



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:24 AM UTC

PDB ID : 1E8G / pdb_00001e8g
Title : STRUCTURE OF THE H61T DOUBLE MUTANT OF VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH FLUORO-CRESOL
Authors : Fraaije, M.W.; Mattevi, A.
Deposited on : 2000-09-20
Resolution : 2.10 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

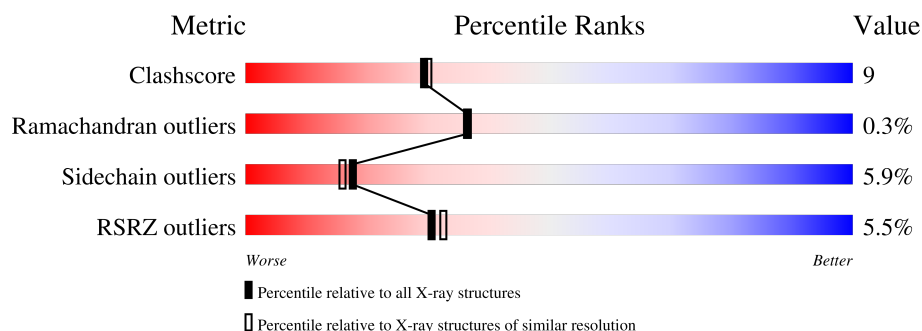
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	4% 71% 22% • • •
1	B	560	6% 70% 22% • • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9209 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	110	0	0
			4348	2791	742	791	24			
1	B	550	Total	C	N	O	S	110	0	0
			4348	2791	742	791	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	HIS	engineered mutation	UNP P56216
B	61	THR	HIS	engineered mutation	UNP P56216

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



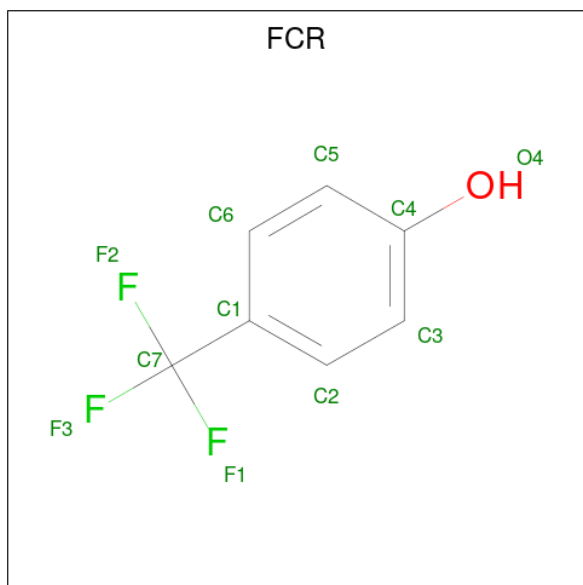
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



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

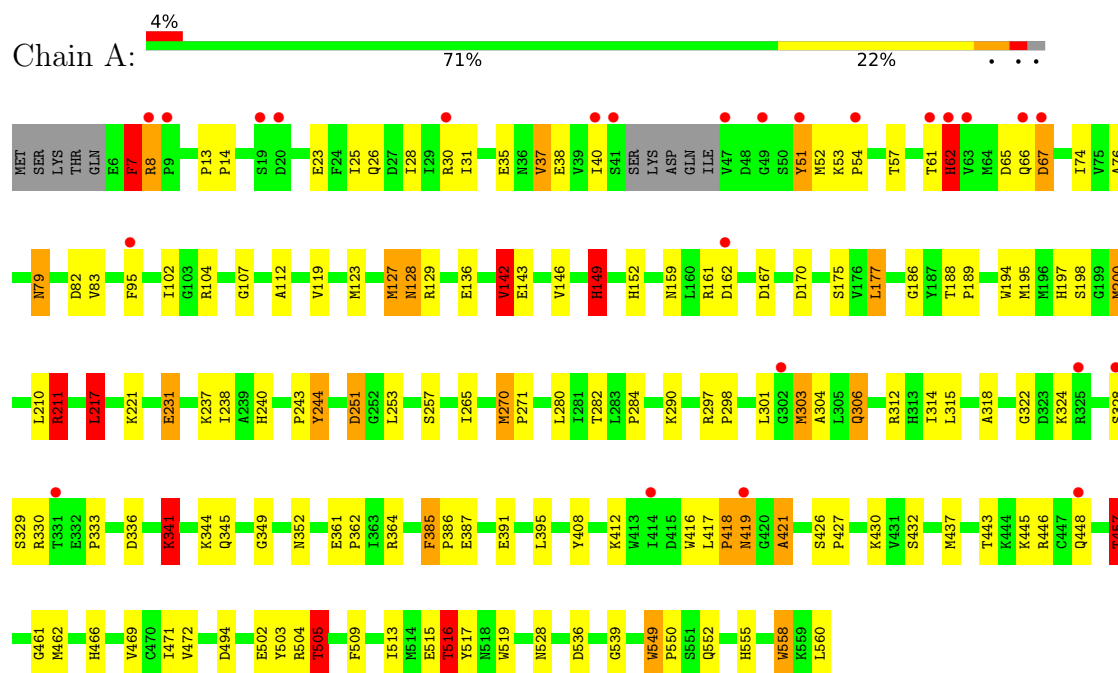
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	204	Total	O	0	0
			204	204		

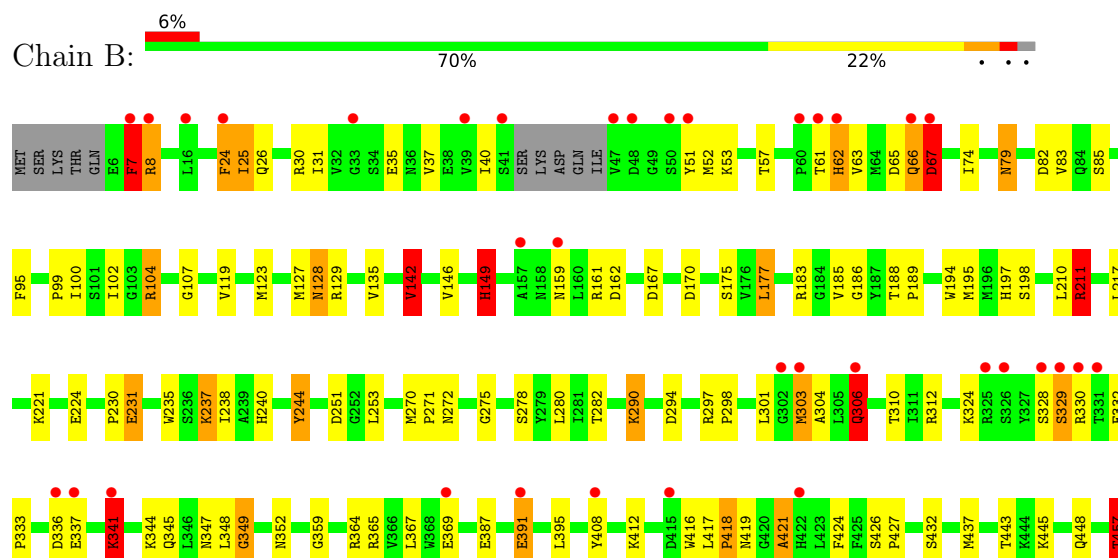
3 Residue-property plots [i](#)

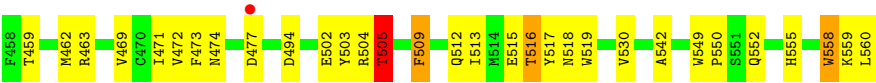
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	130.29Å 130.29Å 132.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 15.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.10) 98.6 (15.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.258 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.009 for -l,-k,-h 0.011 for -h,-l,-k 0.000 for -h,l,k 0.023 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9209	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 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	1.20	18/4466 (0.4%)	1.93	109/6070 (1.8%)
1	B	1.34	23/4466 (0.5%)	1.86	105/6070 (1.7%)
All	All	1.27	41/8932 (0.5%)	1.89	214/12140 (1.8%)

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	3	1
1	B	4	1
All	All	7	2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GLN	CA-CB	-35.65	0.94	1.53
1	B	161	ARG	CB-CG	-31.77	0.57	1.52
1	B	52	MET	CB-CG	30.66	2.44	1.52
1	A	52	MET	CB-CG	30.66	2.44	1.52
1	A	161	ARG	CB-CG	-30.18	0.61	1.52
1	B	344	LYS	CB-CG	-24.14	0.80	1.52
1	B	65	ASP	CA-CB	-23.69	1.16	1.53
1	A	344	LYS	CB-CG	-22.07	0.86	1.52
1	B	341	LYS	CB-CG	-20.15	0.92	1.52
1	A	341	LYS	CB-CG	-20.14	0.92	1.52
1	A	53	LYS	CA-CB	17.01	1.75	1.53
1	A	7	PHE	CA-CB	16.68	1.80	1.53
1	B	7	PHE	CA-CB	15.70	1.78	1.53
1	B	53	LYS	CA-CB	14.04	1.71	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLN	CA-CB	-13.69	1.31	1.53
1	B	53	LYS	CB-CG	13.31	1.92	1.52
1	A	53	LYS	CB-CG	13.28	1.92	1.52
1	B	8	ARG	CA-CB	-13.03	1.34	1.52
1	A	67	ASP	CA-CB	-11.09	1.39	1.54
1	B	221	LYS	CG-CD	-10.30	1.21	1.52
1	A	30	ARG	CA-CB	-10.07	1.37	1.53
1	B	332	GLU	CA-CB	-9.96	1.39	1.53
1	A	8	ARG	CA-CB	-9.24	1.40	1.52
1	A	445	LYS	CG-CD	8.91	1.79	1.52
1	B	67	ASP	CA-CB	-8.80	1.38	1.53
1	A	65	ASP	CA-CB	-7.98	1.40	1.53
1	B	341	LYS	CA-CB	-7.14	1.42	1.53
1	B	26	GLN	CA-CB	-6.76	1.42	1.53
1	B	159	ASN	CA-CB	-6.42	1.44	1.53
1	A	23	GLU	CB-CG	6.31	1.71	1.52
1	A	221	LYS	CG-CD	-5.98	1.34	1.52
1	B	445	LYS	CG-CD	5.61	1.69	1.52
1	B	30	ARG	CA-CB	-5.49	1.44	1.53
1	B	128	ASN	CA-CB	5.41	1.61	1.54
1	B	7	PHE	CB-CG	5.39	1.63	1.50
1	A	7	PHE	CB-CG	5.38	1.63	1.50
1	B	349	GLY	N-CA	5.36	1.49	1.44
1	A	159	ASN	CA-CB	-5.33	1.46	1.53
1	B	303	MET	CA-CB	5.15	1.60	1.53
1	A	8	ARG	CB-CG	5.12	1.67	1.52
1	B	8	ARG	CB-CG	5.11	1.67	1.52

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CD-NE-CZ	30.42	166.99	124.40
1	A	211	ARG	CD-NE-CZ	29.60	165.84	124.40
1	A	67	ASP	CB-CA-C	27.02	150.85	110.04
1	A	37	VAL	CA-C-O	-21.86	98.89	120.31
1	B	67	ASP	CB-CA-C	20.33	150.88	110.42
1	A	7	PHE	N-CA-C	17.86	133.66	111.69
1	B	7	PHE	N-CA-C	16.40	135.25	112.45
1	B	330	ARG	N-CA-CB	-16.10	86.98	110.17
1	A	52	MET	CA-CB-CG	-16.02	82.07	114.10
1	B	52	MET	CA-CB-CG	-15.68	82.73	114.10
1	A	53	LYS	CB-CG-CD	-15.45	75.77	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	LYS	CB-CG-CD	-15.45	75.77	111.30
1	B	303	MET	CB-CA-C	15.18	143.84	110.76
1	A	330	ARG	N-CA-CB	-15.15	88.36	110.17
1	B	221	LYS	CB-CG-CD	14.17	143.90	111.30
1	B	162	ASP	CA-CB-CG	-13.02	99.58	112.60
1	B	66	GLN	N-CA-CB	12.83	128.83	109.97
1	A	7	PHE	N-CA-CB	-12.58	91.46	110.20
1	B	185	VAL	CA-C-N	12.54	132.35	121.82
1	B	185	VAL	C-N-CA	12.54	132.35	121.82
1	B	211	ARG	CA-CB-CG	12.44	138.98	114.10
1	A	53	LYS	N-CA-CB	12.22	129.18	111.21
1	A	419	ASN	CA-CB-CG	-12.18	100.42	112.60
1	B	65	ASP	CB-CA-C	11.71	135.73	110.19
1	A	303	MET	CB-CA-C	11.66	136.18	110.76
1	B	7	PHE	N-CA-CB	-11.47	93.16	110.26
1	B	161	ARG	CA-CB-CG	11.45	137.00	114.10
1	A	67	ASP	N-CA-CB	-11.35	96.75	114.45
1	A	221	LYS	CB-CG-CD	11.01	136.61	111.30
1	B	53	LYS	N-CA-CB	10.87	129.34	111.30
1	A	364	ARG	CD-NE-CZ	10.73	139.42	124.40
1	B	221	LYS	CG-CD-CE	10.65	135.80	111.30
1	B	35	GLU	CB-CG-CD	-10.59	94.59	112.60
1	A	161	ARG	CB-CG-CD	10.44	135.32	111.30
1	A	161	ARG	CA-CB-CG	10.38	134.86	114.10
1	A	162	ASP	CA-CB-CG	-10.36	102.24	112.60
1	B	303	MET	N-CA-CB	-10.25	94.10	113.89
1	A	35	GLU	CB-CG-CD	-10.01	95.58	112.60
1	A	37	VAL	O-C-N	-9.97	113.36	123.03
1	B	161	ARG	CB-CG-CD	9.81	133.87	111.30
1	A	65	ASP	CA-CB-CG	-9.76	102.84	112.60
1	B	66	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	A	66	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	A	221	LYS	CG-CD-CE	9.48	133.09	111.30
1	B	128	ASN	N-CA-CB	-9.38	97.93	110.88
1	A	128	ASN	N-CA-CB	-9.36	96.89	110.65
1	A	128	ASN	N-CA-C	9.24	125.73	113.72
1	A	344	LYS	CA-CB-CG	-9.14	95.82	114.10
1	B	231	GLU	CB-CG-CD	9.11	128.09	112.60
1	B	128	ASN	CB-CA-C	-9.10	94.09	109.38
1	A	128	ASN	CB-CA-C	-9.06	94.34	109.55
1	B	412	LYS	CB-CG-CD	-9.01	90.59	111.30
1	A	211	ARG	CA-CB-CG	8.88	131.86	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	VAL	N-CA-CB	-8.81	95.45	111.92
1	A	66	GLN	CB-CA-C	8.69	124.14	109.72
1	B	303	MET	CA-CB-CG	8.68	131.47	114.10
1	B	306	GLN	OE1-CD-NE2	-8.68	113.92	122.60
1	B	560	LEU	CA-C-O	-8.63	106.12	120.80
1	B	306	GLN	CB-CG-CD	8.56	127.16	112.60
1	A	149	HIS	CA-CB-CG	-8.53	105.27	113.80
1	A	211	ARG	CB-CG-CD	8.45	130.74	111.30
1	B	127	MET	CA-C-N	8.42	135.46	122.23
1	B	127	MET	C-N-CA	8.42	135.46	122.23
1	B	142	VAL	N-CA-CB	-8.32	96.35	111.92
1	B	149	HIS	CA-CB-CG	-8.23	105.57	113.80
1	B	344	LYS	CA-CB-CG	-8.22	97.66	114.10
1	A	505	THR	N-CA-CB	8.19	124.50	111.56
1	B	230	PRO	CA-C-N	8.16	131.56	120.38
1	B	230	PRO	C-N-CA	8.16	131.56	120.38
1	A	30	ARG	N-CA-CB	8.16	121.84	110.01
1	A	306	GLN	CB-CG-CD	8.14	126.44	112.60
1	A	426	SER	N-CA-C	8.06	123.13	108.94
1	B	419	ASN	CA-CB-CG	-8.06	104.54	112.60
1	A	505	THR	CB-CA-C	-7.95	93.04	111.09
1	A	7	PHE	CA-CB-CG	7.94	121.74	113.80
1	B	128	ASN	N-CA-C	7.74	124.88	114.12
1	A	344	LYS	CB-CG-CD	-7.71	93.57	111.30
1	B	494	ASP	CA-CB-CG	7.69	120.29	112.60
1	B	505	THR	CB-CA-C	-7.64	93.76	111.95
1	B	364	ARG	CD-NE-CZ	7.63	135.08	124.40
1	A	560	LEU	CA-C-O	-7.48	108.09	120.80
1	A	217	LEU	CA-C-O	7.42	124.11	119.29
1	B	348	LEU	CA-C-N	-7.30	115.93	122.43
1	B	348	LEU	C-N-CA	-7.30	115.93	122.43
1	B	7	PHE	CA-CB-CG	7.29	121.08	113.80
1	A	270	MET	CA-C-O	7.24	125.04	119.46
1	B	53	LYS	CB-CA-C	7.15	124.42	111.12
1	A	127	MET	CA-C-N	7.13	133.60	122.26
1	A	127	MET	C-N-CA	7.13	133.60	122.26
1	B	107	GLY	N-CA-C	-7.09	106.26	114.69
1	B	67	ASP	N-CA-CB	-7.04	98.59	110.49
1	A	536	ASP	CA-C-N	6.98	126.96	119.28
1	A	536	ASP	C-N-CA	6.98	126.96	119.28
1	B	66	GLN	CG-CD-NE2	6.97	126.86	116.40
1	A	412	LYS	CB-CG-CD	-6.96	95.29	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	MET	CA-CB-CG	6.95	128.00	114.10
1	A	129	ARG	N-CA-C	6.87	121.06	110.20
1	B	129	ARG	N-CA-C	6.87	121.05	110.20
1	B	457	THR	CB-CA-C	-6.80	94.47	109.56
1	A	457	THR	CB-CA-C	-6.79	95.13	110.07
1	A	412	LYS	CA-CB-CG	-6.78	100.54	114.10
1	A	243	PRO	N-CA-C	6.74	122.40	113.57
1	A	66	GLN	CG-CD-NE2	6.70	126.44	116.40
1	A	23	GLU	CA-CB-CG	-6.68	100.74	114.10
1	B	66	GLN	CA-C-O	6.55	128.50	121.16
1	A	143	GLU	CA-C-N	6.55	126.32	119.05
1	A	143	GLU	C-N-CA	6.55	126.32	119.05
1	A	31	ILE	N-CA-C	6.54	116.57	110.42
1	B	426	SER	N-CA-C	6.54	120.44	108.94
1	A	231	GLU	CB-CG-CD	6.49	123.64	112.60
1	A	306	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	A	421	ALA	N-CA-C	-6.48	99.18	109.23
1	B	62	HIS	CA-CB-CG	6.48	120.28	113.80
1	A	471	ILE	CA-C-N	-6.43	114.81	123.10
1	A	471	ILE	C-N-CA	-6.43	114.81	123.10
1	A	38	GLU	N-CA-C	6.34	118.75	108.41
1	A	509	PHE	CA-CB-CG	-6.34	107.46	113.80
1	B	558	TRP	N-CA-C	6.29	121.14	112.90
1	B	304	ALA	N-CA-C	-6.23	105.16	112.89
1	B	237	LYS	N-CA-C	6.19	118.82	111.33
1	A	136	GLU	CA-CB-CG	6.15	126.40	114.10
1	B	474	ASN	CA-CB-CG	6.15	118.75	112.60
1	A	457	THR	CA-CB-OG1	6.13	118.80	109.60
1	A	211	ARG	CG-CD-NE	6.12	125.47	112.00
1	B	244	TYR	N-CA-C	6.08	117.99	111.36
1	A	558	TRP	N-CA-C	6.06	120.84	112.90
1	B	505	THR	N-CA-CB	6.04	121.30	111.21
1	B	462	MET	CA-CB-CG	-6.03	102.04	114.10
1	B	37	VAL	CA-C-O	-6.03	113.97	120.36
1	A	62	HIS	CA-CB-CG	6.01	119.81	113.80
1	B	104	ARG	CD-NE-CZ	5.96	132.75	124.40
1	A	504	ARG	CA-C-O	-5.96	114.34	120.89
1	B	504	ARG	CA-C-O	-5.95	113.41	120.43
1	B	344	LYS	CB-CG-CD	-5.94	97.64	111.30
1	A	461	GLY	N-CA-C	-5.93	103.53	112.60
1	A	53	LYS	CB-CA-C	5.92	122.66	111.29
1	B	515	GLU	CA-C-N	5.92	128.81	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	515	GLU	C-N-CA	5.92	128.81	120.28
1	A	26	GLN	N-CA-CB	5.87	118.75	110.12
1	A	51	TYR	N-CA-C	-5.86	104.48	111.69
1	A	251	ASP	N-CA-C	5.84	118.40	111.33
1	A	385	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	539	GLY	O-C-N	-5.81	117.80	122.51
1	A	170	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	466	HIS	CA-CB-CG	5.77	119.57	113.80
1	A	107	GLY	N-CA-C	-5.74	107.86	114.69
1	B	177	LEU	CA-CB-CG	5.73	136.37	116.30
1	A	516	THR	N-CA-CB	-5.72	101.42	110.28
1	B	211	ARG	CG-CD-NE	5.72	124.58	112.00
1	B	162	ASP	CB-CG-OD2	-5.71	105.26	118.40
1	A	30	ARG	CB-CG-CD	5.71	124.44	111.30
1	B	30	ARG	CB-CG-CD	5.71	124.43	111.30
1	A	159	ASN	CA-CB-CG	5.68	118.28	112.60
1	B	170	ASP	CA-CB-CG	-5.68	106.92	112.60
1	B	518	ASN	N-CA-C	5.68	119.52	112.59
1	B	367	LEU	CA-C-O	5.67	126.43	120.42
1	B	185	VAL	CA-C-O	5.65	127.00	120.67
1	A	200	MET	CA-CB-CG	5.64	125.39	114.10
1	B	542	ALA	N-CA-CB	-5.61	105.43	111.66
1	B	135	VAL	N-CA-C	5.58	115.66	110.42
1	A	177	LEU	CA-CB-CG	5.56	135.76	116.30
1	A	412	LYS	CA-C-O	-5.56	113.82	120.10
1	B	65	ASP	N-CA-CB	-5.55	102.78	110.38
1	A	244	TYR	N-CA-C	5.54	118.24	111.82
1	A	243	PRO	CB-CA-C	-5.53	104.03	112.11
1	B	509	PHE	CA-CB-CG	-5.53	108.27	113.80
1	B	278	SER	O-C-N	5.50	129.10	122.94
1	B	24	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	530	VAL	CA-C-O	-5.45	115.28	120.95
1	B	505	THR	CA-CB-OG1	5.40	117.70	109.60
1	A	515	GLU	CA-C-O	5.39	126.01	119.38
1	B	211	ARG	CB-CG-CD	5.39	123.70	111.30
1	A	322	GLY	CA-C-O	-5.38	116.33	121.49
1	A	112	ALA	N-CA-C	5.38	116.47	109.64
1	B	100	ILE	CA-C-O	-5.36	116.05	121.67
1	B	290	LYS	CB-CG-CD	5.36	123.62	111.30
1	A	284	PRO	N-CA-C	5.32	121.08	113.47
1	B	66	GLN	CB-CA-C	5.32	118.75	109.65
1	A	528	ASN	CA-CB-CG	-5.30	107.30	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	VAL	CA-C-N	5.28	130.45	123.00
1	A	37	VAL	C-N-CA	5.28	130.45	123.00
1	B	127	MET	CA-C-O	5.27	127.29	121.39
1	B	30	ARG	N-CA-CB	5.25	117.63	110.01
1	A	271	PRO	CA-C-O	-5.25	115.35	121.34
1	A	549	TRP	CA-C-N	5.19	125.64	120.14
1	A	549	TRP	C-N-CA	5.19	125.64	120.14
1	A	446	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	304	ALA	N-CA-C	-5.17	105.71	112.23
1	A	385	PHE	N-CA-C	-5.15	102.67	110.50
1	A	462	MET	N-CA-C	5.14	116.88	111.28
1	B	471	ILE	CA-C-N	-5.13	116.49	123.10
1	B	471	ILE	C-N-CA	-5.13	116.49	123.10
1	A	303	MET	N-CA-CB	-5.12	104.01	113.89
1	B	235	TRP	CA-C-O	-5.12	115.36	121.56
1	A	177	LEU	CB-CG-CD1	5.12	126.06	110.70
1	B	424	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	183	ARG	O-C-N	-5.11	116.45	122.58
1	B	477	ASP	CA-C-N	5.11	128.48	120.82
1	B	477	ASP	C-N-CA	5.11	128.48	120.82
1	A	494	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	347	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	A	314	ILE	N-CA-C	5.09	116.42	110.62
1	B	426	SER	CA-C-N	5.06	125.06	120.21
1	B	426	SER	C-N-CA	5.06	125.06	120.21
1	A	76	ALA	CB-CA-C	5.05	116.90	110.34
1	A	66	GLN	CA-C-O	5.05	126.74	121.19
1	B	421	ALA	N-CA-C	-5.03	101.55	109.50
1	B	512	GLN	OE1-CD-NE2	5.03	127.63	122.60
1	B	177	LEU	CA-C-O	-5.03	115.52	120.70
1	A	430	LYS	CA-C-O	-5.02	116.04	121.87
1	B	211	ARG	N-CA-CB	5.01	119.11	110.68
1	B	349	GLY	N-CA-C	-5.01	105.70	112.57
1	B	462	MET	N-CA-C	5.01	116.56	111.14
1	A	555	HIS	CA-CB-CG	5.00	118.80	113.80

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	53	LYS	CA
1	A	67	ASP	CA
1	A	303	MET	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	B	53	LYS	CA
1	B	66	GLN	CA
1	B	67	ASP	CA
1	B	303	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	PHE	Sidechain
1	B	7	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4348	0	4290	78	2
1	B	4348	0	4290	80	2
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	11	0	4	0	0
3	B	11	0	5	0	0
4	A	181	0	0	6	0
4	B	204	0	0	6	0
All	All	9209	0	8651	146	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 9.

All (146) 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:550:PRO:HB2	1:A:552:GLN:HE21	1.33	0.93
1:A:349:GLY:H	1:A:352:ASN:HD21	1.11	0.92
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.36	0.89
1:B:349:GLY:H	1:B:352:ASN:HD21	1.25	0.82
1:A:253:LEU:HD11	1:B:253:LEU:HD21	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:THR:HG21	4:A:2147:HOH:O	1.83	0.78
1:B:550:PRO:HB2	1:B:552:GLN:NE2	1.98	0.78
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.68	0.76
1:B:516:THR:HG21	4:B:2164:HOH:O	1.89	0.72
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.73	0.70
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.06	0.69
1:A:200:MET:HE3	1:A:265:ILE:HD12	1.77	0.67
1:B:341:LYS:O	1:B:345:GLN:HG3	1.96	0.65
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.78	0.65
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.78	0.64
1:A:61:THR:HB	1:A:421:ALA:HB1	1.78	0.64
1:A:188:THR:HB	1:A:189:PRO:HD2	1.79	0.63
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.81	0.63
1:A:194:TRP:O	1:A:197:HIS:HD2	1.82	0.62
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.81	0.61
1:B:188:THR:HB	1:B:189:PRO:CD	2.31	0.61
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.82	0.61
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.00	0.61
1:A:152:HIS:HD2	4:A:2127:HOH:O	1.84	0.60
1:B:61:THR:HB	1:B:421:ALA:HB1	1.84	0.60
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.36	0.60
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.38	0.59
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.01	0.59
1:B:290:LYS:HB2	1:B:437:MET:HG3	1.85	0.59
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.84	0.58
1:A:244:TYR:OH	1:B:195:MET:HG2	2.02	0.58
1:A:83:VAL:HG21	1:A:123:MET:HE1	1.85	0.58
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.18	0.58
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.38	0.57
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.89	0.56
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.85	0.56
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.71	0.56
1:A:79:ASN:ND2	1:A:82:ASP:H	2.03	0.56
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.87	0.56
1:A:195:MET:HG2	1:B:244:TYR:OH	2.05	0.56
1:A:253:LEU:CD1	1:B:253:LEU:HD21	2.34	0.56
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.41	0.56
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.41	0.55
1:B:194:TRP:O	1:B:197:HIS:HD2	1.89	0.55
1:B:387:GLU:CD	1:B:387:GLU:H	2.15	0.55
1:B:365:ARG:HD2	4:B:2130:HOH:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.89	0.54
1:B:457:THR:HG21	4:B:2126:HOH:O	2.06	0.54
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.42	0.54
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.91	0.54
1:A:40:ILE:HD11	1:A:74:ILE:HD13	1.89	0.54
1:A:513:ILE:O	1:A:516:THR:HB	2.08	0.54
1:A:188:THR:HB	1:A:189:PRO:CD	2.38	0.54
1:A:123:MET:O	1:A:127:MET:HB2	2.08	0.53
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.38	0.53
1:B:99:PRO:HD2	4:B:2024:HOH:O	2.09	0.53
1:A:457:THR:HG21	4:A:2108:HOH:O	2.07	0.53
1:A:57:THR:HG22	1:A:74:ILE:CD1	2.38	0.53
1:B:513:ILE:O	1:B:516:THR:HB	2.09	0.53
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.88	0.53
1:B:237:LYS:HG3	1:B:238:ILE:HG12	1.90	0.52
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.90	0.52
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.25	0.52
1:A:198:SER:O	1:A:240:HIS:HD2	1.93	0.52
1:A:79:ASN:HD22	1:A:82:ASP:H	1.57	0.51
1:A:290:LYS:HB2	1:A:437:MET:HG3	1.92	0.51
1:A:333:PRO:HB2	1:A:448:GLN:NE2	2.26	0.51
1:A:341:LYS:O	1:A:345:GLN:HG3	2.10	0.51
1:B:188:THR:CB	1:B:189:PRO:CD	2.88	0.51
1:B:333:PRO:HB2	1:B:448:GLN:NE2	2.26	0.51
1:B:79:ASN:ND2	1:B:82:ASP:H	2.08	0.50
1:A:61:THR:CB	1:A:421:ALA:HB1	2.42	0.50
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.94	0.50
1:B:83:VAL:HG21	1:B:123:MET:HE1	1.94	0.50
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.94	0.49
1:A:253:LEU:HD21	1:B:253:LEU:CD1	2.42	0.49
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.95	0.49
1:B:505:THR:HG23	4:B:2166:HOH:O	2.12	0.49
1:B:79:ASN:HD22	1:B:82:ASP:H	1.61	0.48
1:B:24:PHE:HD1	1:B:25:ILE:HD13	1.78	0.48
1:B:306:GLN:HG3	4:B:2124:HOH:O	2.13	0.48
1:A:149:HIS:HD1	1:A:408:TYR:HH	1.61	0.48
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.96	0.48
1:A:257:SER:HA	4:A:2096:HOH:O	2.13	0.48
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.96	0.47
1:B:198:SER:O	1:B:240:HIS:HD2	1.97	0.47
1:B:324:LYS:HG3	1:B:416:TRP:CZ2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:THR:HG22	1:B:352:ASN:HD22	1.80	0.47
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.45	0.47
1:A:387:GLU:H	1:A:387:GLU:CD	2.22	0.46
1:B:79:ASN:HD22	1:B:79:ASN:C	2.23	0.46
1:A:79:ASN:HD22	1:A:79:ASN:C	2.23	0.46
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.97	0.46
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.44	0.46
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.97	0.46
1:A:189:PRO:HG2	1:A:270:MET:CE	2.45	0.46
1:B:188:THR:HB	1:B:189:PRO:HD2	1.97	0.45
1:B:312:ARG:CG	1:B:457:THR:HG23	2.44	0.45
1:B:427:PRO:HA	1:B:502:GLU:HA	1.98	0.45
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.52	0.45
1:A:324:LYS:HG3	1:A:416:TRP:CZ2	2.52	0.45
1:B:40:ILE:HD11	1:B:74:ILE:HD13	1.98	0.45
1:A:188:THR:CB	1:A:189:PRO:CD	2.93	0.44
1:A:349:GLY:H	1:A:352:ASN:ND2	1.94	0.44
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.99	0.44
1:B:149:HIS:HD1	1:B:408:TYR:HH	1.65	0.44
1:A:280:LEU:HB3	1:A:395:LEU:HD22	2.00	0.44
1:B:210:LEU:C	1:B:210:LEU:HD23	2.41	0.44
1:B:555:HIS:CG	1:B:559:LYS:HE3	2.53	0.44
1:B:463:ARG:HH11	1:B:463:ARG:HG3	1.82	0.44
1:A:210:LEU:HD23	1:A:211:ARG:N	2.33	0.43
1:A:188:THR:CB	1:A:189:PRO:HD2	2.48	0.43
1:B:51:TYR:CZ	1:B:104:ARG:HD3	2.53	0.43
1:A:13:PRO:HG3	1:A:95:PHE:CZ	2.53	0.43
1:B:61:THR:CB	1:B:421:ALA:HB1	2.47	0.43
1:A:361:GLU:HB3	1:A:362:PRO:HD3	2.01	0.43
1:A:427:PRO:HA	1:A:502:GLU:HA	2.01	0.43
1:A:549:TRP:HA	1:A:550:PRO:HD3	1.86	0.43
1:B:210:LEU:HD23	1:B:211:ARG:N	2.34	0.43
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.54	0.43
1:B:290:LYS:HE3	1:B:294:ASP:OD2	2.19	0.43
1:B:280:LEU:HB3	1:B:395:LEU:HD22	2.01	0.43
1:B:63:VAL:HG12	1:B:473:PHE:CZ	2.53	0.42
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.49	0.42
1:B:310:THR:HG22	1:B:459:THR:HG22	2.01	0.42
1:A:237:LYS:HG3	1:A:238:ILE:HG12	2.00	0.42
1:B:24:PHE:CD1	1:B:25:ILE:HD13	2.55	0.42
1:B:271:PRO:O	1:B:272:ASN:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TYR:CZ	1:A:104:ARG:HD3	2.54	0.41
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.50	0.41
1:B:224:GLU:H	1:B:224:GLU:CD	2.27	0.41
1:B:275:GLY:HA3	1:B:359:GLY:O	2.21	0.41
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.56	0.41
1:A:62:HIS:HB2	4:A:2007:HOH:O	2.19	0.41
1:A:210:LEU:HD23	1:A:210:LEU:C	2.45	0.41
1:B:365:ARG:O	1:B:369:GLU:HG3	2.20	0.41
1:B:337:GLU:H	1:B:337:GLU:CD	2.29	0.41
1:B:270:MET:HA	1:B:271:PRO:HD3	1.92	0.41
1:A:238:ILE:HG22	1:A:238:ILE:O	2.22	0.40
1:A:505:THR:HG23	4:A:2131:HOH:O	2.20	0.40
1:A:51:TYR:O	1:A:54:PRO:HD3	2.22	0.40
1:A:385:PHE:HB3	1:A:386:PRO:HD2	2.02	0.40
1:A:552:GLN:H	1:A:552:GLN:CD	2.30	0.40
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.57	0.40
1:A:315:LEU:HA	1:A:318:ALA:HB3	2.04	0.40
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.56	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:37:VAL:O	1:B:391:GLU:OE2[6_655]	1.80	0.40
1:A:419:ASN:OD1	1:B:329:SER:OG[6_655]	2.09	0.11

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	546/560 (98%)	524 (96%)	21 (4%)	1 (0%)	43 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	546/560 (98%)	527 (96%)	17 (3%)	2 (0%)	30	28
All	All	1092/1120 (98%)	1051 (96%)	38 (4%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ASP
1	A	418	PRO
1	B	418	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/481 (98%)	442 (94%)	28 (6%)	17	15
1	B	470/481 (98%)	443 (94%)	27 (6%)	18	17
All	All	940/962 (98%)	885 (94%)	55 (6%)	18	16

All (55) 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	28	ILE
1	A	62	HIS
1	A	67	ASP
1	A	79	ASN
1	A	128	ASN
1	A	142	VAL
1	A	149	HIS
1	A	177	LEU
1	A	211	ARG
1	A	217	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	231	GLU
1	A	301	LEU
1	A	303	MET
1	A	306	GLN
1	A	328	SER
1	A	329	SER
1	A	336	ASP
1	A	341	LYS
1	A	391	GLU
1	A	432	SER
1	A	457	THR
1	A	472	VAL
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	B	7	PHE
1	B	8	ARG
1	B	25	ILE
1	B	62	HIS
1	B	66	GLN
1	B	67	ASP
1	B	79	ASN
1	B	128	ASN
1	B	142	VAL
1	B	149	HIS
1	B	177	LEU
1	B	211	ARG
1	B	231	GLU
1	B	301	LEU
1	B	303	MET
1	B	306	GLN
1	B	328	SER
1	B	329	SER
1	B	336	ASP
1	B	341	LYS
1	B	391	GLU
1	B	432	SER
1	B	457	THR
1	B	472	VAL
1	B	503	TYR
1	B	505	THR
1	B	516	THR

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	448	GLN
1	A	467	HIS
1	A	485	GLN
1	A	520	ASN
1	A	538	ASN
1	A	552	GLN
1	B	79	ASN
1	B	84	GLN
1	B	128	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	448	GLN
1	B	467	HIS
1	B	520	ASN
1	B	538	ASN
1	B	552	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	2.04	10 (17%)	85,89,89	1.69	20 (23%)
2	FAD	A	600	-	58,58,58	2.16	10 (17%)	85,89,89	1.42	15 (17%)
3	FCR	A	601	-	11,11,11	0.93	0	16,16,16	1.85	5 (31%)
3	FCR	B	601	-	11,11,11	0.76	0	16,16,16	1.65	3 (18%)

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	-	-	2/34/50/50	0/6/6/6
2	FAD	A	600	-	-	5/34/50/50	0/6/6/6
3	FCR	A	601	-	-	0/6/6/6	0/1/1/1
3	FCR	B	601	-	-	0/6/6/6	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-11.63	1.46	1.59
2	B	600	FAD	P-O3P	-9.25	1.49	1.59
2	B	600	FAD	PA-O3P	-4.86	1.54	1.59
2	B	600	FAD	PA-O2A	-4.37	1.35	1.55
2	B	600	FAD	C5'-C4'	4.28	1.57	1.51
2	A	600	FAD	PA-O2A	-4.00	1.36	1.55
2	B	600	FAD	O5'-C5'	3.60	1.58	1.44
2	A	600	FAD	O5'-C5'	3.57	1.58	1.44
2	B	600	FAD	P-O2P	-3.41	1.39	1.55
2	A	600	FAD	PA-O3P	-3.29	1.55	1.59
2	A	600	FAD	C5'-C4'	3.25	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O2P	-2.99	1.41	1.55
2	A	600	FAD	C6-C7	-2.99	1.35	1.39
2	B	600	FAD	O2-C2	-2.75	1.18	1.24
2	B	600	FAD	C6-C7	-2.54	1.36	1.39
2	A	600	FAD	O2-C2	-2.48	1.19	1.24
2	B	600	FAD	C1'-C2'	2.45	1.56	1.52
2	A	600	FAD	PA-O5B	-2.42	1.49	1.59
2	A	600	FAD	C5X-N5	-2.09	1.35	1.39
2	B	600	FAD	O4'-C4'	2.04	1.47	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O2P-P-O3P	5.35	121.74	107.27
2	B	600	FAD	O4'-C4'-C3'	4.93	120.79	109.25
2	A	600	FAD	O2P-P-O3P	4.30	118.91	107.27
3	A	601	FCR	F1-C7-C1	3.96	121.37	112.90
3	B	601	FCR	F1-C7-C1	3.86	121.16	112.90
2	B	600	FAD	N6A-C6A-N1A	3.37	125.88	118.38
3	A	601	FCR	F2-C7-C1	-3.34	105.75	112.90
2	B	600	FAD	C4-N3-C2	-3.18	119.99	125.64
2	A	600	FAD	C2A-N1A-C6A	3.15	123.90	118.73
2	A	600	FAD	C4-N3-C2	-3.10	120.14	125.64
2	B	600	FAD	C2A-N1A-C6A	3.06	123.75	118.73
2	B	600	FAD	P-O5'-C5'	2.99	138.49	121.35
2	B	600	FAD	O5B-PA-O1A	-2.94	97.30	108.94
2	A	600	FAD	C4X-C10-N1	-2.72	117.92	124.59
3	B	601	FCR	F2-C7-C1	-2.68	107.16	112.90
2	B	600	FAD	O3P-PA-O1A	2.66	118.72	110.70
3	B	601	FCR	F3-C7-C1	-2.66	107.19	112.90
2	B	600	FAD	C5A-C4A-N9A	-2.64	102.94	105.81
2	B	600	FAD	O2P-P-O1P	2.61	124.58	112.44
2	A	600	FAD	N3A-C2A-N1A	-2.61	124.64	128.58
2	B	600	FAD	C5'-C4'-C3'	-2.59	107.34	112.22
2	B	600	FAD	O3'-C3'-C2'	-2.57	103.09	108.93
2	A	600	FAD	O4B-C1B-N9A	-2.57	103.16	108.09
2	A	600	FAD	P-O5'-C5'	2.57	136.05	121.35
2	B	600	FAD	C4X-C10-N1	-2.51	118.44	124.59
2	A	600	FAD	C10-N1-C2	2.46	122.17	116.85
3	A	601	FCR	F3-C7-C1	-2.36	107.84	112.90
2	B	600	FAD	O2P-P-O5'	-2.35	96.93	107.57
3	A	601	FCR	C5-C4-C3	2.31	123.44	119.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O3P-P-O1P	-2.31	103.76	110.70
2	A	600	FAD	C5A-C4A-N9A	-2.30	103.30	105.81
2	B	600	FAD	C4A-N9A-C8A	2.25	108.10	105.74
2	A	600	FAD	C1'-N10-C9A	-2.23	116.29	120.63
2	A	600	FAD	N3A-C4A-N9A	2.21	130.92	127.17
2	B	600	FAD	O2-C2-N3	-2.18	114.40	118.58
2	A	600	FAD	C4-C4X-C10	2.16	120.63	116.93
3	A	601	FCR	C6-C5-C4	-2.15	117.61	119.88
2	B	600	FAD	C10-N1-C2	2.13	121.46	116.85
2	A	600	FAD	O4'-C4'-C3'	2.09	114.15	109.25
2	A	600	FAD	C4X-C10-N10	2.05	119.42	116.48
2	B	600	FAD	C4X-C10-N10	2.02	119.38	116.48
2	B	600	FAD	C4-C4X-C10	2.02	120.39	116.93
2	B	600	FAD	O4'-C4'-C5'	-2.02	105.54	109.99

There are no chirality outliers.

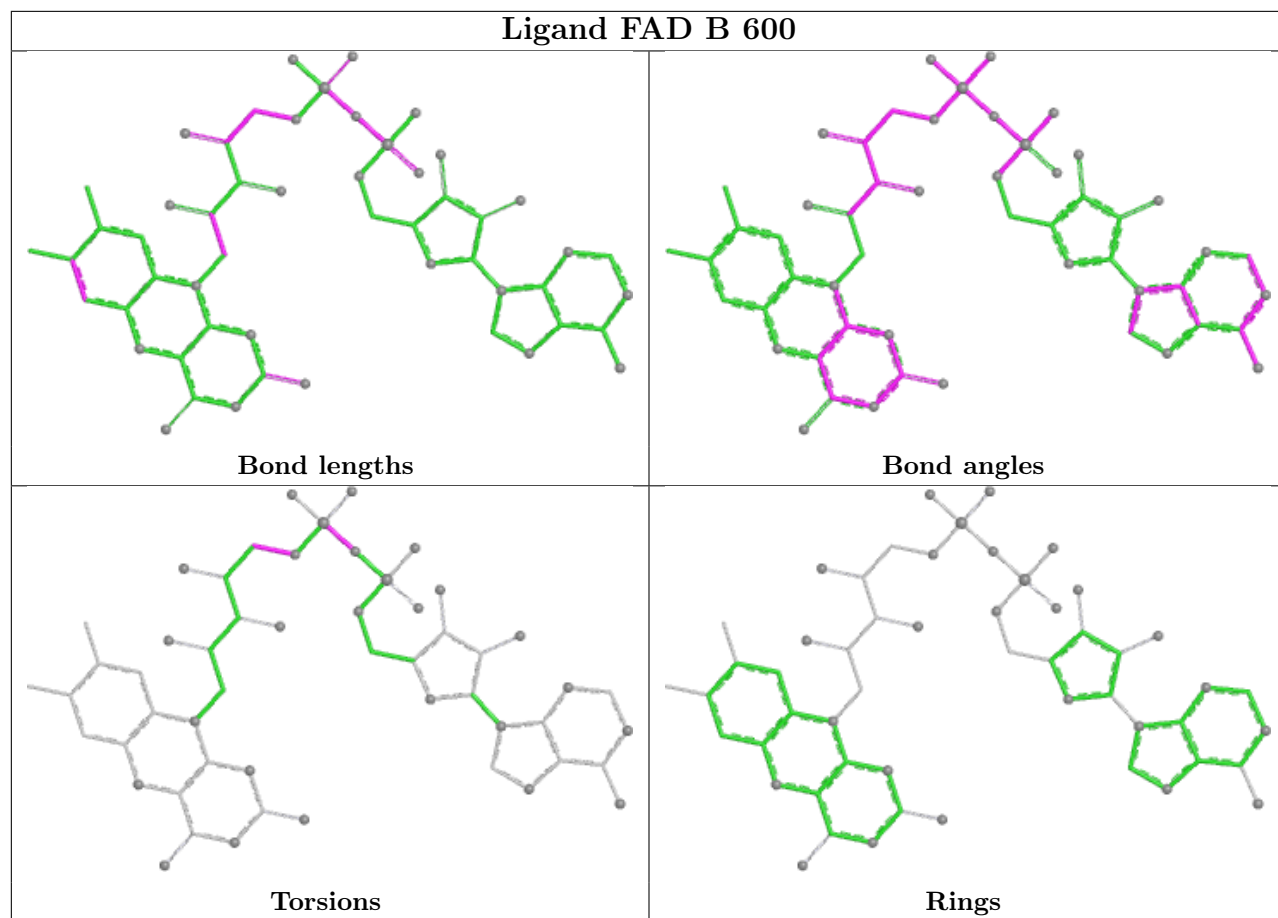
All (7) torsion outliers are listed below:

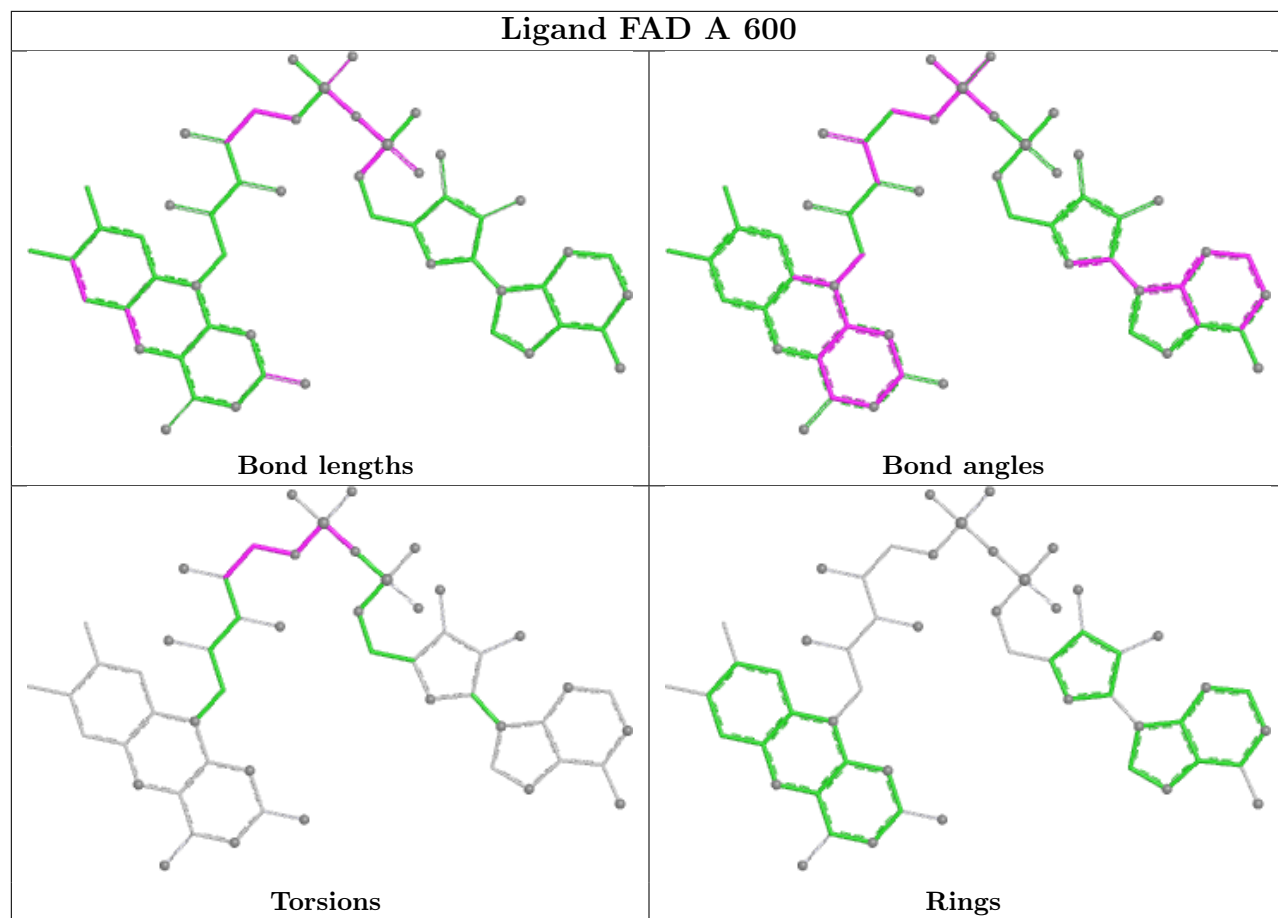
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5'-O5'-P-O1P
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	PA-O3P-P-O2P
2	A	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	PA-O3P-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	550/560 (98%)	0.37	25 (4%)	38 40	22, 41, 63, 79	24 (4%)
1	B	550/560 (98%)	0.40	36 (6%)	25 26	22, 41, 63, 79	24 (4%)
All	All	1100/1120 (98%)	0.38	61 (5%)	30 32	22, 41, 63, 79	48 (4%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	THR	5.6
1	A	49	GLY	4.0
1	B	48	ASP	3.8
1	B	329	SER	3.7
1	A	62	HIS	3.7
1	A	67	ASP	3.7
1	A	47	VAL	3.6
1	B	369	GLU	3.6
1	B	391	GLU	3.5
1	A	66	GLN	3.4
1	A	331	THR	3.4
1	A	328	SER	3.4
1	B	66	GLN	3.4
1	B	61	THR	3.3
1	B	62	HIS	3.1
1	B	330	ARG	3.0
1	B	7	PHE	2.9
1	B	337	GLU	2.8
1	B	67	ASP	2.8
1	A	19	SER	2.8
1	A	41	SER	2.7
1	B	303	MET	2.6
1	B	47	VAL	2.6
1	B	33	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	159	ASN	2.6
1	B	415	ASP	2.5
1	B	408	TYR	2.5
1	B	331	THR	2.5
1	B	422	HIS	2.4
1	B	341	LYS	2.4
1	A	419	ASN	2.4
1	B	60	PRO	2.4
1	A	30	ARG	2.4
1	A	54	PRO	2.4
1	B	51	TYR	2.3
1	A	414	ILE	2.3
1	A	325	ARG	2.3
1	B	328	SER	2.3
1	B	41	SER	2.3
1	B	326	SER	2.3
1	A	8	ARG	2.3
1	A	20	ASP	2.2
1	A	302	GLY	2.2
1	B	8	ARG	2.2
1	A	9	PRO	2.2
1	B	336	ASP	2.2
1	B	302	GLY	2.2
1	B	16	LEU	2.2
1	B	24	PHE	2.1
1	B	477	ASP	2.1
1	B	157	ALA	2.1
1	A	40	ILE	2.1
1	B	50	SER	2.1
1	A	51	TYR	2.1
1	B	325	ARG	2.1
1	A	95	PHE	2.1
1	B	306	GLN	2.0
1	A	63	VAL	2.0
1	B	39	VAL	2.0
1	A	448	GLN	2.0
1	A	162	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

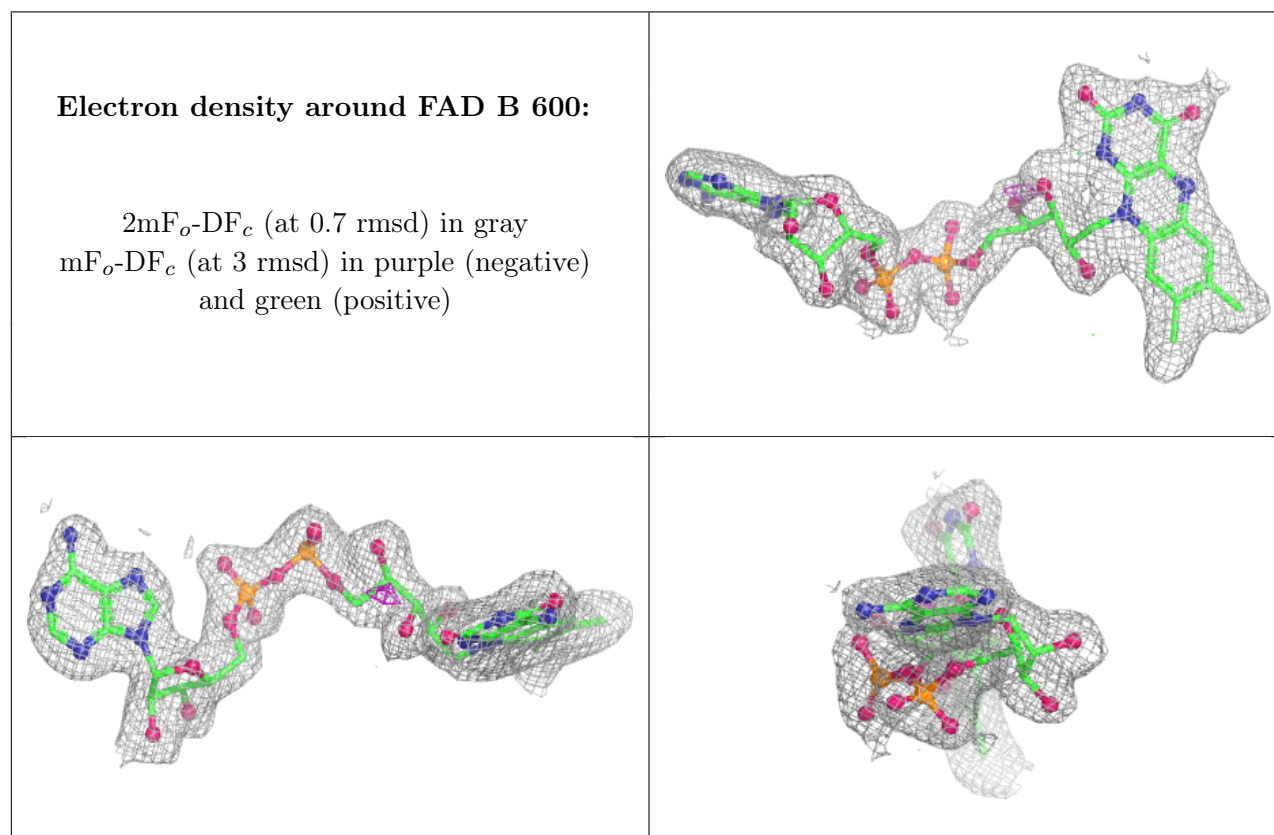
There are no oligosaccharides in this entry.

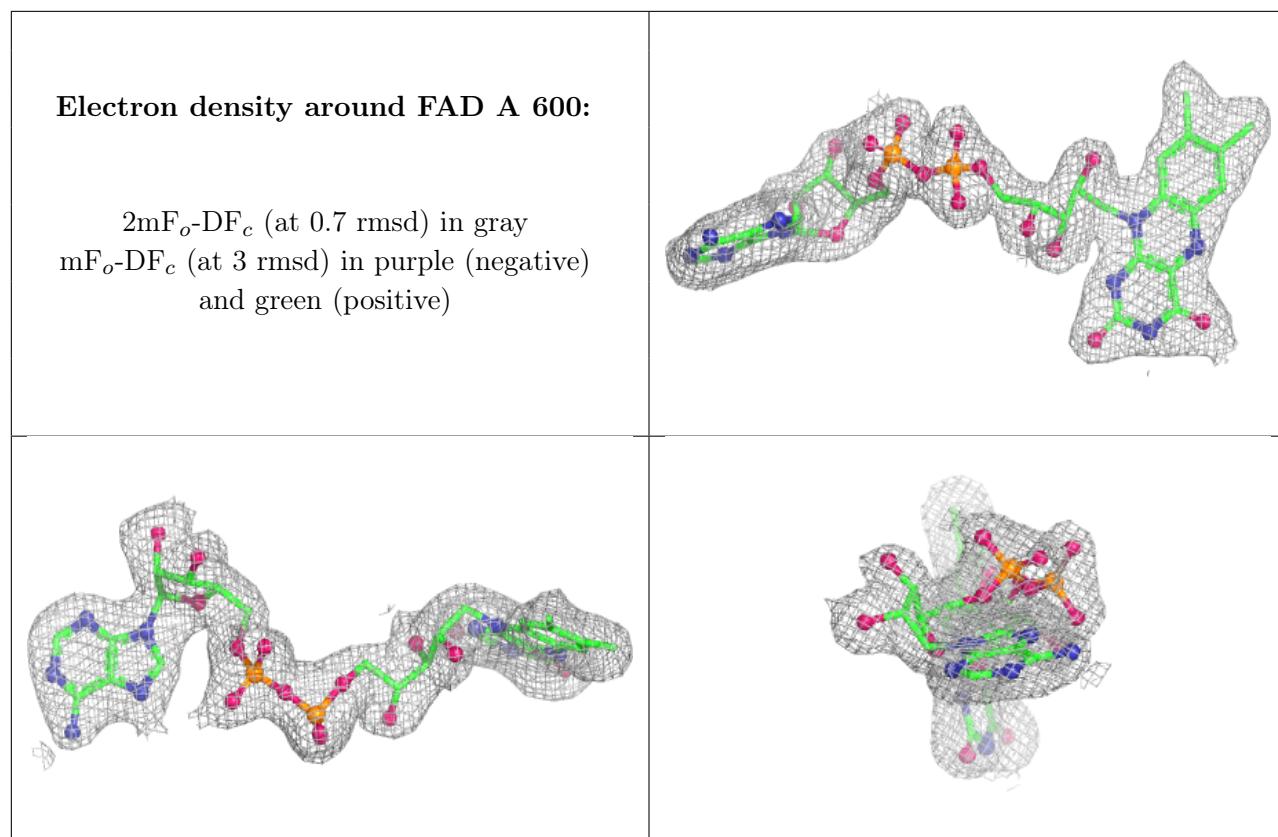
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FCR	B	601	11/11	0.82	0.12	42,44,49,50	0
3	FCR	A	601	11/11	0.85	0.10	42,45,48,49	0
2	FAD	B	600	53/53	0.94	0.08	36,39,43,44	0
2	FAD	A	600	53/53	0.95	0.07	36,39,44,44	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.