



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:45 PM UTC

PDB ID : 1MRZ / pdb_00001mrz
Title : Crystal structure of a flavin binding protein from Thermotoga Maritima, TM379
Authors : Wang, W.; Kim, R.; Jancarik, J.; Yokota, H.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2002-09-19
Resolution : 1.90 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

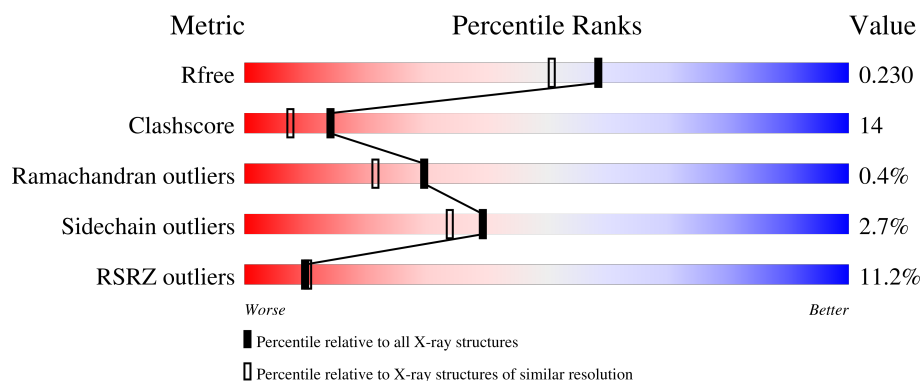
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	293	12% 66% 24% • 9%
1	B	293	8% 73% 17% • 8%

2 Entry composition [i](#)

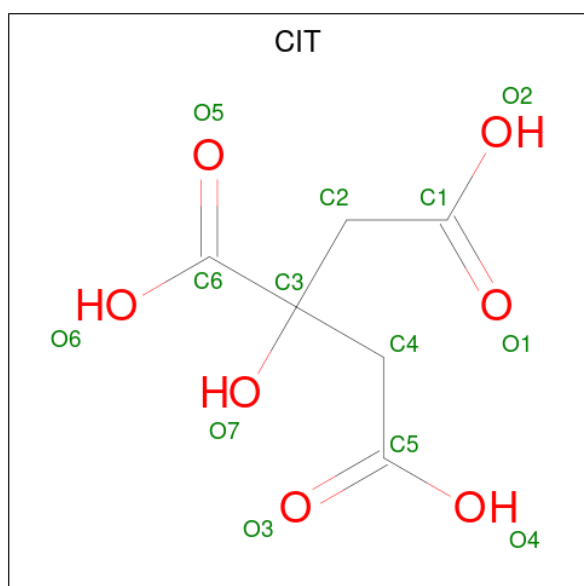
There are 3 unique types of molecules in this entry. The entry contains 4814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Riboflavin kinase/FMN adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2157	1388	373	390	6			
1	B	270	Total	C	N	O	S	0	0	0
			2189	1413	373	397	6			

- 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		

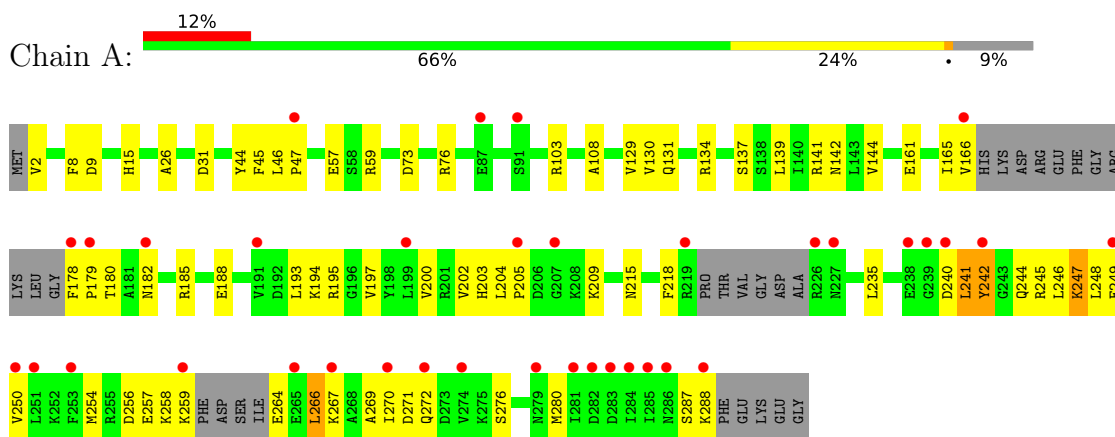
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total 210	O 210	0	0
3	B	232	Total 232	O 232	0	0

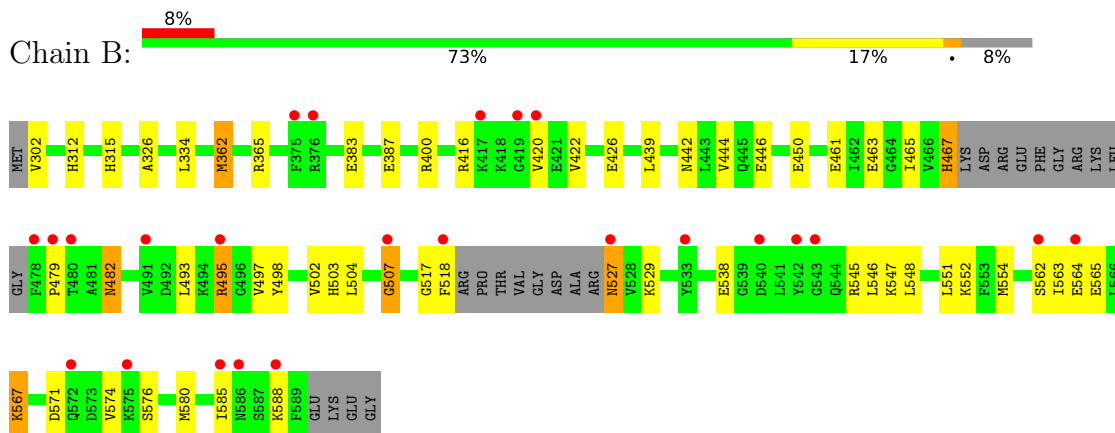
3 Residue-property plots

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: Riboflavin kinase/FMN adenylyltransferase



- Molecule 1: Riboflavin kinase/FMN adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.21Å 83.09Å 67.85Å 90.00° 116.93° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-1.90) 97.6 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.217 , 0.233 0.217 , 0.230	Depositor DCC
R_{free} test set	5167 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4814	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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	0.42	0/2193	0.85	1/2942 (0.0%)
1	B	0.43	1/2229 (0.0%)	0.81	2/2994 (0.1%)
All	All	0.42	1/4422 (0.0%)	0.83	3/5936 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	MET	SD-CE	-6.16	1.64	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	GLY	N-CA-C	-5.62	107.03	114.95
1	A	266	LEU	N-CA-C	-5.59	105.18	111.28
1	B	422	VAL	N-CA-C	5.19	115.59	108.12

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	2157	0	2201	74	0
1	B	2189	0	2221	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	5	3	0
2	B	13	0	5	2	0
3	A	210	0	0	8	0
3	B	232	0	0	5	0
All	All	4814	0	4432	125	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 14.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ARG:H	1:B:495:ARG:HD3	1.18	1.06
1:A:241:LEU:HD12	1:A:241:LEU:H	1.22	1.04
1:A:241:LEU:HD22	1:A:246:LEU:HD11	1.60	0.82
1:B:562:SER:HB3	1:B:565:GLU:HG3	1.60	0.81
1:A:15:HIS:NE2	2:A:295:CIT:H21	1.97	0.80
1:B:465:ILE:HD13	1:B:545:ARG:HG2	1.66	0.78
1:A:270:ILE:HG13	1:A:271:ASP:N	1.97	0.78
1:B:497:VAL:HG12	1:B:554:MET:HE3	1.68	0.76
1:B:495:ARG:H	1:B:495:ARG:CD	1.92	0.75
1:B:517:GLY:O	1:B:518:PHE:HB2	1.88	0.74
1:B:567:LYS:O	1:B:567:LYS:HE3	1.88	0.73
1:B:467:HIS:C	1:B:467:HIS:CD2	2.69	0.71
2:A:295:CIT:H22	3:A:602:HOH:O	1.90	0.71
1:B:400:ARG:HH21	1:B:426:GLU:HG2	1.56	0.71
1:A:178:PHE:CE2	1:A:270:ILE:HB	2.27	0.70
1:A:202:VAL:HG22	1:A:248:LEU:HD22	1.74	0.69
1:A:178:PHE:HE2	1:A:270:ILE:HB	1.58	0.68
1:B:302:VAL:HG11	1:B:326:ALA:HB2	1.77	0.67
1:B:527:ASN:HB2	3:B:884:HOH:O	1.94	0.67
1:A:204:LEU:HD12	1:A:241:LEU:HD21	1.78	0.66
1:B:495:ARG:HD3	1:B:495:ARG:N	2.00	0.65
1:B:482:ASN:OD1	1:B:529:LYS:HE3	1.97	0.65
1:A:9:ASP:HA	1:A:59:ARG:HD2	1.81	0.63
1:A:59:ARG:HD3	3:A:613:HOH:O	1.99	0.62
1:A:270:ILE:HG13	1:A:271:ASP:H	1.65	0.62
1:A:266:LEU:O	1:A:270:ILE:HG23	2.00	0.61
1:A:142:ASN:HD22	1:B:507:GLY:HA3	1.64	0.61
1:A:142:ASN:ND2	1:B:507:GLY:HA3	2.16	0.61
1:B:416:ARG:HA	1:B:420:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:HIS:NE2	2:B:595:CIT:H22	2.17	0.59
1:B:585:ILE:HA	1:B:588:LYS:HE2	1.85	0.59
1:A:205:PRO:HG2	1:A:244:GLN:NE2	2.17	0.59
1:A:178:PHE:N	1:A:179:PRO:CA	2.66	0.58
1:B:302:VAL:CG1	1:B:326:ALA:HB2	2.34	0.58
1:A:139:LEU:C	1:A:139:LEU:HD23	2.30	0.57
1:A:130:VAL:O	1:A:131:GLN:HB2	2.04	0.57
1:B:467:HIS:C	1:B:467:HIS:HD2	2.14	0.56
1:A:247:LYS:NZ	1:A:247:LYS:HB2	2.21	0.56
1:B:450:GLU:CG	1:B:552:LYS:HG2	2.37	0.55
1:B:465:ILE:CD1	1:B:545:ARG:HG2	2.34	0.55
1:B:502:VAL:HG22	1:B:548:LEU:HD22	1.88	0.54
1:A:45:PHE:O	1:B:588:LYS:HG2	2.08	0.54
1:A:205:PRO:HG2	1:A:244:GLN:HE21	1.72	0.54
1:A:166:VAL:HG12	1:A:182:ASN:O	2.08	0.54
1:B:482:ASN:HD22	1:B:482:ASN:N	2.06	0.53
1:A:287:SER:O	1:A:288:LYS:C	2.50	0.53
1:A:47:PRO:HD2	3:A:919:HOH:O	2.08	0.53
1:A:178:PHE:N	1:A:179:PRO:HA	2.24	0.53
1:B:400:ARG:NH1	3:B:709:HOH:O	2.42	0.53
1:A:178:PHE:N	1:A:179:PRO:C	2.66	0.52
1:A:57:GLU:OE2	1:A:245:ARG:NH2	2.42	0.52
1:A:270:ILE:CG1	1:A:271:ASP:N	2.71	0.52
1:A:165:ILE:O	1:A:166:VAL:HB	2.09	0.51
1:A:258:LYS:HG2	1:A:259:LYS:N	2.25	0.51
1:A:178:PHE:HD1	1:A:180:THR:CG2	2.24	0.50
1:B:465:ILE:HD11	1:B:545:ARG:NH1	2.26	0.50
1:B:551:LEU:O	1:B:552:LYS:HG3	2.12	0.50
1:A:241:LEU:H	1:A:241:LEU:CD1	1.96	0.50
1:B:461:GLU:HG3	3:B:941:HOH:O	2.12	0.49
1:A:73:ASP:HB3	1:A:76:ARG:HB2	1.94	0.49
1:A:166:VAL:HA	1:A:242:TYR:O	2.12	0.49
1:B:439:LEU:HD23	1:B:439:LEU:C	2.38	0.49
1:A:45:PHE:O	1:B:588:LYS:HE3	2.13	0.49
1:A:269:ALA:HA	1:A:272:GLN:OE1	2.13	0.48
1:A:267:LYS:C	1:A:270:ILE:HG12	2.37	0.48
1:B:576:SER:O	1:B:580:MET:HG3	2.13	0.48
1:A:178:PHE:HD1	1:A:180:THR:HG23	1.79	0.48
1:A:44:TYR:OH	1:A:188:GLU:OE2	2.16	0.48
1:A:276:SER:O	1:A:280:MET:HG3	2.14	0.48
1:B:442:ASN:OD1	1:B:446:GLU:OE2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HD12	1:A:165:ILE:N	2.29	0.47
1:A:194:LYS:HE2	1:A:256:ASP:OD2	2.14	0.47
1:A:195:ARG:NH1	1:A:218:PHE:CD2	2.83	0.47
1:A:178:PHE:N	1:A:180:THR:HG23	2.29	0.47
1:B:574:VAL:HG23	3:B:971:HOH:O	2.15	0.47
1:A:46:LEU:HD23	1:B:588:LYS:CE	2.44	0.47
1:A:8:PHE:HA	1:A:15:HIS:CE1	2.49	0.46
1:A:197:VAL:HG22	1:A:215:ASN:ND2	2.31	0.46
1:B:571:ASP:O	1:B:574:VAL:HG22	2.16	0.46
1:A:161:GLU:OE2	1:A:247:LYS:HD3	2.16	0.46
1:A:165:ILE:HG22	1:A:166:VAL:HG23	1.97	0.45
1:B:504:LEU:HD23	1:B:546:LEU:HD21	1.99	0.45
1:B:362:MET:HG2	1:B:365:ARG:HH12	1.81	0.45
1:A:258:LYS:O	1:A:259:LYS:C	2.60	0.45
1:A:241:LEU:HB3	1:A:244:GLN:HB2	1.99	0.45
1:A:247:LYS:HB2	1:A:247:LYS:HZ2	1.81	0.45
1:A:267:LYS:O	1:A:270:ILE:HG12	2.17	0.45
1:A:2:VAL:HG11	1:A:26:ALA:HB2	1.98	0.44
1:B:362:MET:HA	1:B:365:ARG:NH1	2.32	0.44
1:A:144:VAL:HG13	1:A:193:LEU:HD23	1.98	0.44
1:B:362:MET:CE	3:B:864:HOH:O	2.65	0.44
1:B:400:ARG:NE	1:B:426:GLU:OE2	2.50	0.44
1:A:137:SER:N	2:A:295:CIT:O2	2.48	0.44
1:A:270:ILE:CG1	1:A:271:ASP:H	2.30	0.44
1:A:194:LYS:HD3	1:A:195:ARG:O	2.18	0.44
1:A:204:LEU:HD12	1:A:241:LEU:CD2	2.47	0.43
1:A:203:HIS:HE2	1:A:249:GLU:CD	2.25	0.43
1:B:312:HIS:H	1:B:315:HIS:HD1	1.67	0.43
1:A:129:VAL:HG22	3:A:769:HOH:O	2.19	0.42
1:A:134:ARG:NH2	1:B:538:GLU:O	2.52	0.42
1:B:503:HIS:HB3	1:B:547:LYS:HB2	2.01	0.42
1:B:383:GLU:O	1:B:387:GLU:HG3	2.19	0.42
1:B:463:GLU:OE2	1:B:545:ARG:NH2	2.41	0.42
1:B:551:LEU:C	1:B:552:LYS:HG3	2.45	0.42
1:B:563:ILE:HG23	1:B:564:GLU:H	1.85	0.42
1:A:203:HIS:CE1	1:A:209:LYS:HE2	2.54	0.42
1:B:563:ILE:HG23	1:B:564:GLU:N	2.35	0.42
1:A:73:ASP:OD2	1:A:76:ARG:HD3	2.20	0.41
1:A:185:ARG:HD3	3:A:764:HOH:O	2.20	0.41
1:A:103:ARG:HD2	1:A:108:ALA:O	2.20	0.41
1:A:165:ILE:HD13	3:A:987:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:HG3	3:A:707:HOH:O	2.20	0.41
1:B:527:ASN:N	1:B:527:ASN:HD22	2.18	0.41
1:A:46:LEU:HA	1:A:47:PRO:HD3	1.94	0.41
1:A:202:VAL:HG12	1:A:204:LEU:HD13	2.03	0.41
1:B:444:VAL:HG13	1:B:493:LEU:HD23	2.03	0.41
1:B:498:TYR:C	1:B:554:MET:HE2	2.46	0.41
1:B:562:SER:HB3	1:B:565:GLU:CG	2.41	0.41
1:B:585:ILE:O	1:B:588:LYS:HD2	2.20	0.41
1:B:585:ILE:O	1:B:588:LYS:CD	2.68	0.41
1:B:312:HIS:HE2	2:B:595:CIT:C1	2.34	0.40
1:A:178:PHE:CD1	1:A:180:THR:CG2	3.04	0.40
1:A:254:MET:HG2	1:A:280:MET:HE1	2.03	0.40
1:A:200:VAL:HG12	1:A:250:VAL:HA	2.03	0.40
1:A:57:GLU:HB2	3:A:779:HOH:O	2.21	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	258/293 (88%)	252 (98%)	5 (2%)	1 (0%)	30	22
1	B	264/293 (90%)	262 (99%)	1 (0%)	1 (0%)	30	22
All	All	522/586 (89%)	514 (98%)	6 (1%)	2 (0%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	TYR
1	B	479	PRO

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	235/257 (91%)	228 (97%)	7 (3%)	36	30
1	B	239/257 (93%)	233 (98%)	6 (2%)	42	37
All	All	474/514 (92%)	461 (97%)	13 (3%)	39	34

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	141	ARG
1	A	235	LEU
1	A	240	ASP
1	A	241	LEU
1	A	247	LYS
1	A	264	GLU
1	B	334	LEU
1	B	467	HIS
1	B	482	ASN
1	B	495	ARG
1	B	527	ASN
1	B	567	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	131	GLN
1	A	142	ASN
1	A	145	GLN
1	A	215	ASN
1	A	244	GLN
1	A	279	ASN
1	B	407	ASN
1	B	442	ASN

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Mol	Chain	Res	Type
1	B	467	HIS
1	B	482	ASN
1	B	527	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	A	295	-	12,12,12	1.00	0	17,17,17	1.76	5 (29%)
2	CIT	B	595	-	12,12,12	0.89	0	17,17,17	1.69	3 (17%)

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	295	-	-	6/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	B	595	-	-	8/16/16/16	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	595	CIT	O6-C6-C3	4.21	121.22	113.14
2	A	295	CIT	O6-C6-C3	3.36	119.58	113.14
2	A	295	CIT	O4-C5-C4	2.87	123.43	114.35
2	B	595	CIT	O4-C5-C4	2.53	122.36	114.35
2	A	295	CIT	C2-C3-C6	-2.52	104.47	110.03
2	A	295	CIT	O2-C1-O1	-2.50	116.90	123.33
2	A	295	CIT	O4-C5-O3	-2.28	117.47	123.33
2	B	595	CIT	C2-C3-C6	-2.12	105.35	110.03

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	295	CIT	O7-C3-C6-O5
2	A	295	CIT	O7-C3-C6-O6
2	A	295	CIT	C4-C3-C6-O5
2	A	295	CIT	C4-C3-C6-O6
2	B	595	CIT	C2-C3-C6-O5
2	B	595	CIT	C2-C3-C6-O6
2	B	595	CIT	O7-C3-C6-O5
2	B	595	CIT	O7-C3-C6-O6
2	B	595	CIT	C3-C4-C5-O3
2	B	595	CIT	C3-C4-C5-O4
2	A	295	CIT	C3-C4-C5-O3
2	A	295	CIT	C3-C4-C5-O4
2	B	595	CIT	C4-C3-C6-O5
2	B	595	CIT	C4-C3-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	295	CIT	3	0
2	B	595	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

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	266/293 (90%)	0.85	36 (13%) 7 7	13, 19, 23, 26	0
1	B	270/293 (92%)	0.53	24 (8%) 15 16	14, 19, 24, 28	0
All	All	536/586 (91%)	0.69	60 (11%) 10 10	13, 19, 24, 28	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	PHE	7.2
1	A	242	TYR	6.9
1	A	284	ILE	5.7
1	A	179	PRO	5.2
1	A	178	PHE	5.2
1	B	542	TYR	5.0
1	A	285	ILE	4.8
1	B	479	PRO	4.3
1	B	540	ASP	4.0
1	B	480	THR	3.9
1	A	272	GLN	3.8
1	A	270	ILE	3.8
1	A	282	ASP	3.6
1	A	239	GLY	3.5
1	A	219	ARG	3.4
1	B	518	PHE	3.4
1	A	281	ILE	3.3
1	B	419	GLY	3.2
1	A	226	ARG	3.2
1	A	288	LYS	3.2
1	A	240	ASP	3.1
1	B	417	LYS	3.1
1	A	286	ASN	3.1
1	A	191	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	543	GLY	2.9
1	B	527	ASN	2.9
1	A	238	GLU	2.8
1	A	279	ASN	2.7
1	A	205	PRO	2.7
1	A	265	GLU	2.7
1	B	375	PHE	2.6
1	B	572	GLN	2.6
1	A	251	LEU	2.6
1	B	495	ARG	2.6
1	B	420	VAL	2.6
1	A	259	LYS	2.5
1	A	267	LYS	2.5
1	A	283	ASP	2.5
1	A	207	GLY	2.5
1	B	588	LYS	2.5
1	A	253	PHE	2.5
1	A	274	VAL	2.4
1	A	227	ASN	2.4
1	A	87	GLU	2.3
1	B	564	GLU	2.3
1	A	199	LEU	2.3
1	A	47	PRO	2.3
1	A	166	VAL	2.3
1	B	507	GLY	2.2
1	B	533	TYR	2.2
1	B	585	ILE	2.2
1	B	575	LYS	2.2
1	A	250	VAL	2.2
1	B	562	SER	2.2
1	A	91	SER	2.1
1	B	491	VAL	2.1
1	B	586	ASN	2.1
1	A	249	GLU	2.1
1	A	182	ASN	2.1
1	B	376	ARG	2.0

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

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	B	595	13/13	0.39	0.23	46,51,54,56	0
2	CIT	A	295	13/13	0.46	0.20	45,49,51,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.