Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 01:04 AM EST

PDB ID	:	2D2Z
Title	:	Crystal structure of Soluble Form Of CLIC4
Authors	:	Li, Y.F.; Li, D.F.; Wang, D.C.
Deposited on	:	2005-09-21
Resolution	:	2.20 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:

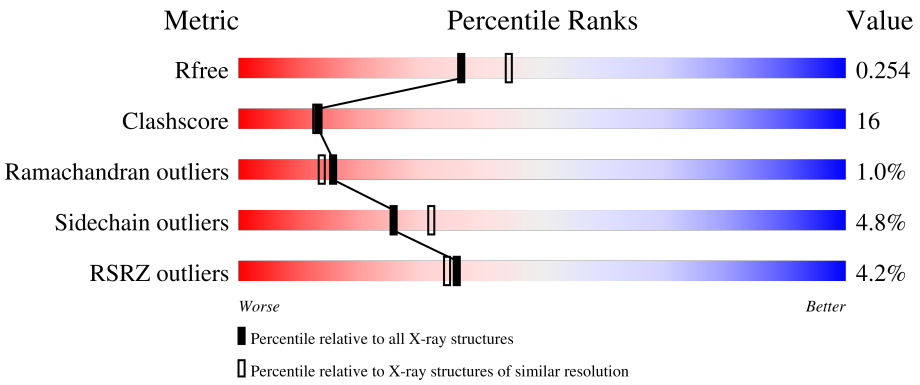
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	261	3% 59% 24% • 15%
1	B	261	6% 55% 32% • 8%
1	C	261	3% 72% 14% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6238 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 Chloride intracellular channel protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	1764	1138	290	328	8	0	0	0
1	B	240	1889	1211	311	359	8	0	0	0
1	C	231	1821	1171	298	344	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	LEU	-	expression tag	UNP Q9Y696
A	255	GLU	-	expression tag	UNP Q9Y696
A	256	HIS	-	expression tag	UNP Q9Y696
A	257	HIS	-	expression tag	UNP Q9Y696
A	258	HIS	-	expression tag	UNP Q9Y696
A	259	HIS	-	expression tag	UNP Q9Y696
A	260	HIS	-	expression tag	UNP Q9Y696
A	261	HIS	-	expression tag	UNP Q9Y696
B	254	LEU	-	expression tag	UNP Q9Y696
B	255	GLU	-	expression tag	UNP Q9Y696
B	256	HIS	-	expression tag	UNP Q9Y696
B	257	HIS	-	expression tag	UNP Q9Y696
B	258	HIS	-	expression tag	UNP Q9Y696
B	259	HIS	-	expression tag	UNP Q9Y696
B	260	HIS	-	expression tag	UNP Q9Y696
B	261	HIS	-	expression tag	UNP Q9Y696
C	254	LEU	-	expression tag	UNP Q9Y696
C	255	GLU	-	expression tag	UNP Q9Y696
C	256	HIS	-	expression tag	UNP Q9Y696
C	257	HIS	-	expression tag	UNP Q9Y696
C	258	HIS	-	expression tag	UNP Q9Y696
C	259	HIS	-	expression tag	UNP Q9Y696
C	260	HIS	-	expression tag	UNP Q9Y696

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Chain	Residue	Modelled	Actual	Comment	Reference
C	261	HIS	-	expression tag	UNP Q9Y696

- Molecule 2 is water.

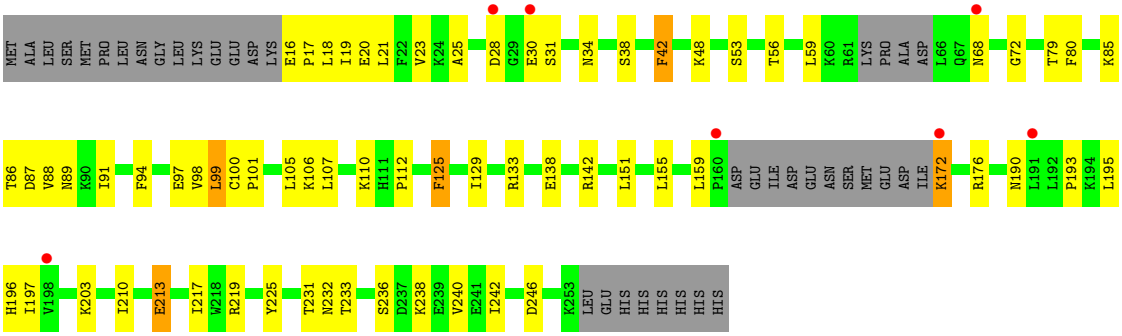
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	229	229	229	0	0
			Total	O		
2	B	254	254	254	0	0
			Total	O		
2	C	281	281	281	0	0

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.

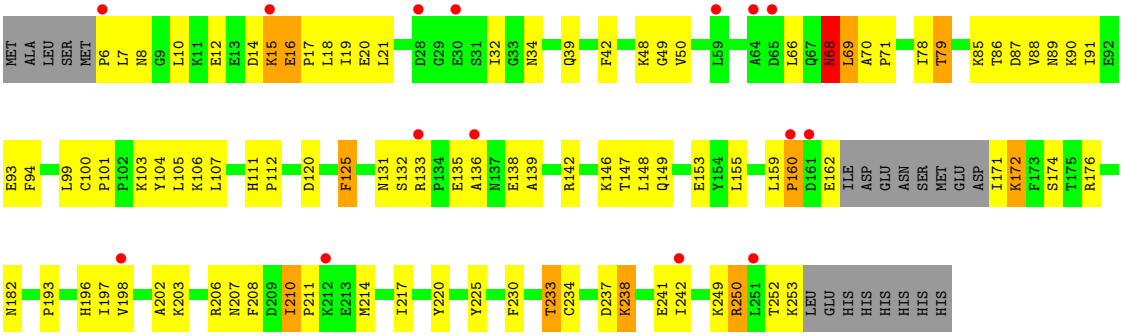
• Molecule 1: Chloride intracellular channel protein 4

Chain A:



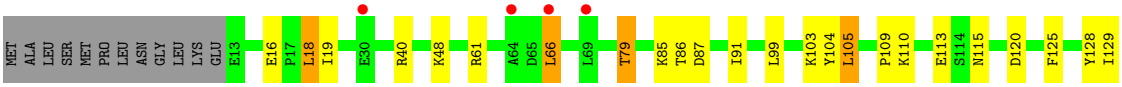
• Molecule 1: Chloride intracellular channel protein 4

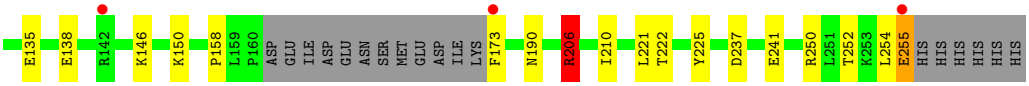
Chain B:



• Molecule 1: Chloride intracellular channel protein 4

Chain C:




E135
E138
R142
K146
K150
P158
L159
P160
ASP
GLU
ILE
ASP
GLU
ASN
SER
MET
GLU
ASP
ILE
LYS
F173
N190
R206
I210
L221
T222
Y225
D237
E241
R250
L251
T252
K253
L254
E255
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.19Å 86.05Å 73.38Å 90.00° 112.99° 90.00°	Depositor
Resolution (Å)	23.49 – 2.20 23.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (23.49-2.20) 99.8 (23.49-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.262 0.212 , 0.254	Depositor DCC
R_{free} test set	4285 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6238	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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)

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	0.36	0/1803	0.57	0/2436
1	B	0.36	0/1929	0.63	3/2607 (0.1%)
1	C	0.39	0/1861	0.63	1/2517 (0.0%)
All	All	0.37	0/5593	0.61	4/7560 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	86	THR	N-CA-C	6.08	127.42	111.00
1	C	206	ARG	N-CA-C	-5.88	95.11	111.00
1	B	6	PRO	N-CA-CB	5.77	110.22	103.30
1	B	210	ILE	N-CA-C	-5.01	97.46	111.00

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	1764	0	1776	54	0
1	B	1889	0	1880	94	0
1	C	1821	0	1813	36	0
2	A	229	0	0	10	0
2	B	254	0	0	13	0
2	C	281	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6238	0	5469	178	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 16.

All (178) 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:174:SER:HB2	2:B:422:HOH:O	1.47	1.15
1:A:98:VAL:HG23	1:A:99:LEU:HD13	1.49	0.95
1:B:50:VAL:HG11	1:B:99:LEU:HD13	1.57	0.86
1:B:34:ASN:HD21	1:B:197:ILE:HD12	1.43	0.84
1:A:193:PRO:O	1:A:197:ILE:HD13	1.80	0.81
1:B:131:ASN:ND2	1:B:133:ARG:H	1.79	0.81
1:C:85:LYS:HB3	1:C:91:ILE:HD12	1.64	0.78
1:B:78:ILE:HG22	1:B:85:LYS:HB2	1.68	0.76
1:B:50:VAL:HG12	1:B:104:TYR:CE1	2.21	0.75
1:B:250:ARG:HD3	1:B:250:ARG:H	1.52	0.75
1:B:211:PRO:HB2	1:B:214:MET:HG3	1.68	0.74
1:B:39:GLN:HG3	1:B:233:THR:HG23	1.69	0.74
1:B:66:LEU:HD23	1:C:250:ARG:NH2	2.04	0.72
1:B:21:LEU:HA	1:B:78:ILE:HD12	1.74	0.68
1:B:237:ASP:O	1:B:241:GLU:HG3	1.94	0.68
1:B:171:ILE:O	1:B:172:LYS:HB2	1.93	0.67
1:B:131:ASN:HD21	1:B:133:ARG:H	1.41	0.67
1:B:230:PHE:O	1:B:233:THR:HG22	1.93	0.67
1:B:176:ARG:HB3	2:B:422:HOH:O	1.96	0.65
1:B:132:SER:HB3	1:B:249:LYS:HB3	1.78	0.65
1:B:162:GLU:OE1	2:B:422:HOH:O	2.14	0.64
1:B:34:ASN:ND2	1:B:197:ILE:HD12	2.11	0.64
1:C:105:LEU:H	1:C:105:LEU:HD23	1.64	0.61
1:B:149:GLN:HA	1:B:214:MET:HE2	1.83	0.61
1:A:238:LYS:O	1:A:242:ILE:HG12	2.00	0.61
1:C:85:LYS:HB3	1:C:91:ILE:CD1	2.31	0.60
1:C:105:LEU:HD23	1:C:105:LEU:N	2.17	0.60
1:A:25:ALA:HB2	1:A:56:THR:HB	1.84	0.59
1:A:172:LYS:NZ	1:A:172:LYS:HB3	2.18	0.59
1:B:203:LYS:O	1:B:207:ASN:HA	2.02	0.59
1:B:250:ARG:HG2	1:B:252:THR:HG23	1.83	0.58
1:B:162:GLU:OE1	1:B:174:SER:HB2	2.02	0.58
1:A:20:GLU:HG3	1:A:53:SER:OG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:CYS:HB2	1:B:101:PRO:CD	2.34	0.57
1:C:18:LEU:HB3	2:C:438:HOH:O	2.05	0.56
1:A:25:ALA:HA	1:A:31:SER:O	2.06	0.56
1:B:19:ILE:HD12	1:B:19:ILE:N	2.21	0.56
1:B:210:ILE:HD12	1:B:210:ILE:H	1.71	0.55
1:C:40:ARG:HD2	1:C:190:ASN:HA	1.87	0.55
1:C:113:GLU:H	1:C:113:GLU:CD	2.10	0.55
1:B:193:PRO:O	1:B:197:ILE:HG12	2.06	0.55
1:C:66:LEU:N	1:C:66:LEU:HD23	2.22	0.55
1:B:50:VAL:CG1	1:B:99:LEU:HD13	2.35	0.55
1:C:18:LEU:O	1:C:19:ILE:HD13	2.07	0.55
1:B:225:TYR:CE2	1:B:230:PHE:HE2	2.25	0.55
1:B:17:PRO:HB2	1:B:19:ILE:HD11	1.88	0.54
1:C:110:LYS:HE2	2:C:290:HOH:O	2.06	0.54
1:B:206:ARG:HH11	1:B:206:ARG:HG2	1.73	0.54
1:B:15:LYS:O	1:B:16:GLU:HB2	2.08	0.54
1:C:128:TYR:CZ	1:C:206:ARG:HG2	2.42	0.54
1:C:237:ASP:O	1:C:241:GLU:HG3	2.07	0.54
1:B:210:ILE:HD12	1:B:210:ILE:N	2.24	0.53
1:B:120:ASP:OD2	1:B:147:THR:HG22	2.07	0.53
1:A:16:GLU:HB3	1:A:17:PRO:HD3	1.91	0.53
1:A:155:LEU:HD12	1:A:217:ILE:HD13	1.91	0.53
1:A:16:GLU:HB3	1:A:17:PRO:CD	2.39	0.53
1:A:59:LEU:HD22	1:B:105:LEU:HD13	1.90	0.53
1:C:40:ARG:CD	1:C:190:ASN:HA	2.39	0.53
1:A:142:ARG:HG3	2:A:406:HOH:O	2.08	0.52
1:B:211:PRO:HD2	1:B:214:MET:SD	2.50	0.52
1:B:176:ARG:CB	2:B:422:HOH:O	2.55	0.52
1:B:100:CYS:HB2	1:B:101:PRO:HD2	1.92	0.52
1:A:196:HIS:HD2	1:A:225:TYR:OH	1.93	0.51
1:B:176:ARG:N	2:B:422:HOH:O	2.15	0.51
1:A:151:LEU:HG	1:A:217:ILE:CD1	2.41	0.51
1:A:18:LEU:C	1:A:19:ILE:HD12	2.31	0.51
1:C:79:THR:HG21	2:C:267:HOH:O	2.10	0.51
1:A:176:ARG:O	1:A:219:ARG:NH2	2.44	0.51
1:A:133:ARG:HH21	1:A:133:ARG:HG2	1.76	0.50
1:B:18:LEU:C	1:B:19:ILE:HD12	2.32	0.50
1:C:103:LYS:HE2	2:C:414:HOH:O	2.12	0.49
1:A:125:PHE:CE1	1:A:129:ILE:HG13	2.48	0.49
1:B:146:LYS:HB2	1:B:146:LYS:NZ	2.27	0.49
1:B:250:ARG:CG	1:B:252:THR:HG23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLU:HB3	2:B:317:HOH:O	2.11	0.49
1:B:106:LYS:HG3	2:B:426:HOH:O	2.13	0.49
1:B:250:ARG:H	1:B:250:ARG:CD	2.22	0.49
1:B:15:LYS:H	1:B:15:LYS:HD3	1.77	0.49
1:C:135:GLU:H	1:C:135:GLU:CD	2.16	0.49
1:A:105:LEU:N	1:A:105:LEU:HD12	2.28	0.49
1:C:48:LYS:NZ	1:C:99:LEU:O	2.38	0.49
1:B:15:LYS:HD3	1:B:15:LYS:N	2.28	0.48
1:B:159:LEU:HG	1:B:160:PRO:HD2	1.95	0.48
1:A:86:THR:O	1:A:87:ASP:HB3	2.13	0.48
1:A:19:ILE:HD11	1:A:80:PHE:CE1	2.48	0.48
1:B:10:LEU:HD13	1:B:10:LEU:O	2.14	0.48
1:B:131:ASN:ND2	1:B:132:SER:N	2.62	0.48
1:A:86:THR:HG22	2:A:349:HOH:O	2.14	0.48
1:A:87:ASP:O	1:A:91:ILE:HG12	2.14	0.48
1:B:39:GLN:CG	1:B:233:THR:HG23	2.40	0.47
1:B:20:GLU:HB2	1:B:79:THR:CG2	2.45	0.47
1:B:68:ASN:O	1:B:69:LEU:HB2	2.13	0.47
1:A:190:ASN:HB2	2:A:268:HOH:O	2.15	0.47
1:B:238:LYS:O	1:B:242:ILE:HG12	2.14	0.47
1:B:7:LEU:HD13	1:C:225:TYR:CE2	2.50	0.47
1:C:210:ILE:HD12	1:C:210:ILE:N	2.29	0.47
1:B:21:LEU:HA	1:B:78:ILE:CD1	2.44	0.46
1:A:28:ASP:C	1:A:30:GLU:H	2.19	0.46
1:C:158:PRO:HG2	1:C:173:PHE:HD2	1.81	0.46
1:A:213:GLU:CD	1:A:213:GLU:H	2.18	0.46
1:A:112:PRO:HB2	1:C:222:THR:HG22	1.97	0.46
1:C:18:LEU:C	1:C:19:ILE:HD13	2.35	0.46
1:B:85:LYS:HE2	1:B:94:PHE:CG	2.52	0.45
1:B:196:HIS:HD2	1:B:225:TYR:OH	1.99	0.45
1:C:103:LYS:HB2	2:C:365:HOH:O	2.14	0.45
1:C:110:LYS:HD3	2:C:538:HOH:O	2.15	0.45
1:B:133:ARG:HH21	1:B:133:ARG:HG3	1.82	0.45
1:C:103:LYS:HD2	1:C:104:TYR:CZ	2.52	0.45
1:A:94:PHE:O	1:A:97:GLU:HB2	2.16	0.45
1:B:131:ASN:ND2	1:B:132:SER:H	2.15	0.45
1:B:202:ALA:HB1	1:B:208:PHE:HB3	1.98	0.45
1:A:72:GLY:HA2	1:B:49:GLY:O	2.17	0.44
1:A:85:LYS:HB3	1:A:91:ILE:HD12	1.99	0.44
1:B:148:LEU:O	1:B:217:ILE:HD11	2.17	0.44
1:A:138:GLU:OE2	1:A:142:ARG:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HD11	2:A:265:HOH:O	2.17	0.44
1:B:39:GLN:OE1	1:B:233:THR:HG23	2.18	0.44
1:B:87:ASP:O	1:B:91:ILE:HG13	2.16	0.44
1:B:253:LYS:HD3	1:B:253:LYS:C	2.37	0.44
1:C:16:GLU:HB2	2:C:310:HOH:O	2.17	0.44
1:A:236:SER:O	1:A:240:VAL:HG23	2.17	0.44
1:B:48:LYS:HE2	1:B:107:LEU:HD12	1.99	0.44
1:A:159:LEU:HD13	1:A:176:ARG:NH1	2.33	0.43
1:A:151:LEU:CD2	1:A:217:ILE:HD12	2.48	0.43
1:A:246:ASP:HB2	2:A:291:HOH:O	2.17	0.43
1:C:254:LEU:O	1:C:255:GLU:C	2.56	0.43
1:B:153:GLU:HA	1:B:153:GLU:OE1	2.18	0.43
1:B:69:LEU:H	1:C:252:THR:HG21	1.83	0.43
1:B:133:ARG:HB2	1:B:136:ALA:HB3	2.01	0.43
1:A:210:ILE:N	1:A:210:ILE:HD12	2.33	0.43
1:B:111:HIS:HA	1:B:112:PRO:HD2	1.88	0.43
1:B:87:ASP:HB3	1:B:90:LYS:HB2	1.99	0.43
1:B:138:GLU:O	1:B:142:ARG:HG3	2.18	0.43
1:B:155:LEU:HD13	1:B:220:TYR:HB2	2.01	0.43
1:B:103:LYS:HD2	2:B:286:HOH:O	2.18	0.43
1:C:109:PRO:HG2	1:C:115:ASN:HD21	1.84	0.42
1:B:196:HIS:HE1	2:B:308:HOH:O	2.01	0.42
1:A:138:GLU:HB2	2:A:301:HOH:O	2.19	0.42
1:A:151:LEU:HD23	1:A:217:ILE:HD12	2.01	0.42
1:B:182:ASN:HB3	2:B:444:HOH:O	2.18	0.42
1:A:100:CYS:HB2	1:A:101:PRO:CD	2.48	0.42
1:C:86:THR:O	1:C:87:ASP:HB3	2.20	0.42
1:A:19:ILE:HD12	1:A:19:ILE:N	2.35	0.42
1:B:88:VAL:HG13	1:B:89:ASN:N	2.34	0.42
1:A:34:ASN:HD21	1:A:197:ILE:HG13	1.85	0.42
1:B:103:LYS:HB3	1:B:103:LYS:HE3	1.82	0.42
1:A:21:LEU:HG	1:A:23:VAL:HG13	2.02	0.42
1:A:23:VAL:HG12	1:A:38:SER:HB3	2.02	0.42
1:A:195:LEU:HB3	2:A:368:HOH:O	2.19	0.42
1:B:206:ARG:HG2	1:B:206:ARG:NH1	2.35	0.42
1:B:131:ASN:O	1:B:206:ARG:NH2	2.52	0.41
1:A:85:LYS:HE3	1:A:94:PHE:CZ	2.55	0.41
1:B:79:THR:O	1:B:79:THR:HG22	2.20	0.41
1:B:89:ASN:O	1:B:93:GLU:HG3	2.19	0.41
1:B:133:ARG:HG3	1:B:133:ARG:NH2	2.36	0.41
1:C:146:LYS:O	1:C:150:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:THR:HG22	1:A:232:ASN:HD22	1.85	0.41
1:B:20:GLU:OE1	1:B:79:THR:HG21	2.20	0.41
1:B:139:ALA:HB3	2:B:499:HOH:O	2.21	0.41
1:B:210:ILE:H	1:B:210:ILE:CD1	2.34	0.41
1:A:110:LYS:HG2	2:A:459:HOH:O	2.20	0.41
1:A:88:VAL:HG13	1:A:89:ASN:N	2.36	0.41
1:B:172:LYS:HE2	2:B:455:HOH:O	2.21	0.41
1:A:85:LYS:HB3	1:A:91:ILE:CD1	2.51	0.41
1:B:101:PRO:HB3	2:B:482:HOH:O	2.19	0.41
1:C:221:LEU:O	1:C:225:TYR:HD2	2.04	0.41
1:B:70:ALA:HB1	1:B:71:PRO:HD2	2.03	0.41
1:C:120:ASP:OD1	1:C:120:ASP:N	2.54	0.41
1:B:71:PRO:HG3	2:C:459:HOH:O	2.21	0.41
1:A:42:PHE:CD1	1:A:233:THR:HG22	2.56	0.41
1:A:107:LEU:HD21	2:A:434:HOH:O	2.20	0.41
1:B:14:ASP:HB3	1:B:15:LYS:H	1.66	0.40
1:C:40:ARG:HD2	1:C:190:ASN:CA	2.51	0.40
1:A:48:LYS:HE2	1:A:107:LEU:HD12	2.03	0.40
1:A:203:LYS:HE3	2:A:478:HOH:O	2.21	0.40
1:B:87:ASP:HB3	1:B:90:LYS:HD2	2.03	0.40
1:B:125:PHE:CG	1:B:198:VAL:HG22	2.56	0.40
1:C:105:LEU:HD11	2:C:357:HOH:O	2.22	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	217/261 (83%)	209 (96%)	7 (3%)	1 (0%)	29 31
1	B	236/261 (90%)	215 (91%)	16 (7%)	5 (2%)	7 4
1	C	227/261 (87%)	219 (96%)	7 (3%)	1 (0%)	34 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	680/783 (87%)	643 (95%)	30 (4%)	7 (1%)	15 14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ASN
1	C	61	ARG
1	B	15	LYS
1	A	68	ASN
1	B	69	LEU
1	B	172	LYS
1	B	16	GLU

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	197/237 (83%)	190 (96%)	7 (4%)	35 45
1	B	209/237 (88%)	196 (94%)	13 (6%)	18 21
1	C	202/237 (85%)	193 (96%)	9 (4%)	27 34
All	All	608/711 (86%)	579 (95%)	29 (5%)	25 32

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	PHE
1	A	79	THR
1	A	99	LEU
1	A	106	LYS
1	A	125	PHE
1	A	172	LYS
1	A	213	GLU
1	B	8	ASN
1	B	12	GLU

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Mol	Chain	Res	Type
1	B	32	ILE
1	B	42	PHE
1	B	68	ASN
1	B	79	THR
1	B	125	PHE
1	B	135	GLU
1	B	160	PRO
1	B	233	THR
1	B	234	CYS
1	B	238	LYS
1	B	250	ARG
1	C	18	LEU
1	C	66	LEU
1	C	79	THR
1	C	105	LEU
1	C	125	PHE
1	C	129	ILE
1	C	138	GLU
1	C	206	ARG
1	C	255	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	111	HIS
1	A	196	HIS
1	A	207	ASN
1	A	232	ASN
1	B	34	ASN
1	B	131	ASN
1	B	196	HIS
1	C	34	ASN
1	C	196	HIS
1	C	232	ASN

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)

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 (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	223/261 (85%)	0.21	7 (3%)	49	47	18, 37, 68, 80	0
1	B	240/261 (91%)	0.29	15 (6%)	20	19	21, 39, 67, 80	0
1	C	231/261 (88%)	-0.03	7 (3%)	50	48	17, 30, 65, 89	0
All	All	694/783 (88%)	0.15	29 (4%)	36	34	17, 35, 68, 89	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	PRO	4.8
1	B	6	PRO	4.1
1	B	64	ALA	3.9
1	C	173	PHE	3.7
1	B	161	ASP	3.6
1	C	69	LEU	3.6
1	A	198	VAL	3.6
1	B	212	LYS	3.4
1	C	64	ALA	3.4
1	A	30	GLU	3.3
1	A	68	ASN	3.2
1	C	255	GLU	3.0
1	B	133	ARG	3.0
1	B	15	LYS	2.8
1	B	30	GLU	2.8
1	A	28	ASP	2.7
1	A	191	LEU	2.6
1	B	198	VAL	2.6
1	A	172	LYS	2.5
1	C	66	LEU	2.3
1	B	136	ALA	2.2
1	C	142	ARG	2.2
1	B	160	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	28	ASP	2.2
1	B	59	LEU	2.1
1	B	242	ILE	2.1
1	C	30	GLU	2.1
1	B	251	LEU	2.0
1	B	65	ASP	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.