



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:58 AM GMT

PDB ID : 3GRS
Title : REFINED STRUCTURE OF GLUTATHIONE REDUCTASE AT 1.54
ANGSTROMS RESOLUTION
Authors : Schulz, G.E.; Karplus, P.A.
Deposited on : 1988-02-05
Resolution : 1.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

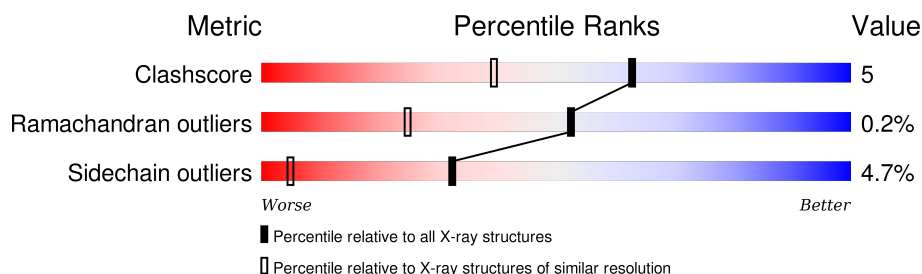
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1627 (1.56-1.52)
Ramachandran outliers	100387	1594 (1.56-1.52)
Sidechain outliers	100360	1592 (1.56-1.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	 74% 18% • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4080 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 GLUTATHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	461	3499	2212	603	660	24	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is water.

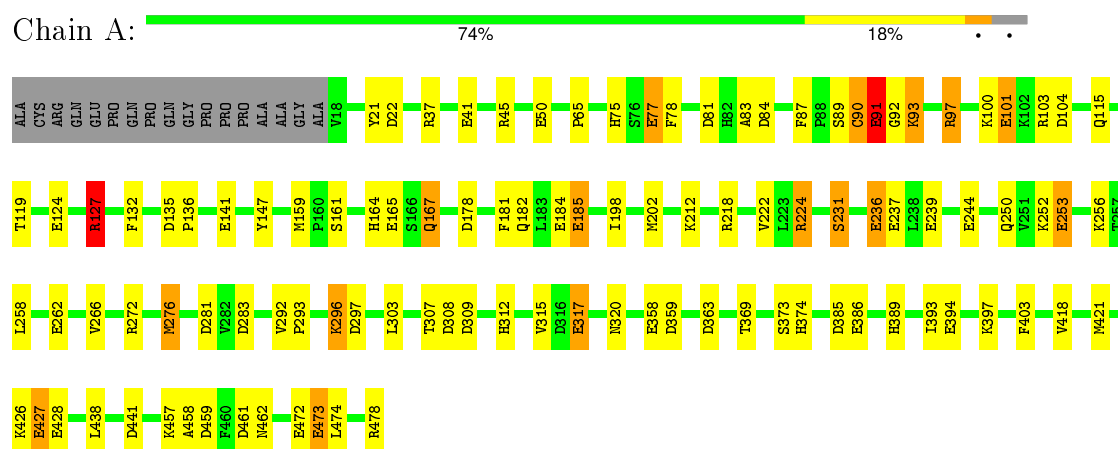
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	523	Total	O	0	0
			523	523		

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.

Note EDS was not executed.

• Molecule 1: GLUTATHIONE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	119.80 Å 84.50 Å 63.20 Å 90.00° 90.00° 58.70°	Depositor
Resolution (Å)	10.00 – 1.54	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.54)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4080	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	1.42	40/3566 (1.1%)	1.35	49/4824 (1.0%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	GLU	CD-OE2	11.32	1.38	1.25
1	A	185	GLU	CD-OE2	10.46	1.37	1.25
1	A	77	GLU	CD-OE2	10.37	1.37	1.25
1	A	253	GLU	CD-OE2	9.77	1.36	1.25
1	A	358	GLU	CD-OE2	9.63	1.36	1.25
1	A	231	SER	CB-OG	-9.59	1.29	1.42
1	A	236	GLU	CD-OE2	9.44	1.36	1.25
1	A	91	GLU	CD-OE2	9.17	1.35	1.25
1	A	317	GLU	CD-OE2	8.55	1.35	1.25
1	A	124	GLU	CD-OE2	8.52	1.35	1.25
1	A	394	GLU	CD-OE2	8.34	1.34	1.25
1	A	262	GLU	CD-OE2	8.05	1.34	1.25
1	A	185	GLU	CG-CD	7.99	1.64	1.51
1	A	473	GLU	CD-OE2	7.70	1.34	1.25
1	A	239	GLU	CD-OE2	7.24	1.33	1.25
1	A	161	SER	CB-OG	-7.18	1.32	1.42
1	A	165	GLU	CD-OE2	7.04	1.33	1.25
1	A	185	GLU	CB-CG	6.97	1.65	1.52
1	A	101	GLU	CD-OE2	6.96	1.33	1.25
1	A	386	GLU	CD-OE2	6.72	1.33	1.25
1	A	428	GLU	CD-OE1	-6.49	1.18	1.25
1	A	472	GLU	CD-OE1	-6.33	1.18	1.25
1	A	141	GLU	CD-OE2	6.26	1.32	1.25
1	A	45	ARG	CZ-NH2	6.05	1.41	1.33
1	A	237	GLU	CD-OE2	5.97	1.32	1.25
1	A	37	ARG	CZ-NH2	5.87	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	GLU	CD-OE1	-5.87	1.19	1.25
1	A	127	ARG	NE-CZ	5.75	1.40	1.33
1	A	127	ARG	CZ-NH2	5.62	1.40	1.33
1	A	427	GLU	CB-CG	5.55	1.62	1.52
1	A	50	GLU	CD-OE2	5.50	1.31	1.25
1	A	97	ARG	NE-CZ	5.48	1.40	1.33
1	A	427	GLU	CG-CD	5.37	1.60	1.51
1	A	41	GLU	CD-OE2	5.34	1.31	1.25
1	A	231	SER	CA-CB	-5.33	1.45	1.52
1	A	45	ARG	CZ-NH1	5.24	1.39	1.33
1	A	389	HIS	CG-CD2	5.14	1.44	1.35
1	A	272	ARG	CZ-NH2	5.09	1.39	1.33
1	A	97	ARG	CZ-NH1	5.07	1.39	1.33
1	A	244	GLU	CD-OE2	5.00	1.31	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	GLU	C-N-CA	-11.84	97.43	122.30
1	A	308	ASP	CB-CG-OD1	9.12	126.51	118.30
1	A	478	ARG	NE-CZ-NH2	8.75	124.68	120.30
1	A	283	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	A	309	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	A	218	ARG	NE-CZ-NH2	8.51	124.56	120.30
1	A	308	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	A	147	TYR	CB-CG-CD2	8.29	125.98	121.00
1	A	218	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	461	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	297	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	A	127	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	A	359	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	147	TYR	CB-CG-CD1	-7.31	116.61	121.00
1	A	22	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	478	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	A	84	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	104	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	359	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	104	ASP	CB-CG-OD1	7.08	124.68	118.30
1	A	385	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	272	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	135	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	224	ARG	NE-CZ-NH2	6.46	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	MET	CB-CA-C	-6.41	97.58	110.40
1	A	281	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	309	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	283	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	178	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	84	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	178	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	459	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	363	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	297	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	81	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	21	TYR	CB-CG-CD1	-5.74	117.55	121.00
1	A	92	GLY	N-CA-C	5.71	127.38	113.10
1	A	441	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	103	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	441	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	92	GLY	CA-C-N	-5.49	105.12	117.20
1	A	461	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	91	GLU	CA-C-N	5.38	126.97	116.20
1	A	159	MET	CA-CB-CG	5.29	122.29	113.30
1	A	22	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	369	THR	CA-CB-CG2	-5.20	105.13	112.40
1	A	281	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	385	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	135	ASP	CB-CG-OD1	5.16	122.94	118.30

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	3499	0	3537	38	1
2	A	5	0	0	0	0
3	A	53	0	31	0	0
4	A	523	0	0	12	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4080	0	3568	38	2

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 5.

All (38) 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:127:ARG:HD2	4:A:725:HOH:O	1.86	0.75
1:A:224:ARG:HD2	4:A:990:HOH:O	1.90	0.72
1:A:266:VAL:HG22	1:A:276:MET:HG2	1.71	0.72
1:A:296:LYS:HB2	4:A:584:HOH:O	1.89	0.71
1:A:93:LYS:O	1:A:93:LYS:HG2	1.95	0.67
1:A:164:HIS:HB2	4:A:930:HOH:O	1.97	0.64
1:A:185:GLU:HG3	4:A:810:HOH:O	2.00	0.60
1:A:91:GLU:HG3	1:A:91:GLU:O	2.02	0.58
1:A:373:SER:HB2	4:A:997:HOH:O	2.05	0.56
1:A:77:GLU:OE1	1:A:374:HIS:ND1	2.39	0.55
1:A:236:GLU:HG2	4:A:934:HOH:O	2.06	0.54
1:A:222:VAL:O	1:A:231:SER:HB2	2.07	0.54
1:A:315:VAL:HA	1:A:320:ASN:O	2.11	0.51
1:A:393:ILE:O	1:A:393:ILE:HG22	2.11	0.50
1:A:421:MET:SD	1:A:457:LYS:HD3	2.52	0.49
1:A:167:GLN:HG2	4:A:648:HOH:O	2.13	0.49
1:A:115:GLN:O	1:A:119:THR:HG23	2.13	0.48
1:A:458:ALA:HA	4:A:756:HOH:O	2.13	0.47
1:A:100:LYS:O	1:A:100:LYS:HG2	2.12	0.46
1:A:198:ILE:O	1:A:202:MET:HG2	2.17	0.45
1:A:403:PHE:CE1	1:A:473:GLU:HG3	2.51	0.45
1:A:462:ASN:ND2	4:A:1003:HOH:O	2.50	0.45
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.82	0.45
1:A:78:PHE:HD2	1:A:78:PHE:HA	1.74	0.45
1:A:252:LYS:HG3	4:A:980:HOH:O	2.16	0.44
1:A:250:GLN:NE2	4:A:924:HOH:O	2.51	0.43
1:A:292:VAL:HG23	1:A:293:PRO:HD2	2.00	0.43
1:A:474:LEU:HD23	1:A:474:LEU:HA	1.91	0.43
1:A:132:PHE:CD2	1:A:303:LEU:HD12	2.54	0.43
1:A:307:THR:HA	1:A:312:HIS:O	2.18	0.43
1:A:418:VAL:O	1:A:418:VAL:HG23	2.19	0.42
1:A:65:PRO:HB2	1:A:181:PHE:CE1	2.55	0.42
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NH1	1:A:101:GLU:OE2	2.52	0.41
1:A:393:ILE:HG23	1:A:393:ILE:HD13	1.86	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.98	0.41
1:A:202:MET:HA	1:A:202:MET:CE	2.51	0.41
1:A:83:ALA:HA	1:A:87:PHE:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:580:HOH:O	4:A:580:HOH:O[2_665]	0.58	1.62
1:A:90:CYS:SG	1:A:90:CYS:SG[2_665]	1.66	0.54

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	459/478 (96%)	443 (96%)	15 (3%)	1 (0%)	52 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	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	382/393 (97%)	364 (95%)	18 (5%)	32 5

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	89	SER
1	A	90	CYS
1	A	91	GLU
1	A	93	LYS
1	A	127	ARG
1	A	167	GLN
1	A	182	GLN
1	A	184	GLU
1	A	212	LYS
1	A	253	GLU
1	A	256	LYS
1	A	276	MET
1	A	296	LYS
1	A	317	GLU
1	A	397	LYS
1	A	426	LYS
1	A	427	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	117	ASN
1	A	182	GLN
1	A	301	ASN
1	A	366	ASN
1	A	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
3	FAD	A	479	-	48,58,58	1.69	6 (12%)	54,89,89	1.73	7 (12%)
2	PO4	A	480	-	4,4,4	0.89	0	6,6,6	0.31	0

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
3	FAD	A	479	-	-	0/30/50/50	0/6/6/6
2	PO4	A	480	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	479	FAD	C10-N10	-4.75	1.33	1.39
3	A	479	FAD	PA-O2A	-4.55	1.35	1.54
3	A	479	FAD	P-O2P	-3.70	1.39	1.54
3	A	479	FAD	C4X-C10	2.21	1.45	1.41
3	A	479	FAD	O5'-C5'	3.89	1.60	1.44
3	A	479	FAD	O4B-C1B	4.84	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	479	FAD	C4X-C4-N3	-5.03	116.72	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	479	FAD	C4B-O4B-C1B	-3.55	105.82	109.72
3	A	479	FAD	O4B-C1B-N9A	-3.31	101.18	108.10
3	A	479	FAD	O5B-PA-O1A	-3.11	97.56	109.62
3	A	479	FAD	C2A-N1A-C6A	2.16	122.62	118.77
3	A	479	FAD	O3P-P-O5'	2.32	109.10	102.94
3	A	479	FAD	C4-N3-C2	6.82	121.14	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.