



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:54 AM UTC

PDB ID : 1GQM / pdb_00001gqm
Title : The structure of S100A12 in a hexameric form and its proposed role in receptor signalling
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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

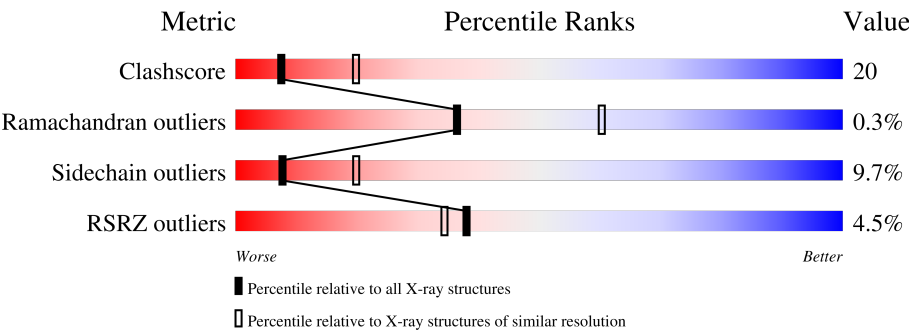
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	91	% 44% 40% 9% . .
1	B	91	% 56% 31% 9% . .
1	C	91	2% 55% 33% 8% .
1	D	91	% 47% 37% 10% . .
1	E	91	60% 27% 8% .
1	F	91	4% 58% 30% 8% .

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Mol	Chain	Length	Quality of chain				
1	G	91		51%	32%	11%	• •
1	H	91		48%	43%	5%	•
1	I	91		44%	40%	10%	• •
1	J	91		47%	37%	8%	• •
1	K	91		49%	37%	8%	• •
1	L	91		33%	37%	43%	14% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8502 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 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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		

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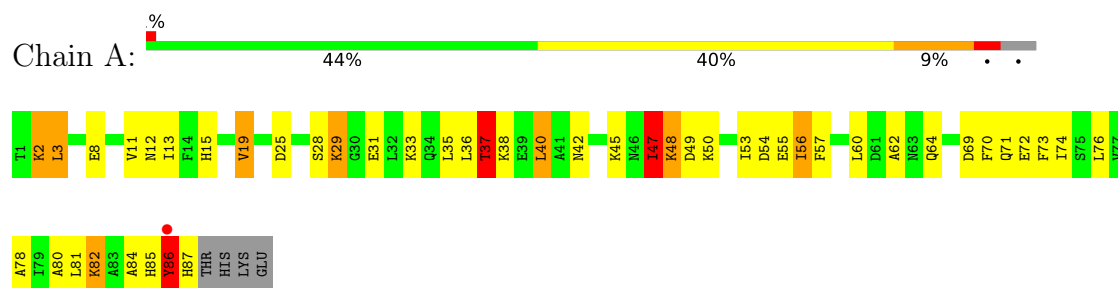
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	O	0	0
			2	2		
3	K	2	Total	O	0	0
			2	2		
3	L	2	Total	O	0	0
			2	2		

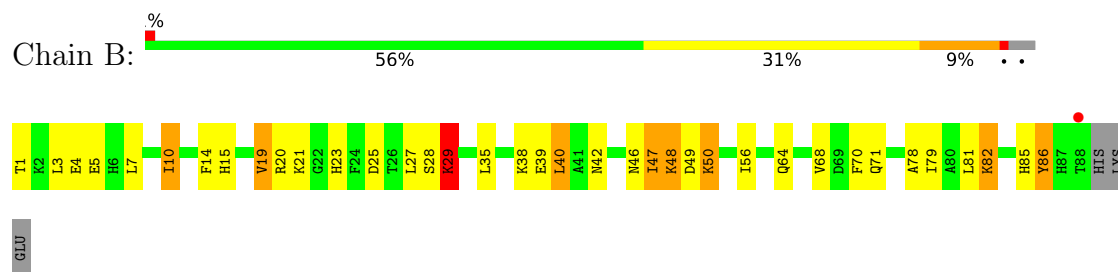
3 Residue-property plots [i](#)

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

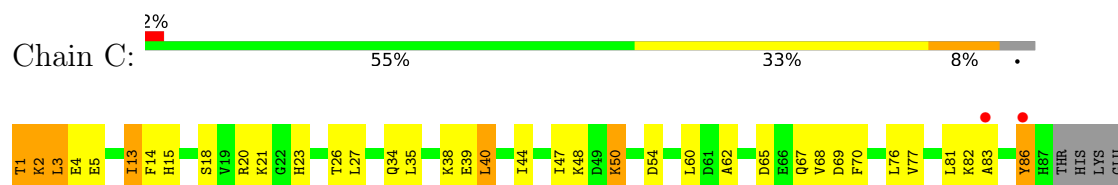
• Molecule 1: CALGRANULIN C



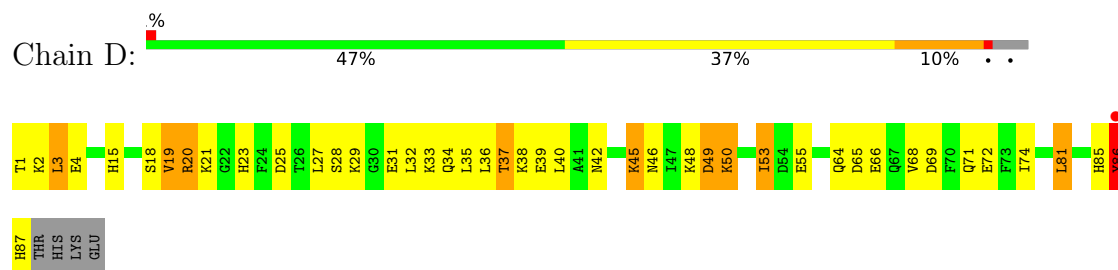
• Molecule 1: CALGRANULIN C



• Molecule 1: CALGRANULIN C

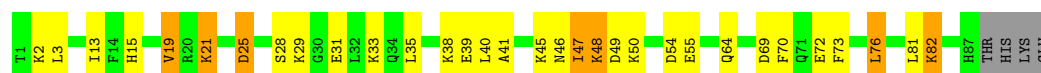


• Molecule 1: CALGRANULIN C



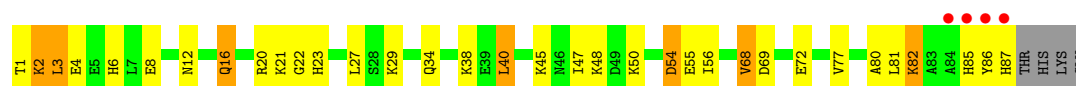
• Molecule 1: CALGRANULIN C

Chain E: 



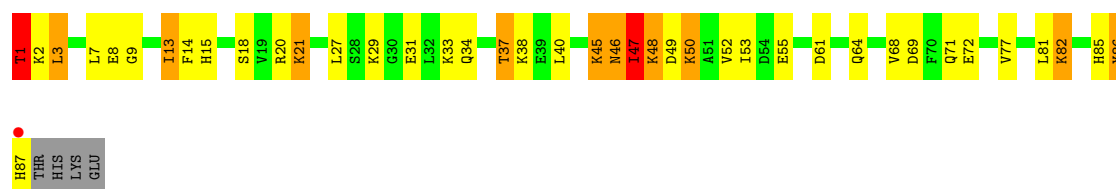
• Molecule 1: CALGRANULIN C

Chain F: 



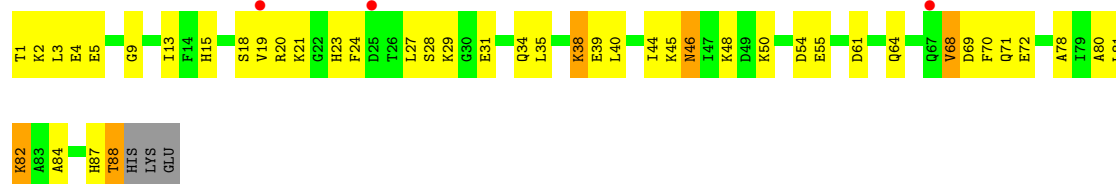
• Molecule 1: CALGRANULIN C

Chain G: 

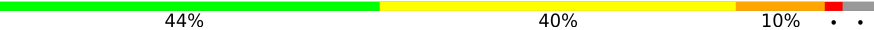


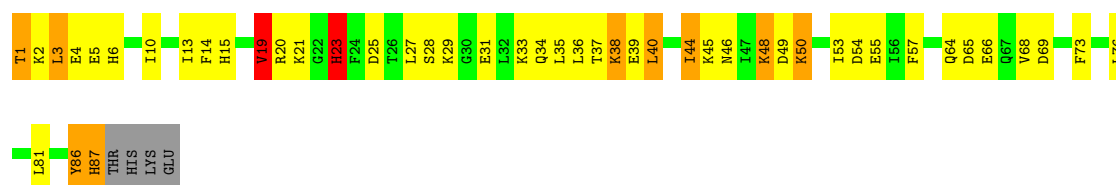
• Molecule 1: CALGRANULIN C

Chain H: 



• Molecule 1: CALGRANULIN C

Chain I: 



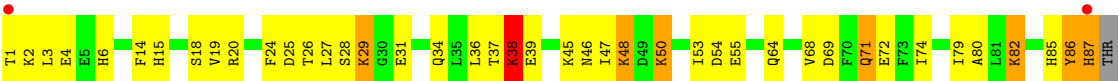
• Molecule 1: CALGRANULIN C

Chain J: 

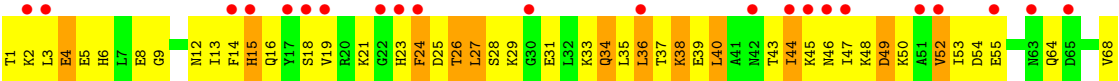




● Molecule 1: CALGRANULIN C



● Molecule 1: CALGRANULIN C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.88Å 100.50Å 112.69Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	19.84 – 2.70 19.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-2.70) 98.1 (19.84-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.217 , 0.281 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8502	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	2.26	6/714 (0.8%)	2.26	17/960 (1.8%)
1	B	1.53	6/721 (0.8%)	1.70	10/970 (1.0%)
1	C	2.15	9/714 (1.3%)	1.86	18/960 (1.9%)
1	D	2.36	9/714 (1.3%)	1.50	9/960 (0.9%)
1	E	1.60	4/714 (0.6%)	1.63	13/960 (1.4%)
1	F	1.81	7/714 (1.0%)	1.76	14/960 (1.5%)
1	G	1.93	9/714 (1.3%)	2.24	20/960 (2.1%)
1	H	1.60	12/721 (1.7%)	1.90	16/970 (1.6%)
1	I	1.86	7/714 (1.0%)	2.47	17/960 (1.8%)
1	J	1.46	5/714 (0.7%)	1.93	16/960 (1.7%)
1	K	1.85	10/714 (1.4%)	2.17	17/960 (1.8%)
1	L	2.50	16/703 (2.3%)	2.57	30/945 (3.2%)
All	All	1.93	100/8571 (1.2%)	2.02	197/11525 (1.7%)

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 (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	HIS	CB-CG	47.93	2.17	1.50
1	A	29	LYS	CD-CE	46.29	2.91	1.52
1	C	50	LYS	CG-CD	37.79	2.65	1.52
1	L	82	LYS	CD-CE	37.15	2.63	1.52
1	L	33	LYS	C-N	25.15	1.67	1.33
1	F	21	LYS	CG-CD	-24.16	0.80	1.52
1	C	82	LYS	CD-CE	23.77	2.23	1.52
1	G	87	HIS	CA-CB	21.55	1.96	1.53
1	G	48	LYS	CB-CG	20.92	2.15	1.52
1	K	48	LYS	CB-CG	20.68	2.14	1.52
1	I	29	LYS	CD-CE	20.45	2.13	1.52
1	E	50	LYS	CG-CD	20.25	2.13	1.52
1	B	82	LYS	CD-CE	-19.84	0.93	1.52
1	L	26	THR	CB-OG1	-18.90	1.13	1.43
1	H	24	PHE	CB-CG	-18.49	1.08	1.50
1	A	86	TYR	CB-CG	-18.38	1.11	1.51
1	I	21	LYS	CG-CD	-17.32	1.00	1.52
1	L	2	LYS	CG-CD	17.10	2.03	1.52
1	G	21	LYS	CG-CD	-17.04	1.01	1.52
1	E	21	LYS	CG-CD	-17.04	1.01	1.52
1	I	86	TYR	CB-CG	-16.33	1.15	1.51
1	H	2	LYS	CG-CD	15.97	2.00	1.52
1	K	50	LYS	CG-CD	15.85	2.00	1.52
1	I	45	LYS	CB-CG	-15.71	1.05	1.52
1	F	86	TYR	CA-CB	15.64	1.78	1.53
1	L	15	HIS	C-N	-15.37	1.13	1.33
1	D	86	TYR	CB-CG	-15.28	1.18	1.51
1	I	87	HIS	CB-CG	-14.69	1.29	1.50
1	G	29	LYS	CD-CE	14.64	1.96	1.52
1	D	50	LYS	CG-CD	-14.33	1.09	1.52
1	K	82	LYS	CD-CE	-14.14	1.10	1.52
1	G	82	LYS	CD-CE	-13.94	1.10	1.52
1	H	46	ASN	CA-CB	13.89	1.74	1.53
1	L	36	LEU	C-N	13.84	1.52	1.33
1	F	87	HIS	CA-CB	-13.44	1.26	1.53
1	K	71	GLN	CA-CB	-13.27	1.32	1.53
1	K	87	HIS	CG-ND1	13.03	1.52	1.38
1	A	8	GLU	CB-CG	-12.81	1.14	1.52
1	B	29	LYS	CD-CE	-12.63	1.14	1.52
1	J	2	LYS	CG-CD	12.45	1.89	1.52
1	K	45	LYS	CB-CG	12.39	1.89	1.52
1	D	21	LYS	CB-CG	-12.11	1.16	1.52
1	J	21	LYS	CD-CE	-11.87	1.16	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	LYS	CG-CD	-11.71	1.17	1.52
1	K	86	TYR	CB-CG	-11.71	1.25	1.51
1	L	5	GLU	CA-CB	10.87	1.70	1.53
1	J	29	LYS	CD-CE	10.83	1.84	1.52
1	C	5	GLU	CA-CB	-10.76	1.36	1.53
1	L	12	ASN	CB-CG	-10.69	1.25	1.52
1	I	48	LYS	CB-CG	10.66	1.84	1.52
1	H	87	HIS	CB-CG	-9.98	1.36	1.50
1	L	16	GLN	C-N	-9.78	1.20	1.33
1	C	23	HIS	CB-CG	9.63	1.63	1.50
1	K	38	LYS	CB-CG	9.47	1.80	1.52
1	L	34	GLN	C-N	-9.19	1.21	1.33
1	C	38	LYS	CB-CG	-8.95	1.25	1.52
1	L	24	PHE	C-N	8.88	1.46	1.33
1	G	50	LYS	CG-CD	8.79	1.78	1.52
1	J	38	LYS	CB-CG	-8.29	1.27	1.52
1	L	45	LYS	CB-CG	8.07	1.76	1.52
1	C	1	THR	CA-C	-7.97	1.36	1.52
1	K	87	HIS	CG-CD2	7.91	1.44	1.35
1	J	86	TYR	CB-CG	-7.55	1.35	1.51
1	F	50	LYS	CG-CD	-7.55	1.29	1.52
1	H	34	GLN	CA-CB	7.54	1.65	1.53
1	D	21	LYS	CG-CD	-7.50	1.29	1.52
1	D	38	LYS	CB-CG	-7.31	1.30	1.52
1	H	50	LYS	CG-CD	-7.09	1.31	1.52
1	L	8	GLU	CB-CG	-6.87	1.31	1.52
1	B	50	LYS	CG-CD	-6.85	1.31	1.52
1	H	38	LYS	CB-CG	-6.73	1.32	1.52
1	G	1	THR	N-CA	-6.68	1.33	1.46
1	C	54	ASP	CB-CG	6.46	1.68	1.52
1	L	24	PHE	CA-CB	6.41	1.63	1.53
1	E	2	LYS	CG-CD	6.34	1.71	1.52
1	K	29	LYS	CD-CE	-6.34	1.33	1.52
1	D	53	ILE	CA-CB	-6.24	1.47	1.54
1	D	2	LYS	CG-CD	6.21	1.71	1.52
1	A	47	ILE	CA-CB	-5.98	1.46	1.54
1	H	78	ALA	CA-CB	-5.89	1.44	1.53
1	L	4	GLU	CG-CD	-5.88	1.37	1.52
1	H	87	HIS	CA-CB	-5.87	1.44	1.53
1	G	61	ASP	CA-C	-5.84	1.47	1.53
1	G	86	TYR	CB-CG	5.80	1.64	1.51
1	A	2	LYS	CG-CD	5.73	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	21	LYS	CB-CG	-5.72	1.35	1.52
1	B	10	ILE	CA-CB	-5.70	1.47	1.54
1	H	82	LYS	CD-CE	-5.42	1.36	1.52
1	F	56	ILE	CA-CB	-5.42	1.47	1.54
1	B	38	LYS	CB-CG	-5.41	1.36	1.52
1	F	68	VAL	CA-CB	-5.35	1.47	1.54
1	B	56	ILE	CA-CB	-5.35	1.48	1.54
1	L	39	GLU	N-CA	5.29	1.53	1.46
1	H	44	ILE	CA-CB	-5.27	1.48	1.54
1	D	74	ILE	CA-CB	-5.26	1.46	1.54
1	C	48	LYS	CB-CG	-5.24	1.36	1.52
1	E	33	LYS	CD-CE	-5.19	1.36	1.52
1	I	54	ASP	CB-CG	5.11	1.64	1.52
1	A	78	ALA	CA-CB	-5.04	1.45	1.53
1	F	45	LYS	CB-CG	5.03	1.67	1.52

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	87	HIS	CB-CG-ND1	-37.92	65.82	122.70
1	L	34	GLN	O-C-N	-30.13	83.22	122.39
1	K	38	LYS	CA-CB-CG	25.78	165.66	114.10
1	G	87	HIS	CB-CA-C	-25.48	61.70	110.10
1	K	38	LYS	CB-CG-CD	24.64	167.98	111.30
1	I	87	HIS	CB-CG-CD2	23.34	161.55	131.20
1	A	86	TYR	CB-CG-CD1	-23.10	86.16	120.80
1	I	87	HIS	CA-CB-CG	22.78	136.58	113.80
1	A	29	LYS	CG-CD-CE	-22.32	59.95	111.30
1	H	24	PHE	CA-CB-CG	21.96	135.76	113.80
1	J	86	TYR	CA-CB-CG	20.85	151.43	113.90
1	I	23	HIS	CA-CB-CG	20.32	134.12	113.80
1	A	86	TYR	CB-CG-CD2	20.05	150.87	120.80
1	L	34	GLN	CA-C-N	19.90	156.62	122.79
1	L	34	GLN	C-N-CA	19.90	156.62	122.79
1	K	45	LYS	CA-CB-CG	-19.78	74.55	114.10
1	G	82	LYS	CG-CD-CE	19.23	155.53	111.30
1	G	87	HIS	CA-CB-CG	-19.01	94.79	113.80
1	G	38	LYS	CA-CB-CG	18.77	151.64	114.10
1	A	8	GLU	CA-CB-CG	18.66	151.42	114.10
1	B	82	LYS	CG-CD-CE	18.42	153.67	111.30
1	H	38	LYS	CA-CB-CG	18.25	150.59	114.10
1	H	87	HIS	CB-CA-C	-18.04	81.95	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	LYS	CA-CB-CG	17.82	149.74	114.10
1	A	48	LYS	CA-CB-CG	17.70	149.49	114.10
1	K	50	LYS	CG-CD-CE	17.60	151.79	111.30
1	D	50	LYS	CB-CG-CD	17.30	151.10	111.30
1	J	38	LYS	CA-CB-CG	17.14	148.38	114.10
1	K	45	LYS	CB-CG-CD	-16.94	72.34	111.30
1	J	86	TYR	CB-CG-CD1	-16.87	95.50	120.80
1	C	50	LYS	CB-CG-CD	-16.81	72.63	111.30
1	L	37	THR	O-C-N	-16.80	104.31	122.12
1	C	21	LYS	CB-CG-CD	16.73	149.78	111.30
1	L	4	GLU	CG-CD-OE2	16.17	155.60	118.40
1	L	4	GLU	CG-CD-OE1	-16.04	81.50	118.40
1	J	86	TYR	CB-CG-CD2	15.99	144.79	120.80
1	L	26	THR	CA-CB-OG1	15.99	133.59	109.60
1	G	86	TYR	CA-CB-CG	-15.89	85.29	113.90
1	F	48	LYS	CA-CB-CG	15.35	144.79	114.10
1	G	29	LYS	CG-CD-CE	-15.01	76.77	111.30
1	L	86	TYR	CB-CG-CD1	-14.79	98.62	120.80
1	J	50	LYS	CG-CD-CE	14.78	145.28	111.30
1	C	23	HIS	CA-CB-CG	14.62	128.41	113.80
1	F	50	LYS	CB-CG-CD	14.49	144.63	111.30
1	B	86	TYR	CB-CG-CD1	-14.23	99.45	120.80
1	I	86	TYR	CB-CG-CD1	-14.16	99.56	120.80
1	L	12	ASN	CA-CB-CG	14.11	126.71	112.60
1	E	29	LYS	CG-CD-CE	-14.04	79.01	111.30
1	L	33	LYS	O-C-N	14.02	136.98	122.12
1	L	36	LEU	O-C-N	13.93	136.52	122.03
1	I	21	LYS	CB-CG-CD	13.58	142.54	111.30
1	L	4	GLU	CB-CG-CD	13.39	135.37	112.60
1	C	50	LYS	CG-CD-CE	13.37	142.06	111.30
1	J	21	LYS	CG-CD-CE	13.23	141.73	111.30
1	L	86	TYR	CB-CG-CD2	12.90	140.15	120.80
1	A	48	LYS	CB-CG-CD	12.58	140.24	111.30
1	C	38	LYS	CA-CB-CG	12.50	139.10	114.10
1	E	21	LYS	CB-CG-CD	12.44	139.91	111.30
1	B	86	TYR	CB-CG-CD2	12.42	139.43	120.80
1	I	23	HIS	CB-CG-ND1	-12.37	104.15	122.70
1	L	82	LYS	CG-CD-CE	-12.31	82.98	111.30
1	D	50	LYS	CG-CD-CE	12.29	139.58	111.30
1	C	82	LYS	CG-CD-CE	-12.04	83.60	111.30
1	K	86	TYR	CB-CG-CD1	-11.99	102.82	120.80
1	A	45	LYS	CA-CB-CG	-11.85	90.39	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	LYS	CA-CB-CG	-11.85	90.39	114.10
1	K	29	LYS	CG-CD-CE	-11.75	84.27	111.30
1	I	29	LYS	CG-CD-CE	-11.74	84.30	111.30
1	H	46	ASN	N-CA-CB	-11.71	94.84	112.28
1	H	45	LYS	CA-CB-CG	11.29	136.69	114.10
1	H	38	LYS	CB-CG-CD	11.23	137.13	111.30
1	F	48	LYS	CB-CG-CD	11.19	137.03	111.30
1	A	38	LYS	CB-CG-CD	11.18	137.02	111.30
1	G	45	LYS	CB-CG-CD	-11.12	85.71	111.30
1	K	48	LYS	CA-CB-CG	-11.08	91.94	114.10
1	K	50	LYS	CB-CG-CD	10.82	136.19	111.30
1	B	48	LYS	CA-CB-CG	10.82	135.73	114.10
1	F	87	HIS	N-CA-CB	-10.73	92.27	110.50
1	L	45	LYS	CA-CB-CG	-10.67	92.75	114.10
1	A	45	LYS	CB-CG-CD	-10.65	86.81	111.30
1	G	38	LYS	CB-CG-CD	10.57	135.60	111.30
1	H	21	LYS	CG-CD-CE	10.47	135.38	111.30
1	L	24	PHE	CA-C-N	10.47	141.53	121.54
1	L	24	PHE	C-N-CA	10.47	141.53	121.54
1	G	87	HIS	N-CA-CB	10.21	127.86	110.50
1	C	48	LYS	CB-CG-CD	10.14	134.62	111.30
1	B	48	LYS	CB-CG-CD	10.06	134.43	111.30
1	J	38	LYS	CB-CG-CD	10.06	134.43	111.30
1	H	24	PHE	CB-CG-CD1	-9.96	103.78	120.70
1	I	23	HIS	CB-CG-CD2	9.90	144.07	131.20
1	I	50	LYS	CB-CG-CD	-9.89	88.55	111.30
1	C	48	LYS	CA-CB-CG	9.61	133.33	114.10
1	F	86	TYR	CB-CA-C	9.59	127.15	110.85
1	G	48	LYS	CA-CB-CG	-9.54	95.03	114.10
1	C	86	TYR	CB-CG-CD1	-9.51	106.53	120.80
1	C	1	THR	CA-C-O	-9.45	104.74	120.80
1	L	86	TYR	CA-CB-CG	9.45	130.91	113.90
1	H	23	HIS	CA-CB-CG	9.44	123.24	113.80
1	C	21	LYS	CG-CD-CE	9.40	132.93	111.30
1	G	82	LYS	CD-CE-NZ	9.36	141.85	111.90
1	G	86	TYR	CB-CG-CD1	-9.36	106.77	120.80
1	D	38	LYS	CA-CB-CG	9.14	132.38	114.10
1	H	54	ASP	CA-CB-CG	-9.13	103.47	112.60
1	A	54	ASP	CB-CG-OD1	9.04	139.20	118.40
1	I	19	VAL	CB-CA-C	-9.01	97.66	112.26
1	J	29	LYS	CG-CD-CE	-8.98	90.66	111.30
1	F	38	LYS	CA-CB-CG	8.93	131.95	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	86	TYR	CB-CG-CD2	8.91	134.16	120.80
1	H	50	LYS	CB-CG-CD	8.70	131.31	111.30
1	F	50	LYS	CG-CD-CE	8.55	130.97	111.30
1	K	54	ASP	CA-CB-CG	-8.52	104.08	112.60
1	H	24	PHE	CB-CG-CD2	8.45	135.06	120.70
1	L	36	LEU	CA-C-N	-8.40	109.03	120.28
1	L	36	LEU	C-N-CA	-8.40	109.03	120.28
1	I	38	LYS	CA-CB-CG	8.29	130.69	114.10
1	E	48	LYS	CB-CG-CD	8.22	130.21	111.30
1	A	86	TYR	CA-CB-CG	8.20	128.66	113.90
1	K	87	HIS	ND1-CG-CD2	-8.13	97.97	106.10
1	G	82	LYS	N-CA-C	-7.99	102.52	111.07
1	B	82	LYS	N-CA-C	-7.94	102.63	111.28
1	E	21	LYS	CG-CD-CE	7.92	129.51	111.30
1	F	45	LYS	CA-CB-CG	-7.90	98.31	114.10
1	E	38	LYS	CA-CB-CG	7.76	129.61	114.10
1	B	50	LYS	CB-CG-CD	7.72	129.06	111.30
1	F	87	HIS	CA-CB-CG	7.68	121.48	113.80
1	E	50	LYS	CB-CG-CD	-7.66	93.68	111.30
1	G	1	THR	N-CA-CB	-7.55	98.66	111.50
1	K	86	TYR	CB-CG-CD2	7.40	131.89	120.80
1	H	50	LYS	CG-CD-CE	7.27	128.02	111.30
1	K	71	GLN	N-CA-CB	7.23	120.72	109.94
1	L	45	LYS	CB-CG-CD	-7.23	94.68	111.30
1	C	38	LYS	CB-CG-CD	7.11	127.65	111.30
1	F	21	LYS	CB-CG-CD	7.05	127.51	111.30
1	C	86	TYR	CB-CG-CD2	7.04	131.36	120.80
1	I	48	LYS	CB-CG-CD	6.97	127.34	111.30
1	D	21	LYS	CG-CD-CE	6.92	127.22	111.30
1	E	45	LYS	CB-CG-CD	-6.89	95.46	111.30
1	G	50	LYS	CG-CD-CE	6.86	127.07	111.30
1	H	21	LYS	CB-CG-CD	-6.75	95.76	111.30
1	B	82	LYS	CD-CE-NZ	6.63	133.11	111.90
1	G	29	LYS	CD-CE-NZ	-6.61	90.76	111.90
1	I	48	LYS	CA-CB-CG	6.57	127.23	114.10
1	A	54	ASP	CA-CB-CG	6.56	119.16	112.60
1	F	86	TYR	N-CA-CB	-6.56	100.46	110.16
1	A	8	GLU	CB-CG-CD	6.53	123.69	112.60
1	F	21	LYS	CG-CD-CE	6.40	126.02	111.30
1	J	24	PHE	N-CA-C	6.37	118.22	111.28
1	E	45	LYS	CA-CB-CG	-6.37	101.37	114.10
1	J	50	LYS	CB-CG-CD	6.32	125.83	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	LYS	CB-CG-CD	6.30	125.79	111.30
1	J	71	GLN	N-CA-C	-6.28	104.35	111.07
1	K	87	HIS	CB-CG-ND1	-6.23	113.35	122.70
1	J	45	LYS	CA-CB-CG	-6.17	101.77	114.10
1	I	21	LYS	CG-CD-CE	6.11	125.35	111.30
1	J	37	THR	N-CA-C	6.07	118.69	111.71
1	K	29	LYS	CD-CE-NZ	-6.07	92.46	111.90
1	C	23	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	E	29	LYS	CD-CE-NZ	-5.78	93.40	111.90
1	E	76	LEU	N-CA-C	-5.77	105.12	111.82
1	L	24	PHE	O-C-N	-5.73	115.91	122.09
1	L	2	LYS	CB-CG-CD	5.72	124.47	111.30
1	H	45	LYS	CB-CG-CD	5.71	124.43	111.30
1	D	86	TYR	CB-CG-CD2	-5.71	112.24	120.80
1	D	68	VAL	CB-CA-C	-5.68	104.02	111.81
1	B	29	LYS	CG-CD-CE	5.68	124.37	111.30
1	B	38	LYS	CA-CB-CG	5.63	125.36	114.10
1	C	86	TYR	CA-CB-CG	5.63	124.03	113.90
1	G	77	VAL	N-CA-C	-5.58	105.08	110.72
1	F	45	LYS	CB-CG-CD	-5.56	98.50	111.30
1	J	3	LEU	N-CA-C	-5.55	105.14	111.07
1	G	86	TYR	CB-CG-CD2	-5.51	112.54	120.80
1	K	86	TYR	CA-CB-CG	5.51	123.81	113.90
1	C	82	LYS	N-CA-C	-5.50	104.92	111.03
1	E	72	GLU	N-CA-C	-5.49	105.45	111.82
1	J	45	LYS	CB-CG-CD	-5.44	98.79	111.30
1	C	54	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	62	ALA	N-CA-C	5.42	117.94	111.71
1	D	21	LYS	CA-CB-CG	-5.36	103.38	114.10
1	C	23	HIS	CB-CG-ND1	5.31	130.67	122.70
1	H	20	ARG	N-CA-C	5.28	117.45	111.11
1	L	16	GLN	CA-C-N	5.28	131.55	122.09
1	L	16	GLN	C-N-CA	5.28	131.55	122.09
1	F	82	LYS	N-CA-C	-5.26	104.79	111.11
1	A	29	LYS	CD-CE-NZ	-5.25	95.10	111.90
1	A	37	THR	N-CA-C	5.24	117.73	111.71
1	J	2	LYS	CG-CD-CE	5.23	123.32	111.30
1	L	49	ASP	N-CA-C	5.20	117.23	108.96
1	E	25	ASP	N-CA-C	5.20	119.72	113.17
1	K	37	THR	N-CA-C	5.17	116.92	111.28
1	D	49	ASP	N-CA-C	5.16	117.17	109.59
1	L	24	PHE	CA-CB-CG	-5.14	108.66	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	2	LYS	CG-CD-CE	5.11	123.06	111.30
1	E	45	LYS	N-CA-C	5.04	117.66	110.24
1	L	37	THR	CA-C-N	-5.04	111.91	121.54
1	L	37	THR	C-N-CA	-5.04	111.91	121.54
1	I	44	ILE	N-CA-CB	-5.04	105.11	111.46
1	G	46	ASN	CB-CA-C	-5.01	103.06	111.23

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
1	L	24	PHE	Mainchain
1	L	34	GLN	Mainchain
1	L	38	LYS	Peptide
1	L	86	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	703	0	707	36	2
1	B	710	0	712	29	2
1	C	703	0	705	26	0
1	D	703	0	707	38	0
1	E	703	0	706	27	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	703	0	707	25	2
1	G	703	0	706	36	0
1	H	710	0	712	29	1
1	I	703	0	707	36	0
1	J	703	0	705	37	0
1	K	703	0	705	34	0
1	L	693	0	697	36	0
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
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	8476	317	4

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 20.

All (317) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:35:LEU:HD23	1:I:35:LEU:C	2.05	0.81
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
1:H:9:GLY:O	1:H:13:ILE:HD12	1.81	0.79
1:A:47:ILE:HG12	1:A:47:ILE:O	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:D:64:GLN:HE22	1:E:55:GLU:CD	1.94	0.76
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:25:ASP:OD1	1:D:25:ASP:O	2.08	0.71
1:H:28:SER:N	1:H:31:GLU:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:82:LYS:CG	1:L:71:GLN:HE22	2.04	0.71
1:F:54:ASP:C	1:F:54:ASP:OD1	2.34	0.70
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:A:55:GLU:CD	1:E:64:GLN:HE22	2.00	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:E:46:ASN:C	1:E:48:LYS:H	2.01	0.67
1:J:23:HIS:HD2	1:J:26:THR:H	1.44	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:15:HIS:O	1:E:19:VAL:HG22	1.97	0.64
1:E:46:ASN:O	1:E:48:LYS:N	2.30	0.64
1:D:33:LYS:O	1:D:37:THR:OG1	2.14	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:A:82:LYS:HD3	1:B:71:GLN:OE1	1.98	0.63
1:H:1:THR:O	1:H:5:GLU:HG3	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
1:H:35:LEU:C	1:H:35:LEU:HD23	2.24	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:E:46:ASN:C	1:E:48:LYS:N	2.55	0.61
1:G:46:ASN:C	1:G:48:LYS:N	2.58	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:55:GLU:CD	1:K:64:GLN:HE22	2.10	0.60
1:D:28:SER:OG	1:D:31:GLU:HG3	2.02	0.60
1:G:71:GLN:HE22	1:H:82:LYS:HG3	1.66	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:D:25:ASP:O	1:D:25:ASP:CG	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:23:HIS:CD2	1:J:23:HIS:C	2.81	0.58
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:J:20:ARG:C	1:J:21:LYS:HG2	2.27	0.58
1:K:82:LYS:HG3	1:L:71:GLN:NE2	2.13	0.57
1:C:39:GLU:O	1:C:40:LEU:HD12	2.03	0.57
1:C:40:LEU:HD11	1:D:3:LEU:HD12	1.85	0.57
1:C:69:ASP:OD1	1:C:69:ASP:C	2.47	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:H	2.13	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:G:69:ASP:OD1	1:G:69:ASP:C	2.48	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:D:65:ASP:O	1:D:66:GLU:HB2	2.04	0.55
1:C:4:GLU:OE1	1:D:42:ASN:ND2	2.32	0.55
1:L:27:LEU:HA	1:L:31:GLU:OE1	2.06	0.55
1:I:38:LYS:O	1:J:1:THR:HG21	2.06	0.55
1:J:23:HIS:HD2	1:J:26:THR:N	2.05	0.55
1:J:1:THR:O	1:J:5:GLU:HG3	2.07	0.55
1:D:45:LYS:H	1:D:45:LYS:CD	2.18	0.55
1:G:7:LEU:CD1	1:H:80:ALA:HB1	2.37	0.54
1:I:73:PHE:CE2	1:I:76:LEU:HD23	2.43	0.54
1:K:15:HIS:HA	1:K:18:SER:OG	2.07	0.54
1:F:1:THR:HG23	1:F:4:GLU:OE1	2.07	0.54
1:G:15:HIS:CE1	3:H:2001:HOH:O	2.61	0.54
1:C:3:LEU:HB2	1:D:39:GLU:HB3	1.89	0.54
1:C:35:LEU:C	1:C:35:LEU:HD23	2.33	0.54
1:A:35:LEU:C	1:A:35:LEU:HD23	2.32	0.54
1:B:20:ARG:HG2	1:B:20:ARG:NH1	2.17	0.54
1:J:23:HIS:CD2	1:J:26:THR:N	2.76	0.54
1:H:46:ASN:C	1:H:48:LYS:N	2.64	0.53
1:H:64:GLN:HE22	1:L:55:GLU:CD	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:O	1:A:82:LYS:C	2.47	0.53
1:F:54:ASP:OD1	1:F:54:ASP:O	2.27	0.53
1:F:81:LEU:O	1:F:82:LYS:C	2.49	0.53
1:H:46:ASN:C	1:H:48:LYS:H	2.17	0.53
1:E:35:LEU:C	1:E:35:LEU:HD23	2.34	0.53
1:H:64:GLN:HA	1:H:64:GLN:OE1	2.07	0.53
1:D:35:LEU:C	1:D:35:LEU:HD23	2.34	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:A:70:PHE:CE2	1:B:85:HIS:HB2	2.44	0.52
1:G:64:GLN:CD	1:I:55:GLU:OE1	2.46	0.52
1:H:35:LEU:O	1:H:39:GLU:HB2	2.09	0.52
1:D:46:ASN:C	1:D:48:LYS:N	2.67	0.51
1:I:3:LEU:HB2	1:J:39:GLU:HB3	1.92	0.51
1:I:35:LEU:C	1:I:35:LEU:CD2	2.79	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:E:70:PHE:CE2	1:F:85:HIS:HB3	2.46	0.51
1:G:85:HIS:HB2	1:H:70:PHE:CE2	2.45	0.51
1:B:49:ASP:OD1	1:B:49:ASP:N	2.42	0.51
1:K:3:LEU:HD23	1:L:40:LEU:HD13	1.92	0.51
1:K:4:GLU:OE2	1:L:43:THR:OG1	2.29	0.51
1:G:46:ASN:O	1:G:47:ILE:C	2.53	0.50
1:D:45:LYS:CD	1:D:45:LYS:N	2.75	0.50
1:I:64:GLN:HE22	1:K:55:GLU:CD	2.20	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:J:31:GLU:HA	1:J:34:GLN:HE21	1.75	0.50
1:K:27:LEU:HA	1:K:31:GLU:OE1	2.12	0.50
1:I:46:ASN:HB3	1:I:49:ASP:OD2	2.11	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:L:44:ILE:HB	1:L:47:ILE:HD13	1.94	0.50
1:G:68:VAL:HA	1:G:72:GLU:OE1	2.11	0.49
1:D:28:SER:O	1:D:29:LYS:C	2.55	0.49
1:F:22:GLY:O	1:F:23:HIS:C	2.53	0.49
1:I:1:THR:O	1:I:5:GLU:HG3	2.12	0.49
1:I:3:LEU:HD23	1:J:13:ILE:CG2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:ARG:O	1:G:21:LYS:HG2	2.12	0.49
1:K:25:ASP:C	1:K:26:THR:CG2	2.86	0.49
1:K:46:ASN:C	1:K:48:LYS:N	2.69	0.49
1:H:69:ASP:OD1	1:H:72:GLU:HG3	2.12	0.49
1:H:68:VAL:HA	1:H:72:GLU:OE1	2.12	0.49
1:A:11:VAL:O	1:A:12:ASN:C	2.53	0.49
1:D:45:LYS:N	1:D:45:LYS:HD3	2.28	0.48
1:G:7:LEU:HD11	1:H:80:ALA:HB1	1.95	0.48
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:J:14:PHE:CE1	1:J:27:LEU:HG	2.48	0.48
1:C:76:LEU:O	1:C:77:VAL:C	2.53	0.48
1:F:29:LYS:NZ	1:F:54:ASP:HB2	2.29	0.48
1:L:15:HIS:HA	1:L:18:SER:OG	2.12	0.48
1:G:15:HIS:HA	1:G:18:SER:OG	2.13	0.48
1:G:49:ASP:HB2	1:G:52:VAL:HG23	1.95	0.48
1:J:35:LEU:C	1:J:35:LEU:HD23	2.38	0.48
1:D:86:TYR:O	1:D:87:HIS:C	2.56	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:D:46:ASN:C	1:D:48:LYS:H	2.21	0.48
1:J:17:TYR:OH	1:J:39:GLU:OE2	2.28	0.48
1:K:82:LYS:CD	1:L:71:GLN:HE22	2.27	0.48
1:H:15:HIS:O	1:H:19:VAL:HG13	2.14	0.47
1:C:13:ILE:O	1:C:14:PHE:C	2.57	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:L:46:ASN:C	1:L:48:LYS:N	2.69	0.46
1:G:14:PHE:HD2	1:G:15:HIS:CD2	2.34	0.46
1:H:28:SER:O	1:H:29:LYS:C	2.59	0.46
1:A:2:LYS:O	1:A:3:LEU:C	2.59	0.46
1:C:60:LEU:O	1:C:62:ALA:N	2.47	0.46
1:B:64:GLN:NE2	1:F:55:GLU:OE2	2.32	0.46
1:I:39:GLU:HB3	1:J:3:LEU:HB2	1.97	0.46
1:G:2:LYS:O	1:G:3:LEU:C	2.59	0.46
1:K:14:PHE:CE1	1:K:27:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:46:ASN:C	1:L:48:LYS:H	2.24	0.45
1:L:28:SER:O	1:L:29:LYS:C	2.59	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:49:ASP:O	1:L:50:LYS:C	2.59	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:B:23:HIS:CD2	1:B:25:ASP:N	2.76	0.45
1:B:35:LEU:HD23	1:B:35:LEU:C	2.42	0.45
1:D:1:THR:HG23	1:D:4:GLU:CD	2.42	0.45
1:E:40:LEU:CD2	1:F:3:LEU:HD13	2.36	0.45
1:G:69:ASP:OD1	1:G:72:GLU:HG3	2.15	0.45
1:H:61:ASP:HA	1:H:72:GLU:OE2	2.17	0.45
1:C:70:PHE:CE2	1:D:85:HIS:CB	3.00	0.44
1:E:69:ASP:OD1	1:E:69:ASP:C	2.60	0.44
1:B:70:PHE:O	1:B:71:GLN:C	2.58	0.44
1:K:79:ILE:O	1:K:80:ALA:C	2.60	0.44
1:E:39:GLU:HB3	1:F:3:LEU:HB2	1.98	0.44
1:E:81:LEU:O	1:E:82:LYS:C	2.59	0.44
1:J:73:PHE:CE2	1:J:76:LEU:HD23	2.53	0.44
1:B:46:ASN:C	1:B:48:LYS:N	2.75	0.44
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.77	0.44
1:B:28:SER:O	1:B:29:LYS:C	2.57	0.44
1:I:81:LEU:HD11	1:J:77:VAL:HG11	1.99	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:B:15:HIS:O	1:B:19:VAL:HG22	2.17	0.44
1:H:55:GLU:CD	1:J:64:GLN:HE22	2.26	0.44
1:J:61:ASP:OD2	1:J:64:GLN:HA	2.18	0.44
1:A:55:GLU:CD	1:E:64:GLN:NE2	2.69	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:J:70:PHE:O	1:J:71:GLN:C	2.60	0.43
1:C:2:LYS:O	1:C:3:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:LEU:HD23	1:H:81:LEU:HA	1.60	0.43
1:A:28:SER:H	1:A:31:GLU:HB2	1.84	0.43
1:E:54:ASP:O	1:E:55:GLU:C	2.59	0.43
1:G:47:ILE:HD12	1:G:47:ILE:HA	1.70	0.43
1:I:14:PHE:HD2	1:I:15:HIS:CD2	2.37	0.43
1:D:49:ASP:O	1:D:50:LYS:C	2.60	0.42
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
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:A:73:PHE:O	1:A:74:ILE:C	2.61	0.42
1:E:46:ASN:O	1:E:47:ILE:C	2.63	0.42
1:A:49:ASP:O	1:A:50:LYS:C	2.63	0.42
1:F:80:ALA:O	1:F:81:LEU:C	2.60	0.42
1:A:56:ILE:O	1:A:57:PHE:C	2.61	0.42
1:A:86:TYR:O	1:A:87:HIS:C	2.63	0.42
1:A:87:HIS:C	1:A:87:HIS:ND1	2.78	0.42
1:D:32:LEU:HG	1:D:36:LEU:HD12	2.01	0.42
1:I:2:LYS:O	1:I:3:LEU:C	2.59	0.42
1:K:46:ASN:C	1:K:48:LYS:H	2.28	0.42
1:A:28:SER:O	1:A:29:LYS:C	2.63	0.42
1:A:33:LYS:HG3	1:A:53:ILE:HD13	2.00	0.42
1:A:80:ALA:HB1	1:B:7:LEU:CD1	2.49	0.42
1:C:3:LEU:CD1	1:D:40:LEU:HD21	2.45	0.42
1:I:40:LEU:HD11	1:J:3:LEU:HD13	2.02	0.42
1:I:46:ASN:C	1:I:48:LYS:N	2.77	0.42
1:J:29:LYS:HG3	1:J:57:PHE:CD2	2.54	0.42
1:K:28:SER:O	1:K:29:LYS:C	2.61	0.42
1:F:47:ILE:HD12	1:F:47:ILE:HA	1.80	0.42
1:A:85:HIS:HB2	1:B:70:PHE:CE2	2.55	0.41
1:K:82:LYS:HD2	1:L:71:GLN:HE22	1.85	0.41
1:A:84:ALA:O	1:A:87:HIS:HD2	1.99	0.41
1:F:20:ARG:NH1	1:F:34:GLN:OE1	2.51	0.41
1:G:20:ARG:C	1:G:21:LYS:HG2	2.45	0.41
1:I:27:LEU:HB2	1:I:68:VAL:HB	2.02	0.41
1:B:81:LEU:HA	1:B:81:LEU:HD23	1.70	0.41
1:B:27:LEU:HB2	1:B:68:VAL:HB	2.02	0.41
1:E:73:PHE:O	1:E:76:LEU:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:81:LEU:O	1:J:82:LYS:C	2.62	0.41
1:I:65:ASP:O	1:I:66:GLU:HB2	2.20	0.41
1:J:73:PHE:O	1:J:76:LEU:N	2.53	0.41
1:J:73:PHE:O	1:J:74:ILE:C	2.62	0.41
1:L:64:GLN:OE1	1:L:64:GLN: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:F:27:LEU:HB2	1:F:68:VAL:HB	2.03	0.41
1:F:81:LEU:HD23	1:F:81:LEU:HA	1.83	0.41
1:G:27:LEU:HA	1:G:31:GLU:OE1	2.21	0.41
1:I:66:GLU:OE1	1:I:66:GLU:HA	2.20	0.41
1:I:69:ASP:OD1	1:I:69:ASP:C	2.63	0.41
1:K:14:PHE:HE1	1:K:27:LEU:HD12	1.85	0.41
1:B:78:ALA:O	1:B:79:ILE:C	2.61	0.41
1:C:65:ASP:C	1:C:65:ASP:OD1	2.63	0.41
1:C:83:ALA:HA	3:C:2002:HOH:O	2.20	0.40
1:J:27:LEU:HA	1:J:31:GLU:OE1	2.21	0.40
1:E:3:LEU:HD23	1:F:40:LEU:CD1	2.51	0.40
1:E:41:ALA:HA	1:E:47:ILE:HG21	2.04	0.40
1:E:81:LEU:HD11	1:F:77:VAL:HG21	2.04	0.40
1:K:38:LYS:O	1:L:1:THR:HG21	2.21	0.40
1:L:46:ASN:O	1:L:48:LYS:N	2.54	0.40
1:D:33:LYS:HD2	1:D:53:ILE:HD13	2.01	0.40
1:D:69:ASP:OD2	1:E:82:LYS:NZ	2.54	0.40
1:J:46:ASN:HD22	1:J:46:ASN:HA	1.70	0.40
1:K:68:VAL:HA	1:K:72:GLU:OE1	2.21	0.40
1:L:27:LEU:HD11	1:L:35:LEU:HD13	2.04	0.40
1:B:14:PHE:CD2	1:B:14:PHE:C	2.98	0.40

All (4) 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	Interatomic distance (Å)	Clash overlap (Å)
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:B:20:ARG:NH2	1:F:12:ASN:OD1[2_655]	2.07	0.13

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%)	10	27
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%)	10	27
1	F	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
1	G	85/91 (93%)	82 (96%)	2 (2%)	1 (1%)	10	27
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%)	36	60

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%)	66 (87%)	10 (13%)	4	10
1	B	77/80 (96%)	70 (91%)	7 (9%)	9	22
1	C	76/80 (95%)	71 (93%)	5 (7%)	15	36
1	D	76/80 (95%)	69 (91%)	7 (9%)	8	22
1	E	76/80 (95%)	72 (95%)	4 (5%)	20	46
1	F	76/80 (95%)	71 (93%)	5 (7%)	15	36
1	G	76/80 (95%)	68 (90%)	8 (10%)	6	17
1	H	77/80 (96%)	71 (92%)	6 (8%)	11	29
1	I	76/80 (95%)	67 (88%)	9 (12%)	5	13
1	J	76/80 (95%)	67 (88%)	9 (12%)	5	13
1	K	76/80 (95%)	70 (92%)	6 (8%)	11	28
1	L	75/80 (94%)	62 (83%)	13 (17%)	2	5
All	All	913/960 (95%)	824 (90%)	89 (10%)	8	20

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	13	ILE
1	A	19	VAL
1	A	25	ASP
1	A	37	THR
1	A	40	LEU
1	A	47	ILE
1	A	56	ILE
1	A	71	GLN
1	A	82	LYS
1	B	19	VAL
1	B	21	LYS
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	13	ILE
1	C	40	LEU
1	C	50	LYS

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Mol	Chain	Res	Type
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	13	ILE
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
1	G	37	THR
1	G	40	LEU
1	G	47	ILE
1	G	50	LYS
1	G	82	LYS
1	H	3	LEU
1	H	38	LYS
1	H	40	LEU
1	H	68	VAL
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	44	ILE
1	I	50	LYS
1	J	3	LEU
1	J	13	ILE
1	J	21	LYS

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Mol	Chain	Res	Type
1	J	23	HIS
1	J	29	LYS
1	J	47	ILE
1	J	50	LYS
1	J	79	ILE
1	J	86	TYR
1	K	1	THR
1	K	38	LYS
1	K	50	LYS
1	K	53	ILE
1	K	71	GLN
1	K	74	ILE
1	L	3	LEU
1	L	4	GLU
1	L	21	LYS
1	L	23	HIS
1	L	25	ASP
1	L	26	THR
1	L	27	LEU
1	L	38	LYS
1	L	40	LEU
1	L	44	ILE
1	L	52	VAL
1	L	54	ASP
1	L	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	67	GLN
1	A	87	HIS
1	B	23	HIS
1	C	46	ASN
1	C	85	HIS
1	D	46	ASN
1	D	87	HIS
1	F	46	ASN
1	G	15	HIS
1	G	46	ASN
1	G	71	GLN
1	I	15	HIS

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Mol	Chain	Res	Type
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	K	46	ASN
1	K	67	GLN
1	L	71	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	33:LYS	C	34:GLN	N	1.67
1	L	16:GLN	C	17:TYR	N	1.20
1	L	15:HIS	C	16:GLN	N	1.13

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	87/91 (95%)	0.04	1 (1%) 78 76	10, 22, 25, 34	9 (10%)
1	B	88/91 (96%)	-0.22	1 (1%) 78 76	10, 22, 27, 34	8 (9%)
1	C	87/91 (95%)	-0.08	2 (2%) 61 58	7, 22, 25, 33	12 (13%)
1	D	87/91 (95%)	-0.05	1 (1%) 78 76	10, 22, 25, 35	8 (9%)
1	E	87/91 (95%)	0.01	0 100 100	13, 22, 26, 31	8 (9%)
1	F	87/91 (95%)	-0.11	4 (4%) 37 34	8, 22, 25, 29	7 (8%)
1	G	87/91 (95%)	-0.09	1 (1%) 78 76	7, 22, 25, 27	10 (11%)
1	H	88/91 (96%)	0.12	3 (3%) 48 44	10, 22, 25, 30	14 (15%)
1	I	87/91 (95%)	-0.01	0 100 100	10, 22, 25, 27	10 (11%)
1	J	87/91 (95%)	0.29	2 (2%) 61 58	10, 22, 25, 31	9 (10%)
1	K	87/91 (95%)	0.06	2 (2%) 61 58	8, 22, 25, 30	12 (13%)
1	L	81/91 (89%)	1.71	30 (37%) 1 0	8, 22, 23, 26	16 (19%)
All	All	1040/1092 (95%)	0.13	47 (4%) 38 34	7, 22, 26, 35	123 (11%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	86	TYR	5.7
1	L	84	ALA	4.6
1	L	85	HIS	4.6
1	L	45	LYS	4.0
1	L	19	VAL	3.9
1	L	23	HIS	3.7
1	F	84	ALA	3.6
1	F	85	HIS	3.5
1	F	86	TYR	3.5
1	L	81	LEU	3.4
1	L	52	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	24	PHE	3.1
1	L	46	ASN	3.1
1	L	44	ILE	3.0
1	L	42	ASN	2.9
1	L	63	ASN	2.9
1	C	86	TYR	2.9
1	L	55	GLU	2.8
1	L	18	SER	2.7
1	D	86	TYR	2.7
1	H	67	GLN	2.6
1	A	86	TYR	2.6
1	H	19	VAL	2.6
1	K	1	THR	2.5
1	L	36	LEU	2.5
1	L	30	GLY	2.5
1	J	87	HIS	2.5
1	L	2	LYS	2.4
1	L	22	GLY	2.4
1	L	14	PHE	2.4
1	L	83	ALA	2.4
1	L	65	ASP	2.3
1	H	25	ASP	2.3
1	L	47	ILE	2.3
1	G	87	HIS	2.2
1	C	83	ALA	2.2
1	L	51	ALA	2.2
1	F	87	HIS	2.2
1	B	88	THR	2.1
1	L	3	LEU	2.1
1	J	86	TYR	2.1
1	K	87	HIS	2.1
1	L	15	HIS	2.1
1	L	82	LYS	2.1
1	L	79	ILE	2.1
1	L	77	VAL	2.1
1	L	17	TYR	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 oligosaccharides 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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	L	1087	1/1	0.84	0.30	24,24,24,24	0
2	CA	A	1089	1/1	0.89	0.23	22,22,22,22	0
2	CA	E	1089	1/1	0.92	0.17	24,24,24,24	0
2	CA	A	1088	1/1	0.93	0.18	23,23,23,23	0
2	CA	E	1088	1/1	0.93	0.17	23,23,23,23	0
2	CA	L	1088	1/1	0.94	0.22	22,22,22,22	0
2	CA	H	1091	1/1	0.95	0.14	22,22,22,22	0
2	CA	F	1089	1/1	0.95	0.08	22,22,22,22	0
2	CA	H	1090	1/1	0.95	0.25	22,22,22,22	0
2	CA	F	1088	1/1	0.96	0.13	24,24,24,24	0
2	CA	C	1089	1/1	0.96	0.23	24,24,24,24	0
2	CA	G	1088	1/1	0.96	0.13	24,24,24,24	0
2	CA	G	1089	1/1	0.96	0.09	21,21,21,21	0
2	CA	C	1091	1/1	0.96	0.14	23,23,23,23	0
2	CA	D	1089	1/1	0.96	0.16	23,23,23,23	0
2	CA	B	1089	1/1	0.96	0.13	24,24,24,24	0
2	CA	B	1091	1/1	0.96	0.12	22,22,22,22	0
2	CA	H	1089	1/1	0.97	0.20	24,24,24,24	0
2	CA	C	1090	1/1	0.97	0.15	22,22,22,22	0
2	CA	C	1088	1/1	0.97	0.12	22,22,22,22	0
2	CA	I	1088	1/1	0.97	0.11	24,24,24,24	0
2	CA	J	1088	1/1	0.97	0.16	22,22,22,22	0
2	CA	K	1089	1/1	0.97	0.15	24,24,24,24	0
2	CA	B	1090	1/1	0.97	0.15	22,22,22,22	0
2	CA	G	1090	1/1	0.97	0.13	21,21,21,21	0
2	CA	K	1088	1/1	0.98	0.10	22,22,22,22	0
2	CA	E	1091	1/1	0.98	0.15	22,22,22,22	0
2	CA	J	1090	1/1	0.98	0.16	22,22,22,22	0
2	CA	J	1091	1/1	0.98	0.17	22,22,22,22	0
2	CA	D	1088	1/1	0.99	0.16	24,24,24,24	0
2	CA	I	1089	1/1	0.99	0.14	22,22,22,22	0
2	CA	A	1090	1/1	0.99	0.13	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	K	1090	1/1	0.99	0.13	22,22,22,22	0
2	CA	K	1091	1/1	0.99	0.17	22,22,22,22	0
2	CA	J	1089	1/1	0.99	0.14	25,25,25,25	0
2	CA	E	1090	1/1	0.99	0.12	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.