



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 02:21 pm GMT

PDB ID : 1S3Q
Title : Crystal structures of a novel open pore ferritin from the hyperthermophilic Archaeon *Archaeoglobus fulgidus*
Authors : Johnson, E.; Cascio, D.; Sawaya, M.; Schroeder, I.
Deposited on : 2004-01-13
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	(not set)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

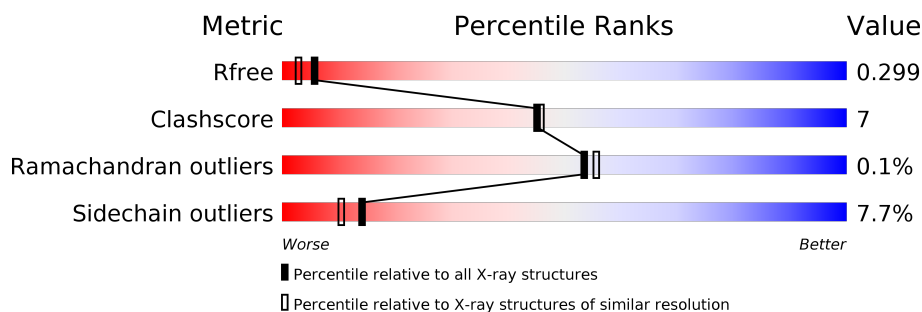
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	173	
1	B	173	
1	C	173	
1	D	173	
1	E	173	
1	F	173	
1	G	173	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	173	<div><div></div><div>80%9%6%</div></div>
1	I	173	<div><div></div><div>78%13%6%</div></div>
1	J	173	<div><div></div><div>79%12%5%</div></div>
1	K	173	<div><div></div><div>71%18%6%</div></div>
1	L	173	<div><div></div><div>77%13%6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17023 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 ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	B	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	C	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	D	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	E	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	F	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	G	163	Total	C	N	O	Se	0	0	0
			1348	865	220	255	8			
1	H	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	I	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	J	164	Total	C	N	O	Se	0	0	0
			1356	870	221	256	9			
1	K	162	Total	C	N	O	Se	0	0	0
			1343	862	219	254	8			
1	L	162	Total	C	N	O	Se	0	0	0
			1342	862	219	253	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
A	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
A	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
A	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
A	54	MSE	MET	MODIFIED RESIDUE	UNP O29424

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
A	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
A	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
A	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
B	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
C	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
D	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
E	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	8	MSE	MET	MODIFIED RESIDUE	UNP O29424

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
F	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
G	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
H	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
I	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
J	109	MSE	MET	MODIFIED RESIDUE	UNP O29424

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
K	111	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	1	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	8	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	29	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	45	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	54	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	57	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	59	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	109	MSE	MET	MODIFIED RESIDUE	UNP O29424
L	111	MSE	MET	MODIFIED RESIDUE	UNP O29424

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	71	Total 71	O 71	0	0
3	C	69	Total 69	O 69	0	0
3	D	72	Total 72	O 72	0	0
3	E	69	Total 69	O 69	0	0
3	F	46	Total 46	O 46	0	0
3	G	93	Total 93	O 93	0	0
3	H	66	Total 66	O 66	0	0
3	I	63	Total 63	O 63	0	0
3	J	83	Total 83	O 83	0	0
3	K	83	Total 83	O 83	0	0
3	L	68	Total 68	O 68	0	0

3 Residue-property plots [i](#)


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

- Molecule 1: ferritin

Chain A: 



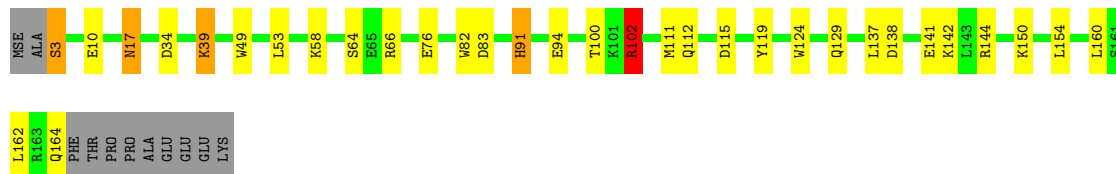
- Molecule 1: ferritin

Chain B: 



- Molecule 1: ferritin

Chain C: 



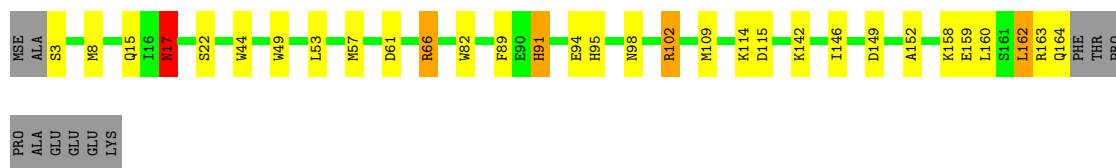
- Molecule 1: ferritin

Chain D: 




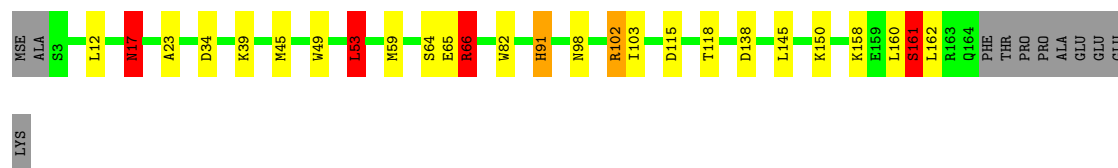
- Molecule 1: ferritin

Chain E: 




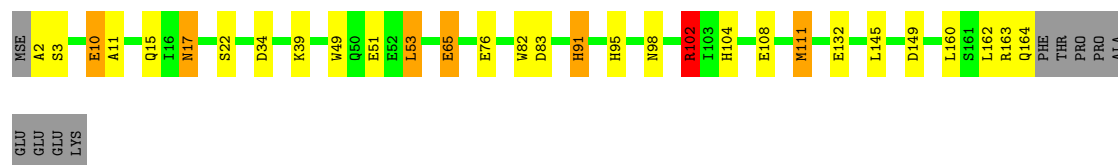
- Molecule 1: ferritin

Chain F:  79% 12% 6%




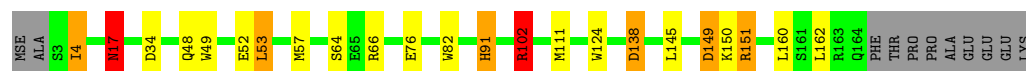
- Molecule 1: ferritin

Chain G:  77% 13% 6%



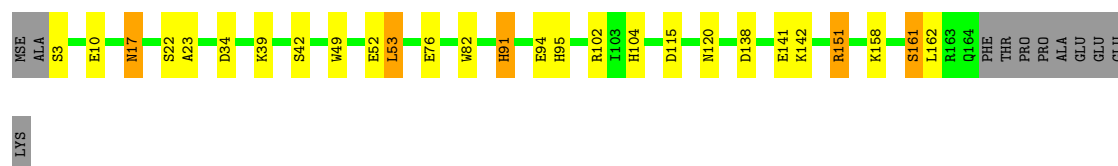
- Molecule 1: ferritin

Chain H:  80% 9% 6%




- Molecule 1: ferritin

Chain I:  78% 13% 6%



- Molecule 1: ferritin

Chain J:  79% 12% 5%



- Molecule 1: ferritin

Chain K:  71% 18% 6%



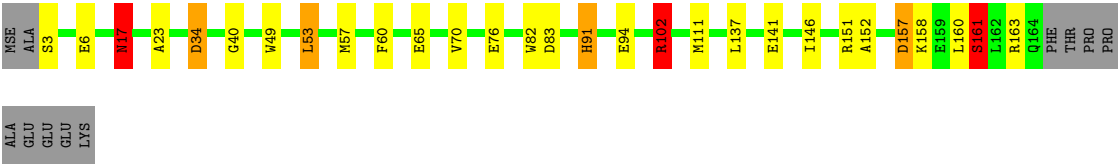
- Molecule 1: ferritin

Chain L:

77%

13%

• • 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	183.44Å 187.83Å 178.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.01 – 2.10 19.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (15.01-2.10) 98.1 (19.92-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.218 0.279 , 0.299	Depositor DCC
R_{free} test set	8740 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17023	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.85	2/1365 (0.1%)	0.86	2/1827 (0.1%)
1	B	0.87	1/1365 (0.1%)	0.85	4/1827 (0.2%)
1	C	0.85	1/1365 (0.1%)	0.86	4/1827 (0.2%)
1	D	0.88	1/1365 (0.1%)	0.90	7/1827 (0.4%)
1	E	0.84	1/1365 (0.1%)	0.88	7/1827 (0.4%)
1	F	0.83	2/1365 (0.1%)	0.85	4/1827 (0.2%)
1	G	0.87	2/1370 (0.1%)	0.87	8/1834 (0.4%)
1	H	0.84	2/1365 (0.1%)	0.88	6/1827 (0.3%)
1	I	0.87	1/1365 (0.1%)	0.83	1/1827 (0.1%)
1	J	0.87	3/1378 (0.2%)	0.95	10/1844 (0.5%)
1	K	0.88	2/1365 (0.1%)	0.93	6/1827 (0.3%)
1	L	0.92	2/1364 (0.1%)	0.88	6/1826 (0.3%)
All	All	0.86	20/16397 (0.1%)	0.88	65/21947 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	2
1	H	0	1
1	I	0	1
1	J	0	4
1	K	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	19

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	ASN	CG-OD1	12.98	1.52	1.24
1	I	17	ASN	CG-OD1	11.06	1.48	1.24
1	L	17	ASN	CG-OD1	10.59	1.47	1.24
1	G	17	ASN	CG-OD1	10.42	1.46	1.24
1	D	17	ASN	CG-OD1	10.29	1.46	1.24
1	E	17	ASN	CG-OD1	10.20	1.46	1.24
1	F	17	ASN	CG-OD1	10.18	1.46	1.24
1	K	17	ASN	CG-OD1	9.95	1.45	1.24
1	B	17	ASN	CG-OD1	9.81	1.45	1.24
1	A	17	ASN	CG-OD1	9.53	1.45	1.24
1	H	17	ASN	CG-OD1	8.86	1.43	1.24
1	J	17	ASN	CG-OD1	8.86	1.43	1.24
1	J	8	MSE	SE-CE	-7.29	1.52	1.95
1	F	45	MSE	CG-SE	-6.13	1.74	1.95
1	J	57	MSE	SE-CE	-5.81	1.61	1.95
1	G	111	MSE	SE-CE	-5.63	1.62	1.95
1	H	57	MSE	SE-CE	-5.55	1.62	1.95
1	L	57	MSE	SE-CE	-5.35	1.63	1.95
1	K	45	MSE	CG-SE	-5.12	1.78	1.95
1	A	8	MSE	SE-CE	-5.00	1.66	1.95

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	66	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	E	149	ASP	CB-CG-OD2	8.66	126.09	118.30
1	E	66	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	C	83	ASP	CB-CG-OD2	8.17	125.66	118.30
1	F	66	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	F	34	ASP	CB-CG-OD2	7.74	125.27	118.30
1	K	102	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	G	149	ASP	CB-CG-OD2	7.33	124.90	118.30
1	D	34	ASP	CB-CG-OD2	7.26	124.83	118.30
1	D	149	ASP	CB-CG-OD2	7.21	124.79	118.30
1	L	34	ASP	CB-CG-OD2	7.17	124.76	118.30
1	C	102	ARG	NE-CZ-NH1	7.09	123.85	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	115	ASP	CB-CG-OD2	7.04	124.64	118.30
1	J	149	ASP	CB-CG-OD2	7.04	124.63	118.30
1	L	102	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	J	66	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	K	102	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	J	8	MSE	CG-SE-CE	-6.61	84.37	98.90
1	K	34	ASP	CB-CG-OD2	6.53	124.17	118.30
1	H	102	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	E	8	MSE	CG-SE-CE	-6.49	84.62	98.90
1	H	53	LEU	CB-CG-CD1	6.41	121.89	111.00
1	D	53	LEU	CB-CG-CD1	6.39	121.86	111.00
1	G	34	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	138	ASP	CB-CG-OD2	6.24	123.92	118.30
1	G	102	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	G	163	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	L	83	ASP	CB-CG-OD2	6.08	123.77	118.30
1	E	66	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	J	53	LEU	CB-CG-CD1	6.01	121.22	111.00
1	D	102	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	K	149	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	34	ASP	CB-CG-OD2	5.92	123.62	118.30
1	J	138	ASP	CB-CG-OD2	5.88	123.59	118.30
1	K	4	ILE	CB-CA-C	-5.85	99.91	111.60
1	A	34	ASP	CB-CG-OD2	5.84	123.55	118.30
1	J	157	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	83	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	17	ASN	CA-CB-CG	-5.65	100.98	113.40
1	H	17	ASN	CA-CB-CG	-5.64	100.98	113.40
1	B	34	ASP	CB-CG-OD2	5.63	123.37	118.30
1	E	61	ASP	CB-CG-OD2	5.63	123.36	118.30
1	E	17	ASN	CA-CB-CG	-5.62	101.04	113.40
1	H	34	ASP	CB-CG-OD2	5.50	123.25	118.30
1	J	83	ASP	CB-CG-OD2	5.50	123.25	118.30
1	G	83	ASP	CB-CG-OD2	5.41	123.17	118.30
1	J	17	ASN	CA-CB-CG	-5.40	101.52	113.40
1	B	83	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	151	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	F	53	LEU	CB-CG-CD1	5.37	120.13	111.00
1	G	53	LEU	CB-CG-CD1	5.37	120.12	111.00
1	L	157	ASP	CB-CG-OD2	5.35	123.11	118.30
1	L	17	ASN	CA-CB-CG	-5.34	101.64	113.40
1	F	138	ASP	CB-CG-OD2	5.33	123.10	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	102	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	H	138	ASP	CB-CG-OD2	5.31	123.08	118.30
1	H	149	ASP	CB-CG-OD2	5.28	123.05	118.30
1	K	138	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	151	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	L	163	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	144	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	G	149	ASP	OD1-CG-OD2	-5.12	113.58	123.30
1	D	61	ASP	CB-CG-OD2	5.09	122.89	118.30
1	E	149	ASP	OD1-CG-OD2	-5.05	113.70	123.30
1	J	115	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	ASN	Sidechain
1	B	17	ASN	Sidechain
1	B	3	SER	Peptide
1	C	17	ASN	Sidechain
1	D	17	ASN	Sidechain
1	E	17	ASN	Sidechain
1	F	161	SER	Mainchain
1	F	17	ASN	Sidechain
1	G	17	ASN	Sidechain
1	G	2	ALA	Peptide
1	H	17	ASN	Sidechain
1	I	17	ASN	Sidechain
1	J	1	MSE	Peptide
1	J	17	ASN	Sidechain
1	J	2	ALA	Mainchain,Peptide
1	K	17	ASN	Sidechain
1	L	161	SER	Mainchain
1	L	17	ASN	Sidechain

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	1343	0	1302	18	0
1	B	1343	0	1302	11	0
1	C	1343	0	1302	26	0
1	D	1343	0	1302	18	0
1	E	1343	0	1302	22	0
1	F	1343	0	1302	19	0
1	G	1348	0	1307	25	0
1	H	1343	0	1302	13	0
1	I	1343	0	1302	15	0
1	J	1356	0	1319	26	0
1	K	1343	0	1302	33	0
1	L	1342	0	1302	17	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
3	A	83	0	0	5	0
3	B	71	0	0	2	0
3	C	69	0	0	2	0
3	D	72	0	0	5	0
3	E	69	0	0	3	0
3	F	46	0	0	3	0
3	G	93	0	0	11	0
3	H	66	0	0	8	0
3	I	63	0	0	5	0
3	J	83	0	0	3	0
3	K	83	0	0	9	0
3	L	68	0	0	4	0
All	All	17023	0	15646	224	0

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

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:ARG:HB2	3:G:967:HOH:O	1.22	1.29
1:H:138:ASP:HB3	3:H:933:HOH:O	1.23	1.27
1:C:102:ARG:NH2	3:C:950:HOH:O	1.59	1.26
1:G:102:ARG:CZ	3:G:975:HOH:O	1.98	1.08
3:A:970:HOH:O	1:F:150:LYS:HG2	1.51	1.08
1:C:102:ARG:HH21	1:C:102:ARG:CG	1.70	1.04
1:C:102:ARG:HG2	1:C:102:ARG:HH21	1.17	1.04
1:G:3:SER:HB3	3:G:966:HOH:O	1.65	0.96
1:G:164:GLN:O	3:G:996:HOH:O	1.84	0.93
1:D:102:ARG:HH21	1:D:102:ARG:HG3	1.34	0.93
1:D:34:ASP:OD1	1:D:39:LYS:HE2	1.69	0.90
1:A:82:TRP:HE1	1:A:91:HIS:HD2	1.17	0.89
1:C:39:LYS:HE2	1:C:39:LYS:HA	1.54	0.88
1:K:102:ARG:HG3	1:K:102:ARG:HH21	1.40	0.87
1:C:3:SER:HB3	1:C:66:ARG:HH12	1.40	0.87
1:G:3:SER:CB	3:G:966:HOH:O	2.21	0.86
1:D:82:TRP:HE1	1:D:91:HIS:HD2	1.15	0.86
1:K:64:SER:OG	3:K:1002:HOH:O	1.94	0.85
1:F:102:ARG:HH21	1:F:102:ARG:HG2	1.45	0.81
1:H:4:ILE:HG12	1:H:66:ARG:HB3	1.62	0.81
1:E:102:ARG:HH21	1:E:102:ARG:HG2	1.47	0.80
1:K:82:TRP:HE1	1:K:91:HIS:HD2	1.26	0.80
1:K:102:ARG:HG2	3:K:954:HOH:O	1.81	0.79
1:C:66:ARG:NH2	1:C:115:ASP:OD1	2.16	0.78
1:J:1:MSE:N	3:J:924:HOH:O	2.17	0.78
1:I:104:HIS:ND1	3:I:973:HOH:O	2.15	0.77
1:A:108:GLU:HA	1:A:111:MSE:HE2	1.65	0.77
1:F:82:TRP:HE1	1:F:91:HIS:CD2	2.03	0.76
1:F:66:ARG:NH2	1:F:115:ASP:OD1	2.17	0.76
1:A:82:TRP:HE1	1:A:91:HIS:CD2	2.01	0.76
1:J:66:ARG:NH2	1:J:115:ASP:OD1	2.18	0.76
1:D:102:ARG:CG	3:D:971:HOH:O	2.33	0.76
1:E:82:TRP:HE1	1:E:91:HIS:HD2	1.29	0.76
1:D:34:ASP:OD1	1:D:39:LYS:CE	2.34	0.76
1:D:102:ARG:HB2	3:D:971:HOH:O	1.85	0.74
1:K:111:MSE:HB3	3:K:924:HOH:O	1.86	0.74
1:E:66:ARG:NH1	1:E:115:ASP:OD1	2.20	0.74
1:D:102:ARG:CB	3:D:971:HOH:O	2.35	0.73
1:I:158:LYS:O	1:I:161:SER:HB2	1.89	0.72
1:C:82:TRP:HE1	1:C:91:HIS:HD2	1.37	0.72
1:K:141:GLU:OE1	3:K:1003:HOH:O	2.08	0.72
1:D:82:TRP:HE1	1:D:91:HIS:CD2	2.04	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:TRP:HE1	1:B:91:HIS:HD2	1.37	0.71
1:L:3:SER:CB	3:L:986:HOH:O	2.38	0.71
1:D:102:ARG:NH2	1:D:102:ARG:HG3	2.06	0.71
1:B:151:ARG:NH2	3:B:963:HOH:O	2.22	0.71
1:K:82:TRP:HE1	1:K:91:HIS:CD2	2.07	0.70
1:F:82:TRP:HE1	1:F:91:HIS:HD2	1.39	0.70
1:F:66:ARG:HH22	1:F:115:ASP:CG	1.95	0.69
1:L:82:TRP:HE1	1:L:91:HIS:CD2	2.09	0.69
1:F:158:LYS:O	1:F:161:SER:HB2	1.91	0.69
1:I:82:TRP:HE1	1:I:91:HIS:HD2	1.40	0.68
1:L:82:TRP:HE1	1:L:91:HIS:HD2	1.40	0.68
1:J:82:TRP:HE1	1:J:91:HIS:HD2	1.39	0.67
1:C:3:SER:HB3	1:C:66:ARG:NH1	2.08	0.67
1:H:82:TRP:HE1	1:H:91:HIS:CD2	2.13	0.67
1:K:102:ARG:HG3	1:K:102:ARG:NH2	2.09	0.66
1:G:22:SER:OG	1:G:95:HIS:HE1	1.78	0.66
1:K:4:ILE:HG12	1:K:66:ARG:HB3	1.77	0.66
1:G:82:TRP:HE1	1:G:91:HIS:CD2	2.12	0.66
1:J:108:GLU:HA	1:J:111:MSE:HE2	1.77	0.66
1:B:82:TRP:HE1	1:B:91:HIS:CD2	2.13	0.66
1:A:34:ASP:OD2	1:A:39:LYS:HE3	1.96	0.66
3:H:978:HOH:O	1:J:142:LYS:HG3	1.95	0.65
1:B:39:LYS:HE2	1:B:39:LYS:HA	1.78	0.65
1:I:82:TRP:HE1	1:I:91:HIS:CD2	2.14	0.65
1:H:82:TRP:HE1	1:H:91:HIS:HD2	1.42	0.65
1:C:82:TRP:HE1	1:C:91:HIS:CD2	2.14	0.65
1:E:3:SER:HB2	3:E:947:HOH:O	1.95	0.65
3:H:978:HOH:O	1:J:142:LYS:CE	2.43	0.65
1:G:82:TRP:HE1	1:G:91:HIS:HD2	1.45	0.64
1:C:102:ARG:HG2	1:C:102:ARG:NH2	1.99	0.64
1:E:82:TRP:HE1	1:E:91:HIS:CD2	2.13	0.64
1:D:34:ASP:OD1	1:D:39:LYS:NZ	2.31	0.63
1:F:23:ALA:CB	1:F:53:LEU:HD13	2.28	0.62
1:L:102:ARG:HH11	1:L:102:ARG:CG	2.12	0.61
1:G:102:ARG:HG2	1:G:102:ARG:NH2	2.15	0.61
1:K:102:ARG:CG	1:K:102:ARG:HH21	2.13	0.61
1:J:82:TRP:HE1	1:J:91:HIS:CD2	2.17	0.61
1:F:102:ARG:CG	1:F:102:ARG:HH21	2.12	0.60
1:C:154:LEU:HD22	1:E:142:LYS:NZ	2.17	0.59
1:L:158:LYS:O	1:L:161:SER:HB2	2.03	0.58
1:K:64:SER:OG	1:L:34:ASP:OD1	2.13	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:ASP:OD2	3:K:960:HOH:O	2.17	0.58
1:E:102:ARG:HH21	1:E:102:ARG:CG	2.16	0.58
1:I:151:ARG:HD2	3:I:981:HOH:O	2.04	0.57
1:C:58:LYS:HE2	1:C:124:TRP:CD2	2.39	0.57
3:H:978:HOH:O	1:J:142:LYS:CG	2.52	0.57
1:C:102:ARG:CG	1:C:102:ARG:NH2	2.43	0.57
1:G:102:ARG:NH2	3:G:975:HOH:O	2.23	0.57
1:D:51:GLU:OE1	1:D:132:GLU:OE2	2.22	0.57
1:A:3:SER:N	3:A:965:HOH:O	2.38	0.57
1:C:39:LYS:CA	1:C:39:LYS:HE2	2.24	0.57
1:I:138:ASP:OD1	1:I:142:LYS:HE2	2.04	0.57
1:A:108:GLU:OE1	1:E:114:LYS:HE2	2.04	0.56
1:G:102:ARG:HH21	1:G:102:ARG:CG	2.18	0.56
1:H:102:ARG:CG	1:H:102:ARG:HH21	2.18	0.56
1:H:149:ASP:OD1	1:H:151:ARG:HG2	2.05	0.56
1:A:4:ILE:HG13	3:A:944:HOH:O	2.06	0.56
1:D:57:MSE:HE2	1:D:57:MSE:HA	1.88	0.56
1:F:59:MSE:HG3	3:F:952:HOH:O	2.04	0.56
1:A:4:ILE:HG12	1:A:66:ARG:HB3	1.88	0.55
1:F:39:LYS:HE2	1:F:39:LYS:HA	1.88	0.55
3:H:978:HOH:O	1:J:142:LYS:HE2	2.03	0.55
1:C:154:LEU:HD22	1:E:142:LYS:HZ2	1.71	0.55
1:J:66:ARG:NH2	1:J:115:ASP:CG	2.61	0.54
1:J:1:MSE:HB3	1:K:133:GLU:OE2	2.08	0.54
1:I:158:LYS:HD3	3:K:977:HOH:O	2.07	0.54
1:H:102:ARG:HG3	1:H:102:ARG:HH21	1.73	0.54
1:G:98:ASN:CB	3:G:998:HOH:O	2.56	0.54
1:I:22:SER:OG	1:I:95:HIS:HE1	1.91	0.54
1:D:65:GLU:HG3	3:D:929:HOH:O	2.07	0.54
1:G:3:SER:HB2	3:G:966:HOH:O	1.99	0.53
1:E:98:ASN:HB3	3:E:977:HOH:O	2.08	0.53
1:G:102:ARG:HG2	1:G:102:ARG:HH21	1.71	0.53
1:E:22:SER:OG	1:E:95:HIS:HE1	1.92	0.53
1:L:102:ARG:HD2	1:L:102:ARG:O	2.08	0.53
1:H:151:ARG:HD2	1:J:151:ARG:HB2	1.90	0.52
1:J:64:SER:HB2	3:J:994:HOH:O	2.10	0.52
1:J:1:MSE:HB2	1:K:133:GLU:OE1	2.09	0.52
1:K:34:ASP:OD1	1:K:39:LYS:HE2	2.10	0.52
1:D:145:LEU:C	1:D:145:LEU:HD23	2.30	0.52
1:I:141:GLU:HG2	3:I:970:HOH:O	2.08	0.52
1:F:102:ARG:CG	1:F:102:ARG:NH2	2.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ARG:HH21	1:D:102:ARG:CG	2.17	0.51
1:K:22:SER:OG	1:K:95:HIS:HE1	1.92	0.51
3:H:978:HOH:O	1:J:142:LYS:CD	2.57	0.51
1:L:102:ARG:HH11	1:L:102:ARG:HG2	1.74	0.51
1:G:98:ASN:HB2	3:G:998:HOH:O	2.08	0.51
1:A:39:LYS:HE2	1:A:39:LYS:HA	1.92	0.51
1:I:23:ALA:CB	1:I:53:LEU:HD13	2.40	0.51
1:C:102:ARG:HG3	1:C:102:ARG:HH21	1.67	0.51
1:E:15:GLN:OE1	1:E:102:ARG:HG3	2.11	0.51
1:J:1:MSE:CB	1:K:133:GLU:OE2	2.59	0.51
1:C:91:HIS:HE1	3:C:930:HOH:O	1.94	0.50
1:J:1:MSE:HB3	1:K:100:THR:HG21	1.93	0.50
1:E:66:ARG:NH1	1:E:115:ASP:CG	2.64	0.50
1:L:137:LEU:O	1:L:141:GLU:HG3	2.10	0.50
1:C:150:LYS:HE3	1:E:146:ILE:O	2.12	0.50
1:I:39:LYS:HA	1:I:39:LYS:HE2	1.93	0.50
1:I:102:ARG:HD3	3:I:972:HOH:O	2.10	0.50
1:G:91:HIS:HE1	3:G:950:HOH:O	1.95	0.50
1:L:102:ARG:NE	3:L:988:HOH:O	2.44	0.50
1:B:158:LYS:O	1:B:161:SER:HB2	2.12	0.50
1:H:124:TRP:HB2	3:H:963:HOH:O	2.11	0.49
1:B:23:ALA:CB	1:B:53:LEU:HD13	2.43	0.49
1:G:145:LEU:C	1:G:145:LEU:HD23	2.32	0.49
1:H:4:ILE:CG1	1:H:66:ARG:HB3	2.40	0.49
1:G:102:ARG:CG	1:G:102:ARG:NH2	2.76	0.48
1:G:108:GLU:HA	1:G:111:MSE:CE	2.43	0.48
1:J:66:ARG:NH2	1:J:115:ASP:OD2	2.46	0.48
1:C:111:MSE:HG2	1:C:119:TYR:CD1	2.48	0.48
1:H:102:ARG:NH2	1:H:102:ARG:HG3	2.29	0.48
1:J:91:HIS:HE1	3:J:945:HOH:O	1.96	0.48
1:L:146:ILE:HG12	1:L:152:ALA:HB1	1.94	0.48
1:B:91:HIS:HE1	3:B:924:HOH:O	1.96	0.47
1:C:102:ARG:HG3	1:C:102:ARG:NH2	2.27	0.47
1:L:102:ARG:CG	1:L:102:ARG:NH1	2.76	0.47
1:K:40:GLY:HA3	1:K:157:ASP:O	2.15	0.47
1:K:95:HIS:HD2	3:K:929:HOH:O	1.97	0.47
1:C:66:ARG:NH2	1:C:115:ASP:CG	2.67	0.47
1:B:3:SER:HA	1:B:66:ARG:HH21	1.79	0.47
1:E:66:ARG:NH1	1:E:115:ASP:OD2	2.47	0.47
1:J:23:ALA:HB2	1:J:52:GLU:HB2	1.96	0.47
1:L:40:GLY:HA3	1:L:157:ASP:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ARG:HH21	1:C:115:ASP:CG	2.17	0.46
1:J:1:MSE:N	1:K:133:GLU:OE1	2.38	0.46
1:I:23:ALA:HB2	1:I:52:GLU:HB2	1.96	0.46
1:K:102:ARG:HD2	1:K:102:ARG:O	2.15	0.46
1:G:15:GLN:OE1	1:G:102:ARG:HG3	2.16	0.46
1:E:146:ILE:HG12	1:E:152:ALA:HB1	1.98	0.45
1:C:137:LEU:O	1:C:141:GLU:HG3	2.16	0.45
1:A:64:SER:CB	1:B:34:ASP:OD1	2.65	0.45
1:A:4:ILE:HG13	1:A:4:ILE:H	1.57	0.45
1:L:23:ALA:CB	1:L:53:LEU:HD13	2.47	0.44
1:A:64:SER:HB2	1:B:34:ASP:OD1	2.17	0.44
1:K:45:MSE:HE1	1:K:92:VAL:HG21	1.99	0.44
1:A:151:ARG:NH1	3:A:983:HOH:O	2.51	0.44
1:B:99:VAL:O	1:B:103:ILE:HD12	2.18	0.43
1:E:66:ARG:HH12	1:E:115:ASP:CG	2.22	0.43
1:K:51:GLU:OE2	1:K:132:GLU:OE2	2.35	0.43
1:G:65:GLU:OE1	3:G:999:HOH:O	2.21	0.43
1:J:1:MSE:HE1	1:K:101:LYS:HA	1.98	0.43
1:F:66:ARG:NH2	1:F:115:ASP:OD2	2.50	0.43
3:A:970:HOH:O	1:F:150:LYS:CG	2.33	0.43
1:G:10:GLU:HG3	1:G:11:ALA:N	2.30	0.43
1:L:91:HIS:HE1	3:L:933:HOH:O	2.02	0.43
1:A:145:LEU:O	1:F:150:LYS:HD3	2.19	0.43
1:D:91:HIS:HE1	3:D:920:HOH:O	2.02	0.43
1:E:3:SER:CB	3:E:947:HOH:O	2.60	0.43
1:G:108:GLU:HA	1:G:111:MSE:HE3	2.01	0.43
1:K:142:LYS:HD2	3:K:997:HOH:O	2.19	0.43
1:C:100:THR:OG1	1:C:129:GLN:HB3	2.19	0.43
1:E:102:ARG:CG	1:E:102:ARG:NH2	2.81	0.43
1:F:91:HIS:CD2	3:F:953:HOH:O	2.71	0.43
1:H:48:GLN:O	1:H:52:GLU:HG2	2.19	0.42
1:C:138:ASP:OD1	1:C:142:LYS:HE2	2.20	0.42
1:F:12:LEU:HD22	3:F:952:HOH:O	2.18	0.42
1:G:51:GLU:OE2	1:G:132:GLU:OE2	2.37	0.42
1:K:34:ASP:OD1	1:K:39:LYS:CE	2.68	0.42
1:I:34:ASP:HB3	3:I:969:HOH:O	2.18	0.42
1:J:65:GLU:HG2	1:K:130:VAL:CG1	2.50	0.42
1:F:66:ARG:NH2	1:F:118:THR:OG1	2.52	0.42
1:A:65:GLU:HG2	1:D:130:VAL:CG1	2.50	0.41
1:E:57:MSE:HA	1:E:57:MSE:HE2	2.01	0.41
1:J:62:PHE:CZ	1:J:66:ARG:HG3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:76:GLU:OE1	3:L:954:HOH:O	2.22	0.41
1:H:91:HIS:HE1	3:H:931:HOH:O	2.02	0.41
1:K:23:ALA:HB2	1:K:52:GLU:HB2	2.03	0.41
1:K:64:SER:HB2	3:K:959:HOH:O	2.20	0.41
1:J:23:ALA:CB	1:J:53:LEU:HD13	2.49	0.41
1:L:60:PHE:CD1	1:L:70:VAL:HG11	2.56	0.41
1:A:34:ASP:OD2	1:A:39:LYS:CE	2.64	0.41
1:J:1:MSE:HB2	1:K:133:GLU:CD	2.40	0.41
1:C:58:LYS:HE2	1:C:124:TRP:CE3	2.56	0.41
1:D:108:GLU:HA	1:D:111:MSE:HE2	2.03	0.41
1:E:159:GLU:O	1:E:162:LEU:HB2	2.21	0.41
1:K:159:GLU:O	1:K:162:LEU:HB2	2.21	0.41
1:A:23:ALA:CB	1:A:53:LEU:HD13	2.50	0.41
1:I:120:ASN:HA	1:I:120:ASN:HD22	1.72	0.41
1:G:104:HIS:O	1:G:108:GLU:HG3	2.21	0.40
1:E:44:TRP:CD1	1:E:163:ARG:HD2	2.56	0.40
1:A:145:LEU:O	1:F:150:LYS:CD	2.69	0.40
1:K:57:MSE:HA	1:K:57:MSE:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/173 (92%)	159 (99%)	1 (1%)	0	100	100
1	B	160/173 (92%)	159 (99%)	1 (1%)	0	100	100
1	C	160/173 (92%)	160 (100%)	0	0	100	100
1	D	160/173 (92%)	157 (98%)	3 (2%)	0	100	100
1	E	160/173 (92%)	158 (99%)	2 (1%)	0	100	100
1	F	160/173 (92%)	158 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	161/173 (93%)	160 (99%)	1 (1%)	0	100	100
1	H	160/173 (92%)	159 (99%)	1 (1%)	0	100	100
1	I	160/173 (92%)	159 (99%)	1 (1%)	0	100	100
1	J	162/173 (94%)	159 (98%)	2 (1%)	1 (1%)	27	23
1	K	160/173 (92%)	158 (99%)	2 (1%)	0	100	100
1	L	160/173 (92%)	158 (99%)	2 (1%)	0	100	100
All	All	1923/2076 (93%)	1904 (99%)	18 (1%)	1 (0%)	53	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	3	SER

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	143/143 (100%)	136 (95%)	7 (5%)	27	25
1	B	143/143 (100%)	134 (94%)	9 (6%)	20	16
1	C	143/143 (100%)	129 (90%)	14 (10%)	9	5
1	D	143/143 (100%)	134 (94%)	9 (6%)	20	16
1	E	143/143 (100%)	131 (92%)	12 (8%)	12	8
1	F	143/143 (100%)	129 (90%)	14 (10%)	9	5
1	G	143/143 (100%)	133 (93%)	10 (7%)	16	13
1	H	143/143 (100%)	129 (90%)	14 (10%)	9	5
1	I	143/143 (100%)	132 (92%)	11 (8%)	14	10
1	J	144/143 (101%)	138 (96%)	6 (4%)	32	32
1	K	143/143 (100%)	129 (90%)	14 (10%)	9	5
1	L	143/143 (100%)	131 (92%)	12 (8%)	12	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1717/1716 (100%)	1585 (92%)	132 (8%)	14	10

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	39	LYS
1	A	49	TRP
1	A	53	LEU
1	A	91	HIS
1	A	94	GLU
1	A	148	GLU
1	B	49	TRP
1	B	53	LEU
1	B	91	HIS
1	B	98	ASN
1	B	113	GLU
1	B	145	LEU
1	B	160	LEU
1	B	161	SER
1	B	162	LEU
1	C	3	SER
1	C	10	GLU
1	C	39	LYS
1	C	49	TRP
1	C	53	LEU
1	C	64	SER
1	C	76	GLU
1	C	91	HIS
1	C	94	GLU
1	C	102	ARG
1	C	112	GLN
1	C	160	LEU
1	C	162	LEU
1	C	164	GLN
1	D	3	SER
1	D	24	TYR
1	D	49	TRP
1	D	53	LEU
1	D	91	HIS
1	D	94	GLU
1	D	102	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	160	LEU
1	D	162	LEU
1	E	17	ASN
1	E	49	TRP
1	E	53	LEU
1	E	89	PHE
1	E	91	HIS
1	E	94	GLU
1	E	102	ARG
1	E	109	MSE
1	E	158	LYS
1	E	160	LEU
1	E	162	LEU
1	E	164	GLN
1	F	17	ASN
1	F	49	TRP
1	F	53	LEU
1	F	64	SER
1	F	65	GLU
1	F	66	ARG
1	F	91	HIS
1	F	98	ASN
1	F	102	ARG
1	F	103	ILE
1	F	145	LEU
1	F	160	LEU
1	F	161	SER
1	F	162	LEU
1	G	10	GLU
1	G	39	LYS
1	G	49	TRP
1	G	53	LEU
1	G	65	GLU
1	G	76	GLU
1	G	91	HIS
1	G	102	ARG
1	G	160	LEU
1	G	162	LEU
1	H	4	ILE
1	H	17	ASN
1	H	49	TRP
1	H	53	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	64	SER
1	H	76	GLU
1	H	91	HIS
1	H	102	ARG
1	H	111	MSE
1	H	145	LEU
1	H	150	LYS
1	H	151	ARG
1	H	160	LEU
1	H	162	LEU
1	I	3	SER
1	I	10	GLU
1	I	42	SER
1	I	49	TRP
1	I	53	LEU
1	I	76	GLU
1	I	91	HIS
1	I	94	GLU
1	I	151	ARG
1	I	161	SER
1	I	162	LEU
1	J	49	TRP
1	J	53	LEU
1	J	91	HIS
1	J	94	GLU
1	J	142	LYS
1	J	160	LEU
1	K	3	SER
1	K	4	ILE
1	K	6	GLU
1	K	39	LYS
1	K	49	TRP
1	K	53	LEU
1	K	94	GLU
1	K	98	ASN
1	K	102	ARG
1	K	111	MSE
1	K	151	ARG
1	K	154	LEU
1	K	160	LEU
1	K	162	LEU
1	L	6	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	17	ASN
1	L	49	TRP
1	L	53	LEU
1	L	65	GLU
1	L	91	HIS
1	L	94	GLU
1	L	102	ARG
1	L	111	MSE
1	L	151	ARG
1	L	160	LEU
1	L	161	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	43	ASN
1	A	91	HIS
1	A	112	GLN
1	B	17	ASN
1	B	91	HIS
1	B	120	ASN
1	C	17	ASN
1	C	43	ASN
1	C	91	HIS
1	C	120	ASN
1	D	17	ASN
1	D	91	HIS
1	D	112	GLN
1	E	43	ASN
1	E	91	HIS
1	E	95	HIS
1	E	112	GLN
1	E	164	GLN
1	F	17	ASN
1	F	50	GLN
1	F	91	HIS
1	F	120	ASN
1	G	17	ASN
1	G	91	HIS
1	G	95	HIS
1	G	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	50	GLN
1	H	91	HIS
1	H	112	GLN
1	H	120	ASN
1	I	17	ASN
1	I	50	GLN
1	I	91	HIS
1	I	95	HIS
1	I	112	GLN
1	I	120	ASN
1	I	164	GLN
1	J	17	ASN
1	J	43	ASN
1	J	91	HIS
1	J	112	GLN
1	K	91	HIS
1	K	95	HIS
1	K	112	GLN
1	L	50	GLN
1	L	91	HIS
1	L	112	GLN
1	L	120	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.