HD13	1.96	0.48
1:G:12:ALA:HB1	1:G:100:ASN:ND2	2.28	0.48
1:H:10:PRO:O	1:H:183:VAL:HG23	2.14	0.48
1:C:92:ARG:CD	1:C:94:LEU:CD2	2.89	0.48
1:D:135:ILE:CD1	1:D:186:ALA:HB2	2.43	0.48
1:A:196:ALA:HB2	1:G:204:PHE:CZ	2.49	0.47
1:D:-2:VAL:HG23	1:D:-2:VAL:O	2.15	0.47
1:A:193:VAL:HA	1:H:19:ARG:HB2	1.97	0.47
1:H:62:ALA:HA	1:H:75:THR:HA	1.97	0.47
1:B:45:ALA:HB3	1:C:200:GLU:HG2	1.97	0.47
1:D:164:LEU:CD1	1:D:170:LEU:HD11	2.45	0.47
1:H:145:ASP:HB3	1:H:148:LYS:HB2	1.97	0.47
1:D:26:CYS:HB3	1:D:51:CYS:HB3	1.83	0.47
1:G:105:ILE:HG21	1:G:178:LEU:HD21	1.97	0.46
1:A:206:LEU:HD23	1:D:34:ASP:CB	2.32	0.46
1:C:34:ASP:C	1:C:36:ALA:H	2.23	0.46
1:F:140:ARG:HG3	1:F:190:TYR:CE2	2.51	0.46
1:D:145:ASP:HB3	1:D:148:LYS:HG3	1.97	0.46
1:E:138:MET:HE2	1:E:138:MET:HB2	1.66	0.46
1:H:62:ALA:CB	1:H:75:THR:HG22	2.46	0.46
1:E:66:GLN:HG2	1:E:71:THR:HG23	1.98	0.46
1:H:33:ARG:O	1:H:34:ASP:C	2.59	0.46
1:C:157:GLN:HG2	1:C:172:PHE:CZ	2.51	0.46
1:C:74:PRO:HG3	1:C:125:LEU:HD22	1.98	0.45
1:C:146:GLU:CD	1:F:19:ARG:HH22	2.24	0.45
1:G:66:GLN:HG3	1:G:71:THR:OG1	2.16	0.45
1:E:137:GLU:O	1:E:152:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:PRO:HD2	1:F:128:TRP:HZ3	1.80	0.45
1:A:29:ARG:HD2	1:A:56:TRP:CZ3	2.51	0.45
1:A:116:PHE:CD2	1:A:178:LEU:HD22	2.51	0.45
1:F:105:ILE:HG21	1:F:178:LEU:HD21	1.97	0.45
1:G:29:ARG:HD3	1:G:80:GLN:O	2.17	0.45
1:E:40:SER:HG	1:E:66:GLN:HB2	1.82	0.45
1:E:160:TRP:O	1:E:161:GLN:C	2.59	0.45
1:E:161:GLN:HA	1:E:164:LEU:HD12	1.98	0.45
1:C:145:ASP:HB3	1:C:148:LYS:HG3	1.97	0.45
1:G:1:MET:HE3	1:G:1:MET:HB2	1.63	0.44
1:F:28:PHE:CE2	1:F:43:ILE:HD11	2.52	0.44
1:F:10:PRO:O	1:F:183:VAL:HG23	2.17	0.44
1:G:10:PRO:O	1:G:183:VAL:HG23	2.17	0.44
1:A:1:MET:HA	1:A:2:PRO:HD3	1.91	0.44
1:B:105:ILE:HG21	1:B:178:LEU:HD21	2.00	0.44
1:H:119:LEU:HD23	1:H:130:PHE:N	2.32	0.44
1:A:204:PHE:HB2	1:D:41:LEU:HB3	1.99	0.44
1:G:12:ALA:HB1	1:G:100:ASN:HD21	1.83	0.44
1:G:106:LEU:HD22	1:G:119:LEU:HD11	1.99	0.44
1:H:116:PHE:CD1	1:H:178:LEU:HD22	2.53	0.44
1:H:139:PRO:HB2	1:H:141:VAL:HG12	2.00	0.44
1:H:37:ASN:HB3	1:H:67:GLN:NE2	2.33	0.44
1:H:169:PRO:HG3	1:H:197:THR:CG2	2.48	0.44
1:A:33:ARG:HH21	1:A:121:PHE:HE2	1.63	0.43
1:B:29:ARG:HD2	1:B:56:TRP:CZ3	2.53	0.43
1:G:140:ARG:HG3	1:G:190:TYR:CD2	2.53	0.43
1:E:6:ALA:O	1:E:8:THR:HG23	2.18	0.43
1:C:161:GLN:HE22	1:C:168:ALA:HB1	1.83	0.43
1:G:191:LEU:HD12	1:G:192:SER:H	1.83	0.43
1:A:44:PRO:HG2	1:A:62:ALA:O	2.18	0.43
1:G:143:ALA:O	1:G:149:ILE:HD11	2.19	0.43
1:G:206:LEU:HB3	1:H:34:ASP:HB2	1.99	0.43
1:A:91:ASP:OD1	1:A:91:ASP:O	2.37	0.43
1:C:26:CYS:HB3	1:C:51:CYS:HB3	1.51	0.43
1:E:74:PRO:HG3	1:E:125:LEU:HD22	2.00	0.43
1:G:152:ARG:HD2	1:G:152:ARG:HA	1.70	0.43
1:H:40:SER:HB3	1:H:66:GLN:HB2	2.00	0.43
1:B:32:TRP:O	1:B:33:ARG:C	2.61	0.43
1:H:62:ALA:CA	1:H:75:THR:HG22	2.48	0.43
1:G:43:ILE:HD13	1:G:63:VAL:HG22	2.01	0.43
1:G:198:HIS:HE1	1:G:200:GLU:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:GLN:O	1:E:161:GLN:HB2	2.20	0.42
1:H:74:PRO:HB2	1:H:76:LEU:HD21	2.01	0.42
1:B:32:TRP:CG	1:C:206:LEU:HD22	2.54	0.42
1:D:178:LEU:HD11	1:D:185:PRO:HB2	2.02	0.42
1:E:1:MET:HB2	1:E:1:MET:HE3	1.66	0.42
1:D:1:MET:HE3	1:D:1:MET:HB2	1.81	0.42
1:A:35:GLU:H	1:A:35:GLU:HG2	1.60	0.42
1:C:63:VAL:O	1:C:74:PRO:HD2	2.20	0.42
1:C:119:LEU:HD22	1:C:130:PHE:HB2	2.02	0.42
1:F:34:ASP:HA	1:F:37:ASN:ND2	2.34	0.42
1:H:106:LEU:HD12	1:H:106:LEU:HA	1.83	0.42
1:F:121:PHE:HD2	1:F:128:TRP:CE2	2.37	0.42
1:F:125:LEU:O	1:F:126:HIS:C	2.63	0.42
1:D:169:PRO:HG3	1:D:197:THR:HB	2.01	0.42
1:A:118:LEU:HD12	1:A:118:LEU:HA	1.85	0.42
1:H:12:ALA:HB1	1:H:100:ASN:ND2	2.35	0.42
1:A:57:LEU:C	1:A:58:GLN:HG2	2.45	0.41
1:F:121:PHE:HA	1:F:128:TRP:HA	2.02	0.41
1:B:60:SER:HA	1:B:76:LEU:O	2.20	0.41
1:G:29:ARG:O	1:G:83:PRO:HD3	2.20	0.41
1:C:143:ALA:O	1:C:149:ILE:HD11	2.21	0.41
1:F:33:ARG:HH12	1:F:101:ALA:CB	2.32	0.41
1:H:47:ASP:OD1	1:H:48:ALA:N	2.54	0.41
1:B:170:LEU:HA	1:B:170:LEU:HD12	1.89	0.41
1:D:63:VAL:O	1:D:73:SER:HA	2.21	0.41
1:H:11:GLN:OE1	1:H:11:GLN:N	2.44	0.41
1:B:206:LEU:HD12	1:B:207:VAL:N	2.35	0.41
1:C:100:ASN:ND2	1:C:102:GLN:OE1	2.54	0.41
1:F:140:ARG:HG3	1:F:190:TYR:CD2	2.55	0.41
1:B:67:GLN:HE21	1:B:67:GLN:HB3	1.65	0.41
1:D:24:GLN:HB2	1:D:51:CYS:SG	2.61	0.41
1:E:140:ARG:HG2	1:E:190:TYR:CE2	2.55	0.41
1:F:83:PRO:HD2	1:F:128:TRP:CZ3	2.55	0.41
1:E:82:TYR:HA	1:E:83:PRO:HD3	1.86	0.41
1:E:205:LYS:HB3	1:F:39:GLY:O	2.20	0.41
1:G:97:VAL:HB	1:G:105:ILE:HB	2.02	0.41
1:A:196:ALA:HB1	1:G:202:SER:HB3	2.04	0.40
1:C:22:LEU:HB2	1:C:26:CYS:SG	2.61	0.40
1:D:-2:VAL:HG23	1:D:0:HIS:NE2	2.37	0.40
1:H:191:LEU:HA	1:H:191:LEU:HD12	1.84	0.40
1:A:199:LEU:HD11	1:G:203:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:C	1:B:37:ASN:N	2.77	0.40
1:C:161:GLN:N	1:C:162:PRO:CD	2.84	0.40
1:C:184:ASP:OD1	1:C:186:ALA:HB3	2.21	0.40
1:D:42:PHE:O	1:D:44:PRO:HD3	2.21	0.40
1:F:92:ARG:HE	1:F:92:ARG:HB2	1.40	0.40
1:H:119:LEU:HD23	1:H:129:ALA:C	2.45	0.40
1:H:161:GLN:N	1:H:162:PRO:CD	2.85	0.40
1:B:206:LEU:HD23	1:C:34:ASP:CB	2.51	0.40
1:C:146:GLU:O	1:C:150:LYS:HD2	2.21	0.40
1:H:97:VAL:HB	1:H:105:ILE:HB	2.03	0.40
1:H:157:GLN:NE2	1:H:170:LEU:HD13	2.37	0.40
1:H:42:PHE:HB3	1:H:64:THR:HB	2.04	0.40
1:A:53:GLU:H	1:A:53:GLU:HG2	1.63	0.40
1:D:205:LYS:O	1:D:206:LEU:C	2.64	0.40

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	201/227 (88%)	194 (96%)	7 (4%)	0	100	100
1	B	205/227 (90%)	195 (95%)	10 (5%)	0	100	100
1	C	205/227 (90%)	197 (96%)	8 (4%)	0	100	100
1	D	206/227 (91%)	197 (96%)	9 (4%)	0	100	100
1	E	205/227 (90%)	201 (98%)	4 (2%)	0	100	100
1	F	202/227 (89%)	191 (95%)	11 (5%)	0	100	100
1	G	204/227 (90%)	197 (97%)	7 (3%)	0	100	100
1	H	201/227 (88%)	195 (97%)	6 (3%)	0	100	100
All	All	1629/1816 (90%)	1567 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	157/176 (89%)	152 (97%)	5 (3%)	34	69
1	B	158/176 (90%)	153 (97%)	5 (3%)	34	69
1	C	161/176 (92%)	148 (92%)	13 (8%)	9	29
1	D	162/176 (92%)	156 (96%)	6 (4%)	29	64
1	E	161/176 (92%)	156 (97%)	5 (3%)	35	70
1	F	157/176 (89%)	149 (95%)	8 (5%)	20	51
1	G	160/176 (91%)	155 (97%)	5 (3%)	35	70
1	H	157/176 (89%)	150 (96%)	7 (4%)	23	56
All	All	1273/1408 (90%)	1219 (96%)	54 (4%)	25	59

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	35	GLU
1	A	40	SER
1	A	92	ARG
1	A	140	ARG
1	B	29	ARG
1	B	53	GLU
1	B	92	ARG
1	B	141	VAL
1	B	170	LEU
1	C	-1	ILE
1	C	7	VAL
1	C	8	THR
1	C	28	PHE
1	C	47	ASP
1	C	65	LEU

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Mol	Chain	Res	Type
1	C	103	ARG
1	C	117	LEU
1	C	141	VAL
1	C	150	LYS
1	C	157	GLN
1	C	182	ARG
1	C	199	LEU
1	D	28	PHE
1	D	122	GLU
1	D	142	ASP
1	D	150	LYS
1	D	206	LEU
1	D	207	VAL
1	E	29	ARG
1	E	92	ARG
1	E	138	MET
1	E	158	THR
1	E	206	LEU
1	F	1	MET
1	F	28	PHE
1	F	43	ILE
1	F	49	LEU
1	F	67	GLN
1	F	92	ARG
1	F	117	LEU
1	F	165	SER
1	G	49	LEU
1	G	67	GLN
1	G	72	LEU
1	G	140	ARG
1	G	157	GLN
1	H	87	VAL
1	H	92	ARG
1	H	148	LYS
1	H	150	LYS
1	H	151	GLN
1	H	163	LEU
1	H	165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	GLN
1	B	58	GLN
1	D	155	GLN
1	E	109	ASN
1	G	67	GLN
1	G	157	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 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	205/227 (90%)	1.33	45 (21%) 3 3	40, 64, 96, 123	1 (0%)
1	B	207/227 (91%)	1.13	33 (15%) 6 5	30, 54, 88, 128	0
1	C	209/227 (92%)	1.35	47 (22%) 3 2	44, 60, 88, 122	0
1	D	210/227 (92%)	1.16	45 (21%) 3 3	41, 57, 87, 120	0
1	E	209/227 (92%)	1.33	44 (21%) 3 3	30, 63, 95, 121	0
1	F	206/227 (90%)	1.34	42 (20%) 3 3	30, 65, 94, 118	0
1	G	208/227 (91%)	0.89	19 (9%) 16 14	44, 60, 90, 115	0
1	H	205/227 (90%)	1.24	39 (19%) 4 3	56, 69, 99, 120	0
All	All	1659/1816 (91%)	1.22	314 (18%) 4 3	30, 62, 95, 128	1 (0%)

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	ALA	6.5
1	C	92	ARG	6.4
1	D	207	VAL	6.1
1	B	37	ASN	6.1
1	C	35	GLU	6.0
1	A	168[A]	ALA	5.7
1	F	54	ASP	5.6
1	G	0	HIS	5.1
1	D	197	THR	4.9
1	B	167	PRO	4.8
1	E	0	HIS	4.8
1	B	166	ALA	4.7
1	A	38	GLY	4.7
1	C	24	GLN	4.7
1	A	24	GLN	4.7
1	F	37	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	8	THR	4.4
1	F	0	HIS	4.4
1	A	37	ASN	4.3
1	F	58	GLN	4.3
1	D	92	ARG	4.3
1	F	207	VAL	4.2
1	A	141	VAL	4.2
1	B	160	TRP	4.2
1	H	91	ASP	4.1
1	G	36	ALA	4.1
1	E	52	GLY	4.1
1	B	206	LEU	4.1
1	D	168	ALA	4.1
1	E	197	THR	4.0
1	A	36	ALA	3.9
1	C	207	VAL	3.9
1	B	115	SER	3.9
1	F	101	ALA	3.9
1	A	47	ASP	3.8
1	D	53	GLU	3.8
1	F	33	ARG	3.7
1	G	168	ALA	3.7
1	C	91	ASP	3.7
1	B	38	GLY	3.7
1	D	60	SER	3.7
1	E	165	SER	3.7
1	D	34	ASP	3.7
1	C	-2	VAL	3.7
1	E	51	CYS	3.7
1	C	37	ASN	3.7
1	H	207	VAL	3.6
1	F	72	LEU	3.6
1	E	144	ALA	3.6
1	C	-3	LEU	3.6
1	A	205	LYS	3.6
1	E	207	VAL	3.6
1	D	205	LYS	3.5
1	A	39	GLY	3.5
1	B	33	ARG	3.5
1	D	163	LEU	3.5
1	A	34	ASP	3.4
1	D	75	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	207	VAL	3.4
1	D	9	SER	3.4
1	D	40	SER	3.4
1	H	33	ARG	3.4
1	A	102	GLN	3.4
1	B	48	ALA	3.3
1	B	113	PRO	3.3
1	C	168	ALA	3.3
1	D	59	GLY	3.3
1	B	159	ALA	3.3
1	B	34	ASP	3.3
1	C	0	HIS	3.3
1	A	165	SER	3.2
1	E	21	SER	3.2
1	A	111	GLN	3.2
1	E	-1	ILE	3.2
1	E	92	ARG	3.2
1	C	180	ALA	3.2
1	B	36	ALA	3.2
1	E	33	ARG	3.2
1	E	-2	VAL	3.1
1	H	65	LEU	3.1
1	C	60	SER	3.1
1	E	58	GLN	3.1
1	A	106	LEU	3.1
1	H	36	ALA	3.1
1	H	168	ALA	3.1
1	F	161	GLN	3.1
1	H	61	GLY	3.1
1	E	119	LEU	3.0
1	F	197	THR	3.0
1	D	165	SER	3.0
1	E	168	ALA	3.0
1	D	150	LYS	3.0
1	F	51	CYS	3.0
1	C	50	ARG	3.0
1	E	54	ASP	3.0
1	D	35	GLU	3.0
1	H	115	SER	3.0
1	C	163	LEU	2.9
1	H	8	THR	2.9
1	D	-3	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	46	GLY	2.9
1	C	54	ASP	2.9
1	C	25	GLY	2.9
1	D	39	GLY	2.9
1	D	43	ILE	2.9
1	E	49	LEU	2.8
1	C	66	GLN	2.8
1	D	66	GLN	2.8
1	H	47	ASP	2.8
1	G	180	ALA	2.8
1	H	69	GLY	2.8
1	F	6	ALA	2.8
1	F	38	GLY	2.8
1	E	53	GLU	2.8
1	G	35	GLU	2.8
1	B	99	ALA	2.8
1	C	7	VAL	2.8
1	A	28	PHE	2.8
1	H	72	LEU	2.8
1	D	37	ASN	2.7
1	F	154	GLN	2.7
1	B	39	GLY	2.7
1	F	5	VAL	2.7
1	F	168	ALA	2.7
1	H	21	SER	2.7
1	B	117	LEU	2.7
1	B	53	GLU	2.7
1	E	30	THR	2.7
1	A	90	GLY	2.7
1	F	124	GLN	2.7
1	C	165	SER	2.7
1	F	165	SER	2.7
1	A	158	THR	2.7
1	C	38	GLY	2.7
1	B	100	ASN	2.7
1	H	3	ALA	2.7
1	A	147	THR	2.7
1	E	70	GLN	2.6
1	A	35	GLU	2.6
1	G	68	GLY	2.6
1	G	188	GLY	2.6
1	D	33	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	177	LYS	2.6
1	E	156	ALA	2.6
1	H	4	ALA	2.6
1	H	133	GLU	2.6
1	H	156	ALA	2.6
1	E	78	PHE	2.6
1	G	-1	ILE	2.6
1	F	30	THR	2.6
1	G	-2	VAL	2.6
1	C	17	ALA	2.6
1	D	164	LEU	2.6
1	A	190	TYR	2.6
1	A	49	LEU	2.6
1	C	22	LEU	2.6
1	C	26	CYS	2.5
1	A	100	ASN	2.5
1	C	109	ASN	2.5
1	A	53	GLU	2.5
1	A	113	PRO	2.5
1	D	198	HIS	2.5
1	D	38	GLY	2.5
1	H	75	THR	2.5
1	E	-3	LEU	2.5
1	H	129	ALA	2.5
1	C	20	PHE	2.5
1	B	102	GLN	2.5
1	C	89	GLY	2.5
1	F	133	GLU	2.5
1	F	164	LEU	2.5
1	F	191	LEU	2.5
1	F	85	ALA	2.5
1	C	34	ASP	2.5
1	E	154	GLN	2.5
1	A	160	TRP	2.5
1	F	27	HIS	2.5
1	H	131	ASN	2.5
1	B	49	LEU	2.5
1	E	26	CYS	2.5
1	D	191	LEU	2.5
1	B	45	ALA	2.5
1	E	101	ALA	2.5
1	H	165	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	55	GLY	2.4
1	H	114	GLY	2.4
1	A	199	LEU	2.4
1	D	93	ALA	2.4
1	F	28	PHE	2.4
1	A	80	GLN	2.4
1	F	169	PRO	2.4
1	E	170	LEU	2.4
1	A	122	GLU	2.4
1	G	93	ALA	2.4
1	C	197	THR	2.4
1	D	162	PRO	2.4
1	E	206	LEU	2.4
1	F	206	LEU	2.4
1	D	61	GLY	2.4
1	B	156	ALA	2.4
1	D	67	GLN	2.4
1	E	139	PRO	2.4
1	D	90	GLY	2.4
1	E	48	ALA	2.4
1	F	17	ALA	2.4
1	C	131	ASN	2.4
1	F	131	ASN	2.4
1	G	37	ASN	2.4
1	C	169	PRO	2.3
1	B	47	ASP	2.3
1	C	-1	ILE	2.3
1	C	28	PHE	2.3
1	A	50	ARG	2.3
1	F	92	ARG	2.3
1	B	197	THR	2.3
1	D	72	LEU	2.3
1	A	108	GLY	2.3
1	C	177	LYS	2.3
1	E	196	ALA	2.3
1	C	171	THR	2.3
1	C	51	CYS	2.3
1	E	25	GLY	2.3
1	B	35	GLU	2.3
1	H	199	LEU	2.3
1	A	124	GLN	2.3
1	C	14	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	34	ASP	2.3
1	F	49	LEU	2.3
1	A	197	THR	2.3
1	E	120	THR	2.3
1	F	205	LYS	2.3
1	E	90	GLY	2.2
1	H	135	ILE	2.2
1	F	118	LEU	2.2
1	E	173	LYS	2.2
1	H	2	PRO	2.2
1	A	96	VAL	2.2
1	H	149	ILE	2.2
1	D	0	HIS	2.2
1	A	33	ARG	2.2
1	D	182	ARG	2.2
1	H	118	LEU	2.2
1	C	13	ASP	2.2
1	A	135	ILE	2.2
1	D	141	VAL	2.2
1	G	61	GLY	2.2
1	C	182	ARG	2.2
1	H	20	PHE	2.2
1	F	48	ALA	2.2
1	C	191	LEU	2.2
1	D	206	LEU	2.2
1	E	104	LEU	2.2
1	E	128	TRP	2.2
1	F	91	ASP	2.2
1	F	7	VAL	2.2
1	F	78	PHE	2.2
1	A	129	ALA	2.2
1	A	159	ALA	2.2
1	G	72	LEU	2.2
1	A	32	TRP	2.2
1	F	90	GLY	2.1
1	G	69	GLY	2.1
1	E	155	GLN	2.1
1	C	41	LEU	2.1
1	G	48	ALA	2.1
1	F	26	CYS	2.1
1	D	52	GLY	2.1
1	F	75	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLN	2.1
1	B	124	GLN	2.1
1	D	204	PHE	2.1
1	B	112	ALA	2.1
1	A	176	GLU	2.1
1	B	169	PRO	2.1
1	H	90	GLY	2.1
1	H	107	GLY	2.1
1	A	115	SER	2.1
1	D	171	THR	2.1
1	E	24	GLN	2.1
1	H	70	GLN	2.1
1	D	41	LEU	2.1
1	A	133	GLU	2.1
1	C	16	PRO	2.1
1	C	33	ARG	2.1
1	G	25	GLY	2.1
1	C	206	LEU	2.1
1	E	66	GLN	2.1
1	H	41	LEU	2.1
1	H	154	GLN	2.1
1	H	174	LEU	2.1
1	G	33	ARG	2.1
1	B	41	LEU	2.0
1	C	106	LEU	2.0
1	A	11	GLN	2.0
1	B	181	ASP	2.0
1	E	47	ASP	2.0
1	F	18	GLN	2.0
1	D	85	ALA	2.0
1	F	3	ALA	2.0
1	G	186	ALA	2.0
1	D	133	GLU	2.0
1	A	105	ILE	2.0
1	E	5	VAL	2.0
1	E	80	GLN	2.0
1	H	111	GLN	2.0
1	D	91	ASP	2.0
1	D	14	SER	2.0
1	D	187	SER	2.0
1	E	40	SER	2.0
1	C	105	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	169	PRO	2.0
1	B	109	ASN	2.0
1	C	100	ASN	2.0
1	H	39	GLY	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.