



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:16 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 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>

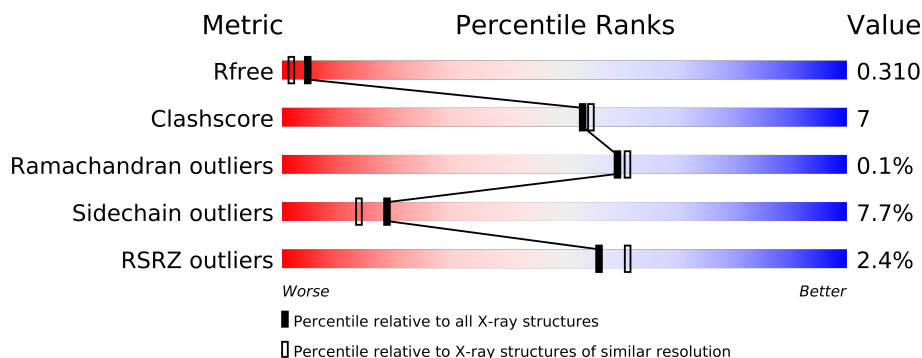
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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	
1	H	173	
1	I	173	
1	J	173	
1	K	173	
1	L	173	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	F	911	-	X
2	ZN	I	918	-	X
2	ZN	K	921	-	X
2	ZN	L	924	-	X

2 Entry composition

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

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

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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

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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

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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

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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.

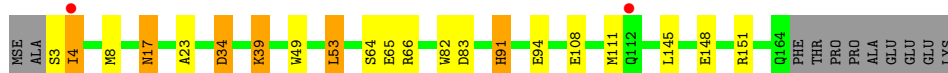
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	71	Total 71	O 71	0	0
3	C	69	Total 69	O 69	0	0
3	D	72	Total 72	O 72	0	0
3	E	69	Total 69	O 69	0	0
3	F	46	Total 46	O 46	0	0
3	G	93	Total 93	O 93	0	0
3	H	66	Total 66	O 66	0	0
3	I	63	Total 63	O 63	0	0
3	J	83	Total 83	O 83	0	0
3	K	83	Total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

3 Residue-property plots

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.

- Molecule 1: ferritin

Chain A: 



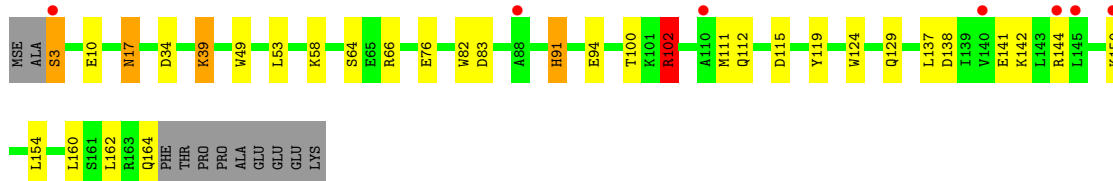
- Molecule 1: ferritin

Chain B: 



- Molecule 1: ferritin

Chain C: 



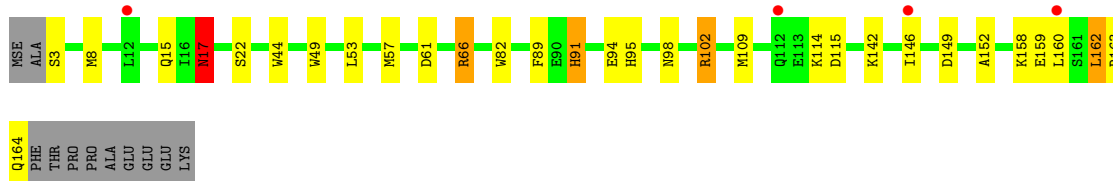
- Molecule 1: ferritin

Chain D: 



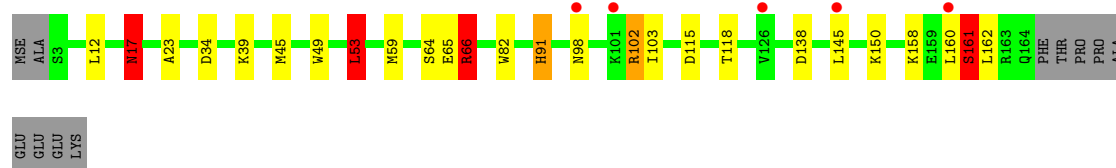
- Molecule 1: ferritin

Chain E: 



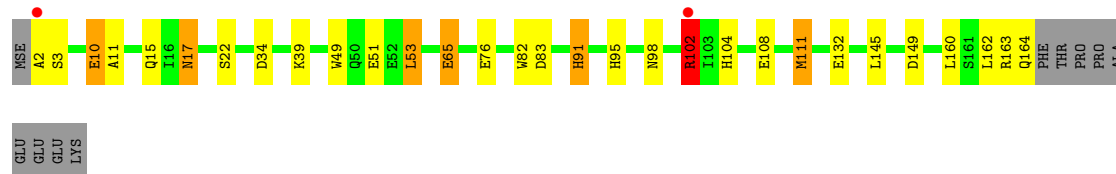
- Molecule 1: ferritin

Chain F:



- Molecule 1: ferritin

Chain G:



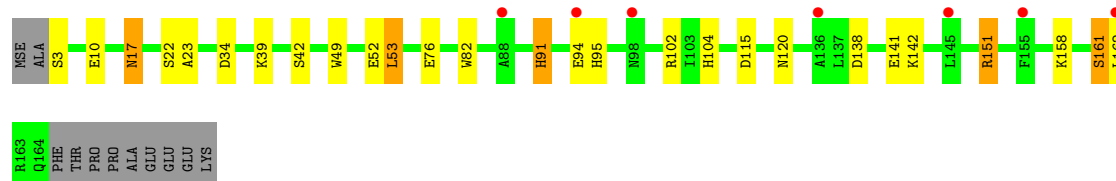
- Molecule 1: ferritin

Chain H:



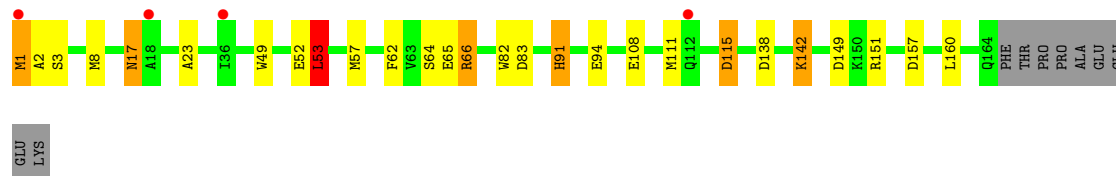
- Molecule 1: ferritin

Chain I:



- Molecule 1: ferritin

Chain J:



- Molecule 1: ferritin

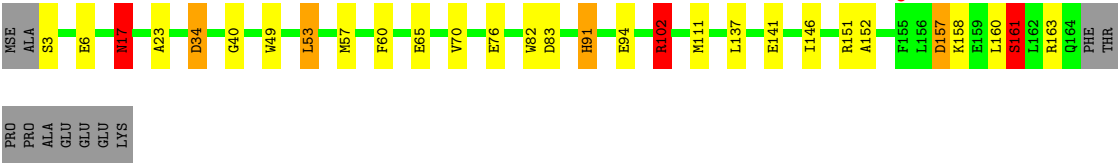
Chain K:





● Molecule 1: ferritin

Chain L:



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) 98.2 (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 0.293 , 0.310	Depositor DCC
R_{free} test set	8746 reflections (5.02%)	DCC
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 , 33.3	EDS
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 174236 reflections	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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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

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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

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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 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	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

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 7.

All (224) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HG2	1:C:102:ARG:HH21	1.17	1.04
1:C:102:ARG:HH21	1:C:102:ARG:CG	1.70	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
1:B:82:TRP:HE1	1:B:91:HIS:HD2	1.37	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:L:82:TRP:HE1	1:L:91:HIS:HD2	1.40	0.68
1:I:82:TRP:HE1	1:I: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
3:H:978:HOH:O	1:J:142:LYS:CE	2.43	0.65
1:E:3:SER:HB2	3:E:947:HOH:O	1.95	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:K:64:SER:OG	1:L:34:ASP:OD1	2.13	0.58
1:L:158:LYS:O	1:L:161:SER:HB2	2.03	0.58
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:151:ARG:HD2	3:I:981:HOH:O	2.04	0.57
3:H:978:HOH:O	1:J:142:LYS:CG	2.52	0.57
1:C:58:LYS:HE2	1:C:124:TRP:CD2	2.39	0.57
1:G:102:ARG:NH2	3:G:975:HOH:O	2.23	0.57
1:C:102:ARG:CG	1:C:102:ARG:NH2	2.43	0.57
1:D:51:GLU:OE1	1:D:132:GLU:OE2	2.22	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:3:SER:N	3:A:965:HOH:O	2.38	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:1:MSE:HB3	1:K:133:GLU:OE2	2.08	0.54
1:J:66:ARG:NH2	1:J:115:ASP:CG	2.61	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:G:102:ARG:HG2	1:G:102:ARG:HH21	1.71	0.53
1:E:98:ASN:HB3	3:E:977:HOH:O	2.08	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:J:1:MSE:HB3	1:K:100:THR:HG21	1.93	0.50
1:C:91:HIS:HE1	3:C:930:HOH:O	1.94	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:I:39:LYS:HA	1:I:39:LYS:HE2	1.93	0.50
1:C:150:LYS:HE3	1:E:146:ILE:O	2.12	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:C:102:ARG:HG3	1:C:102:ARG:NH2	2.27	0.47
1:B:91:HIS:HE1	3:B:924:HOH:O	1.96	0.47
1:L:102:ARG:CG	1:L:102:ARG:NH1	2.76	0.47
1:K:95:HIS:HD2	3:K:929:HOH:O	1.97	0.47
1:K:40:GLY:HA3	1:K:157:ASP:O	2.15	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
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:K:102:ARG:HD2	1:K:102:ARG:O	2.15	0.46
1:I:23:ALA:HB2	1:I:52:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:66:ARG:HH12	1:E:115:ASP:CG	2.22	0.43
1:B:99:VAL:O	1:B:103:ILE:HD12	2.18	0.43
1:K:51:GLU:OE2	1:K:132:GLU:OE2	2.35	0.43
1:J:1:MSE:HE1	1:K:101:LYS:HA	1.98	0.43
1:G:65:GLU:OE1	3:G:999:HOH:O	2.21	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: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:C:100:THR:OG1	1:C:129:GLN:HB3	2.19	0.43
1:H:48:GLN:O	1:H:52:GLU:HG2	2.19	0.42
1:F:12:LEU:HD22	3:F:952:HOH:O	2.18	0.42
1:C:138:ASP:OD1	1:C:142:LYS:HE2	2.20	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:J:62:PHE:CZ	1:J:66:ARG:HG3	2.55	0.41
1:E:57:MSE:HA	1:E:57:MSE:HE2	2.01	0.41
1:L:76:GLU:OE1	3:L:954:HOH:O	2.22	0.41
1:A:65:GLU:HG2	1:D:130:VAL:CG1	2.50	0.41
1:K:64:SER:HB2	3:K:959:HOH:O	2.20	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:J:23:ALA:CB	1:J:53:LEU:HD13	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:60:PHE:CD1	1:L:70:VAL:HG11	2.56	0.41
1:J:1:MSE:HB2	1:K:133:GLU:CD	2.40	0.41
1:A:34:ASP:OD2	1:A:39:LYS:CE	2.64	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:K:159:GLU:O	1:K:162:LEU:HB2	2.21	0.41
1:E:159:GLU:O	1:E:162:LEU:HB2	2.21	0.41
1:I:120:ASN:HA	1:I:120:ASN:HD22	1.72	0.41
1:A:23:ALA:CB	1:A:53:LEU:HD13	2.50	0.41
1:G:104:HIS:O	1:G:108:GLU:HG3	2.21	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
1:E:44:TRP:CD1	1:E:163:ARG:HD2	2.56	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
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%)	33	28
1	K	160/173 (92%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	160/173 (92%)	158 (99%)	2 (1%)	0	100	100
All	All	1923/2076 (93%)	1904 (99%)	18 (1%)	1 (0%)	59	61

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%)	35	31
1	B	143/143 (100%)	134 (94%)	9 (6%)	25	21
1	C	143/143 (100%)	129 (90%)	14 (10%)	12	7
1	D	143/143 (100%)	134 (94%)	9 (6%)	25	21
1	E	143/143 (100%)	131 (92%)	12 (8%)	16	10
1	F	143/143 (100%)	129 (90%)	14 (10%)	12	7
1	G	143/143 (100%)	133 (93%)	10 (7%)	21	17
1	H	143/143 (100%)	129 (90%)	14 (10%)	12	7
1	I	143/143 (100%)	132 (92%)	11 (8%)	18	13
1	J	144/143 (101%)	138 (96%)	6 (4%)	40	38
1	K	143/143 (100%)	129 (90%)	14 (10%)	12	7
1	L	143/143 (100%)	131 (92%)	12 (8%)	16	10
All	All	1717/1716 (100%)	1585 (92%)	132 (8%)	18	13

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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 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.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/173 (93%)	0.68	2 (1%) 75 80	19, 24, 36, 44	0
1	B	162/173 (93%)	0.62	0 100 100	19, 26, 37, 49	0
1	C	162/173 (93%)	0.93	7 (4%) 34 38	21, 27, 37, 52	0
1	D	162/173 (93%)	0.74	0 100 100	19, 24, 36, 42	0
1	E	162/173 (93%)	0.74	4 (2%) 54 59	20, 25, 36, 43	0
1	F	162/173 (93%)	0.73	5 (3%) 47 52	21, 28, 38, 43	0
1	G	163/173 (94%)	0.63	2 (1%) 75 80	19, 24, 37, 58	0
1	H	162/173 (93%)	0.71	3 (1%) 64 68	21, 27, 38, 46	0
1	I	162/173 (93%)	0.96	7 (4%) 34 38	19, 26, 38, 45	0
1	J	164/173 (94%)	0.81	4 (2%) 56 61	18, 24, 36, 61	0
1	K	162/173 (93%)	0.73	2 (1%) 75 80	18, 24, 35, 44	0
1	L	162/173 (93%)	0.71	1 (0%) 86 90	19, 25, 36, 42	0
All	All	1947/2076 (93%)	0.75	37 (1%) 56 68	18, 25, 37, 61	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	1	MSE	5.8
1	C	3	SER	3.8
1	G	2	ALA	3.1
1	I	145	LEU	3.0
1	I	155	PHE	2.6
1	F	145	LEU	2.6
1	C	144	ARG	2.6
1	H	151	ARG	2.5
1	C	145	LEU	2.5
1	E	146	ILE	2.4
1	I	98	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	111	MSE	2.4
1	F	98	ASN	2.4
1	A	4	ILE	2.3
1	C	150	LYS	2.2
1	F	101	LYS	2.2
1	H	150	LYS	2.2
1	C	140	VAL	2.2
1	I	88	ALA	2.2
1	C	110	ALA	2.2
1	H	65	GLU	2.2
1	G	102	ARG	2.1
1	A	112	GLN	2.1
1	I	136	ALA	2.1
1	J	18	ALA	2.1
1	F	126	VAL	2.1
1	E	160	LEU	2.1
1	F	160	LEU	2.1
1	K	146	ILE	2.1
1	J	112	GLN	2.1
1	L	155	PHE	2.1
1	I	94	GLU	2.0
1	I	162	LEU	2.0
1	C	88	ALA	2.0
1	E	12	LEU	2.0
1	J	36	ILE	2.0
1	E	112	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	K	921	1/1	0.20	4.87	29,29,29,29	1
2	ZN	I	918	1/1	0.22	4.23	46,46,46,46	1
2	ZN	L	924	1/1	0.22	3.69	38,38,38,38	1
2	ZN	F	911	1/1	0.19	2.31	35,35,35,35	1
2	ZN	D	907	1/1	0.20	1.82	28,28,28,28	1
2	ZN	E	910	1/1	0.20	1.39	38,38,38,38	1
2	ZN	J	920	1/1	0.19	1.31	36,36,36,36	1
2	ZN	E	909	1/1	0.20	1.03	33,33,33,33	1
2	ZN	I	917	1/1	0.19	0.86	32,32,32,32	1
2	ZN	L	923	1/1	0.17	0.76	31,31,31,31	1
2	ZN	K	922	1/1	0.17	0.73	34,34,34,34	1
2	ZN	C	906	1/1	0.16	0.64	41,41,41,41	1
2	ZN	C	905	1/1	0.16	0.32	34,34,34,34	1
2	ZN	J	919	1/1	0.17	0.19	30,30,30,30	1
2	ZN	H	915	1/1	0.16	-0.10	34,34,34,34	1
2	ZN	G	914	1/1	0.14	-1.02	35,35,35,35	1
2	ZN	D	908	1/1	0.14	-1.22	37,37,37,37	1
2	ZN	A	901	1/1	0.15	-1.54	26,26,26,26	1
2	ZN	G	913	1/1	0.13	-1.72	28,28,28,28	1
2	ZN	H	916	1/1	0.11	-1.75	43,43,43,43	1
2	ZN	F	912	1/1	0.13	-1.89	50,50,50,50	1
2	ZN	A	902	1/1	0.12	-2.70	38,38,38,38	1
2	ZN	B	903	1/1	0.12	-2.95	29,29,29,29	1
2	ZN	B	904	1/1	0.12	-3.19	43,43,43,43	1

6.5 Other polymers ⓘ

There are no such residues in this entry.