Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 10:14 AM EDT

PDB ID	:	3TB5
Title	:	Crystal Structure of the Enterococcus faecalis Methionine aminopeptidase apo form
Authors	:	Kishor, C.; Gumpena, R.; Reddi, R.; Addlagatta, A.
Deposited on	:	2011-08-05
Resolution	:	2.30 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 (i)) were used in the production of this report:

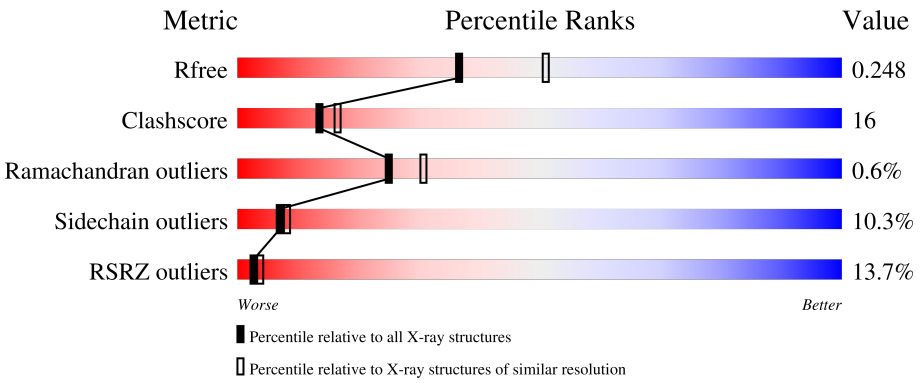
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	264	3%, 70%, 21%, • • •
1	B	264	2%, 65%, 25%, 5%, • •
1	C	264	32%, 51%, 23%, •, 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5897 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 Methionine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	2033	1290	335	392	16	0	11	0
1	B	254	2034	1290	335	391	18	0	11	0
1	C	207	1619	1021	272	311	15	0	2	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	LEU	-	expression tag	UNP C7VIN6
A	256	GLU	-	expression tag	UNP C7VIN6
A	257	HIS	-	expression tag	UNP C7VIN6
A	258	HIS	-	expression tag	UNP C7VIN6
A	259	HIS	-	expression tag	UNP C7VIN6
A	260	PRO	-	expression tag	UNP C7VIN6
A	261	PRO	-	expression tag	UNP C7VIN6
A	262	THR	-	expression tag	UNP C7VIN6
A	263	GLU	-	expression tag	UNP C7VIN6
A	264	GLU	-	expression tag	UNP C7VIN6
B	255	LEU	-	expression tag	UNP C7VIN6
B	256	GLU	-	expression tag	UNP C7VIN6
B	257	HIS	-	expression tag	UNP C7VIN6
B	258	HIS	-	expression tag	UNP C7VIN6
B	259	HIS	-	expression tag	UNP C7VIN6
B	260	PRO	-	expression tag	UNP C7VIN6
B	261	PRO	-	expression tag	UNP C7VIN6
B	262	THR	-	expression tag	UNP C7VIN6
B	263	GLU	-	expression tag	UNP C7VIN6
B	264	GLU	-	expression tag	UNP C7VIN6
C	255	LEU	-	expression tag	UNP C7VIN6
C	256	GLU	-	expression tag	UNP C7VIN6
C	257	HIS	-	expression tag	UNP C7VIN6

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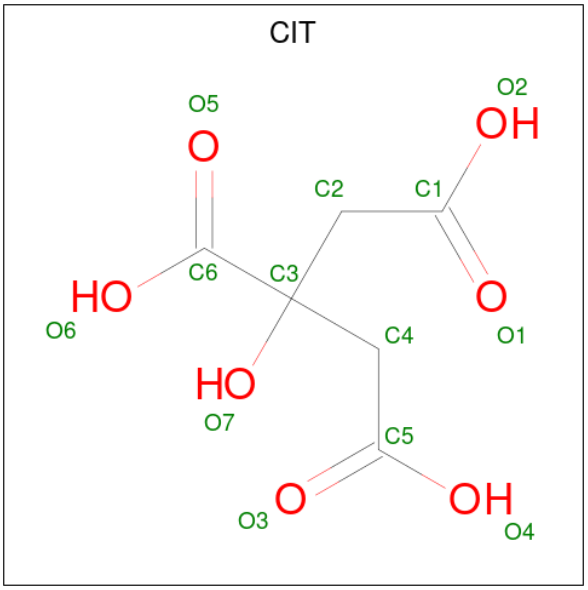
Chain	Residue	Modelled	Actual	Comment	Reference
C	258	HIS	-	expression tag	UNP C7VIN6
C	259	HIS	-	expression tag	UNP C7VIN6
C	260	PRO	-	expression tag	UNP C7VIN6
C	261	PRO	-	expression tag	UNP C7VIN6
C	262	THR	-	expression tag	UNP C7VIN6
C	263	GLU	-	expression tag	UNP C7VIN6
C	264	GLU	-	expression tag	UNP C7VIN6

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			26	12	14		
2	B	1	Total	C	O	0	1
			26	12	14		

- Molecule 3 is water.

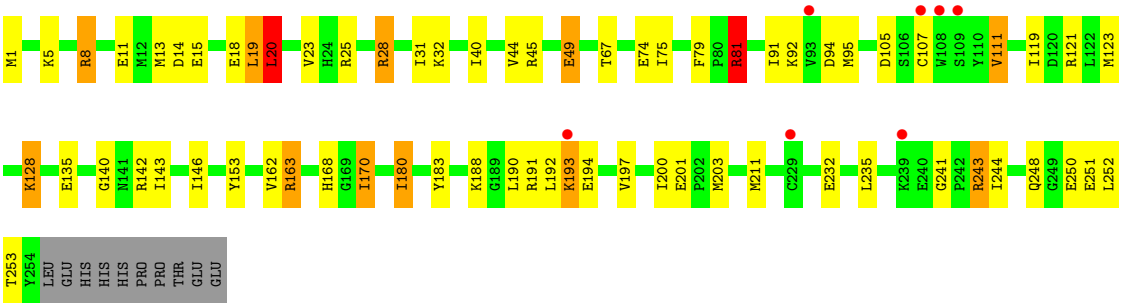
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	74	Total	O	0	0
			74	74		
3	C	8	Total	O	0	0
			8	8		

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.

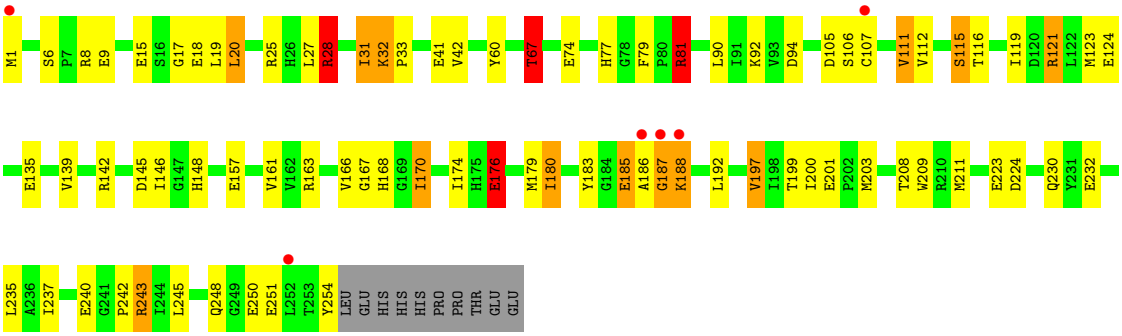
• Molecule 1: Methionine aminopeptidase

Chain A:



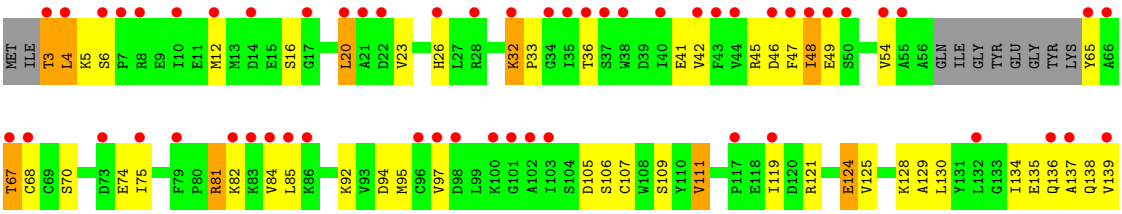
• Molecule 1: Methionine aminopeptidase

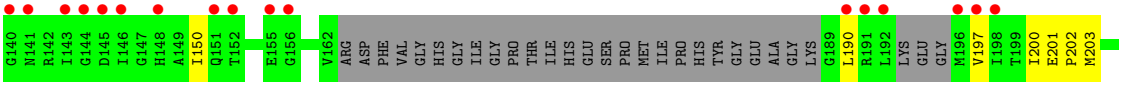
Chain B:

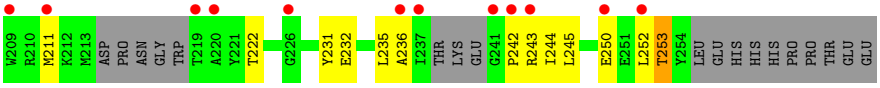


• Molecule 1: Methionine aminopeptidase

Chain C:




G140 N141 R142 I143 G144 D145 I146 G147 H148 A149 I150 Q151 T152 E155 G156 V162 ARG ASP PHE VAL GLY HIS GLY ILE GLY PRO THR ILE HIS GLU SER PRO MET ILE PRO HIS TYR GLY GLU ALA GLY LYS G189 L190 R191 L192 LYS GLU GLY M196 V197 I198 T199 I200 E201 P202 M203


W209 R210 M211 K212 M213 ASP PRO ASN GLY TRP T219 A220 Y221 T222 G226 Y231 E232 L235 A236 I237 THR LYS GLU G241 P242 R243 I244 L245 E250 E251 L252 T253 Y254 LEU GLU HIS HIS HIS PRO PRO THR GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.74Å 132.13Å 85.30Å 90.00° 133.36° 90.00°	Depositor
Resolution (Å)	36.47 – 2.30 36.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.47-2.30) 99.9 (36.47-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.197 , 0.255 0.195 , 0.248	Depositor DCC
R_{free} test set	2157 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.104 for h+2*l,k,-h-l 0.025 for -h-2*l,-k,l 0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5897	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: CIT

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	1.24	4/2105 (0.2%)	1.20	12/2846 (0.4%)
1	B	1.25	6/2106 (0.3%)	1.14	14/2844 (0.5%)
1	C	0.84	0/1650	0.82	2/2221 (0.1%)
All	All	1.14	10/5861 (0.2%)	1.09	28/7911 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	GLU	CG-CD	7.98	1.64	1.51
1	A	49	GLU	CB-CG	-6.84	1.39	1.52
1	A	44	VAL	CB-CG1	5.96	1.65	1.52
1	B	115	SER	CB-OG	-5.93	1.34	1.42
1	B	254	TYR	CD2-CE2	5.90	1.48	1.39
1	A	163	ARG	CZ-NH2	5.55	1.40	1.33
1	B	176	GLU	CG-CD	-5.28	1.44	1.51
1	A	135	GLU	CG-CD	5.13	1.59	1.51
1	B	187	GLY	N-CA	-5.04	1.38	1.46
1	B	42	VAL	CB-CG2	5.00	1.63	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	ARG	NE-CZ-NH1	13.51	127.05	120.30
1	B	81	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	A	81	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	A	81	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	163	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	B	111	VAL	CB-CA-C	-8.55	95.15	111.40
1	B	187	GLY	N-CA-C	-7.93	93.27	113.10
1	A	28	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	C	4	LEU	CA-CB-CG	7.29	132.05	115.30
1	B	121	ARG	CG-CD-NE	-7.20	96.68	111.80
1	A	111	VAL	CB-CA-C	-7.06	97.98	111.40
1	A	20	LEU	CA-CB-CG	6.61	130.49	115.30
1	A	243	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	49	GLU	CB-CA-C	6.31	123.03	110.40
1	A	94	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	243	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	20	LEU	CB-CG-CD2	-5.60	101.49	111.00
1	B	111	VAL	CG1-CB-CG2	5.57	119.81	110.90
1	A	243	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	81	ARG	CD-NE-CZ	5.52	131.32	123.60
1	C	252	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	243	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	81	ARG	CD-NE-CZ	5.21	130.89	123.60
1	A	121	ARG	CG-CD-NE	-5.19	100.90	111.80
1	B	28	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	203	MET	CG-SD-CE	-5.12	92.01	100.20
1	B	111	VAL	CA-CB-CG2	5.08	118.52	110.90
1	B	67	THR	N-CA-CB	-5.06	100.69	110.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	LYS	Peptide
1	B	188	LYS	Peptide

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	2033	0	2019	64	0
1	B	2034	0	2022	77	0
1	C	1619	0	1600	41	0
2	A	26	0	10	2	0
2	B	26	0	10	4	0
3	A	77	0	0	2	0
3	B	74	0	0	4	0
3	C	8	0	0	0	0
All	All	5897	0	5661	182	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 (182) 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:A:119:ILE:HG22	1:A:123:MET:CE	1.72	1.18
1:A:119:ILE:CG2	1:A:123:MET:CE	2.23	1.17
1:B:148:HIS:CB	1:B:186:ALA:HB2	1.77	1.13
1:B:111:VAL:HG11	1:B:115:SER:HB3	1.12	1.11
1:B:148:HIS:HB3	1:B:186:ALA:HB2	1.17	1.10
1:A:119:ILE:CG2	1:A:123:MET:HE2	1.84	1.07
1:B:90:LEU:HD13	1:B:123[A]:MET:HE3	1.36	1.06
1:A:168:HIS:NE2	2:A:265[A]:CIT:H41	1.74	1.01
1:B:31[A]:ILE:HD11	1:B:112:VAL:HG22	1.38	0.99
1:A:119:ILE:HG22	1:A:123:MET:HE2	1.37	0.98
1:B:148:HIS:HB3	1:B:186:ALA:CB	1.99	0.93
1:C:250:GLU:O	1:C:253:THR:HB	1.72	0.90
1:A:162:VAL:HG11	1:A:203:MET:HE1	1.52	0.89
1:B:148:HIS:CB	1:B:186:ALA:CB	2.52	0.87
1:A:119:ILE:CG2	1:A:123:MET:HE1	2.04	0.85
1:A:75:ILE:CG2	1:A:203:MET:HE2	2.08	0.83
1:A:8:ARG:HG3	1:A:8:ARG:HH11	1.44	0.83
1:C:111:VAL:CG1	1:C:119:ILE:HG21	2.09	0.82
1:B:251:GLU:O	3:B:315:HOH:O	1.98	0.82
1:B:111:VAL:CG1	1:B:115:SER:HB3	2.03	0.81
1:C:201:GLU:HB3	1:C:232:GLU:HG3	1.62	0.81
1:A:75:ILE:CG2	1:A:203:MET:CE	2.59	0.81
1:B:111:VAL:HG11	1:B:115:SER:CB	2.04	0.81
1:B:6:SER:OG	1:B:9:GLU:HG3	1.83	0.79
1:A:250:GLU:O	1:A:253:THR:HB	1.82	0.79
1:A:146:ILE:HG21	1:A:180[A]:ILE:HD11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HG22	1:C:203:MET:HE3	1.63	0.77
1:C:107:CYS:H	1:C:232:GLU:HB3	1.49	0.76
1:A:119:ILE:HG23	1:A:123:MET:HE2	1.64	0.76
1:C:124:GLU:O	1:C:125:VAL:HB	1.88	0.73
1:A:8:ARG:HH11	1:A:8:ARG:CG	2.01	0.73
1:B:180[A]:ILE:HD11	1:B:200:ILE:HG12	1.69	0.73
1:B:170:ILE:HG22	1:B:197:VAL:HG22	1.71	0.73
1:A:244:ILE:O	3:A:325:HOH:O	2.07	0.72
1:B:148:HIS:HB2	1:B:186:ALA:HB2	1.73	0.71
1:A:119:ILE:HG23	1:A:123:MET:CE	2.16	0.71
1:B:31[A]:ILE:HD11	1:B:112:VAL:CG2	2.17	0.71
1:B:79:PHE:O	1:B:81:ARG:HD3	1.91	0.71
1:C:3:THR:HB	1:C:197:VAL:H	1.56	0.70
1:C:134:ILE:HG12	1:C:235:LEU:HD11	1.73	0.70
1:A:128:LYS:HE3	1:A:153:TYR:OH	1.92	0.70
1:B:142:ARG:HH11	1:B:188:LYS:HB3	1.56	0.70
1:B:145:ASP:HA	1:B:186:ALA:HB1	1.75	0.68
1:C:41:GLU:OE1	1:C:67:THR:HB	1.94	0.68
1:B:201:GLU:OE1	2:B:265[A]:CIT:O2	2.12	0.67
1:A:143:ILE:HD12	1:A:190:LEU:HB3	1.75	0.66
1:B:27:LEU:O	1:B:31[A]:ILE:HG22	1.96	0.65
1:A:75:ILE:HG22	1:A:203:MET:HE3	1.77	0.65
1:A:31[B]:ILE:HD11	1:A:91:ILE:HG21	1.79	0.65
1:B:170:ILE:HD13	1:B:199:THR:HG23	1.78	0.65
1:C:111:VAL:HG13	1:C:119:ILE:HG21	1.80	0.64
1:A:75:ILE:CG2	1:A:203:MET:HE3	2.27	0.64
1:B:119:ILE:HG22	1:B:123[A]:MET:SD	2.38	0.63
1:B:180[A]:ILE:CD1	1:B:200:ILE:HG12	2.28	0.63
1:A:119:ILE:HG22	1:A:123:MET:HE3	1.72	0.63
1:B:41:GLU:OE1	1:B:67:THR:HB	1.97	0.63
1:A:140:GLY:O	1:A:191:ARG:HD2	1.99	0.63
1:B:90:LEU:HD13	1:B:123[A]:MET:CE	2.22	0.62
1:C:47:PHE:HD1	1:C:48:ILE:H	1.48	0.62
1:A:162:VAL:HG11	1:A:203:MET:CE	2.28	0.62
1:B:27:LEU:O	1:B:31[A]:ILE:CG2	2.47	0.62
1:B:107:CYS:H	1:B:232:GLU:HB3	1.63	0.62
1:A:75:ILE:HG22	1:A:203:MET:CE	2.29	0.61
1:A:75:ILE:HG21	1:A:203:MET:CE	2.30	0.61
1:B:18:GLU:OE2	1:B:25:ARG:NH2	2.33	0.60
1:B:28:ARG:NH1	1:B:248:GLN:HE21	1.99	0.60
1:A:45:ARG:O	1:A:49:GLU:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:O	1:A:81:ARG:HD3	2.04	0.58
1:B:123[A]:MET:SD	3:B:284:HOH:O	2.57	0.57
1:C:137:ALA:O	1:C:242:PRO:HB3	2.06	0.56
1:A:251:GLU:O	1:A:252:LEU:HB2	2.06	0.55
1:B:124:GLU:HA	1:B:124:GLU:OE1	2.05	0.55
1:B:163:ARG:HB2	1:B:183:TYR:CE2	2.41	0.55
1:A:163:ARG:HG3	1:A:183:TYR:CE2	2.42	0.54
1:A:170[B]:ILE:CG1	1:A:197[B]:VAL:HG22	2.38	0.54
1:B:15[A]:GLU:HG3	3:B:322:HOH:O	2.06	0.54
1:C:75:ILE:HG22	1:C:203:MET:CE	2.37	0.54
1:B:105:ASP:OD2	1:B:170:ILE:HD11	2.08	0.54
1:C:111:VAL:CG1	1:C:119:ILE:CG2	2.83	0.54
1:B:145:ASP:HA	1:B:186:ALA:CB	2.37	0.54
1:A:111:VAL:HG22	1:A:123:MET:CE	2.37	0.53
1:A:170[B]:ILE:HG13	1:A:197[B]:VAL:HG22	1.91	0.53
1:B:74:GLU:OE2	1:B:81:ARG:NH2	2.36	0.52
1:B:139:VAL:HG12	1:B:237:ILE:HG22	1.91	0.52
1:B:185:GLU:C	1:B:187:GLY:H	2.11	0.52
1:B:168:HIS:HE1	1:B:170:ILE:HD11	1.75	0.52
1:B:142:ARG:CD	1:B:188:LYS:HB3	2.39	0.52
1:C:75:ILE:CG2	1:C:203:MET:HE3	2.38	0.52
1:A:241[B]:GLY:C	3:A:326:HOH:O	2.46	0.52
1:A:142:ARG:HH11	1:A:191:ARG:CZ	2.23	0.52
1:C:74:GLU:OE2	1:C:81:ARG:NH2	2.43	0.52
1:C:23:VAL:HG22	1:C:47:PHE:CD1	2.46	0.51
1:C:111:VAL:HG13	1:C:119:ILE:CG2	2.40	0.51
1:A:105:ASP:OD2	1:A:170[A]:ILE:HD11	2.11	0.50
1:B:94:ASP:OD2	2:B:265[A]:CIT:O6	2.29	0.50
1:B:167:GLY:C	1:B:180[A]:ILE:HG23	2.32	0.50
1:C:42:VAL:O	1:C:46:ASP:HB2	2.11	0.50
1:C:45:ARG:O	1:C:49:GLU:HG2	2.12	0.50
1:C:70:SER:O	1:C:92:LYS:HE2	2.12	0.50
1:A:31[B]:ILE:HD12	1:A:40:ILE:HD11	1.94	0.49
1:B:17:GLY:HA3	1:B:245:LEU:O	2.12	0.49
1:A:75:ILE:HG21	1:A:203:MET:HE2	1.88	0.49
1:A:11:GLU:O	1:A:15[B]:GLU:HG3	2.13	0.49
1:B:111:VAL:HG22	1:B:123[A]:MET:CE	2.42	0.49
1:A:146:ILE:HG21	1:A:180[A]:ILE:CD1	2.39	0.48
1:C:129:ALA:HB1	1:C:150:ILE:HG23	1.94	0.48
1:B:148:HIS:CG	1:B:186:ALA:CB	2.97	0.48
1:B:148:HIS:CG	1:B:186:ALA:HB3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:C	1:C:136:GLN:H	2.15	0.48
1:B:92:LYS:N	1:B:92:LYS:HD3	2.28	0.47
1:B:168:HIS:CE1	1:B:170:ILE:CD1	2.97	0.47
1:B:148:HIS:HB2	1:B:186:ALA:CB	2.39	0.47
1:B:20:LEU:CD2	1:B:106:SER:HB3	2.45	0.47
1:B:142:ARG:HD2	1:B:188:LYS:HB3	1.96	0.47
1:C:48:ILE:HG22	1:C:49:GLU:N	2.30	0.47
1:C:201:GLU:HB3	1:C:232:GLU:CG	2.38	0.47
1:C:36:THR:HG22	1:C:82:LYS:O	2.15	0.46
1:C:236:ALA:HB2	1:C:245:LEU:HD21	1.98	0.46
1:B:77:HIS:NE2	2:B:265[B]:CIT:H42	2.30	0.46
1:A:92:LYS:N	1:A:92:LYS:HD3	2.31	0.46
1:A:111:VAL:HG13	1:A:119:ILE:HG21	1.97	0.46
1:C:200:ILE:HG22	1:C:202:PRO:HD3	1.97	0.46
1:B:168:HIS:NE2	2:B:265[A]:CIT:H22	2.30	0.46
1:B:176:GLU:HG2	3:B:303:HOH:O	2.15	0.46
1:A:142:ARG:NH1	1:A:191:ARG:CZ	2.79	0.46
1:B:187:GLY:C	1:B:188:LYS:HG2	2.35	0.45
1:C:20:LEU:HD23	1:C:97:VAL:CG2	2.47	0.45
1:A:163:ARG:HG3	1:A:183:TYR:CZ	2.51	0.45
1:C:75:ILE:CG2	1:C:203:MET:CE	2.94	0.45
1:B:28:ARG:HH11	1:B:248:GLN:NE2	2.15	0.45
1:C:92:LYS:HG3	1:C:109:SER:OG	2.17	0.45
1:C:20:LEU:HD23	1:C:97:VAL:HB	1.99	0.45
1:B:32:LYS:HB2	1:B:33:PRO:HD2	1.99	0.44
1:A:193:LYS:HE2	1:A:193:LYS:HB3	1.74	0.44
1:B:119:ILE:CG2	1:B:123[A]:MET:CE	2.95	0.44
1:C:81:ARG:N	1:C:81:ARG:HD2	2.32	0.44
1:B:148:HIS:CD2	1:B:186:ALA:HB3	2.53	0.44
1:C:124:GLU:O	1:C:125:VAL:CB	2.56	0.44
1:A:107:CYS:H	1:A:232:GLU:HB3	1.82	0.44
1:C:130:LEU:HD22	1:C:231:TYR:HB3	1.99	0.44
1:B:119:ILE:CG2	1:B:123[A]:MET:SD	3.06	0.43
1:C:32:LYS:CB	1:C:33:PRO:CD	2.97	0.43
1:B:20:LEU:HD22	1:B:106:SER:HB3	2.01	0.43
1:B:90:LEU:CD1	1:B:123[A]:MET:HE3	2.25	0.43
1:B:163:ARG:HG2	1:B:209:TRP:CE3	2.52	0.43
1:C:68:CYS:HB2	1:C:94:ASP:HB3	1.99	0.43
1:A:13:MET:HE1	1:A:197[A]:VAL:HG21	2.00	0.43
1:C:105:ASP:OD1	1:C:106:SER:N	2.52	0.43
1:A:5:LYS:HD3	1:A:197[B]:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:O	1:B:31[A]:ILE:HG23	2.18	0.42
1:B:60:TYR:CG	1:B:174:ILE:HD11	2.54	0.42
1:B:146:ILE:HD13	1:B:180[A]:ILE:HD12	2.01	0.42
1:A:168:HIS:CD2	2:A:265[A]:CIT:H41	2.52	0.42
1:B:28:ARG:NH1	1:B:248:GLN:NE2	2.67	0.42
1:C:20:LEU:HD12	1:C:106:SER:CB	2.49	0.42
1:A:190:LEU:HG	1:A:191:ARG:N	2.35	0.42
1:B:163:ARG:HE	1:B:163:ARG:HB3	1.67	0.42
1:B:208:THR:HG22	1:B:224:ASP:CG	2.39	0.41
1:A:20:LEU:HD13	1:A:95:MET:SD	2.61	0.41
1:A:19:LEU:O	1:A:23:VAL:HG23	2.20	0.41
1:B:166:VAL:HG21	1:B:179[B]:MET:HB3	2.02	0.41
1:A:25:ARG:O	1:A:28:ARG:HG3	2.20	0.41
1:A:74:GLU:OE2	1:A:81:ARG:NH2	2.45	0.41
1:A:75:ILE:HG23	1:A:203:MET:HE2	1.99	0.41
1:B:119:ILE:CG2	1:B:123[A]:MET:HE1	2.51	0.41
1:B:121:ARG:NH2	1:B:157:GLU:OE1	2.54	0.41
1:A:14:ASP:O	1:A:18[B]:GLU:HG3	2.20	0.41
1:A:28:ARG:NH1	1:A:248:GLN:HE21	2.18	0.41
1:B:139:VAL:HG12	1:B:237:ILE:CG2	2.50	0.41
1:C:235:LEU:HD13	1:C:244:ILE:HA	2.02	0.41
1:B:115:SER:HB2	1:B:116:THR:H	1.66	0.41
1:C:32:LYS:HB2	1:C:33:PRO:CD	2.52	0.40
1:A:180[A]:ILE:HD11	1:A:200:ILE:HG12	2.03	0.40
1:A:8:ARG:CG	1:A:8:ARG:NH1	2.70	0.40
1:A:201:GLU:CB	1:A:232:GLU:HB2	2.51	0.40
1:B:201:GLU:HB2	1:B:230:GLN:HE21	1.87	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	263/264 (100%)	259 (98%)	4 (2%)	0	100	100
1	B	263/264 (100%)	257 (98%)	5 (2%)	1 (0%)	34	42
1	C	196/264 (74%)	182 (93%)	11 (6%)	3 (2%)	10	10
All	All	722/792 (91%)	698 (97%)	20 (3%)	4 (1%)	25	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ILE
1	C	135	GLU
1	B	242	PRO
1	C	6	SER

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	223/223 (100%)	205 (92%)	18 (8%)	11	15
1	B	223/223 (100%)	199 (89%)	24 (11%)	6	7
1	C	178/223 (80%)	152 (85%)	26 (15%)	3	3
All	All	624/669 (93%)	556 (89%)	68 (11%)	7	7

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ARG
1	A	19	LEU
1	A	20	LEU
1	A	32	LYS
1	A	67	THR
1	A	81	ARG
1	A	128	LYS
1	A	170[A]	ILE

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Mol	Chain	Res	Type
1	A	170[B]	ILE
1	A	180[A]	ILE
1	A	180[B]	ILE
1	A	192	LEU
1	A	193	LYS
1	A	194	GLU
1	A	211	MET
1	A	235	LEU
1	A	243	ARG
1	B	1	MET
1	B	8	ARG
1	B	19	LEU
1	B	28	ARG
1	B	31[A]	ILE
1	B	31[B]	ILE
1	B	32	LYS
1	B	67	THR
1	B	81	ARG
1	B	161	VAL
1	B	170	ILE
1	B	176	GLU
1	B	180[A]	ILE
1	B	180[B]	ILE
1	B	185	GLU
1	B	192	LEU
1	B	197	VAL
1	B	211	MET
1	B	223[A]	GLU
1	B	223[B]	GLU
1	B	235	LEU
1	B	243	ARG
1	B	250[A]	GLU
1	B	250[B]	GLU
1	C	3	THR
1	C	4	LEU
1	C	5	LYS
1	C	12	MET
1	C	16	SER
1	C	20	LEU
1	C	26	HIS
1	C	32	LYS
1	C	54	VAL

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Mol	Chain	Res	Type
1	C	65	TYR
1	C	67	THR
1	C	81	ARG
1	C	84	VAL
1	C	85	LEU
1	C	95	MET
1	C	111	VAL
1	C	121	ARG
1	C	124	GLU
1	C	128	LYS
1	C	138	GLN
1	C	139	VAL
1	C	190	LEU
1	C	211	MET
1	C	222	THR
1	C	243	ARG
1	C	253	THR

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

Mol	Chain	Res	Type
1	A	248	GLN
1	B	248	GLN
1	C	138	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CIT	A	265[B]	-	12,12,12	1.03	0	17,17,17	1.80	4 (23%)
2	CIT	B	265[A]	-	12,12,12	1.06	0	17,17,17	1.46	2 (11%)
2	CIT	A	265[A]	-	12,12,12	1.08	0	17,17,17	1.90	4 (23%)
2	CIT	B	265[B]	-	12,12,12	1.05	0	17,17,17	1.80	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	265[B]	-	-	6/16/16/16	-
2	CIT	B	265[A]	-	-	7/16/16/16	-
2	CIT	A	265[A]	-	-	11/16/16/16	-
2	CIT	B	265[B]	-	-	3/16/16/16	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	265[B]	CIT	O6-C6-C3	4.60	121.04	113.05
2	A	265[A]	CIT	O6-C6-C3	4.16	120.27	113.05
2	B	265[B]	CIT	C2-C3-C6	-3.81	101.92	110.11
2	B	265[B]	CIT	O6-C6-C3	3.23	118.65	113.05
2	A	265[A]	CIT	C3-C2-C1	-2.94	106.71	113.81
2	A	265[A]	CIT	C4-C3-C6	-2.78	104.12	110.11
2	A	265[A]	CIT	C3-C4-C5	-2.65	107.40	113.81
2	A	265[B]	CIT	O4-C5-C4	2.57	122.59	114.35
2	B	265[A]	CIT	O6-C6-C3	2.39	117.19	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	265[B]	CIT	O7-C3-C6	-2.35	105.56	108.86
2	B	265[B]	CIT	O4-C5-C4	2.29	121.72	114.35
2	B	265[B]	CIT	O4-C5-O3	-2.21	117.79	123.30
2	B	265[B]	CIT	O2-C1-O1	-2.16	117.91	123.30
2	A	265[B]	CIT	O4-C5-O3	-2.05	118.20	123.30
2	B	265[A]	CIT	O7-C3-C2	-2.04	104.63	109.40

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	265[A]	CIT	O7-C3-C6-O6
2	A	265[B]	CIT	C2-C3-C6-O5
2	A	265[B]	CIT	C2-C3-C6-O6
2	A	265[B]	CIT	O7-C3-C6-O5
2	A	265[B]	CIT	O7-C3-C6-O6
2	B	265[A]	CIT	C1-C2-C3-C6
2	B	265[A]	CIT	C2-C3-C4-C5
2	B	265[A]	CIT	O7-C3-C4-C5
2	B	265[A]	CIT	C6-C3-C4-C5
2	B	265[B]	CIT	C1-C2-C3-O7
2	B	265[B]	CIT	C1-C2-C3-C4
2	B	265[B]	CIT	C1-C2-C3-C6
2	A	265[A]	CIT	C2-C3-C4-C5
2	A	265[A]	CIT	O7-C3-C4-C5
2	A	265[A]	CIT	C6-C3-C4-C5
2	B	265[A]	CIT	C1-C2-C3-O7
2	B	265[A]	CIT	C1-C2-C3-C4
2	A	265[A]	CIT	C2-C3-C6-O5
2	A	265[A]	CIT	O7-C3-C6-O5
2	A	265[A]	CIT	C2-C3-C6-O6
2	A	265[A]	CIT	C4-C3-C6-O5
2	A	265[A]	CIT	C4-C3-C6-O6
2	A	265[B]	CIT	C4-C3-C6-O5
2	A	265[B]	CIT	C4-C3-C6-O6
2	B	265[A]	CIT	C4-C3-C6-O5
2	A	265[A]	CIT	O2-C1-C2-C3
2	A	265[A]	CIT	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	265[A]	CIT	3	0
2	A	265[A]	CIT	2	0
2	B	265[B]	CIT	1	0

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	254/264 (96%)	0.05	7 (2%)	53	60	12, 22, 45, 57	0
1	B	254/264 (96%)	-0.11	6 (2%)	59	66	14, 24, 45, 57	0
1	C	207/264 (78%)	1.87	85 (41%)	0	0	44, 66, 90, 99	0
All	All	715/792 (90%)	0.52	98 (13%)	3	4	12, 27, 80, 99	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	ALA	6.7
1	C	96	CYS	6.2
1	C	7	PRO	6.0
1	C	143	ILE	5.8
1	C	4	LEU	5.6
1	C	79	PHE	5.5
1	C	144	GLY	5.3
1	C	82	LYS	4.8
1	C	6	SER	4.6
1	C	50	SER	4.6
1	B	186	ALA	4.5
1	C	139	VAL	4.4
1	C	101	GLY	4.3
1	C	3	THR	4.3
1	C	48	ILE	4.2
1	C	97	VAL	4.0
1	C	211	MET	4.0
1	C	42	VAL	4.0
1	C	190	LEU	3.8
1	C	148[A]	HIS	3.7
1	C	102	ALA	3.7
1	C	38	TRP	3.7
1	C	54	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	47	PHE	3.6
1	C	98	ASP	3.6
1	C	196[A]	MET	3.5
1	C	22	ASP	3.5
1	C	242	PRO	3.4
1	C	43	PHE	3.4
1	C	152	THR	3.4
1	C	46	ASP	3.4
1	C	36	THR	3.3
1	C	236	ALA	3.2
1	C	65	TYR	3.2
1	C	198	ILE	3.2
1	C	117	PRO	3.1
1	C	17	GLY	3.1
1	C	26	HIS	3.0
1	C	37	SER	3.0
1	C	75	ILE	3.0
1	C	68	CYS	3.0
1	B	252	LEU	3.0
1	C	132	LEU	3.0
1	B	1	MET	2.9
1	C	145	ASP	2.9
1	C	137	ALA	2.9
1	C	85	LEU	2.8
1	C	35	ILE	2.8
1	C	55	ALA	2.8
1	C	192	LEU	2.8
1	C	237	ILE	2.7
1	C	220	ALA	2.7
1	C	86	LYS	2.7
1	C	209	TRP	2.7
1	C	140	GLY	2.7
1	C	151	GLN	2.7
1	C	156	GLY	2.7
1	C	44	VAL	2.6
1	C	14	ASP	2.6
1	C	49	GLU	2.5
1	C	141	ASN	2.5
1	C	100	LYS	2.5
1	C	136	GLN	2.5
1	C	191	ARG	2.5
1	C	219	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	187	GLY	2.4
1	C	241	GLY	2.4
1	C	67	THR	2.4
1	C	28	ARG	2.3
1	C	146	ILE	2.3
1	B	188	LYS	2.3
1	A	107	CYS	2.3
1	C	119	ILE	2.3
1	A	229	CYS	2.3
1	A	193	LYS	2.3
1	C	12	MET	2.3
1	C	84	VAL	2.3
1	C	21	ALA	2.3
1	C	252	LEU	2.3
1	C	226	GLY	2.3
1	C	8	ARG	2.3
1	C	32	LYS	2.2
1	C	73	ASP	2.2
1	C	83	LYS	2.2
1	C	40	ILE	2.2
1	B	107	CYS	2.2
1	C	197	VAL	2.2
1	C	243	ARG	2.2
1	C	155	GLU	2.1
1	A	93	VAL	2.1
1	C	250	GLU	2.1
1	C	34	GLY	2.1
1	A	239	LYS	2.1
1	A	109	SER	2.1
1	C	10	ILE	2.1
1	C	103	ILE	2.0
1	A	108	TRP	2.0
1	C	20	LEU	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
2	CIT	A	265[A]	13/13	0.89	0.23	44,48,52,52	13
2	CIT	A	265[B]	13/13	0.89	0.23	39,42,43,44	13
2	CIT	B	265[A]	13/13	0.90	0.19	36,40,42,43	13
2	CIT	B	265[B]	13/13	0.90	0.19	33,38,39,40	13

6.5 Other polymers (i)

There are no such residues in this entry.