wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 09:27 PM EDT

PDB ID	:	5LID
Title	:	X-ray structure of a pentameric ligand gated ion channel from Erwinia chrysanthemi (ELIC) in complex with bromopromazine
Authors	:	Nys, M.; Wijckmans, E.; Farinha, A.; Brams, M.; Spurny, R.; Ulens, C.
Deposited on	:	2016-07-14
Resolution	:	4.50 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 (i) 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 (1)) were used in the production of this report:

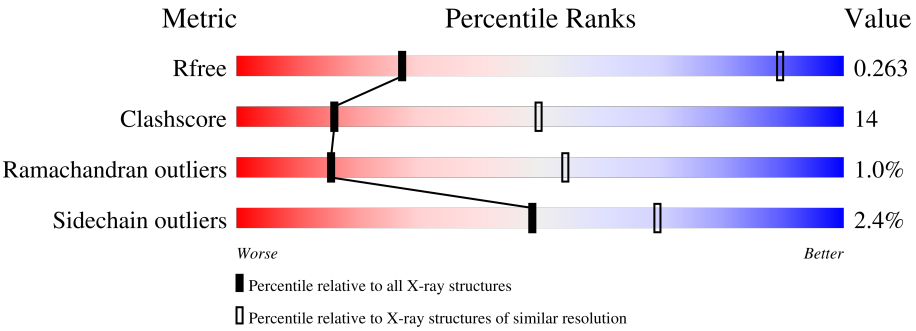
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	307	73% 25% ·
1	B	307	65% 33% ·
1	C	307	65% 33% ··
1	D	307	66% 32% ·
1	E	307	64% 34% ·
1	F	307	68% 32%
1	G	307	65% 33% ·

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Mol	Chain	Length	Quality of chain
1	H	307	64% 36%
1	I	307	65% 34%
1	J	307	67% 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25070 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7

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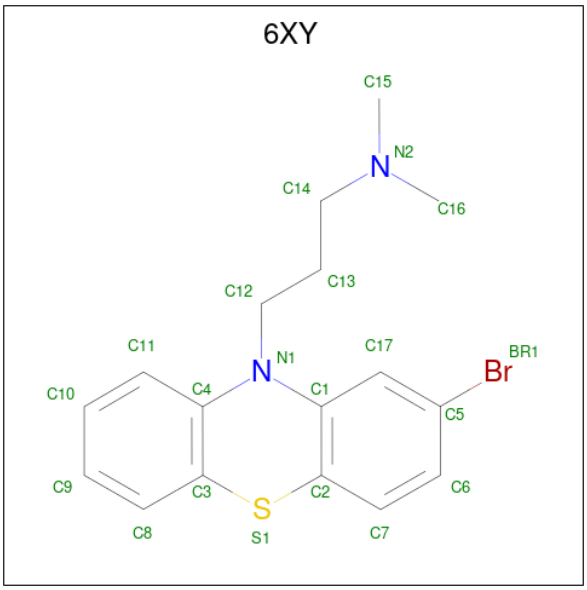
Chain	Residue	Modelled	Actual	Comment	Reference
E	289	ASN	MET	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is bromopromazine (three-letter code: 6XY) (formula: $C_{17}H_{19}BrN_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br 1 1	0	0
2	A	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	C	1	Total Br 1 1	0	0
2	C	1	Total Br 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Br 1 1	0	0
2	D	1	Total Br 1 1	0	0
2	E	1	Total Br 1 1	0	0
2	E	1	Total Br 1 1	0	0
2	F	1	Total Br 1 1	0	0
2	F	1	Total Br 1 1	0	0
2	G	1	Total Br 1 1	0	0
2	G	1	Total Br 1 1	0	0
2	H	1	Total Br 1 1	0	0
2	H	1	Total Br 1 1	0	0
2	I	1	Total Br 1 1	0	0
2	I	1	Total Br 1 1	0	0
2	J	1	Total Br 1 1	0	0
2	J	1	Total Br 1 1	0	0

3 Residue-property plots (i)

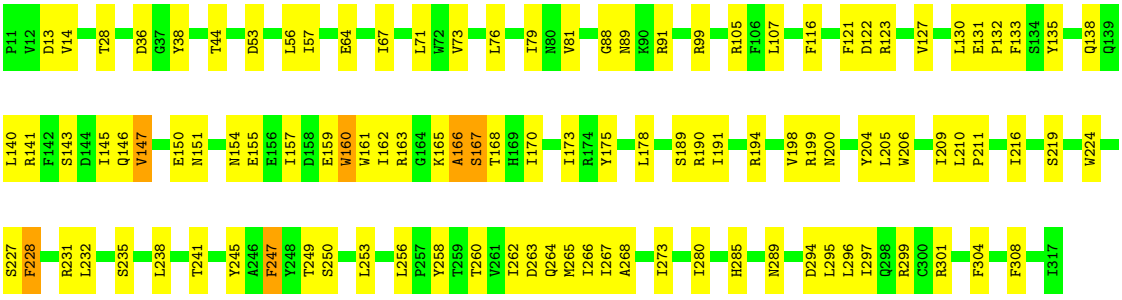
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Cys-loop ligand-gated ion channel

Chain A:

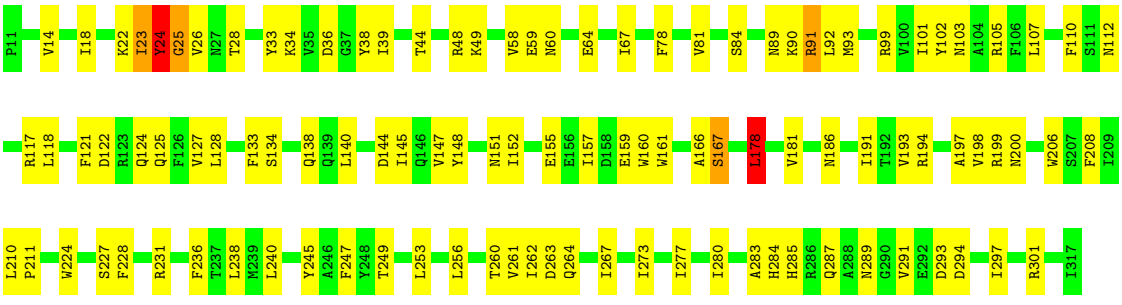
• Molecule 1: Cys-loop ligand-gated ion channel

Chain B:



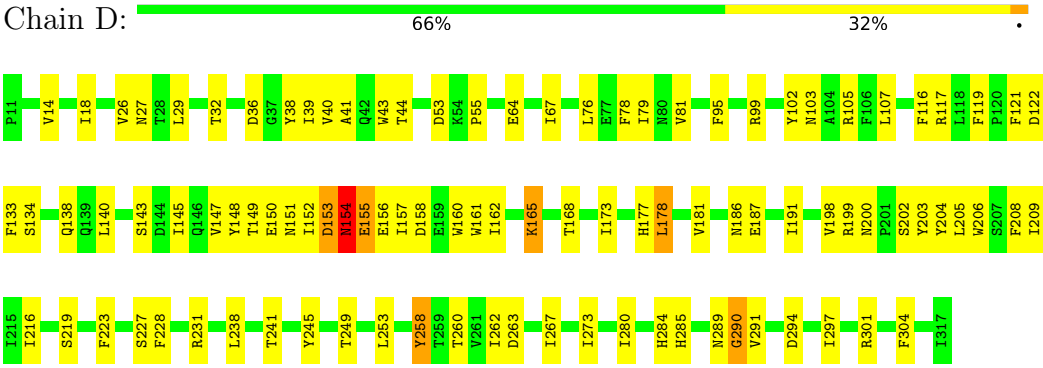
• Molecule 1: Cys-loop ligand-gated ion channel

Chain C:



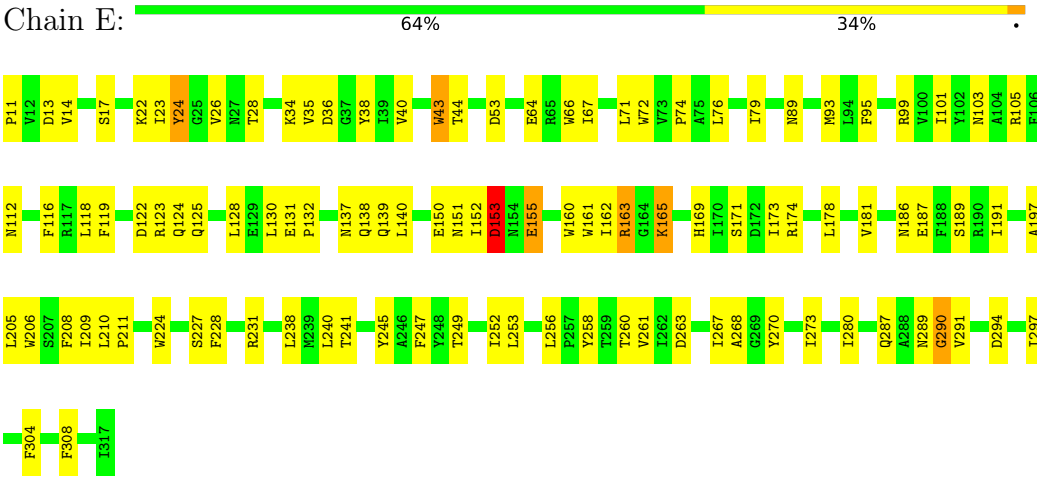
• Molecule 1: Cys-loop ligand-gated ion channel

Chain D:



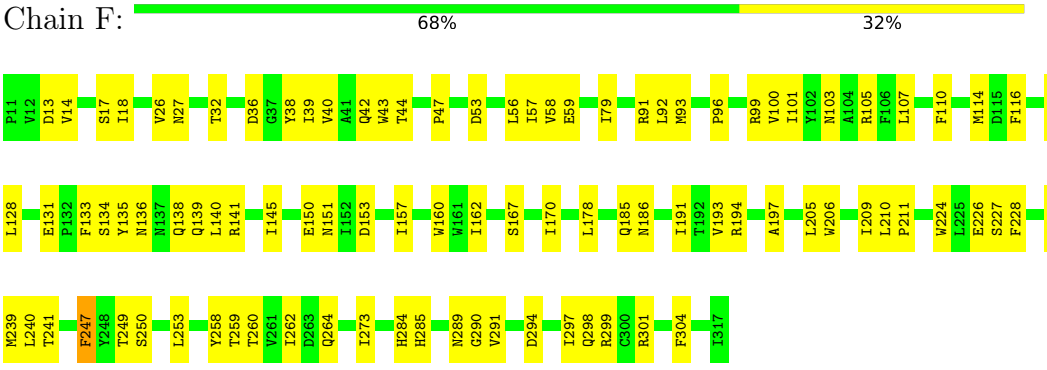
• Molecule 1: Cys-loop ligand-gated ion channel

Chain E:



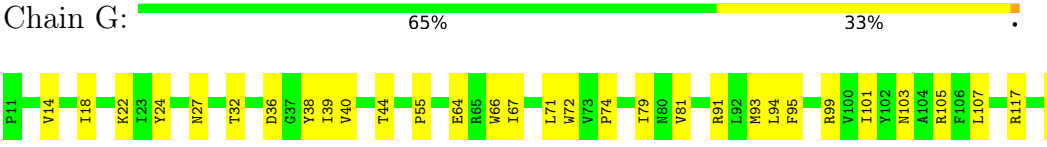
• Molecule 1: Cys-loop ligand-gated ion channel

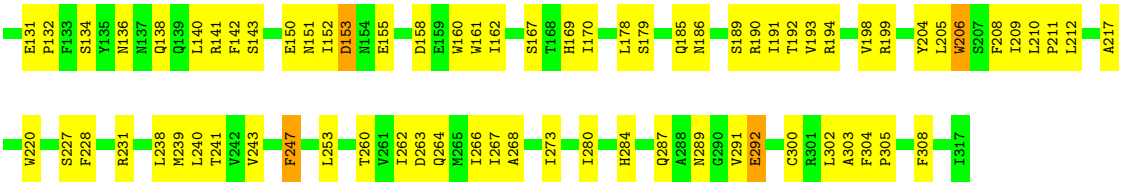
Chain F:



• Molecule 1: Cys-loop ligand-gated ion channel

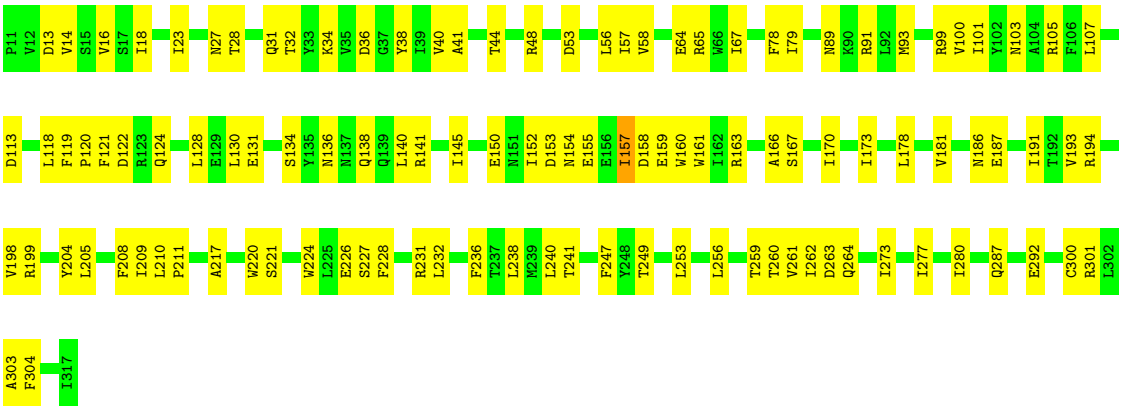
Chain G:





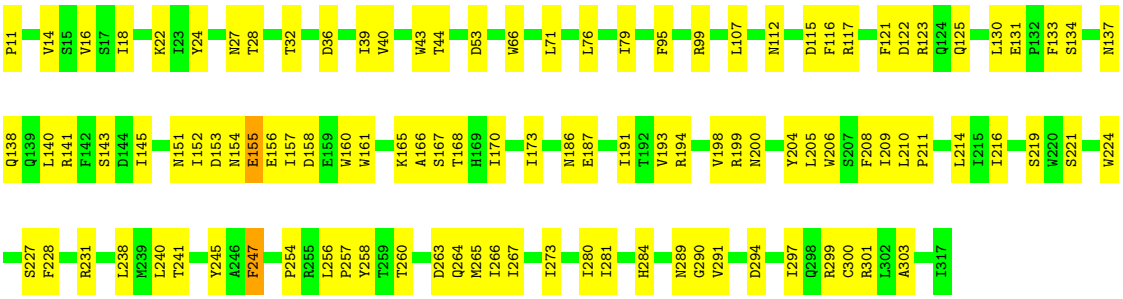
• Molecule 1: Cys-loop ligand-gated ion channel

Chain H:



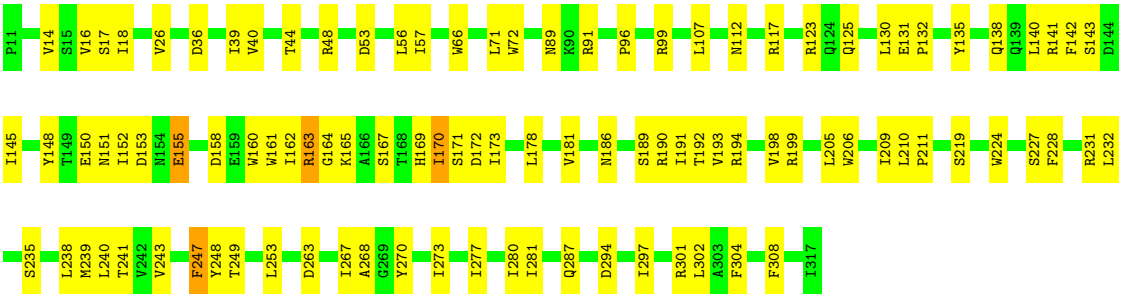
• Molecule 1: Cys-loop ligand-gated ion channel

Chain I:



• Molecule 1: Cys-loop ligand-gated ion channel

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.72Å 267.91Å 111.33Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	49.54 – 4.50 49.54 – 3.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.54-4.50) 99.6 (49.54-3.69)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.257 0.215 , 0.263	Depositor DCC
R_{free} test set	3118 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	161.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 144.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25070	wwPDB-VP
Average B, all atoms (Å^2)	214.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 6XY

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	0.29	0/2573	0.52	0/3507
1	B	0.27	0/2573	0.55	0/3507
1	C	0.29	0/2573	0.58	1/3507 (0.0%)
1	D	0.30	0/2573	0.58	1/3507 (0.0%)
1	E	0.31	0/2573	0.57	0/3507
1	F	0.27	0/2573	0.51	0/3507
1	G	0.27	0/2573	0.52	0/3507
1	H	0.28	0/2573	0.52	0/3507
1	I	0.32	0/2573	0.53	0/3507
1	J	0.29	0/2573	0.51	0/3507
All	All	0.29	0/25730	0.54	2/35070 (0.0%)

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	I	0	1
1	J	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	LEU	CA-CB-CG	7.97	133.63	115.30
1	D	154	ASN	N-CA-C	-5.35	96.55	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	GLY	Peptide
1	I	155	GLU	Peptide
1	J	155	GLU	Peptide
1	J	164	GLY	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	2505	0	2478	57	0
1	B	2505	0	2478	77	0
1	C	2505	0	2478	88	0
1	D	2505	0	2478	84	0
1	E	2505	0	2478	85	0
1	F	2505	0	2478	66	0
1	G	2505	0	2478	75	0
1	H	2505	0	2478	80	0
1	I	2505	0	2478	84	0
1	J	2505	0	2478	81	0
2	A	2	0	0	3	0
2	B	2	0	0	0	0
2	C	2	0	0	4	0
2	D	2	0	0	2	0
2	E	2	0	0	6	0
2	F	2	0	0	5	0
2	G	2	0	0	2	0
2	H	2	0	0	3	0
2	I	2	0	0	2	0
2	J	2	0	0	6	0
All	All	25070	0	24780	721	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 14.

The worst 5 of 721 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:160:TRP:CZ3	2:J:402:6XY:BR1	2.36	1.33
1:E:160:TRP:CD1	2:E:402:6XY:BR1	2.50	1.19
1:E:160:TRP:NE1	2:E:402:6XY:BR1	2.33	1.16
1:F:160:TRP:NE1	2:F:402:6XY:BR1	2.40	1.08
1:C:24:TYR:HA	2:C:402:6XY:BR1	2.14	1.03

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	305/307 (99%)	268 (88%)	33 (11%)	4 (1%)	12 48
1	B	305/307 (99%)	269 (88%)	32 (10%)	4 (1%)	12 48
1	C	305/307 (99%)	268 (88%)	32 (10%)	5 (2%)	9 45
1	D	305/307 (99%)	268 (88%)	34 (11%)	3 (1%)	15 54
1	E	305/307 (99%)	267 (88%)	34 (11%)	4 (1%)	12 48
1	F	305/307 (99%)	270 (88%)	33 (11%)	2 (1%)	22 62
1	G	305/307 (99%)	270 (88%)	34 (11%)	1 (0%)	41 76
1	H	305/307 (99%)	266 (87%)	36 (12%)	3 (1%)	15 54
1	I	305/307 (99%)	269 (88%)	33 (11%)	3 (1%)	15 54
1	J	305/307 (99%)	275 (90%)	28 (9%)	2 (1%)	22 62
All	All	3050/3070 (99%)	2690 (88%)	329 (11%)	31 (1%)	15 54

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	166	ALA
1	A	291	VAL

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Mol	Chain	Res	Type
1	B	166	ALA
1	C	24	TYR

5.3.2 Protein sidechains (i)

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	275/275 (100%)	270 (98%)	5 (2%)	59	77
1	B	275/275 (100%)	268 (98%)	7 (2%)	47	68
1	C	275/275 (100%)	268 (98%)	7 (2%)	47	68
1	D	275/275 (100%)	266 (97%)	9 (3%)	38	61
1	E	275/275 (100%)	266 (97%)	9 (3%)	38	61
1	F	275/275 (100%)	270 (98%)	5 (2%)	59	77
1	G	275/275 (100%)	269 (98%)	6 (2%)	52	71
1	H	275/275 (100%)	269 (98%)	6 (2%)	52	71
1	I	275/275 (100%)	269 (98%)	6 (2%)	52	71
1	J	275/275 (100%)	269 (98%)	6 (2%)	52	71
All	All	2750/2750 (100%)	2684 (98%)	66 (2%)	49	69

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	206	TRP
1	I	299	ARG
1	J	304	PHE
1	D	178	LEU
1	D	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	103	ASN

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Mol	Chain	Res	Type
1	J	151	ASN
1	D	151	ASN
1	E	124	GLN
1	E	151	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 20 are modelled with single atom - 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.