



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:15 PM GMT

PDB ID : 1GQM  
Title : THE STRUCTURE OF S100A12 IN A HEXAMERIC FORM  
Authors : Moroz, O.V.; Antson, A.A.; Dodson, E.G.; Burrell, H.J.; Grist, S.J.; Lloyd, R.M.; Maitland, N.J.; Dodson, G.G.; Wilson, K.S.; Lukanidin, E.; Bronstein, I.B.  
Deposited on : 2001-11-26  
Resolution : 2.70 Å(reported)

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

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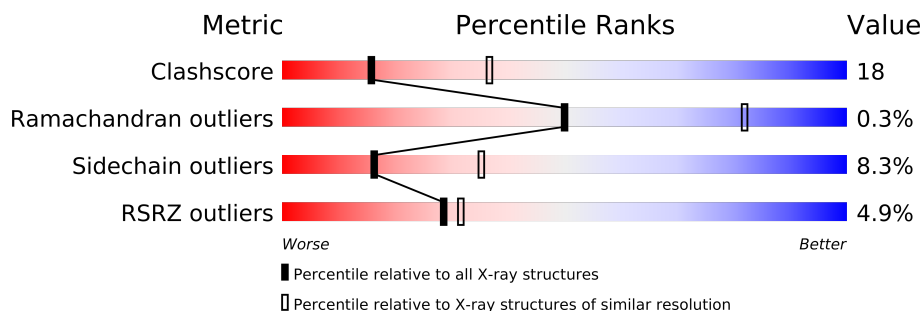
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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  $\geq 3$ , 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	91	
1	B	91	
1	C	91	
1	D	91	
1	E	91	
1	F	91	
1	G	91	
1	H	91	
1	I	91	
1	J	91	
1	K	91	
1	L	91	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8502 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 CALGRANULIN C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	35	0	0
			703	450	119	134			
1	B	88	Total	C	N	O	30	0	0
			710	454	120	136			
1	C	87	Total	C	N	O	48	0	0
			703	450	119	134			
1	D	87	Total	C	N	O	32	0	0
			703	450	119	134			
1	E	87	Total	C	N	O	25	0	0
			703	450	119	134			
1	F	87	Total	C	N	O	32	0	0
			703	450	119	134			
1	G	87	Total	C	N	O	39	0	0
			703	450	119	134			
1	H	88	Total	C	N	O	56	0	0
			710	454	120	136			
1	I	87	Total	C	N	O	40	0	0
			703	450	119	134			
1	J	87	Total	C	N	O	31	0	0
			703	450	119	134			
1	K	87	Total	C	N	O	47	0	0
			703	450	119	134			
1	L	86	Total	C	N	O	104	0	0
			693	444	116	133			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Ca	0	0
			3	3		
2	J	4	Total	Ca	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Ca 2	0	0
2	K	4	Total 4	Ca 4	0	0
2	E	4	Total 4	Ca 4	0	0
2	H	3	Total 3	Ca 3	0	0
2	B	3	Total 3	Ca 3	0	0
2	I	2	Total 2	Ca 2	0	0
2	C	4	Total 4	Ca 4	0	0
2	A	3	Total 3	Ca 3	0	0
2	L	2	Total 2	Ca 2	0	0
2	F	2	Total 2	Ca 2	0	0

- Molecule 3 is water.

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

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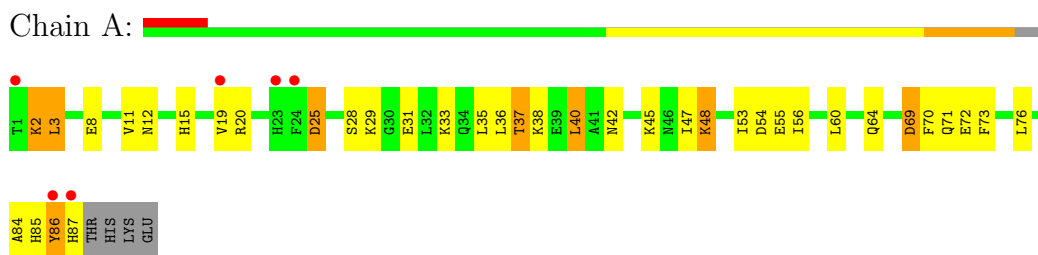
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	O	0	0
			2	2		
3	K	2	Total	O	0	0
			2	2		
3	L	2	Total	O	0	0
			2	2		

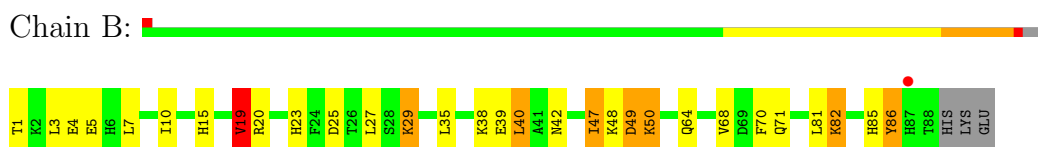
### 3 Residue-property plots

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.

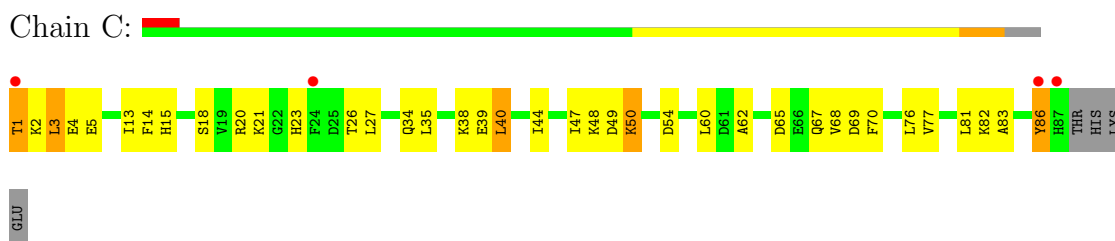
#### • Molecule 1: CALGRANULIN C



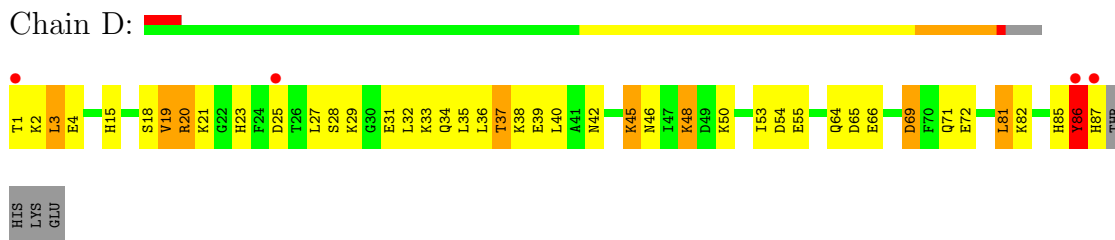
#### • Molecule 1: CALGRANULIN C



#### • Molecule 1: CALGRANULIN C



#### • Molecule 1: CALGRANULIN C



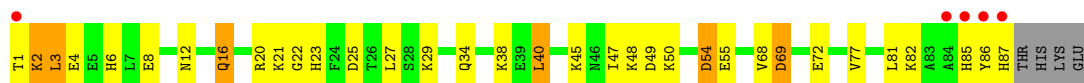
#### • Molecule 1: CALGRANULIN C





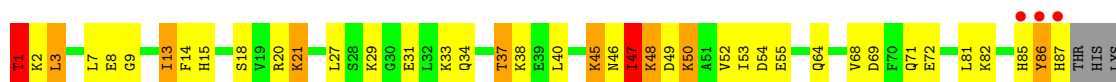
• Molecule 1: CALGRANULIN C

Chain F:



• Molecule 1: CALGRANULIN C

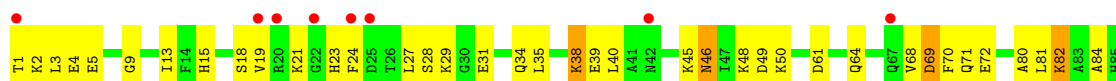
Chain G:



GLU

• Molecule 1: CALGRANULIN C

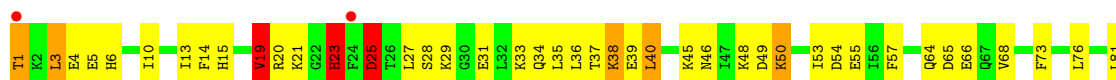
Chain H:



Y86  
H87  
T88  
HIS  
LYS  
GLU

• Molecule 1: CALGRANULIN C

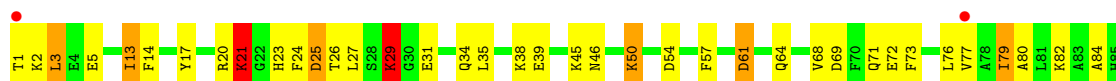
Chain I:



Y86  
H87  
THR  
HIS  
LYS  
GLU

• Molecule 1: CALGRANULIN C

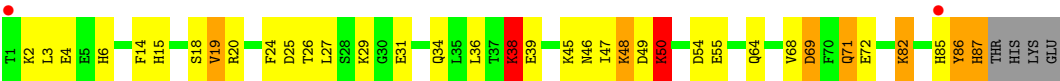
Chain J:



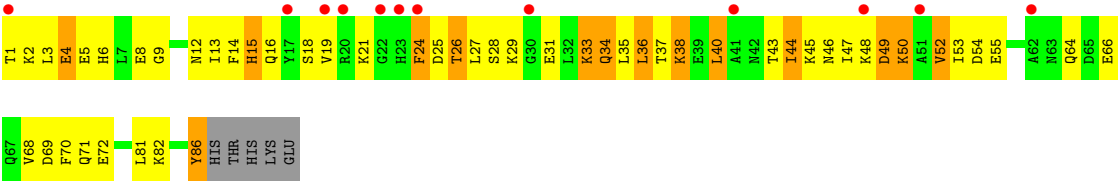
Y86  
H87  
THR  
HIS  
LYS  
GLU

• Molecule 1: CALGRANULIN C

Chain K:



● Molecule 1: CALGRANULIN C





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.88Å 100.50Å 112.69Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	19.84 – 2.70 19.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-2.70) 98.3 (19.83-2.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.217 , 0.281 0.228 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 2.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 32374 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: CA

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	2.60	4/714 (0.6%)	3.10	17/960 (1.8%)
1	B	1.43	4/721 (0.6%)	2.02	11/970 (1.1%)
1	C	2.01	9/714 (1.3%)	1.81	16/960 (1.7%)
1	D	2.04	9/714 (1.3%)	1.28	8/960 (0.8%)
1	E	1.34	4/714 (0.6%)	1.35	14/960 (1.5%)
1	F	1.46	5/714 (0.7%)	1.46	14/960 (1.5%)
1	G	1.84	8/714 (1.1%)	2.07	18/960 (1.9%)
1	H	1.53	9/721 (1.2%)	1.76	15/970 (1.5%)
1	I	1.90	7/714 (1.0%)	2.12	15/960 (1.6%)
1	J	1.35	6/714 (0.8%)	2.40	14/960 (1.5%)
1	K	1.77	11/714 (1.5%)	2.14	17/960 (1.8%)
1	L	2.33	15/703 (2.1%)	2.56	24/945 (2.5%)
All	All	1.84	91/8571 (1.1%)	2.07	183/11525 (1.6%)

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	1
1	C	0	2
1	D	0	1
1	G	0	2
1	I	0	3
1	K	0	2
1	L	0	4
All	All	0	16

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	LYS	CD-CE	56.03	2.91	1.51
1	L	82	LYS	CD-CE	45.06	2.63	1.51
1	D	23	HIS	CB-CG	37.33	2.17	1.50
1	C	50	LYS	CG-CD	33.34	2.65	1.52
1	C	82	LYS	CD-CE	29.00	2.23	1.51
1	A	86	TYR	CB-CG	-26.96	1.11	1.51
1	H	24	PHE	CB-CG	-25.43	1.08	1.51
1	I	29	LYS	CD-CE	25.02	2.13	1.51
1	I	86	TYR	CB-CG	-23.94	1.15	1.51
1	B	82	LYS	CD-CE	-23.33	0.93	1.51
1	G	48	LYS	CB-CG	23.21	2.15	1.52
1	K	48	LYS	CB-CG	22.94	2.14	1.52
1	D	86	TYR	CB-CG	-22.41	1.18	1.51
1	F	21	LYS	CG-CD	-21.31	0.80	1.52
1	A	8	GLU	CB-CG	-20.07	1.14	1.52
1	G	87	HIS	CA-CB	19.36	1.96	1.53
1	G	29	LYS	CD-CE	18.05	1.96	1.51
1	E	50	LYS	CG-CD	17.86	2.13	1.52
1	I	45	LYS	CB-CG	-17.50	1.05	1.52
1	K	86	TYR	CB-CG	-17.17	1.25	1.51
1	K	82	LYS	CD-CE	-16.49	1.10	1.51
1	G	82	LYS	CD-CE	-16.25	1.10	1.51
1	I	21	LYS	CG-CD	-15.29	1.00	1.52
1	L	2	LYS	CG-CD	15.09	2.03	1.52
1	G	21	LYS	CG-CD	-15.03	1.01	1.52
1	E	21	LYS	CG-CD	-15.03	1.01	1.52
1	L	26	THR	CB-OG1	-14.87	1.13	1.43
1	L	33	LYS	C-N	14.71	1.67	1.34
1	B	29	LYS	CD-CE	-14.68	1.14	1.51
1	H	2	LYS	CG-CD	14.09	2.00	1.52
1	K	50	LYS	CG-CD	13.98	2.00	1.52
1	J	21	LYS	CD-CE	-13.77	1.16	1.51
1	K	45	LYS	CB-CG	13.73	1.89	1.52
1	D	21	LYS	CB-CG	-13.50	1.16	1.52
1	J	29	LYS	CD-CE	13.47	1.84	1.51
1	D	50	LYS	CG-CD	-12.65	1.09	1.52
1	F	87	HIS	CA-CB	-12.44	1.26	1.53
1	I	48	LYS	CB-CG	11.80	1.84	1.52
1	I	87	HIS	CB-CG	-11.37	1.29	1.50
1	L	12	ASN	CB-CG	-11.18	1.25	1.51
1	J	86	TYR	CB-CG	-11.07	1.35	1.51
1	F	86	TYR	CA-CB	11.00	1.78	1.53
1	J	2	LYS	CG-CD	10.98	1.89	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	8	GLU	CB-CG	-10.69	1.31	1.52
1	K	38	LYS	CB-CG	10.48	1.80	1.52
1	C	21	LYS	CG-CD	-10.33	1.17	1.52
1	C	38	LYS	CB-CG	-9.98	1.25	1.52
1	L	4	GLU	CG-CD	-9.74	1.37	1.51
1	K	71	GLN	CA-CB	-9.65	1.32	1.53
1	J	38	LYS	CB-CG	-9.25	1.27	1.52
1	L	45	LYS	CB-CG	8.93	1.76	1.52
1	L	15	HIS	C-N	-8.80	1.13	1.34
1	G	86	TYR	CB-CG	8.52	1.64	1.51
1	H	46	ASN	CA-CB	8.26	1.74	1.53
1	D	38	LYS	CB-CG	-8.16	1.30	1.52
1	C	5	GLU	CA-CB	-7.94	1.36	1.53
1	C	54	ASP	CB-CG	7.83	1.68	1.51
1	L	36	LEU	C-N	7.83	1.52	1.34
1	G	50	LYS	CG-CD	7.75	1.78	1.52
1	H	87	HIS	CB-CG	-7.71	1.36	1.50
1	L	5	GLU	CA-CB	7.55	1.70	1.53
1	C	23	HIS	CB-CG	7.55	1.63	1.50
1	H	38	LYS	CB-CG	-7.52	1.32	1.52
1	K	29	LYS	CD-CE	-7.12	1.33	1.51
1	F	50	LYS	CG-CD	-6.66	1.29	1.52
1	D	21	LYS	CG-CD	-6.61	1.29	1.52
1	C	1	THR	CA-C	-6.44	1.36	1.52
1	G	1	THR	N-CA	-6.39	1.33	1.46
1	H	21	LYS	CB-CG	-6.39	1.35	1.52
1	K	87	HIS	CG-ND1	6.29	1.52	1.38
1	H	50	LYS	CG-CD	-6.25	1.31	1.52
1	D	82	LYS	CD-CE	6.24	1.66	1.51
1	I	54	ASP	CB-CG	6.22	1.64	1.51
1	B	38	LYS	CB-CG	-6.05	1.36	1.52
1	B	50	LYS	CG-CD	-6.05	1.31	1.52
1	H	82	LYS	CD-CE	-6.03	1.36	1.51
1	L	16	GLN	C-N	-5.95	1.20	1.34
1	C	48	LYS	CB-CG	-5.86	1.36	1.52
1	E	33	LYS	CD-CE	-5.75	1.36	1.51
1	E	2	LYS	CG-CD	5.60	1.71	1.52
1	F	45	LYS	CB-CG	5.55	1.67	1.52
1	K	54	ASP	CB-CG	5.55	1.63	1.51
1	D	2	LYS	CG-CD	5.48	1.71	1.52
1	L	66	GLU	CB-CG	5.35	1.62	1.52
1	L	34	GLN	C-N	-5.34	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	24	PHE	C-N	5.25	1.46	1.34
1	K	87	HIS	CG-CD2	5.18	1.44	1.35
1	H	34	GLN	CA-CB	5.14	1.65	1.53
1	J	82	LYS	CD-CE	-5.11	1.38	1.51
1	A	2	LYS	CG-CD	5.06	1.69	1.52
1	D	48	LYS	CB-CG	5.05	1.66	1.52

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	TYR	CB-CG-CD1	-58.08	86.16	121.00
1	A	86	TYR	CB-CG-CD2	49.79	150.87	121.00
1	J	86	TYR	CB-CG-CD1	-42.50	95.50	121.00
1	J	86	TYR	CB-CG-CD2	39.65	144.79	121.00
1	L	86	TYR	CB-CG-CD1	-37.30	98.62	121.00
1	B	86	TYR	CB-CG-CD1	-35.91	99.45	121.00
1	I	86	TYR	CB-CG-CD1	-35.73	99.56	121.00
1	L	86	TYR	CB-CG-CD2	31.91	140.15	121.00
1	B	86	TYR	CB-CG-CD2	30.71	139.43	121.00
1	K	86	TYR	CB-CG-CD1	-30.30	102.82	121.00
1	L	34	GLN	O-C-N	-24.68	83.22	122.70
1	G	87	HIS	CB-CA-C	-24.35	61.70	110.40
1	H	24	PHE	CB-CG-CD1	-24.32	103.78	120.80
1	C	86	TYR	CB-CG-CD1	-24.12	106.53	121.00
1	K	38	LYS	CA-CB-CG	23.75	165.66	113.40
1	G	86	TYR	CB-CG-CD1	-23.72	106.77	121.00
1	A	54	ASP	CB-CG-OD1	23.22	139.20	118.30
1	I	87	HIS	CB-CG-ND1	-22.95	65.82	123.20
1	I	86	TYR	CB-CG-CD2	21.94	134.16	121.00
1	K	38	LYS	CB-CG-CD	21.68	167.98	111.60
1	H	24	PHE	CB-CG-CD2	20.37	135.06	120.80
1	J	86	TYR	CA-CB-CG	20.02	151.43	113.40
1	L	4	GLU	CG-CD-OE2	18.65	155.60	118.30
1	L	4	GLU	CG-CD-OE1	-18.40	81.50	118.30
1	K	86	TYR	CB-CG-CD2	18.16	131.89	121.00
1	K	45	LYS	CA-CB-CG	-17.66	74.55	113.40
1	G	38	LYS	CA-CB-CG	17.38	151.64	113.40
1	A	29	LYS	CG-CD-CE	-17.32	59.95	111.90
1	A	8	GLU	CA-CB-CG	17.28	151.42	113.40
1	C	86	TYR	CB-CG-CD2	17.26	131.36	121.00
1	H	38	LYS	CA-CB-CG	16.91	150.59	113.40
1	A	38	LYS	CA-CB-CG	16.52	149.74	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LYS	CA-CB-CG	16.41	149.49	113.40
1	J	38	LYS	CA-CB-CG	15.90	148.38	113.40
1	D	50	LYS	CB-CG-CD	15.19	151.10	111.60
1	K	45	LYS	CB-CG-CD	-15.10	72.34	111.60
1	C	50	LYS	CB-CG-CD	-14.99	72.63	111.60
1	G	86	TYR	CA-CB-CG	-14.79	85.29	113.40
1	C	21	LYS	CB-CG-CD	14.69	149.78	111.60
1	D	86	TYR	CB-CG-CD2	-14.60	112.24	121.00
1	G	82	LYS	CG-CD-CE	14.54	155.53	111.90
1	L	34	GLN	CA-C-N	14.28	148.60	117.20
1	F	48	LYS	CA-CB-CG	14.27	144.79	113.40
1	H	87	HIS	CB-CA-C	-14.22	81.95	110.40
1	G	86	TYR	CB-CG-CD2	-14.10	112.54	121.00
1	L	34	GLN	C-N-CA	13.97	156.62	121.70
1	B	82	LYS	CG-CD-CE	13.92	153.67	111.90
1	I	87	HIS	CA-CB-CG	13.52	136.58	113.60
1	K	50	LYS	CG-CD-CE	13.30	151.79	111.90
1	G	82	LYS	CD-CE-NZ	13.11	141.85	111.70
1	F	50	LYS	CB-CG-CD	12.71	144.63	111.60
1	A	54	ASP	CB-CG-OD2	-12.60	106.96	118.30
1	I	23	HIS	CA-CB-CG	12.07	134.12	113.60
1	I	21	LYS	CB-CG-CD	11.90	142.54	111.60
1	G	29	LYS	CG-CD-CE	-11.71	76.77	111.90
1	L	26	THR	CA-CB-OG1	11.71	133.59	109.00
1	C	38	LYS	CA-CB-CG	11.68	139.10	113.40
1	L	37	THR	O-C-N	-11.50	104.31	122.70
1	J	50	LYS	CG-CD-CE	11.13	145.28	111.90
1	G	87	HIS	CA-CB-CG	-11.06	94.79	113.60
1	A	48	LYS	CB-CG-CD	11.01	140.24	111.60
1	E	29	LYS	CG-CD-CE	-10.96	79.01	111.90
1	E	21	LYS	CB-CG-CD	10.89	139.91	111.60
1	H	45	LYS	CA-CB-CG	10.59	136.69	113.40
1	A	45	LYS	CA-CB-CG	-10.46	90.39	113.40
1	G	45	LYS	CA-CB-CG	-10.46	90.39	113.40
1	F	87	HIS	N-CA-CB	-10.19	92.27	110.60
1	B	48	LYS	CA-CB-CG	10.15	135.73	113.40
1	C	50	LYS	CG-CD-CE	10.05	142.06	111.90
1	G	45	LYS	CB-CG-CD	-9.96	85.71	111.60
1	J	21	LYS	CG-CD-CE	9.95	141.73	111.90
1	I	87	HIS	CB-CG-CD2	9.92	161.55	130.80
1	H	38	LYS	CB-CG-CD	9.82	137.13	111.60
1	F	48	LYS	CB-CG-CD	9.78	137.03	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	LYS	CB-CG-CD	9.78	137.02	111.60
1	K	48	LYS	CA-CB-CG	-9.76	91.94	113.40
1	L	82	LYS	CG-CD-CE	-9.64	82.98	111.90
1	G	87	HIS	N-CA-CB	9.59	127.86	110.60
1	A	45	LYS	CB-CG-CD	-9.54	86.81	111.60
1	B	49	ASP	CB-CG-OD2	9.53	126.87	118.30
1	K	50	LYS	CB-CG-CD	9.46	136.19	111.60
1	C	82	LYS	CG-CD-CE	-9.43	83.60	111.90
1	L	45	LYS	CA-CB-CG	-9.39	92.75	113.40
1	B	82	LYS	CD-CE-NZ	9.31	133.11	111.70
1	G	38	LYS	CB-CG-CD	9.23	135.60	111.60
1	D	50	LYS	CG-CD-CE	9.22	139.58	111.90
1	L	86	TYR	CA-CB-CG	9.21	130.91	113.40
1	K	29	LYS	CG-CD-CE	-9.21	84.27	111.90
1	I	29	LYS	CG-CD-CE	-9.20	84.30	111.90
1	H	24	PHE	CA-CB-CG	9.11	135.76	113.90
1	G	29	LYS	CD-CE-NZ	-9.10	90.76	111.70
1	C	48	LYS	CA-CB-CG	9.06	133.33	113.40
1	L	33	LYS	O-C-N	8.93	136.98	122.70
1	I	50	LYS	CB-CG-CD	-8.86	88.55	111.60
1	C	48	LYS	CB-CG-CD	8.85	134.62	111.60
1	B	48	LYS	CB-CG-CD	8.78	134.43	111.60
1	J	38	LYS	CB-CG-CD	8.78	134.43	111.60
1	H	46	ASN	N-CA-CB	-8.76	94.84	110.60
1	C	23	HIS	CA-CB-CG	8.71	128.41	113.60
1	L	33	LYS	CA-C-N	-8.70	98.06	117.20
1	L	36	LEU	O-C-N	8.64	136.52	122.70
1	D	38	LYS	CA-CB-CG	8.63	132.38	113.40
1	C	65	ASP	CB-CG-OD2	8.47	125.93	118.30
1	F	38	LYS	CA-CB-CG	8.43	131.95	113.40
1	F	86	TYR	CB-CA-C	8.38	127.15	110.40
1	K	29	LYS	CD-CE-NZ	-8.36	92.46	111.70
1	G	48	LYS	CA-CB-CG	-8.35	95.03	113.40
1	H	49	ASP	CB-CG-OD2	8.31	125.78	118.30
1	A	86	TYR	CA-CB-CG	8.03	128.66	113.40
1	E	29	LYS	CD-CE-NZ	-7.96	93.40	111.70
1	L	24	PHE	C-N-CA	7.93	141.53	121.70
1	I	38	LYS	CA-CB-CG	7.86	130.69	113.40
1	L	4	GLU	CB-CG-CD	7.84	135.37	114.20
1	H	21	LYS	CG-CD-CE	7.83	135.38	111.90
1	F	49	ASP	CB-CG-OD2	7.68	125.21	118.30
1	I	23	HIS	CB-CG-ND1	-7.62	104.15	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	50	LYS	CB-CG-CD	7.58	131.31	111.60
1	L	37	THR	CA-C-N	7.52	133.74	117.20
1	E	54	ASP	CB-CG-OD2	7.42	124.98	118.30
1	E	38	LYS	CA-CB-CG	7.37	129.61	113.40
1	K	19	VAL	CB-CA-C	-7.36	97.43	111.40
1	C	1	THR	CA-C-O	-7.32	104.74	120.10
1	I	19	VAL	CB-CA-C	-7.23	97.66	111.40
1	A	29	LYS	CD-CE-NZ	-7.22	95.10	111.70
1	E	48	LYS	CB-CG-CD	7.16	130.21	111.60
1	E	19	VAL	CB-CA-C	-7.15	97.81	111.40
1	J	54	ASP	CB-CG-OD2	7.12	124.71	118.30
1	J	29	LYS	CG-CD-CE	-7.08	90.66	111.90
1	B	19	VAL	CB-CA-C	-7.02	98.07	111.40
1	C	21	LYS	CG-CD-CE	7.01	132.93	111.90
1	E	50	LYS	CB-CG-CD	-6.89	93.68	111.60
1	J	61	ASP	CB-CG-OD2	6.88	124.49	118.30
1	F	45	LYS	CA-CB-CG	-6.86	98.31	113.40
1	K	69	ASP	CB-CG-OD2	6.84	124.46	118.30
1	I	25	ASP	CB-CG-OD2	6.83	124.45	118.30
1	L	69	ASP	CB-CG-OD2	6.82	124.44	118.30
1	J	29	LYS	CD-CE-NZ	-6.72	96.23	111.70
1	B	50	LYS	CB-CG-CD	6.72	129.06	111.60
1	L	36	LEU	CA-C-N	-6.67	102.53	117.20
1	L	45	LYS	CB-CG-CD	-6.51	94.68	111.60
1	F	50	LYS	CG-CD-CE	6.36	130.97	111.90
1	G	54	ASP	CB-CG-OD2	6.29	123.96	118.30
1	I	48	LYS	CA-CB-CG	6.29	127.23	113.40
1	E	45	LYS	CB-CG-CD	-6.21	95.46	111.60
1	F	69	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	38	LYS	CB-CG-CD	6.17	127.65	111.60
1	C	49	ASP	CB-CG-OD2	6.14	123.82	118.30
1	G	1	THR	N-CA-CB	-6.13	98.66	110.30
1	D	69	ASP	CB-CG-OD2	6.12	123.81	118.30
1	F	21	LYS	CB-CG-CD	6.12	127.51	111.60
1	E	49	ASP	CB-CG-OD2	6.11	123.80	118.30
1	H	21	LYS	CB-CG-CD	-6.09	95.76	111.60
1	I	48	LYS	CB-CG-CD	6.05	127.34	111.60
1	L	12	ASN	CA-CB-CG	6.05	126.71	113.40
1	E	21	LYS	CG-CD-CE	5.87	129.51	111.90
1	E	33	LYS	CD-CE-NZ	5.76	124.95	111.70
1	D	54	ASP	CB-CG-OD2	5.74	123.46	118.30
1	K	87	HIS	ND1-CG-CD2	-5.74	97.97	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	61	ASP	CB-CG-OD2	5.72	123.45	118.30
1	H	23	HIS	CA-CB-CG	5.67	123.24	113.60
1	F	86	TYR	N-CA-CB	-5.63	100.46	110.60
1	K	71	GLN	N-CA-CB	5.62	120.72	110.60
1	C	86	TYR	CA-CB-CG	5.59	124.03	113.40
1	F	25	ASP	CB-CG-OD1	5.58	123.33	118.30
1	L	49	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	69	ASP	CB-CG-OD2	5.49	123.24	118.30
1	K	86	TYR	CA-CB-CG	5.48	123.81	113.40
1	J	50	LYS	CB-CG-CD	5.47	125.83	111.60
1	E	45	LYS	CA-CB-CG	-5.47	101.37	113.40
1	D	21	LYS	CB-CG-CD	5.46	125.79	111.60
1	B	29	LYS	CD-CE-NZ	-5.45	99.16	111.70
1	B	38	LYS	CA-CB-CG	5.44	125.36	113.40
1	J	25	ASP	CB-CG-OD2	5.38	123.14	118.30
1	H	50	LYS	CG-CD-CE	5.37	128.02	111.90
1	K	49	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	54	ASP	OD1-CG-OD2	-5.30	113.22	123.30
1	J	45	LYS	CA-CB-CG	-5.29	101.77	113.40
1	A	25	ASP	CB-CG-OD2	5.24	123.02	118.30
1	H	69	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	21	LYS	CG-CD-CE	5.11	127.22	111.90
1	L	36	LEU	C-N-CA	-5.07	109.03	121.70
1	G	50	LYS	CG-CD-CE	5.06	127.07	111.90
1	F	45	LYS	CB-CG-CD	-5.04	98.50	111.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	TYR	Sidechain
1	B	86	TYR	Sidechain
1	C	1	THR	Mainchain
1	C	86	TYR	Sidechain
1	D	86	TYR	Sidechain
1	G	1	THR	Mainchain
1	G	86	TYR	Sidechain
1	I	23	HIS	Sidechain
1	I	86	TYR	Sidechain
1	I	87	HIS	Sidechain
1	K	86	TYR	Sidechain
1	K	87	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	L	24	PHE	Mainchain
1	L	34	GLN	Mainchain
1	L	38	LYS	Peptide
1	L	86	TYR	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	703	0	707	29	2
1	B	710	0	712	24	2
1	C	703	0	705	24	0
1	D	703	0	707	37	0
1	E	703	0	706	23	1
1	F	703	0	707	24	2
1	G	703	0	706	35	0
1	H	710	0	712	28	1
1	I	703	0	707	34	0
1	J	703	0	705	33	0
1	K	703	0	705	31	3
1	L	693	0	695	37	3
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	2	0	0	0	0
2	E	4	0	0	0	0
2	F	2	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	2	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	2	0	0	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	2	0	0	1	0
3	G	4	0	0	2	0
3	H	1	0	0	2	0
3	I	1	0	0	1	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
All	All	8502	0	8474	289	7

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 18.

All (289) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:8:GLU:HG2	3:F:2001:HOH:O	1.06	1.24
1:C:20:ARG:NH1	1:C:34:GLN:OE1	1.81	1.12
1:I:3:LEU:HD23	1:J:13:ILE:HG21	1.39	1.01
1:A:36:LEU:HB3	1:A:47:ILE:HD11	1.38	1.01
1:K:20:ARG:NH1	1:K:34:GLN:OE1	1.96	0.97
1:I:33:LYS:HG3	1:I:53:ILE:HD13	1.40	0.97
1:I:33:LYS:HG3	1:I:53:ILE:CD1	1.98	0.94
1:B:1:THR:HG23	1:B:4:GLU:OE1	1.69	0.92
1:J:23:HIS:CD2	1:J:25:ASP:H	1.87	0.92
1:E:46:ASN:HB3	1:E:49:ASP:OD2	1.68	0.92
1:E:40:LEU:HD21	1:F:3:LEU:HD13	1.52	0.91
1:G:20:ARG:NH1	1:G:34:GLN:OE1	2.04	0.90
1:K:82:LYS:HG3	1:L:71:GLN:HE22	1.36	0.90
1:A:55:GLU:OE2	1:E:64:GLN:NE2	2.03	0.90
1:A:33:LYS:O	1:A:37:THR:HG23	1.74	0.87
1:K:2:LYS:HB3	1:L:13:ILE:HD11	1.57	0.86
1:J:23:HIS:CD2	1:J:25:ASP:N	2.43	0.85
1:B:23:HIS:CD2	1:B:25:ASP:H	1.97	0.83
1:G:33:LYS:HG3	1:G:53:ILE:HD13	1.60	0.83
1:F:2:LYS:HE2	1:F:6:HIS:NE2	1.93	0.83
1:C:70:PHE:HZ	1:D:81:LEU:HD22	1.41	0.83
1:I:33:LYS:O	1:I:37:THR:HG23	1.78	0.83
1:B:20:ARG:HG2	1:B:20:ARG:HH11	1.45	0.82
1:G:64:GLN:NE2	1:I:55:GLU:OE1	2.06	0.81
1:A:3:LEU:HD13	1:B:40:LEU:HD11	1.64	0.80
1:D:69:ASP:OD1	1:D:72:GLU:HG3	1.81	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:9:GLY:O	1:H:13:ILE:HD12	1.81	0.79
1:A:47:ILE:O	1:A:47:ILE:HG12	1.79	0.79
1:L:28:SER:OG	1:L:31:GLU:HG3	1.82	0.78
1:G:81:LEU:HD22	1:H:70:PHE:HZ	1.49	0.78
1:A:64:GLN:NE2	1:D:55:GLU:OE2	2.11	0.78
1:J:69:ASP:OD1	1:J:72:GLU:HG3	1.84	0.77
1:I:35:LEU:C	1:I:35:LEU:HD23	2.05	0.77
1:B:1:THR:O	1:B:5:GLU:HG3	1.87	0.75
1:I:1:THR:HG23	1:I:4:GLU:OE1	1.87	0.74
1:I:28:SER:OG	1:I:31:GLU:HG3	1.89	0.73
1:A:69:ASP:OD1	1:A:72:GLU:HG3	1.89	0.72
1:K:6:HIS:NE2	1:L:9:GLY:HA3	2.04	0.72
1:G:8:GLU:HG3	3:G:2001:HOH:O	1.89	0.72
1:H:84:ALA:O	1:H:88:THR:HG23	1.89	0.72
1:D:64:GLN:HE22	1:E:55:GLU:CD	1.94	0.71
1:K:82:LYS:CG	1:L:71:GLN:HE22	2.04	0.71
1:H:28:SER:N	1:H:31:GLU:OE1	2.23	0.71
1:D:25:ASP:OD1	1:D:25:ASP:O	2.08	0.71
1:C:70:PHE:CZ	1:D:81:LEU:HD22	2.24	0.70
1:C:3:LEU:HD13	1:D:40:LEU:HD21	1.75	0.69
1:L:40:LEU:HD23	1:L:44:ILE:HD11	1.75	0.69
1:K:69:ASP:OD1	1:K:72:GLU:HG3	1.94	0.68
1:G:33:LYS:O	1:G:37:THR:OG1	2.12	0.68
1:G:45:LYS:O	1:G:46:ASN:HB2	1.92	0.67
1:J:23:HIS:NE2	1:J:25:ASP:N	2.42	0.67
1:I:15:HIS:O	1:I:19:VAL:HG22	1.95	0.67
1:J:23:HIS:HD2	1:J:26:THR:H	1.44	0.66
1:F:54:ASP:OD1	1:F:54:ASP:C	2.34	0.66
1:C:15:HIS:HA	1:C:18:SER:OG	1.95	0.66
1:I:20:ARG:NH1	1:I:34:GLN:OE1	2.30	0.65
1:E:3:LEU:HD23	1:F:40:LEU:HD13	1.78	0.64
1:E:46:ASN:O	1:E:48:LYS:N	2.30	0.64
1:E:15:HIS:O	1:E:19:VAL:HG22	1.97	0.64
1:D:33:LYS:O	1:D:37:THR:OG1	2.14	0.64
1:A:55:GLU:CD	1:E:64:GLN:HE22	2.00	0.64
1:D:15:HIS:O	1:D:19:VAL:HG22	1.98	0.64
1:H:15:HIS:HA	1:H:18:SER:OG	1.98	0.64
1:H:1:THR:O	1:H:5:GLU:HG3	1.98	0.63
1:A:82:LYS:HD3	1:B:71:GLN:OE1	1.98	0.63
1:I:33:LYS:CG	1:I:53:ILE:HD13	2.23	0.63
1:A:15:HIS:O	1:A:19:VAL:HG13	1.99	0.63
1:C:4:GLU:HG3	1:D:39:GLU:O	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:46:ASN:C	1:E:48:LYS:H	2.01	0.62
1:L:36:LEU:HD22	1:L:47:ILE:HD11	1.79	0.62
1:A:84:ALA:O	1:A:87:HIS:CD2	2.53	0.61
1:A:3:LEU:HD13	1:B:40:LEU:CD1	2.31	0.60
1:D:1:THR:HG23	1:D:4:GLU:OE1	2.01	0.60
1:G:71:GLN:HE22	1:H:82:LYS:HG3	1.66	0.60
1:D:28:SER:OG	1:D:31:GLU:HG3	2.02	0.60
1:L:52:VAL:HG12	1:L:53:ILE:N	2.15	0.60
1:L:47:ILE:HA	1:L:52:VAL:HG11	1.84	0.59
1:G:81:LEU:HD22	1:H:70:PHE:CZ	2.34	0.59
1:G:46:ASN:O	1:G:48:LYS:N	2.36	0.59
1:K:39:GLU:HA	1:L:1:THR:HG21	1.83	0.59
1:G:71:GLN:HG2	3:I:2001:HOH:O	2.03	0.59
1:J:84:ALA:HA	1:J:87:HIS:CD2	2.37	0.59
1:K:36:LEU:HD22	1:K:47:ILE:HD11	1.85	0.58
1:E:28:SER:OG	1:E:31:GLU:HG3	2.03	0.58
1:H:27:LEU:HA	1:H:31:GLU:OE1	2.04	0.58
1:H:35:LEU:C	1:H:35:LEU:HD23	2.24	0.58
1:K:82:LYS:HG3	1:L:71:GLN:NE2	2.13	0.57
1:D:65:ASP:O	1:D:66:GLU:HB2	2.04	0.57
1:C:40:LEU:HD11	1:D:3:LEU:HD12	1.85	0.57
1:C:39:GLU:O	1:C:40:LEU:HD12	2.03	0.57
1:E:46:ASN:C	1:E:48:LYS:N	2.55	0.57
1:L:14:PHE:HE1	1:L:27:LEU:HG	1.70	0.57
1:G:46:ASN:C	1:G:48:LYS:N	2.58	0.56
1:G:15:HIS:HE1	3:H:2001:HOH:O	1.88	0.56
1:C:70:PHE:HZ	1:D:81:LEU:CD2	2.13	0.56
1:D:15:HIS:HA	1:D:18:SER:OG	2.06	0.56
1:D:32:LEU:HG	1:D:36:LEU:CD1	2.36	0.56
1:B:1:THR:OG1	1:B:4:GLU:HB2	2.06	0.56
1:K:2:LYS:CB	1:L:13:ILE:HD11	2.34	0.56
1:G:71:GLN:NE2	1:J:71:GLN:HE22	2.04	0.55
1:G:55:GLU:CD	1:K:64:GLN:HE22	2.10	0.55
1:L:27:LEU:HA	1:L:31:GLU:OE1	2.06	0.55
1:C:4:GLU:OE1	1:D:42:ASN:ND2	2.32	0.55
1:J:23:HIS:HD2	1:J:26:THR:N	2.05	0.55
1:I:38:LYS:O	1:J:1:THR:HG21	2.06	0.55
1:J:1:THR:O	1:J:5:GLU:HG3	2.07	0.55
1:D:25:ASP:CG	1:D:25:ASP:O	2.45	0.55
1:D:45:LYS:CD	1:D:45:LYS:H	2.18	0.55
1:G:7:LEU:CD1	1:H:80:ALA:HB1	2.37	0.54
1:K:15:HIS:HA	1:K:18:SER:OG	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:73:PHE:CE2	1:I:76:LEU:HD23	2.43	0.54
1:G:15:HIS:CE1	3:H:2001:HOH:O	2.61	0.54
1:F:1:THR:HG23	1:F:4:GLU:OE1	2.07	0.54
1:C:3:LEU:HB2	1:D:39:GLU:HB3	1.89	0.54
1:J:23:HIS:CD2	1:J:26:THR:N	2.76	0.54
1:B:20:ARG:NH1	1:B:20:ARG:HG2	2.17	0.54
1:H:64:GLN:HA	1:H:64:GLN:OE1	2.07	0.54
1:F:54:ASP:OD1	1:F:54:ASP:O	2.27	0.53
1:J:20:ARG:C	1:J:21:LYS:HG2	2.27	0.53
1:J:23:HIS:CD2	1:J:23:HIS:C	2.81	0.53
1:J:68:VAL:HA	1:J:72:GLU:OE1	2.09	0.53
1:E:40:LEU:HD21	1:F:3:LEU:CD1	2.32	0.53
1:L:18:SER:HA	1:L:27:LEU:HD23	1.91	0.53
1:C:69:ASP:OD1	1:C:69:ASP:C	2.47	0.52
1:G:69:ASP:C	1:G:69:ASP:OD1	2.48	0.52
1:A:70:PHE:CE2	1:B:85:HIS:HB2	2.44	0.52
1:G:46:ASN:C	1:G:48:LYS:H	2.13	0.52
1:H:35:LEU:O	1:H:39:GLU:HB2	2.09	0.52
1:I:3:LEU:HB2	1:J:39:GLU:HB3	1.92	0.51
1:A:73:PHE:CE2	1:A:76:LEU:HD23	2.44	0.51
1:H:46:ASN:O	1:H:48:LYS:N	2.44	0.51
1:H:69:ASP:N	1:H:72:GLU:OE1	2.39	0.51
1:C:44:ILE:HB	1:C:47:ILE:HD13	1.93	0.51
1:G:85:HIS:HB2	1:H:70:PHE:CE2	2.45	0.51
1:E:70:PHE:CE2	1:F:85:HIS:HB3	2.46	0.51
1:K:3:LEU:HD23	1:L:40:LEU:HD13	1.92	0.51
1:B:49:ASP:N	1:B:49:ASP:OD1	2.42	0.51
1:K:4:GLU:OE2	1:L:43:THR:OG1	2.29	0.51
1:A:81:LEU:O	1:A:82:LYS:C	2.47	0.50
1:D:45:LYS:CD	1:D:45:LYS:N	2.75	0.50
1:J:79:ILE:HG22	1:J:80:ALA:N	2.27	0.50
1:B:1:THR:CG2	1:B:4:GLU:OE1	2.53	0.50
1:K:27:LEU:HA	1:K:31:GLU:OE1	2.12	0.50
1:J:31:GLU:HA	1:J:34:GLN:HE21	1.75	0.50
1:K:6:HIS:CD2	1:L:9:GLY:HA3	2.47	0.50
1:K:19:VAL:HG12	1:K:24:PHE:HB3	1.93	0.50
1:I:46:ASN:HB3	1:I:49:ASP:OD2	2.11	0.50
1:J:17:TYR:OH	1:J:39:GLU:OE2	2.28	0.50
1:L:44:ILE:HB	1:L:47:ILE:HD13	1.94	0.50
1:H:46:ASN:C	1:H:48:LYS:N	2.64	0.50
1:G:68:VAL:HA	1:G:72:GLU:OE1	2.11	0.49
1:I:3:LEU:HD23	1:J:13:ILE:CG2	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:1:THR:O	1:I:5:GLU:HG3	2.12	0.49
1:G:20:ARG:O	1:G:21:LYS:HG2	2.12	0.49
1:H:69:ASP:OD1	1:H:72:GLU:HG3	2.12	0.49
1:C:35:LEU:C	1:C:35:LEU:HD23	2.33	0.49
1:H:68:VAL:HA	1:H:72:GLU:OE1	2.12	0.49
1:A:35:LEU:C	1:A:35:LEU:HD23	2.32	0.49
1:H:64:GLN:HE22	1:L:55:GLU:CD	2.16	0.49
1:I:3:LEU:CD2	1:J:13:ILE:HG21	2.27	0.48
1:I:33:LYS:HG3	1:I:53:ILE:HD11	1.89	0.48
1:D:45:LYS:HD3	1:D:45:LYS:N	2.28	0.48
1:G:7:LEU:HD11	1:H:80:ALA:HB1	1.95	0.48
1:J:14:PHE:CE1	1:J:27:LEU:HG	2.48	0.48
1:L:15:HIS:HA	1:L:18:SER:OG	2.12	0.48
1:F:29:LYS:NZ	1:F:54:ASP:HB2	2.29	0.48
1:H:46:ASN:C	1:H:48:LYS:H	2.17	0.48
1:F:81:LEU:O	1:F:82:LYS:C	2.49	0.48
1:G:15:HIS:HA	1:G:18:SER:OG	2.13	0.48
1:E:35:LEU:C	1:E:35:LEU:HD23	2.34	0.48
1:G:49:ASP:HB2	1:G:52:VAL:HG23	1.95	0.48
1:D:35:LEU:C	1:D:35:LEU:HD23	2.34	0.48
1:E:70:PHE:CE2	1:F:85:HIS:CB	2.97	0.48
1:C:70:PHE:CE2	1:D:85:HIS:HB2	2.47	0.48
1:A:40:LEU:HD13	1:B:3:LEU:HD23	1.95	0.48
1:A:42:ASN:N	1:B:4:GLU:OE2	2.40	0.48
1:K:82:LYS:CD	1:L:71:GLN:HE22	2.27	0.48
1:I:25:ASP:OD1	1:I:25:ASP:N	2.28	0.47
1:H:15:HIS:O	1:H:19:VAL:HG13	2.14	0.47
1:D:46:ASN:C	1:D:48:LYS:N	2.67	0.47
1:A:81:LEU:HA	1:A:81:LEU:HD23	1.56	0.47
1:C:27:LEU:HB2	1:C:68:VAL:HB	1.97	0.47
1:A:3:LEU:HB2	1:B:39:GLU:HB3	1.96	0.47
1:H:1:THR:HG23	1:H:4:GLU:OE1	2.15	0.47
1:I:14:PHE:CD2	1:I:15:HIS:CD2	3.03	0.46
1:I:35:LEU:CD2	1:I:35:LEU:C	2.79	0.46
1:G:14:PHE:HD2	1:G:15:HIS:CD2	2.34	0.46
1:L:46:ASN:C	1:L:48:LYS:N	2.69	0.46
1:C:60:LEU:O	1:C:62:ALA:N	2.47	0.46
1:I:39:GLU:HB3	1:J:3:LEU:HB2	1.97	0.46
1:B:64:GLN:NE2	1:F:55:GLU:OE2	2.32	0.46
1:K:14:PHE:CE1	1:K:27:LEU:HD12	2.51	0.46
1:K:6:HIS:ND1	1:L:6:HIS:HA	2.31	0.46
1:K:14:PHE:HD2	1:K:15:HIS:CD2	2.34	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:64:GLN:HE22	1:K:55:GLU:CD	2.20	0.45
1:G:46:ASN:O	1:G:47:ILE:C	2.53	0.45
1:H:84:ALA:O	1:H:88:THR:CG2	2.62	0.45
1:K:14:PHE:CD2	1:K:15:HIS:CD2	3.05	0.45
1:L:19:VAL:HG22	1:L:19:VAL:O	2.16	0.45
1:F:69:ASP:OD1	1:F:72:GLU:HG3	2.17	0.45
1:E:40:LEU:CD2	1:F:3:LEU:HD13	2.36	0.45
1:B:23:HIS:CD2	1:B:25:ASP:N	2.76	0.45
1:G:69:ASP:OD1	1:G:72:GLU:HG3	2.15	0.45
1:D:28:SER:O	1:D:29:LYS:C	2.55	0.45
1:H:61:ASP:HA	1:H:72:GLU:OE2	2.17	0.45
1:F:22:GLY:O	1:F:23:HIS:C	2.53	0.45
1:K:25:ASP:C	1:K:26:THR:CG2	2.86	0.44
1:K:46:ASN:C	1:K:48:LYS:N	2.69	0.44
1:C:70:PHE:CE2	1:D:85:HIS:CB	3.00	0.44
1:C:76:LEU:O	1:C:77:VAL:C	2.53	0.44
1:E:39:GLU:HB3	1:F:3:LEU:HB2	1.98	0.44
1:J:73:PHE:CE2	1:J:76:LEU:HD23	2.53	0.44
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.77	0.44
1:A:11:VAL:O	1:A:12:ASN:C	2.53	0.44
1:I:81:LEU:HD11	1:J:77:VAL:HG11	1.99	0.44
1:D:46:ASN:C	1:D:48:LYS:H	2.21	0.44
1:F:68:VAL:HA	1:F:72:GLU:OE1	2.18	0.44
1:I:6:HIS:O	1:I:10:ILE:HG13	2.18	0.44
1:K:85:HIS:CB	1:L:70:PHE:CE2	3.00	0.44
1:J:35:LEU:C	1:J:35:LEU:HD23	2.38	0.44
1:J:61:ASP:OD2	1:J:64:GLN:HA	2.18	0.44
1:B:15:HIS:O	1:B:19:VAL:HG22	2.17	0.44
1:D:86:TYR:O	1:D:87:HIS:C	2.56	0.43
1:G:8:GLU:CG	3:G:2001:HOH:O	2.59	0.43
1:L:68:VAL:HA	1:L:72:GLU:OE1	2.18	0.43
1:G:14:PHE:CD2	1:G:15:HIS:CD2	3.06	0.43
1:J:24:PHE:CD1	1:J:24:PHE:N	2.84	0.43
1:A:82:LYS:HE3	1:A:82:LYS:HB2	1.28	0.43
1:K:14:PHE:CE1	1:K:27:LEU:CD1	3.01	0.43
1:G:64:GLN:CD	1:I:55:GLU:OE1	2.46	0.43
1:H:81:LEU:HA	1:H:81:LEU:HD23	1.60	0.43
1:G:47:ILE:HA	1:G:47:ILE:HD12	1.70	0.43
1:I:14:PHE:HD2	1:I:15:HIS:CD2	2.37	0.43
1:A:28:SER:H	1:A:31:GLU:HB2	1.84	0.43
1:L:27:LEU:HD22	1:L:31:GLU:HB3	2.00	0.42
1:A:60:LEU:O	1:A:72:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:27:LEU:HA	1:D:31:GLU:OE1	2.20	0.42
1:I:57:PHE:CE1	1:I:68:VAL:HG23	2.54	0.42
1:C:13:ILE:O	1:C:14:PHE:C	2.57	0.42
1:D:32:LEU:HG	1:D:36:LEU:HD12	2.01	0.42
1:A:33:LYS:HG3	1:A:53:ILE:HD13	2.00	0.42
1:C:3:LEU:CD1	1:D:40:LEU:HD21	2.45	0.42
1:A:80:ALA:HB1	1:B:7:LEU:CD1	2.49	0.42
1:I:40:LEU:HD11	1:J:3:LEU:HD13	2.02	0.42
1:J:29:LYS:HG3	1:J:57:PHE:CD2	2.54	0.42
1:F:47:ILE:HA	1:F:47:ILE:HD12	1.80	0.42
1:K:82:LYS:HD2	1:L:71:GLN:HE22	1.85	0.41
1:H:28:SER:O	1:H:29:LYS:C	2.59	0.41
1:A:85:HIS:HB2	1:B:70:PHE:CE2	2.55	0.41
1:A:84:ALA:O	1:A:87:HIS:HD2	1.99	0.41
1:I:27:LEU:HB2	1:I:68:VAL:HB	2.02	0.41
1:F:20:ARG:NH1	1:F:34:GLN:OE1	2.51	0.41
1:A:2:LYS:O	1:A:3:LEU:C	2.59	0.41
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.70	0.41
1:E:73:PHE:O	1:E:76:LEU:N	2.50	0.41
1:B:27:LEU:HB2	1:B:68:VAL:HB	2.02	0.41
1:D:20:ARG:NH1	1:D:34:GLN:OE1	2.53	0.41
1:G:9:GLY:O	1:G:13:ILE:HD12	2.20	0.41
1:I:35:LEU:HD23	1:I:36:LEU:N	2.36	0.41
1:G:2:LYS:O	1:G:3:LEU:C	2.59	0.41
1:J:73:PHE:O	1:J:76:LEU:N	2.53	0.41
1:I:65:ASP:O	1:I:66:GLU:HB2	2.20	0.41
1:L:64:GLN:OE1	1:L:64:GLN:HA	2.20	0.41
1:K:14:PHE:HE1	1:K:27:LEU:HD12	1.85	0.41
1:F:81:LEU:HD23	1:F:81:LEU:HA	1.83	0.41
1:L:46:ASN:C	1:L:48:LYS:H	2.24	0.41
1:F:27:LEU:HB2	1:F:68:VAL:HB	2.03	0.41
1:I:66:GLU:OE1	1:I:66:GLU:HA	2.20	0.41
1:B:10:ILE:HD13	1:B:10:ILE:HG21	1.77	0.41
1:C:26:THR:OG1	1:C:67:GLN:OE1	2.30	0.41
1:G:27:LEU:HA	1:G:31:GLU:OE1	2.21	0.41
1:L:28:SER:O	1:L:29:LYS:C	2.59	0.41
1:B:35:LEU:C	1:B:35:LEU:HD23	2.42	0.41
1:J:27:LEU:HA	1:J:31:GLU:OE1	2.21	0.40
1:C:83:ALA:HA	3:C:2002:HOH:O	2.20	0.40
1:E:81:LEU:HD11	1:F:77:VAL:HG21	2.04	0.40
1:E:3:LEU:HD23	1:F:40:LEU:CD1	2.51	0.40
1:K:38:LYS:O	1:L:1:THR:HG21	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:46:ASN:O	1:L:48:LYS:N	2.54	0.40
1:E:41:ALA:HA	1:E:47:ILE:HG21	2.04	0.40
1:D:69:ASP:OD2	1:E:82:LYS:NZ	2.54	0.40
1:D:33:LYS:HD2	1:D:53:ILE:HD13	2.01	0.40
1:L:49:ASP:O	1:L:50:LYS:C	2.59	0.40
1:L:27:LEU:HD11	1:L:35:LEU:HD13	2.04	0.40
1:L:52:VAL:CG1	1:L:53:ILE:N	2.78	0.40
1:K:68:VAL:HA	1:K:72:GLU:OE1	2.21	0.40
1:J:46:ASN:HA	1:J:46:ASN:HD22	1.70	0.40
1:E:81:LEU:O	1:E:82:LYS:C	2.59	0.40
1:D:1:THR:HG23	1:D:4:GLU:CD	2.42	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:50:LYS:NZ	1:L:33:LYS:NZ[1_455]	0.88	1.32
1:E:21:LYS:CE	1:H:88:THR:O[2_545]	1.79	0.41
1:A:48:LYS:O	1:B:50:LYS:NZ[1_455]	1.97	0.23
1:A:2:LYS:NZ	1:F:16:GLN:NE2[2_655]	1.98	0.22
1:K:50:LYS:CE	1:L:33:LYS:NZ[1_455]	2.05	0.15
1:B:20:ARG:NH2	1:F:12:ASN:OD1[2_655]	2.07	0.13
1:K:50:LYS:NZ	1:L:33:LYS:CE[1_455]	2.14	0.06

## 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	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
1	B	86/91 (94%)	84 (98%)	1 (1%)	1 (1%)	19	45
1	C	85/91 (93%)	82 (96%)	3 (4%)	0	100	100
1	D	85/91 (93%)	81 (95%)	4 (5%)	0	100	100
1	E	85/91 (93%)	84 (99%)	0	1 (1%)	19	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
1	G	85/91 (93%)	82 (96%)	2 (2%)	1 (1%)	19	45
1	H	86/91 (94%)	82 (95%)	4 (5%)	0	100	100
1	I	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
1	J	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
1	K	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
1	L	84/91 (92%)	79 (94%)	5 (6%)	0	100	100
All	All	1021/1092 (94%)	990 (97%)	28 (3%)	3 (0%)	50	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	47	ILE
1	G	47	ILE
1	B	47	ILE

### 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	76/80 (95%)	68 (90%)	8 (10%)	10	22
1	B	77/80 (96%)	71 (92%)	6 (8%)	18	40
1	C	76/80 (95%)	72 (95%)	4 (5%)	32	62
1	D	76/80 (95%)	69 (91%)	7 (9%)	13	29
1	E	76/80 (95%)	73 (96%)	3 (4%)	43	76
1	F	76/80 (95%)	71 (93%)	5 (7%)	24	50
1	G	76/80 (95%)	69 (91%)	7 (9%)	13	29
1	H	77/80 (96%)	72 (94%)	5 (6%)	24	51
1	I	76/80 (95%)	67 (88%)	9 (12%)	8	18
1	J	76/80 (95%)	69 (91%)	7 (9%)	13	29
1	K	76/80 (95%)	73 (96%)	3 (4%)	43	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	75/80 (94%)	63 (84%)	12 (16%)	3	9
All	All	913/960 (95%)	837 (92%)	76 (8%)	16	35

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	20	ARG
1	A	25	ASP
1	A	37	THR
1	A	40	LEU
1	A	56	ILE
1	A	71	GLN
1	A	82	LYS
1	B	19	VAL
1	B	29	LYS
1	B	40	LEU
1	B	42	ASN
1	B	47	ILE
1	B	82	LYS
1	C	2	LYS
1	C	3	LEU
1	C	40	LEU
1	C	50	LYS
1	D	3	LEU
1	D	19	VAL
1	D	20	ARG
1	D	37	THR
1	D	45	LYS
1	D	71	GLN
1	D	81	LEU
1	E	19	VAL
1	E	25	ASP
1	E	82	LYS
1	F	2	LYS
1	F	3	LEU
1	F	16	GLN
1	F	40	LEU
1	F	54	ASP
1	G	1	THR
1	G	3	LEU
1	G	13	ILE

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Mol	Chain	Res	Type
1	G	37	THR
1	G	40	LEU
1	G	47	ILE
1	G	50	LYS
1	H	3	LEU
1	H	38	LYS
1	H	40	LEU
1	H	71	GLN
1	H	88	THR
1	I	1	THR
1	I	3	LEU
1	I	13	ILE
1	I	19	VAL
1	I	23	HIS
1	I	25	ASP
1	I	40	LEU
1	I	50	LYS
1	I	87	HIS
1	J	3	LEU
1	J	13	ILE
1	J	21	LYS
1	J	29	LYS
1	J	50	LYS
1	J	79	ILE
1	J	86	TYR
1	K	38	LYS
1	K	50	LYS
1	K	71	GLN
1	L	3	LEU
1	L	4	GLU
1	L	21	LYS
1	L	25	ASP
1	L	26	THR
1	L	38	LYS
1	L	40	LEU
1	L	44	ILE
1	L	50	LYS
1	L	52	VAL
1	L	54	ASP
1	L	81	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	87	HIS
1	B	23	HIS
1	C	46	ASN
1	C	85	HIS
1	D	15	HIS
1	D	46	ASN
1	F	46	ASN
1	G	15	HIS
1	G	46	ASN
1	G	71	GLN
1	I	15	HIS
1	I	46	ASN
1	J	34	GLN
1	J	46	ASN
1	J	71	GLN
1	J	87	HIS
1	K	15	HIS
1	L	71	GLN

### 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 36 ligands modelled in this entry, 36 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	87/91 (95%)	0.24	6 (6%) 17 18	21, 22, 25, 34	9 (10%)
1	B	88/91 (96%)	0.17	1 (1%) 77 82	20, 22, 27, 34	8 (9%)
1	C	87/91 (95%)	-0.04	4 (4%) 31 35	21, 22, 25, 33	12 (13%)
1	D	87/91 (95%)	0.04	4 (4%) 31 35	19, 22, 25, 35	8 (9%)
1	E	87/91 (95%)	0.22	2 (2%) 57 64	18, 22, 26, 31	8 (9%)
1	F	87/91 (95%)	0.27	5 (5%) 23 25	19, 22, 25, 29	7 (8%)
1	G	87/91 (95%)	0.13	3 (3%) 43 48	17, 22, 25, 27	10 (11%)
1	H	88/91 (96%)	0.21	9 (10%) 7 7	21, 22, 25, 30	14 (15%)
1	I	87/91 (95%)	-0.00	2 (2%) 57 64	21, 22, 25, 27	10 (11%)
1	J	87/91 (95%)	0.23	3 (3%) 43 48	21, 22, 25, 31	9 (10%)
1	K	87/91 (95%)	0.16	2 (2%) 57 64	19, 22, 25, 30	12 (13%)
1	L	81/91 (89%)	0.76	12 (14%) 3 3	21, 22, 24, 26	16 (19%)
All	All	1040/1092 (95%)	0.20	53 (5%) 28 30	17, 22, 26, 35	123 (11%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	19	VAL	5.2
1	J	87	HIS	5.2
1	F	85	HIS	4.6
1	C	87	HIS	4.5
1	D	87	HIS	4.2
1	L	23	HIS	4.0
1	K	85	HIS	3.8
1	I	24	PHE	3.8
1	G	87	HIS	3.8
1	H	25	ASP	3.8
1	L	22	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	62	ALA	3.7
1	H	19	VAL	3.4
1	L	1	THR	3.3
1	D	1	THR	3.2
1	H	1	THR	3.2
1	A	87	HIS	3.2
1	A	24	PHE	3.2
1	C	86	TYR	3.1
1	L	24	PHE	3.0
1	I	1	THR	3.0
1	C	24	PHE	3.0
1	A	86	TYR	3.0
1	F	84	ALA	2.9
1	A	1	THR	2.8
1	L	41	ALA	2.8
1	G	85	HIS	2.8
1	H	86	TYR	2.8
1	L	48	LYS	2.8
1	F	1	THR	2.7
1	B	87	HIS	2.6
1	L	17	TYR	2.6
1	F	86	TYR	2.6
1	L	51	ALA	2.5
1	G	86	TYR	2.5
1	J	1	THR	2.5
1	K	1	THR	2.4
1	L	30	GLY	2.4
1	A	19	VAL	2.4
1	H	67	GLN	2.4
1	F	87	HIS	2.3
1	H	24	PHE	2.3
1	E	24	PHE	2.3
1	D	86	TYR	2.3
1	H	22	GLY	2.2
1	L	20	ARG	2.2
1	D	25	ASP	2.2
1	H	20	ARG	2.2
1	H	42	ASN	2.1
1	C	1	THR	2.1
1	A	23	HIS	2.1
1	J	77	VAL	2.0
1	E	77	VAL	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	I	1088	1/1	0.13	-0.79	24,24,24,24	0
2	CA	C	1090	1/1	0.12	-0.80	22,22,22,22	0
2	CA	G	1089	1/1	0.13	-0.99	21,21,21,21	0
2	CA	F	1089	1/1	0.13	-1.08	22,22,22,22	0
2	CA	H	1090	1/1	0.09	-1.32	22,22,22,22	0
2	CA	H	1089	1/1	0.14	-1.36	24,24,24,24	0
2	CA	L	1087	1/1	0.19	-1.39	24,24,24,24	0
2	CA	D	1089	1/1	0.12	-1.46	23,23,23,23	0
2	CA	E	1089	1/1	0.10	-1.60	24,24,24,24	0
2	CA	L	1088	1/1	0.07	-1.62	22,22,22,22	0
2	CA	J	1089	1/1	0.11	-1.63	25,25,25,25	0
2	CA	C	1089	1/1	0.06	-1.74	24,24,24,24	0
2	CA	D	1088	1/1	0.10	-1.78	24,24,24,24	0
2	CA	J	1090	1/1	0.08	-1.79	22,22,22,22	0
2	CA	G	1088	1/1	0.12	-1.83	24,24,24,24	0
2	CA	K	1090	1/1	0.06	-2.08	22,22,22,22	0
2	CA	A	1088	1/1	0.08	-2.09	23,23,23,23	0
2	CA	A	1090	1/1	0.09	-2.19	22,22,22,22	0
2	CA	E	1090	1/1	0.08	-2.38	21,21,21,21	0
2	CA	J	1088	1/1	0.06	-2.38	22,22,22,22	0
2	CA	K	1088	1/1	0.06	-2.42	22,22,22,22	0
2	CA	A	1089	1/1	0.04	-2.45	22,22,22,22	0
2	CA	C	1088	1/1	0.05	-2.51	22,22,22,22	0
2	CA	F	1088	1/1	0.10	-2.69	24,24,24,24	0
2	CA	G	1090	1/1	0.10	-2.70	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	K	1091	1/1	0.08	-3.01	22,22,22,22	0
2	CA	B	1089	1/1	0.09	-3.02	24,24,24,24	0
2	CA	E	1088	1/1	0.07	-3.06	23,23,23,23	0
2	CA	J	1091	1/1	0.06	-3.08	22,22,22,22	0
2	CA	I	1089	1/1	0.06	-3.71	22,22,22,22	0
2	CA	B	1090	1/1	0.05	-3.84	22,22,22,22	0
2	CA	C	1091	1/1	0.04	-3.87	23,23,23,23	0
2	CA	H	1091	1/1	0.07	-4.15	22,22,22,22	0
2	CA	B	1091	1/1	0.08	-4.18	22,22,22,22	0
2	CA	K	1089	1/1	0.07	-4.33	24,24,24,24	0
2	CA	E	1091	1/1	0.05	-23.84	22,22,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.