



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:28 AM UTC

PDB ID : 1YY5 / pdb_00001yy5
Title : Crystal structure of Fms1, a polyamine oxidase from Yeast
Authors : Huang, Q.; Liu, Q.; Hao, Q.
Deposited on : 2005-02-23
Resolution : 2.30 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

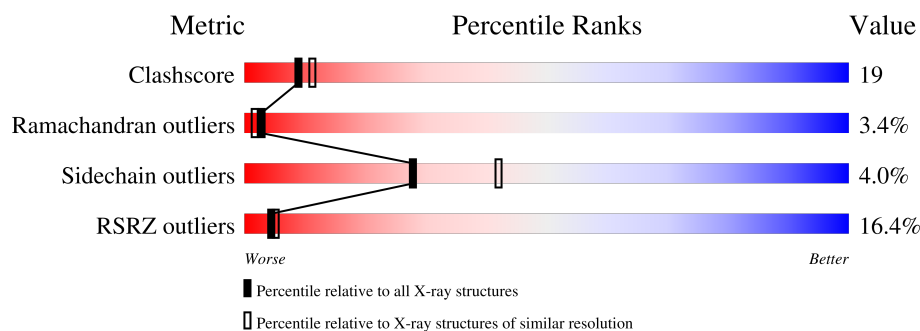
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	513	
1	B	513	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8083 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 FMS1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	86	0	0
			3997	2526	699	750	22			
1	B	487	Total	C	N	O	S	126	0	0
			3908	2472	679	735	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	509	LEU	-	expression tag	UNP P50264
A	510	GLU	-	expression tag	UNP P50264
A	511	HIS	-	expression tag	UNP P50264
A	512	HIS	-	expression tag	UNP P50264
A	513	HIS	-	expression tag	UNP P50264
B	509	LEU	-	expression tag	UNP P50264
B	510	GLU	-	expression tag	UNP P50264
B	511	HIS	-	expression tag	UNP P50264
B	512	HIS	-	expression tag	UNP P50264
B	513	HIS	-	expression tag	UNP P50264

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

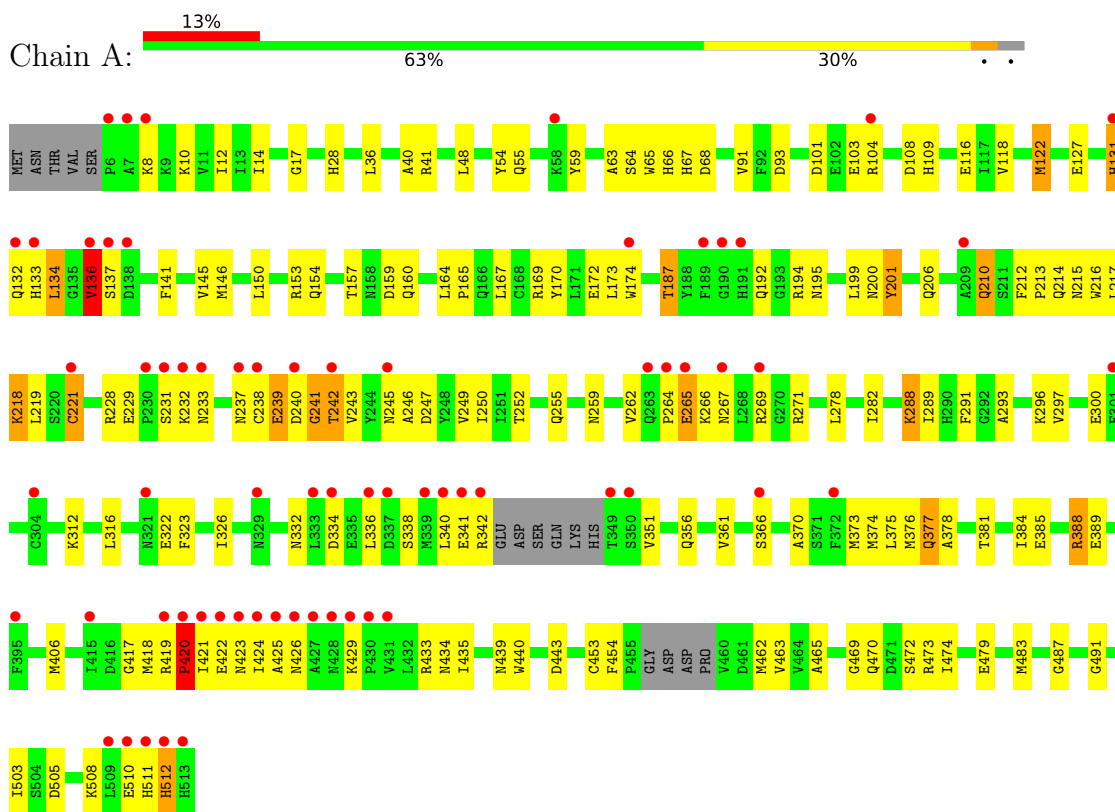
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	34	Total O 34 34	0	0

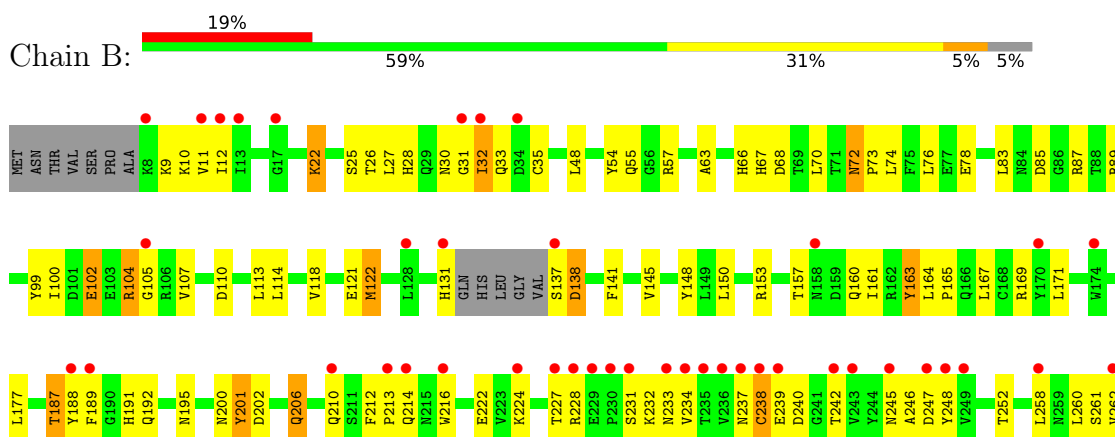
3 Residue-property plots

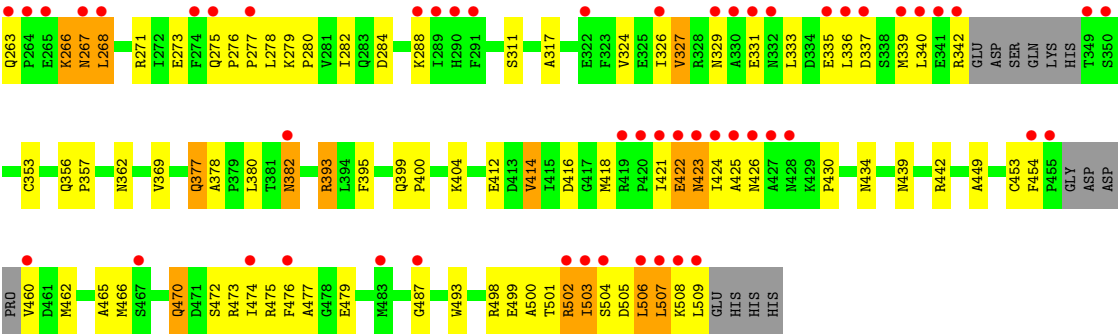
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: FMS1 protein



• Molecule 1: FMS1 protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.71Å 215.37Å 118.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-2.30) 90.2 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.290 0.246 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8083	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/4080	0.96	15/5515 (0.3%)
1	B	0.43	0/3985	0.92	15/5385 (0.3%)
All	All	0.44	0/8065	0.94	30/10900 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	THR	N-CA-C	7.72	119.33	111.07
1	A	454	PHE	N-CA-C	-7.58	100.20	110.36
1	A	288	LYS	N-CA-C	7.18	121.35	112.59
1	A	133	HIS	N-CA-C	6.95	121.05	107.98
1	B	163	TYR	N-CA-C	6.88	120.16	111.69
1	B	470	GLN	N-CA-C	-6.84	103.89	111.82
1	A	351	VAL	N-CA-C	6.71	118.25	108.58
1	A	66	HIS	N-CA-C	-6.70	97.81	108.73
1	B	238	CYS	N-CA-C	-6.46	100.93	110.48
1	B	201	TYR	N-CA-C	-6.16	104.67	111.82
1	B	66	HIS	N-CA-C	-6.13	97.71	108.20
1	A	201	TYR	N-CA-C	-6.08	105.35	112.89
1	B	83	LEU	N-CA-C	-6.02	104.64	112.23
1	B	453	CYS	N-CA-C	5.92	118.60	109.07
1	A	440	TRP	N-CA-C	5.79	118.37	111.71
1	B	378	ALA	N-CA-C	-5.78	102.49	109.83
1	B	105	GLY	N-CA-C	-5.76	104.37	111.45
1	B	100	ILE	N-CA-C	5.49	115.76	107.75
1	A	453	CYS	N-CA-C	5.48	118.17	109.24
1	B	317	ALA	N-CA-C	-5.46	103.69	110.41
1	A	366	SER	N-CA-C	5.35	117.86	111.71
1	A	136	VAL	N-CA-C	5.33	120.43	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	VAL	N-CA-C	5.32	115.95	109.30
1	B	102	GLU	N-CA-C	5.18	117.33	111.11
1	A	65	TRP	N-CA-C	5.17	118.00	109.72
1	A	491	GLY	N-CA-C	-5.12	106.29	112.49
1	B	329	ASN	N-CA-C	5.09	117.96	111.69
1	A	40	ALA	N-CA-C	5.09	116.91	111.36
1	B	327	VAL	N-CA-C	-5.07	105.77	110.53
1	A	17	GLY	N-CA-C	-5.05	104.28	112.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3997	0	3916	126	2
1	B	3908	0	3842	159	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
3	A	38	0	0	1	0
3	B	34	0	0	1	0
All	All	8083	0	7820	284	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 19.

All (284) 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:B:278:LEU:HA	1:B:470:GLN:HE22	1.30	0.96
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.49	0.92
1:A:146:MET:HE3	1:A:336:LEU:HD21	1.51	0.90
1:A:122:MET:HE1	1:A:145:VAL:HG22	1.54	0.90
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.37	0.89
1:A:426:ASN:HB3	1:A:429:LYS:HB2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:HG22	1:B:336:LEU:HD12	1.58	0.85
1:B:122:MET:HE1	1:B:145:VAL:HG22	1.59	0.83
1:A:377:GLN:NE2	1:A:377:GLN:H	1.79	0.80
1:A:376:MET:HE1	1:A:384:ILE:HG21	1.63	0.78
1:B:85:ASP:OD1	1:B:87:ARG:HG3	1.85	0.77
1:A:388:ARG:HB2	1:A:388:ARG:HH11	1.50	0.76
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.00	0.76
1:B:382:ASN:H	1:B:382:ASN:ND2	1.82	0.75
1:A:240:ASP:OD2	1:A:242:THR:HG23	1.87	0.74
1:A:146:MET:HE2	1:A:340:LEU:HD11	1.69	0.74
1:B:72:ASN:C	1:B:72:ASN:HD22	1.96	0.73
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.71	0.72
1:A:388:ARG:NH2	1:A:439:ASN:HB2	2.05	0.72
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.70	0.71
1:B:227:THR:HG23	1:B:275:GLN:HB3	1.72	0.71
1:B:475:ARG:NH1	1:B:502:ARG:CZ	2.53	0.71
1:B:85:ASP:CG	1:B:87:ARG:HG3	2.16	0.71
1:B:377:GLN:H	1:B:377:GLN:NE2	1.89	0.70
1:A:463:VAL:HG21	1:A:483:MET:HE2	1.71	0.70
1:A:389:GLU:OE1	1:A:389:GLU:HA	1.92	0.69
1:A:423:ASN:HD21	1:A:426:ASN:ND2	1.94	0.66
1:A:417:GLY:O	1:A:433:ARG:HD3	1.96	0.66
1:A:41:ARG:HD2	3:A:816:HOH:O	1.95	0.66
1:A:423:ASN:HD21	1:A:426:ASN:HD22	1.42	0.66
1:B:475:ARG:HH12	1:B:502:ARG:NE	1.93	0.66
1:B:439:ASN:HD21	1:B:442:ARG:HH11	1.44	0.65
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.61	0.65
1:A:247:ASP:O	1:A:473:ARG:HD2	1.97	0.65
1:A:289:ILE:HD11	1:A:462:MET:HG2	1.78	0.65
1:A:326:ILE:HD11	1:A:342:ARG:HH21	1.62	0.65
1:B:157:THR:O	1:B:161:ILE:HG13	1.97	0.65
1:B:104:ARG:HG3	1:B:104:ARG:NH1	2.07	0.65
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.26	0.64
1:A:213:PRO:O	1:A:216:TRP:HB2	1.98	0.64
1:B:475:ARG:HH12	1:B:502:ARG:CZ	2.11	0.62
1:B:393:ARG:NH1	1:B:393:ARG:HG2	2.14	0.62
1:A:288:LYS:O	1:A:289:ILE:HG23	1.98	0.62
1:B:122:MET:CE	1:B:145:VAL:HG22	2.29	0.62
1:B:475:ARG:NH1	1:B:502:ARG:NE	2.48	0.61
1:A:322:GLU:CG	1:A:342:ARG:HH22	2.12	0.61
1:B:9:LYS:O	1:B:246:ALA:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PRO:HG2	1:B:216:TRP:CD2	2.35	0.61
1:A:377:GLN:H	1:A:377:GLN:HE21	1.46	0.61
1:B:476:PHE:O	1:B:499:GLU:HG3	1.99	0.61
1:B:11:VAL:HG21	1:B:503:ILE:HG21	1.83	0.61
1:B:189:PHE:HE1	1:B:191:HIS:NE2	1.99	0.61
1:B:462:MET:SD	1:B:466:MET:HE3	2.41	0.61
1:B:141:PHE:O	1:B:145:VAL:HG23	2.00	0.60
1:B:63:ALA:HA	2:B:804:FAD:N5	2.14	0.60
1:B:454:PHE:H	1:B:454:PHE:HD2	1.44	0.60
1:B:233:ASN:HB3	1:B:245:ASN:HD21	1.65	0.60
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.32	0.60
1:A:63:ALA:HA	2:A:803:FAD:N5	2.16	0.59
1:B:67:HIS:ND1	1:B:195:ASN:ND2	2.51	0.59
1:A:104:ARG:NH2	1:A:159:ASP:OD2	2.34	0.59
1:A:67:HIS:ND1	1:A:195:ASN:ND2	2.51	0.58
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.38	0.58
1:B:393:ARG:HG2	1:B:393:ARG:HH11	1.68	0.58
1:A:150:LEU:O	1:A:153:ARG:HD2	2.04	0.58
1:A:297:VAL:HG23	1:A:376:MET:HE3	1.86	0.58
1:A:54:TYR:CD2	1:A:55:GLN:HG3	2.39	0.58
1:A:423:ASN:ND2	1:A:426:ASN:HD22	2.02	0.57
1:A:41:ARG:NH1	1:A:443:ASP:OD2	2.35	0.57
1:B:10:LYS:O	1:B:247:ASP:HB2	2.04	0.57
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.85	0.57
1:A:146:MET:CE	1:A:336:LEU:HD21	2.31	0.57
1:B:233:ASN:HB3	1:B:245:ASN:ND2	2.20	0.56
1:A:297:VAL:CG2	1:A:376:MET:HE3	2.35	0.56
1:B:267:ASN:O	1:B:268:LEU:O	2.23	0.56
1:B:122:MET:HG2	1:B:148:TYR:CD2	2.40	0.56
1:B:333:LEU:O	1:B:337:ASP:HB2	2.06	0.56
1:B:382:ASN:H	1:B:382:ASN:HD22	1.53	0.56
1:A:54:TYR:CZ	1:A:433:ARG:HG3	2.41	0.56
1:B:150:LEU:O	1:B:153:ARG:HG2	2.06	0.56
1:B:228:ARG:HH12	1:B:232:LYS:HA	1.71	0.55
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.42	0.55
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.06	0.55
1:A:167:LEU:HA	1:A:316:LEU:HD22	1.90	0.54
1:A:217:LEU:HD21	1:A:219:LEU:HD21	1.89	0.54
1:B:122:MET:HE2	1:B:145:VAL:HG13	1.89	0.54
1:B:212:PHE:HB2	1:B:213:PRO:HD2	1.89	0.54
1:A:406:MET:HE2	1:A:406:MET:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:TYR:CE2	1:B:473:ARG:HG2	2.42	0.54
1:A:141:PHE:CD2	1:A:187:THR:HG21	2.42	0.54
1:B:335:GLU:O	1:B:339:MET:HG3	2.06	0.54
1:B:508:LYS:O	1:B:509:LEU:C	2.49	0.54
1:B:165:PRO:O	1:B:169:ARG:HG3	2.08	0.54
1:B:278:LEU:CA	1:B:470:GLN:HE22	2.13	0.54
1:B:276:PRO:HB2	1:B:277:PRO:HD2	1.90	0.53
1:B:418:MET:HE3	1:B:434:ASN:HA	1.90	0.53
1:A:14:ILE:HD12	1:A:14:ILE:N	2.24	0.53
1:A:48:LEU:HD23	1:A:63:ALA:HB3	1.90	0.53
1:A:41:ARG:HG2	1:A:41:ARG:NH1	2.24	0.53
1:B:399:GLN:HB3	1:B:400:PRO:HD3	1.91	0.53
1:B:326:ILE:HG22	1:B:336:LEU:CD1	2.36	0.53
1:A:64:SER:OG	1:A:296:LYS:NZ	2.42	0.53
1:A:278:LEU:HA	1:A:470:GLN:HE22	1.72	0.53
1:A:322:GLU:HG3	1:A:342:ARG:HH22	1.72	0.52
1:A:322:GLU:HG2	1:A:342:ARG:HH22	1.75	0.52
1:A:12:ILE:HB	1:A:249:VAL:HG12	1.92	0.52
1:B:72:ASN:C	1:B:72:ASN:ND2	2.66	0.52
1:B:118:VAL:HG23	1:B:164:LEU:HD13	1.91	0.52
1:A:157:THR:OG1	1:A:160:GLN:HG3	2.10	0.52
1:B:324:VAL:O	1:B:327:VAL:N	2.41	0.52
1:A:239:GLU:C	1:A:241:GLY:H	2.17	0.52
1:A:508:LYS:C	1:A:510:GLU:H	2.16	0.51
1:B:104:ARG:HD2	1:B:107:VAL:HG12	1.92	0.51
1:A:28:HIS:ND1	1:A:212:PHE:HA	2.26	0.51
1:A:421:ILE:HG22	1:A:421:ILE:O	2.09	0.51
1:B:137:SER:O	1:B:138:ASP:HB3	2.10	0.51
1:A:164:LEU:N	1:A:165:PRO:HD2	2.25	0.51
1:B:57:ARG:HD3	1:B:369:VAL:HG13	1.92	0.51
1:A:67:HIS:HA	1:A:195:ASN:HD22	1.76	0.50
1:B:502:ARG:HG2	1:B:502:ARG:HH11	1.77	0.50
1:B:222:GLU:O	1:B:238:CYS:HA	2.11	0.50
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.76	0.50
1:A:278:LEU:HA	1:A:470:GLN:NE2	2.27	0.50
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.24	0.49
1:B:72:ASN:HD21	1:B:74:LEU:HB3	1.78	0.49
1:B:475:ARG:NH1	1:B:502:ARG:NH2	2.60	0.49
1:B:167:LEU:HD23	1:B:167:LEU:C	2.37	0.49
1:B:32:ILE:HG22	1:B:33:GLN:N	2.27	0.49
1:A:68:ASP:HB3	1:A:192:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:OG1	1:B:160:GLN:HG3	2.13	0.49
1:A:141:PHE:CE2	1:A:187:THR:HG21	2.48	0.48
1:B:78:GLU:OE1	1:B:89:ARG:HD3	2.13	0.48
1:B:507:LEU:O	1:B:508:LYS:C	2.56	0.48
1:A:8:LYS:CD	1:A:245:ASN:HD22	2.26	0.48
1:A:154:GLN:O	1:A:154:GLN:HG2	2.12	0.48
1:B:189:PHE:HE1	1:B:191:HIS:CE1	2.31	0.48
1:A:237:ASN:OD1	1:A:243:VAL:HG13	2.13	0.48
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.43	0.48
1:B:263:GLN:H	1:B:271:ARG:HH12	1.61	0.48
1:B:475:ARG:HH12	1:B:502:ARG:NH2	2.12	0.48
1:A:232:LYS:HB3	1:A:473:ARG:HH21	1.79	0.48
1:A:214:GLN:C	1:A:216:TRP:H	2.21	0.48
1:A:381:THR:O	1:A:385:GLU:HG3	2.13	0.48
1:B:12:ILE:HG13	1:B:246:ALA:CB	2.44	0.48
1:B:232:LYS:O	1:B:473:ARG:NH1	2.47	0.48
1:A:375:LEU:N	1:A:375:LEU:HD12	2.29	0.48
1:A:250:ILE:HD11	1:A:503:ILE:HD12	1.96	0.48
1:B:356:GLN:HB2	1:B:357:PRO:HD2	1.96	0.48
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.13	0.48
1:A:252:THR:O	2:A:803:FAD:H51A	2.14	0.47
1:B:267:ASN:O	1:B:268:LEU:C	2.57	0.47
1:B:72:ASN:HD22	1:B:73:PRO:N	2.13	0.47
1:A:418:MET:HA	1:A:433:ARG:O	2.15	0.47
1:B:113:LEU:O	1:B:114:LEU:C	2.57	0.47
1:A:206:GLN:O	1:A:210:GLN:HB2	2.15	0.47
1:B:288:LYS:HA	1:B:454:PHE:HZ	1.80	0.47
1:A:259:ASN:O	1:A:262:VAL:HG22	2.14	0.46
1:B:54:TYR:O	1:B:57:ARG:HG3	2.15	0.46
1:B:224:LYS:HE2	1:B:237:ASN:CB	2.46	0.46
1:B:502:ARG:HG2	1:B:502:ARG:NH1	2.30	0.46
1:B:99:TYR:CE2	1:B:167:LEU:HG	2.51	0.46
1:B:260:LEU:C	1:B:262:VAL:H	2.22	0.46
1:B:280:PRO:O	1:B:284:ASP:OD1	2.33	0.46
1:A:12:ILE:O	1:A:249:VAL:HA	2.15	0.46
1:A:474:ILE:HD12	1:A:474:ILE:N	2.30	0.46
1:B:500:ALA:O	1:B:501:THR:C	2.58	0.46
1:A:12:ILE:HG12	1:A:246:ALA:HB2	1.98	0.46
1:B:22:LYS:HG2	1:B:493:TRP:CD1	2.51	0.46
1:B:506:LEU:O	1:B:507:LEU:C	2.59	0.46
1:B:102:GLU:O	1:B:404:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:O	1:A:172:GLU:HG3	2.16	0.46
1:B:70:LEU:HB2	1:B:192:GLN:O	2.16	0.46
1:A:59:TYR:OH	1:A:300:GLU:HG2	2.17	0.45
1:A:237:ASN:OD1	1:A:243:VAL:HG22	2.15	0.45
1:A:167:LEU:O	1:A:170:TYR:HD2	1.99	0.45
1:A:264:PRO:O	1:A:265:GLU:HG3	2.15	0.45
1:A:255:GLN:OE1	1:A:289:ILE:HD12	2.16	0.45
1:A:266:LYS:HA	1:A:271:ARG:NH1	2.31	0.45
1:A:282:ILE:HG12	1:A:465:ALA:HB1	1.98	0.45
1:B:11:VAL:HG22	1:B:248:TYR:HB2	1.98	0.45
1:B:54:TYR:CD2	1:B:55:GLN:HG3	2.52	0.45
1:A:134:LEU:C	1:A:136:VAL:H	2.25	0.45
1:B:393:ARG:NH1	1:B:393:ARG:CG	2.80	0.45
1:B:228:ARG:NH1	1:B:232:LYS:HA	2.31	0.45
1:A:116:GLU:OE2	1:A:116:GLU:N	2.34	0.44
1:B:22:LYS:O	1:B:25:SER:HB3	2.17	0.44
1:A:167:LEU:C	1:A:167:LEU:HD23	2.43	0.44
1:B:279:LYS:HB2	1:B:280:PRO:HD2	1.99	0.44
1:B:395:PHE:O	1:B:399:GLN:HB2	2.17	0.44
1:A:338:SER:O	1:A:341:GLU:HB2	2.17	0.44
1:B:202:ASP:O	1:B:206:GLN:HB2	2.17	0.44
1:B:171:LEU:HD13	1:B:187:THR:HG22	1.98	0.44
1:A:127:GLU:O	1:A:131:HIS:HB2	2.18	0.44
1:A:101:ASP:OD2	1:A:103:GLU:HB3	2.18	0.44
1:B:104:ARG:NH1	1:B:104:ARG:CG	2.75	0.44
1:B:240:ASP:OD2	1:B:240:ASP:C	2.61	0.44
1:A:146:MET:HE1	1:A:323:PHE:CE1	2.53	0.44
1:A:214:GLN:C	1:A:216:TRP:N	2.76	0.44
1:A:439:ASN:CG	1:A:439:ASN:O	2.61	0.44
1:B:247:ASP:O	1:B:473:ARG:HD3	2.18	0.44
1:B:260:LEU:O	1:B:262:VAL:N	2.50	0.44
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.82	0.44
1:B:72:ASN:ND2	1:B:74:LEU:H	2.17	0.43
1:A:63:ALA:HA	2:A:803:FAD:C4X	2.48	0.43
1:A:91:VAL:HG13	1:A:91:VAL:O	2.17	0.43
1:A:116:GLU:H	1:A:116:GLU:CD	2.23	0.43
1:A:264:PRO:O	1:A:265:GLU:CB	2.65	0.43
1:B:340:LEU:O	1:B:342:ARG:N	2.50	0.43
1:A:218:LYS:HD2	1:A:221:CYS:HB3	1.99	0.43
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.34	0.43
1:B:163:TYR:O	1:B:164:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:O	1:A:312:LYS:HE2	2.18	0.43
1:B:231:SER:O	1:B:232:LYS:C	2.61	0.43
1:B:26:THR:O	1:B:27:LEU:C	2.61	0.43
1:A:289:ILE:HD11	1:A:462:MET:CG	2.47	0.43
1:A:434:ASN:ND2	1:A:435:ILE:H	2.16	0.43
1:B:273:GLU:OE1	1:B:273:GLU:HA	2.19	0.43
1:B:501:THR:O	1:B:504:SER:HB2	2.19	0.43
1:B:266:LYS:HA	1:B:271:ARG:HD3	2.00	0.42
1:B:331:GLU:HB2	1:B:335:GLU:HG3	2.00	0.42
1:B:353:CYS:SG	1:B:400:PRO:HB2	2.59	0.42
1:B:362:ASN:C	1:B:362:ASN:ND2	2.76	0.42
1:A:374:MET:HE1	1:A:376:MET:HE2	2.01	0.42
1:B:311:SER:HA	1:B:362:ASN:HB3	2.01	0.42
1:A:322:GLU:HG3	1:A:342:ARG:NH2	2.35	0.42
1:B:11:VAL:HA	1:B:248:TYR:O	2.19	0.42
1:B:228:ARG:N	1:B:275:GLN:O	2.43	0.42
1:B:504:SER:O	1:B:505:ASP:C	2.62	0.42
1:B:240:ASP:OD2	1:B:242:THR:HG23	2.19	0.42
1:A:54:TYR:CE1	1:A:433:ARG:HB3	2.55	0.42
1:A:108:ASP:O	1:A:109:HIS:C	2.62	0.42
1:B:169:ARG:C	1:B:171:LEU:N	2.77	0.42
1:B:189:PHE:O	1:B:189:PHE:CD1	2.73	0.42
1:B:248:TYR:CE1	1:B:507:LEU:HD21	2.55	0.42
1:B:28:HIS:O	1:B:31:GLY:N	2.52	0.42
1:B:35:CYS:H	1:B:216:TRP:NE1	2.18	0.42
1:B:266:LYS:HA	1:B:271:ARG:NE	2.34	0.42
1:A:199:LEU:HA	1:A:199:LEU:HD23	1.76	0.42
1:B:131:HIS:ND1	1:B:131:HIS:C	2.78	0.42
1:A:8:LYS:HD3	1:A:245:ASN:HD22	1.85	0.41
1:A:356:GLN:N	1:A:356:GLN:CD	2.78	0.41
1:B:30:ASN:HD22	1:B:504:SER:HB3	1.85	0.41
1:B:68:ASP:OD1	1:B:191:HIS:ND1	2.53	0.41
1:B:258:LEU:HD21	1:B:476:PHE:CE2	2.55	0.41
1:A:288:LYS:O	1:A:289:ILE:CG2	2.66	0.41
1:B:423:ASN:C	1:B:425:ALA:H	2.28	0.41
1:A:505:ASP:O	1:A:508:LYS:HB3	2.20	0.41
1:A:194:ARG:HE	1:B:121:GLU:CD	2.28	0.41
1:B:30:ASN:C	1:B:32:ILE:H	2.27	0.41
1:B:63:ALA:HA	2:B:804:FAD:C4X	2.49	0.41
1:B:161:ILE:CG2	1:B:327:VAL:HG21	2.50	0.41
1:A:213:PRO:HB2	1:A:216:TRP:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLU:O	1:A:512:HIS:N	2.54	0.41
1:B:141:PHE:CE1	1:B:187:THR:HG21	2.55	0.41
1:B:227:THR:HG23	1:B:275:GLN:CB	2.48	0.41
1:A:332:ASN:OD1	1:A:334:ASP:HB2	2.20	0.41
1:A:377:GLN:NE2	1:A:377:GLN:N	2.58	0.41
1:B:26:THR:HB	1:B:500:ALA:HB1	2.03	0.41
1:B:414:VAL:HA	1:B:430:PRO:HG2	2.02	0.41
1:B:449:ALA:HB3	3:B:818:HOH:O	2.20	0.41
1:B:502:ARG:O	1:B:503:ILE:C	2.63	0.41
1:B:210:GLN:O	1:B:210:GLN:CD	2.64	0.41
1:B:416:ASP:OD1	1:B:416:ASP:C	2.63	0.41
1:A:238:CYS:HB2	1:A:240:ASP:OD2	2.21	0.41
1:A:388:ARG:HH11	1:A:388:ARG:CB	2.24	0.41
1:A:41:ARG:HH11	1:A:41:ARG:CG	2.27	0.40
1:A:167:LEU:HA	1:A:316:LEU:CD2	2.51	0.40
1:A:470:GLN:HB3	1:A:474:ILE:HB	2.02	0.40
1:B:260:LEU:C	1:B:262:VAL:N	2.78	0.40
1:A:153:ARG:HG2	1:A:154:GLN:N	2.35	0.40
1:A:228:ARG:HD2	1:A:233:ASN:O	2.22	0.40
1:A:229:GLU:C	1:A:231:SER:N	2.78	0.40
1:B:22:LYS:HG2	1:B:493:TRP:NE1	2.36	0.40
1:B:68:ASP:HB3	1:B:192:GLN:HB2	2.02	0.40
1:B:266:LYS:HA	1:B:271:ARG:CD	2.51	0.40
1:A:419:ARG:O	1:A:420:PRO:C	2.64	0.40
1:B:234:VAL:O	1:B:245:ASN:HA	2.21	0.40
1:B:141:PHE:HE1	1:B:188:TYR:CE1	2.39	0.40
1:A:361:VAL:HB	1:A:373:MET:HB3	2.04	0.40
1:A:424:ILE:O	1:A:424:ILE:HG22	2.21	0.40
1:B:72:ASN:O	1:B:76:LEU:HG	2.22	0.40
1:B:164:LEU:N	1:B:165:PRO:HD2	2.36	0.40
1:B:252:THR:HG22	1:B:477:ALA:HB3	2.03	0.40
1:B:278:LEU:HD23	1:B:470:GLN:NE2	2.37	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)
1:A:269:ARG:NH2	1:A:269:ARG:NH2[4_555]	1.89	0.31
1:A:267:ASN:OD1	1:A:267:ASN:OD1[4_555]	1.90	0.30

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	492/513 (96%)	444 (90%)	34 (7%)	14 (3%)	4	2
1	B	479/513 (93%)	406 (85%)	54 (11%)	19 (4%)	2	1
All	All	971/1026 (95%)	850 (88%)	88 (9%)	33 (3%)	3	2

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	265	GLU
1	A	422	GLU
1	A	511	HIS
1	B	200	ASN
1	B	267	ASN
1	B	268	LEU
1	B	422	GLU
1	B	426	ASN
1	B	506	LEU
1	A	420	PRO
1	A	512	HIS
1	B	421	ILE
1	B	423	ASN
1	B	424	ILE
1	B	502	ARG
1	A	200	ASN
1	A	370	ALA
1	A	472	SER
1	B	261	SER
1	B	266	LYS
1	B	472	SER
1	B	507	LEU
1	A	137	SER
1	B	138	ASP

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Mol	Chain	Res	Type
1	B	498	ARG
1	A	215	ASN
1	A	425	ALA
1	B	187	THR
1	B	503	ILE
1	A	241	GLY
1	B	32	ILE
1	A	469	GLY

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	439/454 (97%)	420 (96%)	19 (4%)	26	39
1	B	431/454 (95%)	415 (96%)	16 (4%)	30	45
All	All	870/908 (96%)	835 (96%)	35 (4%)	28	42

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	36	LEU
1	A	118	VAL
1	A	122	MET
1	A	131	HIS
1	A	132	GLN
1	A	134	LEU
1	A	173	LEU
1	A	174	TRP
1	A	201	TYR
1	A	210	GLN
1	A	218	LYS
1	A	221	CYS
1	A	239	GLU
1	A	242	THR

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Mol	Chain	Res	Type
1	A	291	PHE
1	A	377	GLN
1	A	388	ARG
1	A	420	PRO
1	B	22	LYS
1	B	72	ASN
1	B	104	ARG
1	B	122	MET
1	B	177	LEU
1	B	201	TYR
1	B	206	GLN
1	B	214	GLN
1	B	239	GLU
1	B	377	GLN
1	B	380	LEU
1	B	382	ASN
1	B	393	ARG
1	B	412	GLU
1	B	422	GLU
1	B	460	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	80	GLN
1	A	131	HIS
1	A	195	ASN
1	A	206	GLN
1	A	245	ASN
1	A	362	ASN
1	A	377	GLN
1	A	426	ASN
1	A	434	ASN
1	A	513	HIS
1	B	30	ASN
1	B	33	GLN
1	B	72	ASN
1	B	120	ASN
1	B	195	ASN
1	B	259	ASN
1	B	283	GLN

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	356	GLN
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	399	GLN
1	B	434	ASN
1	B	439	ASN
1	B	468	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	A	803	-	58,58,58	1.35	7 (12%)	85,89,89	2.25	10 (11%)
2	FAD	B	804	-	58,58,58	1.38	7 (12%)	85,89,89	2.26	13 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	803	-	-	5/34/50/50	0/6/6/6
2	FAD	B	804	-	-	9/34/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	804	FAD	PA-O3P	4.75	1.64	1.59
2	A	803	FAD	PA-O3P	4.11	1.63	1.59
2	B	804	FAD	C4X-N5	3.99	1.39	1.30
2	A	803	FAD	C4X-N5	3.93	1.39	1.30
2	B	804	FAD	P-O3P	2.76	1.62	1.59
2	A	803	FAD	C5B-C4B	2.58	1.59	1.51
2	A	803	FAD	P-O3P	2.43	1.62	1.59
2	B	804	FAD	C2A-N1A	2.41	1.38	1.33
2	A	803	FAD	C9-C8	2.36	1.42	1.39
2	B	804	FAD	C5B-C4B	2.27	1.58	1.51
2	B	804	FAD	C6-C7	2.23	1.42	1.39
2	B	804	FAD	C9A-C5X	2.21	1.44	1.41
2	A	803	FAD	C2A-N1A	2.19	1.37	1.33
2	A	803	FAD	C9A-C5X	2.03	1.44	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	FAD	O3P-PA-O1A	-12.91	71.87	110.70
2	B	804	FAD	O3P-PA-O1A	-12.10	74.32	110.70
2	B	804	FAD	O2A-PA-O5B	-7.80	72.23	107.57
2	A	803	FAD	O2A-PA-O5B	-7.63	73.00	107.57
2	A	803	FAD	O5B-PA-O1A	6.89	136.26	108.94
2	B	804	FAD	O5B-PA-O1A	6.56	134.94	108.94
2	B	804	FAD	O2A-PA-O1A	-6.44	82.48	112.44
2	B	804	FAD	O2A-PA-O3P	6.00	123.48	107.27
2	A	803	FAD	O2A-PA-O1A	-5.97	84.68	112.44
2	A	803	FAD	O2A-PA-O3P	5.58	122.37	107.27
2	B	804	FAD	O3'-C3'-C4'	-3.18	101.71	108.93
2	B	804	FAD	C9A-C5X-N5	-2.83	119.45	122.45
2	A	803	FAD	C9A-C5X-N5	-2.74	119.55	122.45
2	B	804	FAD	C4'-C3'-C2'	2.72	118.10	113.57
2	A	803	FAD	O3'-C3'-C4'	-2.66	102.90	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	804	FAD	O4B-C1B-C2B	-2.36	101.57	106.62
2	B	804	FAD	C5'-C4'-C3'	-2.34	107.80	112.22
2	A	803	FAD	O4B-C1B-C2B	-2.28	101.73	106.62
2	A	803	FAD	C4X-C10-N10	2.17	119.59	116.48
2	A	803	FAD	N3A-C2A-N1A	-2.12	125.37	128.58
2	B	804	FAD	C4-C4X-N5	2.05	121.04	118.21
2	B	804	FAD	N3A-C2A-N1A	-2.04	125.49	128.58
2	B	804	FAD	C10-C4X-N5	-2.01	120.71	124.81

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	803	FAD	C5B-O5B-PA-O1A
2	B	804	FAD	C5B-O5B-PA-O1A
2	B	804	FAD	C3B-C4B-C5B-O5B
2	A	803	FAD	O4B-C4B-C5B-O5B
2	A	803	FAD	C3B-C4B-C5B-O5B
2	B	804	FAD	O4B-C4B-C5B-O5B
2	B	804	FAD	C2'-C3'-C4'-O4'
2	B	804	FAD	O3'-C3'-C4'-O4'
2	A	803	FAD	PA-O3P-P-O5'
2	B	804	FAD	PA-O3P-P-O5'
2	B	804	FAD	O3'-C3'-C4'-C5'
2	B	804	FAD	C2'-C3'-C4'-C5'
2	B	804	FAD	C4B-C5B-O5B-PA
2	A	803	FAD	C4B-C5B-O5B-PA

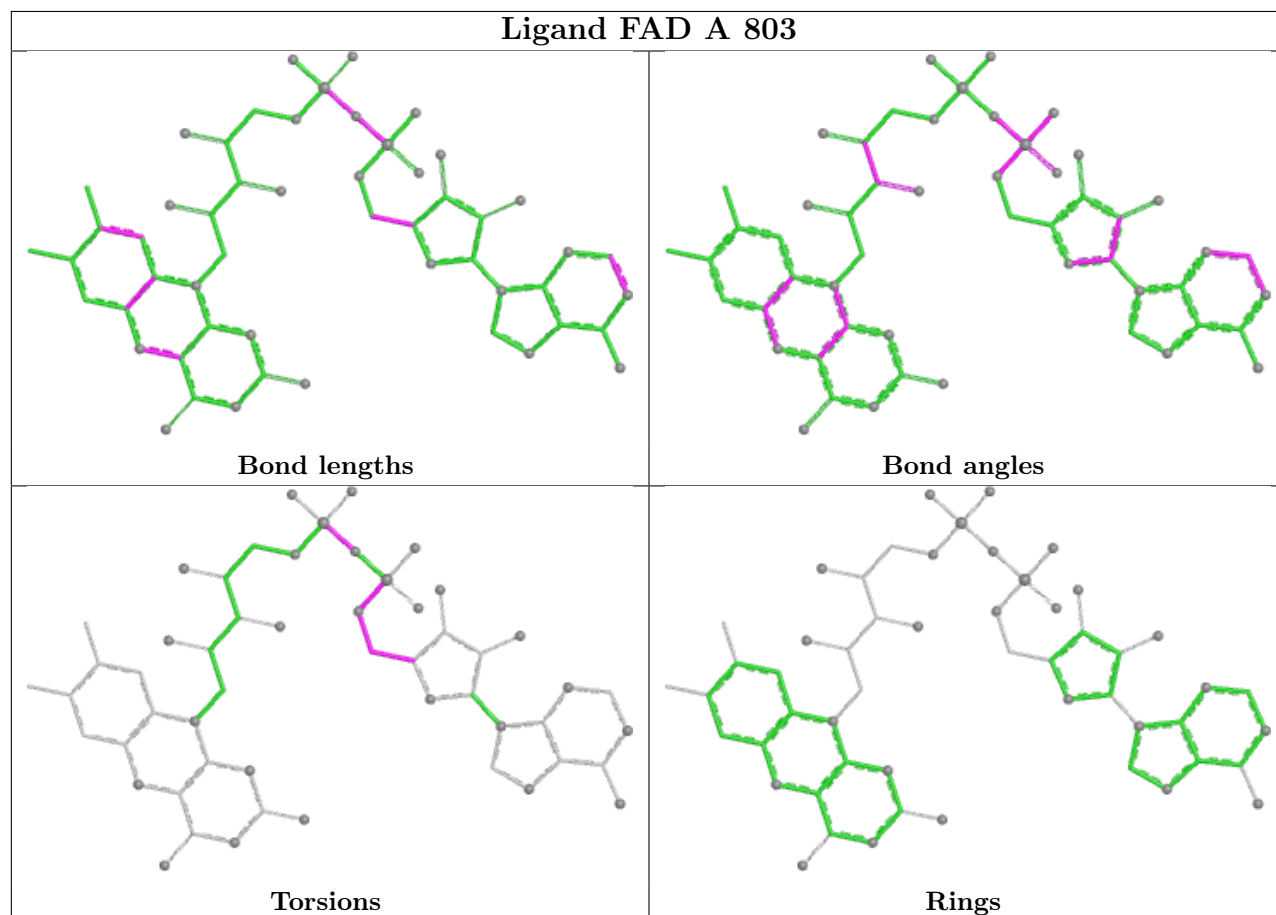
There are no ring outliers.

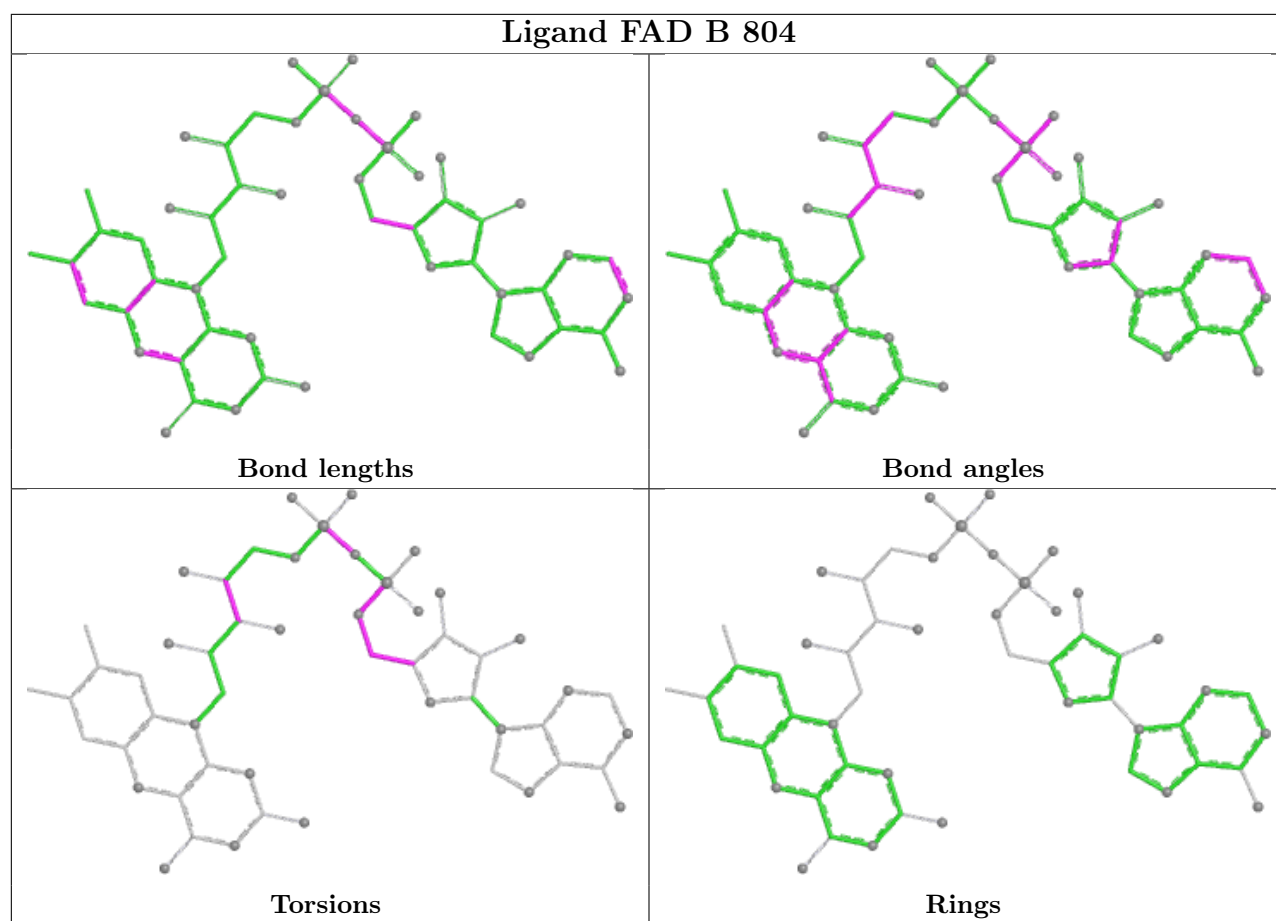
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	FAD	3	0
2	B	804	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/513 (97%)	1.01	67 (13%) 7 8	16, 46, 72, 116	22 (4%)
1	B	487/513 (94%)	1.14	95 (19%) 3 3	20, 47, 78, 93	33 (6%)
All	All	985/1026 (96%)	1.07	162 (16%) 4 5	16, 46, 76, 116	55 (5%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	VAL	8.9
1	B	264	PRO	7.5
1	A	424	ILE	7.5
1	B	509	LEU	6.9
1	B	350	SER	6.3
1	A	509	LEU	6.2
1	B	265	GLU	6.2
1	A	421	ILE	5.6
1	A	230	PRO	5.6
1	A	431	VAL	5.2
1	B	506	LEU	4.9
1	A	512	HIS	4.8
1	B	342	ARG	4.8
1	A	189	PHE	4.7
1	A	511	HIS	4.7
1	B	427	ALA	4.6
1	B	238	CYS	4.5
1	B	454	PHE	4.5
1	B	507	LEU	4.5
1	A	7	ALA	4.4
1	B	229	GLU	4.3
1	A	425	ALA	4.3
1	B	230	PRO	4.2
1	B	289	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	503	ILE	4.1
1	B	236	VAL	4.1
1	A	427	ALA	4.0
1	B	426	ASN	4.0
1	B	382	ASN	3.9
1	A	6	PRO	3.9
1	B	32	ILE	3.9
1	B	424	ILE	3.8
1	B	31	GLY	3.8
1	A	132	GLN	3.7
1	A	342	ARG	3.7
1	B	421	ILE	3.7
1	A	349	THR	3.7
1	B	326	ILE	3.7
1	B	341	GLU	3.7
1	A	233	ASN	3.7
1	B	423	ASN	3.7
1	A	333	LEU	3.6
1	A	136	VAL	3.6
1	A	430	PRO	3.6
1	A	510	GLU	3.6
1	A	420	PRO	3.5
1	B	189	PHE	3.5
1	A	231	SER	3.5
1	B	428	ASN	3.5
1	B	174	TRP	3.4
1	B	420	PRO	3.4
1	A	137	SER	3.4
1	B	331	GLU	3.3
1	B	233	ASN	3.3
1	A	350	SER	3.3
1	B	137	SER	3.3
1	A	190	GLY	3.3
1	A	428	ASN	3.3
1	B	235	THR	3.2
1	B	277	PRO	3.2
1	B	339	MET	3.1
1	B	349	THR	3.1
1	A	426	ASN	3.1
1	B	11	VAL	3.1
1	B	188	TYR	3.0
1	B	322	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	423	ASN	3.0
1	B	476	PHE	3.0
1	B	231	SER	3.0
1	B	267	ASN	3.0
1	B	213	PRO	2.9
1	A	221	CYS	2.9
1	A	337	ASP	2.9
1	B	210	GLN	2.9
1	B	422	GLU	2.9
1	B	8	LYS	2.9
1	A	131	HIS	2.9
1	A	238	CYS	2.9
1	A	138	ASP	2.8
1	A	513	HIS	2.8
1	B	237	ASN	2.8
1	B	340	LEU	2.8
1	A	334	ASP	2.8
1	A	265	GLU	2.8
1	B	228	ARG	2.7
1	A	304	CYS	2.7
1	A	191	HIS	2.7
1	B	243	VAL	2.7
1	A	429	LYS	2.7
1	B	131	HIS	2.7
1	B	455	PRO	2.7
1	B	330	ALA	2.6
1	A	321	ASN	2.6
1	B	249	VAL	2.6
1	B	290	HIS	2.6
1	A	415	ILE	2.6
1	B	467	SER	2.6
1	A	269	ARG	2.5
1	B	508	LYS	2.5
1	A	340	LEU	2.5
1	B	34	ASP	2.5
1	A	422	GLU	2.5
1	B	239	GLU	2.5
1	B	247	ASP	2.4
1	A	174	TRP	2.4
1	A	245	ASN	2.4
1	A	339	MET	2.4
1	B	335	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	242	THR	2.4
1	B	262	VAL	2.4
1	A	264	PRO	2.3
1	A	329	ASN	2.3
1	B	487	GLY	2.3
1	B	227	THR	2.3
1	A	419	ARG	2.3
1	B	474	ILE	2.3
1	B	214	GLN	2.3
1	B	17	GLY	2.2
1	B	12	ILE	2.2
1	A	240	ASP	2.2
1	B	224	LYS	2.2
1	B	288	LYS	2.2
1	B	242	THR	2.2
1	B	425	ALA	2.2
1	B	170	TYR	2.2
1	B	128	LEU	2.2
1	B	234	VAL	2.2
1	B	332	ASN	2.2
1	B	419	ARG	2.2
1	B	216	TRP	2.2
1	B	502	ARG	2.2
1	B	504	SER	2.2
1	B	248	TYR	2.1
1	B	258	LEU	2.1
1	A	237	ASN	2.1
1	A	8	LYS	2.1
1	B	268	LEU	2.1
1	A	395	PHE	2.1
1	A	232	LYS	2.1
1	A	336	LEU	2.1
1	A	341	GLU	2.1
1	B	336	LEU	2.1
1	B	329	ASN	2.1
1	A	133	HIS	2.1
1	A	301	PHE	2.1
1	A	104	ARG	2.1
1	A	366	SER	2.1
1	B	483	MET	2.1
1	B	13	ILE	2.1
1	B	275	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	274	PHE	2.1
1	B	291	PHE	2.1
1	A	263	GLN	2.0
1	A	267	ASN	2.0
1	B	158	ASN	2.0
1	B	337	ASP	2.0
1	B	105	GLY	2.0
1	A	372	PHE	2.0
1	A	58	LYS	2.0
1	A	209	ALA	2.0
1	B	263	GLN	2.0
1	B	245	ASN	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](#)

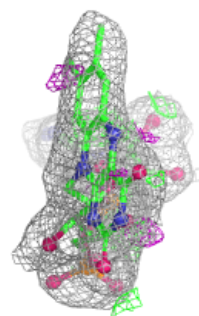
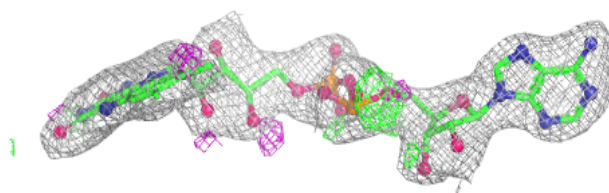
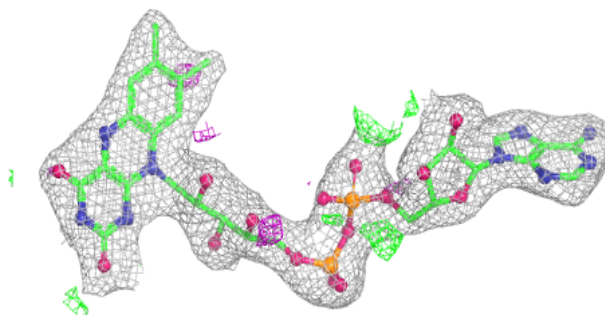
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	803	53/53	0.92	0.10	27,35,45,52	0
2	FAD	B	804	53/53	0.92	0.10	25,41,48,56	0

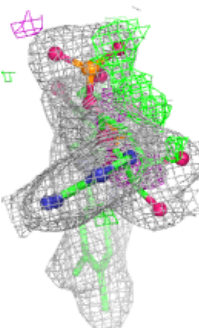
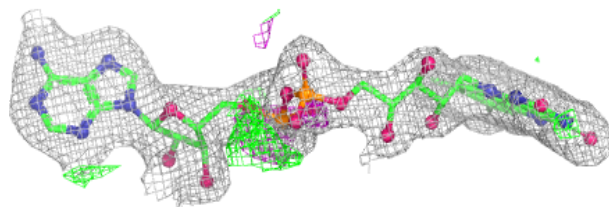
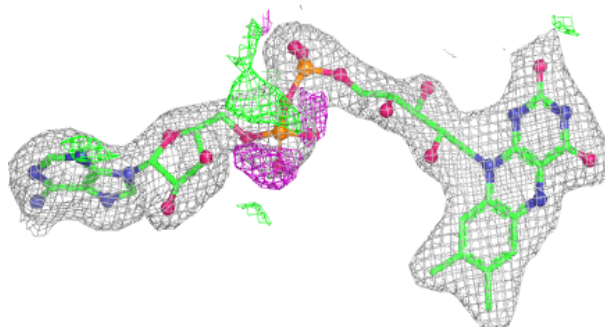
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 803:

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

**Electron density around FAD B 804:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.