



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:28 PM UTC

PDB ID : 5NJY / pdb_00005njy
Title : X-ray structure of the H235Q mutant of GLIC
Authors : Hu, H.; Fourati, Z.; Delarue, M.
Deposited on : 2017-03-30
Resolution : 2.95 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

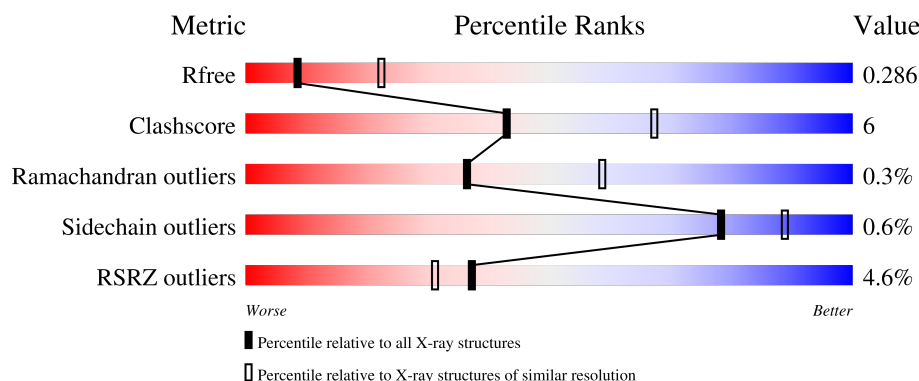
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	327	3% 80% 14% • 5%
1	B	327	3% 79% 15% • 5%
1	C	327	6% 81% 13% • 5%
1	D	327	3% 80% 15% • 5%
1	E	327	7% 81% 13% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12603 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2518	1657	403	454	4			
1	B	311	Total	C	N	O	S	0	0	0
			2518	1657	403	454	4			
1	C	311	Total	C	N	O	S	0	0	0
			2518	1657	403	454	4			
1	D	311	Total	C	N	O	S	0	0	0
			2518	1657	403	454	4			
1	E	311	Total	C	N	O	S	0	0	0
			2518	1657	403	454	4			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLN	HIS	engineered mutation	UNP Q7NDN8
A	318	GLY	-	expression tag	UNP Q7NDN8
A	319	TYR	-	expression tag	UNP Q7NDN8
A	320	PRO	-	expression tag	UNP Q7NDN8
A	321	TYR	-	expression tag	UNP Q7NDN8
A	322	ASP	-	expression tag	UNP Q7NDN8
A	323	VAL	-	expression tag	UNP Q7NDN8
A	324	PRO	-	expression tag	UNP Q7NDN8
A	325	ASP	-	expression tag	UNP Q7NDN8
A	326	TYR	-	expression tag	UNP Q7NDN8
A	327	ALA	-	expression tag	UNP Q7NDN8
B	235	GLN	HIS	engineered mutation	UNP Q7NDN8
B	318	GLY	-	expression tag	UNP Q7NDN8
B	319	TYR	-	expression tag	UNP Q7NDN8
B	320	PRO	-	expression tag	UNP Q7NDN8
B	321	TYR	-	expression tag	UNP Q7NDN8
B	322	ASP	-	expression tag	UNP Q7NDN8
B	323	VAL	-	expression tag	UNP Q7NDN8
B	324	PRO	-	expression tag	UNP Q7NDN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	325	ASP	-	expression tag	UNP Q7NDN8
B	326	TYR	-	expression tag	UNP Q7NDN8
B	327	ALA	-	expression tag	UNP Q7NDN8
C	235	GLN	HIS	engineered mutation	UNP Q7NDN8
C	318	GLY	-	expression tag	UNP Q7NDN8
C	319	TYR	-	expression tag	UNP Q7NDN8
C	320	PRO	-	expression tag	UNP Q7NDN8
C	321	TYR	-	expression tag	UNP Q7NDN8
C	322	ASP	-	expression tag	UNP Q7NDN8
C	323	VAL	-	expression tag	UNP Q7NDN8
C	324	PRO	-	expression tag	UNP Q7NDN8
C	325	ASP	-	expression tag	UNP Q7NDN8
C	326	TYR	-	expression tag	UNP Q7NDN8
C	327	ALA	-	expression tag	UNP Q7NDN8
D	235	GLN	HIS	engineered mutation	UNP Q7NDN8
D	318	GLY	-	expression tag	UNP Q7NDN8
D	319	TYR	-	expression tag	UNP Q7NDN8
D	320	PRO	-	expression tag	UNP Q7NDN8
D	321	TYR	-	expression tag	UNP Q7NDN8
D	322	ASP	-	expression tag	UNP Q7NDN8
D	323	VAL	-	expression tag	UNP Q7NDN8
D	324	PRO	-	expression tag	UNP Q7NDN8
D	325	ASP	-	expression tag	UNP Q7NDN8
D	326	TYR	-	expression tag	UNP Q7NDN8
D	327	ALA	-	expression tag	UNP Q7NDN8
E	235	GLN	HIS	engineered mutation	UNP Q7NDN8
E	318	GLY	-	expression tag	UNP Q7NDN8
E	319	TYR	-	expression tag	UNP Q7NDN8
E	320	PRO	-	expression tag	UNP Q7NDN8
E	321	TYR	-	expression tag	UNP Q7NDN8
E	322	ASP	-	expression tag	UNP Q7NDN8
E	323	VAL	-	expression tag	UNP Q7NDN8
E	324	PRO	-	expression tag	UNP Q7NDN8
E	325	ASP	-	expression tag	UNP Q7NDN8
E	326	TYR	-	expression tag	UNP Q7NDN8
E	327	ALA	-	expression tag	UNP Q7NDN8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0

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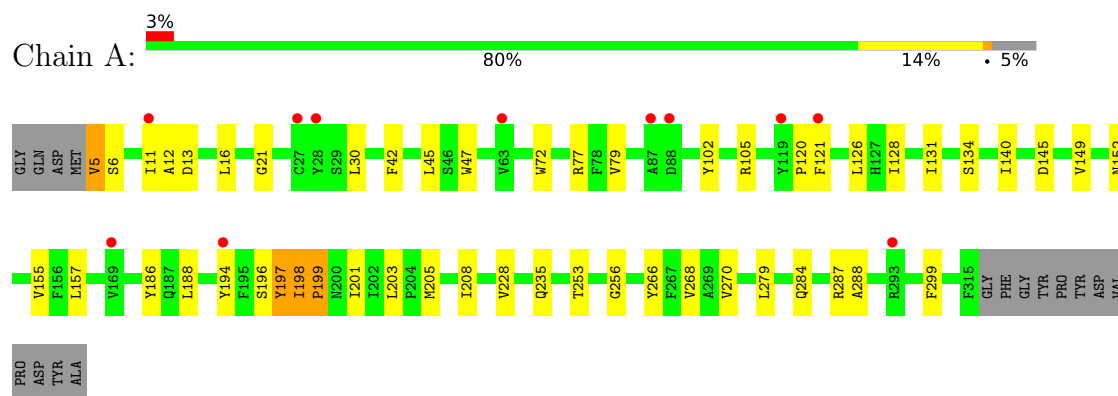
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total 5	O 5	0	0
2	C	3	Total 3	O 3	0	0
2	D	2	Total 2	O 2	0	0
2	E	1	Total 1	O 1	0	0

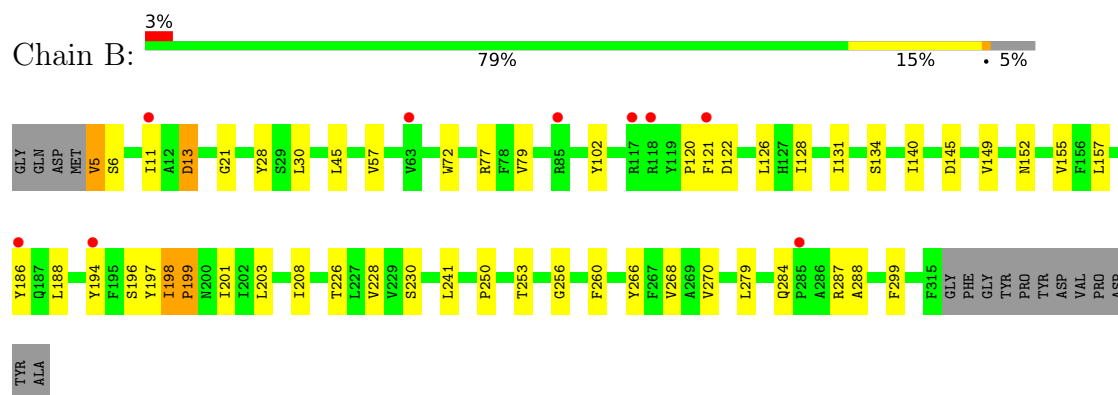
3 Residue-property plots

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.

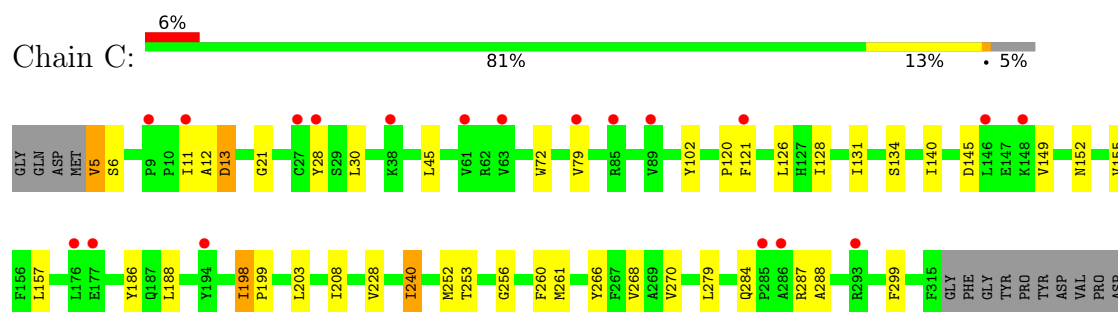
• Molecule 1: Proton-gated ion channel



• Molecule 1: Proton-gated ion channel



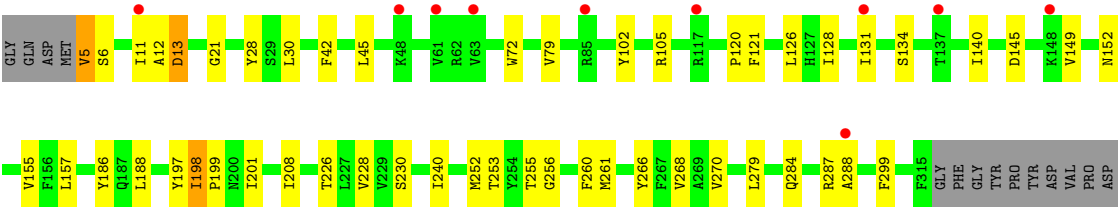
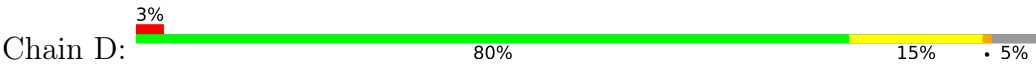
• Molecule 1: Proton-gated ion channel



TYR

ALA

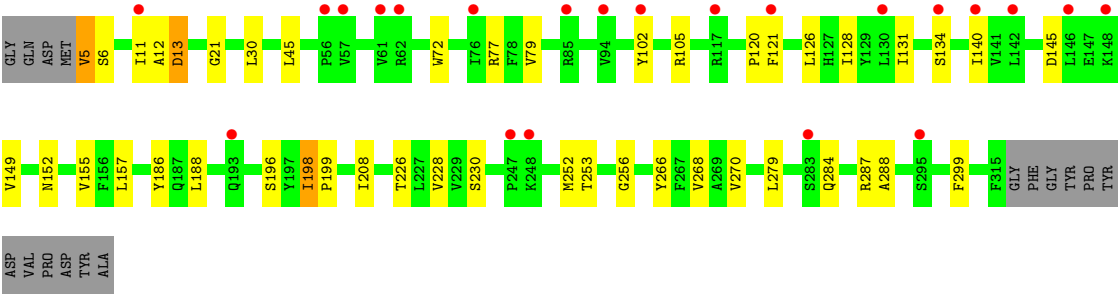
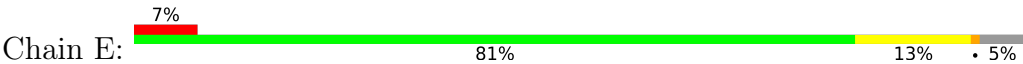
● Molecule 1: Proton-gated ion channel



TYR

ALA

● Molecule 1: Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.93Å 134.24Å 160.63Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 20.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.95) 97.3 (20.00-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.93Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.224 , 0.243 0.270 , 0.286	Depositor DCC
R_{free} test set	3890 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12603	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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	0.86	2/2584 (0.1%)	1.27	11/3533 (0.3%)
1	B	0.88	1/2584 (0.0%)	1.27	12/3533 (0.3%)
1	C	0.85	0/2584	1.26	9/3533 (0.3%)
1	D	0.83	0/2584	1.25	10/3533 (0.3%)
1	E	0.84	0/2584	1.26	7/3533 (0.2%)
All	All	0.85	3/12920 (0.0%)	1.26	49/17665 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ILE	CA-CB	5.67	1.57	1.54
1	B	198	ILE	CA-CB	5.42	1.56	1.54
1	A	197	TYR	CA-C	-5.01	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	ILE	N-CA-CB	11.26	118.07	110.52
1	A	197	TYR	N-CA-C	-8.70	101.38	111.03
1	D	11	ILE	CA-C-N	6.67	134.28	121.54
1	D	11	ILE	C-N-CA	6.67	134.28	121.54
1	A	198	ILE	N-CA-CB	6.59	115.59	110.45
1	C	11	ILE	CA-C-N	6.55	134.06	121.54
1	C	11	ILE	C-N-CA	6.55	134.06	121.54
1	E	11	ILE	CA-C-N	6.47	133.91	121.54
1	E	11	ILE	C-N-CA	6.47	133.91	121.54
1	B	11	ILE	CA-C-N	6.35	133.76	122.45
1	B	11	ILE	C-N-CA	6.35	133.76	122.45
1	A	199	PRO	CA-C-N	-6.06	113.03	122.37
1	A	199	PRO	C-N-CA	-6.06	113.03	122.37
1	A	145	ASP	CA-C-N	6.01	129.16	120.38
1	A	145	ASP	C-N-CA	6.01	129.16	120.38
1	B	13	ASP	CA-CB-CG	6.01	118.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	ASP	CA-C-N	5.98	129.11	120.38
1	E	145	ASP	C-N-CA	5.98	129.11	120.38
1	C	13	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	145	ASP	CA-C-N	5.78	128.81	120.38
1	D	145	ASP	C-N-CA	5.78	128.81	120.38
1	A	12	ALA	N-CA-C	-5.77	98.44	107.73
1	E	13	ASP	CA-CB-CG	5.74	118.34	112.60
1	C	145	ASP	CA-C-N	5.71	128.72	120.38
1	C	145	ASP	C-N-CA	5.71	128.72	120.38
1	D	198	ILE	CA-C-O	-5.70	114.87	118.69
1	B	145	ASP	CA-C-N	5.67	128.66	120.38
1	B	145	ASP	C-N-CA	5.67	128.66	120.38
1	A	11	ILE	CA-C-N	5.66	134.23	122.41
1	A	11	ILE	C-N-CA	5.66	134.23	122.41
1	C	198	ILE	CA-C-O	-5.61	114.93	118.69
1	D	13	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	198	ILE	CA-C-O	-5.55	114.97	118.69
1	D	12	ALA	N-CA-C	-5.38	99.35	110.80
1	B	198	ILE	CA-C-O	-5.34	114.65	118.71
1	E	12	ALA	N-CA-C	-5.29	99.53	110.80
1	C	12	ALA	N-CA-C	-5.29	99.54	110.80
1	A	42	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	28	TYR	CA-C-N	5.11	131.31	121.54
1	C	28	TYR	C-N-CA	5.11	131.31	121.54
1	B	28	TYR	CA-C-N	5.11	131.30	121.54
1	B	28	TYR	C-N-CA	5.11	131.30	121.54
1	D	28	TYR	CA-C-N	5.10	131.29	121.54
1	D	28	TYR	C-N-CA	5.10	131.29	121.54
1	B	122	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	42	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	199	PRO	CA-C-N	-5.05	114.59	122.37
1	B	199	PRO	C-N-CA	-5.05	114.59	122.37
1	E	198	ILE	CA-C-O	-5.04	115.31	118.69

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	2518	0	2539	42	0
1	B	2518	0	2539	37	0
1	C	2518	0	2539	31	0
1	D	2518	0	2539	32	0
1	E	2518	0	2539	28	0
2	A	2	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
All	All	12603	0	12695	157	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 6.

All (157) 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:E:198:ILE:HG13	1:E:199:PRO:HD3	1.41	1.02
1:A:198:ILE:HG13	1:A:199:PRO:HD3	1.42	0.99
1:C:198:ILE:HG13	1:C:199:PRO:HD3	1.45	0.98
1:B:198:ILE:HG13	1:B:199:PRO:HD3	1.48	0.96
1:D:198:ILE:HG13	1:D:199:PRO:HD3	1.48	0.94
1:A:194:TYR:HE2	1:A:197:TYR:HA	1.34	0.91
1:C:5:VAL:HG23	1:C:6:SER:H	1.39	0.87
1:B:5:VAL:HG23	1:B:6:SER:H	1.39	0.85
1:E:5:VAL:HG23	1:E:6:SER:H	1.44	0.82
1:A:5:VAL:HG23	1:A:6:SER:H	1.44	0.82
1:D:5:VAL:HG23	1:D:6:SER:H	1.43	0.82
1:A:194:TYR:CE2	1:A:197:TYR:HA	2.18	0.79
1:A:196:SER:HA	1:A:199:PRO:HD2	1.66	0.76
1:A:194:TYR:CD1	1:B:250:PRO:HA	2.22	0.75
1:E:198:ILE:CG1	1:E:199:PRO:HD3	2.17	0.73
1:C:198:ILE:CG1	1:C:199:PRO:HD3	2.19	0.72
1:A:198:ILE:CG1	1:A:199:PRO:HD3	2.20	0.71
1:A:194:TYR:HD1	1:B:250:PRO:HA	1.57	0.70
1:A:134:SER:HA	1:A:140:ILE:HD12	1.74	0.70
1:C:134:SER:HA	1:C:140:ILE:HD12	1.75	0.69
1:A:120:PRO:HD2	1:A:121:PHE:CE2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TYR:CE2	1:A:197:TYR:CA	2.77	0.67
1:B:134:SER:HA	1:B:140:ILE:HD12	1.75	0.67
1:B:120:PRO:HD2	1:B:121:PHE:CE2	2.29	0.67
1:E:134:SER:HA	1:E:140:ILE:HD12	1.76	0.66
1:D:134:SER:HA	1:D:140:ILE:HD12	1.76	0.66
1:B:197:TYR:HD1	1:B:201:ILE:HD13	1.60	0.66
1:B:253:THR:HB	1:B:256:GLY:H	1.62	0.65
1:A:253:THR:HB	1:A:256:GLY:H	1.62	0.65
1:A:194:TYR:HE2	1:A:197:TYR:CA	2.07	0.64
1:B:198:ILE:CG1	1:B:199:PRO:HD3	2.25	0.64
1:E:253:THR:HB	1:E:256:GLY:H	1.64	0.63
1:C:5:VAL:HG22	1:C:72:TRP:HB2	1.81	0.63
1:B:5:VAL:CG2	1:B:6:SER:H	2.13	0.62
1:C:5:VAL:HG23	1:C:6:SER:N	2.12	0.62
1:D:198:ILE:CG1	1:D:199:PRO:HD3	2.25	0.62
1:C:5:VAL:CG2	1:C:6:SER:N	2.63	0.62
1:D:120:PRO:HD2	1:D:121:PHE:CE2	2.35	0.62
1:D:253:THR:HB	1:D:256:GLY:H	1.65	0.61
1:D:5:VAL:HG23	1:D:6:SER:N	2.14	0.61
1:C:253:THR:HB	1:C:256:GLY:H	1.65	0.61
1:D:5:VAL:CG2	1:D:6:SER:N	2.63	0.61
1:B:5:VAL:CG2	1:B:6:SER:N	2.63	0.61
1:E:120:PRO:HD2	1:E:121:PHE:CE2	2.36	0.60
1:A:5:VAL:CG2	1:A:6:SER:N	2.63	0.60
1:A:5:VAL:CG2	1:A:6:SER:H	2.12	0.60
1:B:268:VAL:HG12	1:B:299:PHE:CZ	2.36	0.60
1:A:128:ILE:HB	1:A:186:TYR:HB2	1.83	0.60
1:B:5:VAL:HG23	1:B:6:SER:N	2.11	0.60
1:C:268:VAL:HG12	1:C:299:PHE:CZ	2.36	0.60
1:D:5:VAL:HG22	1:D:72:TRP:HB2	1.84	0.60
1:D:128:ILE:HB	1:D:186:TYR:HB2	1.84	0.60
1:E:5:VAL:CG2	1:E:6:SER:N	2.64	0.60
1:B:5:VAL:HG22	1:B:72:TRP:HB2	1.83	0.60
1:E:128:ILE:HB	1:E:186:TYR:HB2	1.83	0.59
1:C:5:VAL:CG2	1:C:6:SER:H	2.12	0.59
1:B:128:ILE:HB	1:B:186:TYR:HB2	1.84	0.59
1:D:268:VAL:HG12	1:D:299:PHE:CZ	2.38	0.59
1:C:120:PRO:HD2	1:C:121:PHE:CE2	2.38	0.59
1:E:268:VAL:HG12	1:E:299:PHE:CZ	2.37	0.58
1:E:5:VAL:HG22	1:E:72:TRP:HB2	1.83	0.58
1:A:268:VAL:HG12	1:A:299:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HB2	1:A:288:ALA:HB2	1.86	0.58
1:A:5:VAL:HG22	1:A:72:TRP:HB2	1.86	0.58
1:C:128:ILE:HB	1:C:186:TYR:HB2	1.85	0.58
1:B:279:LEU:HB2	1:B:288:ALA:HB2	1.85	0.57
1:E:5:VAL:CG2	1:E:6:SER:H	2.15	0.57
1:D:279:LEU:HB2	1:D:288:ALA:HB2	1.87	0.56
1:E:279:LEU:HB2	1:E:288:ALA:HB2	1.87	0.56
1:E:5:VAL:HG23	1:E:6:SER:N	2.15	0.56
1:A:5:VAL:CG2	1:A:72:TRP:HB2	2.36	0.56
1:B:5:VAL:CG2	1:B:72:TRP:HB2	2.36	0.56
1:C:279:LEU:HB2	1:C:288:ALA:HB2	1.87	0.55
1:D:5:VAL:CG2	1:D:72:TRP:HB2	2.36	0.55
1:A:194:TYR:CE2	1:A:197:TYR:N	2.75	0.55
1:E:5:VAL:CG2	1:E:72:TRP:HB2	2.36	0.55
1:C:126:LEU:HB2	1:C:188:LEU:HB3	1.89	0.54
1:C:5:VAL:CG2	1:C:72:TRP:HB2	2.38	0.54
1:A:196:SER:CA	1:A:199:PRO:HD2	2.36	0.53
1:D:126:LEU:HB2	1:D:188:LEU:HB3	1.89	0.53
1:A:5:VAL:HG23	1:A:6:SER:N	2.17	0.53
1:D:5:VAL:CG2	1:D:6:SER:H	2.14	0.52
1:A:126:LEU:HB2	1:A:188:LEU:HB3	1.90	0.52
1:E:126:LEU:HB2	1:E:188:LEU:HB3	1.91	0.52
1:D:105:ARG:HH11	1:E:77:ARG:HE	1.58	0.51
1:B:126:LEU:HB2	1:B:188:LEU:HB3	1.93	0.51
1:A:105:ARG:HH11	1:B:77:ARG:HE	1.60	0.50
1:B:194:TYR:HE1	1:B:196:SER:HB3	1.77	0.49
1:C:208:ILE:HG22	1:C:266:TYR:OH	2.13	0.49
1:D:208:ILE:HG22	1:D:266:TYR:OH	2.14	0.48
1:B:199:PRO:HB2	1:C:252:MET:CE	2.43	0.48
1:B:194:TYR:CE1	1:B:196:SER:HB3	2.48	0.48
1:A:194:TYR:CE2	1:A:196:SER:C	2.92	0.48
1:C:228:VAL:HG11	1:C:270:VAL:HG23	1.96	0.48
1:A:208:ILE:HG22	1:A:266:TYR:OH	2.14	0.48
1:D:197:TYR:HD1	1:D:201:ILE:HD13	1.79	0.47
1:B:208:ILE:HG22	1:B:266:TYR:OH	2.14	0.47
1:E:21:GLY:HA2	1:E:149:VAL:HG22	1.96	0.47
1:A:120:PRO:HD2	1:A:121:PHE:CD2	2.50	0.47
1:E:208:ILE:HG22	1:E:266:TYR:OH	2.15	0.47
1:A:203:LEU:HD13	1:B:260:PHE:HZ	1.79	0.47
1:D:30:LEU:HD12	1:D:157:LEU:HD21	1.97	0.47
1:D:21:GLY:HA2	1:D:149:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD12	1:A:157:LEU:HD21	1.97	0.47
1:B:197:TYR:CD1	1:B:201:ILE:HD13	2.46	0.46
1:C:203:LEU:HD13	1:D:260:PHE:HZ	1.80	0.46
1:A:197:TYR:HD1	1:A:201:ILE:HD13	1.81	0.46
1:D:284:GLN:NE2	1:D:287:ARG:HE	2.14	0.46
1:A:77:ARG:HE	1:E:105:ARG:HH11	1.63	0.46
1:B:21:GLY:HA2	1:B:149:VAL:HG22	1.97	0.46
1:C:21:GLY:HA2	1:C:149:VAL:HG22	1.97	0.45
1:C:199:PRO:HB2	1:D:252:MET:CE	2.45	0.45
1:C:79:VAL:HG22	1:C:131:ILE:HB	1.99	0.45
1:E:30:LEU:HD12	1:E:157:LEU:HD21	1.98	0.45
1:A:79:VAL:HG22	1:A:131:ILE:HB	1.99	0.45
1:A:284:GLN:NE2	1:A:287:ARG:HE	2.15	0.45
1:C:30:LEU:HD12	1:C:157:LEU:HD21	1.98	0.45
1:B:199:PRO:HB2	1:C:252:MET:HE1	1.98	0.45
1:A:21:GLY:HA2	1:A:149:VAL:HG22	1.97	0.44
1:B:284:GLN:NE2	1:B:287:ARG:HE	2.15	0.44
1:B:30:LEU:HD12	1:B:157:LEU:HD21	2.00	0.44
1:B:120:PRO:HD2	1:B:121:PHE:CD2	2.51	0.44
1:E:284:GLN:NE2	1:E:287:ARG:HE	2.15	0.44
1:C:284:GLN:NE2	1:C:287:ARG:HE	2.15	0.44
1:D:79:VAL:HG22	1:D:131:ILE:HB	2.00	0.43
1:D:261:MET:HE2	1:D:261:MET:HB3	1.92	0.43
1:E:79:VAL:HG22	1:E:131:ILE:HB	1.99	0.43
1:B:203:LEU:HD13	1:C:260:PHE:HZ	1.82	0.43
1:B:45:LEU:HB2	1:B:102:TYR:HB3	2.01	0.43
1:D:228:VAL:HG11	1:D:270:VAL:HG23	2.00	0.43
1:E:226:THR:O	1:E:230:SER:HB2	2.18	0.43
1:E:228:VAL:HG11	1:E:270:VAL:HG23	2.01	0.43
1:A:45:LEU:HB2	1:A:102:TYR:HB3	2.00	0.43
1:C:198:ILE:CD1	1:C:199:PRO:HD3	2.49	0.43
1:A:205:MET:HE2	1:A:235:GLN:HE22	1.85	0.42
1:E:196:SER:HA	1:E:199:PRO:HD2	2.02	0.42
1:D:152:ASN:HB3	1:D:155:VAL:HG23	2.02	0.42
1:E:45:LEU:HB2	1:E:102:TYR:HB3	2.01	0.42
1:E:152:ASN:HB3	1:E:155:VAL:HG23	2.01	0.42
1:B:241:LEU:HD13	1:C:240:ILE:HG13	2.02	0.41
1:C:152:ASN:HB3	1:C:155:VAL:HG23	2.01	0.41
1:C:45:LEU:HB2	1:C:102:TYR:HB3	2.01	0.41
1:D:45:LEU:HB2	1:D:102:TYR:HB3	2.01	0.41
1:B:228:VAL:HG11	1:B:270:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:C	1:A:199:PRO:HD2	2.46	0.41
1:B:152:ASN:HB3	1:B:155:VAL:HG23	2.02	0.41
1:D:197:TYR:OH	1:D:255:THR:HG23	2.21	0.41
1:A:228:VAL:HG11	1:A:270:VAL:HG23	2.03	0.41
1:C:261:MET:HE2	1:C:261:MET:HB3	1.88	0.41
1:D:199:PRO:HB2	1:E:252:MET:CE	2.52	0.40
1:A:152:ASN:HB3	1:A:155:VAL:HG23	2.04	0.40
1:A:194:TYR:HD2	1:A:197:TYR:HB2	1.85	0.40
1:B:226:THR:O	1:B:230:SER:HB2	2.21	0.40
1:D:120:PRO:HD2	1:D:121:PHE:CD2	2.56	0.40
1:D:226:THR:O	1:D:230:SER:HB2	2.21	0.40
1:B:79:VAL:HG22	1:B:131:ILE:HB	2.02	0.40
1:A:16:LEU:HD11	1:A:47:TRP:HB2	2.04	0.40

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	309/327 (94%)	292 (94%)	16 (5%)	1 (0%)	36	59
1	B	309/327 (94%)	293 (95%)	15 (5%)	1 (0%)	36	59
1	C	309/327 (94%)	293 (95%)	15 (5%)	1 (0%)	36	59
1	D	309/327 (94%)	292 (94%)	16 (5%)	1 (0%)	36	59
1	E	309/327 (94%)	295 (96%)	13 (4%)	1 (0%)	36	59
All	All	1545/1635 (94%)	1465 (95%)	75 (5%)	5 (0%)	36	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	ASP

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Mol	Chain	Res	Type
1	E	13	ASP
1	A	13	ASP
1	C	13	ASP
1	D	13	ASP

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	279/292 (96%)	278 (100%)	1 (0%)	84	92
1	B	279/292 (96%)	277 (99%)	2 (1%)	76	87
1	C	279/292 (96%)	277 (99%)	2 (1%)	76	87
1	D	279/292 (96%)	277 (99%)	2 (1%)	76	87
1	E	279/292 (96%)	278 (100%)	1 (0%)	84	92
All	All	1395/1460 (96%)	1387 (99%)	8 (1%)	78	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	B	5	VAL
1	B	57	VAL
1	C	5	VAL
1	C	240	ILE
1	D	5	VAL
1	D	240	ILE
1	E	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	239	ASN

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Mol	Chain	Res	Type
1	A	277	HIS
1	A	284	GLN
1	B	152	ASN
1	B	200	ASN
1	B	239	ASN
1	B	277	HIS
1	B	284	GLN
1	C	152	ASN
1	C	200	ASN
1	C	239	ASN
1	C	284	GLN
1	D	200	ASN
1	D	239	ASN
1	D	277	HIS
1	D	284	GLN
1	E	152	ASN
1	E	200	ASN
1	E	239	ASN
1	E	277	HIS
1	E	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	311/327 (95%)	0.29	11 (3%) 47 40	85, 137, 225, 261	0
1	B	311/327 (95%)	0.27	9 (2%) 53 46	82, 130, 193, 220	0
1	C	311/327 (95%)	0.44	19 (6%) 27 22	89, 139, 220, 258	0
1	D	311/327 (95%)	0.33	10 (3%) 50 43	96, 155, 233, 261	0
1	E	311/327 (95%)	0.38	22 (7%) 22 19	91, 148, 233, 257	0
All	All	1555/1635 (95%)	0.34	71 (4%) 37 31	82, 142, 225, 261	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	140	ILE	4.9
1	E	76	ILE	4.4
1	A	194	TYR	4.1
1	D	63	VAL	4.0
1	B	63	VAL	3.8
1	E	11	ILE	3.7
1	C	146	LEU	3.7
1	C	11	ILE	3.5
1	C	27	CYS	3.5
1	B	121	PHE	3.5
1	E	248	LYS	3.4
1	D	11	ILE	3.3
1	E	247	PRO	3.1
1	C	28	TYR	3.0
1	A	11	ILE	3.0
1	A	88	ASP	3.0
1	C	177	GLU	3.0
1	E	134	SER	3.0
1	E	56	PRO	2.9
1	A	63	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	148	LYS	2.8
1	D	61	VAL	2.8
1	B	11	ILE	2.8
1	E	61	VAL	2.8
1	C	63	VAL	2.8
1	C	194	TYR	2.7
1	C	121	PHE	2.7
1	E	283	SER	2.6
1	C	285	PRO	2.6
1	E	57	VAL	2.6
1	E	130	LEU	2.6
1	D	117	ARG	2.5
1	A	28	TYR	2.5
1	A	293	ARG	2.5
1	C	89	VAL	2.5
1	C	148	LYS	2.5
1	D	148	LYS	2.5
1	E	62	ARG	2.5
1	E	193	GLN	2.4
1	E	146	LEU	2.4
1	C	61	VAL	2.4
1	E	102	TYR	2.4
1	B	85	ARG	2.4
1	D	288	ALA	2.4
1	E	94	VAL	2.3
1	C	38	LYS	2.3
1	C	85	ARG	2.3
1	C	9	PRO	2.3
1	C	79	VAL	2.3
1	B	117	ARG	2.3
1	C	286	ALA	2.2
1	A	27	CYS	2.2
1	B	186	TYR	2.2
1	D	48	LYS	2.2
1	C	176	LEU	2.2
1	E	142	LEU	2.2
1	D	85	ARG	2.2
1	D	137	THR	2.1
1	A	119	TYR	2.1
1	C	293	ARG	2.1
1	E	85	ARG	2.1
1	D	131	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	285	PRO	2.1
1	A	121	PHE	2.1
1	E	295	SER	2.1
1	E	121	PHE	2.1
1	B	194	TYR	2.1
1	A	169	VAL	2.0
1	B	118	ARG	2.0
1	E	117	ARG	2.0
1	A	87	ALA	2.0

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.