



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:50 PM UTC

PDB ID : 9BJ7 / pdb_00009bj7
Title : Crystal structure of the N-terminal truncated AbiV (residues 24-201)
Authors : Zhu, X.; Moineau, S.; Shi, R.
Deposited on : 2024-04-25
Resolution : 2.64 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:

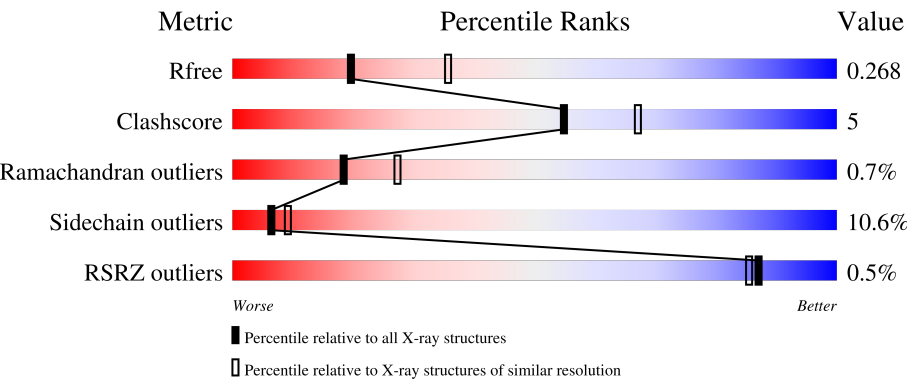
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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.





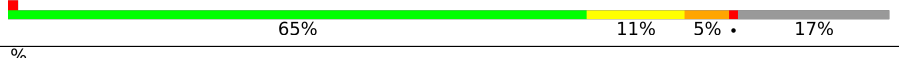

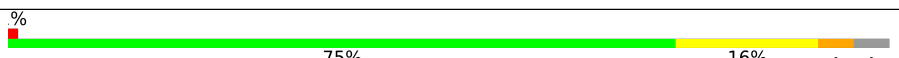

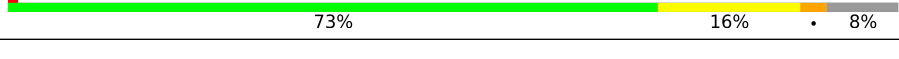

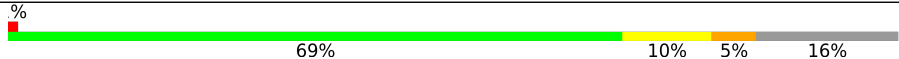

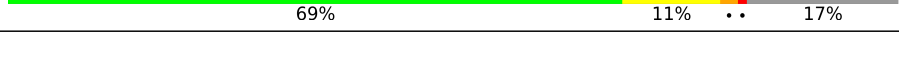
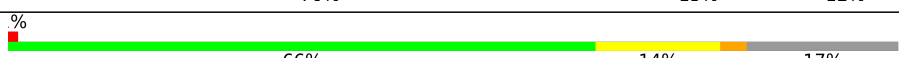




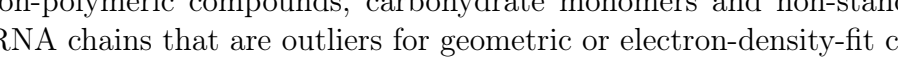
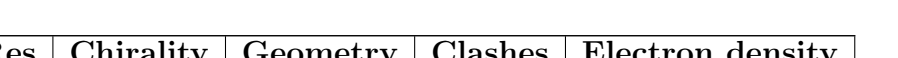
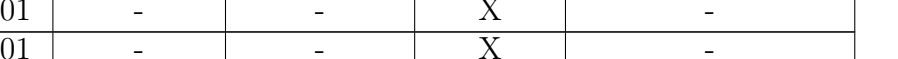
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	184	<div><div></div><div>76%12%10%</div></div>
1	B	184	<div><div>%</div><div>65%12%18%</div></div>
1	C	184	<div><div>%</div><div>75%14%9%</div></div>
1	D	184	<div><div>%</div><div>66%13%18%</div></div>
1	E	184	<div><div></div><div>71%15%12%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	184	
1	G	184	
1	H	184	
1	I	184	
1	J	184	
1	K	184	
1	L	184	
1	M	184	
1	N	184	
1	O	184	
1	P	184	
1	Q	184	
1	R	184	
1	S	184	
1	T	184	
1	U	184	
1	V	184	
1	W	184	
1	X	184	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	G	301	-	-	X	-
2	SO4	R	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30045 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 AbiV family abortive infection protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1293	817	208	263	5			
1	B	151	Total	C	N	O	S	0	0	0
			1177	745	182	245	5			
1	C	167	Total	C	N	O	S	0	0	0
			1310	826	213	266	5			
1	D	151	Total	C	N	O	S	0	0	0
			1177	745	182	245	5			
1	E	161	Total	C	N	O	S	0	0	0
			1259	798	196	260	5			
1	F	152	Total	C	N	O	S	0	0	0
			1186	751	184	246	5			
1	G	163	Total	C	N	O	S	0	0	0
			1281	810	206	261	4			
1	H	152	Total	C	N	O	S	0	0	0
			1187	751	185	246	5			
1	I	166	Total	C	N	O	S	0	0	0
			1307	825	213	265	4			
1	J	153	Total	C	N	O	S	0	0	0
			1198	760	186	247	5			
1	K	176	Total	C	N	O	S	0	0	0
			1386	875	225	281	5			
1	L	156	Total	C	N	O	S	0	0	0
			1221	772	193	251	5			
1	M	170	Total	C	N	O	S	0	0	0
			1333	844	211	273	5			
1	N	155	Total	C	N	O	S	0	0	0
			1211	766	190	250	5			
1	O	170	Total	C	N	O	S	0	0	0
			1333	844	211	273	5			
1	P	155	Total	C	N	O	S	0	0	0
			1211	766	190	250	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	161	Total	C	N	O	S	0	0	0
			1259	798	196	260	5			
1	R	152	Total	C	N	O	S	0	0	0
			1186	751	184	246	5			
1	S	161	Total	C	N	O	S	0	0	0
			1259	798	196	260	5			
1	T	152	Total	C	N	O	S	0	0	0
			1186	751	184	246	5			
1	U	166	Total	C	N	O	S	0	0	0
			1307	825	213	265	4			
1	V	152	Total	C	N	O	S	0	0	0
			1188	754	183	246	5			
1	W	169	Total	C	N	O	S	0	0	0
			1332	839	218	271	4			
1	X	148	Total	C	N	O	S	0	0	0
			1155	731	178	242	4			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	HIS	-	expression tag	UNP Q9AGY3
A	203	HIS	-	expression tag	UNP Q9AGY3
A	204	HIS	-	expression tag	UNP Q9AGY3
A	205	HIS	-	expression tag	UNP Q9AGY3
A	206	HIS	-	expression tag	UNP Q9AGY3
A	207	HIS	-	expression tag	UNP Q9AGY3
B	202	HIS	-	expression tag	UNP Q9AGY3
B	203	HIS	-	expression tag	UNP Q9AGY3
B	204	HIS	-	expression tag	UNP Q9AGY3
B	205	HIS	-	expression tag	UNP Q9AGY3
B	206	HIS	-	expression tag	UNP Q9AGY3
B	207	HIS	-	expression tag	UNP Q9AGY3
C	202	HIS	-	expression tag	UNP Q9AGY3
C	203	HIS	-	expression tag	UNP Q9AGY3
C	204	HIS	-	expression tag	UNP Q9AGY3
C	205	HIS	-	expression tag	UNP Q9AGY3
C	206	HIS	-	expression tag	UNP Q9AGY3
C	207	HIS	-	expression tag	UNP Q9AGY3
D	202	HIS	-	expression tag	UNP Q9AGY3
D	203	HIS	-	expression tag	UNP Q9AGY3
D	204	HIS	-	expression tag	UNP Q9AGY3
D	205	HIS	-	expression tag	UNP Q9AGY3
D	206	HIS	-	expression tag	UNP Q9AGY3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	207	HIS	-	expression tag	UNP Q9AGY3
E	202	HIS	-	expression tag	UNP Q9AGY3
E	203	HIS	-	expression tag	UNP Q9AGY3
E	204	HIS	-	expression tag	UNP Q9AGY3
E	205	HIS	-	expression tag	UNP Q9AGY3
E	206	HIS	-	expression tag	UNP Q9AGY3
E	207	HIS	-	expression tag	UNP Q9AGY3
F	202	HIS	-	expression tag	UNP Q9AGY3
F	203	HIS	-	expression tag	UNP Q9AGY3
F	204	HIS	-	expression tag	UNP Q9AGY3
F	205	HIS	-	expression tag	UNP Q9AGY3
F	206	HIS	-	expression tag	UNP Q9AGY3
F	207	HIS	-	expression tag	UNP Q9AGY3
G	202	HIS	-	expression tag	UNP Q9AGY3
G	203	HIS	-	expression tag	UNP Q9AGY3
G	204	HIS	-	expression tag	UNP Q9AGY3
G	205	HIS	-	expression tag	UNP Q9AGY3
G	206	HIS	-	expression tag	UNP Q9AGY3
G	207	HIS	-	expression tag	UNP Q9AGY3
H	202	HIS	-	expression tag	UNP Q9AGY3
H	203	HIS	-	expression tag	UNP Q9AGY3
H	204	HIS	-	expression tag	UNP Q9AGY3
H	205	HIS	-	expression tag	UNP Q9AGY3
H	206	HIS	-	expression tag	UNP Q9AGY3
H	207	HIS	-	expression tag	UNP Q9AGY3
I	202	HIS	-	expression tag	UNP Q9AGY3
I	203	HIS	-	expression tag	UNP Q9AGY3
I	204	HIS	-	expression tag	UNP Q9AGY3
I	205	HIS	-	expression tag	UNP Q9AGY3
I	206	HIS	-	expression tag	UNP Q9AGY3
I	207	HIS	-	expression tag	UNP Q9AGY3
J	202	HIS	-	expression tag	UNP Q9AGY3
J	203	HIS	-	expression tag	UNP Q9AGY3
J	204	HIS	-	expression tag	UNP Q9AGY3
J	205	HIS	-	expression tag	UNP Q9AGY3
J	206	HIS	-	expression tag	UNP Q9AGY3
J	207	HIS	-	expression tag	UNP Q9AGY3
K	202	HIS	-	expression tag	UNP Q9AGY3
K	203	HIS	-	expression tag	UNP Q9AGY3
K	204	HIS	-	expression tag	UNP Q9AGY3
K	205	HIS	-	expression tag	UNP Q9AGY3
K	206	HIS	-	expression tag	UNP Q9AGY3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	207	HIS	-	expression tag	UNP Q9AGY3
L	202	HIS	-	expression tag	UNP Q9AGY3
L	203	HIS	-	expression tag	UNP Q9AGY3
L	204	HIS	-	expression tag	UNP Q9AGY3
L	205	HIS	-	expression tag	UNP Q9AGY3
L	206	HIS	-	expression tag	UNP Q9AGY3
L	207	HIS	-	expression tag	UNP Q9AGY3
M	202	HIS	-	expression tag	UNP Q9AGY3
M	203	HIS	-	expression tag	UNP Q9AGY3
M	204	HIS	-	expression tag	UNP Q9AGY3
M	205	HIS	-	expression tag	UNP Q9AGY3
M	206	HIS	-	expression tag	UNP Q9AGY3
M	207	HIS	-	expression tag	UNP Q9AGY3
N	202	HIS	-	expression tag	UNP Q9AGY3
N	203	HIS	-	expression tag	UNP Q9AGY3
N	204	HIS	-	expression tag	UNP Q9AGY3
N	205	HIS	-	expression tag	UNP Q9AGY3
N	206	HIS	-	expression tag	UNP Q9AGY3
N	207	HIS	-	expression tag	UNP Q9AGY3
O	202	HIS	-	expression tag	UNP Q9AGY3
O	203	HIS	-	expression tag	UNP Q9AGY3
O	204	HIS	-	expression tag	UNP Q9AGY3
O	205	HIS	-	expression tag	UNP Q9AGY3
O	206	HIS	-	expression tag	UNP Q9AGY3
O	207	HIS	-	expression tag	UNP Q9AGY3
P	202	HIS	-	expression tag	UNP Q9AGY3
P	203	HIS	-	expression tag	UNP Q9AGY3
P	204	HIS	-	expression tag	UNP Q9AGY3
P	205	HIS	-	expression tag	UNP Q9AGY3
P	206	HIS	-	expression tag	UNP Q9AGY3
P	207	HIS	-	expression tag	UNP Q9AGY3
Q	202	HIS	-	expression tag	UNP Q9AGY3
Q	203	HIS	-	expression tag	UNP Q9AGY3
Q	204	HIS	-	expression tag	UNP Q9AGY3
Q	205	HIS	-	expression tag	UNP Q9AGY3
Q	206	HIS	-	expression tag	UNP Q9AGY3
Q	207	HIS	-	expression tag	UNP Q9AGY3
R	202	HIS	-	expression tag	UNP Q9AGY3
R	203	HIS	-	expression tag	UNP Q9AGY3
R	204	HIS	-	expression tag	UNP Q9AGY3
R	205	HIS	-	expression tag	UNP Q9AGY3
R	206	HIS	-	expression tag	UNP Q9AGY3

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Chain	Residue	Modelled	Actual	Comment	Reference
R	207	HIS	-	expression tag	UNP Q9AGY3
S	202	HIS	-	expression tag	UNP Q9AGY3
S	203	HIS	-	expression tag	UNP Q9AGY3
S	204	HIS	-	expression tag	UNP Q9AGY3
S	205	HIS	-	expression tag	UNP Q9AGY3
S	206	HIS	-	expression tag	UNP Q9AGY3
S	207	HIS	-	expression tag	UNP Q9AGY3
T	202	HIS	-	expression tag	UNP Q9AGY3
T	203	HIS	-	expression tag	UNP Q9AGY3
T	204	HIS	-	expression tag	UNP Q9AGY3
T	205	HIS	-	expression tag	UNP Q9AGY3
T	206	HIS	-	expression tag	UNP Q9AGY3
T	207	HIS	-	expression tag	UNP Q9AGY3
U	202	HIS	-	expression tag	UNP Q9AGY3
U	203	HIS	-	expression tag	UNP Q9AGY3
U	204	HIS	-	expression tag	UNP Q9AGY3
U	205	HIS	-	expression tag	UNP Q9AGY3
U	206	HIS	-	expression tag	UNP Q9AGY3
U	207	HIS	-	expression tag	UNP Q9AGY3
V	202	HIS	-	expression tag	UNP Q9AGY3
V	203	HIS	-	expression tag	UNP Q9AGY3
V	204	HIS	-	expression tag	UNP Q9AGY3
V	205	HIS	-	expression tag	UNP Q9AGY3
V	206	HIS	-	expression tag	UNP Q9AGY3
V	207	HIS	-	expression tag	UNP Q9AGY3
W	202	HIS	-	expression tag	UNP Q9AGY3
W	203	HIS	-	expression tag	UNP Q9AGY3
W	204	HIS	-	expression tag	UNP Q9AGY3
W	205	HIS	-	expression tag	UNP Q9AGY3
W	206	HIS	-	expression tag	UNP Q9AGY3
W	207	HIS	-	expression tag	UNP Q9AGY3
X	202	HIS	-	expression tag	UNP Q9AGY3
X	203	HIS	-	expression tag	UNP Q9AGY3
X	204	HIS	-	expression tag	UNP Q9AGY3
X	205	HIS	-	expression tag	UNP Q9AGY3
X	206	HIS	-	expression tag	UNP Q9AGY3
X	207	HIS	-	expression tag	UNP Q9AGY3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	4	Total	O	0	0
			4	4		
3	C	2	Total	O	0	0
			2	2		
3	D	3	Total	O	0	0
			3	3		
3	E	1	Total	O	0	0
			1	1		

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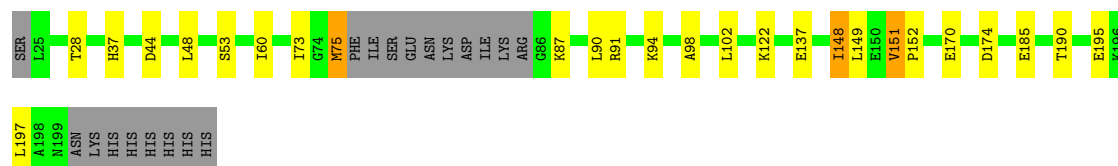
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	4	Total O 4 4	0	0
3	G	4	Total O 4 4	0	0
3	H	1	Total O 1 1	0	0
3	I	4	Total O 4 4	0	0
3	J	5	Total O 5 5	0	0
3	K	3	Total O 3 3	0	0
3	L	4	Total O 4 4	0	0
3	M	5	Total O 5 5	0	0
3	N	1	Total O 1 1	0	0
3	O	5	Total O 5 5	0	0
3	P	1	Total O 1 1	0	0
3	R	3	Total O 3 3	0	0
3	T	2	Total O 2 2	0	0
3	U	4	Total O 4 4	0	0
3	V	3	Total O 3 3	0	0
3	W	1	Total O 1 1	0	0
3	X	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.

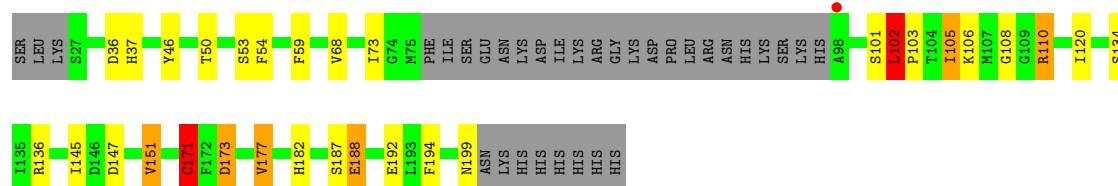
- Molecule 1: AbiV family abortive infection protein

Chain A: 




- Molecule 1: AbiV family abortive infection protein

Chain B: 



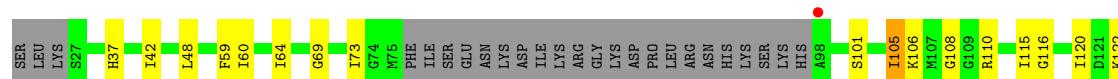
- Molecule 1: AbiV family abortive infection protein

Chain C: 



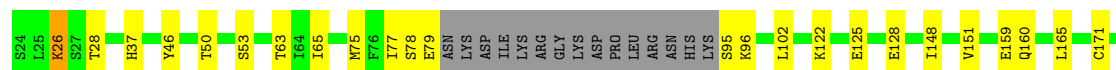
- Molecule 1: AbiV family abortive infection protein

Chain D: 

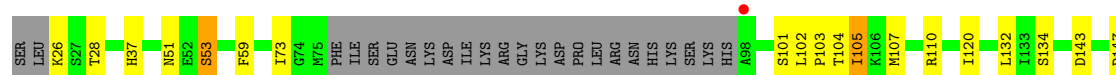




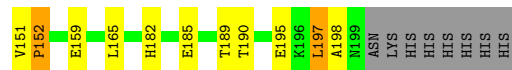
- Molecule 1: AbiV family abortive infection protein



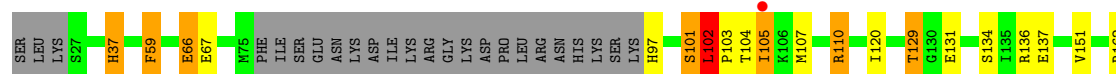
- Molecule 1: AbiV family abortive infection protein



- Molecule 1: AbiV family abortive infection protein

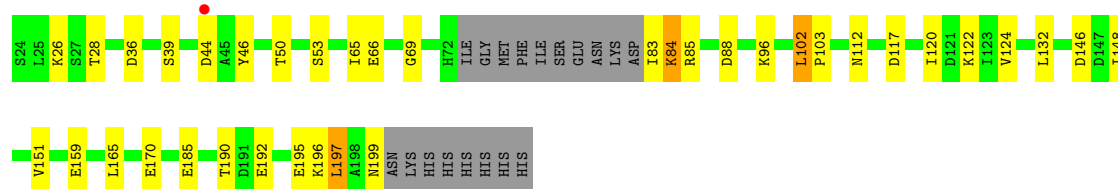


- Molecule 1: AbiV family abortive infection protein

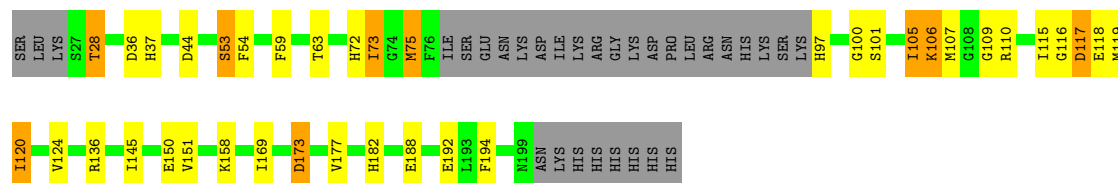


- Molecule 1: AbiV family abortive infection protein

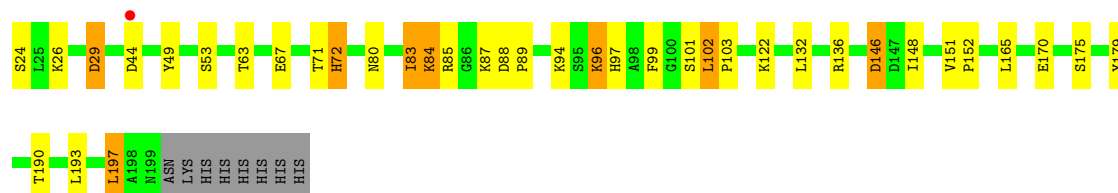
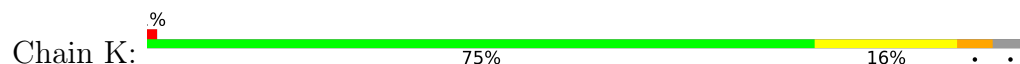




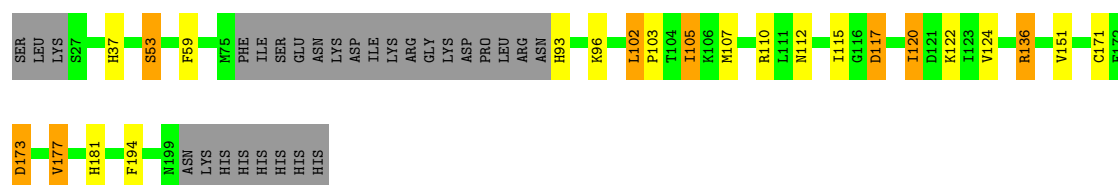
- Molecule 1: AbiV family abortive infection protein



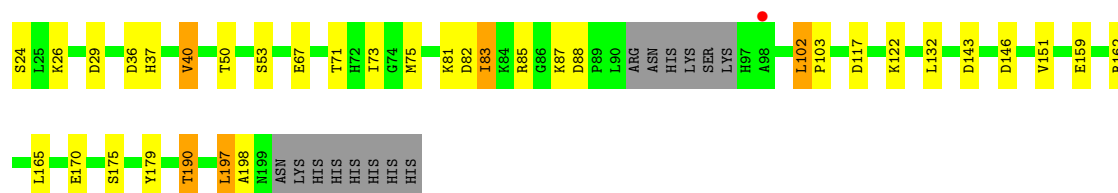
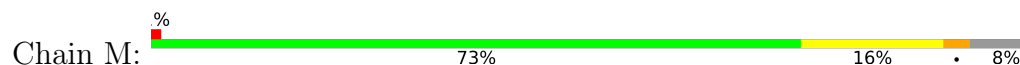
- Molecule 1: AbiV family abortive infection protein



- Molecule 1: AbiV family abortive infection protein

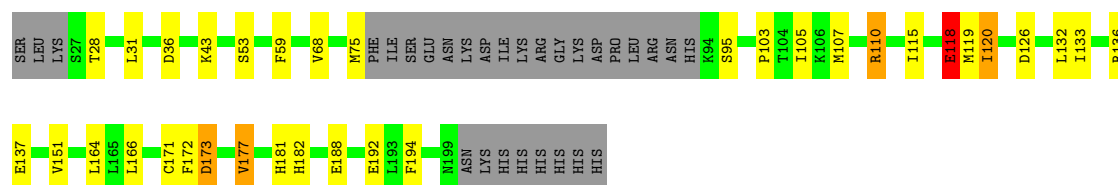


- Molecule 1: AbiV family abortive infection protein




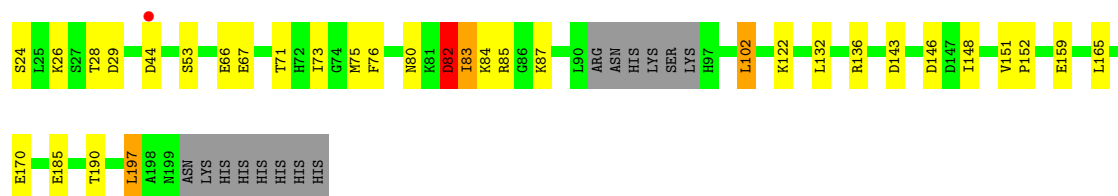
- Molecule 1: AbiV family abortive infection protein

Chain N: 



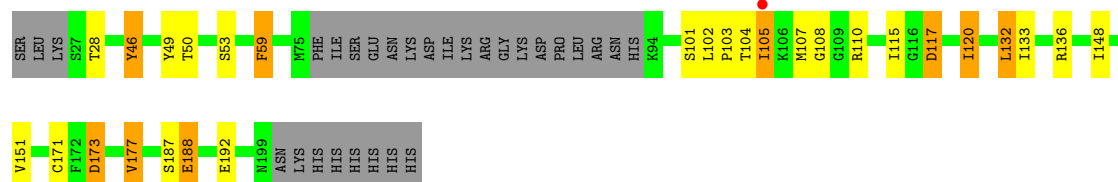
• Molecule 1: AbiV family abortive infection protein

Chain O: 



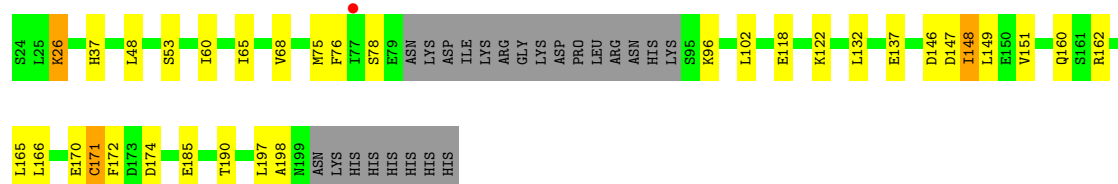
• Molecule 1: AbiV family abortive infection protein

Chain P: 



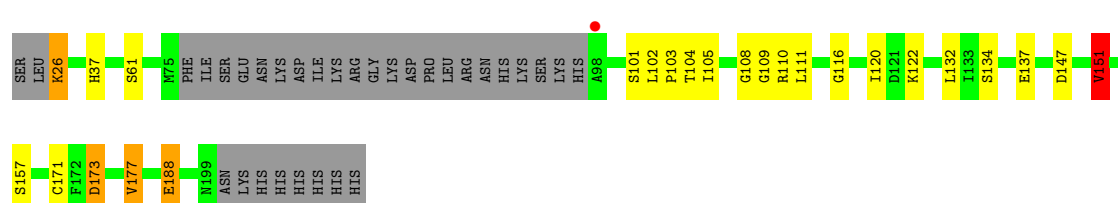
• Molecule 1: AbiV family abortive infection protein

Chain Q: 

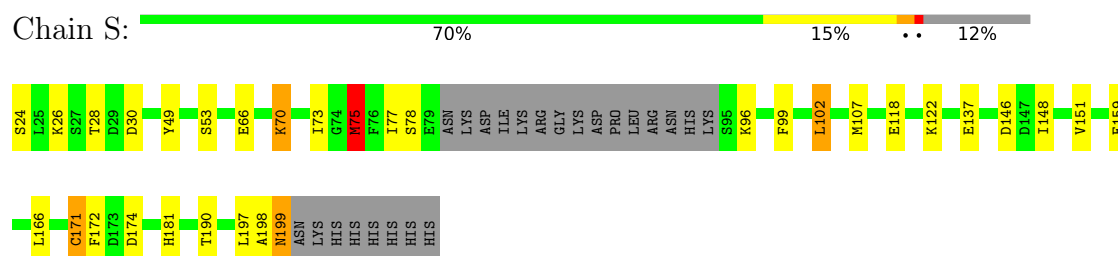


• Molecule 1: AbiV family abortive infection protein

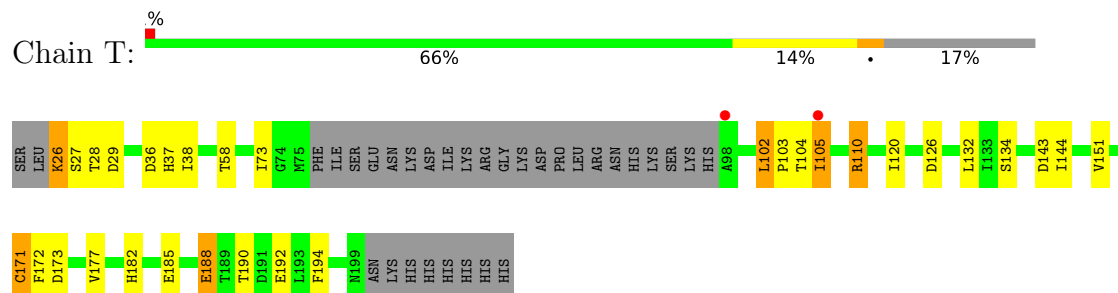
Chain R: 



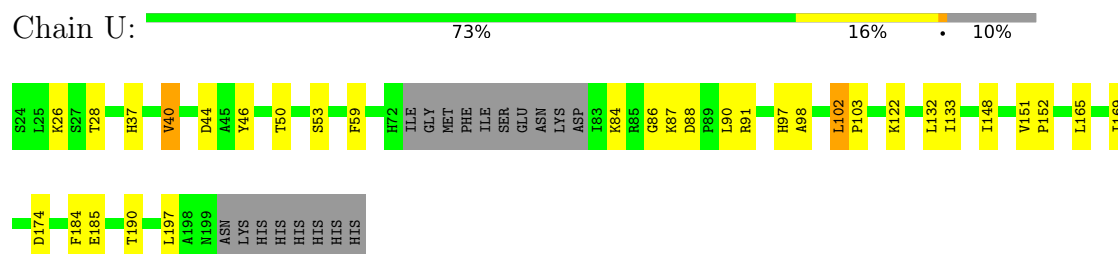
- Molecule 1: AbiV family abortive infection protein



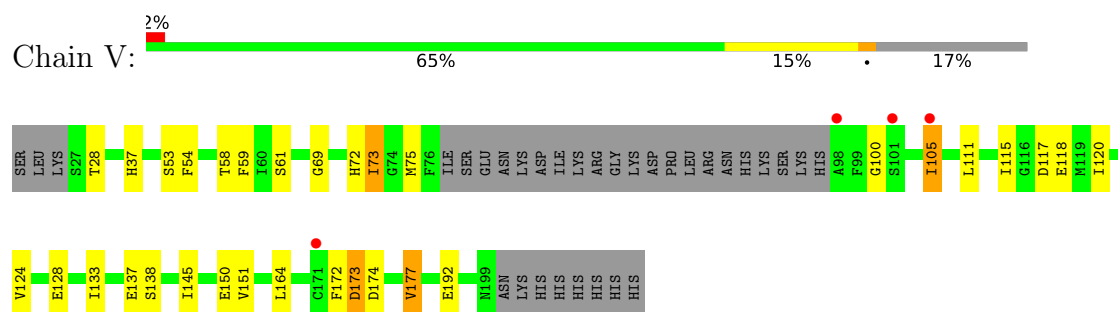
- Molecule 1: AbiV family abortive infection protein



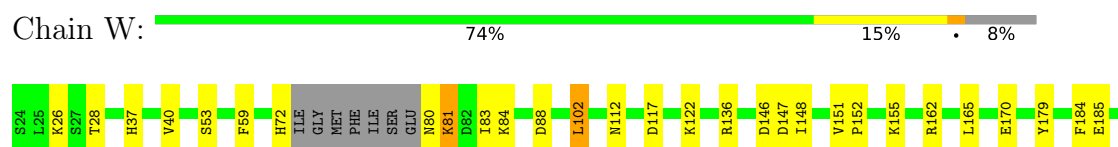
- Molecule 1: AbiV family abortive infection protein



- Molecule 1: AbiV family abortive infection protein

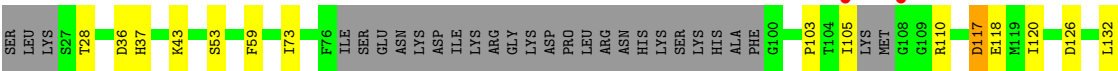


- Molecule 1: AbiV family abortive infection protein





● Molecule 1: AbiV family abortive infection protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.44Å 106.90Å 146.23Å 90.96° 89.95° 95.02°	Depositor
Resolution (Å)	106.70 – 2.64 106.70 – 2.64	Depositor EDS
% Data completeness (in resolution range)	92.9 (106.70-2.64) 92.9 (106.70-2.64)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.225 , 0.268 0.229 , 0.268	Depositor DCC
R_{free} test set	6016 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30045	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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 60.68 % 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 1.4683e-05. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.15	1/1311 (0.1%)	1.60	0/1766
1	B	1.17	3/1192 (0.3%)	1.53	1/1609 (0.1%)
1	C	1.12	0/1328	1.63	3/1788 (0.2%)
1	D	1.14	3/1192 (0.3%)	1.57	2/1609 (0.1%)
1	E	1.16	1/1276 (0.1%)	1.58	6/1720 (0.3%)
1	F	1.17	2/1201 (0.2%)	1.54	3/1620 (0.2%)
1	G	1.15	3/1299 (0.2%)	1.62	2/1751 (0.1%)
1	H	1.17	3/1203 (0.2%)	1.57	2/1624 (0.1%)
1	I	1.12	1/1325 (0.1%)	1.61	9/1784 (0.5%)
1	J	1.18	2/1215 (0.2%)	1.64	6/1640 (0.4%)
1	K	1.13	1/1406 (0.1%)	1.59	3/1893 (0.2%)
1	L	1.20	0/1238	1.60	5/1669 (0.3%)
1	M	1.12	0/1351	1.61	8/1820 (0.4%)
1	N	1.17	1/1227 (0.1%)	1.61	9/1654 (0.5%)
1	O	1.12	0/1351	1.59	5/1820 (0.3%)
1	P	1.20	1/1227 (0.1%)	1.61	2/1654 (0.1%)
1	Q	1.15	1/1276 (0.1%)	1.61	4/1720 (0.2%)
1	R	1.14	2/1201 (0.2%)	1.61	6/1620 (0.4%)
1	S	1.14	1/1276 (0.1%)	1.60	6/1720 (0.3%)
1	T	1.15	1/1201 (0.1%)	1.59	6/1620 (0.4%)
1	U	1.14	0/1325	1.65	6/1784 (0.3%)
1	V	1.14	1/1204 (0.1%)	1.63	4/1625 (0.2%)
1	W	1.12	0/1350	1.63	3/1817 (0.2%)
1	X	1.17	1/1169 (0.1%)	1.61	3/1578 (0.2%)
All	All	1.15	29/30344 (0.1%)	1.60	104/40905 (0.3%)

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	37	HIS	CE1-NE2	7.21	1.39	1.32
1	R	37	HIS	CE1-NE2	6.87	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	HIS	CE1-NE2	6.83	1.39	1.32
1	D	37	HIS	CE1-NE2	6.46	1.39	1.32
1	P	46	TYR	C-O	-6.30	1.16	1.24

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	174	ASP	CA-CB-CG	8.54	121.14	112.60
1	W	88	ASP	CA-CB-CG	8.22	120.82	112.60
1	M	88	ASP	CA-CB-CG	7.50	120.10	112.60
1	J	117	ASP	CA-CB-CG	7.49	120.09	112.60
1	U	88	ASP	CA-CB-CG	7.24	119.84	112.60

There are no chirality outliers.

There are no planarity outliers.

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	1293	0	1287	14	0
1	B	1177	0	1161	14	0
1	C	1310	0	1305	12	0
1	D	1177	0	1161	14	0
1	E	1259	0	1246	14	0
1	F	1186	0	1174	12	0
1	G	1281	0	1275	10	0
1	H	1187	0	1168	17	0
1	I	1307	0	1306	11	0
1	J	1198	0	1177	24	0
1	K	1386	0	1384	16	0
1	L	1221	0	1206	17	0
1	M	1333	0	1326	10	0
1	N	1211	0	1199	16	0
1	O	1333	0	1326	11	0
1	P	1211	0	1199	17	0
1	Q	1259	0	1246	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1186	0	1174	9	0
1	S	1259	0	1246	16	0
1	T	1186	0	1174	11	0
1	U	1307	0	1306	16	0
1	V	1188	0	1170	18	0
1	W	1332	0	1329	12	0
1	X	1155	0	1133	9	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	1	0
2	G	10	0	0	3	0
2	Q	5	0	0	0	0
2	R	5	0	0	3	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
3	C	2	0	0	1	0
3	D	3	0	0	0	0
3	E	1	0	0	1	0
3	F	4	0	0	3	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
3	I	4	0	0	0	0
3	J	5	0	0	1	0
3	K	3	0	0	0	0
3	L	4	0	0	0	0
3	M	5	0	0	0	0
3	N	1	0	0	0	0
3	O	5	0	0	0	0
3	P	1	0	0	0	0
3	R	3	0	0	1	0
3	T	2	0	0	0	0
3	U	4	0	0	0	0
3	V	3	0	0	0	0
3	W	1	0	0	0	0
3	X	4	0	0	0	0
All	All	30045	0	29678	289	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 289 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:R:108:GLY:HA3	2:R:301:SO4:O2	1.50	1.12
1:H:102:LEU:HD13	1:H:167:TYR:OH	1.56	1.06
1:L:136:ARG:HG2	1:L:136:ARG:HH21	1.30	0.95
1:G:125:GLU:O	1:G:129:THR:HG23	1.69	0.91
1:K:24:SER:HB3	1:K:72:HIS:O	1.75	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/184 (88%)	156 (97%)	5 (3%)	0	100	100
1	B	147/184 (80%)	144 (98%)	1 (1%)	2 (1%)	9	12
1	C	163/184 (89%)	156 (96%)	6 (4%)	1 (1%)	21	31
1	D	147/184 (80%)	143 (97%)	4 (3%)	0	100	100
1	E	157/184 (85%)	153 (98%)	4 (2%)	0	100	100
1	F	148/184 (80%)	138 (93%)	9 (6%)	1 (1%)	18	27
1	G	159/184 (86%)	155 (98%)	3 (2%)	1 (1%)	21	31
1	H	148/184 (80%)	141 (95%)	4 (3%)	3 (2%)	6	8
1	I	162/184 (88%)	156 (96%)	6 (4%)	0	100	100
1	J	149/184 (81%)	144 (97%)	5 (3%)	0	100	100
1	K	174/184 (95%)	165 (95%)	8 (5%)	1 (1%)	21	31
1	L	152/184 (83%)	143 (94%)	8 (5%)	1 (1%)	18	27
1	M	166/184 (90%)	161 (97%)	4 (2%)	1 (1%)	21	31
1	N	151/184 (82%)	145 (96%)	5 (3%)	1 (1%)	18	27
1	O	166/184 (90%)	161 (97%)	2 (1%)	3 (2%)	6	9
1	P	151/184 (82%)	147 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	157/184 (85%)	148 (94%)	8 (5%)	1 (1%)	21	31
1	R	148/184 (80%)	143 (97%)	3 (2%)	2 (1%)	9	12
1	S	157/184 (85%)	150 (96%)	6 (4%)	1 (1%)	21	31
1	T	148/184 (80%)	144 (97%)	2 (1%)	2 (1%)	9	12
1	U	162/184 (88%)	155 (96%)	7 (4%)	0	100	100
1	V	148/184 (80%)	143 (97%)	4 (3%)	1 (1%)	18	27
1	W	165/184 (90%)	156 (94%)	7 (4%)	2 (1%)	10	15
1	X	142/184 (77%)	138 (97%)	2 (1%)	2 (1%)	9	12
All	All	3728/4416 (84%)	3585 (96%)	117 (3%)	26 (1%)	18	27

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	ARG
1	F	102	LEU
1	H	110	ARG
1	N	110	ARG
1	O	82	ASP

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	147/166 (89%)	133 (90%)	14 (10%)	8	12
1	B	134/166 (81%)	119 (89%)	15 (11%)	6	8
1	C	149/166 (90%)	133 (89%)	16 (11%)	6	9
1	D	134/166 (81%)	123 (92%)	11 (8%)	10	17
1	E	144/166 (87%)	127 (88%)	17 (12%)	5	6
1	F	135/166 (81%)	121 (90%)	14 (10%)	7	9
1	G	146/166 (88%)	125 (86%)	21 (14%)	3	3
1	H	135/166 (81%)	116 (86%)	19 (14%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	149/166 (90%)	134 (90%)	15 (10%)	7	10
1	J	136/166 (82%)	123 (90%)	13 (10%)	8	12
1	K	158/166 (95%)	140 (89%)	18 (11%)	5	7
1	L	139/166 (84%)	129 (93%)	10 (7%)	13	21
1	M	152/166 (92%)	134 (88%)	18 (12%)	5	6
1	N	138/166 (83%)	124 (90%)	14 (10%)	7	10
1	O	152/166 (92%)	134 (88%)	18 (12%)	5	6
1	P	138/166 (83%)	122 (88%)	16 (12%)	5	7
1	Q	144/166 (87%)	127 (88%)	17 (12%)	5	6
1	R	135/166 (81%)	122 (90%)	13 (10%)	8	12
1	S	144/166 (87%)	126 (88%)	18 (12%)	4	6
1	T	135/166 (81%)	122 (90%)	13 (10%)	8	12
1	U	149/166 (90%)	138 (93%)	11 (7%)	13	20
1	V	135/166 (81%)	121 (90%)	14 (10%)	7	9
1	W	152/166 (92%)	136 (90%)	16 (10%)	6	9
1	X	132/166 (80%)	120 (91%)	12 (9%)	9	13
All	All	3412/3984 (86%)	3049 (89%)	363 (11%)	6	9

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	190	THR
1	S	102	LEU
1	P	107	MET
1	Q	151	VAL
1	T	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	97	HIS
1	T	37	HIS
1	P	199	ASN
1	R	37	HIS
1	T	112	ASN

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](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	R	301	-	4,4,4	0.29	0	6,6,6	0.31	0
2	SO4	Q	301	-	4,4,4	0.61	0	6,6,6	0.25	0
2	SO4	G	301	-	4,4,4	0.35	0	6,6,6	0.38	0
2	SO4	A	301	-	4,4,4	0.54	0	6,6,6	0.36	0
2	SO4	G	302	-	4,4,4	0.41	0	6,6,6	0.13	0
2	SO4	E	301	-	4,4,4	0.46	0	6,6,6	0.36	0
2	SO4	C	301	-	4,4,4	0.40	0	6,6,6	0.27	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	301	SO4	3	0
2	G	301	SO4	3	0
2	E	301	SO4	1	0

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	165/184 (89%)	-0.27	0 100 100	41, 67, 105, 121	0
1	B	151/184 (82%)	-0.11	1 (0%) 84 82	36, 65, 108, 129	0
1	C	167/184 (90%)	-0.13	1 (0%) 85 83	46, 73, 109, 124	0
1	D	151/184 (82%)	0.05	1 (0%) 84 82	42, 74, 117, 144	0
1	E	161/184 (87%)	-0.29	0 100 100	41, 66, 106, 139	0
1	F	152/184 (82%)	-0.16	1 (0%) 84 82	40, 66, 111, 124	0
1	G	163/184 (88%)	-0.12	0 100 100	48, 76, 111, 136	0
1	H	152/184 (82%)	0.01	1 (0%) 84 82	44, 75, 117, 140	0
1	I	166/184 (90%)	-0.20	1 (0%) 85 83	41, 69, 103, 120	0
1	J	153/184 (83%)	-0.08	0 100 100	37, 69, 119, 128	0
1	K	176/184 (95%)	-0.05	1 (0%) 85 83	44, 75, 121, 161	0
1	L	156/184 (84%)	-0.08	0 100 100	39, 69, 113, 139	0
1	M	170/184 (92%)	-0.17	1 (0%) 85 83	40, 71, 111, 128	0
1	N	155/184 (84%)	-0.11	0 100 100	39, 70, 118, 149	0
1	O	170/184 (92%)	-0.12	1 (0%) 85 83	45, 74, 113, 131	0
1	P	155/184 (84%)	-0.11	1 (0%) 85 83	38, 70, 119, 142	0
1	Q	161/184 (87%)	-0.13	1 (0%) 85 83	42, 70, 111, 139	0
1	R	152/184 (82%)	-0.09	1 (0%) 84 82	41, 71, 112, 132	0
1	S	161/184 (87%)	-0.23	0 100 100	46, 71, 110, 134	0
1	T	152/184 (82%)	-0.04	2 (1%) 75 72	44, 71, 115, 135	0
1	U	166/184 (90%)	-0.07	0 100 100	46, 76, 111, 134	0
1	V	152/184 (82%)	0.04	4 (2%) 57 52	45, 81, 131, 152	0
1	W	169/184 (91%)	-0.05	0 100 100	44, 76, 118, 128	0
1	X	148/184 (80%)	0.08	2 (1%) 73 70	43, 77, 132, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3824/4416 (86%)	-0.10	20 (0%) 87 85	36, 72, 117, 161	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	98	ALA	2.7
1	Q	77	ILE	2.7
1	T	105	ILE	2.7
1	X	108	GLY	2.7
1	K	44	ASP	2.6

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	R	301	5/5	0.81	0.20	65,76,88,88	0
2	SO4	G	302	5/5	0.84	0.17	78,79,91,97	0
2	SO4	C	301	5/5	0.88	0.20	66,67,77,85	0
2	SO4	G	301	5/5	0.89	0.18	67,68,77,86	0
2	SO4	E	301	5/5	0.91	0.14	57,62,83,86	0
2	SO4	Q	301	5/5	0.91	0.17	59,59,74,86	0
2	SO4	A	301	5/5	0.91	0.17	58,59,73,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.