



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:52 AM UTC

PDB ID : 1ZC2 / pdb_00001zc2
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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

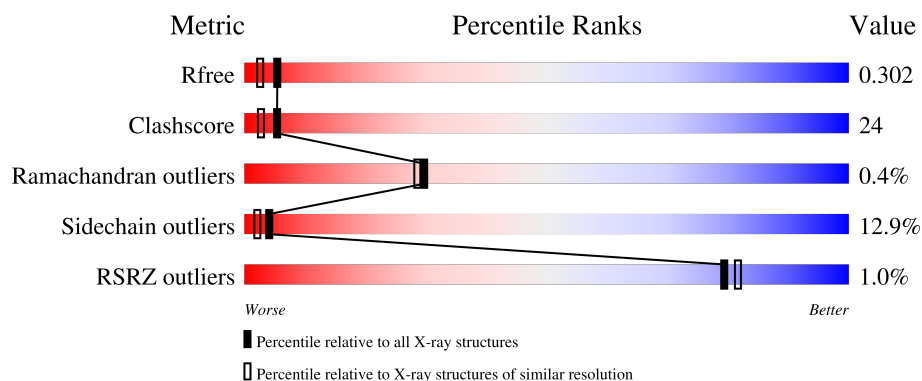
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	361	
1	B	361	

2 Entry composition [i](#)

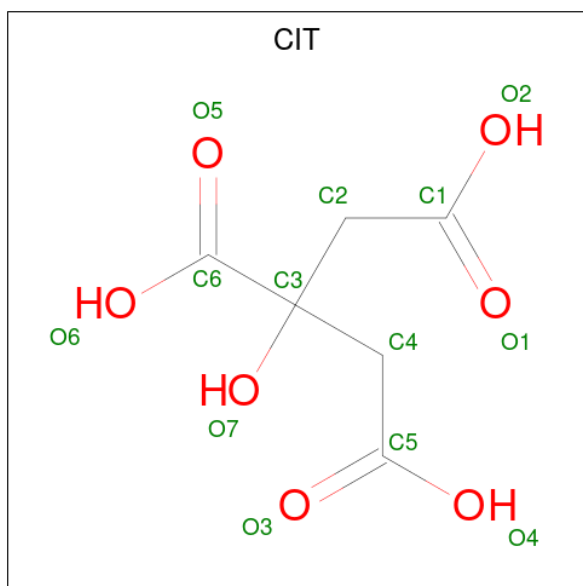
There are 3 unique types of molecules in this entry. The entry contains 6033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

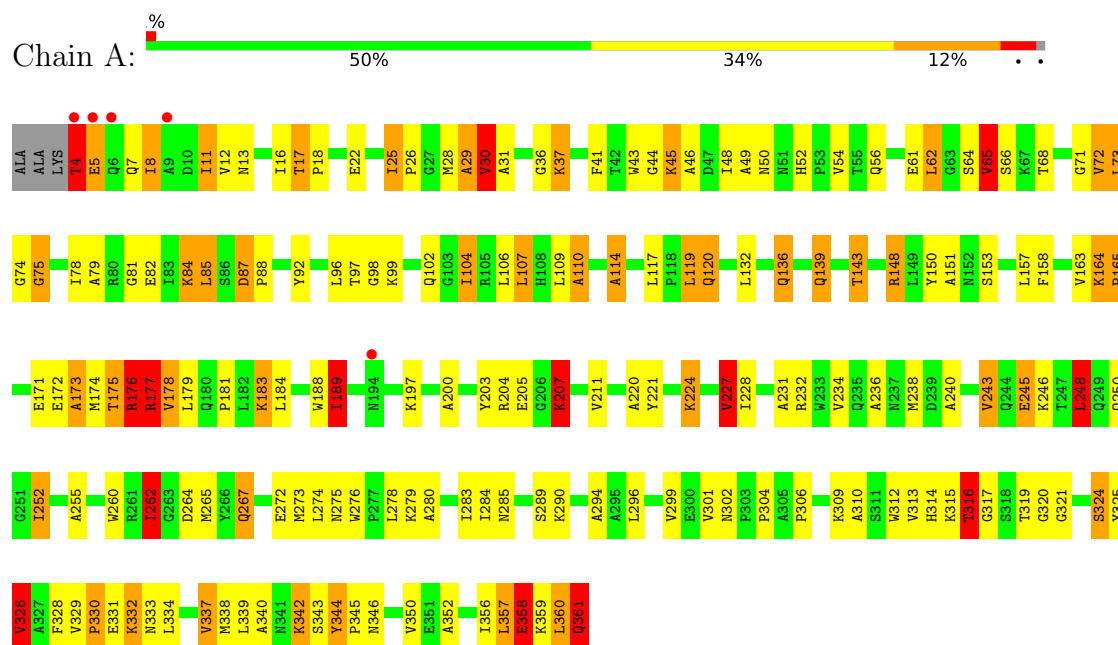
- Molecule 3 is water.

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

3 Residue-property plots

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: beta-lactamase class C



• Molecule 1: beta-lactamase class C



G320	G321	F322	Y325	V326	A327	F328	V329	P330	E331	K332	N333	L334	G335	I336	V337	A340	N341	K342	S343	Y344	P345	N346	F347	V348	R349	V350	E351	A352	A353	W354	R355	I356	L357	E358	K359	L360	Q361
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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 43.85 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.85-2.09) 98.5 (43.85-2.09)	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 (5.00%)	wwPDB-VP
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 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	2.05	71/2875 (2.5%)	1.69	49/3918 (1.3%)
1	B	2.02	66/2841 (2.3%)	1.77	67/3876 (1.7%)
All	All	2.03	137/5716 (2.4%)	1.73	116/7794 (1.5%)

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	VAL	CA-CB	16.21	1.78	1.54
1	B	284	ILE	CA-CB	-9.97	1.41	1.54
1	A	68	THR	CA-CB	9.80	1.69	1.53
1	B	79	ALA	CA-CB	-9.78	1.36	1.53
1	B	30	VAL	C-O	9.77	1.33	1.24
1	A	172	GLU	C-O	9.33	1.34	1.24
1	B	315	LYS	CA-C	9.31	1.62	1.52
1	B	224	LYS	CE-NZ	9.07	1.76	1.49
1	B	162	ALA	N-CA	-8.90	1.35	1.46
1	A	224	LYS	N-CA	-8.75	1.34	1.45
1	B	111	THR	N-CA	8.51	1.56	1.46
1	B	190	THR	CA-CB	-8.06	1.42	1.53
1	B	217	ASP	C-O	-8.04	1.14	1.24
1	A	346	ASN	C-O	-8.02	1.17	1.24
1	B	220	ALA	N-CA	7.89	1.56	1.46
1	A	29	ALA	CA-CB	-7.88	1.39	1.53
1	A	50	ASN	CB-CG	7.69	1.71	1.52
1	A	79	ALA	CA-C	7.68	1.63	1.52
1	B	89	VAL	C-O	-7.65	1.15	1.24
1	A	272	GLU	CA-C	-7.58	1.43	1.52
1	A	275	ASN	CA-C	-7.57	1.42	1.52
1	B	46	ALA	C-O	7.52	1.33	1.24
1	A	321	GLY	C-O	7.47	1.34	1.23
1	A	301	VAL	CA-C	-7.37	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ARG	N-CA	7.34	1.55	1.46
1	B	14	ARG	CA-CB	7.21	1.66	1.53
1	B	58	THR	CA-C	-7.21	1.43	1.52
1	A	178	VAL	N-CA	7.15	1.55	1.46
1	B	334	LEU	C-O	7.15	1.32	1.24
1	B	308	VAL	CA-CB	7.13	1.62	1.54
1	B	173	ALA	CA-CB	-7.11	1.42	1.53
1	B	81	GLY	C-O	-7.10	1.14	1.24
1	B	292	ALA	CA-C	7.10	1.62	1.52
1	B	255	ALA	CA-CB	7.09	1.65	1.53
1	A	344	TYR	C-O	7.07	1.33	1.24
1	B	268	GLY	N-CA	7.01	1.53	1.45
1	A	302	ASN	C-O	-7.00	1.19	1.25
1	A	119	LEU	C-O	-7.00	1.16	1.24
1	A	280	ALA	CA-C	-6.97	1.43	1.52
1	A	337	VAL	CA-CB	6.94	1.62	1.54
1	A	79	ALA	CA-CB	6.87	1.64	1.53
1	B	72	VAL	CA-CB	6.85	1.62	1.54
1	A	71	GLY	C-O	-6.73	1.15	1.23
1	A	164	LYS	C-O	-6.71	1.18	1.24
1	B	309	LYS	N-CA	6.66	1.54	1.46
1	B	25	ILE	CA-C	6.64	1.59	1.52
1	B	280	ALA	CA-C	-6.61	1.44	1.52
1	B	261	ARG	C-O	-6.60	1.16	1.24
1	A	294	ALA	CA-CB	6.57	1.63	1.53
1	A	267	GLN	C-O	6.56	1.32	1.24
1	B	85	LEU	CA-C	6.51	1.61	1.52
1	B	175	THR	C-O	6.49	1.31	1.24
1	A	110	ALA	N-CA	-6.45	1.38	1.46
1	B	191	VAL	CA-CB	-6.39	1.46	1.54
1	B	157	LEU	CA-CB	-6.35	1.43	1.53
1	B	217	ASP	CA-C	-6.33	1.44	1.52
1	A	88	PRO	C-O	6.27	1.31	1.23
1	A	75	GLY	C-O	6.24	1.31	1.23
1	B	32	VAL	CA-CB	6.23	1.61	1.54
1	B	209	VAL	C-O	6.20	1.30	1.23
1	B	16	ILE	CA-CB	6.14	1.62	1.54
1	B	326	VAL	C-O	6.14	1.31	1.24
1	A	304	PRO	CA-C	6.14	1.59	1.52
1	B	279	LYS	C-O	-6.12	1.16	1.23
1	A	177	ARG	N-CA	6.11	1.54	1.46
1	B	200	ALA	CA-CB	-6.11	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ILE	C-O	-6.08	1.16	1.24
1	A	139	GLN	CA-C	6.07	1.59	1.52
1	A	17	THR	CA-CB	6.04	1.62	1.53
1	B	132	LEU	CA-C	5.99	1.60	1.52
1	B	351	GLU	CA-C	-5.98	1.45	1.52
1	A	188	TRP	C-O	-5.90	1.16	1.23
1	A	200	ALA	CA-C	5.88	1.60	1.53
1	A	153	SER	C-O	5.87	1.31	1.24
1	A	173	ALA	CA-CB	-5.79	1.44	1.53
1	A	4	THR	N-CA	5.78	1.57	1.46
1	B	66	SER	CA-C	-5.77	1.45	1.52
1	B	356	ILE	CA-CB	5.77	1.60	1.54
1	A	132	LEU	CA-C	5.75	1.60	1.52
1	B	292	ALA	CA-CB	-5.74	1.43	1.53
1	B	189	ILE	CA-CB	-5.71	1.47	1.54
1	B	69	PHE	CD2-CE2	5.69	1.55	1.38
1	A	68	THR	N-CA	-5.66	1.38	1.46
1	B	77	ALA	C-O	5.63	1.30	1.24
1	B	224	LYS	N-CA	-5.56	1.39	1.46
1	A	81	GLY	N-CA	5.56	1.53	1.45
1	A	326	VAL	C-O	5.56	1.29	1.24
1	B	235	GLN	CA-C	-5.56	1.45	1.52
1	A	189	ILE	CA-CB	-5.54	1.47	1.54
1	A	306	PRO	C-O	5.53	1.31	1.24
1	B	333	ASN	C-O	5.52	1.31	1.23
1	B	250	GLN	CB-CG	5.51	1.69	1.52
1	A	25	ILE	C-O	5.51	1.32	1.24
1	A	107	LEU	CA-C	5.49	1.60	1.52
1	B	164	LYS	CA-C	5.49	1.59	1.52
1	A	299	VAL	CA-CB	5.46	1.60	1.54
1	A	46	ALA	CA-C	-5.45	1.45	1.52
1	B	253	ALA	CA-CB	5.42	1.62	1.53
1	A	37	LYS	CD-CE	5.41	1.68	1.52
1	B	195	GLU	CA-C	5.40	1.59	1.52
1	B	250	GLN	CA-CB	5.40	1.61	1.53
1	A	31	ALA	CA-CB	-5.39	1.41	1.53
1	A	245	GLU	C-O	-5.38	1.17	1.24
1	B	275	ASN	CA-C	-5.37	1.46	1.52
1	B	151	ALA	CA-C	-5.35	1.46	1.52
1	A	45	LYS	CE-NZ	5.32	1.65	1.49
1	B	307	ALA	CA-C	5.29	1.59	1.52
1	A	30	VAL	C-O	5.28	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	ILE	CA-CB	5.28	1.61	1.55
1	A	356	ILE	CA-CB	5.25	1.60	1.54
1	B	298	ALA	CA-CB	-5.24	1.45	1.53
1	A	316	THR	C-O	5.24	1.30	1.23
1	A	279	LYS	C-O	5.22	1.30	1.24
1	A	360	LEU	N-CA	-5.22	1.41	1.46
1	A	346	ASN	N-CA	5.20	1.51	1.46
1	B	121	ILE	CA-C	5.18	1.57	1.52
1	B	42	THR	C-O	-5.17	1.17	1.23
1	B	223	VAL	N-CA	5.17	1.52	1.46
1	A	68	THR	C-O	5.16	1.30	1.24
1	B	65	VAL	C-O	5.15	1.30	1.24
1	A	143	THR	CA-C	5.15	1.59	1.53
1	A	8	ILE	CA-CB	5.15	1.60	1.54
1	B	51	ASN	C-O	5.15	1.31	1.23
1	B	73	LEU	CA-CB	5.14	1.61	1.53
1	A	236	ALA	CA-CB	-5.12	1.45	1.53
1	A	284	ILE	CA-CB	-5.12	1.48	1.54
1	A	117	LEU	CA-C	5.11	1.58	1.53
1	A	262	ILE	CA-CB	5.10	1.60	1.53
1	A	179	LEU	C-O	5.10	1.30	1.24
1	A	74	GLY	C-O	-5.09	1.17	1.23
1	B	174	MET	CA-CB	5.08	1.61	1.53
1	A	84	LYS	N-CA	5.07	1.52	1.46
1	A	71	GLY	CA-C	5.07	1.57	1.52
1	B	313	VAL	CB-CG1	5.05	1.69	1.52
1	A	85	LEU	CG-CD1	-5.01	1.36	1.52
1	A	66	SER	C-O	5.00	1.30	1.24
1	A	174	MET	C-O	-5.00	1.18	1.24

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	NE-CZ-NH2	10.64	128.78	119.20
1	B	249	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	B	215	GLN	OE1-CD-NE2	-10.01	112.59	122.60
1	B	267	GLN	OE1-CD-NE2	-9.67	112.93	122.60
1	B	48	ILE	N-CA-C	8.99	119.02	110.30
1	B	227	VAL	CB-CA-C	-8.91	99.92	112.22
1	B	285	ASN	N-CA-C	-8.58	101.87	111.82
1	A	148	ARG	NE-CZ-NH1	-8.51	112.99	121.50
1	B	160	ALA	N-CA-C	-8.12	101.50	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	GLN	CA-C-N	8.11	131.47	122.55
1	B	267	GLN	C-N-CA	8.11	131.47	122.55
1	B	11	ILE	CB-CA-C	-7.92	101.67	112.04
1	A	148	ARG	CD-NE-CZ	7.86	135.41	124.40
1	B	54	VAL	CB-CA-C	-7.67	99.09	111.59
1	A	177	ARG	NE-CZ-NH1	7.51	129.01	121.50
1	B	249	GLN	CG-CD-NE2	7.28	127.32	116.40
1	A	87	ASP	CA-C-N	-7.21	112.36	119.78
1	A	87	ASP	C-N-CA	-7.21	112.36	119.78
1	B	151	ALA	N-CA-C	7.17	119.75	107.93
1	A	49	ALA	N-CA-C	7.13	119.92	111.71
1	B	267	GLN	CG-CD-NE2	7.12	127.08	116.40
1	B	227	VAL	N-CA-C	-6.97	103.68	110.72
1	B	107	LEU	N-CA-C	-6.89	103.00	111.33
1	A	13	ASN	N-CA-C	6.86	118.41	111.07
1	A	97	THR	CA-C-N	-6.73	108.22	121.41
1	A	97	THR	C-N-CA	-6.73	108.22	121.41
1	A	22	GLU	N-CA-C	6.69	119.58	111.82
1	A	151	ALA	N-CA-C	6.54	119.92	108.75
1	A	243	VAL	CB-CA-C	6.50	119.51	111.25
1	B	235	GLN	N-CA-C	6.50	118.03	111.07
1	B	215	GLN	CG-CD-NE2	6.50	126.15	116.40
1	A	97	THR	N-CA-C	-6.45	102.20	110.53
1	B	95	GLU	N-CA-C	-6.44	105.39	113.18
1	B	125	VAL	CB-CA-C	6.42	120.30	111.31
1	B	298	ALA	CA-C-N	-6.42	114.84	122.93
1	B	298	ALA	C-N-CA	-6.42	114.84	122.93
1	B	308	VAL	CB-CA-C	6.41	119.76	110.98
1	B	8	ILE	N-CA-C	-6.38	104.05	111.00
1	A	227	VAL	CB-CA-C	-6.36	101.95	112.26
1	B	268	GLY	N-CA-C	-6.35	101.38	112.55
1	B	273	MET	CB-CG-SD	6.34	131.73	112.70
1	B	21	GLN	N-CA-C	6.30	118.15	111.28
1	A	278	LEU	CA-C-N	-6.28	113.82	122.93
1	A	278	LEU	C-N-CA	-6.28	113.82	122.93
1	A	148	ARG	CG-CD-NE	-6.27	98.20	112.00
1	A	178	VAL	CG1-CB-CG2	-6.22	97.11	110.80
1	B	307	ALA	N-CA-C	6.16	119.28	110.10
1	A	72	VAL	N-CA-C	6.14	116.89	110.62
1	B	233	TRP	N-CA-C	-6.07	104.22	111.69
1	B	248	LEU	N-CA-C	-6.07	104.95	112.90
1	B	13	ASN	N-CA-C	6.00	117.82	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	MET	N-CA-C	5.99	119.31	109.72
1	B	232	ARG	NE-CZ-NH1	-5.97	115.53	121.50
1	A	231	ALA	N-CA-C	-5.88	104.87	111.28
1	B	74	GLY	CA-C-N	5.82	126.44	119.98
1	B	74	GLY	C-N-CA	5.82	126.44	119.98
1	A	358	GLU	N-CA-C	-5.80	105.70	112.89
1	B	97	THR	N-CA-C	-5.80	101.38	110.36
1	B	29	ALA	CA-C-N	-5.79	113.49	122.69
1	B	29	ALA	C-N-CA	-5.79	113.49	122.69
1	A	97	THR	O-C-N	-5.74	115.60	122.65
1	A	260	TRP	CA-C-N	5.73	131.07	123.05
1	A	260	TRP	C-N-CA	5.73	131.07	123.05
1	A	62	LEU	CB-CG-CD1	5.72	127.86	110.70
1	A	136	GLN	N-CA-C	5.68	117.48	111.28
1	A	220	ALA	N-CA-C	5.67	120.20	113.12
1	A	357	LEU	N-CA-C	5.63	118.35	111.82
1	B	352	ALA	N-CA-C	5.62	117.08	111.07
1	A	328	PHE	N-CA-C	5.58	117.58	108.76
1	B	246	LYS	N-CA-C	5.58	117.36	111.28
1	A	350	VAL	CB-CA-C	-5.56	104.85	111.97
1	B	177	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	178	VAL	CA-C-N	5.55	127.98	120.65
1	B	178	VAL	C-N-CA	5.55	127.98	120.65
1	B	177	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	B	148	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	B	332	LYS	CA-C-N	5.51	130.40	122.35
1	B	332	LYS	C-N-CA	5.51	130.40	122.35
1	B	217	ASP	CA-C-N	5.50	129.07	120.82
1	B	217	ASP	C-N-CA	5.50	129.07	120.82
1	A	143	THR	CB-CA-C	5.49	118.11	109.27
1	A	317	GLY	N-CA-C	5.45	119.27	110.87
1	B	358	GLU	N-CA-C	-5.44	105.35	111.28
1	A	207	LYS	CB-CA-C	5.41	116.18	108.76
1	B	281	ASP	N-CA-C	5.40	118.66	111.75
1	A	359	LYS	CA-C-N	5.38	129.21	120.23
1	A	359	LYS	C-N-CA	5.38	129.21	120.23
1	A	178	VAL	N-CA-C	5.33	120.43	109.34
1	A	234	VAL	N-CA-CB	5.33	118.58	110.58
1	A	114	ALA	N-CA-C	5.31	117.82	111.71
1	A	361	GLN	CB-CA-C	5.31	120.19	110.10
1	B	121	ILE	N-CA-CB	5.29	115.44	109.99
1	B	333	ASN	N-CA-C	-5.29	104.83	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	LEU	N-CA-C	5.27	117.77	111.71
1	A	54	VAL	CB-CA-C	-5.24	103.29	111.26
1	B	314	HIS	CA-C-N	5.23	130.06	121.58
1	B	314	HIS	C-N-CA	5.23	130.06	121.58
1	B	139	GLN	CA-C-N	5.18	125.18	119.90
1	B	139	GLN	C-N-CA	5.18	125.18	119.90
1	A	66	SER	N-CA-C	-5.16	106.24	112.54
1	B	312	TRP	CA-C-O	-5.16	115.06	120.58
1	B	48	ILE	CA-C-N	5.16	127.19	120.28
1	B	48	ILE	C-N-CA	5.16	127.19	120.28
1	A	98	GLY	N-CA-C	-5.13	101.01	113.18
1	A	285	ASN	N-CA-CB	5.13	117.67	110.12
1	A	275	ASN	N-CA-C	-5.13	102.27	109.96
1	B	111	THR	CA-C-O	5.11	125.52	119.48
1	A	12	VAL	CA-C-N	5.08	127.05	120.44
1	A	12	VAL	C-N-CA	5.08	127.05	120.44
1	B	341	ASN	CA-C-N	5.06	129.78	121.58
1	B	341	ASN	C-N-CA	5.06	129.78	121.58
1	A	248	LEU	N-CA-C	-5.05	104.76	112.04
1	B	176	ARG	N-CA-C	5.05	119.16	112.89
1	B	217	ASP	N-CA-CB	5.05	117.47	109.94
1	B	258	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	A	245	GLU	CA-CB-CG	5.04	124.18	114.10

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	110	0
1	B	2764	0	2730	158	0
2	A	13	0	5	3	0
2	B	13	0	5	2	0
3	A	219	0	0	40	0
3	B	226	0	0	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6033	0	5522	267	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 24.

All (267) 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:CB	1:A:65:VAL:CA	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:A:61:GLU:CD	1:A:211:VAL:HG23	2.01	0.85
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:25:ILE:HG23	3:A:509:HOH:O	1.76	0.84
1:A:227:VAL:HG22	3:A:607: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:GLU:CD	1:A:177:ARG:HH22	1.92	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
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: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:A:56:GLN:HE21	1:A:228:ILE:HD11	1.54	0.71
1:B:30:VAL:HG13	1:B:43:TRP:HZ3	1.53	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:268:GLY:CA	1:B:273:MET:HE1	2.23	0.68
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:O	1:B:54:VAL:CG2	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:CA	1:A:65:VAL:CG1	2.72	0.66
1:B:227:VAL:HG22	3:B:532:HOH:O	1.95	0.66
1:B:250:GLN:HA	1:B:250:GLN:HE21	1.59	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:34:TYR:CE1	3:B:704:HOH:O	2.49	0.65
1:B:45:LYS:HD3	1:B:48:ILE:HD13	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:73:LEU:HD11	1:A:163:VAL:HG12	1.81	0.61
1:B:33:ILE:HG23	1:B:335:GLY:CA	2.30	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:159:GLY:O	1:B:160:ALA:C	2.45	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:B:28:MET:HE3	1:B:340:ALA:HB2	1.86	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:136:GLN:NE2	1:B:136:GLN:HA	2.22	0.55
1:B:355:ARG:HD2	3:B:678:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLU:HG2	3:B:692:HOH:O	2.05	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:351:GLU:CD	1:B:355:ARG:HH12	2.14	0.55
1:B:329:VAL:CG1	3:B:712:HOH:O	2.53	0.54
1:B:33:ILE:HG12	1:B:238:MET:HE1	1.88	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:A:273:MET:HG3	1:A:313:VAL:HG22	1.89	0.53
1:A:310:ALA:HB2	1:A:331:GLU:CD	2.32	0.53
1:B:204:ARG:NH2	1:B:320:GLY:HA2	2.22	0.53
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:178:VAL:C	1:A:181:PRO:HD2	2.33	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:20:MET:HG2	1:B:28:MET:HG3	1.90	0.52
1:B:55:THR:HG23	1:B:57:GLN:N	2.17	0.52
1:A:28:MET:HE3	1:A:340:ALA:HB2	1.92	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:A:72:VAL:HG13	1:A:252:ILE:HD13	1.92	0.50
1:B:45:LYS:HD3	3:B:690:HOH:O	2.12	0.50
1:A:84:LYS:HE3	3:A:701:HOH:O	2.12	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:B:67:LYS:NZ	1:B:152:ASN:OD1	2.26	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: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:268:GLY:HA3	1:B:273:MET:HE1	1.93	0.49
1:A:204:ARG:C	1:A:205:GLU:HG2	2.38	0.49
1:A:150:TYR:OH	2:A:501:CIT:O7	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:HG23	1:B:335:GLY:H	1.74	0.49
1:B:287:SER:HB3	3:B:727:HOH:O	2.11	0.49
1:B:84:LYS:O	1:B:87:ASP:HB2	2.12	0.49
1:B:271:TRP:HH2	1:B:326:VAL:HG11	1.78	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:B:124:ASP:HB3	3:B:694:HOH:O	2.13	0.48
1:B:302:ASN:HA	1:B:303:PRO:C	2.39	0.48
1:B:352:ALA:O	1:B:356:ILE:HG13	2.13	0.48
1:A:26:PRO:O	1:A:44:GLY:HA3	2.14	0.48
1:B:316:THR:HG22	1:B:325:TYR:CD1	2.49	0.48
1:A:329:VAL:HG12	1:A:332:LYS:HB2	1.96	0.48
1:B:65:VAL:C	1:B:67:LYS:N	2.71	0.48
1:A:30:VAL:HG13	1:A:43:TRP:HZ3	1.78	0.47
1:B:6:GLN:CB	3:B:563:HOH:O	2.62	0.47
1:A:73:LEU:CD1	1:A:163:VAL:CG1	2.92	0.47
1:A:110:ALA:HB2	1:A:158:PHE:CD2	2.49	0.47
1:A:240:ALA:HB2	1:A:252:ILE:HG21	1.97	0.47
1:B:97:THR:O	1:B:136:GLN:NE2	2.34	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:A:73:LEU:CD1	1:A:163:VAL:HG12	2.45	0.47
1:B:272:GLU:HB2	3:B:630:HOH:O	2.13	0.47
1:B:287:SER:HB2	3:B:727:HOH:O	2.10	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:351:GLU:O	1:B:354:TRP:HB3	2.15	0.47
1:B:91:LYS:HG2	1:B:92:TYR:CE2	2.50	0.47
1:B:270:GLY:N	3:B:653:HOH:O	2.47	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:B:102:GLN:CD	3:B:683:HOH:O	2.58	0.46
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:78:ILE:HD11	1:B:85:LEU:HD13	1.96	0.46
1:B:121:ILE:HB	3:B:705:HOH:O	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:NH2	1:B:308:VAL:HG13	2.30	0.46
1:A:157:LEU:O	1:A:158:PHE:C	2.58	0.46
1:A:17:THR:HB	1:A:18:PRO:HD3	1.99	0.45
1:B:269:LEU:C	3:B:653:HOH:O	2.58	0.45
1:A:87:ASP:N	3:A:524:HOH:O	2.50	0.45
1:A:203:TYR:HA	1:A:207:LYS:O	2.16	0.45
1:B:184:LEU:CD2	1:B:232:ARG:HG3	2.47	0.45
1:A:183:LYS:HE3	3:A:705:HOH:O	2.16	0.45
1:A:211:VAL:CG2	1:A:319:THR:HG21	2.47	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: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: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
1:B:319:THR:HG1	1:B:322:PHE:HB2	1.82	0.44
1:B:218:ALA:HB3	3:B:685:HOH:O	2.17	0.44
1:B:232:ARG:HB2	3:B:681:HOH:O	2.17	0.44
1:B:99:LYS:CD	3:B:660:HOH:O	2.50	0.44
1:A:342:LYS:HZ2	1:A:342:LYS:HG2	1.74	0.43
1:A:5:GLU:HB2	3:A:685:HOH:O	2.18	0.43
1:B:90:THR:O	1:B:91:LYS:C	2.58	0.43
1:B:164:LYS:HB2	1:B:165:PRO:HD3	2.00	0.43
1:A:319:THR:O	1:A:320:GLY:C	2.61	0.43
1:A:338:MET:HE1	1:A:352:ALA:HB3	2.01	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:A:92:TYR:CE1	1:A:106:LEU:HD11	2.54	0.43
1:B:33:ILE:HD11	1:B:36:GLY:CA	2.49	0.43
1:A:85:LEU:HB3	1:A:107:LEU:HB2	2.01	0.42
1:B:58:THR:HA	1:B:198:ASP:O	2.19	0.42
1:A:243:VAL:CG1	1:A:248:LEU:HD13	2.48	0.42
1:B:351:GLU:CG	1:B:355:ARG:NH1	2.41	0.42
1:B:43:TRP:O	1:B:54:VAL:HG11	2.19	0.42
1:A:334:LEU:HG	1:A:357:LEU:HD22	2.00	0.42
1:B:56:GLN:HE21	1:B:228:ILE:HD11	1.84	0.42
1:A:176:ARG:HH11	1:A:176:ARG:CG	2.32	0.42
1:B:72:VAL:CG1	1:B:252:ILE:CD1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PRO:HB2	1:B:125:VAL:CG1	2.50	0.42
1:B:316:THR:HG22	1:B:325:TYR:HD1	1.83	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:43:TRP:C	1:B:54:VAL:HG21	2.45	0.41
1:A:72:VAL:HG13	1:A:252:ILE:CD1	2.50	0.41
1:B:331:GLU:CA	3:B:712:HOH:O	2.65	0.41
1:A:265:MET:HE1	3:A:673:HOH:O	2.20	0.41
1:B:250:GLN:NE2	3:B:597:HOH:O	2.54	0.41
1:A:65:VAL:CA	1:A:65:VAL:CG2	2.86	0.41
1:A:96:LEU:CD2	1:A:136:GLN:HE21	2.34	0.41
1:B:283:ILE:HD13	1:B:283:ILE:HG21	1.78	0.41
1:B:315:LYS:HA	1:B:315:LYS:HD2	1.60	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:A:120:GLN:HE21	1:A:120:GLN:HB2	1.09	0.40
1:B:332:LYS:HE3	1:B:332:LYS:HB3	1.79	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: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
1:B:99:LYS:HG2	3:B:683:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	21	18
1	B	354/361 (98%)	330 (93%)	23 (6%)	1 (0%)	36	36
All	All	710/722 (98%)	670 (94%)	37 (5%)	3 (0%)	30	28

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%)	247 (85%)	43 (15%)	3	1
1	B	284/291 (98%)	253 (89%)	31 (11%)	6	4
All	All	574/582 (99%)	500 (87%)	74 (13%)	4	2

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	GLU
1	A	16	ILE
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

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Mol	Chain	Res	Type
1	A	139	GLN
1	A	143	THR
1	A	165	PRO
1	A	175	THR
1	A	176	ARG
1	A	177	ARG
1	A	183	LYS
1	A	184	LEU
1	A	189	ILE
1	A	207	LYS
1	A	227	VAL
1	A	245	GLU
1	A	246	LYS
1	A	248	LEU
1	A	250	GLN
1	A	252	ILE
1	A	262	ILE
1	A	289	SER
1	A	296	LEU
1	A	316	THR
1	A	324	SER
1	A	326	VAL
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	16	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	99	LYS
1	B	107	LEU

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Mol	Chain	Res	Type
1	B	121	ILE
1	B	125	VAL
1	B	155	ILE
1	B	164	LYS
1	B	179	LEU
1	B	209	VAL
1	B	227	VAL
1	B	232	ARG
1	B	252	ILE
1	B	254	LEU
1	B	273	MET
1	B	278	LEU
1	B	308	VAL
1	B	326	VAL
1	B	332	LYS
1	B	333	ASN
1	B	349	ARG
1	B	360	LEU
1	B	361	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	50	ASN
1	A	52	HIS
1	A	56	GLN
1	A	120	GLN
1	A	133	HIS
1	A	136	GLN
1	A	139	GLN
1	A	180	GLN
1	A	361	GLN
1	B	21	GLN
1	B	56	GLN
1	B	136	GLN
1	B	137	ASN
1	B	193	GLN
1	B	196	GLN
1	B	235	GLN
1	B	250	GLN
1	B	285	ASN

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Mol	Chain	Res	Type
1	B	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	502	-	12,12,12	1.49	3 (25%)	17,17,17	2.33	6 (35%)
2	CIT	A	501	-	12,12,12	2.55	5 (41%)	17,17,17	2.75	10 (58%)

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	B	502	-	-	0/16/16/16	-
2	CIT	A	501	-	-	1/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CIT	C4-C3	5.27	1.60	1.54
2	A	501	CIT	C3-C6	4.19	1.57	1.53
2	A	501	CIT	O5-C6	3.75	1.33	1.22
2	B	502	CIT	O5-C6	2.64	1.30	1.22
2	A	501	CIT	O3-C5	2.52	1.30	1.22
2	A	501	CIT	C4-C5	2.33	1.57	1.50
2	B	502	CIT	C4-C3	2.23	1.56	1.54
2	B	502	CIT	C3-C6	2.11	1.55	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	CIT	O3-C5-C4	-4.80	109.35	122.95
2	A	501	CIT	O7-C3-C6	-4.77	102.19	108.96
2	B	502	CIT	O4-C5-C4	4.34	128.11	114.35
2	A	501	CIT	O6-C6-C3	4.20	121.20	113.14
2	A	501	CIT	O3-C5-C4	-4.15	111.19	122.95
2	B	502	CIT	O6-C6-C3	3.72	120.28	113.14
2	A	501	CIT	C2-C3-C6	3.57	117.94	110.03
2	A	501	CIT	C3-C2-C1	3.46	123.39	113.92
2	A	501	CIT	O4-C5-C4	3.42	125.18	114.35
2	B	502	CIT	O5-C6-C3	-3.21	115.88	122.09
2	A	501	CIT	O7-C3-C2	-3.14	102.21	109.38
2	A	501	CIT	O2-C1-O1	-2.58	116.70	123.33
2	B	502	CIT	C3-C2-C1	2.57	120.94	113.92
2	B	502	CIT	O7-C3-C4	-2.55	103.56	109.38
2	A	501	CIT	C4-C3-C6	2.18	114.87	110.03
2	A	501	CIT	O2-C1-C2	2.07	120.90	114.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C1-C2-C3-C6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	CIT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CIT	3	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%)	0.05	5 (1%) 73 75	4, 17, 33, 45	0
1	B	356/361 (98%)	0.06	2 (0%) 85 87	6, 17, 34, 46	0
All	All	714/722 (98%)	0.06	7 (0%) 79 81	4, 17, 34, 46	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	GLN	2.7
1	A	4	THR	2.6
1	A	9	ALA	2.2
1	A	194	ASN	2.2
1	A	5	GLU	2.1
1	B	11	ILE	2.1
1	A	6	GLN	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CIT	A	501	13/13	0.86	0.10	19,27,31,33	0
2	CIT	B	502	13/13	0.86	0.11	26,31,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.