



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 09:46 AM GMT

PDB ID : 2JD8
Title : CRYSTAL STRUCTURE OF THE ZN-SOAKED FERRITIN FROM THE
HYPERTHERMOPHILIC ARCHAEAL ANAEROBE PYROCOCCLUS FU-
RIOSUS
Authors : Tatur, J.; Hagen, W.R.; Matias, P.M.
Deposited on : 2007-01-05
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

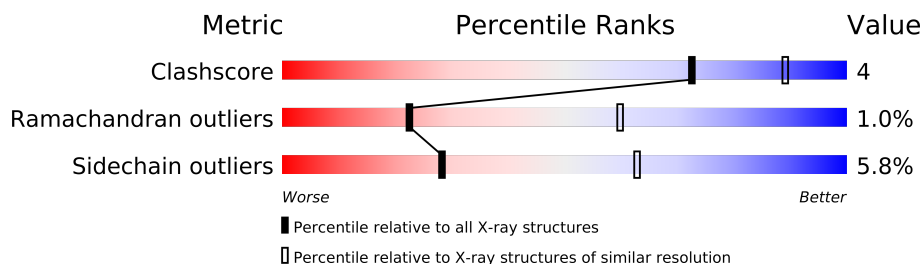
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)



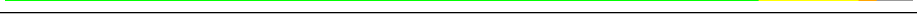
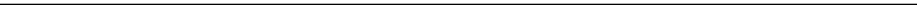





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	174	
1	1	174	
1	2	174	
1	3	174	
1	4	174	
1	5	174	
1	6	174	
1	7	174	
1	8	174	
1	9	174	
1	A	174	
1	B	174	
1	C	174	
1	D	174	
1	E	174	
1	F	174	
1	G	174	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	174	
1	I	174	
1	J	174	
1	K	174	
1	L	174	
1	M	174	
1	N	174	
1	O	174	
1	P	174	
1	Q	174	
1	R	174	
1	S	174	
1	T	174	
1	U	174	
1	V	174	
1	W	174	
1	X	174	
1	Y	174	
1	Z	174	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50351 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FERRITIN HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	1	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	2	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	3	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	4	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	5	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	6	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	7	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	8	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	9	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	A	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	B	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	C	167	Total	C	N	O	S	0	1	0
			1391	902	223	261	5			
1	D	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	E	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	F	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	H	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	I	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	J	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	K	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	L	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	M	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	N	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	O	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	P	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	Q	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	R	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	S	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	T	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	U	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	V	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	W	167	Total	C	N	O	S	0	1	0
			1388	900	221	262	5			
1	X	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	Y	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			
1	Z	167	Total	C	N	O	S	0	0	0
			1383	897	220	261	5			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total 2 Zn 2	0	0
2	K	2	Total 2 Zn 2	0	0
2	B	2	Total 2 Zn 2	0	0
2	6	2	Total 2 Zn 2	0	0
2	W	2	Total 2 Zn 2	0	0
2	N	2	Total 2 Zn 2	0	0
2	X	2	Total 2 Zn 2	0	0
2	2	2	Total 2 Zn 2	0	0
2	S	2	Total 2 Zn 2	0	0
2	J	2	Total 2 Zn 2	0	0
2	E	2	Total 2 Zn 2	0	0
2	V	2	Total 2 Zn 2	0	0
2	A	2	Total 2 Zn 2	0	0
2	5	2	Total 2 Zn 2	0	0
2	R	2	Total 2 Zn 2	0	0
2	M	2	Total 2 Zn 2	0	0
2	1	2	Total 2 Zn 2	0	0
2	D	2	Total 2 Zn 2	0	0
2	I	2	Total 2 Zn 2	0	0
2	Z	2	Total 2 Zn 2	0	0
2	4	2	Total 2 Zn 2	0	0
2	U	2	Total 2 Zn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	9	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	0	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	Q	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	7	2	Total 2	Zn 2	0	0
2	T	2	Total 2	Zn 2	0	0
2	8	2	Total 2	Zn 2	0	0
2	O	2	Total 2	Zn 2	0	0
2	Y	2	Total 2	Zn 2	0	0
2	3	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Fe 1	0	0
3	K	1	Total 1	Fe 1	0	0
3	B	1	Total 1	Fe 1	0	0
3	6	1	Total 1	Fe 1	0	0
3	W	1	Total 1	Fe 1	0	0

Continued on next page...

Continued from previous page...

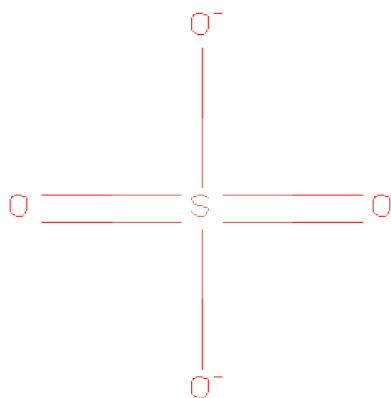
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	1	Total 1	Fe 1	0	0
3	X	1	Total 1	Fe 1	0	0
3	2	1	Total 1	Fe 1	0	0
3	S	1	Total 1	Fe 1	0	0
3	J	1	Total 1	Fe 1	0	0
3	E	1	Total 1	Fe 1	0	0
3	V	1	Total 1	Fe 1	0	0
3	A	1	Total 1	Fe 1	0	0
3	5	1	Total 1	Fe 1	0	0
3	R	1	Total 1	Fe 1	0	0
3	M	1	Total 1	Fe 1	0	0
3	1	1	Total 1	Fe 1	0	0
3	D	1	Total 1	Fe 1	0	0
3	I	1	Total 1	Fe 1	0	0
3	Z	1	Total 1	Fe 1	0	0
3	4	1	Total 1	Fe 1	0	0
3	U	1	Total 1	Fe 1	0	0
3	9	1	Total 1	Fe 1	0	0
3	L	1	Total 1	Fe 1	0	0
3	0	1	Total 1	Fe 1	0	0
3	G	1	Total 1	Fe 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Q	1	Total 1	Fe 1	0	0
3	H	1	Total 1	Fe 1	0	0
3	C	1	Total 1	Fe 1	0	0
3	7	1	Total 1	Fe 1	0	0
3	T	1	Total 1	Fe 1	0	0
3	8	1	Total 1	Fe 1	0	0
3	O	1	Total 1	Fe 1	0	0
3	Y	1	Total 1	Fe 1	0	0
3	3	1	Total 1	Fe 1	0	0
3	F	1	Total 1	Fe 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1	1	Total 5	O 4	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	2	1	Total	O	S	0	0
			5	4	1		
4	3	1	Total	O	S	0	0
			5	4	1		
4	3	1	Total	O	S	0	0
			5	4	1		
4	3	1	Total	O	S	0	0
			5	4	1		
4	4	1	Total	O	S	0	0
			5	4	1		
4	5	1	Total	O	S	0	0
			5	4	1		
4	5	1	Total	O	S	0	0
			5	4	1		
4	6	1	Total	O	S	0	0
			5	4	1		
4	7	1	Total	O	S	0	0
			5	4	1		
4	8	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		
4	S	1	Total	O	S	0	0
			5	4	1		
4	S	1	Total	O	S	0	0
			5	4	1		
4	T	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	W	1	Total	O	S	0	0
			5	4	1		
4	W	1	Total	O	S	0	0
			5	4	1		
4	W	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	Y	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	Z	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	0	6	Total	O		0	0
			6	6			
5	1	1	Total	O		0	0
			1	1			
5	2	7	Total	O		0	0
			7	7			
5	3	7	Total	O		0	0
			7	7			
5	5	5	Total	O		0	0
			5	5			
5	7	6	Total	O		0	0
			6	6			
5	8	3	Total	O		0	0
			3	3			
5	9	4	Total	O		0	0
			4	4			
5	A	5	Total	O		0	0
			5	5			
5	B	11	Total	O		0	0
			11	11			
5	C	8	Total	O		0	0
			8	8			
5	D	2	Total	O		0	0
			2	2			
5	E	9	Total	O		0	0
			9	9			
5	F	7	Total	O		0	0
			7	7			
5	G	7	Total	O		0	0
			7	7			
5	H	1	Total	O		0	0
			1	1			
5	I	2	Total	O		0	0
			2	2			
5	J	9	Total	O		0	0
			9	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	4	Total O 4 4	0	0
5	L	2	Total O 2 2	0	0
5	M	2	Total O 2 2	0	0
5	N	1	Total O 1 1	0	0
5	P	2	Total O 2 2	0	0
5	Q	6	Total O 6 6	0	0
5	R	2	Total O 2 2	0	0
5	S	4	Total O 4 4	0	0
5	T	4	Total O 4 4	0	0
5	U	8	Total O 8 8	0	0
5	V	4	Total O 4 4	0	0
5	W	7	Total O 7 7	0	0
5	X	4	Total O 4 4	0	0
5	Y	10	Total O 10 10	0	0
5	Z	2	Total O 2 2	0	0

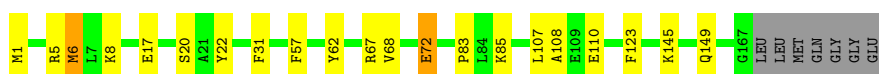
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: FERRITIN HOMOLOG

Chain 0: 



• Molecule 1: FERRITIN HOMOLOG

Chain 1: 



GLU

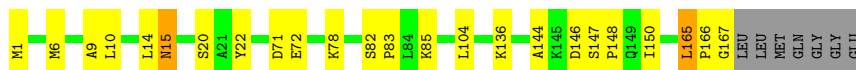
• Molecule 1: FERRITIN HOMOLOG

Chain 2: 



• Molecule 1: FERRITIN HOMOLOG

Chain 3: 



• Molecule 1: FERRITIN HOMOLOG

Chain 4: 



• Molecule 1: FERRITIN HOMOLOG

Chain 5: 



- Molecule 1: FERRITIN HOMOLOG

Chain 6:



- Molecule 1: FERRITIN HOMOLOG

Chain 7:



- Molecule 1: FERRITIN HOMOLOG

Chain 8:



- Molecule 1: FERRITIN HOMOLOG

Chain 9:



- Molecule 1: FERRITIN HOMOLOG

Chain A:



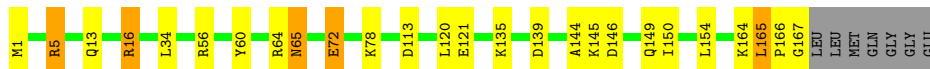
- Molecule 1: FERRITIN HOMOLOG

Chain B:



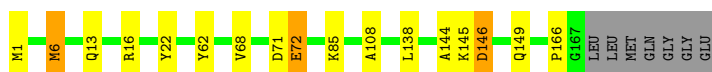
- Molecule 1: FERRITIN HOMOLOG

Chain C:



- Molecule 1: FERRITIN HOMOLOG

Chain D:



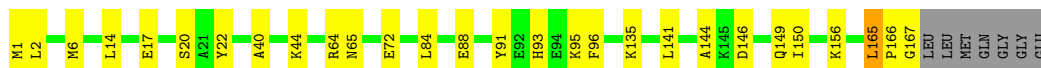
- Molecule 1: FERRITIN HOMOLOG

Chain E:



- Molecule 1: FERRITIN HOMOLOG

Chain F:



- Molecule 1: FERRITIN HOMOLOG

Chain G:



- Molecule 1: FERRITIN HOMOLOG

Chain H:



- Molecule 1: FERRITIN HOMOLOG

Chain I:



- Molecule 1: FERRITIN HOMOLOG

Chain J:



- Molecule 1: FERRITIN HOMOLOG

Chain K:



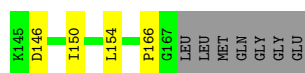
- Molecule 1: FERRITIN HOMOLOG

Chain L:



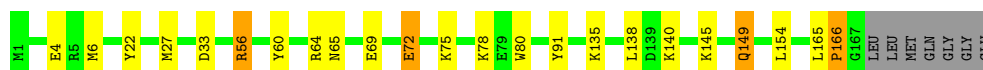
- Molecule 1: FERRITIN HOMOLOG

Chain M:



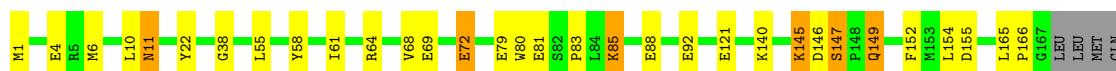
- Molecule 1: FERRITIN HOMOLOG

Chain N:



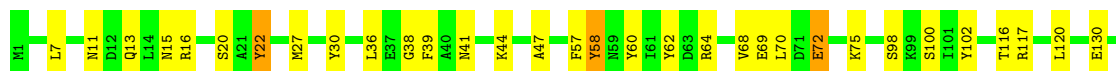
- Molecule 1: FERRITIN HOMOLOG

Chain O:



- Molecule 1: FERRITIN HOMOLOG

Chain P:



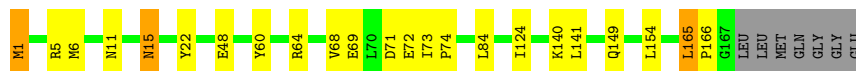
- Molecule 1: FERRITIN HOMOLOG

Chain Q:



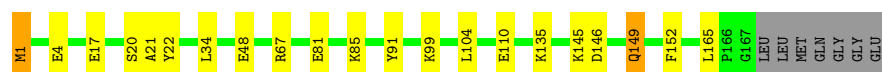
- Molecule 1: FERRITIN HOMOLOG

Chain R:



- Molecule 1: FERRITIN HOMOLOG

Chain S:



- Molecule 1: FERRITIN HOMOLOG

Chain T:



- Molecule 1: FERRITIN HOMOLOG

Chain U:



- Molecule 1: FERRITIN HOMOLOG

Chain V:



- Molecule 1: FERRITIN HOMOLOG

Chain W:



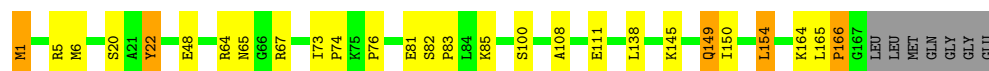
- Molecule 1: FERRITIN HOMOLOG

Chain X:



- Molecule 1: FERRITIN HOMOLOG

Chain Y:



- Molecule 1: FERRITIN HOMOLOG

Chain Z:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	255.37Å 342.06Å 265.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	204.12 – 2.80	Depositor
% Data completeness (in resolution range)	98.7 (204.12-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.200 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	50351	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FE, 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	0	0.68	0/1417	0.72	0/1908
1	1	0.69	0/1417	0.69	0/1908
1	2	0.70	0/1417	0.69	0/1908
1	3	0.76	0/1417	0.77	0/1908
1	4	0.73	0/1417	0.72	0/1908
1	5	0.66	0/1425	0.67	1/1919 (0.1%)
1	6	0.72	0/1417	0.71	1/1908 (0.1%)
1	7	0.73	0/1417	0.75	2/1908 (0.1%)
1	8	0.72	0/1425	0.74	0/1919
1	9	0.67	0/1417	0.66	0/1908
1	A	0.79	0/1417	0.78	0/1908
1	B	0.79	1/1425 (0.1%)	0.80	2/1919 (0.1%)
1	C	0.79	0/1428	0.77	2/1922 (0.1%)
1	D	0.76	0/1417	0.78	1/1908 (0.1%)
1	E	0.76	0/1425	0.72	0/1919
1	F	0.80	0/1417	0.76	1/1908 (0.1%)
1	G	0.82	0/1425	0.76	0/1919
1	H	0.68	0/1425	0.66	0/1919
1	I	0.75	1/1417 (0.1%)	0.74	1/1908 (0.1%)
1	J	0.73	0/1425	0.72	0/1919
1	K	0.69	0/1417	0.69	0/1908
1	L	0.73	0/1417	0.72	0/1908
1	M	0.71	0/1425	0.74	1/1919 (0.1%)
1	N	0.68	0/1417	0.69	0/1908
1	O	0.76	0/1425	0.72	0/1919
1	P	0.76	0/1417	0.73	0/1908
1	Q	0.74	0/1425	0.71	0/1919
1	R	0.65	0/1417	0.67	0/1908
1	S	0.78	1/1417 (0.1%)	0.74	1/1908 (0.1%)
1	T	0.79	0/1425	0.77	0/1919
1	U	0.80	0/1425	0.76	0/1919
1	V	0.79	1/1417 (0.1%)	0.81	0/1908

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	W	0.83	0/1425	0.79	0/1919
1	X	0.75	0/1417	0.77	1/1908 (0.1%)
1	Y	0.79	0/1417	0.80	0/1908
1	Z	0.65	0/1417	0.68	0/1908
All	All	0.74	4/51127 (0.0%)	0.73	14/68845 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	T	0	1
1	U	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	15	ASN	CB-CG	6.07	1.65	1.51
1	B	129	GLU	CG-CD	5.42	1.60	1.51
1	S	4	GLU	CG-CD	5.32	1.59	1.51
1	V	15	ASN	CB-CG	5.22	1.63	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	64	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	7	161	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	S	1	MET	CG-SD-CE	5.61	109.18	100.20
1	C	16	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	7	67	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	6	23	LEU	CA-CB-CG	5.42	127.76	115.30
1	M	64	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	113	ASP	CB-CG-OD1	5.21	122.98	118.30
1	5	2	LEU	CA-CB-CG	5.11	127.06	115.30
1	F	2	LEU	CA-CB-CG	5.07	126.96	115.30
1	X	117	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	I	6	MET	CG-SD-CE	-5.05	92.12	100.20
1	D	71	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	1	MET	Peptide
1	T	78	LYS	Peptide
1	U	1	MET	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1383	0	1352	10	0
1	1	1383	0	1352	14	0
1	2	1383	0	1352	11	0
1	3	1383	0	1352	13	0
1	4	1383	0	1352	13	0
1	5	1388	0	1358	16	0
1	6	1383	0	1352	16	0
1	7	1383	0	1352	13	0
1	8	1388	0	1358	12	0
1	9	1383	0	1352	15	0
1	A	1383	0	1352	11	0
1	B	1388	0	1358	12	0
1	C	1391	0	1365	15	0
1	D	1383	0	1352	9	0
1	E	1388	0	1358	10	0
1	F	1383	0	1352	14	0
1	G	1388	0	1358	14	0
1	H	1388	0	1358	15	0
1	I	1383	0	1352	11	0
1	J	1388	0	1358	9	0
1	K	1383	0	1352	9	0
1	L	1383	0	1352	5	0
1	M	1388	0	1358	25	0
1	N	1383	0	1352	20	0
1	O	1388	0	1358	22	0
1	P	1383	0	1352	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1388	0	1358	10	0
1	R	1383	0	1352	13	0
1	S	1383	0	1352	7	0
1	T	1388	0	1358	7	0
1	U	1388	0	1358	5	0
1	V	1383	0	1352	9	0
1	W	1388	0	1358	17	0
1	X	1383	0	1352	7	0
1	Y	1383	0	1352	18	0
1	Z	1383	0	1352	9	0
2	0	2	0	0	0	0
2	1	2	0	0	0	0
2	2	2	0	0	0	0
2	3	2	0	0	0	0
2	4	2	0	0	0	0
2	5	2	0	0	0	0
2	6	2	0	0	0	0
2	7	2	0	0	0	0
2	8	2	0	0	0	0
2	9	2	0	0	0	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	2	0	0	0	0
2	X	2	0	0	0	0
2	Y	2	0	0	0	0
2	Z	2	0	0	0	0
3	0	1	0	0	0	0
3	1	1	0	0	0	0
3	2	1	0	0	0	0
3	3	1	0	0	0	0
3	4	1	0	0	0	0
3	5	1	0	0	0	0
3	6	1	0	0	0	0
3	7	1	0	0	0	0
3	8	1	0	0	0	0
3	9	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
4	1	5	0	0	0	0
4	2	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	15	0	0	0	0
4	4	5	0	0	1	0
4	5	10	0	0	0	0
4	6	5	0	0	0	0
4	7	5	0	0	0	0
4	8	5	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	1	0
4	D	5	0	0	1	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	I	10	0	0	0	0
4	J	15	0	0	1	0
4	K	10	0	0	0	0
4	M	5	0	0	1	0
4	O	10	0	0	0	0
4	Q	5	0	0	0	0
4	S	10	0	0	0	0
4	T	5	0	0	1	0
4	V	10	0	0	0	0
4	W	15	0	0	1	0
4	X	5	0	0	0	0
4	Y	5	0	0	0	0
4	Z	5	0	0	0	0
5	0	6	0	0	0	0
5	1	1	0	0	0	0
5	2	7	0	0	0	0
5	3	7	0	0	0	0
5	5	5	0	0	0	0
5	7	6	0	0	0	0
5	8	3	0	0	1	0
5	9	4	0	0	0	0
5	A	5	0	0	0	0
5	B	11	0	0	0	0
5	C	8	0	0	0	0
5	D	2	0	0	0	0
5	E	9	0	0	0	0
5	F	7	0	0	0	0
5	G	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
5	I	2	0	0	0	0
5	J	9	0	0	0	0
5	K	4	0	0	0	0
5	L	2	0	0	0	0
5	M	2	0	0	0	0
5	N	1	0	0	0	0
5	P	2	0	0	0	0
5	Q	6	0	0	0	0
5	R	2	0	0	1	0
5	S	4	0	0	0	0
5	T	4	0	0	0	0
5	U	8	0	0	0	0
5	V	4	0	0	0	0
5	W	7	0	0	0	0
5	X	4	0	0	0	0
5	Y	10	0	0	1	0
5	Z	2	0	0	0	0
All	All	50351	0	48763	417	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (417) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:LEU:O	1:A:3:SER:HB3	1.51	1.05
1:1:58:TYR:OH	1:J:32:GLU:HG3	1.61	0.99
1:N:56:ARG:HG2	1:N:56:ARG:HH11	1.27	0.96
1:K:149:GLN:HE21	1:K:149:GLN:H	1.17	0.92
1:N:56:ARG:HH11	1:N:56:ARG:CG	1.84	0.91
1:M:91:TYR:CZ	1:M:135:LYS:HD3	2.06	0.90
1:N:138:LEU:HD23	1:N:138:LEU:C	1.95	0.87
1:9:149:GLN:H	1:9:149:GLN:HE21	1.26	0.81
1:6:149:GLN:HE21	1:6:149:GLN:H	1.29	0.80
1:N:138:LEU:O	1:N:138:LEU:HD23	1.85	0.77
1:M:15[B]:ASN:HD21	1:M:71:ASP:H	1.30	0.77
1:O:11:ASN:HD21	1:O:68:VAL:HA	1.50	0.76
1:3:78:LYS:HE3	1:L:69:GLU:HB2	1.67	0.75
1:P:116:THR:O	1:P:120:LEU:HD12	1.84	0.75
1:P:116:THR:HG22	1:P:120:LEU:HD11	1.69	0.73
1:G:149:GLN:H	1:G:149:GLN:HE21	1.37	0.72
1:X:91:TYR:CZ	1:X:135:LYS:HD3	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:9:78:LYS:HE3	1:R:69:GLU:OE1	1.90	0.71
1:V:14:LEU:C	1:V:14:LEU:HD23	2.11	0.70
1:3:15:ASN:HD21	1:3:71:ASP:H	1.38	0.70
1:1:58:TYR:OH	1:J:32:GLU:CG	2.38	0.69
1:C:72:GLU:OE1	1:U:72:GLU:OE1	2.12	0.68
1:D:62:TYR:CE2	1:D:68:VAL:HG23	2.29	0.68
1:M:15[B]:ASN:ND2	1:M:71:ASP:H	1.90	0.68
1:3:15:ASN:ND2	1:3:71:ASP:H	1.91	0.68
1:N:56:ARG:HG2	1:N:56:ARG:NH1	2.06	0.68
1:N:149:GLN:NE2	1:N:149:GLN:H	1.93	0.67
1:Y:149:GLN:HE21	1:Y:149:GLN:H	1.42	0.66
1:R:15:ASN:HD21	1:R:71:ASP:H	1.40	0.66
1:9:15:ASN:HD21	1:9:71:ASP:H	1.44	0.66
1:W:4:GLU:HG2	1:W:8:LYS:HE3	1.79	0.65
1:H:144:ALA:HB2	1:H:150:ILE:HG21	1.77	0.65
1:P:149:GLN:HE21	1:Z:149:GLN:HG3	1.62	0.65
1:C:5[A]:ARG:HD3	1:C:5[A]:ARG:H	1.62	0.65
1:O:11:ASN:ND2	1:O:61:ILE:HD13	2.12	0.63
1:I:40:ALA:O	1:I:44:LYS:HG3	1.97	0.63
1:B:149:GLN:HE21	1:B:149:GLN:H	1.46	0.63
1:E:149:GLN:HE21	1:X:149:GLN:HG3	1.64	0.63
1:3:144:ALA:HB2	1:3:150:ILE:HG21	1.79	0.63
1:D:138:LEU:O	1:D:138:LEU:HD23	1.99	0.62
1:O:11:ASN:OD1	1:O:69:GLU:N	2.31	0.62
1:N:149:GLN:HE21	1:N:149:GLN:H	1.44	0.62
1:Q:165:LEU:O	1:Q:167:GLY:N	2.30	0.62
1:W:6:MET:HE3	1:W:108:ALA:HA	1.82	0.62
1:8:81:GLU:HB2	1:8:85:LYS:HD3	1.81	0.61
1:F:149:GLN:HG2	1:S:149:GLN:HG3	1.82	0.61
1:X:135:LYS:NZ	1:X:139:ASP:OD1	2.33	0.61
1:N:56:ARG:NH1	1:N:56:ARG:CG	2.52	0.61
1:I:88:GLU:HG3	1:I:138:LEU:HD11	1.82	0.61
1:R:11:ASN:ND2	1:R:69:GLU:H	1.98	0.61
1:Y:81:GLU:HB2	1:Y:85:LYS:HG3	1.83	0.60
1:O:11:ASN:HD22	1:O:61:ILE:HD13	1.67	0.60
1:H:144:ALA:O	1:H:146:ASP:N	2.34	0.59
1:Y:6:MET:HE3	1:Y:108:ALA:HB2	1.82	0.59
1:5:72:GLU:OE2	1:N:72:GLU:OE1	2.21	0.59
1:4:13:GLN:HA	1:4:13:GLN:OE1	2.03	0.59
1:4:40:ALA:O	1:4:44:LYS:HG3	2.02	0.59
1:P:13:GLN:OE1	1:P:13:GLN:HA	2.02	0.59
1:H:144:ALA:HB2	1:H:150:ILE:CG2	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:144:ALA:HB2	1:C:150:ILE:HG21	1.83	0.59
1:N:138:LEU:CD2	1:N:138:LEU:C	2.70	0.59
1:4:72:GLU:OE1	1:M:72:GLU:OE1	2.20	0.59
1:O:6:MET:HE2	1:O:10:LEU:HG	1.85	0.59
1:G:15[B]:ASN:HD21	1:G:71:ASP:H	1.50	0.58
1:5:13:GLN:OE1	1:5:16:ARG:HD2	2.03	0.58
1:Y:64:ARG:O	1:Y:65:ASN:HB3	2.03	0.58
1:F:84:LEU:HA	1:F:141:LEU:HD13	1.83	0.58
1:P:117:ARG:HH11	1:P:117:ARG:HG3	1.66	0.58
1:M:13:GLN:HE22	1:M:100:SER:HB2	1.68	0.58
1:Q:144:ALA:HB2	1:Q:150:ILE:HG21	1.85	0.58
1:G:15[B]:ASN:ND2	1:G:71:ASP:H	2.01	0.58
1:2:73:ILE:HB	1:K:73:ILE:HB	1.85	0.58
1:G:149:GLN:NE2	1:G:149:GLN:H	2.01	0.57
1:N:140:LYS:HB3	1:N:154:LEU:HD11	1.87	0.57
1:1:91:TYR:CZ	1:1:135:LYS:HD3	2.39	0.57
1:N:91:TYR:CZ	1:N:135:LYS:HD3	2.40	0.57
1:1:46:GLN:NE2	1:1:130:GLU:OE1	2.37	0.56
1:6:37:GLU:OE2	1:M:136:LYS:HE2	2.04	0.56
1:9:107:LEU:O	1:9:111:GLU:HG3	2.04	0.56
1:Z:3:SER:OG	1:Z:6:MET:HB2	2.05	0.56
1:E:140:LYS:HD3	1:E:154:LEU:HD21	1.87	0.56
1:7:165:LEU:O	1:7:167:GLY:N	2.39	0.56
1:6:32:GLU:HG2	1:6:40:ALA:HB1	1.88	0.56
1:4:70:LEU:HD12	1:M:26:ALA:HB2	1.87	0.56
1:X:17:GLU:O	1:X:20:SER:HB2	2.06	0.55
1:F:91:TYR:CZ	1:F:135:LYS:HD3	2.42	0.55
1:P:13:GLN:OE1	1:P:16:ARG:HD2	2.07	0.55
1:O:140:LYS:HD3	1:O:154:LEU:HD21	1.89	0.55
1:7:70:LEU:HD13	1:P:22:TYR:CE1	2.41	0.55
1:R:11:ASN:HD21	1:R:68:VAL:HA	1.72	0.55
1:Y:1:MET:HG2	5:Y:2004:HOH:O	2.07	0.55
1:A:152:PHE:HD1	1:W:143:PHE:HE2	1.55	0.55
1:S:91:TYR:CZ	1:S:135:LYS:HD3	2.42	0.55
1:O:72:GLU:OE1	1:I:72:GLU:OE1	2.25	0.55
1:7:22:TYR:CZ	1:P:70:LEU:HB3	2.41	0.55
1:G:15[A]:ASN:ND2	1:G:71:ASP:HB2	2.21	0.54
1:7:22:TYR:CE1	1:P:70:LEU:HD13	2.42	0.54
1:B:144:ALA:HB1	1:B:150:ILE:HB	1.88	0.54
1:5:69:GLU:OE2	1:N:75:LYS:NZ	2.34	0.54
1:O:6:MET:HE2	1:O:107:LEU:HD23	1.89	0.54
1:D:138:LEU:HD23	1:D:138:LEU:C	2.29	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:65:ASN:ND2	4:D:1170:SO4:O1	2.38	0.54
1:Q:99:LYS:HE2	1:Q:103:GLU:OE2	2.08	0.54
1:9:42:TRP:CD1	1:9:158:LEU:HD22	2.43	0.53
1:9:149:GLN:N	1:9:149:GLN:HE21	2.03	0.53
1:8:25:PHE:O	1:8:28:ALA:HB3	2.08	0.53
1:O:121:GLU:HA	1:O:121:GLU:OE1	2.09	0.53
1:V:138:LEU:O	1:V:138:LEU:HD23	2.08	0.53
1:T:144:ALA:O	1:T:145:LYS:C	2.46	0.53
1:J:149:GLN:H	1:J:149:GLN:HE21	1.56	0.53
1:8:72:GLU:HG2	5:8:2002:HOH:O	2.07	0.53
1:3:144:ALA:HB2	1:3:150:ILE:CG2	2.38	0.53
1:Y:138:LEU:HD23	1:Y:138:LEU:O	2.09	0.53
1:K:131:GLU:OE1	1:R:1:MET:HE1	2.09	0.53
1:H:114:TYR:HB3	1:R:124:ILE:HD13	1.91	0.52
1:F:14:LEU:HD23	1:F:14:LEU:O	2.09	0.52
1:9:38:GLY:HA3	1:9:155:ASP:O	2.10	0.52
1:9:147:SER:OG	1:9:150:ILE:HG13	2.09	0.52
1:Q:149:GLN:H	1:Q:149:GLN:NE2	2.06	0.52
1:P:62:TYR:CE2	1:P:68:VAL:HG23	2.45	0.52
1:G:22:TYR:CD1	1:G:76:PRO:HD3	2.44	0.52
1:Y:5:ARG:HD2	1:Y:111:GLU:OE2	2.10	0.52
1:Y:22:TYR:CE2	1:Y:76:PRO:HD3	2.45	0.52
1:D:72:GLU:OE1	1:V:72:GLU:OE1	2.27	0.52
1:C:64:ARG:O	1:C:65:ASN:HB3	2.10	0.52
1:Y:82:SER:HB2	1:Y:83:PRO:HD2	1.90	0.52
1:R:140:LYS:HD3	1:R:154:LEU:HD21	1.92	0.52
1:W:9:ALA:HB1	1:W:104:LEU:HD21	1.91	0.51
1:S:48:GLU:OE2	1:S:165:LEU:HB2	2.10	0.51
1:U:107:LEU:O	1:U:111:GLU:HG3	2.10	0.51
1:9:15:ASN:ND2	1:9:71:ASP:H	2.06	0.51
1:9:5:ARG:HD3	1:9:107:LEU:HD11	1.93	0.51
1:4:26:ALA:HB2	1:M:70:LEU:HD12	1.93	0.51
1:5:165:LEU:HB3	1:5:166:PRO:HD3	1.92	0.51
1:G:138:LEU:HD23	1:G:138:LEU:C	2.31	0.51
1:6:137:ILE:O	1:6:137:ILE:HG22	2.11	0.51
1:Y:149:GLN:NE2	1:Y:149:GLN:H	2.08	0.51
1:P:13:GLN:HG3	1:P:57:PHE:CZ	2.46	0.51
1:W:13:GLN:HB2	1:W:104:LEU:HD11	1.92	0.51
1:G:111:GLU:O	1:G:112:LYS:HB2	2.10	0.51
1:L:13:GLN:OE1	1:L:13:GLN:HA	2.11	0.51
1:5:48:GLU:OE1	1:5:164:LYS:N	2.35	0.51
1:R:149:GLN:HB2	5:R:2001:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:91:TYR:CZ	1:T:135:LYS:HD3	2.46	0.50
1:L:38:GLY:HA3	1:L:155:ASP:O	2.12	0.50
1:K:149:GLN:NE2	1:K:149:GLN:H	1.99	0.50
1:P:117:ARG:NH1	1:P:117:ARG:HG3	2.27	0.50
1:K:140:LYS:HB3	1:K:154:LEU:HD11	1.94	0.50
1:X:107:LEU:O	1:X:111:GLU:HG3	2.11	0.50
1:P:148:PRO:HD2	1:P:149:GLN:OE1	2.11	0.50
1:8:27:MET:O	1:8:30:TYR:HB3	2.12	0.50
1:B:44:LYS:HB2	1:B:163:PRO:HG3	1.94	0.50
1:6:23:LEU:O	1:6:26:ALA:HB3	2.11	0.50
1:4:78:LYS:HE3	1:M:69:GLU:OE1	2.13	0.49
1:D:62:TYR:CE2	1:D:68:VAL:CG2	2.94	0.49
1:I:11:ASN:HD21	1:I:68:VAL:HA	1.78	0.49
1:M:144:ALA:HB1	1:M:150:ILE:HB	1.94	0.49
1:I:22:TYR:CD2	1:I:76:PRO:HD3	2.47	0.49
1:1:58:TYR:CZ	1:J:32:GLU:HG3	2.45	0.49
1:4:17:GLU:O	1:4:20:SER:HB2	2.11	0.49
1:R:60:TYR:CZ	1:R:64:ARG:HG3	2.47	0.49
1:6:20:SER:O	1:6:21:ALA:C	2.49	0.49
1:9:13:GLN:OE1	1:9:13:GLN:HA	2.13	0.49
1:2:156:LYS:O	1:2:159:SER:OG	2.26	0.49
1:B:107:LEU:O	1:B:111:GLU:HG3	2.13	0.49
1:G:149:GLN:O	1:G:153:MET:HG3	2.12	0.48
1:K:64:ARG:HA	1:K:64:ARG:HD2	1.68	0.48
1:Q:144:ALA:HB2	1:Q:150:ILE:CG2	2.42	0.48
1:4:25:PHE:O	1:4:28:ALA:HB3	2.12	0.48
1:7:72:GLU:OE1	1:P:72:GLU:OE1	2.32	0.48
1:1:37:GLU:OE2	1:I:136:LYS:HD3	2.14	0.48
1:Q:84:LEU:O	1:Q:88:GLU:HG3	2.13	0.48
1:6:32:GLU:HG2	1:6:40:ALA:CB	2.43	0.48
1:P:130:GLU:O	1:P:134:VAL:HG23	2.13	0.48
1:C:13:GLN:OE1	1:C:16:ARG:HD2	2.13	0.48
1:P:36:LEU:HB3	1:P:39:PHE:HD1	1.77	0.48
1:J:40:ALA:O	1:J:44:LYS:HG3	2.13	0.48
1:5:149:GLN:O	1:5:153:MET:HG3	2.13	0.48
1:F:144:ALA:HB2	1:F:150:ILE:HG21	1.95	0.48
1:P:68:VAL:HG12	1:P:69:GLU:N	2.28	0.48
1:H:17:GLU:O	1:H:20:SER:HB2	2.14	0.48
1:M:114:TYR:HB2	1:P:102:TYR:CE1	2.48	0.48
1:O:38:GLY:HA3	1:O:155:ASP:O	2.13	0.48
1:5:69:GLU:HG3	1:N:78:LYS:HD2	1.96	0.48
1:M:4:GLU:N	4:M:1170:SO4:O3	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:57:PHE:CE2	1:0:123:PHE:CZ	3.02	0.48
1:3:14:LEU:C	1:3:14:LEU:HD23	2.34	0.48
1:2:25:PHE:O	1:2:28:ALA:HB3	2.13	0.48
1:M:84:LEU:HA	1:M:141:LEU:HD13	1.96	0.48
1:V:62:TYR:CE2	1:V:68:VAL:HG23	2.49	0.48
1:P:60:TYR:CZ	1:P:64:ARG:HG3	2.48	0.48
1:F:40:ALA:O	1:F:44:LYS:HG3	2.14	0.47
1:O:149:GLN:HE21	1:O:149:GLN:H	1.60	0.47
1:6:61:ILE:HG21	1:6:68:VAL:HG23	1.95	0.47
1:0:6:MET:CE	1:0:107:LEU:HD23	2.44	0.47
1:V:14:LEU:HD23	1:V:14:LEU:O	2.14	0.47
1:P:149:GLN:NE2	1:Z:149:GLN:HG3	2.28	0.47
1:V:14:LEU:C	1:V:14:LEU:CD2	2.83	0.47
1:M:91:TYR:OH	1:M:135:LYS:HD3	2.13	0.47
1:B:144:ALA:CB	1:B:150:ILE:HB	2.44	0.47
1:P:144:ALA:O	1:P:145:LYS:C	2.52	0.47
1:I:91:TYR:CZ	1:I:135:LYS:HD3	2.49	0.47
1:T:143:PHE:CD2	1:T:143:PHE:C	2.88	0.47
1:C:72:GLU:N	4:C:1171:SO4:O3	2.37	0.47
1:Y:6:MET:HE3	1:Y:108:ALA:CB	2.43	0.47
1:C:60:TYR:CZ	1:C:64:ARG:HG3	2.50	0.47
1:P:64:ARG:HD2	1:P:64:ARG:HA	1.66	0.47
1:5:91:TYR:CZ	1:5:135:LYS:HD3	2.50	0.47
1:O:149:GLN:NE2	1:O:149:GLN:H	2.12	0.47
1:9:40:ALA:O	1:9:44:LYS:HG3	2.15	0.47
1:B:3:SER:HB2	1:B:6:MET:H	1.80	0.47
1:O:55:LEU:O	1:O:58:TYR:HB3	2.14	0.47
1:N:165:LEU:O	1:N:166:PRO:C	2.53	0.47
1:O:149:GLN:O	1:O:152:PHE:HB3	2.15	0.47
1:T:165:LEU:O	1:T:166:PRO:C	2.54	0.46
1:2:165:LEU:HB3	1:2:166:PRO:HD3	1.98	0.46
1:3:82:SER:O	1:3:83:PRO:C	2.52	0.46
1:J:17:GLU:O	1:J:20:SER:HB2	2.16	0.46
1:G:65:ASN:ND2	4:J:1171:SO4:O1	2.44	0.46
1:A:72:GLU:O	1:A:72:GLU:HG3	2.13	0.46
1:H:58:TYR:C	1:H:58:TYR:CD1	2.88	0.46
1:O:85:LYS:HE2	1:O:88:GLU:OE1	2.15	0.46
1:M:13:GLN:NE2	1:M:100:SER:HB2	2.30	0.46
1:X:60:TYR:CZ	1:X:64:ARG:HG3	2.50	0.46
1:C:78:LYS:O	1:U:67:ARG:NH2	2.48	0.46
1:C:135:LYS:HE3	1:C:139:ASP:OD2	2.15	0.46
1:F:64:ARG:HD2	1:F:64:ARG:HA	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:165:LEU:O	1:G:166:PRO:C	2.53	0.46
1:G:16:ARG:O	1:G:20:SER:HB2	2.15	0.46
1:M:6:MET:HE3	1:M:108:ALA:HB2	1.98	0.46
1:O:67:ARG:NH2	1:I:30:TYR:HA	2.30	0.46
1:Z:56:ARG:HG2	1:Z:56:ARG:HH11	1.81	0.46
1:B:135:LYS:HE3	1:B:139:ASP:OD2	2.16	0.46
1:R:73:ILE:HA	1:R:74:PRO:HD2	1.80	0.46
1:M:138:LEU:HD21	1:M:142:LYS:HE3	1.98	0.46
1:2:91:TYR:CZ	1:2:135:LYS:HD3	2.51	0.46
1:E:138:LEU:O	1:E:138:LEU:HD23	2.16	0.46
1:F:93:HIS:O	1:F:96:PHE:HB3	2.16	0.46
4:4:1670:SO4:O3	1:8:135:LYS:NZ	2.35	0.46
1:7:84:LEU:HA	1:7:141:LEU:HD13	1.99	0.45
1:F:165:LEU:O	1:F:167:GLY:N	2.49	0.45
1:7:70:LEU:O	1:P:75:LYS:HG3	2.17	0.45
1:O:72:GLU:HG3	1:O:72:GLU:O	2.15	0.45
1:3:6:MET:CE	1:3:10:LEU:HG	2.47	0.45
1:Y:165:LEU:HA	1:Y:165:LEU:HD12	1.56	0.45
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.76	0.45
1:Y:48:GLU:OE2	1:Y:165:LEU:HB2	2.16	0.45
1:O:17:GLU:O	1:O:20:SER:HB2	2.16	0.45
1:W:144:ALA:O	1:W:147:SER:HB3	2.17	0.45
1:O:64:ARG:HA	1:O:64:ARG:HD2	1.75	0.45
1:5:152:PHE:O	1:5:155:ASP:HB3	2.16	0.45
1:L:46:GLN:NE2	1:L:130:GLU:OE1	2.49	0.45
1:Z:138:LEU:HD23	1:Z:138:LEU:C	2.37	0.45
1:9:46:GLN:NE2	1:9:130:GLU:OE1	2.45	0.45
1:M:138:LEU:C	1:M:138:LEU:HD23	2.37	0.45
1:M:60:TYR:CZ	1:M:64:ARG:HG3	2.51	0.45
1:W:58:TYR:CD1	1:W:58:TYR:C	2.90	0.45
1:W:64:ARG:O	1:W:65:ASN:HB3	2.16	0.45
1:B:165:LEU:O	1:B:166:PRO:C	2.53	0.45
1:D:6:MET:HE3	1:D:108:ALA:HA	1.99	0.45
1:1:107:LEU:O	1:1:111:GLU:HG3	2.17	0.45
1:E:138:LEU:C	1:E:138:LEU:HD23	2.37	0.45
1:3:9:ALA:HB1	1:3:104:LEU:HD21	1.99	0.44
1:M:107:LEU:O	1:M:111:GLU:HG3	2.16	0.44
1:P:38:GLY:HA2	1:P:159:SER:HB3	1.98	0.44
1:7:22:TYR:OH	1:P:70:LEU:HB3	2.17	0.44
1:Y:154:LEU:HA	1:Y:154:LEU:HD23	1.83	0.44
1:N:27:MET:HG2	1:N:80:TRP:CH2	2.52	0.44
1:P:44:LYS:O	1:P:47:ALA:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:120:LEU:O	1:C:121:GLU:C	2.55	0.44
1:A:107:LEU:O	1:A:108:ALA:C	2.54	0.44
1:I:22:TYR:CE2	1:I:76:PRO:HD3	2.53	0.44
1:2:151:LEU:HD23	1:H:143:PHE:HZ	1.82	0.44
1:8:12:ASP:O	1:8:16:ARG:HG3	2.17	0.44
1:Z:91:TYR:CE1	1:Z:135:LYS:HB2	2.53	0.44
1:5:48:GLU:HG2	1:N:165:LEU:HD11	1.98	0.44
1:5:149:GLN:HG2	1:L:149:GLN:HG3	1.98	0.44
1:P:135:LYS:HE3	1:P:139:ASP:OD2	2.17	0.44
1:8:95:LYS:O	1:8:99:LYS:HG3	2.18	0.44
1:F:17:GLU:O	1:F:20:SER:HB2	2.17	0.44
1:C:64:ARG:O	1:C:65:ASN:CB	2.66	0.44
1:S:81:GLU:HB2	1:S:85:LYS:HG3	2.00	0.44
1:5:78:LYS:HE3	1:N:69:GLU:HB2	1.99	0.43
1:1:2:LEU:HA	1:1:2:LEU:HD23	1.90	0.43
1:3:165:LEU:O	1:3:167:GLY:N	2.51	0.43
1:1:32:GLU:HG2	1:J:62:TYR:CD2	2.53	0.43
1:Y:6:MET:HE3	1:Y:108:ALA:CA	2.47	0.43
1:F:144:ALA:HB1	1:F:150:ILE:HB	2.00	0.43
1:O:81:GLU:HB2	1:O:85:LYS:HG2	2.00	0.43
1:1:144:ALA:O	1:1:145:LYS:C	2.56	0.43
1:2:81:GLU:HB3	1:2:85:LYS:HG3	2.00	0.43
1:2:30:TYR:CZ	1:2:34:LEU:HD11	2.53	0.43
1:G:149:GLN:N	1:G:149:GLN:HE21	2.11	0.43
1:H:144:ALA:O	1:H:145:LYS:C	2.56	0.43
1:4:135:LYS:HG2	1:9:65:ASN:ND2	2.32	0.43
1:K:144:ALA:O	1:K:145:LYS:C	2.57	0.43
1:X:31:PHE:O	1:X:32:GLU:C	2.55	0.43
1:E:147:SER:OG	1:E:150:ILE:HG13	2.18	0.43
1:F:144:ALA:HB2	1:F:150:ILE:CG2	2.49	0.43
1:1:42:TRP:CD1	1:1:158:LEU:HD22	2.53	0.43
1:H:124:ILE:HD13	1:K:114:TYR:HB3	2.00	0.43
1:S:17:GLU:O	1:S:20:SER:HB2	2.17	0.43
1:A:60:TYR:O	1:A:61:ILE:C	2.57	0.43
1:7:64:ARG:O	1:7:65:ASN:HB2	2.19	0.43
1:A:140:LYS:HD3	1:A:154:LEU:HD21	1.99	0.43
1:6:91:TYR:CZ	1:6:135:LYS:HD3	2.54	0.43
1:H:147:SER:HA	1:H:148:PRO:HD2	1.89	0.43
1:W:6:MET:HE3	1:W:108:ALA:CA	2.48	0.43
1:A:33:ASP:OD1	1:S:67:ARG:HD3	2.19	0.43
1:T:16:ARG:NE	4:T:1668:SO4:O3	2.36	0.43
1:P:27:MET:O	1:P:30:TYR:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:LEU:O	1:A:3:SER:CB	2.37	0.43
1:F:91:TYR:CZ	1:F:95:LYS:HE3	2.54	0.43
1:M:20:SER:O	1:M:24:TYR:CD2	2.72	0.43
1:6:42:TRP:CD1	1:6:158:LEU:HD22	2.54	0.43
1:U:154:LEU:HD23	1:U:154:LEU:HA	1.79	0.43
1:R:84:LEU:HA	1:R:141:LEU:HD13	2.00	0.43
1:5:65:ASN:OD1	1:6:135:LYS:HE3	2.19	0.42
1:N:60:TYR:CZ	1:N:64:ARG:HG3	2.54	0.42
1:J:91:TYR:CZ	1:J:95:LYS:HE3	2.54	0.42
1:D:13:GLN:OE1	1:D:16:ARG:NH1	2.48	0.42
1:3:9:ALA:CB	1:3:104:LEU:HD21	2.50	0.42
1:W:82:SER:O	1:W:83:PRO:C	2.57	0.42
1:6:64:ARG:HD2	1:6:64:ARG:HA	1.64	0.42
1:D:138:LEU:CD2	1:D:138:LEU:C	2.87	0.42
1:A:152:PHE:CD1	1:W:143:PHE:HE2	2.35	0.42
1:B:17:GLU:O	1:B:20:SER:HB2	2.20	0.42
1:U:13:GLN:NE2	1:U:101:ILE:HD11	2.35	0.42
1:6:32:GLU:HG3	1:O:58:TYR:OH	2.19	0.42
1:7:64:ARG:HD2	1:7:64:ARG:HA	1.92	0.42
1:E:81:GLU:HB2	1:E:85:LYS:HG3	2.01	0.42
1:0:31:PHE:HE1	1:0:83:PRO:HB3	1.84	0.42
1:5:104:LEU:HD22	1:5:120:LEU:HD11	2.00	0.42
1:7:135:LYS:NZ	1:7:139:ASP:OD2	2.49	0.42
1:W:109:GLU:HG3	1:W:117:ARG:HD3	2.01	0.42
1:B:22:TYR:CZ	1:T:70:LEU:HB3	2.55	0.42
1:D:144:ALA:O	1:D:146:ASP:N	2.53	0.42
1:C:165:LEU:HA	1:C:165:LEU:HD12	1.87	0.42
1:W:34:LEU:HD12	1:W:34:LEU:HA	1.82	0.42
1:Y:165:LEU:O	1:Y:166:PRO:C	2.56	0.42
1:W:5:ARG:HD2	1:W:111:GLU:OE2	2.20	0.42
1:8:6:MET:HE3	1:8:108:ALA:HA	2.01	0.42
1:E:34:LEU:HD23	1:E:34:LEU:HA	1.80	0.42
1:3:82:SER:O	1:3:85:LYS:N	2.53	0.42
1:C:165:LEU:O	1:C:167:GLY:N	2.52	0.42
1:P:7:LEU:HD12	1:P:11:ASN:ND2	2.35	0.42
1:2:138:LEU:HD23	1:2:138:LEU:C	2.40	0.42
1:2:149:GLN:O	1:2:153:MET:HG3	2.19	0.42
1:Z:64:ARG:HA	1:Z:64:ARG:HD2	1.86	0.42
1:0:62:TYR:CE2	1:0:68:VAL:HG23	2.55	0.42
1:4:165:LEU:O	1:4:166:PRO:C	2.58	0.42
1:O:79:GLU:C	1:O:80:TRP:CE3	2.93	0.42
1:G:138:LEU:O	1:G:138:LEU:HD23	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:64:ARG:O	1:F:65:ASN:HB3	2.20	0.41
1:Y:150:ILE:O	1:Y:154:LEU:HB2	2.20	0.41
1:5:67:ARG:HD3	1:N:33:ASP:OD1	2.20	0.41
1:Q:64:ARG:O	1:Q:65:ASN:CB	2.69	0.41
1:V:144:ALA:O	1:V:145:LYS:C	2.59	0.41
1:8:140:LYS:HB3	1:8:154:LEU:HD11	2.02	0.41
1:6:41:ASN:HA	1:6:44:LYS:HD3	2.02	0.41
1:E:165:LEU:O	1:E:166:PRO:C	2.59	0.41
1:Z:82:SER:O	1:Z:83:PRO:C	2.56	0.41
1:3:147:SER:O	1:3:148:PRO:C	2.58	0.41
1:1:10:LEU:HD23	1:1:10:LEU:HA	1.97	0.41
1:7:104:LEU:HD22	1:7:120:LEU:HD11	2.01	0.41
1:H:140:LYS:HD3	1:H:154:LEU:HD21	2.02	0.41
1:E:154:LEU:HD23	1:E:154:LEU:HA	1.83	0.41
1:O:55:LEU:HD23	1:O:55:LEU:HA	1.78	0.41
1:W:9:ALA:HB1	1:W:104:LEU:CD2	2.51	0.41
1:K:153:MET:O	1:K:157:GLU:HG3	2.20	0.41
1:0:6:MET:HE3	1:0:108:ALA:HB2	2.02	0.41
1:Y:73:ILE:HA	1:Y:74:PRO:HD3	1.95	0.41
1:M:13:GLN:NE2	1:M:16:ARG:HH11	2.19	0.41
1:J:104:LEU:HB3	1:J:120:LEU:HD11	2.02	0.41
1:6:58:TYR:CD1	1:6:58:TYR:C	2.94	0.41
1:6:78:LYS:HG3	1:6:78:LYS:O	2.20	0.41
1:V:18:LEU:HA	1:V:18:LEU:HD23	1.79	0.41
1:9:143:PHE:CG	1:9:143:PHE:O	2.73	0.41
1:8:24:TYR:CD2	1:8:46:GLN:HG3	2.56	0.41
1:C:64:ARG:HA	1:C:64:ARG:HD2	1.84	0.41
1:O:11:ASN:HD22	1:O:61:ILE:CD1	2.33	0.41
1:W:4:GLU:HB3	4:W:1668:SO4:O4	2.21	0.41
1:4:70:LEU:HB3	1:M:22:TYR:CZ	2.56	0.41
1:Q:149:GLN:HE21	1:Q:149:GLN:H	1.69	0.41
1:8:6:MET:CE	1:8:108:ALA:HA	2.51	0.41
1:8:111:GLU:O	1:8:112:LYS:HB2	2.20	0.41
1:B:55:LEU:HA	1:B:55:LEU:HD23	1.90	0.41
1:O:145:LYS:C	1:O:147:SER:H	2.24	0.41
1:H:165:LEU:O	1:H:166:PRO:C	2.59	0.41
1:V:165:LEU:O	1:V:166:PRO:C	2.59	0.41
1:P:58:TYR:CD1	1:P:58:TYR:C	2.94	0.41
1:0:67:ARG:HH22	1:I:30:TYR:HA	1.85	0.41
1:H:73:ILE:HA	1:H:74:PRO:HD3	1.95	0.41
1:E:40:ALA:O	1:E:44:LYS:HG3	2.21	0.41
1:M:46:GLN:O	1:M:50:GLU:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:165:LEU:HB3	1:Q:166:PRO:HD3	2.02	0.40
1:C:144:ALA:HB2	1:C:150:ILE:CG2	2.48	0.40
1:R:64:ARG:HD2	1:R:64:ARG:HA	1.87	0.40
1:S:20:SER:O	1:S:21:ALA:C	2.60	0.40
1:1:77:PRO:HB2	1:1:80:TRP:CZ2	2.55	0.40
1:R:48:GLU:OE2	1:R:165:LEU:HB2	2.21	0.40
1:H:60:TYR:CZ	1:H:64:ARG:HG3	2.55	0.40
1:H:3:SER:O	1:H:6:MET:N	2.54	0.40
1:Q:56:ARG:NH1	1:Q:56:ARG:HG2	2.36	0.40
1:1:165:LEU:HA	1:1:165:LEU:HD12	1.76	0.40
1:O:6:MET:HE2	1:O:6:MET:O	2.21	0.40
1:Z:56:ARG:HG2	1:Z:56:ARG:NH1	2.37	0.40
1:P:41:ASN:HA	1:P:44:LYS:HD2	2.04	0.40
1:I:13:GLN:HG3	1:I:57:PHE:CZ	2.57	0.40
1:5:165:LEU:HB3	1:5:166:PRO:CD	2.51	0.40
1:B:143:PHE:HE2	1:W:152:PHE:HB2	1.86	0.40
1:M:23:LEU:O	1:M:27:MET:HG3	2.20	0.40
1:2:48:GLU:OE2	1:2:163:PRO:HB2	2.21	0.40
1:T:64:ARG:HD2	1:T:64:ARG:HA	1.85	0.40
1:7:55:LEU:HA	1:7:55:LEU:HD23	1.89	0.40
1:4:165:LEU:HD12	1:4:165:LEU:HA	1.85	0.40
1:4:67:ARG:NH1	1:4:68:VAL:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	165/174 (95%)	157 (95%)	7 (4%)	1 (1%)	33	72
1	1	165/174 (95%)	161 (98%)	3 (2%)	1 (1%)	33	72
1	2	165/174 (95%)	160 (97%)	3 (2%)	2 (1%)	19	54
1	3	165/174 (95%)	161 (98%)	3 (2%)	1 (1%)	33	72
1	4	165/174 (95%)	158 (96%)	6 (4%)	1 (1%)	33	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	166/174 (95%)	158 (95%)	7 (4%)	1 (1%)	33	72
1	6	165/174 (95%)	162 (98%)	2 (1%)	1 (1%)	33	72
1	7	165/174 (95%)	160 (97%)	3 (2%)	2 (1%)	19	54
1	8	166/174 (95%)	161 (97%)	3 (2%)	2 (1%)	19	54
1	9	165/174 (95%)	157 (95%)	6 (4%)	2 (1%)	19	54
1	A	165/174 (95%)	158 (96%)	2 (1%)	5 (3%)	7	22
1	B	166/174 (95%)	160 (96%)	5 (3%)	1 (1%)	33	72
1	C	166/174 (95%)	159 (96%)	4 (2%)	3 (2%)	13	39
1	D	165/174 (95%)	159 (96%)	4 (2%)	2 (1%)	19	54
1	E	166/174 (95%)	161 (97%)	4 (2%)	1 (1%)	33	72
1	F	165/174 (95%)	159 (96%)	5 (3%)	1 (1%)	33	72
1	G	166/174 (95%)	161 (97%)	3 (2%)	2 (1%)	19	54
1	H	166/174 (95%)	158 (95%)	7 (4%)	1 (1%)	33	72
1	I	165/174 (95%)	159 (96%)	5 (3%)	1 (1%)	33	72
1	J	166/174 (95%)	160 (96%)	5 (3%)	1 (1%)	33	72
1	K	165/174 (95%)	161 (98%)	3 (2%)	1 (1%)	33	72
1	L	165/174 (95%)	158 (96%)	6 (4%)	1 (1%)	33	72
1	M	166/174 (95%)	150 (90%)	14 (8%)	2 (1%)	19	54
1	N	165/174 (95%)	157 (95%)	6 (4%)	2 (1%)	19	54
1	O	166/174 (95%)	157 (95%)	6 (4%)	3 (2%)	13	39
1	P	165/174 (95%)	156 (94%)	7 (4%)	2 (1%)	19	54
1	Q	166/174 (95%)	158 (95%)	5 (3%)	3 (2%)	13	39
1	R	165/174 (95%)	159 (96%)	4 (2%)	2 (1%)	19	54
1	S	165/174 (95%)	160 (97%)	4 (2%)	1 (1%)	33	72
1	T	166/174 (95%)	163 (98%)	2 (1%)	1 (1%)	33	72
1	U	166/174 (95%)	159 (96%)	4 (2%)	3 (2%)	13	39
1	V	165/174 (95%)	157 (95%)	6 (4%)	2 (1%)	19	54
1	W	166/174 (95%)	163 (98%)	2 (1%)	1 (1%)	33	72
1	X	165/174 (95%)	161 (98%)	2 (1%)	2 (1%)	19	54
1	Y	165/174 (95%)	160 (97%)	3 (2%)	2 (1%)	19	54
1	Z	165/174 (95%)	155 (94%)	9 (6%)	1 (1%)	33	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5954/6264 (95%)	5723 (96%)	170 (3%)	61 (1%)	22 60

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	145	LYS
1	1	145	LYS
1	7	145	LYS
1	A	3	SER
1	H	145	LYS
1	K	145	LYS
1	N	145	LYS
1	P	145	LYS
1	S	145	LYS
1	T	145	LYS
1	U	145	LYS
1	W	145	LYS
1	3	166	PRO
1	4	145	LYS
1	7	166	PRO
1	8	145	LYS
1	D	145	LYS
1	E	145	LYS
1	G	145	LYS
1	O	145	LYS
1	O	146	ASP
1	Q	145	LYS
1	V	145	LYS
1	X	145	LYS
1	Z	143	PHE
1	5	145	LYS
1	8	166	PRO
1	9	145	LYS
1	A	146	ASP
1	A	166	PRO
1	D	166	PRO
1	F	166	PRO
1	G	166	PRO
1	Q	166	PRO
1	R	165	LEU
1	Y	145	LYS
1	2	144	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	166	PRO
1	A	165	LEU
1	C	65	ASN
1	J	166	PRO
1	M	115	SER
1	M	166	PRO
1	U	166	PRO
1	V	166	PRO
1	9	166	PRO
1	A	147	SER
1	C	145	LYS
1	I	145	LYS
1	N	166	PRO
1	Q	143	PHE
1	U	143	PHE
1	Y	166	PRO
1	6	166	PRO
1	C	166	PRO
1	B	166	PRO
1	O	166	PRO
1	P	166	PRO
1	X	166	PRO
1	L	166	PRO
1	R	166	PRO

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	0	142/147 (97%)	133 (94%)	9 (6%)	25	59
1	1	142/147 (97%)	131 (92%)	11 (8%)	18	45
1	2	142/147 (97%)	138 (97%)	4 (3%)	56	88
1	3	142/147 (97%)	134 (94%)	8 (6%)	30	64
1	4	142/147 (97%)	136 (96%)	6 (4%)	40	77
1	5	143/147 (97%)	139 (97%)	4 (3%)	56	88
1	6	142/147 (97%)	135 (95%)	7 (5%)	35	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	142/147 (97%)	129 (91%)	13 (9%)	13	36
1	8	143/147 (97%)	137 (96%)	6 (4%)	40	77
1	9	142/147 (97%)	134 (94%)	8 (6%)	30	64
1	A	142/147 (97%)	136 (96%)	6 (4%)	40	77
1	B	143/147 (97%)	132 (92%)	11 (8%)	18	45
1	C	143/147 (97%)	132 (92%)	11 (8%)	18	45
1	D	142/147 (97%)	135 (95%)	7 (5%)	35	71
1	E	143/147 (97%)	133 (93%)	10 (7%)	21	52
1	F	142/147 (97%)	134 (94%)	8 (6%)	30	64
1	G	143/147 (97%)	133 (93%)	10 (7%)	21	52
1	H	143/147 (97%)	135 (94%)	8 (6%)	30	64
1	I	142/147 (97%)	135 (95%)	7 (5%)	35	71
1	J	143/147 (97%)	139 (97%)	4 (3%)	56	88
1	K	142/147 (97%)	130 (92%)	12 (8%)	15	41
1	L	142/147 (97%)	135 (95%)	7 (5%)	35	71
1	M	143/147 (97%)	132 (92%)	11 (8%)	18	45
1	N	142/147 (97%)	135 (95%)	7 (5%)	35	71
1	O	143/147 (97%)	132 (92%)	11 (8%)	18	45
1	P	142/147 (97%)	131 (92%)	11 (8%)	18	45
1	Q	143/147 (97%)	134 (94%)	9 (6%)	25	59
1	R	142/147 (97%)	136 (96%)	6 (4%)	40	77
1	S	142/147 (97%)	133 (94%)	9 (6%)	25	59
1	T	143/147 (97%)	133 (93%)	10 (7%)	21	52
1	U	143/147 (97%)	135 (94%)	8 (6%)	30	64
1	V	142/147 (97%)	132 (93%)	10 (7%)	21	52
1	W	143/147 (97%)	137 (96%)	6 (4%)	40	77
1	X	142/147 (97%)	138 (97%)	4 (3%)	56	88
1	Y	142/147 (97%)	134 (94%)	8 (6%)	30	64
1	Z	142/147 (97%)	134 (94%)	8 (6%)	30	64
All	All	5126/5292 (97%)	4831 (94%)	295 (6%)	28	63

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	1	MET
1	0	5	ARG
1	0	6	MET
1	0	8	LYS
1	0	22	TYR
1	0	72	GLU
1	0	85	LYS
1	0	110	GLU
1	0	149	GLN
1	1	1	MET
1	1	4	GLU
1	1	5	ARG
1	1	6	MET
1	1	22	TYR
1	1	72	GLU
1	1	79	GLU
1	1	100	SER
1	1	115	SER
1	1	149	GLN
1	1	154	LEU
1	2	65	ASN
1	2	98	SER
1	2	146	ASP
1	2	149	GLN
1	3	1	MET
1	3	15	ASN
1	3	20	SER
1	3	22	TYR
1	3	72	GLU
1	3	136	LYS
1	3	146	ASP
1	3	165	LEU
1	4	1	MET
1	4	6	MET
1	4	22	TYR
1	4	72	GLU
1	4	146	ASP
1	4	164	LYS
1	5	22	TYR
1	5	72	GLU
1	5	104	LEU
1	5	154	LEU
1	6	6	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	22	TYR
1	6	72	GLU
1	6	88	GLU
1	6	104	LEU
1	6	110	GLU
1	6	149	GLN
1	7	7	LEU
1	7	15	ASN
1	7	20	SER
1	7	22	TYR
1	7	72	GLU
1	7	92	GLU
1	7	100	SER
1	7	104	LEU
1	7	109	GLU
1	7	119	PHE
1	7	133	SER
1	7	154	LEU
1	7	164	LYS
1	8	1	MET
1	8	5	ARG
1	8	22	TYR
1	8	104	LEU
1	8	133	SER
1	8	154	LEU
1	9	5	ARG
1	9	15	ASN
1	9	65	ASN
1	9	72	GLU
1	9	136	LYS
1	9	143	PHE
1	9	149	GLN
1	9	165	LEU
1	A	3	SER
1	A	22	TYR
1	A	85	LYS
1	A	100	SER
1	A	110	GLU
1	A	149	GLN
1	B	5	ARG
1	B	20	SER
1	B	22	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	34	LEU
1	B	67	ARG
1	B	72	GLU
1	B	81	GLU
1	B	145	LYS
1	B	149	GLN
1	B	154	LEU
1	B	166	PRO
1	C	1	MET
1	C	5[A]	ARG
1	C	5[B]	ARG
1	C	34	LEU
1	C	56	ARG
1	C	72	GLU
1	C	146	ASP
1	C	149	GLN
1	C	154	LEU
1	C	164	LYS
1	C	165	LEU
1	D	1	MET
1	D	6	MET
1	D	22	TYR
1	D	72	GLU
1	D	85	LYS
1	D	146	ASP
1	D	149	GLN
1	E	4	GLU
1	E	6	MET
1	E	22	TYR
1	E	67	ARG
1	E	72	GLU
1	E	92	GLU
1	E	104	LEU
1	E	110	GLU
1	E	149	GLN
1	E	165	LEU
1	F	1	MET
1	F	6	MET
1	F	22	TYR
1	F	72	GLU
1	F	88	GLU
1	F	146	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	156	LYS
1	F	165	LEU
1	G	1	MET
1	G	5	ARG
1	G	22	TYR
1	G	67	ARG
1	G	78	LYS
1	G	81	GLU
1	G	100	SER
1	G	110	GLU
1	G	149	GLN
1	G	164	LYS
1	H	1	MET
1	H	6	MET
1	H	22	TYR
1	H	58	TYR
1	H	72	GLU
1	H	110	GLU
1	H	147	SER
1	H	165	LEU
1	I	13	GLN
1	I	22	TYR
1	I	58	TYR
1	I	72	GLU
1	I	104	LEU
1	I	136	LYS
1	I	143	PHE
1	J	22	TYR
1	J	72	GLU
1	J	149	GLN
1	J	165	LEU
1	K	1	MET
1	K	6	MET
1	K	22	TYR
1	K	33	ASP
1	K	72	GLU
1	K	81	GLU
1	K	100	SER
1	K	104	LEU
1	K	119	PHE
1	K	149	GLN
1	K	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	165	LEU
1	L	1	MET
1	L	6	MET
1	L	22	TYR
1	L	72	GLU
1	L	104	LEU
1	L	149	GLN
1	L	164	LYS
1	M	1	MET
1	M	6	MET
1	M	22	TYR
1	M	69	GLU
1	M	72	GLU
1	M	99	LYS
1	M	100	SER
1	M	103	GLU
1	M	104	LEU
1	M	146	ASP
1	M	154	LEU
1	N	4	GLU
1	N	6	MET
1	N	22	TYR
1	N	56	ARG
1	N	65	ASN
1	N	72	GLU
1	N	149	GLN
1	O	1	MET
1	O	4	GLU
1	O	11	ASN
1	O	22	TYR
1	O	72	GLU
1	O	83	PRO
1	O	85	LYS
1	O	92	GLU
1	O	147	SER
1	O	149	GLN
1	O	165	LEU
1	P	15	ASN
1	P	20	SER
1	P	22	TYR
1	P	58	TYR
1	P	72	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	98	SER
1	P	100	SER
1	P	133	SER
1	P	149	GLN
1	P	153	MET
1	P	156	LYS
1	Q	1	MET
1	Q	6	MET
1	Q	22	TYR
1	Q	67	ARG
1	Q	75	LYS
1	Q	100	SER
1	Q	146	ASP
1	Q	149	GLN
1	Q	156	LYS
1	R	1	MET
1	R	5	ARG
1	R	6	MET
1	R	15	ASN
1	R	22	TYR
1	R	72	GLU
1	S	1	MET
1	S	22	TYR
1	S	34	LEU
1	S	99	LYS
1	S	104	LEU
1	S	110	GLU
1	S	146	ASP
1	S	149	GLN
1	S	152	PHE
1	T	1	MET
1	T	22	TYR
1	T	34	LEU
1	T	72	GLU
1	T	95	LYS
1	T	110	GLU
1	T	121	GLU
1	T	143	PHE
1	T	152	PHE
1	T	154	LEU
1	U	1	MET
1	U	22	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	34	LEU
1	U	72	GLU
1	U	104	LEU
1	U	149	GLN
1	U	154	LEU
1	U	165	LEU
1	V	1	MET
1	V	4	GLU
1	V	6	MET
1	V	20	SER
1	V	22	TYR
1	V	72	GLU
1	V	103	GLU
1	V	110	GLU
1	V	149	GLN
1	V	154	LEU
1	W	34	LEU
1	W	58	TYR
1	W	119	PHE
1	W	136	LYS
1	W	149	GLN
1	W	154	LEU
1	X	5	ARG
1	X	22	TYR
1	X	65	ASN
1	X	149	GLN
1	Y	1	MET
1	Y	20	SER
1	Y	22	TYR
1	Y	67	ARG
1	Y	100	SER
1	Y	149	GLN
1	Y	154	LEU
1	Y	164	LYS
1	Z	1	MET
1	Z	5	ARG
1	Z	6	MET
1	Z	11	ASN
1	Z	22	TYR
1	Z	72	GLU
1	Z	110	GLU
1	Z	149	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	15	ASN
1	1	15	ASN
1	2	149	GLN
1	3	15	ASN
1	4	149	GLN
1	6	149	GLN
1	8	149	GLN
1	9	15	ASN
1	9	65	ASN
1	9	149	GLN
1	A	15	ASN
1	A	149	GLN
1	B	149	GLN
1	E	149	GLN
1	F	15	ASN
1	G	149	GLN
1	H	149	GLN
1	I	11	ASN
1	I	149	GLN
1	J	149	GLN
1	K	149	GLN
1	L	15	ASN
1	L	149	GLN
1	M	13	GLN
1	M	149	GLN
1	N	149	GLN
1	O	149	GLN
1	P	15	ASN
1	Q	149	GLN
1	R	11	ASN
1	R	15	ASN
1	R	149	GLN
1	S	149	GLN
1	U	149	GLN
1	W	149	GLN
1	X	149	GLN
1	Y	149	GLN
1	Z	65	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 152 ligands modelled in this entry, 108 are monoatomic - leaving 44 for Mogul analysis.

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	$\# Z > 2$
4	SO4	1	1670	-	4,4,4	0.12	0	6,6,6	0.43	0
4	SO4	2	1670	-	4,4,4	0.11	0	6,6,6	0.29	0
4	SO4	3	1670	-	4,4,4	0.22	0	6,6,6	0.41	0
4	SO4	3	1671	-	4,4,4	0.09	0	6,6,6	0.20	0
4	SO4	3	1672	-	4,4,4	0.16	0	6,6,6	0.30	0
4	SO4	4	1670	-	4,4,4	0.16	0	6,6,6	0.36	0
4	SO4	5	1670	-	4,4,4	0.13	0	6,6,6	0.11	0
4	SO4	5	1671	-	4,4,4	0.08	0	6,6,6	0.28	0
4	SO4	6	1670	-	4,4,4	0.26	0	6,6,6	0.43	0
4	SO4	7	1670	-	4,4,4	0.10	0	6,6,6	0.15	0
4	SO4	8	1670	-	4,4,4	0.10	0	6,6,6	0.10	0
4	SO4	A	1170	-	4,4,4	0.11	0	6,6,6	0.35	0
4	SO4	A	1171	-	4,4,4	0.27	0	6,6,6	0.22	0
4	SO4	B	1170	-	4,4,4	0.20	0	6,6,6	0.39	0
4	SO4	B	1171	-	4,4,4	0.19	0	6,6,6	0.23	0
4	SO4	C	1170	-	4,4,4	0.03	0	6,6,6	0.07	0
4	SO4	C	1171	-	4,4,4	0.24	0	6,6,6	0.39	0
4	SO4	D	1170	-	4,4,4	0.16	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	1170	-	4,4,4	0.13	0	6,6,6	0.31	0
4	SO4	F	1170	-	4,4,4	0.13	0	6,6,6	0.52	0
4	SO4	G	1170	-	4,4,4	0.14	0	6,6,6	0.37	0
4	SO4	H	1170	-	4,4,4	0.09	0	6,6,6	0.22	0
4	SO4	I	1170	-	4,4,4	0.25	0	6,6,6	0.54	0
4	SO4	I	1171	-	4,4,4	0.21	0	6,6,6	0.55	0
4	SO4	J	1170	-	4,4,4	0.15	0	6,6,6	0.27	0
4	SO4	J	1171	-	4,4,4	0.15	0	6,6,6	0.26	0
4	SO4	J	1172	-	4,4,4	0.17	0	6,6,6	0.56	0
4	SO4	K	1170	-	4,4,4	0.13	0	6,6,6	0.15	0
4	SO4	K	1171	-	4,4,4	0.11	0	6,6,6	0.14	0
4	SO4	M	1170	-	4,4,4	0.11	0	6,6,6	0.18	0
4	SO4	O	1170	-	4,4,4	0.14	0	6,6,6	0.28	0
4	SO4	O	1171	-	4,4,4	0.10	0	6,6,6	0.09	0
4	SO4	Q	1170	-	4,4,4	0.20	0	6,6,6	0.17	0
4	SO4	S	1668	-	4,4,4	0.07	0	6,6,6	0.28	0
4	SO4	S	1669	-	4,4,4	0.33	0	6,6,6	0.37	0
4	SO4	T	1668	-	4,4,4	0.19	0	6,6,6	0.51	0
4	SO4	V	1668	-	4,4,4	0.31	0	6,6,6	0.57	0
4	SO4	V	1669	-	4,4,4	0.30	0	6,6,6	0.46	0
4	SO4	W	1668	-	4,4,4	0.17	0	6,6,6	0.26	0
4	SO4	W	1669	-	4,4,4	0.17	0	6,6,6	0.39	0
4	SO4	W	1670	-	4,4,4	0.10	0	6,6,6	0.24	0
4	SO4	X	1668	-	4,4,4	0.24	0	6,6,6	0.25	0
4	SO4	Y	1668	-	4,4,4	0.18	0	6,6,6	0.31	0
4	SO4	Z	1668	-	4,4,4	0.17	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	1	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	2	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	3	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	3	1671	-	-	0/0/0/0	0/0/0/0
4	SO4	3	1672	-	-	0/0/0/0	0/0/0/0
4	SO4	4	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	5	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	5	1671	-	-	0/0/0/0	0/0/0/0
4	SO4	6	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	7	1670	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	8	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1171	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1171	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1171	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	G	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	H	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	I	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	I	1171	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1171	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1172	-	-	0/0/0/0	0/0/0/0
4	SO4	K	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	K	1171	-	-	0/0/0/0	0/0/0/0
4	SO4	M	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	O	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	O	1171	-	-	0/0/0/0	0/0/0/0
4	SO4	Q	1170	-	-	0/0/0/0	0/0/0/0
4	SO4	S	1668	-	-	0/0/0/0	0/0/0/0
4	SO4	S	1669	-	-	0/0/0/0	0/0/0/0
4	SO4	T	1668	-	-	0/0/0/0	0/0/0/0
4	SO4	V	1668	-	-	0/0/0/0	0/0/0/0
4	SO4	V	1669	-	-	0/0/0/0	0/0/0/0
4	SO4	W	1668	-	-	0/0/0/0	0/0/0/0
4	SO4	W	1669	-	-	0/0/0/0	0/0/0/0
4	SO4	W	1670	-	-	0/0/0/0	0/0/0/0
4	SO4	X	1668	-	-	0/0/0/0	0/0/0/0
4	SO4	Y	1668	-	-	0/0/0/0	0/0/0/0
4	SO4	Z	1668	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.