



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 1W1L / pdb_00001w1l
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-
ALCOHOL OXIDASE: Phe454Tyr Mutant
Authors : Van Den Heuvel, R.H.
Deposited on : 2004-06-22
Resolution : 2.70 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

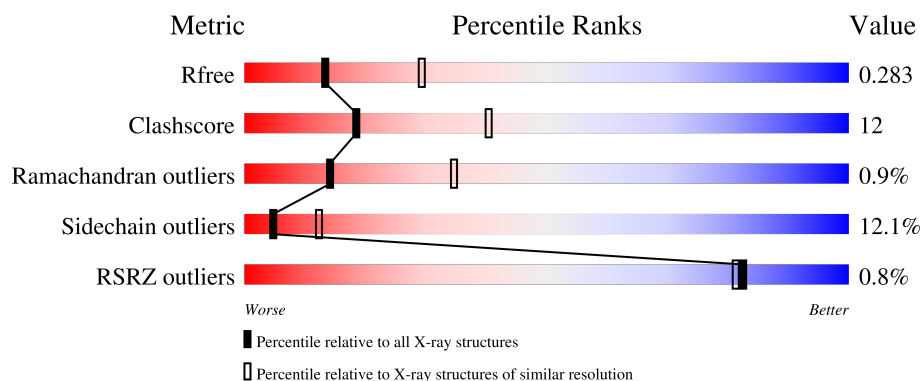
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	560	 61% 31% 6% .
1	B	560	 72% 22% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8832 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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4352	2793	744	791	24			
1	B	550	Total	C	N	O	S	0	0	0
			4352	2793	744	791	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	TYR	PHE	engineered mutation	UNP P56216
B	454	TYR	PHE	engineered mutation	UNP P56216

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



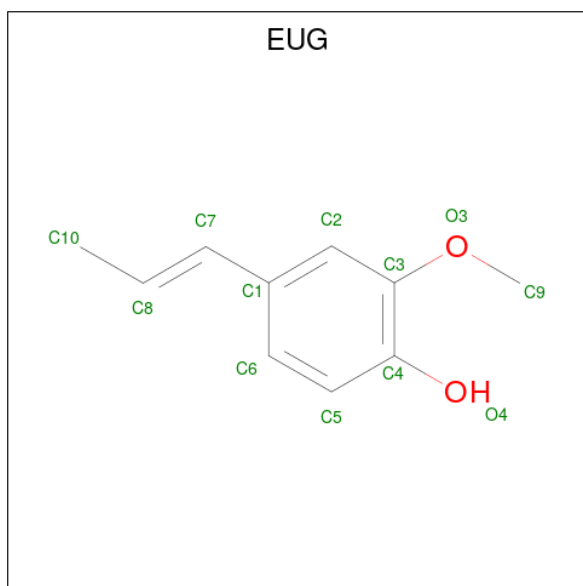
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (CCD ID: EUG) (formula: C₁₀H₁₂O₂).

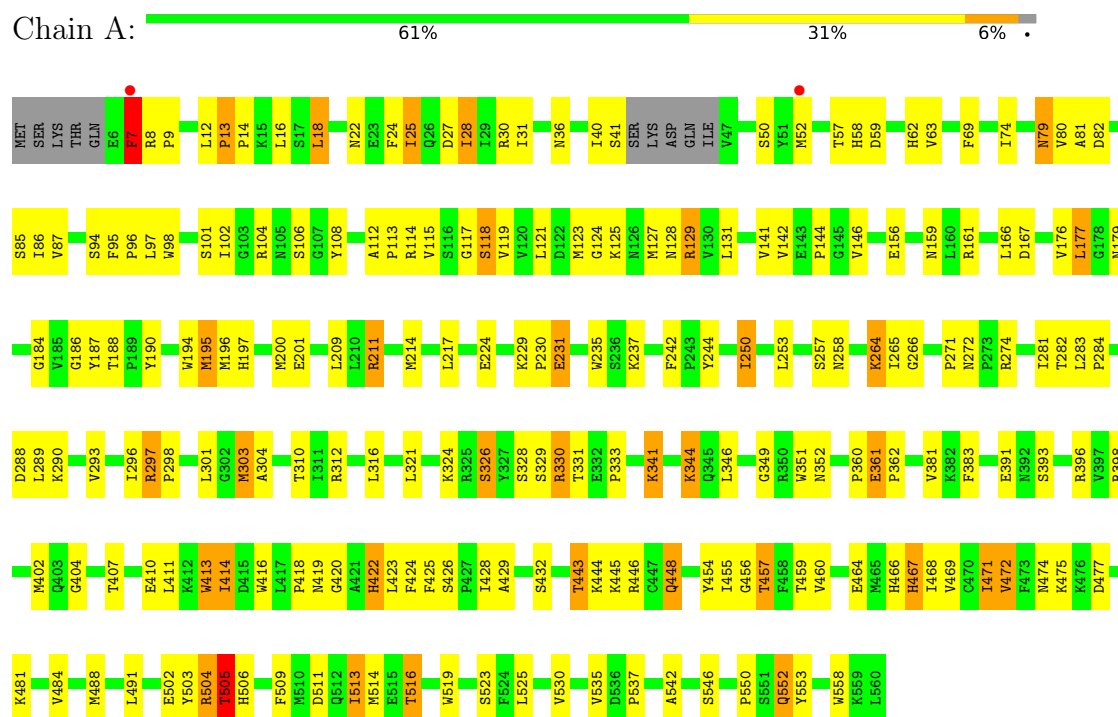


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

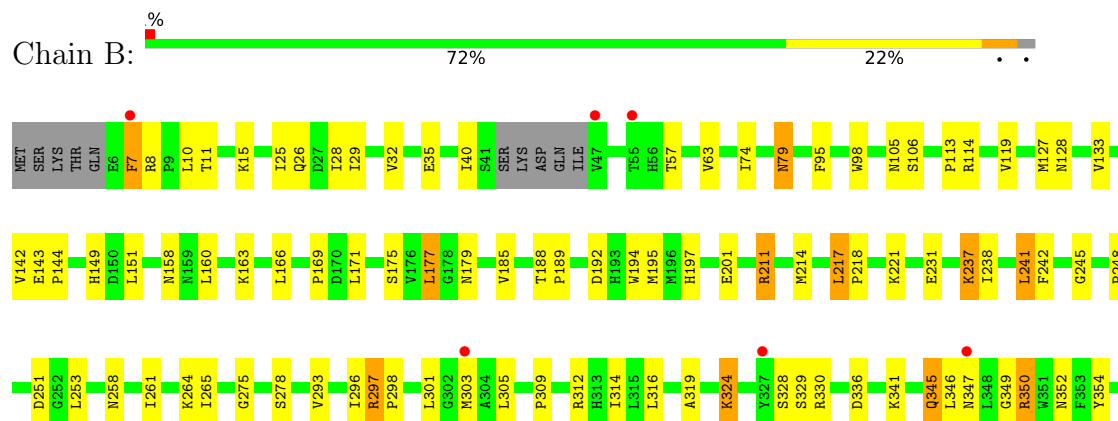
3 Residue-property plots

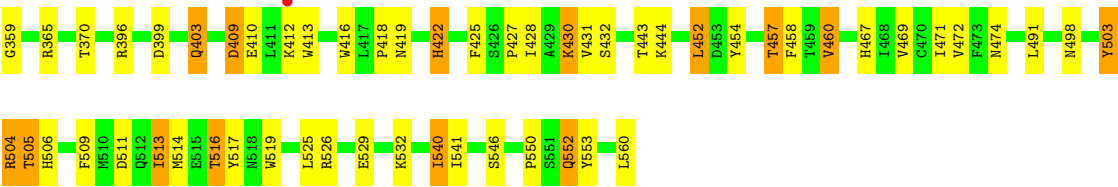
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: VANILLYL-ALCOHOL OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	129.90Å 129.90Å 133.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.00-2.70) 97.5 (40.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.203 , 0.293 0.203 , 0.283	Depositor DCC
R_{free} test set	1508 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h 0.020 for -l,-k,-h 0.021 for -h,-l,-k 0.008 for -h,l,k 0.037 for -h,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8832	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, EUG

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	0.92	4/4471 (0.1%)	1.14	14/6077 (0.2%)
1	B	0.70	1/4471 (0.0%)	1.04	6/6077 (0.1%)
All	All	0.82	5/8942 (0.1%)	1.09	20/12154 (0.2%)

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	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	MET	SD-CE	7.85	1.99	1.79
1	A	303	MET	SD-CE	7.02	1.97	1.79
1	A	52	MET	SD-CE	6.88	1.96	1.79
1	A	13	PRO	CA-C	6.29	1.55	1.51
1	A	530	VAL	CA-CB	5.59	1.60	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	THR	N-CA-C	7.11	117.63	108.24
1	A	460	VAL	N-CA-C	6.47	116.72	106.88
1	B	460	VAL	N-CA-C	6.45	115.89	106.55
1	A	471	ILE	CA-C-N	-6.09	115.24	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ILE	C-N-CA	-6.09	115.24	123.10
1	A	290	LYS	N-CA-C	6.07	117.56	111.07
1	B	237	LYS	N-CA-C	5.87	117.75	111.36
1	A	505	THR	N-CA-C	5.86	116.02	108.34
1	B	540	ILE	N-CA-C	5.73	118.69	112.96
1	A	446	ARG	N-CA-C	5.58	117.04	111.07
1	A	7	PHE	N-CA-C	5.46	119.95	113.12
1	A	404	GLY	CA-C-N	-5.42	118.68	122.59
1	A	404	GLY	C-N-CA	-5.42	118.68	122.59
1	B	350	ARG	N-CA-C	-5.37	105.46	112.23
1	A	448	GLN	N-CA-C	-5.33	105.38	111.14
1	A	118	SER	N-CA-C	-5.33	103.50	110.53
1	A	12	LEU	CA-C-N	5.33	123.55	119.66
1	A	12	LEU	C-N-CA	5.33	123.55	119.66
1	A	304	ALA	N-CA-C	-5.21	105.78	111.82
1	B	7	PHE	N-CA-C	5.10	119.38	112.04

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	MET	Peptide
1	A	141	VAL	Peptide
1	B	127	MET	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4352	0	4288	133	0
1	B	4352	0	4288	85	0
2	A	53	0	29	2	0
2	B	53	0	29	1	0
3	A	11	0	7	0	0
3	B	11	0	7	1	0
All	All	8832	0	8648	209	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 12.

All (209) 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)
2:A:600:FAD:C5B	2:A:600:FAD:O5B	1.66	1.42
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.50	0.93
1:B:513:ILE:O	1:B:516:THR:HB	1.76	0.83
1:A:443:THR:HA	1:A:491:LEU:HD21	1.63	0.81
1:A:552:GLN:NE2	1:A:552:GLN:H	1.79	0.81
1:A:177:LEU:HB2	1:A:265:ILE:HG21	1.64	0.80
1:A:310:THR:HG22	1:A:459:THR:HG22	1.63	0.79
1:A:211:ARG:HG3	1:B:519:TRP:CZ3	2.18	0.78
1:A:177:LEU:HB2	1:A:265:ILE:CG2	2.13	0.77
1:A:257:SER:HB3	1:B:248:PRO:HB3	1.66	0.77
1:A:349:GLY:H	1:A:352:ASN:HD21	1.35	0.74
1:A:454:TYR:OH	1:A:467:HIS:HE1	1.69	0.74
1:A:250:ILE:O	1:A:253:LEU:HB2	1.86	0.74
1:B:214:MET:HE2	1:B:245:GLY:HA2	1.71	0.72
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.20	0.70
1:B:297:ARG:HG3	1:B:431:VAL:O	1.92	0.70
1:A:454:TYR:OH	1:A:467:HIS:CE1	2.46	0.69
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.74	0.68
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.09	0.68
1:B:312:ARG:NH2	1:B:410:GLU:OE1	2.27	0.68
1:A:14:PRO:HG3	1:A:558:TRP:HZ2	1.59	0.67
1:B:79:ASN:C	1:B:79:ASN:HD22	2.03	0.67
1:A:513:ILE:O	1:A:516:THR:HB	1.94	0.66
1:A:24:PHE:HD2	1:A:25:ILE:HD12	1.60	0.66
1:A:328:SER:OG	1:A:330:ARG:HB2	1.96	0.66
1:A:312:ARG:HG3	1:A:457:THR:HG23	1.78	0.66
1:B:504:ARG:O	1:B:505:THR:HG23	1.95	0.66
1:A:80:VAL:HG11	1:A:209:LEU:HD11	1.77	0.66
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.78	0.65
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.61	0.65
1:A:514:MET:HE3	1:A:525:LEU:HD13	1.78	0.64
1:A:195:MET:O	1:A:196:MET:HE2	1.97	0.64
1:B:349:GLY:H	1:B:352:ASN:HD21	1.44	0.64
1:B:275:GLY:HA3	1:B:359:GLY:O	1.98	0.64
1:A:237:LYS:NZ	1:B:498:ASN:O	2.31	0.63
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.33	0.63
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:OE2	1:A:211:ARG:HD3	1.99	0.61
1:A:24:PHE:CD2	1:A:25:ILE:HD12	2.36	0.61
1:A:36:ASN:OD1	1:A:125:LYS:NZ	2.35	0.60
1:A:106:SER:HB2	1:A:422:HIS:HE1	1.67	0.60
1:A:108:TYR:CZ	1:A:504:ARG:HG2	2.37	0.60
1:A:7:PHE:HA	1:A:22:ASN:OD1	2.02	0.59
1:A:398:ARG:NH1	1:A:410:GLU:OE2	2.35	0.59
1:B:552:GLN:NE2	1:B:552:GLN:H	2.01	0.59
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.85	0.58
1:B:454:TYR:C	1:B:454:TYR:CD2	2.81	0.58
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.19	0.58
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.34	0.58
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.40	0.57
1:A:505:THR:OG1	1:A:513:ILE:HD12	2.05	0.57
1:B:177:LEU:HB2	1:B:265:ILE:CG2	2.34	0.56
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.89	0.56
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.40	0.56
1:B:177:LEU:C	1:B:177:LEU:HD12	2.30	0.56
1:A:101:SER:O	1:A:124:GLY:HA3	2.06	0.56
1:A:398:ARG:O	1:A:402:MET:HG3	2.06	0.56
1:A:129:ARG:HH21	1:A:131:LEU:HD21	1.70	0.56
1:A:31:ILE:HD13	1:A:85:SER:HB3	1.88	0.55
1:A:115:VAL:HG13	1:A:558:TRP:CH2	2.41	0.55
1:B:28:ILE:O	1:B:32:VAL:HG22	2.06	0.55
1:A:454:TYR:C	1:A:454:TYR:CD2	2.84	0.55
1:A:244:TYR:OH	1:B:195:MET:HG2	2.06	0.55
1:A:464:GLU:HG2	1:B:242:PHE:HB2	1.88	0.55
1:B:177:LEU:HB2	1:B:265:ILE:HG21	1.89	0.55
1:A:82:ASP:O	1:A:86:ILE:HD12	2.06	0.55
1:B:428:ILE:HD11	1:B:503:TYR:HB3	1.88	0.54
1:A:411:LEU:O	1:A:414:ILE:HB	2.07	0.54
1:A:177:LEU:HB2	1:A:265:ILE:HG22	1.89	0.54
1:A:552:GLN:H	1:A:552:GLN:HE21	1.51	0.54
1:A:211:ARG:HG3	1:B:519:TRP:CH2	2.43	0.54
1:B:194:TRP:O	1:B:197:HIS:HD2	1.91	0.53
1:B:201:GLU:CB	1:B:264:LYS:HB2	2.38	0.53
1:B:403:GLN:O	1:B:403:GLN:HG3	2.08	0.53
1:B:514:MET:HE2	1:B:546:SER:O	2.08	0.53
1:A:96:PRO:HG3	1:A:553:TYR:OH	2.08	0.53
1:A:312:ARG:HG2	1:A:316:LEU:HD23	1.90	0.53
1:A:443:THR:HG21	1:A:469:VAL:CG2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HD11	1:B:541:ILE:HD12	1.91	0.52
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.91	0.52
1:A:506:HIS:HB3	1:A:509:PHE:HD2	1.74	0.52
1:A:502:GLU:HB2	1:A:513:ILE:HD13	1.91	0.52
1:B:114:ARG:NH2	1:B:511:ASP:OD2	2.35	0.52
1:A:69:PHE:HB2	1:A:112:ALA:HB1	1.92	0.52
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.45	0.51
1:A:194:TRP:O	1:A:197:HIS:HD2	1.93	0.51
1:A:349:GLY:H	1:A:352:ASN:ND2	2.08	0.51
1:A:101:SER:HB3	1:A:144:PRO:O	2.11	0.51
1:A:244:TYR:OH	1:B:192:ASP:OD1	2.28	0.51
1:A:419:ASN:O	1:A:474:ASN:HA	2.11	0.51
1:A:477:ASP:O	1:A:481:LYS:HG3	2.11	0.51
1:A:114:ARG:NH2	1:A:511:ASP:OD2	2.42	0.50
1:A:58:HIS:C	1:A:112:ALA:HB2	2.36	0.50
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.94	0.50
1:A:24:PHE:O	1:A:27:ASP:HB2	2.12	0.50
2:B:1561:FAD:N1	2:B:1561:FAD:O3'	2.36	0.50
1:A:535:VAL:O	1:A:537:PRO:HD3	2.11	0.50
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.93	0.50
1:B:409:ASP:N	1:B:409:ASP:OD1	2.44	0.50
1:A:237:LYS:HB3	1:B:430:LYS:HD2	1.94	0.50
1:B:133:VAL:HG11	1:B:160:LEU:HD13	1.92	0.50
1:B:258:ASN:OD1	1:B:532:LYS:HD3	2.12	0.50
1:A:211:ARG:HD2	1:A:235:TRP:CH2	2.48	0.49
1:B:201:GLU:HB3	1:B:264:LYS:HB2	1.95	0.49
1:A:62:HIS:H	1:A:62:HIS:CD2	2.29	0.49
1:A:281:ILE:HG12	1:A:383:PHE:HD1	1.76	0.49
2:A:600:FAD:O5B	2:A:600:FAD:C4B	2.55	0.49
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.47	0.49
1:B:316:LEU:HD23	1:B:457:THR:HG23	1.94	0.49
1:B:106:SER:HB3	1:B:422:HIS:HE1	1.77	0.49
1:A:9:PRO:HA	1:A:40:ILE:O	2.12	0.48
1:A:18:LEU:O	1:A:22:ASN:ND2	2.46	0.48
1:A:146:VAL:O	1:A:176:VAL:HG23	2.14	0.48
1:A:471:ILE:HG21	1:A:484:VAL:HG13	1.95	0.48
1:A:271:PRO:O	1:A:272:ASN:C	2.56	0.48
1:A:197:HIS:HA	1:A:266:GLY:O	2.14	0.48
1:A:330:ARG:NH2	1:A:333:PRO:O	2.46	0.48
1:A:293:VAL:HA	1:A:296:ILE:HD12	1.95	0.47
1:A:349:GLY:N	1:A:352:ASN:HD21	2.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD2	1:A:62:HIS:HA	2.15	0.47
1:A:360:PRO:HB2	1:A:362:PRO:HD2	1.97	0.47
1:A:445:LYS:O	1:A:448:GLN:HB3	2.14	0.47
1:A:79:ASN:C	1:A:79:ASN:HD22	2.23	0.47
1:B:238:ILE:HA	1:B:241:LEU:HD12	1.98	0.46
1:B:296:ILE:HG23	1:B:305:LEU:CD1	2.45	0.46
1:A:224:GLU:CD	1:A:224:GLU:H	2.23	0.46
1:A:414:ILE:O	1:A:420:GLY:HA3	2.15	0.46
1:A:201:GLU:OE1	1:A:264:LYS:NZ	2.40	0.46
1:B:346:LEU:O	1:B:347:ASN:HB2	2.15	0.46
1:A:97:LEU:HD13	1:A:121:LEU:HD22	1.97	0.46
1:A:242:PHE:CZ	1:A:244:TYR:HB2	2.51	0.45
1:A:79:ASN:C	1:A:79:ASN:ND2	2.74	0.45
1:B:514:MET:HE3	1:B:525:LEU:HD13	1.97	0.45
1:B:79:ASN:C	1:B:79:ASN:ND2	2.74	0.45
1:A:79:ASN:HD21	1:A:81:ALA:HB3	1.81	0.45
1:A:258:ASN:HB2	1:A:542:ALA:HB3	1.99	0.45
1:A:422:HIS:CD2	1:A:424:PHE:CZ	3.04	0.45
1:A:514:MET:HE2	1:A:546:SER:O	2.16	0.45
1:B:319:ALA:CB	1:B:413:TRP:HB2	2.47	0.45
1:B:506:HIS:HB3	1:B:509:PHE:HD2	1.81	0.45
1:B:201:GLU:HB2	1:B:264:LYS:HB2	1.98	0.45
1:B:425:PHE:HB3	1:B:469:VAL:HB	1.98	0.45
1:B:427:PRO:HG2	1:B:467:HIS:HB3	1.98	0.45
1:B:458:PHE:CE1	1:B:467:HIS:CD2	3.06	0.45
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.98	0.44
1:B:314:ILE:O	1:B:314:ILE:HG13	2.17	0.44
1:A:281:ILE:HG12	1:A:383:PHE:CD1	2.51	0.44
1:B:443:THR:HA	1:B:491:LEU:HD21	1.98	0.44
1:B:526:ARG:HH21	1:B:529:GLU:CD	2.26	0.44
1:A:123:MET:HE3	1:A:123:MET:HB3	1.85	0.44
1:A:288:ASP:O	1:A:289:LEU:C	2.60	0.44
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.52	0.44
1:A:188:THR:C	1:A:190:TYR:N	2.76	0.44
1:A:188:THR:C	1:A:190:TYR:H	2.26	0.44
1:A:428:ILE:HG22	1:A:429:ALA:N	2.33	0.44
1:B:217:LEU:HD13	1:B:218:PRO:HD2	1.99	0.44
1:A:341:LYS:HA	1:A:344:LYS:HE2	2.00	0.43
1:B:297:ARG:NH1	1:B:298:PRO:HD3	2.33	0.43
1:A:474:ASN:OD1	1:A:474:ASN:C	2.61	0.43
1:A:443:THR:HA	1:A:491:LEU:CD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:HA	1:B:296:ILE:HD12	2.01	0.43
1:B:188:THR:HB	1:B:189:PRO:HD2	2.00	0.43
1:A:28:ILE:HD13	1:A:86:ILE:HG12	2.01	0.42
1:B:550:PRO:HG2	1:B:553:TYR:CD1	2.54	0.42
1:B:175:SER:O	1:B:179:ASN:HB2	2.19	0.42
1:A:102:ILE:HG21	1:A:104:ARG:HD2	2.02	0.42
1:A:211:ARG:HG3	1:B:519:TRP:CE3	2.52	0.42
1:B:194:TRP:O	1:B:197:HIS:CD2	2.71	0.42
1:B:309:PRO:O	1:B:460:VAL:HG23	2.20	0.42
1:A:214:MET:HE1	1:B:517:TYR:OH	2.19	0.42
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.80	0.42
1:B:185:VAL:HB	3:B:1562:EUG:C9	2.50	0.42
1:B:552:GLN:HE21	1:B:552:GLN:H	1.66	0.42
1:A:321:LEU:HD12	1:A:346:LEU:HD22	2.02	0.42
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.82	0.42
1:B:151:LEU:HD23	1:B:166:LEU:HD22	2.01	0.42
1:A:179:ASN:OD1	1:A:184:GLY:HA3	2.20	0.42
1:A:425:PHE:HB2	1:A:488:MET:SD	2.60	0.42
1:A:535:VAL:C	1:A:537:PRO:HD3	2.45	0.42
1:A:456:GLY:HA2	1:A:468:ILE:O	2.20	0.41
1:A:459:THR:OG1	1:A:466:HIS:HB2	2.20	0.41
1:A:310:THR:HB	1:A:457:THR:CG2	2.49	0.41
1:A:129:ARG:NH2	1:A:131:LEU:HD21	2.35	0.41
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.86	0.41
1:B:40:ILE:HD11	1:B:74:ILE:HD12	2.02	0.41
1:A:167:ASP:OD2	1:A:188:THR:OG1	2.30	0.41
1:A:13:PRO:HD3	1:A:117:GLY:O	2.21	0.41
1:B:297:ARG:CB	1:B:298:PRO:CD	2.92	0.41
1:B:319:ALA:HB3	1:B:413:TRP:HB2	2.02	0.41
1:B:350:ARG:HD2	1:B:350:ARG:HA	1.97	0.41
1:A:324:LYS:C	1:A:326:SER:N	2.78	0.41
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.51	0.41
1:B:177:LEU:HB2	1:B:265:ILE:HG22	2.03	0.41
1:B:278:SER:OG	1:B:399:ASP:OD1	2.33	0.41
1:A:211:ARG:CG	1:B:519:TRP:CZ3	2.98	0.41
1:B:452:LEU:HD11	1:B:471:ILE:HG23	2.03	0.41
1:A:360:PRO:O	1:A:361:GLU:C	2.64	0.40
1:A:297:ARG:O	1:A:301:LEU:HB2	2.20	0.40
1:A:310:THR:CG2	1:A:459:THR:HG22	2.42	0.40
1:A:413:TRP:CH2	1:A:422:HIS:HD2	2.39	0.40
1:B:312:ARG:HD3	1:B:354:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLY:C	1:A:187:TYR:CG	2.99	0.40
1:B:324:LYS:HG3	1:B:416:TRP:CZ2	2.56	0.40
1:A:444:LYS:O	1:A:445:LYS:C	2.62	0.40
1:B:419:ASN:HB2	1:B:474:ASN:OD1	2.21	0.40
1:A:86:ILE:O	1:A:87:VAL:C	2.63	0.40
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.86	0.40
1:B:214:MET:HE2	1:B:245:GLY:CA	2.48	0.40
1:B:238:ILE:O	1:B:238:ILE:HG22	2.21	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	546/560 (98%)	492 (90%)	48 (9%)	6 (1%)	11	29
1	B	546/560 (98%)	514 (94%)	28 (5%)	4 (1%)	18	41
All	All	1092/1120 (98%)	1006 (92%)	76 (7%)	10 (1%)	14	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLU
1	B	418	PRO
1	A	159	ASN
1	B	105	ASN
1	A	274	ARG
1	A	418	PRO
1	A	361	GLU
1	B	345	GLN
1	B	169	PRO
1	A	230	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/482 (98%)	410 (87%)	60 (13%)	4	11
1	B	470/482 (98%)	416 (88%)	54 (12%)	5	14
All	All	940/964 (98%)	826 (88%)	114 (12%)	5	12

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	8	ARG
1	A	16	LEU
1	A	18	LEU
1	A	25	ILE
1	A	28	ILE
1	A	30	ARG
1	A	41	SER
1	A	50	SER
1	A	63	VAL
1	A	79	ASN
1	A	94	SER
1	A	118	SER
1	A	128	ASN
1	A	129	ARG
1	A	142	VAL
1	A	156	GLU
1	A	161	ARG
1	A	166	LEU
1	A	177	LEU
1	A	195	MET
1	A	200	MET
1	A	211	ARG
1	A	217	LEU
1	A	229	LYS
1	A	231	GLU
1	A	250	ILE

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Mol	Chain	Res	Type
1	A	264	LYS
1	A	297	ARG
1	A	303	MET
1	A	326	SER
1	A	329	SER
1	A	330	ARG
1	A	331	THR
1	A	341	LYS
1	A	344	LYS
1	A	381	VAL
1	A	391	GLU
1	A	393	SER
1	A	396	ARG
1	A	407	THR
1	A	413	TRP
1	A	414	ILE
1	A	422	HIS
1	A	423	LEU
1	A	426	SER
1	A	432	SER
1	A	443	THR
1	A	455	ILE
1	A	457	THR
1	A	467	HIS
1	A	472	VAL
1	A	475	LYS
1	A	503	TYR
1	A	504	ARG
1	A	505	THR
1	A	513	ILE
1	A	516	THR
1	A	523	SER
1	A	552	GLN
1	B	7	PHE
1	B	8	ARG
1	B	10	LEU
1	B	11	THR
1	B	15	LYS
1	B	25	ILE
1	B	26	GLN
1	B	29	ILE
1	B	35	GLU

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Mol	Chain	Res	Type
1	B	63	VAL
1	B	79	ASN
1	B	128	ASN
1	B	142	VAL
1	B	149	HIS
1	B	158	ASN
1	B	163	LYS
1	B	171	LEU
1	B	177	LEU
1	B	211	ARG
1	B	217	LEU
1	B	221	LYS
1	B	231	GLU
1	B	237	LYS
1	B	241	LEU
1	B	253	LEU
1	B	297	ARG
1	B	301	LEU
1	B	324	LYS
1	B	328	SER
1	B	329	SER
1	B	330	ARG
1	B	336	ASP
1	B	341	LYS
1	B	345	GLN
1	B	365	ARG
1	B	370	THR
1	B	396	ARG
1	B	403	GLN
1	B	409	ASP
1	B	412	LYS
1	B	422	HIS
1	B	430	LYS
1	B	432	SER
1	B	444	LYS
1	B	452	LEU
1	B	457	THR
1	B	472	VAL
1	B	503	TYR
1	B	504	ARG
1	B	513	ILE
1	B	516	THR

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Mol	Chain	Res	Type
1	B	540	ILE
1	B	552	GLN
1	B	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	79	ASN
1	A	84	GLN
1	A	91	ASN
1	A	128	ASN
1	A	153	ASN
1	A	158	ASN
1	A	197	HIS
1	A	352	ASN
1	A	467	HIS
1	A	520	ASN
1	A	538	ASN
1	A	552	GLN
1	A	555	HIS
1	B	79	ASN
1	B	128	ASN
1	B	153	ASN
1	B	158	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	467	HIS
1	B	485	GLN
1	B	520	ASN
1	B	552	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](#)

4 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	1561	1	58,58,58	1.20	7 (12%)	85,89,89	1.59	15 (17%)
2	FAD	A	600	1	58,58,58	1.37	6 (10%)	85,89,89	1.72	21 (24%)
3	EUG	A	1562	-	11,11,12	1.71	1 (9%)	14,14,15	1.34	2 (14%)
3	EUG	B	1562	-	11,11,12	1.56	1 (9%)	14,14,15	1.35	2 (14%)

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	1561	1	-	6/34/50/50	0/6/6/6
2	FAD	A	600	1	-	7/34/50/50	0/6/6/6
3	EUG	A	1562	-	-	2/4/4/5	0/1/1/1
3	EUG	B	1562	-	-	2/4/4/5	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	O5B-C5B	5.83	1.66	1.44
3	A	1562	EUG	C4-C3	4.90	1.48	1.40
3	B	1562	EUG	C4-C3	4.73	1.48	1.40
2	B	1561	FAD	C4X-N5	3.44	1.38	1.30
2	A	600	FAD	C4X-N5	3.43	1.38	1.30
2	A	600	FAD	C10-N1	3.07	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1561	FAD	C2A-N1A	2.89	1.39	1.33
2	B	1561	FAD	C2A-N3A	2.85	1.39	1.33
2	A	600	FAD	C2A-N3A	2.81	1.38	1.33
2	A	600	FAD	C2A-N1A	2.54	1.38	1.33
2	B	1561	FAD	P-O3P	2.46	1.62	1.59
2	B	1561	FAD	C10-N1	2.39	1.38	1.33
2	B	1561	FAD	PA-O3P	2.33	1.62	1.59
2	A	600	FAD	C5A-N7A	-2.15	1.35	1.39
2	B	1561	FAD	C5A-N7A	-2.05	1.35	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1561	FAD	N3A-C2A-N1A	-6.18	119.23	128.58
2	A	600	FAD	N3A-C2A-N1A	-5.88	119.69	128.58
2	A	600	FAD	C5A-C4A-N3A	-4.48	120.55	126.72
2	B	1561	FAD	C5A-C4A-N3A	-4.17	120.97	126.72
2	B	1561	FAD	N9A-C8A-N7A	-3.59	108.85	113.94
2	A	600	FAD	C5X-C9A-N10	3.52	121.15	117.97
2	A	600	FAD	N9A-C8A-N7A	-3.40	109.11	113.94
2	B	1561	FAD	C2A-N3A-C4A	3.39	120.12	111.83
3	A	1562	EUG	O3-C3-C4	3.33	119.55	114.55
2	A	600	FAD	C5A-C6A-N6A	-3.30	115.11	123.29
3	B	1562	EUG	O3-C3-C4	3.28	119.47	114.55
2	A	600	FAD	C2A-N3A-C4A	3.23	119.73	111.83
2	A	600	FAD	N3A-C4A-N9A	3.21	132.63	127.17
2	B	1561	FAD	C5A-N7A-C8A	3.19	108.47	103.45
2	A	600	FAD	C5A-N7A-C8A	3.06	108.26	103.45
2	B	1561	FAD	N3A-C4A-N9A	3.03	132.33	127.17
2	B	1561	FAD	C4X-C10-N10	2.89	120.61	116.48
2	A	600	FAD	O4-C4-C4X	-2.89	118.91	126.53
2	A	600	FAD	C9A-C5X-N5	-2.81	119.47	122.45
3	B	1562	EUG	C9-O3-C3	2.66	121.42	117.51
2	A	600	FAD	O2A-PA-O5B	2.65	119.59	107.57
2	A	600	FAD	O4-C4-N3	-2.65	115.13	120.11
2	B	1561	FAD	O4-C4-C4X	-2.63	119.60	126.53
2	A	600	FAD	PA-O5B-C5B	2.57	136.10	121.35
2	B	1561	FAD	C10-C4X-N5	-2.56	119.59	124.81
2	B	1561	FAD	C4-N3-C2	-2.51	121.18	125.64
2	B	1561	FAD	C9A-C5X-N5	-2.49	119.81	122.45
2	A	600	FAD	C4X-C4-N3	2.41	119.38	113.25
2	A	600	FAD	C4-N3-C2	-2.41	121.37	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1561	FAD	C3B-C2B-C1B	2.34	105.89	101.46
2	A	600	FAD	C4X-C10-N10	2.29	119.76	116.48
2	B	1561	FAD	O2P-P-O3P	2.28	113.44	107.27
2	B	1561	FAD	C4X-C4-N3	2.27	119.02	113.25
2	A	600	FAD	C8M-C8-C7	2.26	125.38	120.76
3	A	1562	EUG	O3-C3-C2	-2.22	120.25	124.08
2	A	600	FAD	C6A-C5A-C4A	2.14	120.10	117.18
2	A	600	FAD	C10-C4X-N5	-2.09	120.55	124.81
2	A	600	FAD	C8M-C8-C9	-2.04	115.99	119.57
2	B	1561	FAD	C9A-C9-C8	2.03	123.31	119.22
2	A	600	FAD	O4'-C4'-C5'	-2.03	105.52	109.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

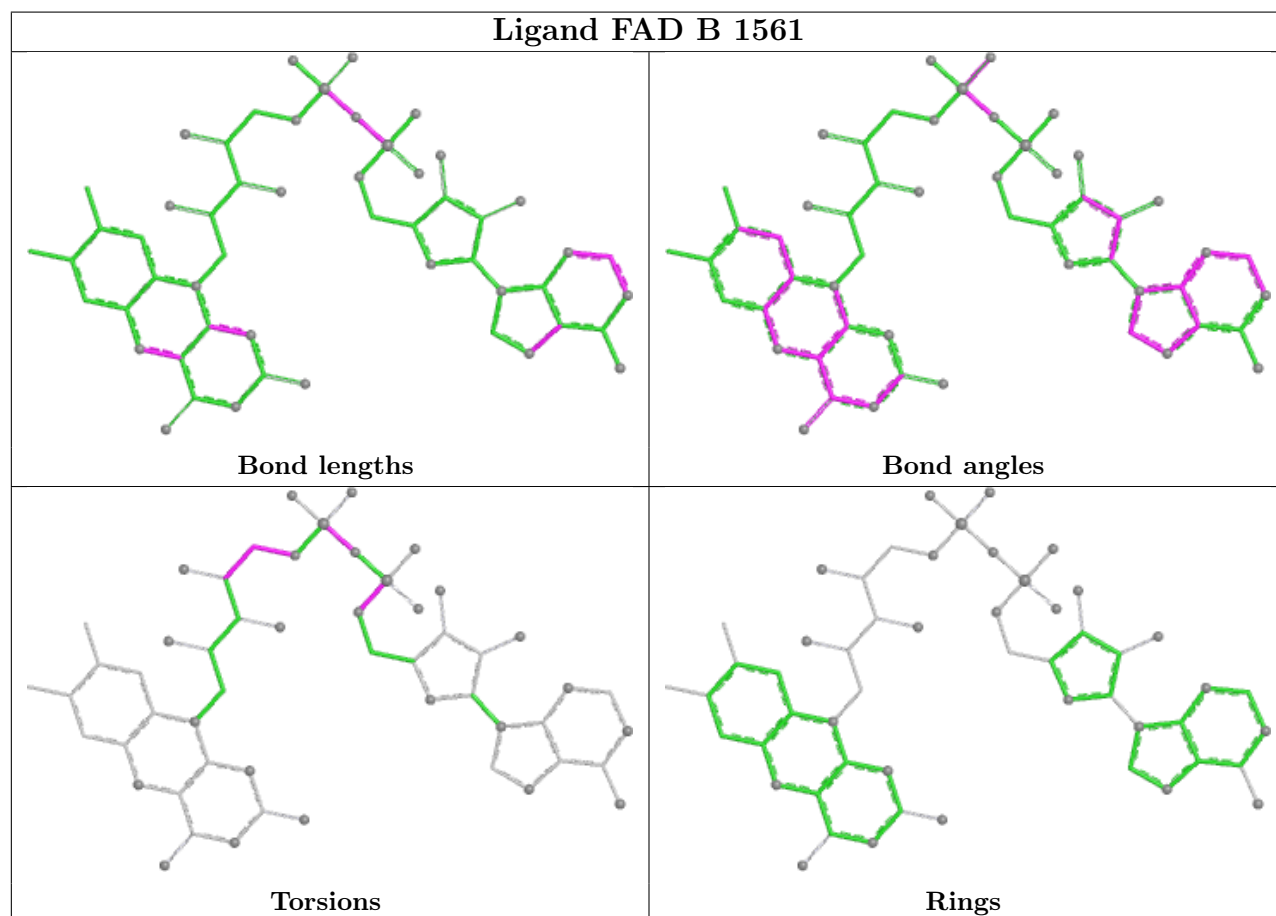
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O1A
2	B	1561	FAD	C5B-O5B-PA-O1A
2	B	1561	FAD	C5B-O5B-PA-O3P
3	A	1562	EUG	C4-C3-O3-C9
3	A	1562	EUG	C2-C3-O3-C9
2	A	600	FAD	O4'-C4'-C5'-O5'
2	B	1561	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	C3'-C4'-C5'-O5'
2	B	1561	FAD	C3'-C4'-C5'-O5'
2	B	1561	FAD	PA-O3P-P-O1P
3	B	1562	EUG	C6-C1-C7-C8
3	B	1562	EUG	C2-C1-C7-C8
2	A	600	FAD	C5B-O5B-PA-O2A
2	A	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C4'-C5'-O5'-P
2	B	1561	FAD	C4'-C5'-O5'-P
2	A	600	FAD	PA-O3P-P-O1P

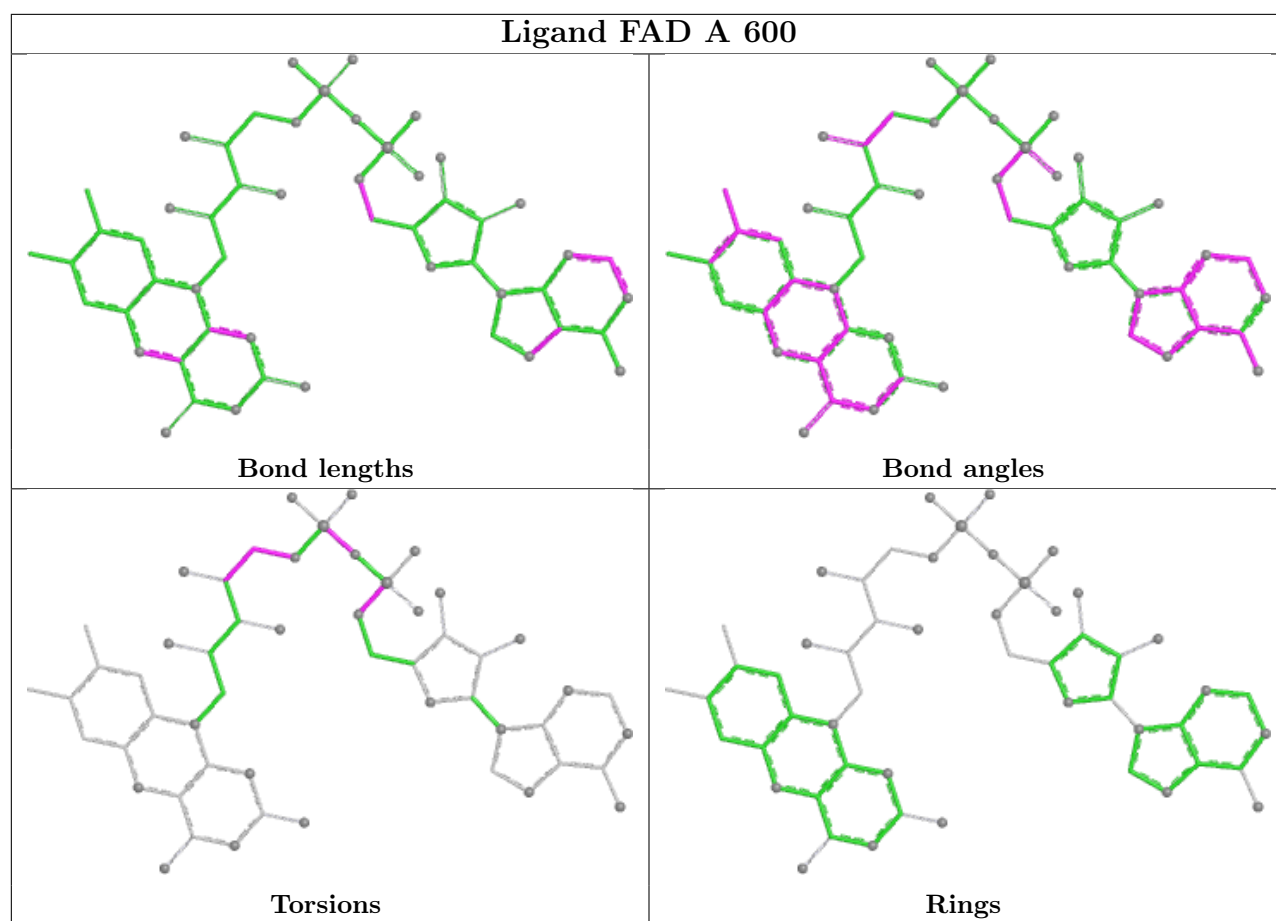
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1561	FAD	1	0
2	A	600	FAD	2	0
3	B	1562	EUG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	550/560 (98%)	-0.39	2 (0%)	88 87	33, 42, 55, 66	0
1	B	550/560 (98%)	0.25	7 (1%)	75 73	44, 60, 90, 102	0
All	All	1100/1120 (98%)	-0.07	9 (0%)	82 81	33, 51, 81, 102	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	MET	3.7
1	B	7	PHE	2.9
1	B	347	ASN	2.7
1	B	47	VAL	2.6
1	B	412	LYS	2.2
1	B	327	TYR	2.2
1	A	52	MET	2.2
1	A	7	PHE	2.1
1	B	55	THR	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,

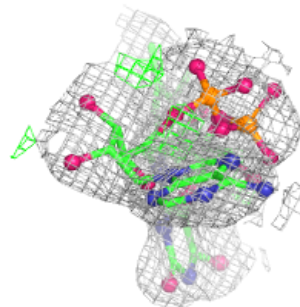
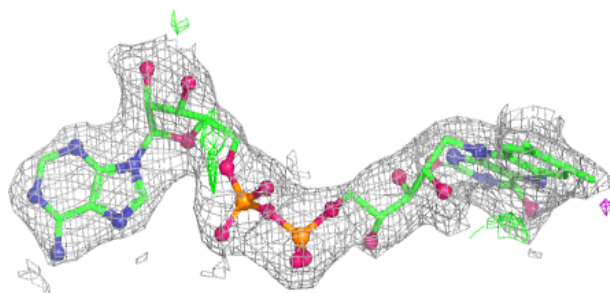
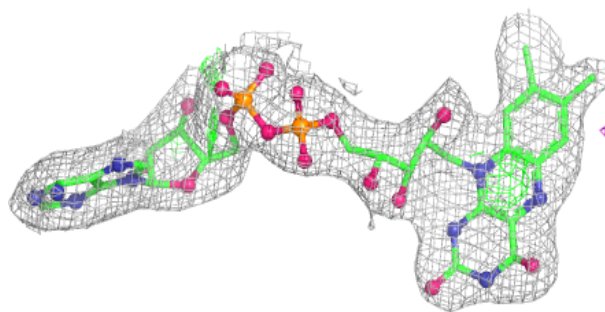
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

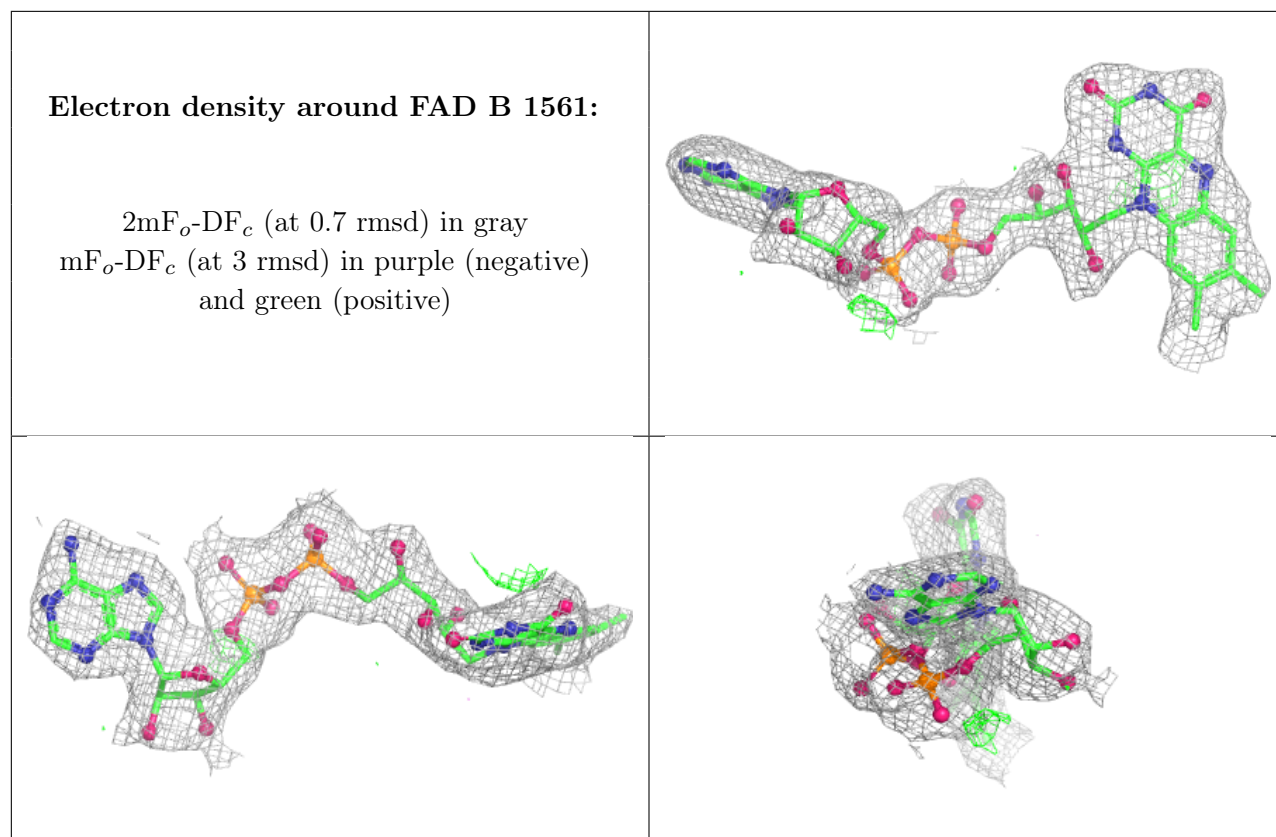
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EUG	A	1562	11/12	0.89	0.18	64,65,67,67	0
3	EUG	B	1562	11/12	0.92	0.13	71,72,74,74	0
2	FAD	A	600	53/53	0.95	0.09	48,55,64,65	0
2	FAD	B	1561	53/53	0.95	0.09	54,59,70,71	0

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 600:

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.