



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:00 PM GMT

PDB ID : 1RP4
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
<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) : 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

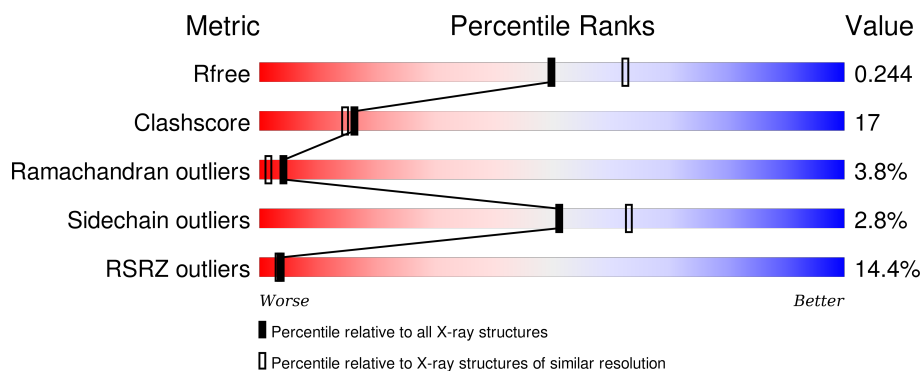
1 Overall quality at a glance

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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.

Mol	Chain	Length	Quality of chain
1	A	389	

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	NEN	A	501	-	-	-	X

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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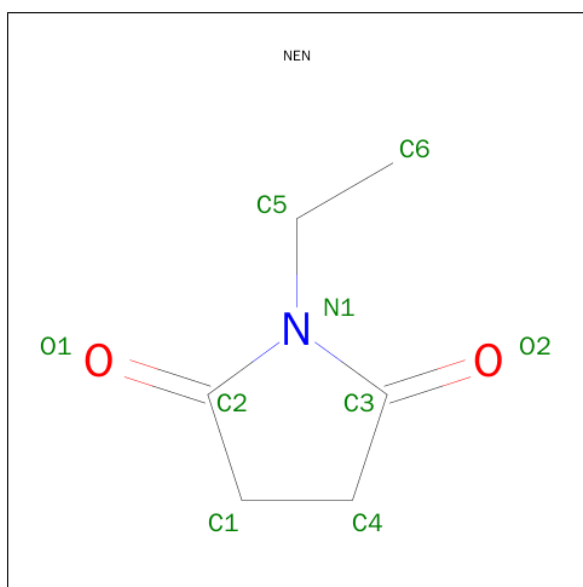
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Chain	Residue	Modelled	Actual	Comment	Reference
A	427	ARG	-	CLONING ARTIFACT	UNP Q03103

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 3 is 1-ETHYL-PYRROLIDINE-2,5-DIONE (three-letter code: NEN) (formula: C₆H₉NO₂).



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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

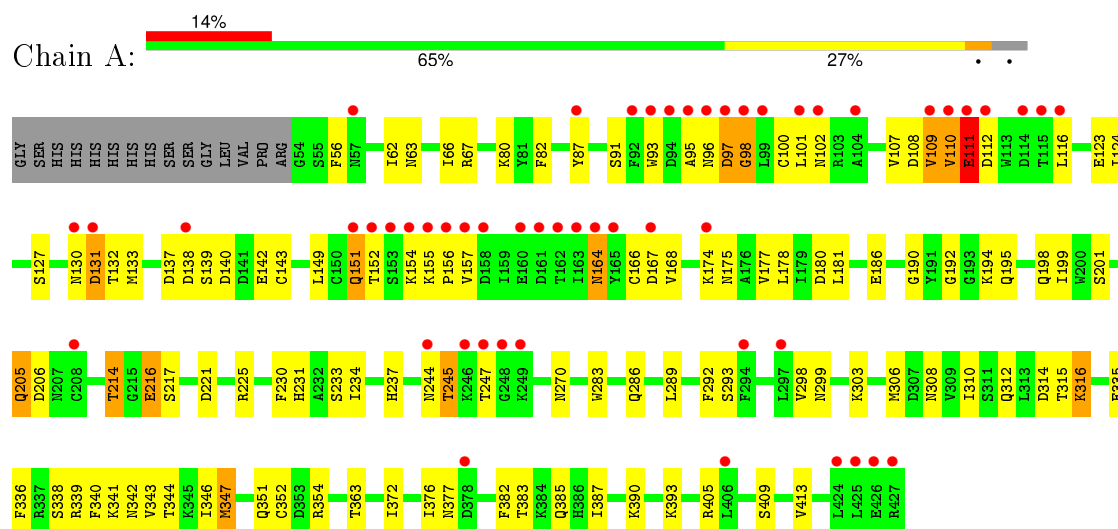
- Molecule 5 is water.

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

3 Residue-property plots [i](#)

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: 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 38.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.20) 98.5 (38.24-2.20)	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%)	DCC
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 , 51.4	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25784 reflections	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, 0.375 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: NEN, FAD, CD

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	0.37	0/3058	0.54	1/4122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	156	PRO	N-CA-CB	5.83	110.30	103.30

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	3003	0	2864	100	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	100	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 17.

All (100) 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:H	1:A:316:LYS:HD2	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:225:ARG:HG3	1:A:270:ASN:ND2	2.16	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: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
1:A:66:ILE:HD12	1:A:67:ARG:N	2.24	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:289:LEU:HD11	1:A:306:MSE:HE2	1.91	0.51
1:A:286:GLN:HB2	1:A:310:ILE:HG21	1.92	0.51
1:A:93:TRP:CZ2	1:A:195:GLN:HG3	2.45	0.51
1:A:289:LEU:HD13	1:A:306:MSE:HE2	1.91	0.51
1:A:151:GLN:HG3	1:A:155:LYS:CB	2.41	0.51
1:A:127:SER:O	1:A:354:ARG:HD2	2.10	0.51
1:A:347:MSE:HA	1:A:347:MSE:CE	2.41	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:216:GLU:HG2	5:A:896:HOH:O	2.12	0.49
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:108:ASP:O	1:A:109:VAL:C	2.51	0.48
1:A:97:ASP:O	1:A:98:GLY:C	2.51	0.48
1:A:130:ASN:CG	1:A:131:ASP:H	2.17	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:303:LYS:C	1:A:303:LYS:HD3	2.36	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:341:LYS:HG3	1:A:342:ASN:N	2.31	0.45
1:A:124:ILE:N	1:A:124:ILE:HD12	2.31	0.45
1:A:217:SER:HB2	5:A:879:HOH:O	2.15	0.45
1:A:206:ASP:HB3	5:A:862:HOH:O	2.16	0.45
1:A:66:ILE:HD12	1:A:66:ILE:C	2.36	0.45
1:A:343:VAL:HG12	1:A:363:THR:HG21	1.99	0.45
1:A:149:LEU:CD1	1:A:292:PHE:HB2	2.43	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:316:LYS:CD	1:A:316:LYS:N	2.66	0.44
1:A:123:GLU:CD	1:A:123:GLU:H	2.21	0.44
1:A:82:PHE:HB2	1:A:181:LEU:HD11	2.00	0.44
1:A:110:VAL:O	1:A:111:GLU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:390:LYS:O	1:A:390:LYS:HG2	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:335:GLU:O	1:A:339:ARG:HG2	2.19	0.42
1:A:164:ASN:OD1	1:A:167:ASP:HB2	2.20	0.41
1:A:164:ASN:O	1:A:168:VAL:HG23	2.20	0.41
1:A:116:LEU:HD22	1:A:245:THR:HB	2.02	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: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:130:ASN:CG	1:A:131:ASP:N	2.75	0.40
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
1:A:67:ARG:HD3	1:A:67:ARG:C	2.41	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%)	4 1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	109	VAL

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Mol	Chain	Res	Type
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%)	315 (97%)	9 (3%)	51 63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	A	164	ASN
1	A	205	GLN
1	A	216	GLU
1	A	316	LYS
1	A	336	PHE
1	A	340	PHE
1	A	347	MSE
1	A	352	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	60	ASN
1	A	164	ASN
1	A	175	ASN
1	A	195	GLN
1	A	205	GLN
1	A	237	HIS
1	A	244	ASN
1	A	270	ASN
1	A	351	GLN
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 carbohydrates 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	$\# Z > 2$
3	NEN	A	501	1	9,9,9	0.57	0	12,12,12	0.88	0
4	FAD	A	634	-	48,58,58	2.56	13 (27%)	54,89,89	4.91	28 (51%)

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	NEN	A	501	1	-	0/2/15/15	0/1/1/1
4	FAD	A	634	-	-	0/30/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	634	FAD	C1'-N10	-5.90	1.42	1.48
4	A	634	FAD	C5A-C4A	-3.52	1.32	1.40
4	A	634	FAD	C5'-C4'	-2.92	1.47	1.51
4	A	634	FAD	C2B-C3B	-2.43	1.46	1.53
4	A	634	FAD	C8A-N7A	-2.38	1.30	1.34
4	A	634	FAD	O4B-C1B	2.49	1.44	1.41
4	A	634	FAD	C9A-C5X	3.43	1.49	1.42
4	A	634	FAD	C5X-N5	4.78	1.43	1.35
4	A	634	FAD	C4-N3	4.90	1.42	1.33
4	A	634	FAD	C4A-N3A	5.06	1.43	1.35
4	A	634	FAD	C2A-N3A	5.31	1.41	1.32
4	A	634	FAD	C4X-N5	6.90	1.44	1.33
4	A	634	FAD	C9A-N10	6.97	1.48	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	634	FAD	N3A-C2A-N1A	-20.63	113.10	128.89
4	A	634	FAD	C4X-C10-N10	-11.51	113.74	120.52
4	A	634	FAD	C5X-C9A-N10	-11.28	109.05	117.62
4	A	634	FAD	C1'-N10-C9A	-5.98	112.15	118.86
4	A	634	FAD	C4-C4X-C10	-5.39	116.49	119.94
4	A	634	FAD	C8M-C8-C9	-5.36	105.70	120.28
4	A	634	FAD	O3P-PA-O5B	-4.85	90.06	102.94
4	A	634	FAD	C7M-C7-C6	-4.62	107.72	120.28
4	A	634	FAD	O5'-P-O1P	-4.38	92.62	109.62
4	A	634	FAD	O3B-C3B-C4B	-3.41	100.82	111.05
4	A	634	FAD	C4B-O4B-C1B	-3.29	106.10	109.72
4	A	634	FAD	C9A-C5X-N5	-2.79	118.23	122.36
4	A	634	FAD	O4B-C4B-C5B	-2.69	99.70	109.32
4	A	634	FAD	O2'-C2'-C1'	-2.69	103.34	109.94
4	A	634	FAD	C7-C6-C5X	-2.59	116.70	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	634	FAD	C4X-C4-N3	-2.12	120.69	123.59
4	A	634	FAD	O4'-C4'-C3'	2.24	114.65	109.02
4	A	634	FAD	O2P-P-O1P	2.33	125.18	112.53
4	A	634	FAD	C6-C7-C8	2.38	124.58	120.04
4	A	634	FAD	O3'-C3'-C4'	2.49	115.01	108.75
4	A	634	FAD	C5B-C4B-C3B	2.58	125.43	115.21
4	A	634	FAD	O2A-PA-O1A	2.90	128.24	112.53
4	A	634	FAD	C7M-C7-C8	3.12	127.58	120.73
4	A	634	FAD	C2A-N1A-C6A	4.04	125.99	118.77
4	A	634	FAD	C4-C4X-N5	5.57	125.48	118.72
4	A	634	FAD	C8M-C8-C7	7.63	137.50	120.73
4	A	634	FAD	C4X-N5-C5X	8.54	126.59	116.76
4	A	634	FAD	C4-N3-C2	11.91	125.55	115.25

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.69	53 (14%) 3 3	28, 53, 95, 102	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	VAL	15.8
1	A	110	VAL	8.2
1	A	99	LEU	6.8
1	A	95	ALA	6.6
1	A	111	GLU	6.2
1	A	153	SER	6.0
1	A	297	LEU	5.4
1	A	427	ARG	5.2
1	A	152	THR	4.9
1	A	156	PRO	4.6
1	A	160	GLU	4.4
1	A	247	THR	4.3
1	A	109	VAL	4.2
1	A	102	ASN	4.2
1	A	116	LEU	4.2
1	A	101	LEU	4.0
1	A	174	LYS	4.0
1	A	164	ASN	4.0
1	A	246	LYS	3.9
1	A	97	ASP	3.9
1	A	158	ASP	3.8
1	A	249	LYS	3.6
1	A	57	ASN	3.6
1	A	93	TRP	3.5
1	A	163	ILE	3.4
1	A	162	THR	3.2
1	A	87	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	161	ASP	3.1
1	A	208	CYS	3.1
1	A	130	ASN	3.1
1	A	426	GLU	3.1
1	A	378	ASP	3.0
1	A	112	ASP	2.9
1	A	425	LEU	2.9
1	A	131	ASP	2.8
1	A	92	PHE	2.8
1	A	248	GLY	2.7
1	A	98	GLY	2.7
1	A	424	LEU	2.6
1	A	94	ASP	2.6
1	A	244	ASN	2.5
1	A	151	GLN	2.4
1	A	115	THR	2.4
1	A	154	LYS	2.3
1	A	114	ASP	2.3
1	A	96	ASN	2.2
1	A	104	ALA	2.2
1	A	138	ASP	2.2
1	A	155	LYS	2.2
1	A	165	TYR	2.1
1	A	167	ASP	2.1
1	A	294	PHE	2.1
1	A	406	LEU	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 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(\AA^2)	Q<0.9
3	NEN	A	501	9/9	0.74	0.41	4.44	92,94,96,97	0
2	CD	A	801	1/1	0.98	0.15	0.39	44,44,44,44	0
4	FAD	A	634	53/53	0.97	0.13	-0.87	29,36,41,43	0
2	CD	A	802	1/1	0.97	0.06	-6.21	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.