W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:33 AM GMT

PDB ID : 3ITJ
Title : Crystal structure of Saccharomyces cerevisiae thioredoxin reductase 1 (Trr1)
Authors : Oliveira, M.A.; Discola, K.F.; Alves, S.V.; Medrano, F.J.; Guimaraes, B.G.; Netto, L.E.S.
Deposited on : 2009-08-28
Resolution : 2.40 Å(reported)

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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.
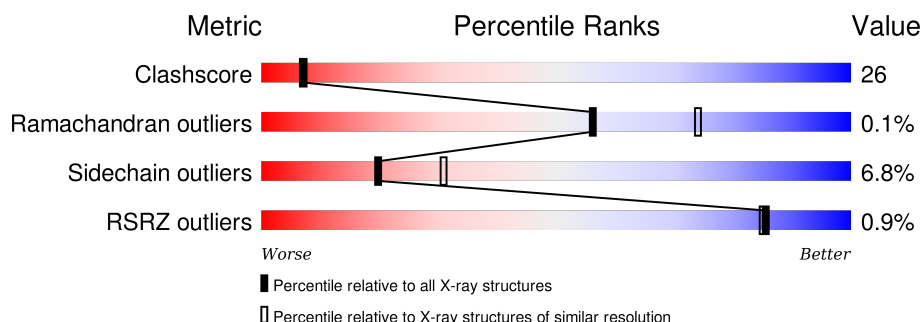
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	338	60% 30% • 6%
1	B	338	59% 31% • 6%
1	C	338	58% 30% • 7%
1	D	338	58% 28% 5% 9%

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
3	CIT	A	501	-	-	X	X
3	CIT	C	505	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9837 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 Thioredoxin reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total 2376	C 1499	N 402	O 463	S 12	0	1	0
1	B	319	Total 2373	C 1496	N 402	O 463	S 12	0	0	0
1	C	314	Total 2299	C 1444	N 388	O 456	S 11	0	0	0
1	D	307	Total 2222	C 1401	N 369	O 442	S 10	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P29509
A	-18	GLY	-	EXPRESSION TAG	UNP P29509
A	-17	SER	-	EXPRESSION TAG	UNP P29509
A	-16	SER	-	EXPRESSION TAG	UNP P29509
A	-15	HIS	-	EXPRESSION TAG	UNP P29509
A	-14	HIS	-	EXPRESSION TAG	UNP P29509
A	-13	HIS	-	EXPRESSION TAG	UNP P29509
A	-12	HIS	-	EXPRESSION TAG	UNP P29509
A	-11	HIS	-	EXPRESSION TAG	UNP P29509
A	-10	HIS	-	EXPRESSION TAG	UNP P29509
A	-9	SER	-	EXPRESSION TAG	UNP P29509
A	-8	SER	-	EXPRESSION TAG	UNP P29509
A	-7	GLY	-	EXPRESSION TAG	UNP P29509
A	-6	LEU	-	EXPRESSION TAG	UNP P29509
A	-5	VAL	-	EXPRESSION TAG	UNP P29509
A	-4	PRO	-	EXPRESSION TAG	UNP P29509
A	-3	ARG	-	EXPRESSION TAG	UNP P29509
A	-2	GLY	-	EXPRESSION TAG	UNP P29509
A	-1	SER	-	EXPRESSION TAG	UNP P29509
A	0	HIS	-	EXPRESSION TAG	UNP P29509
B	-19	MET	-	EXPRESSION TAG	UNP P29509

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP P29509
B	-17	SER	-	EXPRESSION TAG	UNP P29509
B	-16	SER	-	EXPRESSION TAG	UNP P29509
B	-15	HIS	-	EXPRESSION TAG	UNP P29509
B	-14	HIS	-	EXPRESSION TAG	UNP P29509
B	-13	HIS	-	EXPRESSION TAG	UNP P29509
B	-12	HIS	-	EXPRESSION TAG	UNP P29509
B	-11	HIS	-	EXPRESSION TAG	UNP P29509
B	-10	HIS	-	EXPRESSION TAG	UNP P29509
B	-9	SER	-	EXPRESSION TAG	UNP P29509
B	-8	SER	-	EXPRESSION TAG	UNP P29509
B	-7	GLY	-	EXPRESSION TAG	UNP P29509
B	-6	LEU	-	EXPRESSION TAG	UNP P29509
B	-5	VAL	-	EXPRESSION TAG	UNP P29509
B	-4	PRO	-	EXPRESSION TAG	UNP P29509
B	-3	ARG	-	EXPRESSION TAG	UNP P29509
B	-2	GLY	-	EXPRESSION TAG	UNP P29509
B	-1	SER	-	EXPRESSION TAG	UNP P29509
B	0	HIS	-	EXPRESSION TAG	UNP P29509
C	-19	MET	-	EXPRESSION TAG	UNP P29509
C	-18	GLY	-	EXPRESSION TAG	UNP P29509
C	-17	SER	-	EXPRESSION TAG	UNP P29509
C	-16	SER	-	EXPRESSION TAG	UNP P29509
C	-15	HIS	-	EXPRESSION TAG	UNP P29509
C	-14	HIS	-	EXPRESSION TAG	UNP P29509
C	-13	HIS	-	EXPRESSION TAG	UNP P29509
C	-12	HIS	-	EXPRESSION TAG	UNP P29509
C	-11	HIS	-	EXPRESSION TAG	UNP P29509
C	-10	HIS	-	EXPRESSION TAG	UNP P29509
C	-9	SER	-	EXPRESSION TAG	UNP P29509
C	-8	SER	-	EXPRESSION TAG	UNP P29509
C	-7	GLY	-	EXPRESSION TAG	UNP P29509
C	-6	LEU	-	EXPRESSION TAG	UNP P29509
C	-5	VAL	-	EXPRESSION TAG	UNP P29509
C	-4	PRO	-	EXPRESSION TAG	UNP P29509
C	-3	ARG	-	EXPRESSION TAG	UNP P29509
C	-2	GLY	-	EXPRESSION TAG	UNP P29509
C	-1	SER	-	EXPRESSION TAG	UNP P29509
C	0	HIS	-	EXPRESSION TAG	UNP P29509
D	-19	MET	-	EXPRESSION TAG	UNP P29509
D	-18	GLY	-	EXPRESSION TAG	UNP P29509
D	-17	SER	-	EXPRESSION TAG	UNP P29509

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP P29509
D	-15	HIS	-	EXPRESSION TAG	UNP P29509
D	-14	HIS	-	EXPRESSION TAG	UNP P29509
D	-13	HIS	-	EXPRESSION TAG	UNP P29509
D	-12	HIS	-	EXPRESSION TAG	UNP P29509
D	-11	HIS	-	EXPRESSION TAG	UNP P29509
D	-10	HIS	-	EXPRESSION TAG	UNP P29509
D	-9	SER	-	EXPRESSION TAG	UNP P29509
D	-8	SER	-	EXPRESSION TAG	UNP P29509
D	-7	GLY	-	EXPRESSION TAG	UNP P29509
D	-6	LEU	-	EXPRESSION TAG	UNP P29509
D	-5	VAL	-	EXPRESSION TAG	UNP P29509
D	-4	PRO	-	EXPRESSION TAG	UNP P29509
D	-3	ARG	-	EXPRESSION TAG	UNP P29509
D	-2	GLY	-	EXPRESSION TAG	UNP P29509
D	-1	SER	-	EXPRESSION TAG	UNP P29509
D	0	HIS	-	EXPRESSION TAG	UNP P29509

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
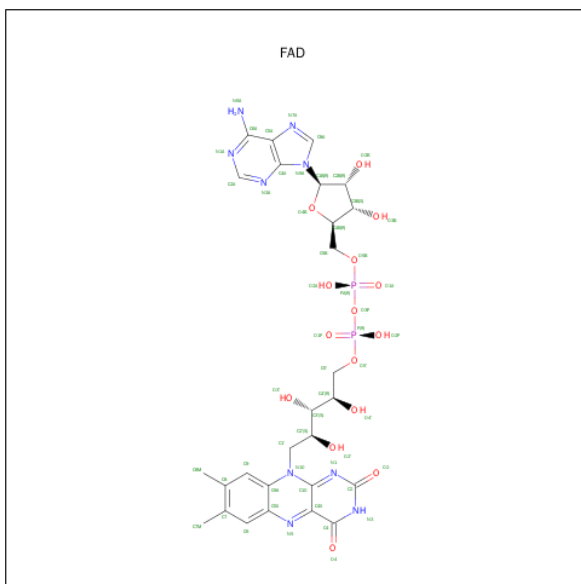
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
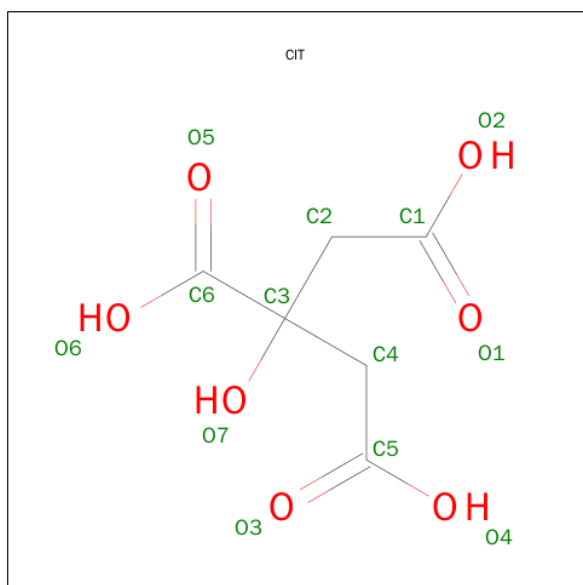
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		

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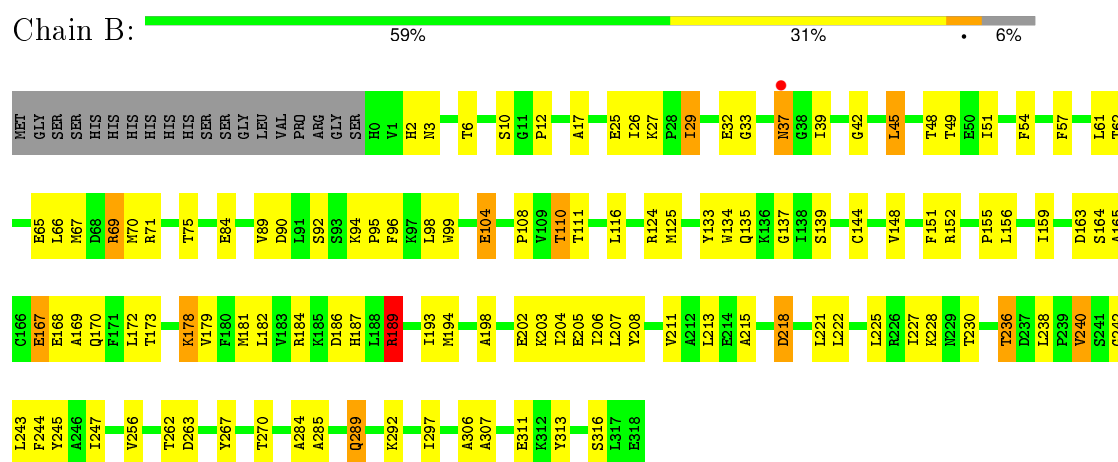| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	76	Total 76	O 76	0	0
4	C	65	Total 65	O 65	0	0
4	D	54	Total 54	O 54	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
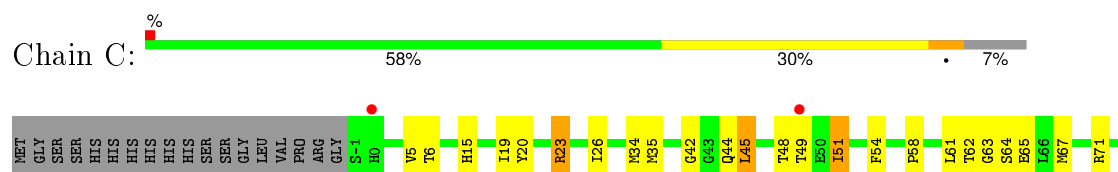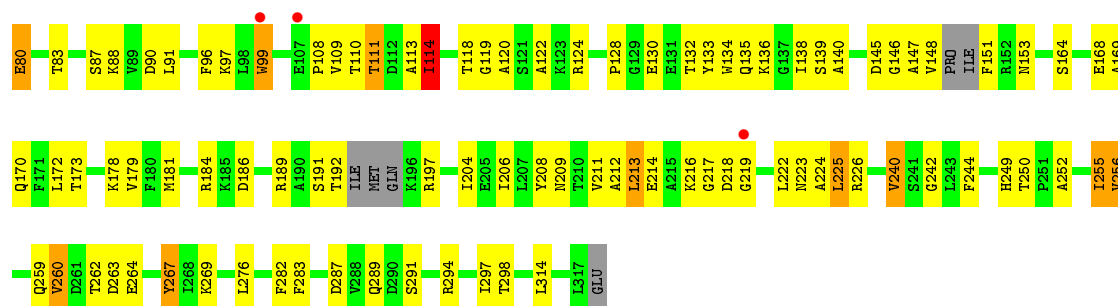
- Molecule 1: Thioredoxin reductase 1

Chain A:

- Molecule 1: Thioredoxin reductase 1

Chain B:

- Molecule 1: Thioredoxin reductase 1

Chain C:

E80 T83 S87 K88 V89 D90 L91 F96 K97 L98 W99 E107 P108 V109 T110 T111 D112 A113 I114 T118 G119 A120 S121 A122 K123 R124 P128 G129 E130 E131 T132 Y133 W134 Q135 K136 G137 I138 S139 A140 D145 G146 A147 V148 PRO ILE F151 R152 N153 S164 E168 A169

Q170 F171 L172 T173 K178 V179 F180 M181 R184 K185 D186 R189 A190 S191 T192 ILE MET GLN K196 R197 I204 E205 I206 L207 Y208 N209 T210 V211 A212 L213 E214 A215 K216 G217 D218 G219 L222 N223 A224 L225 R226 V240 S241 G242 L243 F244 H249 T250 P251 A252 I255 V256

Q259 V260 D261 T262 D263 E264 Y267 I268 K269 L276 F282 F283 D287 V288 Q289 D290 S291 R294 I297 T298 L314 L317 GLU

• Molecule 1: Thioredoxin reductase 1

Chain D:

%

58% 28% 5% 9%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS V1 H2 N3 T6 I7 S10 L21 I26 E32 N37 G42 G43 Q44 L45 T48 I51 P55 L61 T62 G63 S64 E65 L66 M67 R71 T83

V86 S87 K88 V89 D90 L91 K94 P95 F96 K97 L98 W99 P108 V109 T110 T111 I114 R124 M125 H126 L127 P128 G129 E130 E131 T132 Y133 W134 G137 I138 S139 A140 C141 A142 V143 C144 P155 L156 A157 D163 S164 E167 E168 F171 L172 T173 V179 F180 M181 L182

V183 R184 K185 D186 H187 A190 SER THR ILE MET GLN LYS R197 N201 E202 K203 I204 E205 I206 L207 Y208 N209 T210 V211 E214 A215 K216 G217 ASP GLY LYS LEU L222 N223 A224 L225 R226 T230 D237 V240 S241 G242 L243 F244 Y245 I255 V256 V260 D263 E264

Y267 T270 S275 L276 F282 F283 V288 Q289 D290 S291 R294 I297 A306 A307 L308 D309 A310 L314 L317 GLU

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.97Å 135.41Å 75.82Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 46.50 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-2.40) 79.0 (46.50-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.06 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.169 , 0.194 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.6	EDS
Estimated twinning fraction	0.783 for H, K, L 0.217 for -H, -K, L 0.000 for -h,-k,l	Xtriage
Reported twinning fraction	0.783 for H, K, L 0.217 for -H, -K, L	Depositor
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Outliers	0 of 40523 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9837	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FAD, 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	1.10	3/2420 (0.1%)	1.03	2/3276 (0.1%)
1	B	1.17	3/2413 (0.1%)	1.07	4/3267 (0.1%)
1	C	1.12	3/2336 (0.1%)	1.08	7/3168 (0.2%)
1	D	1.11	3/2261 (0.1%)	1.06	6/3076 (0.2%)
All	All	1.13	12/9430 (0.1%)	1.06	19/12787 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	GLU	CG-CD	6.54	1.61	1.51
1	C	20	TYR	CD1-CE1	-6.22	1.30	1.39
1	B	167	GLU	CG-CD	5.88	1.60	1.51
1	A	300	ALA	CA-CB	5.72	1.64	1.52
1	B	165	ALA	CA-CB	5.67	1.64	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	217	GLY	N-CA-C	10.59	139.56	113.10
1	C	114	ILE	CG1-CB-CG2	-9.13	91.32	111.40
1	C	225	LEU	CB-CG-CD2	-7.23	98.71	111.00
1	D	294	ARG	CG-CD-NE	-6.65	97.84	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ILE	CG1-CB-CG2	-6.57	96.95	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	185	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2376	0	2382	113	0
1	B	2373	0	2375	129	0
1	C	2299	0	2234	113	0
1	D	2222	0	2130	129	0
2	A	53	0	31	4	0
2	B	53	0	31	9	0
2	C	53	0	31	2	0
2	D	53	0	31	2	0
3	A	13	0	5	7	0
3	B	26	0	10	8	0
3	C	26	0	10	6	0
3	D	13	0	5	2	0
4	A	82	0	0	7	0
4	B	76	0	0	4	0
4	C	65	0	0	4	0
4	D	54	0	0	4	0
All	All	9837	0	9275	493	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 26.

The worst 5 of 493 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:D:216:LYS:CB	1:D:224:ALA:H	1.26	1.45
1:D:201:ASN:ND2	1:D:203:LYS:H	1.37	1.20
1:C:191:SER:O	1:C:192:THR:HB	1.44	1.16
1:C:147:ALA:HB1	1:C:151:PHE:CB	1.75	1.15
1:C:249:HIS:ND1	3:C:505:CIT:O4	1.77	1.15

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	316/338 (94%)	300 (95%)	15 (5%)	1 (0%)	46	63
1	B	317/338 (94%)	301 (95%)	16 (5%)	0	100	100
1	C	308/338 (91%)	296 (96%)	12 (4%)	0	100	100
1	D	301/338 (89%)	280 (93%)	21 (7%)	0	100	100
All	All	1242/1352 (92%)	1177 (95%)	64 (5%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA

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	249/270 (92%)	233 (94%)	16 (6%)	22	34
1	B	247/270 (92%)	229 (93%)	18 (7%)	17	27
1	C	232/270 (86%)	215 (93%)	17 (7%)	17	27
1	D	222/270 (82%)	207 (93%)	15 (7%)	20	31
All	All	950/1080 (88%)	884 (93%)	66 (7%)	20	30

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	236	THR
1	C	51	ILE
1	D	211	VAL
1	B	240	VAL
1	B	297	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	170	GLN
1	B	289	GLN
1	C	289	GLN
1	B	37	ASN
1	C	259	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 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	FAD	A	400	-	48,58,58	1.47	7 (14%)	54,89,89	2.17	14 (25%)
3	CIT	A	501	-	3,12,12	2.12	2 (66%)	3,17,17	6.56	3 (100%)
2	FAD	B	401	-	48,58,58	1.19	5 (10%)	54,89,89	2.31	10 (18%)
3	CIT	B	502	-	3,12,12	1.48	1 (33%)	3,17,17	3.21	1 (33%)
3	CIT	B	506	-	3,12,12	1.80	1 (33%)	3,17,17	2.75	1 (33%)
2	FAD	C	402	-	48,58,58	1.15	5 (10%)	54,89,89	2.51	15 (27%)
3	CIT	C	503	-	3,12,12	1.71	1 (33%)	3,17,17	2.50	1 (33%)
3	CIT	C	505	-	3,12,12	1.08	0	3,17,17	2.97	3 (100%)
2	FAD	D	403	-	48,58,58	1.33	7 (14%)	54,89,89	2.57	13 (24%)
3	CIT	D	504	-	3,12,12	0.58	0	3,17,17	3.18	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	FAD	A	400	-	-	0/30/50/50	0/6/6/6
3	CIT	A	501	-	-	0/6/16/16	0/0/0/0
2	FAD	B	401	-	-	0/30/50/50	0/6/6/6
3	CIT	B	502	-	-	0/6/16/16	0/0/0/0
3	CIT	B	506	-	-	0/6/16/16	0/0/0/0
2	FAD	C	402	-	-	0/30/50/50	0/6/6/6
3	CIT	C	503	-	-	0/6/16/16	0/0/0/0
3	CIT	C	505	-	-	0/6/16/16	0/0/0/0
2	FAD	D	403	-	-	0/30/50/50	0/6/6/6
3	CIT	D	504	-	-	0/6/16/16	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	506	CIT	C2-C3	-3.02	1.50	1.54
2	C	402	FAD	C10-N10	-2.72	1.36	1.39
2	A	400	FAD	C10-N10	-2.68	1.36	1.39
2	A	400	FAD	O4B-C4B	-2.54	1.39	1.45
3	A	501	CIT	C4-C3	-2.51	1.50	1.54

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	402	FAD	N3A-C2A-N1A	-12.49	119.33	128.89
2	D	403	FAD	N3A-C2A-N1A	-12.44	119.37	128.89
2	B	401	FAD	N3A-C2A-N1A	-11.89	119.79	128.89
2	A	400	FAD	N3A-C2A-N1A	-8.68	122.25	128.89
2	B	401	FAD	C2B-C1B-N9A	-7.20	103.28	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	FAD	4	0
3	A	501	CIT	7	0
2	B	401	FAD	9	0
3	B	502	CIT	4	0
3	B	506	CIT	4	0
2	C	402	FAD	2	0
3	C	503	CIT	3	0
3	C	505	CIT	3	0
2	D	403	FAD	2	0
3	D	504	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	317/338 (93%)	-0.24	2 (0%)	90 90	9, 19, 31, 41	0
1	B	319/338 (94%)	-0.25	1 (0%)	94 94	10, 19, 31, 38	0
1	C	314/338 (92%)	-0.13	5 (1%)	74 74	10, 20, 33, 46	0
1	D	307/338 (90%)	-0.06	3 (0%)	84 83	9, 19, 32, 40	0
All	All	1257/1352 (92%)	-0.17	11 (0%)	85 85	9, 19, 33, 46	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	110	THR	3.4
1	B	37	ASN	2.6
1	C	107	GLU	2.6
1	D	171	PHE	2.4
1	A	37	ASN	2.3

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(Å^2)	Q<0.9
3	CIT	A	501	13/13	0.88	0.18	2.75	26,39,49,51	0
3	CIT	C	505	13/13	0.84	0.20	2.50	31,39,46,50	0
3	CIT	C	503	13/13	0.79	0.17	1.67	44,49,52,56	0
3	CIT	D	504	13/13	0.86	0.17	0.41	55,58,64,65	0
3	CIT	B	506	13/13	0.95	0.13	0.04	28,35,40,44	0
2	FAD	D	403	53/53	0.97	0.13	-0.19	11,22,28,31	1
2	FAD	A	400	53/53	0.97	0.12	-0.28	5,19,27,30	1
2	FAD	C	402	53/53	0.97	0.13	-0.34	12,23,29,35	1
2	FAD	B	401	53/53	0.96	0.13	-0.40	7,22,31,35	1
3	CIT	B	502	13/13	0.91	0.11	-1.03	33,37,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.