



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:08 AM UTC

PDB ID : 4ZOQ / pdb_00004zoq
Title : Crystal Structure of a Lanthipeptide Protease
Authors : Dong, S.H.; Nair, S.K.
Deposited on : 2015-05-06
Resolution : 2.35 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

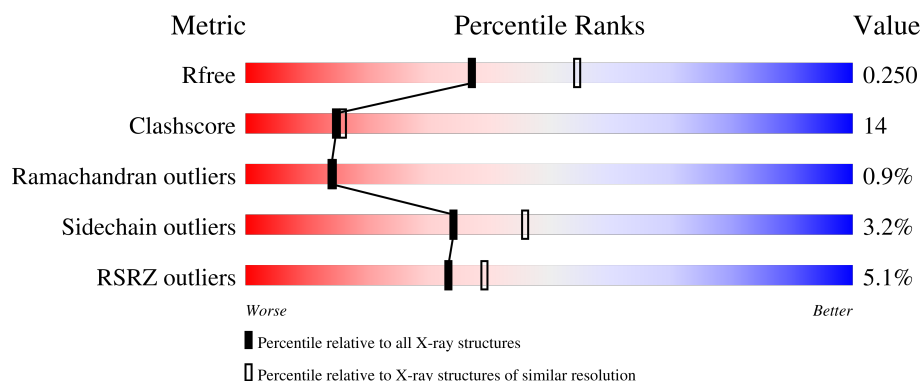
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	100	0% 37% 23% • 39%
1	B	100	47% 12% • 40%
1	C	100	2% 38% 19% • 40%
1	D	100	8% 27% 28% 5% 40%
1	E	100	25% 25% 21% 13% • 39%

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Mol	Chain	Length	Quality of chain
1	F	100	14%26%25%11%38%
1	G	100	28%17%32%12%38%
1	H	100	33%17%27%7%11%38%
2	I	343	%79%18%..
2	J	343	%82%16%.
2	K	343	%79%17%..
2	L	343	%78%19%..
2	M	343	3%74%21%..
2	N	343	3%75%21%..
2	O	343	2%77%18%..
2	P	343	3%75%19%..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25562 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 Intracellular serine protease.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	0	0	0
			486	314	79	93			
1	B	60	Total	C	N	O	0	0	0
			477	309	78	90			
1	C	60	Total	C	N	O	0	0	0
			477	309	78	90			
1	D	60	Total	C	N	O	0	0	0
			473	306	77	90			
1	E	61	Total	C	N	O	0	0	0
			478	309	78	91			
1	F	62	Total	C	N	O	0	0	0
			487	314	79	94			
1	G	62	Total	C	N	O	0	0	0
			483	312	79	92			
1	H	62	Total	C	N	O	0	0	0
			487	315	80	92			

- Molecule 2 is a protein called Intracellular serine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			
2	J	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			
2	K	335	Total	C	N	O	S	0	0	0
			2571	1612	449	500	10			
2	L	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			
2	M	333	Total	C	N	O	S	0	0	0
			2557	1607	447	494	9			
2	N	335	Total	C	N	O	S	0	0	0
			2571	1612	449	500	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	335	Total	C	N	O	S	0	0	0
			2571	1612	449	500	10			
2	P	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			

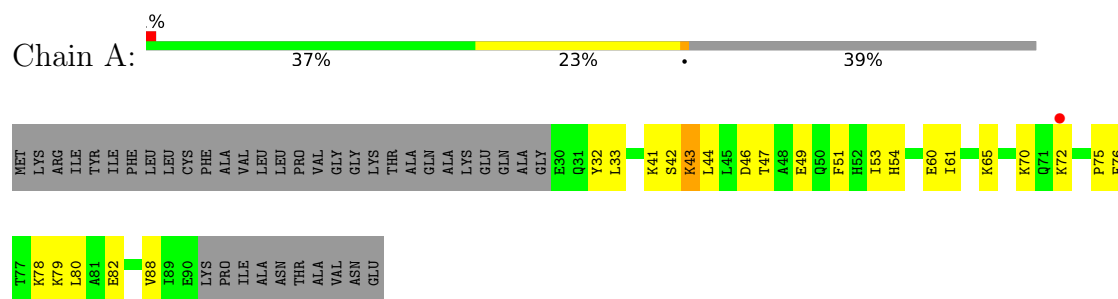
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	I	176	Total	O	0	0
			176	176		
3	B	20	Total	O	0	0
			20	20		
3	J	150	Total	O	0	0
			150	150		
3	C	21	Total	O	0	0
			21	21		
3	K	164	Total	O	0	0
			164	164		
3	D	4	Total	O	0	0
			4	4		
3	L	98	Total	O	0	0
			98	98		
3	E	9	Total	O	0	0
			9	9		
3	M	109	Total	O	0	0
			109	109		
3	F	3	Total	O	0	0
			3	3		
3	N	113	Total	O	0	0
			113	113		
3	G	5	Total	O	0	0
			5	5		
3	O	110	Total	O	0	0
			110	110		
3	H	3	Total	O	0	0
			3	3		
3	P	97	Total	O	0	0
			97	97		

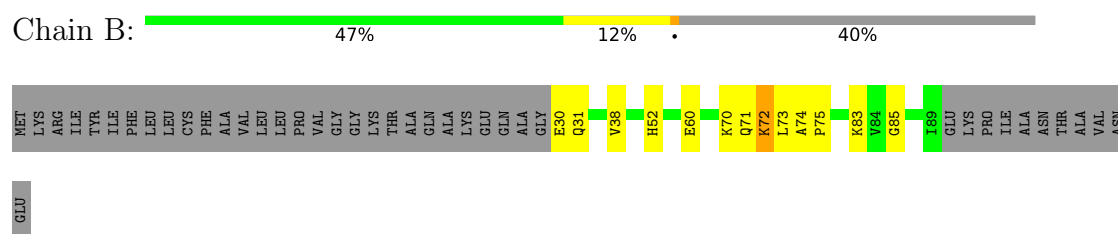
3 Residue-property plots [i](#)

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.

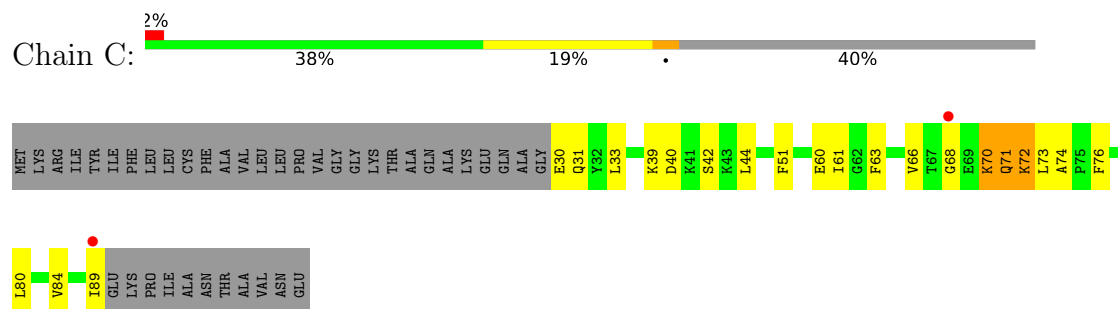
- Molecule 1: Intracellular serine protease



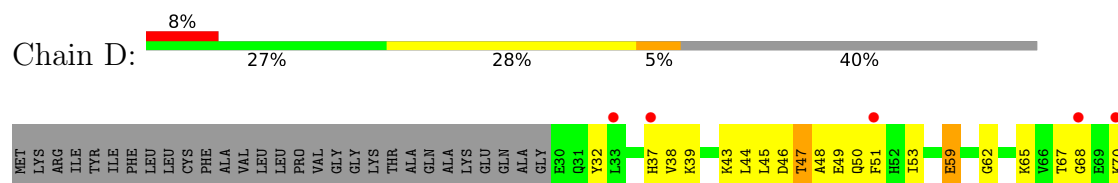
- Molecule 1: Intracellular serine protease



- Molecule 1: Intracellular serine protease

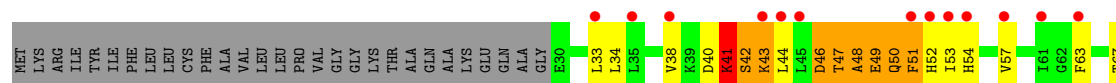


- Molecule 1: Intracellular serine protease

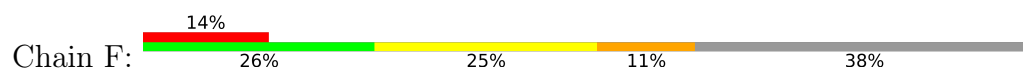




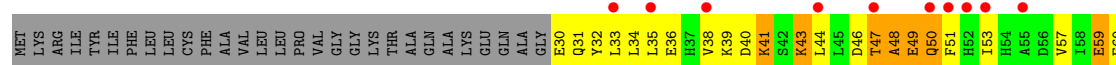
- Molecule 1: Intracellular serine protease



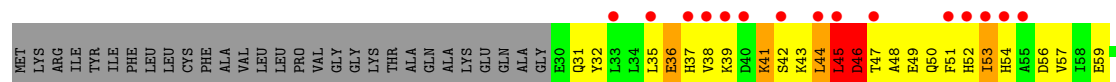
- Molecule 1: Intracellular serine protease



- Molecule 1: Intracellular serine protease

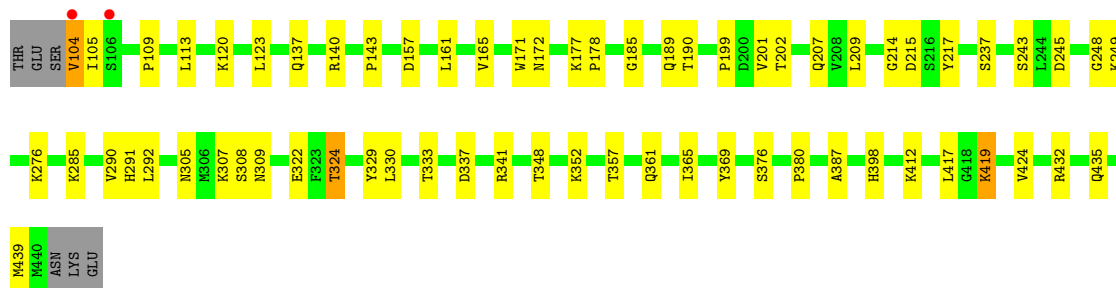


- Molecule 1: Intracellular serine protease

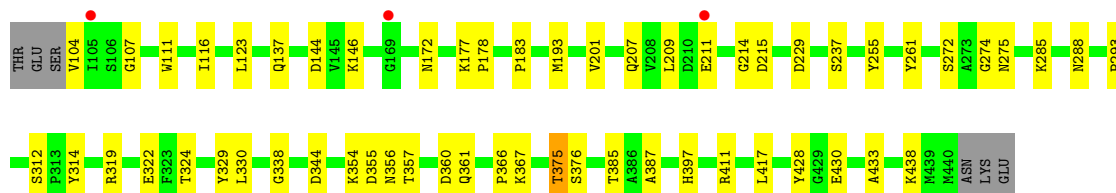
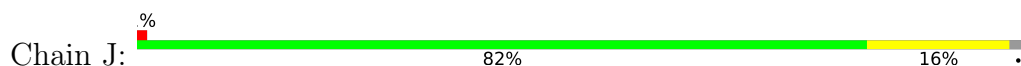


- Molecule 2: Intracellular serine protease

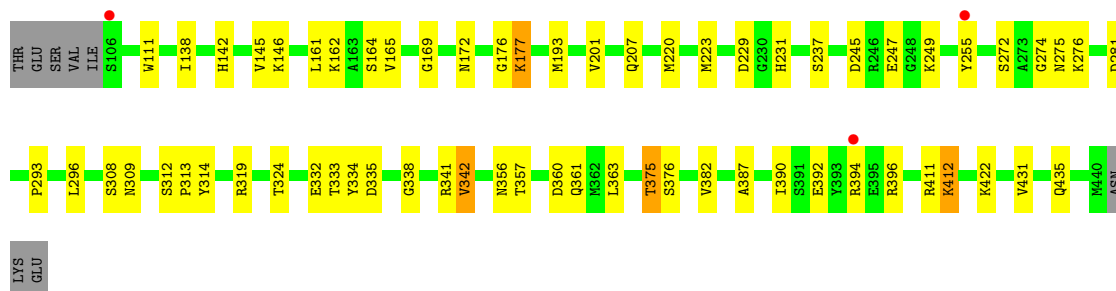
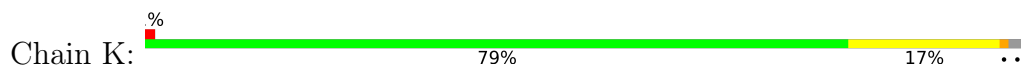




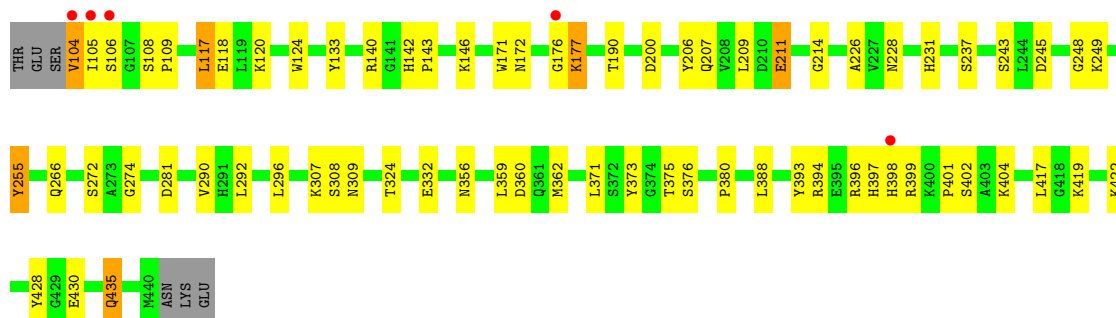
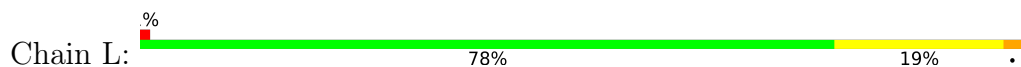
- Molecule 2: Intracellular serine protease



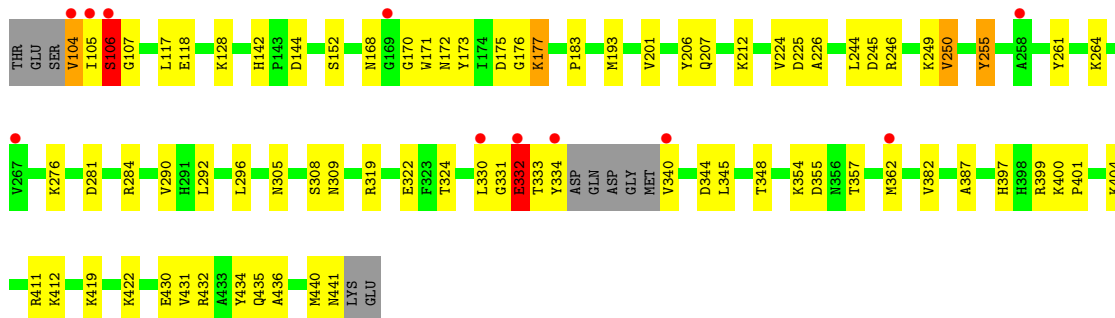
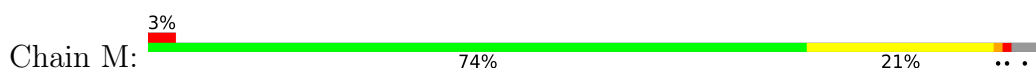
- Molecule 2: Intracellular serine protease



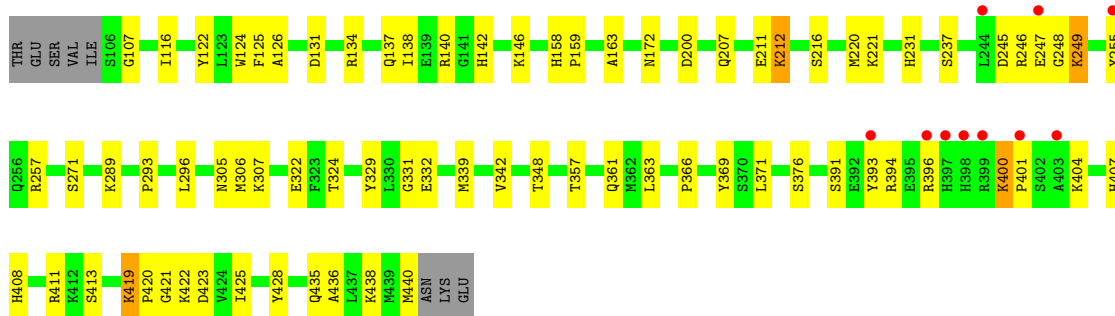
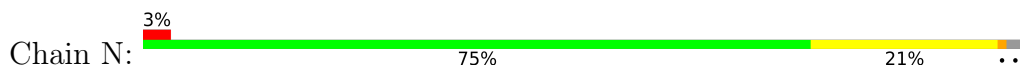
- Molecule 2: Intracellular serine protease



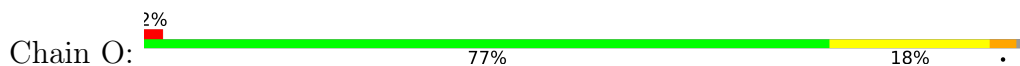
- Molecule 2: Intracellular serine protease



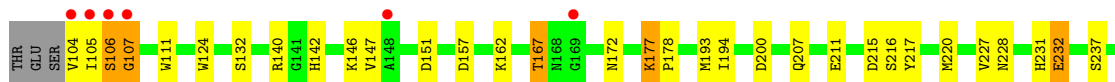
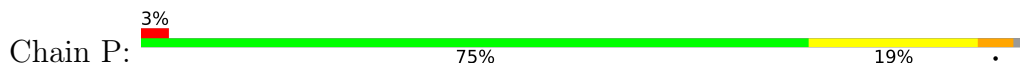
• Molecule 2: Intracellular serine protease

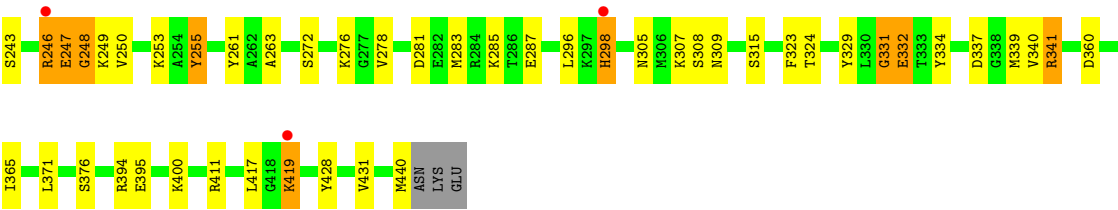


• Molecule 2: Intracellular serine protease



• Molecule 2: Intracellular serine protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.04Å 112.78Å 114.77Å 82.17° 89.68° 82.85°	Depositor
Resolution (Å)	38.03 – 2.35 38.03 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.03-2.35) 98.5 (38.03-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.200 , 0.250 0.202 , 0.250	Depositor DCC
R_{free} test set	7186 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25562	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	0/493	1.10	2/661 (0.3%)
1	B	0.54	0/484	0.96	3/649 (0.5%)
1	C	0.53	0/484	1.17	5/649 (0.8%)
1	D	0.64	0/480	1.38	7/645 (1.1%)
1	E	0.76	0/485	1.66	11/652 (1.7%)
1	F	0.81	1/494 (0.2%)	1.38	5/664 (0.8%)
1	G	0.74	0/490	1.55	8/659 (1.2%)
1	H	1.12	3/494 (0.6%)	2.22	28/663 (4.2%)
2	I	0.65	0/2639	0.88	2/3576 (0.1%)
2	J	0.63	0/2639	0.93	2/3576 (0.1%)
2	K	0.68	0/2624	0.99	4/3555 (0.1%)
2	L	0.61	0/2639	0.97	9/3576 (0.3%)
2	M	0.63	0/2609	0.99	10/3535 (0.3%)
2	N	0.61	0/2624	0.95	2/3555 (0.1%)
2	O	0.60	0/2624	0.94	1/3555 (0.0%)
2	P	0.59	0/2639	1.00	7/3576 (0.2%)
All	All	0.65	4/24941 (0.0%)	1.05	106/33746 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	4
1	G	0	1
1	H	0	6
2	L	0	1
2	M	0	1
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	83	LYS	N-CA	6.25	1.54	1.46
1	H	82	GLU	CA-C	6.21	1.61	1.52
1	H	71	GLN	CA-C	5.41	1.60	1.52
1	F	90	GLU	CA-C	5.07	1.59	1.52

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	LYS	N-CA-C	15.04	142.84	110.80
2	P	331	GLY	N-CA-C	-12.56	95.49	112.82
1	H	71	GLN	N-CA-C	11.99	136.33	110.80
2	N	248	GLY	N-CA-C	-11.32	99.15	112.73
1	E	41	LYS	N-CA-C	-11.19	99.10	111.07
1	H	83	LYS	CA-C-N	10.89	141.57	121.97
1	H	83	LYS	C-N-CA	10.89	141.57	121.97
1	G	74	ALA	CA-C-N	-10.85	108.08	120.12
1	G	74	ALA	C-N-CA	-10.85	108.08	120.12
1	H	44	LEU	N-CA-C	-10.36	100.65	113.18
1	H	77	THR	N-CA-C	-9.93	100.30	111.71
1	H	80	LEU	CA-CB-CG	9.56	149.77	116.30
2	M	331	GLY	N-CA-C	-9.22	97.22	110.96
2	K	335	ASP	N-CA-C	8.88	121.92	111.71
2	J	397	HIS	N-CA-C	-8.80	95.64	109.72
1	H	74	ALA	CA-C-N	-8.67	110.88	119.64
1	H	74	ALA	C-N-CA	-8.67	110.88	119.64
1	C	68	GLY	N-CA-C	-8.59	99.26	110.69
1	F	78	LYS	N-CA-C	-8.58	102.81	113.28
1	F	88	VAL	CA-C-N	-8.57	109.06	122.69
1	F	88	VAL	C-N-CA	-8.57	109.06	122.69
1	E	81	ALA	N-CA-C	-8.57	102.09	112.54
1	H	78	LYS	CA-CB-CG	8.44	130.98	114.10
1	D	74	ALA	CA-C-N	-8.37	109.72	118.85
1	D	74	ALA	C-N-CA	-8.37	109.72	118.85
1	H	78	LYS	CB-CG-CD	8.17	130.08	111.30
1	D	68	GLY	N-CA-C	-8.12	99.16	111.42
1	E	80	LEU	N-CA-C	-8.03	103.46	113.18
1	E	51	PHE	CA-C-N	7.63	133.22	122.46
1	E	51	PHE	C-N-CA	7.63	133.22	122.46
2	M	332	GLU	N-CA-C	-7.60	103.98	113.18
1	H	69	GLU	N-CA-C	7.58	120.93	110.24
1	H	70	LYS	CA-C-N	7.38	135.63	121.54
1	H	70	LYS	C-N-CA	7.38	135.63	121.54
2	L	117	LEU	CA-C-N	-7.20	112.44	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	117	LEU	C-N-CA	-7.20	112.44	123.17
1	E	48	ALA	N-CA-C	7.07	118.88	111.03
2	J	107	GLY	N-CA-C	-6.98	97.95	112.04
1	G	50	GLN	N-CA-C	-6.94	104.81	113.20
1	F	90	GLU	N-CA-C	6.87	119.79	111.40
1	G	43	LYS	N-CA-C	-6.87	104.87	113.18
1	H	71	GLN	N-CA-CB	-6.86	98.89	110.49
2	L	176	GLY	N-CA-C	-6.81	99.35	112.02
2	P	419	LYS	CA-C-N	6.69	128.20	119.84
2	P	419	LYS	C-N-CA	6.69	128.20	119.84
1	G	84	VAL	CB-CA-C	-6.63	100.42	111.29
2	K	333	THR	N-CA-C	6.58	119.17	109.24
2	K	176	GLY	N-CA-C	-6.47	99.99	112.02
1	H	79	LYS	N-CA-C	-6.45	104.47	113.37
1	A	43	LYS	N-CA-C	-6.38	105.50	113.28
1	G	57	VAL	N-CA-C	6.30	117.00	108.17
1	H	45	LEU	CA-CB-CG	-6.27	94.36	116.30
2	L	177	LYS	CA-C-N	6.26	126.22	119.78
2	L	177	LYS	C-N-CA	6.26	126.22	119.78
1	E	57	VAL	N-CA-C	6.22	116.88	108.17
1	C	74	ALA	CA-C-N	-6.21	113.29	119.56
1	C	74	ALA	C-N-CA	-6.21	113.29	119.56
2	P	107	GLY	N-CA-C	-6.20	100.17	110.95
1	D	79	LYS	N-CA-C	-6.17	105.39	113.17
1	B	72	LYS	N-CA-C	6.09	120.55	113.18
1	H	72	LYS	N-CA-C	5.91	118.93	107.71
1	H	44	LEU	CB-CG-CD2	-5.89	93.04	110.70
1	H	72	LYS	CB-CA-C	-5.87	103.13	111.76
1	H	49	GLU	N-CA-C	-5.86	106.10	113.18
1	E	50	GLN	N-CA-C	-5.78	106.20	113.20
2	M	107	GLY	N-CA-C	-5.74	102.02	111.38
1	A	80	LEU	N-CA-C	-5.72	105.03	112.23
1	D	47	THR	N-CA-C	-5.71	105.14	111.71
1	G	79	LYS	CG-CD-CE	-5.70	98.20	111.30
1	F	47	THR	N-CA-C	-5.68	105.23	111.82
2	M	176	GLY	N-CA-C	-5.67	101.72	111.47
1	E	77	THR	N-CA-C	5.64	118.20	111.71
1	H	83	LYS	O-C-N	5.64	130.09	122.59
1	H	75	PRO	CA-C-N	-5.59	113.62	122.23
1	H	75	PRO	C-N-CA	-5.59	113.62	122.23
2	M	419	LYS	CA-C-N	5.56	126.43	119.98
2	M	419	LYS	C-N-CA	5.56	126.43	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	419	LYS	CA-C-N	5.54	126.77	119.84
2	I	419	LYS	C-N-CA	5.54	126.77	119.84
2	P	248	GLY	N-CA-C	-5.49	106.13	112.50
1	E	47	THR	N-CA-C	-5.43	105.91	112.54
1	H	37	HIS	N-CA-CB	5.41	120.79	111.00
2	P	332	GLU	N-CA-C	-5.37	99.35	110.80
2	M	106	SER	N-CA-C	5.36	122.22	110.80
2	M	357	THR	N-CA-C	5.36	117.44	110.53
1	C	84	VAL	N-CA-C	-5.29	100.74	108.99
1	B	74	ALA	CA-C-N	-5.25	114.25	119.56
1	B	74	ALA	C-N-CA	-5.25	114.25	119.56
1	H	83	LYS	CB-CA-C	-5.25	99.97	110.42
2	N	425	ILE	CB-CA-C	-5.24	105.05	111.92
2	L	106	SER	N-CA-C	5.24	117.62	109.60
2	M	331	GLY	CA-C-N	-5.22	111.39	121.58
2	M	331	GLY	C-N-CA	-5.22	111.39	121.58
1	D	72	LYS	N-CA-C	-5.19	106.90	113.18
1	C	71	GLN	N-CA-C	-5.15	103.81	110.19
2	L	117	LEU	N-CA-C	5.10	117.74	111.82
1	H	82	GLU	CA-C-N	5.09	131.26	121.54
1	H	82	GLU	C-N-CA	5.09	131.26	121.54
1	G	84	VAL	N-CA-C	5.08	119.91	109.34
1	D	44	LEU	N-CA-C	-5.07	105.84	112.23
2	L	142	HIS	CA-C-N	5.04	125.32	119.47
2	L	142	HIS	C-N-CA	5.04	125.32	119.47
1	E	54	HIS	N-CA-C	5.03	117.46	109.96
2	K	341	ARG	N-CA-C	5.03	117.10	108.90
2	O	333	THR	N-CA-C	-5.02	104.47	111.30
2	P	247	GLU	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	79	LYS	Peptide
1	E	46	ASP	Peptide
1	E	77	THR	Peptide
1	E	79	LYS	Peptide
1	E	83	LYS	Peptide
1	G	71	GLN	Peptide
1	H	36	GLU	Peptide
1	H	45	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	H	46	ASP	Peptide
1	H	77	THR	Peptide
1	H	80	LEU	Peptide
1	H	82	GLU	Peptide
2	L	118	GLU	Peptide
2	M	106	SER	Peptide

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	486	0	499	19	0
1	B	477	0	493	11	0
1	C	477	0	493	14	0
1	D	473	0	482	24	0
1	E	478	0	484	32	0
1	F	487	0	490	45	0
1	G	483	0	486	51	0
1	H	487	0	497	62	0
2	I	2586	0	2557	46	0
2	J	2586	0	2557	38	0
2	K	2571	0	2537	49	0
2	L	2586	0	2557	50	0
2	M	2557	0	2534	57	1
2	N	2571	0	2537	68	0
2	O	2571	0	2537	68	1
2	P	2586	0	2557	63	0
3	A	18	0	0	8	0
3	B	20	0	0	6	0
3	C	21	0	0	3	0
3	D	4	0	0	1	0
3	E	9	0	0	0	0
3	F	3	0	0	3	0
3	G	5	0	0	3	0
3	H	3	0	0	2	0
3	I	176	0	0	12	0
3	J	150	0	0	12	1
3	K	164	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	98	0	0	7	0
3	M	109	0	0	20	0
3	N	113	0	0	14	0
3	O	110	0	0	12	1
3	P	97	0	0	13	0
All	All	25562	0	24297	672	2

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 14.

All (672) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:LEU:HD11	1:G:86:ALA:HB1	1.31	1.09
1:H:41:LYS:HG3	1:H:45:LEU:HD13	1.30	1.08
1:B:30:GLU:N	3:B:201:HOH:O	1.89	1.02
2:L:272:SER:HB2	2:L:375:THR:HG23	1.40	1.00
2:J:274:GLY:H	2:J:375:THR:HG21	1.27	0.99
2:O:272:SER:HB2	2:O:375:THR:HG23	1.47	0.96
1:H:80:LEU:O	1:H:82:GLU:N	1.99	0.96
1:H:35:LEU:HD11	1:H:44:LEU:HD21	1.48	0.95
2:O:341:ARG:NH1	3:O:502:HOH:O	2.02	0.90
1:G:87:ASP:OD2	3:G:501:HOH:O	1.88	0.90
2:K:274:GLY:H	2:K:375:THR:HG21	1.34	0.90
2:M:183:PRO:O	2:M:354:LYS:NZ	2.06	0.89
2:N:211:GLU:O	3:N:501:HOH:O	1.90	0.88
2:N:246:ARG:NH1	2:N:247:GLU:OE2	2.07	0.86
1:G:77:THR:HB	1:G:88:VAL:HG21	1.55	0.86
1:G:83:LYS:HG3	1:G:84:VAL:HG13	1.58	0.86
1:F:79:LYS:HE2	1:F:80:LEU:HG	1.58	0.85
2:J:272:SER:HB2	2:J:375:THR:HG22	1.57	0.85
2:P:395:GLU:OE1	3:P:502:HOH:O	1.96	0.83
2:P:315:SER:O	3:P:501:HOH:O	1.95	0.83
2:O:274:GLY:H	2:O:375:THR:HG21	1.43	0.82
2:M:104:VAL:HG22	2:M:105:ILE:HD12	1.61	0.82
2:L:417:LEU:O	3:L:502:HOH:O	1.96	0.82
1:H:71:GLN:HG3	1:H:72:LYS:HG3	1.62	0.82
2:O:336:GLN:HE22	2:O:341:ARG:HE	1.28	0.82
1:G:46:ASP:N	3:G:502:HOH:O	2.07	0.81
2:I:157:ASP:O	2:I:352:LYS:NZ	2.12	0.81
2:M:355:ASP:O	3:M:501:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LYS:NZ	3:B:205:HOH:O	2.12	0.81
2:O:336:GLN:NE2	2:O:341:ARG:HE	1.78	0.81
2:K:276:LYS:NZ	3:K:505:HOH:O	2.14	0.81
1:H:41:LYS:O	1:H:43:LYS:N	2.14	0.81
2:N:271:SER:OG	3:N:503:HOH:O	1.99	0.80
2:N:421:GLY:O	3:N:502:HOH:O	1.97	0.80
2:J:361:GLN:NE2	3:J:505:HOH:O	2.15	0.80
2:N:255:TYR:HB3	2:N:296:LEU:HD11	1.64	0.80
2:I:419:LYS:O	3:I:501:HOH:O	1.99	0.80
2:O:332:GLU:N	3:O:505:HOH:O	2.15	0.80
1:G:36:GLU:CD	1:G:85:GLY:HA3	2.07	0.80
1:B:85:GLY:O	3:B:202:HOH:O	2.00	0.79
1:H:76:PHE:HB3	1:H:79:LYS:HG2	1.64	0.79
2:P:281:ASP:OD1	3:P:503:HOH:O	1.99	0.79
2:L:281:ASP:OD2	3:L:503:HOH:O	2.01	0.78
1:F:76:PHE:O	1:F:79:LYS:N	2.16	0.78
2:I:276:LYS:NZ	3:I:503:HOH:O	2.16	0.78
2:K:332:GLU:O	3:K:501:HOH:O	2.02	0.78
2:I:398:HIS:CE1	2:L:171:TRP:CG	2.71	0.78
1:F:77:THR:HG21	1:F:88:VAL:HG21	1.66	0.77
2:P:232:GLU:OE2	2:P:394:ARG:NH2	2.17	0.77
2:J:144:ASP:O	3:J:502:HOH:O	2.02	0.77
2:K:275:ASN:OD1	2:K:375:THR:HB	1.85	0.77
1:H:81:ALA:HA	1:H:83:LYS:HE2	1.67	0.77
1:F:73:LEU:HA	1:F:76:PHE:HB3	1.68	0.76
1:H:71:GLN:HG3	1:H:72:LYS:CG	2.15	0.76
1:H:78:LYS:HG3	1:H:80:LEU:HB3	1.66	0.75
2:K:281:ASP:OD2	3:K:502:HOH:O	2.05	0.75
2:J:104:VAL:N	3:J:510:HOH:O	2.19	0.75
2:L:402:SER:OG	3:L:501:HOH:O	1.91	0.74
1:F:73:LEU:HA	1:F:76:PHE:CB	2.17	0.74
2:J:215:ASP:OD2	3:J:503:HOH:O	2.05	0.74
2:N:396:ARG:NH2	3:N:506:HOH:O	2.21	0.74
1:E:49:GLU:HA	1:E:52:HIS:HA	1.68	0.73
1:E:79:LYS:NZ	1:E:82:GLU:O	2.21	0.73
1:A:70:LYS:O	3:A:201:HOH:O	2.06	0.73
2:J:288:ASN:OD1	3:J:504:HOH:O	2.07	0.73
1:F:42:SER:O	3:F:201:HOH:O	2.06	0.72
2:K:162:LYS:O	3:K:503:HOH:O	2.07	0.72
2:L:274:GLY:H	2:L:375:THR:HG21	1.54	0.72
1:E:47:THR:HA	1:E:50:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:SER:OG	1:E:43:LYS:N	2.23	0.72
1:F:79:LYS:HG3	1:F:80:LEU:H	1.53	0.72
2:O:419:LYS:O	3:O:503:HOH:O	2.08	0.72
2:P:167:THR:OG1	3:P:504:HOH:O	2.06	0.72
2:J:272:SER:HB2	2:J:375:THR:CG2	2.18	0.71
2:I:417:LEU:O	3:I:501:HOH:O	2.07	0.71
2:N:216:SER:HB3	2:N:255:TYR:HE1	1.55	0.71
1:H:78:LYS:HG3	1:H:80:LEU:CB	2.21	0.70
2:J:275:ASN:OD1	2:J:375:THR:HB	1.91	0.70
2:K:142:HIS:ND1	3:K:508:HOH:O	2.24	0.70
2:L:237:SER:HB3	2:L:376:SER:HB2	1.73	0.70
2:P:227:VAL:O	3:P:506:HOH:O	2.09	0.70
1:H:80:LEU:O	1:H:83:LYS:N	2.24	0.69
2:K:272:SER:HB2	2:K:375:THR:HG22	1.73	0.69
1:E:40:ASP:OD2	1:E:84:VAL:HG21	1.91	0.69
2:N:305:ASN:HD22	2:N:324:THR:HG23	1.58	0.69
2:I:245:ASP:OD1	3:I:502:HOH:O	2.11	0.69
1:B:60:GLU:OE1	3:B:204:HOH:O	2.11	0.69
2:N:411:ARG:HD2	2:N:428:TYR:CE1	2.27	0.69
2:P:278:VAL:HG21	2:P:283:MET:HE3	1.75	0.69
1:H:45:LEU:HD11	1:H:57:VAL:HG21	1.74	0.68
2:J:183:PRO:HD2	3:J:577:HOH:O	1.93	0.68
1:H:48:ALA:HA	1:H:51:PHE:HD2	1.58	0.68
2:O:160:ASP:OD1	3:O:504:HOH:O	2.11	0.68
2:K:247:GLU:OE1	3:K:504:HOH:O	2.11	0.68
2:M:276:LYS:NZ	3:M:505:HOH:O	2.26	0.68
2:P:440:MET:O	3:P:507:HOH:O	2.11	0.67
1:E:46:ASP:OD1	1:E:50:GLN:N	2.27	0.67
2:K:272:SER:HB2	2:K:375:THR:CG2	2.25	0.67
1:H:41:LYS:HZ2	1:H:57:VAL:HB	1.59	0.67
2:L:419:LYS:O	3:L:502:HOH:O	2.11	0.67
2:K:165:VAL:O	3:K:503:HOH:O	2.13	0.67
2:M:249:LYS:HD2	3:M:537:HOH:O	1.95	0.67
2:N:332:GLU:OE1	3:N:504:HOH:O	2.13	0.66
2:P:337:ASP:O	3:P:508:HOH:O	2.12	0.66
1:C:71:GLN:O	1:C:73:LEU:N	2.26	0.66
2:M:332:GLU:O	2:M:333:THR:HG23	1.95	0.66
2:O:336:GLN:HE22	2:O:341:ARG:NE	1.94	0.66
2:P:142:HIS:CE1	2:P:395:GLU:HG3	2.31	0.66
1:A:42:SER:OG	3:A:202:HOH:O	2.12	0.66
2:M:183:PRO:HD2	3:M:527:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:ASP:OD1	3:H:201:HOH:O	2.13	0.66
1:F:90:GLU:HG2	1:F:91:LYS:H	1.61	0.65
2:O:331:GLY:O	2:O:333:THR:N	2.30	0.65
1:C:42:SER:OG	3:C:201:HOH:O	2.14	0.65
1:E:46:ASP:OD1	1:E:49:GLU:N	2.30	0.65
1:F:90:GLU:HG2	1:F:91:LYS:N	2.11	0.65
2:P:142:HIS:NE2	2:P:395:GLU:HG3	2.12	0.65
2:K:138:ILE:O	3:K:506:HOH:O	2.15	0.64
2:L:104:VAL:HG22	2:L:105:ILE:HD12	1.80	0.64
2:P:287:GLU:OE2	3:P:509:HOH:O	2.15	0.64
1:A:46:ASP:OD1	3:A:203:HOH:O	2.15	0.63
2:P:337:ASP:HB3	2:P:339:MET:H	1.62	0.63
2:J:201:VAL:HG21	2:J:387:ALA:HB1	1.81	0.63
2:N:220:MET:HE2	2:N:255:TYR:CD1	2.34	0.63
1:G:73:LEU:HD23	1:G:79:LYS:HD3	1.81	0.63
2:I:412:LYS:HB2	2:I:439:MET:HE1	1.80	0.63
1:C:30:GLU:N	3:C:204:HOH:O	2.31	0.63
2:M:344:ASP:OD1	3:M:502:HOH:O	2.15	0.63
1:H:69:GLU:HG3	1:H:71:GLN:HB3	1.81	0.63
2:N:142:HIS:CD2	2:N:391:SER:HB3	2.34	0.62
1:H:31:GLN:HB3	1:H:89:ILE:O	1.98	0.62
1:F:43:LYS:HD3	1:F:83:LYS:HE2	1.81	0.62
1:F:56:ASP:OD2	2:N:221:LYS:NZ	2.30	0.61
2:M:332:GLU:O	2:M:332:GLU:HG3	2.00	0.61
1:B:72:LYS:C	1:B:75:PRO:HD2	2.26	0.61
2:K:237:SER:HB3	2:K:376:SER:HB2	1.82	0.61
1:G:73:LEU:HG	1:G:75:PRO:HD2	1.83	0.61
2:P:215:ASP:OD2	2:P:217:TYR:HB3	2.01	0.61
2:O:106:SER:N	3:O:515:HOH:O	2.33	0.61
2:I:104:VAL:N	3:I:508:HOH:O	2.34	0.60
2:K:342:VAL:HG21	2:K:363:LEU:HD11	1.83	0.60
1:H:80:LEU:HD22	1:H:83:LYS:HD3	1.83	0.60
2:L:435:GLN:HA	2:L:435:GLN:OE1	2.01	0.60
2:J:355:ASP:HA	2:J:367:LYS:HE2	1.84	0.60
1:C:63:PHE:CD2	2:K:220:MET:HE1	2.36	0.60
2:K:164:SER:OG	3:K:507:HOH:O	2.16	0.60
1:H:78:LYS:NZ	1:H:80:LEU:HB2	2.15	0.60
2:I:249:LYS:O	3:I:504:HOH:O	2.16	0.60
2:K:255:TYR:CZ	2:K:293:PRO:HB3	2.36	0.60
1:D:53:ILE:HG23	1:D:67:THR:O	2.02	0.60
2:N:116:ILE:HD12	2:N:366:PRO:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:VAL:HG21	1:G:59:GLU:O	2.01	0.59
1:H:69:GLU:HG3	1:H:71:GLN:CB	2.31	0.59
2:L:117:LEU:O	2:L:120:LYS:HG3	2.02	0.59
2:N:131:ASP:OD2	2:N:134:ARG:HD2	2.01	0.59
1:G:79:LYS:HA	1:G:82:GLU:OE2	2.01	0.59
2:J:319:ARG:NE	3:J:517:HOH:O	2.34	0.59
2:K:255:TYR:CD2	2:K:296:LEU:HD11	2.37	0.59
2:J:146:LYS:NZ	2:J:229:ASP:O	2.33	0.59
1:D:71:GLN:O	1:D:75:PRO:HD3	2.03	0.59
2:M:401:PRO:HG2	3:M:549:HOH:O	2.02	0.59
1:H:83:LYS:HD2	1:H:85:GLY:HA2	1.84	0.59
2:L:266:GLN:OE1	3:L:505:HOH:O	2.17	0.59
2:K:274:GLY:N	2:K:375:THR:HG21	2.13	0.59
1:F:77:THR:HA	1:F:79:LYS:HG2	1.85	0.59
1:H:41:LYS:HD3	1:H:59:GLU:CD	2.28	0.59
1:D:37:HIS:CD2	1:D:39:LYS:H	2.20	0.59
1:F:44:LEU:HD12	1:F:79:LYS:HZ3	1.68	0.59
1:H:41:LYS:HG3	1:H:45:LEU:CD1	2.20	0.59
2:J:417:LEU:O	3:J:506:HOH:O	2.16	0.59
2:L:172:ASN:HA	2:L:207:GLN:HB3	1.84	0.59
1:F:72:LYS:O	1:F:76:PHE:HB2	2.02	0.59
2:L:308:SER:OG	2:L:332:GLU:OE2	2.20	0.58
2:P:255:TYR:HB3	2:P:296:LEU:HD11	1.84	0.58
2:M:334:TYR:HA	3:M:540:HOH:O	2.02	0.58
2:O:109:PRO:HD2	2:O:120:LYS:HE3	1.84	0.58
2:O:336:GLN:NE2	2:O:341:ARG:NE	2.51	0.58
1:E:52:HIS:O	1:E:53:ILE:HD13	2.03	0.58
2:M:340:VAL:N	3:M:510:HOH:O	2.36	0.58
1:E:69:GLU:HG2	1:E:71:GLN:H	1.67	0.58
2:N:342:VAL:HG21	2:N:363:LEU:HD11	1.85	0.58
2:I:357:THR:O	2:I:361:GLN:HG3	2.03	0.58
1:A:43:LYS:HG3	3:A:202:HOH:O	2.04	0.58
2:N:422:LYS:HG3	2:N:428:TYR:CD1	2.39	0.58
2:I:177:LYS:HG3	2:I:178:PRO:HD2	1.86	0.58
1:F:79:LYS:HE2	1:F:80:LEU:CG	2.32	0.58
2:O:274:GLY:N	2:O:375:THR:HG21	2.16	0.57
2:P:157:ASP:CG	2:P:162:LYS:HD2	2.29	0.57
2:M:152:SER:HB2	3:M:527:HOH:O	2.03	0.57
1:F:79:LYS:CG	1:F:80:LEU:H	2.17	0.57
1:G:35:LEU:HD12	1:G:36:GLU:H	1.69	0.57
1:G:43:LYS:O	1:G:83:LYS:HE2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:281:ASP:O	2:P:285:LYS:HG2	2.04	0.57
2:N:419:LYS:HG2	2:N:421:GLY:H	1.70	0.57
1:A:51:PHE:O	1:A:72:LYS:HE3	2.05	0.57
2:K:357:THR:O	2:K:361:GLN:HG2	2.05	0.57
2:N:306:MET:HE3	2:N:329:TYR:HB3	1.87	0.57
2:I:291:HIS:NE2	3:I:506:HOH:O	2.33	0.57
2:K:392:GLU:OE2	2:K:396:ARG:NH2	2.38	0.57
2:M:441:ASN:HB3	3:M:542:HOH:O	2.05	0.57
1:G:82:GLU:OE2	1:G:82:GLU:N	2.38	0.57
2:O:142:HIS:HE2	2:O:395:GLU:CG	2.17	0.57
2:O:255:TYR:HB3	2:O:296:LEU:HD21	1.87	0.57
1:H:50:GLN:O	1:H:50:GLN:HG2	2.03	0.57
2:I:398:HIS:CE1	2:L:171:TRP:CD1	2.93	0.57
1:D:83:LYS:HG2	1:D:84:VAL:HG12	1.87	0.57
2:I:201:VAL:HG11	2:I:387:ALA:HB1	1.86	0.57
2:N:411:ARG:NH1	3:N:505:HOH:O	2.38	0.57
1:G:69:GLU:OE1	1:G:71:GLN:HG3	2.05	0.56
1:A:79:LYS:HA	1:A:82:GLU:HG3	1.87	0.56
2:L:362:MET:HE1	2:M:345:LEU:HD21	1.87	0.56
1:D:37:HIS:HD2	1:D:39:LYS:H	1.54	0.56
1:F:44:LEU:HD12	1:F:79:LYS:NZ	2.20	0.56
1:G:76:PHE:HD1	1:G:79:LYS:HE2	1.69	0.56
2:O:237:SER:HB3	2:O:376:SER:HB2	1.86	0.56
1:D:49:GLU:O	1:D:49:GLU:HG2	2.05	0.56
2:K:145:VAL:HG22	2:K:394:ARG:HH11	1.70	0.56
2:N:255:TYR:CE2	2:N:293:PRO:HB3	2.40	0.56
1:D:38:VAL:HG13	1:D:59:GLU:O	2.06	0.56
2:N:142:HIS:HD2	2:N:391:SER:HB3	1.70	0.56
2:J:137:GLN:O	2:J:137:GLN:HG2	2.05	0.56
2:L:356:ASN:HB2	2:L:360:ASP:OD2	2.06	0.55
2:M:400:LYS:NZ	3:M:515:HOH:O	2.39	0.55
1:E:79:LYS:C	1:E:82:GLU:H	2.14	0.55
2:O:142:HIS:HE2	2:O:395:GLU:HG3	1.71	0.55
2:J:338:GLY:O	3:J:509:HOH:O	2.18	0.55
1:H:36:GLU:OE1	2:P:253:LYS:NZ	2.39	0.55
1:H:46:ASP:C	1:H:48:ALA:N	2.65	0.55
2:M:128:LYS:HE2	2:M:309:ASN:OD1	2.07	0.55
2:P:341:ARG:NE	3:P:505:HOH:O	2.07	0.55
2:J:237:SER:HB3	2:J:376:SER:HB2	1.87	0.55
1:E:46:ASP:HA	1:E:48:ALA:H	1.72	0.55
2:K:319:ARG:O	2:K:422:LYS:HE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:HIS:HD2	1:D:38:VAL:N	2.05	0.54
2:N:423:ASP:OD1	3:N:502:HOH:O	2.18	0.54
2:P:177:LYS:HB2	2:P:178:PRO:HD2	1.89	0.54
2:N:220:MET:HE2	2:N:255:TYR:HD1	1.72	0.54
1:E:34:LEU:HB2	1:E:63:PHE:CE1	2.42	0.54
1:F:61:ILE:O	2:N:257:ARG:NH1	2.41	0.54
2:J:255:TYR:CE2	2:J:293:PRO:HB3	2.43	0.54
2:N:305:ASN:ND2	2:N:324:THR:HG23	2.23	0.54
1:G:47:THR:HA	1:G:50:GLN:OE1	2.07	0.54
2:K:255:TYR:CE2	2:K:293:PRO:HB3	2.43	0.54
2:I:237:SER:HB3	2:I:376:SER:HB2	1.90	0.54
1:F:76:PHE:O	1:F:78:LYS:N	2.42	0.54
2:P:157:ASP:HA	2:P:162:LYS:HG2	1.90	0.54
2:L:274:GLY:N	2:L:375:THR:HG21	2.23	0.53
2:N:216:SER:HB3	2:N:255:TYR:CE1	2.41	0.53
1:G:73:LEU:CD2	1:G:79:LYS:HD3	2.38	0.53
2:O:142:HIS:HE2	2:O:395:GLU:CD	2.16	0.53
2:O:142:HIS:CE1	2:P:105:ILE:HG13	2.44	0.53
1:H:41:LYS:NZ	1:H:57:VAL:HB	2.22	0.53
1:H:72:LYS:C	1:H:73:LEU:HD12	2.33	0.53
1:H:77:THR:O	1:H:78:LYS:HB2	2.08	0.53
1:H:90:GLU:H	2:P:247:GLU:CD	2.16	0.53
2:P:246:ARG:HG3	2:P:247:GLU:HB2	1.90	0.53
2:J:274:GLY:N	2:J:375:THR:HG21	2.11	0.53
2:L:140:ARG:HD3	2:L:200:ASP:OD2	2.08	0.53
1:G:60:GLU:OE1	1:G:60:GLU:N	2.38	0.53
1:G:78:LYS:HG3	1:G:78:LYS:O	2.09	0.53
1:F:45:LEU:N	3:F:201:HOH:O	2.42	0.53
2:O:275:ASN:ND2	3:O:507:HOH:O	2.19	0.53
2:P:246:ARG:CG	2:P:247:GLU:N	2.71	0.53
2:I:113:LEU:HD21	2:I:123:LEU:HD11	1.91	0.53
2:K:356:ASN:HB2	2:K:360:ASP:OD2	2.09	0.53
2:L:108:SER:HB2	2:L:109:PRO:HD2	1.91	0.53
2:M:173:TYR:OH	2:M:225:ASP:OD2	2.22	0.53
1:C:71:GLN:C	1:C:73:LEU:H	2.17	0.53
1:F:47:THR:HG21	1:F:79:LYS:HE3	1.90	0.52
1:A:49:GLU:OE2	3:A:205:HOH:O	2.19	0.52
1:F:48:ALA:HA	1:F:76:PHE:CE1	2.44	0.52
2:J:209:LEU:HD23	2:J:214:GLY:HA3	1.90	0.52
1:E:89:ILE:HD11	2:M:250:VAL:HG12	1.91	0.52
2:M:104:VAL:HG22	2:M:105:ILE:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:333:THR:H	2:I:341:ARG:HH12	1.55	0.52
2:K:361:GLN:NE2	3:K:518:HOH:O	2.42	0.52
1:F:34:LEU:HD11	2:N:257:ARG:NH1	2.25	0.52
1:F:73:LEU:HA	1:F:76:PHE:HB2	1.89	0.52
2:J:172:ASN:HA	2:J:207:GLN:HB3	1.91	0.52
2:P:211:GLU:CD	2:P:211:GLU:H	2.18	0.52
2:I:157:ASP:C	2:I:352:LYS:HZ3	2.13	0.52
1:H:75:PRO:C	1:H:77:THR:H	2.18	0.52
1:A:60:GLU:OE1	3:A:204:HOH:O	2.18	0.52
2:K:146:LYS:HB3	2:K:231:HIS:CD2	2.45	0.52
1:F:54:HIS:HB3	1:F:67:THR:OG1	2.10	0.52
1:G:48:ALA:O	1:G:53:ILE:HB	2.10	0.52
2:O:201:VAL:HG21	2:O:387:ALA:HB1	1.92	0.52
1:D:78:LYS:HA	1:D:81:ALA:HB3	1.92	0.51
2:O:332:GLU:HB3	2:O:335:ASP:OD1	2.09	0.51
1:D:73:LEU:O	1:D:77:THR:HG23	2.10	0.51
1:E:50:GLN:HG3	1:E:51:PHE:CD1	2.45	0.51
2:M:170:GLY:HA2	3:M:521:HOH:O	2.10	0.51
1:G:72:LYS:O	1:G:73:LEU:HB2	2.11	0.51
1:H:74:ALA:O	1:H:77:THR:HB	2.10	0.51
2:L:209:LEU:HD23	2:L:214:GLY:HA3	1.91	0.51
1:G:79:LYS:HA	1:G:82:GLU:CD	2.35	0.51
2:O:232:GLU:OE1	2:O:394:ARG:NH2	2.43	0.51
2:O:396:ARG:HH12	2:O:440:MET:HB3	1.75	0.51
2:P:246:ARG:HG2	2:P:247:GLU:N	2.26	0.51
1:E:82:GLU:CG	1:E:83:LYS:H	2.23	0.51
2:N:211:GLU:H	2:N:211:GLU:CD	2.18	0.51
1:G:43:LYS:C	3:G:502:HOH:O	2.52	0.51
1:F:47:THR:CG2	1:F:79:LYS:HE3	2.40	0.51
1:H:32:TYR:CE1	1:H:65:LYS:HB2	2.46	0.51
2:P:308:SER:O	2:P:309:ASN:HB2	2.09	0.51
2:K:172:ASN:HA	2:K:207:GLN:HB3	1.93	0.51
1:D:50:GLN:O	1:D:51:PHE:HD1	1.94	0.51
1:H:35:LEU:CD1	1:H:44:LEU:HD21	2.32	0.51
2:P:216:SER:O	2:P:220:MET:HG3	2.11	0.51
2:I:419:LYS:NZ	3:I:518:HOH:O	2.42	0.50
1:G:83:LYS:HG2	1:G:84:VAL:HG22	1.93	0.50
1:C:33:LEU:HD12	1:C:66:VAL:HG11	1.91	0.50
2:M:244:LEU:HD11	3:M:525:HOH:O	2.11	0.50
1:A:32:TYR:CE2	1:A:65:LYS:HB2	2.47	0.50
2:O:172:ASN:HA	2:O:207:GLN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:177:LYS:HG2	2:O:178:PRO:O	2.11	0.50
2:O:393:TYR:OH	2:O:399:ARG:NH2	2.44	0.50
2:P:105:ILE:HG22	2:P:106:SER:O	2.12	0.50
2:I:337:ASP:OD2	2:I:341:ARG:NH2	2.44	0.50
2:J:183:PRO:O	2:J:354:LYS:NZ	2.39	0.50
2:J:319:ARG:NH1	3:J:523:HOH:O	2.44	0.50
2:M:201:VAL:HG21	2:M:387:ALA:HB1	1.94	0.50
1:G:73:LEU:HB3	1:G:76:PHE:HB2	1.92	0.50
1:G:80:LEU:HD22	1:G:83:LYS:HE3	1.94	0.50
2:O:245:ASP:O	2:O:249:LYS:HG3	2.11	0.50
2:O:331:GLY:HA2	3:O:506:HOH:O	2.11	0.50
2:I:307:LYS:NZ	3:I:516:HOH:O	2.41	0.50
2:I:143:PRO:HD2	2:L:228:ASN:O	2.12	0.50
2:K:411:ARG:NH1	2:K:412:LYS:NZ	2.60	0.50
1:F:39:LYS:HE3	1:F:39:LYS:HA	1.92	0.50
2:N:394:ARG:HE	2:N:400:LYS:N	2.10	0.50
1:G:33:LEU:HD21	1:G:80:LEU:HD12	1.94	0.50
2:K:382:VAL:HG13	2:K:431:VAL:HG21	1.93	0.49
1:E:76:PHE:CZ	1:E:80:LEU:HD21	2.47	0.49
1:B:38:VAL:N	3:B:206:HOH:O	2.44	0.49
2:M:172:ASN:HA	2:M:207:GLN:HB3	1.93	0.49
2:O:146:LYS:HB3	2:O:231:HIS:CD2	2.46	0.49
1:H:53:ILE:HG22	1:H:54:HIS:H	1.77	0.49
2:I:322:GLU:HG3	3:I:512:HOH:O	2.10	0.49
2:M:255:TYR:HB3	2:M:296:LEU:HD11	1.94	0.49
2:M:432:ARG:NH2	2:M:435:GLN:HG2	2.26	0.49
1:G:61:ILE:HB	2:O:257:ARG:HG3	1.94	0.49
2:O:149:LEU:HD11	2:O:194:ILE:CD1	2.43	0.49
2:O:411:ARG:HD2	2:O:428:TYR:CE1	2.47	0.49
1:H:76:PHE:C	1:H:78:LYS:N	2.67	0.49
2:L:245:ASP:O	2:L:249:LYS:HG3	2.11	0.49
1:H:35:LEU:HB3	3:H:202:HOH:O	2.12	0.49
2:K:177:LYS:N	3:K:512:HOH:O	2.29	0.49
1:D:32:TYR:CE1	1:D:65:LYS:HB2	2.48	0.49
2:O:172:ASN:HB3	2:O:177:LYS:O	2.13	0.49
2:L:146:LYS:HB3	2:L:231:HIS:CD2	2.48	0.49
2:M:334:TYR:HB3	3:M:511:HOH:O	2.13	0.49
1:G:33:LEU:HD12	1:G:34:LEU:N	2.28	0.49
2:O:142:HIS:NE2	2:O:395:GLU:HG3	2.28	0.49
2:P:246:ARG:NH1	2:P:247:GLU:OE1	2.42	0.49
2:I:137:GLN:NE2	2:L:143:PRO:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HD13	1:C:80:LEU:HD21	1.95	0.49
2:P:124:TRP:CD2	2:P:307:LYS:HE2	2.48	0.49
2:P:394:ARG:HH21	2:P:400:LYS:HE3	1.78	0.49
2:L:422:LYS:HD2	2:L:428:TYR:CE1	2.48	0.49
2:J:324:THR:HG22	2:J:430:GLU:HA	1.95	0.49
1:G:32:TYR:CE2	1:G:65:LYS:HB2	2.47	0.49
2:M:104:VAL:HG22	2:M:105:ILE:H	1.76	0.49
1:G:73:LEU:HG	1:G:75:PRO:CD	2.43	0.49
1:G:43:LYS:HB3	1:G:83:LYS:HD2	1.95	0.48
1:H:78:LYS:C	1:H:80:LEU:N	2.71	0.48
2:L:397:HIS:O	2:L:399:ARG:N	2.46	0.48
2:P:360:ASP:HB3	2:P:365:ILE:HB	1.95	0.48
2:I:143:PRO:O	2:I:202:THR:OG1	2.25	0.48
2:M:290:VAL:HG13	2:M:292:LEU:HG	1.95	0.48
1:F:77:THR:O	1:F:77:THR:HG22	2.13	0.48
1:H:73:LEU:HA	1:H:76:PHE:CE1	2.47	0.48
2:N:140:ARG:HD3	2:N:200:ASP:OD2	2.13	0.48
2:N:357:THR:O	2:N:361:GLN:HG3	2.13	0.48
2:O:335:ASP:N	3:O:506:HOH:O	2.17	0.48
1:H:78:LYS:HZ3	1:H:80:LEU:HB2	1.77	0.48
2:P:237:SER:HB3	2:P:376:SER:HB2	1.96	0.48
2:P:172:ASN:HA	2:P:207:GLN:HB3	1.95	0.48
2:P:276:LYS:NZ	3:P:519:HOH:O	2.47	0.48
2:L:190:THR:HG23	2:L:380:PRO:HG3	1.94	0.48
2:M:104:VAL:HG22	2:M:105:ILE:CD1	2.40	0.48
1:F:38:VAL:HG13	1:F:59:GLU:O	2.13	0.48
2:N:107:GLY:HA2	3:N:539:HOH:O	2.14	0.48
2:N:413:SER:HB2	2:N:435:GLN:HB3	1.95	0.48
2:N:422:LYS:CD	2:N:422:LYS:N	2.77	0.48
1:H:44:LEU:HG	1:H:45:LEU:HD12	1.96	0.48
1:E:50:GLN:C	1:E:51:PHE:HD1	2.22	0.47
1:A:72:LYS:C	1:A:75:PRO:HD2	2.38	0.47
2:J:344:ASP:OD1	3:J:512:HOH:O	2.20	0.47
1:D:45:LEU:O	1:D:48:ALA:HB3	2.14	0.47
2:L:422:LYS:HD2	2:L:428:TYR:CZ	2.48	0.47
1:E:76:PHE:CE1	1:E:80:LEU:HD11	2.49	0.47
2:P:243:SER:O	2:P:248:GLY:HA3	2.14	0.47
2:I:190:THR:HG23	2:I:380:PRO:HG3	1.96	0.47
1:G:43:LYS:C	1:G:83:LYS:HE2	2.39	0.47
2:O:142:HIS:NE2	2:O:395:GLU:OE2	2.45	0.47
2:K:411:ARG:NH1	2:K:412:LYS:HZ3	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:LEU:HG	1:E:80:LEU:HD23	1.97	0.47
2:N:339:MET:HA	2:N:339:MET:HE2	1.96	0.47
2:P:107:GLY:HA3	2:P:132:SER:O	2.15	0.47
1:C:61:ILE:HA	3:C:205:HOH:O	2.14	0.47
1:E:82:GLU:HG3	1:E:83:LYS:H	1.80	0.47
2:O:254:ALA:O	2:O:257:ARG:HG2	2.13	0.47
1:B:72:LYS:O	1:B:75:PRO:HD2	2.15	0.47
2:L:371:LEU:HD12	2:L:371:LEU:HA	1.69	0.47
2:M:193:MET:HE1	2:M:348:THR:HA	1.96	0.47
2:P:140:ARG:HD3	2:P:200:ASP:OD2	2.15	0.47
2:P:334:TYR:HB2	2:P:340:VAL:HG22	1.97	0.47
2:P:419:LYS:HA	2:P:419:LYS:HD3	1.72	0.47
2:I:209:LEU:HD23	2:I:214:GLY:HA3	1.97	0.47
2:K:313:PRO:HB2	2:K:334:TYR:CE2	2.50	0.47
1:F:79:LYS:HG3	1:F:80:LEU:HG	1.97	0.47
1:F:89:ILE:HD12	2:N:247:GLU:HB2	1.97	0.47
2:N:138:ILE:C	3:N:509:HOH:O	2.58	0.47
1:H:35:LEU:HD21	1:H:44:LEU:CD2	2.45	0.47
1:G:46:ASP:O	1:G:50:GLN:HB2	2.15	0.47
2:O:337:ASP:N	3:O:509:HOH:O	2.38	0.47
1:E:50:GLN:HG3	1:E:51:PHE:HD1	1.79	0.47
2:N:237:SER:HB3	2:N:376:SER:HB2	1.97	0.47
2:N:255:TYR:HE2	2:N:293:PRO:HB3	1.80	0.47
2:K:223:MET:SD	2:K:255:TYR:CE2	3.08	0.46
1:E:79:LYS:HG2	1:E:82:GLU:HA	1.97	0.46
2:L:308:SER:O	2:L:309:ASN:HB2	2.15	0.46
2:M:382:VAL:HG13	2:M:431:VAL:HG21	1.96	0.46
1:D:77:THR:OG1	1:D:78:LYS:N	2.48	0.46
1:E:80:LEU:C	1:E:82:GLU:N	2.71	0.46
2:I:333:THR:H	2:I:341:ARG:NH1	2.13	0.46
2:K:412:LYS:HA	2:K:412:LYS:HD2	1.57	0.46
2:M:175:ASP:O	2:M:177:LYS:HG3	2.15	0.46
1:G:49:GLU:CD	1:G:49:GLU:H	2.23	0.46
2:K:146:LYS:NZ	2:K:229:ASP:O	2.40	0.46
2:I:245:ASP:O	2:I:249:LYS:HG3	2.15	0.46
2:M:411:ARG:NH1	3:M:506:HOH:O	2.28	0.46
2:O:356:ASN:HB2	2:O:360:ASP:OD2	2.15	0.46
2:I:140:ARG:HG2	2:I:199:PRO:HG2	1.98	0.46
1:E:48:ALA:HB1	1:E:53:ILE:O	2.16	0.46
2:O:341:ARG:CZ	3:O:502:HOH:O	2.50	0.46
1:H:78:LYS:HG3	1:H:80:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:162:LYS:HB3	2:P:162:LYS:HE2	1.74	0.46
1:F:77:THR:CG2	1:F:88:VAL:HG21	2.43	0.46
2:L:373:TYR:CE1	2:M:362:MET:HG3	2.50	0.46
2:L:393:TYR:CD1	2:L:401:PRO:HB3	2.51	0.46
2:I:171:TRP:N	3:I:505:HOH:O	2.27	0.45
1:D:37:HIS:CD2	1:D:38:VAL:N	2.83	0.45
1:F:34:LEU:HD11	2:N:257:ARG:HH12	1.80	0.45
2:O:109:PRO:CD	2:O:120:LYS:HE3	2.45	0.45
2:O:305:ASN:OD1	2:O:324:THR:HG23	2.16	0.45
1:H:78:LYS:CG	1:H:80:LEU:HB3	2.41	0.45
2:J:312:SER:HB3	2:J:314:TYR:CE2	2.51	0.45
2:L:124:TRP:CZ3	2:L:307:LYS:HA	2.51	0.45
2:M:308:SER:O	2:M:309:ASN:HB2	2.17	0.45
2:O:393:TYR:CD1	2:O:401:PRO:HB3	2.51	0.45
1:C:39:LYS:NZ	1:C:40:ASP:OD1	2.49	0.45
2:L:117:LEU:HD12	2:N:420:PRO:HG2	1.98	0.45
2:M:404:LYS:HD2	2:M:404:LYS:HA	1.80	0.45
1:G:73:LEU:HB3	1:G:76:PHE:CB	2.46	0.45
1:H:35:LEU:C	1:H:36:GLU:HG3	2.41	0.45
2:K:308:SER:O	2:K:309:ASN:HB2	2.17	0.45
2:I:329:TYR:CG	2:I:330:LEU:N	2.82	0.45
1:E:34:LEU:HB2	1:E:63:PHE:HE1	1.80	0.45
1:G:35:LEU:HD12	1:G:36:GLU:N	2.30	0.45
2:P:147:VAL:HG11	2:P:194:ILE:HD13	1.98	0.45
2:M:142:HIS:HB3	2:M:144:ASP:OD1	2.17	0.45
2:M:322:GLU:HG2	2:M:422:LYS:HE3	1.98	0.45
2:M:436:ALA:O	2:M:440:MET:HG3	2.16	0.45
1:F:30:GLU:HA	1:F:66:VAL:O	2.15	0.45
1:F:76:PHE:O	1:F:79:LYS:HG2	2.17	0.45
2:O:255:TYR:HB3	2:O:296:LEU:HD11	1.97	0.45
2:P:329:TYR:CD2	2:P:331:GLY:O	2.70	0.45
2:L:397:HIS:C	2:L:399:ARG:H	2.25	0.45
2:N:172:ASN:HA	2:N:207:GLN:HB3	1.98	0.45
1:G:41:LYS:O	1:G:44:LEU:HB3	2.17	0.45
1:A:33:LEU:CD2	1:A:88:VAL:HG22	2.47	0.45
2:L:373:TYR:CD1	2:M:362:MET:HG3	2.52	0.45
2:M:330:LEU:HD22	2:M:345:LEU:HD11	1.99	0.45
1:G:69:GLU:CD	1:G:71:GLN:HG3	2.42	0.45
2:P:167:THR:N	3:P:504:HOH:O	2.23	0.45
2:N:306:MET:HE1	2:N:331:GLY:O	2.17	0.45
1:G:76:PHE:HA	1:G:79:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:296:LEU:O	3:P:510:HOH:O	2.21	0.45
2:K:145:VAL:HG22	2:K:394:ARG:NH1	2.31	0.44
1:E:46:ASP:HA	1:E:48:ALA:N	2.32	0.44
2:O:124:TRP:CD2	2:O:307:LYS:HE2	2.52	0.44
2:O:142:HIS:HB3	2:O:144:ASP:OD1	2.17	0.44
2:P:111:TRP:HH2	2:P:193:MET:HE1	1.82	0.44
2:K:201:VAL:HG21	2:K:387:ALA:HB1	1.98	0.44
2:K:245:ASP:O	2:K:249:LYS:HG3	2.17	0.44
1:D:70:LYS:HA	1:D:73:LEU:HD12	1.99	0.44
2:N:305:ASN:HD22	2:N:324:THR:CG2	2.28	0.44
1:G:40:ASP:OD2	1:G:84:VAL:HG11	2.17	0.44
2:P:305:ASN:OD1	2:P:324:THR:HG23	2.17	0.44
2:I:172:ASN:HA	2:I:207:GLN:HB3	1.99	0.44
2:I:245:ASP:CG	3:I:502:HOH:O	2.58	0.44
2:I:439:MET:HE3	2:I:439:MET:HB3	1.60	0.44
2:K:435:GLN:OE1	2:K:435:GLN:HA	2.17	0.44
2:N:322:GLU:HG3	3:N:515:HOH:O	2.17	0.44
1:H:78:LYS:C	1:H:80:LEU:H	2.26	0.44
1:H:89:ILE:HG12	2:P:247:GLU:HG3	2.00	0.44
2:P:151:ASP:OD2	3:P:511:HOH:O	2.21	0.44
2:J:116:ILE:HD12	2:J:366:PRO:HG3	1.98	0.44
2:N:124:TRP:CZ3	2:N:307:LYS:HA	2.52	0.44
2:I:290:VAL:HG13	2:I:292:LEU:HG	2.00	0.44
1:C:89:ILE:HG23	2:K:247:GLU:HB3	1.97	0.44
2:N:245:ASP:O	2:N:249:LYS:HG3	2.18	0.44
1:G:31:GLN:HB3	1:G:89:ILE:O	2.18	0.44
2:O:393:TYR:CG	2:O:401:PRO:HB3	2.52	0.44
2:J:111:TRP:CZ3	2:J:123:LEU:HD21	2.53	0.44
2:L:243:SER:O	2:L:248:GLY:HA3	2.18	0.44
1:H:80:LEU:HD22	1:H:83:LYS:CB	2.47	0.44
2:J:177:LYS:HB2	2:J:178:PRO:HD2	1.99	0.44
2:J:385:THR:HG23	2:J:433:ALA:HA	2.00	0.44
2:L:255:TYR:HB3	2:L:296:LEU:HD11	1.98	0.44
1:E:43:LYS:HB3	1:E:43:LYS:HE2	1.74	0.44
2:M:397:HIS:HB3	2:M:399:ARG:NH1	2.32	0.44
2:N:411:ARG:HG3	2:N:428:TYR:CD1	2.53	0.44
1:H:83:LYS:HB2	1:H:84:VAL:H	0.93	0.44
2:N:422:LYS:H	2:N:422:LYS:HD3	1.83	0.44
2:K:293:PRO:HD2	3:K:523:HOH:O	2.18	0.44
1:F:89:ILE:HG12	1:F:90:GLU:H	1.83	0.44
2:O:158:HIS:HA	2:O:159:PRO:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:LEU:HB2	1:H:78:LYS:HE2	1.99	0.44
2:J:329:TYR:CG	2:J:330:LEU:N	2.86	0.43
1:D:78:LYS:HA	1:D:81:ALA:CB	2.48	0.43
1:E:53:ILE:HG23	1:E:67:THR:O	2.17	0.43
1:H:32:TYR:HB2	1:H:89:ILE:HB	2.00	0.43
2:L:140:ARG:NH2	3:L:518:HOH:O	2.50	0.43
2:M:245:ASP:O	2:M:249:LYS:HG3	2.18	0.43
2:N:408:HIS:ND1	3:N:505:HOH:O	2.19	0.43
2:N:438:LYS:HE3	2:N:438:LYS:HB3	1.90	0.43
2:P:309:ASN:O	2:P:417:LEU:HD13	2.17	0.43
1:A:61:ILE:HA	3:A:211:HOH:O	2.17	0.43
1:E:33:LEU:HA	1:E:87:ASP:O	2.19	0.43
2:N:212:LYS:HE3	3:N:586:HOH:O	2.18	0.43
2:N:163:ALA:HB3	3:N:564:HOH:O	2.17	0.43
1:G:51:PHE:CD1	1:G:79:LYS:NZ	2.74	0.43
2:K:111:TRP:HH2	2:K:193:MET:HE1	1.83	0.43
2:L:109:PRO:HD3	2:L:133:TYR:CE2	2.53	0.43
1:H:71:GLN:HG3	1:H:72:LYS:HG2	1.95	0.43
2:J:111:TRP:HH2	2:J:193:MET:HE1	1.83	0.43
2:J:322:GLU:HG3	3:J:527:HOH:O	2.19	0.43
1:E:72:LYS:C	1:E:75:PRO:HD2	2.44	0.43
1:F:32:TYR:CE1	1:F:65:LYS:HB2	2.53	0.43
1:F:89:ILE:HG12	1:F:90:GLU:N	2.32	0.43
2:N:436:ALA:O	2:N:440:MET:HG3	2.19	0.43
2:O:396:ARG:HH12	2:O:440:MET:C	2.27	0.43
1:A:53:ILE:HG23	1:A:72:LYS:HE3	2.00	0.43
2:P:146:LYS:HB3	2:P:231:HIS:CD2	2.54	0.43
2:I:161:LEU:O	2:I:165:VAL:HG23	2.18	0.43
1:C:73:LEU:HA	1:C:76:PHE:HB3	2.00	0.43
1:F:41:LYS:HE3	1:F:41:LYS:HB3	1.77	0.43
1:H:44:LEU:C	1:H:46:ASP:HA	2.44	0.43
1:H:84:VAL:HB	1:H:85:GLY:H	1.15	0.43
1:F:88:VAL:O	2:N:247:GLU:OE1	2.37	0.43
2:I:432:ARG:CZ	2:I:435:GLN:HG3	2.49	0.42
1:G:30:GLU:C	1:G:31:GLN:HG3	2.44	0.42
1:G:51:PHE:CE1	1:G:79:LYS:NZ	2.74	0.42
2:O:142:HIS:CE1	2:O:395:GLU:HG3	2.53	0.42
2:O:432:ARG:CZ	2:O:435:GLN:HG3	2.48	0.42
1:H:80:LEU:O	1:H:81:ALA:C	2.60	0.42
2:L:211:GLU:CD	2:L:211:GLU:H	2.27	0.42
2:O:318:GLY:CA	2:O:424:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:LYS:H	1:H:79:LYS:HG3	1.53	0.42
1:A:51:PHE:O	1:A:72:LYS:CE	2.67	0.42
2:I:104:VAL:HG22	2:I:105:ILE:HD12	2.00	0.42
1:B:31:GLN:HG3	1:B:73:LEU:HD13	2.01	0.42
2:L:422:LYS:NZ	3:L:521:HOH:O	2.52	0.42
2:M:225:ASP:HA	3:M:517:HOH:O	2.19	0.42
1:B:52:HIS:O	1:B:52:HIS:ND1	2.51	0.42
1:B:60:GLU:HG2	2:J:261:TYR:CZ	2.55	0.42
1:C:31:GLN:CD	1:C:70:LYS:HZ1	2.27	0.42
2:N:306:MET:HE2	2:N:306:MET:HB3	1.85	0.42
2:O:232:GLU:CD	2:O:394:ARG:NH2	2.78	0.42
1:A:47:THR:HG22	1:A:76:PHE:HD1	1.84	0.42
1:B:70:LYS:C	3:B:203:HOH:O	2.62	0.42
1:D:32:TYR:HB2	1:D:89:ILE:HB	2.02	0.42
1:F:50:GLN:O	1:F:51:PHE:HD1	2.03	0.42
2:O:360:ASP:HB3	2:O:365:ILE:HB	2.00	0.42
2:I:215:ASP:OD2	2:I:217:TYR:HB3	2.20	0.42
2:M:264:LYS:NZ	3:M:513:HOH:O	2.38	0.42
1:H:69:GLU:HG3	1:H:71:GLN:HB2	2.01	0.42
2:P:246:ARG:O	2:P:250:VAL:HG23	2.20	0.42
2:P:411:ARG:HD2	2:P:428:TYR:CE1	2.55	0.42
2:O:308:SER:O	2:O:309:ASN:HB2	2.18	0.42
2:O:317:GLN:OE1	2:O:425:ILE:HG12	2.19	0.42
2:O:411:ARG:HD2	2:O:428:TYR:CZ	2.55	0.42
1:D:46:ASP:O	1:D:50:GLN:HB3	2.20	0.42
2:M:171:TRP:HD1	2:M:173:TYR:CE2	2.38	0.42
1:F:80:LEU:HB3	1:F:84:VAL:HG23	2.02	0.42
2:N:394:ARG:HE	2:N:400:LYS:HB3	1.84	0.42
1:G:78:LYS:O	1:G:82:GLU:OE2	2.37	0.42
1:H:75:PRO:C	1:H:77:THR:N	2.77	0.42
2:J:411:ARG:HD2	2:J:428:TYR:CE1	2.55	0.42
1:C:60:GLU:OE1	1:C:60:GLU:N	2.47	0.42
2:O:142:HIS:HB2	2:O:145:VAL:HG23	2.01	0.42
2:O:328:GLY:N	3:O:508:HOH:O	2.23	0.42
2:I:348:THR:O	2:I:369:TYR:HA	2.19	0.41
2:K:169:GLY:HA3	3:K:642:HOH:O	2.20	0.41
2:L:394:ARG:HA	2:L:399:ARG:O	2.20	0.41
2:M:212:LYS:HE3	2:M:212:LYS:HB2	1.84	0.41
2:M:281:ASP:OD1	2:M:319:ARG:NH1	2.53	0.41
1:F:46:ASP:N	3:F:201:HOH:O	2.05	0.41
2:N:158:HIS:HA	2:N:159:PRO:HD2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HA	1:A:75:PRO:HD2	2.01	0.41
2:M:284:ARG:NE	3:M:525:HOH:O	2.53	0.41
2:P:371:LEU:HA	2:P:371:LEU:HD12	1.85	0.41
2:I:185:GLY:O	2:I:189:GLN:HG3	2.21	0.41
2:K:390:ILE:O	2:K:394:ARG:HG3	2.20	0.41
1:H:39:LYS:O	1:H:39:LYS:HG2	2.20	0.41
2:P:323:PHE:HB3	2:P:431:VAL:HG23	2.02	0.41
2:O:397:HIS:N	2:O:397:HIS:CD2	2.87	0.41
1:C:51:PHE:O	1:C:72:LYS:HB3	2.21	0.41
2:L:396:ARG:HD3	2:L:397:HIS:CE1	2.55	0.41
1:E:41:LYS:O	1:E:42:SER:C	2.63	0.41
1:F:47:THR:HG21	1:F:79:LYS:HB2	2.02	0.41
1:G:35:LEU:CD2	1:G:38:VAL:HA	2.51	0.41
1:G:82:GLU:N	1:G:82:GLU:CD	2.75	0.41
2:I:109:PRO:HD2	2:I:120:LYS:HE2	2.03	0.41
2:L:404:LYS:HE2	2:L:404:LYS:HB3	1.79	0.41
2:N:125:PHE:CG	2:N:126:ALA:N	2.89	0.41
1:H:77:THR:O	1:H:78:LYS:CB	2.67	0.41
2:P:263:ALA:CB	2:P:298:HIS:CD2	3.04	0.41
1:A:78:LYS:NZ	3:A:207:HOH:O	2.37	0.41
2:I:243:SER:O	2:I:248:GLY:HA3	2.21	0.41
2:K:312:SER:HB3	2:K:314:TYR:CE2	2.56	0.41
2:L:324:THR:HG22	2:L:430:GLU:HA	2.01	0.41
2:L:359:LEU:HD13	2:M:330:LEU:HD21	2.02	0.41
2:M:224:VAL:HG13	2:M:261:TYR:CE2	2.55	0.41
2:N:289:LYS:HZ2	2:N:289:LYS:HG2	1.69	0.41
2:N:322:GLU:OE1	2:N:407:HIS:NE2	2.31	0.41
2:P:228:ASN:OD1	2:P:261:TYR:OH	2.23	0.41
2:P:272:SER:HB3	2:P:376:SER:HA	2.03	0.41
2:J:357:THR:O	2:J:361:GLN:HG2	2.21	0.41
1:D:37:HIS:CD2	1:D:37:HIS:C	2.99	0.41
2:N:122:TYR:CD1	2:N:371:LEU:HD11	2.56	0.41
2:O:324:THR:HG22	2:O:430:GLU:HA	2.03	0.41
2:O:412:LYS:HZ2	2:O:412:LYS:HG3	1.78	0.41
1:H:35:LEU:HD11	1:H:44:LEU:CD2	2.34	0.41
1:A:41:LYS:O	1:A:44:LEU:HB3	2.21	0.41
2:K:338:GLY:HA3	3:K:556:HOH:O	2.21	0.41
1:D:62:GLY:HA2	3:D:203:HOH:O	2.20	0.41
1:D:78:LYS:HB3	1:D:78:LYS:HE2	1.88	0.41
2:M:206:TYR:OH	2:M:226:ALA:HA	2.20	0.41
2:N:146:LYS:HB3	2:N:231:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:LEU:HD23	1:G:80:LEU:HA	1.57	0.41
2:O:352:LYS:HB3	3:O:541:HOH:O	2.20	0.41
2:O:396:ARG:HB3	2:O:397:HIS:HD2	1.86	0.41
1:H:46:ASP:C	1:H:48:ALA:H	2.28	0.41
1:A:33:LEU:HD23	1:A:88:VAL:HG22	2.03	0.41
2:I:308:SER:O	2:I:309:ASN:HB2	2.21	0.41
2:J:356:ASN:HB2	2:J:360:ASP:OD2	2.21	0.41
1:D:47:THR:HG22	1:D:76:PHE:CE1	2.56	0.41
2:L:290:VAL:HG13	2:L:292:LEU:HG	2.02	0.41
2:M:281:ASP:HA	3:M:526:HOH:O	2.20	0.41
2:M:305:ASN:OD1	2:M:324:THR:HG23	2.21	0.41
2:N:348:THR:O	2:N:369:TYR:HA	2.20	0.41
1:G:38:VAL:O	1:G:40:ASP:N	2.54	0.41
1:G:48:ALA:C	1:G:50:GLN:H	2.28	0.41
2:P:246:ARG:CG	2:P:247:GLU:HB2	2.50	0.41
1:E:73:LEU:O	1:E:77:THR:HG23	2.21	0.40
2:I:305:ASN:OD1	2:I:324:THR:HG23	2.21	0.40
2:N:393:TYR:HD2	2:N:401:PRO:HD3	1.86	0.40
2:N:419:LYS:O	3:N:502:HOH:O	2.22	0.40
2:O:397:HIS:HB3	2:O:399:ARG:HE	1.86	0.40
2:K:161:LEU:O	2:K:165:VAL:HG23	2.22	0.40
1:D:81:ALA:HA	1:D:84:VAL:O	2.22	0.40
2:M:324:THR:HG22	2:M:430:GLU:HA	2.03	0.40
1:F:80:LEU:O	1:F:83:LYS:N	2.52	0.40
2:P:394:ARG:NE	2:P:400:LYS:HG2	2.37	0.40
2:L:206:TYR:OH	2:L:226:ALA:HA	2.22	0.40
2:M:106:SER:C	3:M:530:HOH:O	2.65	0.40
2:N:411:ARG:HG3	2:N:428:TYR:CG	2.57	0.40
2:O:394:ARG:C	2:P:105:ILE:HD11	2.47	0.40

All (2) 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)
3:J:620:HOH:O	3:O:535:HOH:O[1_455]	2.02	0.18
2:M:434:TYR:OH	2:O:336:GLN:O[1_456]	2.09	0.11

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	59/100 (59%)	59 (100%)	0	0	100	100
1	B	58/100 (58%)	56 (97%)	2 (3%)	0	100	100
1	C	58/100 (58%)	54 (93%)	2 (3%)	2 (3%)	3	1
1	D	58/100 (58%)	54 (93%)	4 (7%)	0	100	100
1	E	59/100 (59%)	53 (90%)	4 (7%)	2 (3%)	3	1
1	F	60/100 (60%)	51 (85%)	6 (10%)	3 (5%)	1	0
1	G	60/100 (60%)	53 (88%)	3 (5%)	4 (7%)	1	0
1	H	60/100 (60%)	44 (73%)	7 (12%)	9 (15%)	0	0
2	I	335/343 (98%)	327 (98%)	8 (2%)	0	100	100
2	J	335/343 (98%)	329 (98%)	6 (2%)	0	100	100
2	K	333/343 (97%)	327 (98%)	5 (2%)	1 (0%)	36	43
2	L	335/343 (98%)	324 (97%)	9 (3%)	2 (1%)	21	24
2	M	329/343 (96%)	321 (98%)	6 (2%)	2 (1%)	21	24
2	N	333/343 (97%)	327 (98%)	6 (2%)	0	100	100
2	O	333/343 (97%)	322 (97%)	9 (3%)	2 (1%)	21	24
2	P	335/343 (98%)	326 (97%)	7 (2%)	2 (1%)	21	24
All	All	3140/3544 (89%)	3027 (96%)	84 (3%)	29 (1%)	14	14

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	LYS
2	L	398	HIS
1	E	42	SER
1	E	82	GLU
2	M	106	SER
1	F	79	LYS

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Mol	Chain	Res	Type
1	G	39	LYS
2	O	337	ASP
1	H	42	SER
1	H	46	ASP
1	H	47	THR
1	H	71	GLN
1	H	83	LYS
2	P	332	GLU
1	G	73	LEU
1	H	41	LYS
1	H	52	HIS
2	L	177	LYS
1	G	48	ALA
1	C	70	LYS
1	H	78	LYS
2	K	177	LYS
1	F	77	THR
1	G	81	ALA
2	P	177	LYS
1	H	84	VAL
1	F	68	GLY
2	M	177	LYS
2	O	331	GLY

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	52/82 (63%)	51 (98%)	1 (2%)	50	65
1	B	51/82 (62%)	50 (98%)	1 (2%)	48	63
1	C	51/82 (62%)	51 (100%)	0	100	100
1	D	50/82 (61%)	46 (92%)	4 (8%)	11	12
1	E	50/82 (61%)	44 (88%)	6 (12%)	5	4
1	F	51/82 (62%)	46 (90%)	5 (10%)	7	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	50/82 (61%)	43 (86%)	7 (14%)	3	3
1	H	51/82 (62%)	42 (82%)	9 (18%)	2	1
2	I	277/283 (98%)	272 (98%)	5 (2%)	51	66
2	J	277/283 (98%)	273 (99%)	4 (1%)	59	73
2	K	275/283 (97%)	271 (98%)	4 (2%)	57	72
2	L	277/283 (98%)	272 (98%)	5 (2%)	51	66
2	M	274/283 (97%)	265 (97%)	9 (3%)	33	44
2	N	275/283 (97%)	269 (98%)	6 (2%)	45	59
2	O	275/283 (97%)	266 (97%)	9 (3%)	33	44
2	P	277/283 (98%)	268 (97%)	9 (3%)	34	46
All	All	2613/2920 (90%)	2529 (97%)	84 (3%)	34	46

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
2	I	104	VAL
2	I	285	LYS
2	I	324	THR
2	I	365	ILE
2	I	424	VAL
1	B	71	GLN
2	J	211	GLU
2	J	285	LYS
2	J	375	THR
2	J	438	LYS
2	K	324	THR
2	K	342	VAL
2	K	375	THR
2	K	412	LYS
1	D	43	LYS
1	D	59	GLU
1	D	78	LYS
1	D	84	VAL
2	L	104	VAL
2	L	211	GLU
2	L	255	TYR
2	L	388	LEU

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Mol	Chain	Res	Type
2	L	435	GLN
1	E	38	VAL
1	E	41	LYS
1	E	43	LYS
1	E	49	GLU
1	E	72	LYS
1	E	78	LYS
2	M	104	VAL
2	M	117	LEU
2	M	118	GLU
2	M	168	ASN
2	M	246	ARG
2	M	250	VAL
2	M	255	TYR
2	M	332	GLU
2	M	412	LYS
1	F	41	LYS
1	F	59	GLU
1	F	72	LYS
1	F	80	LEU
1	F	89	ILE
2	N	137	GLN
2	N	212	LYS
2	N	249	LYS
2	N	400	LYS
2	N	404	LYS
2	N	419	LYS
1	G	41	LYS
1	G	47	THR
1	G	49	GLU
1	G	59	GLU
1	G	73	LEU
1	G	78	LYS
1	G	82	GLU
2	O	149	LEU
2	O	201	VAL
2	O	255	TYR
2	O	257	ARG
2	O	264	LYS
2	O	371	LEU
2	O	397	HIS
2	O	412	LYS

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Mol	Chain	Res	Type
2	O	424	VAL
1	H	38	VAL
1	H	45	LEU
1	H	53	ILE
1	H	71	GLN
1	H	72	LYS
1	H	79	LYS
1	H	80	LEU
1	H	84	VAL
1	H	88	VAL
2	P	104	VAL
2	P	106	SER
2	P	167	THR
2	P	232	GLU
2	P	246	ARG
2	P	249	LYS
2	P	255	TYR
2	P	298	HIS
2	P	341	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	137	GLN
2	I	408	HIS
2	J	189	GLN
2	K	235	ASN
1	D	31	GLN
1	D	37	HIS
2	L	189	GLN
2	L	195	ASN
2	L	298	HIS
1	E	31	GLN
1	E	50	GLN
2	M	408	HIS
1	F	37	HIS
2	N	142	HIS
2	N	235	ASN
2	N	305	ASN
2	N	408	HIS
2	O	235	ASN
2	O	336	GLN

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Mol	Chain	Res	Type
2	O	408	HIS
2	P	189	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	61/100 (61%)	0.52	1 (1%) 70 76	39, 59, 79, 88	0
1	B	60/100 (60%)	0.40	0 100 100	43, 60, 82, 88	0
1	C	60/100 (60%)	0.46	2 (3%) 49 56	44, 60, 79, 90	0
1	D	60/100 (60%)	1.11	8 (13%) 7 8	50, 80, 107, 116	0
1	E	61/100 (61%)	1.91	25 (40%) 0 0	57, 95, 110, 122	0
1	F	62/100 (62%)	1.41	14 (22%) 2 1	57, 92, 110, 115	0
1	G	62/100 (62%)	1.83	28 (45%) 0 0	61, 95, 121, 124	0
1	H	62/100 (62%)	2.23	33 (53%) 0 0	68, 110, 136, 144	0
2	I	337/343 (98%)	-0.26	2 (0%) 85 89	26, 37, 53, 77	0
2	J	337/343 (98%)	-0.21	3 (0%) 81 84	27, 38, 56, 74	0
2	K	335/343 (97%)	-0.16	3 (0%) 81 84	28, 38, 52, 80	0
2	L	337/343 (98%)	0.14	5 (1%) 72 77	33, 45, 63, 119	0
2	M	333/343 (97%)	0.24	11 (3%) 49 56	29, 44, 71, 95	0
2	N	335/343 (97%)	0.20	10 (2%) 52 59	29, 46, 75, 95	0
2	O	335/343 (97%)	0.15	7 (2%) 63 68	30, 47, 72, 103	0
2	P	337/343 (98%)	0.46	9 (2%) 56 63	34, 54, 78, 115	0
All	All	3174/3544 (89%)	0.25	161 (5%) 33 39	26, 46, 95, 144	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	84	VAL	6.4
2	P	104	VAL	6.4
2	M	105	ILE	6.2
2	M	104	VAL	5.4
2	P	105	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
2	L	104	VAL	4.9
1	H	75	PRO	4.7
2	M	106	SER	4.6
1	E	44	LEU	4.6
2	L	105	ILE	4.5
1	H	53	ILE	4.2
1	H	51	PHE	4.1
1	E	53	ILE	4.1
1	G	73	LEU	4.0
2	P	106	SER	3.8
1	H	86	ALA	3.8
1	H	76	PHE	3.8
1	G	44	LEU	3.8
1	E	73	LEU	3.7
1	E	45	LEU	3.7
2	K	255	TYR	3.7
1	H	35	LEU	3.6
1	E	84	VAL	3.6
1	H	33	LEU	3.6
2	O	336	GLN	3.6
1	H	38	VAL	3.6
1	H	74	ALA	3.6
2	K	394	ARG	3.5
1	H	47	THR	3.5
1	F	84	VAL	3.5
1	G	51	PHE	3.5
1	F	89	ILE	3.4
2	I	104	VAL	3.4
1	H	73	LEU	3.4
1	E	51	PHE	3.3
2	N	255	TYR	3.3
2	O	334	TYR	3.3
1	E	86	ALA	3.2
1	G	74	ALA	3.2
2	N	247	GLU	3.2
2	M	334	TYR	3.2
1	G	77	THR	3.2
2	N	393	TYR	3.2
1	H	81	ALA	3.1
2	L	398	HIS	3.1
2	N	397	HIS	3.1
2	M	332	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	76	PHE	3.0
1	D	70	LYS	3.0
1	G	80	LEU	3.0
1	G	53	ILE	3.0
1	H	85	GLY	3.0
1	E	63	PHE	3.0
1	H	45	LEU	3.0
1	E	89	ILE	3.0
1	D	68	GLY	3.0
1	G	84	VAL	2.9
1	H	80	LEU	2.9
2	M	362	MET	2.9
1	F	77	THR	2.9
1	F	75	PRO	2.8
1	G	76	PHE	2.8
1	F	70	LYS	2.8
2	K	106	SER	2.8
1	H	37	HIS	2.8
1	F	51	PHE	2.8
2	N	403	ALA	2.8
1	E	77	THR	2.8
1	D	85	GLY	2.8
1	E	33	LEU	2.8
1	A	72	LYS	2.8
1	H	72	LYS	2.8
1	H	78	LYS	2.8
2	J	105	ILE	2.7
2	L	106	SER	2.7
1	G	55	ALA	2.7
1	D	51	PHE	2.7
1	G	38	VAL	2.7
1	E	80	LEU	2.7
1	H	44	LEU	2.7
2	N	398	HIS	2.7
1	H	55	ALA	2.7
2	O	333	THR	2.7
1	F	73	LEU	2.7
1	E	52	HIS	2.6
1	G	70	LYS	2.6
1	F	80	LEU	2.6
1	F	91	LYS	2.6
1	E	74	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	68	GLY	2.6
1	F	53	ILE	2.6
1	E	35	LEU	2.6
1	E	57	VAL	2.6
1	D	73	LEU	2.5
1	E	88	VAL	2.5
1	H	79	LYS	2.5
1	G	67	THR	2.5
1	G	86	ALA	2.5
1	G	52	HIS	2.5
2	N	401	PRO	2.5
1	G	91	LYS	2.5
2	P	419	LYS	2.5
2	P	298	HIS	2.5
2	N	396	ARG	2.4
1	G	88	VAL	2.4
2	O	438	LYS	2.4
2	O	335	ASP	2.4
1	G	68	GLY	2.4
2	M	267	VAL	2.4
2	M	340	VAL	2.4
1	G	72	LYS	2.4
1	H	83	LYS	2.4
1	G	35	LEU	2.4
1	E	78	LYS	2.3
2	P	169	GLY	2.3
1	H	66	VAL	2.3
1	F	45	LEU	2.3
1	G	33	LEU	2.3
1	G	83	LYS	2.3
2	I	106	SER	2.3
1	E	38	VAL	2.3
1	C	68	GLY	2.3
2	L	176	GLY	2.3
1	D	84	VAL	2.3
1	C	89	ILE	2.2
1	G	75	PRO	2.2
1	E	85	GLY	2.2
2	J	169	GLY	2.2
2	O	331	GLY	2.2
2	P	107	GLY	2.2
1	H	54	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	43	LYS	2.2
1	G	50	GLN	2.2
2	M	258	ALA	2.2
1	E	61	ILE	2.2
2	N	244	LEU	2.2
2	M	169	GLY	2.2
1	H	89	ILE	2.2
1	E	83	LYS	2.2
1	G	69	GLU	2.2
1	H	52	HIS	2.2
1	H	42	SER	2.2
1	F	88	VAL	2.1
1	G	66	VAL	2.1
1	H	39	LYS	2.1
1	G	47	THR	2.1
1	H	67	THR	2.1
1	D	33	LEU	2.1
2	M	330	LEU	2.1
1	F	86	ALA	2.1
2	P	148	ALA	2.1
1	D	37	HIS	2.1
2	O	439	MET	2.1
2	J	211	GLU	2.1
1	E	54	HIS	2.1
1	G	61	ILE	2.1
1	H	40	ASP	2.1
1	F	68	GLY	2.1
2	N	399	ARG	2.0
1	H	77	THR	2.0
2	P	246	ARG	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.