



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 10:04 PM EDT

PDB ID : 3K49
Title : Puf3 RNA binding domain bound to Cox17 RNA 3' UTR recognition sequence site B
Authors : Zhu, D.; Stumpf, C.R.; Krahn, J.M.; Wickens, M.; Hall, T.M.T.
Deposited on : 2009-10-05
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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 : 2.35
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

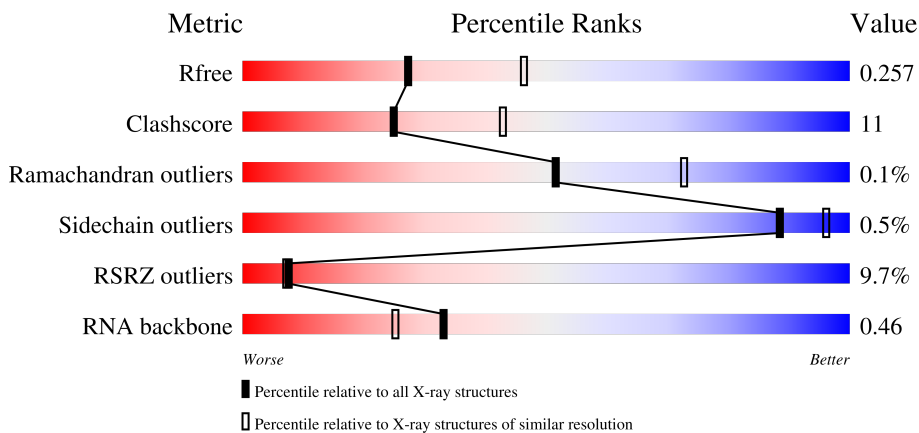
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

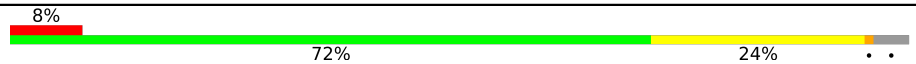

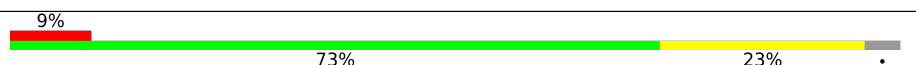
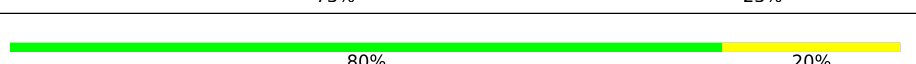
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 $\leq 5\%$. 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	369	
1	C	369	
1	E	369	
2	B	10	

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Mol	Chain	Length	Quality of chain	
2	D	10	 70%	 30%
2	F	10	 70%	 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9635 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 mRNA-binding protein PUF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	353	2847	1808	482	547	10	0	0	0
1	C	353	2847	1808	482	547	10	0	0	0
1	E	353	2847	1808	482	547	10	0	0	0

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*CP*UP*GP*UP*AP*AP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	10	208	95	37	67	9	0	0	0
2	D	10	208	95	37	67	9	0	0	0
2	F	10	208	95	37	67	9	0	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	E	1	Total C O 13 6 7	0	0

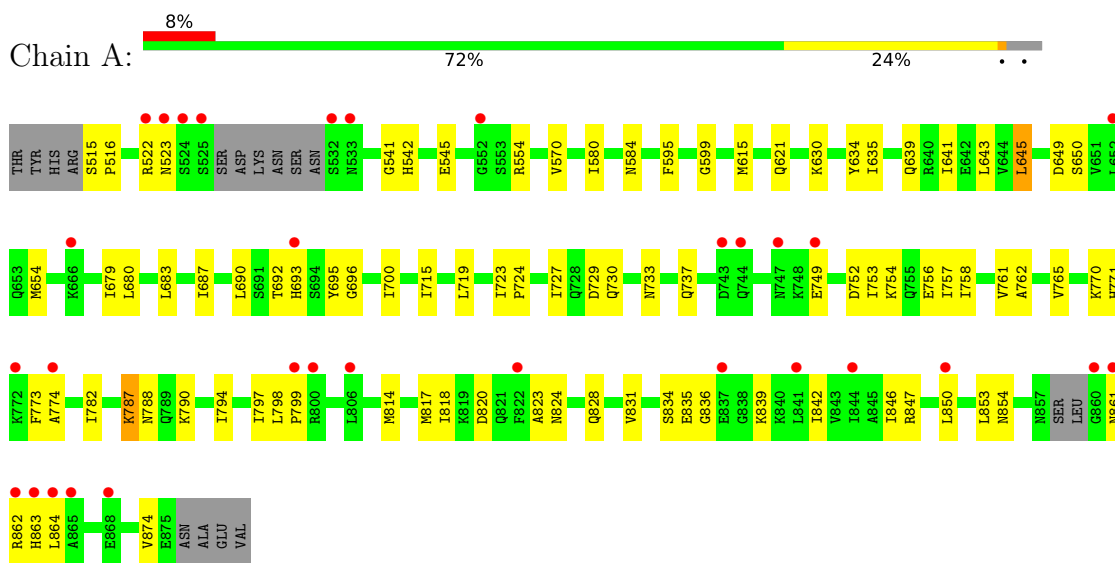
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	132	Total O 132 132	0	0
4	B	10	Total O 10 10	0	0
4	C	120	Total O 120 120	0	0
4	D	9	Total O 9 9	0	0
4	E	154	Total O 154 154	0	0
4	F	6	Total O 6 6	0	0

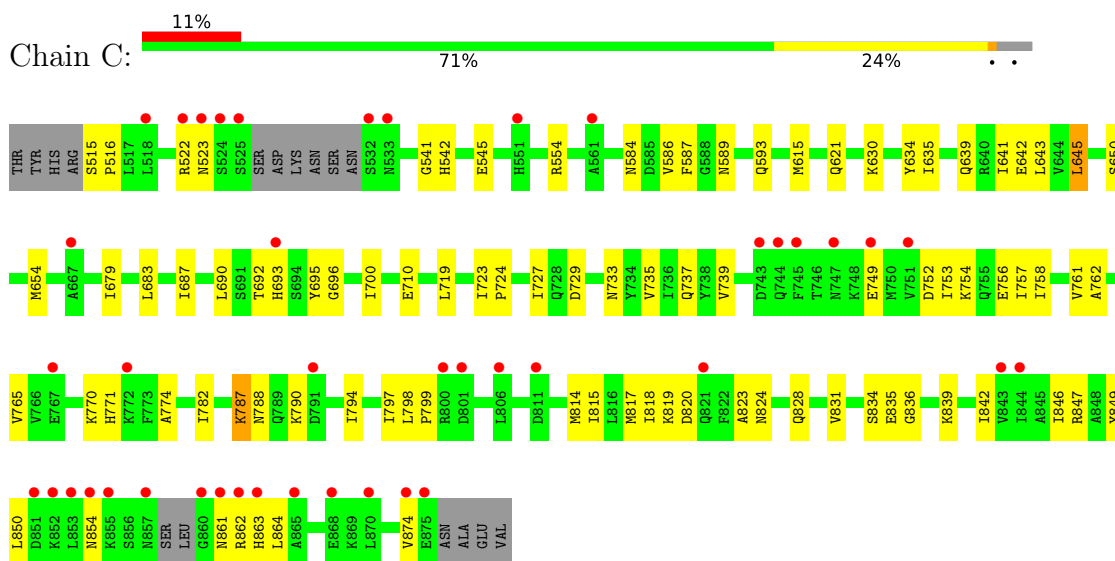
3 Residue-property plots [i](#)

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.

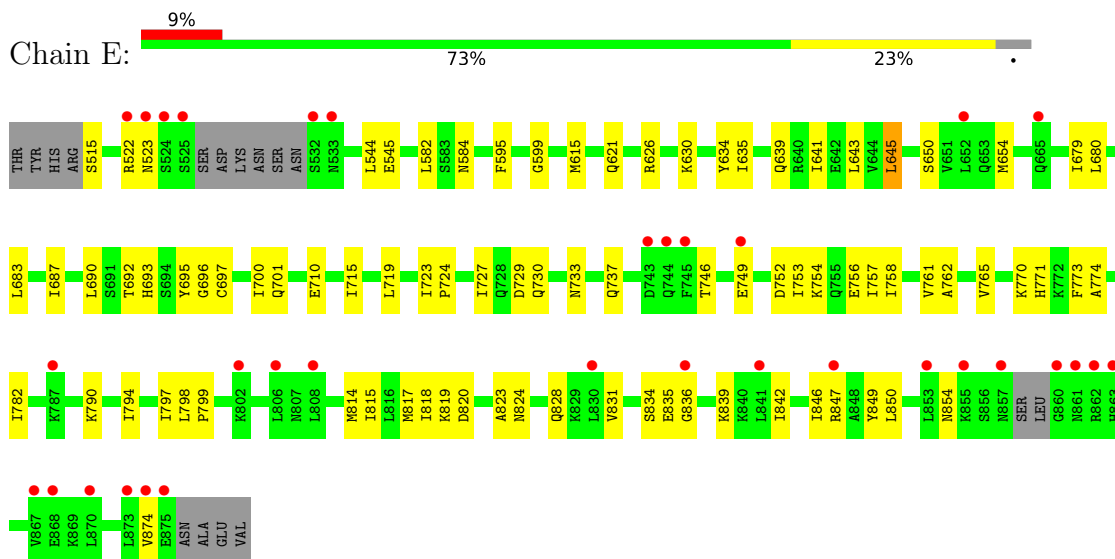
- Molecule 1: mRNA-binding protein PUF3



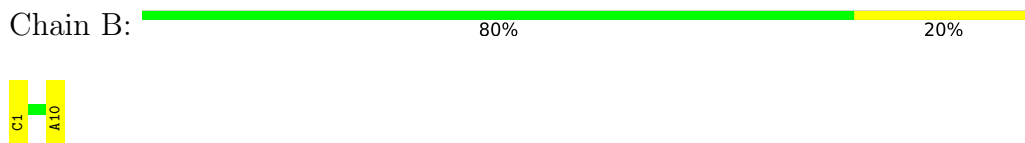
- Molecule 1: mRNA-binding protein PUF3



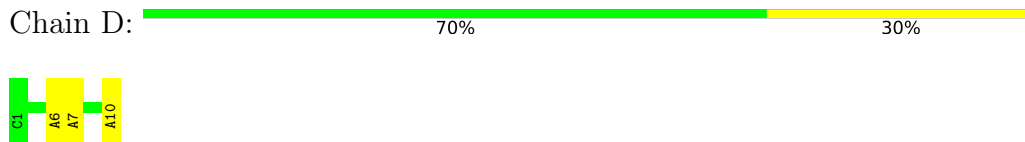
- Molecule 1: mRNA-binding protein PUF3



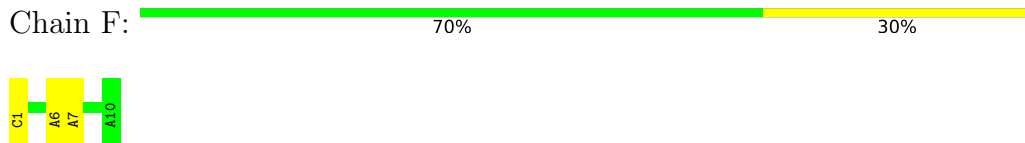
- Molecule 2: RNA (5'-R(*CP*CP*UP*GP*UP*AP*AP*AP*UP*A)-3')



- Molecule 2: RNA (5'-R(*CP*CP*UP*GP*UP*AP*AP*AP*UP*A)-3')



- Molecule 2: RNA (5'-R(*CP*CP*UP*GP*UP*AP*AP*AP*UP*A)-3')



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.13Å 87.07Å 125.18Å 90.00° 116.48° 90.00°	Depositor
Resolution (Å)	36.61 – 2.50 36.61 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.3 (36.61-2.50) 93.4 (36.61-2.48)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.48Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.263 0.224 , 0.257	Depositor DCC
R_{free} test set	2429 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtrriage
Anisotropy	0.931	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.074 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-1 0.087 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-1	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9635	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/2888	0.49	0/3885
1	C	0.39	0/2888	0.49	0/3885
1	E	0.40	0/2888	0.51	0/3885
2	B	0.58	0/232	1.10	1/359 (0.3%)
2	D	0.52	0/232	0.89	0/359
2	F	0.59	0/232	1.08	1/359 (0.3%)
All	All	0.41	0/9360	0.56	2/12732 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	C	C5-C6-N1	6.49	124.25	121.00
2	F	1	C	C6-N1-C1'	-5.01	114.79	120.80

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	2847	0	2876	66	1
1	C	2847	0	2876	69	1
1	E	2847	0	2876	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	208	0	109	1	0
2	D	208	0	109	3	0
2	F	208	0	109	1	0
3	A	13	0	5	0	0
3	C	13	0	5	0	0
3	E	13	0	5	1	0
4	A	132	0	0	1	0
4	B	10	0	0	0	0
4	C	120	0	0	0	1
4	D	9	0	0	0	0
4	E	154	0	0	0	1
4	F	6	0	0	0	0
All	All	9635	0	8970	196	2

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 11.

All (196) 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:584:ASN:ND2	1:A:621:GLN:HE22	1.80	0.79
1:E:584:ASN:ND2	1:E:621:GLN:HE22	1.85	0.74
1:A:753:ILE:HD13	1:A:756:GLU:OE2	1.89	0.72
1:C:584:ASN:ND2	1:C:621:GLN:HE22	1.86	0.71
1:E:753:ILE:HD13	1:E:756:GLU:OE2	1.91	0.69
1:C:541:GLY:HA3	1:C:542:HIS:HD2	1.58	0.69
1:C:753:ILE:HD13	1:C:756:GLU:OE2	1.92	0.68
1:C:824:ASN:O	1:C:828:GLN:HG3	1.94	0.68
1:A:541:GLY:HA3	1:A:542:HIS:CD2	2.29	0.68
1:C:541:GLY:HA3	1:C:542:HIS:CD2	2.28	0.68
1:A:541:GLY:HA3	1:A:542:HIS:HD2	1.59	0.67
1:E:824:ASN:O	1:E:828:GLN:HG3	1.95	0.67
1:A:696:GLY:O	1:A:700:ILE:HG12	1.95	0.66
1:A:824:ASN:O	1:A:828:GLN:HG3	1.94	0.66
1:E:696:GLY:O	1:E:700:ILE:HG12	1.96	0.66
1:C:862:ARG:HB3	1:C:864:LEU:HG	1.79	0.65
1:C:765:VAL:HG11	1:C:797:ILE:HD11	1.78	0.64
1:A:765:VAL:HG11	1:A:797:ILE:HD11	1.78	0.64
1:E:819:LYS:HE2	1:E:849:TYR:HE1	1.64	0.63
1:A:861:ASN:HB3	1:A:863:HIS:CE1	2.35	0.62
1:C:819:LYS:HE2	1:C:849:TYR:HE1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:GLY:O	1:C:700:ILE:HG12	1.99	0.62
1:C:554:ARG:NH2	2:D:10:A:C4	2.68	0.62
1:C:541:GLY:CA	1:C:542:HIS:HD2	2.12	0.62
1:E:765:VAL:HG11	1:E:797:ILE:HD11	1.81	0.62
1:C:541:GLY:C	1:C:542:HIS:CD2	2.75	0.60
1:A:541:GLY:CA	1:A:542:HIS:HD2	2.14	0.59
1:A:770:LYS:HA	1:A:820:ASP:OD2	2.02	0.59
1:E:770:LYS:HA	1:E:820:ASP:OD2	2.03	0.59
1:A:733:ASN:O	1:A:737:GLN:HG3	2.03	0.58
1:C:770:LYS:HA	1:C:820:ASP:OD2	2.02	0.58
1:C:542:HIS:CD2	1:C:542:HIS:N	2.70	0.58
1:C:733:ASN:O	1:C:737:GLN:HG3	2.03	0.58
1:E:842:ILE:O	1:E:846:ILE:HG13	2.04	0.57
1:A:541:GLY:C	1:A:542:HIS:CD2	2.78	0.57
1:E:650:SER:O	1:E:654:MET:HG2	2.04	0.57
1:C:757:ILE:O	1:C:761:VAL:HG23	2.05	0.57
1:A:842:ILE:O	1:A:846:ILE:HG13	2.05	0.56
1:A:615:MET:HG3	1:A:643:LEU:O	2.04	0.56
1:A:757:ILE:O	1:A:761:VAL:HG23	2.05	0.56
1:C:650:SER:O	1:C:654:MET:HG2	2.05	0.56
1:C:842:ILE:O	1:C:846:ILE:HG13	2.05	0.56
1:E:630:LYS:HE2	1:E:634:TYR:CE2	2.41	0.56
1:A:835:GLU:HG2	1:A:836:GLY:N	2.19	0.56
1:C:835:GLU:HG2	1:C:836:GLY:N	2.21	0.56
1:C:749:GLU:O	1:C:753:ILE:HG12	2.06	0.56
1:C:861:ASN:HB3	1:C:863:HIS:CE1	2.41	0.56
1:C:771:HIS:HB3	1:C:774:ALA:HB3	1.87	0.55
1:A:584:ASN:CG	1:A:621:GLN:HE22	2.09	0.55
1:A:853:LEU:HD21	1:A:862:ARG:HD2	1.89	0.55
1:E:771:HIS:HB3	1:E:774:ALA:HB3	1.86	0.55
1:A:771:HIS:HB3	1:A:774:ALA:HB3	1.88	0.55
1:E:835:GLU:HG2	1:E:836:GLY:N	2.21	0.55
1:E:630:LYS:HE2	1:E:634:TYR:HE2	1.72	0.55
1:E:749:GLU:O	1:E:753:ILE:HG12	2.07	0.55
1:C:541:GLY:CA	1:C:542:HIS:CD2	2.89	0.54
1:A:542:HIS:CD2	1:A:542:HIS:N	2.75	0.54
1:A:554:ARG:NH2	2:B:10:A:C4	2.76	0.54
1:E:626:ARG:NH1	3:E:3:CIT:O1	2.40	0.54
1:E:733:ASN:O	1:E:737:GLN:HG3	2.07	0.54
1:A:749:GLU:O	1:A:753:ILE:HG12	2.07	0.54
1:A:650:SER:O	1:A:654:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:ARG:HG3	1:C:874:VAL:HG11	1.90	0.53
1:A:765:VAL:CG1	1:A:797:ILE:HD11	2.37	0.53
1:E:765:VAL:CG1	1:E:797:ILE:HD11	2.39	0.53
1:A:862:ARG:HB3	1:A:864:LEU:HG	1.90	0.53
1:C:765:VAL:CG1	1:C:797:ILE:HD11	2.38	0.53
1:A:834:SER:O	1:A:839:LYS:HD2	2.09	0.53
1:E:584:ASN:CG	1:E:621:GLN:HE22	2.12	0.52
1:C:615:MET:HG3	1:C:643:LEU:O	2.09	0.52
1:A:630:LYS:HE2	1:A:634:TYR:CE2	2.44	0.52
1:A:584:ASN:CG	1:A:621:GLN:NE2	2.62	0.52
1:C:834:SER:O	1:C:839:LYS:HD2	2.10	0.52
1:C:630:LYS:HE2	1:C:634:TYR:CE2	2.45	0.51
1:E:850:LEU:O	1:E:854:ASN:HB2	2.10	0.51
1:E:757:ILE:O	1:E:761:VAL:HG23	2.10	0.51
2:D:6:A:O2'	2:D:7:A:H5'	2.11	0.51
1:C:850:LEU:O	1:C:854:ASN:HB2	2.10	0.50
1:E:584:ASN:CG	1:E:621:GLN:NE2	2.65	0.50
1:A:723:ILE:HB	1:A:724:PRO:HD3	1.92	0.50
1:A:522:ARG:HG3	1:A:523:ASN:N	2.26	0.50
1:A:850:LEU:O	1:A:854:ASN:HB2	2.12	0.50
1:E:615:MET:HG3	1:E:643:LEU:O	2.11	0.50
2:F:6:A:O2'	2:F:7:A:H5'	2.11	0.50
1:E:819:LYS:HE2	1:E:849:TYR:CE1	2.46	0.50
1:A:834:SER:HB3	1:A:839:LYS:HB2	1.94	0.50
1:C:834:SER:HB3	1:C:839:LYS:HB2	1.94	0.50
1:E:820:ASP:HB3	1:E:823:ALA:HB3	1.94	0.49
1:C:630:LYS:HE2	1:C:634:TYR:HE2	1.77	0.49
1:E:522:ARG:HG3	1:E:523:ASN:N	2.27	0.49
1:E:834:SER:O	1:E:839:LYS:HD2	2.12	0.49
1:C:820:ASP:HB3	1:C:823:ALA:HB3	1.95	0.49
1:A:787:LYS:HD2	1:A:788:ASN:N	2.27	0.49
1:A:794:ILE:HG22	1:A:798:LEU:HG	1.95	0.49
1:A:541:GLY:CA	1:A:542:HIS:CD2	2.91	0.49
1:E:834:SER:HB3	1:E:839:LYS:HB2	1.95	0.49
1:A:692:THR:HG22	1:A:729:ASP:OD1	2.13	0.48
1:C:723:ILE:HB	1:C:724:PRO:HD3	1.94	0.48
1:A:641:ILE:HG13	1:A:645:LEU:HD12	1.95	0.48
1:A:687:ILE:HG22	1:A:719:LEU:HD21	1.95	0.48
1:A:847:ARG:HG3	1:A:874:VAL:HG11	1.95	0.48
1:E:794:ILE:HG22	1:E:798:LEU:HG	1.96	0.48
1:A:630:LYS:HE2	1:A:634:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ILE:HG13	1:C:645:LEU:HD12	1.96	0.48
1:C:692:THR:HG22	1:C:729:ASP:OD1	2.13	0.48
1:C:819:LYS:HE2	1:C:849:TYR:CE1	2.46	0.48
1:E:641:ILE:HG13	1:E:645:LEU:HD12	1.96	0.47
1:A:820:ASP:HB3	1:A:823:ALA:HB3	1.96	0.47
1:C:554:ARG:NH2	2:D:10:A:C5	2.82	0.47
1:E:762:ALA:O	1:E:765:VAL:HG23	2.14	0.47
1:C:787:LYS:HD2	1:C:788:ASN:N	2.29	0.47
1:C:794:ILE:HG22	1:C:798:LEU:HG	1.96	0.47
1:E:847:ARG:HG3	1:E:874:VAL:HG11	1.96	0.47
1:C:754:LYS:O	1:C:758:ILE:HG12	2.14	0.47
1:E:752:ASP:O	1:E:756:GLU:HG3	2.14	0.47
1:C:790:LYS:O	1:C:794:ILE:HG13	2.15	0.47
1:E:723:ILE:HB	1:E:724:PRO:HD3	1.96	0.47
1:A:515:SER:HB2	1:A:545:GLU:OE2	2.15	0.47
1:A:762:ALA:O	1:A:765:VAL:HG23	2.15	0.47
1:A:814:MET:O	1:A:818:ILE:HG13	2.14	0.47
1:E:515:SER:HB2	1:E:545:GLU:OE2	2.15	0.46
1:E:814:MET:O	1:E:818:ILE:HG13	2.15	0.46
1:A:635:ILE:HD12	1:A:639:GLN:HB3	1.98	0.46
1:C:586:VAL:HG13	1:C:587:PHE:N	2.31	0.46
1:E:697:CYS:O	1:E:701:GLN:HG3	2.15	0.46
1:A:595:PHE:O	1:A:599:GLY:HA3	2.17	0.45
1:C:584:ASN:CG	1:C:621:GLN:NE2	2.70	0.45
1:E:693:HIS:HE1	1:E:695:TYR:CD1	2.34	0.45
1:A:798:LEU:HA	1:A:799:PRO:HD2	1.81	0.45
1:C:814:MET:O	1:C:818:ILE:HG13	2.16	0.45
1:C:522:ARG:HG3	1:C:523:ASN:N	2.32	0.45
1:A:570:VAL:HG23	4:A:201:HOH:O	2.17	0.45
1:A:782:ILE:O	1:A:790:LYS:HE2	2.17	0.45
1:C:515:SER:HB2	1:C:545:GLU:OE2	2.16	0.45
1:C:584:ASN:CG	1:C:621:GLN:HE22	2.18	0.45
1:A:754:LYS:O	1:A:758:ILE:HG12	2.16	0.45
1:A:752:ASP:O	1:A:756:GLU:HG3	2.17	0.45
1:C:589:ASN:O	1:C:593:GLN:HG3	2.17	0.44
1:E:815:ILE:CG2	1:E:819:LYS:HE3	2.47	0.44
1:C:683:LEU:HG	1:C:690:LEU:CD1	2.47	0.44
1:E:635:ILE:HD12	1:E:639:GLN:HB3	1.98	0.44
1:E:687:ILE:HG22	1:E:719:LEU:HD21	2.00	0.44
1:C:752:ASP:O	1:C:756:GLU:HG3	2.18	0.44
1:A:679:ILE:O	1:A:683:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:ALA:O	1:C:765:VAL:HG23	2.18	0.43
1:C:815:ILE:CG2	1:C:819:LYS:HE3	2.48	0.43
1:C:815:ILE:O	1:C:819:LYS:HG3	2.17	0.43
1:A:797:ILE:HD13	1:A:817:MET:SD	2.58	0.43
1:C:693:HIS:HE1	1:C:695:TYR:CD1	2.37	0.43
1:E:692:THR:HG22	1:E:729:ASP:OD1	2.18	0.43
1:A:693:HIS:HE1	1:A:695:TYR:CD1	2.36	0.43
1:C:798:LEU:HA	1:C:799:PRO:HD2	1.81	0.43
1:A:790:LYS:O	1:A:794:ILE:HG13	2.18	0.43
1:E:790:LYS:O	1:E:794:ILE:HG13	2.18	0.43
1:E:815:ILE:O	1:E:819:LYS:HG3	2.19	0.42
1:A:683:LEU:HG	1:A:690:LEU:CD1	2.49	0.42
1:C:515:SER:HA	1:C:516:PRO:HD3	1.84	0.42
1:C:679:ILE:O	1:C:683:LEU:HD13	2.19	0.42
1:A:831:VAL:O	1:A:839:LYS:HE3	2.20	0.42
1:C:782:ILE:O	1:C:790:LYS:HE2	2.20	0.42
1:E:687:ILE:HD13	1:E:715:ILE:HA	2.01	0.42
1:E:798:LEU:HA	1:E:798:LEU:HD23	1.77	0.42
1:C:687:ILE:HG22	1:C:719:LEU:HD21	2.01	0.42
1:E:595:PHE:O	1:E:599:GLY:HA3	2.20	0.42
1:E:782:ILE:O	1:E:790:LYS:HE2	2.18	0.42
1:C:635:ILE:HD12	1:C:639:GLN:HB3	2.01	0.42
1:C:831:VAL:O	1:C:839:LYS:HE3	2.19	0.42
1:C:847:ARG:CG	1:C:874:VAL:HG11	2.49	0.42
1:C:683:LEU:HG	1:C:690:LEU:HD11	2.02	0.42
1:E:680:LEU:HD12	1:E:680:LEU:HA	1.88	0.42
1:C:735:VAL:O	1:C:739:VAL:HG23	2.20	0.41
1:E:730:GLN:HB3	1:E:773:PHE:CZ	2.55	0.41
1:E:798:LEU:HA	1:E:799:PRO:HD2	1.81	0.41
1:E:683:LEU:HG	1:E:690:LEU:CD1	2.50	0.41
1:A:723:ILE:O	1:A:727:ILE:HG13	2.21	0.41
1:C:710:GLU:H	1:C:710:GLU:CD	2.23	0.41
1:E:754:LYS:O	1:E:758:ILE:HG12	2.20	0.41
1:E:723:ILE:O	1:E:727:ILE:HG13	2.21	0.41
1:A:515:SER:HA	1:A:516:PRO:HD3	1.84	0.41
1:A:756:GLU:HG3	1:A:756:GLU:H	1.76	0.41
1:C:723:ILE:O	1:C:727:ILE:HG13	2.21	0.41
1:E:544:LEU:HD12	1:E:582:LEU:HD11	2.03	0.41
1:E:683:LEU:HG	1:E:690:LEU:HD11	2.03	0.41
1:E:797:ILE:HD13	1:E:817:MET:SD	2.61	0.41
1:A:687:ILE:HD13	1:A:715:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:797:ILE:HD13	1:C:817:MET:SD	2.61	0.41
1:C:834:SER:HB3	1:C:839:LYS:CB	2.51	0.41
1:E:679:ILE:O	1:E:683:LEU:HD13	2.21	0.41
1:C:798:LEU:HD21	1:C:842:ILE:HG13	2.03	0.40
1:E:710:GLU:H	1:E:710:GLU:CD	2.25	0.40
1:A:580:ILE:HD13	1:A:580:ILE:HA	1.88	0.40
1:A:683:LEU:HG	1:A:690:LEU:HD11	2.02	0.40
1:E:831:VAL:O	1:E:839:LYS:HE3	2.21	0.40
1:A:834:SER:HB3	1:A:839:LYS:CB	2.51	0.40
1:A:680:LEU:HA	1:A:680:LEU:HD12	1.82	0.40
1:A:730:GLN:HB3	1:A:773:PHE:CZ	2.56	0.40

All (2) 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)
4:C:103:HOH:O	4:E:410:HOH:O[2_555]	2.13	0.07
1:A:649:ASP:OD2	1:C:642:GLU:OE1[4_444]	2.14	0.06

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	347/369 (94%)	335 (96%)	12 (4%)	0	100	100
1	C	347/369 (94%)	335 (96%)	12 (4%)	0	100	100
1	E	347/369 (94%)	335 (96%)	11 (3%)	1 (0%)	41	61
All	All	1041/1107 (94%)	1005 (96%)	35 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	746	THR

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	324/339 (96%)	322 (99%)	2 (1%)	86	95
1	C	324/339 (96%)	322 (99%)	2 (1%)	86	95
1	E	324/339 (96%)	323 (100%)	1 (0%)	92	97
All	All	972/1017 (96%)	967 (100%)	5 (0%)	88	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	645	LEU
1	A	787	LYS
1	C	645	LEU
1	C	787	LYS
1	E	645	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	HIS
1	A	621	GLN
1	A	863	HIS
1	C	542	HIS
1	C	550	GLN
1	C	621	GLN
1	E	550	GLN
1	E	621	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	9/10 (90%)	0	0
2	D	9/10 (90%)	0	0
2	F	9/10 (90%)	0	0
All	All	27/30 (90%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

3 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	$\# Z > 2$
3	CIT	A	1	-	12,12,12	0.99	0	17,17,17	1.49	3 (17%)
3	CIT	E	3	-	12,12,12	1.04	0	17,17,17	1.45	2 (11%)
3	CIT	C	2	-	12,12,12	1.02	0	17,17,17	1.40	1 (5%)

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
3	CIT	A	1	-	-	7/16/16/16	-
3	CIT	E	3	-	-	8/16/16/16	-
3	CIT	C	2	-	-	9/16/16/16	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	CIT	O6-C6-C3	3.89	119.81	113.05
3	C	2	CIT	O6-C6-C3	3.82	119.68	113.05
3	E	3	CIT	O6-C6-C3	3.73	119.53	113.05
3	A	1	CIT	O2-C1-O1	-2.12	118.01	123.30
3	A	1	CIT	O2-C1-C2	2.10	121.11	114.35
3	E	3	CIT	C3-C2-C1	-2.08	108.77	113.81

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	CIT	C2-C3-C4-C5
3	A	1	CIT	O7-C3-C4-C5
3	A	1	CIT	C6-C3-C4-C5
3	A	1	CIT	C2-C3-C6-O5
3	A	1	CIT	C2-C3-C6-O6
3	A	1	CIT	O7-C3-C6-O5
3	A	1	CIT	O7-C3-C6-O6
3	C	2	CIT	O7-C3-C6-O5
3	C	2	CIT	O7-C3-C6-O6
3	C	2	CIT	C4-C3-C6-O5
3	C	2	CIT	C4-C3-C6-O6
3	E	3	CIT	C2-C3-C6-O5
3	E	3	CIT	C2-C3-C6-O6
3	E	3	CIT	O7-C3-C6-O5
3	E	3	CIT	O7-C3-C6-O6
3	E	3	CIT	C1-C2-C3-O7
3	E	3	CIT	C1-C2-C3-C6
3	C	2	CIT	O7-C3-C4-C5
3	E	3	CIT	C1-C2-C3-C4
3	C	2	CIT	C2-C3-C6-O5
3	C	2	CIT	C2-C3-C6-O6
3	C	2	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	C	2	CIT	C6-C3-C4-C5
3	E	3	CIT	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	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

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, 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	353/369 (95%)	0.54	31 (8%) 10 10	28, 54, 112, 127	0
1	C	353/369 (95%)	0.68	42 (11%) 4 4	28, 55, 113, 137	0
1	E	353/369 (95%)	0.58	33 (9%) 8 8	29, 54, 113, 132	0
2	B	10/10 (100%)	-0.42	0 100 100	43, 57, 96, 106	0
2	D	10/10 (100%)	-0.47	0 100 100	45, 57, 96, 105	0
2	F	10/10 (100%)	-0.55	0 100 100	43, 56, 96, 105	0
All	All	1089/1137 (95%)	0.57	106 (9%) 7 7	28, 54, 113, 137	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	860	GLY	15.0
1	E	861	ASN	9.7
1	E	525	SER	9.5
1	C	853	LEU	8.8
1	C	861	ASN	8.4
1	C	855	LYS	8.1
1	A	860	GLY	7.9
1	C	525	SER	7.6
1	C	533	ASN	7.1
1	A	861	ASN	6.5
1	C	524	SER	6.2
1	C	874	VAL	6.1
1	C	532	SER	5.8
1	A	525	SER	5.8
1	E	523	ASN	5.5
1	A	744	GLN	5.5
1	E	806	LEU	5.4
1	A	524	SER	5.1
1	E	862	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	522	ARG	4.8
1	C	791	ASP	4.7
1	E	524	SER	4.5
1	E	853	LEU	4.5
1	E	802	LYS	4.2
1	A	743	ASP	4.1
1	A	533	ASN	4.1
1	C	865	ALA	4.1
1	E	863	HIS	4.1
1	C	801	ASP	4.0
1	A	747	ASN	4.0
1	A	850	LEU	3.9
1	C	523	ASN	3.9
1	E	874	VAL	3.9
1	A	863	HIS	3.8
1	A	837	GLU	3.8
1	A	532	SER	3.8
1	C	744	GLN	3.7
1	A	652	LEU	3.7
1	C	821	GLN	3.7
1	C	743	ASP	3.7
1	C	522	ARG	3.6
1	C	863	HIS	3.6
1	E	745	PHE	3.5
1	C	854	ASN	3.5
1	E	868	GLU	3.5
1	E	787	LYS	3.5
1	E	870	LEU	3.5
1	E	744	GLN	3.5
1	E	841	LEU	3.4
1	C	860	GLY	3.3
1	C	800	ARG	3.3
1	C	747	ASN	3.3
1	C	857	ASN	3.2
1	E	808	LEU	3.2
1	A	749	GLU	3.2
1	C	868	GLU	3.1
1	A	522	ARG	3.1
1	C	811	ASP	3.1
1	A	862	ARG	3.1
1	A	523	ASN	3.1
1	E	867	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	743	ASP	3.0
1	E	857	ASN	3.0
1	E	533	ASN	2.9
1	E	855	LYS	2.9
1	E	532	SER	2.9
1	C	862	ARG	2.9
1	C	806	LEU	2.9
1	C	749	GLU	2.8
1	C	667	ALA	2.8
1	A	822	PHE	2.7
1	C	693	HIS	2.7
1	C	852	LYS	2.7
1	A	799	PRO	2.7
1	C	518	LEU	2.7
1	E	652	LEU	2.6
1	A	552	GLY	2.6
1	A	800	ARG	2.6
1	A	868	GLU	2.6
1	A	841	LEU	2.6
1	C	551	HIS	2.5
1	C	767	GLU	2.5
1	E	875	GLU	2.5
1	C	745	PHE	2.4
1	A	864	LEU	2.4
1	C	772	LYS	2.4
1	C	870	LEU	2.4
1	A	772	LYS	2.3
1	E	665	GLN	2.3
1	E	836	GLY	2.3
1	A	865	ALA	2.2
1	E	830	LEU	2.2
1	C	844	ILE	2.2
1	E	749	GLU	2.2
1	A	806	LEU	2.2
1	C	561	ALA	2.2
1	C	751	VAL	2.2
1	E	873	LEU	2.1
1	C	875	GLU	2.1
1	A	844	ILE	2.1
1	A	774	ALA	2.1
1	A	693	HIS	2.1
1	E	847	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	843	VAL	2.0
1	C	851	ASP	2.0
1	A	666	LYS	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
3	CIT	A	1	13/13	0.48	0.36	95,118,128,132	0
3	CIT	C	2	13/13	0.67	0.28	86,100,108,110	0
3	CIT	E	3	13/13	0.85	0.18	70,87,95,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.