



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:15 PM UTC

PDB ID : 3UQ5 / pdb_00003uq5
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) mutant L240A F247L (L9A F16L) in the presence of 10 mM cysteamine
Authors : Gonzalez-Gutierrez, G.; Lukk, T.; Agarwal, V.; Papke, D.; Nair, S.K.; Grosman, C.
Deposited on : 2011-11-19
Resolution : 4.20 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

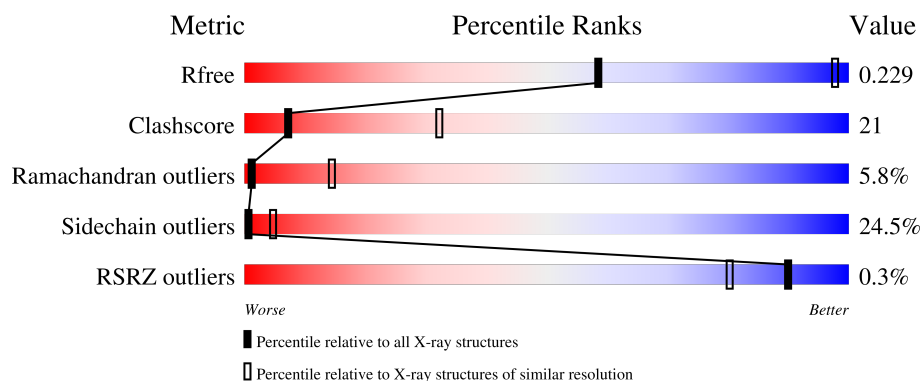
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	324	42% 38% 14% • 5%
1	B	324	39% 40% 15% • 5%
1	C	324	% 41% 38% 14% • 5%
1	D	324	41% 39% 14% • 5%
1	E	324	41% 39% 13% • 5%

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Mol	Chain	Length	Quality of chain
1	F	324	42%37%14%5%
1	G	324	41%39%13%5%
1	H	324	42%38%14%5%
1	I	324	%39%39%15%5%
1	J	324	41%38%15%5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24991 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 Gamma-aminobutyric-acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP E0SJQ4
A	0	SER	-	expression tag	UNP E0SJQ4
A	240	ALA	LEU	engineered mutation	UNP E0SJQ4
A	247	LEU	PHE	engineered mutation	UNP E0SJQ4
B	-1	GLY	-	expression tag	UNP E0SJQ4
B	0	SER	-	expression tag	UNP E0SJQ4
B	240	ALA	LEU	engineered mutation	UNP E0SJQ4
B	247	LEU	PHE	engineered mutation	UNP E0SJQ4
C	-1	GLY	-	expression tag	UNP E0SJQ4

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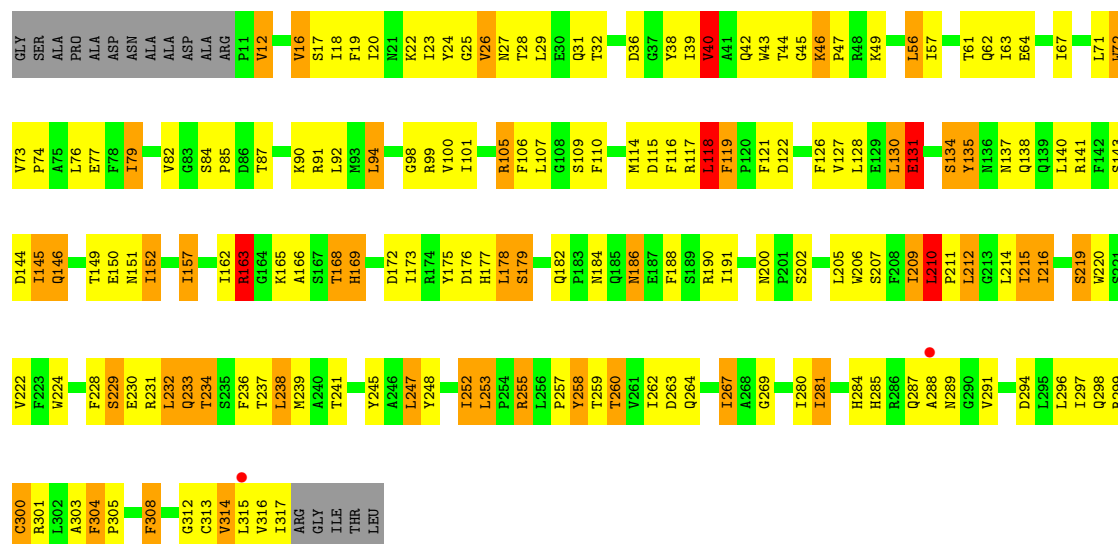
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP E0SJQ4
C	240	ALA	LEU	engineered mutation	UNP E0SJQ4
C	247	LEU	PHE	engineered mutation	UNP E0SJQ4
D	-1	GLY	-	expression tag	UNP E0SJQ4
D	0	SER	-	expression tag	UNP E0SJQ4
D	240	ALA	LEU	engineered mutation	UNP E0SJQ4
D	247	LEU	PHE	engineered mutation	UNP E0SJQ4
E	-1	GLY	-	expression tag	UNP E0SJQ4
E	0	SER	-	expression tag	UNP E0SJQ4
E	240	ALA	LEU	engineered mutation	UNP E0SJQ4
E	247	LEU	PHE	engineered mutation	UNP E0SJQ4
F	-1	GLY	-	expression tag	UNP E0SJQ4
F	0	SER	-	expression tag	UNP E0SJQ4
F	240	ALA	LEU	engineered mutation	UNP E0SJQ4
F	247	LEU	PHE	engineered mutation	UNP E0SJQ4
G	-1	GLY	-	expression tag	UNP E0SJQ4
G	0	SER	-	expression tag	UNP E0SJQ4
G	240	ALA	LEU	engineered mutation	UNP E0SJQ4
G	247	LEU	PHE	engineered mutation	UNP E0SJQ4
H	-1	GLY	-	expression tag	UNP E0SJQ4
H	0	SER	-	expression tag	UNP E0SJQ4
H	240	ALA	LEU	engineered mutation	UNP E0SJQ4
H	247	LEU	PHE	engineered mutation	UNP E0SJQ4
I	-1	GLY	-	expression tag	UNP E0SJQ4
I	0	SER	-	expression tag	UNP E0SJQ4
I	240	ALA	LEU	engineered mutation	UNP E0SJQ4
I	247	LEU	PHE	engineered mutation	UNP E0SJQ4
J	-1	GLY	-	expression tag	UNP E0SJQ4
J	0	SER	-	expression tag	UNP E0SJQ4
J	240	ALA	LEU	engineered mutation	UNP E0SJQ4
J	247	LEU	PHE	engineered mutation	UNP E0SJQ4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

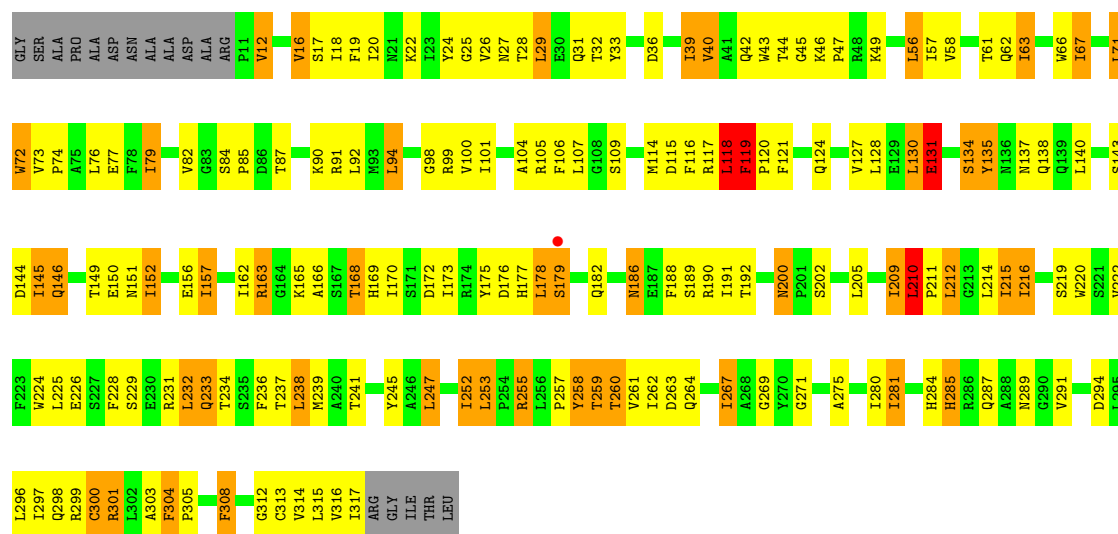
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Na 1 1	0	0



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

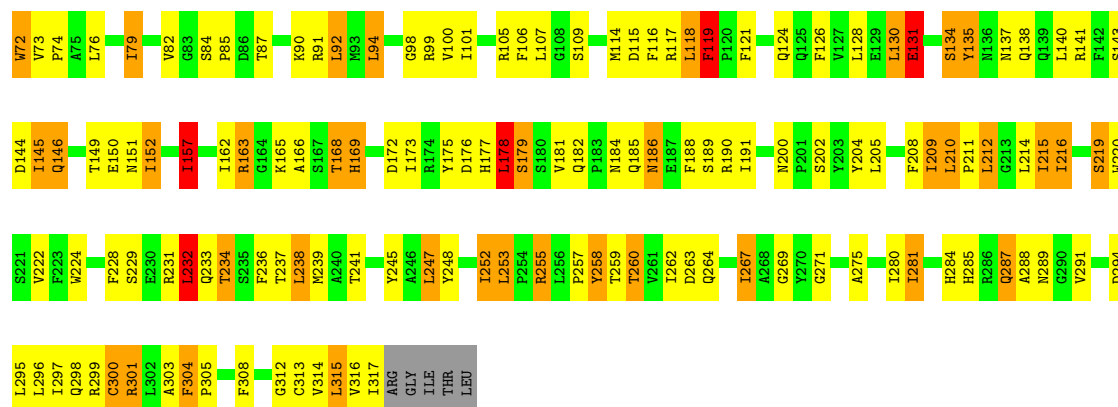


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



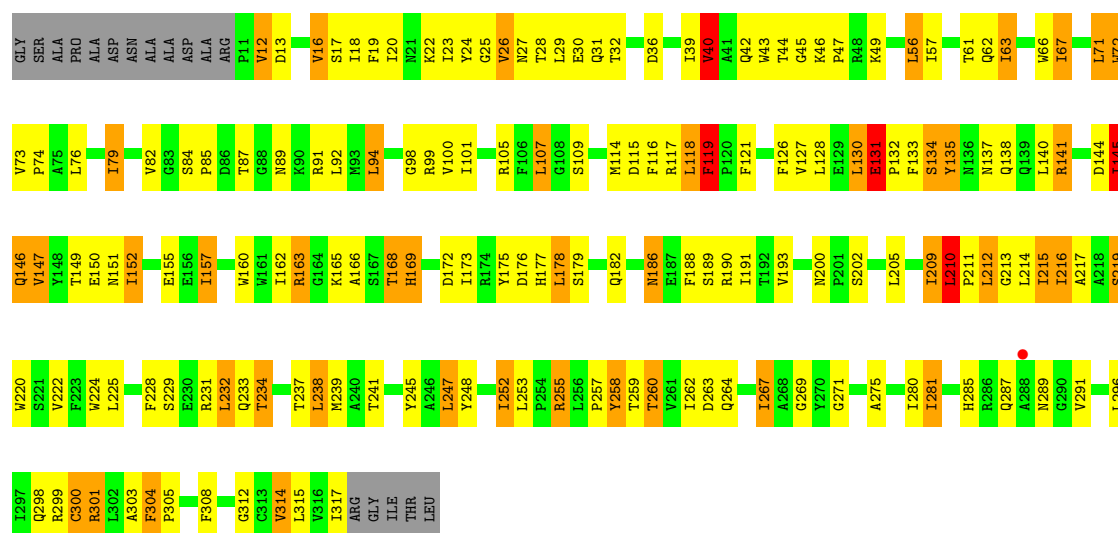
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1





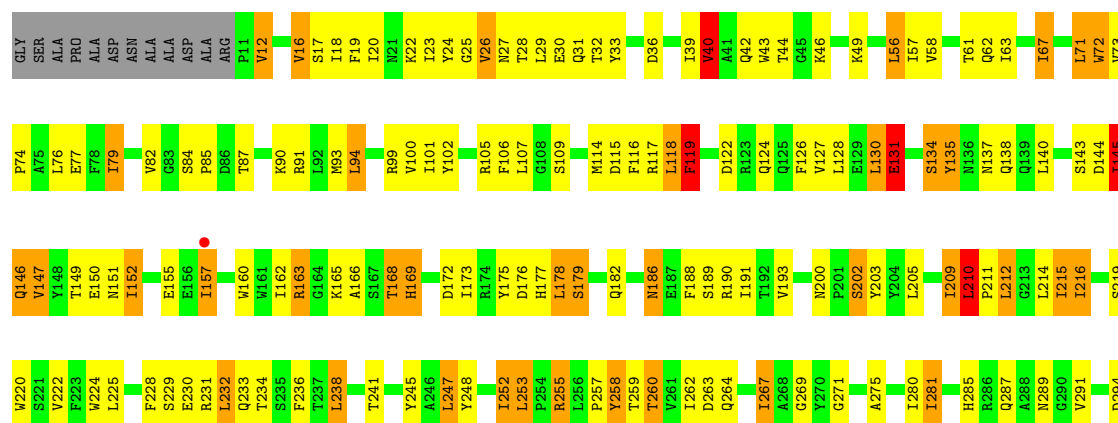
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain F: 42% 37% 14% 5%



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

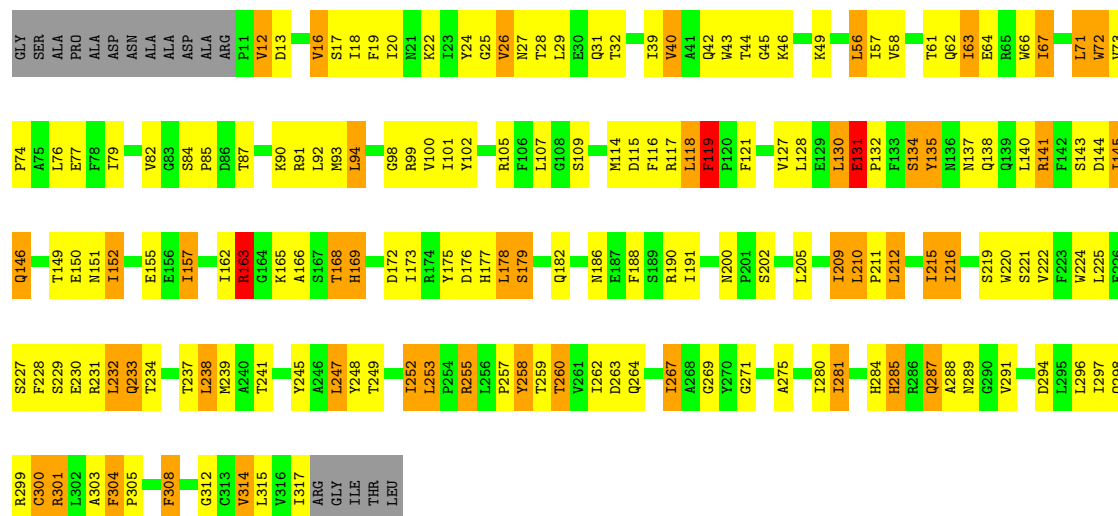
Chain G: 41% 39% 13% 5%





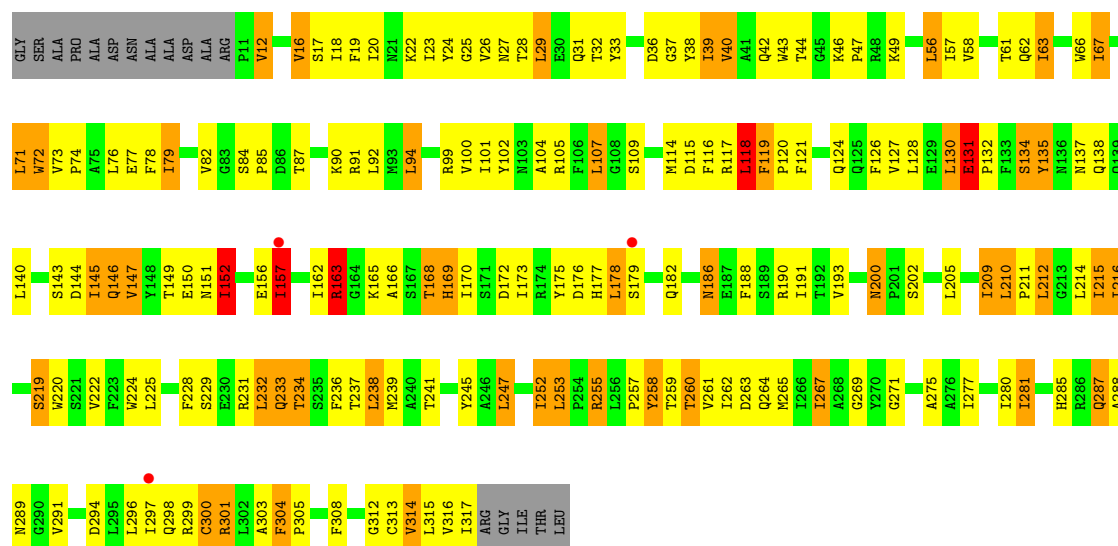
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain H: 42% 38% 14% 5%



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain I: 39% 39% 15% 5%



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain J: 41% 38% 15% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.57Å 267.43Å 111.16Å 90.00° 108.64° 90.00°	Depositor
Resolution (Å)	19.99 – 4.20 19.99 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-4.20) 98.9 (19.99-4.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 4.21Å)	Xtriage
Refinement program	PHENIX dev_897, REFMAC	Depositor
R, R_{free}	0.220 , 0.249 0.200 , 0.229	Depositor DCC
R_{free} test set	2103 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	117.0	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24991	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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:
NA

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	0.69	0/2566	1.12	15/3498 (0.4%)
1	B	0.75	0/2566	1.17	21/3498 (0.6%)
1	C	0.74	1/2566 (0.0%)	1.14	22/3498 (0.6%)
1	D	0.75	0/2566	1.16	20/3498 (0.6%)
1	E	0.72	0/2566	1.13	20/3498 (0.6%)
1	F	0.73	0/2566	1.14	20/3498 (0.6%)
1	G	0.73	0/2566	1.15	25/3498 (0.7%)
1	H	0.74	0/2566	1.14	17/3498 (0.5%)
1	I	0.76	0/2566	1.18	18/3498 (0.5%)
1	J	0.75	1/2566 (0.0%)	1.15	18/3498 (0.5%)
All	All	0.74	2/25660 (0.0%)	1.15	196/34980 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	288	ALA	CA-CB	-6.20	1.44	1.53
1	J	149	THR	CA-CB	5.12	1.61	1.53

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	12	VAL	N-CA-C	10.66	123.26	109.30
1	B	12	VAL	N-CA-C	9.57	122.29	109.37
1	D	12	VAL	N-CA-C	9.12	121.68	109.37
1	I	12	VAL	CB-CA-C	-8.00	99.07	111.71
1	G	238	LEU	N-CA-C	-7.55	104.59	113.88

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASN	Peptide
1	B	137	ASN	Peptide
1	C	137	ASN	Peptide
1	D	137	ASN	Peptide
1	E	137	ASN	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	2499	0	2474	109	0
1	B	2499	0	2474	124	0
1	C	2499	0	2474	114	0
1	D	2499	0	2474	118	0
1	E	2499	0	2474	106	0
1	F	2499	0	2474	106	0
1	G	2499	0	2473	112	0
1	H	2499	0	2473	111	0
1	I	2499	0	2473	126	0
1	J	2499	0	2474	115	0
2	F	1	0	0	0	0
All	All	24991	0	24737	1027	0

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 21.

The worst 5 of 1027 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:J:62:GLN:HE21	1:J:62:GLN:HA	1.10	1.10
1:D:140:LEU:HD22	1:D:191:ILE:HD11	1.52	0.91
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.38	0.89
1:H:224:TRP:HE1	1:H:301:ARG:HB3	1.38	0.89
1:C:224:TRP:HE1	1:C:301:ARG:HB3	1.38	0.87

There are no symmetry-related clashes.

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	305/324 (94%)	235 (77%)	53 (17%)	17 (6%)	1	15
1	B	305/324 (94%)	230 (75%)	56 (18%)	19 (6%)	1	13
1	C	305/324 (94%)	233 (76%)	56 (18%)	16 (5%)	1	16
1	D	305/324 (94%)	233 (76%)	55 (18%)	17 (6%)	1	15
1	E	305/324 (94%)	235 (77%)	50 (16%)	20 (7%)	1	12
1	F	305/324 (94%)	235 (77%)	51 (17%)	19 (6%)	1	13
1	G	305/324 (94%)	232 (76%)	57 (19%)	16 (5%)	1	16
1	H	305/324 (94%)	234 (77%)	52 (17%)	19 (6%)	1	13
1	I	305/324 (94%)	235 (77%)	55 (18%)	15 (5%)	1	16
1	J	305/324 (94%)	232 (76%)	55 (18%)	18 (6%)	1	14
All	All	3050/3240 (94%)	2334 (76%)	540 (18%)	176 (6%)	1	14

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	169	HIS
1	A	202	SER
1	B	119	PHE
1	B	151	ASN

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	274/284 (96%)	206 (75%)	68 (25%)	1	4
1	B	274/284 (96%)	205 (75%)	69 (25%)	0	4
1	C	274/284 (96%)	206 (75%)	68 (25%)	1	4
1	D	274/284 (96%)	208 (76%)	66 (24%)	1	5
1	E	274/284 (96%)	206 (75%)	68 (25%)	1	4
1	F	274/284 (96%)	208 (76%)	66 (24%)	1	5
1	G	274/284 (96%)	209 (76%)	65 (24%)	1	5
1	H	274/284 (96%)	208 (76%)	66 (24%)	1	5
1	I	274/284 (96%)	206 (75%)	68 (25%)	1	4
1	J	274/284 (96%)	206 (75%)	68 (25%)	1	4
All	All	2740/2840 (96%)	2068 (76%)	672 (24%)	1	5

5 of 672 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	281	ILE
1	I	168	THR
1	H	39	ILE
1	G	267	ILE
1	H	247	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	264	GLN
1	I	284	HIS
1	G	284	HIS
1	H	284	HIS
1	J	68	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	307/324 (94%)	-0.39	1 (0%) 90 80	83, 137, 287, 353	0
1	B	307/324 (94%)	-0.33	1 (0%) 90 80	80, 134, 284, 357	0
1	C	307/324 (94%)	-0.37	2 (0%) 84 70	80, 135, 285, 355	0
1	D	307/324 (94%)	-0.29	1 (0%) 90 80	79, 135, 285, 354	0
1	E	307/324 (94%)	-0.35	0 100 100	79, 138, 287, 356	0
1	F	307/324 (94%)	-0.37	1 (0%) 90 80	81, 137, 284, 360	0
1	G	307/324 (94%)	-0.39	1 (0%) 90 80	81, 135, 281, 354	0
1	H	307/324 (94%)	-0.37	0 100 100	82, 136, 286, 357	0
1	I	307/324 (94%)	-0.30	3 (0%) 79 63	80, 135, 286, 351	0
1	J	307/324 (94%)	-0.38	0 100 100	81, 136, 282, 356	0
All	All	3070/3240 (94%)	-0.35	10 (0%) 90 80	79, 136, 287, 360	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	SER	4.5
1	B	315	LEU	4.2
1	A	179	SER	4.0
1	I	157	ILE	3.0
1	I	297	ILE	2.4

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	NA	F	323	1/1	0.99	0.17	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.