



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:23 am BST

PDB ID : 4LTP
Title : Bacterial sodium channel in high calcium, I222 space group, crystal 2
Authors : Shaya, D.; Findeisen, F.; Abderemane-Ali, F.; Arrigoni, C.; Wong, S.; Reddy
Nurva, S.; Loussouarn, G.; Minor, D.L.
Deposited on : 2013-07-23
Resolution : 3.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

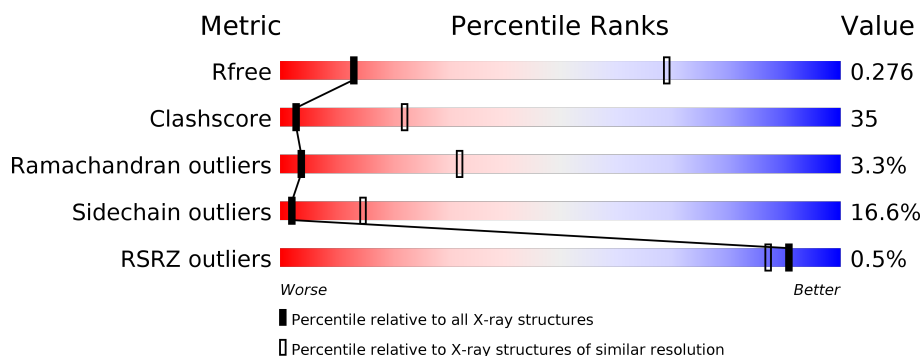
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 on 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	152	<div> <div></div> <div> <div></div> <div>44%</div> <div>37%</div> <div>10%</div> <div>9%</div> </div> </div>
1	B	152	<div> <div></div> <div> <div></div> <div>37%</div> <div>48%</div> <div>6%</div> <div>9%</div> </div> </div>
1	C	152	<div> <div></div> <div> <div></div> <div>45%</div> <div>39%</div> <div>6%</div> <div>9%</div> </div> </div>
1	D	152	<div> <div></div> <div> <div></div> <div>46%</div> <div>34%</div> <div>11%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4090 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1029	687	156	180	6			
1	B	138	Total	C	N	O	S	0	0	0
			1025	687	155	177	6			
1	C	138	Total	C	N	O	S	0	0	0
			1015	681	155	173	6			
1	D	138	Total	C	N	O	S	0	0	0
			1010	678	155	171	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
A	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
A	139	SER	-	EXPRESSION TAG	UNP Q0ABW0
A	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
A	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
A	142	SER	-	EXPRESSION TAG	UNP Q0ABW0
B	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
B	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
B	139	SER	-	EXPRESSION TAG	UNP Q0ABW0
B	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
B	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
B	142	SER	-	EXPRESSION TAG	UNP Q0ABW0
C	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
C	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
C	139	SER	-	EXPRESSION TAG	UNP Q0ABW0
C	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
C	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
C	142	SER	-	EXPRESSION TAG	UNP Q0ABW0
D	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
D	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
D	139	SER	-	EXPRESSION TAG	UNP Q0ABW0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
D	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
D	142	SER	-	EXPRESSION TAG	UNP Q0ABW0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	4	Total Ca 4 4	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

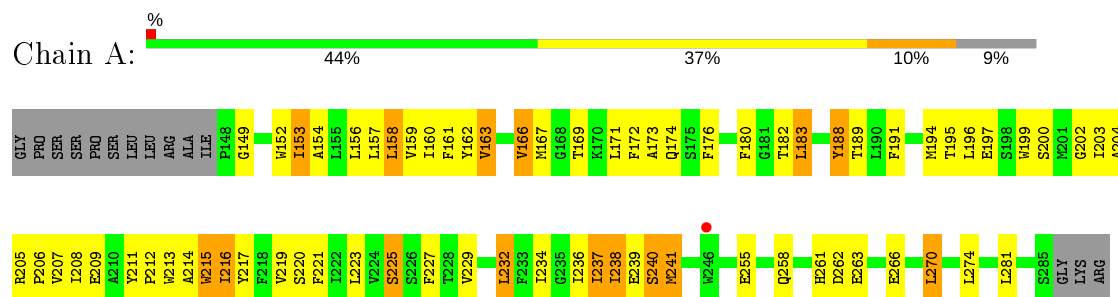
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

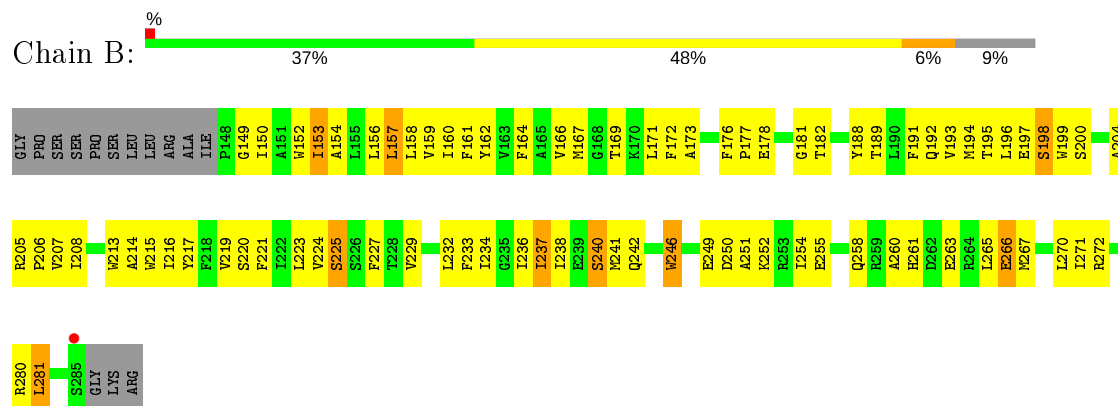
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

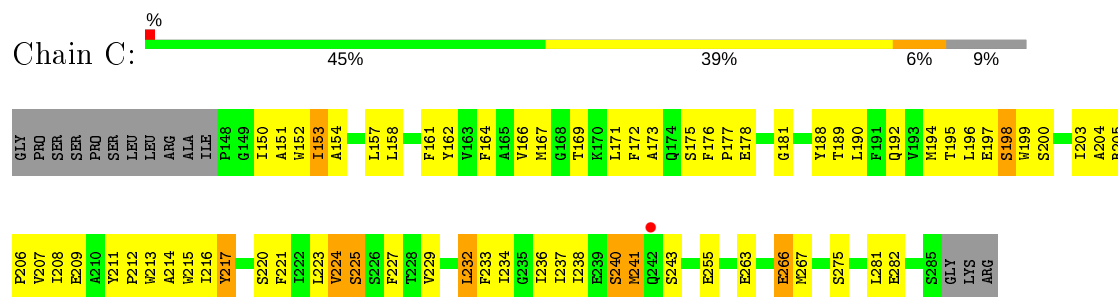
• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein



GLY	PRO	SER	SER	PRO	SER	LEU	LEU	ARG	ALA	ILE	P148	G149	I150	A151	W152	I153	A154	I155	L156	L157	L158	V159	I160	F161	Y162		V166	M167		L171		Q174	S175	F176		T182	L183		M187		Q192	V193	M194	T195	L196	E197	S198	W199	S200	M201	G202	I203	A204	R205	P206	V207	I208	E209	A210
Y211	P212	W213	A214	W215	I216	Y217	F218	V219	S220	F221	I222	L223	V224	S225	S226	F227	T228	V229	L230	M231	L232	F233	I234	G235	L236	I237		S240	M241		E255		A260	H261	D262	E263		E266	M267	L268		L274		L281		S285	GLY	LYS	ARG										

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	147.26 Å 161.50 Å 161.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.80 15.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-3.80) 98.4 (15.00-3.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.77 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.225 , 0.273 0.226 , 0.276	Depositor DCC
R_{free} test set	949 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	172.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 195.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.166 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4090	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.60	0/1057	0.75	0/1447
1	B	0.58	0/1053	0.79	0/1442
1	C	0.60	0/1043	0.78	0/1429
1	D	0.56	0/1038	0.79	0/1423
All	All	0.59	0/4191	0.78	0/5741

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	1029	0	957	87	0
1	B	1025	0	958	75	0
1	C	1015	0	943	88	0
1	D	1010	0	937	83	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	4090	0	3795	277	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 35.

All (277) 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:237:ILE:HA	1:C:234:ILE:HD11	1.09	1.08
1:A:234:ILE:HD11	1:D:237:ILE:HA	1.38	1.04
1:B:205:ARG:HB2	1:B:206:PRO:HD3	1.42	1.00
1:B:237:ILE:CA	1:C:234:ILE:HD11	1.93	0.98
1:A:237:ILE:HA	1:B:234:ILE:HD11	1.46	0.96
1:A:236:ILE:O	1:A:240:SER:HB2	1.64	0.95
1:B:197:GLU:OE2	1:C:200:SER:HB3	1.67	0.94
1:A:270:LEU:HD21	1:B:272:ARG:HG3	1.51	0.93
1:B:281:LEU:HD11	1:C:282:GLU:HG2	1.52	0.92
1:C:162:TYR:O	1:C:166:VAL:HG23	1.69	0.92
1:A:171:LEU:HD23	1:A:213:TRP:HH2	1.35	0.92
1:C:176:PHE:CE1	1:C:207:VAL:HA	2.07	0.90
1:D:200:SER:HA	1:D:204:ALA:HB3	1.53	0.90
1:B:157:LEU:HA	1:B:160:ILE:HD12	1.50	0.90
1:B:167:MET:O	1:B:171:LEU:HD13	1.72	0.90
1:B:236:ILE:O	1:B:240:SER:HB2	1.73	0.89
1:D:157:LEU:HA	1:D:160:ILE:HD12	1.54	0.89
1:A:203:ILE:O	1:A:206:PRO:HD2	1.73	0.88
1:B:281:LEU:CD1	1:C:282:GLU:HG2	2.04	0.88
1:C:167:MET:O	1:C:171:LEU:HD13	1.74	0.87
1:C:237:ILE:O	1:C:241:MET:HB2	1.76	0.86
1:A:238:ILE:HD11	1:D:240:SER:HB3	1.57	0.86
1:A:215:TRP:O	1:A:219:VAL:HG23	1.76	0.85
1:D:176:PHE:CZ	1:D:207:VAL:HA	2.13	0.83
1:A:205:ARG:HE	1:D:192:GLN:NE2	1.75	0.83
1:C:263:GLU:OE2	1:D:261:HIS:CE1	2.33	0.81
1:D:215:TRP:CD1	1:D:216:ILE:N	2.49	0.80
1:A:171:LEU:CD2	1:A:213:TRP:HH2	1.97	0.78
1:B:223:LEU:O	1:B:227:PHE:HB2	1.83	0.78
1:A:171:LEU:HD23	1:A:213:TRP:CH2	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:HB	1:B:196:LEU:HD13	1.66	0.76
1:C:263:GLU:OE2	1:D:261:HIS:NE2	2.19	0.75
1:D:204:ALA:HA	1:D:218:PHE:CE1	2.21	0.75
1:B:162:TYR:O	1:B:166:VAL:HG23	1.88	0.74
1:B:266:GLU:HG3	1:B:267:MET:N	2.02	0.74
1:A:221:PHE:O	1:A:225:SER:HB3	1.88	0.74
1:C:233:PHE:CE2	1:C:237:ILE:HD11	2.21	0.73
1:A:195:THR:HB	1:B:196:LEU:CD1	2.17	0.73
1:A:176:PHE:CZ	1:A:207:VAL:HA	2.25	0.72
1:C:195:THR:HB	1:D:196:LEU:HD13	1.72	0.71
1:D:223:LEU:O	1:D:227:PHE:HB2	1.91	0.71
1:B:215:TRP:CG	1:B:216:ILE:N	2.58	0.70
1:D:150:ILE:C	1:D:152:TRP:H	1.95	0.70
1:A:157:LEU:HA	1:A:160:ILE:HD12	1.73	0.70
1:A:215:TRP:CD1	1:A:216:ILE:N	2.60	0.69
1:C:176:PHE:CZ	1:C:207:VAL:HA	2.27	0.69
1:C:197:GLU:OE1	1:D:198:SER:HA	1.93	0.69
1:A:241:MET:HB3	1:D:241:MET:HE1	1.74	0.69
1:A:149:GLY:H	1:A:152:TRP:HB2	1.59	0.68
1:C:205:ARG:HB2	1:C:206:PRO:HD3	1.75	0.68
1:A:196:LEU:HD13	1:D:195:THR:HB	1.77	0.67
1:D:215:TRP:CG	1:D:216:ILE:N	2.63	0.67
1:A:237:ILE:CA	1:B:234:ILE:HD11	2.22	0.67
1:A:171:LEU:CD2	1:A:213:TRP:CH2	2.75	0.67
1:B:215:TRP:CD1	1:B:216:ILE:N	2.63	0.67
1:A:153:ILE:HG22	1:A:156:LEU:HD23	1.77	0.67
1:D:167:MET:O	1:D:171:LEU:HD13	1.93	0.67
1:D:266:GLU:HG3	1:D:267:MET:N	2.09	0.66
1:C:241:MET:CE	1:D:241:MET:HB3	2.26	0.66
1:A:211:TYR:HB3	1:A:213:TRP:NE1	2.11	0.66
1:D:205:ARG:HB2	1:D:206:PRO:HD3	1.76	0.66
1:B:214:ALA:O	1:B:217:TYR:HB3	1.96	0.66
1:D:266:GLU:HG3	1:D:267:MET:H	1.61	0.65
1:A:223:LEU:O	1:A:227:PHE:HB2	1.96	0.65
1:B:260:ALA:HA	1:B:263:GLU:H	1.60	0.65
1:C:172:PHE:HE1	1:C:217:TYR:CE2	2.14	0.65
1:B:240:SER:HB3	1:C:238:ILE:HD11	1.78	0.65
1:D:194:MET:HG3	1:D:225:SER:OG	1.95	0.65
1:A:270:LEU:HD23	1:B:271:ILE:HG22	1.77	0.65
1:A:205:ARG:HH21	1:D:192:GLN:NE2	1.95	0.65
1:B:177:PRO:HD2	1:B:178:GLU:H	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HB2	1:B:206:PRO:CD	2.24	0.64
1:A:153:ILE:HB	1:A:232:LEU:HD12	1.79	0.64
1:A:236:ILE:O	1:A:240:SER:CB	2.44	0.63
1:B:195:THR:HB	1:C:196:LEU:HD13	1.79	0.63
1:D:171:LEU:HD23	1:D:213:TRP:CH2	2.33	0.63
1:A:167:MET:O	1:A:171:LEU:HD13	1.98	0.63
1:D:203:ILE:O	1:D:206:PRO:HD2	1.99	0.63
1:C:223:LEU:O	1:C:227:PHE:HB2	1.99	0.62
1:C:150:ILE:C	1:C:152:TRP:H	2.02	0.62
1:A:215:TRP:CG	1:A:216:ILE:N	2.67	0.62
1:B:213:TRP:O	1:B:216:ILE:HG22	1.99	0.62
1:D:196:LEU:HD22	1:D:199:TRP:CD1	2.34	0.62
1:D:237:ILE:O	1:D:241:MET:HB2	2.00	0.61
1:C:208:ILE:HA	1:C:211:TYR:O	2.00	0.61
1:A:167:MET:O	1:A:171:LEU:CD1	2.49	0.61
1:A:234:ILE:HD11	1:D:237:ILE:CA	2.25	0.61
1:A:234:ILE:HG13	1:A:237:ILE:HD12	1.80	0.61
1:B:191:PHE:O	1:B:195:THR:HG23	2.00	0.61
1:C:177:PRO:HD2	1:C:178:GLU:H	1.64	0.61
1:B:200:SER:HA	1:B:204:ALA:HB3	1.83	0.60
1:A:211:TYR:HB3	1:A:213:TRP:CE2	2.37	0.60
1:D:231:ASN:O	1:D:234:ILE:HG22	2.01	0.60
1:D:233:PHE:CE2	1:D:237:ILE:HD11	2.37	0.60
1:B:205:ARG:CB	1:B:206:PRO:HD3	2.26	0.60
1:C:197:GLU:HG3	1:D:199:TRP:H	1.66	0.60
1:A:205:ARG:HE	1:D:192:GLN:HE22	1.47	0.59
1:A:169:THR:O	1:A:173:ALA:HB2	2.02	0.59
1:A:258:GLN:HG3	1:A:258:GLN:O	2.02	0.58
1:D:166:VAL:HG22	1:D:183:LEU:HD21	1.84	0.58
1:C:200:SER:HA	1:C:204:ALA:HB3	1.85	0.58
1:A:205:ARG:HB2	1:A:206:PRO:HD3	1.85	0.58
1:A:208:ILE:HD11	1:A:215:TRP:HA	1.85	0.58
1:C:169:THR:O	1:C:173:ALA:HB2	2.01	0.58
1:B:169:THR:O	1:B:173:ALA:HB2	2.03	0.58
1:A:241:MET:HB3	1:D:241:MET:CE	2.33	0.58
1:A:237:ILE:O	1:A:241:MET:N	2.26	0.58
1:B:177:PRO:CD	1:B:178:GLU:H	2.17	0.58
1:C:225:SER:O	1:C:229:VAL:HG23	2.05	0.57
1:D:263:GLU:O	1:D:266:GLU:HG3	2.04	0.57
1:A:199:TRP:CZ3	1:A:200:SER:HB2	2.40	0.56
1:D:153:ILE:HG22	1:D:156:LEU:HD23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:SER:HA	1:A:223:LEU:HD12	1.87	0.56
1:D:167:MET:O	1:D:171:LEU:CD1	2.53	0.56
1:C:177:PRO:CD	1:C:178:GLU:H	2.18	0.56
1:C:198:SER:HB2	1:D:201:MET:HG3	1.86	0.56
1:C:171:LEU:CD2	1:C:213:TRP:HH2	2.19	0.55
1:C:221:PHE:O	1:C:225:SER:HB3	2.06	0.55
1:C:215:TRP:CG	1:C:216:ILE:N	2.74	0.55
1:C:263:GLU:OE2	1:D:261:HIS:CD2	2.60	0.55
1:C:213:TRP:O	1:C:216:ILE:HG22	2.06	0.54
1:A:206:PRO:O	1:A:209:GLU:HB3	2.08	0.54
1:C:164:PHE:CD1	1:C:221:PHE:HD1	2.26	0.54
1:D:221:PHE:O	1:D:225:SER:HB3	2.08	0.54
1:A:203:ILE:C	1:A:206:PRO:HD2	2.26	0.54
1:A:237:ILE:HG22	1:A:241:MET:HG3	1.90	0.54
1:B:176:PHE:CZ	1:B:207:VAL:HA	2.43	0.54
1:C:177:PRO:O	1:C:181:GLY:HA3	2.07	0.53
1:D:156:LEU:O	1:D:159:VAL:HB	2.09	0.53
1:B:208:ILE:HD11	1:B:215:TRP:HA	1.90	0.53
1:B:249:GLU:O	1:B:252:LYS:N	2.41	0.53
1:C:169:THR:O	1:C:173:ALA:CB	2.57	0.53
1:C:237:ILE:HA	1:D:234:ILE:HD11	1.91	0.53
1:A:200:SER:HA	1:A:204:ALA:HB3	1.91	0.53
1:D:220:SER:HA	1:D:223:LEU:HD12	1.90	0.53
1:C:172:PHE:CD2	1:C:211:TYR:HD1	2.27	0.53
1:A:194:MET:HG3	1:A:225:SER:OG	2.09	0.52
1:B:225:SER:O	1:B:229:VAL:HG23	2.10	0.52
1:D:197:GLU:O	1:D:198:SER:C	2.47	0.52
1:B:192:GLN:NE2	1:C:205:ARG:HH21	2.06	0.52
1:D:215:TRP:O	1:D:219:VAL:HG23	2.09	0.52
1:A:199:TRP:CE3	1:A:200:SER:HB2	2.45	0.51
1:A:270:LEU:HD23	1:B:271:ILE:CG2	2.39	0.51
1:A:169:THR:O	1:A:173:ALA:CB	2.59	0.51
1:D:150:ILE:O	1:D:152:TRP:N	2.44	0.51
1:B:177:PRO:O	1:B:181:GLY:N	2.40	0.51
1:B:234:ILE:C	1:B:236:ILE:H	2.13	0.51
1:C:172:PHE:HD2	1:C:211:TYR:CD1	2.28	0.51
1:C:164:PHE:CD2	1:C:217:TYR:HE1	2.28	0.50
1:C:164:PHE:CE1	1:C:221:PHE:HA	2.46	0.50
1:C:172:PHE:CD2	1:C:211:TYR:CD1	2.99	0.50
1:B:234:ILE:HG13	1:B:237:ILE:HD12	1.94	0.50
1:B:172:PHE:HB3	1:B:176:PHE:HD1	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LEU:HD23	1:D:213:TRP:HH2	1.75	0.50
1:B:197:GLU:OE1	1:C:198:SER:HA	2.10	0.50
1:C:220:SER:OG	1:C:221:PHE:N	2.44	0.50
1:C:241:MET:HE1	1:D:241:MET:HB3	1.94	0.50
1:C:216:ILE:CG2	1:C:217:TYR:N	2.75	0.50
1:A:199:TRP:O	1:A:203:ILE:HB	2.12	0.50
1:C:192:GLN:NE2	1:D:205:ARG:HH21	2.10	0.50
1:A:205:ARG:HE	1:D:192:GLN:HE21	1.56	0.49
1:C:176:PHE:CD1	1:C:207:VAL:HG22	2.47	0.49
1:C:224:VAL:HG12	1:C:225:SER:N	2.26	0.49
1:C:267:MET:HG3	1:D:268:LEU:HD23	1.93	0.49
1:B:169:THR:O	1:B:173:ALA:CB	2.60	0.49
1:A:205:ARG:NE	1:D:192:GLN:NE2	2.53	0.49
1:C:215:TRP:CD1	1:C:216:ILE:N	2.80	0.49
1:C:234:ILE:HG13	1:C:237:ILE:HD12	1.95	0.49
1:D:162:TYR:C	1:D:162:TYR:CD2	2.86	0.49
1:B:242:GLN:HA	1:B:246:TRP:CB	2.43	0.49
1:C:216:ILE:HG23	1:C:217:TYR:N	2.27	0.49
1:A:156:LEU:O	1:A:159:VAL:HB	2.13	0.48
1:B:164:PHE:HD2	1:B:217:TYR:CE1	2.31	0.48
1:C:266:GLU:HG3	1:C:267:MET:N	2.28	0.48
1:A:199:TRP:CH2	1:A:200:SER:HB2	2.48	0.48
1:A:219:VAL:O	1:A:223:LEU:HG	2.13	0.48
1:B:261:HIS:O	1:B:265:LEU:CB	2.61	0.48
1:C:203:ILE:O	1:C:207:VAL:HG23	2.13	0.48
1:A:172:PHE:HB2	1:A:180:PHE:CD1	2.48	0.48
1:B:241:MET:HG2	1:C:238:ILE:HG12	1.94	0.48
1:A:237:ILE:O	1:A:241:MET:HB2	2.14	0.48
1:C:240:SER:HA	1:C:243:SER:OG	2.14	0.48
1:D:210:ALA:O	1:D:212:PRO:HD3	2.14	0.48
1:D:225:SER:O	1:D:229:VAL:HG23	2.13	0.47
1:A:166:VAL:HG22	1:A:183:LEU:HD21	1.95	0.47
1:A:162:TYR:O	1:A:166:VAL:HG23	2.14	0.47
1:B:156:LEU:O	1:B:159:VAL:HB	2.13	0.47
1:D:162:TYR:O	1:D:166:VAL:HG23	2.14	0.47
1:B:172:PHE:O	1:B:173:ALA:C	2.52	0.47
1:B:189:THR:O	1:B:193:VAL:HG23	2.14	0.47
1:C:190:LEU:O	1:C:194:MET:HB2	2.14	0.47
1:A:238:ILE:C	1:A:240:SER:H	2.18	0.47
1:A:261:HIS:CE1	1:D:263:GLU:OE2	2.68	0.47
1:B:149:GLY:O	1:B:152:TRP:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HD12	1:D:274:LEU:HA	1.66	0.47
1:C:189:THR:O	1:C:192:GLN:HB3	2.15	0.47
1:C:171:LEU:CD2	1:C:213:TRP:CH2	2.98	0.46
1:B:156:LEU:O	1:B:160:ILE:HG13	2.15	0.46
1:D:236:ILE:O	1:D:240:SER:HB2	2.16	0.46
1:A:154:ALA:O	1:A:158:LEU:HB2	2.15	0.46
1:D:171:LEU:HD23	1:D:213:TRP:CZ3	2.51	0.46
1:C:267:MET:HB2	1:D:268:LEU:HD21	1.97	0.46
1:A:188:TYR:O	1:A:191:PHE:N	2.49	0.46
1:A:214:ALA:O	1:A:217:TYR:HB3	2.16	0.46
1:D:208:ILE:HD11	1:D:215:TRP:HA	1.97	0.46
1:B:154:ALA:O	1:B:158:LEU:HB2	2.16	0.46
1:A:241:MET:SD	1:D:241:MET:SD	3.15	0.45
1:A:241:MET:CB	1:D:241:MET:CE	2.93	0.45
1:D:219:VAL:O	1:D:223:LEU:HG	2.17	0.45
1:A:197:GLU:HG3	1:B:199:TRP:H	1.82	0.45
1:A:171:LEU:HD21	1:A:213:TRP:CH2	2.49	0.45
1:C:154:ALA:O	1:C:158:LEU:HD12	2.15	0.45
1:D:205:ARG:O	1:D:209:GLU:N	2.44	0.45
1:B:249:GLU:O	1:B:251:ALA:N	2.50	0.45
1:A:238:ILE:O	1:A:240:SER:N	2.49	0.45
1:A:197:GLU:HG3	1:B:199:TRP:CD1	2.52	0.45
1:C:204:ALA:C	1:C:208:ILE:HD12	2.37	0.45
1:B:159:VAL:HG12	1:B:160:ILE:N	2.31	0.44
1:B:215:TRP:O	1:B:219:VAL:HG23	2.17	0.44
1:B:221:PHE:O	1:B:225:SER:HB3	2.17	0.44
1:C:229:VAL:O	1:C:233:PHE:N	2.27	0.44
1:B:177:PRO:CD	1:B:178:GLU:N	2.80	0.44
1:B:238:ILE:C	1:B:240:SER:H	2.20	0.44
1:A:219:VAL:HG12	1:A:223:LEU:HD11	1.99	0.44
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.82	0.44
1:C:164:PHE:HD2	1:C:217:TYR:HE1	1.66	0.44
1:B:150:ILE:C	1:B:152:TRP:H	2.21	0.44
1:D:233:PHE:HE2	1:D:237:ILE:HD11	1.80	0.44
1:D:260:ALA:HA	1:D:263:GLU:H	1.82	0.44
1:C:167:MET:O	1:C:171:LEU:CD1	2.54	0.44
1:A:237:ILE:HG23	1:B:237:ILE:HD12	2.00	0.43
1:C:172:PHE:HD2	1:C:211:TYR:CE1	2.35	0.43
1:B:249:GLU:C	1:B:251:ALA:N	2.71	0.43
1:A:205:ARG:NH2	1:D:192:GLN:NE2	2.66	0.43
1:C:263:GLU:CD	1:D:261:HIS:CD2	2.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:SER:O	1:B:224:VAL:HG23	2.18	0.43
1:D:154:ALA:O	1:D:158:LEU:HB2	2.19	0.43
1:D:214:ALA:O	1:D:217:TYR:HB3	2.18	0.43
1:D:263:GLU:O	1:D:266:GLU:CG	2.65	0.43
1:A:203:ILE:O	1:A:206:PRO:CD	2.57	0.42
1:A:236:ILE:HG22	1:B:234:ILE:HD13	2.01	0.42
1:C:192:GLN:HG3	1:D:200:SER:HB3	2.01	0.42
1:C:153:ILE:HB	1:C:232:LEU:HD12	2.00	0.42
1:D:150:ILE:C	1:D:152:TRP:N	2.66	0.42
1:A:227:PHE:C	1:A:229:VAL:H	2.23	0.42
1:A:202:GLY:O	1:A:206:PRO:HG2	2.18	0.42
1:C:241:MET:SD	1:D:241:MET:HB3	2.60	0.42
1:B:280:ARG:O	1:B:281:LEU:HD12	2.20	0.42
1:C:216:ILE:CG2	1:C:217:TYR:H	2.32	0.41
1:A:159:VAL:O	1:A:163:VAL:HG23	2.20	0.41
1:B:233:PHE:CE2	1:B:237:ILE:HD11	2.55	0.41
1:D:183:LEU:O	1:D:187:MET:HG2	2.20	0.41
1:A:188:TYR:O	1:A:189:THR:C	2.59	0.41
1:A:211:TYR:HA	1:A:212:PRO:HD2	1.75	0.41
1:B:188:TYR:OH	1:C:204:ALA:HB1	2.20	0.41
1:B:194:MET:HG3	1:B:225:SER:OG	2.19	0.41
1:C:172:PHE:HE1	1:C:217:TYR:CD2	2.38	0.41
1:C:196:LEU:HA	1:C:199:TRP:HB3	2.01	0.41
1:C:233:PHE:CD2	1:C:237:ILE:HD11	2.56	0.41
1:A:154:ALA:O	1:A:158:LEU:HD12	2.21	0.41
1:D:208:ILE:HG12	1:D:215:TRP:N	2.35	0.41
1:D:215:TRP:NE1	1:D:216:ILE:HB	2.35	0.41
1:D:220:SER:O	1:D:221:PHE:C	2.59	0.41
1:C:171:LEU:HD21	1:C:213:TRP:CH2	2.56	0.41
1:C:172:PHE:CE2	1:C:211:TYR:HD1	2.39	0.41
1:C:214:ALA:O	1:C:217:TYR:HB3	2.20	0.41
1:C:209:GLU:OE2	1:C:209:GLU:HA	2.21	0.41
1:C:164:PHE:HA	1:C:167:MET:HB2	2.02	0.41
1:A:200:SER:HB3	1:D:197:GLU:OE2	2.20	0.40
1:D:156:LEU:HD21	1:D:160:ILE:HD11	2.03	0.40
1:B:160:ILE:O	1:B:164:PHE:HB2	2.21	0.40
1:C:208:ILE:O	1:C:212:PRO:HA	2.21	0.40
1:B:153:ILE:HG13	1:B:153:ILE:H	1.59	0.40
1:C:234:ILE:C	1:C:236:ILE:H	2.23	0.40
1:A:263:GLU:OE2	1:B:261:HIS:CE1	2.75	0.40
1:C:188:TYR:O	1:C:189:THR:C	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ILE:N	1:C:234:ILE:HD11	2.35	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	136/152 (90%)	110 (81%)	21 (15%)	5 (4%)	3	29
1	B	136/152 (90%)	106 (78%)	25 (18%)	5 (4%)	3	29
1	C	136/152 (90%)	112 (82%)	20 (15%)	4 (3%)	4	34
1	D	136/152 (90%)	113 (83%)	19 (14%)	4 (3%)	4	34
All	All	544/608 (90%)	441 (81%)	85 (16%)	18 (3%)	4	32

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	SER
1	C	198	SER
1	D	151	ALA
1	A	163	VAL
1	A	174	GLN
1	A	238	ILE
1	A	239	GLU
1	B	250	ASP
1	A	188	TYR
1	D	198	SER
1	B	258	GLN
1	C	151	ALA
1	C	217	TYR
1	D	174	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	270	LEU
1	D	260	ALA
1	B	246	TRP
1	C	224	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	96/131 (73%)	78 (81%)	18 (19%)	1	10
1	B	95/131 (72%)	82 (86%)	13 (14%)	3	22
1	C	92/131 (70%)	80 (87%)	12 (13%)	4	23
1	D	91/131 (70%)	72 (79%)	19 (21%)	1	8
All	All	374/524 (71%)	312 (83%)	62 (17%)	2	15

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ILE
1	A	158	LEU
1	A	161	PHE
1	A	166	VAL
1	A	182	THR
1	A	183	LEU
1	A	215	TRP
1	A	216	ILE
1	A	225	SER
1	A	232	LEU
1	A	237	ILE
1	A	240	SER
1	A	241	MET
1	A	255	GLU
1	A	262	ASP
1	A	266	GLU
1	A	270	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	281	LEU
1	B	153	ILE
1	B	157	LEU
1	B	161	PHE
1	B	182	THR
1	B	198	SER
1	B	225	SER
1	B	232	LEU
1	B	237	ILE
1	B	240	SER
1	B	254	ILE
1	B	255	GLU
1	B	266	GLU
1	B	281	LEU
1	C	153	ILE
1	C	157	LEU
1	C	161	PHE
1	C	175	SER
1	C	225	SER
1	C	232	LEU
1	C	240	SER
1	C	241	MET
1	C	255	GLU
1	C	266	GLU
1	C	275	SER
1	C	281	LEU
1	D	153	ILE
1	D	156	LEU
1	D	157	LEU
1	D	158	LEU
1	D	161	PHE
1	D	162	TYR
1	D	166	VAL
1	D	167	MET
1	D	175	SER
1	D	182	THR
1	D	183	LEU
1	D	194	MET
1	D	215	TRP
1	D	216	ILE
1	D	225	SER
1	D	241	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	255	GLU
1	D	266	GLU
1	D	281	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	GLN
1	C	192	GLN
1	D	192	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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	138/152 (90%)	-0.81	1 (0%) 87 83	110, 187, 245, 312	0
1	B	138/152 (90%)	-0.75	1 (0%) 87 83	131, 194, 250, 286	0
1	C	138/152 (90%)	-0.87	1 (0%) 87 83	113, 184, 238, 300	0
1	D	138/152 (90%)	-0.83	0 100 100	130, 177, 242, 290	0
All	All	552/608 (90%)	-0.81	3 (0%) 91 87	110, 186, 247, 312	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	TRP	2.9
1	B	285	SER	2.5
1	C	242	GLN	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 carbohydrates 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(\AA^2)	Q<0.9
2	CA	A	304	1/1	0.58	0.11	221,221,221,221	0
2	CA	A	303	1/1	0.95	0.19	162,162,162,162	0
2	CA	A	302	1/1	0.95	0.41	163,163,163,163	0
2	CA	C	301	1/1	0.98	0.12	123,123,123,123	0
2	CA	D	301	1/1	0.98	0.15	166,166,166,166	0
2	CA	B	301	1/1	0.98	0.46	97,97,97,97	0
2	CA	A	301	1/1	0.99	0.41	143,143,143,143	0

6.5 Other polymers [i](#)

There are no such residues in this entry.