



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:44 AM UTC

PDB ID : 5J5Z / pdb_00005j5z
Title : Crystal structure of the D444V disease-causing mutant of the human dihydroipoamide dehydrogenase
Authors : Szabo, E.; Mizsei, R.; Zambo, Z.; Torocsik, B.; Weiss, M.S.; Adam-Vizi, V.; Ambrus, A.
Deposited on : 2016-04-04
Resolution : 1.84 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

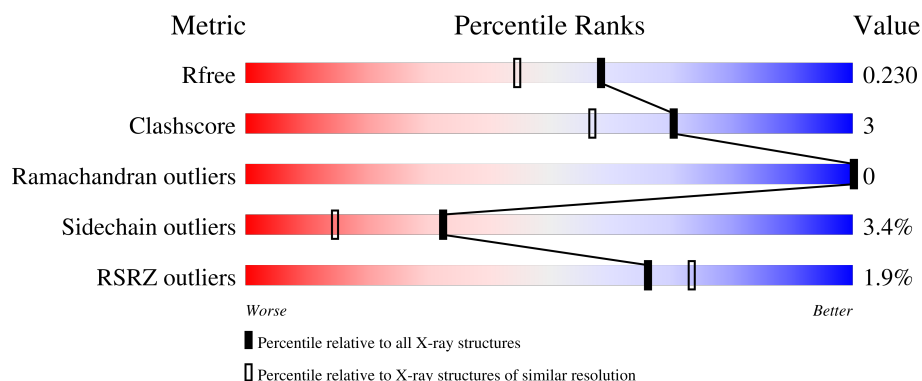
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	496	2% 76% 18% • •
1	B	496	2% 78% 17% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7848 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 Dihydrolipoyl dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	7	0
			3598	2270	624	682	22			
1	B	482	Total	C	N	O	S	0	5	0
			3611	2279	624	686	22			

There are 46 discrepancies between the modelled and reference sequences:

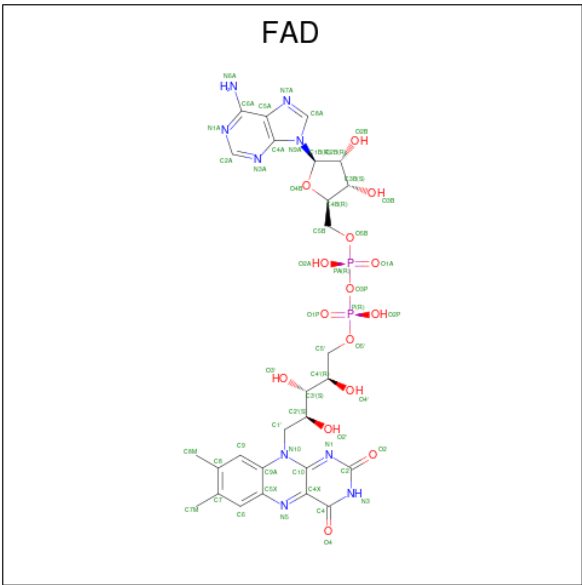
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P09622
A	-20	ALA	-	expression tag	UNP P09622
A	-19	SER	-	expression tag	UNP P09622
A	-18	TRP	-	expression tag	UNP P09622
A	-17	SER	-	expression tag	UNP P09622
A	-16	HIS	-	expression tag	UNP P09622
A	-15	PRO	-	expression tag	UNP P09622
A	-14	GLN	-	expression tag	UNP P09622
A	-13	PHE	-	expression tag	UNP P09622
A	-12	GLU	-	expression tag	UNP P09622
A	-11	LYS	-	expression tag	UNP P09622
A	-10	GLY	-	expression tag	UNP P09622
A	-9	ALA	-	expression tag	UNP P09622
A	-8	LEU	-	expression tag	UNP P09622
A	-7	GLU	-	expression tag	UNP P09622
A	-6	VAL	-	expression tag	UNP P09622
A	-5	LEU	-	expression tag	UNP P09622
A	-4	PHE	-	expression tag	UNP P09622
A	-3	GLN	-	expression tag	UNP P09622
A	-2	GLY	-	expression tag	UNP P09622
A	-1	PRO	-	expression tag	UNP P09622
A	0	GLY	-	expression tag	UNP P09622
A	444	VAL	ASP	engineered mutation	UNP P09622
B	-21	MET	-	initiating methionine	UNP P09622
B	-20	ALA	-	expression tag	UNP P09622

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP P09622
B	-18	TRP	-	expression tag	UNP P09622
B	-17	SER	-	expression tag	UNP P09622
B	-16	HIS	-	expression tag	UNP P09622
B	-15	PRO	-	expression tag	UNP P09622
B	-14	GLN	-	expression tag	UNP P09622
B	-13	PHE	-	expression tag	UNP P09622
B	-12	GLU	-	expression tag	UNP P09622
B	-11	LYS	-	expression tag	UNP P09622
B	-10	GLY	-	expression tag	UNP P09622
B	-9	ALA	-	expression tag	UNP P09622
B	-8	LEU	-	expression tag	UNP P09622
B	-7	GLU	-	expression tag	UNP P09622
B	-6	VAL	-	expression tag	UNP P09622
B	-5	LEU	-	expression tag	UNP P09622
B	-4	PHE	-	expression tag	UNP P09622
B	-3	GLN	-	expression tag	UNP P09622
B	-2	GLY	-	expression tag	UNP P09622
B	-1	PRO	-	expression tag	UNP P09622
B	0	GLY	-	expression tag	UNP P09622
B	444	VAL	ASP	engineered mutation	UNP P09622

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

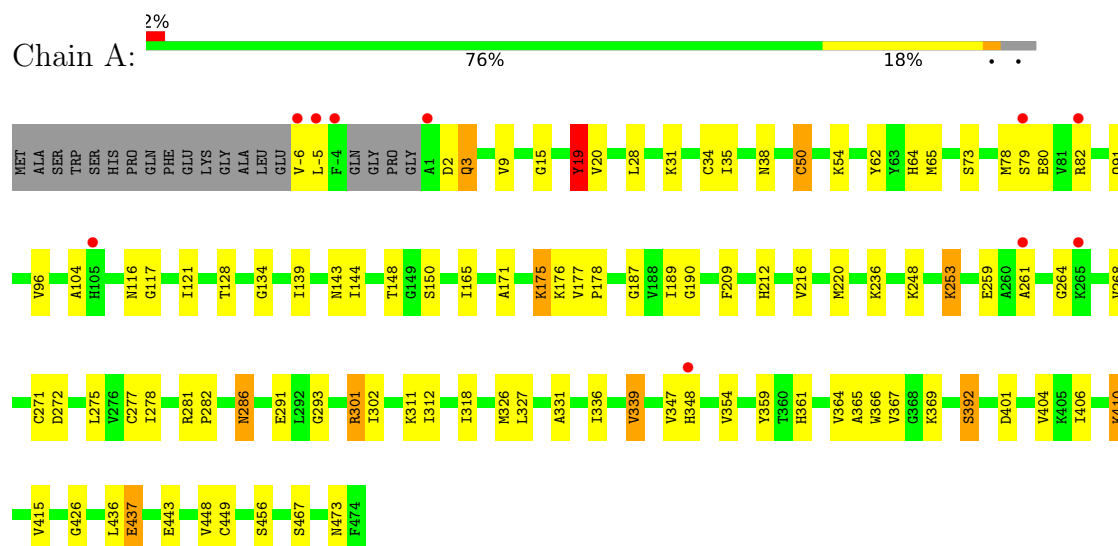
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	276	Total	O	0	4
			279	279		
5	B	219	Total	O	0	1
			220	220		

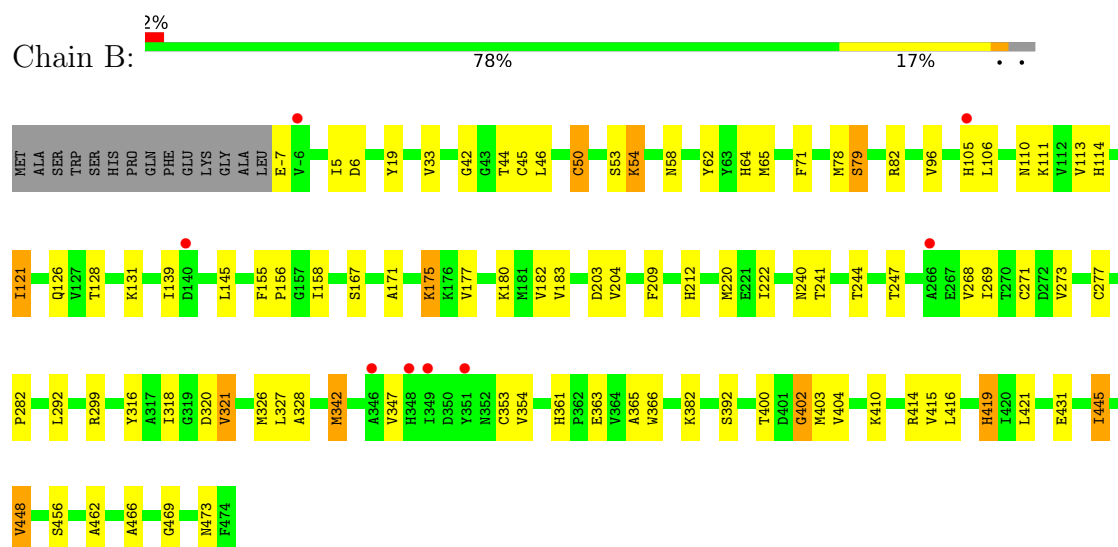
3 Residue-property plots

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: Dihydrolipoyl dehydrogenase, mitochondrial



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.03Å 168.94Å 61.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 1.84 48.38 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.38-1.84) 98.2 (48.38-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.181 , 0.226 0.189 , 0.230	Depositor DCC
R_{free} test set	2101 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.6	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	0.97	EDS
Total number of atoms	7848	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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, GOL, PO4

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	1.83	62/3661 (1.7%)	1.41	11/4941 (0.2%)
1	B	1.74	51/3679 (1.4%)	1.40	23/4968 (0.5%)
All	All	1.79	113/7340 (1.5%)	1.40	34/9909 (0.3%)

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	ILE	CA-C	9.58	1.60	1.53
1	B	128	THR	CA-CB	9.29	1.66	1.53
1	A	369	LYS	C-O	9.25	1.34	1.23
1	A	437	GLU	C-O	-8.87	1.13	1.24
1	B	171	ALA	N-CA	8.43	1.56	1.46
1	B	299	ARG	C-O	-8.33	1.12	1.24
1	A	187	GLY	C-O	-8.32	1.15	1.23
1	B	361	HIS	C-O	-8.32	1.18	1.25
1	A	354	VAL	N-CA	-8.18	1.40	1.46
1	A	175	LYS	C-O	-7.85	1.13	1.24
1	B	156	PRO	N-CA	7.82	1.56	1.47
1	B	320	ASP	CA-C	7.70	1.63	1.52
1	B	139	ILE	CA-C	-7.58	1.42	1.52
1	B	419	HIS	CA-C	-7.32	1.43	1.52
1	A	19	TYR	C-O	7.26	1.32	1.24
1	A	268	VAL	C-O	-7.25	1.16	1.24
1	A	271	CYS	C-O	7.12	1.32	1.23
1	A	275	LEU	CA-C	-7.04	1.44	1.52
1	B	121	ILE	CA-C	7.00	1.60	1.53
1	A	302	ILE	N-CA	-6.99	1.41	1.46
1	B	448	VAL	CA-CB	6.95	1.63	1.54
1	B	365	ALA	CA-C	-6.94	1.43	1.52
1	A	50	CYS	N-CA	6.86	1.54	1.46
1	A	177	VAL	C-O	-6.86	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	HIS	CA-C	6.84	1.61	1.52
1	A	9	VAL	CA-CB	6.73	1.63	1.54
1	B	204	VAL	C-O	-6.69	1.17	1.24
1	A	361	HIS	C-O	-6.50	1.19	1.25
1	B	456	SER	CB-OG	6.50	1.55	1.42
1	A	73	SER	C-O	-6.42	1.16	1.24
1	A	410	LYS	N-CA	6.41	1.54	1.46
1	B	42	GLY	N-CA	6.39	1.53	1.45
1	A	117	GLY	C-O	6.36	1.31	1.24
1	A	448	VAL	CA-CB	6.33	1.60	1.54
1	B	45	CYS	C-O	6.26	1.31	1.24
1	B	382	LYS	N-CA	6.25	1.53	1.45
1	A	449	CYS	CA-CB	6.25	1.60	1.52
1	B	50	CYS	N-CA	6.25	1.53	1.46
1	A	291	GLU	CD-OE1	6.17	1.37	1.25
1	A	148	THR	N-CA	6.09	1.54	1.46
1	A	443	GLU	N-CA	6.06	1.53	1.46
1	B	110	ASN	CA-C	6.04	1.61	1.52
1	A	2	ASP	CA-C	6.02	1.60	1.52
1	B	363	GLU	CA-C	-6.00	1.44	1.53
1	A	64	HIS	CA-C	5.97	1.60	1.52
1	A	15	GLY	N-CA	5.94	1.52	1.44
1	B	410	LYS	CA-C	-5.91	1.45	1.52
1	B	421	LEU	N-CA	-5.91	1.39	1.46
1	A	437	GLU	CD-OE1	5.89	1.36	1.25
1	A	34	CYS	C-O	-5.89	1.17	1.24
1	A	38	ASN	C-O	-5.88	1.16	1.23
1	B	347	VAL	CA-C	5.87	1.58	1.53
1	A	128	THR	CA-CB	5.86	1.61	1.53
1	B	327	LEU	CA-C	-5.85	1.45	1.52
1	B	392	SER	C-O	-5.85	1.17	1.24
1	A	116	ASN	CA-C	-5.79	1.45	1.53
1	A	406	ILE	C-O	5.78	1.30	1.24
1	B	404	VAL	CA-C	-5.77	1.45	1.52
1	B	244	THR	N-CA	5.77	1.53	1.46
1	A	406	ILE	N-CA	-5.72	1.39	1.46
1	B	415	VAL	CA-C	5.71	1.59	1.52
1	A	331	ALA	CA-C	-5.71	1.45	1.52
1	A	178	PRO	CA-C	-5.70	1.45	1.52
1	B	106	LEU	CA-C	5.67	1.60	1.52
1	A	347	VAL	C-O	-5.65	1.18	1.24
1	B	416	LEU	N-CA	5.64	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	ALA	N-CA	5.64	1.53	1.46
1	A	121	ILE	C-O	-5.63	1.17	1.24
1	B	469	GLY	C-O	-5.59	1.16	1.24
1	A	367	VAL	C-O	5.56	1.30	1.23
1	A	278	ILE	C-O	-5.55	1.18	1.24
1	A	327	LEU	CA-C	-5.54	1.46	1.52
1	B	327	LEU	N-CA	5.51	1.52	1.45
1	B	244	THR	C-O	-5.51	1.16	1.24
1	A	366	TRP	N-CA	-5.50	1.39	1.46
1	A	361	HIS	N-CA	5.49	1.52	1.46
1	B	96	VAL	N-CA	5.49	1.52	1.46
1	A	364	VAL	CA-C	-5.48	1.46	1.52
1	A	3	GLN	CA-C	5.45	1.58	1.52
1	B	114	HIS	CA-C	5.44	1.59	1.52
1	A	467	SER	C-O	-5.41	1.17	1.24
1	A	456	SER	CB-OG	5.40	1.52	1.42
1	A	91	GLN	CA-C	5.38	1.59	1.52
1	A	401	ASP	CG-OD2	5.38	1.35	1.25
1	A	96	VAL	CA-CB	-5.36	1.48	1.54
1	B	342	MET	C-O	-5.35	1.17	1.24
1	A	176	LYS	N-CA	-5.33	1.39	1.45
1	B	145	LEU	CA-C	-5.30	1.46	1.52
1	B	53	SER	CA-C	5.29	1.59	1.52
1	A	150	SER	C-O	-5.26	1.17	1.23
1	B	111	LYS	N-CA	5.25	1.54	1.46
1	A	365	ALA	CA-C	-5.25	1.45	1.52
1	B	171	ALA	C-O	5.24	1.30	1.24
1	A	436	LEU	N-CA	5.23	1.52	1.46
1	B	183	VAL	CA-CB	5.23	1.60	1.54
1	A	171	ALA	N-CA	5.23	1.52	1.46
1	A	339	VAL	CA-CB	-5.22	1.47	1.54
1	B	126	GLN	N-CA	-5.22	1.39	1.46
1	B	421	LEU	CA-C	-5.22	1.46	1.52
1	A	104	ALA	N-CA	5.21	1.52	1.46
1	A	404	VAL	N-CA	-5.19	1.39	1.46
1	A	144	ILE	C-O	-5.11	1.18	1.24
1	A	253	LYS	C-O	5.08	1.30	1.23
1	B	175	LYS	C-O	-5.06	1.17	1.24
1	B	82	ARG	N-CA	5.05	1.52	1.45
1	B	273	VAL	C-O	5.05	1.29	1.24
1	B	167	SER	CA-C	5.04	1.59	1.53
1	B	241	THR	N-CA	-5.04	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	VAL	N-CA	-5.03	1.40	1.46
1	A	143	ASN	CG-ND2	-5.03	1.22	1.33
1	B	44	THR	N-CA	-5.01	1.40	1.46
1	A	473	ASN	CG-ND2	-5.00	1.22	1.33
1	B	180	LYS	C-O	5.00	1.30	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	ASN	N-CA-C	8.35	123.03	113.02
1	B	347	VAL	N-CA-C	7.86	118.28	106.42
1	A	359	TYR	N-CA-C	7.54	120.97	112.97
1	B	392	SER	N-CA-C	7.15	119.07	111.28
1	A	392	SER	N-CA-C	7.11	118.68	111.07
1	B	58	ASN	N-CA-C	-6.97	103.61	111.14
1	A	286	ASN	N-CA-C	6.88	121.05	112.24
1	B	177	VAL	N-CA-C	-6.57	102.52	108.95
1	A	190	GLY	N-CA-C	6.53	120.56	112.73
1	B	400	THR	N-CA-C	6.52	120.89	112.41
1	B	44	THR	N-CA-C	-6.38	104.25	111.14
1	B	46	LEU	N-CA-C	6.36	118.22	111.28
1	B	402	GLY	N-CA-C	6.20	122.64	112.84
1	B	462	ALA	N-CA-C	-6.16	104.67	111.82
1	A	415	VAL	CA-C-O	-5.88	114.31	121.13
1	A	336	ILE	CB-CA-C	-5.76	104.47	112.02
1	B	318	ILE	CB-CG1-CD1	5.73	125.83	113.80
1	B	354	VAL	N-CA-C	5.66	112.71	107.56
1	B	177	VAL	CA-C-N	-5.57	114.23	120.14
1	B	177	VAL	C-N-CA	-5.57	114.23	120.14
1	A	473	ASN	N-CA-C	5.52	119.64	113.02
1	A	134	GLY	CA-C-N	5.44	125.14	119.92
1	A	134	GLY	C-N-CA	5.44	125.14	119.92
1	A	318	ILE	CB-CG1-CD1	5.39	125.13	113.80
1	B	366	TRP	N-CA-C	5.34	116.96	108.79
1	B	431	GLU	N-CA-C	-5.33	105.55	111.36
1	B	414	ARG	CG-CD-NE	-5.32	100.29	112.00
1	B	328	ALA	N-CA-C	5.31	116.76	111.07
1	B	71	PHE	N-CA-C	5.27	117.02	111.28
1	B	268	VAL	N-CA-C	-5.16	100.69	108.12
1	B	204	VAL	N-CA-C	5.14	115.52	108.12
1	B	131	LYS	N-CA-C	5.08	117.96	110.59
1	B	54	LYS	CB-CG-CD	5.06	122.94	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	GLY	N-CA-C	5.05	118.36	112.50

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	3598	0	3660	28	0
1	B	3611	0	3670	20	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	24	0	32	2	0
5	A	279	0	0	8	0
5	B	220	0	0	3	0
All	All	7848	0	7424	48	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 3.

All (48) 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:65[B]:MET:HA	1:A:65[B]:MET:HE2	1.49	0.94
1:A:259:GLU:HB2	1:A:264:GLY:O	1.82	0.80
1:A:82[B]:ARG:HG2	1:A:82[B]:ARG:HH21	1.51	0.75
1:A:212:HIS:CG	1:A:220:MET:HE1	2.24	0.73
1:B:105[B]:HIS:CD2	5:B:611:HOH:O	2.48	0.67
1:A:82[B]:ARG:HH21	1:A:82[B]:ARG:CG	2.07	0.66
1:B:155:PHE:CD1	1:B:158:ILE:HD12	2.31	0.66
1:B:402:GLY:HA2	1:B:403[B]:MET:HE3	1.77	0.66
1:A:326[B]:MET:HE1	5:A:824:HOH:O	2.00	0.62
1:A:437:GLU:OE1	5:A:602:HOH:O	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:GOL:O2	5:A:601:HOH:O	2.16	0.60
1:A:65[B]:MET:HE2	1:A:65[B]:MET:CA	2.30	0.58
1:B:445:ILE:HD13	1:B:445:ILE:N	2.21	0.55
1:B:403[B]:MET:HE1	5:B:812:HOH:O	2.05	0.55
1:A:165:ILE:HD12	1:A:248:LYS:HE2	1.90	0.53
1:A:348[B]:HIS:HE1	5:A:848:HOH:O	1.93	0.52
1:A:82[B]:ARG:CG	1:A:82[B]:ARG:NH2	2.70	0.52
1:A:79:SER:OG	1:B:79:SER:OG	2.25	0.51
1:B:62:TYR:HD1	1:B:65:MET:HE2	1.75	0.51
1:A:437:GLU:HG2	1:B:448:VAL:HG22	1.93	0.50
1:A:392:SER:HB2	5:A:611:HOH:O	2.11	0.49
1:B:121:ILE:HG21	1:B:292:LEU:HD11	1.95	0.49
1:B:155:PHE:CE1	1:B:158:ILE:HD12	2.47	0.49
1:A:281:ARG:HB2	1:A:282:PRO:HD2	1.94	0.49
5:A:753[B]:HOH:O	1:B:353:CYS:O	2.20	0.48
1:B:33:VAL:HG22	1:B:113:VAL:HB	1.96	0.48
4:A:503[A]:GOL:H12	5:A:642:HOH:O	2.13	0.48
1:A:209:PHE:CE1	1:A:261:ALA:HB1	2.48	0.48
1:A:65[B]:MET:HA	1:A:65[B]:MET:CE	2.33	0.46
1:A:236:LYS:HB2	1:A:236:LYS:HE2	1.77	0.45
1:A:253:LYS:HE2	1:A:272:ASP:OD1	2.17	0.45
1:A:286:ASN:HB3	5:A:663:HOH:O	2.17	0.45
1:B:326[B]:MET:HE1	5:B:738:HOH:O	2.16	0.45
1:A:282:PRO:HG3	1:A:301:ARG:HG3	1.99	0.44
1:A:28:LEU:HD12	1:A:339:VAL:HG12	2.00	0.44
1:B:282:PRO:HB3	1:B:321:VAL:HA	2.01	0.43
1:A:62:TYR:CD1	1:A:65[A]:MET:CE	3.01	0.43
1:A:293:GLY:O	1:A:311:LYS:HE2	2.17	0.43
1:A:189:ILE:HG22	1:A:277[B]:CYS:SG	2.58	0.43
1:B:316:TYR:CD1	1:B:342:MET:HE2	2.54	0.43
1:B:203:ASP:OD1	1:B:203:ASP:C	2.61	0.43
1:A:78:MET:HE3	1:A:78:MET:HB2	1.82	0.41
1:B:212:HIS:CG	1:B:220:MET:HE1	2.54	0.41
1:A:19:TYR:CD1	1:A:19:TYR:C	2.98	0.41
1:B:182:VAL:HG23	1:B:271:CYS:HB3	2.03	0.41
1:B:222:ILE:HG13	1:B:419:HIS:HB3	2.03	0.41
1:B:209:PHE:O	1:B:240:ASN:HA	2.21	0.40
1:A:35:ILE:HD11	1:A:139:ILE:HD13	2.04	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	480/496 (97%)	468 (98%)	12 (2%)	0	100	100
1	B	485/496 (98%)	471 (97%)	14 (3%)	0	100	100
All	All	965/992 (97%)	939 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	383/390 (98%)	371 (97%)	12 (3%)	35	18
1	B	384/390 (98%)	369 (96%)	15 (4%)	28	11
All	All	767/780 (98%)	740 (96%)	27 (4%)	32	14

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	VAL
1	A	-5	LEU
1	A	3	GLN
1	A	19	TYR
1	A	31	LYS
1	A	50	CYS
1	A	54	LYS
1	A	80	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	175	LYS
1	A	216	VAL
1	A	301	ARG
1	A	410	LYS
1	B	-7	GLU
1	B	5	ILE
1	B	6	ASP
1	B	19	TYR
1	B	50	CYS
1	B	54	LYS
1	B	78	MET
1	B	79	SER
1	B	175	LYS
1	B	247	THR
1	B	269	ILE
1	B	277[A]	CYS
1	B	277[B]	CYS
1	B	321	VAL
1	B	445	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	143	ASN
1	A	227	GLN
1	A	231	GLN
1	A	240	ASN
1	A	286	ASN
1	A	397	ASN
1	A	409	GLN
1	A	473	ASN
1	B	64	HIS
1	B	227	GLN
1	B	231	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
4	GOL	A	504	-	5,5,5	0.42	0	5,5,5	0.33	0
3	PO4	A	502	-	4,4,4	1.28	0	6,6,6	1.12	0
3	PO4	B	502	-	4,4,4	0.46	0	6,6,6	1.22	1 (16%)
4	GOL	A	505	-	5,5,5	1.15	0	5,5,5	0.83	0
2	FAD	A	501	-	58,58,58	2.20	17 (29%)	85,89,89	1.95	23 (27%)
4	GOL	A	503[B]	-	5,5,5	0.70	0	5,5,5	1.60	1 (20%)
4	GOL	A	503[A]	-	5,5,5	0.50	0	5,5,5	1.96	1 (20%)
2	FAD	B	501	-	58,58,58	2.05	18 (31%)	85,89,89	2.11	24 (28%)

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
4	GOL	A	504	-	-	4/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
2	FAD	A	501	-	-	2/34/50/50	0/6/6/6
4	GOL	A	503[B]	-	-	4/4/4/4	-
4	GOL	A	503[A]	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	501	-	-	2/34/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C8A-N7A	7.47	1.46	1.31
2	A	501	FAD	P-O3P	6.78	1.66	1.59
2	A	501	FAD	C9A-C5X	5.51	1.50	1.41
2	B	501	FAD	C9A-C5X	5.30	1.49	1.41
2	B	501	FAD	O4-C4	4.72	1.32	1.23
2	B	501	FAD	C8A-N7A	4.59	1.40	1.31
2	B	501	FAD	C10-N10	4.44	1.46	1.37
2	B	501	FAD	C5A-C4A	4.25	1.46	1.39
2	B	501	FAD	C2A-N3A	3.65	1.40	1.33
2	A	501	FAD	C5A-N7A	-3.57	1.32	1.39
2	B	501	FAD	P-O3P	3.39	1.63	1.59
2	A	501	FAD	C5A-C6A	3.37	1.50	1.41
2	A	501	FAD	PA-O3P	-3.28	1.56	1.59
2	B	501	FAD	C4X-N5	3.22	1.37	1.30
2	A	501	FAD	C1'-C2'	-3.15	1.48	1.52
2	A	501	FAD	C9-C8	-3.08	1.35	1.39
2	A	501	FAD	C10-N10	2.90	1.43	1.37
2	A	501	FAD	C2A-N1A	2.83	1.39	1.33
2	B	501	FAD	C6-C5X	-2.67	1.35	1.40
2	A	501	FAD	C5'-C4'	-2.55	1.48	1.51
2	B	501	FAD	C9-C8	-2.51	1.36	1.39
2	A	501	FAD	P-O2P	-2.49	1.43	1.55
2	B	501	FAD	C5A-C6A	2.36	1.47	1.41
2	A	501	FAD	C9A-N10	-2.27	1.37	1.41
2	A	501	FAD	C4X-C4	2.27	1.52	1.44
2	B	501	FAD	C2-N3	-2.21	1.34	1.39
2	B	501	FAD	C4-N3	-2.17	1.34	1.38
2	A	501	FAD	C4-N3	-2.16	1.34	1.38
2	B	501	FAD	PA-O1A	2.16	1.58	1.50
2	A	501	FAD	O4B-C1B	2.16	1.47	1.42
2	B	501	FAD	C4X-C4	2.14	1.52	1.44
2	B	501	FAD	C2-N1	2.13	1.41	1.36
2	B	501	FAD	O4B-C1B	2.06	1.46	1.42
2	B	501	FAD	C6-C7	2.06	1.42	1.39
2	A	501	FAD	C2-N3	-2.02	1.34	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C5X-C9A-N10	6.48	123.83	117.97
2	B	501	FAD	O4-C4-N3	5.51	130.48	120.11
2	A	501	FAD	N9A-C8A-N7A	-5.29	106.43	113.94
2	B	501	FAD	O4-C4-C4X	-4.92	113.56	126.53
2	A	501	FAD	N6A-C6A-N1A	4.47	128.34	118.38
2	A	501	FAD	C5X-C9A-N10	4.36	121.91	117.97
2	B	501	FAD	O4B-C1B-N9A	-4.23	99.96	108.09
2	A	501	FAD	C5A-C4A-N3A	-4.19	120.94	126.72
2	B	501	FAD	C4A-N9A-C8A	4.19	110.14	105.74
2	A	501	FAD	C4A-N9A-C8A	4.14	110.09	105.74
2	B	501	FAD	C9A-C5X-N5	-4.06	118.15	122.45
2	A	501	FAD	O4-C4-C4X	-3.87	116.31	126.53
2	A	501	FAD	C5A-C6A-N6A	-3.86	113.73	123.29
2	B	501	FAD	O2-C2-N1	-3.85	115.40	121.80
2	B	501	FAD	C5A-C6A-N6A	-3.82	113.83	123.29
2	B	501	FAD	C1'-N10-C9A	3.81	128.03	120.63
2	B	501	FAD	N6A-C6A-N1A	3.77	126.77	118.38
2	A	501	FAD	C9A-C5X-N5	-3.77	118.46	122.45
2	A	501	FAD	C1'-N10-C9A	3.73	127.88	120.63
2	B	501	FAD	C5A-C4A-N3A	-3.63	121.72	126.72
2	B	501	FAD	N3A-C4A-N9A	3.61	133.31	127.17
4	A	503[A]	GOL	C3-C2-C1	-3.31	99.64	111.80
2	A	501	FAD	O4B-C1B-N9A	-3.24	101.87	108.09
2	B	501	FAD	O2-C2-N3	3.18	124.68	118.58
2	B	501	FAD	N9A-C8A-N7A	-3.10	109.54	113.94
2	A	501	FAD	O4-C4-N3	3.00	125.75	120.11
2	B	501	FAD	C4B-O4B-C1B	-2.96	102.94	109.47
2	B	501	FAD	C9A-N10-C10	-2.89	116.34	120.75
2	A	501	FAD	O5B-PA-O1A	-2.86	97.58	108.94
2	A	501	FAD	C4A-N9A-C1B	-2.86	119.94	126.63
2	A	501	FAD	N3A-C4A-N9A	2.77	131.87	127.17
2	B	501	FAD	C9-C9A-C5X	-2.74	115.19	120.03
2	A	501	FAD	O3'-C3'-C2'	-2.70	102.80	108.93
2	B	501	FAD	N3A-C2A-N1A	-2.64	124.59	128.58
3	B	502	PO4	O4-P-O2	2.42	115.45	107.91
2	B	501	FAD	O5B-PA-O1A	-2.37	99.53	108.94
2	B	501	FAD	C9A-C9-C8	2.34	123.93	119.22
2	A	501	FAD	O2P-P-O3P	-2.30	101.05	107.27
2	B	501	FAD	C4A-N9A-C1B	-2.30	121.25	126.63
2	B	501	FAD	C2A-N3A-C4A	2.17	117.13	111.83
4	A	503[B]	GOL	C3-C2-C1	-2.13	104.00	111.80
2	A	501	FAD	O3P-P-O1P	2.12	117.10	110.70
2	A	501	FAD	O2A-PA-O5B	2.12	117.17	107.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	O4B-C1B-C2B	-2.11	102.10	106.62
2	A	501	FAD	C5A-N7A-C8A	2.10	106.75	103.45
2	A	501	FAD	C9-C8-C7	2.09	122.75	119.69
2	A	501	FAD	C2B-C1B-N9A	2.05	118.40	113.30
2	B	501	FAD	C10-N1-C2	2.05	121.28	116.85
2	B	501	FAD	O4'-C4'-C5'	2.02	114.44	109.99
2	A	501	FAD	O4B-C4B-C3B	2.00	109.12	105.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503[B]	GOL	O1-C1-C2-O2
4	A	503[B]	GOL	O1-C1-C2-C3
4	A	503[B]	GOL	C1-C2-C3-O3
4	A	504	GOL	O1-C1-C2-C3
4	A	504	GOL	O1-C1-C2-O2
4	A	503[A]	GOL	O1-C1-C2-C3
4	A	504	GOL	C1-C2-C3-O3
4	A	505	GOL	C1-C2-C3-O3
4	A	503[B]	GOL	O2-C2-C3-O3
4	A	503[A]	GOL	O1-C1-C2-O2
4	A	505	GOL	O2-C2-C3-O3
2	A	501	FAD	O4B-C4B-C5B-O5B
4	A	504	GOL	O2-C2-C3-O3
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	O4B-C4B-C5B-O5B

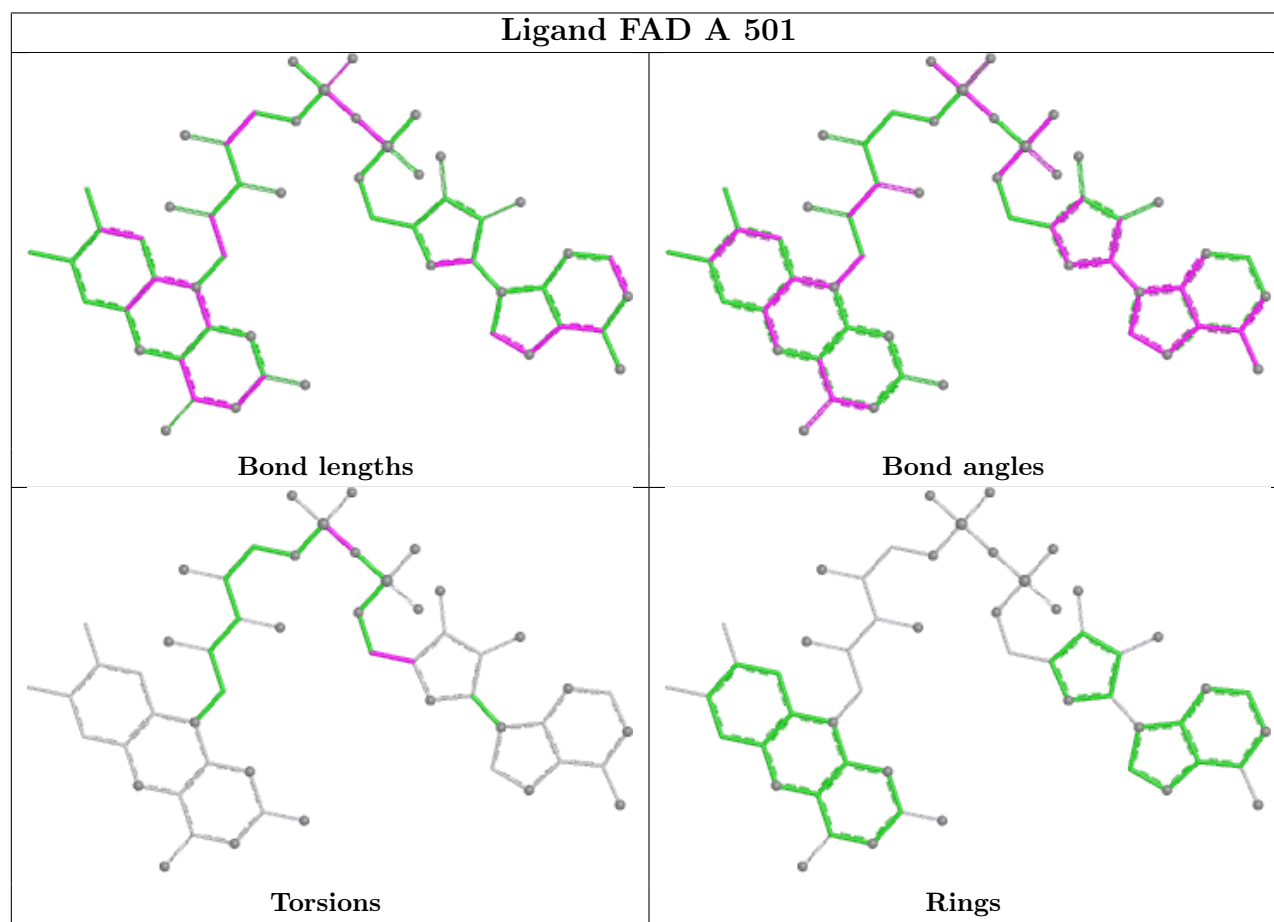
There are no ring outliers.

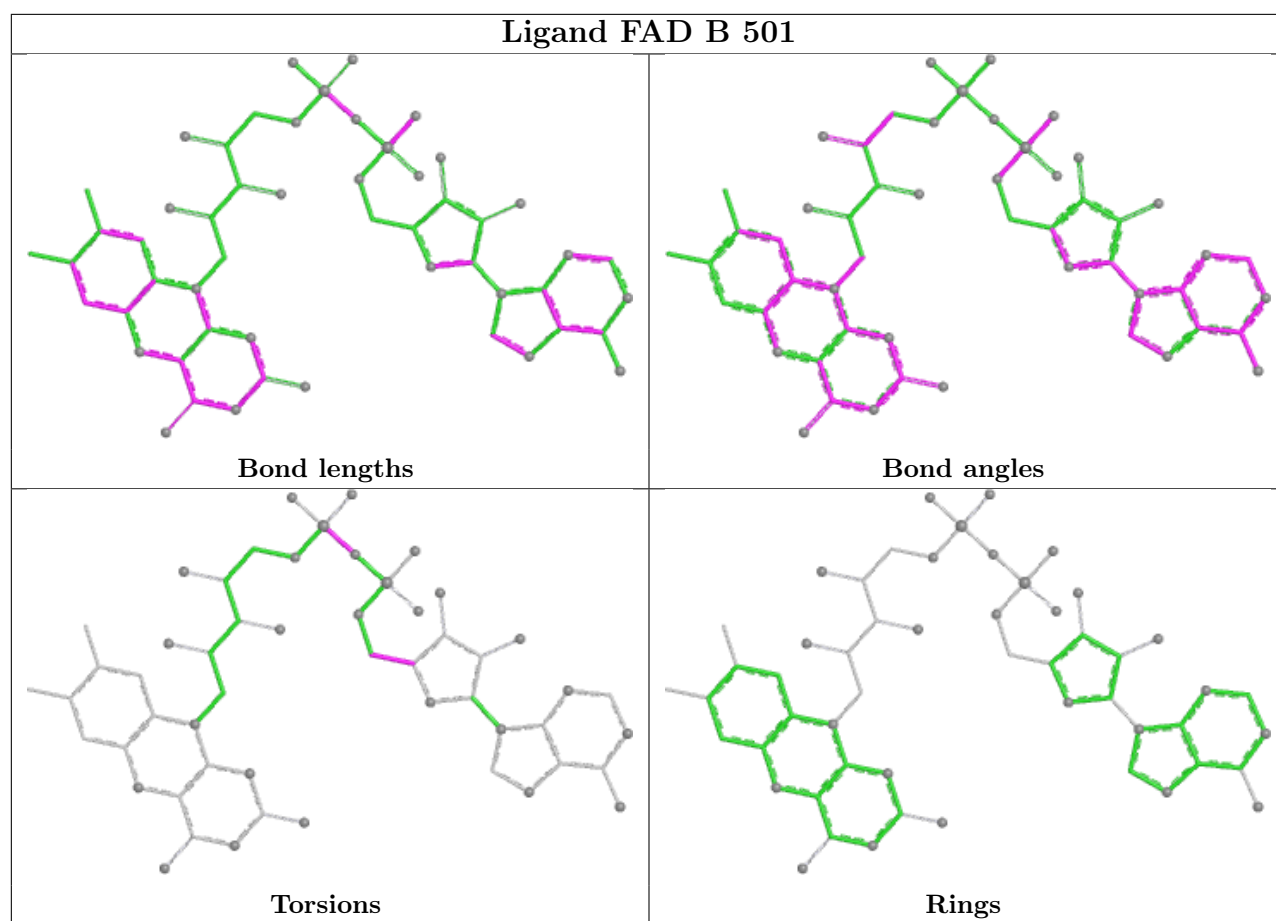
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	GOL	1	0
4	A	503[A]	GOL	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	477/496 (96%)	-0.10	10 (2%) 63 71	13, 34, 56, 88	7 (1%)
1	B	482/496 (97%)	0.04	8 (1%) 69 77	15, 38, 65, 85	5 (1%)
All	All	959/992 (96%)	-0.03	18 (1%) 66 73	13, 36, 62, 88	12 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-6	VAL	6.2
1	A	-5	LEU	5.3
1	B	348[A]	HIS	5.2
1	B	346	ALA	4.0
1	A	105[A]	HIS	3.6
1	B	105[A]	HIS	3.5
1	A	-4	PHE	3.2
1	A	261	ALA	3.1
1	B	351	TYR	2.7
1	A	82[A]	ARG	2.6
1	A	265	LYS	2.4
1	B	266	ALA	2.3
1	A	1	ALA	2.2
1	B	140	ASP	2.2
1	B	349	ILE	2.2
1	A	348[A]	HIS	2.1
1	A	79	SER	2.1
1	B	-6	VAL	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](#)

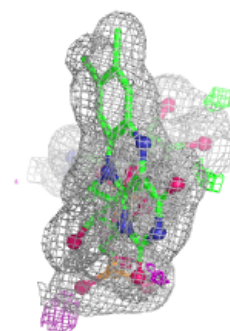
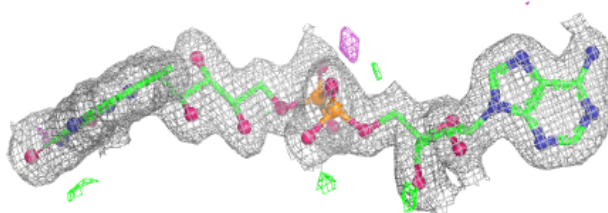
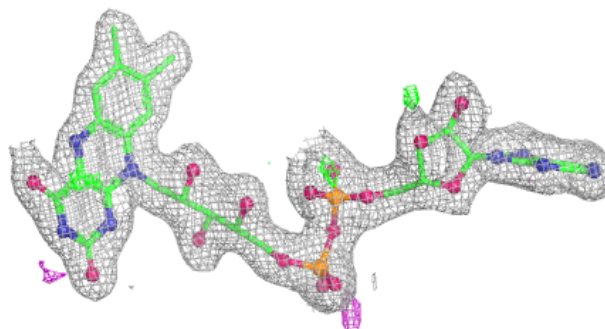
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	505	6/6	0.77	0.20	40,44,51,52	6
3	PO4	B	502	5/5	0.81	0.10	75,77,81,87	0
4	GOL	A	503[B]	6/6	0.82	0.14	26,36,37,37	6
4	GOL	A	503[A]	6/6	0.82	0.14	26,31,33,33	6
4	GOL	A	504	6/6	0.84	0.14	73,86,90,94	0
3	PO4	A	502	5/5	0.84	0.12	49,59,75,84	0
2	FAD	B	501	53/53	0.98	0.04	25,27,29,30	0
2	FAD	A	501	53/53	0.99	0.04	22,24,25,26	0

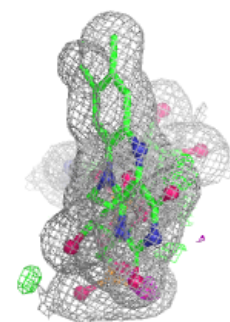
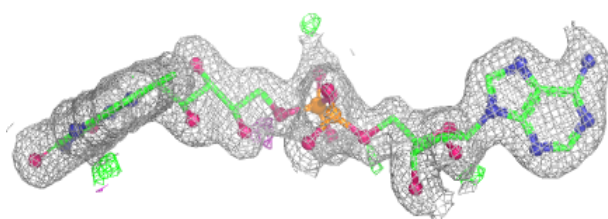
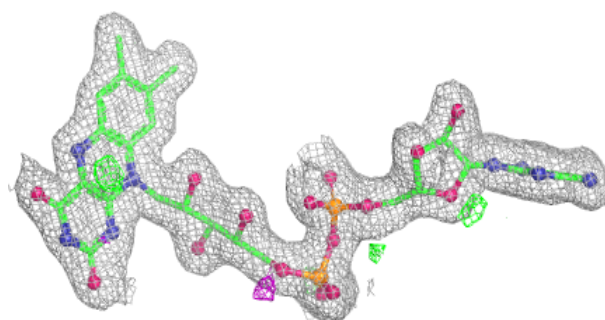
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 501:

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

**Electron density around FAD A 501:**

$2mF_o-DF_c$ (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.