



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:48 PM UTC

PDB ID : 1RP4 / pdb_00001rp4
Title : Structure of Ero1p, Source of Disulfide Bonds for Oxidative Protein Folding in the Cell
Authors : Gross, E.; Kastner, D.B.; Kaiser, C.A.; Fass, D.
Deposited on : 2003-12-03
Resolution : 2.20 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

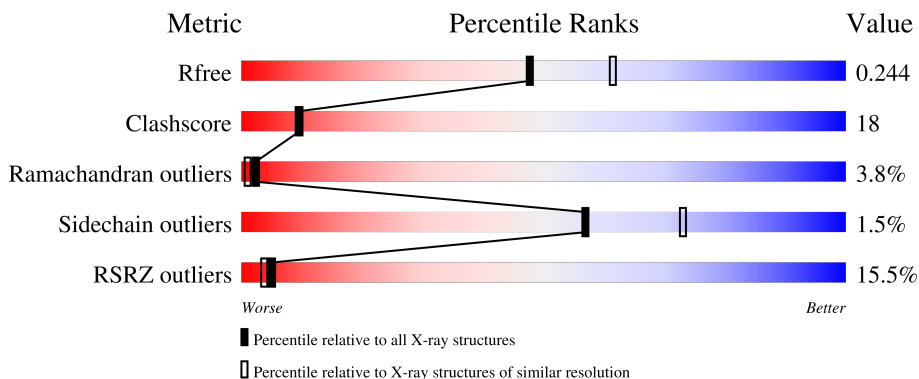
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	389	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3169 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 Hypothetical 65.0 kDa protein in COX14-COS3 intergenic region precursor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	Se	0	0	0
			3003	1911	496	578	11	7			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	cloning artifact	UNP Q03103
A	40	SER	-	cloning artifact	UNP Q03103
A	41	HIS	-	expression tag	UNP Q03103
A	42	HIS	-	expression tag	UNP Q03103
A	43	HIS	-	expression tag	UNP Q03103
A	44	HIS	-	expression tag	UNP Q03103
A	45	HIS	-	expression tag	UNP Q03103
A	46	HIS	-	expression tag	UNP Q03103
A	47	SER	-	cloning artifact	UNP Q03103
A	48	SER	-	cloning artifact	UNP Q03103
A	49	GLY	-	cloning artifact	UNP Q03103
A	50	LEU	-	cloning artifact	UNP Q03103
A	51	VAL	-	cloning artifact	UNP Q03103
A	52	PRO	-	cloning artifact	UNP Q03103
A	53	ARG	-	cloning artifact	UNP Q03103
A	54	GLY	-	cloning artifact	UNP Q03103
A	55	SER	-	cloning artifact	UNP Q03103
A	133	MSE	MET	modified residue	UNP Q03103
A	258	MSE	MET	modified residue	UNP Q03103
A	271	MSE	MET	modified residue	UNP Q03103
A	306	MSE	MET	modified residue	UNP Q03103
A	347	MSE	MET	modified residue	UNP Q03103
A	415	MSE	MET	modified residue	UNP Q03103
A	419	MSE	MET	modified residue	UNP Q03103
A	425	LEU	-	cloning artifact	UNP Q03103
A	426	GLU	-	cloning artifact	UNP Q03103

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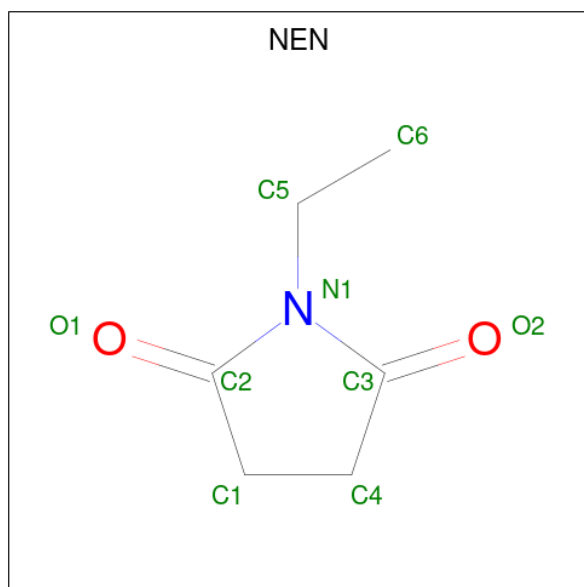
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Chain	Residue	Modelled	Actual	Comment	Reference
A	427	ARG	-	cloning artifact	UNP Q03103

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	Cd		0	0
			2	2			

- Molecule 3 is 1-ETHYL-PYRROLIDINE-2,5-DIONE (CCD ID: NEN) (formula: C₆H₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

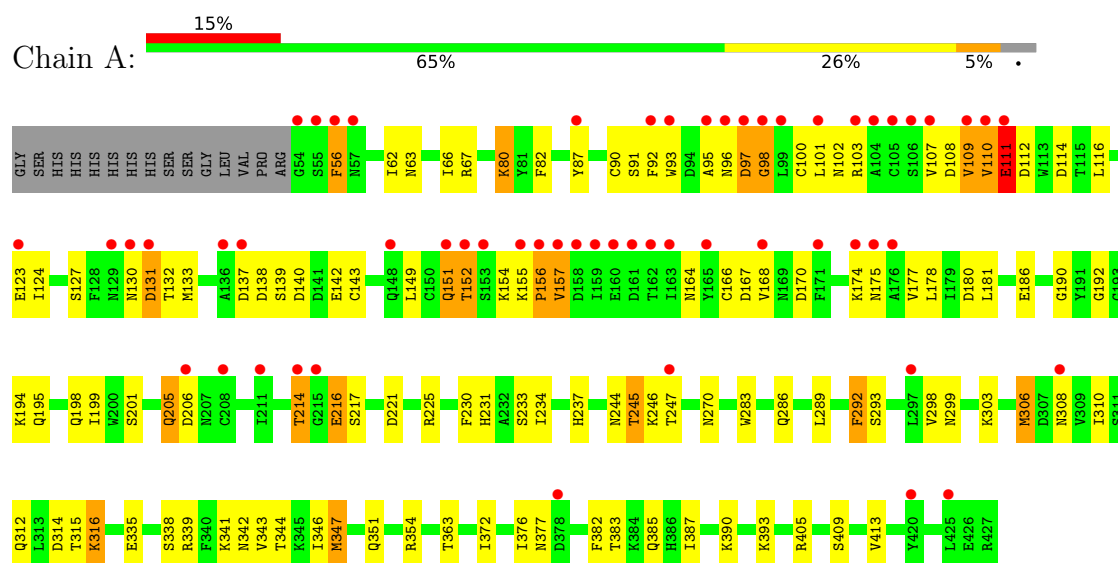
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	102	Total O 102 102	0	0

3 Residue-property plots [i](#)

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: Hypothetical 65.0 kDa protein in COX14-COS3 intergenic region precursor



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.47Å 134.33Å 102.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.20) 98.5 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.244 0.217 , 0.244	Depositor DCC
R_{free} test set	1756 reflections (6.81%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3169	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NEN, CD, 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	0.43	0/3058	0.87	5/4122 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	PRO	N-CA-CB	10.18	110.30	102.36
1	A	292	PHE	N-CA-C	5.98	120.19	113.01
1	A	306	MSE	N-CA-C	-5.48	105.32	112.23
1	A	80	LYS	N-CA-C	5.22	119.28	113.01
1	A	56	PHE	N-CA-C	-5.09	105.91	111.82

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	3003	0	2864	106	0
2	A	2	0	0	0	0
3	A	9	0	8	0	0
4	A	53	0	31	1	0
5	A	102	0	0	17	0
All	All	3169	0	2903	106	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 18.

All (106) 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:316:LYS:HD2	1:A:316:LYS:H	1.13	1.04
1:A:316:LYS:HD2	1:A:316:LYS:N	1.89	0.87
1:A:195:GLN:HE22	1:A:351:GLN:HG2	1.47	0.79
1:A:225:ARG:HH11	1:A:270:ASN:HD21	1.30	0.78
1:A:149:LEU:HD12	1:A:292:PHE:HB2	1.67	0.75
1:A:405:ARG:HD3	5:A:880:HOH:O	1.87	0.73
1:A:194:LYS:O	1:A:198:GLN:HG3	1.90	0.72
1:A:133:MSE:HE3	1:A:177:VAL:HG21	1.72	0.70
1:A:214:THR:HG23	5:A:821:HOH:O	1.93	0.69
1:A:138:ASP:HB3	1:A:164:ASN:ND2	2.10	0.67
1:A:221:ASP:HB2	5:A:894:HOH:O	1.96	0.66
1:A:225:ARG:NH1	1:A:270:ASN:HD21	1.93	0.65
1:A:142:GLU:HA	1:A:393:LYS:HB3	1.81	0.63
1:A:298:VAL:HG23	5:A:898:HOH:O	1.98	0.63
1:A:289:LEU:CD1	1:A:306:MSE:HE2	2.29	0.62
1:A:225:ARG:HH11	1:A:270:ASN:ND2	1.97	0.62
1:A:377:ASN:HA	5:A:901:HOH:O	2.00	0.61
1:A:344:THR:HA	5:A:885:HOH:O	1.99	0.61
1:A:110:VAL:HG12	1:A:111:GLU:OE1	2.01	0.60
1:A:195:GLN:NE2	1:A:351:GLN:HG2	2.16	0.60
1:A:154:LYS:HA	5:A:904:HOH:O	2.01	0.59
1:A:56:PHE:HB2	5:A:836:HOH:O	2.02	0.59
1:A:101:LEU:HD12	1:A:102:ASN:H	1.67	0.59
1:A:225:ARG:HG3	1:A:270:ASN:ND2	2.16	0.59
1:A:107:VAL:HB	1:A:109:VAL:HG23	1.83	0.59
1:A:382:PHE:O	1:A:385:GLN:HG3	2.02	0.58
1:A:137:ASP:OD2	1:A:139:SER:HB2	2.02	0.58
1:A:186:GLU:HB3	5:A:845:HOH:O	2.05	0.57
1:A:107:VAL:CG1	1:A:192:GLY:HA3	2.35	0.57
1:A:107:VAL:HG12	1:A:192:GLY:HA3	1.88	0.56
1:A:293:SER:HB2	1:A:299:ASN:O	2.05	0.55
1:A:244:ASN:HD21	1:A:247:THR:HG23	1.72	0.54
1:A:338:SER:O	1:A:341:LYS:HG2	2.07	0.54
1:A:140:ASP:OD2	1:A:178:LEU:HD21	2.08	0.54
1:A:110:VAL:HG11	1:A:116:LEU:HD11	1.89	0.53
1:A:133:MSE:CE	1:A:177:VAL:HG21	2.39	0.53
1:A:233:SER:O	1:A:237:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HD12	1:A:67:ARG:N	2.24	0.53
1:A:108:ASP:O	1:A:109:VAL:C	2.51	0.52
1:A:97:ASP:O	1:A:98:GLY:C	2.51	0.52
1:A:130:ASN:CG	1:A:131:ASP:H	2.17	0.52
1:A:405:ARG:HB3	5:A:880:HOH:O	2.09	0.52
1:A:409:SER:O	1:A:413:VAL:HG23	2.10	0.52
1:A:289:LEU:HD11	1:A:306:MSE:CE	2.40	0.52
1:A:347:MSE:SE	5:A:885:HOH:O	2.78	0.52
1:A:286:GLN:HB2	1:A:310:ILE:HG21	1.92	0.51
1:A:289:LEU:HD11	1:A:306:MSE:HE2	1.91	0.51
1:A:93:TRP:CZ2	1:A:195:GLN:HG3	2.45	0.51
1:A:127:SER:O	1:A:354:ARG:HD2	2.10	0.51
1:A:151:GLN:HG3	1:A:155:LYS:CB	2.41	0.51
1:A:289:LEU:HD13	1:A:306:MSE:HE2	1.91	0.51
1:A:66:ILE:HD12	1:A:66:ILE:C	2.36	0.51
1:A:347:MSE:HA	1:A:347:MSE:CE	2.41	0.51
1:A:303:LYS:C	1:A:303:LYS:HD3	2.36	0.51
1:A:201:SER:O	1:A:205:GLN:HB2	2.12	0.50
1:A:95:ALA:HA	1:A:351:GLN:HE22	1.76	0.50
1:A:237:HIS:CE1	1:A:405:ARG:NH1	2.79	0.50
1:A:195:GLN:HE22	1:A:351:GLN:H	1.60	0.50
1:A:283:TRP:CH2	1:A:314:ASP:HB2	2.47	0.49
1:A:123:GLU:CD	1:A:123:GLU:H	2.21	0.49
1:A:216:GLU:HG2	5:A:896:HOH:O	2.12	0.49
1:A:110:VAL:O	1:A:111:GLU:C	2.55	0.48
1:A:244:ASN:ND2	1:A:247:THR:HG23	2.28	0.48
1:A:237:HIS:ND1	5:A:845:HOH:O	2.34	0.48
1:A:347:MSE:HB2	5:A:885:HOH:O	2.14	0.47
1:A:230:PHE:CE1	1:A:234:ILE:HD11	2.50	0.47
1:A:237:HIS:CE1	1:A:405:ARG:HH11	2.34	0.46
1:A:231:HIS:HE1	4:A:634:FAD:H51A	1.80	0.46
1:A:383:THR:O	1:A:387:ILE:HG13	2.16	0.46
1:A:132:THR:HB	1:A:180:ASP:HB3	1.98	0.46
1:A:109:VAL:HG12	1:A:110:VAL:N	2.31	0.46
1:A:124:ILE:HD12	1:A:124:ILE:N	2.31	0.45
1:A:217:SER:HB2	5:A:879:HOH:O	2.15	0.45
1:A:130:ASN:CG	1:A:131:ASP:N	2.75	0.45
1:A:206:ASP:HB3	5:A:862:HOH:O	2.16	0.45
1:A:343:VAL:HG12	1:A:363:THR:HG21	1.99	0.45
1:A:67:ARG:C	1:A:67:ARG:HD3	2.41	0.45
1:A:149:LEU:CD1	1:A:292:PHE:HB2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:HG3	1:A:342:ASN:N	2.31	0.45
1:A:237:HIS:HE1	1:A:405:ARG:NH1	2.15	0.44
1:A:62:ILE:HD11	1:A:315:THR:HB	1.99	0.44
1:A:82:PHE:HB2	1:A:181:LEU:HD11	2.00	0.44
1:A:316:LYS:N	1:A:316:LYS:CD	2.66	0.44
1:A:143:CYS:HB3	1:A:166:CYS:HA	2.00	0.43
1:A:100:CYS:HB2	1:A:351:GLN:HG3	2.00	0.43
1:A:244:ASN:C	1:A:246:LYS:H	2.26	0.43
1:A:390:LYS:HG2	1:A:390:LYS:O	2.19	0.43
1:A:63:ASN:O	1:A:67:ARG:HB2	2.19	0.43
1:A:372:ILE:HG23	1:A:376:ILE:HD12	2.01	0.43
1:A:303:LYS:HB3	5:A:824:HOH:O	2.18	0.42
1:A:107:VAL:HG22	1:A:190:GLY:O	2.19	0.42
1:A:168:VAL:C	1:A:170:ASP:H	2.27	0.42
1:A:335:GLU:O	1:A:339:ARG:HG2	2.19	0.42
1:A:151:GLN:O	1:A:152:THR:C	2.62	0.42
1:A:116:LEU:HD22	1:A:245:THR:HB	2.02	0.41
1:A:164:ASN:O	1:A:168:VAL:HG23	2.20	0.41
1:A:164:ASN:OD1	1:A:167:ASP:HB2	2.20	0.41
1:A:156:PRO:O	1:A:157:VAL:C	2.63	0.41
1:A:90:CYS:C	1:A:92:PHE:H	2.28	0.41
1:A:308:ASN:O	1:A:312:GLN:HG3	2.19	0.41
1:A:195:GLN:O	1:A:199:ILE:HG13	2.20	0.41
1:A:103:ARG:HH22	1:A:114:ASP:CG	2.29	0.41
1:A:343:VAL:O	1:A:346:ILE:HG22	2.21	0.41
1:A:87:TYR:CD2	1:A:174:LYS:HD2	2.56	0.41
1:A:80:LYS:HB2	1:A:80:LYS:HE3	1.95	0.40
1:A:110:VAL:O	1:A:112:ASP:N	2.54	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	372/389 (96%)	336 (90%)	22 (6%)	14 (4%)	2 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	109	VAL
1	A	111	GLU
1	A	152	THR
1	A	91	SER
1	A	97	ASP
1	A	131	ASP
1	A	151	GLN
1	A	157	VAL
1	A	175	ASN
1	A	214	THR
1	A	245	THR
1	A	98	GLY
1	A	110	VAL

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	324/341 (95%)	319 (98%)	5 (2%)	57 73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	A	205	GLN
1	A	216	GLU
1	A	316	LYS
1	A	347	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	60	ASN
1	A	164	ASN
1	A	195	GLN
1	A	198	GLN
1	A	205	GLN
1	A	237	HIS
1	A	244	ASN
1	A	270	ASN
1	A	326	ASN
1	A	351	GLN
1	A	377	ASN
1	A	414	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	FAD	A	634	-	58,58,58	2.00	13 (22%)	85,89,89	3.67	47 (55%)
3	NEN	A	501	1	9,9,9	0.59	0	12,12,12	1.07	1 (8%)

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
4	FAD	A	634	-	-	9/34/50/50	0/6/6/6
3	NEN	A	501	1	-	0/2/15/15	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	634	FAD	C4X-N5	6.22	1.44	1.30
4	A	634	FAD	C9A-C5X	5.25	1.49	1.41
4	A	634	FAD	C4A-N3A	4.65	1.43	1.34
4	A	634	FAD	C2A-N3A	4.31	1.41	1.33
4	A	634	FAD	C9A-N10	4.18	1.48	1.41
4	A	634	FAD	C5A-C4A	-3.65	1.32	1.39
4	A	634	FAD	C5'-C4'	-3.41	1.47	1.51
4	A	634	FAD	C8A-N9A	3.04	1.42	1.37
4	A	634	FAD	C10-N1	2.52	1.38	1.33
4	A	634	FAD	C2B-C3B	-2.43	1.46	1.53
4	A	634	FAD	O4-C4	2.33	1.28	1.23
4	A	634	FAD	C1'-N10	-2.33	1.42	1.47
4	A	634	FAD	C6-C7	2.11	1.42	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	634	FAD	N3A-C2A-N1A	-10.23	113.10	128.58
4	A	634	FAD	C5X-C9A-N10	-9.87	109.05	117.97
4	A	634	FAD	C9-C9A-N10	9.58	134.74	121.85
4	A	634	FAD	C9A-N10-C10	8.72	134.05	120.75
4	A	634	FAD	C8M-C8-C7	8.20	137.50	120.76
4	A	634	FAD	C4A-N9A-C8A	-7.93	97.41	105.74
4	A	634	FAD	C8M-C8-C9	-7.87	105.70	119.57
4	A	634	FAD	C7M-C7-C6	-6.73	107.72	119.57
4	A	634	FAD	C5A-C4A-N9A	6.62	113.02	105.81
4	A	634	FAD	C10-N1-C2	5.73	129.25	116.85
4	A	634	FAD	C4-C4X-N5	5.27	125.48	118.21
4	A	634	FAD	C5X-N5-C4X	5.25	126.59	118.09
4	A	634	FAD	O2-C2-N3	4.84	127.87	118.58
4	A	634	FAD	N3-C2-N1	-4.50	109.94	119.50
4	A	634	FAD	C2A-N1A-C6A	4.42	125.99	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	634	FAD	C1'-N10-C9A	-4.36	112.15	120.63
4	A	634	FAD	O5'-P-O1P	-4.12	92.62	108.94
4	A	634	FAD	O3P-PA-O1A	-4.01	98.63	110.70
4	A	634	FAD	C9A-C5X-N5	-3.98	118.23	122.45
4	A	634	FAD	C2A-N3A-C4A	3.85	121.23	111.83
4	A	634	FAD	C2'-C1'-N10	3.74	127.87	110.20
4	A	634	FAD	O3B-C3B-C4B	-3.57	100.82	111.08
4	A	634	FAD	O2A-PA-O1A	3.40	128.24	112.44
4	A	634	FAD	C10-C4X-N5	-3.34	117.99	124.81
4	A	634	FAD	C7M-C7-C8	3.34	127.58	120.76
4	A	634	FAD	C6-C7-C8	3.33	124.58	119.69
4	A	634	FAD	N10-C10-N1	3.30	128.22	118.51
4	A	634	FAD	O4B-C4B-C5B	-3.01	99.70	109.33
4	A	634	FAD	C4X-C4-N3	2.92	120.69	113.25
4	A	634	FAD	C1B-N9A-C8A	2.92	133.57	127.09
4	A	634	FAD	C5B-C4B-C3B	2.84	125.43	115.21
4	A	634	FAD	C5A-C4A-N3A	-2.81	122.85	126.72
4	A	634	FAD	O5'-C5'-C4'	2.78	116.79	109.36
4	A	634	FAD	O2P-P-O1P	2.74	125.18	112.44
4	A	634	FAD	O3'-C3'-C4'	2.68	115.01	108.93
4	A	634	FAD	C4X-C10-N1	-2.67	118.04	124.59
4	A	634	FAD	C9A-C9-C8	2.43	124.10	119.22
4	A	634	FAD	O4'-C4'-C3'	2.31	114.65	109.25
3	A	501	NEN	C1-C4-C3	-2.28	102.91	105.24
4	A	634	FAD	O4B-C1B-C2B	2.23	111.39	106.62
4	A	634	FAD	C5X-C6-C7	-2.23	116.70	120.83
4	A	634	FAD	O3P-P-O1P	2.22	117.38	110.70
4	A	634	FAD	N9A-C8A-N7A	2.21	117.08	113.94
4	A	634	FAD	C9-C9A-C5X	-2.18	116.17	120.03
4	A	634	FAD	C2B-C3B-C4B	2.09	106.64	102.61
4	A	634	FAD	C5'-C4'-C3'	2.07	116.11	112.22
4	A	634	FAD	O4-C4-N3	-2.06	116.24	120.11
4	A	634	FAD	C9-C8-C7	-2.01	116.74	119.69

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	634	FAD	C5B-O5B-PA-O1A
4	A	634	FAD	O4B-C4B-C5B-O5B
4	A	634	FAD	C3B-C4B-C5B-O5B
4	A	634	FAD	PA-O3P-P-O5'

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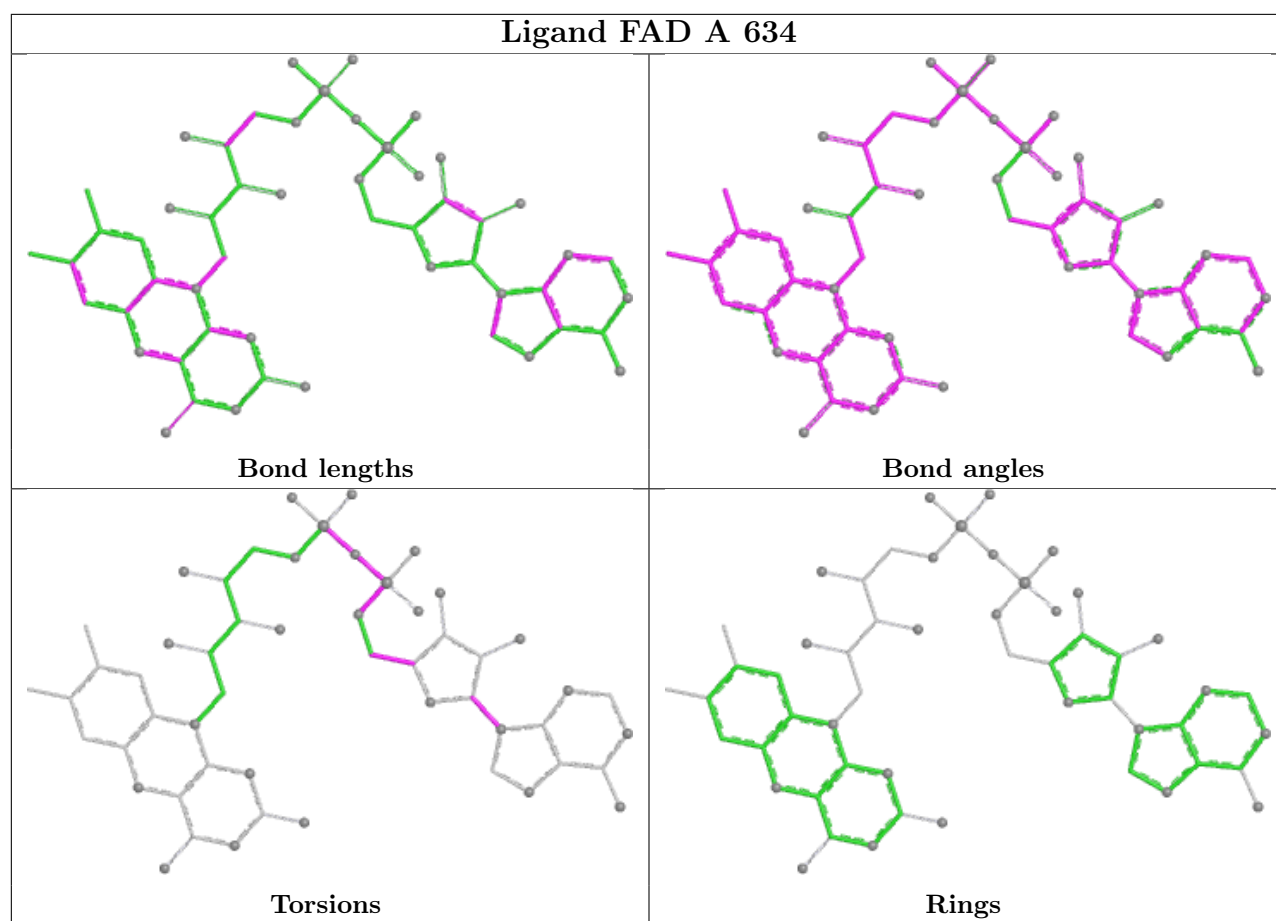
Mol	Chain	Res	Type	Atoms
4	A	634	FAD	C5B-O5B-PA-O2A
4	A	634	FAD	C5B-O5B-PA-O3P
4	A	634	FAD	C2B-C1B-N9A-C8A
4	A	634	FAD	O4B-C1B-N9A-C8A
4	A	634	FAD	P-O3P-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	634	FAD	1	0

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 ⓘ

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	367/389 (94%)	0.81	57 (15%) 5 4	28, 53, 95, 102	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	VAL	8.2
1	A	163	ILE	5.0
1	A	99	LEU	5.0
1	A	109	VAL	4.9
1	A	156	PRO	4.9
1	A	208	CYS	4.5
1	A	130	ASN	4.4
1	A	95	ALA	4.3
1	A	110	VAL	3.9
1	A	155	LYS	3.9
1	A	162	THR	3.8
1	A	152	THR	3.7
1	A	57	ASN	3.7
1	A	165	TYR	3.7
1	A	153	SER	3.6
1	A	123	GLU	3.3
1	A	92	PHE	3.2
1	A	98	GLY	3.1
1	A	161	ASP	3.0
1	A	160	GLU	3.0
1	A	297	LEU	3.0
1	A	106	SER	3.0
1	A	131	ASP	3.0
1	A	171	PHE	2.9
1	A	104	ALA	2.9
1	A	111	GLU	2.9
1	A	87	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	136	ALA	2.9
1	A	214	THR	2.9
1	A	97	ASP	2.9
1	A	215	GLY	2.8
1	A	425	LEU	2.8
1	A	175	ASN	2.8
1	A	55	SER	2.8
1	A	151	GLN	2.7
1	A	159	ILE	2.6
1	A	93	TRP	2.6
1	A	107	VAL	2.6
1	A	54	GLY	2.6
1	A	168	VAL	2.6
1	A	158	ASP	2.5
1	A	148	GLN	2.5
1	A	96	ASN	2.5
1	A	56	PHE	2.4
1	A	211	ILE	2.4
1	A	105	CYS	2.4
1	A	378	ASP	2.3
1	A	129	ASN	2.3
1	A	101	LEU	2.3
1	A	174	LYS	2.3
1	A	308	ASN	2.2
1	A	103	ARG	2.2
1	A	206	ASP	2.2
1	A	420	TYR	2.1
1	A	137	ASP	2.1
1	A	247	THR	2.0
1	A	176	ALA	2.0

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](#)

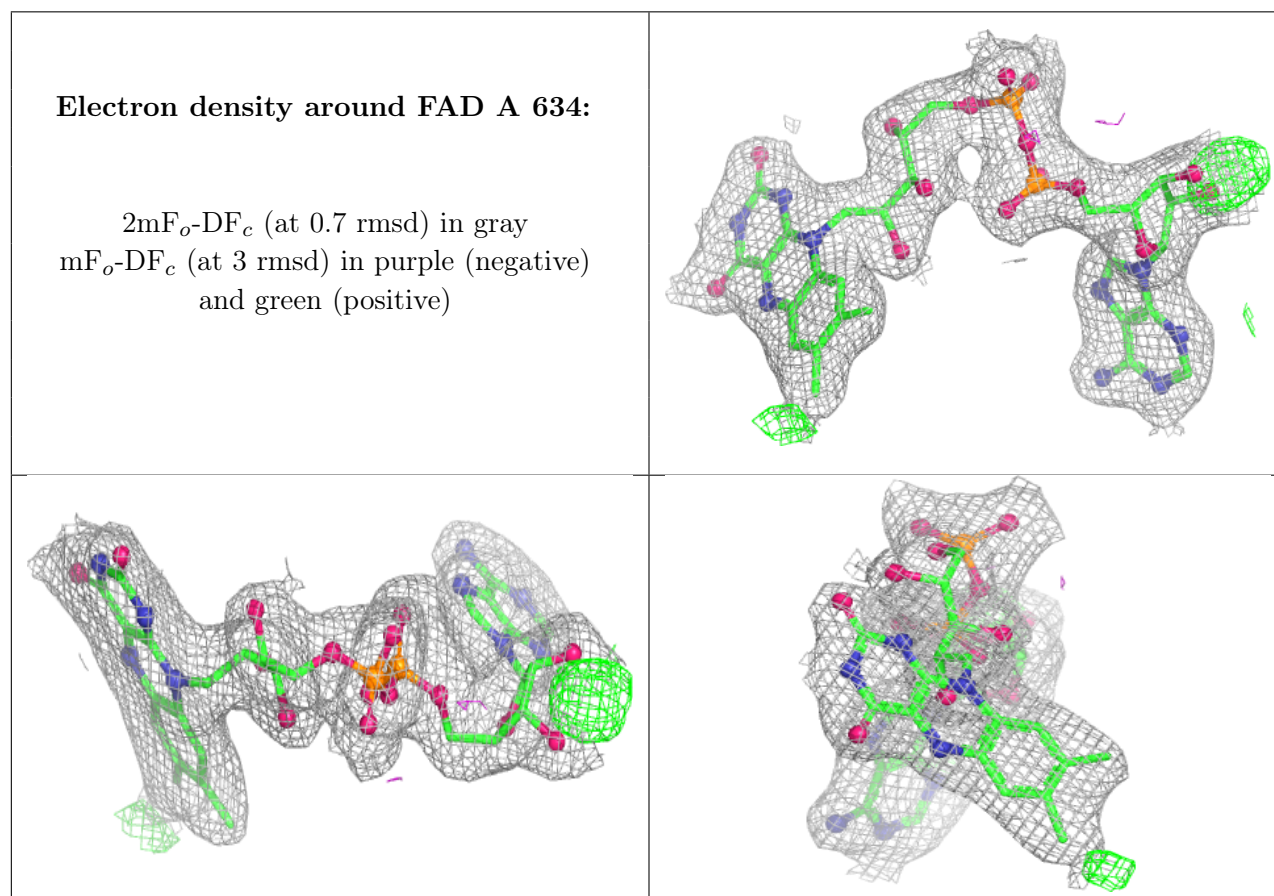
There are no oligosaccharides in this entry.

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
3	NEN	A	501	9/9	0.53	0.26	92,94,96,97	0
4	FAD	A	634	53/53	0.96	0.07	29,36,41,43	0
2	CD	A	801	1/1	0.98	0.06	44,44,44,44	0
2	CD	A	802	1/1	0.98	0.10	89,89,89,89	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.