



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:36 AM JST

PDB ID : 6AJU / pdb_00006aju
Title : Rat Xanthine oxidoreductase
Authors : Okamoto, K.; Kawaguchi, Y.
Deposited on : 2018-08-28
Resolution : 1.94 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

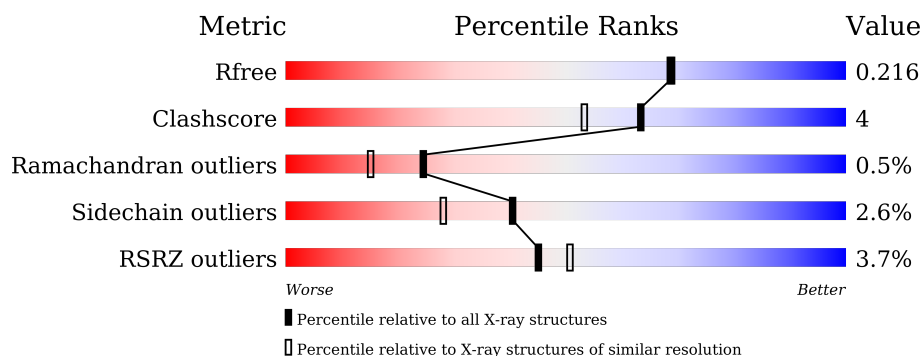
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	1331	3% 86% 9% ..
1	F	1331	4% 86% 9% ..

2 Entry composition [i](#)

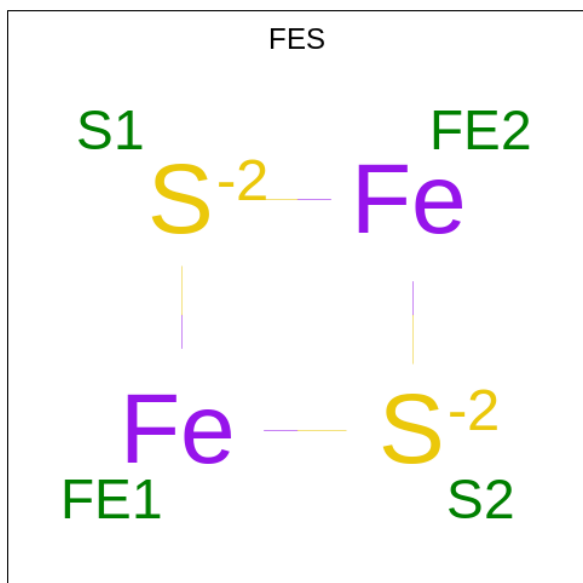
There are 6 unique types of molecules in this entry. The entry contains 21334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

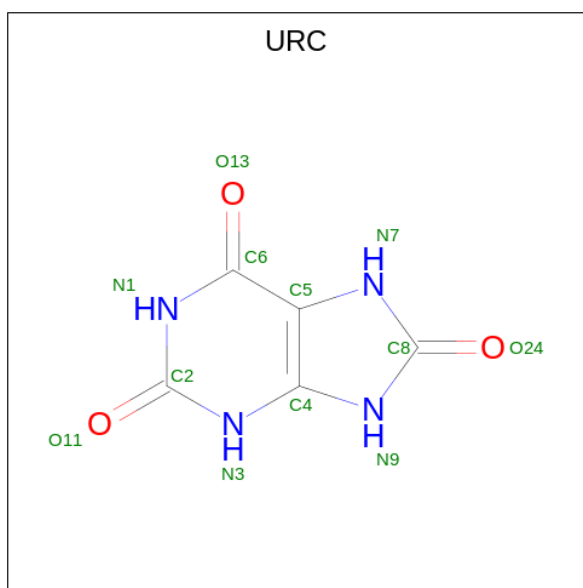
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1287	Total	C	N	O	S	0	0	0
			9945	6306	1710	1865	64			
1	F	1287	Total	C	N	O	S	0	0	0
			9945	6306	1710	1865	64			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



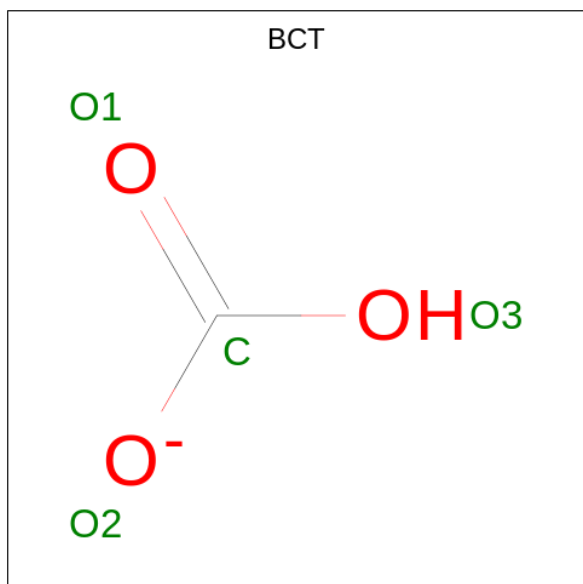
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	F	1	Total	Fe	S	0	0
			4	2	2		
2	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	5	4	3		
3	F	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 4 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



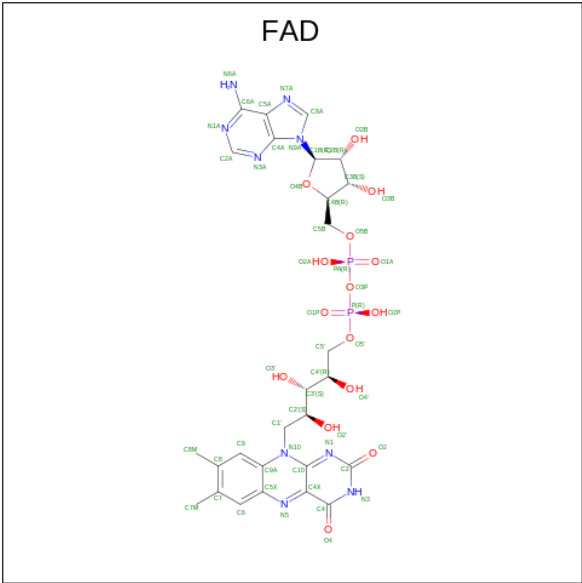
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

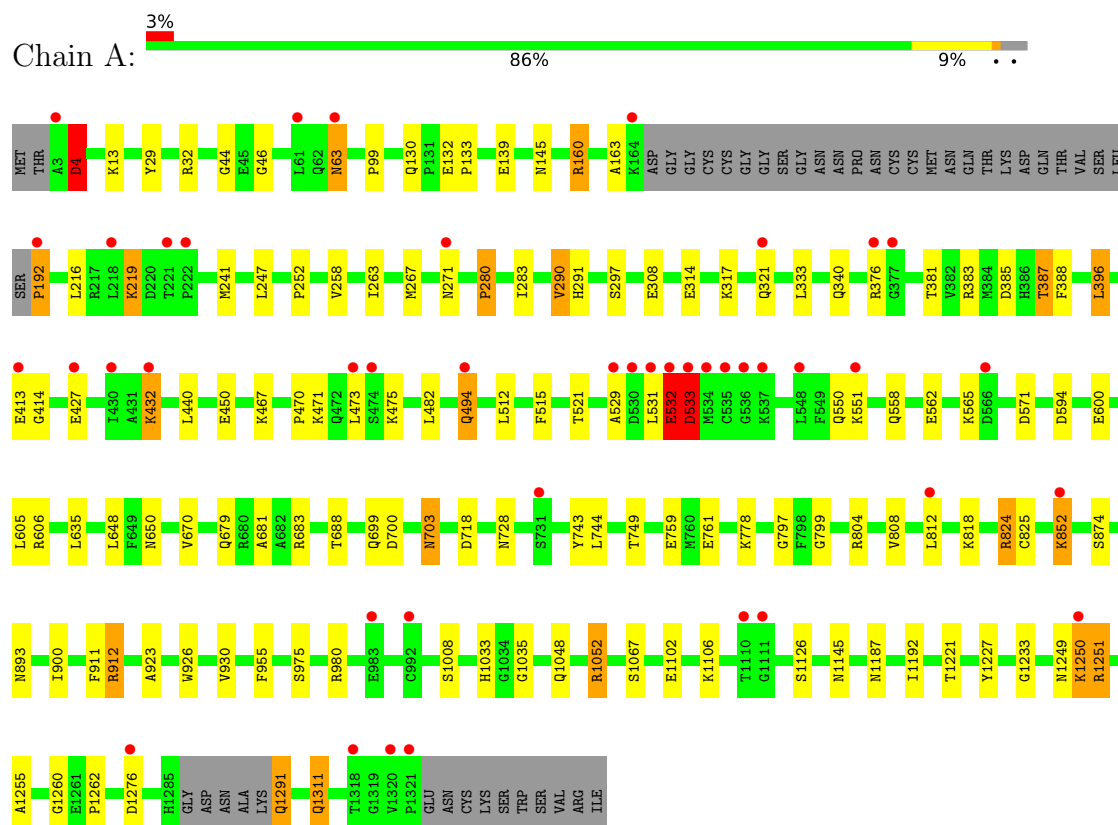
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	684	Total	O	0	0
			684	684		
6	F	606	Total	O	0	0
			606	606		

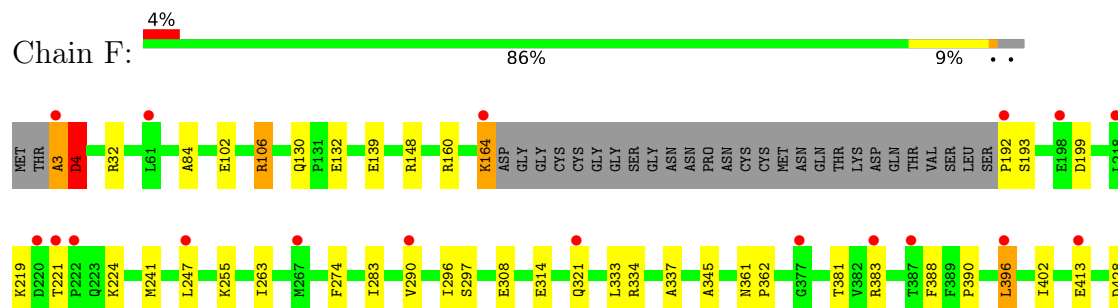
3 Residue-property plots [i](#)

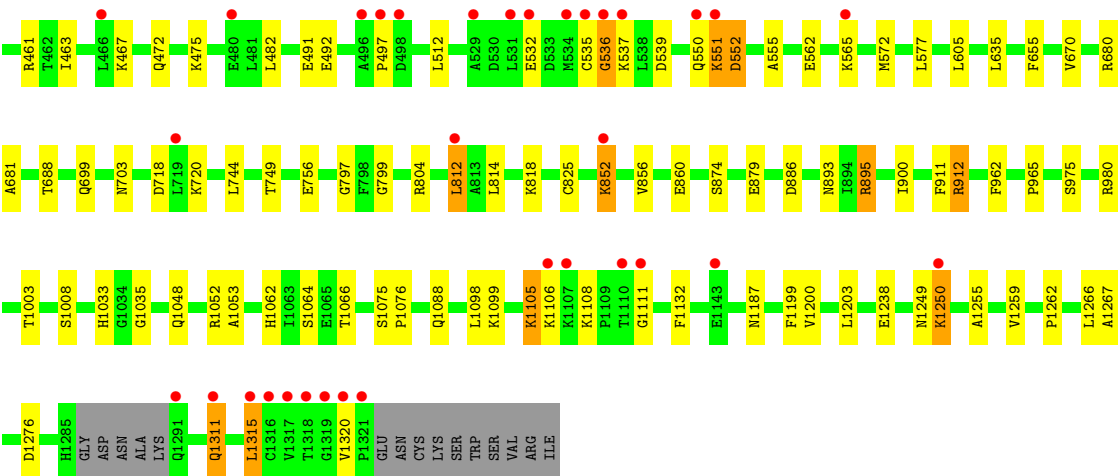
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.72Å 138.08Å 222.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.89 – 1.94 38.89 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.89-1.94) 99.8 (38.89-1.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.76 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.172 , 0.208 0.183 , 0.216	Depositor DCC
R_{free} test set	11236 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21334	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: FES, BCT, URC, 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	1.00	10/10155 (0.1%)	1.06	13/13743 (0.1%)
1	F	0.97	8/10155 (0.1%)	1.04	9/13743 (0.1%)
All	All	0.99	18/20310 (0.1%)	1.05	22/27486 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	F	0	11
All	All	0	19

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	463	ILE	N-CA	6.62	1.53	1.46
1	A	1260	GLY	N-CA	6.30	1.53	1.45
1	A	600	GLU	CD-OE2	6.11	1.36	1.25
1	F	1200	VAL	C-O	-6.01	1.16	1.24
1	F	1111	GLY	N-CA	5.88	1.52	1.44
1	A	648	LEU	N-CA	-5.66	1.39	1.46
1	A	930	VAL	C-O	5.62	1.30	1.24
1	A	29	TYR	C-O	5.54	1.30	1.24
1	A	139	GLU	N-CA	5.48	1.52	1.46
1	A	44	GLY	C-O	5.46	1.31	1.23
1	A	521	THR	N-CA	5.28	1.52	1.46
1	F	1066	THR	N-CA	-5.18	1.39	1.46
1	A	258	VAL	C-O	-5.10	1.18	1.24
1	F	84	ALA	N-CA	-5.09	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	856	VAL	N-CA	-5.08	1.40	1.46
1	F	879	GLU	N-CA	-5.05	1.40	1.46
1	A	427	GLU	CD-OE1	5.02	1.34	1.25
1	F	536	GLY	N-CA	5.01	1.52	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1262	PRO	N-CA-C	7.31	119.61	110.70
1	A	4	ASP	CA-CB-CG	7.02	119.62	112.60
1	F	4	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	562	GLU	CB-CG-CD	6.56	123.75	112.60
1	A	515	PHE	CA-CB-CG	-6.50	107.30	113.80
1	F	139	GLU	CB-CG-CD	6.41	123.49	112.60
1	A	533	ASP	CB-CA-C	6.03	122.41	110.42
1	F	221	THR	CB-CA-C	5.93	117.79	108.84
1	A	1262	PRO	N-CA-C	5.88	117.87	110.70
1	A	700	ASP	CA-CB-CG	5.83	118.43	112.60
1	F	756	GLU	CB-CA-C	-5.79	99.22	109.70
1	A	280	PRO	N-CA-CB	-5.64	97.33	103.25
1	F	562	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	532	GLU	CA-C-O	-5.44	113.66	122.20
1	F	886	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	192	PRO	N-CA-CB	5.41	108.96	103.00
1	A	252	PRO	CA-C-N	5.27	127.86	120.28
1	A	252	PRO	C-N-CA	5.27	127.86	120.28
1	A	139	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	761	GLU	CB-CA-C	5.12	119.07	109.71
1	F	1088	GLN	CA-C-N	5.02	125.51	119.94
1	F	1088	GLN	C-N-CA	5.02	125.51	119.94

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	ARG	Sidechain
1	A	1251	ARG	Sidechain
1	A	160	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	383	ARG	Sidechain
1	A	532	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	804	ARG	Sidechain
1	F	1052	ARG	Sidechain
1	F	106	ARG	Sidechain
1	F	148	ARG	Sidechain
1	F	160	ARG	Sidechain
1	F	3	ALA	Peptide
1	F	32	ARG	Sidechain
1	F	334	ARG	Sidechain
1	F	383	ARG	Sidechain
1	F	680	ARG	Sidechain
1	F	804	ARG	Sidechain
1	F	895	ARG	Sidechain

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	9945	0	9957	87	0
1	F	9945	0	9957	73	0
2	A	8	0	0	1	0
2	F	8	0	0	0	0
3	A	12	0	4	1	0
3	F	12	0	4	0	0
4	A	4	0	0	0	0
4	F	4	0	0	0	0
5	A	53	0	31	1	0
5	F	53	0	31	2	0
6	A	684	0	0	16	0
6	F	606	0	0	8	0
All	All	21334	0	19984	159	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 (159) 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:F:164:LYS:HA	6:F:3569:HOH:O	1.41	1.17
1:A:1067:SER:HB2	6:A:3101:HOH:O	0.96	1.13
1:A:160:ARG:HD3	6:A:3302:HOH:O	1.57	1.02
1:A:718:ASP:H	1:A:893:ASN:HD22	1.11	0.96
1:A:749:THR:HB	1:A:812:LEU:HD12	1.47	0.96
1:A:271:ASN:OD1	1:A:683:ARG:NH1	1.99	0.95
1:A:1311:GLN:HE21	1:A:1311:GLN:H	1.21	0.88
1:A:749:THR:HB	1:A:812:LEU:CD1	2.05	0.87
1:A:812:LEU:HD21	1:A:825:CYS:CB	2.05	0.86
1:A:1067:SER:CB	6:A:3101:HOH:O	1.68	0.84
1:A:267:MET:HE1	6:A:3551:HOH:O	1.77	0.82
1:A:1291:GLN:N	6:A:3102:HOH:O	2.11	0.81
1:F:130:GLN:HE21	1:F:132:GLU:H	1.24	0.81
1:A:812:LEU:HD21	1:A:825:CYS:HB2	1.62	0.79
1:A:216:LEU:O	1:A:219:LYS:HG3	1.81	0.79
1:A:1276:ASP:HB3	6:A:3195:HOH:O	1.83	0.79
1:F:1311:GLN:HE21	1:F:1311:GLN:H	1.31	0.77
1:A:130:GLN:HE21	1:A:132:GLU:H	1.29	0.75
1:A:271:ASN:CG	1:A:683:ARG:HH11	1.97	0.73
1:A:718:ASP:H	1:A:893:ASN:ND2	1.87	0.73
1:F:718:ASP:H	1:F:893:ASN:HD22	1.37	0.73
1:A:812:LEU:HD21	1:A:825:CYS:HB3	1.71	0.71
1:F:532:GLU:OE2	1:F:537:LYS:NZ	2.20	0.69
1:F:106:ARG:HH22	1:F:199:ASP:HB2	1.58	0.69
1:F:532:GLU:O	1:F:535:CYS:O	2.11	0.68
1:A:192:PRO:HD2	6:A:3611:HOH:O	1.94	0.68
1:A:241:MET:HE2	1:A:283:ILE:HG21	1.76	0.67
1:A:388:PHE:HA	1:A:396:LEU:HD13	1.78	0.66
1:F:1048:GLN:HE22	1:F:1187:ASN:HD22	1.45	0.65
1:F:812:LEU:HD11	1:F:825:CYS:HB3	1.79	0.63
1:A:321:GLN:HE21	1:A:414:GLY:H	1.47	0.62
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.25	0.62
1:F:1105:LYS:HE3	6:F:3205:HOH:O	1.99	0.62
1:A:63:ASN:HB3	6:A:3714:HOH:O	2.00	0.61
1:F:321:GLN:HG2	1:F:413:GLU:CD	2.26	0.61
1:A:494:GLN:HE21	1:A:494:GLN:HA	1.67	0.60
1:F:975:SER:O	1:F:980:ARG:HD3	2.02	0.60
1:A:699:GLN:HE21	1:A:703:ASN:HD22	1.49	0.60
1:F:388:PHE:CD1	1:F:396:LEU:HD22	2.36	0.59
1:F:192:PRO:HD2	6:F:3621:HOH:O	2.01	0.59
1:F:718:ASP:H	1:F:893:ASN:ND2	1.99	0.59
1:A:728:ASN:HD21	1:A:852:LYS:CE	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.51	0.59
1:A:975:SER:O	1:A:980:ARG:HD3	2.02	0.58
1:A:688:THR:HG23	6:A:3293:HOH:O	2.04	0.58
1:F:1250:LYS:HG3	6:F:3497:HOH:O	2.02	0.58
1:A:571:ASP:OD2	1:A:1052:ARG:HD2	2.04	0.58
1:A:385:ASP:OD1	1:A:387:THR:HB	2.05	0.57
1:A:606:ARG:HD3	1:A:679:GLN:HA	1.87	0.56
1:A:529:ALA:HB3	1:A:531:LEU:CD1	2.35	0.56
1:F:255:LYS:HE2	1:F:274:PHE:CE1	2.40	0.56
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.88	0.55
1:F:1033:HIS:HD2	1:F:1035:GLY:H	1.55	0.55
1:F:572:MET:HE2	1:F:577:LEU:HD13	1.88	0.54
1:F:321:GLN:HG2	1:F:413:GLU:OE2	2.08	0.54
1:A:291:HIS:HE1	1:A:314:GLU:OE2	1.90	0.54
1:A:571:ASP:CG	1:A:1052:ARG:HD2	2.33	0.54
1:F:635:LEU:HD21	1:F:818:LYS:HD3	1.90	0.54
1:A:321:GLN:NE2	1:A:414:GLY:H	2.05	0.53
1:F:3:ALA:HB1	6:F:3603:HOH:O	2.08	0.53
1:F:605:LEU:HD22	1:F:812:LEU:CD2	2.39	0.53
1:F:396:LEU:C	1:F:396:LEU:HD23	2.33	0.52
1:F:749:THR:O	1:F:812:LEU:HD12	2.08	0.52
1:F:1033:HIS:CD2	1:F:1035:GLY:H	2.27	0.52
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.57	0.52
1:A:1048:GLN:NE2	1:A:1187:ASN:HD22	2.07	0.52
1:F:1259:VAL:HG22	1:F:1259:VAL:O	2.10	0.52
1:A:271:ASN:CG	1:A:683:ARG:HD3	2.34	0.51
1:A:728:ASN:HD21	1:A:852:LYS:HE2	1.75	0.51
1:A:605:LEU:HD13	1:A:812:LEU:HD23	1.92	0.51
1:A:160:ARG:CD	6:A:3302:HOH:O	2.35	0.51
1:F:241:MET:HE2	1:F:283:ILE:HG21	1.93	0.51
1:F:321:GLN:HG2	1:F:413:GLU:OE1	2.11	0.50
1:F:551:LYS:O	1:F:552:ASP:HB2	2.11	0.50
1:F:852:LYS:HE3	1:F:852:LYS:HA	1.93	0.50
1:A:396:LEU:C	1:A:396:LEU:HD23	2.37	0.50
1:F:812:LEU:HD23	1:F:812:LEU:N	2.27	0.49
1:F:1048:GLN:NE2	1:F:1187:ASN:HD22	2.07	0.49
1:A:290:VAL:HG22	1:A:297:SER:HB2	1.95	0.49
1:A:808:VAL:HG12	1:A:812:LEU:HD11	1.94	0.49
1:A:551:LYS:HE2	1:A:1233:GLY:O	2.12	0.49
1:F:106:ARG:HH22	1:F:199:ASP:CB	2.25	0.49
1:F:874:SER:HB3	1:F:900:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1311:GLN:H	1:F:1311:GLN:NE2	2.06	0.49
1:F:308:GLU:HG3	1:F:333:LEU:HD13	1.95	0.48
1:F:1003:THR:HG22	1:F:1266:LEU:HD21	1.95	0.48
1:A:852:LYS:HE2	1:A:852:LYS:HA	1.95	0.48
1:F:390:PRO:C	1:F:461:ARG:NH1	2.73	0.47
1:F:1203:LEU:C	1:F:1203:LEU:HD23	2.40	0.47
1:F:799:GLY:HA2	6:F:3319:HOH:O	2.16	0.46
1:A:635:LEU:HD21	1:A:818:LYS:HD3	1.97	0.46
1:A:1250:LYS:HG3	6:A:3620:HOH:O	2.16	0.46
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.15	0.46
1:A:63:ASN:OD1	1:A:63:ASN:N	2.49	0.46
1:F:1249:ASN:O	1:F:1255:ALA:HA	2.16	0.46
1:F:749:THR:O	1:F:812:LEU:CD1	2.64	0.46
1:F:900:ILE:HD12	1:F:900:ILE:N	2.31	0.46
1:F:296:ILE:CD1	1:F:314:GLU:HG3	2.45	0.46
1:F:1311:GLN:HE21	1:F:1311:GLN:N	2.06	0.46
1:F:1315:LEU:HD13	6:F:3135:HOH:O	2.15	0.46
1:F:290:VAL:CG2	1:F:297:SER:HB2	2.46	0.46
1:F:605:LEU:HD22	1:F:812:LEU:HD21	1.98	0.46
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.34	0.45
1:F:1053:ALA:O	1:F:1098:LEU:HD11	2.16	0.45
1:F:337:ALA:HA	1:F:428:ASP:OD1	2.17	0.45
1:A:321:GLN:HG2	1:A:413:GLU:OE2	2.16	0.45
1:A:749:THR:CB	1:A:812:LEU:HD12	2.32	0.45
1:A:812:LEU:CD2	1:A:825:CYS:CB	2.88	0.45
1:F:699:GLN:NE2	1:F:703:ASN:OD1	2.46	0.45
1:A:911:PHE:O	1:A:912:ARG:C	2.59	0.44
1:A:440:LEU:HB3	1:A:450:GLU:HB2	2.00	0.44
1:A:874:SER:HB3	1:A:900:ILE:HG21	2.00	0.44
1:F:670:VAL:HG11	1:F:681:ALA:HB3	1.99	0.44
1:A:1102:GLU:HG2	1:A:1106:LYS:HE3	1.99	0.44
1:A:145:ASN:ND2	1:A:340:GLN:HE22	2.16	0.44
1:A:1126:SER:HB2	1:F:1132:PHE:CG	2.53	0.44
1:F:688:THR:HG23	6:F:3539:HOH:O	2.16	0.44
1:A:1276:ASP:CB	6:A:3195:HOH:O	2.54	0.44
1:A:1311:GLN:H	1:A:1311:GLN:NE2	2.02	0.43
3:A:3003:URC:O24	6:A:3103:HOH:O	2.21	0.43
1:F:361:ASN:N	1:F:362:PRO:CD	2.81	0.43
1:A:308:GLU:HG3	1:A:333:LEU:HD13	2.00	0.43
1:F:962:PHE:CE2	1:F:965:PRO:HD3	2.53	0.43
1:F:467:LYS:HD3	1:F:492:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:LEU:CD2	1:A:825:CYS:HB2	2.40	0.43
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.34	0.43
1:A:759:GLU:OE2	1:F:1062:HIS:NE2	2.46	0.43
1:F:345:ALA:HB1	5:F:3005:FAD:H4'	2.00	0.43
1:A:133:PRO:O	1:A:163:ALA:HA	2.19	0.43
1:F:539:ASP:OD1	1:F:539:ASP:C	2.61	0.43
1:F:472:GLN:HA	1:F:475:LYS:HE3	2.00	0.42
1:F:860:GLU:HA	1:F:895:ARG:O	2.18	0.42
1:A:263:ILE:HD11	5:A:3005:FAD:H3B	2.01	0.42
1:F:555:ALA:O	1:F:1238:GLU:HA	2.20	0.42
1:A:470:PRO:O	1:A:473:LEU:HG	2.20	0.42
1:F:551:LYS:O	1:F:552:ASP:CB	2.68	0.42
1:A:471:LYS:O	1:A:475:LYS:HE3	2.20	0.42
1:F:263:ILE:HD11	5:F:3005:FAD:H3B	2.01	0.42
1:A:432:LYS:HD3	1:A:432:LYS:HA	1.93	0.42
1:A:650:ASN:OD1	1:A:778:LYS:NZ	2.53	0.42
1:A:799:GLY:HA2	6:A:3247:HOH:O	2.19	0.42
1:A:46:GLY:HA2	2:A:3002:FES:S1	2.60	0.41
1:F:655:PHE:HE2	1:F:814:LEU:HD23	1.85	0.41
1:A:812:LEU:HD11	1:A:825:CYS:HB3	2.01	0.41
1:F:1199:PHE:CE1	1:F:1267:ALA:HA	2.55	0.41
1:A:594:ASP:OD1	1:A:824:ARG:HD3	2.20	0.41
1:A:955:PHE:HA	1:A:1145:ASN:OD1	2.21	0.41
1:F:812:LEU:HD21	1:F:825:CYS:CB	2.51	0.41
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	2.02	0.41
1:A:1250:LYS:HD3	1:A:1251:ARG:N	2.35	0.41
1:F:1075:SER:HB3	1:F:1076:PRO:HD2	2.02	0.41
1:F:102:GLU:HG2	1:F:106:ARG:HD3	2.03	0.41
1:F:911:PHE:O	1:F:912:ARG:C	2.63	0.41
1:F:605:LEU:HD13	1:F:812:LEU:CD2	2.50	0.41
1:A:267:MET:CE	6:A:3551:HOH:O	2.53	0.40
1:A:532:GLU:O	1:A:533:ASP:HB3	2.22	0.40
1:A:160:ARG:NH1	6:A:3126:HOH:O	2.54	0.40
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.02	0.40
1:A:728:ASN:HD21	1:A:852:LYS:HE3	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1281/1331 (96%)	1241 (97%)	35 (3%)	5 (0%)	30	22
1	F	1281/1331 (96%)	1230 (96%)	43 (3%)	8 (1%)	21	11
All	All	2562/2662 (96%)	2471 (96%)	78 (3%)	13 (0%)	24	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	ASP
1	A	1008	SER
1	F	552	ASP
1	F	1008	SER
1	A	4	ASP
1	A	912	ARG
1	F	4	ASP
1	F	912	ARG
1	F	797	GLY
1	A	797	GLY
1	F	497	PRO
1	F	536	GLY
1	F	1320	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	1087/1124 (97%)	1059 (97%)	28 (3%)	40	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	1087/1124 (97%)	1059 (97%)	28 (3%)	40	28
All	All	2174/2248 (97%)	2118 (97%)	56 (3%)	40	28

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	13	LYS
1	A	63	ASN
1	A	99	PRO
1	A	219	LYS
1	A	247	LEU
1	A	280	PRO
1	A	290	VAL
1	A	317	LYS
1	A	381	THR
1	A	387	THR
1	A	396	LEU
1	A	432	LYS
1	A	467	LYS
1	A	482	LEU
1	A	494	GLN
1	A	512	LEU
1	A	533	ASP
1	A	550	GLN
1	A	565	LYS
1	A	703	ASN
1	A	743	TYR
1	A	744	LEU
1	A	824	ARG
1	A	852	LYS
1	A	1250	LYS
1	A	1291	GLN
1	A	1311	GLN
1	F	4	ASP
1	F	164	LYS
1	F	193	SER
1	F	219	LYS
1	F	224	LYS
1	F	247	LEU
1	F	381	THR
1	F	396	LEU

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Mol	Chain	Res	Type
1	F	402	ILE
1	F	482	LEU
1	F	491	GLU
1	F	512	LEU
1	F	550	GLN
1	F	551	LYS
1	F	565	LYS
1	F	720	LYS
1	F	744	LEU
1	F	812	LEU
1	F	852	LYS
1	F	1064	SER
1	F	1099	LYS
1	F	1105	LYS
1	F	1106	LYS
1	F	1108	LYS
1	F	1250	LYS
1	F	1276	ASP
1	F	1311	GLN
1	F	1315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	145	ASN
1	A	260	ASN
1	A	291	HIS
1	A	321	GLN
1	A	332	GLN
1	A	350	ASN
1	A	472	GLN
1	A	494	GLN
1	A	556	ASN
1	A	585	GLN
1	A	699	GLN
1	A	705	ASN
1	A	728	ASN
1	A	869	ASN
1	A	893	ASN
1	A	1033	HIS
1	A	1048	GLN

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Mol	Chain	Res	Type
1	A	1088	GLN
1	A	1173	ASN
1	A	1212	HIS
1	A	1294	GLN
1	A	1311	GLN
1	F	63	ASN
1	F	130	GLN
1	F	143	GLN
1	F	145	ASN
1	F	157	GLN
1	F	291	HIS
1	F	332	GLN
1	F	449	GLN
1	F	472	GLN
1	F	483	GLN
1	F	550	GLN
1	F	556	ASN
1	F	558	GLN
1	F	585	GLN
1	F	705	ASN
1	F	893	ASN
1	F	1033	HIS
1	F	1048	GLN
1	F	1173	ASN
1	F	1194	GLN
1	F	1220	HIS
1	F	1294	GLN
1	F	1311	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

10 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	FES	A	3002	1	0,4,4	-	-	-		
5	FAD	A	3005	-	56,58,58	1.57	11 (19%)	81,89,89	1.71	18 (22%)
2	FES	A	3001	1	0,4,4	-	-	-		
4	BCT	F	3004	-	2,3,3	0.80	0	2,3,3	1.02	0
2	FES	F	3002	1	0,4,4	-	-	-		
4	BCT	A	3004	-	2,3,3	0.87	0	2,3,3	1.14	0
3	URC	A	3003	-	11,13,13	1.90	4 (36%)	12,19,19	2.45	6 (50%)
3	URC	F	3003	-	11,13,13	2.54	4 (36%)	12,19,19	2.02	4 (33%)
2	FES	F	3001	1	0,4,4	-	-	-		
5	FAD	F	3005	-	56,58,58	1.61	10 (17%)	81,89,89	1.57	16 (19%)

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	FES	A	3002	1	-	-	0/1/1/1
5	FAD	A	3005	-	-	5/34/50/50	0/6/6/6
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	F	3002	1	-	-	0/1/1/1
3	URC	A	3003	-	-	-	0/2/2/2
3	URC	F	3003	-	-	-	0/2/2/2
2	FES	F	3001	1	-	-	0/1/1/1
5	FAD	F	3005	-	-	4/34/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3003	URC	O13-C6	5.57	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3005	FAD	C9A-C5X	5.44	1.50	1.41
5	A	3005	FAD	C9A-C5X	4.84	1.49	1.41
3	F	3003	URC	O24-C8	4.17	1.32	1.23
5	F	3005	FAD	C5A-C4A	4.15	1.46	1.39
5	A	3005	FAD	C4X-N5	3.71	1.38	1.30
5	A	3005	FAD	C8A-N7A	3.56	1.38	1.31
5	F	3005	FAD	C5X-N5	-3.52	1.32	1.39
3	A	3003	URC	O24-C8	3.47	1.30	1.23
5	F	3005	FAD	C5A-N7A	-3.34	1.32	1.39
5	A	3005	FAD	C8-C7	3.12	1.48	1.40
5	F	3005	FAD	C5A-C6A	2.88	1.49	1.41
5	A	3005	FAD	C5X-N5	-2.85	1.34	1.39
3	A	3003	URC	O11-C2	2.84	1.29	1.23
5	F	3005	FAD	C4A-N9A	-2.61	1.31	1.37
3	A	3003	URC	C6-N1	-2.61	1.34	1.38
5	A	3005	FAD	C9A-N10	2.52	1.45	1.41
5	A	3005	FAD	C4A-N3A	2.49	1.39	1.34
5	A	3005	FAD	O4-C4	2.47	1.28	1.23
5	F	3005	FAD	C2-N3	-2.44	1.33	1.39
3	A	3003	URC	O13-C6	2.42	1.28	1.23
5	F	3005	FAD	O2-C2	2.39	1.28	1.24
5	A	3005	FAD	C5A-C4A	2.20	1.43	1.39
5	F	3005	FAD	C4-N3	-2.16	1.34	1.38
5	A	3005	FAD	O3'-C3'	2.12	1.48	1.43
3	F	3003	URC	C8-N9	-2.11	1.35	1.39
3	F	3003	URC	C5-C6	2.10	1.47	1.42
5	F	3005	FAD	C7M-C7	2.05	1.55	1.51
5	A	3005	FAD	C2-N3	-2.02	1.34	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3005	FAD	C5A-C4A-N3A	-5.20	119.97	126.75
3	A	3003	URC	N7-C8-N9	4.73	114.68	107.19
5	A	3005	FAD	N3A-C4A-N9A	4.61	134.69	127.08
5	F	3005	FAD	C5A-C4A-N3A	-3.96	121.58	126.75
5	A	3005	FAD	C9A-C5X-N5	-3.83	118.27	122.43
5	F	3005	FAD	N3A-C4A-N9A	3.61	133.04	127.08
3	F	3003	URC	N7-C8-N9	3.60	112.88	107.19
5	F	3005	FAD	C5A-N7A-C8A	3.55	108.56	103.51
5	F	3005	FAD	C4A-C5A-N7A	-3.42	106.45	110.62
3	A	3003	URC	N3-C2-N1	3.40	121.27	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3005	FAD	C5X-C9A-N10	3.35	121.42	117.95
5	A	3005	FAD	C5A-C6A-N6A	-3.28	116.28	123.43
5	F	3005	FAD	C2B-C1B-N9A	3.24	121.52	113.30
3	F	3003	URC	N3-C2-N1	3.23	120.99	115.80
5	F	3005	FAD	C4A-N9A-C8A	3.14	109.13	105.73
3	A	3003	URC	O24-C8-N9	-3.14	119.79	125.39
5	F	3005	FAD	C9A-C5X-N5	-3.04	119.13	122.43
5	A	3005	FAD	C2B-C1B-N9A	3.04	120.99	113.30
3	F	3003	URC	N9-C4-N3	3.02	135.15	122.78
5	A	3005	FAD	C2A-N3A-C4A	2.93	118.67	111.75
5	F	3005	FAD	C4-C4X-N5	2.90	122.36	118.23
3	A	3003	URC	N9-C4-N3	2.89	134.59	122.78
5	A	3005	FAD	O3'-C3'-C4'	2.88	115.76	108.81
5	A	3005	FAD	C4A-N9A-C8A	2.61	108.56	105.73
5	F	3005	FAD	N9A-C8A-N7A	-2.56	110.41	113.91
5	A	3005	FAD	N3A-C2A-N1A	-2.49	124.71	128.60
5	A	3005	FAD	C9A-N10-C10	-2.48	116.90	120.77
3	A	3003	URC	O13-C6-C5	-2.48	121.55	127.24
5	F	3005	FAD	C2A-N1A-C6A	2.46	123.00	118.77
5	A	3005	FAD	C6-C5X-C9A	2.46	122.42	118.94
5	A	3005	FAD	O4-C4-C4X	-2.40	120.24	126.60
5	A	3005	FAD	C4A-N9A-C1B	-2.34	121.02	126.59
5	A	3005	FAD	C5'-C4'-C3'	2.32	116.68	112.20
3	F	3003	URC	O13-C6-C5	-2.29	122.00	127.24
5	A	3005	FAD	N6A-C6A-N1A	2.27	123.32	118.35
5	A	3005	FAD	C5X-N5-C4X	2.23	121.79	118.07
5	A	3005	FAD	O4'-C4'-C3'	-2.20	103.75	109.10
3	A	3003	URC	C5-C6-N1	2.15	118.72	112.31
5	F	3005	FAD	C2B-C3B-C4B	2.13	106.79	102.64
5	F	3005	FAD	C4A-N9A-C1B	-2.10	121.58	126.59
5	F	3005	FAD	O4'-C4'-C3'	-2.10	104.00	109.10
5	F	3005	FAD	C6A-C5A-N7A	2.08	135.90	132.02
5	F	3005	FAD	O4B-C1B-N9A	-2.07	103.99	108.06
5	F	3005	FAD	C5X-N5-C4X	2.03	121.45	118.07

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3005	FAD	N10-C1'-C2'-O2'
5	A	3005	FAD	N10-C1'-C2'-C3'
5	F	3005	FAD	N10-C1'-C2'-O2'

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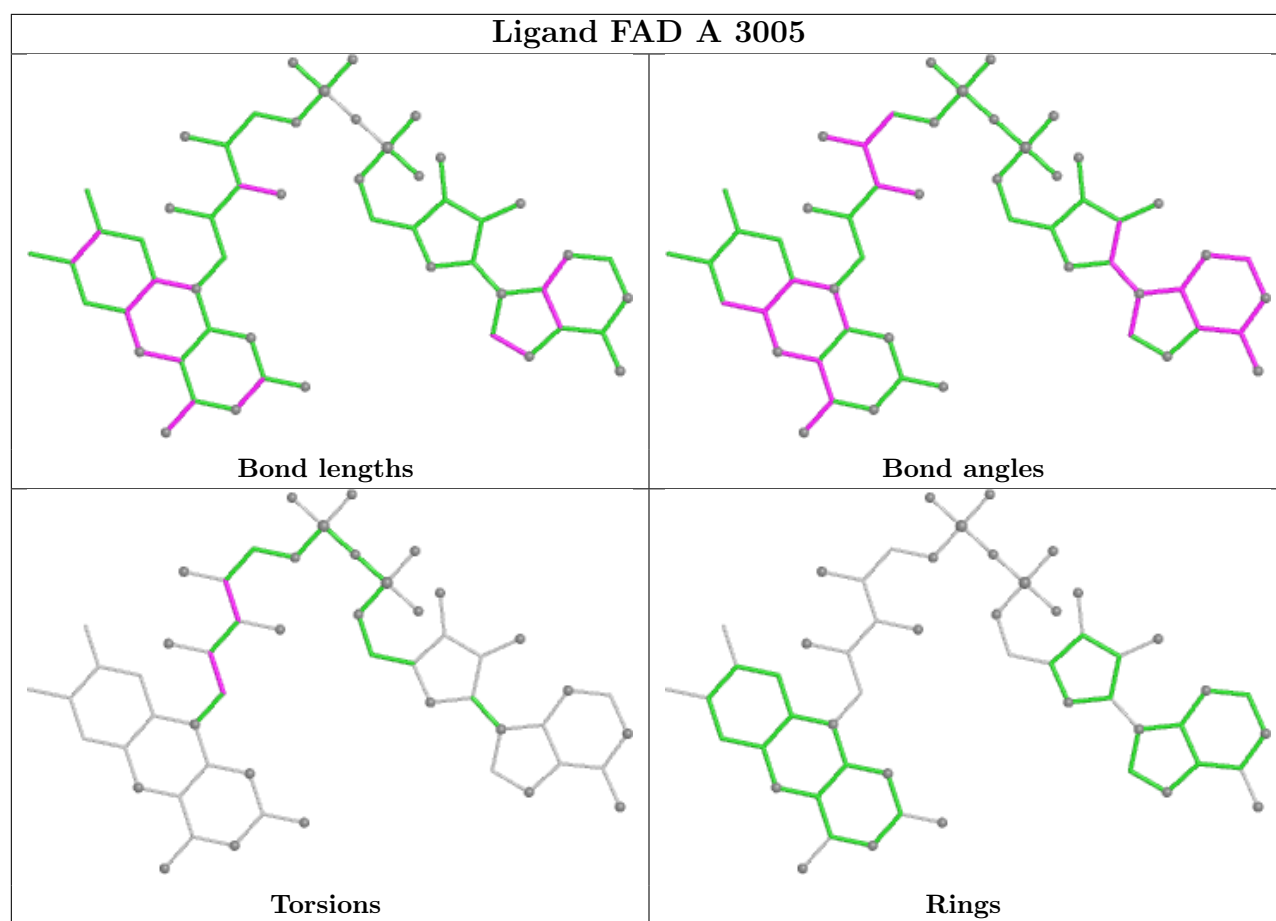
Mol	Chain	Res	Type	Atoms
5	F	3005	FAD	N10-C1'-C2'-C3'
5	A	3005	FAD	C2'-C3'-C4'-O4'
5	A	3005	FAD	C2'-C3'-C4'-C5'
5	F	3005	FAD	C2'-C3'-C4'-C5'
5	F	3005	FAD	C2'-C3'-C4'-O4'
5	A	3005	FAD	O3'-C3'-C4'-O4'

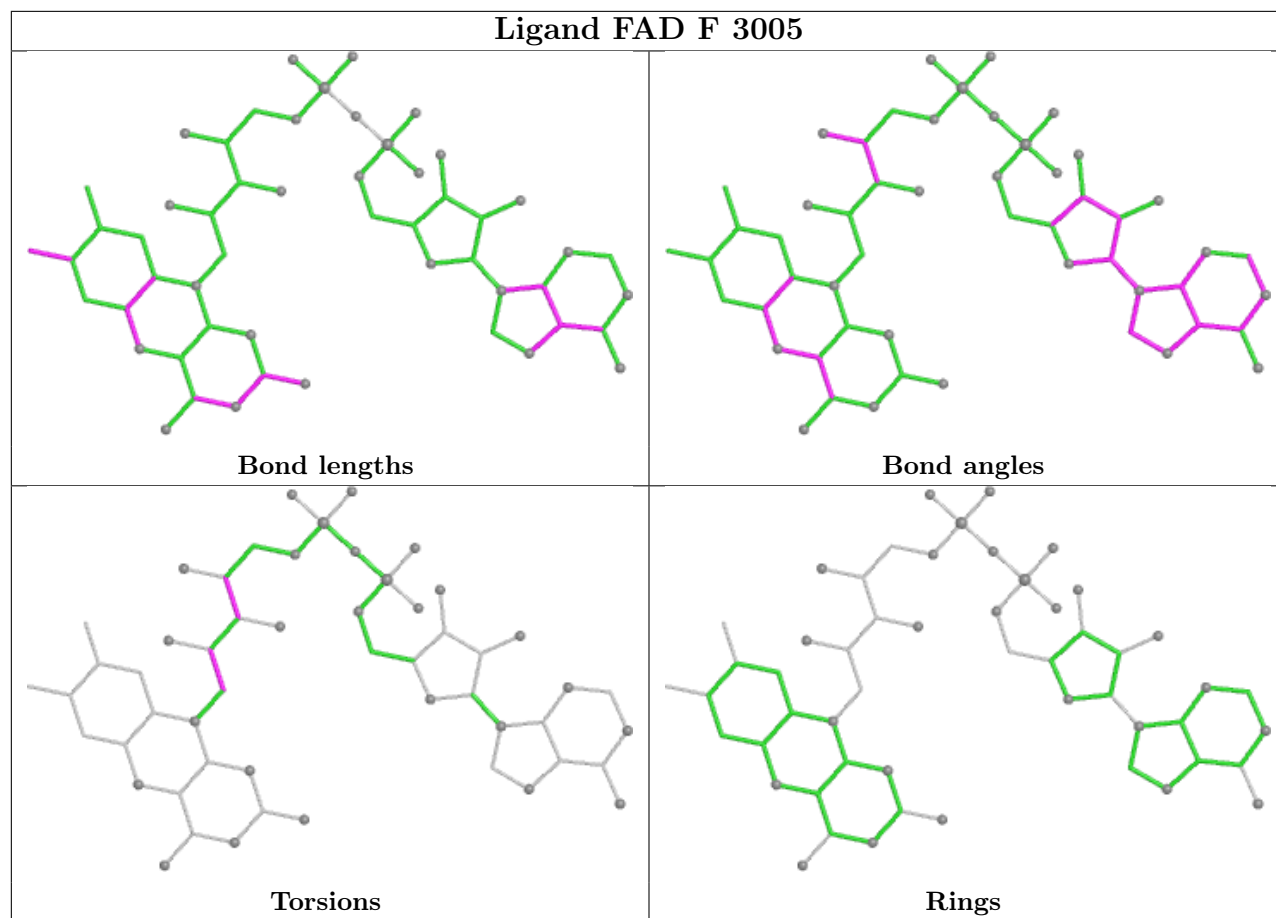
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	FES	1	0
5	A	3005	FAD	1	0
3	A	3003	URC	1	0
5	F	3005	FAD	2	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	1287/1331 (96%)	-0.08	43 (3%) 49 55	12, 20, 40, 70	0
1	F	1287/1331 (96%)	0.08	51 (3%) 42 47	12, 23, 46, 134	0
All	All	2574/2662 (96%)	0.00	94 (3%) 45 51	12, 21, 44, 134	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1320	VAL	8.2
1	F	1319	GLY	7.9
1	F	1321	PRO	7.2
1	F	1318	THR	6.3
1	F	3	ALA	5.2
1	F	551	LYS	5.2
1	F	536	GLY	5.2
1	F	1111	GLY	5.0
1	A	1321	PRO	4.9
1	F	192	PRO	4.6
1	F	1317	VAL	4.4
1	A	1111	GLY	4.3
1	A	533	ASP	3.9
1	A	218	LEU	3.8
1	F	1110	THR	3.7
1	A	63	ASN	3.6
1	A	1110	THR	3.6
1	A	221	THR	3.6
1	A	61	LEU	3.6
1	F	466	LEU	3.5
1	A	164	LYS	3.4
1	A	1320	VAL	3.3
1	F	497	PRO	3.3
1	A	551	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	321	GLN	3.2
1	A	534	MET	3.2
1	F	290	VAL	3.1
1	F	1250	LYS	3.1
1	F	61	LEU	3.1
1	F	531	LEU	2.9
1	A	3	ALA	2.9
1	A	222	PRO	2.9
1	F	480	GLU	2.9
1	A	537	LYS	2.9
1	A	430	ILE	2.9
1	F	1291	GLN	2.8
1	F	496	ALA	2.7
1	F	529	ALA	2.7
1	A	535	CYS	2.7
1	F	164	LYS	2.7
1	A	536	GLY	2.6
1	F	1311	GLN	2.6
1	A	376	ARG	2.6
1	A	532	GLU	2.6
1	A	1250	LYS	2.6
1	A	529	ALA	2.6
1	F	396	LEU	2.5
1	F	812	LEU	2.5
1	A	377	GLY	2.5
1	F	537	LYS	2.5
1	F	221	THR	2.5
1	A	494	GLN	2.5
1	F	413	GLU	2.5
1	A	531	LEU	2.5
1	A	427	GLU	2.5
1	F	377	GLY	2.5
1	A	271	ASN	2.4
1	A	812	LEU	2.4
1	A	992	CYS	2.4
1	F	534	MET	2.4
1	A	1318	THR	2.4
1	F	383	ARG	2.4
1	F	535	CYS	2.4
1	A	473	LEU	2.4
1	F	1143	GLU	2.3
1	F	1107	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	566	ASP	2.3
1	F	1315	LEU	2.3
1	A	852	LYS	2.3
1	F	1106	LYS	2.3
1	A	432	LYS	2.3
1	F	218	LEU	2.3
1	F	565	LYS	2.3
1	F	719	LEU	2.3
1	F	198	GLU	2.2
1	F	222	PRO	2.2
1	F	532	GLU	2.2
1	A	530	ASP	2.2
1	F	852	LYS	2.2
1	A	983	GLU	2.1
1	F	220	ASP	2.1
1	A	474	SER	2.1
1	A	731	SER	2.1
1	F	267	MET	2.1
1	F	387	THR	2.1
1	A	413	GLU	2.1
1	A	192	PRO	2.1
1	A	548	LEU	2.1
1	A	1276	ASP	2.1
1	F	498	ASP	2.1
1	F	247	LEU	2.0
1	F	1316	CYS	2.0
1	A	321	GLN	2.0
1	F	550	GLN	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.

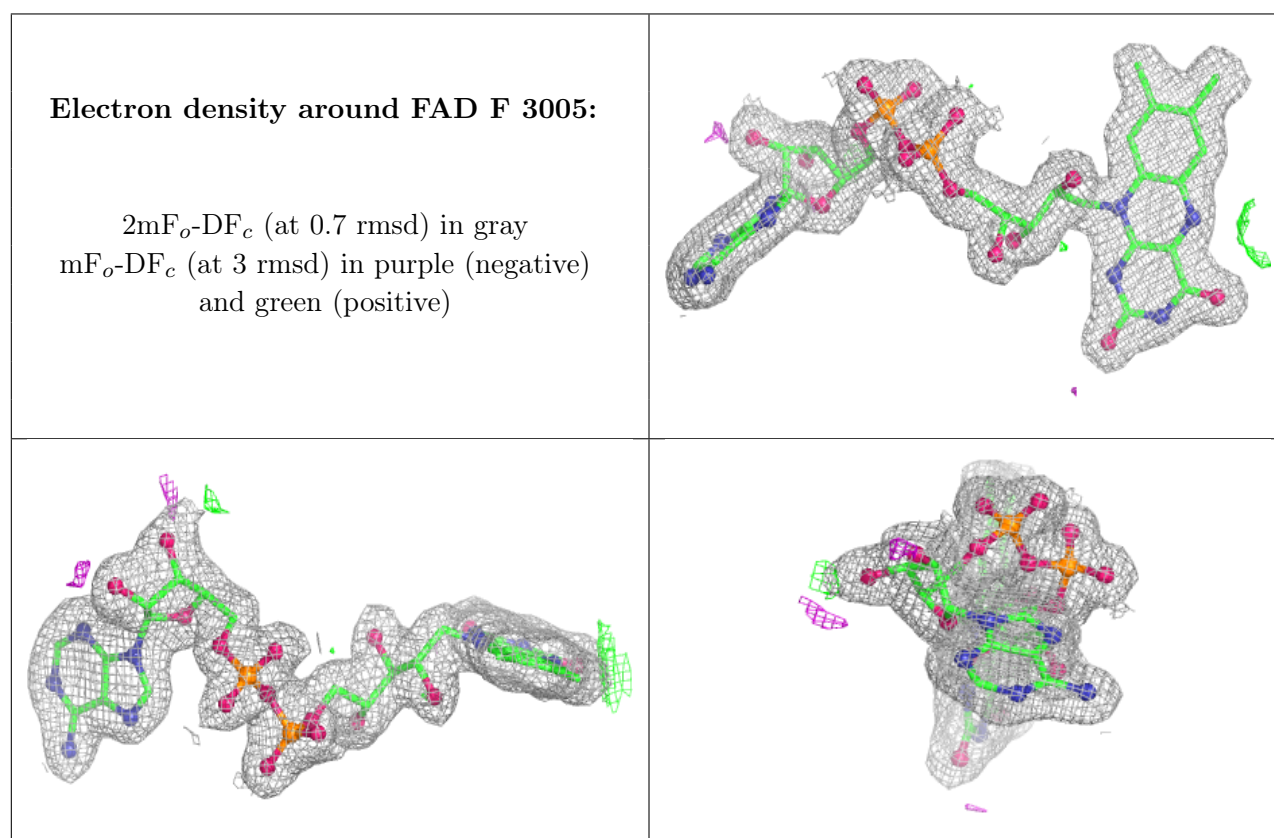
6.4 Ligands [i](#)

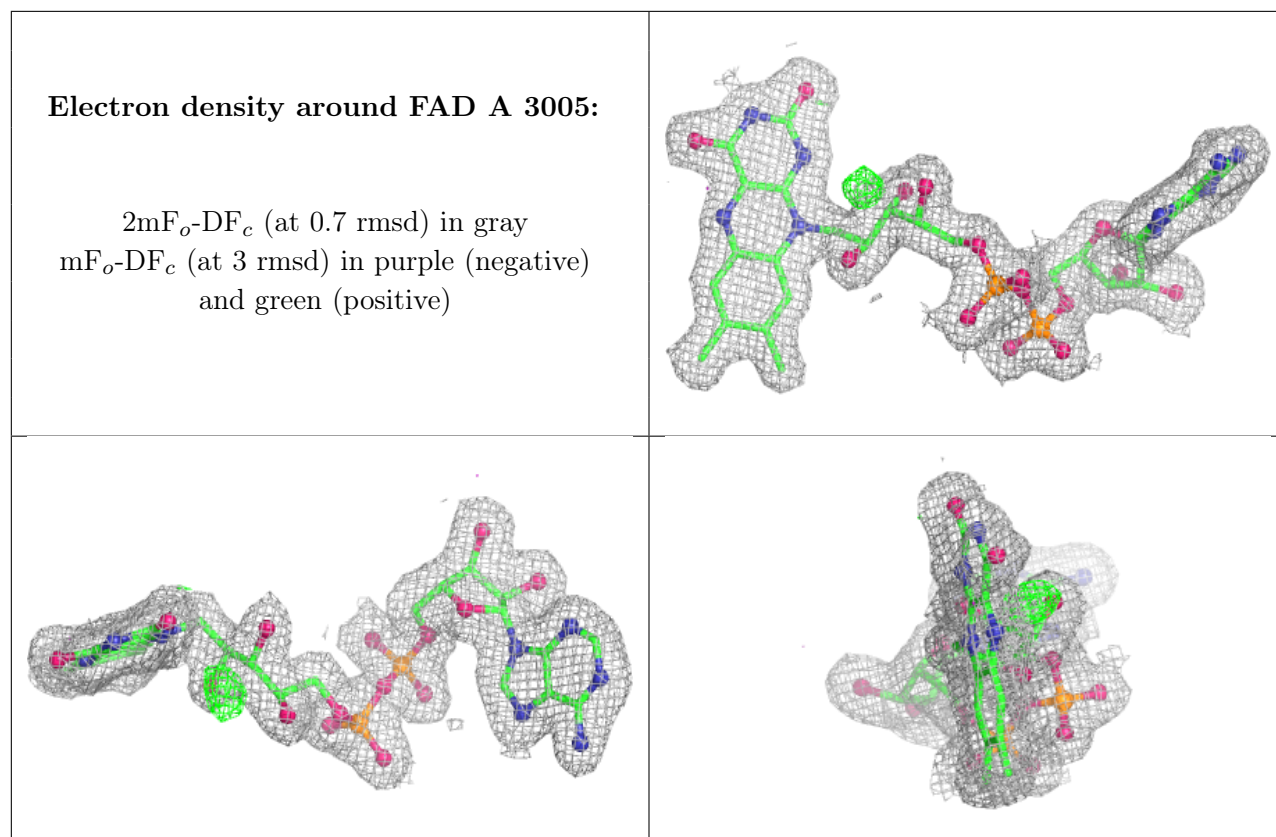
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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($\text{\AA}^2$)	Q<0.9
3	URC	A	3003	12/12	0.96	0.05	17,18,19,20	0
3	URC	F	3003	12/12	0.96	0.06	18,20,21,21	0
5	FAD	F	3005	53/53	0.97	0.06	18,23,25,26	0
5	FAD	A	3005	53/53	0.98	0.05	15,17,19,22	0
4	BCT	A	3004	4/4	0.98	0.04	14,16,17,19	0
2	FES	F	3001	4/4	0.99	0.04	17,17,18,19	0
4	BCT	F	3004	4/4	0.99	0.04	18,20,21,23	0
2	FES	A	3002	4/4	1.00	0.01	13,13,13,14	0
2	FES	A	3001	4/4	1.00	0.04	15,16,17,17	0
2	FES	F	3002	4/4	1.00	0.02	15,15,15,15	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.