



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:06 PM UTC

PDB ID : 4JPZ / pdb_00004jpz
Title : Voltage-gated sodium channel 1.2 C-terminal domain in complex with FGF13U and Ca²⁺/calmodulin
Authors : Wang, C.; Chung, B.C.; Yan, H.; Wang, H.G.; Lee, S.Y.; Pitt, G.S.
Deposited on : 2013-03-19
Resolution : 3.02 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

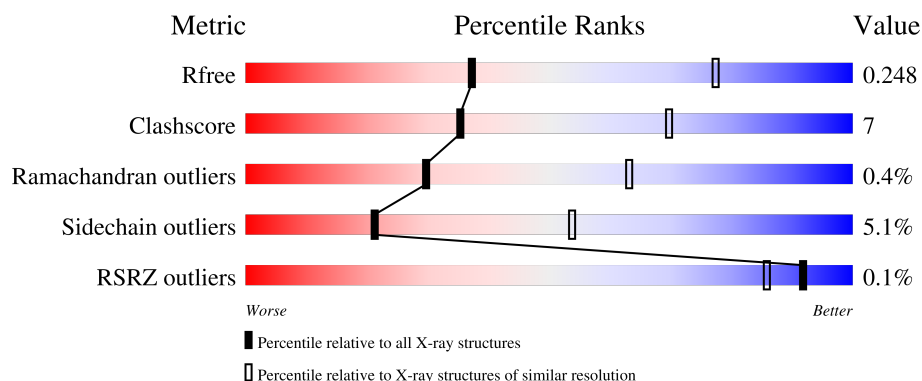
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	192	
1	E	192	
2	B	184	
2	H	184	
3	C	149	

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Mol	Chain	Length	Quality of chain
3	I	149	 74%19% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6991 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 Fibroblast growth factor 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1194	770	198	221	5			
1	E	148	Total	C	N	O	S	0	0	0
			1194	770	198	221	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q92913
A	2	ALA	-	expression tag	UNP Q92913
A	3	LEU	-	expression tag	UNP Q92913
A	4	LEU	-	expression tag	UNP Q92913
A	6	LYS	ARG	SEE REMARK 999	UNP Q92913
A	7	SER	ARG	SEE REMARK 999	UNP Q92913
A	8	TYR	ARG	SEE REMARK 999	UNP Q92913
A	9	SER	PRO	SEE REMARK 999	UNP Q92913
E	1	MET	-	expression tag	UNP Q92913
E	2	ALA	-	expression tag	UNP Q92913
E	3	LEU	-	expression tag	UNP Q92913
E	4	LEU	-	expression tag	UNP Q92913
E	6	LYS	ARG	SEE REMARK 999	UNP Q92913
E	7	SER	ARG	SEE REMARK 999	UNP Q92913
E	8	TYR	ARG	SEE REMARK 999	UNP Q92913
E	9	SER	PRO	SEE REMARK 999	UNP Q92913

- Molecule 2 is a protein called Sodium channel protein type 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1156	744	189	216	7			
2	H	142	Total	C	N	O	S	0	0	0
			1156	744	189	216	7			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1754	MET	-	expression tag	UNP Q99250
B	1755	GLY	-	expression tag	UNP Q99250
B	1756	SER	-	expression tag	UNP Q99250
B	1757	SER	-	expression tag	UNP Q99250
B	1758	HIS	-	expression tag	UNP Q99250
B	1759	HIS	-	expression tag	UNP Q99250
B	1760	HIS	-	expression tag	UNP Q99250
B	1761	HIS	-	expression tag	UNP Q99250
B	1762	HIS	-	expression tag	UNP Q99250
B	1763	HIS	-	expression tag	UNP Q99250
B	1764	SER	-	expression tag	UNP Q99250
B	1765	SER	-	expression tag	UNP Q99250
B	1766	GLY	-	expression tag	UNP Q99250
B	1767	LEU	-	expression tag	UNP Q99250
B	1768	VAL	-	expression tag	UNP Q99250
B	1769	PRO	-	expression tag	UNP Q99250
B	1770	ARG	-	expression tag	UNP Q99250
B	1771	GLY	-	expression tag	UNP Q99250
B	1772	SER	-	expression tag	UNP Q99250
B	1773	HIS	-	expression tag	UNP Q99250
B	1774	MET	-	expression tag	UNP Q99250
B	1775	ALA	-	expression tag	UNP Q99250
B	1776	SER	-	expression tag	UNP Q99250
H	1754	MET	-	expression tag	UNP Q99250
H	1755	GLY	-	expression tag	UNP Q99250
H	1756	SER	-	expression tag	UNP Q99250
H	1757	SER	-	expression tag	UNP Q99250
H	1758	HIS	-	expression tag	UNP Q99250
H	1759	HIS	-	expression tag	UNP Q99250
H	1760	HIS	-	expression tag	UNP Q99250
H	1761	HIS	-	expression tag	UNP Q99250
H	1762	HIS	-	expression tag	UNP Q99250
H	1763	HIS	-	expression tag	UNP Q99250
H	1764	SER	-	expression tag	UNP Q99250
H	1765	SER	-	expression tag	UNP Q99250
H	1766	GLY	-	expression tag	UNP Q99250
H	1767	LEU	-	expression tag	UNP Q99250
H	1768	VAL	-	expression tag	UNP Q99250
H	1769	PRO	-	expression tag	UNP Q99250
H	1770	ARG	-	expression tag	UNP Q99250
H	1771	GLY	-	expression tag	UNP Q99250
H	1772	SER	-	expression tag	UNP Q99250

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1773	HIS	-	expression tag	UNP Q99250
H	1774	MET	-	expression tag	UNP Q99250
H	1775	ALA	-	expression tag	UNP Q99250
H	1776	SER	-	expression tag	UNP Q99250

- Molecule 3 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	143	Total	C	N	O	S	0	0	0
			1124	689	181	245	9			
3	I	143	Total	C	N	O	S	0	0	0
			1128	692	182	245	9			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

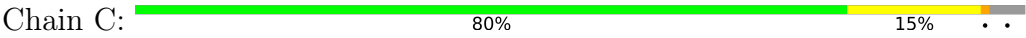
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	4	Total	Ca	0	0
			4	4		
4	I	4	Total	Ca	0	0
			4	4		

- Molecule 5 is water.

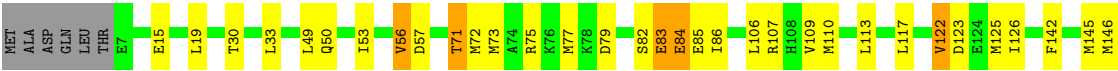
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	6	Total	O	0	0
			6	6		
5	C	6	Total	O	0	0
			6	6		
5	E	5	Total	O	0	0
			5	5		
5	H	6	Total	O	0	0
			6	6		



● Molecule 3: Calmodulin



● Molecule 3: Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.13Å 86.11Å 109.40Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	48.23 – 3.02 48.23 – 3.02	Depositor EDS
% Data completeness (in resolution range)	91.8 (48.23-3.02) 92.3 (48.23-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.212 , 0.246 0.216 , 0.248	Depositor DCC
R_{free} test set	1902 reflections (6.87%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6991	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.38	0/1223	0.83	2/1650 (0.1%)
1	E	0.46	0/1223	0.85	3/1650 (0.2%)
2	B	0.41	0/1179	0.84	3/1588 (0.2%)
2	H	0.43	0/1179	0.83	0/1588
3	C	0.39	0/1136	0.90	2/1525 (0.1%)
3	I	0.38	0/1140	0.87	1/1529 (0.1%)
All	All	0.41	0/7080	0.85	11/9530 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	86	ILE	N-CA-C	-11.34	101.61	112.83
3	I	86	ILE	N-CA-C	-10.68	102.26	112.83
3	C	84	GLU	N-CA-C	-8.21	103.24	113.18
2	B	1866	LEU	N-CA-C	5.92	118.63	111.40
1	E	136	LYS	CA-C-N	5.25	125.56	119.47
1	E	136	LYS	C-N-CA	5.25	125.56	119.47
1	A	144	LYS	CA-C-N	5.22	125.20	120.03
1	A	144	LYS	C-N-CA	5.22	125.20	120.03
2	B	1788	GLU	CA-C-N	5.17	126.31	119.84
2	B	1788	GLU	C-N-CA	5.17	126.31	119.84
1	E	110	GLN	N-CA-C	5.15	117.57	111.33

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	1194	0	1194	21	0
1	E	1194	0	1194	11	0
2	B	1156	0	1170	25	0
2	H	1156	0	1170	14	0
3	C	1124	0	1047	13	0
3	I	1128	0	1058	23	0
4	C	4	0	0	0	0
4	I	4	0	0	0	0
5	A	8	0	0	1	0
5	B	6	0	0	2	0
5	C	6	0	0	0	0
5	E	5	0	0	0	0
5	H	6	0	0	1	0
All	All	6991	0	6833	102	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 7.

All (102) 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)
3:I:107:ARG:NH2	3:I:123:ASP:OD1	2.16	0.78
3:I:82:SER:O	3:I:84:GLU:N	2.16	0.78
3:I:83:GLU:O	3:I:85:GLU:N	2.16	0.78
2:B:1846:MET:HG2	2:B:1852:ILE:HG12	1.68	0.76
2:B:1839:LEU:HA	2:B:1842:MET:HE2	1.69	0.75
3:I:79:ASP:HB3	3:I:82:SER:HB3	1.71	0.73
3:I:109:VAL:HG13	3:I:113:LEU:HD12	1.71	0.71
2:B:1875:LEU:HG	2:B:1879:MET:HE3	1.74	0.70
1:E:16:ILE:HG22	1:E:51:LEU:HB2	1.74	0.70
3:C:110:MET:HE3	3:C:117:LEU:HD11	1.75	0.68
2:H:1875:LEU:HG	2:H:1879:MET:HE2	1.75	0.67
3:C:87:ARG:NH2	3:C:144:GLN:OE1	2.28	0.66
3:I:117:LEU:HB2	3:I:122:VAL:HG23	1.78	0.65
3:I:110:MET:HE3	3:I:117:LEU:HD11	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1880:GLU:HG2	2:H:1884:MET:HE2	1.81	0.62
2:B:1840:ILE:HD11	2:B:1901:LYS:HG3	1.80	0.62
3:I:30:THR:HG21	3:I:50:GLN:HG3	1.81	0.62
1:A:16:ILE:HD12	1:A:145:PRO:HB3	1.82	0.60
3:I:33:LEU:HD22	3:I:49:LEU:HD22	1.83	0.60
1:A:78:LEU:HD13	1:A:126:ILE:HD11	1.83	0.60
3:C:36:VAL:O	3:C:39:SER:OG	2.18	0.60
3:C:117:LEU:HB2	3:C:122:VAL:HG23	1.84	0.59
1:E:78:LEU:HD13	1:E:126:ILE:HD11	1.85	0.59
1:A:82:GLU:HG3	1:A:83:LEU:HD12	1.83	0.59
3:I:56:VAL:HG11	3:I:72:MET:HB2	1.85	0.59
1:E:121:ASN:HD21	1:E:125:GLU:HB2	1.67	0.59
3:C:107:ARG:HB2	3:C:126:ILE:HD11	1.85	0.58
1:A:57:ARG:HA	1:A:57:ARG:HE	1.69	0.58
2:B:1862:THR:HG21	2:B:1879:MET:HE1	1.86	0.57
2:H:1815:PHE:CD1	2:H:1846:MET:HE1	2.40	0.57
2:H:1915:ALA:HA	2:H:1918:ARG:NH1	2.20	0.56
1:A:11:PRO:HA	1:A:150:MET:HB3	1.87	0.54
2:B:1914:ARG:NH1	5:B:2003:HOH:O	2.32	0.54
2:B:1795:PHE:CE1	2:B:1879:MET:HE2	2.43	0.54
1:A:57:ARG:NH1	2:B:1856:ASP:OD2	2.40	0.54
2:B:1794:ASP:O	2:B:1797:MET:HG3	2.07	0.54
2:B:1837:VAL:O	2:B:1840:ILE:HG22	2.08	0.53
2:B:1795:PHE:HE1	2:B:1879:MET:HE2	1.74	0.52
1:E:103:SER:HB3	1:E:117:TYR:CE1	2.45	0.52
2:H:1847:VAL:HG13	5:H:2005:HOH:O	2.10	0.51
1:A:25:GLY:O	1:A:40:LYS:HE3	2.11	0.51
1:A:16:ILE:HD11	1:A:18:THR:HB	1.92	0.51
2:B:1802:TRP:HA	2:B:1821:PHE:HE1	1.76	0.51
2:H:1794:ASP:O	2:H:1797:MET:HG3	2.12	0.49
1:A:16:ILE:HG23	2:B:1895:PRO:HG2	1.93	0.49
3:I:107:ARG:HD2	3:I:126:ILE:HD12	1.94	0.48
2:H:1922:LYS:HA	3:I:77:MET:HE2	1.94	0.48
1:A:19:LYS:HG3	1:A:48:LEU:HD23	1.95	0.48
1:E:62:GLN:HB2	1:E:69:TYR:CD1	2.49	0.48
2:H:1923:GLN:O	2:H:1927:LYS:HB2	2.13	0.48
1:A:117:TYR:CZ	1:A:134:LYS:HB2	2.49	0.48
1:A:85:THR:HG22	1:A:86:PRO:HD2	1.96	0.47
1:A:93:SER:HB3	5:A:207:HOH:O	2.14	0.47
3:C:107:ARG:HG3	3:C:122:VAL:HG11	1.96	0.47
1:E:117:TYR:OH	1:E:134:LYS:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1825:LEU:O	2:H:1830:LEU:HB2	2.14	0.47
1:A:30:LEU:HD11	1:A:80:THR:HG21	1.97	0.47
1:E:73:ASN:HD21	1:E:77:TYR:HB2	1.80	0.46
2:B:1797:MET:HE1	2:B:1825:LEU:HA	1.97	0.46
3:I:107:ARG:HB2	3:I:126:ILE:HD11	1.97	0.46
1:A:103:SER:HB3	1:A:117:TYR:CE1	2.51	0.46
3:I:30:THR:HG23	3:I:53:ILE:HD12	1.98	0.46
3:C:111:THR:HG23	3:C:122:VAL:HG21	1.98	0.46
2:B:1830:LEU:O	2:B:1864:ARG:NH2	2.50	0.45
2:B:1919:TYR:CZ	3:C:145:MET:HE3	2.52	0.45
3:C:87:ARG:O	3:C:91:ARG:HG3	2.17	0.45
3:I:106:LEU:HD21	3:I:125:MET:HE3	1.99	0.44
2:B:1840:ILE:HA	2:B:1900:LEU:HD23	1.99	0.44
1:A:103:SER:HB3	1:A:117:TYR:CD1	2.53	0.44
3:I:56:VAL:HG21	3:I:72:MET:HG3	1.98	0.44
1:A:128:LYS:HD3	1:A:131:HIS:CE1	2.53	0.44
2:B:1839:LEU:HD23	2:B:1842:MET:HE1	1.99	0.43
2:H:1811:GLN:HG2	2:H:1883:PHE:CZ	2.53	0.43
3:I:71:THR:O	3:I:75:ARG:HG3	2.18	0.43
1:A:153:GLU:HA	1:A:154:PRO:HD3	1.78	0.43
1:E:91:LYS:HB2	1:E:105:MET:SD	2.59	0.43
2:H:1790:LEU:HD21	2:H:1865:VAL:HG11	2.00	0.43
3:I:142:PHE:CE2	3:I:146:MET:HE2	2.54	0.43
2:B:1897:THR:HG23	5:B:2006:HOH:O	2.19	0.42
3:C:10:ILE:HA	3:C:13:PHE:HD2	1.85	0.42
3:I:73:MET:HE3	3:I:73:MET:HB3	1.90	0.42
3:I:110:MET:HE2	3:I:125:MET:SD	2.60	0.42
2:H:1919:TYR:CZ	3:I:145:MET:HE3	2.55	0.42
1:E:12:GLN:HB3	1:E:150:MET:HE3	2.02	0.41
1:E:57:ARG:O	1:E:91:LYS:HD2	2.20	0.41
2:H:1848:SER:HA	2:H:1849:GLY:HA2	1.72	0.41
3:I:110:MET:HG3	3:I:125:MET:HE1	2.02	0.41
1:A:109:GLN:HG2	1:A:112:SER:HB3	2.02	0.41
2:B:1818:LEU:HD21	2:B:1839:LEU:HD22	2.02	0.41
3:C:56:VAL:HG11	3:C:72:MET:HB2	2.02	0.41
3:C:110:MET:HG3	3:C:125:MET:HE1	2.02	0.41
1:A:83:LEU:HB3	1:A:157:HIS:ND1	2.36	0.41
2:B:1840:ILE:HG13	2:B:1901:LYS:HA	2.02	0.40
2:H:1829:LEU:HD23	2:H:1829:LEU:HA	1.79	0.40
2:B:1848:SER:HA	2:B:1849:GLY:HA2	1.68	0.40
1:A:33:ASP:OD1	1:A:33:ASP:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1924:LYS:HE3	2:B:1927:LYS:HD3	2.03	0.40
3:C:110:MET:HE3	3:C:117:LEU:CD1	2.46	0.40
1:E:62:GLN:HB2	1:E:69:TYR:CE1	2.57	0.40
2:B:1802:TRP:CZ2	2:B:1854:CYS:HB2	2.57	0.40
2:B:1840:ILE:CD1	2:B:1901:LYS:HG3	2.51	0.40
3:I:15:GLU:O	3:I:19:LEU:HG	2.21	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	146/192 (76%)	137 (94%)	9 (6%)	0	100	100
1	E	146/192 (76%)	140 (96%)	6 (4%)	0	100	100
2	B	140/184 (76%)	133 (95%)	6 (4%)	1 (1%)	18	51
2	H	140/184 (76%)	132 (94%)	8 (6%)	0	100	100
3	C	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
3	I	141/149 (95%)	136 (96%)	3 (2%)	2 (1%)	9	34
All	All	854/1050 (81%)	814 (95%)	37 (4%)	3 (0%)	30	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	83	GLU
3	I	84	GLU
2	B	1789	PRO

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	130/168 (77%)	120 (92%)	10 (8%)	12	38
1	E	130/168 (77%)	122 (94%)	8 (6%)	16	47
2	B	128/163 (78%)	122 (95%)	6 (5%)	23	56
2	H	128/163 (78%)	124 (97%)	4 (3%)	35	67
3	C	121/127 (95%)	114 (94%)	7 (6%)	18	49
3	I	122/127 (96%)	118 (97%)	4 (3%)	33	65
All	All	759/916 (83%)	720 (95%)	39 (5%)	21	54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	35	THR
1	A	45	THR
1	A	51	LEU
1	A	57	ARG
1	A	80	THR
1	A	85	THR
1	A	126	ILE
1	A	142	LEU
1	A	155	SER
2	B	1790	LEU
2	B	1801	VAL
2	B	1840	ILE
2	B	1858	LEU
2	B	1924	LYS
2	B	1928	VAL
3	C	19	LEU
3	C	33	LEU
3	C	56	VAL
3	C	77	MET
3	C	82	SER
3	C	83	GLU

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Mol	Chain	Res	Type
3	C	122	VAL
1	E	16	ILE
1	E	39	THR
1	E	45	THR
1	E	59	VAL
1	E	78	LEU
1	E	85	THR
1	E	109	GLN
1	E	142	LEU
2	H	1797	MET
2	H	1813	ILE
2	H	1924	LYS
2	H	1928	VAL
3	I	56	VAL
3	I	57	ASP
3	I	71	THR
3	I	122	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	42	GLN
3	C	108	HIS
3	C	136	GLN
1	E	12	GLN
2	H	1811	GLN
2	H	1887	ASN
3	I	136	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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	148/192 (77%)	-0.38	0 100 100	39, 71, 99, 121	0
1	E	148/192 (77%)	-0.67	1 (0%) 84 66	24, 41, 73, 92	0
2	B	142/184 (77%)	-0.54	0 100 100	39, 61, 99, 113	0
2	H	142/184 (77%)	-0.56	0 100 100	29, 50, 89, 133	0
3	C	143/149 (95%)	-0.46	0 100 100	38, 71, 110, 130	0
3	I	143/149 (95%)	-0.28	0 100 100	48, 87, 122, 129	0
All	All	866/1050 (82%)	-0.48	1 (0%) 92 86	24, 64, 109, 133	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	11	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	I	201	1/1	0.94	0.04	123,123,123,123	0
4	CA	I	203	1/1	0.95	0.05	78,78,78,78	0
4	CA	I	202	1/1	0.96	0.07	112,112,112,112	0
4	CA	C	204	1/1	0.97	0.04	88,88,88,88	0
4	CA	I	204	1/1	0.97	0.06	76,76,76,76	0
4	CA	C	203	1/1	0.98	0.05	71,71,71,71	0
4	CA	C	201	1/1	0.98	0.04	97,97,97,97	0
4	CA	C	202	1/1	0.99	0.06	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.