



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:56 AM UTC

PDB ID : 3VYI / pdb_00003vyi
Title : Crystal Structure of a trimeric coiled-coil (I/I-type) assembly domain from the voltage-gated proton channel mutant
Authors : Fujiwara, Y.; Takeshita, K.; Nakagawa, A.
Deposited on : 2012-09-25
Resolution : 2.31 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

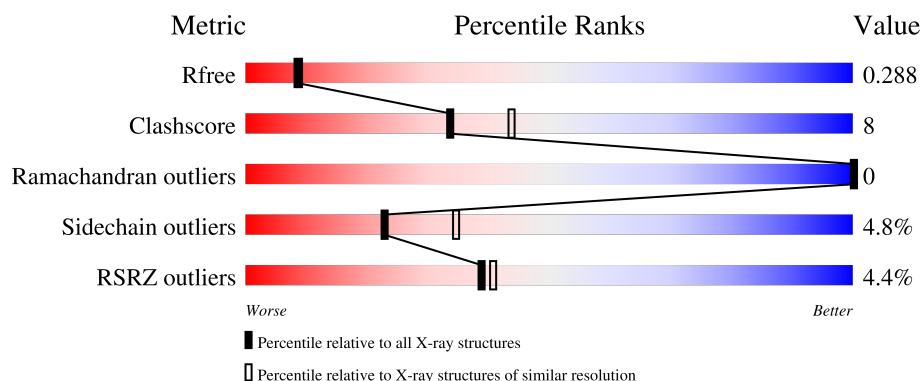
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.



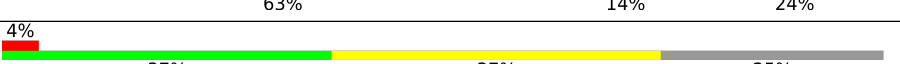
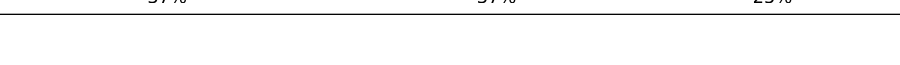
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	51	2% 73% 18% 10%
1	B	51	4% 69% 22% 10%
1	C	51	2% 76% 16% • 6%
1	D	51	2% 71% 22% • 6%
1	E	51	2% 69% 22% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	51	
1	G	51	
1	H	51	
1	I	51	
1	J	51	
1	K	51	
1	L	51	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4529 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 Voltage-gated hydrogen channel 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	46	Total	C	N	O	0	0	0
			384	241	71	72			
1	B	46	Total	C	N	O	0	0	0
			384	241	71	72			
1	D	48	Total	C	N	O	0	0	0
			392	245	73	74			
1	C	48	Total	C	N	O	0	0	0
			396	247	73	76			
1	E	46	Total	C	N	O	0	0	0
			384	241	71	72			
1	F	49	Total	C	N	O	0	0	0
			400	249	74	77			
1	H	40	Total	C	N	O	0	0	0
			341	215	63	63			
1	G	40	Total	C	N	O	0	0	0
			338	212	62	64			
1	I	40	Total	C	N	O	0	0	0
			338	212	62	64			
1	J	42	Total	C	N	O	0	0	0
			356	223	66	67			
1	K	39	Total	C	N	O	0	0	0
			332	210	62	60			
1	L	38	Total	C	N	O	0	0	0
			324	203	60	61			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	-	expression tag	UNP Q3U2S8
A	227	ILE	LEU	engineered mutation	UNP Q3U2S8
A	230	ASN	ILE	engineered mutation	UNP Q3U2S8
A	231	ILE	ASN	engineered mutation	UNP Q3U2S8
A	232	ASN	ILE	engineered mutation	UNP Q3U2S8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ILE	LEU	engineered mutation	UNP Q3U2S8
A	241	ILE	LEU	engineered mutation	UNP Q3U2S8
A	245	ILE	CYS	engineered mutation	UNP Q3U2S8
A	248	ILE	LYS	engineered mutation	UNP Q3U2S8
A	255	ILE	LEU	engineered mutation	UNP Q3U2S8
A	259	ILE	LEU	engineered mutation	UNP Q3U2S8
B	219	GLY	-	expression tag	UNP Q3U2S8
B	227	ILE	LEU	engineered mutation	UNP Q3U2S8
B	230	ASN	ILE	engineered mutation	UNP Q3U2S8
B	231	ILE	ASN	engineered mutation	UNP Q3U2S8
B	232	ASN	ILE	engineered mutation	UNP Q3U2S8
B	234	ILE	LEU	engineered mutation	UNP Q3U2S8
B	241	ILE	LEU	engineered mutation	UNP Q3U2S8
B	245	ILE	CYS	engineered mutation	UNP Q3U2S8
B	248	ILE	LYS	engineered mutation	UNP Q3U2S8
B	255	ILE	LEU	engineered mutation	UNP Q3U2S8
B	259	ILE	LEU	engineered mutation	UNP Q3U2S8
D	219	GLY	-	expression tag	UNP Q3U2S8
D	227	ILE	LEU	engineered mutation	UNP Q3U2S8
D	230	ASN	ILE	engineered mutation	UNP Q3U2S8
D	231	ILE	ASN	engineered mutation	UNP Q3U2S8
D	232	ASN	ILE	engineered mutation	UNP Q3U2S8
D	234	ILE	LEU	engineered mutation	UNP Q3U2S8
D	241	ILE	LEU	engineered mutation	UNP Q3U2S8
D	245	ILE	CYS	engineered mutation	UNP Q3U2S8
D	248	ILE	LYS	engineered mutation	UNP Q3U2S8
D	255	ILE	LEU	engineered mutation	UNP Q3U2S8
D	259	ILE	LEU	engineered mutation	UNP Q3U2S8
C	219	GLY	-	expression tag	UNP Q3U2S8
C	227	ILE	LEU	engineered mutation	UNP Q3U2S8
C	230	ASN	ILE	engineered mutation	UNP Q3U2S8
C	231	ILE	ASN	engineered mutation	UNP Q3U2S8
C	232	ASN	ILE	engineered mutation	UNP Q3U2S8
C	234	ILE	LEU	engineered mutation	UNP Q3U2S8
C	241	ILE	LEU	engineered mutation	UNP Q3U2S8
C	245	ILE	CYS	engineered mutation	UNP Q3U2S8
C	248	ILE	LYS	engineered mutation	UNP Q3U2S8
C	255	ILE	LEU	engineered mutation	UNP Q3U2S8
C	259	ILE	LEU	engineered mutation	UNP Q3U2S8
E	219	GLY	-	expression tag	UNP Q3U2S8
E	227	ILE	LEU	engineered mutation	UNP Q3U2S8
E	230	ASN	ILE	engineered mutation	UNP Q3U2S8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	231	ILE	ASN	engineered mutation	UNP Q3U2S8
E	232	ASN	ILE	engineered mutation	UNP Q3U2S8
E	234	ILE	LEU	engineered mutation	UNP Q3U2S8
E	241	ILE	LEU	engineered mutation	UNP Q3U2S8
E	245	ILE	CYS	engineered mutation	UNP Q3U2S8
E	248	ILE	LYS	engineered mutation	UNP Q3U2S8
E	255	ILE	LEU	engineered mutation	UNP Q3U2S8
E	259	ILE	LEU	engineered mutation	UNP Q3U2S8
F	219	GLY	-	expression tag	UNP Q3U2S8
F	227	ILE	LEU	engineered mutation	UNP Q3U2S8
F	230	ASN	ILE	engineered mutation	UNP Q3U2S8
F	231	ILE	ASN	engineered mutation	UNP Q3U2S8
F	232	ASN	ILE	engineered mutation	UNP Q3U2S8
F	234	ILE	LEU	engineered mutation	UNP Q3U2S8
F	241	ILE	LEU	engineered mutation	UNP Q3U2S8
F	245	ILE	CYS	engineered mutation	UNP Q3U2S8
F	248	ILE	LYS	engineered mutation	UNP Q3U2S8
F	255	ILE	LEU	engineered mutation	UNP Q3U2S8
F	259	ILE	LEU	engineered mutation	UNP Q3U2S8
H	219	GLY	-	expression tag	UNP Q3U2S8
H	227	ILE	LEU	engineered mutation	UNP Q3U2S8
H	230	ASN	ILE	engineered mutation	UNP Q3U2S8
H	231	ILE	ASN	engineered mutation	UNP Q3U2S8
H	232	ASN	ILE	engineered mutation	UNP Q3U2S8
H	234	ILE	LEU	engineered mutation	UNP Q3U2S8
H	241	ILE	LEU	engineered mutation	UNP Q3U2S8
H	245	ILE	CYS	engineered mutation	UNP Q3U2S8
H	248	ILE	LYS	engineered mutation	UNP Q3U2S8
H	255	ILE	LEU	engineered mutation	UNP Q3U2S8
H	259	ILE	LEU	engineered mutation	UNP Q3U2S8
G	219	GLY	-	expression tag	UNP Q3U2S8
G	227	ILE	LEU	engineered mutation	UNP Q3U2S8
G	230	ASN	ILE	engineered mutation	UNP Q3U2S8
G	231	ILE	ASN	engineered mutation	UNP Q3U2S8
G	232	ASN	ILE	engineered mutation	UNP Q3U2S8
G	234	ILE	LEU	engineered mutation	UNP Q3U2S8
G	241	ILE	LEU	engineered mutation	UNP Q3U2S8
G	245	ILE	CYS	engineered mutation	UNP Q3U2S8
G	248	ILE	LYS	engineered mutation	UNP Q3U2S8
G	255	ILE	LEU	engineered mutation	UNP Q3U2S8
G	259	ILE	LEU	engineered mutation	UNP Q3U2S8
I	219	GLY	-	expression tag	UNP Q3U2S8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	227	ILE	LEU	engineered mutation	UNP Q3U2S8
I	230	ASN	ILE	engineered mutation	UNP Q3U2S8
I	231	ILE	ASN	engineered mutation	UNP Q3U2S8
I	232	ASN	ILE	engineered mutation	UNP Q3U2S8
I	234	ILE	LEU	engineered mutation	UNP Q3U2S8
I	241	ILE	LEU	engineered mutation	UNP Q3U2S8
I	245	ILE	CYS	engineered mutation	UNP Q3U2S8
I	248	ILE	LYS	engineered mutation	UNP Q3U2S8
I	255	ILE	LEU	engineered mutation	UNP Q3U2S8
I	259	ILE	LEU	engineered mutation	UNP Q3U2S8
J	219	GLY	-	expression tag	UNP Q3U2S8
J	227	ILE	LEU	engineered mutation	UNP Q3U2S8
J	230	ASN	ILE	engineered mutation	UNP Q3U2S8
J	231	ILE	ASN	engineered mutation	UNP Q3U2S8
J	232	ASN	ILE	engineered mutation	UNP Q3U2S8
J	234	ILE	LEU	engineered mutation	UNP Q3U2S8
J	241	ILE	LEU	engineered mutation	UNP Q3U2S8
J	245	ILE	CYS	engineered mutation	UNP Q3U2S8
J	248	ILE	LYS	engineered mutation	UNP Q3U2S8
J	255	ILE	LEU	engineered mutation	UNP Q3U2S8
J	259	ILE	LEU	engineered mutation	UNP Q3U2S8
K	219	GLY	-	expression tag	UNP Q3U2S8
K	227	ILE	LEU	engineered mutation	UNP Q3U2S8
K	230	ASN	ILE	engineered mutation	UNP Q3U2S8
K	231	ILE	ASN	engineered mutation	UNP Q3U2S8
K	232	ASN	ILE	engineered mutation	UNP Q3U2S8
K	234	ILE	LEU	engineered mutation	UNP Q3U2S8
K	241	ILE	LEU	engineered mutation	UNP Q3U2S8
K	245	ILE	CYS	engineered mutation	UNP Q3U2S8
K	248	ILE	LYS	engineered mutation	UNP Q3U2S8
K	255	ILE	LEU	engineered mutation	UNP Q3U2S8
K	259	ILE	LEU	engineered mutation	UNP Q3U2S8
L	219	GLY	-	expression tag	UNP Q3U2S8
L	227	ILE	LEU	engineered mutation	UNP Q3U2S8
L	230	ASN	ILE	engineered mutation	UNP Q3U2S8
L	231	ILE	ASN	engineered mutation	UNP Q3U2S8
L	232	ASN	ILE	engineered mutation	UNP Q3U2S8
L	234	ILE	LEU	engineered mutation	UNP Q3U2S8
L	241	ILE	LEU	engineered mutation	UNP Q3U2S8
L	245	ILE	CYS	engineered mutation	UNP Q3U2S8
L	248	ILE	LYS	engineered mutation	UNP Q3U2S8
L	255	ILE	LEU	engineered mutation	UNP Q3U2S8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	259	ILE	LEU	engineered mutation	UNP Q3U2S8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	22	Total O 22 22	0	0
2	D	12	Total O 12 12	0	0
2	C	15	Total O 15 15	0	0
2	E	26	Total O 26 26	0	0
2	F	16	Total O 16 16	0	0
2	H	10	Total O 10 10	0	0
2	G	13	Total O 13 13	0	0
2	I	11	Total O 11 11	0	0
2	J	3	Total O 3 3	0	0
2	K	8	Total O 8 8	0	0
2	L	10	Total O 10 10	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 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: Voltage-gated hydrogen channel 1



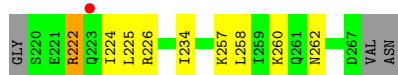
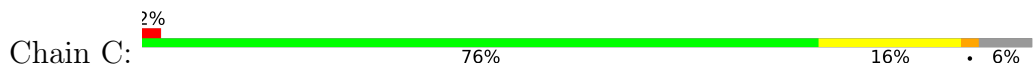
- Molecule 1: Voltage-gated hydrogen channel 1



- Molecule 1: Voltage-gated hydrogen channel 1



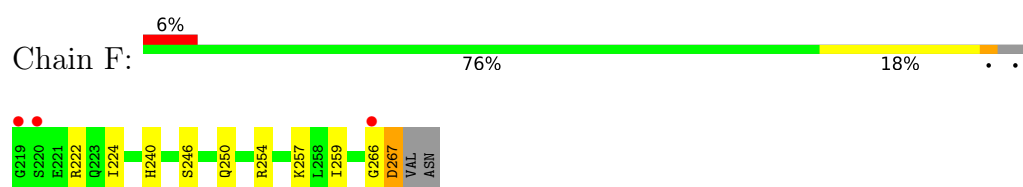
- Molecule 1: Voltage-gated hydrogen channel 1



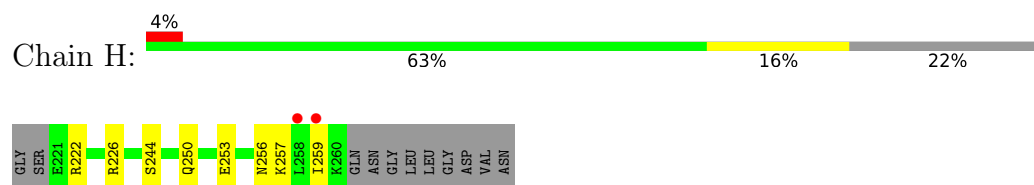
- Molecule 1: Voltage-gated hydrogen channel 1



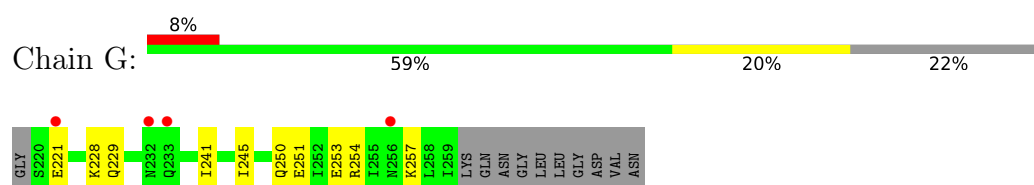
- Molecule 1: Voltage-gated hydrogen channel 1



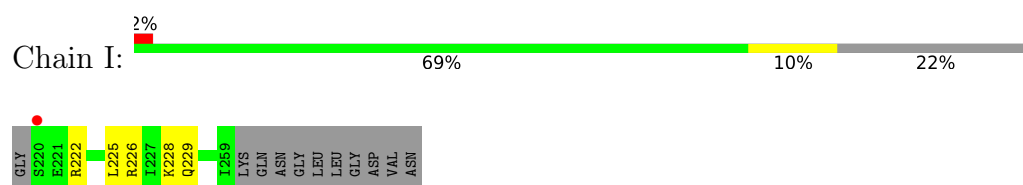
- Molecule 1: Voltage-gated hydrogen channel 1



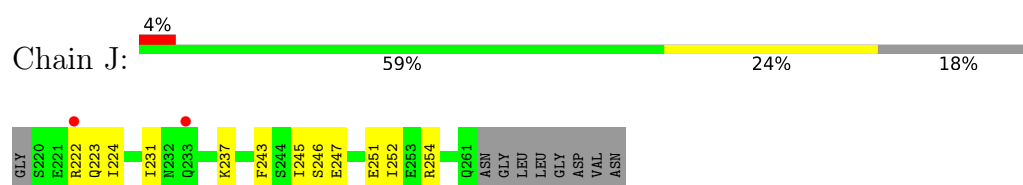
- Molecule 1: Voltage-gated hydrogen channel 1



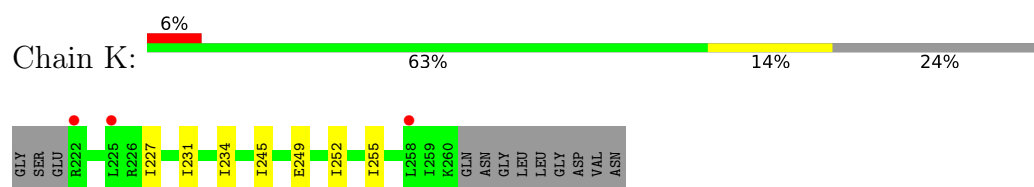
- Molecule 1: Voltage-gated hydrogen channel 1



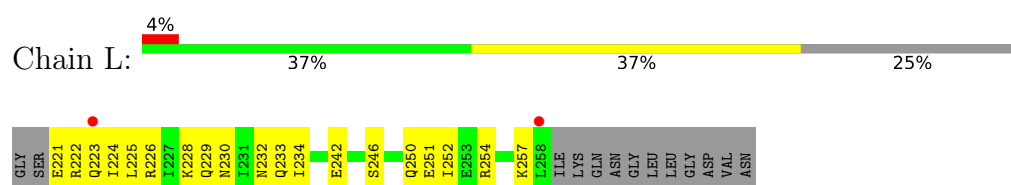
- Molecule 1: Voltage-gated hydrogen channel 1



- Molecule 1: Voltage-gated hydrogen channel 1



- Molecule 1: Voltage-gated hydrogen channel 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.27Å 84.01Å 88.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 2.31 39.11 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.11-2.31) 98.4 (39.11-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.232 , 0.295 0.228 , 0.288	Depositor DCC
R_{free} test set	1398 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4529	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9742e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.56	0/385	0.85	0/513
1	B	0.61	0/385	0.76	0/513
1	C	0.53	0/397	0.84	0/529
1	D	0.56	0/393	0.80	0/523
1	E	0.57	0/385	0.79	0/513
1	F	0.57	0/401	0.84	0/534
1	G	0.63	0/339	0.88	0/452
1	H	0.50	0/342	0.81	0/455
1	I	0.51	0/339	0.75	0/452
1	J	0.60	0/357	0.76	0/475
1	K	0.56	0/333	0.79	0/443
1	L	0.59	0/325	0.85	0/433
All	All	0.57	0/4381	0.81	0/5835

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	384	0	409	6	0
1	B	384	0	409	13	0
1	C	396	0	416	6	0
1	D	392	0	415	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	384	0	409	14	0
1	F	400	0	419	6	0
1	G	338	0	357	7	0
1	H	341	0	365	3	0
1	I	338	0	357	2	0
1	J	356	0	378	10	0
1	K	332	0	359	5	0
1	L	324	0	341	20	0
2	A	14	0	0	0	0
2	B	22	0	0	0	0
2	C	15	0	0	0	0
2	D	12	0	0	0	0
2	E	26	0	0	0	0
2	F	16	0	0	0	0
2	G	13	0	0	0	0
2	H	10	0	0	0	0
2	I	11	0	0	1	0
2	J	3	0	0	0	0
2	K	8	0	0	1	0
2	L	10	0	0	0	0
All	All	4529	0	4634	69	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 8.

All (69) 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:B:229:GLN:HG3	1:L:233:GLN:HE21	1.39	0.88
1:B:229:GLN:HG3	1:L:233:GLN:NE2	2.06	0.70
1:B:229:GLN:HG2	1:E:240:HIS:CE1	2.30	0.67
1:A:256:ASN:OD1	1:B:254:ARG:NH2	2.29	0.60
1:E:247:GLU:HG2	1:L:225:LEU:HD23	1.83	0.60
1:E:255:ILE:O	1:E:259:ILE:HG12	2.05	0.57
1:I:225:LEU:HD23	1:I:228:LYS:HE2	1.87	0.56
1:F:266:GLY:O	1:F:267:ASP:HB2	2.04	0.56
1:I:226:ARG:NH1	2:I:305:HOH:O	2.38	0.56
1:F:246:SER:O	1:F:250:GLN:HG2	2.05	0.56
1:L:224:ILE:HG22	1:L:228:LYS:HE2	1.88	0.55
1:E:251:GLU:HG2	1:L:222:ARG:HH22	1.72	0.54
1:E:243:PHE:CG	1:L:229:GLN:HG3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:LYS:NZ	1:L:250:GLN:OE1	2.43	0.52
1:D:225:LEU:O	1:D:229:GLN:HG3	2.11	0.51
1:E:243:PHE:CD2	1:L:229:GLN:HG3	2.46	0.50
1:L:223:GLN:H	1:L:223:GLN:CD	2.19	0.50
1:B:243:PHE:CD2	1:G:229:GLN:HG3	2.47	0.49
1:D:258:LEU:HD22	1:F:259:ILE:HD13	1.94	0.49
1:L:251:GLU:OE2	1:L:254:ARG:NH2	2.46	0.49
1:L:222:ARG:HD2	1:L:226:ARG:CZ	2.42	0.49
1:A:227:ILE:O	1:A:231:ILE:HG12	2.12	0.49
1:G:250:GLN:HA	1:G:253:GLU:HG2	1.95	0.48
1:J:231:ILE:HG23	1:K:234:ILE:HD11	1.94	0.48
1:K:245:ILE:O	1:K:249:GLU:HG3	2.13	0.48
1:A:265:LEU:HD13	1:B:258:LEU:HD22	1.93	0.48
1:J:222:ARG:HD2	1:J:222:ARG:HA	1.58	0.48
1:H:256:ASN:O	1:H:259:ILE:HG13	2.14	0.48
1:K:252:ILE:HG21	1:L:251:GLU:HG2	1.96	0.47
1:B:265:LEU:HB2	1:C:262:ASN:HD21	1.80	0.47
1:D:237:LYS:HB2	1:D:237:LYS:HE3	1.65	0.46
1:D:255:ILE:O	1:D:259:ILE:HG12	2.15	0.46
1:B:226:ARG:NH2	1:D:249:GLU:OE2	2.41	0.46
1:L:230:ASN:O	1:L:234:ILE:HG12	2.16	0.45
1:K:227:ILE:O	1:K:231:ILE:HG12	2.16	0.45
1:H:222:ARG:O	1:H:226:ARG:HG3	2.17	0.45
1:E:239:GLN:NE2	1:L:232:ASN:OD1	2.49	0.44
1:B:238:ILE:HD11	1:C:234:ILE:HG23	2.00	0.44
1:E:234:ILE:O	1:E:238:ILE:HG12	2.18	0.44
1:C:226:ARG:HD3	2:K:303:HOH:O	2.17	0.44
1:D:258:LEU:HD12	1:F:267:ASP:N	2.33	0.44
1:C:257:LYS:HB2	1:C:257:LYS:HE3	1.84	0.44
1:J:223:GLN:HG3	1:L:224:ILE:HG21	2.00	0.44
1:D:241:ILE:O	1:D:245:ILE:HG12	2.17	0.43
1:J:251:GLU:HG2	1:L:252:ILE:HG21	1.99	0.43
1:J:243:PHE:O	1:J:247:GLU:HG2	2.18	0.43
1:E:221:GLU:H	1:E:221:GLU:CD	2.27	0.43
1:G:241:ILE:O	1:G:245:ILE:HG12	2.19	0.43
1:J:251:GLU:OE1	1:J:254:ARG:HD3	2.19	0.43
1:L:221:GLU:HG2	1:L:224:ILE:HG13	2.01	0.42
1:J:237:LYS:NZ	1:L:242:GLU:OE2	2.42	0.42
1:A:255:ILE:O	1:A:259:ILE:HG12	2.20	0.42
1:G:251:GLU:CD	1:G:254:ARG:HD3	2.45	0.42
1:D:227:ILE:HD11	1:F:224:ILE:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ILE:HD11	1:E:238:ILE:HD11	2.01	0.42
1:A:245:ILE:HD11	1:B:241:ILE:HG23	2.02	0.41
1:J:251:GLU:HA	1:J:254:ARG:HG2	2.03	0.41
1:J:252:ILE:HG23	1:K:255:ILE:HD11	2.02	0.41
1:B:243:PHE:CG	1:G:229:GLN:HG3	2.54	0.41
1:B:226:ARG:HH22	1:D:249:GLU:CD	2.24	0.41
1:F:240:HIS:NE2	1:H:250:GLN:OE1	2.52	0.41
1:A:249:GLU:OE2	1:E:226:ARG:NH2	2.50	0.41
1:C:224:ILE:HD13	1:C:224:ILE:HA	1.87	0.41
1:G:221:GLU:CD	1:G:221:GLU:H	2.28	0.41
1:J:245:ILE:HD13	1:J:245:ILE:HA	1.89	0.41
1:E:243:PHE:CE1	1:L:225:LEU:HG	2.55	0.41
1:B:229:GLN:HG2	1:E:240:HIS:NE2	2.36	0.41
1:C:222:ARG:HG3	1:C:226:ARG:NH2	2.37	0.41
1:E:243:PHE:CD1	1:L:229:GLN:HG3	2.55	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	44/51 (86%)	44 (100%)	0	0	100	100
1	B	44/51 (86%)	44 (100%)	0	0	100	100
1	C	46/51 (90%)	46 (100%)	0	0	100	100
1	D	46/51 (90%)	45 (98%)	1 (2%)	0	100	100
1	E	44/51 (86%)	44 (100%)	0	0	100	100
1	F	47/51 (92%)	47 (100%)	0	0	100	100
1	G	38/51 (74%)	38 (100%)	0	0	100	100
1	H	38/51 (74%)	38 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	38/51 (74%)	37 (97%)	1 (3%)	0	100	100
1	J	40/51 (78%)	39 (98%)	1 (2%)	0	100	100
1	K	37/51 (72%)	36 (97%)	1 (3%)	0	100	100
1	L	36/51 (71%)	35 (97%)	1 (3%)	0	100	100
All	All	498/612 (81%)	493 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	44/47 (94%)	43 (98%)	1 (2%)	44	63
1	B	44/47 (94%)	41 (93%)	3 (7%)	14	20
1	C	45/47 (96%)	41 (91%)	4 (9%)	9	12
1	D	44/47 (94%)	42 (96%)	2 (4%)	24	37
1	E	44/47 (94%)	44 (100%)	0	100	100
1	F	45/47 (96%)	41 (91%)	4 (9%)	9	12
1	G	39/47 (83%)	38 (97%)	1 (3%)	40	59
1	H	39/47 (83%)	36 (92%)	3 (8%)	12	16
1	I	39/47 (83%)	37 (95%)	2 (5%)	21	32
1	J	41/47 (87%)	39 (95%)	2 (5%)	22	34
1	K	38/47 (81%)	38 (100%)	0	100	100
1	L	37/47 (79%)	35 (95%)	2 (5%)	20	29
All	All	499/564 (88%)	475 (95%)	24 (5%)	23	35

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	233	GLN
1	B	247	GLU
1	B	257	LYS
1	D	225	LEU
1	D	233	GLN
1	C	222	ARG
1	C	225	LEU
1	C	258	LEU
1	C	260	LYS
1	F	222	ARG
1	F	254	ARG
1	F	257	LYS
1	F	267	ASP
1	H	244	SER
1	H	253	GLU
1	H	257	LYS
1	G	257	LYS
1	I	222	ARG
1	I	229	GLN
1	J	224	ILE
1	J	246	SER
1	L	246	SER
1	L	257	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	223	GLN
1	B	229	GLN
1	B	233	GLN
1	E	229	GLN
1	G	223	GLN
1	G	229	GLN
1	G	239	GLN
1	I	223	GLN
1	I	233	GLN
1	K	239	GLN
1	K	250	GLN
1	L	223	GLN
1	L	229	GLN
1	L	239	GLN

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	46/51 (90%)	0.51	1 (2%) 62 64	32, 44, 56, 61	0
1	B	46/51 (90%)	0.33	2 (4%) 40 41	22, 40, 54, 72	0
1	C	48/51 (94%)	0.38	1 (2%) 63 65	28, 43, 57, 70	0
1	D	48/51 (94%)	0.37	1 (2%) 63 65	31, 43, 59, 68	0
1	E	46/51 (90%)	0.24	1 (2%) 62 64	24, 39, 57, 68	0
1	F	49/51 (96%)	0.63	3 (6%) 27 29	29, 43, 59, 65	0
1	G	40/51 (78%)	0.56	4 (10%) 12 14	28, 42, 65, 68	0
1	H	40/51 (78%)	0.70	2 (5%) 34 35	32, 46, 70, 75	0
1	I	40/51 (78%)	0.71	1 (2%) 58 60	38, 50, 65, 67	0
1	J	42/51 (82%)	0.99	2 (4%) 35 37	41, 54, 69, 81	0
1	K	39/51 (76%)	0.81	3 (7%) 19 21	31, 47, 72, 81	0
1	L	38/51 (74%)	0.75	2 (5%) 32 34	31, 44, 66, 71	0
All	All	522/612 (85%)	0.57	23 (4%) 39 41	22, 45, 67, 81	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	258	LEU	4.2
1	L	258	LEU	4.1
1	D	219	GLY	3.9
1	H	258	LEU	3.7
1	F	219	GLY	3.2
1	L	223	GLN	3.1
1	J	233	GLN	3.0
1	G	221	GLU	3.0
1	K	225	LEU	2.9
1	K	222	ARG	2.8
1	E	265	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	265	LEU	2.7
1	H	259	ILE	2.7
1	F	220	SER	2.6
1	G	256	ASN	2.5
1	F	266	GLY	2.4
1	I	220	SER	2.3
1	G	232	ASN	2.3
1	J	222	ARG	2.2
1	C	223	GLN	2.2
1	B	265	LEU	2.2
1	B	221	GLU	2.1
1	G	233	GLN	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.