



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 04:19 PM EDT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

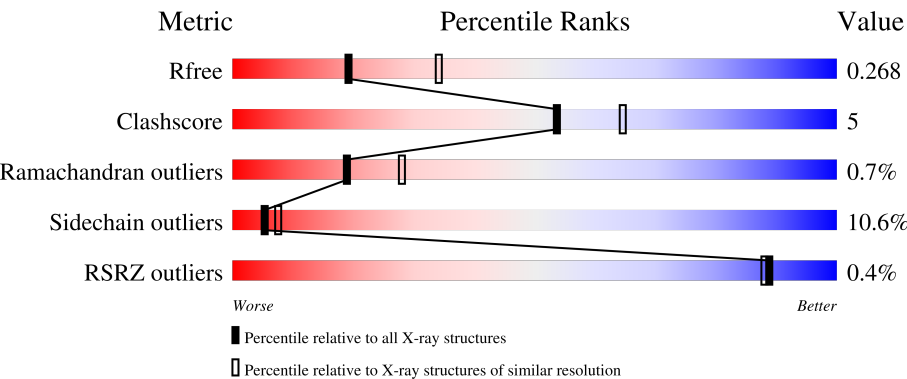
MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 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.













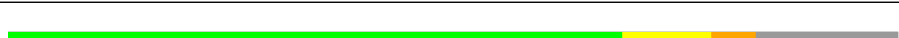


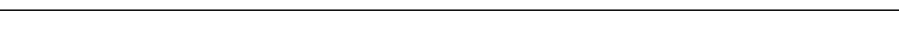
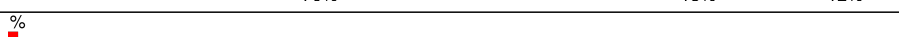
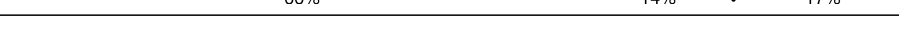



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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  $\geq 3$ , 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	
1	B	184	
1	C	184	
1	D	184	
1	E	184	

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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: O<sub>4</sub>S).





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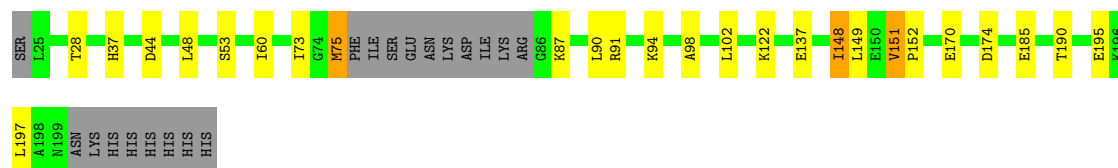
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	4	Total O 4 4	0	0
3	G	4	Total O 4 4	0	0
3	H	1	Total O 1 1	0	0
3	I	4	Total O 4 4	0	0
3	J	5	Total O 5 5	0	0
3	K	3	Total O 3 3	0	0
3	L	4	Total O 4 4	0	0
3	M	5	Total O 5 5	0	0
3	N	1	Total O 1 1	0	0
3	O	5	Total O 5 5	0	0
3	P	1	Total O 1 1	0	0
3	R	3	Total O 3 3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

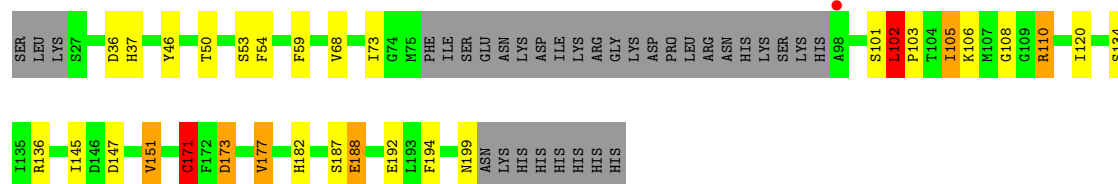
- Molecule 1: AbiV family abortive infection protein

Chain A: 



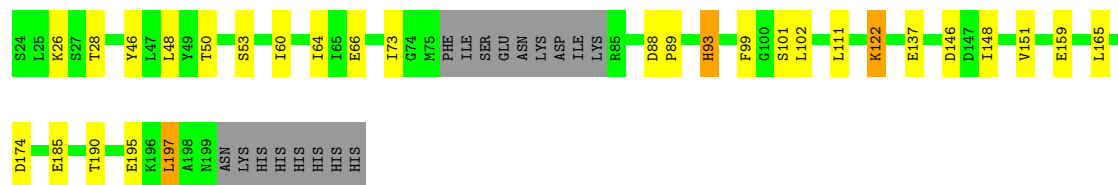
- Molecule 1: AbiV family abortive infection protein

Chain B: 



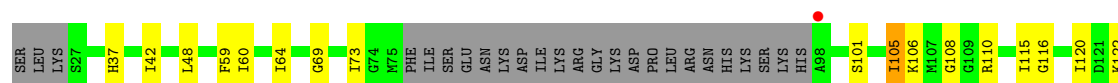
- Molecule 1: AbiV family abortive infection protein

Chain C: 



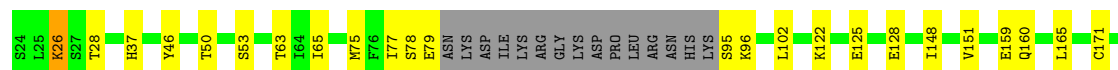
- Molecule 1: AbiV family abortive infection protein

Chain D: 

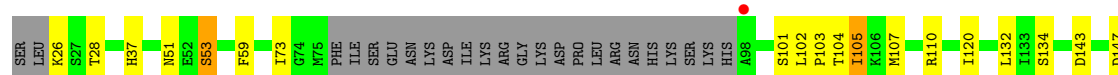




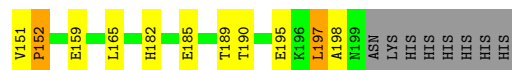
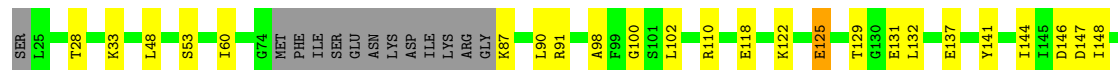
- Molecule 1: AbiV family abortive infection protein



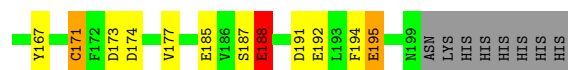
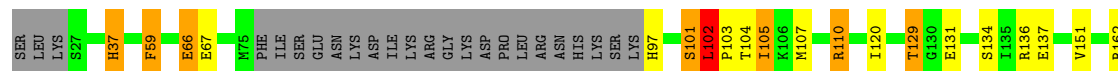
- Molecule 1: AbiV family abortive infection protein



- Molecule 1: AbiV family abortive infection protein

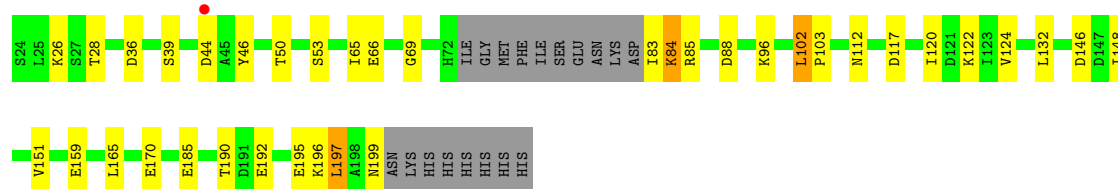


- Molecule 1: AbiV family abortive infection protein

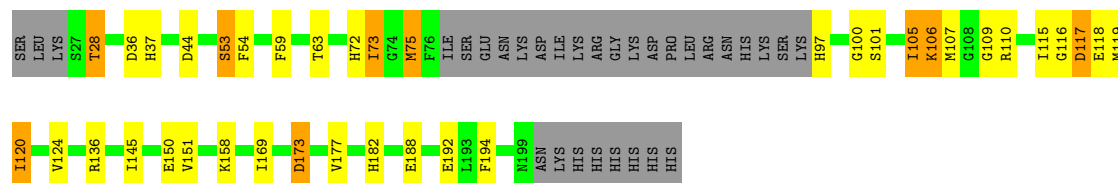


- Molecule 1: AbiV family abortive infection protein

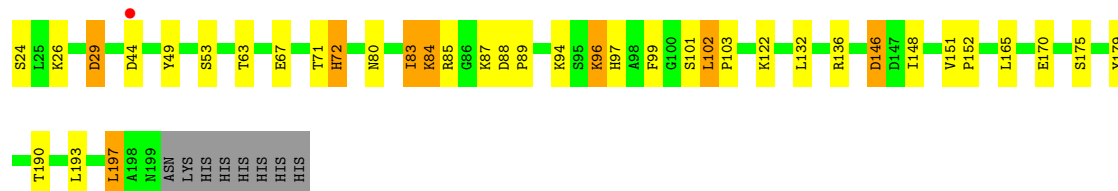
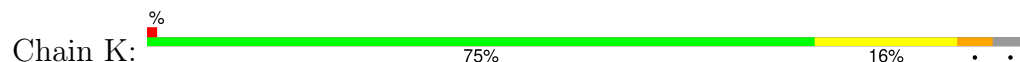




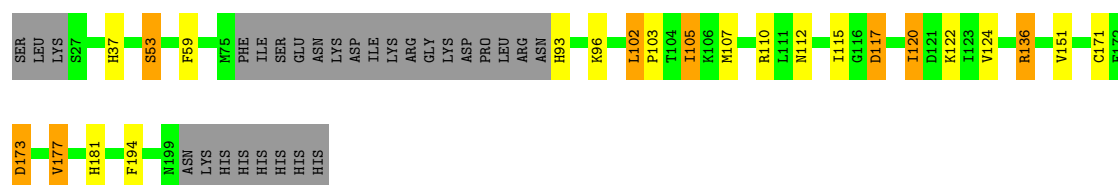
- Molecule 1: AbiV family abortive infection protein



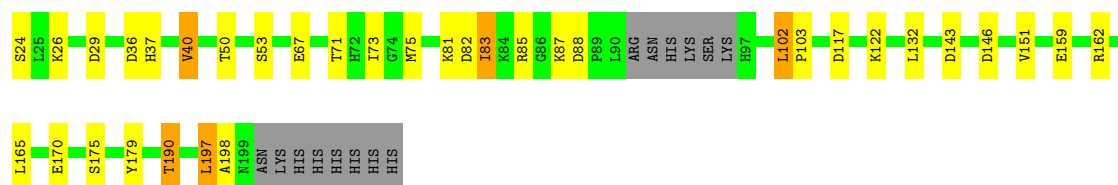
- Molecule 1: AbiV family abortive infection protein



- Molecule 1: AbiV family abortive infection protein



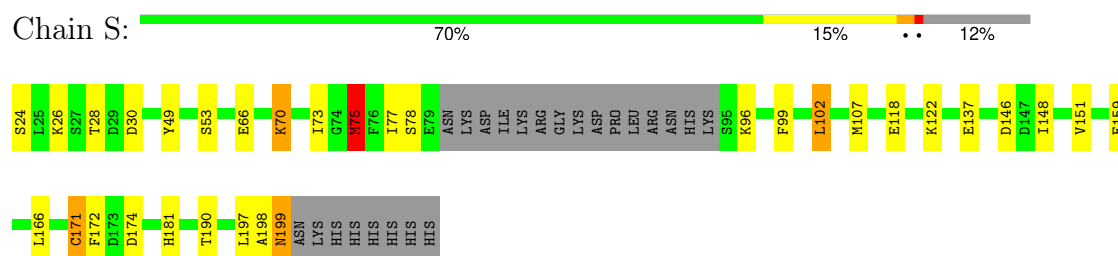
- Molecule 1: AbiV family abortive infection protein



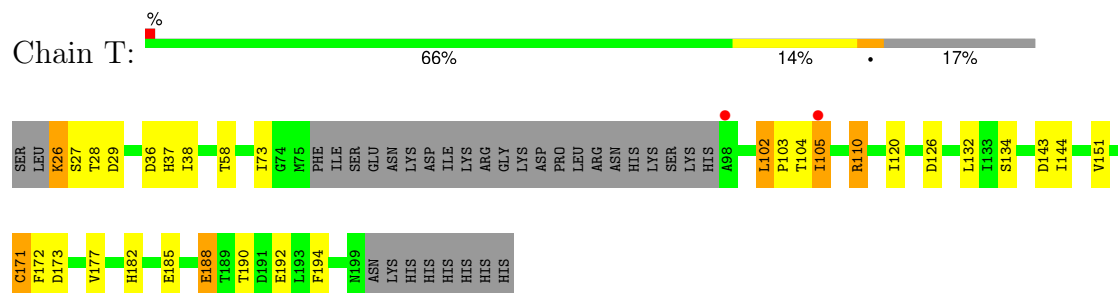
- Molecule 1: AbiV family abortive infection protein



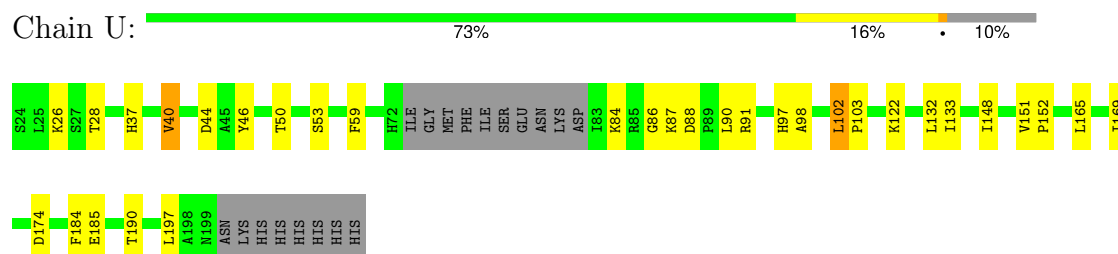
- Molecule 1: AbiV family abortive infection protein



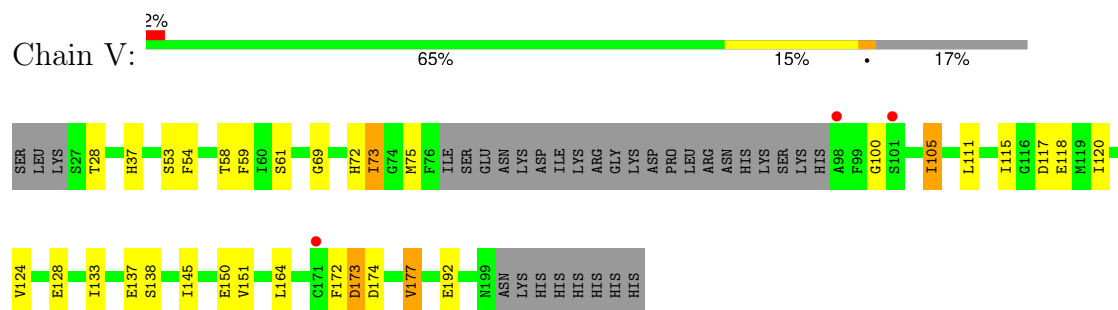
- Molecule 1: AbiV family abortive infection protein



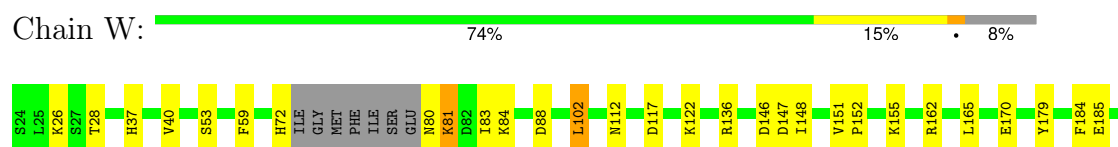
- Molecule 1: AbiV family abortive infection protein



- Molecule 1: AbiV family abortive infection protein

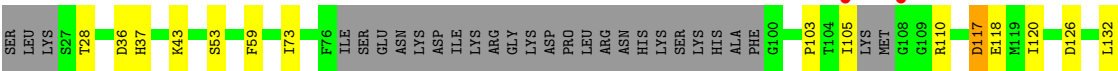


- Molecule 1: AbiV family abortive infection protein





● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	51.9	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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%)

All (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
1	J	37	HIS	CE1-NE2	6.20	1.38	1.32
1	F	37	HIS	CE1-NE2	6.15	1.38	1.32
1	E	37	HIS	CE1-NE2	6.01	1.38	1.32
1	J	169	ILE	C-O	-5.97	1.17	1.24
1	G	198	ALA	C-O	5.96	1.31	1.24
1	F	59	PHE	C-O	5.80	1.30	1.24
1	B	68	VAL	C-O	-5.78	1.17	1.24
1	V	59	PHE	C-O	5.75	1.30	1.24
1	I	65	ILE	C-O	-5.50	1.17	1.24
1	S	49	TYR	C-O	-5.49	1.17	1.24
1	B	54	PHE	C-O	5.47	1.30	1.24
1	A	37	HIS	CE1-NE2	5.43	1.38	1.32
1	X	157	SER	CA-CB	-5.39	1.45	1.53
1	D	162	ARG	C-O	5.33	1.30	1.24
1	H	37	HIS	CE1-NE2	5.32	1.37	1.32
1	T	37	HIS	CE1-NE2	5.26	1.37	1.32
1	G	98	ALA	C-O	5.23	1.30	1.24
1	H	162	ARG	C-O	5.20	1.30	1.24
1	D	152	PRO	C-O	-5.18	1.17	1.24
1	H	59	PHE	C-O	5.13	1.29	1.24
1	G	110	ARG	C-O	5.10	1.30	1.24
1	K	63	THR	C-O	-5.04	1.18	1.24
1	R	61	SER	C-O	5.02	1.29	1.24
1	N	164	LEU	C-O	-5.01	1.17	1.24

All (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
1	R	151	VAL	CB-CA-C	7.18	116.37	109.33
1	D	116	GLY	CA-C-N	6.97	129.95	120.54
1	D	116	GLY	C-N-CA	6.97	129.95	120.54
1	Q	65	ILE	CA-C-O	-6.84	114.15	121.27
1	X	174	ASP	CA-CB-CG	6.70	119.30	112.60
1	T	58	THR	CA-CB-OG1	-6.64	99.64	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	117	ASP	CA-CB-CG	6.55	119.15	112.60
1	X	126	ASP	CA-CB-CG	6.47	119.07	112.60
1	M	190	THR	CA-CB-OG1	-6.30	100.14	109.60
1	R	151	VAL	N-CA-CB	-6.29	104.90	111.64
1	F	171	CYS	CB-CA-C	-6.28	100.76	110.81
1	I	65	ILE	CA-C-O	-6.23	114.25	120.85
1	I	88	ASP	CA-CB-CG	6.22	118.82	112.60
1	I	66	GLU	CB-CA-C	-6.10	101.31	110.88
1	F	143	ASP	CA-CB-CG	6.08	118.68	112.60
1	R	151	VAL	O-C-N	-6.02	117.89	121.69
1	L	181	HIS	CA-CB-CG	-5.98	107.82	113.80
1	S	30	ASP	CA-CB-CG	5.98	118.58	112.60
1	W	72	HIS	CA-CB-CG	5.97	119.77	113.80
1	O	159	GLU	CA-C-N	5.96	129.38	120.31
1	O	159	GLU	C-N-CA	5.96	129.38	120.31
1	E	193	LEU	N-CA-C	-5.85	104.59	110.97
1	X	117	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	64	ILE	CA-C-O	-5.83	115.21	121.27
1	I	103	PRO	CB-CA-C	-5.74	104.41	111.64
1	H	188	GLU	CA-C-N	5.67	128.13	120.65
1	H	188	GLU	C-N-CA	5.67	128.13	120.65
1	V	172	PHE	CA-C-N	5.67	127.87	120.28
1	V	172	PHE	C-N-CA	5.67	127.87	120.28
1	U	103	PRO	CB-CA-C	-5.65	104.52	111.64
1	T	190	THR	CA-C-O	-5.63	113.74	120.10
1	N	126	ASP	CA-CB-CG	5.62	118.22	112.60
1	W	184	PHE	CA-CB-CG	-5.61	108.19	113.80
1	S	172	PHE	CA-CB-CG	5.55	119.35	113.80
1	K	136	ARG	N-CA-C	-5.54	104.93	110.97
1	O	152	PRO	CA-C-N	5.50	127.92	120.38
1	O	152	PRO	C-N-CA	5.50	127.92	120.38
1	S	171	CYS	CA-C-N	5.48	127.89	120.44
1	S	171	CYS	C-N-CA	5.48	127.89	120.44
1	J	100	GLY	CA-C-O	-5.48	117.30	122.39
1	G	152	PRO	CA-C-N	5.46	128.35	120.38
1	G	152	PRO	C-N-CA	5.46	128.35	120.38
1	C	111	LEU	O-C-N	5.45	127.97	122.09
1	T	143	ASP	CA-CB-CG	5.45	118.05	112.60
1	N	181	HIS	CA-CB-CG	-5.44	108.36	113.80
1	K	72	HIS	CB-CA-C	5.42	119.11	109.72
1	P	59	PHE	CA-CB-CG	-5.41	108.39	113.80
1	J	116	GLY	CA-C-O	-5.41	117.66	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	49	TYR	CA-C-O	-5.37	114.86	120.55
1	N	188	GLU	CA-C-N	5.36	127.41	120.44
1	N	188	GLU	C-N-CA	5.36	127.41	120.44
1	R	116	GLY	CA-C-N	5.35	127.76	120.54
1	R	116	GLY	C-N-CA	5.35	127.76	120.54
1	M	36	ASP	N-CA-C	-5.33	105.38	111.14
1	R	157	SER	CA-C-O	-5.31	115.18	121.66
1	I	196	LYS	CA-C-N	5.30	127.38	120.28
1	I	196	LYS	C-N-CA	5.30	127.38	120.28
1	Q	76	PHE	CA-C-N	5.29	129.43	120.64
1	Q	76	PHE	C-N-CA	5.29	129.43	120.64
1	N	172	PHE	CA-C-N	5.28	128.09	120.38
1	N	172	PHE	C-N-CA	5.28	128.09	120.38
1	L	53	SER	CA-C-O	-5.28	116.05	122.64
1	F	191	ASP	CA-CB-CG	5.25	117.84	112.60
1	T	126	ASP	CA-CB-CG	5.25	117.84	112.60
1	U	86	GLY	CA-C-O	-5.22	116.26	121.90
1	M	159	GLU	CA-C-N	5.21	127.69	120.29
1	M	159	GLU	C-N-CA	5.21	127.69	120.29
1	C	88	ASP	CA-CB-CG	5.19	117.79	112.60
1	Q	172	PHE	CA-CB-CG	5.18	118.98	113.80
1	E	63	THR	CA-CB-OG1	-5.14	101.89	109.60
1	J	63	THR	CA-CB-OG1	-5.14	101.89	109.60
1	E	125	GLU	CB-CG-CD	5.14	121.34	112.60
1	B	171	CYS	CB-CA-C	-5.13	102.82	110.88
1	E	195	GLU	CA-C-O	-5.13	115.43	120.82
1	U	174	ASP	CA-CB-CG	5.13	117.73	112.60
1	T	28	THR	N-CA-C	-5.11	106.55	112.89
1	I	69	GLY	CA-C-O	-5.11	115.49	120.75
1	J	28	THR	CB-CA-C	5.10	118.16	109.24
1	N	166	LEU	N-CA-C	-5.10	105.64	111.14
1	U	40	VAL	CA-C-O	-5.10	115.83	121.29
1	M	198	ALA	CA-C-N	5.09	130.86	121.70
1	M	198	ALA	C-N-CA	5.09	130.86	121.70
1	N	118	GLU	CA-C-N	5.09	127.10	120.28
1	N	118	GLU	C-N-CA	5.09	127.10	120.28
1	P	188	GLU	N-CA-C	-5.08	105.66	111.14
1	L	122	LYS	CA-C-N	5.07	127.40	120.46
1	L	122	LYS	C-N-CA	5.07	127.40	120.46
1	O	29	ASP	CA-C-O	-5.07	115.50	120.82
1	V	54	PHE	CA-C-O	-5.07	115.18	120.55
1	U	169	ILE	CA-C-O	-5.06	115.80	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	44	ASP	CB-CA-C	5.05	119.28	110.79
1	V	61	SER	N-CA-C	-5.05	105.66	111.07
1	M	40	VAL	CA-C-O	-5.05	115.89	121.29
1	I	159	GLU	CA-C-N	5.02	127.94	120.31
1	I	159	GLU	C-N-CA	5.02	127.94	120.31
1	S	75	MET	CA-C-N	5.02	127.50	120.28
1	S	75	MET	C-N-CA	5.02	127.50	120.28
1	T	171	CYS	CB-CA-C	-5.01	102.79	110.81
1	E	65	ILE	CA-C-O	-5.01	115.74	120.95

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
1	R	1186	0	1174	9	0
1	S	1259	0	1246	16	0
1	T	1186	0	1174	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:110:ARG:HG2	1:B:194:PHE:CE1	2.15	0.82
1:A:90:LEU:HD22	1:V:73:ILE:HG22	1.62	0.79
1:N:133:ILE:CD1	1:S:77:ILE:HG12	2.13	0.79
1:D:110:ARG:HG2	1:D:194:PHE:CE1	2.18	0.78
1:C:93:HIS:CG	1:J:73:ILE:HD11	2.19	0.77
1:C:93:HIS:HB3	1:J:73:ILE:HD11	1.66	0.77
1:X:103:PRO:HG3	1:X:171:CYS:SG	2.24	0.77
1:G:100:GLY:O	1:K:84:LYS:HE2	1.83	0.77
1:F:110:ARG:HG2	1:F:194:PHE:CE1	2.20	0.76
1:B:151:VAL:HG13	3:B:304:HOH:O	1.86	0.75
1:U:165:LEU:HD23	1:U:197:LEU:HD11	1.69	0.75
1:C:93:HIS:CB	1:J:73:ILE:HD11	2.17	0.74
1:X:173:ASP:O	1:X:177:VAL:HG12	1.90	0.72
1:C:93:HIS:CG	1:J:73:ILE:CD1	2.74	0.71
1:L:136:ARG:HH21	1:L:136:ARG:CG	2.04	0.69
1:E:77:ILE:HG23	1:P:133:ILE:HD11	1.73	0.69
1:L:115:ILE:HD11	1:L:120:ILE:HG13	1.75	0.69
1:L:136:ARG:HG2	1:L:136:ARG:NH2	2.03	0.69
1:L:110:ARG:HG2	1:L:194:PHE:CZ	2.28	0.68
1:A:90:LEU:CD2	1:V:73:ILE:HG22	2.22	0.67
1:J:110:ARG:HG2	1:J:194:PHE:CZ	2.30	0.67
1:E:77:ILE:O	1:E:77:ILE:CG2	2.42	0.67
1:W:165:LEU:HD23	1:W:197:LEU:HD11	1.77	0.67
1:Q:170:GLU:HA	1:Q:170:GLU:OE1	1.95	0.66
1:W:37:HIS:O	1:W:40:VAL:HB	1.96	0.66
1:C:48:LEU:HD12	1:C:60:ILE:HD12	1.76	0.66
1:H:102:LEU:CD1	1:H:167:TYR:OH	2.41	0.66
1:E:79:GLU:HG3	1:E:79:GLU:O	1.96	0.66
1:H:188:GLU:HA	1:H:188:GLU:OE2	1.96	0.66
1:A:90:LEU:HD22	1:V:73:ILE:CG2	2.27	0.65
1:O:73:ILE:HD12	1:O:83:ILE:HD11	1.77	0.65
1:W:199:ASN:C	1:W:199:ASN:HD22	2.05	0.65
1:J:173:ASP:O	1:J:177:VAL:HG12	1.96	0.64
1:J:106:LYS:H	1:J:106:LYS:HD2	1.63	0.64
1:D:188:GLU:OE2	1:D:188:GLU:HA	1.98	0.64
1:R:103:PRO:HD3	1:R:171:CYS:SG	2.38	0.63
1:P:115:ILE:HD11	1:P:120:ILE:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:165:LEU:HD23	1:Q:197:LEU:HD11	1.81	0.62
1:P:105:ILE:HD13	1:P:105:ILE:O	1.99	0.62
1:X:103:PRO:CG	1:X:171:CYS:SG	2.88	0.61
1:F:110:ARG:HG2	1:F:194:PHE:CZ	2.36	0.61
1:V:173:ASP:O	1:V:177:VAL:HG12	2.01	0.61
1:F:53:SER:HB3	3:F:302:HOH:O	2.01	0.61
1:X:146:ASP:O	1:X:147:ASP:HB2	1.99	0.61
1:T:110:ARG:HG2	1:T:194:PHE:CZ	2.35	0.60
1:E:77:ILE:O	1:E:77:ILE:HG22	2.00	0.60
1:L:103:PRO:HG3	1:L:171:CYS:HA	1.83	0.60
1:C:122:LYS:HG2	3:C:402:HOH:O	2.00	0.60
1:N:31:LEU:HD22	1:N:75:MET:HE3	1.83	0.59
1:S:107:MET:HB2	1:U:184:PHE:HE2	1.67	0.59
1:I:165:LEU:HD23	1:I:197:LEU:HD11	1.84	0.59
1:N:133:ILE:HD11	1:S:77:ILE:HG23	1.82	0.59
2:R:301:SO4:O3	1:S:181:HIS:HB2	2.03	0.59
1:E:77:ILE:HG12	1:P:133:ILE:HD13	1.85	0.59
1:T:110:ARG:HG2	1:T:194:PHE:CE1	2.37	0.59
1:T:105:ILE:HG21	1:T:120:ILE:HG21	1.85	0.58
1:B:188:GLU:OE2	1:B:188:GLU:HA	2.02	0.58
1:M:67:GLU:O	1:M:71:THR:HG23	2.04	0.58
1:L:105:ILE:HG21	1:L:120:ILE:HG21	1.86	0.58
1:K:67:GLU:O	1:K:71:THR:HG23	2.03	0.58
1:J:97:HIS:CE1	3:J:301:HOH:O	2.56	0.57
1:L:103:PRO:HD3	1:L:171:CYS:SG	2.44	0.57
1:V:115:ILE:HD11	1:V:120:ILE:CD1	2.35	0.57
1:U:44:ASP:OD1	1:V:53:SER:OG	2.22	0.57
1:O:67:GLU:O	1:O:71:THR:HG23	2.04	0.57
1:J:110:ARG:HG2	1:J:194:PHE:CE1	2.39	0.57
1:J:145:ILE:HD12	1:J:150:GLU:OE1	2.04	0.57
1:R:108:GLY:CA	2:R:301:SO4:O2	2.39	0.57
1:I:112:ASN:OD1	1:I:117:ASP:OD1	2.23	0.56
1:A:151:VAL:O	1:A:152:PRO:C	2.47	0.56
1:N:133:ILE:HD13	1:S:77:ILE:HG12	1.87	0.56
1:N:173:ASP:O	1:N:177:VAL:HG12	2.04	0.56
1:O:165:LEU:HD23	1:O:197:LEU:HD11	1.85	0.56
1:H:129:THR:HG22	1:H:131:GLU:H	1.71	0.56
1:K:96:LYS:HE2	1:K:96:LYS:H	1.70	0.55
1:S:107:MET:HB2	1:U:184:PHE:CE2	2.41	0.55
1:N:133:ILE:HD12	1:S:77:ILE:HG12	1.89	0.55
1:F:51:ASN:HB3	3:F:303:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:29:ASP:OD1	1:P:108:GLY:O	2.25	0.55
1:E:79:GLU:O	1:E:79:GLU:CG	2.54	0.55
1:J:72:HIS:ND1	1:J:75:MET:CE	2.69	0.55
1:E:165:LEU:HD23	1:E:197:LEU:HD11	1.88	0.55
1:P:173:ASP:O	1:P:177:VAL:HG12	2.07	0.55
1:A:170:GLU:OE1	1:A:170:GLU:HA	2.06	0.54
1:B:103:PRO:HD3	1:B:171:CYS:SG	2.48	0.54
1:T:103:PRO:HD3	1:T:171:CYS:SG	2.47	0.54
1:J:106:LYS:HD3	1:J:109:GLY:HA3	1.88	0.54
1:V:120:ILE:O	1:V:124:VAL:HG23	2.07	0.54
1:N:110:ARG:HG2	1:N:194:PHE:CZ	2.42	0.54
1:C:66:GLU:HG3	1:C:99:PHE:CE2	2.43	0.54
1:W:152:PRO:HG2	1:X:37:HIS:CE1	2.43	0.54
1:B:110:ARG:HG2	1:B:194:PHE:CZ	2.42	0.53
1:D:48:LEU:HD12	1:D:60:ILE:HD12	1.89	0.53
1:L:110:ARG:HG2	1:L:194:PHE:CE1	2.44	0.53
1:H:110:ARG:HG2	1:H:194:PHE:CZ	2.43	0.53
1:B:36:ASP:OD1	1:B:182:HIS:HE1	1.92	0.53
1:B:108:GLY:HA3	2:E:301:SO4:O2	2.08	0.53
1:F:188:GLU:HA	1:F:188:GLU:OE2	2.09	0.52
1:S:77:ILE:O	1:S:77:ILE:CG2	2.57	0.52
1:N:95:SER:HB3	1:U:90:LEU:O	2.09	0.52
1:Q:166:LEU:HD21	1:Q:197:LEU:HB3	1.91	0.52
1:H:191:ASP:O	1:H:195:GLU:HG3	2.09	0.52
1:J:36:ASP:OD1	1:J:182:HIS:HE1	1.93	0.52
1:B:173:ASP:O	1:B:177:VAL:HG12	2.10	0.51
1:H:129:THR:CG2	1:H:131:GLU:HB2	2.39	0.51
1:I:170:GLU:OE1	1:I:170:GLU:HA	2.11	0.51
1:W:26:LYS:NZ	1:X:147:ASP:O	2.43	0.51
1:L:103:PRO:CD	1:L:171:CYS:SG	2.98	0.51
1:T:36:ASP:OD1	1:T:182:HIS:HE1	1.93	0.51
1:H:136:ARG:O	1:H:137:GLU:C	2.54	0.51
1:A:90:LEU:CD2	1:V:73:ILE:CG2	2.88	0.51
1:G:91:ARG:HB2	1:G:91:ARG:NH1	2.26	0.50
1:Q:48:LEU:HD12	1:Q:60:ILE:HD12	1.93	0.50
1:V:105:ILE:HD13	1:V:105:ILE:H	1.76	0.50
1:B:106:LYS:HD3	1:E:182:HIS:CE1	2.45	0.50
1:G:48:LEU:HD12	1:G:60:ILE:HD12	1.94	0.50
1:K:193:LEU:O	1:K:197:LEU:HB2	2.11	0.50
1:J:115:ILE:HD11	1:J:120:ILE:HG13	1.93	0.50
1:J:120:ILE:O	1:J:124:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:44:ASP:OD1	1:L:53:SER:OG	2.29	0.49
1:D:115:ILE:HD11	1:D:120:ILE:HG13	1.94	0.49
1:R:188:GLU:HA	1:R:188:GLU:OE2	2.11	0.49
1:U:59:PHE:C	1:U:59:PHE:CD2	2.90	0.49
1:W:170:GLU:OE1	1:W:170:GLU:HA	2.13	0.49
1:O:73:ILE:HG21	1:O:83:ILE:CD1	2.42	0.49
1:N:59:PHE:CD1	1:N:136:ARG:HG2	2.47	0.49
1:P:103:PRO:HD3	1:P:171:CYS:SG	2.52	0.49
1:M:103:PRO:HG3	1:M:175:SER:OG	2.13	0.49
1:P:117:ASP:OD1	1:P:117:ASP:N	2.42	0.49
1:X:146:ASP:O	1:X:147:ASP:CB	2.60	0.49
1:G:141:TYR:HA	1:H:67:GLU:OE1	2.12	0.49
1:O:44:ASP:OD1	1:P:53:SER:OG	2.31	0.48
1:L:120:ILE:O	1:L:124:VAL:HG23	2.13	0.48
1:R:151:VAL:HG13	3:R:402:HOH:O	2.12	0.48
1:D:173:ASP:O	1:D:177:VAL:HG12	2.13	0.48
1:E:77:ILE:HG12	1:P:133:ILE:CD1	2.43	0.48
1:D:108:GLY:HA3	2:G:301:SO4:O2	2.13	0.48
1:M:165:LEU:HD23	1:M:197:LEU:HD11	1.95	0.48
1:W:112:ASN:OD1	1:W:117:ASP:OD1	2.32	0.48
1:M:162:ARG:HG3	1:M:197:LEU:HD22	1.96	0.48
1:T:188:GLU:OE2	1:T:188:GLU:HA	2.14	0.47
1:O:75:MET:HB2	1:O:82:ASP:HB2	1.97	0.47
1:G:152:PRO:HG2	1:H:37:HIS:CE1	2.49	0.47
1:L:59:PHE:CD1	1:L:136:ARG:HG3	2.49	0.47
1:P:59:PHE:CD1	1:P:136:ARG:HG2	2.49	0.47
1:L:136:ARG:CG	1:L:136:ARG:NH2	2.71	0.47
1:M:170:GLU:HA	1:M:170:GLU:OE1	2.14	0.47
1:K:152:PRO:HG2	1:L:37:HIS:CE1	2.50	0.47
1:T:110:ARG:CG	1:T:194:PHE:CE1	2.97	0.47
1:L:93:HIS:HA	1:L:96:LYS:HE3	1.97	0.47
1:Q:162:ARG:HH21	1:Q:198:ALA:HA	1.79	0.46
1:U:37:HIS:O	1:U:40:VAL:HB	2.15	0.46
1:R:109:GLY:O	1:R:111:LEU:N	2.49	0.46
1:T:38:ILE:HG21	1:T:172:PHE:CD1	2.50	0.46
1:H:110:ARG:HG2	1:H:194:PHE:CE1	2.51	0.46
1:A:91:ARG:NH2	1:V:128:GLU:OE1	2.48	0.46
1:X:59:PHE:CD1	1:X:136:ARG:HG2	2.50	0.46
1:L:173:ASP:O	1:L:177:VAL:HG12	2.15	0.46
1:O:170:GLU:HA	1:O:170:GLU:OE1	2.16	0.46
1:H:66:GLU:HG3	1:H:66:GLU:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LYS:HB2	1:E:26:LYS:HE2	1.78	0.45
1:Q:68:VAL:HG11	1:Q:171:CYS:SG	2.56	0.45
1:O:132:LEU:HD23	1:O:132:LEU:HA	1.88	0.45
1:W:162:ARG:HG3	1:W:197:LEU:HD22	1.99	0.45
1:F:103:PRO:HD3	1:F:171:CYS:SG	2.55	0.45
1:G:165:LEU:HD23	1:G:197:LEU:HD11	1.98	0.45
1:G:132:LEU:HD23	1:G:132:LEU:HA	1.85	0.45
1:S:198:ALA:O	1:S:199:ASN:C	2.60	0.45
1:R:132:LEU:HD23	1:R:132:LEU:HA	1.88	0.45
1:K:83:ILE:HD12	1:K:179:TYR:CG	2.52	0.45
1:R:173:ASP:O	1:R:177:VAL:HG12	2.17	0.45
1:S:166:LEU:HD21	1:S:197:LEU:HB3	1.98	0.45
1:C:159:GLU:CD	1:C:159:GLU:H	2.25	0.45
1:M:73:ILE:HD13	1:M:83:ILE:HD13	1.97	0.45
1:K:103:PRO:HG3	1:K:175:SER:OG	2.17	0.44
1:F:105:ILE:HG21	1:F:120:ILE:HG21	1.98	0.44
1:I:120:ILE:O	1:I:124:VAL:HG23	2.17	0.44
1:S:75:MET:HG3	1:U:87:LYS:HD2	1.98	0.44
1:B:46:TYR:O	1:B:50:THR:HG23	2.17	0.44
1:D:69:GLY:HA2	1:D:101:SER:HB3	1.99	0.44
1:J:105:ILE:HD13	1:J:105:ILE:H	1.81	0.44
1:R:26:LYS:NZ	1:R:26:LYS:CB	2.80	0.44
1:D:42:ILE:HG12	1:D:64:ILE:HD13	1.98	0.44
1:H:105:ILE:HG21	1:H:120:ILE:HG21	1.98	0.44
1:D:108:GLY:CA	2:G:301:SO4:O2	2.65	0.44
1:C:89:PRO:O	1:J:101:SER:HA	2.17	0.44
1:O:102:LEU:HD13	1:O:102:LEU:HA	1.85	0.44
1:G:91:ARG:HB2	1:G:91:ARG:HH11	1.83	0.44
1:S:77:ILE:O	1:S:77:ILE:HG22	2.18	0.44
1:N:36:ASP:OD1	1:N:182:HIS:HE1	2.00	0.44
1:N:115:ILE:HD11	1:N:120:ILE:HG13	1.99	0.43
1:A:44:ASP:OD1	1:B:53:SER:OG	2.35	0.43
1:E:95:SER:O	1:E:95:SER:OG	2.31	0.43
1:U:97:HIS:HD2	1:U:98:ALA:N	2.15	0.43
1:H:105:ILE:HD13	1:H:105:ILE:H	1.82	0.43
1:K:97:HIS:CD2	1:K:99:PHE:HB2	2.54	0.43
1:M:132:LEU:HD23	1:M:132:LEU:HA	1.83	0.43
1:T:132:LEU:HD23	1:T:132:LEU:HA	1.89	0.43
1:I:192:GLU:O	1:I:195:GLU:HG2	2.18	0.43
1:O:28:THR:HG22	1:O:76:PHE:CD2	2.54	0.43
1:K:165:LEU:HD23	1:K:197:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:HIS:O	1:M:40:VAL:HB	2.18	0.43
1:V:69:GLY:O	1:V:73:ILE:HG23	2.19	0.43
1:D:105:ILE:HD13	1:D:105:ILE:H	1.82	0.43
1:N:103:PRO:HG3	1:N:171:CYS:SG	2.58	0.43
1:O:82:ASP:O	1:O:82:ASP:CG	2.62	0.43
1:P:46:TYR:CZ	1:P:50:THR:HG21	2.53	0.43
1:S:24:SER:HB2	1:T:144:ILE:CD1	2.49	0.43
1:J:118:GLU:HG2	1:J:119:MET:N	2.32	0.43
1:B:102:LEU:HA	1:B:103:PRO:HD2	1.91	0.43
1:N:103:PRO:CG	1:N:171:CYS:SG	3.07	0.43
1:P:177:VAL:CG2	1:P:187:SER:HB3	2.49	0.43
1:V:145:ILE:HD12	1:V:150:GLU:OE1	2.19	0.43
1:W:83:ILE:HD13	1:W:179:TYR:CG	2.54	0.43
1:H:103:PRO:HD3	1:H:171:CYS:SG	2.59	0.42
1:A:90:LEU:HD11	1:V:72:HIS:CD2	2.54	0.42
1:D:59:PHE:CD1	1:D:136:ARG:HG2	2.53	0.42
1:J:72:HIS:ND1	1:J:75:MET:HE3	2.32	0.42
1:Q:148:ILE:HD13	1:Q:149:LEU:O	2.19	0.42
1:D:110:ARG:HG2	1:D:194:PHE:CZ	2.53	0.42
1:D:125:GLU:O	1:D:129:THR:OG1	2.37	0.42
1:K:170:GLU:OE1	1:K:170:GLU:HA	2.19	0.42
1:U:97:HIS:CD2	1:U:98:ALA:N	2.87	0.42
1:F:107:MET:HE2	1:F:107:MET:HB3	1.97	0.42
1:V:111:LEU:HG	1:V:120:ILE:HD11	2.01	0.42
1:M:83:ILE:HD12	1:M:179:TYR:CG	2.55	0.42
1:U:165:LEU:CD2	1:U:197:LEU:HD11	2.45	0.42
1:F:151:VAL:HG13	3:F:304:HOH:O	2.19	0.42
1:D:42:ILE:CG1	1:D:64:ILE:HD13	2.50	0.42
1:H:59:PHE:CD1	1:H:136:ARG:HG2	2.55	0.42
1:U:97:HIS:HE1	1:U:133:ILE:HD11	1.85	0.42
1:X:36:ASP:OD1	1:X:182:HIS:HE1	2.03	0.42
1:U:46:TYR:CZ	1:U:50:THR:HG21	2.54	0.42
1:H:102:LEU:HA	1:H:103:PRO:HD2	1.95	0.41
1:J:54:PHE:CZ	1:J:158:LYS:HD2	2.55	0.41
1:J:59:PHE:CD1	1:J:136:ARG:HG2	2.55	0.41
1:I:46:TYR:O	1:I:50:THR:HG23	2.20	0.41
1:J:72:HIS:HA	1:J:75:MET:HE2	2.02	0.41
1:C:46:TYR:O	1:C:50:THR:HG23	2.20	0.41
1:I:102:LEU:HD13	1:I:102:LEU:HA	1.85	0.41
1:A:148:ILE:HD13	1:A:149:LEU:O	2.20	0.41
1:I:132:LEU:HD23	1:I:132:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:31:LEU:CD2	1:N:75:MET:HE3	2.49	0.41
1:Q:26:LYS:HB3	1:Q:26:LYS:HE2	1.86	0.41
1:S:70:LYS:HA	1:S:73:ILE:HD12	2.02	0.41
1:B:105:ILE:HG21	1:B:120:ILE:HD13	2.01	0.41
1:F:110:ARG:CG	1:F:194:PHE:CE1	2.99	0.41
1:F:177:VAL:O	1:F:177:VAL:CG1	2.68	0.41
1:P:132:LEU:HD23	1:P:132:LEU:HA	1.83	0.41
1:W:59:PHE:CD2	1:W:59:PHE:C	2.99	0.41
1:W:199:ASN:C	1:W:199:ASN:ND2	2.77	0.41
1:S:66:GLU:HG3	1:S:99:PHE:CZ	2.55	0.41
1:S:102:LEU:HD13	1:S:102:LEU:HA	1.85	0.41
1:U:102:LEU:HD13	1:U:102:LEU:HA	1.94	0.41
1:P:177:VAL:HG21	1:P:187:SER:CB	2.51	0.41
1:Q:132:LEU:HD23	1:Q:132:LEU:HA	1.90	0.41
1:A:48:LEU:HD12	1:A:60:ILE:HD12	2.03	0.41
1:E:46:TYR:O	1:E:50:THR:HG23	2.21	0.41
1:A:73:ILE:HD11	1:A:98:ALA:CA	2.51	0.41
1:E:77:ILE:CG2	1:P:133:ILE:HD11	2.47	0.41
1:N:118:GLU:HG2	1:N:119:MET:N	2.36	0.41
1:U:152:PRO:HG2	1:V:37:HIS:CE1	2.56	0.41
1:E:171:CYS:HB2	3:E:401:HOH:O	2.21	0.40
1:F:132:LEU:HA	1:F:132:LEU:HD23	1.88	0.40
1:I:36:ASP:O	1:I:39:SER:HB3	2.22	0.40
1:I:44:ASP:OD1	1:J:53:SER:OG	2.31	0.40
1:K:102:LEU:HD13	1:K:102:LEU:HA	1.91	0.40
1:K:132:LEU:HD23	1:K:132:LEU:HA	1.79	0.40
1:C:165:LEU:HD23	1:C:197:LEU:HD11	2.03	0.40
1:P:49:TYR:CD1	1:P:49:TYR:C	2.98	0.40
1:U:132:LEU:HD23	1:U:132:LEU:HA	1.86	0.40
1:A:75:MET:HE3	1:A:94:LYS:HD3	2.03	0.40
1:G:182:HIS:N	2:G:301:SO4:O3	2.42	0.40
1:K:88:ASP:HA	1:K:89:PRO:HD2	1.93	0.40
1:T:26:LYS:HB2	1:T:27:SER:H	1.76	0.40
1:V:58:THR:HG23	1:V:164:LEU:HD12	2.03	0.40
1:A:90:LEU:CD1	1:V:72:HIS:CD2	3.05	0.40
1:B:59:PHE:CD1	1:B:136:ARG:HG2	2.57	0.40
1:M:102:LEU:HD13	1:M:102:LEU:HA	1.88	0.40
1:V:115:ILE:HD11	1:V:120:ILE:HD13	2.02	0.40
1:W:102:LEU:HD13	1:W:102:LEU:HA	1.88	0.40
1:C:93:HIS:HB3	1:J:73:ILE:CD1	2.46	0.40
1:I:83:ILE:C	1:I:84:LYS:HG3	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:ASP:O	1:N:177:VAL:CG1	2.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	22	32
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%)	19	28
1	G	159/184 (86%)	155 (98%)	3 (2%)	1 (1%)	22	32
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%)	22	32
1	L	152/184 (83%)	143 (94%)	8 (5%)	1 (1%)	19	28
1	M	166/184 (90%)	161 (97%)	4 (2%)	1 (1%)	22	32
1	N	151/184 (82%)	145 (96%)	5 (3%)	1 (1%)	19	28
1	O	166/184 (90%)	161 (97%)	2 (1%)	3 (2%)	7	9
1	P	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
1	Q	157/184 (85%)	148 (94%)	8 (5%)	1 (1%)	22	32
1	R	148/184 (80%)	143 (97%)	3 (2%)	2 (1%)	9	12
1	S	157/184 (85%)	150 (96%)	6 (4%)	1 (1%)	22	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	19	28
1	W	165/184 (90%)	156 (94%)	7 (4%)	2 (1%)	11	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%)	19	28

All (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
1	R	110	ARG
1	T	110	ARG
1	X	110	ARG
1	H	102	LEU
1	B	102	LEU
1	C	146	ASP
1	G	146	ASP
1	K	146	ASP
1	L	102	LEU
1	M	146	ASP
1	Q	146	ASP
1	R	102	LEU
1	T	102	LEU
1	W	146	ASP
1	X	147	ASP
1	O	80	ASN
1	O	146	ASP
1	S	146	ASP
1	W	81	LYS
1	H	101	SER
1	V	100	GLY



### 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%)	7	10
1	B	134/166 (81%)	119 (89%)	15 (11%)	5	6
1	C	149/166 (90%)	133 (89%)	16 (11%)	5	7
1	D	134/166 (81%)	123 (92%)	11 (8%)	9	14
1	E	144/166 (87%)	127 (88%)	17 (12%)	4	5
1	F	135/166 (81%)	121 (90%)	14 (10%)	5	8
1	G	146/166 (88%)	125 (86%)	21 (14%)	2	2
1	H	135/166 (81%)	116 (86%)	19 (14%)	3	3
1	I	149/166 (90%)	134 (90%)	15 (10%)	6	8
1	J	136/166 (82%)	123 (90%)	13 (10%)	7	9
1	K	158/166 (95%)	140 (89%)	18 (11%)	4	6
1	L	139/166 (84%)	129 (93%)	10 (7%)	12	18
1	M	152/166 (92%)	134 (88%)	18 (12%)	4	5
1	N	138/166 (83%)	124 (90%)	14 (10%)	6	8
1	O	152/166 (92%)	134 (88%)	18 (12%)	4	5
1	P	138/166 (83%)	122 (88%)	16 (12%)	4	6
1	Q	144/166 (87%)	127 (88%)	17 (12%)	4	5
1	R	135/166 (81%)	122 (90%)	13 (10%)	7	9
1	S	144/166 (87%)	126 (88%)	18 (12%)	3	4
1	T	135/166 (81%)	122 (90%)	13 (10%)	7	9
1	U	149/166 (90%)	138 (93%)	11 (7%)	11	18
1	V	135/166 (81%)	121 (90%)	14 (10%)	5	8
1	W	152/166 (92%)	136 (90%)	16 (10%)	5	8
1	X	132/166 (80%)	120 (91%)	12 (9%)	7	11
All	All	3412/3984 (86%)	3049 (89%)	363 (11%)	5	7

All (363) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	53	SER
1	A	75	MET
1	A	87	LYS
1	A	102	LEU
1	A	122	LYS
1	A	137	GLU
1	A	148	ILE
1	A	151	VAL
1	A	174	ASP
1	A	185	GLU
1	A	190	THR
1	A	195	GLU
1	A	197	LEU
1	B	73	ILE
1	B	101	SER
1	B	102	LEU
1	B	105	ILE
1	B	134	SER
1	B	145	ILE
1	B	147	ASP
1	B	151	VAL
1	B	171	CYS
1	B	173	ASP
1	B	177	VAL
1	B	187	SER
1	B	188	GLU
1	B	192	GLU
1	B	199	ASN
1	C	26	LYS
1	C	28	THR
1	C	53	SER
1	C	73	ILE
1	C	93	HIS
1	C	101	SER
1	C	102	LEU
1	C	122	LYS
1	C	137	GLU
1	C	148	ILE
1	C	151	VAL
1	C	174	ASP
1	C	185	GLU
1	C	190	THR

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Mol	Chain	Res	Type
1	C	195	GLU
1	C	197	LEU
1	D	73	ILE
1	D	105	ILE
1	D	106	LYS
1	D	122	LYS
1	D	129	THR
1	D	132	LEU
1	D	151	VAL
1	D	173	ASP
1	D	174	ASP
1	D	177	VAL
1	D	188	GLU
1	E	26	LYS
1	E	28	THR
1	E	53	SER
1	E	75	MET
1	E	78	SER
1	E	96	LYS
1	E	102	LEU
1	E	122	LYS
1	E	128	GLU
1	E	148	ILE
1	E	151	VAL
1	E	159	GLU
1	E	160	GLN
1	E	174	ASP
1	E	185	GLU
1	E	190	THR
1	E	195	GLU
1	F	26	LYS
1	F	28	THR
1	F	53	SER
1	F	73	ILE
1	F	101	SER
1	F	104	THR
1	F	105	ILE
1	F	134	SER
1	F	147	ASP
1	F	151	VAL
1	F	171	CYS
1	F	173	ASP

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Mol	Chain	Res	Type
1	F	177	VAL
1	F	188	GLU
1	G	28	THR
1	G	33	LYS
1	G	53	SER
1	G	87	LYS
1	G	90	LEU
1	G	102	LEU
1	G	118	GLU
1	G	122	LYS
1	G	125	GLU
1	G	131	GLU
1	G	137	GLU
1	G	144	ILE
1	G	147	ASP
1	G	148	ILE
1	G	151	VAL
1	G	159	GLU
1	G	185	GLU
1	G	189	THR
1	G	190	THR
1	G	195	GLU
1	G	197	LEU
1	H	66	GLU
1	H	97	HIS
1	H	101	SER
1	H	102	LEU
1	H	104	THR
1	H	105	ILE
1	H	107	MET
1	H	129	THR
1	H	134	SER
1	H	151	VAL
1	H	171	CYS
1	H	173	ASP
1	H	174	ASP
1	H	177	VAL
1	H	185	GLU
1	H	187	SER
1	H	188	GLU
1	H	192	GLU
1	H	195	GLU

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Mol	Chain	Res	Type
1	I	26	LYS
1	I	28	THR
1	I	53	SER
1	I	84	LYS
1	I	85	ARG
1	I	96	LYS
1	I	102	LEU
1	I	122	LYS
1	I	146	ASP
1	I	148	ILE
1	I	151	VAL
1	I	185	GLU
1	I	190	THR
1	I	197	LEU
1	I	199	ASN
1	J	28	THR
1	J	53	SER
1	J	73	ILE
1	J	75	MET
1	J	105	ILE
1	J	106	LYS
1	J	107	MET
1	J	117	ASP
1	J	120	ILE
1	J	151	VAL
1	J	173	ASP
1	J	188	GLU
1	J	192	GLU
1	K	26	LYS
1	K	29	ASP
1	K	53	SER
1	K	80	ASN
1	K	83	ILE
1	K	84	LYS
1	K	85	ARG
1	K	87	LYS
1	K	94	LYS
1	K	96	LYS
1	K	101	SER
1	K	102	LEU
1	K	122	LYS
1	K	146	ASP

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Mol	Chain	Res	Type
1	K	148	ILE
1	K	151	VAL
1	K	190	THR
1	K	197	LEU
1	L	102	LEU
1	L	105	ILE
1	L	107	MET
1	L	112	ASN
1	L	117	ASP
1	L	120	ILE
1	L	136	ARG
1	L	151	VAL
1	L	173	ASP
1	L	177	VAL
1	M	24	SER
1	M	26	LYS
1	M	29	ASP
1	M	50	THR
1	M	53	SER
1	M	75	MET
1	M	81	LYS
1	M	82	ASP
1	M	83	ILE
1	M	85	ARG
1	M	87	LYS
1	M	102	LEU
1	M	117	ASP
1	M	122	LYS
1	M	143	ASP
1	M	151	VAL
1	M	190	THR
1	M	197	LEU
1	N	28	THR
1	N	43	LYS
1	N	53	SER
1	N	68	VAL
1	N	105	ILE
1	N	107	MET
1	N	118	GLU
1	N	120	ILE
1	N	132	LEU
1	N	137	GLU

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Mol	Chain	Res	Type
1	N	151	VAL
1	N	173	ASP
1	N	177	VAL
1	N	192	GLU
1	O	24	SER
1	O	26	LYS
1	O	53	SER
1	O	66	GLU
1	O	82	ASP
1	O	83	ILE
1	O	84	LYS
1	O	85	ARG
1	O	87	LYS
1	O	102	LEU
1	O	122	LYS
1	O	136	ARG
1	O	143	ASP
1	O	148	ILE
1	O	151	VAL
1	O	185	GLU
1	O	190	THR
1	O	197	LEU
1	P	28	THR
1	P	101	SER
1	P	102	LEU
1	P	104	THR
1	P	105	ILE
1	P	107	MET
1	P	110	ARG
1	P	117	ASP
1	P	120	ILE
1	P	132	LEU
1	P	148	ILE
1	P	151	VAL
1	P	173	ASP
1	P	177	VAL
1	P	188	GLU
1	P	192	GLU
1	Q	26	LYS
1	Q	53	SER
1	Q	75	MET
1	Q	78	SER

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Mol	Chain	Res	Type
1	Q	96	LYS
1	Q	102	LEU
1	Q	118	GLU
1	Q	122	LYS
1	Q	137	GLU
1	Q	147	ASP
1	Q	148	ILE
1	Q	151	VAL
1	Q	160	GLN
1	Q	171	CYS
1	Q	174	ASP
1	Q	185	GLU
1	Q	190	THR
1	R	26	LYS
1	R	101	SER
1	R	104	THR
1	R	105	ILE
1	R	120	ILE
1	R	122	LYS
1	R	134	SER
1	R	137	GLU
1	R	147	ASP
1	R	151	VAL
1	R	173	ASP
1	R	177	VAL
1	R	188	GLU
1	S	26	LYS
1	S	28	THR
1	S	53	SER
1	S	70	LYS
1	S	75	MET
1	S	78	SER
1	S	96	LYS
1	S	102	LEU
1	S	118	GLU
1	S	122	LYS
1	S	137	GLU
1	S	148	ILE
1	S	151	VAL
1	S	159	GLU
1	S	171	CYS
1	S	174	ASP

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Mol	Chain	Res	Type
1	S	190	THR
1	S	199	ASN
1	T	26	LYS
1	T	29	ASP
1	T	73	ILE
1	T	102	LEU
1	T	104	THR
1	T	105	ILE
1	T	134	SER
1	T	151	VAL
1	T	173	ASP
1	T	177	VAL
1	T	185	GLU
1	T	188	GLU
1	T	192	GLU
1	U	26	LYS
1	U	28	THR
1	U	53	SER
1	U	84	LYS
1	U	91	ARG
1	U	102	LEU
1	U	122	LYS
1	U	148	ILE
1	U	151	VAL
1	U	185	GLU
1	U	190	THR
1	V	28	THR
1	V	73	ILE
1	V	75	MET
1	V	105	ILE
1	V	117	ASP
1	V	118	GLU
1	V	133	ILE
1	V	137	GLU
1	V	138	SER
1	V	151	VAL
1	V	173	ASP
1	V	174	ASP
1	V	177	VAL
1	V	192	GLU
1	W	28	THR
1	W	53	SER

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Mol	Chain	Res	Type
1	W	80	ASN
1	W	81	LYS
1	W	84	LYS
1	W	102	LEU
1	W	122	LYS
1	W	136	ARG
1	W	147	ASP
1	W	148	ILE
1	W	151	VAL
1	W	155	LYS
1	W	185	GLU
1	W	190	THR
1	W	197	LEU
1	W	199	ASN
1	X	28	THR
1	X	43	LYS
1	X	53	SER
1	X	73	ILE
1	X	105	ILE
1	X	117	ASP
1	X	118	GLU
1	X	120	ILE
1	X	132	LEU
1	X	147	ASP
1	X	151	VAL
1	X	177	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	B	72	HIS
1	B	182	HIS
1	B	199	ASN
1	C	112	ASN
1	D	37	HIS
1	E	112	ASN
1	F	37	HIS
1	F	72	HIS
1	F	112	ASN
1	G	97	HIS
1	G	112	ASN

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Mol	Chain	Res	Type
1	H	37	HIS
1	H	72	HIS
1	I	32	ASN
1	I	112	ASN
1	J	182	HIS
1	K	80	ASN
1	K	112	ASN
1	L	37	HIS
1	L	72	HIS
1	L	182	HIS
1	M	72	HIS
1	M	80	ASN
1	N	37	HIS
1	N	182	HIS
1	O	112	ASN
1	P	37	HIS
1	P	97	HIS
1	P	199	ASN
1	Q	112	ASN
1	Q	160	GLN
1	R	37	HIS
1	R	199	ASN
1	S	112	ASN
1	T	37	HIS
1	T	72	HIS
1	T	112	ASN
1	T	182	HIS
1	U	97	HIS
1	V	160	GLN
1	V	182	HIS
1	W	72	HIS
1	W	112	ASN
1	W	199	ASN
1	X	112	ASN
1	X	182	HIS

### 5.3.3 RNA ⓘ

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	A	301	-	4,4,4	0.54	0	6,6,6	0.36	0
2	SO4	C	301	-	4,4,4	0.40	0	6,6,6	0.27	0
2	SO4	E	301	-	4,4,4	0.46	0	6,6,6	0.36	0
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	G	302	-	4,4,4	0.41	0	6,6,6	0.13	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	E	301	SO4	1	0
2	R	301	SO4	3	0
2	G	301	SO4	3	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	165/184 (89%)	-0.40	0 100 100	41, 67, 105, 121	0
1	B	151/184 (82%)	-0.24	1 (0%) 84 82	36, 65, 108, 129	0
1	C	167/184 (90%)	-0.26	0 100 100	46, 73, 109, 124	0
1	D	151/184 (82%)	-0.09	1 (0%) 84 82	42, 74, 117, 144	0
1	E	161/184 (87%)	-0.43	0 100 100	41, 66, 106, 139	0
1	F	152/184 (82%)	-0.29	1 (0%) 84 82	40, 66, 111, 124	0
1	G	163/184 (88%)	-0.25	0 100 100	48, 76, 111, 136	0
1	H	152/184 (82%)	-0.12	0 100 100	44, 75, 117, 140	0
1	I	166/184 (90%)	-0.34	1 (0%) 85 84	41, 69, 103, 120	0
1	J	153/184 (83%)	-0.22	0 100 100	37, 69, 119, 128	0
1	K	176/184 (95%)	-0.19	1 (0%) 85 84	44, 75, 121, 161	0
1	L	156/184 (84%)	-0.22	0 100 100	39, 69, 113, 139	0
1	M	170/184 (92%)	-0.31	0 100 100	40, 71, 111, 128	0
1	N	155/184 (84%)	-0.25	0 100 100	39, 70, 118, 149	0
1	O	170/184 (92%)	-0.25	1 (0%) 85 84	45, 74, 113, 131	0
1	P	155/184 (84%)	-0.24	0 100 100	38, 70, 119, 142	0
1	Q	161/184 (87%)	-0.27	1 (0%) 85 84	42, 70, 111, 139	0
1	R	152/184 (82%)	-0.22	1 (0%) 84 82	41, 71, 112, 132	0
1	S	161/184 (87%)	-0.37	0 100 100	46, 71, 110, 134	0
1	T	152/184 (82%)	-0.18	2 (1%) 74 73	44, 71, 115, 135	0
1	U	166/184 (90%)	-0.21	0 100 100	46, 76, 111, 134	0
1	V	152/184 (82%)	-0.10	3 (1%) 64 63	45, 81, 131, 152	0
1	W	169/184 (91%)	-0.18	0 100 100	44, 76, 118, 128	0
1	X	148/184 (80%)	-0.05	2 (1%) 73 72	43, 77, 132, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3824/4416 (86%)	-0.24	15 (0%) 89 88	36, 72, 117, 161	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	98	ALA	2.6
1	Q	77	ILE	2.6
1	T	105	ILE	2.6
1	K	44	ASP	2.5
1	X	108	GLY	2.5
1	F	98	ALA	2.4
1	X	105	ILE	2.4
1	V	98	ALA	2.2
1	R	98	ALA	2.2
1	B	98	ALA	2.2
1	O	44	ASP	2.2
1	D	98	ALA	2.2
1	I	44	ASP	2.1
1	V	101	SER	2.1
1	V	171	CYS	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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.