



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 08:19 PM JST

PDB ID : 5H16  
Title : Crystal structure of the complex of Phosphopantetheine adenylyltransferase from *Acinetobacter baumannii* with citrate at 2.3 Å resolution.  
Authors : Gupta, A.; Singh, P.K.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2016-10-08  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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

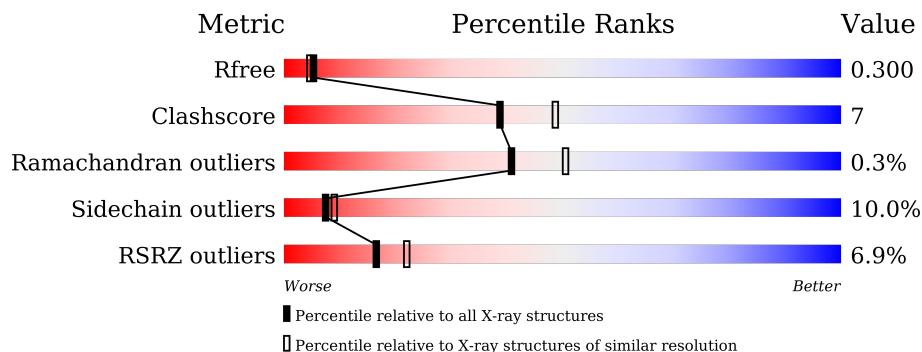
# 1 Overall quality at a glance

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  $\geq 3$ , 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	163	 5% 78% 17% 6%
1	B	163	 11% 77% 20% ..
1	C	163	 5% 80% 15% ..
1	D	163	 7% 81% 12% 5% ..
1	E	163	 5% 83% 14% .
1	F	163	 8% 83% 13% ..

## 2 Entry composition [i](#)

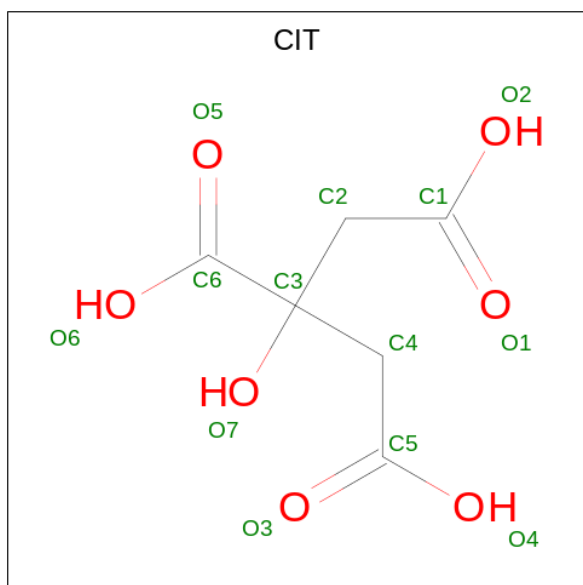
There are 3 unique types of molecules in this entry. The entry contains 7990 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	163	Total 1305	C 838	N 227	O 237	S 3	0	0	0
1	B	161	Total 1291	C 830	N 225	O 234	S 2	0	0	0
1	C	161	Total 1291	C 830	N 225	O 234	S 2	0	0	0
1	D	161	Total 1291	C 830	N 225	O 234	S 2	0	0	0
1	E	163	Total 1305	C 838	N 227	O 237	S 3	0	0	0
1	F	163	Total 1305	C 838	N 227	O 237	S 3	0	0	0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

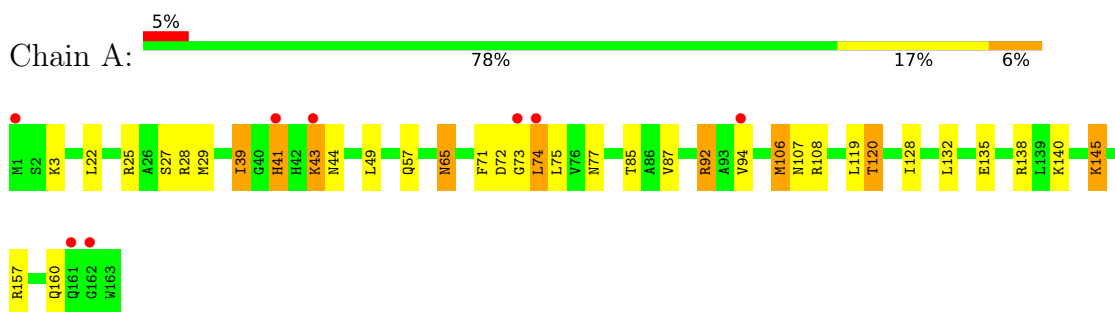
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	12	Total	O	0	0
			12	12		
3	C	22	Total	O	0	0
			22	22		
3	D	21	Total	O	0	0
			21	21		
3	E	16	Total	O	0	0
			16	16		
3	F	26	Total	O	0	0
			26	26		

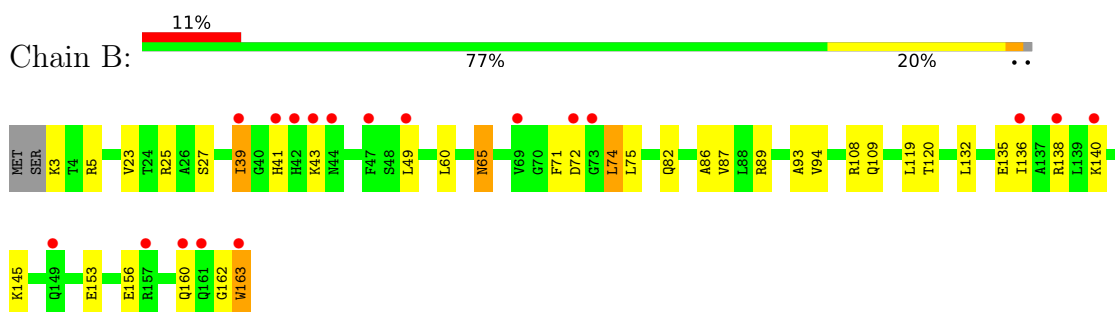
### 3 Residue-property plots [i](#)

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.

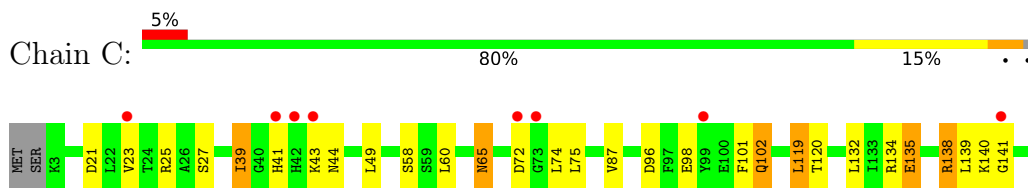
- Molecule 1: Phosphopantetheine adenylyltransferase



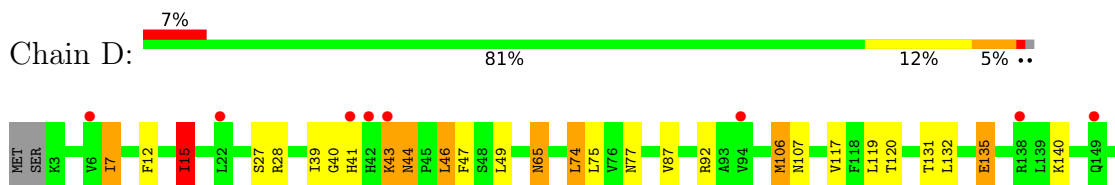
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase

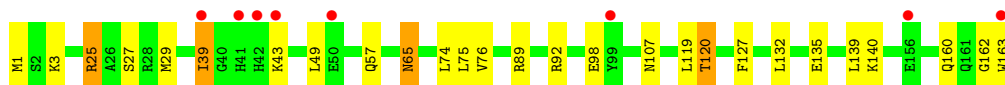
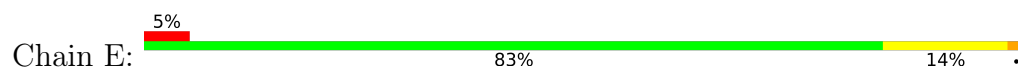


- Molecule 1: Phosphopantetheine adenylyltransferase

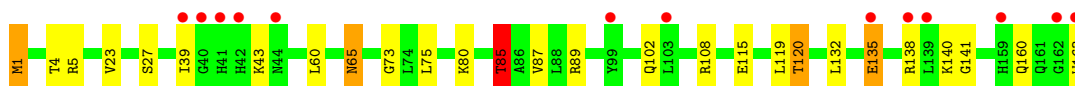
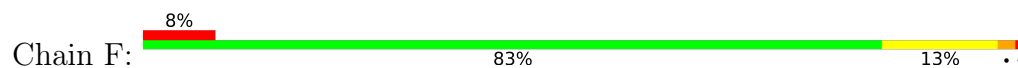




- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.59Å 109.81Å 121.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.56 – 2.30 40.78 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (81.56-2.30) 98.8 (40.78-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.261 , 0.302 0.262 , 0.300	Depositor DCC
$R_{free}$ test set	955 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtrriage
Anisotropy	0.378	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.67	0/1335	0.88	4/1806 (0.2%)
1	B	0.63	0/1321	0.88	5/1788 (0.3%)
1	C	0.69	0/1321	0.91	4/1788 (0.2%)
1	D	0.72	1/1321 (0.1%)	0.96	4/1788 (0.2%)
1	E	0.69	0/1335	0.93	5/1806 (0.3%)
1	F	0.73	0/1335	0.91	3/1806 (0.2%)
All	All	0.69	1/7968 (0.0%)	0.91	25/10782 (0.2%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	GLY	C-O	-6.00	1.14	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	ARG	CG-CD-NE	9.69	132.15	111.80
1	E	25	ARG	NE-CZ-NH1	-7.97	116.32	120.30
1	C	134	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	D	92	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	157	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	74	LEU	CB-CG-CD2	6.79	122.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	B	25	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	C	135	GLU	CA-CB-CG	6.41	127.50	113.40
1	F	85	THR	CA-CB-CG2	6.12	120.96	112.40
1	C	72	ASP	N-CA-C	-6.04	94.68	111.00
1	E	89	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	F	89	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	D	28	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	F	80	LYS	CD-CE-NZ	5.55	124.48	111.70
1	E	75	LEU	CB-CG-CD1	5.52	120.39	111.00
1	A	145	LYS	CB-CG-CD	5.50	125.90	111.60
1	D	135	GLU	CG-CD-OE1	5.41	129.11	118.30
1	B	89	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	162	GLY	N-CA-C	-5.27	99.92	113.10
1	B	138	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	138	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	28	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	E	25	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	D	15	ILE	N-CA-CB	5.01	122.31	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	41	HIS	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	1305	0	1295	30	0
1	B	1291	0	1278	23	0
1	C	1291	0	1278	23	0
1	D	1291	0	1278	20	0
1	E	1305	0	1295	13	0
1	F	1305	0	1295	28	0
2	A	13	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	1	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
3	A	27	0	0	7	0
3	B	12	0	0	5	0
3	C	22	0	0	1	0
3	D	21	0	0	0	0
3	E	16	0	0	0	0
3	F	26	0	0	1	0
All	All	7990	0	7749	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (117) 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:71:PHE:CD2	1:B:72:ASP:O	2.24	0.90
1:A:71:PHE:CD2	1:A:72:ASP:O	2.25	0.90
1:F:5:ARG:H	1:F:85:THR:HG23	1.41	0.85
1:A:43:LYS:O	1:A:43:LYS:HD3	1.81	0.80
1:F:5:ARG:H	1:F:85:THR:CG2	1.95	0.77
1:A:74:LEU:HD11	1:C:141:GLY:HA2	1.67	0.77
1:C:75:LEU:HD11	1:C:87:VAL:HG21	1.68	0.74
1:F:75:LEU:HD11	1:F:87:VAL:HG21	1.69	0.74
1:A:25:ARG:HD2	1:F:115:GLU:OE1	1.87	0.73
1:D:39:ILE:HD13	1:D:49:LEU:HD22	1.74	0.70
1:A:75:LEU:HD11	1:A:87:VAL:HG11	1.75	0.69
1:C:138:ARG:HD2	1:C:163:TRP:CZ3	2.28	0.69
1:C:39:ILE:HD12	1:C:49:LEU:HD22	1.75	0.68
1:A:41:HIS:CE1	1:C:139:LEU:HD11	2.30	0.66
1:B:75:LEU:HD11	1:B:87:VAL:HG11	1.78	0.66
2:A:201:CIT:O7	3:A:301:HOH:O	2.03	0.66
1:D:12:PHE:HB3	1:D:15:ILE:HG22	1.76	0.66
1:E:39:ILE:HD12	1:E:49:LEU:HD22	1.77	0.66
1:C:101:PHE:HD1	1:C:102:GLN:OE1	1.79	0.65
1:D:74:LEU:HD11	1:F:141:GLY:HA2	1.78	0.64
1:B:153:GLU:HA	1:B:156:GLU:OE1	1.99	0.63
1:B:39:ILE:HD12	1:B:49:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ILE:HD13	1:D:87:VAL:HG23	1.81	0.62
1:B:86:ALA:HB2	1:E:29:MET:HE1	1.79	0.62
1:F:5:ARG:N	1:F:85:THR:HG23	2.14	0.62
1:A:43:LYS:HD3	1:A:43:LYS:C	2.20	0.61
1:B:94:VAL:HG22	1:C:98:GLU:CD	2.19	0.61
1:D:7:ILE:CD1	1:D:87:VAL:HG23	2.31	0.61
1:F:4:THR:HA	1:F:85:THR:HG21	1.82	0.61
1:A:39:ILE:HD12	1:A:49:LEU:HD22	1.82	0.60
1:B:27:SER:HB2	1:B:65:ASN:HD21	1.66	0.60
1:C:27:SER:HB2	1:C:65:ASN:HD21	1.67	0.60
1:F:23:VAL:HG21	1:F:60:LEU:CD2	2.32	0.60
1:F:27:SER:HB2	1:F:65:ASN:HD21	1.67	0.59
1:D:27:SER:HB2	1:D:65:ASN:HD21	1.68	0.58
1:B:108:ARG:NH2	3:B:301:HOH:O	2.28	0.58
1:A:27:SER:HB2	1:A:65:ASN:HD21	1.68	0.58
1:E:27:SER:HB2	1:E:65:ASN:HD21	1.67	0.57
1:D:12:PHE:HD2	1:D:15:ILE:HG22	1.70	0.56
1:A:41:HIS:CG	1:C:139:LEU:HD21	2.41	0.56
1:D:12:PHE:CD2	1:D:15:ILE:HG22	2.40	0.56
1:E:25:ARG:NH1	1:E:120:THR:O	2.34	0.56
1:A:44:ASN:OD1	1:A:44:ASN:N	2.38	0.56
1:A:92:ARG:NH2	1:A:128:ILE:O	2.39	0.56
1:A:85:THR:HB	3:A:319:HOH:O	2.07	0.55
1:C:23:VAL:HG11	1:C:60:LEU:CD2	2.36	0.55
1:B:23:VAL:HG21	1:B:60:LEU:CD2	2.37	0.55
1:C:65:ASN:HD22	1:C:65:ASN:H	1.54	0.55
1:B:108:ARG:NH1	3:B:301:HOH:O	2.36	0.55
1:A:43:LYS:O	1:A:43:LYS:CD	2.53	0.54
1:F:65:ASN:H	1:F:65:ASN:HD22	1.55	0.54
1:A:25:ARG:NH1	1:A:120:THR:O	2.33	0.53
1:D:65:ASN:HD22	1:D:65:ASN:H	1.56	0.53
1:A:92:ARG:NH1	2:A:201:CIT:O5	2.41	0.53
1:A:65:ASN:H	1:A:65:ASN:HD22	1.55	0.52
1:A:108:ARG:NH1	3:A:305:HOH:O	2.37	0.52
1:D:131:THR:N	2:D:201:CIT:O3	2.42	0.52
1:B:65:ASN:H	1:B:65:ASN:HD22	1.58	0.52
1:B:136:ILE:HA	1:C:74:LEU:HD21	1.92	0.51
1:A:74:LEU:HD11	1:C:141:GLY:CA	2.39	0.51
1:C:39:ILE:HD12	1:C:49:LEU:CD2	2.40	0.51
1:F:23:VAL:HG21	1:F:60:LEU:CD1	2.41	0.51
1:F:135:GLU:OE1	1:F:138:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:VAL:HG13	1:E:107:ASN:OD1	2.12	0.50
1:E:127:PHE:HA	1:F:102:GLN:HE21	1.76	0.50
1:B:23:VAL:HG21	1:B:60:LEU:CD1	2.42	0.50
1:A:74:LEU:HD13	1:A:77:ASN:ND2	2.27	0.50
1:A:72:ASP:OD1	3:A:302:HOH:O	2.20	0.50
1:D:74:LEU:HD13	1:D:77:ASN:ND2	2.27	0.49
1:B:93:ALA:HB2	3:B:309:HOH:O	2.11	0.49
1:D:7:ILE:HD13	1:D:7:ILE:O	2.12	0.49
1:E:139:LEU:HD22	1:F:73:GLY:HA2	1.95	0.49
1:A:39:ILE:HD12	1:A:49:LEU:CD2	2.43	0.49
1:A:73:GLY:N	3:A:306:HOH:O	2.46	0.49
1:C:21:ASP:OD2	3:C:301:HOH:O	2.18	0.49
1:C:101:PHE:CD1	1:C:102:GLN:OE1	2.64	0.48
1:F:138:ARG:HD3	1:F:163:TRP:CH2	2.49	0.48
3:A:309:HOH:O	1:F:120:THR:CG2	2.61	0.48
1:D:74:LEU:HD11	1:F:141:GLY:CA	2.43	0.48
1:B:39:ILE:HD12	1:B:49:LEU:CD2	2.43	0.47
1:F:23:VAL:CG2	1:F:60:LEU:CD2	2.92	0.47
1:E:39:ILE:HD12	1:E:49:LEU:CD2	2.43	0.47
1:E:162:GLY:O	1:E:163:TRP:C	2.54	0.46
1:D:43:LYS:HG3	1:D:44:ASN:N	2.31	0.46
1:E:65:ASN:HD22	1:E:65:ASN:H	1.64	0.46
1:E:74:LEU:HG	1:E:76:VAL:HG22	1.97	0.45
1:A:25:ARG:NH2	1:F:115:GLU:OE2	2.48	0.45
1:A:106:MET:HG3	1:A:107:ASN:N	2.32	0.45
1:D:43:LYS:HG3	1:D:44:ASN:H	1.82	0.45
1:D:106:MET:HG3	1:D:107:ASN:N	2.32	0.44
1:A:71:PHE:CE2	1:A:72:ASP:O	2.70	0.44
3:B:301:HOH:O	1:E:120:THR:HG22	2.17	0.44
1:C:23:VAL:HG11	1:C:60:LEU:CD1	2.47	0.44
1:D:7:ILE:HD11	1:D:75:LEU:HD21	2.00	0.44
1:F:108:ARG:HD3	3:F:314:HOH:O	2.16	0.44
1:B:93:ALA:HB1	1:C:98:GLU:CD	2.38	0.43
1:B:5:ARG:HH11	1:B:82:GLN:HE22	1.67	0.43
1:F:23:VAL:CG2	1:F:60:LEU:HD22	2.48	0.43
1:A:41:HIS:ND1	1:C:139:LEU:HD21	2.34	0.43
1:B:94:VAL:HG22	1:C:98:GLU:OE1	2.19	0.43
1:B:71:PHE:CE2	1:B:72:ASP:O	2.70	0.43
1:B:108:ARG:CZ	3:B:301:HOH:O	2.66	0.43
1:A:29:MET:HE1	1:F:115:GLU:HG2	2.01	0.42
1:B:23:VAL:CG2	1:B:60:LEU:CD2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD11	1:D:117:VAL:HG12	2.01	0.42
1:B:94:VAL:HG22	1:C:98:GLU:OE2	2.20	0.42
1:F:23:VAL:HG21	1:F:60:LEU:HD22	2.00	0.42
1:F:1:MET:HA	1:F:1:MET:CE	2.49	0.41
1:A:29:MET:CE	1:F:115:GLU:HG2	2.50	0.41
1:E:3:LYS:N	1:E:3:LYS:HD2	2.35	0.41
1:F:4:THR:HA	1:F:85:THR:CG2	2.49	0.41
1:B:163:TRP:HA	1:B:163:TRP:CE3	2.56	0.41
1:C:119:LEU:CD1	1:D:117:VAL:HG12	2.51	0.41
1:D:46:LEU:HD12	1:D:47:PHE:CE2	2.56	0.41
1:A:65:ASN:HD22	1:A:65:ASN:N	2.20	0.40
1:F:135:GLU:OE1	1:F:138:ARG:CZ	2.69	0.40
3:A:309:HOH:O	1:F:120:THR:HG23	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	161/163 (99%)	156 (97%)	4 (2%)	1 (1%)	25	31
1	B	159/163 (98%)	154 (97%)	4 (2%)	1 (1%)	25	31
1	C	159/163 (98%)	154 (97%)	4 (2%)	1 (1%)	25	31
1	D	159/163 (98%)	156 (98%)	3 (2%)	0	100	100
1	E	161/163 (99%)	156 (97%)	5 (3%)	0	100	100
1	F	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
All	All	960/978 (98%)	933 (97%)	24 (2%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	B	41	HIS
1	C	41	HIS

### 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	141/141 (100%)	124 (88%)	17 (12%)	5 5
1	B	139/141 (99%)	125 (90%)	14 (10%)	7 9
1	C	139/141 (99%)	124 (89%)	15 (11%)	6 7
1	D	139/141 (99%)	125 (90%)	14 (10%)	7 9
1	E	141/141 (100%)	128 (91%)	13 (9%)	9 11
1	F	141/141 (100%)	130 (92%)	11 (8%)	12 16
All	All	840/846 (99%)	756 (90%)	84 (10%)	7 9

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	22	LEU
1	A	39	ILE
1	A	43	LYS
1	A	57	GLN
1	A	65	ASN
1	A	74	LEU
1	A	92	ARG
1	A	94	VAL
1	A	106	MET
1	A	119	LEU
1	A	120	THR
1	A	132	LEU
1	A	135	GLU
1	A	140	LYS
1	A	145	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	160	GLN
1	B	3	LYS
1	B	39	ILE
1	B	43	LYS
1	B	65	ASN
1	B	74	LEU
1	B	109	GLN
1	B	119	LEU
1	B	120	THR
1	B	132	LEU
1	B	135	GLU
1	B	140	LYS
1	B	145	LYS
1	B	160	GLN
1	B	163	TRP
1	C	39	ILE
1	C	43	LYS
1	C	44	ASN
1	C	58	SER
1	C	65	ASN
1	C	96	ASP
1	C	102	GLN
1	C	119	LEU
1	C	120	THR
1	C	132	LEU
1	C	135	GLU
1	C	138	ARG
1	C	140	LYS
1	C	145	LYS
1	C	163	TRP
1	D	7	ILE
1	D	15	ILE
1	D	43	LYS
1	D	44	ASN
1	D	46	LEU
1	D	65	ASN
1	D	74	LEU
1	D	106	MET
1	D	119	LEU
1	D	120	THR
1	D	132	LEU
1	D	135	GLU

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Mol	Chain	Res	Type
1	D	140	LYS
1	D	160	GLN
1	E	1	MET
1	E	39	ILE
1	E	43	LYS
1	E	57	GLN
1	E	65	ASN
1	E	92	ARG
1	E	98	GLU
1	E	119	LEU
1	E	120	THR
1	E	132	LEU
1	E	135	GLU
1	E	140	LYS
1	E	160	GLN
1	F	1	MET
1	F	39	ILE
1	F	43	LYS
1	F	65	ASN
1	F	85	THR
1	F	119	LEU
1	F	120	THR
1	F	132	LEU
1	F	135	GLU
1	F	140	LYS
1	F	160	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	57	GLN
1	A	65	ASN
1	A	82	GLN
1	A	160	GLN
1	B	57	GLN
1	B	65	ASN
1	B	82	GLN
1	B	102	GLN
1	C	57	GLN
1	C	65	ASN
1	C	82	GLN

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Mol	Chain	Res	Type
1	C	160	GLN
1	D	57	GLN
1	D	65	ASN
1	D	82	GLN
1	E	57	GLN
1	E	65	ASN
1	E	82	GLN
1	E	160	GLN
1	F	57	GLN
1	F	65	ASN
1	F	82	GLN
1	F	102	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](#)

6 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	E	201	-	12,12,12	1.03	0	17,17,17	1.59	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CIT	F	201	-	12,12,12	2.12	2 (16%)	17,17,17	4.54	9 (52%)
2	CIT	C	201	-	12,12,12	1.19	0	17,17,17	1.70	5 (29%)
2	CIT	B	201	-	12,12,12	1.17	2 (16%)	17,17,17	1.46	4 (23%)
2	CIT	D	201	-	12,12,12	1.46	2 (16%)	17,17,17	2.05	6 (35%)
2	CIT	A	201	-	12,12,12	2.63	2 (16%)	17,17,17	4.58	9 (52%)

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	E	201	-	-	11/16/16/16	-
2	CIT	F	201	-	-	5/16/16/16	-
2	CIT	C	201	-	-	6/16/16/16	-
2	CIT	B	201	-	-	5/16/16/16	-
2	CIT	D	201	-	-	3/16/16/16	-
2	CIT	A	201	-	-	5/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	CIT	C3-C6	6.63	1.60	1.53
2	A	201	CIT	C4-C3	-5.15	1.47	1.53
2	F	201	CIT	C4-C3	-5.08	1.47	1.53
2	F	201	CIT	C3-C6	3.89	1.57	1.53
2	D	201	CIT	C3-C6	-3.28	1.50	1.53
2	D	201	CIT	O4-C5	-2.39	1.22	1.30
2	B	201	CIT	O4-C5	-2.16	1.23	1.30
2	B	201	CIT	C3-C6	-2.02	1.51	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	CIT	O7-C3-C6	-12.63	91.14	108.86
2	A	201	CIT	C4-C3-C2	9.19	133.12	109.16
2	A	201	CIT	O7-C3-C6	-8.66	96.71	108.86
2	F	201	CIT	C4-C3-C2	7.96	129.94	109.16
2	A	201	CIT	C2-C3-C6	-7.58	93.81	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	CIT	O6-C6-C3	7.04	125.27	113.05
2	A	201	CIT	C4-C3-C6	-6.39	96.38	110.11
2	F	201	CIT	C2-C3-C6	-5.88	97.47	110.11
2	F	201	CIT	O6-C6-C3	5.86	123.23	113.05
2	D	201	CIT	O5-C6-C3	-4.61	115.73	122.25
2	F	201	CIT	O7-C3-C2	4.42	119.75	109.40
2	D	201	CIT	O6-C6-C3	4.09	120.15	113.05
2	A	201	CIT	O7-C3-C2	4.01	118.78	109.40
2	F	201	CIT	C4-C3-C6	-3.29	103.04	110.11
2	C	201	CIT	O4-C5-C4	3.25	124.79	114.35
2	D	201	CIT	O4-C5-O3	-3.21	115.31	123.30
2	A	201	CIT	O6-C6-O5	-3.01	114.24	123.82
2	C	201	CIT	C3-C2-C1	-2.97	106.63	113.81
2	B	201	CIT	O6-C6-C3	2.78	117.88	113.05
2	D	201	CIT	C2-C3-C6	-2.69	104.33	110.11
2	E	201	CIT	O3-C5-C4	-2.68	115.11	122.94
2	B	201	CIT	O1-C1-C2	-2.62	115.30	122.94
2	E	201	CIT	O5-C6-C3	-2.61	118.56	122.25
2	F	201	CIT	O2-C1-O1	-2.57	116.89	123.30
2	B	201	CIT	O5-C6-C3	-2.53	118.67	122.25
2	C	201	CIT	O3-C5-C4	-2.40	115.93	122.94
2	E	201	CIT	O4-C5-C4	2.38	121.98	114.35
2	D	201	CIT	C4-C3-C2	2.37	115.34	109.16
2	E	201	CIT	O2-C1-C2	2.29	121.71	114.35
2	C	201	CIT	O1-C1-C2	-2.27	116.30	122.94
2	C	201	CIT	O5-C6-C3	-2.26	119.05	122.25
2	B	201	CIT	O4-C5-O3	-2.19	117.84	123.30
2	A	201	CIT	C3-C4-C5	-2.18	108.54	113.81
2	F	201	CIT	O2-C1-C2	2.18	121.34	114.35
2	A	201	CIT	O2-C1-C2	2.17	121.31	114.35
2	D	201	CIT	O4-C5-C4	2.14	121.23	114.35
2	F	201	CIT	O6-C6-O5	-2.11	117.11	123.82

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	CIT	C2-C3-C4-C5
2	A	201	CIT	C6-C3-C4-C5
2	B	201	CIT	C1-C2-C3-O7
2	B	201	CIT	C1-C2-C3-C4
2	B	201	CIT	C1-C2-C3-C6

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Mol	Chain	Res	Type	Atoms
2	E	201	CIT	C1-C2-C3-C4
2	E	201	CIT	C1-C2-C3-C6
2	F	201	CIT	C2-C3-C4-C5
2	D	201	CIT	C1-C2-C3-C4
2	F	201	CIT	C6-C3-C4-C5
2	D	201	CIT	C1-C2-C3-C6
2	E	201	CIT	C1-C2-C3-O7
2	F	201	CIT	C1-C2-C3-O7
2	C	201	CIT	C1-C2-C3-C6
2	E	201	CIT	O7-C3-C6-O5
2	A	201	CIT	C4-C3-C6-O6
2	E	201	CIT	C2-C3-C6-O5
2	E	201	CIT	C2-C3-C6-O6
2	E	201	CIT	C4-C3-C6-O5
2	F	201	CIT	C4-C3-C6-O5
2	C	201	CIT	C1-C2-C3-C4
2	C	201	CIT	C2-C3-C6-O5
2	C	201	CIT	C2-C3-C6-O6
2	F	201	CIT	C4-C3-C6-O6
2	A	201	CIT	C1-C2-C3-O7
2	E	201	CIT	O7-C3-C6-O6
2	A	201	CIT	C4-C3-C6-O5
2	E	201	CIT	C4-C3-C6-O6
2	C	201	CIT	C3-C4-C5-O3
2	C	201	CIT	C3-C4-C5-O4
2	E	201	CIT	C3-C4-C5-O3
2	B	201	CIT	O1-C1-C2-C3
2	E	201	CIT	C3-C4-C5-O4
2	B	201	CIT	O2-C1-C2-C3
2	D	201	CIT	C1-C2-C3-O7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	CIT	1	0
2	A	201	CIT	2	0

## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	163/163 (100%)	0.41	8 (4%) 29 36	20, 31, 56, 101	0
1	B	161/163 (98%)	0.78	18 (11%) 5 7	21, 38, 84, 142	0
1	C	161/163 (98%)	0.49	8 (4%) 28 35	20, 32, 56, 149	0
1	D	161/163 (98%)	0.53	12 (7%) 14 19	21, 35, 70, 100	0
1	E	163/163 (100%)	0.45	8 (4%) 29 36	20, 35, 57, 131	0
1	F	163/163 (100%)	0.53	13 (7%) 12 16	19, 31, 61, 130	0
All	All	972/978 (99%)	0.53	67 (6%) 16 22	19, 34, 68, 149	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	HIS	10.7
1	B	41	HIS	8.4
1	B	73	GLY	7.4
1	B	42	HIS	7.2
1	C	41	HIS	6.6
1	E	41	HIS	5.8
1	F	42	HIS	5.6
1	F	41	HIS	5.4
1	B	43	LYS	5.2
1	D	163	TRP	5.2
1	C	42	HIS	5.0
1	B	157	ARG	4.9
1	B	163	TRP	4.7
1	E	42	HIS	4.4
1	D	162	GLY	4.3
1	B	72	ASP	4.1
1	C	99	TYR	3.7
1	C	72	ASP	3.6
1	A	1	MET	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	141	GLY	3.6
1	F	163	TRP	3.4
1	E	99	TYR	3.4
1	B	160	GLN	3.4
1	F	39	ILE	3.4
1	B	47	PHE	3.3
1	F	162	GLY	3.2
1	A	43	LYS	3.2
1	F	138	ARG	3.1
1	A	73	GLY	3.0
1	D	160	GLN	3.0
1	D	161	GLN	3.0
1	F	135	GLU	2.9
1	C	23	VAL	2.9
1	D	41	HIS	2.8
1	D	42	HIS	2.8
1	B	149	GLN	2.7
1	B	161	GLN	2.7
1	F	40	GLY	2.6
1	B	69	VAL	2.6
1	B	39	ILE	2.4
1	A	162	GLY	2.4
1	D	6	VAL	2.4
1	D	43	LYS	2.3
1	D	138	ARG	2.3
1	A	94	VAL	2.3
1	F	99	TYR	2.2
1	E	50	GLU	2.2
1	B	138	ARG	2.2
1	A	74	LEU	2.2
1	A	161	GLN	2.2
1	C	43	LYS	2.2
1	F	139	LEU	2.2
1	E	39	ILE	2.2
1	C	73	GLY	2.2
1	D	149	GLN	2.1
1	B	44	ASN	2.1
1	B	140	LYS	2.1
1	E	43	LYS	2.1
1	F	44	ASN	2.1
1	E	163	TRP	2.1
1	F	159	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	94	VAL	2.1
1	B	136	ILE	2.0
1	D	22	LEU	2.0
1	B	49	LEU	2.0
1	E	156	GLU	2.0
1	F	103	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CIT	A	201	13/13	0.81	0.16	30,40,42,43	0
2	CIT	C	201	13/13	0.83	0.18	41,51,54,56	0
2	CIT	F	201	13/13	0.84	0.17	28,38,46,46	0
2	CIT	E	201	13/13	0.88	0.12	38,46,52,52	0
2	CIT	D	201	13/13	0.88	0.16	39,52,57,59	0
2	CIT	B	201	13/13	0.89	0.17	47,52,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.