



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:36 AM UTC

PDB ID : 4Z2T / pdb_00004z2t
Title : Crystal Structure of 2-hydroxybiphenyl 3-monooxygenase W225Y from *Pseudomonas azelaica*
Authors : Kanteev, M.; Bregman-Cohen, A.; Fishman, A.
Deposited on : 2015-03-30
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

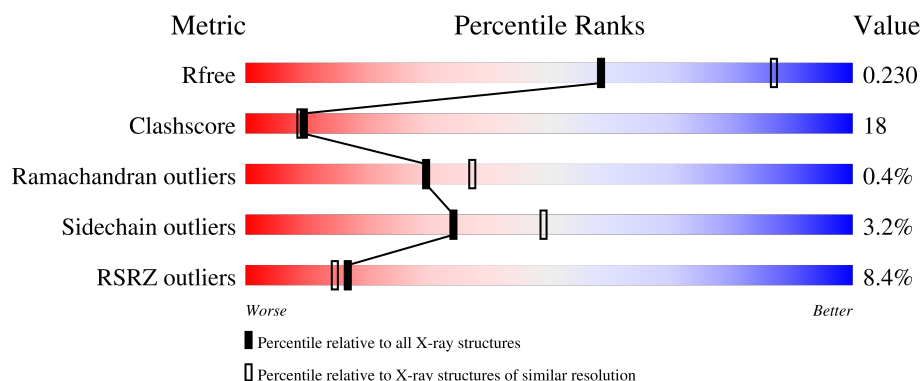
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	592	7% 65% 27% 6%
1	B	592	9% 67% 25% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9201 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.

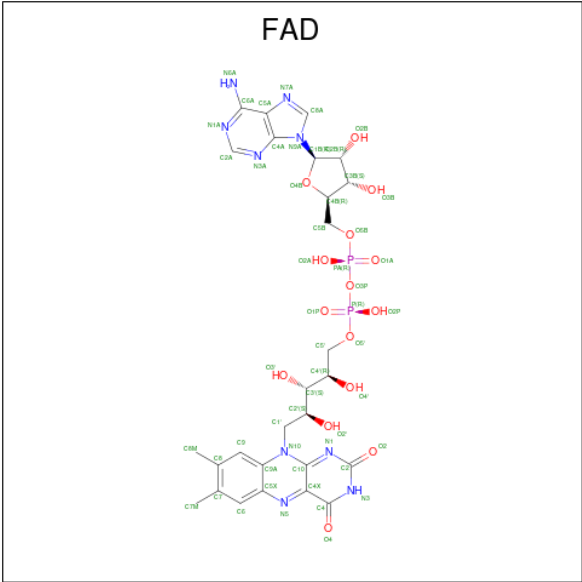
- Molecule 1 is a protein called 2-hydroxybiphenyl-3-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4301	2717	756	808	20			
1	B	564	Total	C	N	O	S	0	0	0
			4339	2741	761	817	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP O06647
A	-4	HIS	-	expression tag	UNP O06647
A	-3	HIS	-	expression tag	UNP O06647
A	-2	HIS	-	expression tag	UNP O06647
A	-1	HIS	-	expression tag	UNP O06647
A	0	HIS	-	expression tag	UNP O06647
A	1	HIS	-	expression tag	UNP O06647
A	225	TYR	TRP	engineered mutation	UNP O06647
B	-5	MET	-	initiating methionine	UNP O06647
B	-4	HIS	-	expression tag	UNP O06647
B	-3	HIS	-	expression tag	UNP O06647
B	-2	HIS	-	expression tag	UNP O06647
B	-1	HIS	-	expression tag	UNP O06647
B	0	HIS	-	expression tag	UNP O06647
B	1	HIS	-	expression tag	UNP O06647
B	225	TYR	TRP	engineered mutation	UNP O06647

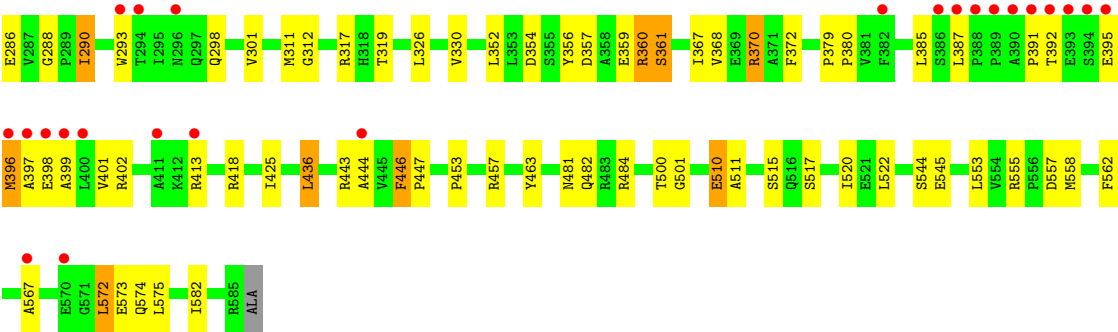
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total	O	0	0
			242	242		
3	B	213	Total	O	0	0
			213	213		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.38Å 130.58Å 78.75Å 90.00° 98.79° 90.00°	Depositor
Resolution (Å)	43.85 – 2.45 43.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.85-2.45) 97.1 (43.85-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.218 , 0.236 0.213 , 0.230	Depositor DCC
R_{free} test set	2792 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9201	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.97% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.26	7/4393 (0.2%)	1.15	27/5951 (0.5%)
1	B	1.12	6/4433 (0.1%)	1.17	35/6007 (0.6%)
All	All	1.19	13/8826 (0.1%)	1.16	62/11958 (0.5%)

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	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	TYR	C-N	-26.59	0.94	1.33
1	A	416	ALA	C-N	-16.60	1.11	1.33
1	A	520	ILE	C-N	-14.99	1.11	1.33
1	A	358	ALA	C-N	-12.01	1.16	1.33
1	B	359	GLU	C-N	11.02	1.49	1.33
1	B	70	LEU	C-N	-10.57	1.18	1.33
1	B	360	ARG	C-N	-9.76	1.13	1.33
1	B	573	GLU	C-N	8.62	1.45	1.33
1	B	69	SER	C-N	-6.73	1.24	1.33
1	A	425	ILE	CA-CB	-6.14	1.45	1.54
1	A	118	LEU	C-O	-5.68	1.19	1.24
1	B	118	LEU	C-O	-5.64	1.19	1.24
1	A	359	GLU	C-N	5.18	1.41	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	GLU	CA-C-N	-15.84	96.40	122.54
1	B	359	GLU	C-N-CA	-15.84	96.40	122.54
1	A	77	MET	CA-C-N	14.15	138.17	120.34
1	A	77	MET	C-N-CA	14.15	138.17	120.34
1	A	77	MET	O-C-N	-14.15	102.94	122.46
1	A	519	GLY	O-C-N	-12.72	110.99	122.57
1	B	69	SER	O-C-N	11.79	134.62	122.12
1	B	354	ASP	N-CA-C	11.47	127.25	112.34
1	B	360	ARG	O-C-N	-10.97	108.62	122.34
1	A	134	ARG	N-CA-C	10.83	126.59	113.16
1	B	198	ILE	N-CA-C	-10.20	88.12	109.34
1	B	134	ARG	N-CA-C	9.68	125.36	113.17
1	B	359	GLU	O-C-N	9.54	133.03	122.15
1	A	195	GLN	N-CA-C	-9.25	102.57	112.93
1	B	78	GLY	N-CA-C	7.91	122.22	112.73
1	A	520	ILE	O-C-N	-7.70	115.10	123.03
1	B	572	LEU	CA-C-N	7.63	130.50	120.28
1	B	572	LEU	C-N-CA	7.63	130.50	120.28
1	B	70	LEU	O-C-N	-7.35	112.67	122.23
1	B	70	LEU	CA-C-N	7.29	131.84	121.42
1	B	70	LEU	C-N-CA	7.29	131.84	121.42
1	B	446	PHE	CA-C-N	7.27	127.27	119.78
1	B	446	PHE	C-N-CA	7.27	127.27	119.78
1	A	446	PHE	CA-C-N	7.19	127.19	119.78
1	A	446	PHE	C-N-CA	7.19	127.19	119.78
1	B	269	GLU	N-CA-C	-7.04	105.22	113.88
1	A	519	GLY	CA-C-N	7.03	133.46	122.70
1	A	519	GLY	C-N-CA	7.03	133.46	122.70
1	A	361	SER	CA-C-N	-6.93	111.84	119.19
1	A	361	SER	C-N-CA	-6.93	111.84	119.19
1	B	453	PRO	CA-C-N	-6.87	111.83	122.69
1	B	453	PRO	C-N-CA	-6.87	111.83	122.69
1	A	520	ILE	N-CA-C	6.68	117.73	107.78
1	B	41	THR	N-CA-C	-6.58	102.32	110.41
1	A	275	HIS	N-CA-C	-6.48	103.72	111.69
1	A	453	PRO	CA-C-N	-6.45	111.72	122.43
1	A	453	PRO	C-N-CA	-6.45	111.72	122.43
1	B	69	SER	CA-C-N	-6.28	109.85	120.58
1	B	69	SER	C-N-CA	-6.28	109.85	120.58
1	B	71	ALA	N-CA-C	6.19	119.99	110.20
1	B	290	ILE	CB-CA-C	-6.18	103.37	110.73
1	B	219	ARG	N-CA-C	6.16	117.86	109.11
1	A	401	VAL	N-CA-C	-6.15	104.85	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	573	GLU	O-C-N	5.95	128.43	122.12
1	B	38	TRP	N-CA-C	5.93	119.13	110.17
1	B	572	LEU	O-C-N	-5.75	116.03	122.12
1	A	41	THR	N-CA-C	-5.73	102.94	110.33
1	B	265	ILE	CB-CA-C	-5.68	103.87	110.91
1	A	268	GLU	N-CA-C	-5.55	106.49	113.20
1	B	77	MET	N-CA-C	5.46	119.20	112.54
1	A	38	TRP	N-CA-C	5.41	118.74	110.36
1	A	520	ILE	CA-C-N	5.28	128.83	121.02
1	A	520	ILE	C-N-CA	5.28	128.83	121.02
1	A	206	ILE	CB-CA-C	-5.25	104.17	110.99
1	A	274	ILE	CB-CA-C	-5.13	103.94	112.26
1	A	288	GLY	CA-C-N	5.09	126.21	119.84
1	A	288	GLY	C-N-CA	5.09	126.21	119.84
1	B	288	GLY	CA-C-N	5.08	126.19	119.84
1	B	288	GLY	C-N-CA	5.08	126.19	119.84
1	B	273	ILE	CB-CA-C	-5.07	105.40	112.04
1	B	206	ILE	CB-CA-C	-5.03	104.20	111.19
1	B	203	SER	N-CA-C	5.02	116.47	108.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	360	ARG	Mainchain

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	4301	0	4251	156	0
1	B	4339	0	4286	152	0
2	A	53	0	31	4	0
2	B	53	0	31	10	0
3	A	242	0	0	3	1
3	B	213	0	0	4	2
All	All	9201	0	8599	309	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (309) 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:70:LEU:O	1:A:245:ARG:NH2	1.76	1.16
1:A:191:PRO:HG2	1:A:301:VAL:CG2	1.79	1.12
1:A:223:MET:HE2	1:A:225:TYR:HE1	1.09	1.07
1:A:270:ALA:HA	1:A:273:ILE:HD12	1.38	1.06
1:B:46:ARG:HH11	1:B:46:ARG:CG	1.68	1.06
1:B:46:ARG:HH11	1:B:46:ARG:HG2	0.89	1.03
1:A:267:LYS:HG2	1:A:268:GLU:H	1.21	1.02
1:B:46:ARG:HG2	1:B:46:ARG:NH1	1.71	1.02
1:A:223:MET:HE2	1:A:225:TYR:CE1	1.96	0.99
1:A:294:THR:HG23	1:A:294:THR:O	1.59	0.97
1:B:443:ARG:O	3:B:701:HOH:O	1.84	0.96
1:B:398:GLU:HB3	1:B:402:ARG:HH12	1.37	0.88
1:A:191:PRO:HG2	1:A:301:VAL:HG23	1.55	0.86
1:A:321:MET:CE	1:A:375:LEU:HD23	2.05	0.86
1:B:46:ARG:HB3	2:B:601:FAD:C5X	2.08	0.84
1:B:198:ILE:HG22	1:B:199:GLY:H	1.41	0.84
1:A:267:LYS:HG2	1:A:268:GLU:N	1.93	0.83
1:A:293:TRP:CZ2	1:A:295:ILE:HD11	2.15	0.82
1:B:157:ARG:HD2	1:B:166:GLU:HG2	1.62	0.81
1:B:398:GLU:HB3	1:B:402:ARG:NH1	1.95	0.80
1:B:206:ILE:HD13	1:B:270:ALA:HB1	1.63	0.80
1:A:294:THR:O	1:A:294:THR:CG2	2.30	0.80
1:A:244:ILE:HB	1:A:249:LYS:HB3	1.64	0.79
1:B:46:ARG:O	2:B:601:FAD:C4X	2.30	0.79
1:B:244:ILE:O	1:B:245:ARG:HD3	1.83	0.79
1:B:197:GLY:O	1:B:198:ILE:HG13	1.83	0.78
1:B:444:ALA:O	1:B:582:ILE:HG12	1.83	0.78
1:B:218:HIS:CD2	1:B:219:ARG:HG2	2.18	0.78
1:A:191:PRO:HG2	1:A:301:VAL:HG22	1.66	0.78
1:A:223:MET:CE	1:A:225:TYR:HE1	1.96	0.78
1:A:402:ARG:HB3	1:A:413:ARG:NH1	1.99	0.78
1:B:457:ARG:NH1	3:B:704:HOH:O	2.16	0.78
1:B:357:ASP:O	1:B:361:SER:HB2	1.83	0.77
1:A:370:ARG:O	1:A:370:ARG:HD3	1.85	0.76
1:B:198:ILE:HG22	1:B:199:GLY:N	2.01	0.76
1:A:227:PHE:HD1	1:A:238:VAL:HG22	1.51	0.76
1:A:227:PHE:CD1	1:A:238:VAL:HG22	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:HG21	1:A:174:ILE:HG13	1.68	0.75
1:A:522:LEU:O	1:A:522:LEU:HD12	1.86	0.75
1:B:154:VAL:HG21	1:B:174:ILE:HG13	1.69	0.74
1:A:267:LYS:CG	1:A:268:GLU:H	1.95	0.74
1:B:144:TYR:OH	1:B:147:HIS:ND1	2.14	0.74
1:A:144:TYR:OH	1:A:147:HIS:HD2	1.71	0.74
1:A:293:TRP:CE2	1:A:295:ILE:HD11	2.23	0.74
1:B:392:THR:O	1:B:395:GLU:HB3	1.87	0.73
1:B:149:GLU:OE2	3:B:702:HOH:O	2.07	0.72
1:B:220:LYS:HG2	1:B:247:TRP:CZ2	2.24	0.71
1:A:508:LYS:O	1:A:512:GLU:HG3	1.90	0.71
1:A:370:ARG:HD3	1:A:370:ARG:C	2.14	0.70
1:B:201:SER:HB3	1:B:256:TYR:O	1.92	0.70
1:A:293:TRP:CH2	1:A:295:ILE:HD11	2.26	0.69
1:A:321:MET:HE3	1:A:375:LEU:HD23	1.72	0.69
1:B:290:ILE:HG22	1:B:290:ILE:O	1.91	0.69
1:B:267:LYS:HG3	1:B:268:GLU:N	2.07	0.69
1:A:20:MET:HG2	1:A:330:VAL:HG13	1.74	0.69
1:B:46:ARG:HB3	2:B:601:FAD:C9A	2.22	0.68
1:A:148:VAL:HG13	1:A:148:VAL:O	1.91	0.68
1:B:20:MET:HG2	1:B:330:VAL:HG13	1.74	0.68
1:A:191:PRO:CG	1:A:301:VAL:CG2	2.65	0.68
1:B:370:ARG:O	1:B:370:ARG:HD3	1.94	0.68
1:B:157:ARG:HD2	1:B:166:GLU:CG	2.24	0.67
1:B:282:GLU:CG	1:B:282:GLU:O	2.42	0.67
1:B:370:ARG:HD3	1:B:370:ARG:C	2.20	0.66
1:B:206:ILE:HD11	1:B:254:TRP:HH2	1.60	0.66
1:B:48:HIS:HD2	1:B:117:ASP:OD1	1.79	0.66
1:B:157:ARG:HD2	1:B:166:GLU:OE2	1.96	0.66
1:B:45:PRO:CB	1:B:119:PRO:HB3	2.26	0.66
1:B:46:ARG:O	2:B:601:FAD:C4	2.44	0.65
1:B:45:PRO:HB2	1:B:119:PRO:HB3	1.77	0.65
1:B:46:ARG:CG	1:B:46:ARG:NH1	2.39	0.65
1:A:28:LEU:HD23	1:A:341:ALA:HB2	1.79	0.65
1:A:392:THR:HG21	3:A:897:HOH:O	1.97	0.65
1:A:267:LYS:HD3	1:A:269:GLU:HG3	1.79	0.64
1:A:273:ILE:O	1:A:277:ILE:HG12	1.97	0.64
1:B:282:GLU:O	1:B:282:GLU:HG3	1.96	0.64
1:A:569:ARG:O	1:A:573:GLU:HG3	1.97	0.64
1:A:28:LEU:HD23	1:A:341:ALA:CB	2.28	0.64
1:A:321:MET:HG2	1:A:374:SER:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:HB2	1:A:380:PRO:HD3	1.80	0.63
1:B:567:ALA:O	1:B:572:LEU:HG	1.99	0.63
1:A:326:LEU:C	1:A:326:LEU:HD23	2.23	0.63
1:B:326:LEU:HD23	1:B:326:LEU:C	2.23	0.62
1:B:267:LYS:C	1:B:269:GLU:H	2.06	0.62
1:B:206:ILE:CD1	1:B:254:TRP:HH2	2.13	0.62
1:B:227:PHE:O	1:B:396:MET:HE1	1.99	0.62
1:B:399:ALA:HA	1:B:402:ARG:CZ	2.30	0.61
1:A:133:LEU:HG	3:A:812:HOH:O	1.99	0.61
1:A:281:ASP:OD1	1:A:281:ASP:O	2.19	0.61
1:A:265:ILE:HG22	1:A:266:THR:N	2.15	0.61
1:A:264:GLU:HG2	1:A:265:ILE:N	2.12	0.61
1:B:195:GLN:HA	1:B:298:GLN:HG2	1.83	0.60
1:B:48:HIS:CD2	1:B:117:ASP:OD1	2.55	0.60
1:B:256:TYR:CE2	1:B:264:GLU:HB2	2.36	0.60
1:A:46:ARG:NH2	2:A:601:FAD:O4'	2.34	0.59
1:B:48:HIS:CE1	1:B:242:ARG:HD2	2.38	0.59
1:A:321:MET:HG2	1:A:374:SER:HB3	1.83	0.59
1:B:48:HIS:HB2	1:B:117:ASP:OD2	2.01	0.59
1:B:70:LEU:O	1:B:245:ARG:NH2	2.35	0.59
1:B:206:ILE:HD11	1:B:254:TRP:CH2	2.37	0.59
1:B:269:GLU:O	1:B:270:ALA:C	2.47	0.58
1:A:511:ALA:HB1	1:A:522:LEU:HD11	1.85	0.58
1:A:365:LYS:HE3	1:A:369:GLU:OE2	2.03	0.58
1:B:241:LEU:HG	1:B:250:TRP:CE3	2.39	0.58
1:B:397:ALA:O	1:B:401:VAL:HG23	2.04	0.58
1:B:244:ILE:O	1:B:245:ARG:CD	2.52	0.57
1:A:58:LEU:HD13	1:A:67:ALA:HB2	1.85	0.57
1:B:418:ARG:O	1:B:418:ARG:HD3	2.03	0.57
1:A:19:ALA:HB1	1:A:127:VAL:HG12	1.86	0.57
1:A:321:MET:HE2	1:A:375:LEU:HD23	1.85	0.57
1:A:48:HIS:NE2	1:A:242:ARG:HD2	2.19	0.57
1:B:557:ASP:O	1:B:558:MET:HB2	2.05	0.57
1:A:373:LYS:O	1:A:376:SER:OG	2.22	0.57
1:A:244:ILE:O	1:A:245:ARG:HD3	2.05	0.57
1:B:19:ALA:HB1	1:B:127:VAL:HG12	1.86	0.56
1:A:557:ASP:O	1:A:558:MET:HB2	2.05	0.56
1:A:154:VAL:HG21	1:A:174:ILE:CG1	2.35	0.56
1:A:211:ASP:C	1:A:211:ASP:OD1	2.46	0.55
1:A:400:LEU:HD23	1:A:400:LEU:O	2.06	0.55
1:B:58:LEU:HD13	1:B:67:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:VAL:HG21	1:B:174:ILE:CG1	2.35	0.55
1:B:210:ALA:O	1:B:248:ASN:HA	2.07	0.55
1:B:268:GLU:O	1:B:268:GLU:HG2	2.06	0.55
1:B:206:ILE:CD1	1:B:254:TRP:CH2	2.90	0.55
1:B:220:LYS:HG2	1:B:247:TRP:HZ2	1.66	0.55
1:B:282:GLU:O	1:B:282:GLU:CD	2.50	0.55
1:A:247:TRP:O	1:A:250:TRP:NE1	2.36	0.55
1:A:441:VAL:O	1:A:442:SER:HB3	2.07	0.55
1:B:218:HIS:NE2	1:B:219:ARG:HG2	2.22	0.54
1:A:516:GLN:OE1	1:A:516:GLN:HA	2.07	0.54
1:B:515:SER:HB2	1:B:520:ILE:O	2.07	0.54
1:B:244:ILE:HD12	1:B:250:TRP:C	2.32	0.54
1:A:267:LYS:CG	1:A:268:GLU:N	2.62	0.54
1:B:16:PRO:HD2	2:B:601:FAD:O2P	2.08	0.54
1:A:397:ALA:O	1:A:401:VAL:HG23	2.07	0.54
1:A:148:VAL:O	1:A:148:VAL:CG1	2.56	0.53
1:B:269:GLU:C	1:B:271:LYS:N	2.64	0.53
1:B:198:ILE:CG2	1:B:199:GLY:H	2.18	0.53
1:B:379:PRO:HB2	1:B:380:PRO:HD3	1.90	0.53
1:A:61:ILE:HG13	1:A:63:LEU:HD12	1.91	0.53
1:A:436:LEU:HB3	1:A:463:TYR:CD1	2.44	0.53
1:A:281:ASP:OD1	1:A:281:ASP:C	2.52	0.53
1:A:448:ASP:OD2	1:A:565:LYS:NZ	2.42	0.53
1:B:48:HIS:CE1	1:B:242:ARG:CD	2.92	0.53
1:B:436:LEU:HB3	1:B:463:TYR:CD1	2.44	0.53
1:B:108:GLU:HG3	1:B:114:ARG:NH2	2.24	0.52
1:A:55:MET:HE2	3:A:855:HOH:O	2.09	0.52
1:A:321:MET:CE	1:A:375:LEU:CD2	2.85	0.52
1:A:492:GLY:O	1:A:493:LYS:HB2	2.09	0.52
1:B:197:GLY:C	1:B:198:ILE:HG13	2.34	0.52
1:A:13:GLY:HA2	2:A:601:FAD:O4B	2.10	0.52
1:B:79:GLU:HB2	1:B:220:LYS:O	2.10	0.51
1:A:194:GLY:O	1:A:297:GLN:O	2.29	0.51
1:B:46:ARG:HB3	2:B:601:FAD:C6	2.40	0.51
1:B:55:MET:HE3	1:B:64:GLU:HG3	1.90	0.51
1:B:154:VAL:O	1:B:170:ARG:HD2	2.10	0.51
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.11	0.51
1:A:402:ARG:HB3	1:A:413:ARG:HH11	1.74	0.51
1:B:269:GLU:O	1:B:272:LYS:N	2.34	0.51
1:B:205:ASN:OD1	1:B:253:VAL:HG13	2.11	0.50
1:A:220:LYS:HG2	1:A:247:TRP:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:MET:SD	1:A:246:PRO:HD3	2.52	0.50
1:B:198:ILE:CG2	1:B:199:GLY:N	2.72	0.50
1:B:301:VAL:HG11	3:B:882:HOH:O	2.12	0.50
1:B:399:ALA:HB2	1:B:402:ARG:NH2	2.27	0.49
1:A:311:MET:HB3	1:A:356:TYR:OH	2.12	0.49
1:A:392:THR:HG22	1:A:393:GLU:N	2.27	0.49
1:B:157:ARG:CD	1:B:166:GLU:HG2	2.39	0.49
1:A:387:LEU:CD2	1:A:388:PRO:HD2	2.42	0.49
1:B:399:ALA:HA	1:B:402:ARG:NH2	2.28	0.49
1:B:45:PRO:HB3	1:B:119:PRO:HB3	1.94	0.49
1:A:154:VAL:O	1:A:170:ARG:HD2	2.12	0.49
1:A:511:ALA:HB1	1:A:522:LEU:CD1	2.42	0.49
1:A:520:ILE:O	1:A:520:ILE:HG23	2.12	0.48
1:A:387:LEU:HD22	1:A:388:PRO:HD2	1.95	0.48
1:A:400:LEU:HD23	1:A:400:LEU:C	2.38	0.48
1:B:55:MET:HB3	1:B:113:SER:HB3	1.96	0.48
1:B:392:THR:O	1:B:395:GLU:CB	2.58	0.48
1:A:280:THR:OG1	1:A:282:GLU:HG2	2.14	0.48
1:B:267:LYS:C	1:B:269:GLU:N	2.70	0.48
1:A:245:ARG:HB2	1:A:249:LYS:HB2	1.94	0.48
1:A:365:LYS:CE	1:A:369:GLU:OE2	2.61	0.48
1:A:321:MET:HG2	1:A:374:SER:HB2	1.93	0.48
1:A:367:ILE:HG13	1:A:368:VAL:N	2.29	0.48
1:A:389:PRO:O	1:A:391:PRO:HD3	2.13	0.48
1:B:267:LYS:CG	1:B:268:GLU:N	2.73	0.48
1:A:220:LYS:HG2	1:A:247:TRP:CZ2	2.49	0.48
1:B:367:ILE:HG13	1:B:368:VAL:N	2.28	0.48
1:A:7:THR:O	1:A:171:ALA:HA	2.14	0.48
1:A:108:GLU:HG3	1:A:114:ARG:NH2	2.29	0.47
1:A:227:PHE:CZ	1:A:381:VAL:HG11	2.48	0.47
1:B:269:GLU:O	1:B:271:LYS:N	2.47	0.47
1:B:352:LEU:HD12	1:B:352:LEU:O	2.14	0.47
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.61	0.47
1:A:265:ILE:CG2	1:A:266:THR:N	2.78	0.47
1:A:401:VAL:C	1:A:403:LEU:H	2.22	0.47
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.66	0.47
2:B:601:FAD:O2'	2:B:601:FAD:O4'	2.30	0.47
1:A:227:PHE:HD1	1:A:238:VAL:CG2	2.25	0.47
1:B:46:ARG:O	2:B:601:FAD:N5	2.47	0.47
1:A:293:TRP:CZ3	1:A:295:ILE:HD11	2.50	0.46
1:B:311:MET:HB3	1:B:356:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:N	1:A:380:PRO:CD	2.78	0.46
1:B:574:GLN:O	1:B:575:LEU:C	2.58	0.46
1:A:553:LEU:HB3	1:A:562:PHE:HB3	1.97	0.46
1:B:13:GLY:HA2	2:B:601:FAD:O4B	2.16	0.46
1:B:267:LYS:O	1:B:269:GLU:N	2.45	0.46
1:B:285:VAL:HG12	1:B:286:GLU:N	2.31	0.46
1:A:418:ARG:O	1:A:418:ARG:HD3	2.16	0.46
1:B:109:LEU:HA	1:B:109:LEU:HD23	1.66	0.46
1:B:544:SER:O	1:B:545:GLU:HB2	2.16	0.46
1:A:48:HIS:CE1	1:A:242:ARG:HD2	2.51	0.46
1:A:278:ILE:HG22	1:A:280:THR:HG22	1.97	0.45
1:A:293:TRP:CD2	1:A:295:ILE:HD11	2.51	0.45
1:B:399:ALA:HB2	1:B:402:ARG:HH22	1.82	0.45
1:B:553:LEU:HB3	1:B:562:PHE:HB3	1.97	0.45
1:A:141:LEU:HD13	1:A:162:VAL:HG23	1.98	0.45
1:B:157:ARG:HD2	1:B:166:GLU:CD	2.41	0.45
1:B:392:THR:OG1	1:B:395:GLU:HB2	2.16	0.45
1:B:7:THR:O	1:B:171:ALA:HA	2.16	0.45
1:A:120:GLN:NE2	1:A:124:GLU:OE2	2.48	0.45
1:B:392:THR:O	1:B:395:GLU:N	2.46	0.45
1:A:178:ASP:OD2	1:A:184:VAL:HG23	2.17	0.45
1:A:321:MET:HE2	1:A:375:LEU:CD2	2.46	0.45
1:B:145:LEU:HD12	1:B:157:ARG:HG3	1.99	0.45
1:A:194:GLY:C	1:A:196:MET:H	2.24	0.45
1:A:269:GLU:O	1:A:272:LYS:HB2	2.16	0.45
1:A:402:ARG:CB	1:A:413:ARG:NH1	2.76	0.45
1:B:277:ILE:HG23	1:B:277:ILE:O	2.17	0.45
1:A:57:ILE:HG12	1:A:334:TYR:CD2	2.51	0.44
1:A:312:GLY:HA3	2:A:601:FAD:O1P	2.17	0.44
1:A:366:GLN:O	1:A:366:GLN:HG2	2.15	0.44
1:A:544:SER:O	1:A:545:GLU:HB2	2.16	0.44
1:B:248:ASN:OD1	1:B:249:LYS:HG3	2.17	0.44
1:A:303:ASN:OD1	1:A:357:ASP:HB2	2.18	0.44
1:B:245:ARG:HD2	1:B:245:ARG:HA	1.55	0.44
1:A:48:HIS:HD2	1:A:117:ASP:OD1	2.00	0.44
1:A:565:LYS:N	1:A:565:LYS:HD2	2.31	0.44
1:A:278:ILE:C	1:A:280:THR:H	2.25	0.44
1:B:244:ILE:HD11	1:B:251:ILE:HB	1.98	0.44
1:B:385:LEU:HB3	1:B:387:LEU:HG	1.99	0.44
1:B:273:ILE:O	1:B:276:GLU:HG2	2.17	0.44
1:B:281:ASP:C	1:B:281:ASP:OD1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:HIS:HB2	1:A:117:ASP:OD2	2.18	0.44
1:B:76:TYR:CD1	1:B:220:LYS:HD3	2.52	0.44
1:B:312:GLY:HA3	2:B:601:FAD:O1P	2.17	0.44
1:A:238:VAL:HG23	1:A:382:PHE:HZ	1.82	0.44
1:B:278:ILE:HG22	1:B:280:THR:HG22	1.98	0.44
1:A:223:MET:CE	1:A:225:TYR:CE1	2.82	0.44
1:B:178:ASP:OD2	1:B:184:VAL:HG23	2.17	0.44
1:B:511:ALA:HB1	1:B:522:LEU:HD11	2.00	0.44
1:A:82:TYR:CD1	1:A:225:TYR:HB2	2.53	0.43
1:A:370:ARG:C	1:A:370:ARG:CD	2.89	0.43
1:A:120:GLN:HG3	1:A:326:LEU:HD12	2.00	0.43
1:B:510:GLU:OE1	1:B:510:GLU:HA	2.19	0.43
1:A:144:TYR:OH	1:A:147:HIS:CD2	2.61	0.43
1:B:200:ASP:OD1	1:B:200:ASP:C	2.61	0.43
1:A:58:LEU:CD1	1:A:67:ALA:HB2	2.48	0.43
1:B:278:ILE:C	1:B:280:THR:H	2.26	0.43
1:B:281:ASP:OD1	1:B:281:ASP:O	2.36	0.43
1:A:326:LEU:HD23	1:A:326:LEU:O	2.18	0.43
1:A:401:VAL:C	1:A:403:LEU:N	2.75	0.43
1:B:446:PHE:HA	1:B:447:PRO:HD3	1.73	0.43
1:A:195:GLN:HA	1:A:298:GLN:HG2	2.01	0.43
1:B:86:LEU:O	1:B:219:ARG:NH2	2.52	0.43
1:B:212:LEU:HD23	1:B:283:ILE:HD13	2.00	0.43
1:A:278:ILE:HG22	1:A:278:ILE:O	2.18	0.43
1:B:241:LEU:HG	1:B:250:TRP:CZ3	2.54	0.43
1:A:63:LEU:HD11	1:A:130:GLU:HG2	2.00	0.42
1:A:402:ARG:HH11	1:A:402:ARG:HD3	1.71	0.42
1:A:401:VAL:O	1:A:403:LEU:N	2.53	0.42
1:B:52:GLN:NE2	1:B:111:SER:HB3	2.34	0.42
1:B:120:GLN:HG3	1:B:326:LEU:HD12	2.01	0.42
1:B:326:LEU:HD23	1:B:326:LEU:O	2.18	0.42
1:A:302:ARG:HA	1:A:357:ASP:OD1	2.19	0.42
1:A:522:LEU:HD12	1:A:522:LEU:C	2.44	0.42
1:B:202:GLY:HA3	1:B:293:TRP:O	2.20	0.42
1:B:481:ASN:O	1:B:482:GLN:HB2	2.18	0.42
1:B:425:ILE:O	1:B:425:ILE:HG13	2.19	0.42
1:A:226:MET:O	1:A:238:VAL:HA	2.20	0.42
1:B:198:ILE:CD1	1:B:372:PHE:HE1	2.32	0.42
1:B:191:PRO:HG2	1:B:301:VAL:HB	2.01	0.42
1:A:51:ASN:OD1	1:A:51:ASN:C	2.62	0.42
1:A:182:SER:HB3	1:A:185:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ALA:HB2	1:B:118:LEU:HB2	2.02	0.41
1:A:16:PRO:HD2	2:A:601:FAD:O2P	2.19	0.41
1:B:387:LEU:HD21	1:B:399:ALA:HB2	2.02	0.41
1:A:89:GLU:OE1	1:A:400:LEU:HD11	2.20	0.41
1:A:83:ALA:HB2	1:A:90:GLU:HA	2.02	0.41
1:A:86:LEU:O	1:A:219:ARG:NH2	2.53	0.41
1:B:83:ALA:HB2	1:B:90:GLU:HA	2.02	0.41
1:B:206:ILE:HD13	1:B:206:ILE:HG21	1.83	0.41
1:A:285:VAL:HG12	1:A:286:GLU:N	2.36	0.41
1:A:379:PRO:N	1:A:380:PRO:HD2	2.35	0.41
1:A:432:HIS:NE2	1:A:436:LEU:HD22	2.36	0.41
1:B:200:ASP:OD1	1:B:201:SER:N	2.53	0.41
1:B:204:ILE:CG2	1:B:254:TRP:CE2	3.03	0.41
1:B:500:THR:OG1	1:B:501:GLY:N	2.54	0.41
1:A:206:ILE:HG21	1:A:206:ILE:HD13	1.83	0.41
1:A:290:ILE:HD13	1:A:290:ILE:HG21	1.86	0.41
1:B:55:MET:CB	1:B:113:SER:HB3	2.51	0.41
1:B:224:TYR:CD2	1:B:224:TYR:N	2.89	0.41
1:A:31:ARG:HD2	1:A:31:ARG:HA	1.86	0.40
1:A:130:GLU:HG3	1:A:134:ARG:HE	1.86	0.40
1:A:264:GLU:HG2	1:A:265:ILE:O	2.22	0.40
1:B:399:ALA:CA	1:B:402:ARG:NH2	2.85	0.40
1:B:402:ARG:HH11	1:B:402:ARG:HG3	1.87	0.40
1:A:36:ASN:OD1	1:A:37:ARG:N	2.54	0.40
1:A:74:LYS:O	1:A:77:MET:HB2	2.22	0.40
1:A:238:VAL:HG23	1:A:382:PHE:CZ	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:816:HOH:O	3:B:816:HOH:O[2_655]	1.33	0.87
3:A:807:HOH:O	3:B:881:HOH:O[4_555]	2.03	0.17

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	551/592 (93%)	527 (96%)	23 (4%)	1 (0%)	43	54
1	B	558/592 (94%)	533 (96%)	22 (4%)	3 (0%)	24	32
All	All	1109/1184 (94%)	1060 (96%)	45 (4%)	4 (0%)	30	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ILE
1	B	391	PRO
1	B	270	ALA
1	A	442	SER

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	448/473 (95%)	435 (97%)	13 (3%)	37	52
1	B	452/473 (96%)	436 (96%)	16 (4%)	32	46
All	All	900/946 (95%)	871 (97%)	29 (3%)	34	49

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	84	THR
1	A	162	VAL
1	A	196	MET
1	A	204	ILE
1	A	245	ARG
1	A	272	LYS
1	A	317	ARG

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Mol	Chain	Res	Type
1	A	319	THR
1	A	370	ARG
1	A	436	LEU
1	A	484	ARG
1	A	555	ARG
1	B	9	VAL
1	B	46	ARG
1	B	243	MET
1	B	245	ARG
1	B	277	ILE
1	B	317	ARG
1	B	319	THR
1	B	361	SER
1	B	370	ARG
1	B	396	MET
1	B	413	ARG
1	B	436	LEU
1	B	484	ARG
1	B	510	GLU
1	B	517	SER
1	B	555	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	459	GLN
1	B	48	HIS
1	B	297	GLN
1	B	513	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	FAD	B	601	-	58,58,58	1.48	11 (18%)	85,89,89	1.58	17 (20%)
2	FAD	A	601	-	58,58,58	1.46	9 (15%)	85,89,89	1.59	18 (21%)

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	B	601	-	-	10/34/50/50	0/6/6/6
2	FAD	A	601	-	-	3/34/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C9A-C5X	5.47	1.50	1.41
2	A	601	FAD	C9A-C5X	5.47	1.50	1.41
2	A	601	FAD	C5A-C4A	4.24	1.46	1.39
2	B	601	FAD	C5A-C4A	4.20	1.46	1.39
2	B	601	FAD	C8-C7	3.32	1.48	1.40
2	A	601	FAD	C8-C7	3.16	1.48	1.40
2	B	601	FAD	C4-N3	-2.60	1.34	1.38
2	B	601	FAD	C5A-C6A	2.58	1.48	1.41
2	A	601	FAD	C4-N3	-2.57	1.34	1.38
2	A	601	FAD	C5A-C6A	2.56	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C5A-N7A	-2.37	1.34	1.39
2	B	601	FAD	C5A-N7A	-2.35	1.34	1.39
2	B	601	FAD	C8A-N7A	2.28	1.36	1.31
2	A	601	FAD	C8A-N7A	2.28	1.36	1.31
2	A	601	FAD	C5X-N5	-2.26	1.35	1.39
2	B	601	FAD	C5X-N5	-2.26	1.35	1.39
2	A	601	FAD	C4A-N9A	-2.11	1.33	1.37
2	B	601	FAD	C4A-N9A	-2.10	1.33	1.37
2	B	601	FAD	PA-O3P	2.03	1.61	1.59
2	B	601	FAD	C2-N3	-2.00	1.34	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C5A-C4A-N3A	-5.51	119.14	126.72
2	B	601	FAD	C5A-C4A-N3A	-5.46	119.20	126.72
2	B	601	FAD	N3A-C4A-N9A	4.37	134.60	127.17
2	A	601	FAD	N3A-C4A-N9A	4.35	134.57	127.17
2	A	601	FAD	N3A-C2A-N1A	-3.94	122.61	128.58
2	A	601	FAD	C2A-N3A-C4A	3.88	121.31	111.83
2	B	601	FAD	N3A-C2A-N1A	-3.85	122.75	128.58
2	B	601	FAD	C2A-N3A-C4A	3.82	121.16	111.83
2	A	601	FAD	C4A-C5A-N7A	-3.49	106.59	110.58
2	B	601	FAD	C4A-C5A-N7A	-3.45	106.64	110.58
2	B	601	FAD	C4A-N9A-C8A	3.21	109.11	105.74
2	A	601	FAD	C4A-N9A-C8A	3.09	108.99	105.74
2	A	601	FAD	C5A-N7A-C8A	2.76	107.79	103.45
2	B	601	FAD	C5A-N7A-C8A	2.74	107.75	103.45
2	B	601	FAD	C4X-C10-N1	-2.64	118.11	124.59
2	A	601	FAD	C4X-C10-N1	-2.64	118.11	124.59
2	A	601	FAD	C4-C4X-N5	2.61	121.81	118.21
2	B	601	FAD	C4-C4X-N5	2.57	121.76	118.21
2	B	601	FAD	N9A-C8A-N7A	-2.56	110.31	113.94
2	B	601	FAD	C4X-C10-N10	2.55	120.14	116.48
2	A	601	FAD	C4X-C10-N10	2.54	120.12	116.48
2	A	601	FAD	N9A-C8A-N7A	-2.54	110.33	113.94
2	A	601	FAD	C6A-C5A-N7A	2.40	136.72	132.09
2	B	601	FAD	C6A-C5A-N7A	2.37	136.66	132.09
2	A	601	FAD	O4-C4-C4X	-2.36	120.30	126.53
2	B	601	FAD	O4-C4-C4X	-2.33	120.37	126.53
2	A	601	FAD	C10-N1-C2	2.27	121.77	116.85
2	B	601	FAD	C10-N1-C2	2.23	121.68	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-N3-C2	-2.15	121.82	125.64
2	A	601	FAD	C4-N3-C2	-2.15	121.83	125.64
2	A	601	FAD	C2A-N1A-C6A	2.12	122.22	118.73
2	B	601	FAD	C4X-C4-N3	2.11	118.63	113.25
2	B	601	FAD	C2A-N1A-C6A	2.11	122.19	118.73
2	A	601	FAD	C4X-C4-N3	2.10	118.61	113.25
2	A	601	FAD	O2-C2-N1	-2.05	118.40	121.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5'-O5'-P-O1P
2	B	601	FAD	C5'-O5'-P-O1P
2	B	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B

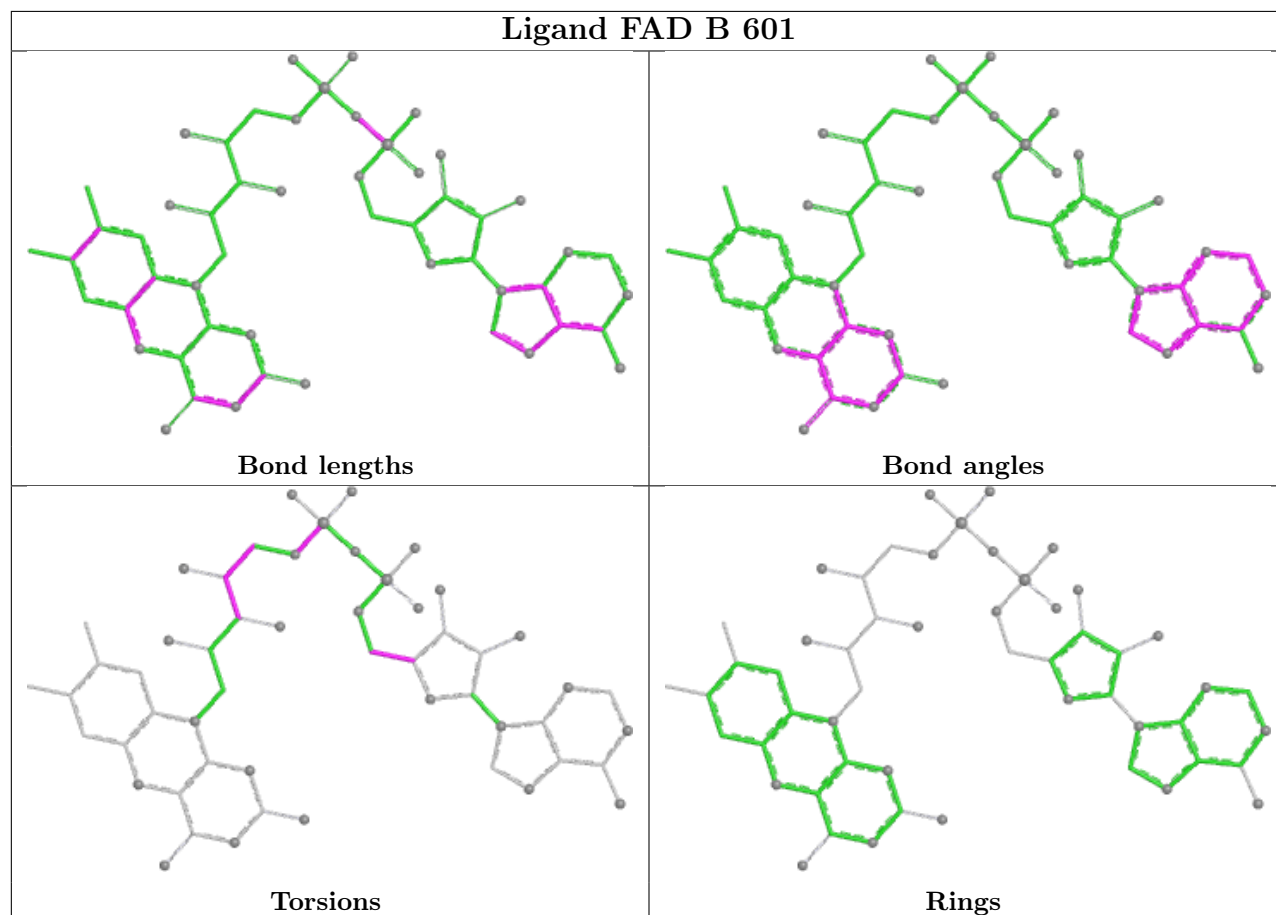
There are no ring outliers.

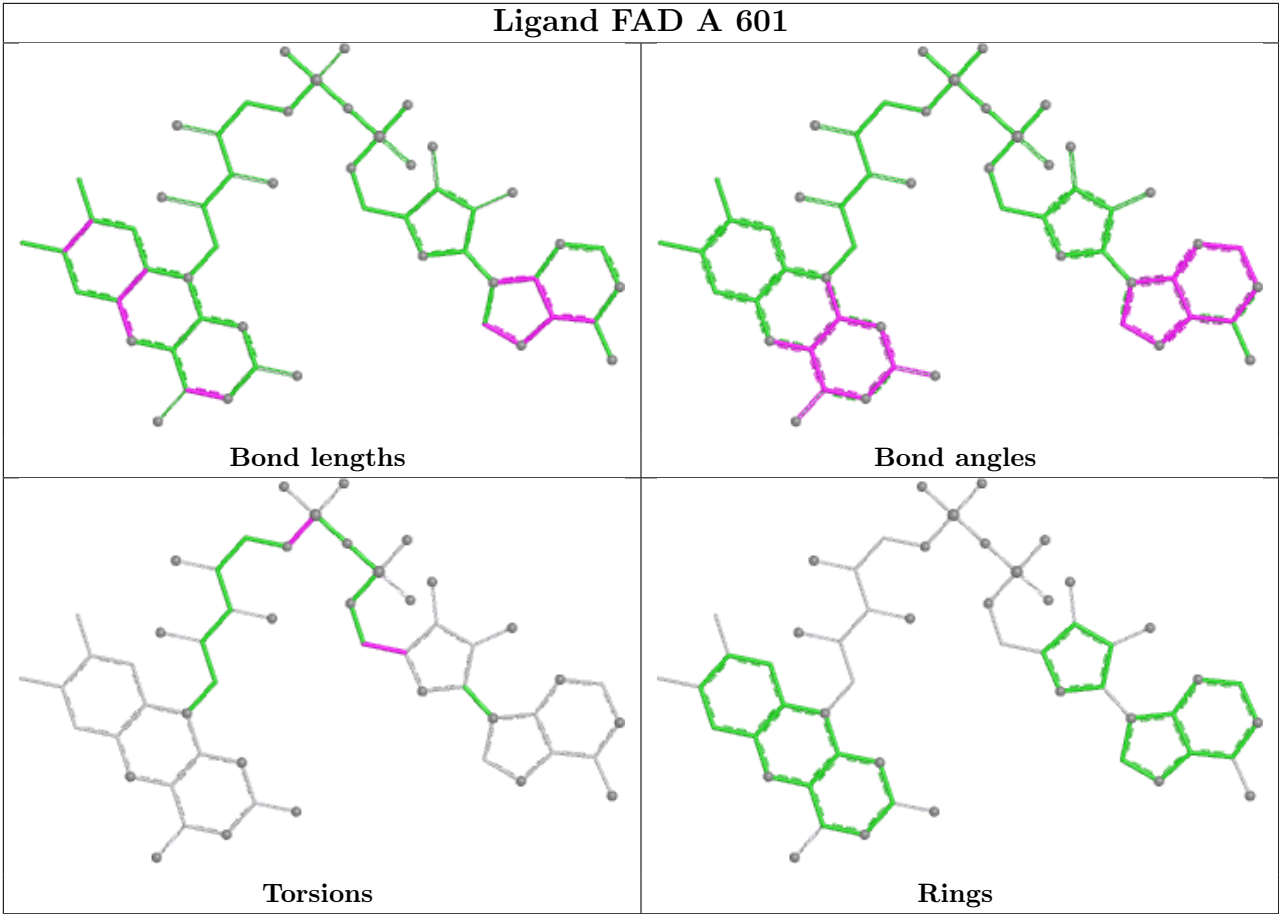
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	10	0
2	A	601	FAD	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	70:LEU	C	71:ALA	N	1.18
1	A	358:ALA	C	359:GLU	N	1.16
1	B	360:ARG	C	361:SER	N	1.13
1	A	416:ALA	C	417:LEU	N	1.11

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	520:ILE	C	521:GLU	N	1.11
1	A	76:TYR	C	77:MET	N	0.94

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	559/592 (94%)	0.27	43 (7%)	19 17	10, 24, 63, 131	0
1	B	564/592 (95%)	0.37	51 (9%)	15 13	11, 25, 73, 140	0
All	All	1123/1184 (94%)	0.32	94 (8%)	17 15	10, 25, 67, 140	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	TYR	7.6
1	A	196	MET	7.5
1	A	197	GLY	7.0
1	A	392	THR	6.8
1	B	198	ILE	6.2
1	B	197	GLY	5.5
1	A	202	GLY	5.4
1	B	196	MET	5.4
1	B	388	PRO	5.3
1	A	270	ALA	5.2
1	A	265	ILE	5.0
1	A	194	GLY	5.0
1	A	269	GLU	5.0
1	B	270	ALA	4.9
1	B	195	GLN	4.9
1	B	397	ALA	4.9
1	B	396	MET	4.8
1	B	387	LEU	4.8
1	A	195	GLN	4.6
1	A	397	ALA	4.5
1	B	200	ASP	4.5
1	B	202	GLY	4.3
1	A	388	PRO	4.3
1	B	46	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	199	GLY	4.3
1	B	194	GLY	4.2
1	B	391	PRO	4.1
1	A	255	GLY	4.0
1	A	266	THR	4.0
1	B	392	THR	4.0
1	A	390	ALA	4.0
1	A	400	LEU	3.9
1	A	389	PRO	3.9
1	A	268	GLU	3.8
1	A	264	GLU	3.8
1	A	391	PRO	3.8
1	B	223	MET	3.7
1	B	264	GLU	3.7
1	B	268	GLU	3.6
1	A	238	VAL	3.6
1	B	390	ALA	3.5
1	B	386	SER	3.5
1	A	393	GLU	3.4
1	A	295	ILE	3.4
1	B	389	PRO	3.3
1	A	227	PHE	3.2
1	B	444	ALA	3.1
1	A	254	TRP	3.1
1	A	394	SER	3.1
1	B	394	SER	3.1
1	B	395	GLU	3.1
1	B	294	THR	2.9
1	A	267	LYS	2.8
1	B	393	GLU	2.8
1	B	281	ASP	2.8
1	B	238	VAL	2.8
1	A	399	ALA	2.8
1	A	282	GLU	2.8
1	B	382	PHE	2.7
1	A	296	ASN	2.7
1	A	409	GLU	2.7
1	B	570	GLU	2.6
1	B	398	GLU	2.6
1	B	254	TRP	2.6
1	B	45	PRO	2.5
1	A	382	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	250	TRP	2.5
1	B	296	ASN	2.5
1	B	227	PHE	2.4
1	B	265	ILE	2.4
1	A	411	ALA	2.4
1	A	291	SER	2.4
1	B	272	LYS	2.4
1	B	411	ALA	2.3
1	B	255	GLY	2.3
1	A	401	VAL	2.3
1	B	282	GLU	2.2
1	A	405	ASP	2.2
1	B	413	ARG	2.2
1	B	293	TRP	2.1
1	B	399	ALA	2.1
1	A	293	TRP	2.1
1	B	248	ASN	2.1
1	A	294	THR	2.1
1	B	567	ALA	2.1
1	A	387	LEU	2.1
1	A	186	GLN	2.0
1	B	157	ARG	2.0
1	B	400	LEU	2.0
1	B	218	HIS	2.0
1	A	46	ARG	2.0
1	A	6	GLU	2.0
1	A	395	GLU	2.0
1	A	396	MET	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,

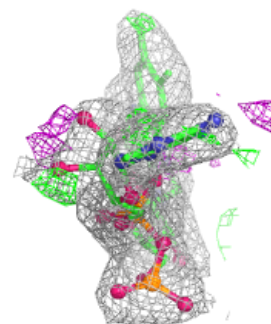
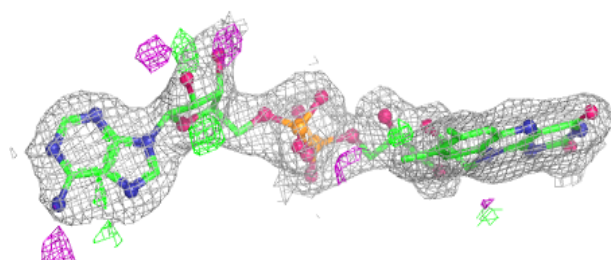
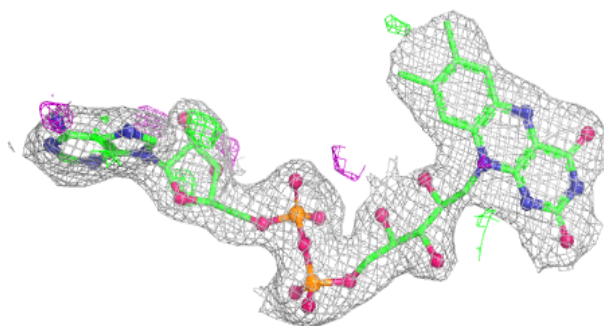
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

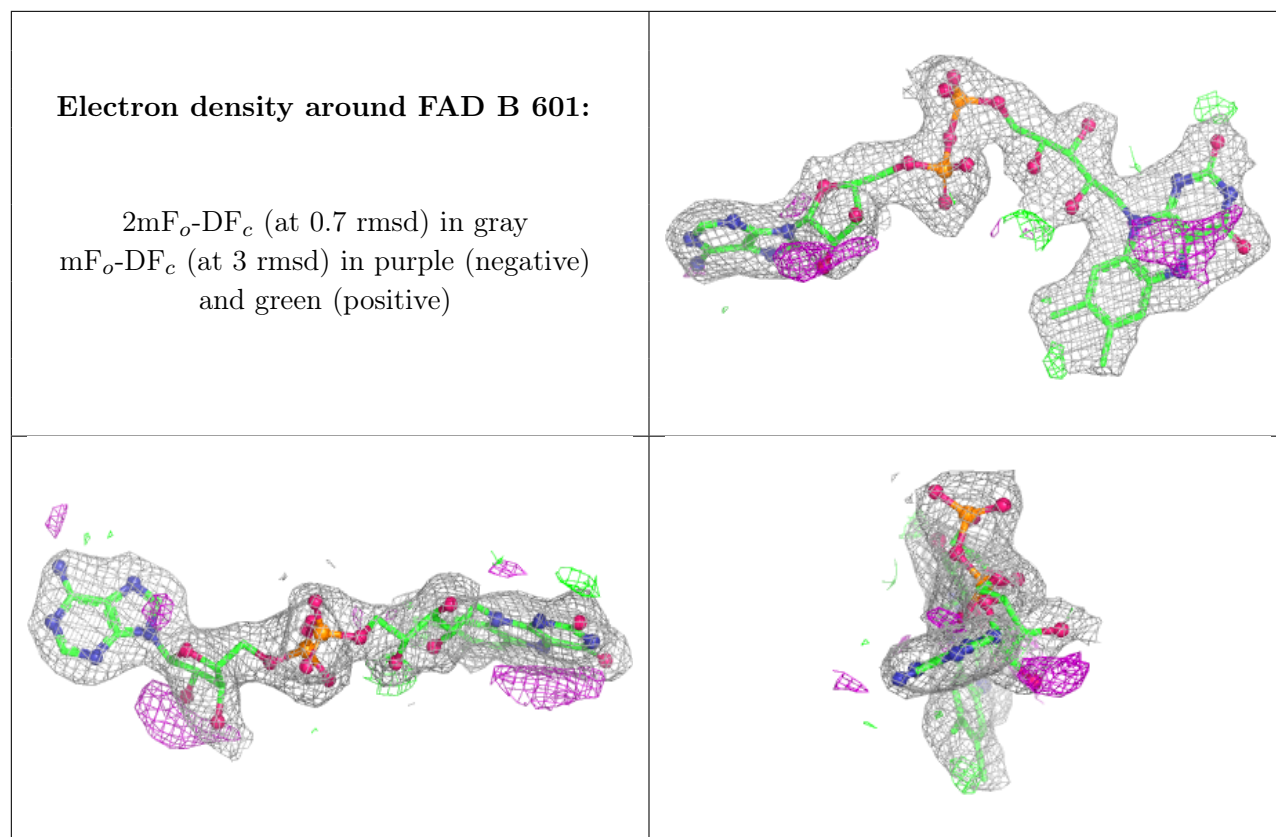
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	601	53/53	0.94	0.10	16,30,42,46	0
2	FAD	B	601	53/53	0.94	0.10	15,31,43,46	0

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.

Electron density around FAD A 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.