



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:23 PM UTC

PDB ID : 3AHR / pdb_00003ahr
Title : Inactive human Ero1
Authors : Inaba, K.; Sitia, R.; Suzuki, M.
Deposited on : 2010-04-26
Resolution : 3.07 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

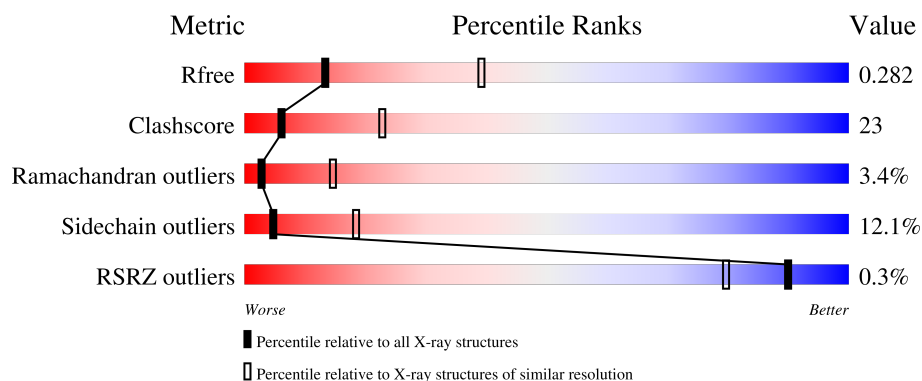
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	465	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3069 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 ERO1-like protein alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	3016	1938	515	548	15	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q96HE7
A	5	GLY	-	expression tag	UNP Q96HE7
A	6	SER	-	expression tag	UNP Q96HE7
A	7	SER	-	expression tag	UNP Q96HE7
A	8	HIS	-	expression tag	UNP Q96HE7
A	9	HIS	-	expression tag	UNP Q96HE7
A	10	HIS	-	expression tag	UNP Q96HE7
A	11	HIS	-	expression tag	UNP Q96HE7
A	12	HIS	-	expression tag	UNP Q96HE7
A	13	HIS	-	expression tag	UNP Q96HE7
A	14	SER	-	expression tag	UNP Q96HE7
A	15	SER	-	expression tag	UNP Q96HE7
A	16	GLY	-	expression tag	UNP Q96HE7
A	17	HIS	-	expression tag	UNP Q96HE7
A	18	ILE	-	expression tag	UNP Q96HE7
A	19	GLU	-	expression tag	UNP Q96HE7
A	20	GLY	-	expression tag	UNP Q96HE7
A	21	ARG	-	expression tag	UNP Q96HE7
A	99	ALA	CYS	engineered mutation	UNP Q96HE7
A	104	ALA	CYS	engineered mutation	UNP Q96HE7
A	166	ALA	CYS	engineered mutation	UNP Q96HE7

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

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	54.70Å 139.09Å 143.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.01 – 3.07 36.01 – 3.07	Depositor EDS
% Data completeness (in resolution range)	98.2 (36.01-3.07) 98.2 (36.01-3.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.303 0.210 , 0.282	Depositor DCC
R_{free} test set	572 reflections (5.40%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3069	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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: 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	0.87	0/3089	1.07	13/4161 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	LYS	N-CA-C	7.83	118.93	107.88
1	A	319	LEU	CA-C-N	5.76	125.23	119.24
1	A	319	LEU	C-N-CA	5.76	125.23	119.24
1	A	434	HIS	N-CA-C	5.64	117.65	109.07
1	A	302	LYS	N-CA-C	-5.51	105.38	111.71
1	A	368	LYS	CB-CA-C	-5.46	110.25	116.54
1	A	354	PHE	CA-C-N	5.40	126.58	119.84
1	A	354	PHE	C-N-CA	5.40	126.58	119.84
1	A	245	ARG	N-CA-C	-5.27	105.59	112.23
1	A	414	ILE	CB-CA-C	-5.25	105.16	111.88
1	A	411	ALA	N-CA-C	-5.25	105.25	110.97
1	A	406	GLN	N-CA-C	-5.20	104.87	111.11
1	A	281	ILE	CB-CA-C	-5.13	105.32	112.04

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	3016	0	2937	135	0
2	A	53	0	31	3	0
All	All	3069	0	2968	136	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 23.

All (136) 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:336:GLN:HA	1:A:339:GLU:HB2	1.33	1.06
1:A:300:ARG:HD3	2:A:1:FAD:C6A	2.06	0.85
1:A:42:TYR:CD2	1:A:43:LEU:N	2.51	0.75
1:A:336:GLN:O	1:A:340:ASN:N	2.19	0.75
1:A:40:SER:OG	1:A:42:TYR:CD2	2.41	0.74
1:A:336:GLN:H	1:A:336:GLN:CD	1.96	0.72
1:A:336:GLN:NE2	1:A:337:ASP:H	1.87	0.71
1:A:87:PHE:HB2	1:A:88:TRP:CE3	2.26	0.70
1:A:56:PHE:O	1:A:60:ARG:HB2	1.93	0.67
1:A:42:TYR:HD2	1:A:43:LEU:H	1.42	0.67
1:A:313:ARG:HG3	1:A:415:LEU:HD21	1.76	0.67
1:A:68:LEU:O	1:A:71:SER:HB3	1.95	0.66
1:A:45:ASP:HA	1:A:249:ARG:NH1	2.10	0.66
1:A:45:ASP:HA	1:A:249:ARG:HH12	1.61	0.65
1:A:36:PHE:CE1	1:A:359:ASP:OD1	2.50	0.64
1:A:90:ASP:C	1:A:92:SER:H	2.05	0.64
1:A:92:SER:O	1:A:93:GLN:HB3	1.98	0.64
1:A:315:LEU:O	1:A:318:VAL:HG12	1.99	0.63
1:A:174:PRO:C	1:A:176:ALA:H	2.05	0.62
1:A:304:LEU:HD11	1:A:453:SER:HB3	1.81	0.62
1:A:66:GLN:O	1:A:70:GLU:HG3	2.00	0.61
1:A:50:VAL:HG12	1:A:54:ASP:OD2	2.00	0.61
1:A:147:GLU:H	1:A:147:GLU:CD	2.09	0.60
1:A:60:ARG:HD2	1:A:350:GLU:OE2	2.01	0.60
1:A:146:GLU:HB3	1:A:147:GLU:OE2	2.02	0.60
1:A:322:PHE:HD1	1:A:327:PHE:CE2	2.20	0.59
1:A:333:ASN:HB2	1:A:336:GLN:NE2	2.17	0.59
1:A:424:MET:HA	1:A:424:MET:HE2	1.86	0.58
1:A:36:PHE:CZ	1:A:359:ASP:OD1	2.57	0.58
1:A:57:ASN:HB2	1:A:308:TYR:OH	2.03	0.58
1:A:328:GLN:NE2	1:A:334:LYS:HE2	2.19	0.58
1:A:296:GLU:O	1:A:300:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:ND2	1:A:83:ARG:HG3	2.20	0.57
1:A:87:PHE:HB2	1:A:88:TRP:CZ3	2.41	0.56
1:A:336:GLN:CD	1:A:336:GLN:N	2.58	0.56
1:A:64:ARG:NH2	1:A:346:GLU:OE2	2.39	0.56
1:A:136:ARG:NH2	1:A:270:GLU:OE2	2.39	0.56
1:A:282:THR:O	1:A:286:GLN:HG3	2.06	0.55
1:A:41:GLY:N	1:A:44:ASP:OD2	2.35	0.55
1:A:336:GLN:HE21	1:A:337:ASP:H	1.54	0.55
1:A:419:LYS:O	1:A:422:ALA:N	2.41	0.54
1:A:316:SER:HB3	1:A:351:ILE:HG22	1.89	0.54
1:A:322:PHE:CD1	1:A:327:PHE:CE2	2.96	0.53
1:A:359:ASP:C	1:A:361:ASN:N	2.64	0.53
1:A:420:LEU:HD22	1:A:433:PHE:HB2	1.89	0.53
1:A:71:SER:HB2	1:A:340:ASN:OD1	2.09	0.53
1:A:401:GLY:O	1:A:405:THR:HG23	2.08	0.52
1:A:460:PHE:O	1:A:461:ARG:C	2.52	0.52
1:A:333:ASN:HB2	1:A:336:GLN:HE22	1.74	0.52
1:A:267:LEU:HB2	1:A:277:TRP:CH2	2.45	0.52
1:A:147:GLU:OE2	1:A:147:GLU:N	2.43	0.52
1:A:250:LEU:HD21	1:A:310:ILE:HG13	1.91	0.52
1:A:335:ILE:H	1:A:335:ILE:HD12	1.74	0.52
1:A:403:LEU:C	1:A:403:LEU:HD23	2.35	0.51
2:A:1:FAD:H8A	2:A:1:FAD:O2A	2.11	0.51
1:A:326:ASP:OD1	1:A:326:ASP:N	2.33	0.51
1:A:419:LYS:O	1:A:421:ILE:N	2.44	0.50
1:A:247:PHE:O	1:A:248:TYR:C	2.55	0.50
1:A:434:HIS:CG	1:A:435:LEU:N	2.80	0.50
1:A:359:ASP:C	1:A:361:ASN:H	2.18	0.50
1:A:271:THR:C	1:A:273:LEU:H	2.19	0.50
1:A:456:GLU:OE1	1:A:456:GLU:HA	2.14	0.48
1:A:202:VAL:HG12	1:A:388:ILE:CD1	2.44	0.48
1:A:259:ASN:HA	1:A:262:LEU:HD23	1.95	0.48
1:A:335:ILE:HD12	1:A:335:ILE:N	2.29	0.48
1:A:441:VAL:O	1:A:445:ASN:HB2	2.14	0.48
1:A:259:ASN:HA	1:A:262:LEU:CD2	2.44	0.48
1:A:429:PRO:HG2	1:A:431:TYR:OH	2.14	0.48
1:A:204:TYR:CE2	1:A:251:ILE:HG22	2.50	0.47
1:A:64:ARG:O	1:A:67:LYS:HB3	2.14	0.47
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.54	0.47
1:A:198:LYS:O	1:A:202:VAL:HG23	2.15	0.47
1:A:336:GLN:HA	1:A:339:GLU:CB	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:HB3	1:A:277:TRP:HZ3	1.80	0.47
1:A:80:ASN:HD21	1:A:83:ARG:HG3	1.79	0.47
1:A:87:PHE:CB	1:A:88:TRP:CE3	2.97	0.46
1:A:319:LEU:N	1:A:320:PRO:CD	2.78	0.46
1:A:366:GLY:C	1:A:368:LYS:H	2.23	0.46
1:A:283:GLU:O	1:A:284:PHE:C	2.54	0.46
1:A:417:SER:O	1:A:421:ILE:HG13	2.15	0.46
1:A:401:GLY:O	1:A:402:LYS:C	2.58	0.46
1:A:202:VAL:HG12	1:A:388:ILE:HD11	1.97	0.46
1:A:58:ASN:OD1	1:A:455:LYS:HA	2.16	0.45
1:A:210:LYS:HE3	1:A:211:PRO:HD2	1.97	0.45
1:A:387:ARG:O	1:A:390:ASP:HB2	2.17	0.45
1:A:300:ARG:HD3	2:A:1:FAD:C5A	2.46	0.45
1:A:336:GLN:C	1:A:338:GLU:N	2.73	0.45
1:A:271:THR:C	1:A:273:LEU:N	2.73	0.45
1:A:374:LEU:HD23	1:A:416:PHE:CZ	2.51	0.45
1:A:138:GLY:O	1:A:395:PHE:HB2	2.17	0.45
1:A:406:GLN:HE22	1:A:438:GLN:HG2	1.82	0.45
1:A:319:LEU:N	1:A:320:PRO:HD2	2.32	0.45
1:A:75:ARG:HG3	1:A:76:TYR:CE2	2.52	0.45
1:A:336:GLN:O	1:A:340:ASN:HB2	2.17	0.45
1:A:267:LEU:HB2	1:A:277:TRP:CZ3	2.51	0.44
1:A:280:ASN:OD1	1:A:280:ASN:C	2.59	0.44
1:A:372:HIS:O	1:A:373:LYS:C	2.61	0.44
1:A:367:ASP:O	1:A:370:GLU:OE1	2.34	0.44
1:A:402:LYS:O	1:A:403:LEU:C	2.56	0.44
1:A:44:ASP:O	1:A:245:ARG:NH1	2.50	0.44
1:A:54:ASP:O	1:A:58:ASN:HB2	2.17	0.44
1:A:374:LEU:HD23	1:A:416:PHE:HZ	1.81	0.44
1:A:421:ILE:HA	1:A:424:MET:HE3	2.00	0.44
1:A:37:CYS:O	1:A:358:PHE:HA	2.18	0.44
1:A:370:GLU:OE1	1:A:370:GLU:N	2.38	0.43
1:A:385:ILE:O	1:A:388:ILE:HB	2.17	0.43
1:A:461:ARG:HH11	1:A:461:ARG:HG3	1.83	0.43
1:A:456:GLU:O	1:A:457:LEU:C	2.62	0.43
1:A:344:LEU:CD2	1:A:348:LEU:HD12	2.48	0.43
1:A:157:LYS:O	1:A:160:ASP:HB2	2.19	0.43
1:A:317:LYS:HD3	1:A:317:LYS:HA	1.89	0.43
1:A:296:GLU:OE1	1:A:296:GLU:HA	2.18	0.43
1:A:76:TYR:HE1	1:A:180:ASP:HB2	1.84	0.42
1:A:362:SER:C	1:A:364:PHE:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:O	1:A:413:LYS:C	2.60	0.42
1:A:336:GLN:O	1:A:337:ASP:C	2.62	0.42
1:A:342:MET:HA	1:A:345:LEU:HD12	2.00	0.42
1:A:421:ILE:O	1:A:424:MET:HB2	2.18	0.42
1:A:245:ARG:NE	1:A:249:ARG:HD2	2.35	0.42
1:A:405:THR:O	1:A:406:GLN:C	2.60	0.41
1:A:152:VAL:O	1:A:155:TRP:HB2	2.20	0.41
1:A:363:PHE:C	1:A:363:PHE:CD1	2.97	0.41
1:A:461:ARG:HG3	1:A:461:ARG:NH1	2.35	0.41
1:A:159:ASP:OD2	1:A:437:ARG:NE	2.50	0.41
1:A:419:LYS:HE3	1:A:419:LYS:HB2	1.96	0.41
1:A:261:HIS:HE1	1:A:449:ARG:O	2.04	0.41
1:A:75:ARG:CZ	1:A:182:LEU:HD12	2.51	0.41
1:A:88:TRP:CH2	1:A:198:LYS:HE2	2.56	0.41
1:A:424:MET:HA	1:A:424:MET:CE	2.49	0.41
1:A:71:SER:CB	1:A:340:ASN:OD1	2.69	0.41
1:A:173:SER:O	1:A:174:PRO:C	2.63	0.41
1:A:40:SER:OG	1:A:42:TYR:HD2	2.00	0.40
1:A:155:TRP:O	1:A:156:THR:C	2.63	0.40
1:A:174:PRO:C	1:A:176:ALA:N	2.73	0.40
1:A:306:PHE:O	1:A:307:LEU:C	2.64	0.40
1:A:133:GLN:O	1:A:136:ARG:HB3	2.21	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	354/465 (76%)	299 (84%)	43 (12%)	12 (3%)	3 14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ILE
1	A	420	LEU
1	A	143	SER
1	A	90	ASP
1	A	175	GLU
1	A	363	PHE
1	A	157	LYS
1	A	174	PRO
1	A	86	PRO
1	A	332	GLY
1	A	425	PRO
1	A	355	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	330/415 (80%)	290 (88%)	40 (12%)	5	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	42	TYR
1	A	66	GLN
1	A	71	SER
1	A	91	ILE
1	A	131	CYS
1	A	132	GLU
1	A	133	GLN
1	A	147	GLU
1	A	149	GLN
1	A	150	LYS
1	A	152	VAL
1	A	162	SER
1	A	163	ASP
1	A	173	SER

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	240	LEU
1	A	269	GLN
1	A	273	LEU
1	A	281	ILE
1	A	298	PRO
1	A	304	LEU
1	A	324	ARG
1	A	326	ASP
1	A	328	GLN
1	A	329	LEU
1	A	333	ASN
1	A	336	GLN
1	A	340	ASN
1	A	351	ILE
1	A	363	PHE
1	A	373	LYS
1	A	374	LEU
1	A	383	ARG
1	A	385	ILE
1	A	419	LYS
1	A	420	LEU
1	A	423	ASN
1	A	424	MET
1	A	438	GLN

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

Mol	Chain	Res	Type
1	A	38	GLN
1	A	57	ASN
1	A	80	ASN
1	A	89	ASN
1	A	93	GLN
1	A	149	GLN
1	A	164	ASN
1	A	259	ASN
1	A	328	GLN
1	A	336	GLN
1	A	404	GLN

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 ⓘ

1 ligand is 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	1	-	58,58,58	1.11	7 (12%)	85,89,89	1.73	23 (27%)

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	1	-	-	9/34/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	FAD	C4X-N5	3.35	1.38	1.30
2	A	1	FAD	C2A-N3A	2.44	1.38	1.33
2	A	1	FAD	C8A-N7A	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	FAD	C2A-N1A	2.36	1.38	1.33
2	A	1	FAD	C4X-C10	-2.25	1.37	1.44
2	A	1	FAD	C5'-C4'	2.21	1.54	1.51
2	A	1	FAD	C1'-C2'	2.17	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	FAD	N3A-C2A-N1A	-4.68	121.49	128.58
2	A	1	FAD	C5A-C4A-N3A	-4.10	121.08	126.72
2	A	1	FAD	N9A-C8A-N7A	-3.43	109.06	113.94
2	A	1	FAD	O2-C2-N1	-3.31	116.31	121.80
2	A	1	FAD	C9A-C5X-N5	-3.31	118.94	122.45
2	A	1	FAD	C4-N3-C2	-3.20	119.97	125.64
2	A	1	FAD	C4X-C10-N10	3.18	121.04	116.48
2	A	1	FAD	C2A-N3A-C4A	3.18	119.59	111.83
2	A	1	FAD	C5A-N7A-C8A	2.95	108.09	103.45
2	A	1	FAD	O2-C2-N3	2.87	124.08	118.58
2	A	1	FAD	O4-C4-C4X	-2.82	119.08	126.53
2	A	1	FAD	O2A-PA-O3P	2.80	114.85	107.27
2	A	1	FAD	O3P-PA-O1A	-2.76	102.40	110.70
2	A	1	FAD	C4A-C5A-N7A	-2.57	107.64	110.58
2	A	1	FAD	C4X-C4-N3	2.55	119.75	113.25
2	A	1	FAD	C10-C4X-N5	-2.47	119.76	124.81
2	A	1	FAD	C4-C4X-N5	2.41	121.53	118.21
2	A	1	FAD	C5X-C9A-N10	2.32	120.07	117.97
2	A	1	FAD	N3A-C4A-N9A	2.31	131.09	127.17
2	A	1	FAD	C5'-C4'-C3'	2.16	116.28	112.22
2	A	1	FAD	C1'-C2'-C3'	2.13	115.43	109.66
2	A	1	FAD	C1'-N10-C9A	2.13	124.77	120.63
2	A	1	FAD	O4'-C4'-C5'	2.05	114.50	109.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	FAD	C5B-O5B-PA-O1A
2	A	1	FAD	C5B-O5B-PA-O3P
2	A	1	FAD	P-O3P-PA-O1A
2	A	1	FAD	C2B-C1B-N9A-C8A
2	A	1	FAD	C5B-O5B-PA-O2A
2	A	1	FAD	C3B-C4B-C5B-O5B

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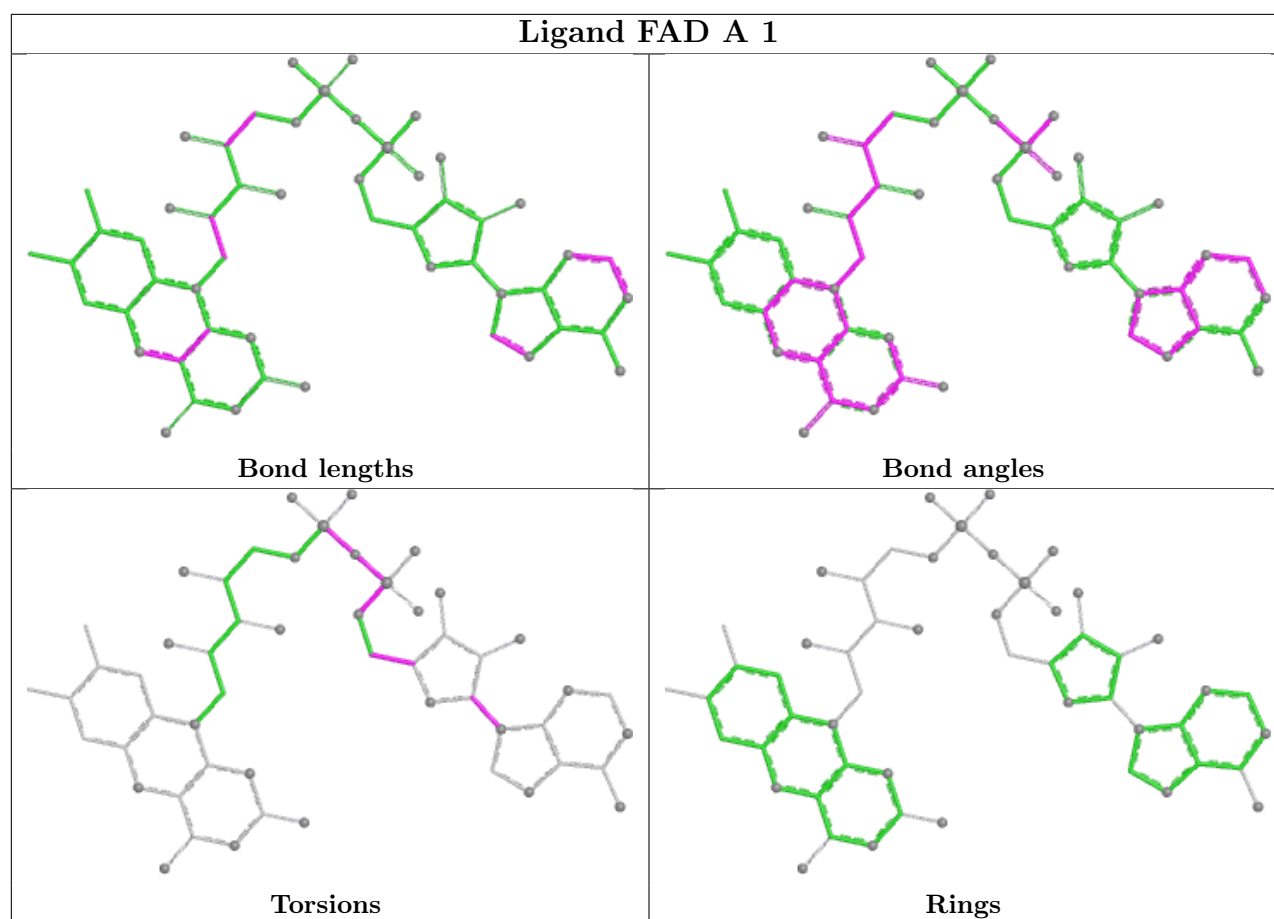
Mol	Chain	Res	Type	Atoms
2	A	1	FAD	P-O3P-PA-O2A
2	A	1	FAD	C2B-C1B-N9A-C4A
2	A	1	FAD	PA-O3P-P-O2P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	FAD	3	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 [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	362/465 (77%)	-0.38	1 (0%) 90 80	39, 65, 102, 111	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	TRP	2.2

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](#)

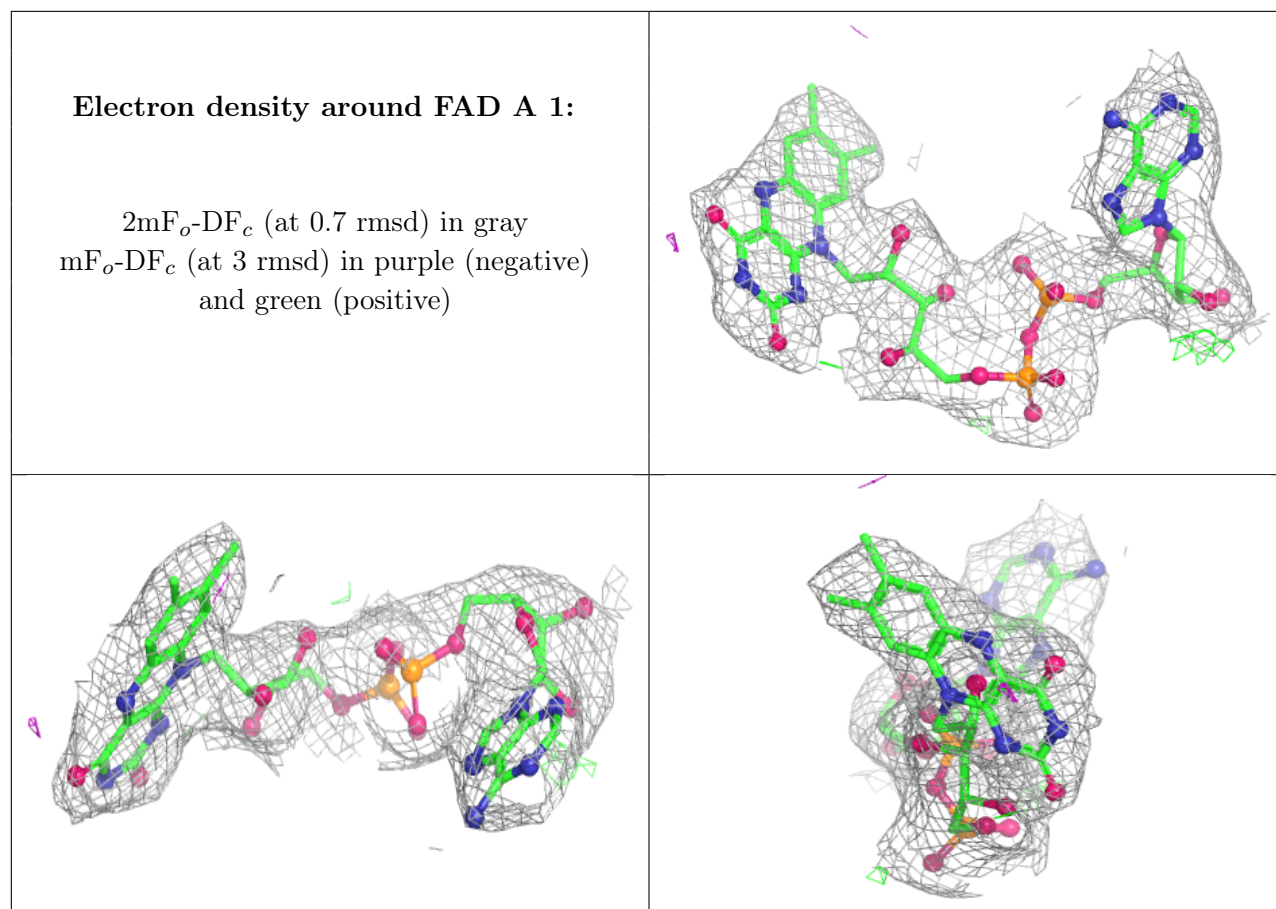
There are no oligosaccharides in this entry.

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	1	53/53	0.97	0.06	35,43,52,53	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 ⓘ

There are no such residues in this entry.