



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1ZC2
Title : Crystal Structure of plasmid-encoded class C beta-lactamase CMY-2 complexed with citrate molecule
Authors : Bauvois, C.; Jacquamet, L.; Fieulaine, S.; Frere, J.-M.; Galleni, M.; Ferrer, J.-L.
Deposited on : 2005-04-10
Resolution : 2.09 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

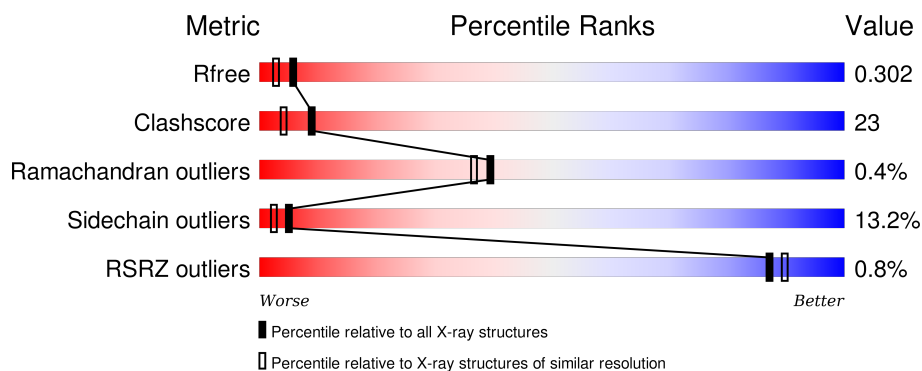
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	361	<div> <div></div> <div>59% 27% 11% ..</div> </div>
1	B	361	<div> <div></div> <div>53% 36% 7% ..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	501	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6033 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 beta-lactamase class C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2798	1797	483	509	9			
1	B	356	Total	C	N	O	S	0	0	0
			2764	1777	475	503	9			

- 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	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	219	Total 219	O 219	0	0
3	B	226	Total 226	O 226	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.71Å 97.10Å 103.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.85 – 2.09 43.94 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.85-2.09) 98.6 (43.94-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.299 0.227 , 0.302	Depositor DCC
R_{free} test set	2170 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	2 of 43385 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6033	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7593e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.67	38/2875 (1.3%)	1.43	29/3918 (0.7%)
1	B	1.65	30/2841 (1.1%)	1.40	26/3876 (0.7%)
All	All	1.66	68/5716 (1.2%)	1.42	55/7794 (0.7%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	VAL	CA-CB	11.27	1.78	1.54
1	B	224	LYS	CE-NZ	11.01	1.76	1.49
1	A	50	ASN	CB-CG	8.80	1.71	1.51
1	B	69	PHE	CD2-CE2	8.23	1.55	1.39
1	B	171	GLU	CD-OE1	8.03	1.34	1.25
1	B	313	VAL	CB-CG1	7.80	1.69	1.52
1	B	308	VAL	CB-CG1	-7.72	1.36	1.52
1	B	170	TYR	CD2-CE2	7.71	1.50	1.39
1	A	326	VAL	CB-CG2	7.68	1.69	1.52
1	B	79	ALA	CA-CB	-7.41	1.36	1.52
1	A	243	VAL	CB-CG1	6.97	1.67	1.52
1	A	37	LYS	CD-CE	6.97	1.68	1.51
1	B	266	TYR	CG-CD2	6.97	1.48	1.39
1	A	344	TYR	CE1-CZ	6.92	1.47	1.38
1	A	158	PHE	CG-CD1	6.57	1.48	1.38
1	A	266	TYR	CE2-CZ	6.53	1.47	1.38
1	A	45	LYS	CE-NZ	6.50	1.65	1.49
1	B	54	VAL	CB-CG2	6.48	1.66	1.52
1	A	321	GLY	C-O	6.47	1.34	1.23
1	A	82	GLU	CD-OE1	6.36	1.32	1.25
1	A	29	ALA	CA-CB	-6.35	1.39	1.52
1	B	325	TYR	CE2-CZ	-6.34	1.30	1.38
1	A	199	TYR	CD2-CE2	6.19	1.48	1.39
1	A	68	THR	CA-CB	6.16	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	TRP	CE3-CZ3	-6.15	1.27	1.38
1	B	250	GLN	CB-CG	6.09	1.69	1.52
1	A	172	GLU	C-O	6.04	1.34	1.23
1	B	255	ALA	CA-CB	5.96	1.65	1.52
1	B	81	GLY	C-O	-5.93	1.14	1.23
1	A	67	LYS	CE-NZ	5.86	1.63	1.49
1	A	22	GLU	CB-CG	-5.81	1.41	1.52
1	B	284	ILE	CA-CB	-5.80	1.41	1.54
1	A	224	LYS	N-CA	-5.78	1.34	1.46
1	B	150	TYR	CD2-CE2	5.78	1.48	1.39
1	A	267	GLN	CG-CD	5.75	1.64	1.51
1	A	326	VAL	CB-CG1	-5.74	1.40	1.52
1	B	313	VAL	CB-CG2	5.71	1.64	1.52
1	B	43	TRP	CZ3-CH2	5.71	1.49	1.40
1	A	300	GLU	CD-OE1	5.70	1.31	1.25
1	B	170	TYR	CD1-CE1	5.64	1.47	1.39
1	A	79	ALA	CA-CB	5.61	1.64	1.52
1	B	112	TYR	CD2-CE2	-5.58	1.30	1.39
1	B	46	ALA	C-O	5.58	1.33	1.23
1	B	162	ALA	N-CA	-5.58	1.35	1.46
1	A	5	GLU	CD-OE1	5.54	1.31	1.25
1	A	4	THR	N-CA	5.44	1.57	1.46
1	B	14	ARG	CA-CB	5.43	1.66	1.53
1	A	300	GLU	CB-CG	5.43	1.62	1.52
1	B	30	VAL	C-O	5.41	1.33	1.23
1	B	233	TRP	CE3-CZ3	-5.40	1.29	1.38
1	B	331	GLU	CD-OE1	5.39	1.31	1.25
1	A	158	PHE	CE2-CZ	5.38	1.47	1.37
1	A	31	ALA	CA-CB	-5.30	1.41	1.52
1	A	344	TYR	C-O	5.23	1.33	1.23
1	A	158	PHE	CE1-CZ	5.21	1.47	1.37
1	A	294	ALA	CA-CB	5.21	1.63	1.52
1	A	250	GLN	CB-CG	5.16	1.66	1.52
1	B	171	GLU	CG-CD	5.16	1.59	1.51
1	B	268	GLY	N-CA	5.16	1.53	1.46
1	A	324	SER	CB-OG	5.16	1.49	1.42
1	A	41	PHE	CE2-CZ	5.14	1.47	1.37
1	A	104	ILE	CB-CG2	-5.14	1.36	1.52
1	B	111	THR	N-CA	5.12	1.56	1.46
1	A	112	TYR	CD1-CE1	-5.11	1.31	1.39
1	B	257	SER	CB-OG	5.10	1.48	1.42
1	A	266	TYR	CG-CD2	5.10	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLY	N-CA	5.07	1.53	1.46
1	B	259	TYR	CD2-CE2	-5.07	1.31	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH1	17.41	129.01	120.30
1	A	148	ARG	NE-CZ-NH2	16.96	128.78	120.30
1	A	148	ARG	NE-CZ-NH1	-14.63	112.99	120.30
1	B	349	ARG	NE-CZ-NH1	11.57	126.08	120.30
1	B	217	ASP	CB-CG-OD2	10.29	127.56	118.30
1	A	62	LEU	CB-CG-CD1	9.92	127.86	111.00
1	B	232	ARG	NE-CZ-NH1	-9.53	115.53	120.30
1	B	349	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	A	177	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	B	176	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	B	288	ASP	CB-CG-OD2	8.80	126.22	118.30
1	B	177	ARG	NE-CZ-NH1	-8.69	115.95	120.30
1	A	178	VAL	CG1-CB-CG2	-8.62	97.11	110.90
1	A	148	ARG	CD-NE-CZ	8.44	135.41	123.60
1	B	161	LEU	CB-CG-CD1	-7.82	97.71	111.00
1	B	177	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	B	148	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	B	261	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	47	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	274	LEU	CA-CB-CG	7.29	132.07	115.30
1	B	258	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	A	97	THR	C-N-CA	-6.71	108.22	122.30
1	A	349	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	217	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	127	ASP	CB-CG-OD2	6.63	124.26	118.30
1	B	54	VAL	CB-CA-C	-6.48	99.09	111.40
1	A	148	ARG	CG-CD-NE	-6.48	98.20	111.80
1	A	258	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	273	MET	CB-CG-SD	6.44	131.73	112.40
1	A	62	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	B	62	LEU	CB-CG-CD1	6.33	121.77	111.00
1	A	184	LEU	CB-CG-CD1	6.30	121.71	111.00
1	A	248	LEU	CB-CG-CD1	6.30	121.71	111.00
1	B	161	LEU	CB-CG-CD2	6.05	121.29	111.00
1	B	227	VAL	CB-CA-C	-6.04	99.92	111.40
1	A	176	ARG	NE-CZ-NH1	5.88	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	LEU	CB-CG-CD1	5.80	120.86	111.00
1	A	119	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	37	LYS	CD-CE-NZ	5.55	124.46	111.70
1	B	76	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	47	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	177	ARG	CD-NE-CZ	5.49	131.29	123.60
1	B	127	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	157	LEU	CB-CG-CD1	5.33	120.07	111.00
1	A	131	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	148	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	107	LEU	CB-CG-CD2	-5.30	101.98	111.00
1	B	258	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	232	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	67	LYS	CD-CE-NZ	-5.23	99.66	111.70
1	A	184	LEU	CB-CG-CD2	5.22	119.88	111.00
1	B	332	LYS	CD-CE-NZ	5.22	123.71	111.70
1	A	349	ARG	CG-CD-NE	5.18	122.67	111.80
1	B	355	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	16	ILE	CG1-CB-CG2	-5.04	100.32	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2798	0	2782	107	0
1	B	2764	0	2730	153	0
2	A	13	0	5	3	0
2	B	13	0	5	2	0
3	A	219	0	0	39	0
3	B	226	0	0	66	0
All	All	6033	0	5522	259	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 23.

All (259) 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:65:VAL:CA	1:A:65:VAL:CB	1.78	1.58
1:B:224:LYS:NZ	1:B:224:LYS:CE	1.76	1.48
1:B:351:GLU:HG2	1:B:355:ARG:NH1	1.52	1.24
1:B:194:ASN:HB3	3:B:679:HOH:O	1.40	1.18
1:B:121:ILE:HD11	1:B:125:VAL:HG22	1.26	1.18
1:B:54:VAL:HB	3:B:693:HOH:O	1.44	1.17
1:A:326:VAL:HG22	3:A:683:HOH:O	1.48	1.09
1:B:351:GLU:CG	1:B:355:ARG:HH12	1.65	1.06
1:A:337:VAL:HG22	3:A:683:HOH:O	1.58	1.04
1:B:33:ILE:HB	3:B:697:HOH:O	1.55	1.04
1:B:351:GLU:HG2	1:B:355:ARG:HH12	0.90	1.02
1:A:358:GLU:HA	3:A:706:HOH:O	1.62	0.99
1:A:358:GLU:HB2	3:A:706:HOH:O	1.63	0.97
1:A:45:LYS:HD2	3:A:712:HOH:O	1.66	0.93
1:B:54:VAL:HG23	1:B:54:VAL:O	1.70	0.92
1:B:121:ILE:HD11	1:B:125:VAL:CG2	2.00	0.91
1:B:248:LEU:HD23	3:B:639:HOH:O	1.69	0.91
1:B:55:THR:HG23	1:B:57:GLN:H	1.35	0.91
1:B:83:ILE:HD11	3:B:724:HOH:O	1.71	0.89
1:A:104:ILE:HG21	3:A:692:HOH:O	1.74	0.87
1:B:48:ILE:HG23	3:B:690:HOH:O	1.75	0.85
1:A:104:ILE:CG2	3:A:692:HOH:O	2.23	0.85
1:A:283:ILE:HG21	3:A:709:HOH:O	1.76	0.85
1:B:99:LYS:HD3	3:B:660:HOH:O	1.77	0.84
1:A:65:VAL:CB	1:A:65:VAL:HA	2.02	0.84
1:A:227:VAL:HG22	3:A:607:HOH:O	1.76	0.84
1:A:25:ILE:HG23	3:A:509:HOH:O	1.76	0.84
1:A:283:ILE:CG2	3:A:709:HOH:O	2.25	0.84
1:A:274:LEU:HD13	3:A:709:HOH:O	1.77	0.84
1:A:61:GLU:CD	1:A:211:VAL:HG23	2.01	0.81
1:A:82:GLU:OE2	1:A:177:ARG:NH2	2.14	0.81
1:A:264:ASP:HB3	3:A:710:HOH:O	1.80	0.80
1:B:346:ASN:HA	1:B:349:ARG:HG3	1.64	0.79
1:B:197:LYS:HG2	3:B:656:HOH:O	1.82	0.78
1:A:358:GLU:CA	3:A:706:HOH:O	2.26	0.78
1:A:310:ALA:HB2	1:A:331:GLU:OE1	1.85	0.77
1:A:106:LEU:HB2	3:A:524:HOH:O	1.83	0.77
1:B:117:LEU:HB3	3:B:585:HOH:O	1.84	0.77
1:A:312:TRP:CD1	3:A:709:HOH:O	2.37	0.77
1:A:255:ALA:HB3	3:A:502:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LYS:HE2	3:A:663:HOH:O	1.86	0.76
1:B:8:ILE:O	1:B:11:ILE:HG13	1.86	0.74
1:B:78:ILE:HD13	3:B:680:HOH:O	1.85	0.74
1:A:52:HIS:HE1	3:A:689:HOH:O	1.71	0.73
1:B:33:ILE:CG2	3:B:697:HOH:O	2.36	0.73
1:B:33:ILE:HG23	1:B:335:GLY:N	2.04	0.72
1:B:44:GLY:O	1:B:54:VAL:HG22	1.89	0.72
1:A:82:GLU:CD	1:A:177:ARG:HH22	1.92	0.72
1:B:331:GLU:N	3:B:712:HOH:O	2.22	0.72
1:B:54:VAL:CB	3:B:693:HOH:O	2.17	0.72
1:B:30:VAL:HG13	1:B:43:TRP:HZ3	1.53	0.71
1:A:56:GLN:HE21	1:A:228:ILE:HD11	1.54	0.71
1:B:25:ILE:HG21	1:B:340:ALA:HB1	1.74	0.69
1:B:329:VAL:HG12	3:B:712:HOH:O	1.92	0.69
1:B:64:SER:O	1:B:67:LYS:HB2	1.93	0.69
1:B:45:LYS:NZ	3:B:555:HOH:O	2.26	0.68
1:A:48:ILE:HG23	3:A:712:HOH:O	1.93	0.68
1:B:78:ILE:CD1	3:B:680:HOH:O	2.39	0.68
1:B:54:VAL:CG2	1:B:54:VAL:O	2.42	0.67
1:A:342:LYS:N	3:A:509:HOH:O	2.28	0.67
1:B:250:GLN:HG2	3:B:650:HOH:O	1.94	0.67
1:A:65:VAL:CG1	1:A:65:VAL:CA	2.72	0.66
1:B:250:GLN:HA	1:B:250:GLN:HE21	1.59	0.66
1:B:227:VAL:HG22	3:B:532:HOH:O	1.95	0.66
1:B:6:GLN:HA	3:B:675:HOH:O	1.96	0.66
1:B:7:GLN:NE2	3:B:717:HOH:O	2.28	0.66
1:B:45:LYS:HD3	1:B:48:ILE:HD13	1.78	0.65
1:B:34:TYR:CE1	3:B:704:HOH:O	2.49	0.65
1:A:232:ARG:NH1	3:A:576:HOH:O	2.27	0.65
1:B:326:VAL:HG22	1:B:337:VAL:HG22	1.79	0.64
1:B:358:GLU:HA	1:B:358:GLU:OE1	1.96	0.64
1:B:96:LEU:HD12	1:B:136:GLN:NE2	2.13	0.64
1:B:83:ILE:CD1	3:B:724:HOH:O	2.38	0.63
1:B:233:TRP:HA	3:B:681:HOH:O	1.96	0.63
1:B:243:VAL:CG1	3:B:639:HOH:O	2.46	0.63
1:A:45:LYS:NZ	3:A:508:HOH:O	2.31	0.63
1:B:287:SER:CB	3:B:727:HOH:O	2.48	0.62
1:B:6:GLN:CA	3:B:675:HOH:O	2.46	0.62
1:B:243:VAL:HG13	3:B:639:HOH:O	1.99	0.62
1:A:276:TRP:HZ2	1:A:361:GLN:HG3	1.64	0.62
1:B:33:ILE:HG23	1:B:335:GLY:CA	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD11	1:A:163:VAL:HG12	1.81	0.61
1:B:233:TRP:CA	3:B:681:HOH:O	2.48	0.61
1:B:11:ILE:HD12	1:B:356:ILE:HG23	1.82	0.60
1:B:310:ALA:HB2	1:B:331:GLU:OE2	2.00	0.60
1:B:150:TYR:CE1	2:B:502:CIT:H42	2.35	0.60
1:B:33:ILE:CB	3:B:697:HOH:O	2.24	0.60
1:B:264:ASP:HB3	1:B:274:LEU:HD23	1.84	0.60
1:A:73:LEU:HD11	1:A:163:VAL:CG1	2.32	0.60
1:B:82:GLU:OE2	1:B:177:ARG:NH2	2.35	0.59
1:A:267:GLN:HB2	3:A:673:HOH:O	2.03	0.59
1:B:332:LYS:HE2	1:B:334:LEU:HD22	1.84	0.59
1:B:319:THR:OG1	1:B:322:PHE:HB2	2.02	0.58
1:A:276:TRP:CZ2	1:A:361:GLN:HG3	2.39	0.58
1:A:4:THR:HG23	1:A:7:GLN:OE1	2.03	0.58
1:A:150:TYR:CE1	2:A:501:CIT:H42	2.38	0.58
1:B:155:ILE:HD11	3:B:653:HOH:O	2.03	0.58
1:A:358:GLU:CB	3:A:706:HOH:O	2.27	0.58
1:B:331:GLU:CB	3:B:712:HOH:O	2.51	0.58
1:B:64:SER:OG	1:B:150:TYR:OH	2.18	0.57
1:B:136:GLN:HA	1:B:136:GLN:HE21	1.70	0.57
1:A:345:PRO:HD3	1:B:285:ASN:ND2	2.19	0.57
1:A:329:VAL:CG1	1:A:332:LYS:HB2	2.34	0.57
1:B:110:ALA:O	1:B:155:ILE:HD12	2.04	0.57
1:A:61:GLU:OE2	1:A:211:VAL:HG23	2.05	0.56
1:A:75:GLY:HA2	1:A:78:ILE:HD12	1.85	0.56
1:B:45:LYS:CD	3:B:690:HOH:O	2.54	0.56
1:A:324:SER:HA	1:A:338:MET:O	2.06	0.56
1:A:104:ILE:CB	3:A:692:HOH:O	2.52	0.55
1:B:170:TYR:HB3	3:B:685:HOH:O	2.06	0.55
1:B:355:ARG:HD2	3:B:678:HOH:O	2.07	0.55
1:B:136:GLN:HA	1:B:136:GLN:NE2	2.22	0.55
1:B:358:GLU:HG2	3:B:692:HOH:O	2.05	0.55
1:B:159:GLY:O	1:B:160:ALA:C	2.45	0.55
1:A:342:LYS:HB3	3:A:509:HOH:O	2.05	0.55
1:B:184:LEU:HD21	3:B:681:HOH:O	2.06	0.55
1:A:171:GLU:O	1:A:175:THR:CG2	2.54	0.55
1:B:329:VAL:CG1	3:B:712:HOH:O	2.53	0.54
1:A:283:ILE:HG22	3:A:709:HOH:O	2.01	0.54
3:A:531:HOH:O	1:B:290:LYS:HD2	2.07	0.54
1:B:204:ARG:NH2	1:B:320:GLY:HA2	2.22	0.53
1:A:273:MET:HG3	1:A:313:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:CB	3:B:713:HOH:O	2.56	0.53
1:B:96:LEU:HD12	1:B:136:GLN:HE21	1.72	0.53
1:A:290:LYS:HE2	3:B:537:HOH:O	2.08	0.53
1:A:197:LYS:HE3	3:A:688:HOH:O	2.08	0.53
1:B:55:THR:HG23	1:B:57:GLN:N	2.17	0.52
1:B:20:MET:HG2	1:B:28:MET:HG3	1.90	0.52
1:B:30:VAL:HG13	1:B:43:TRP:CZ3	2.41	0.51
1:A:316:THR:HG23	2:A:501:CIT:H21	1.92	0.51
1:B:72:VAL:HG13	1:B:252:ILE:CD1	2.41	0.51
1:B:313:VAL:O	1:B:327:ALA:HA	2.11	0.51
1:A:82:GLU:HB3	1:A:165:PRO:HB2	1.93	0.51
1:B:17:THR:HB	1:B:18:PRO:HD3	1.91	0.50
1:B:158:PHE:HZ	3:B:724:HOH:O	1.95	0.50
1:B:45:LYS:HD3	3:B:690:HOH:O	2.12	0.50
1:A:72:VAL:HG13	1:A:252:ILE:HD13	1.92	0.50
1:A:164:LYS:HB2	1:A:165:PRO:HD3	1.92	0.50
1:B:35:GLN:NE2	3:B:704:HOH:O	2.44	0.50
1:A:84:LYS:HE3	3:A:701:HOH:O	2.12	0.50
1:B:67:LYS:NZ	1:B:152:ASN:OD1	2.26	0.50
1:B:351:GLU:CD	1:B:355:ARG:HH12	2.14	0.50
1:B:232:ARG:HD3	3:B:640:HOH:O	2.10	0.50
1:B:180:GLN:HB3	3:B:673:HOH:O	2.12	0.50
1:A:104:ILE:HB	3:A:692:HOH:O	2.11	0.49
1:B:33:ILE:HG12	1:B:238:MET:HE1	1.93	0.49
1:A:45:LYS:CD	3:A:712:HOH:O	2.43	0.49
1:B:54:VAL:CG1	3:B:693:HOH:O	2.56	0.49
1:B:33:ILE:HG23	1:B:335:GLY:H	1.74	0.49
1:A:150:TYR:OH	2:A:501:CIT:O7	2.26	0.49
1:B:287:SER:HB3	3:B:727:HOH:O	2.11	0.49
1:B:271:TRP:HH2	1:B:326:VAL:HG11	1.78	0.49
1:B:84:LYS:O	1:B:87:ASP:HB2	2.12	0.49
1:A:310:ALA:HB2	1:A:331:GLU:CD	2.32	0.49
1:A:238:MET:HG3	1:A:330:PRO:HA	1.94	0.49
1:A:64:SER:OG	1:A:150:TYR:OH	2.30	0.48
1:A:171:GLU:O	1:A:175:THR:HG22	2.12	0.48
1:B:88:PRO:O	1:B:91:LYS:HB3	2.13	0.48
1:A:64:SER:HB3	1:A:315:LYS:HZ2	1.78	0.48
1:A:178:VAL:C	1:A:181:PRO:HD2	2.33	0.48
1:B:124:ASP:HB3	3:B:694:HOH:O	2.13	0.48
1:B:352:ALA:O	1:B:356:ILE:HG13	2.13	0.48
1:B:316:THR:HG22	1:B:325:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:O	1:A:44:GLY:HA3	2.14	0.48
1:A:329:VAL:HG12	1:A:332:LYS:HB2	1.96	0.48
1:B:6:GLN:CB	3:B:563:HOH:O	2.62	0.47
1:A:30:VAL:HG13	1:A:43:TRP:HZ3	1.78	0.47
1:B:97:THR:O	1:B:136:GLN:NE2	2.34	0.47
1:A:73:LEU:CD1	1:A:163:VAL:CG1	2.92	0.47
1:A:240:ALA:HB2	1:A:252:ILE:HG21	1.97	0.47
1:A:110:ALA:HB2	1:A:158:PHE:CD2	2.49	0.47
1:A:324:SER:HB3	1:A:339:LEU:HD23	1.96	0.47
1:B:6:GLN:CB	3:B:686:HOH:O	2.63	0.47
1:A:64:SER:HB3	1:A:315:LYS:NZ	2.29	0.47
1:B:351:GLU:O	1:B:354:TRP:HB3	2.15	0.47
1:B:287:SER:HB2	3:B:727:HOH:O	2.10	0.47
1:A:73:LEU:CD1	1:A:163:VAL:HG12	2.45	0.47
1:B:316:THR:CG2	1:B:325:TYR:CD1	2.98	0.47
1:B:345:PRO:HB2	1:B:348:VAL:HG23	1.97	0.47
1:B:272:GLU:HB2	3:B:630:HOH:O	2.13	0.47
1:B:270:GLY:N	3:B:653:HOH:O	2.47	0.47
1:B:91:LYS:HG2	1:B:92:TYR:CE2	2.50	0.47
1:B:316:THR:CG2	1:B:325:TYR:HD1	2.28	0.47
1:A:109:LEU:HD13	1:A:157:LEU:HB3	1.97	0.47
1:A:8:ILE:O	1:A:11:ILE:HB	2.14	0.46
1:B:110:ALA:O	1:B:155:ILE:CD1	2.63	0.46
1:B:121:ILE:HB	3:B:705:HOH:O	2.14	0.46
1:B:78:ILE:HD11	1:B:85:LEU:HD13	1.96	0.46
1:B:255:ALA:HB3	3:B:567:HOH:O	2.13	0.46
1:B:72:VAL:HG13	1:B:252:ILE:HD13	1.97	0.46
1:B:258:ARG:NH2	1:B:308:VAL:HG13	2.30	0.46
1:A:17:THR:HB	1:A:18:PRO:HD3	1.99	0.45
1:A:87:ASP:N	3:A:524:HOH:O	2.50	0.45
1:B:184:LEU:CD2	1:B:232:ARG:HG3	2.47	0.45
1:A:203:TYR:HA	1:A:207:LYS:O	2.16	0.45
1:B:33:ILE:HD11	1:B:36:GLY:HA2	1.99	0.45
1:B:45:LYS:CD	1:B:48:ILE:HD13	2.45	0.45
1:A:211:VAL:CG2	1:A:319:THR:HG21	2.47	0.45
1:A:183:LYS:HE3	3:A:705:HOH:O	2.16	0.45
1:B:163:VAL:HG21	1:B:170:TYR:HA	1.99	0.45
1:A:148:ARG:CD	3:A:673:HOH:O	2.65	0.44
1:A:204:ARG:C	1:A:205:GLU:HG2	2.38	0.44
1:B:233:TRP:N	3:B:681:HOH:O	2.48	0.44
1:A:183:LYS:HE2	3:A:576:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:HB2	3:B:681:HOH:O	2.17	0.44
1:B:218:ALA:HB3	3:B:685:HOH:O	2.17	0.44
1:A:61:GLU:OE1	1:A:211:VAL:HG23	2.18	0.44
1:B:99:LYS:CD	3:B:660:HOH:O	2.50	0.44
1:B:302:ASN:HA	1:B:303:PRO:C	2.39	0.43
1:B:164:LYS:HB2	1:B:165:PRO:HD3	2.00	0.43
1:A:5:GLU:HB2	3:A:685:HOH:O	2.18	0.43
1:B:25:ILE:HD11	1:B:344:TYR:CD1	2.53	0.43
1:B:150:TYR:CZ	2:B:502:CIT:H42	2.54	0.43
1:A:171:GLU:O	1:A:175:THR:HG23	2.17	0.43
1:B:260:TRP:O	1:B:266:TYR:HA	2.18	0.43
1:A:7:GLN:O	1:A:11:ILE:HG12	2.19	0.43
1:B:33:ILE:HD11	1:B:36:GLY:CA	2.49	0.43
1:A:92:TYR:CE1	1:A:106:LEU:HD11	2.54	0.43
1:B:65:VAL:C	1:B:67:LYS:N	2.71	0.42
1:B:58:THR:HA	1:B:198:ASP:O	2.19	0.42
1:A:85:LEU:HB3	1:A:107:LEU:HB2	2.01	0.42
1:B:351:GLU:CG	1:B:355:ARG:NH1	2.41	0.42
1:A:243:VAL:CG1	1:A:248:LEU:HD13	2.48	0.42
1:B:43:TRP:O	1:B:54:VAL:HG11	2.19	0.42
1:B:56:GLN:HE21	1:B:228:ILE:HD11	1.84	0.42
1:A:334:LEU:HG	1:A:357:LEU:HD22	2.00	0.42
1:B:122:PRO:HB2	1:B:125:VAL:CG1	2.50	0.42
1:B:102:GLN:CD	3:B:683:HOH:O	2.58	0.42
1:B:72:VAL:CG1	1:B:252:ILE:CD1	2.97	0.42
1:B:316:THR:HG22	1:B:325:TYR:HD1	1.83	0.42
1:A:176:ARG:CG	1:A:176:ARG:HH11	2.32	0.42
1:B:246:LYS:NZ	3:B:682:HOH:O	2.48	0.42
1:B:342:LYS:NZ	3:B:536:HOH:O	2.52	0.42
1:B:112:TYR:HB3	1:B:149:LEU:O	2.20	0.42
1:A:104:ILE:CD1	1:A:114:ALA:HB1	2.50	0.42
1:A:148:ARG:HD3	1:A:262:ILE:HG13	2.01	0.42
1:A:189:ILE:O	1:A:224:LYS:NZ	2.53	0.42
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.86	0.41
1:B:306:PRO:HB3	3:B:726:HOH:O	2.19	0.41
1:B:331:GLU:CA	3:B:712:HOH:O	2.65	0.41
1:A:72:VAL:HG13	1:A:252:ILE:CD1	2.50	0.41
1:B:69:PHE:HB3	1:B:174:MET:HE3	2.03	0.41
1:B:250:GLN:NE2	3:B:597:HOH:O	2.54	0.41
1:A:157:LEU:O	1:A:158:PHE:C	2.58	0.41
1:A:65:VAL:CA	1:A:65:VAL:CG2	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LYS:HA	1:B:315:LYS:HD2	1.60	0.41
1:B:283:ILE:HD13	1:B:283:ILE:HG21	1.78	0.41
1:A:96:LEU:CD2	1:A:136:GLN:HE21	2.34	0.41
1:B:269:LEU:C	3:B:653:HOH:O	2.58	0.41
1:A:29:ALA:HA	1:A:41:PHE:O	2.21	0.41
1:B:258:ARG:CZ	1:B:308:VAL:CG1	2.98	0.41
1:B:332:LYS:HB3	1:B:332:LYS:HE3	1.79	0.40
1:A:120:GLN:HE21	1:A:120:GLN:HB2	1.09	0.40
1:A:329:VAL:HG11	1:A:332:LYS:HB2	2.02	0.40
1:B:23:GLN:O	1:B:342:LYS:HE2	2.21	0.40
1:B:99:LYS:HG2	3:B:683:HOH:O	2.22	0.40
1:A:173:ALA:O	1:A:177:ARG:HB2	2.21	0.40
1:A:314:HIS:ND1	1:A:325:TYR:OH	2.36	0.40
1:A:343:SER:CB	3:A:603:HOH:O	2.69	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	356/361 (99%)	340 (96%)	14 (4%)	2 (1%)	30	24
1	B	354/361 (98%)	330 (93%)	23 (6%)	1 (0%)	46	45
All	All	710/722 (98%)	670 (94%)	37 (5%)	3 (0%)	39	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLY
1	A	221	TYR
1	B	252	ILE

5.3.2 Protein sidechains ⓘ

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	290/291 (100%)	246 (85%)	44 (15%)	3	1
1	B	284/291 (98%)	252 (89%)	32 (11%)	7	4
All	All	574/582 (99%)	498 (87%)	76 (13%)	5	2

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	GLU
1	A	30	VAL
1	A	37	LYS
1	A	62	LEU
1	A	65	VAL
1	A	73	LEU
1	A	99	LYS
1	A	102	GLN
1	A	104	ILE
1	A	119	LEU
1	A	120	GLN
1	A	139	GLN
1	A	143	THR
1	A	148	ARG
1	A	165	PRO
1	A	175	THR
1	A	176	ARG
1	A	183	LYS
1	A	184	LEU
1	A	189	ILE
1	A	197	LYS
1	A	199	TYR
1	A	207	LYS
1	A	227	VAL
1	A	245	GLU
1	A	246	LYS

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Mol	Chain	Res	Type
1	A	248	LEU
1	A	250	GLN
1	A	252	ILE
1	A	278	LEU
1	A	289	SER
1	A	296	LEU
1	A	314	HIS
1	A	315	LYS
1	A	324	SER
1	A	330	PRO
1	A	332	LYS
1	A	333	ASN
1	A	342	LYS
1	A	344	TYR
1	A	358	GLU
1	A	360	LEU
1	A	361	GLN
1	B	11	ILE
1	B	19	LEU
1	B	30	VAL
1	B	33	ILE
1	B	45	LYS
1	B	54	VAL
1	B	55	THR
1	B	62	LEU
1	B	85	LEU
1	B	94	PRO
1	B	99	LYS
1	B	107	LEU
1	B	121	ILE
1	B	123	ASP
1	B	164	LYS
1	B	179	LEU
1	B	209	VAL
1	B	227	VAL
1	B	232	ARG
1	B	242	HIS
1	B	252	ILE
1	B	254	LEU
1	B	273	MET
1	B	278	LEU
1	B	281	ASP

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Mol	Chain	Res	Type
1	B	308	VAL
1	B	314	HIS
1	B	332	LYS
1	B	333	ASN
1	B	349	ARG
1	B	360	LEU
1	B	361	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	23	GLN
1	A	52	HIS
1	A	56	GLN
1	A	120	GLN
1	A	136	GLN
1	A	250	GLN
1	A	361	GLN
1	B	21	GLN
1	B	56	GLN
1	B	136	GLN
1	B	137	ASN
1	B	196	GLN
1	B	235	GLN
1	B	250	GLN
1	B	285	ASN
1	B	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	501	-	3,12,12	2.26	1 (33%)	3,17,17	3.35	2 (66%)
2	CIT	B	502	-	3,12,12	1.53	1 (33%)	3,17,17	2.54	2 (66%)

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	501	-	-	0/6/16/16	0/0/0/0
2	CIT	B	502	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	CIT	O7-C3	2.24	1.46	1.43
2	A	501	CIT	C4-C3	3.79	1.60	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	CIT	C3-C4-C5	-2.28	111.31	114.96
2	A	501	CIT	C3-C4-C5	2.42	118.83	114.96
2	B	502	CIT	C3-C2-C1	3.74	120.94	114.96
2	A	501	CIT	C3-C2-C1	5.27	123.39	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CIT	3	0
2	B	502	CIT	2	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	358/361 (99%)	0.01	5 (1%) 78 82	4, 17, 33, 45	0
1	B	356/361 (98%)	-0.01	1 (0%) 94 95	6, 17, 34, 46	0
All	All	714/722 (98%)	0.00	6 (0%) 87 90	4, 17, 34, 46	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ARG	3.3
1	B	39	TYR	2.5
1	A	39	TYR	2.2
1	A	4	THR	2.1
1	A	361	GLN	2.0
1	A	8	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CIT	A	501	13/13	0.85	0.17	2.11	19,27,31,33	0
2	CIT	B	502	13/13	0.84	0.16	1.55	26,31,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.