



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:20 PM UTC

PDB ID : 1E0Y / pdb_00001e0y
Title : Structure of the D170S/T457E double mutant of vanillyl-alcohol oxidase
Authors : Van Der heuvel, R.H.H.; Van Berkel, W.J.H.; Mattevi, A.
Deposited on : 2000-04-11
Resolution : 2.75 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

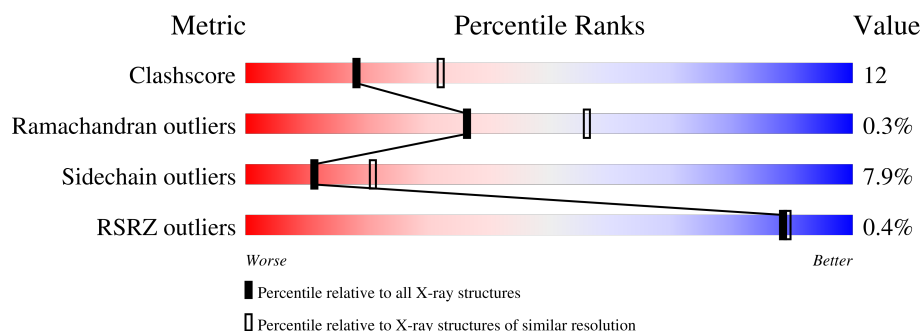
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	60%29%7% . .
1	B	560	58%33%6% . .

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8753 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.

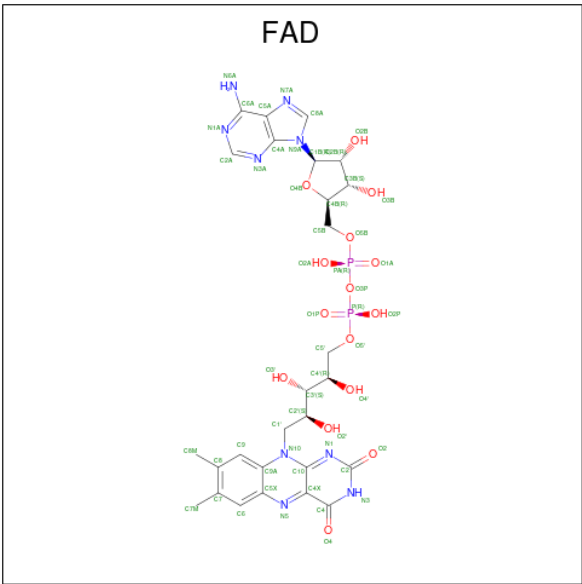
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	3	0	0
			4287	2753	730	781	23			
1	B	550	Total	C	N	O	S	0	0	0
			4269	2740	726	780	23			

There are 6 discrepancies between the modelled and reference sequences:

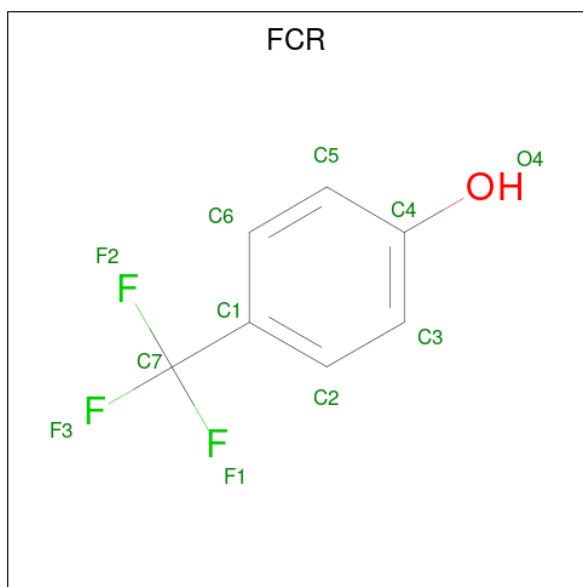
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	GLY	ARG	conflict	UNP P56216
A	457	GLU	THR	engineered mutation	UNP P56216
A	170	SER	ASP	engineered mutation	UNP P56216
B	274	GLY	ARG	conflict	UNP P56216
B	457	GLU	THR	engineered mutation	UNP P56216
B	170	SER	ASP	engineered mutation	UNP P56216

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



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

- Molecule 3 is ALPHA,ALPHA,ALPHA-TRIFLUORO-P-CRESOL (CCD ID: FCR) (formula: C₇H₅F₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	F	O	0	0
			11	7	3	1		

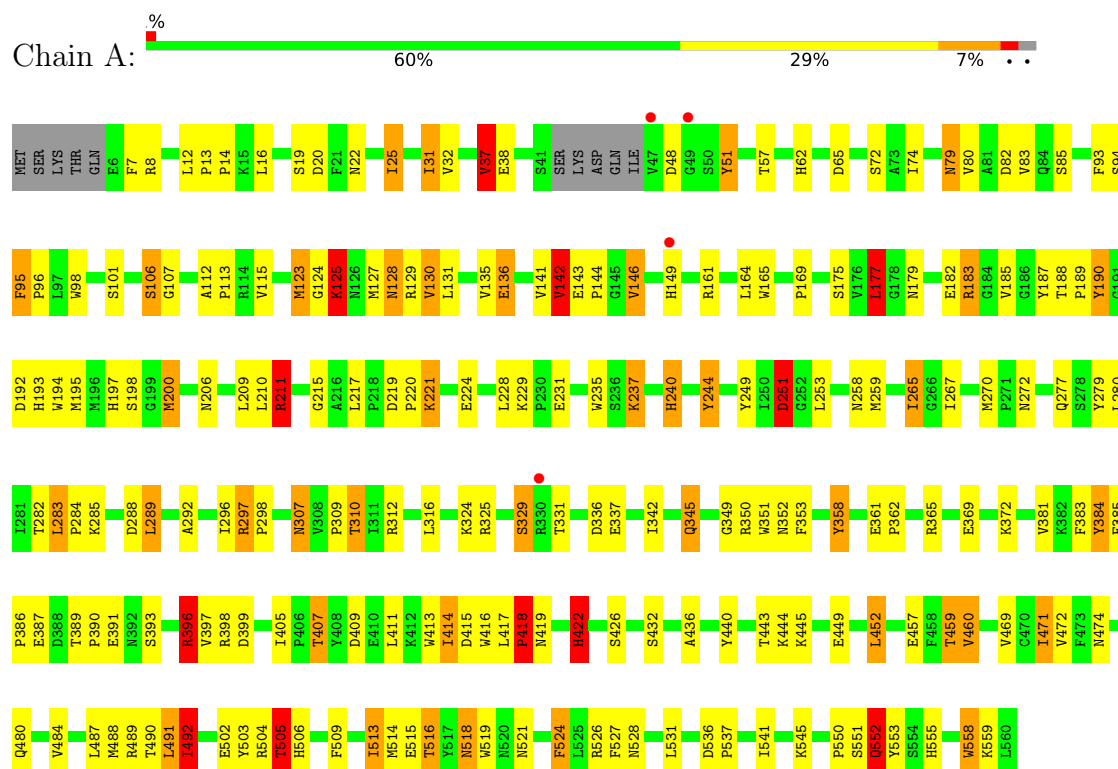
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	38	Total	O	0	0
			38	38		

3 Residue-property plots [i](#)

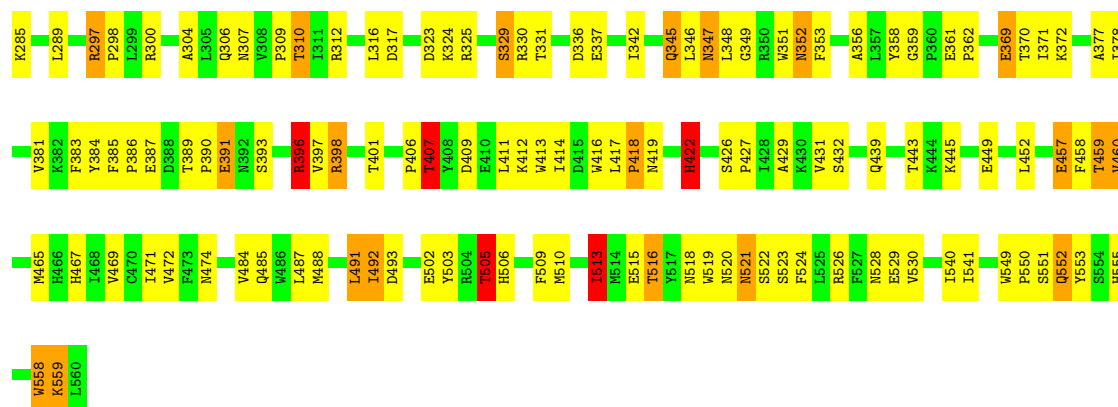
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	131.28Å 131.28Å 134.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.75) 96.8 (20.00-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.287 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h 0.017 for -l,-k,-h 0.025 for -h,-l,-k 0.006 for -h,l,k 0.038 for -h,k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8753	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 3.95% 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, FCR

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	0.67	3/4406 (0.1%)	1.99	142/5997 (2.4%)
1	B	0.62	2/4387 (0.0%)	1.97	138/5972 (2.3%)
All	All	0.65	5/8793 (0.1%)	1.98	280/11969 (2.3%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	LYS	CG-CD	11.19	1.86	1.52
1	B	422	HIS	CE1-NE2	6.15	1.38	1.32
1	A	422	HIS	CD2-NE2	6.06	1.44	1.37
1	B	422	HIS	CD2-NE2	5.85	1.44	1.37
1	A	422	HIS	CE1-NE2	5.63	1.38	1.32

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CD-NE-CZ	20.15	152.61	124.40
1	A	211	ARG	CD-NE-CZ	17.45	148.83	124.40
1	B	211	ARG	CA-CB-CG	14.91	143.93	114.10
1	A	211	ARG	CA-CB-CG	14.82	143.75	114.10
1	B	7	PHE	N-CA-C	14.53	132.45	111.96
1	B	127	MET	CA-C-N	13.64	143.95	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	MET	C-N-CA	13.64	143.95	122.26
1	B	65	ASP	CA-CB-CG	13.31	125.91	112.60
1	A	37	VAL	CA-C-O	-13.28	107.02	121.09
1	A	258	ASN	OD1-CG-ND2	-13.24	109.36	122.60
1	A	258	ASN	CA-CB-CG	12.66	125.26	112.60
1	B	183	ARG	CD-NE-CZ	12.16	141.43	124.40
1	A	127	MET	CA-C-N	11.83	141.07	122.26
1	A	127	MET	C-N-CA	11.83	141.07	122.26
1	B	422	HIS	CE1-NE2-CD2	-11.23	97.77	109.00
1	A	65	ASP	CA-CB-CG	10.83	123.43	112.60
1	B	48	ASP	CA-CB-CG	10.07	122.67	112.60
1	A	258	ASN	CB-CG-ND2	10.03	131.45	116.40
1	A	259	MET	CA-C-O	-10.03	109.11	120.24
1	A	422	HIS	CE1-NE2-CD2	-10.01	98.99	109.00
1	A	48	ASP	CA-CB-CG	10.01	122.61	112.60
1	B	128	ASN	N-CA-C	9.93	126.63	113.72
1	B	336	ASP	CA-CB-CG	-9.85	102.75	112.60
1	B	258	ASN	CA-CB-CG	9.78	122.38	112.60
1	A	190	TYR	CA-C-N	9.77	130.97	120.03
1	A	190	TYR	C-N-CA	9.77	130.97	120.03
1	A	244	TYR	N-CA-C	9.67	123.03	111.82
1	A	492	ILE	N-CA-CB	9.63	120.74	110.62
1	B	128	ASN	N-CA-CB	-9.62	96.52	110.65
1	A	31	ILE	N-CA-C	9.51	119.53	110.30
1	B	258	ASN	CB-CG-ND2	9.49	130.64	116.40
1	A	37	VAL	O-C-N	-9.47	112.83	122.30
1	A	336	ASP	CA-CB-CG	-9.45	103.15	112.60
1	A	128	ASN	N-CA-C	9.41	125.96	113.72
1	B	509	PHE	CA-CB-CG	-9.16	104.64	113.80
1	B	215	GLY	N-CA-C	-9.13	103.36	115.32
1	B	492	ILE	N-CA-CB	9.08	120.16	110.62
1	B	244	TYR	N-CA-C	9.02	122.29	111.82
1	A	183	ARG	CD-NE-CZ	9.01	137.01	124.40
1	A	249	TYR	CA-C-N	8.98	135.47	121.19
1	A	249	TYR	C-N-CA	8.98	135.47	121.19
1	A	128	ASN	N-CA-CB	-8.97	97.47	110.65
1	B	398	ARG	CD-NE-CZ	8.95	136.93	124.40
1	B	242	PHE	CA-CB-CG	8.79	122.59	113.80
1	A	65	ASP	N-CA-CB	8.79	122.83	110.26
1	B	300	ARG	NE-CZ-NH2	8.75	127.08	119.20
1	B	128	ASN	CB-CA-C	-8.63	95.06	109.55
1	A	509	PHE	CA-CB-CG	-8.61	105.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	GLN	CA-C-N	8.50	136.57	123.23
1	A	552	GLN	C-N-CA	8.50	136.57	123.23
1	A	128	ASN	CB-CA-C	-8.47	95.33	109.55
1	B	31	ILE	N-CA-C	8.43	118.52	110.42
1	A	125	LYS	CA-C-O	-8.34	111.58	120.92
1	A	545	LYS	CA-C-O	8.16	129.85	120.96
1	A	515	GLU	CA-C-N	8.15	131.20	120.28
1	A	515	GLU	C-N-CA	8.15	131.20	120.28
1	B	325	ARG	CD-NE-CZ	8.01	135.62	124.40
1	B	240	HIS	CA-CB-CG	-7.92	105.88	113.80
1	B	170	SER	N-CA-C	7.92	121.89	111.75
1	A	149	HIS	CA-CB-CG	-7.75	106.05	113.80
1	A	536	ASP	CA-C-N	7.75	127.65	119.05
1	A	536	ASP	C-N-CA	7.75	127.65	119.05
1	A	249	TYR	CA-C-O	7.66	129.97	121.39
1	B	124	GLY	N-CA-C	7.65	121.91	112.73
1	B	62	HIS	N-CA-C	7.57	120.72	109.59
1	B	185	VAL	CA-C-N	7.50	129.43	121.48
1	B	185	VAL	C-N-CA	7.50	129.43	121.48
1	B	279	TYR	N-CA-C	7.50	119.55	108.60
1	A	524	PHE	CA-C-O	-7.46	112.64	120.55
1	B	460	VAL	N-CA-C	7.38	118.44	107.15
1	A	426	SER	N-CA-C	7.33	123.08	110.02
1	B	258	ASN	CB-CG-OD1	-7.27	106.27	120.80
1	B	129	ARG	N-CA-C	7.13	121.46	110.20
1	A	383	PHE	N-CA-C	7.12	120.14	109.25
1	B	22	ASN	CA-C-O	-7.06	113.07	120.55
1	A	62	HIS	N-CA-C	7.03	119.92	109.59
1	A	129	ARG	N-CA-C	7.02	121.28	110.20
1	A	7	PHE	CA-C-O	-6.94	111.69	119.67
1	A	504	ARG	CA-C-O	-6.94	112.98	120.75
1	A	62	HIS	CA-CB-CG	6.84	120.64	113.80
1	B	426	SER	N-CA-C	6.83	122.17	110.02
1	B	249	TYR	CA-C-O	6.80	129.19	121.58
1	B	383	PHE	N-CA-C	6.79	119.75	108.96
1	B	297	ARG	NE-CZ-NH2	6.74	125.26	119.20
1	A	265	ILE	CA-C-O	6.71	126.59	121.09
1	B	422	HIS	ND1-CE1-NE2	6.70	115.10	108.40
1	B	31	ILE	CA-C-O	-6.67	114.10	121.17
1	B	558	TRP	CA-C-O	-6.67	111.83	118.97
1	B	386	PRO	CA-C-N	6.66	129.50	120.38
1	B	386	PRO	C-N-CA	6.66	129.50	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	CD-NE-CZ	6.64	133.70	124.40
1	B	145	GLY	N-CA-C	6.64	121.98	114.67
1	B	300	ARG	CA-C-O	6.60	127.50	120.70
1	A	405	ILE	CA-C-O	6.59	123.04	119.15
1	A	399	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	7	PHE	N-CA-C	6.55	121.81	113.55
1	A	460	VAL	N-CA-C	6.49	117.86	107.73
1	B	32	VAL	N-CA-C	6.47	118.37	112.29
1	B	398	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	B	384	TYR	N-CA-C	6.41	119.59	108.76
1	A	528	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	459	THR	CB-CA-C	6.37	120.73	109.72
1	B	413	TRP	CA-CB-CG	6.34	125.66	113.60
1	B	179	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	251	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	540	ILE	CA-C-N	-6.28	115.16	122.95
1	B	540	ILE	C-N-CA	-6.28	115.16	122.95
1	B	127	MET	CA-C-O	6.28	129.22	122.13
1	A	161	ARG	CA-C-O	-6.27	111.90	119.49
1	B	347	ASN	OD1-CG-ND2	6.27	128.87	122.60
1	B	65	ASP	N-CA-CB	6.26	119.21	110.26
1	B	393	SER	N-CA-C	6.26	118.62	110.43
1	A	215	GLY	N-CA-C	-6.23	105.83	115.73
1	B	119	VAL	CA-C-O	-6.23	113.80	120.59
1	B	211	ARG	CG-CD-NE	6.23	125.70	112.00
1	A	136	GLU	CA-CB-CG	6.22	126.54	114.10
1	B	513	ILE	CA-C-O	-6.21	114.81	121.27
1	A	283	LEU	CB-CA-C	6.21	117.29	110.15
1	B	541	ILE	N-CA-CB	6.21	119.05	111.60
1	B	505	THR	N-CA-C	6.20	117.30	108.74
1	A	123	MET	CA-C-O	6.12	127.03	120.24
1	A	490	THR	N-CA-C	-6.11	104.31	110.97
1	A	518	ASN	CA-CB-CG	6.08	118.68	112.60
1	A	385	PHE	N-CA-C	-6.08	102.43	110.40
1	A	471	ILE	CA-C-O	-6.07	113.04	120.69
1	A	25	ILE	CA-C-O	-6.07	114.96	121.27
1	A	146	VAL	CB-CA-C	-6.07	104.74	111.35
1	A	37	VAL	CB-CA-C	-6.06	105.11	111.23
1	B	528	ASN	CA-CB-CG	-6.06	106.54	112.60
1	A	384	TYR	N-CA-C	6.05	118.76	108.90
1	B	524	PHE	CA-C-O	-6.04	114.15	120.55
1	A	237	LYS	N-CA-C	6.03	118.34	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	558	TRP	N-CA-C	6.03	121.68	113.97
1	A	325	ARG	CD-NE-CZ	6.01	132.81	124.40
1	B	526	ARG	CG-CD-NE	6.00	125.19	112.00
1	A	369	GLU	CA-C-O	-5.98	114.72	121.00
1	A	552	GLN	N-CA-C	5.96	120.55	113.16
1	A	413	TRP	CA-CB-CG	5.94	124.89	113.60
1	B	37	VAL	CA-C-O	-5.94	114.49	120.31
1	A	558	TRP	N-CA-C	5.94	121.58	113.97
1	A	211	ARG	CG-CD-NE	5.92	125.03	112.00
1	B	422	HIS	CG-CD2-NE2	5.92	113.12	107.20
1	A	490	THR	CA-C-O	-5.92	114.79	121.00
1	A	297	ARG	CA-C-N	5.89	125.43	119.19
1	A	297	ARG	C-N-CA	5.89	125.43	119.19
1	B	530	VAL	CA-C-O	-5.87	114.95	121.17
1	B	192	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	521	ASN	CA-CB-CG	-5.86	106.74	112.60
1	A	422	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	A	545	LYS	CA-C-N	5.85	130.88	122.40
1	A	545	LYS	C-N-CA	5.85	130.88	122.40
1	A	22	ASN	CA-C-O	-5.84	114.36	120.55
1	B	330	ARG	N-CA-CB	-5.84	100.57	109.92
1	B	93	PHE	CA-C-O	-5.83	112.23	119.28
1	B	352	ASN	CA-CB-CG	-5.81	106.79	112.60
1	A	551	SER	N-CA-C	5.80	119.17	111.75
1	A	125	LYS	CA-CB-CG	5.79	125.67	114.10
1	B	515	GLU	CA-C-N	5.79	129.10	120.31
1	B	515	GLU	C-N-CA	5.79	129.10	120.31
1	B	251	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	300	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	B	149	HIS	CA-C-O	5.76	126.86	120.82
1	A	386	PRO	CA-C-N	5.75	128.26	120.38
1	A	386	PRO	C-N-CA	5.75	128.26	120.38
1	A	393	SER	N-CA-C	5.74	117.95	110.43
1	B	385	PHE	N-CA-C	-5.74	102.88	110.40
1	A	240	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	192	ASP	N-CA-CB	-5.73	102.33	110.58
1	A	209	LEU	CA-C-O	-5.73	114.52	121.05
1	B	529	GLU	CA-C-N	5.70	127.74	120.56
1	B	529	GLU	C-N-CA	5.70	127.74	120.56
1	A	72	SER	N-CA-C	-5.69	105.44	112.90
1	B	142	VAL	N-CA-CB	-5.68	101.42	111.93
1	B	203	VAL	N-CA-CB	5.67	117.85	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLY	N-CA-C	-5.65	107.58	114.92
1	A	521	ASN	CA-CB-CG	-5.64	106.96	112.60
1	A	537	PRO	CA-C-O	-5.63	111.07	119.86
1	A	541	ILE	N-CA-CB	5.63	118.23	111.31
1	A	177	LEU	CA-CB-CG	5.61	135.92	116.30
1	A	452	LEU	N-CA-C	5.60	118.53	109.40
1	A	459	THR	N-CA-C	-5.60	100.06	109.07
1	A	164	LEU	CA-C-O	-5.59	114.66	120.70
1	A	164	LEU	N-CA-C	5.59	118.51	109.40
1	A	307	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	279	TYR	N-CA-C	5.56	117.25	108.96
1	A	436	ALA	CA-C-O	-5.56	114.95	120.90
1	A	491	LEU	CA-C-O	-5.55	114.66	120.55
1	B	125	LYS	CA-C-O	-5.54	114.72	120.92
1	A	206	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	179	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	38	GLU	CA-C-O	-5.49	114.34	120.54
1	A	396	ARG	CD-NE-CZ	5.48	132.08	124.40
1	A	142	VAL	N-CA-CB	-5.48	101.67	111.92
1	B	190	TYR	CA-C-N	5.47	127.03	120.13
1	B	190	TYR	C-N-CA	5.47	127.03	120.13
1	A	398	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	B	378	ILE	CB-CA-C	-5.47	104.56	110.85
1	A	249	TYR	CB-CA-C	5.46	120.79	111.68
1	B	526	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	A	267	ILE	CB-CG1-CD1	5.45	125.24	113.80
1	B	125	LYS	CB-CG-CD	5.45	123.83	111.30
1	B	356	ALA	CA-C-O	5.43	126.83	120.75
1	B	306	GLN	N-CA-C	5.41	117.26	111.36
1	A	277	GLN	N-CA-CB	5.41	118.99	110.71
1	B	56	HIS	CA-CB-CG	5.41	119.21	113.80
1	A	383	PHE	N-CA-CB	-5.40	101.07	109.87
1	B	107	GLY	N-CA-C	-5.39	107.91	114.92
1	B	329	SER	CA-C-N	5.39	128.74	120.82
1	B	329	SER	C-N-CA	5.39	128.74	120.82
1	B	491	LEU	CA-C-O	-5.38	115.17	120.82
1	A	165	TRP	CA-CB-CG	5.38	123.82	113.60
1	A	358	TYR	CA-C-O	-5.37	114.90	120.70
1	B	551	SER	N-CA-C	5.34	118.59	111.75
1	B	86	ILE	CA-C-O	-5.34	115.40	120.95
1	A	285	LYS	N-CA-C	5.33	118.42	109.95
1	B	348	LEU	CA-C-O	-5.32	115.67	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ALA	CA-C-O	5.31	126.06	119.79
1	A	130	VAL	N-CA-C	-5.30	99.97	107.98
1	A	142	VAL	N-CA-C	5.29	117.38	108.81
1	B	20	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	272	ASN	N-CA-C	-5.28	102.22	109.71
1	B	133	VAL	N-CA-CB	5.27	118.62	112.35
1	A	95	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	228	LEU	CA-C-O	-5.24	115.07	121.05
1	A	505	THR	N-CA-C	5.24	115.97	108.74
1	B	245	GLY	CA-C-O	-5.22	115.03	121.56
1	A	552	GLN	O-C-N	-5.22	115.17	122.37
1	B	412	LYS	N-CA-C	5.21	117.70	111.71
1	A	135	VAL	N-CA-C	5.19	115.41	110.53
1	B	96	PRO	O-C-N	5.18	129.32	123.10
1	B	317	ASP	CA-C-N	5.18	127.48	120.38
1	B	317	ASP	C-N-CA	5.18	127.48	120.38
1	B	161	ARG	CA-C-O	-5.17	114.41	120.20
1	A	193	HIS	CA-C-N	5.17	127.52	120.54
1	A	193	HIS	C-N-CA	5.17	127.52	120.54
1	B	136	GLU	CA-CB-CG	5.17	124.44	114.10
1	B	254	PHE	CA-C-N	-5.16	115.20	122.94
1	B	254	PHE	C-N-CA	-5.16	115.20	122.94
1	B	209	LEU	CA-C-O	-5.16	114.71	120.54
1	B	407	THR	CB-CA-C	-5.14	101.65	111.48
1	B	114	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	372	LYS	CA-C-O	5.12	127.02	121.02
1	B	385	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	383	PHE	N-CA-CB	-5.11	101.58	110.17
1	B	459	THR	CB-CA-C	5.11	118.58	110.19
1	A	372	LYS	CA-C-O	5.11	127.00	121.02
1	B	285	LYS	N-CA-C	5.11	118.07	109.95
1	B	211	ARG	N-CA-CB	5.10	119.71	110.83
1	B	249	TYR	CB-CA-C	5.10	120.25	111.68
1	A	210	LEU	CA-C-O	-5.10	114.48	120.60
1	A	329	SER	CA-C-N	5.10	128.32	120.82
1	A	329	SER	C-N-CA	5.10	128.32	120.82
1	B	149	HIS	CA-CB-CG	-5.09	108.70	113.80
1	B	377	ALA	CA-C-N	5.09	131.60	123.46
1	B	377	ALA	C-N-CA	5.09	131.60	123.46
1	B	493	ASP	N-CA-C	5.09	116.52	111.07
1	B	417	LEU	CA-C-N	5.08	126.19	119.84
1	B	417	LEU	C-N-CA	5.08	126.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	THR	CB-CA-C	-5.08	99.87	111.95
1	B	406	PRO	N-CA-C	5.07	118.82	110.55
1	A	288	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	369	GLU	CA-C-O	-5.07	113.26	120.51
1	B	559	LYS	CA-C-O	-5.07	116.29	121.87
1	B	25	ILE	CA-C-O	-5.06	115.69	120.95
1	A	93	PHE	CA-C-O	-5.06	113.16	119.28
1	B	114	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	51	TYR	N-CA-C	-5.04	107.30	113.50
1	B	187	TYR	CA-C-O	-5.04	113.40	119.15
1	A	289	LEU	N-CA-C	-5.04	105.79	111.28
1	B	323	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	235	TRP	CA-CB-CG	5.02	123.14	113.60
1	A	526	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	169	PRO	N-CA-C	-5.02	103.65	111.13
1	B	283	LEU	CB-CA-C	5.02	115.92	110.15
1	B	396	ARG	CA-C-N	5.02	126.84	120.72
1	B	396	ARG	C-N-CA	5.02	126.84	120.72
1	A	32	VAL	N-CA-C	5.01	117.79	112.83
1	A	415	ASP	CA-CB-CG	-5.01	107.59	112.60
1	A	350	ARG	CA-C-O	5.01	125.46	119.60
1	A	244	TYR	CA-C-O	-5.00	114.22	119.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	VAL	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4287	0	4166	105	2
1	B	4269	0	4137	113	1
2	A	53	0	29	2	0
2	B	53	0	29	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	5	0	0
4	A	42	0	0	1	0
4	B	38	0	0	2	0
All	All	8753	0	8366	206	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 12.

All (206) 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:297:ARG:HB3	1:B:298:PRO:HD3	1.56	0.86
1:A:349:GLY:H	1:A:352:ASN:HD21	1.27	0.83
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.94	0.82
1:B:83:VAL:HG21	1:B:123:MET:HE1	1.61	0.81
1:B:397:VAL:HG13	1:B:407:THR:HG21	1.66	0.78
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.64	0.77
1:B:349:GLY:H	1:B:352:ASN:HD21	1.35	0.75
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.02	0.74
1:A:83:VAL:HG21	1:A:123:MET:HE1	1.68	0.74
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.71	0.73
1:A:365:ARG:HD2	4:A:2032:HOH:O	1.88	0.73
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.69	0.73
1:A:513:ILE:O	1:A:516:THR:HB	1.89	0.73
1:B:131:LEU:HD12	1:B:141:VAL:HG12	1.70	0.72
1:A:79:ASN:ND2	1:A:82:ASP:H	1.88	0.72
1:B:513:ILE:O	1:B:516:THR:HB	1.89	0.72
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.73	0.70
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.73	0.70
1:B:389:THR:HB	1:B:390:PRO:HD2	1.74	0.70
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.75	0.69
1:B:310:THR:HG22	1:B:459:THR:HG22	1.74	0.69
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.74	0.68
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.57	0.67
1:B:312:ARG:HG2	1:B:316:LEU:HD23	1.75	0.67
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.79	0.65
1:B:505:THR:HG22	1:B:506:HIS:H	1.61	0.65
1:B:361:GLU:HB3	1:B:362:PRO:HD3	1.78	0.65
1:A:131:LEU:HD12	1:A:141:VAL:HG12	1.76	0.65
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.62	0.65
1:A:397:VAL:HG13	1:A:407:THR:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HG2	1:A:270:MET:CE	2.28	0.64
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.14	0.62
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.81	0.62
1:B:342:ILE:HA	1:B:345:GLN:HG3	1.80	0.62
1:B:282:THR:HG22	1:B:352:ASN:HD22	1.64	0.62
1:B:182:GLU:O	1:B:183:ARG:HB2	2.00	0.61
1:B:387:GLU:HA	1:B:396:ARG:NH2	2.15	0.61
1:A:310:THR:HG22	1:A:459:THR:HG22	1.82	0.61
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.31	0.60
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.82	0.60
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.37	0.60
1:B:79:ASN:ND2	1:B:82:ASP:H	1.99	0.59
1:B:407:THR:HG22	1:B:409:ASP:OD1	2.03	0.59
1:A:492:ILE:HG12	1:A:513:ILE:HG13	1.84	0.58
1:B:552:GLN:NE2	1:B:552:GLN:H	2.01	0.58
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.85	0.58
1:A:342:ILE:HA	1:A:345:GLN:HG3	1.84	0.58
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.85	0.58
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.86	0.58
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.70	0.57
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.20	0.57
1:A:292:ALA:O	1:A:296:ILE:HG13	2.05	0.57
1:A:79:ASN:HD22	1:A:82:ASP:H	1.52	0.56
1:A:200:MET:HE3	1:A:265:ILE:HD12	1.87	0.56
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.87	0.56
1:B:337:GLU:H	1:B:337:GLU:CD	2.13	0.56
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.40	0.56
1:B:106:SER:HB2	1:B:422:HIS:HE1	1.68	0.56
1:A:253:LEU:HD11	1:B:253:LEU:HD21	1.88	0.56
1:A:106:SER:HB2	1:A:422:HIS:HE1	1.72	0.55
1:A:552:GLN:NE2	1:A:552:GLN:H	2.04	0.55
1:B:307:ASN:HB3	1:B:358:TYR:HE2	1.72	0.55
1:A:387:GLU:HA	1:A:396:ARG:NH2	2.22	0.54
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.37	0.54
1:A:514:MET:HE1	1:A:524:PHE:HE1	1.73	0.54
1:A:312:ARG:HG2	1:A:316:LEU:HD23	1.90	0.54
1:B:187:TYR:O	1:B:307:ASN:HB2	2.09	0.53
1:B:505:THR:HG23	4:B:2025:HOH:O	2.07	0.53
1:A:419:ASN:HB2	1:A:474:ASN:OD1	2.09	0.53
1:B:389:THR:HB	1:B:390:PRO:CD	2.38	0.53
1:B:188:THR:HB	1:B:189:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.44	0.53
1:A:505:THR:HG22	1:A:506:HIS:H	1.72	0.53
1:A:407:THR:HG22	1:A:409:ASP:OD1	2.10	0.52
1:A:307:ASN:HB3	1:A:358:TYR:HE2	1.75	0.52
1:B:289:LEU:HD22	1:B:351:TRP:CZ2	2.45	0.52
1:A:324:LYS:HB2	1:A:416:TRP:CE2	2.46	0.51
1:B:492:ILE:HG12	1:B:513:ILE:HG13	1.91	0.51
1:A:502:GLU:OE1	1:A:513:ILE:HG12	2.11	0.51
1:A:389:THR:HB	1:A:390:PRO:HD2	1.92	0.51
1:A:182:GLU:O	1:A:183:ARG:HB2	2.11	0.50
1:A:445:LYS:O	1:A:449:GLU:HG3	2.11	0.50
1:A:124:GLY:O	1:A:125:LYS:C	2.54	0.50
1:A:387:GLU:CD	1:A:387:GLU:H	2.20	0.49
2:A:600:FAD:H8A	2:A:600:FAD:O5B	2.12	0.49
1:B:64:MET:HE1	1:B:485:GLN:NE2	2.26	0.49
1:B:431:VAL:HG22	1:B:465:MET:HG3	1.94	0.49
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.42	0.49
1:A:505:THR:HG21	1:A:513:ILE:CD1	2.42	0.49
1:A:115:VAL:HG13	1:A:558:TRP:CH2	2.47	0.49
1:B:177:LEU:HB2	1:B:265:ILE:CG2	2.43	0.49
1:B:181:VAL:O	1:B:255:SER:HB2	2.13	0.49
1:A:177:LEU:HB2	1:A:265:ILE:HG22	1.94	0.48
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.48	0.48
1:B:80:VAL:HG11	1:B:231:GLU:HB3	1.95	0.48
1:B:419:ASN:HB2	1:B:474:ASN:OD1	2.12	0.48
1:A:142:VAL:HG22	1:A:146:VAL:CG2	2.41	0.48
1:B:79:ASN:HD22	1:B:82:ASP:H	1.60	0.48
1:B:79:ASN:HD22	1:B:79:ASN:C	2.21	0.48
1:A:79:ASN:HD22	1:A:79:ASN:C	2.20	0.48
1:A:452:LEU:HD12	1:A:487:LEU:CD2	2.44	0.48
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.96	0.48
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.48	0.48
1:B:452:LEU:HD12	1:B:487:LEU:CD2	2.44	0.47
1:B:275:GLY:HA3	1:B:359:GLY:O	2.14	0.47
1:B:307:ASN:HB3	1:B:358:TYR:CE2	2.49	0.47
1:B:398:ARG:HA	1:B:401:THR:HB	1.95	0.47
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.49	0.47
1:A:414:ILE:HD11	2:A:600:FAD:HM73	1.95	0.47
1:B:491:LEU:O	1:B:492:ILE:C	2.57	0.47
1:A:309:PRO:HG2	1:A:460:VAL:CB	2.44	0.47
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:PRO:O	1:B:460:VAL:HG23	2.14	0.47
1:A:188:THR:HB	1:A:189:PRO:CD	2.45	0.46
1:B:177:LEU:HB2	1:B:265:ILE:HG22	1.96	0.46
1:A:177:LEU:HB2	1:A:265:ILE:CG2	2.45	0.46
1:B:142:VAL:HG22	1:B:146:VAL:CG2	2.45	0.46
1:B:445:LYS:O	1:B:449:GLU:HG3	2.16	0.46
1:A:337:GLU:CD	1:A:337:GLU:H	2.24	0.46
1:B:189:PRO:HG2	1:B:270:MET:CE	2.46	0.46
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.99	0.46
1:B:283:LEU:HA	1:B:284:PRO:HD3	1.70	0.46
1:B:346:LEU:O	1:B:347:ASN:HB2	2.16	0.46
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.98	0.46
1:B:214:MET:HE2	1:B:245:GLY:HA2	1.98	0.46
1:A:194:TRP:O	1:A:197:HIS:HD2	1.99	0.45
1:B:224:GLU:CD	1:B:224:GLU:H	2.24	0.45
1:B:510:MET:HE2	4:B:2035:HOH:O	2.16	0.45
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.98	0.45
1:A:16:LEU:HD11	1:A:20:ASP:HB3	1.98	0.45
1:B:16:LEU:HD11	1:B:20:ASP:HB3	1.99	0.45
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.98	0.45
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.81	0.45
1:A:518:ASN:O	1:A:519:TRP:C	2.58	0.45
1:B:64:MET:HE1	1:B:485:GLN:HE22	1.82	0.45
1:B:188:THR:CB	1:B:189:PRO:CD	2.95	0.45
1:A:187:TYR:O	1:A:307:ASN:HB2	2.16	0.44
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.52	0.44
1:B:24:PHE:O	1:B:28:ILE:HG12	2.17	0.44
1:A:280:LEU:HB3	1:A:384:TYR:HB2	1.98	0.44
1:B:57:THR:HG22	1:B:74:ILE:CD1	2.45	0.44
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.33	0.44
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.52	0.44
1:A:224:GLU:CD	1:A:224:GLU:H	2.25	0.44
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.52	0.44
1:B:521:ASN:O	1:B:522:SER:HB2	2.17	0.44
1:A:309:PRO:O	1:A:460:VAL:HG23	2.18	0.44
1:A:309:PRO:HB2	1:A:353:PHE:CE1	2.53	0.44
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.98	0.44
1:B:124:GLY:O	1:B:125:LYS:C	2.61	0.43
1:B:309:PRO:HB2	1:B:353:PHE:CE1	2.53	0.43
1:B:488:MET:O	1:B:492:ILE:HD12	2.17	0.43
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:HB3	1:A:358:TYR:CE2	2.53	0.43
1:A:488:MET:O	1:A:492:ILE:HD12	2.17	0.43
1:A:37:VAL:O	1:A:37:VAL:HG12	2.19	0.43
1:A:443:THR:HA	1:A:491:LEU:HD21	2.00	0.43
1:B:188:THR:HB	1:B:189:PRO:HD3	2.01	0.43
2:B:600:FAD:H8A	2:B:600:FAD:O5B	2.18	0.43
1:A:136:GLU:O	1:B:297:ARG:NH1	2.51	0.43
1:B:457:GLU:HG2	1:B:458:PHE:N	2.31	0.43
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.79	0.43
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.53	0.43
1:A:198:SER:O	1:A:240:HIS:HA	2.19	0.43
1:A:440:TYR:CE2	1:A:444:LYS:HE2	2.53	0.43
1:B:427:PRO:HD2	1:B:467:HIS:O	2.19	0.43
1:A:96:PRO:HG3	1:A:553:TYR:OH	2.19	0.42
1:B:96:PRO:HG3	1:B:553:TYR:OH	2.19	0.42
1:B:369:GLU:O	1:B:370:THR:C	2.62	0.42
1:A:80:VAL:HG11	1:A:231:GLU:HB3	2.01	0.42
1:A:471:ILE:HG21	1:A:484:VAL:HG13	2.01	0.42
1:B:51:TYR:CD2	1:B:411:LEU:HD11	2.54	0.42
1:B:93:PHE:O	1:B:94:SER:HB2	2.19	0.42
1:A:229:LYS:HD2	1:A:231:GLU:OE2	2.19	0.42
1:B:505:THR:OG1	1:B:513:ILE:HD13	2.20	0.42
1:A:31:ILE:HD13	1:A:85:SER:HB3	2.01	0.42
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.50	0.42
1:B:90:ALA:HB1	1:B:95:PHE:O	2.17	0.42
1:A:12:LEU:HB3	1:A:13:PRO:HD2	2.00	0.42
1:A:51:TYR:CD2	1:A:411:LEU:HD11	2.54	0.42
1:B:12:LEU:HB3	1:B:13:PRO:HD2	2.01	0.42
1:A:219:ASP:HA	1:A:220:PRO:HD3	1.67	0.42
1:B:90:ALA:HB2	1:B:97:LEU:HD21	2.01	0.42
1:B:387:GLU:H	1:B:387:GLU:CD	2.27	0.42
1:B:555:HIS:HB3	1:B:559:LYS:HE3	2.01	0.42
1:B:225:THR:HG21	1:B:234:PRO:HG3	2.02	0.41
1:A:25:ILE:HD13	1:A:25:ILE:HA	1.86	0.41
1:A:253:LEU:HD21	1:B:253:LEU:CD1	2.45	0.41
1:B:361:GLU:N	1:B:362:PRO:CD	2.83	0.41
1:B:520:ASN:HD22	1:B:520:ASN:HA	1.63	0.41
1:A:188:THR:CB	1:A:189:PRO:CD	2.98	0.41
1:A:244:TYR:CE2	1:B:183:ARG:HD2	2.55	0.41
1:B:324:LYS:HB2	1:B:416:TRP:CE2	2.55	0.41
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PRO:HA	1:A:14:PRO:HD3	1.88	0.41
1:A:143:GLU:O	1:A:144:PRO:C	2.63	0.41
1:A:195:MET:SD	1:B:195:MET:SD	3.19	0.41
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.56	0.41
1:B:502:GLU:OE1	1:B:513:ILE:HG12	2.20	0.41
1:B:471:ILE:HG21	1:B:484:VAL:HG13	2.03	0.41
1:B:552:GLN:H	1:B:552:GLN:HE21	1.69	0.41
1:A:101:SER:O	1:A:124:GLY:HA3	2.21	0.40
1:B:518:ASN:O	1:B:519:TRP:C	2.63	0.40
1:A:389:THR:HB	1:A:390:PRO:CD	2.51	0.40
1:B:219:ASP:HA	1:B:220:PRO:HD3	1.91	0.40
1:B:272:ASN:HA	1:B:273:PRO:HD3	1.96	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:221:LYS:NZ	1:A:489:ARG:CD[4_565]	1.98	0.22
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	2.00	0.20

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	461/560 (82%)	431 (94%)	29 (6%)	1 (0%)	43	64
1	B	546/560 (98%)	512 (94%)	32 (6%)	2 (0%)	30	50
All	All	1007/1120 (90%)	943 (94%)	61 (6%)	3 (0%)	36	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	PRO
1	B	418	PRO
1	B	371	ILE

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	455/481 (95%)	418 (92%)	37 (8%)	11	20
1	B	452/481 (94%)	417 (92%)	35 (8%)	12	22
All	All	907/962 (94%)	835 (92%)	72 (8%)	11	21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	19	SER
1	A	79	ASN
1	A	94	SER
1	A	106	SER
1	A	125	LYS
1	A	128	ASN
1	A	130	VAL
1	A	142	VAL
1	A	175	SER
1	A	177	LEU
1	A	185	VAL
1	A	200	MET
1	A	211	ARG
1	A	237	LYS
1	A	251	ASP
1	A	310	THR
1	A	329	SER
1	A	331	THR
1	A	345	GLN
1	A	381	VAL

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Mol	Chain	Res	Type
1	A	391	GLU
1	A	396	ARG
1	A	407	THR
1	A	414	ILE
1	A	418	PRO
1	A	422	HIS
1	A	432	SER
1	A	457	GLU
1	A	472	VAL
1	A	480	GLN
1	A	492	ILE
1	A	503	TYR
1	A	505	THR
1	A	513	ILE
1	A	516	THR
1	A	552	GLN
1	B	19	SER
1	B	79	ASN
1	B	94	SER
1	B	106	SER
1	B	125	LYS
1	B	128	ASN
1	B	130	VAL
1	B	142	VAL
1	B	175	SER
1	B	177	LEU
1	B	185	VAL
1	B	200	MET
1	B	211	ARG
1	B	237	LYS
1	B	251	ASP
1	B	310	THR
1	B	329	SER
1	B	331	THR
1	B	345	GLN
1	B	381	VAL
1	B	391	GLU
1	B	396	ARG
1	B	407	THR
1	B	414	ILE
1	B	418	PRO
1	B	422	HIS

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Mol	Chain	Res	Type
1	B	432	SER
1	B	457	GLU
1	B	472	VAL
1	B	503	TYR
1	B	505	THR
1	B	513	ILE
1	B	516	THR
1	B	523	SER
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	158	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	B	79	ASN
1	B	128	ASN
1	B	158	ASN
1	B	197	HIS
1	B	233	GLN
1	B	240	HIS
1	B	352	ASN
1	B	439	GLN
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 [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](#)

3 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	600	1	58,58,58	2.72	7 (12%)	85,89,89	1.31	8 (9%)
2	FAD	A	600	1	58,58,58	2.70	7 (12%)	85,89,89	1.38	11 (12%)
3	FCR	B	601	-	11,11,11	0.96	0	16,16,16	1.58	2 (12%)

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	600	1	-	7/34/50/50	0/6/6/6
2	FAD	A	600	1	-	8/34/50/50	0/6/6/6
3	FCR	B	601	-	-	0/6/6/6	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	P-O3P	-16.63	1.41	1.59
2	A	600	FAD	P-O3P	-16.24	1.42	1.59
2	A	600	FAD	PA-O3P	-7.56	1.51	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	PA-O3P	-7.13	1.51	1.59
2	A	600	FAD	PA-O2A	-4.31	1.35	1.55
2	B	600	FAD	PA-O2A	-4.18	1.36	1.55
2	B	600	FAD	O5'-C5'	3.38	1.57	1.44
2	A	600	FAD	O5'-C5'	3.36	1.57	1.44
2	A	600	FAD	P-O2P	-2.96	1.41	1.55
2	B	600	FAD	P-O2P	-2.92	1.41	1.55
2	A	600	FAD	C6-C7	-2.51	1.36	1.39
2	B	600	FAD	C6-C7	-2.46	1.36	1.39
2	A	600	FAD	O2-C2	-2.32	1.19	1.24
2	B	600	FAD	O2-C2	-2.14	1.20	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O2P-P-O3P	4.64	119.81	107.27
2	A	600	FAD	O4B-C1B-N9A	-4.30	99.83	108.09
3	B	601	FCR	F1-C7-C1	4.15	121.78	112.90
2	B	600	FAD	C4'-C3'-C2'	-3.54	107.67	113.57
2	A	600	FAD	O5B-PA-O1A	-3.53	94.93	108.94
2	A	600	FAD	C4'-C3'-C2'	-3.51	107.73	113.57
2	B	600	FAD	O5B-PA-O1A	-3.42	95.38	108.94
2	B	600	FAD	C4-N3-C2	-3.02	120.28	125.64
2	B	600	FAD	C2A-N1A-C6A	2.93	123.55	118.73
2	A	600	FAD	C2A-N1A-C6A	2.80	123.32	118.73
2	A	600	FAD	C4-N3-C2	-2.69	120.87	125.64
2	A	600	FAD	C5'-C4'-C3'	-2.47	107.56	112.22
2	A	600	FAD	O2-C2-N3	-2.43	113.93	118.58
2	A	600	FAD	O3B-C3B-C4B	2.36	117.85	111.08
2	A	600	FAD	O4-C4-N3	-2.20	115.97	120.11
3	B	601	FCR	F3-C7-C1	-2.16	108.27	112.90
2	B	600	FAD	O3P-PA-O1A	2.14	117.13	110.70
2	A	600	FAD	C10-C4X-N5	-2.08	120.56	124.81
2	A	600	FAD	P-O5'-C5'	2.07	133.21	121.35
2	B	600	FAD	P-O5'-C5'	2.02	132.94	121.35
2	B	600	FAD	N3-C2-N1	2.01	123.77	119.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5'-O5'-P-O1P

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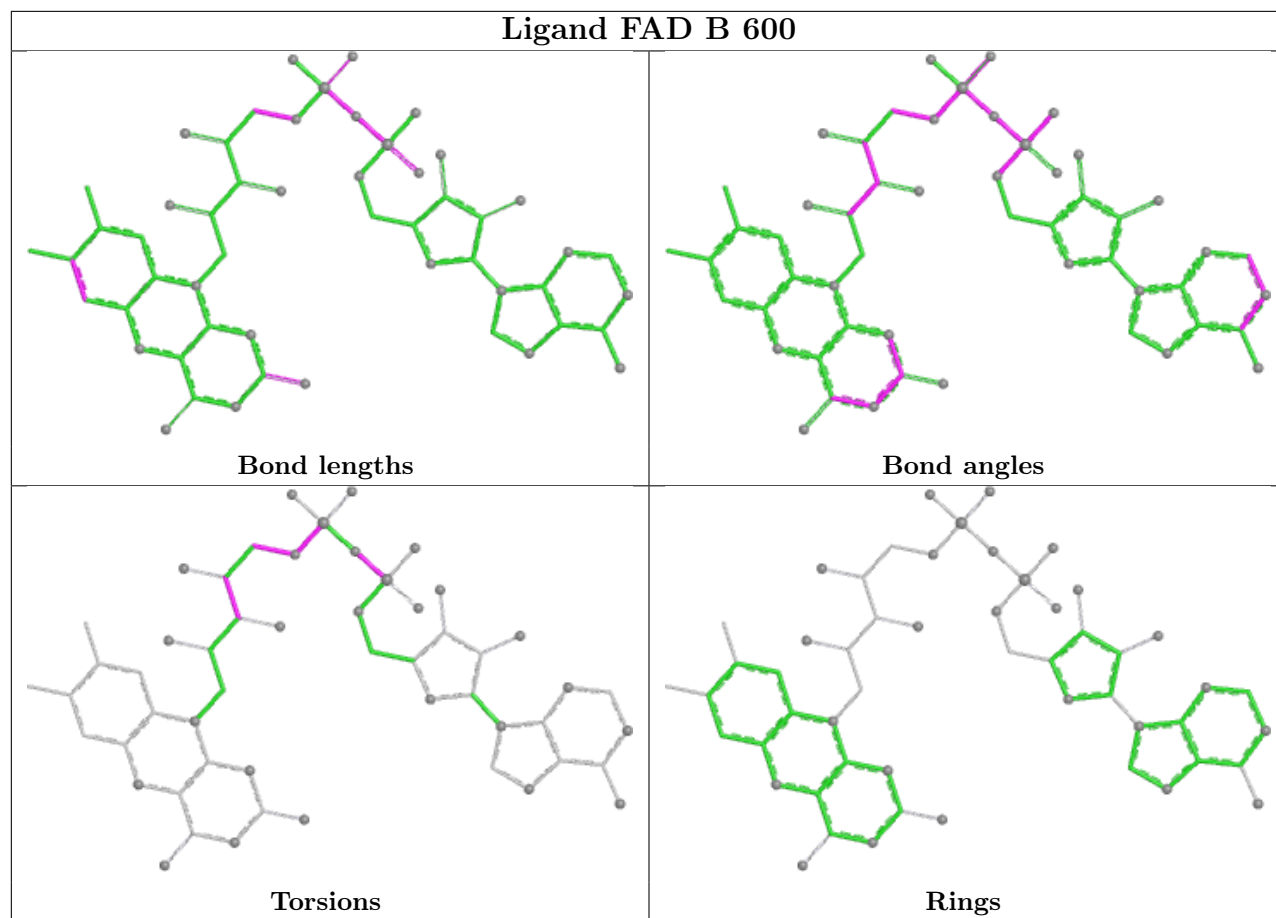
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5'-O5'-P-O2P
2	A	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	C5'-O5'-P-O3P
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	O3'-C3'-C4'-O4'
2	B	600	FAD	C5'-O5'-P-O2P
2	A	600	FAD	O3'-C3'-C4'-C5'
2	B	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	P-O3P-PA-O2A
2	B	600	FAD	O3'-C3'-C4'-C5'

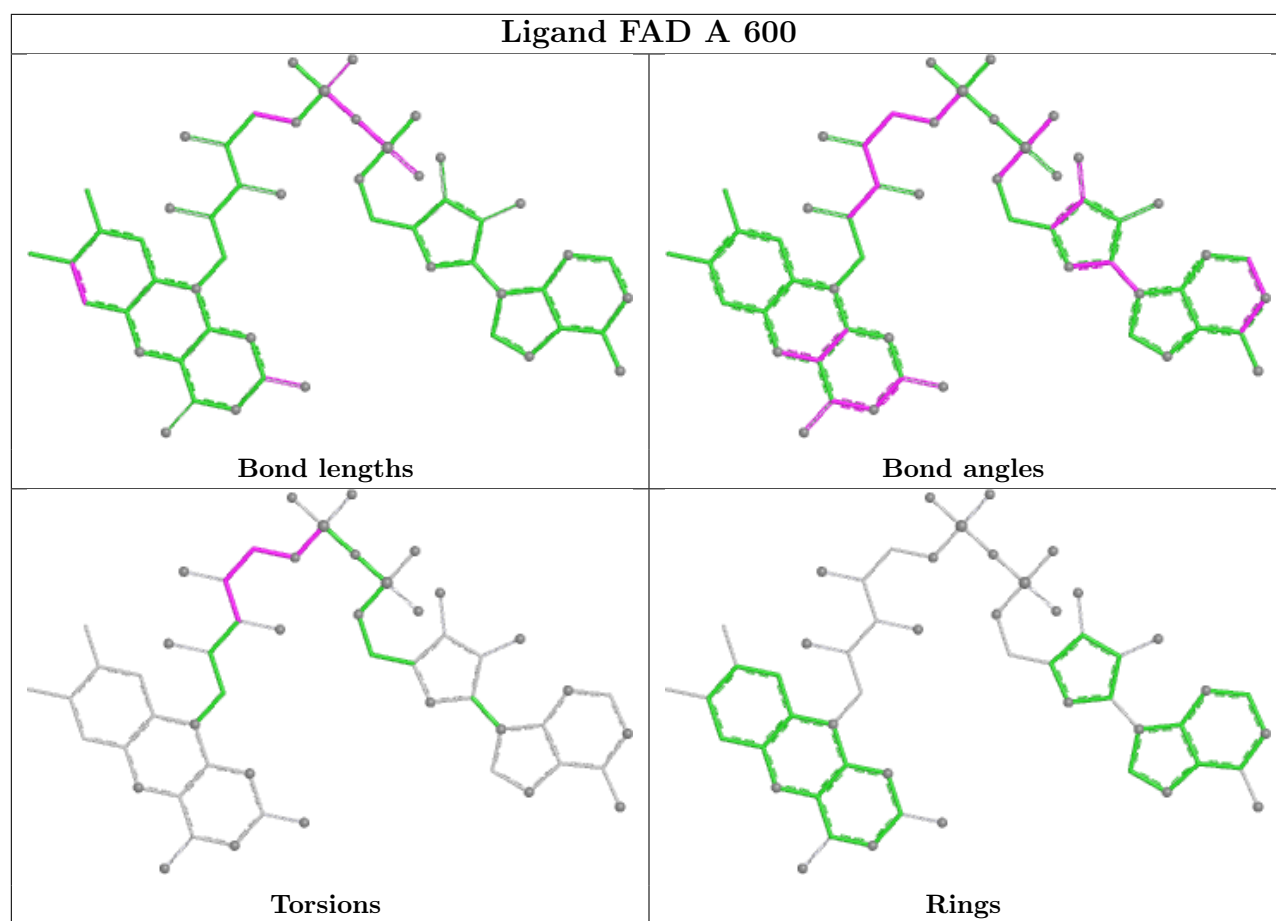
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	1	0
2	A	600	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 [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%)	0.05	4 (0%) 84 84	32, 49, 73, 88	1 (0%)
1	B	550/560 (98%)	0.07	0 100 100	33, 49, 73, 86	0
All	All	1100/1120 (98%)	0.06	4 (0%) 88 89	32, 49, 73, 88	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	ARG	2.4
1	A	47	VAL	2.3
1	A	149	HIS	2.2
1	A	49	GLY	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
3	FCR	B	601	11/11	0.66	0.19	72,74,78,78	0

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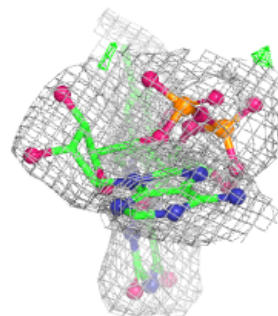
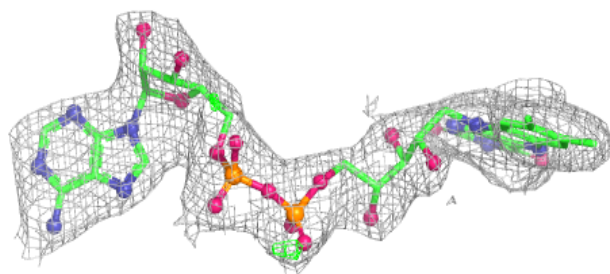
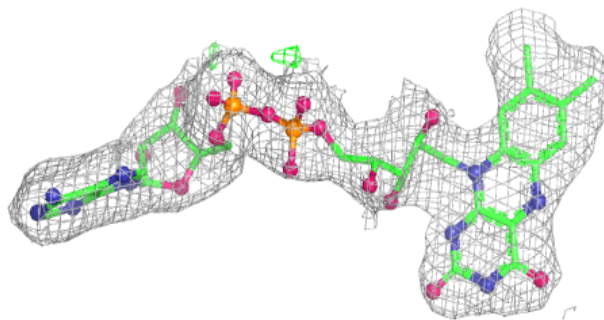
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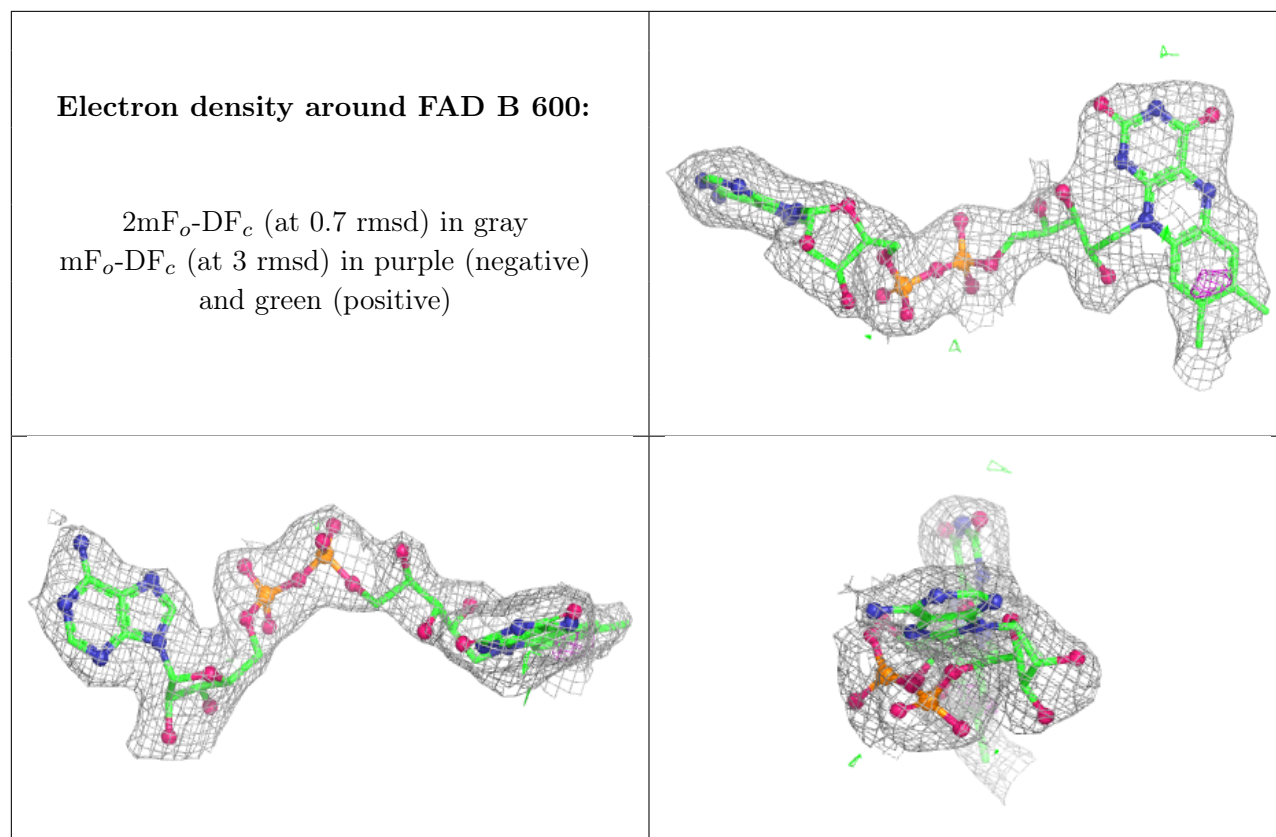
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	600	53/53	0.92	0.09	46,49,53,54	0
2	FAD	B	600	53/53	0.93	0.09	46,49,53,54	0

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.