



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:53 AM UTC

PDB ID : 1GER / pdb_00001ger
Title : THE STRUCTURE OF GLUTATHIONE REDUCTASE FROM ES-
CHERICHIA COLI AT 1.86 ANGSTROMS RESOLUTION: COMPARISON
WITH THE ENZYME FROM HUMAN ERYTHROCYTES
Authors : Mittl, P.R.E.; Schulz, G.E.
Deposited on : 1994-01-18
Resolution : 1.86 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

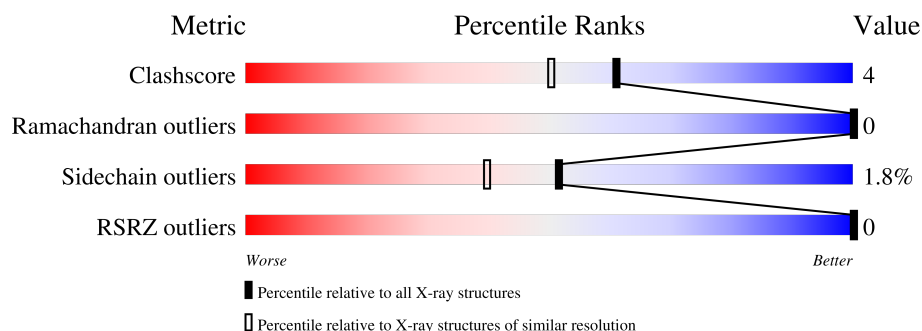
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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.

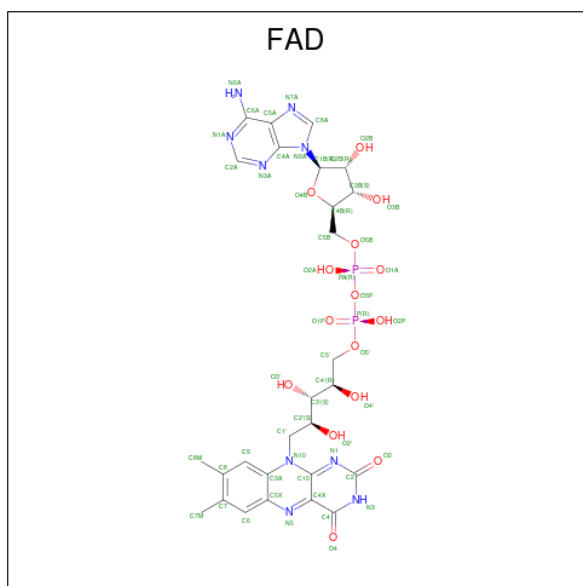
Mol	Chain	Length	Quality of chain
1	A	450	
1	B	450	

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
1	A	448	Total 3415	C 2156	N 589	O 652	S 18	0	1	0
1	B	449	Total 3422	C 2160	N 590	O 654	S 18	0	1	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

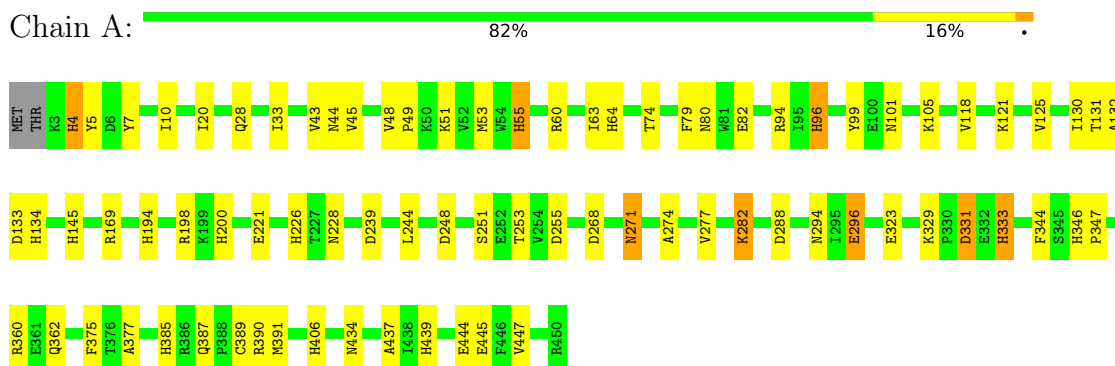
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	315	Total 315	O 315	0	0
3	B	330	Total 330	O 330	0	0

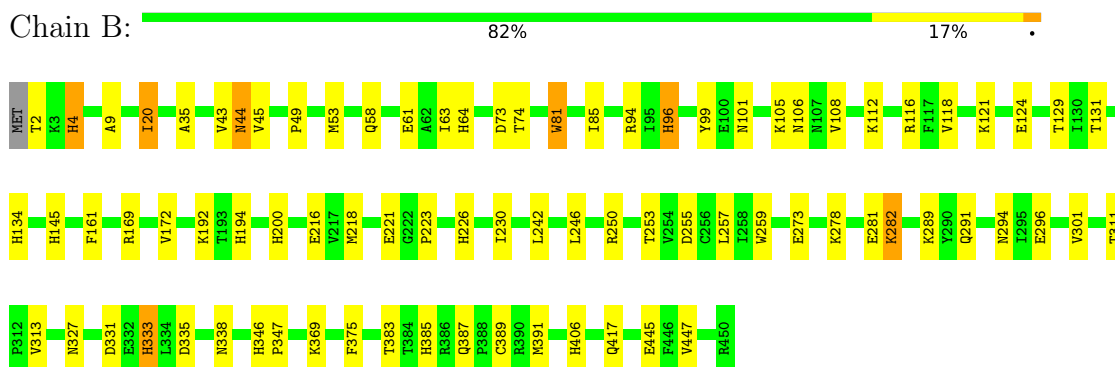
3 Residue-property plots

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: GLUTATHIONE REDUCTASE



• Molecule 1: GLUTATHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, α , β , γ	120.50Å 73.60Å 60.50Å 90.00° 90.00° 83.00°	Depositor
Resolution (Å)	7.00 – 1.86 7.00 – 1.86	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.86) 93.1 (7.00-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.168 , (Not available) 0.159 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7588	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 21.55 % 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 6.8521e-03.*

¹Theoretical 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: 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	1.10	19/3490 (0.5%)	1.65	31/4737 (0.7%)
1	B	1.15	19/3497 (0.5%)	1.65	35/4747 (0.7%)
All	All	1.13	38/6987 (0.5%)	1.65	66/9484 (0.7%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	VAL	CA-CB	7.54	1.63	1.54
1	B	333	HIS	CD2-NE2	-7.49	1.29	1.37
1	A	194	HIS	CD2-NE2	-7.38	1.29	1.37
1	A	333	HIS	CD2-NE2	-7.34	1.29	1.37
1	B	194	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	145	HIS	CD2-NE2	-6.87	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	145	HIS	CD2-NE2	-6.76	1.30	1.37
1	B	4	HIS	CD2-NE2	-6.67	1.30	1.37
1	B	385	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	346	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	406	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	226	HIS	CG-ND1	-6.15	1.31	1.38
1	B	406	HIS	CG-ND1	-6.11	1.31	1.38
1	B	301	VAL	CA-CB	6.08	1.65	1.55
1	A	48	VAL	CA-CB	6.03	1.61	1.54
1	A	64	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	439	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	134	HIS	CD2-NE2	-5.93	1.31	1.37
1	B	64	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	4	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	346	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	447	VAL	CA-CB	5.76	1.62	1.54
1	B	230	ILE	CA-CB	-5.75	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	VAL	CA-CB	5.74	1.62	1.54
1	B	108	VAL	CA-CB	5.66	1.61	1.54
1	A	200	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	55	HIS	CD2-NE2	-5.62	1.31	1.37
1	B	200	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	10	ILE	CA-C	5.40	1.59	1.53
1	A	406	HIS	CD2-NE2	-5.37	1.31	1.37
1	A	385	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	145	HIS	CG-ND1	-5.24	1.32	1.38
1	B	383	THR	CA-CB	5.16	1.61	1.53
1	A	96	HIS	CD2-NE2	-5.16	1.32	1.37
1	A	45	VAL	CA-CB	5.15	1.61	1.54
1	B	226	HIS	CD2-NE2	-5.07	1.32	1.37
1	A	333	HIS	CG-ND1	-5.01	1.32	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	VAL	N-CA-C	-12.53	100.79	111.56
1	A	94	ARG	NE-CZ-NH2	-12.31	108.12	119.20
1	B	94	ARG	NE-CZ-NH2	-12.07	108.33	119.20
1	A	118	VAL	N-CA-C	-10.02	102.15	111.67
1	A	434	ASN	CA-CB-CG	-7.97	104.63	112.60
1	B	194	HIS	CB-CG-CD2	-7.64	121.26	131.20
1	A	94	ARG	NE-CZ-NH1	7.48	128.98	121.50
1	A	94	ARG	CG-CD-NE	-7.46	95.58	112.00
1	B	94	ARG	CG-CD-NE	-7.29	95.97	112.00
1	A	385	HIS	CB-CG-CD2	-7.24	121.79	131.20
1	A	346	HIS	CB-CG-CD2	-7.20	121.83	131.20
1	B	94	ARG	NE-CZ-NH1	7.19	128.69	121.50
1	B	172	VAL	N-CA-C	-6.72	98.70	108.11
1	A	268	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	125	VAL	N-CA-C	-6.62	99.20	108.27
1	B	161	PHE	CA-CB-CG	-6.59	107.21	113.80
1	B	73	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	385	HIS	CB-CG-CD2	-6.57	122.65	131.20
1	A	134	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	A	439	HIS	CB-CG-CD2	-6.48	122.77	131.20
1	A	194	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	B	346	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	B	2	THR	N-CA-CB	-6.39	100.64	111.50
1	B	296	GLU	CB-CG-CD	6.31	123.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	145	HIS	CB-CG-CD2	-6.23	123.11	131.20
1	A	28	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	B	64	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	B	134	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	B	346	HIS	CA-CB-CG	-6.09	107.70	113.80
1	B	289	LYS	CA-CB-CG	6.04	126.19	114.10
1	B	145	HIS	CA-CB-CG	-6.00	107.81	113.80
1	B	338	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	253	THR	CA-CB-OG1	-5.87	100.79	109.60
1	A	96	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	B	335	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	64	HIS	N-CA-CB	-5.70	102.15	110.47
1	A	248	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	291	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	390	ARG	CA-CB-CG	-5.67	102.77	114.10
1	A	346	HIS	CB-CG-ND1	5.65	131.17	122.70
1	A	271	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	B	44	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	60	ARG	CA-CB-CG	-5.49	103.12	114.10
1	B	313	VAL	CA-C-O	-5.42	114.51	120.96
1	A	64	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	288	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	80	ASN	OD1-CG-ND2	5.39	127.99	122.60
1	B	106	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	B	291	GLN	CG-CD-NE2	5.38	124.47	116.40
1	B	311	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	406	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	B	81	TRP	CG-CD2-CE3	5.37	139.27	133.90
1	B	61	GLU	CA-CB-CG	-5.37	103.36	114.10
1	A	82	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	344	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	44	ASN	CB-CG-ND2	5.33	124.39	116.40
1	A	362	GLN	N-CA-C	5.32	118.00	111.82
1	B	112	LYS	CB-CG-CD	5.30	123.49	111.30
1	B	96	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	B	417	GLN	N-CA-C	5.24	116.67	111.07
1	A	271	ASN	CA-C-O	5.18	127.71	121.65
1	A	79	PHE	N-CA-C	-5.17	98.97	108.02
1	A	239	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	58	GLN	CG-CD-NE2	5.05	123.98	116.40
1	B	216	GLU	CB-CA-C	-5.05	102.73	110.81

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	3415	0	3375	31	0
1	B	3422	0	3382	28	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	315	0	0	2	0
3	B	330	0	0	4	0
All	All	7588	0	6819	58	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 4.

All (58) 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:4:HIS:HD2	1:B:131:THR:HG23	1.39	0.85
1:A:74:THR:HB	3:B:593:HOH:O	1.84	0.77
1:B:74:THR:HB	3:B:593:HOH:O	1.85	0.75
1:B:4:HIS:CD2	1:B:131:THR:HG23	2.23	0.73
1:B:389[A]:CYS:SG	1:B:391:MET:HE3	2.30	0.70
1:A:389[A]:CYS:SG	1:A:391:MET:HE3	2.33	0.69
1:A:4:HIS:HD2	1:A:131:THR:HG23	1.57	0.67
1:B:389[B]:CYS:SG	1:B:391:MET:HE3	2.35	0.66
1:B:331:ASP:O	1:B:333:HIS:HD2	1.82	0.62
1:A:4:HIS:CD2	1:A:131:THR:HG23	2.35	0.61
1:A:375:PHE:CE1	1:A:445:GLU:HG3	2.35	0.61
1:A:282:LYS:HD2	1:A:282:LYS:H	1.68	0.59
1:B:44:ASN:OD1	1:B:96:HIS:HE1	1.87	0.57
1:A:389[A]:CYS:HG	1:A:391:MET:HE3	1.70	0.55
1:A:377:ALA:HB2	1:A:389[B]:CYS:SG	2.47	0.55
1:B:375:PHE:CE1	1:B:445:GLU:HG3	2.43	0.53
1:B:389[A]:CYS:HG	1:B:391:MET:HE3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HE3	3:A:661:HOH:O	2.11	0.50
1:B:278:LYS:HE3	1:B:294:ASN:HB3	1.94	0.49
1:A:44:ASN:OD1	1:A:96:HIS:HE1	1.94	0.49
1:A:63:ILE:HG12	1:B:63:ILE:HG12	1.93	0.49
1:A:296:GLU:H	1:A:296:GLU:CD	2.22	0.48
1:A:375:PHE:CZ	1:A:445:GLU:HG3	2.48	0.48
1:B:169:ARG:HD3	1:B:255:ASP:OD2	2.14	0.48
1:B:35:ALA:HB1	3:B:733:HOH:O	2.13	0.48
1:B:218:MET:HG2	1:B:223:PRO:HD2	1.94	0.47
1:B:43:VAL:HG21	1:B:99:TYR:HE2	1.79	0.47
1:A:347:PRO:HB3	1:A:387:GLN:OE1	2.16	0.46
1:B:101:ASN:OD1	1:B:105:LYS:HE2	2.15	0.46
1:A:169:ARG:HD3	1:A:255:ASP:OD2	2.15	0.46
1:A:96:HIS:HD2	3:A:569:HOH:O	1.99	0.45
1:B:49:PRO:O	1:B:53:MET:HG2	2.16	0.45
1:A:5:TYR:O	1:A:132:ALA:HA	2.17	0.44
1:B:389[B]:CYS:HG	1:B:391:MET:HE3	1.81	0.44
1:A:49:PRO:O	1:A:53:MET:HG2	2.17	0.44
1:A:360:ARG:HG2	1:A:360:ARG:HH11	1.83	0.44
1:B:242:LEU:O	1:B:253:THR:HA	2.19	0.43
1:B:281:GLU:HB2	1:B:282:LYS:HE3	2.00	0.43
1:A:323:GLU:HB3	1:A:329:LYS:HD2	1.99	0.43
1:A:271:ASN:OD1	1:A:274:ALA:HB2	2.19	0.43
1:B:81:TRP:O	1:B:85:ILE:HG12	2.18	0.43
1:A:51:LYS:HE2	1:A:55:HIS:CE1	2.54	0.43
1:B:246:LEU:HD12	1:B:250:ARG:HB2	2.00	0.43
1:B:44:ASN:OD1	1:B:96:HIS:CE1	2.69	0.43
1:A:101:ASN:OD1	1:A:105:LYS:HE2	2.18	0.43
1:A:198:ARG:O	1:A:228:ASN:HA	2.19	0.43
1:A:43:VAL:HG21	1:A:99:TYR:HE2	1.84	0.42
1:A:244:LEU:O	1:A:251:SER:HA	2.20	0.42
1:B:257:LEU:HD21	1:B:259:TRP:CZ2	2.55	0.41
1:A:331:ASP:O	1:A:333:HIS:HD2	2.03	0.41
1:A:33:ILE:HD11	1:A:130:ILE:HD11	2.02	0.41
1:A:437:ALA:HB1	1:A:444:GLU:HB2	2.03	0.41
1:B:347:PRO:HB3	1:B:387:GLN:OE1	2.21	0.41
1:A:277:VAL:HA	1:A:294:ASN:OD1	2.21	0.41
1:A:7:TYR:CD2	1:A:20:ILE:HD12	2.56	0.40
1:B:369:LYS:HA	1:B:369:LYS:HD2	1.98	0.40
1:B:9:ALA:HB2	1:B:20:ILE:HD13	2.03	0.40
1:B:116:ARG:HD3	3:B:746:HOH:O	2.20	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	447/450 (99%)	431 (96%)	16 (4%)	0	100	100
1	B	448/450 (100%)	434 (97%)	14 (3%)	0	100	100
All	All	895/900 (99%)	865 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	361/362 (100%)	356 (99%)	5 (1%)	59	49
1	B	362/362 (100%)	354 (98%)	8 (2%)	45	32
All	All	723/724 (100%)	710 (98%)	13 (2%)	51	40

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

Mol	Chain	Res	Type
1	A	133	ASP
1	A	221	GLU
1	A	282	LYS
1	A	296	GLU
1	A	331	ASP

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Mol	Chain	Res	Type
1	B	20	ILE
1	B	121	LYS
1	B	124	GLU
1	B	129	THR
1	B	192	LYS
1	B	221	GLU
1	B	273	GLU
1	B	282	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	28	GLN
1	A	55	HIS
1	A	64	HIS
1	A	96	HIS
1	A	237	ASN
1	A	327	ASN
1	A	333	HIS
1	B	4	HIS
1	B	55	HIS
1	B	77	ASN
1	B	96	HIS
1	B	200	HIS
1	B	237	ASN
1	B	327	ASN
1	B	333	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 oligosaccharides 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	451	-	58,58,58	1.26	6 (10%)	85,89,89	1.20	9 (10%)
2	FAD	B	451	-	58,58,58	1.26	8 (13%)	85,89,89	1.05	5 (5%)

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	451	-	-	4/34/50/50	0/6/6/6
2	FAD	B	451	-	-	3/34/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	FAD	P-O3P	-3.88	1.55	1.59
2	B	451	FAD	PA-O3P	-3.34	1.55	1.59
2	B	451	FAD	P-O3P	-3.01	1.56	1.59
2	A	451	FAD	C5A-C4A	2.96	1.44	1.39
2	B	451	FAD	C9A-N10	-2.72	1.36	1.41
2	A	451	FAD	C5X-N5	-2.71	1.34	1.39
2	A	451	FAD	P-O2P	-2.55	1.43	1.55
2	B	451	FAD	C4'-C3'	2.44	1.57	1.53
2	A	451	FAD	C6-C7	2.22	1.42	1.39
2	B	451	FAD	C5X-N5	-2.19	1.35	1.39
2	A	451	FAD	PA-O2A	-2.17	1.45	1.55
2	B	451	FAD	C10-N1	2.07	1.37	1.33
2	B	451	FAD	C4X-N5	2.04	1.35	1.30
2	B	451	FAD	C1'-C2'	2.02	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	451	FAD	O2A-PA-O3P	3.11	115.67	107.27
2	B	451	FAD	O2A-PA-O3P	3.04	115.50	107.27
2	A	451	FAD	O4B-C1B-C2B	-2.92	100.37	106.62
2	B	451	FAD	C5'-C4'-C3'	-2.64	107.25	112.22
2	A	451	FAD	C4-N3-C2	-2.55	121.11	125.64
2	A	451	FAD	N3A-C2A-N1A	2.47	132.31	128.58
2	A	451	FAD	C4A-C5A-N7A	-2.38	107.86	110.58
2	B	451	FAD	C4-N3-C2	-2.27	121.61	125.64
2	A	451	FAD	C10-C4X-N5	-2.26	120.19	124.81
2	B	451	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
2	B	451	FAD	C5A-N7A-C8A	2.19	106.89	103.45
2	A	451	FAD	C10-N1-C2	2.09	121.38	116.85
2	A	451	FAD	C9-C9A-N10	2.02	124.57	121.85
2	A	451	FAD	O4'-C4'-C5'	-2.01	105.56	109.99

There are no chirality outliers.

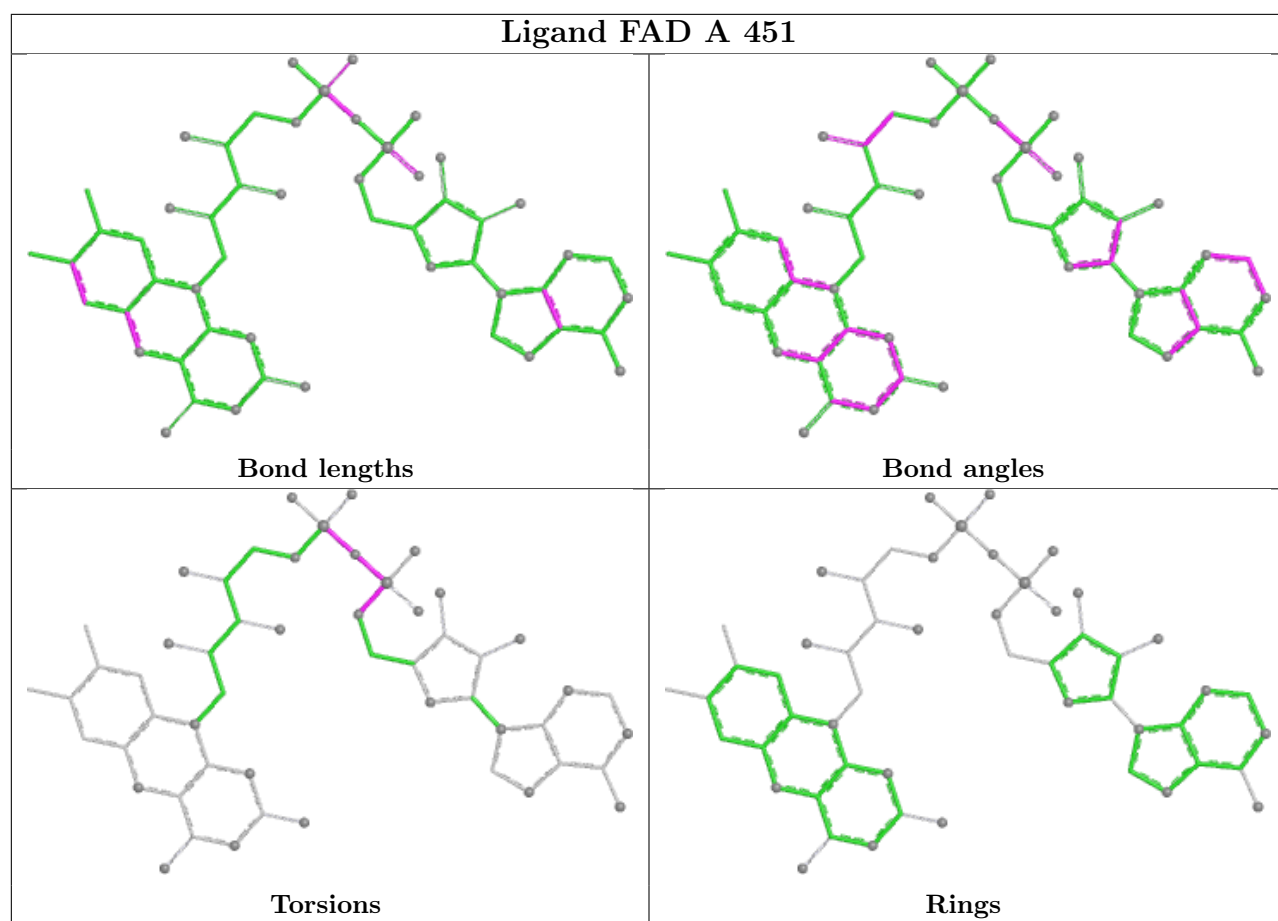
All (7) torsion outliers are listed below:

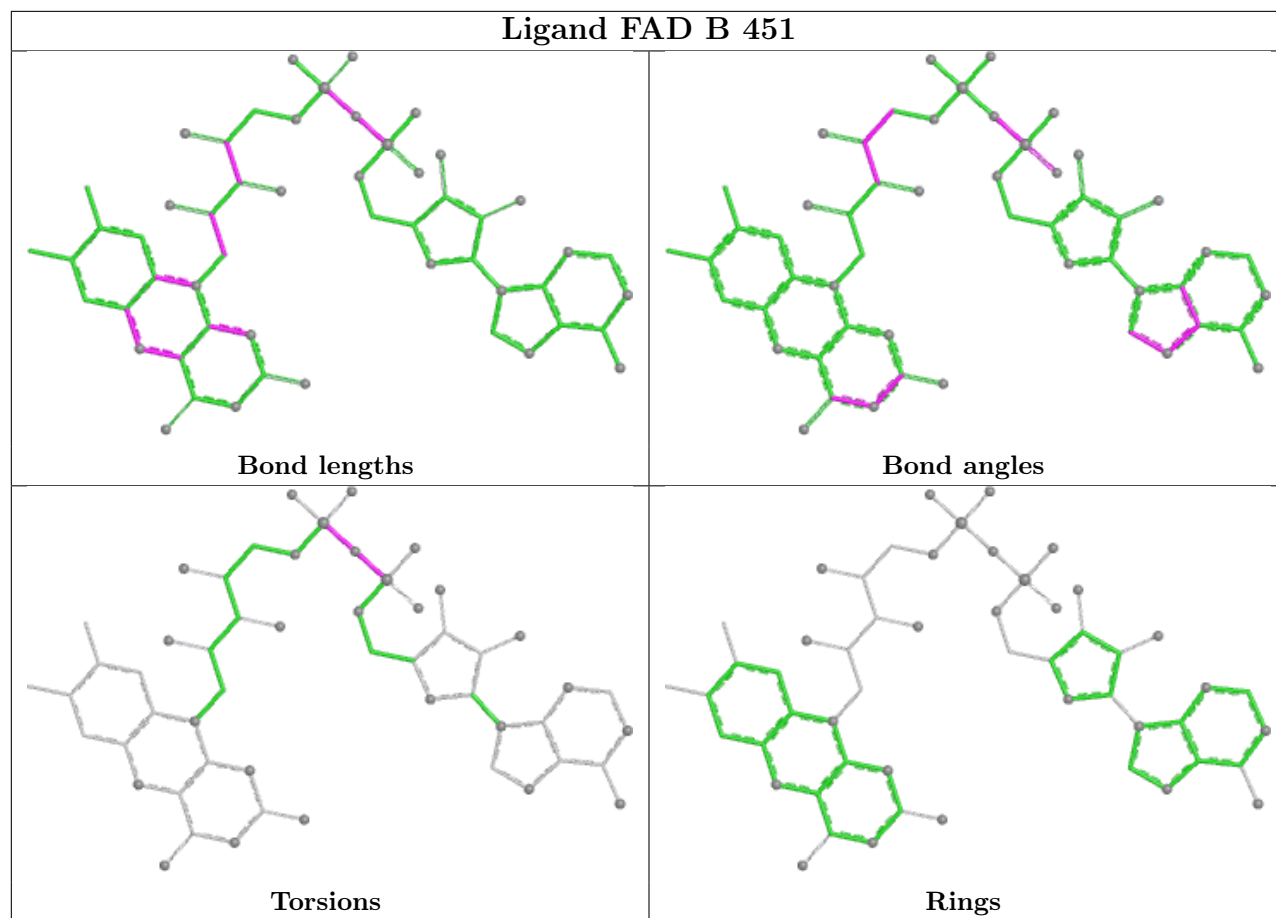
Mol	Chain	Res	Type	Atoms
2	B	451	FAD	P-O3P-PA-O1A
2	A	451	FAD	PA-O3P-P-O5'
2	B	451	FAD	PA-O3P-P-O5'
2	A	451	FAD	P-O3P-PA-O1A
2	A	451	FAD	P-O3P-PA-O2A
2	A	451	FAD	C5B-O5B-PA-O1A
2	B	451	FAD	P-O3P-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	448/450 (99%)	-1.03	0 100 100	9, 20, 50, 70	1 (0%)
1	B	449/450 (99%)	-1.09	0 100 100	7, 18, 44, 71	1 (0%)
All	All	897/900 (99%)	-1.06	0 100 100	7, 19, 48, 71	2 (0%)

There are no RSRZ outliers to report.

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](#)

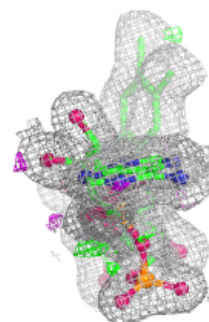
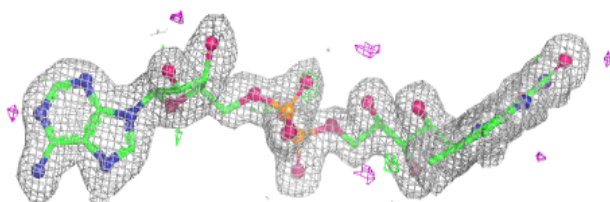
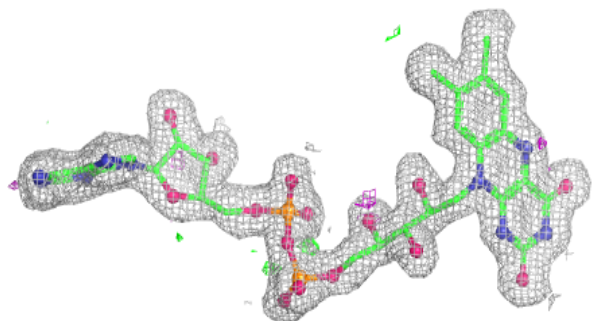
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	451	53/53	0.99	0.03	5,11,24,44	0
2	FAD	B	451	53/53	0.99	0.03	3,10,19,23	0

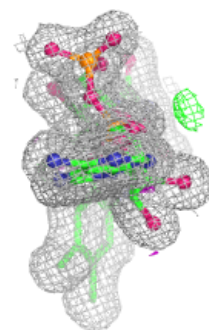
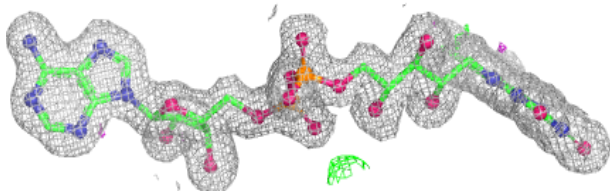
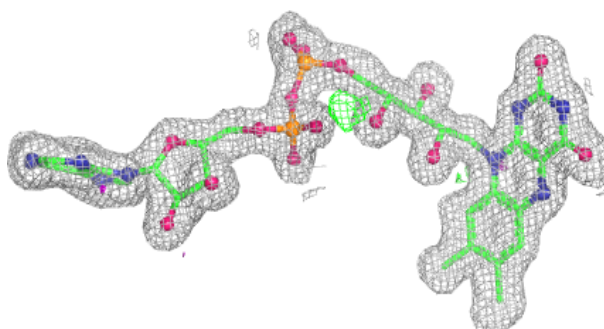
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 451:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD B 451:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.