Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 02:47 AM EDT

PDB ID	:	1ORQ
Title	:	X-ray structure of a voltage-dependent potassium channel in complex with an Fab
Authors	:	Jiang, Y.; Lee, A.; Chen, J.; Ruta, V.; Cadene, M.; Chait, B.T.; MacKinnon, R.
Deposited on	:	2003-03-14
Resolution	:	3.20 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 (i) 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 (1)) were used in the production of this report:

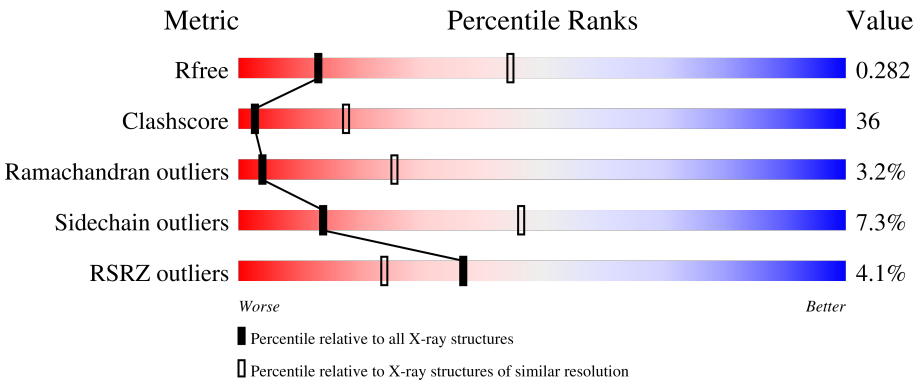
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	215	% 46% 48% 6%
2	B	219	% 44% 49% 7%
3	C	223	10% 43% 52% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	K	C	5	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5059 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 6E1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1652	1024	278	342	8	0	0	0

- Molecule 2 is a protein called 6E1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	219	1674	1060	272	335	7	0	0	0

- Molecule 3 is a protein called potassium channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	223	1714	1145	268	295	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	46	CYS	TYR	engineered mutation	UNP Q9YDF8

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
4	A	3	3	3	0	0
4	B	1	1	1	0	0
4	C	3	3	3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	C	6	6	6	0	0

- Molecule 6 is water.

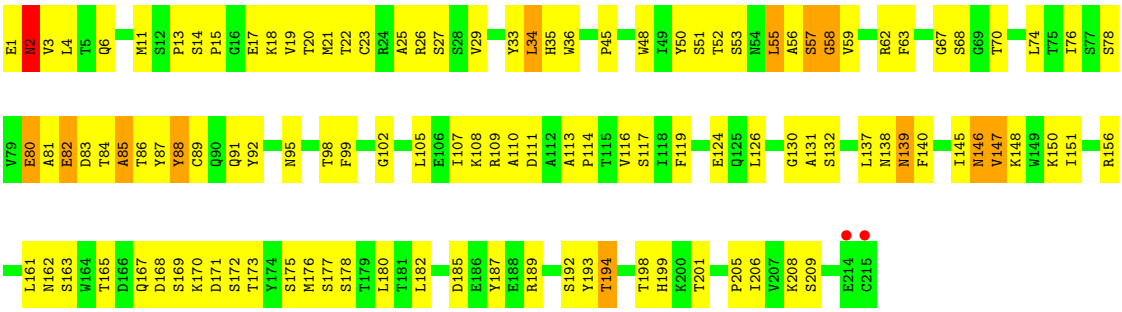
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	2	2	2	0	0
			Total	O		
6	B	2	2	2	0	0
			Total	O		
6	C	2	2	2	0	0

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.

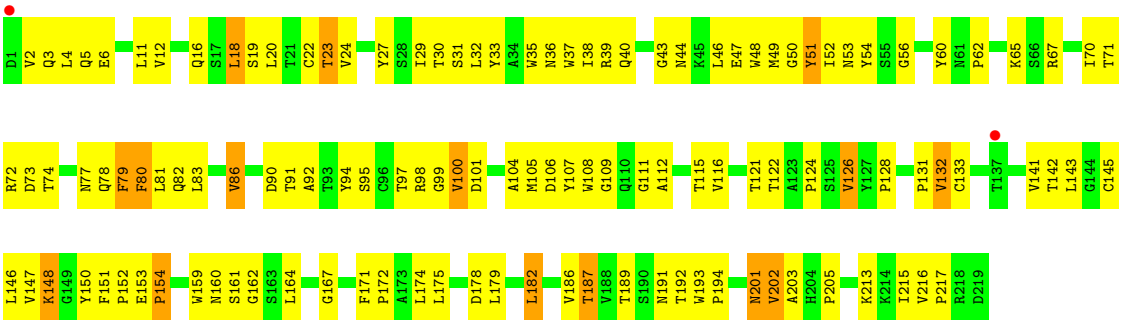
• Molecule 1: 6E1 Fab light chain

Chain A:



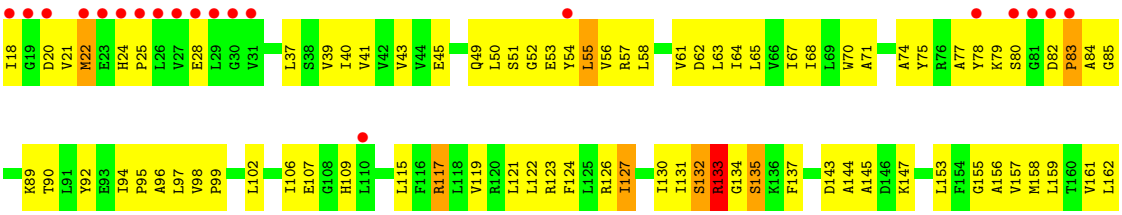
• Molecule 2: 6E1 Fab heavy chain

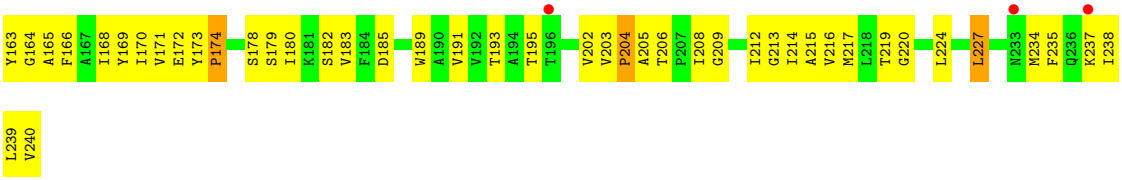
Chain B:



• Molecule 3: potassium channel

Chain C:




Y163
G164
A165
F166
A167
I168
Y169
I170
V171
E172
Y173
P174
S178
S179
I180
K181
S182
V183
F184
D185
W189
A190
V191
V192
T193
A194
T195
T196
V202
V203
P204
A205
T206
P207
I208
G209
I212
G213
I214
A215
V216
M217
L218
T219
G220
L224
L227
N233
M234
F235
Q236
K237
I238
L239
V240

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	189.44Å 189.44Å 150.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.20 29.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.95-3.20) 98.8 (29.95-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.18Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.253 , 0.298 0.247 , 0.282	Depositor DCC
R_{free} test set	1150 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5059	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CD, K

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	0.49	0/1692	0.72	0/2299
2	B	0.48	0/1719	0.73	0/2354
3	C	0.44	0/1751	0.62	0/2389
All	All	0.47	0/5162	0.69	0/7042

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	1652	0	1567	120	1
2	B	1674	0	1623	139	0
3	C	1714	0	1816	125	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
5	C	6	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
All	All	5059	0	5006	362	1

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 36.

All (362) 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)
2:B:100:VAL:HG12	2:B:101:ASP:H	1.09	1.17
3:C:18:ILE:HG23	3:C:22:MET:HG2	1.35	1.05
2:B:36:ASN:HB3	2:B:51:TYR:HB3	1.38	1.04
3:C:18:ILE:HA	3:C:22:MET:HA	1.41	0.98
1:A:113:ALA:HB2	1:A:201:THR:HG21	1.46	0.94
1:A:194:THR:HB	1:A:209:SER:HB2	1.52	0.91
3:C:214:ILE:HA	3:C:217:MET:HE3	1.52	0.91
2:B:124:PRO:HB3	2:B:150:TYR:HB3	1.53	0.90
1:A:11:MET:HG2	1:A:13:PRO:HD3	1.54	0.89
1:A:95:ASN:ND2	2:B:62:PRO:HD3	1.90	0.87
2:B:100:VAL:HG12	2:B:101:ASP:N	1.91	0.86
2:B:143:LEU:HD23	2:B:215:ILE:HG21	1.59	0.83
1:A:62:ARG:HD2	1:A:80:GLU:OE2	1.78	0.82
2:B:153:GLU:OE1	2:B:154:PRO:HA	1.80	0.82
1:A:208:LYS:HA	1:A:208:LYS:HE2	1.60	0.81
3:C:195:THR:HG22	3:C:224:LEU:HD21	1.62	0.81
3:C:165:ALA:O	3:C:168:ILE:HG22	1.81	0.81
2:B:100:VAL:CG1	2:B:101:ASP:H	1.92	0.80
2:B:2:VAL:HB	2:B:107:TYR:CE1	2.19	0.77
1:A:2:ASN:ND2	1:A:27:SER:H	1.83	0.77
2:B:161:SER:H	2:B:201:ASN:ND2	1.82	0.77
2:B:161:SER:H	2:B:201:ASN:HD21	1.32	0.76
1:A:55:LEU:HD12	1:A:55:LEU:H	1.53	0.74
2:B:132:VAL:HG12	2:B:133:CYS:H	1.51	0.74
2:B:36:ASN:HB3	2:B:51:TYR:CB	2.18	0.74
2:B:132:VAL:HG12	2:B:133:CYS:N	2.05	0.71
3:C:195:THR:HG22	3:C:224:LEU:CD2	2.19	0.71
2:B:2:VAL:HB	2:B:107:TYR:CD1	2.26	0.71
2:B:153:GLU:OE1	2:B:153:GLU:HA	1.90	0.71
2:B:30:THR:CG2	2:B:74:THR:HG22	2.19	0.70
1:A:161:LEU:HD21	2:B:174:LEU:HB3	1.71	0.70
2:B:95:SER:HB3	2:B:111:GLY:HA2	1.71	0.70
3:C:49:GLN:HE22	3:C:53:GLU:HG2	1.55	0.70
3:C:57:ARG:NH1	3:C:58:LEU:HA	2.07	0.70
2:B:81:LEU:HD12	2:B:82:GLN:N	2.07	0.69
1:A:2:ASN:HD21	1:A:27:SER:H	1.37	0.69
2:B:72:ARG:HA	2:B:79:PHE:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH1	1:A:80:GLU:OE1	2.25	0.69
2:B:128:PRO:HG3	2:B:213:LYS:HG2	1.74	0.68
3:C:83:PRO:HG2	3:C:84:ALA:H	1.58	0.68
2:B:143:LEU:HD23	2:B:215:ILE:CG2	2.24	0.67
2:B:23:THR:HB	2:B:78:GLN:HE21	1.58	0.67
3:C:49:GLN:NE2	3:C:53:GLU:HG2	2.08	0.67
3:C:173:TYR:N	3:C:174:PRO:HD2	2.09	0.67
3:C:53:GLU:HB3	3:C:56:VAL:HB	1.75	0.67
3:C:238:ILE:HG23	3:C:239:LEU:HD12	1.77	0.67
1:A:109:ARG:HG2	1:A:110:ALA:H	1.60	0.66
2:B:48:TRP:CZ2	2:B:50:GLY:HA2	2.30	0.66
2:B:30:THR:HG21	2:B:74:THR:HG22	1.78	0.66
3:C:172:GLU:OE1	3:C:209:GLY:HA3	1.96	0.66
1:A:206:ILE:H	1:A:206:ILE:HD12	1.61	0.66
1:A:199:HIS:CE1	1:A:201:THR:H	2.13	0.65
3:C:51:SER:O	3:C:57:ARG:HG3	1.97	0.65
3:C:63:LEU:HG	3:C:67:ILE:HD11	1.78	0.65
2:B:18:LEU:HD22	2:B:19:SER:N	2.11	0.65
1:A:137:LEU:HD22	1:A:176:MET:CE	2.27	0.65
3:C:144:ALA:O	3:C:147:LYS:HB3	1.96	0.65
2:B:33:TYR:HD2	2:B:100:VAL:HA	1.62	0.65
3:C:57:ARG:HD2	3:C:57:ARG:O	1.97	0.64
2:B:80:PHE:CE1	3:C:55:LEU:HD13	2.32	0.64
1:A:151:ILE:HD11	1:A:180:LEU:HD21	1.80	0.64
1:A:116:VAL:HG22	1:A:137:LEU:HG	1.80	0.64
1:A:35:HIS:CE1	2:B:104:ALA:HB2	2.33	0.63
1:A:109:ARG:HD2	1:A:173:THR:HG22	1.78	0.63
3:C:94:ILE:HG22	3:C:97:LEU:HB2	1.80	0.63
3:C:132:SER:O	3:C:134:GLY:N	2.31	0.63
2:B:20:LEU:O	2:B:80:PHE:HB3	1.99	0.63
2:B:35:TRP:CH2	2:B:98:ARG:HG3	2.33	0.62
2:B:142:THR:C	2:B:143:LEU:HD12	2.20	0.62
1:A:48:TRP:CE2	1:A:59:VAL:HG13	2.33	0.62
1:A:95:ASN:HD22	2:B:62:PRO:HD3	1.64	0.62
2:B:2:VAL:HG12	2:B:3:GLN:N	2.14	0.62
2:B:4:LEU:HB3	2:B:22:CYS:SG	2.39	0.62
2:B:6:GLU:OE2	2:B:109:GLY:HA3	2.00	0.62
2:B:174:LEU:C	2:B:174:LEU:HD23	2.21	0.62
3:C:64:ILE:O	3:C:68:ILE:HG12	1.99	0.62
1:A:14:SER:OG	1:A:15:PRO:HD2	2.00	0.61
2:B:189:THR:O	2:B:192:THR:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:VAL:O	3:C:195:THR:HG23	1.99	0.61
1:A:161:LEU:HD23	2:B:174:LEU:HD13	1.82	0.61
3:C:126:ARG:O	3:C:130:ILE:HG13	2.00	0.61
3:C:204:PRO:O	3:C:205:ALA:HB3	1.99	0.61
3:C:40:ILE:HG23	3:C:215:ALA:HB2	1.82	0.61
3:C:122:LEU:HD23	3:C:122:LEU:C	2.21	0.61
1:A:84:THR:HG21	1:A:167:GLN:HB3	1.83	0.61
2:B:167:GLY:O	2:B:186:VAL:HA	2.01	0.61
1:A:21:MET:CE	1:A:74:LEU:HD22	2.31	0.60
1:A:137:LEU:HD22	1:A:176:MET:HE2	1.82	0.60
2:B:81:LEU:HD12	2:B:82:GLN:H	1.65	0.60
2:B:162:GLY:C	2:B:164:LEU:H	2.04	0.60
3:C:75:TYR:CE1	3:C:79:LYS:HE3	2.37	0.60
1:A:194:THR:HG22	1:A:209:SER:OG	2.02	0.59
2:B:37:TRP:CD1	2:B:81:LEU:HB2	2.38	0.59
3:C:18:ILE:HG23	3:C:22:MET:CG	2.23	0.59
1:A:17:GLU:HG2	1:A:18:LYS:O	2.01	0.59
2:B:33:TYR:HB3	2:B:99:GLY:O	2.03	0.59
1:A:35:HIS:CE1	1:A:51:SER:H	2.21	0.59
2:B:22:CYS:HB2	2:B:37:TRP:CH2	2.37	0.59
2:B:215:ILE:N	2:B:215:ILE:HD12	2.18	0.59
2:B:27:TYR:HH	2:B:33:TYR:HE1	1.49	0.58
2:B:126:VAL:HG11	2:B:202:VAL:HG11	1.85	0.58
1:A:81:ALA:O	1:A:83:ASP:N	2.37	0.58
1:A:161:LEU:CG	2:B:174:LEU:HD22	2.34	0.58
2:B:105:MET:HE3	2:B:108:TRP:CZ2	2.39	0.58
3:C:164:GLY:HA3	3:C:216:VAL:HG13	1.85	0.58
3:C:65:LEU:O	3:C:68:ILE:HB	2.04	0.58
3:C:37:LEU:O	3:C:41:VAL:HG23	2.04	0.58
1:A:4:LEU:HD22	1:A:23:CYS:SG	2.44	0.58
1:A:113:ALA:HB2	1:A:201:THR:CG2	2.27	0.58
2:B:73:ASP:OD1	3:C:54:TYR:HB3	2.03	0.57
3:C:203:VAL:HG23	3:C:204:PRO:HD2	1.86	0.57
1:A:109:ARG:HG2	1:A:110:ALA:N	2.19	0.57
2:B:193:TRP:CG	2:B:194:PRO:HA	2.39	0.57
2:B:31:SER:O	2:B:32:LEU:HB2	2.05	0.57
1:A:199:HIS:CE1	1:A:201:THR:OG1	2.58	0.56
2:B:178:ASP:O	2:B:179:LEU:HD23	2.05	0.56
3:C:178:SER:C	3:C:180:ILE:H	2.08	0.56
1:A:62:ARG:HD2	1:A:80:GLU:CD	2.24	0.56
2:B:60:TYR:HE1	2:B:70:ILE:H	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:ILE:C	3:C:20:ASP:H	2.09	0.56
1:A:87:TYR:O	1:A:102:GLY:HA2	2.05	0.56
2:B:126:VAL:HG11	2:B:202:VAL:CG1	2.36	0.56
3:C:134:GLY:HA3	3:C:137:PHE:HB3	1.87	0.56
3:C:107:GLU:OE2	3:C:123:ARG:HD3	2.06	0.55
3:C:97:LEU:HD23	3:C:97:LEU:O	2.06	0.55
1:A:161:LEU:HG	2:B:174:LEU:HD22	1.87	0.55
1:A:33:TYR:HD2	1:A:92:TYR:HB3	1.71	0.55
1:A:151:ILE:HD12	1:A:156:ARG:HE	1.71	0.55
2:B:51:TYR:CD1	2:B:51:TYR:C	2.79	0.55
1:A:161:LEU:CD2	2:B:174:LEU:HD13	2.37	0.55
1:A:176:MET:HG2	1:A:177:SER:N	2.22	0.54
2:B:11:LEU:HD12	2:B:115:THR:O	2.07	0.54
2:B:193:TRP:CZ2	2:B:217:PRO:HD3	2.42	0.54
3:C:127:ILE:O	3:C:131:ILE:HG13	2.07	0.54
3:C:132:SER:OG	3:C:133:ARG:N	2.41	0.54
2:B:43:GLY:O	2:B:44:ASN:HB2	2.07	0.54
3:C:57:ARG:HD2	3:C:57:ARG:C	2.26	0.54
1:A:114:PRO:HA	1:A:140:PHE:HB3	1.89	0.54
1:A:80:GLU:HG2	1:A:83:ASP:OD2	2.08	0.54
1:A:145:ILE:HG13	1:A:199:HIS:HB2	1.89	0.54
3:C:95:PRO:HG3	3:C:133:ARG:HH22	1.71	0.54
3:C:135:SER:H	3:C:137:PHE:H	1.55	0.54
3:C:145:ALA:C	3:C:147:LYS:H	2.11	0.54
2:B:91:THR:HG23	2:B:115:THR:HA	1.90	0.53
3:C:189:TRP:HB2	3:C:202:VAL:CG1	2.38	0.53
1:A:126:LEU:HD23	1:A:130:GLY:O	2.09	0.53
3:C:102:LEU:O	3:C:106:ILE:HG13	2.08	0.53
1:A:4:LEU:HD23	1:A:25:ALA:HB2	1.90	0.53
3:C:193:THR:CG2	3:C:217:MET:HG2	2.38	0.53
2:B:24:VAL:HG11	2:B:29:ILE:CG2	2.39	0.53
1:A:168:ASP:O	1:A:172:SER:HA	2.09	0.53
3:C:189:TRP:HD1	3:C:202:VAL:O	1.92	0.52
1:A:171:ASP:OD2	1:A:173:THR:HG23	2.09	0.52
1:A:95:ASN:HD21	2:B:62:PRO:HD3	1.72	0.52
2:B:16:GLN:O	2:B:86:VAL:HG22	2.09	0.52
2:B:24:VAL:HG11	2:B:29:ILE:HG23	1.91	0.52
2:B:29:ILE:O	2:B:54:TYR:HA	2.10	0.52
3:C:82:ASP:CG	3:C:85:GLY:HA3	2.29	0.52
1:A:80:GLU:O	1:A:83:ASP:HB2	2.10	0.52
1:A:81:ALA:C	1:A:83:ASP:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:CG1	2:B:133:CYS:H	2.22	0.52
3:C:115:LEU:O	3:C:119:VAL:HG23	2.09	0.52
1:A:86:THR:HG22	1:A:88:TYR:CE2	2.45	0.52
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.33	0.52
3:C:18:ILE:N	3:C:18:ILE:HD12	2.24	0.52
1:A:148:LYS:HZ2	1:A:150:LYS:HD3	1.75	0.52
1:A:170:LYS:NZ	1:A:170:LYS:HB3	2.24	0.52
2:B:145:CYS:HB2	2:B:159:TRP:CH2	2.45	0.52
3:C:64:ILE:HA	3:C:67:ILE:HD12	1.92	0.52
3:C:119:VAL:O	3:C:123:ARG:HG3	2.10	0.52
3:C:157:VAL:HG12	3:C:158:MET:N	2.24	0.52
2:B:33:TYR:HE2	2:B:100:VAL:HG13	1.75	0.51
1:A:21:MET:HE1	1:A:74:LEU:HD22	1.93	0.51
3:C:171:VAL:HG11	3:C:208:ILE:HG22	1.93	0.51
1:A:35:HIS:ND1	1:A:50:TYR:HA	2.25	0.51
3:C:206:THR:HG22	3:C:208:ILE:H	1.76	0.51
3:C:204:PRO:O	3:C:205:ALA:CB	2.59	0.51
1:A:81:ALA:HB1	1:A:169:SER:O	2.12	0.50
1:A:171:ASP:CG	1:A:173:THR:HG23	2.31	0.50
2:B:12:VAL:CG2	2:B:116:VAL:HG22	2.41	0.50
2:B:97:THR:HA	2:B:107:TYR:O	2.10	0.50
2:B:141:VAL:HG12	2:B:143:LEU:CD1	2.42	0.50
2:B:71:THR:OG1	3:C:55:LEU:HD11	2.12	0.50
3:C:157:VAL:O	3:C:161:VAL:HG23	2.12	0.50
1:A:17:GLU:O	1:A:78:SER:HA	2.12	0.50
3:C:24:HIS:HB3	3:C:25:PRO:HD3	1.93	0.50
1:A:4:LEU:HD13	1:A:89:CYS:SG	2.51	0.49
3:C:21:VAL:HG12	3:C:21:VAL:O	2.12	0.49
3:C:145:ALA:C	3:C:147:LYS:N	2.65	0.49
2:B:6:GLU:CB	2:B:112:ALA:HB2	2.42	0.49
3:C:41:VAL:O	3:C:45:GLU:HB2	2.12	0.49
1:A:6:GLN:HA	1:A:22:THR:O	2.11	0.49
3:C:172:GLU:OE1	3:C:206:THR:HB	2.12	0.49
3:C:166:PHE:O	3:C:169:TYR:HB3	2.12	0.49
2:B:215:ILE:HG22	2:B:215:ILE:O	2.11	0.49
3:C:189:TRP:HB2	3:C:202:VAL:HG12	1.95	0.49
2:B:33:TYR:CE2	2:B:100:VAL:HG13	2.47	0.49
3:C:53:GLU:CB	3:C:56:VAL:HB	2.42	0.49
2:B:11:LEU:HB2	2:B:152:PRO:HG3	1.95	0.49
2:B:12:VAL:HG21	2:B:86:VAL:HG21	1.95	0.49
2:B:39:ARG:NE	2:B:47:GLU:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:GLY:O	3:C:89:LYS:HG3	2.12	0.49
3:C:163:TYR:O	3:C:164:GLY:C	2.51	0.49
1:A:119:PHE:CD1	1:A:119:PHE:N	2.80	0.48
1:A:137:LEU:HD22	1:A:176:MET:HE1	1.95	0.48
1:A:162:ASN:OD1	1:A:178:SER:CB	2.62	0.48
3:C:220:GLY:O	3:C:224:LEU:HB2	2.13	0.48
3:C:94:ILE:HG22	3:C:94:ILE:O	2.13	0.48
3:C:238:ILE:CG2	3:C:239:LEU:HD12	2.41	0.48
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.78	0.48
2:B:106:ASP:O	2:B:107:TYR:HD2	1.96	0.48
3:C:168:ILE:HG13	3:C:172:GLU:HG3	1.95	0.48
3:C:171:VAL:HG12	3:C:171:VAL:O	2.13	0.48
1:A:162:ASN:OD1	1:A:178:SER:HB2	2.13	0.48
2:B:79:PHE:CD1	2:B:79:PHE:N	2.81	0.48
3:C:126:ARG:HG2	3:C:130:ILE:HD11	1.94	0.48
3:C:169:TYR:CZ	3:C:183:VAL:HG22	2.49	0.48
1:A:29:VAL:HG11	1:A:91:GLN:HB2	1.95	0.48
1:A:88:TYR:CD1	2:B:46:LEU:HD12	2.48	0.48
3:C:124:PHE:C	3:C:126:ARG:H	2.17	0.48
1:A:99:PHE:HZ	2:B:105:MET:HE1	1.78	0.48
3:C:95:PRO:O	3:C:99:PRO:HD2	2.14	0.48
1:A:18:LYS:O	1:A:19:VAL:HB	2.13	0.48
3:C:213:GLY:O	3:C:217:MET:HG3	2.14	0.48
1:A:151:ILE:HD12	1:A:156:ARG:NE	2.29	0.47
2:B:67:ARG:HH22	2:B:90:ASP:CG	2.15	0.47
1:A:161:LEU:HD21	2:B:174:LEU:HD22	1.96	0.47
2:B:48:TRP:CH2	2:B:50:GLY:HA2	2.49	0.47
1:A:198:THR:HA	1:A:205:PRO:HB3	1.96	0.47
2:B:142:THR:OG1	2:B:187:THR:HG23	2.13	0.47
3:C:206:THR:HG22	3:C:209:GLY:H	1.79	0.47
1:A:81:ALA:C	1:A:83:ASP:N	2.68	0.47
2:B:126:VAL:HB	2:B:147:VAL:HG22	1.95	0.47
3:C:219:THR:HG22	3:C:220:GLY:N	2.28	0.47
1:A:62:ARG:CD	1:A:80:GLU:OE1	2.63	0.47
1:A:84:THR:O	1:A:85:ALA:HB2	2.14	0.47
2:B:143:LEU:HD12	2:B:143:LEU:N	2.28	0.47
3:C:235:PHE:C	3:C:237:LYS:H	2.18	0.47
1:A:36:TRP:CG	1:A:74:LEU:HD12	2.50	0.47
1:A:56:ALA:O	1:A:57:SER:O	2.33	0.47
2:B:51:TYR:HD1	2:B:52:ILE:N	2.13	0.47
1:A:137:LEU:HD23	1:A:145:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ILE:HG23	2:B:52:ILE:O	2.15	0.46
2:B:162:GLY:C	2:B:164:LEU:N	2.68	0.46
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.80	0.46
2:B:6:GLU:HB2	2:B:112:ALA:HB2	1.97	0.46
2:B:2:VAL:CG1	2:B:3:GLN:N	2.79	0.46
1:A:1:GLU:O	1:A:3:VAL:HG23	2.16	0.46
1:A:91:GLN:HE21	1:A:98:THR:CB	2.28	0.46
1:A:113:ALA:HB1	1:A:114:PRO:HD2	1.97	0.46
1:A:163:SER:OG	2:B:172:PRO:HD2	2.16	0.46
1:A:27:SER:O	1:A:70:THR:HG22	2.15	0.46
2:B:100:VAL:CG1	2:B:101:ASP:N	2.62	0.46
2:B:40:GLN:O	2:B:92:ALA:HB1	2.16	0.46
3:C:178:SER:O	3:C:179:SER:HB2	2.15	0.46
1:A:167:GLN:NE2	1:A:172:SER:O	2.46	0.46
3:C:162:LEU:O	3:C:165:ALA:HB3	2.16	0.46
2:B:146:LEU:HD22	2:B:148:LYS:HD2	1.97	0.45
1:A:167:GLN:HE21	1:A:172:SER:C	2.20	0.45
2:B:215:ILE:N	2:B:215:ILE:CD1	2.79	0.45
2:B:53:ASN:O	2:B:56:GLY:N	2.37	0.45
2:B:193:TRP:CD1	2:B:194:PRO:HA	2.51	0.45
2:B:27:TYR:OH	2:B:33:TYR:HE1	1.98	0.45
1:A:34:LEU:HD13	1:A:35:HIS:N	2.32	0.45
2:B:141:VAL:HG12	2:B:143:LEU:HD11	1.99	0.45
3:C:117:ARG:HB2	3:C:117:ARG:HH11	1.82	0.45
3:C:157:VAL:C	3:C:159:LEU:N	2.70	0.45
1:A:91:GLN:HE21	1:A:98:THR:HB	1.82	0.45
1:A:110:ALA:O	1:A:111:ASP:C	2.55	0.45
2:B:2:VAL:HB	2:B:107:TYR:HE1	1.76	0.44
3:C:124:PHE:C	3:C:126:ARG:N	2.70	0.44
1:A:1:GLU:O	1:A:3:VAL:N	2.50	0.44
1:A:182:LEU:HD11	1:A:193:TYR:HE2	1.83	0.44
2:B:51:TYR:C	2:B:51:TYR:HD1	2.21	0.44
3:C:155:GLY:O	3:C:156:ALA:C	2.55	0.44
2:B:153:GLU:CD	2:B:154:PRO:HA	2.36	0.44
1:A:45:PRO:HD2	2:B:108:TRP:CE3	2.52	0.44
1:A:57:SER:OG	1:A:58:GLY:N	2.50	0.44
1:A:76:ILE:HG22	1:A:78:SER:O	2.18	0.44
1:A:105:LEU:HD23	1:A:105:LEU:C	2.37	0.44
2:B:94:TYR:N	2:B:94:TYR:CD1	2.86	0.44
3:C:39:VAL:O	3:C:43:VAL:HG23	2.17	0.44
1:A:137:LEU:HD13	1:A:176:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:PHE:CD1	2:B:152:PRO:HA	2.53	0.44
2:B:4:LEU:HD12	2:B:4:LEU:N	2.33	0.44
2:B:39:ARG:HD3	2:B:49:MET:CE	2.47	0.44
3:C:18:ILE:CG2	3:C:22:MET:HG2	2.26	0.44
3:C:172:GLU:C	3:C:174:PRO:HD2	2.38	0.44
2:B:24:VAL:O	2:B:77:ASN:ND2	2.43	0.43
2:B:193:TRP:CH2	2:B:217:PRO:HB3	2.53	0.43
1:A:126:LEU:CD2	1:A:131:ALA:HB2	2.48	0.43
3:C:168:ILE:O	3:C:172:GLU:HB2	2.17	0.43
3:C:171:VAL:HG11	3:C:208:ILE:CG2	2.48	0.43
2:B:160:ASN:HD22	2:B:164:LEU:HD12	1.83	0.43
2:B:193:TRP:HH2	2:B:217:PRO:HB3	1.83	0.43
3:C:133:ARG:HD3	3:C:133:ARG:C	2.38	0.43
2:B:189:THR:HG22	2:B:191:ASN:OD1	2.19	0.43
3:C:51:SER:HB3	3:C:163:TYR:HE1	1.84	0.43
3:C:195:THR:HA	3:C:224:LEU:HD23	2.00	0.43
3:C:206:THR:HG22	3:C:208:ILE:N	2.34	0.43
1:A:185:ASP:HB3	1:A:189:ARG:HH12	1.83	0.43
1:A:187:TYR:HA	1:A:193:TYR:OH	2.19	0.43
3:C:94:ILE:CG2	3:C:97:LEU:HB2	2.46	0.43
3:C:182:SER:HB2	3:C:185:ASP:H	1.84	0.43
3:C:50:LEU:HG	3:C:163:TYR:CE1	2.54	0.43
3:C:57:ARG:C	3:C:57:ARG:CD	2.87	0.43
3:C:126:ARG:HG2	3:C:130:ILE:CD1	2.49	0.43
3:C:173:TYR:N	3:C:174:PRO:CD	2.78	0.43
3:C:212:ILE:O	3:C:216:VAL:HG23	2.19	0.43
1:A:124:GLU:HG2	2:B:213:LYS:NZ	2.33	0.43
2:B:6:GLU:HG2	2:B:95:SER:HA	2.00	0.43
3:C:52:GLY:O	3:C:54:TYR:CD1	2.72	0.43
1:A:51:SER:O	1:A:53:SER:N	2.51	0.43
2:B:146:LEU:CD2	2:B:148:LYS:HD2	2.48	0.43
3:C:75:TYR:HE1	3:C:79:LYS:HE3	1.80	0.43
3:C:182:SER:HB2	3:C:185:ASP:OD1	2.19	0.43
1:A:161:LEU:CD2	2:B:174:LEU:HD22	2.49	0.42
2:B:83:LEU:HD23	2:B:83:LEU:HA	1.75	0.42
2:B:132:VAL:CG1	2:B:133:CYS:N	2.74	0.42
1:A:67:GLY:O	1:A:68:SER:HB3	2.18	0.42
1:A:199:HIS:HE1	1:A:201:THR:OG1	2.02	0.42
3:C:202:VAL:O	3:C:202:VAL:HG12	2.17	0.42
1:A:140:PHE:CD1	1:A:140:PHE:C	2.92	0.42
3:C:178:SER:C	3:C:180:ILE:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:HG22	2:B:116:VAL:HG22	2.00	0.42
2:B:182:LEU:C	2:B:182:LEU:HD23	2.39	0.42
3:C:90:THR:C	3:C:92:TYR:N	2.72	0.42
2:B:171:PHE:HA	2:B:172:PRO:HD3	1.91	0.42
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.34	0.42
1:A:194:THR:HG22	1:A:209:SER:HG	1.83	0.42
2:B:38:ILE:HG21	2:B:108:TRP:CH2	2.54	0.42
2:B:19:SER:O	2:B:20:LEU:HD23	2.20	0.41
2:B:128:PRO:HG3	2:B:213:LYS:CG	2.47	0.41
3:C:153:LEU:HD22	3:C:227:LEU:HD23	2.01	0.41
2:B:101:ASP:OD2	3:C:117:ARG:HB2	2.20	0.41
2:B:160:ASN:C	2:B:162:GLY:H	2.24	0.41
3:C:163:TYR:N	3:C:163:TYR:CD2	2.87	0.41
3:C:78:TYR:C	3:C:80:SER:H	2.24	0.41
3:C:163:TYR:O	3:C:166:PHE:N	2.54	0.41
1:A:86:THR:CG2	1:A:88:TYR:CE2	3.04	0.41
1:A:99:PHE:CZ	2:B:105:MET:HE1	2.55	0.41
3:C:57:ARG:O	3:C:61:VAL:HG23	2.20	0.41
3:C:123:ARG:O	3:C:126:ARG:HB3	2.21	0.41
2:B:18:LEU:HD22	2:B:18:LEU:C	2.40	0.41
3:C:67:ILE:O	3:C:71:ALA:HB3	2.21	0.41
1:A:63:PHE:CE2	1:A:76:ILE:HG12	2.56	0.41
3:C:96:ALA:C	3:C:99:PRO:HD2	2.41	0.41
3:C:98:VAL:N	3:C:99:PRO:HD2	2.35	0.41
3:C:178:SER:O	3:C:180:ILE:N	2.50	0.41
3:C:237:LYS:HA	3:C:240:VAL:HG12	2.03	0.41
3:C:74:ALA:O	3:C:77:ALA:HB3	2.20	0.41
1:A:146:ASN:HD22	1:A:147:VAL:N	2.19	0.40
1:A:57:SER:O	1:A:59:VAL:N	2.54	0.40
2:B:202:VAL:CG2	2:B:203:ALA:N	2.84	0.40
1:A:20:THR:CG2	1:A:21:MET:N	2.84	0.40
1:A:107:ILE:CG2	1:A:108:LYS:N	2.83	0.40
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.79	0.40
3:C:83:PRO:CG	3:C:84:ALA:H	2.30	0.40
1:A:126:LEU:HD21	1:A:131:ALA:HB2	2.02	0.40
1:A:138:ASN:O	1:A:139:ASN:C	2.59	0.40
1:A:165:THR:HG23	2:B:171:PHE:CD1	2.57	0.40
2:B:30:THR:HG21	2:B:74:THR:CG2	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH1	1:A:82:GLU:OE2[5_755]	2.09	0.11

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	213/215 (99%)	184 (86%)	22 (10%)	7 (3%)	4 25
2	B	217/219 (99%)	186 (86%)	27 (12%)	4 (2%)	8 41
3	C	221/223 (99%)	172 (78%)	39 (18%)	10 (4%)	2 18
All	All	651/657 (99%)	542 (83%)	88 (14%)	21 (3%)	4 26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	57	SER
3	C	22	MET
3	C	133	ARG
3	C	135	SER
1	A	58	GLY
1	A	82	GLU
1	A	139	ASN
2	B	65	LYS
2	B	131	PRO
3	C	55	LEU
3	C	121	LEU
3	C	132	SER
1	A	2	ASN
1	A	85	ALA
3	C	83	PRO
3	C	174	PRO
3	C	204	PRO
2	B	100	VAL

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Mol	Chain	Res	Type
2	B	132	VAL
3	C	170	ILE

5.3.2 Protein sidechains (i)

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	189/189 (100%)	177 (94%)	12 (6%)	18 52
2	B	194/194 (100%)	175 (90%)	19 (10%)	8 31
3	C	182/182 (100%)	172 (94%)	10 (6%)	21 57
All	All	565/565 (100%)	524 (93%)	41 (7%)	14 46

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	34	LEU
1	A	55	LEU
1	A	80	GLU
1	A	88	TYR
1	A	117	SER
1	A	132	SER
1	A	146	ASN
1	A	147	VAL
1	A	175	SER
1	A	192	SER
1	A	194	THR
2	B	5	GLN
2	B	18	LEU
2	B	23	THR
2	B	51	TYR
2	B	79	PHE
2	B	80	PHE
2	B	86	VAL
2	B	121	THR

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Mol	Chain	Res	Type
2	B	122	THR
2	B	126	VAL
2	B	148	LYS
2	B	154	PRO
2	B	175	LEU
2	B	182	LEU
2	B	187	THR
2	B	201	ASN
2	B	202	VAL
2	B	205	PRO
2	B	216	VAL
3	C	28	GLU
3	C	62	ASP
3	C	70	TRP
3	C	109	HIS
3	C	117	ARG
3	C	127	ILE
3	C	133	ARG
3	C	143	ASP
3	C	227	LEU
3	C	234	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	90	GLN
1	A	91	GLN
1	A	95	ASN
1	A	138	ASN
1	A	146	ASN
2	B	78	GLN
2	B	82	GLN
2	B	84	HIS
2	B	160	ASN
2	B	201	ASN
3	C	49	GLN
3	C	152	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 13 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	215/215 (100%)	-0.16	2 (0%)	84	75	39, 64, 91, 113	0
2	B	219/219 (100%)	-0.11	2 (0%)	84	75	35, 62, 95, 126	0
3	C	223/223 (100%)	0.27	23 (10%)	6	4	54, 85, 123, 143	0
All	All	657/657 (100%)	0.00	27 (4%)	37	24	35, 69, 117, 143	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	26	LEU	6.2
1	A	215	CYS	5.0
3	C	20	ASP	4.5
3	C	237	LYS	4.5
3	C	25	PRO	4.2
3	C	80	SER	4.0
3	C	81	GLY	4.0
3	C	27	VAL	3.8
2	B	137	THR	3.8
3	C	30	GLY	3.6
3	C	18	ILE	3.3
3	C	19	GLY	3.2
2	B	1	ASP	3.1
3	C	23	GLU	3.0
3	C	28	GLU	2.8
3	C	54	TYR	2.8
3	C	24	HIS	2.6
3	C	83	PRO	2.5
1	A	214	GLU	2.5
3	C	22	MET	2.3
3	C	31	VAL	2.3
3	C	110	LEU	2.3
3	C	82	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	78	TYR	2.3
3	C	29	LEU	2.2
3	C	233	ASN	2.2
3	C	196	THR	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 monosaccharides 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(Å^2)	Q<0.9
5	K	C	2	1/1	0.67	0.25	81,81,81,81	1
5	K	C	5	1/1	0.76	1.61	114,114,114,114	1
4	CD	C	8	1/1	0.78	0.21	201,201,201,201	0
5	K	C	6	1/1	0.83	0.52	135,135,135,135	1
4	CD	A	217	1/1	0.91	0.11	120,120,120,120	0
5	K	C	3	1/1	0.94	0.36	71,71,71,71	1
5	K	C	4	1/1	0.94	0.30	50,50,50,50	1
4	CD	C	7	1/1	0.95	0.16	126,126,126,126	0
4	CD	C	9	1/1	0.96	0.04	127,127,127,127	0
4	CD	A	216	1/1	0.96	0.47	99,99,99,99	1
4	CD	A	218	1/1	0.98	0.07	147,147,147,147	0
5	K	C	1	1/1	0.99	0.25	72,72,72,72	1
4	CD	B	220	1/1	1.00	0.16	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.