



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:06 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 wwPDB X-ray Structure Validation Summary 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

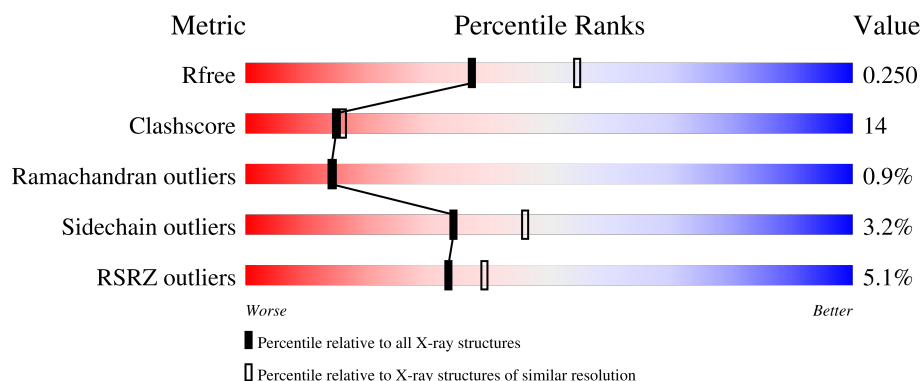
1 Overall quality at a glance

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 [i](#)

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			

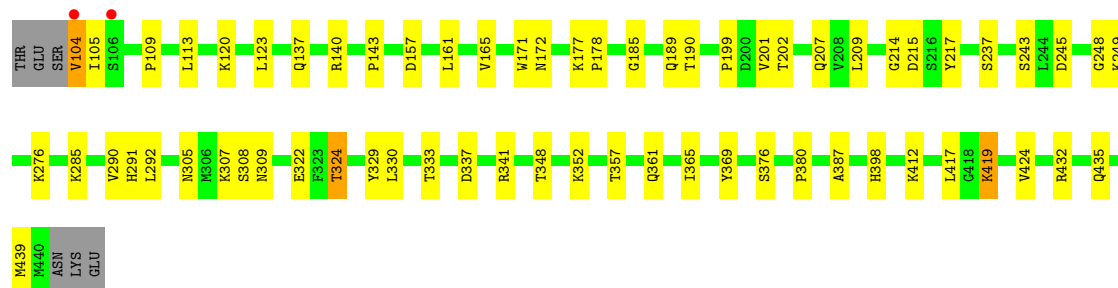
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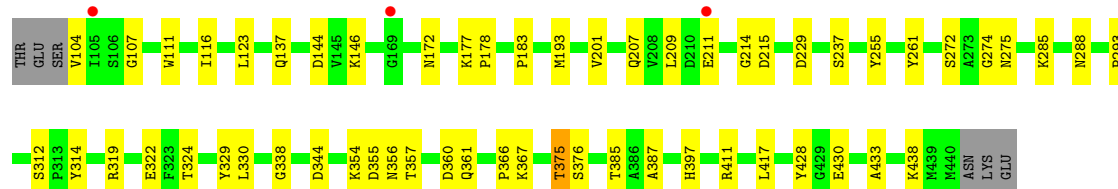
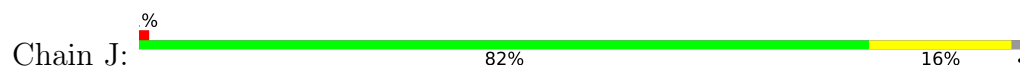
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	335	Total	C	N	O	S	0	0	0
			2571	1612	449	500	10			
2	P	337	Total	C	N	O	S	0	0	0
			2586	1623	451	502	10			

- Molecule 3 is water.

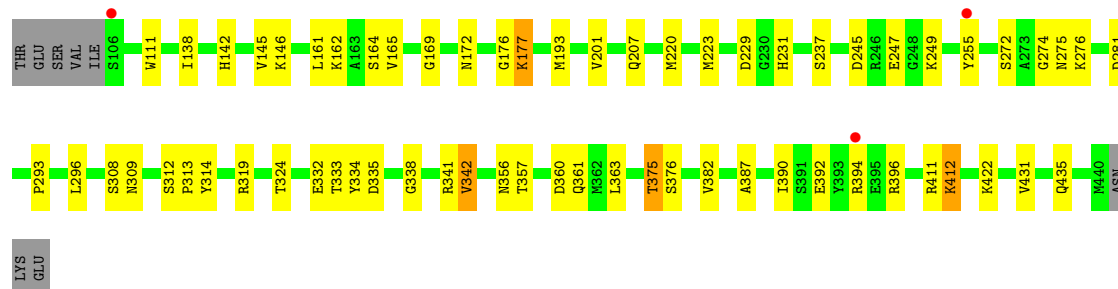
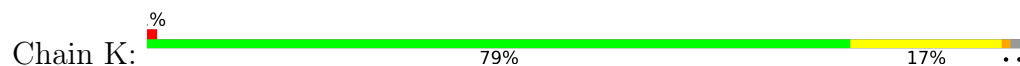
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	I	176	Total	O	0	0
			176	176		
3	B	20	Total	O	0	0
			20	20		
3	J	150	Total	O	0	0
			150	150		
3	C	21	Total	O	0	0
			21	21		
3	K	164	Total	O	0	0
			164	164		
3	D	4	Total	O	0	0
			4	4		
3	L	98	Total	O	0	0
			98	98		
3	E	9	Total	O	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		



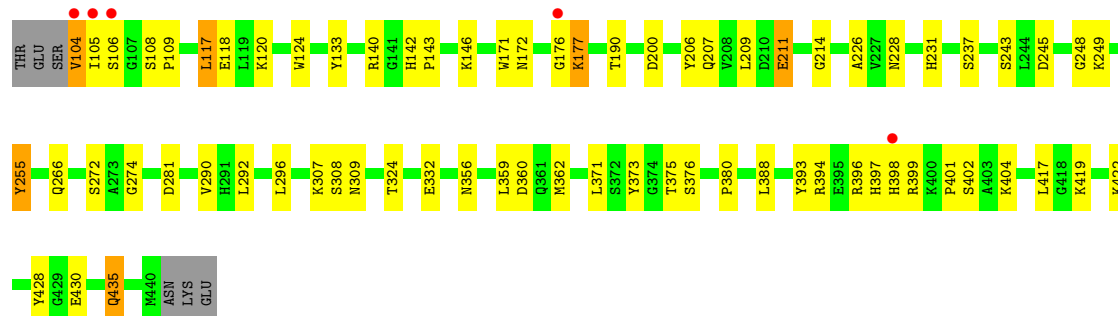
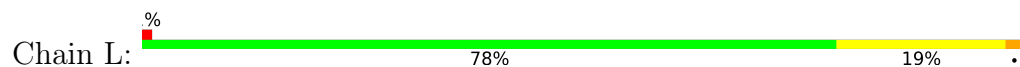
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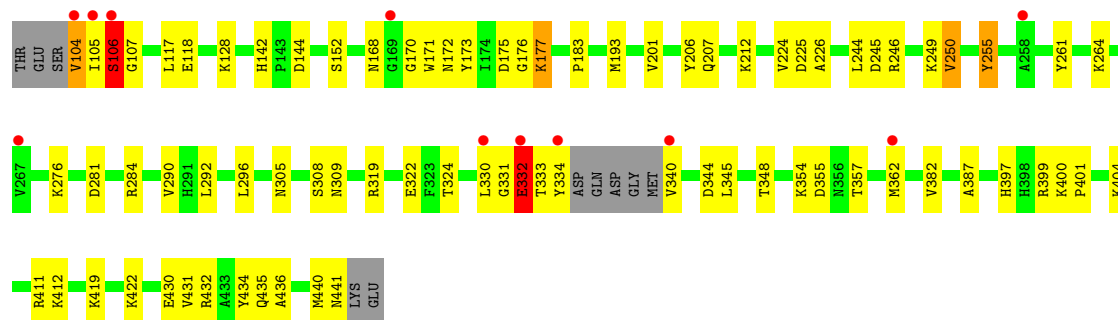
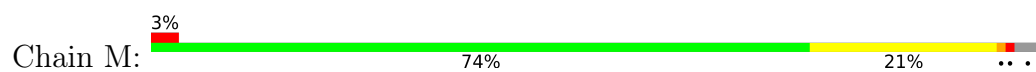
- Molecule 2: Intracellular serine protease



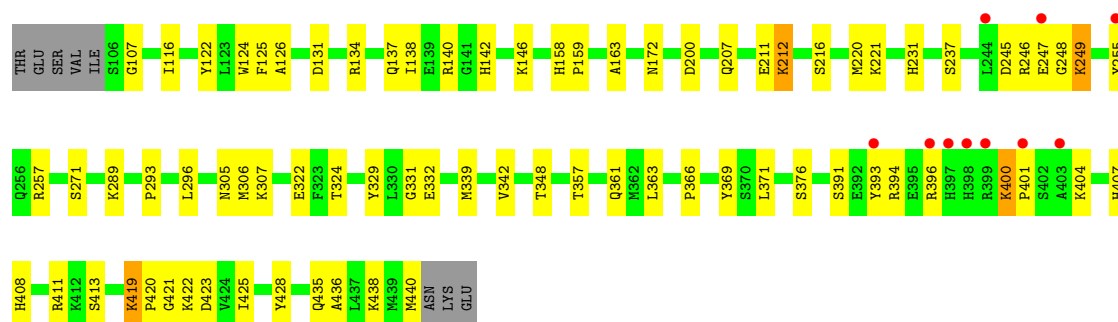
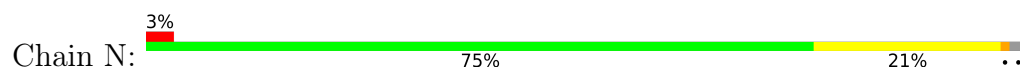
- Molecule 2: Intracellular serine protease



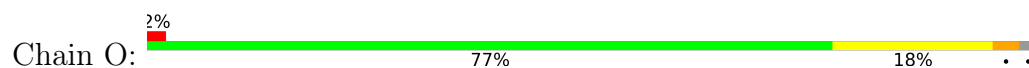
- Molecule 2: Intracellular serine protease



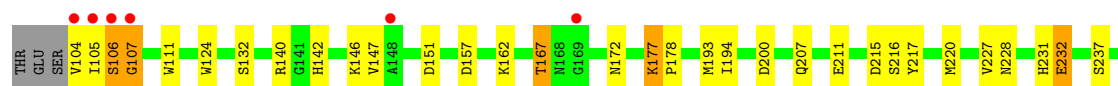
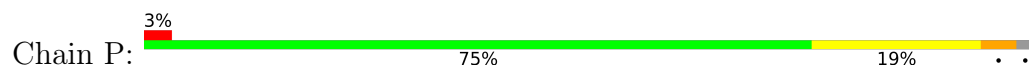
• Molecule 2: Intracellular serine protease

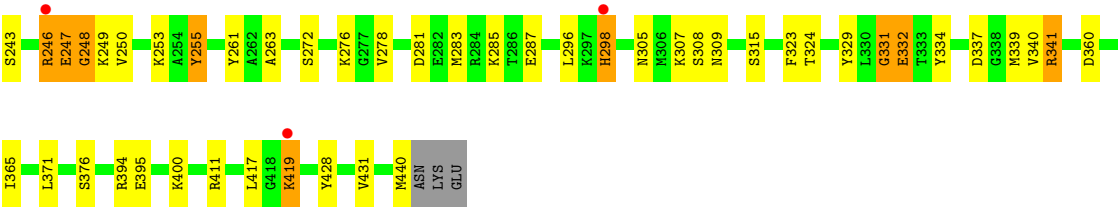


• Molecule 2: Intracellular serine protease



• 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

The worst 5 of 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

There are no chirality outliers.

5 of 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
2	L	118	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

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 [i](#)

5.3.1 Protein backbone [i](#)

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

5 of 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

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
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

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	149	LEU

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Mol	Chain	Res	Type
1	H	79	LYS
2	O	255	TYR
2	O	424	VAL
2	P	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	235	ASN
2	O	235	ASN
2	P	189	GLN
2	O	336	GLN
2	N	408	HIS

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

The worst 5 of 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

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

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

6.3 Carbohydrates [i](#)

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.