



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:30 AM UTC

PDB ID : 4YEU / pdb_00004yeu
Title : ELIC-GLIC chimera in the resting conformation
Authors : Schmandt, N.; Vivien, Y.; Lodowski, D.; Chakrapani, S.
Deposited on : 2015-02-24
Resolution : 4.60 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

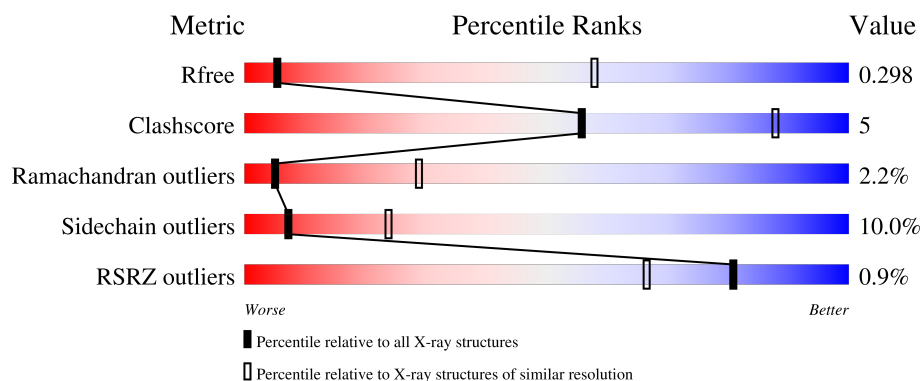
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	312	2% 77% 20% .
1	B	312	% 76% 22% .
1	C	312	% 77% 20% .
1	D	312	% 79% 18% .
1	E	312	% 77% 21% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12825 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,Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	B	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	C	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	D	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	E	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			

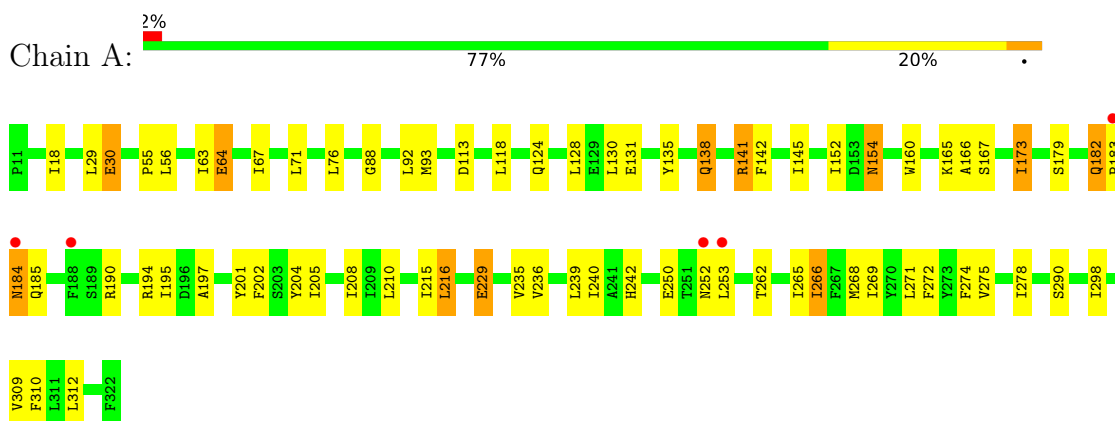
There are 5 discrepancies between the modelled and reference sequences:

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

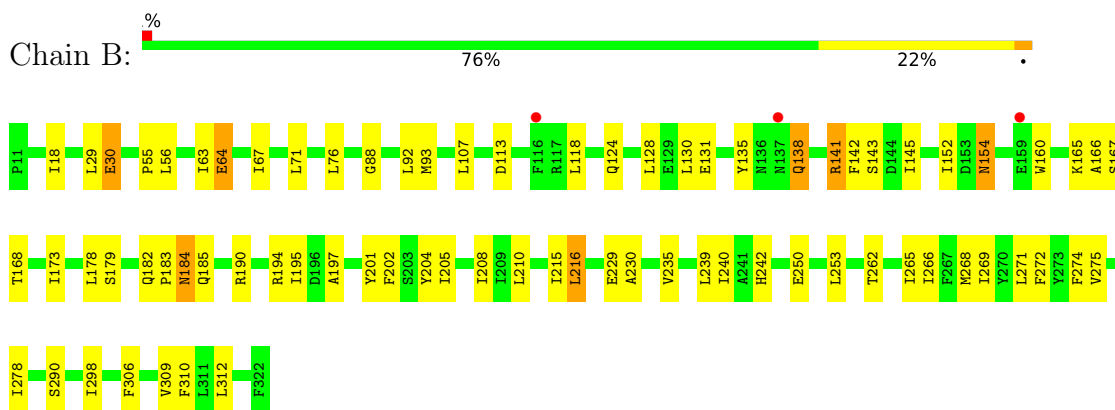
3 Residue-property plots

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: Cys-loop ligand-gated ion channel,Proton-gated ion channel



- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel

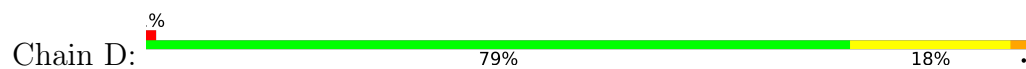


- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel

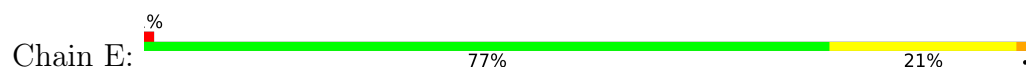




- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel



- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.44Å 217.96Å 229.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.60 20.00 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-4.60) 97.8 (20.00-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 4.64Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.242 , 0.248 0.281 , 0.298	Depositor DCC
R_{free} test set	956 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	254.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 114.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12825	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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	0.70	0/2638	1.26	5/3600 (0.1%)
1	B	0.70	0/2638	1.27	4/3600 (0.1%)
1	C	0.70	0/2638	1.27	5/3600 (0.1%)
1	D	0.71	1/2638 (0.0%)	1.29	8/3600 (0.2%)
1	E	0.70	0/2638	1.27	6/3600 (0.2%)
All	All	0.70	1/13190 (0.0%)	1.27	28/18000 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	182	GLN	CA-C	6.13	1.57	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	PHE	CA-CB-CG	6.28	120.08	113.80
1	D	208	ILE	CB-CG1-CD1	6.05	126.52	113.80
1	D	182	GLN	N-CA-C	5.81	119.66	108.45
1	D	252	ASN	CA-CB-CG	5.65	118.25	112.60
1	C	250	GLU	CB-CG-CD	5.51	121.97	112.60
1	E	252	ASN	CA-CB-CG	5.43	118.03	112.60
1	E	250	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	154	ASN	CA-CB-CG	5.40	118.00	112.60
1	B	154	ASN	CA-CB-CG	5.32	117.92	112.60
1	D	154	ASN	CA-CB-CG	5.32	117.92	112.60
1	C	252	ASN	CA-CB-CG	5.28	117.88	112.60
1	D	138	GLN	CA-C-N	5.26	128.17	120.71
1	D	138	GLN	C-N-CA	5.26	128.17	120.71
1	A	252	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	138	GLN	CA-C-N	5.18	128.07	120.71
1	A	138	GLN	C-N-CA	5.18	128.07	120.71
1	E	135	TYR	N-CA-C	5.18	116.86	108.41
1	A	135	TYR	N-CA-C	5.17	116.83	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	TYR	N-CA-C	5.16	116.83	108.41
1	D	181	VAL	N-CA-C	5.16	120.07	109.34
1	E	138	GLN	CA-C-N	5.14	128.01	120.71
1	E	138	GLN	C-N-CA	5.14	128.01	120.71
1	B	138	GLN	CA-C-N	5.10	127.95	120.71
1	B	138	GLN	C-N-CA	5.10	127.95	120.71
1	C	138	GLN	CA-C-N	5.08	127.92	120.71
1	C	138	GLN	C-N-CA	5.08	127.92	120.71
1	D	135	TYR	N-CA-C	5.05	116.64	108.41
1	C	135	TYR	N-CA-C	5.02	116.59	108.41

There are no chirality outliers.

There are no planarity outliers.

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	2565	0	2545	25	0
1	B	2565	0	2545	28	0
1	C	2565	0	2545	26	0
1	D	2565	0	2545	26	0
1	E	2565	0	2545	25	0
All	All	12825	0	12725	119	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 5.

All (119) 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:D:208:ILE:HD12	1:D:249:VAL:HG22	1.46	0.97
1:D:182:GLN:HB3	1:D:185:GLN:HB3	1.57	0.85
1:D:167:SER:HB3	1:D:194:ARG:HG3	1.71	0.73
1:E:167:SER:HB3	1:E:194:ARG:HG3	1.71	0.72
1:B:167:SER:HB3	1:B:194:ARG:HG3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:SER:HB3	1:C:194:ARG:HG3	1.71	0.72
1:A:167:SER:HB3	1:A:194:ARG:HG3	1.71	0.70
1:D:182:GLN:HG3	1:D:184:ASN:H	1.59	0.67
1:C:215:ILE:HD12	1:C:242:HIS:HA	1.82	0.61
1:D:215:ILE:HD12	1:D:242:HIS:HA	1.82	0.61
1:A:215:ILE:HD12	1:A:242:HIS:HA	1.81	0.61
1:B:215:ILE:HD12	1:B:242:HIS:HA	1.83	0.60
1:E:215:ILE:HD12	1:E:242:HIS:HA	1.83	0.60
1:A:166:ALA:HB2	1:A:195:ILE:HG12	1.85	0.58
1:C:166:ALA:HB2	1:C:195:ILE:HG12	1.87	0.57
1:A:239:LEU:HD21	1:E:215:ILE:HG22	1.87	0.56
1:B:166:ALA:HB2	1:B:195:ILE:HG12	1.86	0.56
1:E:166:ALA:HB2	1:E:195:ILE:HG12	1.86	0.56
1:D:166:ALA:HB2	1:D:195:ILE:HG12	1.87	0.55
1:B:215:ILE:HG22	1:C:239:LEU:HD21	1.89	0.54
1:A:229:GLU:HG3	1:E:230:ALA:HB2	1.88	0.54
1:C:215:ILE:HG22	1:D:239:LEU:HD21	1.88	0.54
1:A:274:PHE:O	1:A:278:ILE:HG12	2.08	0.53
1:A:215:ILE:HG22	1:B:239:LEU:HD21	1.89	0.53
1:B:274:PHE:O	1:B:278:ILE:HG12	2.08	0.53
1:E:274:PHE:O	1:E:278:ILE:HG12	2.09	0.53
1:C:274:PHE:O	1:C:278:ILE:HG12	2.09	0.53
1:D:274:PHE:O	1:D:278:ILE:HG12	2.10	0.51
1:C:216:LEU:HD13	1:C:269:ILE:HG23	1.93	0.50
1:B:216:LEU:HD13	1:B:269:ILE:HG23	1.94	0.49
1:B:178:LEU:HD22	1:B:182:GLN:NE2	2.28	0.49
1:D:216:LEU:HD13	1:D:269:ILE:HG23	1.94	0.49
1:A:216:LEU:HD13	1:A:269:ILE:HG23	1.94	0.49
1:D:215:ILE:HG22	1:E:239:LEU:HD21	1.95	0.48
1:E:216:LEU:HD13	1:E:269:ILE:HG23	1.94	0.48
1:E:265:ILE:O	1:E:269:ILE:HG13	2.13	0.48
1:A:266:ILE:HA	1:A:269:ILE:HD12	1.95	0.48
1:B:266:ILE:HA	1:B:269:ILE:HD12	1.96	0.48
1:D:266:ILE:HA	1:D:269:ILE:HD12	1.96	0.48
1:A:265:ILE:O	1:A:269:ILE:HG13	2.14	0.47
1:B:160:TRP:HB3	1:B:197:ALA:HB1	1.96	0.47
1:C:266:ILE:HA	1:C:269:ILE:HD12	1.95	0.47
1:E:266:ILE:HA	1:E:269:ILE:HD12	1.96	0.47
1:A:160:TRP:HB3	1:A:197:ALA:HB1	1.96	0.47
1:B:131:GLU:HB2	1:B:190:ARG:HG3	1.96	0.47
1:D:160:TRP:HB3	1:D:197:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLU:HA	1:E:67:ILE:HD12	1.97	0.47
1:E:131:GLU:HB2	1:E:190:ARG:HG3	1.97	0.47
1:C:230:ALA:HB2	1:D:229:GLU:HG3	1.97	0.47
1:D:265:ILE:O	1:D:269:ILE:HG13	2.14	0.47
1:E:160:TRP:HB3	1:E:197:ALA:HB1	1.97	0.47
1:A:131:GLU:HB2	1:A:190:ARG:HG3	1.96	0.47
1:D:131:GLU:HB2	1:D:190:ARG:HG3	1.96	0.47
1:A:64:GLU:HA	1:A:67:ILE:HD12	1.97	0.46
1:C:131:GLU:HB2	1:C:190:ARG:HG3	1.97	0.46
1:E:55:PRO:HG2	1:E:93:MET:HE2	1.98	0.46
1:A:271:LEU:O	1:A:275:VAL:HG23	2.15	0.46
1:B:271:LEU:O	1:B:275:VAL:HG23	2.16	0.46
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.97	0.46
1:C:64:GLU:HA	1:C:67:ILE:HD12	1.96	0.46
1:C:265:ILE:O	1:C:269:ILE:HG13	2.16	0.46
1:B:265:ILE:O	1:B:269:ILE:HG13	2.14	0.46
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.97	0.46
1:E:271:LEU:O	1:E:275:VAL:HG23	2.16	0.46
1:A:182:GLN:N	1:A:183:PRO:HD3	2.31	0.46
1:A:204:TYR:HD1	1:A:208:ILE:HD12	1.80	0.46
1:D:64:GLU:HA	1:D:67:ILE:HD12	1.97	0.46
1:D:173:ILE:HD13	1:D:190:ARG:HB3	1.98	0.46
1:D:55:PRO:HG2	1:D:93:MET:HE2	1.98	0.45
1:B:107:LEU:HD13	1:C:83:GLY:H	1.81	0.45
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.97	0.45
1:C:160:TRP:HB3	1:C:197:ALA:HB1	1.97	0.45
1:C:178:LEU:HD22	1:C:182:GLN:NE2	2.30	0.45
1:C:182:GLN:N	1:C:183:PRO:HD3	2.31	0.45
1:D:63:ILE:HG12	1:D:92:LEU:HD12	1.97	0.45
1:D:271:LEU:O	1:D:275:VAL:HG23	2.16	0.45
1:D:230:ALA:HB2	1:E:229:GLU:HG3	1.98	0.45
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.98	0.45
1:B:204:TYR:HD1	1:B:208:ILE:HD12	1.82	0.45
1:B:29:LEU:HD23	1:B:30:GLU:HG2	1.99	0.45
1:B:182:GLN:N	1:B:183:PRO:HD3	2.32	0.45
1:A:236:VAL:HG11	1:E:237:SER:HB2	1.99	0.45
1:C:271:LEU:O	1:C:275:VAL:HG23	2.18	0.44
1:B:230:ALA:HB2	1:C:229:GLU:HG3	1.99	0.44
1:A:63:ILE:HG12	1:A:92:LEU:HD12	1.99	0.44
1:E:204:TYR:HD1	1:E:208:ILE:HD12	1.81	0.44
1:A:55:PRO:HG2	1:A:93:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:HG12	1:B:92:LEU:HD12	1.99	0.44
1:C:268:MET:HE3	1:C:310:PHE:CE1	2.52	0.44
1:B:55:PRO:HG2	1:B:93:MET:HE2	1.98	0.44
1:C:55:PRO:HG2	1:C:93:MET:HE2	1.99	0.44
1:D:182:GLN:HA	1:D:183:PRO:HD3	1.96	0.44
1:E:182:GLN:N	1:E:183:PRO:HD3	2.32	0.44
1:A:268:MET:HE3	1:A:310:PHE:CE1	2.53	0.44
1:B:64:GLU:HA	1:B:67:ILE:HD12	1.98	0.44
1:B:306:PHE:HA	1:B:309:VAL:HG12	2.00	0.43
1:C:204:TYR:HD1	1:C:208:ILE:HD12	1.82	0.43
1:E:63:ILE:HG12	1:E:92:LEU:HD12	1.99	0.43
1:A:29:LEU:HD23	1:A:30:GLU:HG2	2.00	0.43
1:C:63:ILE:HG12	1:C:92:LEU:HD12	1.99	0.42
1:B:268:MET:HE3	1:B:310:PHE:CE1	2.55	0.42
1:E:268:MET:HE3	1:E:310:PHE:CE1	2.55	0.42
1:C:141:ARG:HE	1:C:142:PHE:HE2	1.68	0.41
1:B:272:PHE:CE2	1:B:309:VAL:HG13	2.55	0.41
1:D:141:ARG:HE	1:D:142:PHE:HE2	1.68	0.41
1:C:309:VAL:HA	1:C:312:LEU:HD12	2.03	0.41
1:D:182:GLN:CB	1:D:185:GLN:HB3	2.41	0.41
1:D:268:MET:HE3	1:D:310:PHE:CE1	2.55	0.41
1:B:143:SER:HB3	1:B:168:THR:HG23	2.03	0.41
1:E:309:VAL:HA	1:E:312:LEU:HD12	2.03	0.41
1:D:184:ASN:HD22	1:D:184:ASN:HA	1.58	0.41
1:E:140:LEU:HD13	1:E:191:ILE:HG13	2.03	0.41
1:A:272:PHE:HZ	1:A:309:VAL:HG12	1.85	0.40
1:B:141:ARG:HE	1:B:142:PHE:HE2	1.67	0.40
1:B:309:VAL:HA	1:B:312:LEU:HD12	2.03	0.40
1:A:309:VAL:HA	1:A:312:LEU:HD12	2.03	0.40
1:A:141:ARG:HE	1:A:142:PHE:HE2	1.68	0.40
1:C:140:LEU:HD13	1:C:191:ILE:HG13	2.04	0.40
1:E:272:PHE:HZ	1:E:309:VAL:HG12	1.87	0.40

There are no symmetry-related clashes.

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	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	5	28
1	B	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	5	28
1	C	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	5	28
1	D	310/312 (99%)	280 (90%)	24 (8%)	6 (2%)	6	32
1	E	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	5	28
All	All	1550/1560 (99%)	1392 (90%)	124 (8%)	34 (2%)	5	29

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	GLU
1	B	250	GLU
1	C	250	GLU
1	D	250	GLU
1	E	250	GLU
1	E	141	ARG
1	A	141	ARG
1	A	202	PHE
1	A	290	SER
1	B	141	ARG
1	B	179	SER
1	B	202	PHE
1	B	290	SER
1	C	141	ARG
1	C	202	PHE
1	D	141	ARG
1	D	202	PHE
1	D	290	SER
1	E	202	PHE
1	E	290	SER
1	A	184	ASN
1	B	184	ASN
1	C	179	SER
1	C	290	SER
1	A	179	SER
1	C	184	ASN
1	E	179	SER

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Mol	Chain	Res	Type
1	E	184	ASN
1	B	88	GLY
1	C	88	GLY
1	D	88	GLY
1	E	88	GLY
1	A	88	GLY
1	D	181	VAL

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	283/283 (100%)	252 (89%)	31 (11%)	6	21
1	B	283/283 (100%)	255 (90%)	28 (10%)	7	24
1	C	283/283 (100%)	255 (90%)	28 (10%)	7	24
1	D	283/283 (100%)	255 (90%)	28 (10%)	7	24
1	E	283/283 (100%)	256 (90%)	27 (10%)	8	25
All	All	1415/1415 (100%)	1273 (90%)	142 (10%)	7	24

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	30	GLU
1	A	56	LEU
1	A	64	GLU
1	A	71	LEU
1	A	76	LEU
1	A	113	ASP
1	A	118	LEU
1	A	124	GLN
1	A	128	LEU
1	A	130	LEU
1	A	138	GLN

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Mol	Chain	Res	Type
1	A	145	ILE
1	A	152	ILE
1	A	154	ASN
1	A	165	LYS
1	A	173	ILE
1	A	182	GLN
1	A	184	ASN
1	A	185	GLN
1	A	201	TYR
1	A	205	ILE
1	A	210	LEU
1	A	216	LEU
1	A	229	GLU
1	A	235	VAL
1	A	240	ILE
1	A	253	LEU
1	A	262	THR
1	A	266	ILE
1	A	298	ILE
1	B	18	ILE
1	B	30	GLU
1	B	56	LEU
1	B	64	GLU
1	B	71	LEU
1	B	76	LEU
1	B	113	ASP
1	B	118	LEU
1	B	124	GLN
1	B	128	LEU
1	B	130	LEU
1	B	138	GLN
1	B	145	ILE
1	B	152	ILE
1	B	154	ASN
1	B	165	LYS
1	B	184	ASN
1	B	185	GLN
1	B	201	TYR
1	B	205	ILE
1	B	210	LEU
1	B	216	LEU
1	B	229	GLU

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Mol	Chain	Res	Type
1	B	235	VAL
1	B	240	ILE
1	B	253	LEU
1	B	262	THR
1	B	298	ILE
1	C	18	ILE
1	C	56	LEU
1	C	64	GLU
1	C	71	LEU
1	C	76	LEU
1	C	113	ASP
1	C	118	LEU
1	C	124	GLN
1	C	128	LEU
1	C	130	LEU
1	C	138	GLN
1	C	145	ILE
1	C	152	ILE
1	C	165	LYS
1	C	173	ILE
1	C	184	ASN
1	C	185	GLN
1	C	201	TYR
1	C	205	ILE
1	C	210	LEU
1	C	216	LEU
1	C	229	GLU
1	C	235	VAL
1	C	240	ILE
1	C	253	LEU
1	C	262	THR
1	C	266	ILE
1	C	298	ILE
1	D	18	ILE
1	D	56	LEU
1	D	64	GLU
1	D	71	LEU
1	D	76	LEU
1	D	113	ASP
1	D	118	LEU
1	D	124	GLN
1	D	128	LEU

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Mol	Chain	Res	Type
1	D	130	LEU
1	D	138	GLN
1	D	145	ILE
1	D	152	ILE
1	D	154	ASN
1	D	165	LYS
1	D	182	GLN
1	D	184	ASN
1	D	185	GLN
1	D	201	TYR
1	D	205	ILE
1	D	210	LEU
1	D	216	LEU
1	D	229	GLU
1	D	235	VAL
1	D	240	ILE
1	D	253	LEU
1	D	262	THR
1	D	298	ILE
1	E	18	ILE
1	E	56	LEU
1	E	64	GLU
1	E	71	LEU
1	E	76	LEU
1	E	113	ASP
1	E	118	LEU
1	E	124	GLN
1	E	128	LEU
1	E	130	LEU
1	E	138	GLN
1	E	145	ILE
1	E	152	ILE
1	E	165	LYS
1	E	182	GLN
1	E	184	ASN
1	E	185	GLN
1	E	201	TYR
1	E	205	ILE
1	E	210	LEU
1	E	216	LEU
1	E	229	GLU
1	E	235	VAL

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Mol	Chain	Res	Type
1	E	240	ILE
1	E	253	LEU
1	E	262	THR
1	E	298	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	62	GLN
1	A	68	ASN
1	A	112	ASN
1	A	136	ASN
1	A	185	GLN
1	A	200	ASN
1	A	207	ASN
1	A	252	ASN
1	A	284	HIS
1	B	42	GLN
1	B	62	GLN
1	B	112	ASN
1	B	146	GLN
1	B	154	ASN
1	B	182	GLN
1	B	185	GLN
1	B	200	ASN
1	B	207	ASN
1	B	252	ASN
1	B	283	GLN
1	B	284	HIS
1	C	42	GLN
1	C	62	GLN
1	C	112	ASN
1	C	154	ASN
1	C	185	GLN
1	C	200	ASN
1	C	252	ASN
1	C	284	HIS
1	D	42	GLN
1	D	62	GLN
1	D	112	ASN
1	D	154	ASN

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Mol	Chain	Res	Type
1	D	184	ASN
1	D	200	ASN
1	D	207	ASN
1	D	252	ASN
1	D	284	HIS
1	E	42	GLN
1	E	62	GLN
1	E	112	ASN
1	E	185	GLN
1	E	200	ASN
1	E	207	ASN
1	E	252	ASN
1	E	284	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	312/312 (100%)	-0.17	5 (1%) 70 55	73, 153, 255, 278	0
1	B	312/312 (100%)	-0.15	3 (0%) 79 64	93, 191, 292, 300	0
1	C	312/312 (100%)	-0.29	2 (0%) 85 73	109, 206, 298, 300	0
1	D	312/312 (100%)	-0.25	2 (0%) 85 73	95, 172, 264, 294	0
1	E	312/312 (100%)	-0.27	2 (0%) 85 73	80, 142, 231, 278	0
All	All	1560/1560 (100%)	-0.23	14 (0%) 81 66	73, 170, 274, 300	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	PHE	3.8
1	A	252	ASN	2.9
1	A	253	LEU	2.6
1	E	120	PRO	2.6
1	A	188	PHE	2.6
1	A	183	PRO	2.5
1	A	184	ASN	2.5
1	C	250	GLU	2.3
1	E	156	GLU	2.3
1	B	159	GLU	2.3
1	C	11	PRO	2.3
1	D	11	PRO	2.1
1	B	137	ASN	2.1
1	D	256	THR	2.1

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.