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Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 10:26 am GMT

PDB ID	:	4NEW
Title	:	Crystal structure of Trypanothione Reductase from Trypanosoma cruzi in complex with inhibitor EP127 (5-{5-[1-(PYRROLIDIN-1-YL)CYCLOHEXYL]-1, 3-THIAZOL-2-YL}-1H-INDOLE)
Authors	:	Persch, E.; Bryson, S.; Pai, E.F.; Krauth-Siegel, R.L.; Diederich, F.
Deposited on	:	2013-10-30
Resolution	:	2.80 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 (i) symbol.

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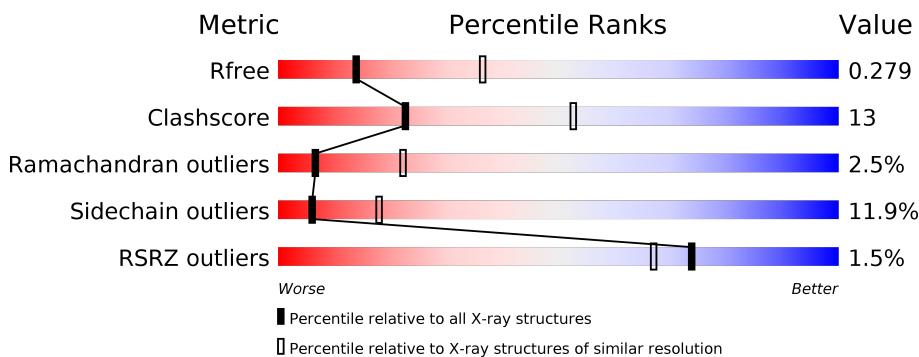
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
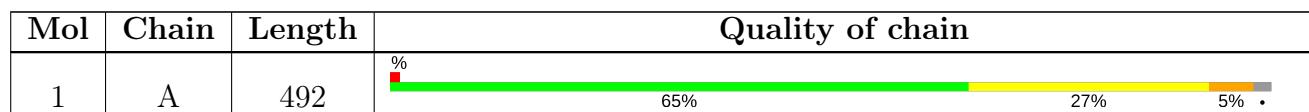
The reported resolution of this entry is 2.80 Å.

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	Percentile Ranks	Value
Rfree		0.279
Clashscore		13
Ramachandran outliers		2.5%
Sidechain outliers		11.9%
RSRZ outliers		1.5%

Worse ← → Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	492	65% 27% 5% ·

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	2JR	A	502	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3787 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.
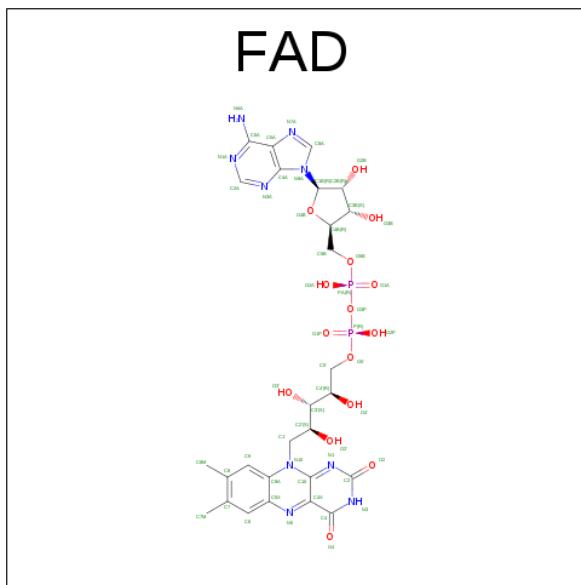
- Molecule 1 is a protein called Trypanothione reductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total 3709	C 2358	N 631	O 699	S 21	0	0	0

There is a discrepancy between the modelled and reference sequences:
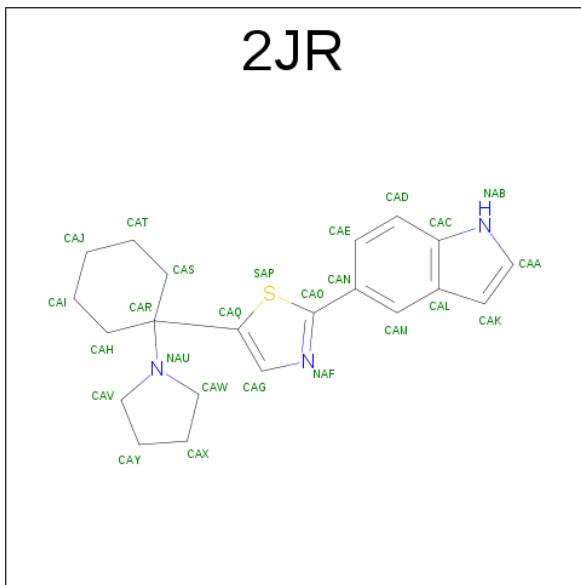
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ASN	LYS	SEE REMARK 999	UNP K4E0T9

- 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 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is 5-{5-[1-(PYRROLIDIN-1-YL)CYCLOHEXYL]-1,3-THIAZOL-2-YL}-1H-INDOLE (three-letter code: 2JR) (formula: $C_{21}H_{25}N_3S$).

2JR
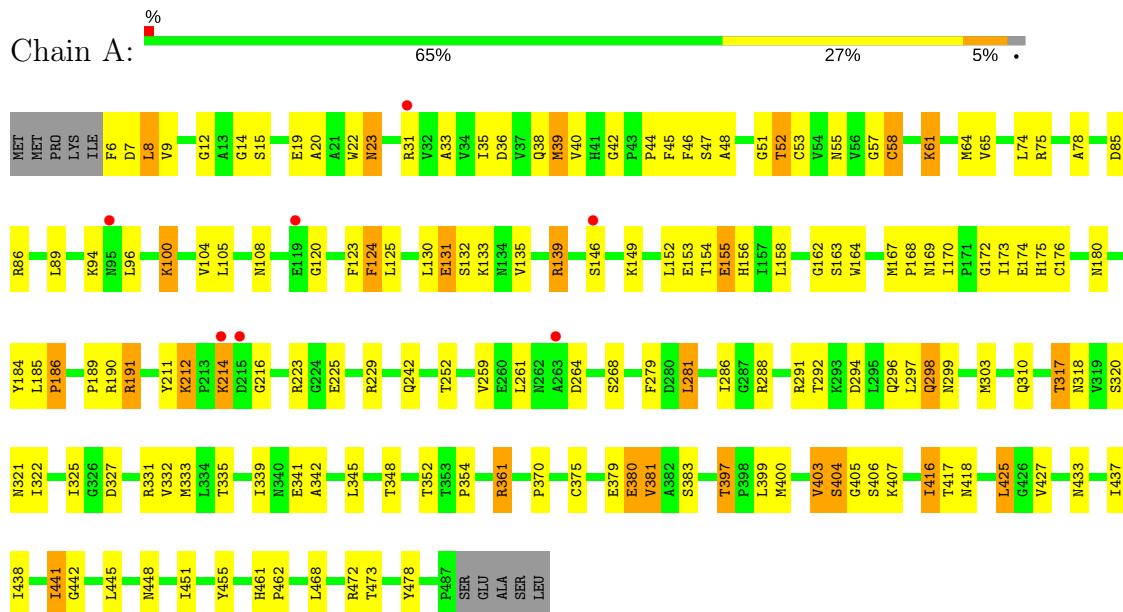
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			25	21	3	1		

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 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: Trypanothione reductase, putative

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	86.85Å 86.85Å 151.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 2.80 16.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (17.00-2.80) 79.9 (16.99-2.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.59Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.232 , 0.278 0.231 , 0.279	Depositor DCC
R_{free} test set	662 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3787	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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, 0.333 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: 2JR, FAD

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	0.44	0/3786	0.64	0/5130

There are no bond length outliers.

There are no bond angle outliers.

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	3709	0	3716	95	0
2	A	53	0	31	7	0
3	A	25	0	25	3	0
All	All	3787	0	3772	97	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 13.

All (97) 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:47:SER:OG	2:A:501:FAD:O3B	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:VAL:HG22	1:A:404:SER:H	1.53	0.74
1:A:75:ARG:NH2	1:A:406:SER:OG	2.23	0.71
1:A:375:CYS:HB3	1:A:441:ILE:HD11	1.74	0.70
1:A:403:VAL:O	1:A:405:GLY:N	2.25	0.69
1:A:379:GLU:OE2	1:A:478:TYR:HE1	1.76	0.69
1:A:139:ARG:HD3	1:A:146:SER:H	1.59	0.68
1:A:168:PRO:HD3	1:A:286:ILE:HD11	1.78	0.66
1:A:39:MET:SD	1:A:125:LEU:HD11	2.37	0.64
1:A:317:THR:HG22	1:A:322:ILE:O	1.98	0.63
1:A:139:ARG:HB3	1:A:146:SER:HB2	1.79	0.63
1:A:379:GLU:OE2	1:A:478:TYR:CE1	2.53	0.62
1:A:397:THR:HG21	1:A:407:LYS:O	2.00	0.62
1:A:189:PRO:HG3	1:A:281:LEU:HD12	1.81	0.61
1:A:296:GLN:OE1	1:A:298:GLN:NE2	2.33	0.61
1:A:15:SER:HB3	1:A:335:THR:HG23	1.82	0.61
1:A:348:THR:HG23	1:A:354:PRO:HB3	1.84	0.60
1:A:74:LEU:O	1:A:86:ARG:NH2	2.35	0.59
1:A:191:ARG:HG3	1:A:279:PHE:HA	1.84	0.59
1:A:158:LEU:HD11	1:A:325:ILE:HG13	1.85	0.58
1:A:123:PHE:HE1	1:A:125:LEU:HD12	1.69	0.58
1:A:38:GLN:NE2	1:A:40:VAL:O	2.35	0.58
1:A:441:ILE:HD12	1:A:445:LEU:HD13	1.85	0.58
1:A:51:GLY:O	1:A:55:ASN:ND2	2.29	0.58
1:A:35:ILE:HG22	2:A:501:FAD:H2A	1.84	0.58
1:A:42:GLY:HA2	1:A:184:TYR:CZ	2.40	0.56
1:A:348:THR:HA	1:A:354:PRO:HA	1.88	0.56
1:A:331:ARG:CG	1:A:332:VAL:H	2.18	0.56
1:A:380:GLU:O	1:A:381:VAL:C	2.44	0.56
1:A:135:VAL:HG22	1:A:153:GLU:HB3	1.88	0.55
1:A:167:MET:HB3	1:A:173:ILE:HD11	1.88	0.55
1:A:172:GLY:HA3	1:A:259:VAL:O	2.07	0.55
1:A:242:GLN:OE1	1:A:370:PRO:HG2	2.07	0.55
1:A:168:PRO:HB2	1:A:170:ILE:HG23	1.89	0.54
1:A:58:CYS:HB3	2:A:501:FAD:C4	2.38	0.53
1:A:176:CYS:SG	1:A:259:VAL:HG21	2.48	0.53
1:A:320:SER:O	1:A:321:ASN:HB2	2.08	0.53
1:A:53:CYS:CB	1:A:58:CYS:SG	2.97	0.52
1:A:33:ALA:HB1	1:A:124:PHE:HE1	1.74	0.52
1:A:96:LEU:HD22	1:A:211:TYR:CZ	2.43	0.52
1:A:105:LEU:HA	1:A:108:ASN:HB2	1.92	0.52
1:A:325:ILE:HG21	1:A:341:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:2JR:H13	3:A:502:2JR:SAP	2.42	0.51
1:A:212:LYS:HG2	1:A:216:GLY:HA3	1.91	0.51
1:A:403:VAL:HG22	1:A:404:SER:N	2.20	0.51
1:A:14:GLY:HA2	1:A:51:GLY:HA3	1.93	0.51
1:A:441:ILE:HG13	1:A:442:GLY:N	2.26	0.50
1:A:20:ALA:HB2	1:A:342:ALA:HB1	1.94	0.50
1:A:46:PHE:CD2	1:A:180:ASN:HB3	2.47	0.50
1:A:7:ASP:O	1:A:156:HIS:HB2	2.12	0.50
1:A:418:ASN:N	1:A:425:LEU:HD22	2.27	0.50
1:A:154:THR:OG1	1:A:155:GLU:N	2.45	0.49
1:A:47:SER:OG	2:A:501:FAD:O2B	2.29	0.49
1:A:438:ILE:HD12	1:A:441:ILE:HG12	1.94	0.49
1:A:416:ILE:HG13	1:A:416:ILE:O	2.13	0.48
1:A:327:ASP:OD1	1:A:333:MET:HB3	2.12	0.48
1:A:47:SER:CB	2:A:501:FAD:HO2A	2.27	0.48
1:A:175:HIS:CE1	1:A:261:LEU:HB2	2.48	0.47
1:A:317:THR:HG21	1:A:322:ILE:HG22	1.95	0.47
1:A:78:ALA:HB2	1:A:86:ARG:NH1	2.29	0.47
1:A:8:LEU:HG	1:A:9:VAL:N	2.28	0.47
1:A:44:PRO:HG2	1:A:45:PHE:CD1	2.50	0.46
1:A:317:THR:HG23	1:A:318:ASN:H	1.81	0.46
1:A:331:ARG:HG3	1:A:332:VAL:N	2.30	0.45
1:A:331:ARG:CG	1:A:332:VAL:N	2.76	0.45
1:A:131:GLU:O	1:A:299:ASN:HB3	2.17	0.45
1:A:33:ALA:HB1	1:A:124:PHE:CE1	2.51	0.45
3:A:502:2JR:H3	3:A:502:2JR:CAG	2.47	0.45
1:A:185:LEU:HA	1:A:186:PRO:HD2	1.87	0.44
1:A:52:THR:HG22	2:A:501:FAD:O2'	2.17	0.44
1:A:417:THR:HG21	1:A:451:ILE:HB	1.99	0.44
1:A:380:GLU:O	1:A:383:SER:N	2.50	0.44
1:A:325:ILE:CG2	1:A:341:GLU:HB3	2.47	0.44
1:A:31:ARG:HA	1:A:120:GLY:O	2.18	0.44
1:A:19:GLU:HG2	1:A:339:ILE:HG23	2.00	0.43
1:A:12:GLY:HA2	2:A:501:FAD:O4B	2.18	0.43
1:A:53:CYS:HA	1:A:57:GLY:HA3	2.00	0.43
1:A:61:LYS:O	1:A:65:VAL:HG23	2.18	0.43
1:A:100:LYS:O	1:A:104:VAL:HG23	2.19	0.43
1:A:433:ASN:O	1:A:437:ILE:HG13	2.19	0.43
1:A:167:MET:HA	1:A:168:PRO:HD2	1.89	0.43
1:A:164:TRP:CE3	1:A:291:ARG:NH1	2.87	0.43
1:A:361:ARG:NH2	1:A:448:ASN:OD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:HG3	1:A:132:SER:N	2.34	0.43
1:A:286:ILE:H	1:A:286:ILE:HG13	1.51	0.42
1:A:22:TRP:CE2	3:A:502:2JR:H2	2.54	0.42
1:A:327:ASP:CG	1:A:333:MET:HB3	2.40	0.42
1:A:162:GLY:HA2	1:A:327:ASP:HB2	2.01	0.42
1:A:427:VAL:HB	1:A:441:ILE:HD13	2.02	0.42
1:A:48:ALA:HB3	1:A:55:ASN:OD1	2.20	0.42
1:A:22:TRP:CD1	1:A:23:ASN:N	2.87	0.41
1:A:78:ALA:HB2	1:A:86:ARG:HH12	1.85	0.41
1:A:163:SER:O	1:A:291:ARG:HD2	2.21	0.41
1:A:64:MET:HA	1:A:96:LEU:HD11	2.03	0.41
1:A:15:SER:CB	1:A:335:THR:HG23	2.51	0.40
1:A:461:HIS:HA	1:A:462:PRO:HA	1.76	0.40
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.77	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	480/492 (98%)	418 (87%)	50 (10%)	12 (2%)	6	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	LYS
1	A	264	ASP
1	A	317	THR
1	A	380	GLU
1	A	381	VAL
1	A	403	VAL
1	A	404	SER

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Mol	Chain	Res	Type
1	A	23	ASN
1	A	85	ASP
1	A	169	ASN
1	A	174	GLU
1	A	186	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	403/412 (98%)	355 (88%)	48 (12%)	6	18

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	8	LEU
1	A	36	ASP
1	A	39	MET
1	A	52	THR
1	A	58	CYS
1	A	61	LYS
1	A	89	LEU
1	A	94	LYS
1	A	100	LYS
1	A	124	PHE
1	A	130	LEU
1	A	131	GLU
1	A	133	LYS
1	A	139	ARG
1	A	149	LYS
1	A	152	LEU
1	A	155	GLU
1	A	190	ARG
1	A	191	ARG
1	A	212	LYS

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Mol	Chain	Res	Type
1	A	214	LYS
1	A	223	ARG
1	A	225	GLU
1	A	229	ARG
1	A	252	THR
1	A	268	SER
1	A	281	LEU
1	A	288	ARG
1	A	292	THR
1	A	294	ASP
1	A	297	LEU
1	A	298	GLN
1	A	303	MET
1	A	310	GLN
1	A	345	LEU
1	A	352	THR
1	A	361	ARG
1	A	397	THR
1	A	399	LEU
1	A	400	MET
1	A	416	ILE
1	A	425	LEU
1	A	441	ILE
1	A	455	TYR
1	A	468	LEU
1	A	472	ARG
1	A	473	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	156	HIS

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	FAD	A	501	-	51,58,58	1.39	5 (9%)	54,89,89	1.98	10 (18%)
3	2JR	A	502	-	25,29,29	3.31	6 (24%)	23,42,42	3.60	8 (34%)

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	501	-	-	0/28/50/50	0/6/6/6
3	2JR	A	502	-	-	0/10/33/33	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	2JR	CAO-SAP	-11.66	1.57	1.73
3	A	502	2JR	CAQ-SAP	-6.23	1.62	1.74
3	A	502	2JR	CAD-CAC	-4.78	1.33	1.41
3	A	502	2JR	CAM-CAL	-3.58	1.33	1.42
3	A	502	2JR	CAO-NAF	2.31	1.34	1.31
2	A	501	FAD	C5A-C4A	3.12	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C8-C7	3.23	1.49	1.41
2	A	501	FAD	C9A-C5X	3.46	1.49	1.42
2	A	501	FAD	C4-C4X	3.88	1.48	1.41
2	A	501	FAD	C4X-C10	4.27	1.48	1.41
3	A	502	2JR	CAR-CAQ	5.76	1.59	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	2JR	CAW-NAU-CAV	-9.35	87.23	106.40
3	A	502	2JR	CAX-CAY-CAV	-6.68	86.09	105.28
2	A	501	FAD	N3A-C2A-N1A	-5.94	123.68	128.86
3	A	502	2JR	CAY-CAX-CAW	-5.39	89.77	105.28
2	A	501	FAD	C4-C4X-C10	-4.20	116.56	119.96
3	A	502	2JR	CAG-CAQ-SAP	-4.12	107.91	112.00
2	A	501	FAD	C4X-C4-N3	-3.51	118.48	123.48
3	A	502	2JR	CAS-CAR-NAU	-2.96	103.51	109.95
2	A	501	FAD	C4A-C5A-N7A	-2.91	106.60	109.41
3	A	502	2JR	CAH-CAR-CAS	-2.22	104.60	108.26
2	A	501	FAD	C1'-N10-C10	2.26	120.82	118.50
2	A	501	FAD	C5X-C9A-N10	2.55	119.55	117.66
2	A	501	FAD	C1'-N10-C9A	2.69	120.81	118.35
2	A	501	FAD	C4-C4X-N5	3.19	122.18	118.68
2	A	501	FAD	C4X-N5-C5X	3.82	120.79	116.76
3	A	502	2JR	CAY-CAV-NAU	6.36	112.89	103.97
3	A	502	2JR	CAX-CAW-NAU	6.61	113.24	103.97
2	A	501	FAD	C4-N3-C2	8.11	122.25	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	7	0
3	A	502	2JR	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 ⓘ

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(Å²)	Q<0.9
1	A	482/492 (97%)	-0.22	7 (1%)	74	67	51, 78, 102, 115	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	ASP	3.3
1	A	263	ALA	3.2
1	A	31	ARG	3.0
1	A	214	LYS	2.8
1	A	119	GLU	2.7
1	A	95	ASN	2.3
1	A	146	SER	2.3

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	2JR	A	502	25/25	0.70	0.42	4.98	93,111,122,129	0
2	FAD	A	501	53/53	0.93	0.19	0.97	64,71,88,90	0

6.5 Other polymers ⓘ

There are no such residues in this entry.