



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 03:49 PM BST

PDB ID : 6AJU  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

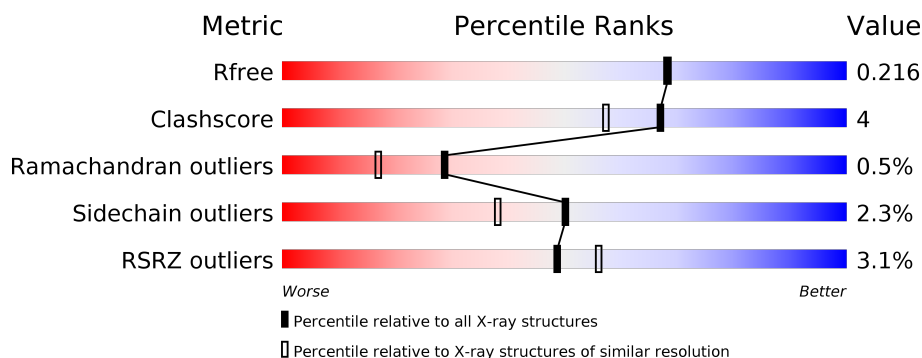
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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  $\geq 3$ , 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	
1	F	1331	

## 2 Entry composition [i](#)

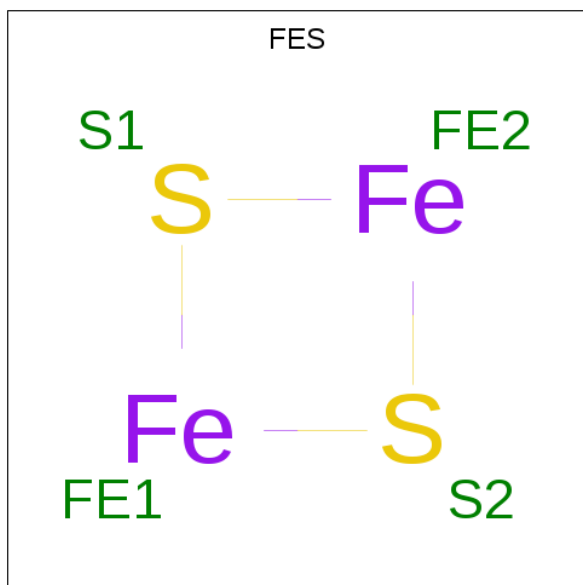
There are 6 unique types of molecules in this entry. The entry contains 21334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

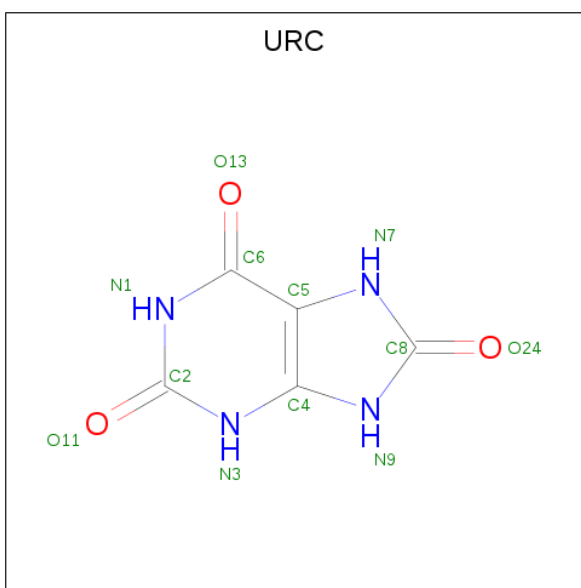
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1287	Total	C	N	O	S	0	0	0
			9945	6306	1710	1865	64			
1	F	1287	Total	C	N	O	S	0	0	0
			9945	6306	1710	1865	64			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



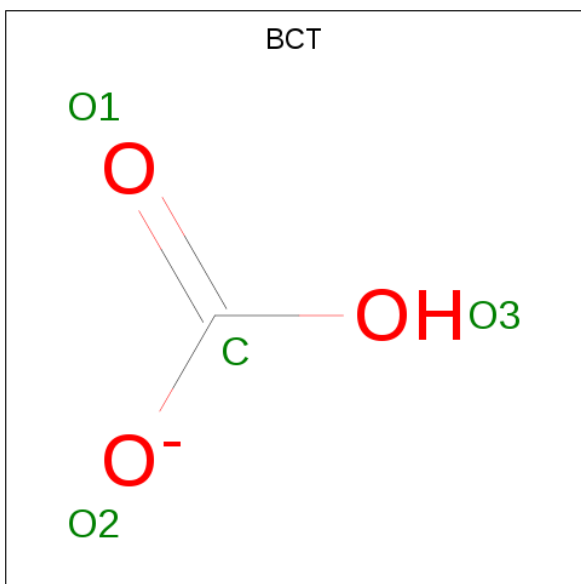
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	F	1	Total	Fe	S	0	0
			4	2	2		
2	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is URIC ACID (three-letter code: 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 (three-letter code: BCT) (formula:  $CHO_3$ ).



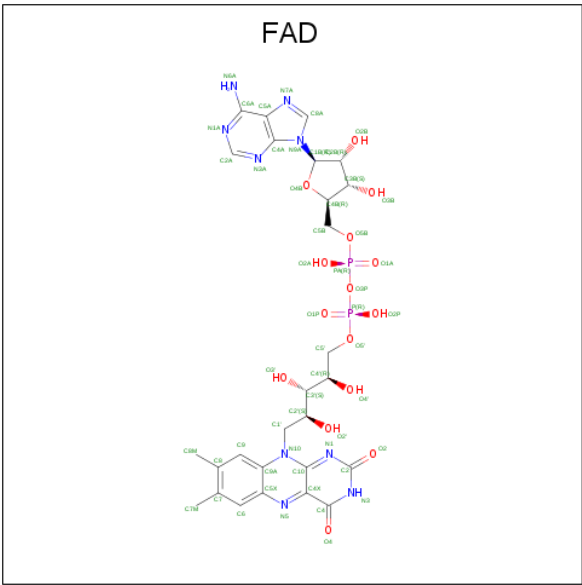
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		

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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 (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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		

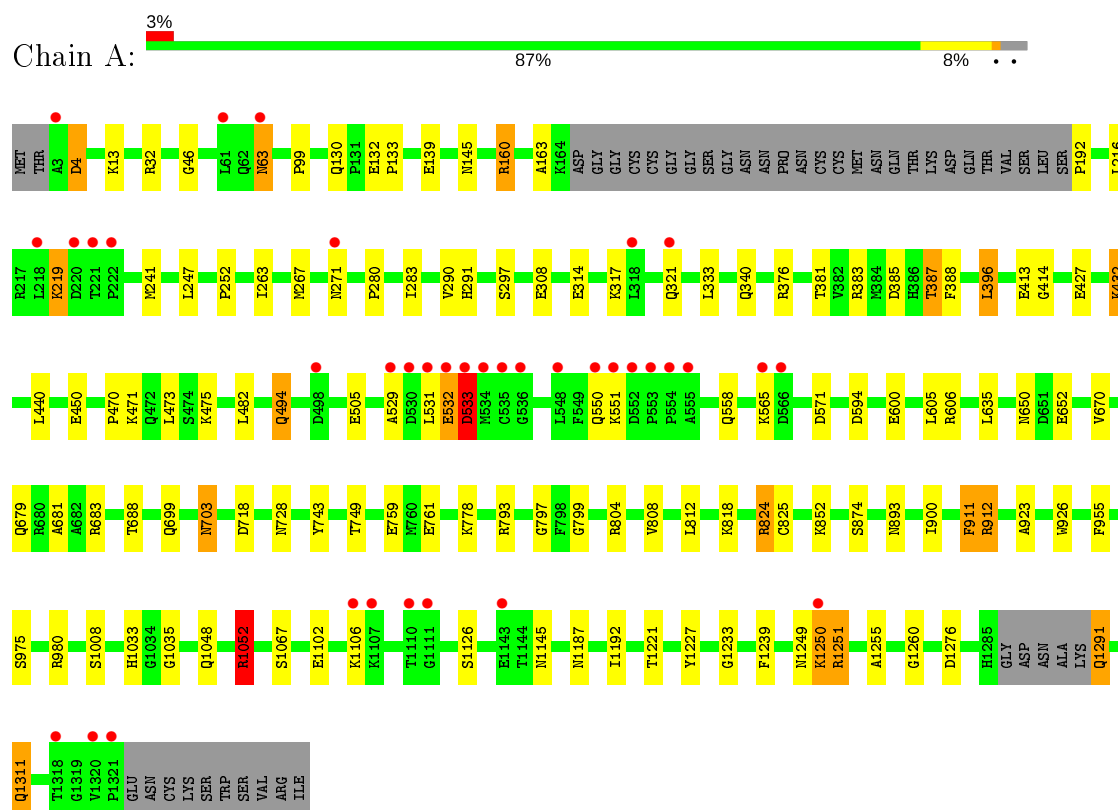
- Molecule 6 is water.

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

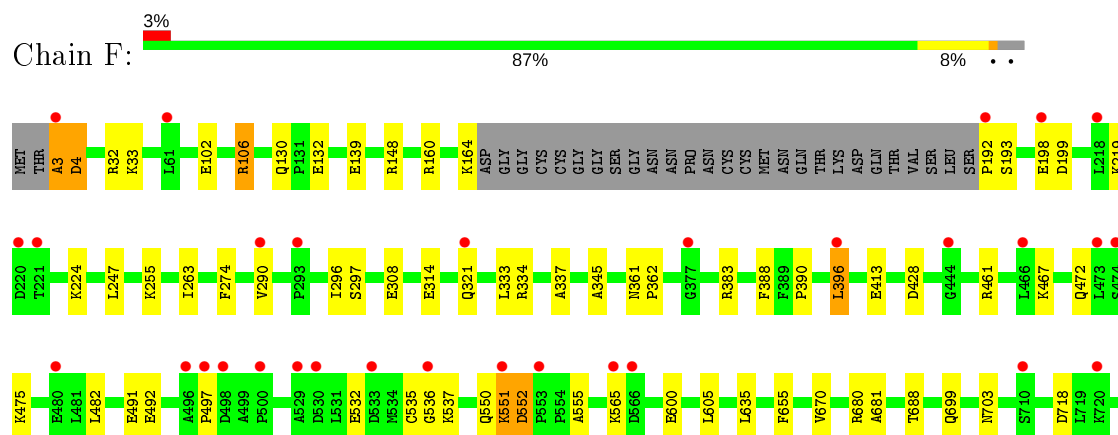
### 3 Residue-property plots [i](#)

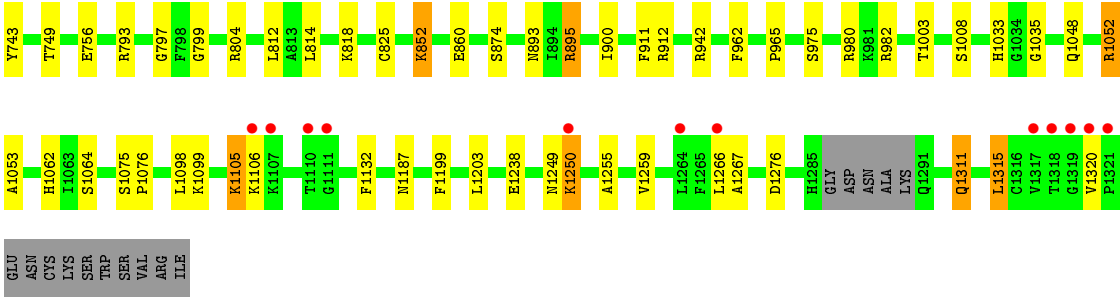
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	11222 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BCT, FES, FAD, URC

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	0.72	7/10155 (0.1%)	0.81	4/13743 (0.0%)
1	F	0.68	3/10155 (0.0%)	0.77	5/13743 (0.0%)
All	All	0.70	10/20310 (0.0%)	0.79	9/27486 (0.0%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	600	GLU	CD-OE2	10.29	1.36	1.25
1	A	427	GLU	CD-OE1	8.40	1.34	1.25
1	F	600	GLU	CD-OE2	8.11	1.34	1.25
1	A	761	GLU	CD-OE1	7.79	1.34	1.25
1	A	139	GLU	CD-OE1	7.25	1.33	1.25
1	F	139	GLU	CD-OE1	6.53	1.32	1.25
1	A	652	GLU	CD-OE2	6.51	1.32	1.25
1	A	505	GLU	CD-OE1	6.09	1.32	1.25
1	F	756	GLU	CD-OE1	5.67	1.31	1.25
1	A	1260	GLY	N-CA	5.09	1.53	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	793	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	1052	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	F	1052	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	A	533	ASP	CB-CA-C	6.00	122.41	110.40
1	A	1052	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	F	756	GLU	CB-CA-C	-5.59	99.22	110.40
1	F	942	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	F	982	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	F	793	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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
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	69	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	155	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 (155) 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: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:1276:ASP:HB3	6:A:3195:HOH:O	1.83	0.79
1:A:216:LEU:O	1:A:219:LYS:HG3	1.81	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:241:MET:HE2	1:A:283:ILE:HG21	1.70	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ARG:HH22	1:F:199:ASP:HB2	1.58	0.69
1:A:271:ASN:CG	1:A:683:ARG:HH11	1.97	0.68
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: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:A:267:MET:HE1	6:A:3551:HOH:O	1.98	0.63
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: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: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:1048:GLN:HE22	1:A:1187:ASN:HD22	1.51	0.59
1:A:728:ASN:HD21	1:A:852:LYS:CE	2.16	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:321:GLN:HG2	1:A:413:GLU:CD	2.25	0.57
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:F:321:GLN:HG2	1:F:413:GLU:CD	2.26	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:A:267:MET:CE	6:A:3551:HOH:O	2.53	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: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:1033:HIS:CD2	1:F:1035:GLY:H	2.27	0.52
1:F:749:THR:O	1:F:812:LEU:HD12	2.08	0.52
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:GLN:NE2	1:A:1187:ASN:HD22	2.07	0.52
1:F:1259:VAL:O	1:F:1259:VAL:HG22	2.10	0.52
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: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:HA	1:F:852:LYS:HE3	1.93	0.50
1:F:1048:GLN:NE2	1:F:1187:ASN:HD22	2.07	0.49
1:F:812:LEU:HD23	1:F:812:LEU:N	2.27	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:571:ASP:CG	1:A:1052:ARG:HD2	2.33	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
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:F:396:LEU:HD23	1:F:396:LEU:C	2.33	0.48
1:A:852:LYS:HA	1:A:852:LYS:HE2	1.95	0.48
1:A:271:ASN:CG	1:A:683:ARG:HD3	2.34	0.47
1:F:799:GLY:HA2	6:F:3319:HOH:O	2.16	0.46
1:A:1250:LYS:HG3	6:A:3620:HOH:O	2.16	0.46
1:A:635:LEU:HD21	1:A:818:LYS:HD3	1.97	0.46
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.15	0.46
1:A:63:ASN:N	1:A:63:ASN:OD1	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: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:296:ILE:CD1	1:F:314:GLU:HG3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:C	1:A:396:LEU:HD23	2.37	0.45
1:F:699:GLN:NE2	1:F:703:ASN:OD1	2.46	0.45
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:NE2	1:A:1311:GLN:H	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
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: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:390:PRO:C	1:F:461:ARG:NH1	2.73	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:1203:LEU:C	1:F:1203:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1250:LYS:HD3	1:A:1251:ARG:N	2.35	0.41
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	2.02	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:605:LEU:HD13	1:F:812:LEU:CD2	2.50	0.41
1:A:911:PHE:O	1:A:912:ARG:C	2.59	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%)	34	24
1	F	1281/1331 (96%)	1230 (96%)	43 (3%)	8 (1%)	25	13
All	All	2562/2662 (96%)	2471 (96%)	78 (3%)	13 (0%)	29	17

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

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Mol	Chain	Res	Type
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%)	1061 (98%)	26 (2%)	49	36
1	F	1087/1124 (97%)	1063 (98%)	24 (2%)	52	39
All	All	2174/2248 (97%)	2124 (98%)	50 (2%)	50	38

All (50) 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	252	PRO
1	A	280	PRO
1	A	317	LYS
1	A	381	THR
1	A	387	THR
1	A	396	LEU
1	A	432	LYS
1	A	482	LEU
1	A	494	GLN
1	A	533	ASP
1	A	550	GLN
1	A	565	LYS

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Mol	Chain	Res	Type
1	A	703	ASN
1	A	743	TYR
1	A	824	ARG
1	A	911	PHE
1	A	1239	PHE
1	A	1250	LYS
1	A	1291	GLN
1	A	1311	GLN
1	F	4	ASP
1	F	33	LYS
1	F	193	SER
1	F	198	GLU
1	F	219	LYS
1	F	224	LYS
1	F	247	LEU
1	F	396	LEU
1	F	482	LEU
1	F	491	GLU
1	F	550	GLN
1	F	551	LYS
1	F	565	LYS
1	F	743	TYR
1	F	852	LYS
1	F	911	PHE
1	F	1064	SER
1	F	1099	LYS
1	F	1105	LYS
1	F	1106	LYS
1	F	1250	LYS
1	F	1276	ASP
1	F	1311	GLN
1	F	1315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	145	ASN
1	A	291	HIS
1	A	321	GLN
1	A	332	GLN
1	A	350	ASN

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Mol	Chain	Res	Type
1	A	449	GLN
1	A	472	GLN
1	A	494	GLN
1	A	585	GLN
1	A	642	ASN
1	A	703	ASN
1	A	728	ASN
1	A	893	ASN
1	A	1033	HIS
1	A	1048	GLN
1	A	1173	ASN
1	A	1212	HIS
1	A	1294	GLN
1	A	1311	GLN
1	F	130	GLN
1	F	145	ASN
1	F	291	HIS
1	F	321	GLN
1	F	332	GLN
1	F	350	ASN
1	F	449	GLN
1	F	472	GLN
1	F	483	GLN
1	F	550	GLN
1	F	585	GLN
1	F	642	ASN
1	F	893	ASN
1	F	1033	HIS
1	F	1048	GLN
1	F	1173	ASN
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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	F	3002	1	0,4,4	0.00	-	-		
2	FES	A	3001	1	0,4,4	0.00	-	-		
2	FES	F	3001	1	0,4,4	0.00	-	-		
4	BCT	A	3004	-	0,3,3	0.00	-	0,3,3	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	-		
4	BCT	F	3004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	F	3005	-	51,58,58	1.84	8 (15%)	60,89,89	2.65	16 (26%)
5	FAD	A	3005	-	51,58,58	1.94	11 (21%)	60,89,89	2.26	18 (30%)
3	URC	F	3003	-	13,13,13	3.97	6 (46%)	11,19,19	3.36	5 (45%)
3	URC	A	3003	-	13,13,13	3.36	7 (53%)	11,19,19	4.19	5 (45%)

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	F	3002	1	-	-	0/1/1/1
2	FES	A	3001	1	-	-	0/1/1/1
2	FES	F	3001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
5	FAD	F	3005	-	-	4/30/50/50	0/6/6/6
5	FAD	A	3005	-	-	5/30/50/50	0/6/6/6
3	URC	F	3003	-	-	-	0/2/2/2
3	URC	A	3003	-	-	-	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3003	URC	C4-N3	-9.18	1.34	1.46
5	F	3005	FAD	C4X-C10	7.85	1.46	1.38
5	A	3005	FAD	C4X-C10	7.17	1.46	1.38
3	A	3003	URC	C4-N9	-7.00	1.36	1.44
3	F	3003	URC	C4-N9	-6.55	1.36	1.44
3	A	3003	URC	C4-N3	-6.26	1.38	1.46
3	F	3003	URC	O13-C6	5.42	1.34	1.23
5	A	3005	FAD	C9A-N10	5.22	1.45	1.38
3	F	3003	URC	O24-C8	4.17	1.32	1.23
3	F	3003	URC	C5-N7	-4.16	1.37	1.45
5	F	3005	FAD	C9A-C5X	3.86	1.50	1.42
5	A	3005	FAD	O4B-C1B	3.69	1.46	1.41
5	F	3005	FAD	C2B-C1B	-3.62	1.48	1.53
5	A	3005	FAD	C4-C4X	3.55	1.47	1.41
3	A	3003	URC	O24-C8	3.47	1.30	1.23
5	A	3005	FAD	C9A-C5X	3.36	1.49	1.42
5	A	3005	FAD	C4X-N5	3.23	1.38	1.33
3	A	3003	URC	C5-C6	-3.21	1.47	1.52
3	A	3003	URC	C5-N7	-3.16	1.39	1.45
5	A	3005	FAD	C8-C7	3.12	1.48	1.40
5	A	3005	FAD	C2B-C1B	-3.09	1.49	1.53
5	F	3005	FAD	C9A-N10	2.96	1.42	1.38
3	F	3003	URC	C5-C6	-2.94	1.47	1.52
3	A	3003	URC	O11-C2	2.84	1.29	1.23
5	A	3005	FAD	C4A-N3A	2.66	1.39	1.35
5	F	3005	FAD	C4-C4X	2.62	1.45	1.41
5	F	3005	FAD	C2-N3	-2.43	1.33	1.38
3	A	3003	URC	O13-C6	2.41	1.28	1.23
5	F	3005	FAD	C5A-C4A	2.20	1.46	1.40
5	A	3005	FAD	O3'-C3'	2.12	1.48	1.43
5	F	3005	FAD	C7M-C7	2.05	1.55	1.51
5	A	3005	FAD	C8A-N7A	2.03	1.38	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3005	FAD	C4-N3-C2	13.19	126.28	115.14
5	A	3005	FAD	C4-N3-C2	8.79	122.56	115.14
3	A	3003	URC	C4-N9-C8	-8.12	107.37	112.89
5	F	3005	FAD	C4-C4X-C10	-7.25	115.15	119.95
3	F	3003	URC	C4-N9-C8	-6.60	108.41	112.89
3	A	3003	URC	N7-C8-N9	6.31	114.68	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3003	URC	C5-C4-N9	6.08	105.46	102.64
5	F	3005	FAD	C1'-N10-C9A	5.54	122.65	118.29
5	A	3005	FAD	C5X-C9A-N10	5.11	121.42	117.72
3	F	3003	URC	C5-C4-N9	5.09	105.00	102.64
5	A	3005	FAD	C4X-N5-C5X	5.02	121.79	116.77
5	F	3005	FAD	C4X-C4-N3	-4.99	116.61	123.43
3	A	3003	URC	N1-C2-N3	4.89	121.27	116.12
5	A	3005	FAD	C1'-N10-C9A	4.84	122.10	118.29
5	F	3005	FAD	C4X-N5-C5X	4.68	121.45	116.77
3	F	3003	URC	N1-C2-N3	4.63	120.99	116.12
5	A	3005	FAD	C4X-C4-N3	-4.60	117.14	123.43
3	F	3003	URC	N7-C8-N9	4.39	112.88	108.76
3	A	3003	URC	O24-C8-N9	-4.28	119.79	125.94
5	A	3005	FAD	C9A-N10-C10	-3.83	116.90	121.91
5	A	3005	FAD	C4-C4X-C10	-3.65	117.53	119.95
5	F	3005	FAD	C4-C4X-N5	3.29	122.36	118.60
5	A	3005	FAD	C1B-N9A-C4A	-3.20	121.02	126.64
5	F	3005	FAD	C9A-N10-C10	-2.88	118.13	121.91
5	F	3005	FAD	C1B-N9A-C4A	-2.88	121.58	126.64
5	A	3005	FAD	O3'-C3'-C4'	2.88	115.76	108.81
5	F	3005	FAD	C4A-C5A-N7A	-2.83	106.45	109.40
5	F	3005	FAD	C5X-C9A-N10	2.77	119.72	117.72
5	A	3005	FAD	C5A-C6A-N6A	-2.68	116.28	120.35
5	A	3005	FAD	C9A-C5X-N5	-2.62	118.27	122.36
5	A	3005	FAD	C6-C5X-C9A	2.57	122.42	119.05
5	A	3005	FAD	N3A-C2A-N1A	-2.54	124.71	128.68
5	A	3005	FAD	C1'-N10-C10	2.53	120.67	118.41
5	F	3005	FAD	C5A-C6A-N1A	-2.49	114.70	120.35
5	F	3005	FAD	C2A-N1A-C6A	2.48	123.00	118.75
5	A	3005	FAD	C5'-C4'-C3'	2.32	116.68	112.20
5	A	3005	FAD	N6A-C6A-N1A	2.29	123.32	118.57
5	A	3005	FAD	O4'-C4'-C3'	-2.20	103.75	109.10
5	F	3005	FAD	C2B-C3B-C4B	2.13	106.79	102.64
5	F	3005	FAD	O4'-C4'-C3'	-2.10	104.00	109.10
5	F	3005	FAD	C9A-C5X-N5	-2.07	119.13	122.36
5	F	3005	FAD	C5A-C6A-N6A	2.05	123.47	120.35
3	F	3003	URC	O11-C2-N3	-2.02	118.90	122.92
5	A	3005	FAD	C10-C4X-N5	2.02	122.65	121.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

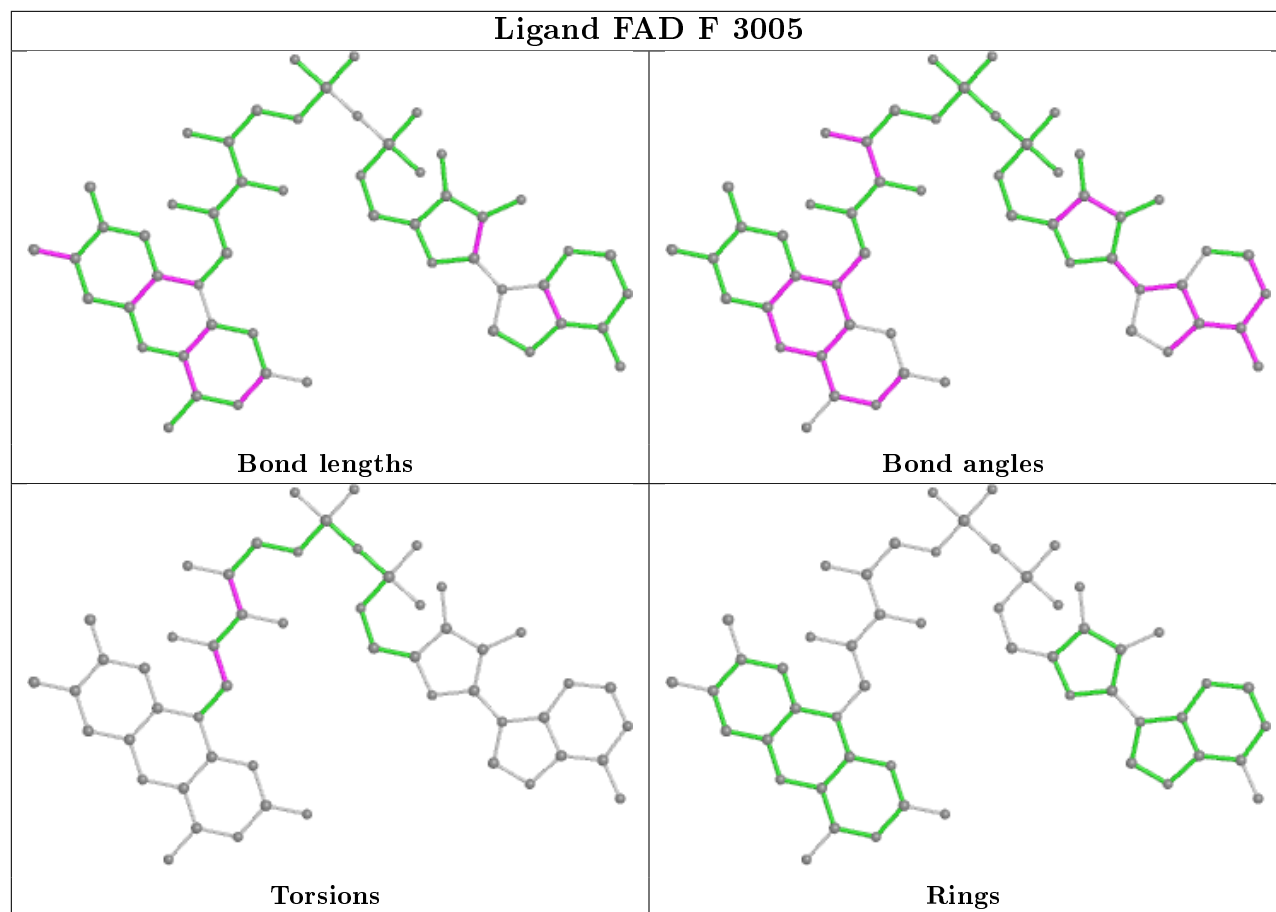
Mol	Chain	Res	Type	Atoms
5	F	3005	FAD	N10-C1'-C2'-O2'
5	F	3005	FAD	N10-C1'-C2'-C3'
5	A	3005	FAD	N10-C1'-C2'-O2'
5	A	3005	FAD	C2'-C3'-C4'-O4'
5	A	3005	FAD	C2'-C3'-C4'-C5'
5	F	3005	FAD	C2'-C3'-C4'-C5'
5	A	3005	FAD	N10-C1'-C2'-C3'
5	F	3005	FAD	C2'-C3'-C4'-O4'
5	A	3005	FAD	O3'-C3'-C4'-O4'

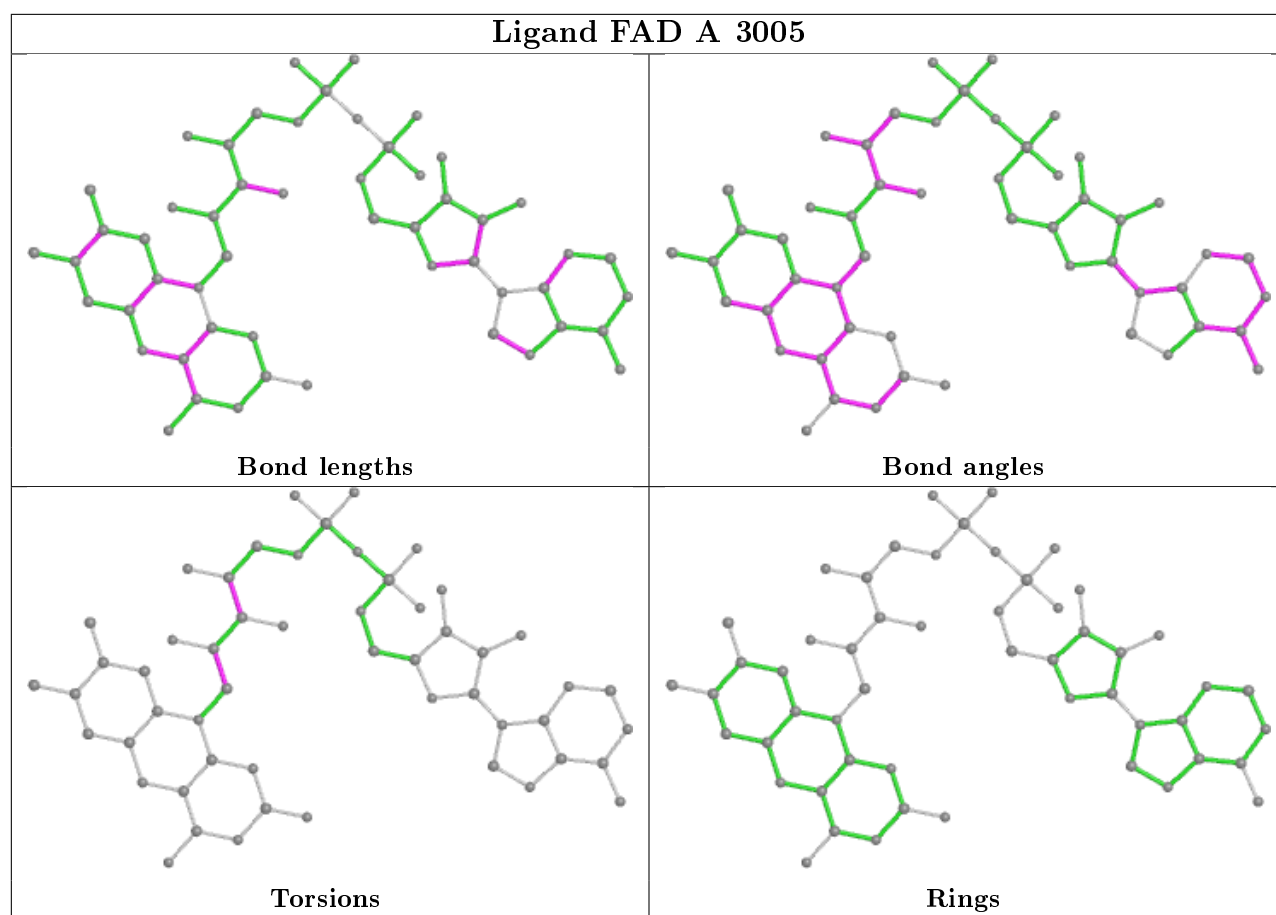
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	FES	1	0
5	F	3005	FAD	2	0
5	A	3005	FAD	1	0
3	A	3003	URC	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1287/1331 (96%)	-0.11	37 (2%) 51 59	12, 20, 40, 70	0
1	F	1287/1331 (96%)	0.04	43 (3%) 46 54	12, 23, 46, 134	0
All	All	2574/2662 (96%)	-0.04	80 (3%) 49 56	12, 21, 44, 134	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1320	VAL	20.6
1	F	1318	THR	17.5
1	F	1319	GLY	15.8
1	F	1321	PRO	12.0
1	F	1111	GLY	4.9
1	F	3	ALA	4.2
1	F	377	GLY	4.2
1	A	218	LEU	4.1
1	A	1111	GLY	4.0
1	A	533	ASP	4.0
1	A	530	ASP	3.9
1	A	534	MET	3.8
1	F	536	GLY	3.7
1	A	532	GLU	3.6
1	A	221	THR	3.5
1	F	1110	THR	3.5
1	F	1317	VAL	3.5
1	F	496	ALA	3.4
1	A	1110	THR	3.3
1	F	497	PRO	3.3
1	A	1106	LYS	3.2
1	A	220	ASP	3.1
1	A	1320	VAL	3.1
1	F	220	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	473	LEU	3.1
1	A	222	PRO	3.1
1	F	551	LYS	3.1
1	A	3	ALA	3.0
1	A	554	PRO	3.0
1	A	1321	PRO	2.9
1	A	536	GLY	2.9
1	A	529	ALA	2.9
1	A	553	PRO	2.8
1	F	61	LEU	2.8
1	F	533	ASP	2.8
1	F	530	ASP	2.7
1	A	531	LEU	2.6
1	A	552	ASP	2.6
1	F	529	ALA	2.6
1	A	551	LYS	2.5
1	F	218	LEU	2.5
1	A	498	ASP	2.5
1	F	396	LEU	2.5
1	F	553	PRO	2.5
1	F	566	ASP	2.5
1	A	535	CYS	2.5
1	A	63	ASN	2.5
1	F	466	LEU	2.5
1	F	192	PRO	2.5
1	F	1106	LYS	2.4
1	F	1250	LYS	2.4
1	F	480	GLU	2.4
1	F	290	VAL	2.4
1	F	293	PRO	2.4
1	A	1143	GLU	2.4
1	A	61	LEU	2.3
1	F	498	ASP	2.3
1	A	550	GLN	2.3
1	F	221	THR	2.3
1	A	555	ALA	2.3
1	A	566	ASP	2.3
1	A	318	LEU	2.3
1	F	321	GLN	2.3
1	A	565	LYS	2.3
1	A	1250	LYS	2.3
1	A	271	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	565	LYS	2.2
1	F	444	GLY	2.2
1	F	710	SER	2.2
1	A	1318	THR	2.2
1	F	474	SER	2.1
1	F	720	LYS	2.1
1	F	1264	LEU	2.1
1	F	500	PRO	2.1
1	A	321	GLN	2.1
1	F	1107	LYS	2.1
1	A	548	LEU	2.1
1	A	1107	LYS	2.0
1	F	1266	LEU	2.0
1	F	198	GLU	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 monosaccharides 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, 95<sup>th</sup> 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.

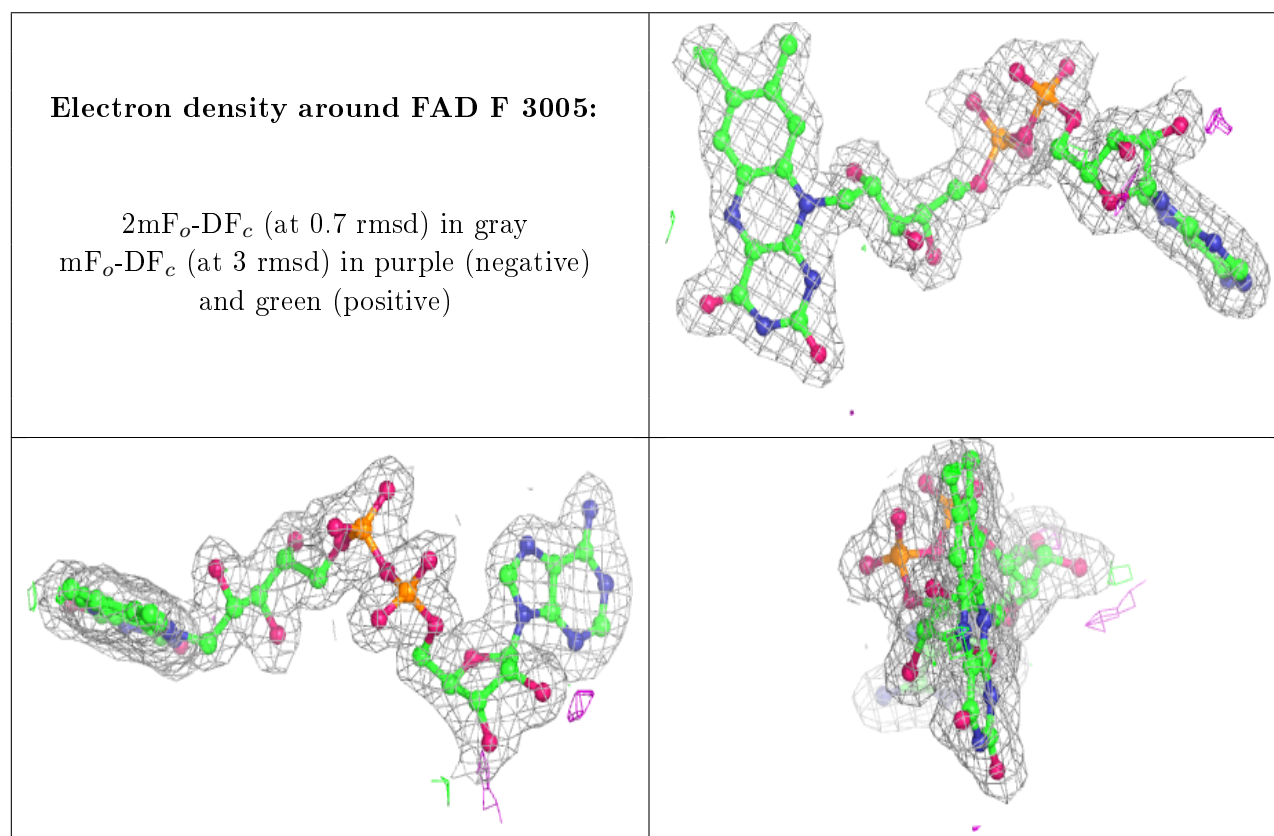
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	URC	F	3003	12/12	0.96	0.10	18,20,21,21	0
4	BCT	A	3004	4/4	0.97	0.10	14,16,17,19	0
3	URC	A	3003	12/12	0.97	0.07	17,18,19,20	0
5	FAD	F	3005	53/53	0.98	0.10	18,23,25,26	0
5	FAD	A	3005	53/53	0.98	0.09	15,17,19,22	0
2	FES	F	3002	4/4	0.99	0.06	15,15,15,15	0
4	BCT	F	3004	4/4	0.99	0.10	18,20,21,23	0
2	FES	F	3001	4/4	0.99	0.04	17,17,18,19	0
2	FES	A	3002	4/4	1.00	0.07	13,13,13,14	0

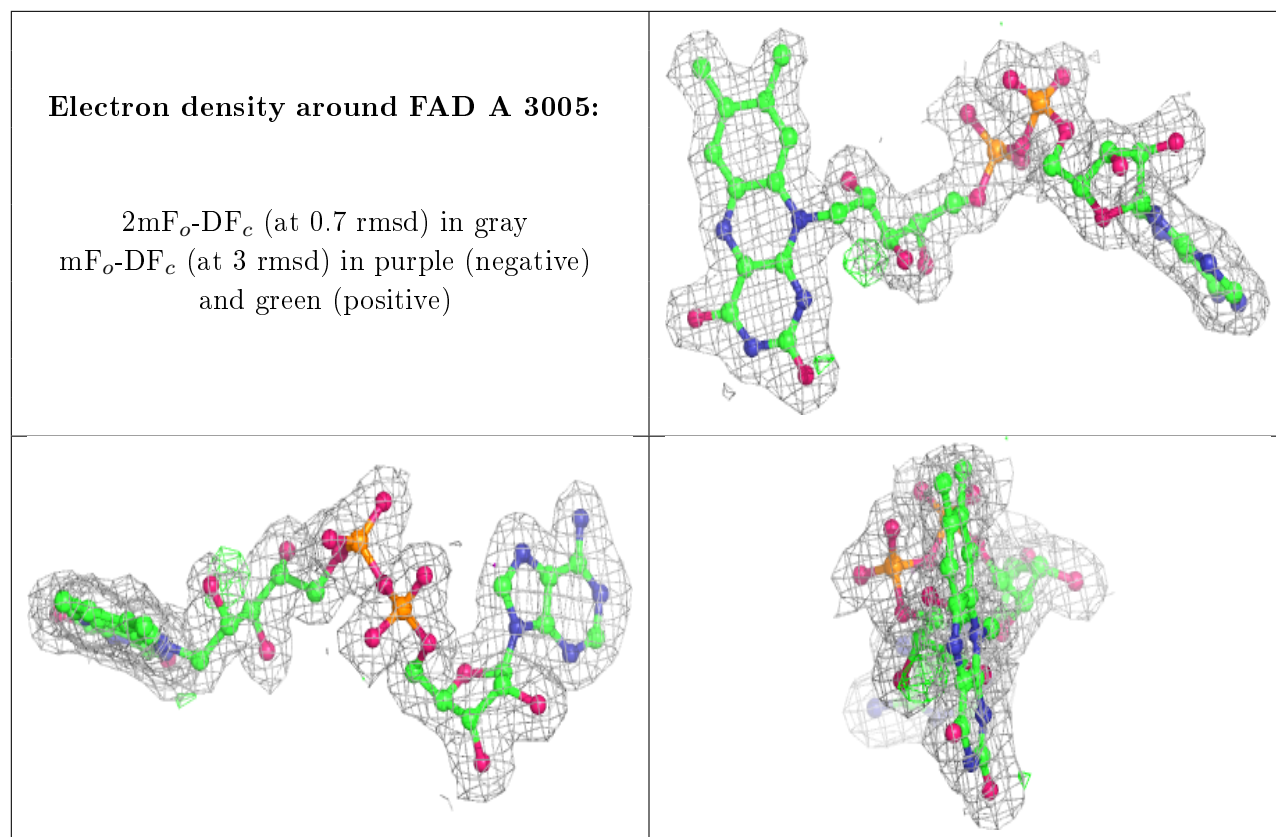
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FES	A	3001	4/4	1.00	0.04	15,16,17,17	0

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.