



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 05:00 PM UTC

PDB ID : 1QLT / pdb_00001qlt
Title : STRUCTURE OF THE H422A MUTANT OF THE FLAVOENZYME
VANILLYL-ALCOHOL OXIDASE
Authors : Mattevi, A.; Fraaije, M.
Deposited on : 1999-09-16
Resolution : 2.20 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	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

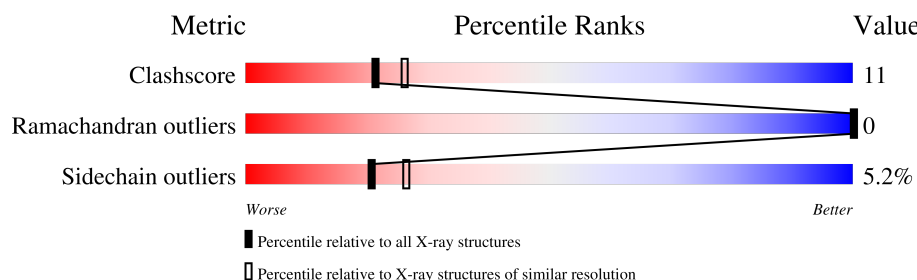
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9178 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.

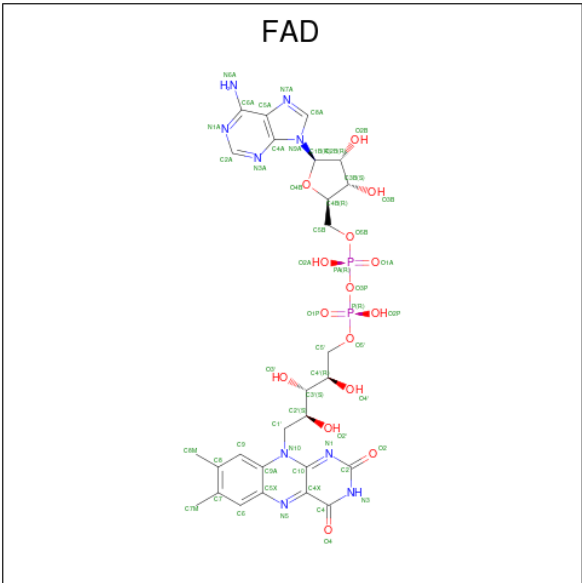
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	68	0	0
			4346	2790	742	790	24			
1	B	550	Total	C	N	O	S	68	0	0
			4346	2790	742	790	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	ALA	HIS	engineered mutation	? ?
B	422	ALA	HIS	engineered mutation	? ?

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



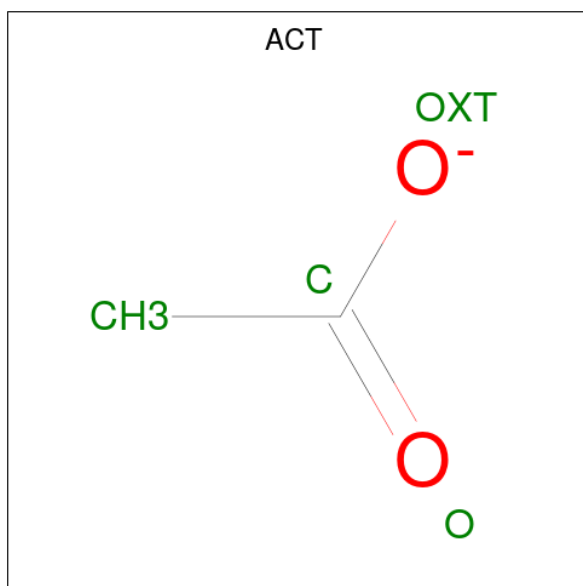
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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 ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

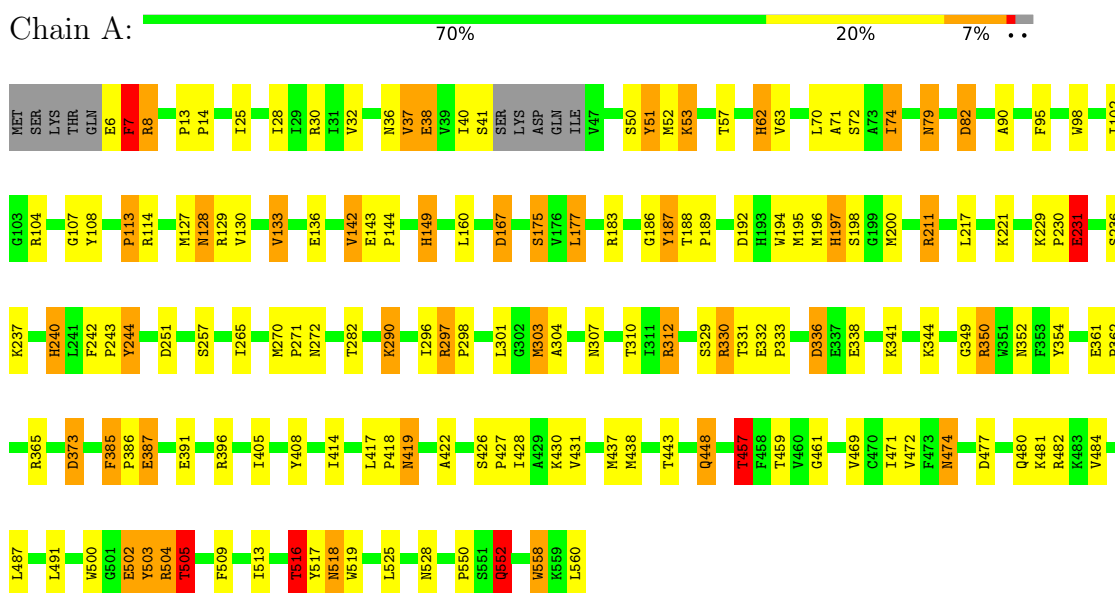
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	207	Total	O	0	0
			207	207		
4	B	165	Total	O	0	0
			165	165		

3 Residue-property plots

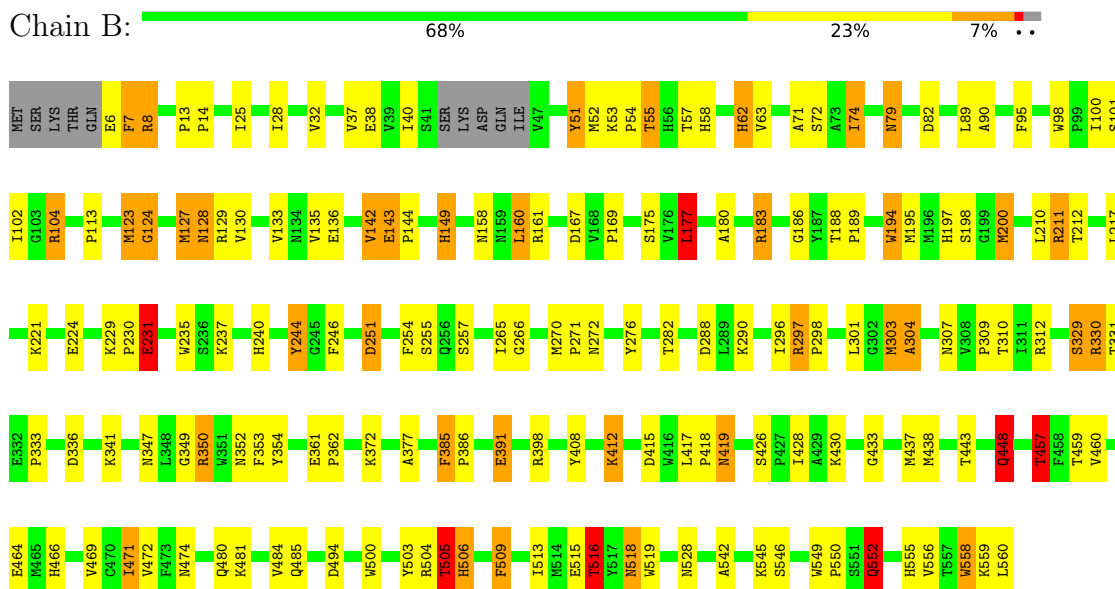
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	129.66Å 129.66Å 132.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.1 (30.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.264	Depositor
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.601	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h 0.017 for -l,-k,-h 0.022 for -h,-l,-k 0.006 for -h,l,k 0.034 for -h,k,-l	Xtriage
Total number of atoms	9178	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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, ACT

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	1.06	12/4464 (0.3%)	2.12	121/6067 (2.0%)
1	B	1.02	12/4464 (0.3%)	2.03	120/6067 (2.0%)
All	All	1.04	24/8928 (0.3%)	2.08	241/12134 (2.0%)

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
1	B	0	1
All	All	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	MET	CB-CG	30.68	2.44	1.52
1	A	52	MET	CB-CG	30.66	2.44	1.52
1	A	53	LYS	CB-CG	13.28	1.92	1.52
1	A	350	ARG	CZ-NH1	-11.12	1.17	1.32
1	B	350	ARG	CZ-NH1	-9.77	1.19	1.32
1	B	221	LYS	CG-CD	-9.21	1.24	1.52
1	A	350	ARG	CZ-NH2	8.08	1.44	1.33
1	A	221	LYS	CG-CD	-7.77	1.29	1.52
1	B	53	LYS	CB-CG	6.69	1.72	1.52
1	B	542	ALA	CA-CB	6.44	1.58	1.52
1	A	365	ARG	CD-NE	-6.14	1.37	1.46
1	B	128	ASN	CA-CB	6.13	1.62	1.54
1	B	542	ALA	C-O	6.07	1.26	1.23
1	B	161	ARG	CB-CG	-5.95	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	LYS	CB-CG	-5.84	1.34	1.52
1	A	504	ARG	CD-NE	-5.73	1.38	1.46
1	A	7	PHE	CB-CG	-5.71	1.37	1.50
1	A	128	ASN	CA-CB	5.55	1.62	1.54
1	A	344	LYS	CB-CG	-5.40	1.36	1.52
1	A	53	LYS	CA-CB	-5.38	1.46	1.53
1	B	266	GLY	CA-C	5.09	1.55	1.52
1	B	341	LYS	CB-CG	-5.06	1.37	1.52
1	B	7	PHE	CB-CG	-5.05	1.39	1.50
1	B	128	ASN	N-CA	-5.05	1.39	1.45

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	GLN	OE1-CD-NE2	-41.90	80.70	122.60
1	A	211	ARG	CD-NE-CZ	35.31	173.83	124.40
1	B	211	ARG	CD-NE-CZ	34.10	172.14	124.40
1	B	448	GLN	OE1-CD-NE2	-26.84	95.75	122.60
1	A	350	ARG	NE-CZ-NH1	-23.07	98.43	121.50
1	A	448	GLN	CG-CD-NE2	22.98	150.88	116.40
1	A	37	VAL	CA-C-O	-21.30	95.75	120.67
1	B	350	ARG	NE-CZ-NH1	-21.30	100.20	121.50
1	A	504	ARG	CD-NE-CZ	20.03	152.44	124.40
1	B	504	ARG	CD-NE-CZ	19.87	152.21	124.40
1	A	7	PHE	CA-CB-CG	16.19	129.99	113.80
1	B	52	MET	CA-CB-CG	-15.97	82.16	114.10
1	A	52	MET	CA-CB-CG	-15.78	82.55	114.10
1	B	448	GLN	CG-CD-NE2	15.51	139.66	116.40
1	A	53	LYS	CB-CG-CD	-15.45	75.77	111.30
1	B	7	PHE	CA-CB-CG	14.26	128.06	113.80
1	B	53	LYS	CB-CG-CD	-13.88	79.38	111.30
1	B	7	PHE	N-CA-C	13.56	126.08	111.03
1	B	127	MET	CA-C-N	13.00	143.43	122.11
1	B	127	MET	C-N-CA	13.00	143.43	122.11
1	A	7	PHE	N-CA-C	12.74	124.86	110.97
1	A	53	LYS	N-CA-CB	11.91	128.72	111.21
1	B	211	ARG	CA-CB-CG	11.61	137.31	114.10
1	A	127	MET	CA-C-N	11.37	140.34	122.26
1	A	127	MET	C-N-CA	11.37	140.34	122.26
1	A	211	ARG	CA-CB-CG	11.25	136.60	114.10
1	B	37	VAL	CA-C-O	-11.03	108.81	120.39
1	A	341	LYS	CA-CB-CG	11.02	136.13	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CB-CG-CD	10.64	135.76	111.30
1	A	128	ASN	N-CA-C	10.45	127.31	113.72
1	B	552	GLN	CA-CB-CG	10.20	134.51	114.10
1	A	350	ARG	NE-CZ-NH2	9.74	127.97	119.20
1	B	221	LYS	CB-CG-CD	9.69	133.58	111.30
1	B	341	LYS	CA-CB-CG	9.68	133.46	114.10
1	A	221	LYS	CB-CG-CD	9.54	133.25	111.30
1	A	128	ASN	N-CA-CB	-9.51	96.67	110.65
1	B	128	ASN	N-CA-C	9.46	126.08	113.97
1	A	552	GLN	CA-CB-CG	9.02	132.13	114.10
1	A	128	ASN	CB-CA-C	-8.91	94.57	109.55
1	B	211	ARG	CB-CG-CD	8.90	131.78	111.30
1	A	6	GLU	CA-C-N	8.89	132.38	120.65
1	A	6	GLU	C-N-CA	8.89	132.38	120.65
1	B	128	ASN	CB-CA-C	-8.85	94.21	109.07
1	B	230	PRO	CA-C-N	8.77	132.39	120.38
1	B	230	PRO	C-N-CA	8.77	132.39	120.38
1	B	142	VAL	N-CA-CB	-8.35	96.92	112.36
1	B	128	ASN	N-CA-CB	-8.19	99.28	110.67
1	A	297	ARG	CD-NE-CZ	8.11	135.76	124.40
1	A	142	VAL	N-CA-CB	-8.06	97.44	112.36
1	B	6	GLU	CA-C-N	8.04	131.56	120.63
1	B	6	GLU	C-N-CA	8.04	131.56	120.63
1	B	560	LEU	CA-C-O	-8.02	107.16	120.80
1	A	37	VAL	CA-C-N	8.01	134.06	122.77
1	A	37	VAL	C-N-CA	8.01	134.06	122.77
1	B	558	TRP	N-CA-C	7.88	123.22	112.90
1	B	505	THR	CB-CA-C	-7.87	93.23	111.09
1	A	560	LEU	CA-C-O	-7.83	107.49	120.80
1	B	485	GLN	OE1-CD-NE2	-7.69	114.91	122.60
1	A	426	SER	N-CA-C	7.66	122.90	108.97
1	B	552	GLN	CB-CG-CD	7.59	125.50	112.60
1	A	552	GLN	CB-CG-CD	7.56	125.45	112.60
1	A	558	TRP	N-CA-C	7.54	122.78	112.90
1	A	51	TYR	N-CA-C	-7.45	103.17	111.82
1	A	336	ASP	CA-CB-CG	-7.42	105.17	112.60
1	A	304	ALA	N-CA-C	-7.38	102.93	112.23
1	B	509	PHE	CA-CB-CG	-7.38	106.42	113.80
1	B	518	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	B	457	THR	CB-CA-C	-7.32	93.32	109.56
1	A	457	THR	CB-CA-C	-7.30	93.36	109.56
1	A	177	LEU	CA-CB-CG	7.28	141.78	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	HIS	CA-CB-CG	-7.26	106.54	113.80
1	B	51	TYR	N-CA-C	-7.25	103.45	111.36
1	A	231	GLU	CA-C-O	7.21	128.41	120.63
1	A	405	ILE	CA-C-O	7.20	123.87	119.19
1	B	149	HIS	CA-CB-CG	-7.15	106.65	113.80
1	B	556	VAL	CA-C-N	7.14	130.15	120.44
1	B	556	VAL	C-N-CA	7.14	130.15	120.44
1	B	528	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	504	ARG	CG-CD-NE	7.11	127.64	112.00
1	B	504	ARG	CG-CD-NE	7.08	127.56	112.00
1	A	505	THR	CB-CA-C	-6.99	95.30	111.95
1	A	474	ASN	CA-CB-CG	6.96	119.56	112.60
1	A	385	PHE	N-CA-C	-6.96	99.92	110.50
1	A	419	ASN	CA-CB-CG	-6.93	105.67	112.60
1	A	129	ARG	CD-NE-CZ	6.87	134.01	124.40
1	B	194	TRP	CA-C-O	-6.86	113.28	120.55
1	A	471	ILE	CA-C-N	-6.82	113.65	123.06
1	A	471	ILE	C-N-CA	-6.82	113.65	123.06
1	B	303	MET	N-CA-C	6.78	120.89	111.74
1	B	419	ASN	CA-CB-CG	-6.73	105.87	112.60
1	A	196	MET	CG-SD-CE	6.60	115.43	100.90
1	B	426	SER	N-CA-C	6.59	120.97	108.97
1	A	240	HIS	CA-CB-CG	-6.56	107.24	113.80
1	A	8	ARG	CB-CG-CD	6.55	126.36	111.30
1	A	230	PRO	CA-C-N	6.48	129.26	120.38
1	A	230	PRO	C-N-CA	6.48	129.26	120.38
1	A	133	VAL	CA-C-N	6.45	131.23	122.84
1	A	133	VAL	C-N-CA	6.45	131.23	122.84
1	B	129	ARG	CD-NE-CZ	6.43	133.40	124.40
1	B	516	THR	O-C-N	-6.43	114.37	122.27
1	B	350	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	B	297	ARG	CG-CD-NE	-6.40	97.91	112.00
1	A	504	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	B	542	ALA	CB-CA-C	-6.39	106.66	111.20
1	A	431	VAL	N-CA-CB	6.37	118.65	112.28
1	A	244	TYR	N-CA-C	6.34	119.18	111.82
1	B	515	GLU	CA-C-N	6.34	129.95	120.31
1	B	515	GLU	C-N-CA	6.34	129.95	120.31
1	B	244	TYR	N-CA-C	6.33	118.26	111.36
1	A	487	LEU	CA-C-O	6.32	127.45	120.82
1	A	243	PRO	CB-CA-C	-6.29	102.92	112.11
1	B	347	ASN	OD1-CG-ND2	6.25	128.85	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	THR	CA-C-N	6.23	130.16	120.00
1	B	212	THR	C-N-CA	6.23	130.16	120.00
1	A	312	ARG	NE-CZ-NH1	-6.23	115.27	121.50
1	A	509	PHE	CA-CB-CG	-6.16	107.64	113.80
1	B	385	PHE	CA-CB-CG	6.15	119.95	113.80
1	B	504	ARG	CA-C-O	-6.14	114.13	120.89
1	A	430	LYS	CG-CD-CE	6.10	125.34	111.30
1	A	72	SER	N-CA-C	-6.10	104.91	112.90
1	B	160	LEU	CA-C-N	6.08	128.71	120.38
1	B	160	LEU	C-N-CA	6.08	128.71	120.38
1	A	296	ILE	N-CA-CB	-6.06	103.78	110.51
1	A	74	ILE	CA-C-O	-6.03	114.09	120.48
1	A	243	PRO	O-C-N	6.02	130.40	122.27
1	A	113	PRO	CA-C-O	-6.00	114.53	121.86
1	A	528	ASN	CA-CB-CG	-5.98	106.62	112.60
1	B	71	ALA	CA-C-O	-5.96	115.06	121.56
1	B	129	ARG	N-CA-C	5.95	119.60	110.20
1	B	303	MET	O-C-N	-5.95	114.44	122.41
1	A	37	VAL	O-C-N	-5.93	116.78	123.18
1	B	135	VAL	N-CA-C	5.91	116.08	110.53
1	A	516	THR	N-CA-CB	-5.87	101.18	110.28
1	B	330	ARG	N-CA-CB	-5.86	101.38	110.57
1	A	136	GLU	CA-CB-CG	5.85	125.80	114.10
1	A	290	LYS	CB-CG-CD	5.85	124.76	111.30
1	B	8	ARG	CB-CG-CD	5.85	124.75	111.30
1	B	304	ALA	N-CA-C	-5.83	104.52	111.69
1	A	482	ARG	CD-NE-CZ	5.83	132.56	124.40
1	B	471	ILE	CA-C-N	-5.83	115.02	123.06
1	B	471	ILE	C-N-CA	-5.83	115.02	123.06
1	B	415	ASP	CA-CB-CG	-5.79	106.81	112.60
1	B	506	HIS	N-CA-CB	-5.79	101.49	110.29
1	B	235	TRP	CA-C-O	-5.79	114.56	121.56
1	B	104	ARG	CD-NE-CZ	5.77	132.48	124.40
1	A	114	ARG	NE-CZ-NH2	-5.75	114.03	119.20
1	B	385	PHE	N-CA-C	-5.73	101.79	110.50
1	A	385	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	505	THR	N-CA-CB	5.72	120.76	111.21
1	A	461	GLY	N-CA-C	-5.70	103.87	112.60
1	B	53	LYS	N-CA-CB	5.68	119.56	111.21
1	B	211	ARG	N-CA-CB	5.66	121.25	111.00
1	B	347	ASN	CA-CB-CG	-5.64	106.96	112.60
1	B	372	LYS	CA-C-O	5.64	126.93	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	A	330	ARG	N-CA-CB	-5.63	101.73	110.57
1	B	177	LEU	CA-CB-CG	5.63	136.01	116.30
1	B	505	THR	N-CA-CB	5.63	120.45	111.56
1	A	6	GLU	CA-C-O	5.62	130.35	120.80
1	A	297	ARG	CG-CD-NE	-5.61	99.65	112.00
1	A	303	MET	N-CA-C	5.61	119.31	111.74
1	B	246	PHE	CA-C-O	-5.60	114.56	121.11
1	B	542	ALA	O-C-N	-5.58	118.96	121.53
1	B	136	GLU	CA-CB-CG	5.57	125.24	114.10
1	B	251	ASP	CA-C-N	5.57	127.10	120.14
1	B	251	ASP	C-N-CA	5.57	127.10	120.14
1	A	197	HIS	O-C-N	-5.55	116.53	122.85
1	A	236	SER	CA-CB-OG	-5.54	100.02	111.10
1	A	192	ASP	CA-CB-CG	-5.51	107.08	112.60
1	A	167	ASP	N-CA-CB	5.51	119.21	110.84
1	A	62	HIS	CA-C-N	5.50	129.35	120.82
1	A	62	HIS	C-N-CA	5.50	129.35	120.82
1	B	307	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	221	LYS	CG-CD-CE	5.50	123.94	111.30
1	B	377	ALA	CA-C-N	5.49	128.73	123.02
1	B	377	ALA	C-N-CA	5.49	128.73	123.02
1	B	183	ARG	CD-NE-CZ	5.49	132.09	124.40
1	B	221	LYS	CG-CD-CE	5.48	123.90	111.30
1	A	237	LYS	CA-C-O	-5.46	115.06	120.90
1	A	38	GLU	N-CA-CB	5.45	119.33	110.77
1	A	457	THR	N-CA-CB	5.45	121.67	111.53
1	A	70	LEU	N-CA-C	5.44	118.31	109.06
1	A	129	ARG	N-CA-C	5.42	118.77	110.20
1	B	516	THR	N-CA-CB	-5.40	101.91	110.28
1	B	180	ALA	O-C-N	5.39	128.30	122.15
1	B	398	ARG	CD-NE-CZ	5.39	131.95	124.40
1	B	124	GLY	N-CA-C	5.38	119.19	112.73
1	A	82	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	237	LYS	CG-CD-CE	5.37	123.65	111.30
1	A	552	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	A	242	PHE	CA-C-N	5.37	124.88	119.19
1	A	242	PHE	C-N-CA	5.37	124.88	119.19
1	B	412	LYS	CA-C-O	-5.36	113.00	119.49
1	A	505	THR	OG1-CB-CG2	5.36	120.02	109.30
1	A	183	ARG	CA-C-N	5.34	128.00	121.06
1	A	183	ARG	C-N-CA	5.34	128.00	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ARG	CA-C-N	5.34	124.98	119.05
1	A	297	ARG	C-N-CA	5.34	124.98	119.05
1	B	231	GLU	CG-CD-OE2	5.34	130.68	118.40
1	B	55	THR	CA-C-O	-5.31	115.54	121.81
1	A	8	ARG	CA-CB-CG	5.30	124.69	114.10
1	B	505	THR	CA-CB-OG1	5.29	117.54	109.60
1	B	130	VAL	N-CA-C	-5.27	99.88	107.37
1	B	123	MET	CA-C-N	5.25	125.81	119.98
1	B	123	MET	C-N-CA	5.25	125.81	119.98
1	B	426	SER	N-CA-CB	-5.24	101.65	111.24
1	A	504	ARG	CA-C-O	-5.22	115.15	120.89
1	A	130	VAL	N-CA-C	-5.21	99.98	107.37
1	B	231	GLU	CA-C-O	5.21	126.25	120.63
1	B	251	ASP	N-CA-C	5.20	117.35	111.11
1	B	350	ARG	NH1-CZ-NH2	5.20	126.06	119.30
1	A	525	LEU	CA-C-O	-5.19	115.35	120.70
1	A	518	ASN	N-CA-C	5.19	118.64	112.72
1	A	265	ILE	CA-C-O	-5.19	116.60	120.96
1	B	255	SER	N-CA-CB	5.19	118.72	110.57
1	B	158	ASN	O-C-N	-5.18	116.13	122.34
1	B	62	HIS	N-CA-C	5.17	117.67	109.96
1	B	296	ILE	N-CA-C	5.16	115.78	110.36
1	A	71	ALA	CA-C-O	-5.15	115.95	121.56
1	A	30	ARG	CA-CB-CG	5.15	124.39	114.10
1	B	143	GLU	N-CA-C	-5.14	104.15	110.31
1	B	100	ILE	CA-C-O	-5.13	116.28	121.67
1	A	187	TYR	N-CA-C	5.12	119.06	112.41
1	B	430	LYS	CG-CD-CE	5.11	123.06	111.30
1	A	396	ARG	CD-NE-CZ	5.11	131.55	124.40
1	B	276	TYR	CA-C-O	-5.11	114.26	120.54
1	A	330	ARG	NE-CZ-NH2	5.09	123.79	119.20
1	B	419	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	B	303	MET	N-CA-CB	-5.08	104.46	112.13
1	B	460	VAL	N-CA-C	5.07	115.64	107.73
1	A	373	ASP	N-CA-C	5.07	116.49	111.07
1	A	38	GLU	CA-C-O	-5.07	114.87	120.24
1	B	38	GLU	CB-CG-CD	5.06	121.20	112.60
1	B	254	PHE	CA-C-O	-5.06	113.31	119.43
1	B	74	ILE	CA-C-O	-5.04	115.14	120.48
1	A	38	GLU	N-CA-C	5.04	116.60	108.34
1	B	72	SER	N-CA-C	-5.04	106.30	112.90
1	A	304	ALA	CA-C-O	5.02	125.72	119.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	HIS	N-CA-C	5.02	117.43	109.96
1	B	494	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	237	LYS	CA-C-O	-5.00	115.55	120.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	ARG	Sidechain
1	B	350	ARG	Sidechain

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	4346	0	4288	85	4
1	B	4346	0	4288	100	4
2	A	53	0	31	6	0
2	B	53	0	31	8	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	207	0	0	5	0
4	B	165	0	0	6	0
All	All	9178	0	8644	186	4

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 11.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:FAD:C5B	2:B:600:FAD:H8A	1.66	1.25
2:A:600:FAD:H51A	2:A:600:FAD:C8A	1.69	1.20
2:A:600:FAD:H8A	2:A:600:FAD:C5B	1.73	1.19
2:B:600:FAD:H51A	2:B:600:FAD:C8A	1.73	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLY:H	1:B:352:ASN:HD21	1.09	0.99
1:A:349:GLY:H	1:A:352:ASN:HD21	0.99	0.97
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.81	0.95
1:B:550:PRO:HB2	1:B:552:GLN:HE22	1.35	0.91
1:B:550:PRO:HB2	1:B:552:GLN:NE2	1.89	0.88
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.56	0.86
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.59	0.85
2:B:600:FAD:H8A	2:B:600:FAD:H51A	0.84	0.80
1:A:550:PRO:HB2	1:A:552:GLN:HE22	1.46	0.79
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.66	0.78
1:A:516:THR:HG21	4:A:2173:HOH:O	1.86	0.76
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.68	0.76
2:B:600:FAD:H9	2:B:600:FAD:O2'	1.90	0.71
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.74	0.70
1:A:167:ASP:OD1	1:A:186:GLY:HA3	1.94	0.68
1:A:428:ILE:HD11	1:A:503:TYR:HB3	1.76	0.66
2:B:600:FAD:C5B	2:B:600:FAD:C8A	2.51	0.65
1:A:349:GLY:N	1:A:352:ASN:HD21	1.83	0.65
1:A:195:MET:HE1	1:B:195:MET:SD	2.37	0.65
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.78	0.65
1:B:79:ASN:ND2	1:B:82:ASP:H	1.95	0.64
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.32	0.64
2:A:600:FAD:H51A	2:A:600:FAD:H8A	0.78	0.64
1:B:79:ASN:HD22	1:B:82:ASP:H	1.44	0.64
1:B:194:TRP:O	1:B:197:HIS:HD2	1.81	0.64
1:B:310:THR:HG22	1:B:459:THR:HG22	1.80	0.63
1:B:480:GLN:O	1:B:484:VAL:HG23	1.99	0.63
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.80	0.63
1:B:505:THR:HG23	4:B:2133:HOH:O	1.99	0.63
1:A:79:ASN:ND2	1:A:82:ASP:H	1.97	0.63
1:B:167:ASP:OD1	1:B:186:GLY:HA3	1.98	0.63
1:A:188:THR:HB	1:A:189:PRO:CD	2.30	0.62
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.29	0.62
1:B:188:THR:HB	1:B:189:PRO:CD	2.30	0.61
1:A:194:TRP:O	1:A:197:HIS:HD2	1.83	0.60
1:B:51:TYR:CE1	1:B:104:ARG:HD3	2.36	0.60
1:B:304:ALA:HB2	4:B:2103:HOH:O	2.01	0.60
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.82	0.60
1:B:516:THR:HG21	4:B:2131:HOH:O	2.01	0.60
1:A:310:THR:HG22	1:A:459:THR:HG22	1.83	0.60
1:B:552:GLN:NE2	1:B:552:GLN:H	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.37	0.59
1:A:513:ILE:O	1:A:516:THR:HB	2.02	0.59
1:B:282:THR:HG22	1:B:352:ASN:HD22	1.67	0.59
1:A:244:TYR:OH	1:B:195:MET:HG2	2.04	0.58
1:B:438:MET:HG2	1:B:500:TRP:HH2	1.67	0.58
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.85	0.58
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.33	0.58
1:A:349:GLY:H	1:A:352:ASN:ND2	1.84	0.58
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.69	0.57
1:B:349:GLY:H	1:B:352:ASN:ND2	1.92	0.57
1:B:133:VAL:HG11	1:B:160:LEU:HD13	1.86	0.57
1:B:51:TYR:CZ	1:B:104:ARG:HD3	2.40	0.57
1:B:229:LYS:HD2	1:B:231:GLU:OE2	2.04	0.56
2:B:600:FAD:O2'	2:B:600:FAD:C9	2.52	0.56
1:A:333:PRO:HB2	1:A:448:GLN:NE2	2.20	0.56
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.42	0.55
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.89	0.55
1:A:438:MET:HG2	1:A:500:TRP:HH2	1.71	0.55
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.42	0.55
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.22	0.55
1:B:149:HIS:HD1	1:B:408:TYR:HH	1.53	0.54
1:B:513:ILE:O	1:B:516:THR:HB	2.06	0.54
1:B:428:ILE:HD11	1:B:503:TYR:HB3	1.88	0.54
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.88	0.54
1:A:195:MET:SD	1:B:195:MET:HE1	2.48	0.54
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.37	0.53
1:B:200:MET:HE3	1:B:265:ILE:HD12	1.90	0.53
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.91	0.53
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.92	0.53
1:B:310:THR:CG2	1:B:459:THR:HG22	2.39	0.53
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.23	0.52
1:B:40:ILE:HD11	1:B:74:ILE:CD1	2.39	0.52
1:A:51:TYR:CZ	1:A:104:ARG:HD3	2.44	0.52
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.91	0.52
1:B:419:ASN:HB2	1:B:474:ASN:OD1	2.09	0.52
1:B:90:ALA:HB1	1:B:95:PHE:O	2.09	0.52
1:B:457:THR:HG21	4:B:2104:HOH:O	2.09	0.51
2:A:600:FAD:C8A	2:A:600:FAD:C5B	2.57	0.51
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.44	0.51
1:A:505:THR:HG23	4:A:2174:HOH:O	2.11	0.51
1:A:40:ILE:HD11	1:A:74:ILE:CD1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HB	2:B:600:FAD:O2P	2.11	0.51
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.40	0.51
1:A:79:ASN:HD22	1:A:82:ASP:H	1.59	0.51
1:B:333:PRO:HB2	1:B:448:GLN:OE1	2.11	0.50
1:B:464:GLU:OE1	1:B:466:HIS:ND1	2.40	0.50
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.47	0.50
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.41	0.50
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.68	0.50
1:A:414:ILE:HD11	2:A:600:FAD:HM81	1.92	0.50
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.47	0.50
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.46	0.50
1:B:271:PRO:O	1:B:272:ASN:C	2.54	0.50
1:A:257:SER:HA	4:A:2107:HOH:O	2.12	0.50
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.41	0.50
1:B:189:PRO:CG	1:B:270:MET:HE1	2.41	0.49
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.95	0.49
1:A:552:GLN:NE2	1:A:552:GLN:H	2.09	0.49
1:A:51:TYR:CE1	1:A:104:ARG:HD3	2.47	0.49
1:A:361:GLU:N	1:A:362:PRO:HD2	2.28	0.49
2:A:600:FAD:H9	2:A:600:FAD:O2'	2.12	0.49
1:B:312:ARG:HD3	1:B:354:TYR:CE1	2.48	0.49
1:B:361:GLU:N	1:B:362:PRO:HD2	2.27	0.49
1:A:62:HIS:O	1:A:481:LYS:HE3	2.13	0.49
1:B:198:SER:O	1:B:240:HIS:HD2	1.96	0.49
1:A:90:ALA:HB1	1:A:95:PHE:O	2.13	0.48
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.95	0.48
1:A:188:THR:CB	1:A:189:PRO:CD	2.91	0.48
1:A:480:GLN:O	1:A:484:VAL:HG23	2.13	0.48
1:A:312:ARG:HD3	1:A:354:TYR:CE1	2.47	0.48
1:B:349:GLY:N	1:B:352:ASN:HD21	1.93	0.48
1:B:28:ILE:O	1:B:32:VAL:HG22	2.14	0.48
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.95	0.47
1:B:188:THR:CB	1:B:189:PRO:CD	2.91	0.47
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.95	0.47
1:A:195:MET:HG2	1:B:244:TYR:OH	2.15	0.47
1:B:518:ASN:O	1:B:519:TRP:C	2.57	0.47
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.97	0.47
1:A:330:ARG:NH2	1:A:333:PRO:O	2.47	0.47
1:A:290:LYS:HB2	1:A:437:MET:CG	2.44	0.47
1:B:471:ILE:HG21	1:B:484:VAL:HG13	1.96	0.47
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:THR:HG22	1:B:506:HIS:H	1.80	0.47
1:A:310:THR:CG2	1:A:459:THR:HG22	2.44	0.46
1:A:387:GLU:HG2	4:A:2136:HOH:O	2.16	0.46
1:B:79:ASN:HD22	1:B:79:ASN:C	2.24	0.46
1:B:309:PRO:HB2	1:B:353:PHE:CE1	2.51	0.46
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.98	0.45
1:A:419:ASN:HB2	1:A:474:ASN:OD1	2.17	0.45
1:A:133:VAL:HG11	1:A:160:LEU:HD13	1.97	0.45
1:A:7:PHE:HB3	4:A:2007:HOH:O	2.16	0.45
1:A:198:SER:O	1:A:240:HIS:HD2	2.00	0.45
1:A:518:ASN:O	1:A:519:TRP:C	2.58	0.45
1:A:107:GLY:HA2	1:A:422:ALA:O	2.17	0.45
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.98	0.45
1:A:28:ILE:O	1:A:32:VAL:HG22	2.16	0.45
1:A:330:ARG:NH1	1:A:338:GLU:OE1	2.50	0.45
1:A:229:LYS:HD2	1:A:231:GLU:OE2	2.18	0.44
1:A:271:PRO:O	1:A:272:ASN:C	2.58	0.44
1:A:427:PRO:HA	1:A:502:GLU:HA	2.00	0.44
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.52	0.44
1:A:187:TYR:O	1:A:307:ASN:HB2	2.17	0.44
1:B:28:ILE:HG12	1:B:89:LEU:HD12	2.00	0.44
1:B:330:ARG:NH2	1:B:333:PRO:O	2.48	0.44
1:A:149:HIS:ND1	1:A:408:TYR:OH	2.45	0.43
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.53	0.43
1:B:62:HIS:O	1:B:481:LYS:HE3	2.18	0.43
1:B:188:THR:HB	1:B:189:PRO:HD2	1.99	0.43
1:A:188:THR:HB	1:A:189:PRO:HD3	2.00	0.43
1:B:51:TYR:O	1:B:54:PRO:HD3	2.19	0.43
1:B:290:LYS:HB2	1:B:437:MET:HG3	2.01	0.43
1:A:108:TYR:CZ	1:A:504:ARG:HG2	2.54	0.42
1:B:123:MET:O	1:B:127:MET:HB2	2.19	0.42
1:B:257:SER:HA	4:B:2154:HOH:O	2.18	0.42
1:B:433:GLY:O	1:B:437:MET:HG2	2.18	0.42
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.55	0.42
1:B:102:ILE:CG1	1:B:175:SER:HB2	2.49	0.42
1:B:417:LEU:HB3	1:B:418:PRO:HD2	2.02	0.42
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.50	0.42
1:B:101:SER:O	1:B:124:GLY:HA3	2.20	0.42
1:B:169:PRO:HB3	2:B:600:FAD:N3	2.34	0.42
1:B:194:TRP:O	1:B:197:HIS:CD2	2.65	0.42
1:A:38:GLU:N	1:A:74:ILE:O	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PRO:HA	1:B:177:LEU:HG	2.01	0.41
1:B:183:ARG:HG2	1:B:194:TRP:HB2	2.02	0.41
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.55	0.41
1:B:312:ARG:CG	1:B:457:THR:HG23	2.48	0.41
1:A:477:ASP:O	1:A:481:LYS:HG3	2.20	0.41
1:B:143:GLU:HB3	1:B:144:PRO:HD2	2.02	0.41
1:B:224:GLU:H	1:B:224:GLU:CD	2.28	0.41
1:B:333:PRO:CB	1:B:448:GLN:OE1	2.68	0.41
1:A:312:ARG:HD3	1:A:354:TYR:CD1	2.56	0.41
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.85	0.41
1:A:332:GLU:HB3	1:A:333:PRO:CD	2.51	0.41
1:A:143:GLU:HB3	1:A:144:PRO:CD	2.52	0.40
1:B:545:LYS:HD2	4:B:2155:HOH:O	2.20	0.40
1:B:545:LYS:O	1:B:546:SER:HB2	2.21	0.40
1:B:210:LEU:HD23	1:B:210:LEU:C	2.46	0.40
1:B:555:HIS:HB3	1:B:559:LYS:HE3	2.04	0.40
1:B:231:GLU:H	1:B:231:GLU:HG3	1.31	0.40
1:A:98:TRP:CG	1:A:113:PRO:HA	2.57	0.40

All (4) 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:37:VAL:O	1:B:391:GLU:OE2[6_655]	1.81	0.39
1:A:50:SER:OG	1:B:412:LYS:NZ[6_655]	1.94	0.26
1:A:419:ASN:OD1	1:B:329:SER:OG[6_655]	2.16	0.04
1:A:373:ASP:OD2	1:B:288:ASP:OD1[4_665]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/560 (98%)	523 (96%)	23 (4%)	0	100	100
1	B	546/560 (98%)	523 (96%)	23 (4%)	0	100	100
All	All	1092/1120 (98%)	1046 (96%)	46 (4%)	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	469/480 (98%)	442 (94%)	27 (6%)	18	22
1	B	469/480 (98%)	447 (95%)	22 (5%)	23	31
All	All	938/960 (98%)	889 (95%)	49 (5%)	21	26

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	8	ARG
1	A	25	ILE
1	A	41	SER
1	A	53	LYS
1	A	63	VAL
1	A	79	ASN
1	A	128	ASN
1	A	142	VAL
1	A	175	SER
1	A	177	LEU
1	A	200	MET
1	A	231	GLU
1	A	301	LEU
1	A	303	MET
1	A	329	SER
1	A	331	THR
1	A	336	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	387	GLU
1	A	391	GLU
1	A	457	THR
1	A	472	VAL
1	A	502	GLU
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	552	GLN
1	B	7	PHE
1	B	8	ARG
1	B	25	ILE
1	B	63	VAL
1	B	79	ASN
1	B	128	ASN
1	B	142	VAL
1	B	177	LEU
1	B	200	MET
1	B	231	GLU
1	B	301	LEU
1	B	303	MET
1	B	329	SER
1	B	331	THR
1	B	336	ASP
1	B	391	GLU
1	B	448	GLN
1	B	457	THR
1	B	472	VAL
1	B	505	THR
1	B	516	THR
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	84	GLN
1	A	128	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	439	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	467	HIS
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	79	ASN
1	B	84	GLN
1	B	126	ASN
1	B	128	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	467	HIS
1	B	520	ASN
1	B	552	GLN
1	B	555	HIS

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	600	-	58,58,58	2.55	12 (20%)	85,89,89	1.85	24 (28%)
2	FAD	A	600	-	58,58,58	2.63	13 (22%)	85,89,89	1.67	24 (28%)
3	ACT	B	601	-	3,3,3	0.95	0	3,3,3	0.29	0
3	ACT	A	601	-	3,3,3	0.88	0	3,3,3	0.83	0

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	-	-	10/34/50/50	0/6/6/6
2	FAD	A	600	-	-	6/34/50/50	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-15.40	1.42	1.59
2	B	600	FAD	P-O3P	-14.66	1.43	1.59
2	A	600	FAD	PA-O3P	-4.81	1.54	1.59
2	B	600	FAD	O5'-C5'	4.58	1.62	1.44
2	A	600	FAD	PA-O2A	-4.52	1.34	1.55
2	B	600	FAD	PA-O3P	-4.45	1.54	1.59
2	B	600	FAD	PA-O2A	-4.17	1.36	1.55
2	A	600	FAD	P-O2P	-3.64	1.38	1.55
2	A	600	FAD	O5'-C5'	3.49	1.57	1.44
2	B	600	FAD	P-O2P	-3.21	1.40	1.55
2	B	600	FAD	O4B-C1B	3.19	1.49	1.42
2	B	600	FAD	C1'-C2'	3.04	1.56	1.52
2	A	600	FAD	PA-O5B	-3.01	1.47	1.59
2	A	600	FAD	O2-C2	-2.80	1.18	1.24
2	A	600	FAD	C6-C7	-2.65	1.36	1.39
2	B	600	FAD	O4'-C4'	2.59	1.48	1.43
2	B	600	FAD	O2-C2	-2.52	1.19	1.24
2	B	600	FAD	C6-C7	-2.36	1.36	1.39
2	A	600	FAD	C5X-N5	-2.23	1.35	1.39
2	A	600	FAD	O4B-C1B	2.23	1.47	1.42
2	B	600	FAD	C2-N3	2.15	1.43	1.39
2	A	600	FAD	C2-N1	-2.15	1.31	1.36
2	A	600	FAD	C10-N10	-2.12	1.32	1.37
2	A	600	FAD	C5A-C6A	2.06	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C5A-C6A	2.05	1.46	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O3P-PA-O1A	4.85	125.28	110.70
2	B	600	FAD	O5B-PA-O1A	-4.23	92.17	108.94
2	B	600	FAD	O2P-P-O3P	4.00	118.09	107.27
2	A	600	FAD	O5B-PA-O1A	-3.96	93.23	108.94
2	A	600	FAD	C2A-N1A-C6A	3.87	125.08	118.73
2	B	600	FAD	C9A-C5X-N5	3.54	126.21	122.45
2	B	600	FAD	C4X-C10-N10	3.39	121.33	116.48
2	A	600	FAD	O4B-C4B-C5B	-3.36	98.58	109.33
2	B	600	FAD	C4A-N9A-C1B	-3.35	118.79	126.63
2	B	600	FAD	N6A-C6A-N1A	3.31	125.75	118.38
2	A	600	FAD	N3A-C2A-N1A	-3.27	123.63	128.58
2	A	600	FAD	O2A-PA-O3P	-3.13	98.82	107.27
2	B	600	FAD	C4-N3-C2	-3.07	120.19	125.64
2	A	600	FAD	C4A-N9A-C1B	-2.87	119.93	126.63
2	A	600	FAD	C4X-C10-N10	2.83	120.53	116.48
2	B	600	FAD	O4B-C4B-C5B	-2.83	100.28	109.33
2	B	600	FAD	O2A-PA-O3P	-2.82	99.66	107.27
2	B	600	FAD	O3P-P-O1P	-2.77	102.38	110.70
2	A	600	FAD	C1B-N9A-C8A	2.74	133.18	127.09
2	B	600	FAD	O3B-C3B-C4B	2.73	118.93	111.08
2	A	600	FAD	O2P-P-O1P	2.66	124.83	112.44
2	B	600	FAD	C1B-N9A-C8A	2.62	132.91	127.09
2	B	600	FAD	C5A-C4A-N9A	-2.58	103.00	105.81
2	B	600	FAD	C2A-N1A-C6A	2.56	122.94	118.73
2	B	600	FAD	C5X-C9A-N10	-2.55	115.66	117.97
2	A	600	FAD	C5A-C4A-N9A	-2.52	103.07	105.81
2	B	600	FAD	O3'-C3'-C2'	-2.51	103.24	108.93
2	B	600	FAD	O4B-C1B-N9A	-2.50	103.29	108.09
2	A	600	FAD	C9A-C9-C8	2.47	124.19	119.22
2	A	600	FAD	O2P-P-O3P	2.47	113.95	107.27
2	B	600	FAD	C2B-C1B-N9A	2.44	119.36	113.30
2	A	600	FAD	O4B-C1B-N9A	-2.42	103.44	108.09
2	B	600	FAD	C4A-N9A-C8A	2.39	108.25	105.74
2	A	600	FAD	C4-N3-C2	-2.36	121.45	125.64
2	A	600	FAD	PA-O5B-C5B	2.32	134.63	121.35
2	B	600	FAD	C4B-O4B-C1B	-2.32	104.35	109.47
2	B	600	FAD	C5A-C4A-N3A	2.30	129.88	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C9-C8-C7	-2.29	116.33	119.69
2	A	600	FAD	O3P-P-O1P	-2.25	103.93	110.70
2	A	600	FAD	O5'-P-O1P	-2.25	100.04	108.94
2	A	600	FAD	O2A-PA-O5B	2.24	117.72	107.57
2	A	600	FAD	C9A-C5X-N5	2.23	124.82	122.45
2	B	600	FAD	N9A-C8A-N7A	-2.22	110.79	113.94
2	A	600	FAD	C6A-C5A-C4A	-2.15	114.25	117.18
2	A	600	FAD	C9-C9A-N10	2.12	124.70	121.85
2	B	600	FAD	C5X-C6-C7	2.10	124.71	120.83
2	A	600	FAD	O3P-PA-O1A	2.09	117.00	110.70
2	A	600	FAD	C10-N1-C2	2.06	121.31	116.85

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5'-O5'-P-O1P
2	A	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C5B-O5B-PA-O1A
2	B	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	C3B-C4B-C5B-O5B
2	B	600	FAD	P-O3P-PA-O2A

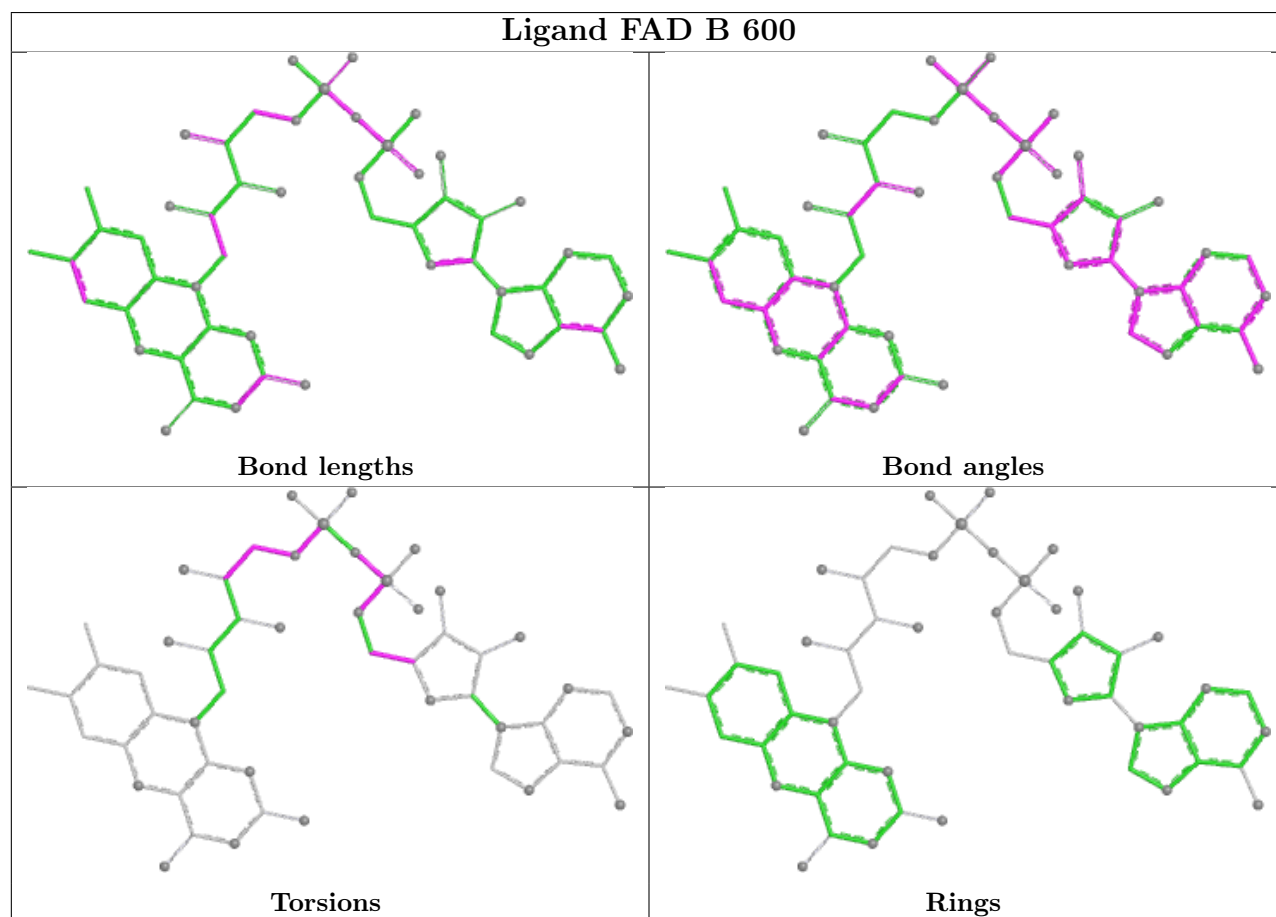
There are no ring outliers.

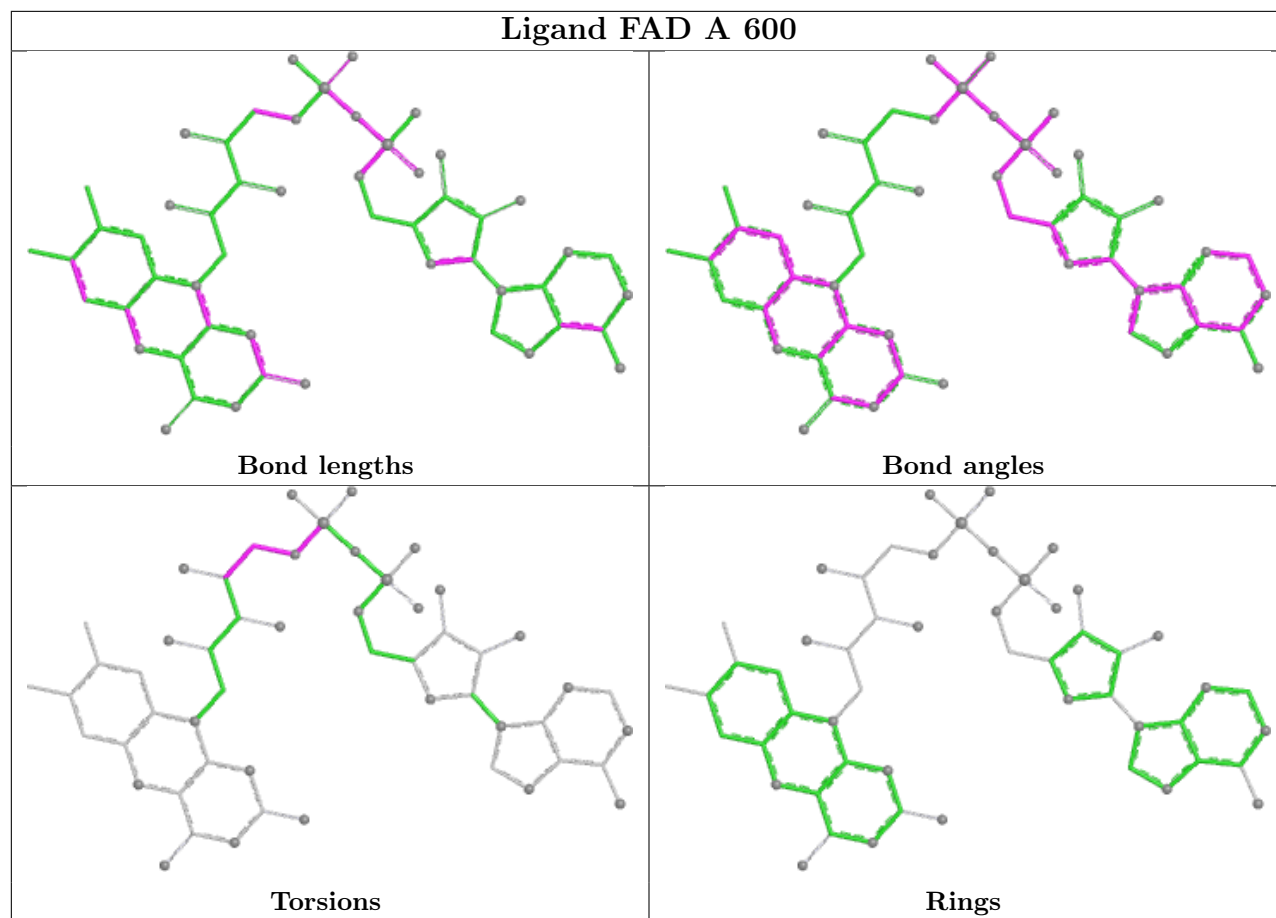
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	8	0
2	A	600	FAD	6	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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.