WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 12:36 am GMT

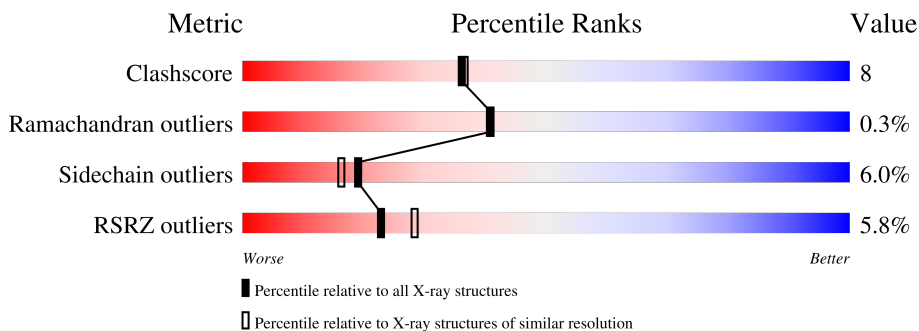|		
PDB ID	:	1E8G
Title	:	STRUCTURE OF THE H61T DOUBLE MUTANT OF VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH FLUORO-CRESOL
Authors	:	Fraaije, M.W.; Mattevi, A.
Deposited on	:	2000-09-20
Resolution	:	2.10 Å(reported)

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1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
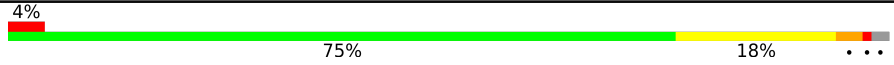*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		6.0%
RSRZ outliers		5.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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% ▮▮▮ 75% 18% ⋯
1	B	560	7% ▮▮▮ 75% 18% ⋯

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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

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

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

- Molecule 3 is ALPHA,ALPHA,ALPHA-TRIFLUORO-P-CRESOL (three-letter code: FCR) (formula: $C_7H_5F_3O$).
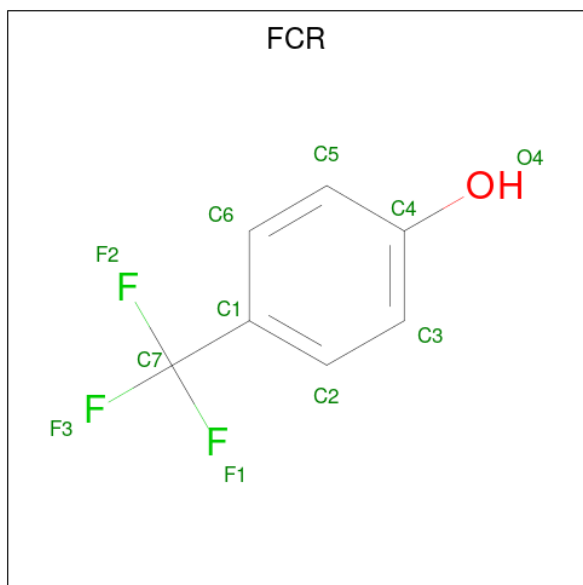
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 11	C 7	F 3	O 1	0	0
3	B	1	Total 11	C 7	F 3	O 1	0	0

- Molecule 4 is water.

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

3　Residue-property plots ⓘ

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

- Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain A:

- Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:
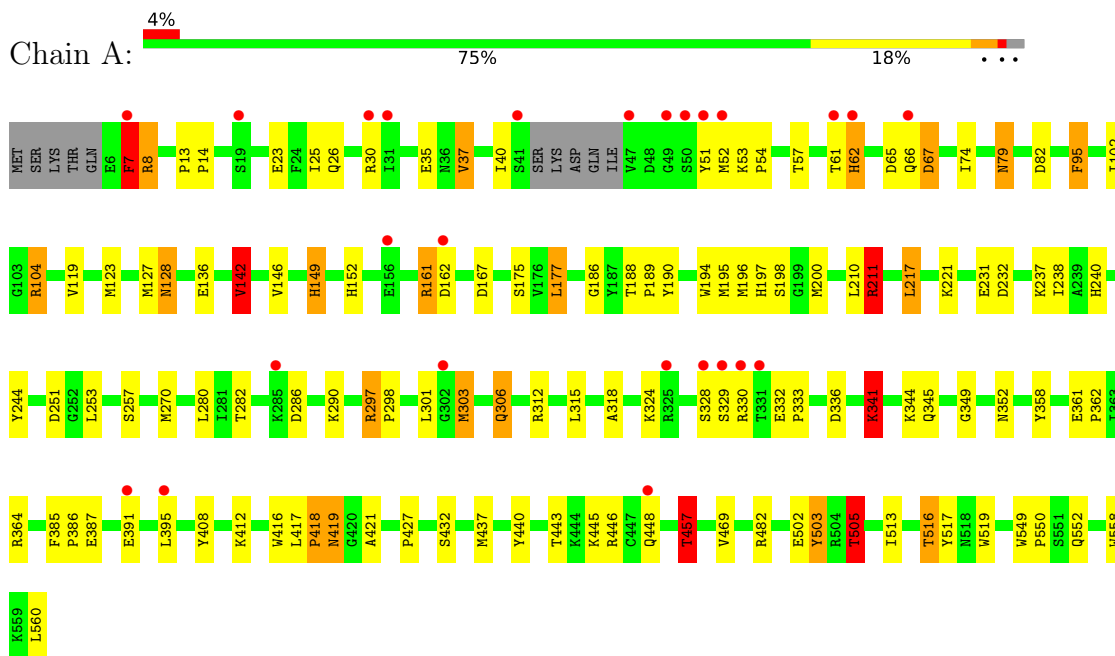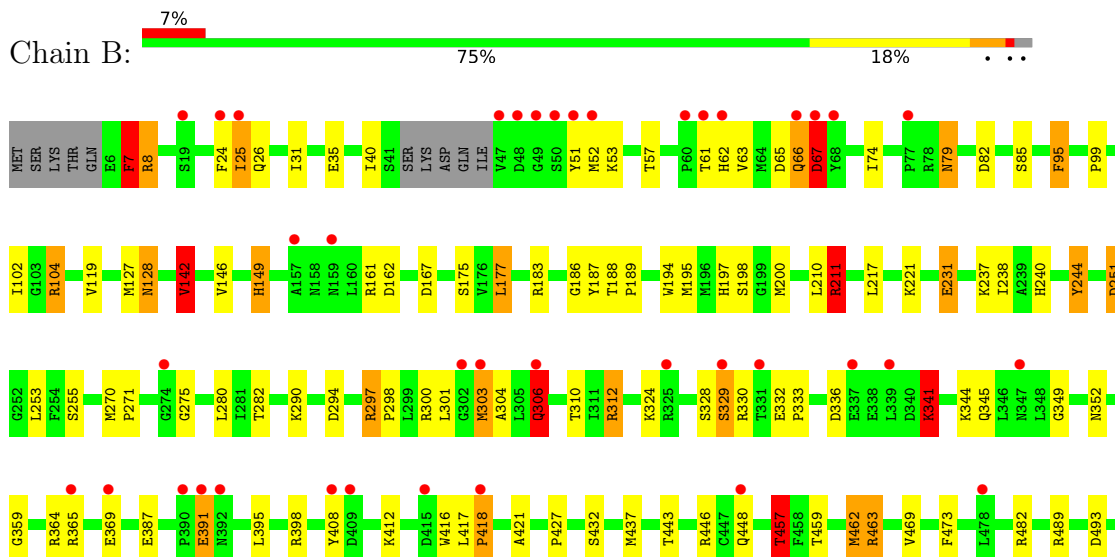
E502 Y503 R504 T505 F509 I513 T516 Y517 N518 W519 W549 P550 S551 Q552 H555 W558 K559 L560

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 14.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.10) 98.9 (14.91-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [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)	0.40 , 65.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.11	17/4466 (0.4%)	1.56	69/6070 (1.1%)
1	B	1.20	17/4466 (0.4%)	1.54	70/6070 (1.2%)
All	All	1.16	34/8932 (0.4%)	1.55	139/12140 (1.1%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	ARG	CB-CG	-35.33	0.57	1.52
1	A	161	ARG	CB-CG	-33.56	0.61	1.52
1	B	52	MET	CB-CG	29.09	2.44	1.51
1	A	52	MET	CB-CG	29.09	2.44	1.51
1	B	66	GLN	CA-CB	-27.20	0.94	1.53
1	B	344	LYS	CB-CG	-26.86	0.80	1.52
1	A	344	LYS	CB-CG	-24.55	0.86	1.52
1	B	341	LYS	CB-CG	-22.43	0.92	1.52
1	A	341	LYS	CB-CG	-22.42	0.92	1.52
1	B	65	ASP	CA-CB	-16.89	1.16	1.53
1	B	53	LYS	CB-CG	14.75	1.92	1.52
1	A	53	LYS	CB-CG	14.72	1.92	1.52
1	A	7	PHE	CA-CB	12.00	1.80	1.53
1	B	7	PHE	CA-CB	11.15	1.78	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CB-CG	10.12	1.71	1.52
1	A	26	GLN	CA-CB	-10.00	1.31	1.53
1	A	53	LYS	CA-CB	9.96	1.75	1.53
1	B	221	LYS	CG-CD	-9.09	1.21	1.52
1	B	8	ARG	CA-CB	-8.79	1.34	1.53
1	A	445	LYS	CG-CD	7.87	1.79	1.52
1	B	53	LYS	CA-CB	7.78	1.71	1.53
1	A	30	ARG	CA-CB	-7.37	1.37	1.53
1	B	67	ASP	CA-CB	-6.98	1.38	1.53
1	B	7	PHE	CB-CG	6.88	1.63	1.51
1	A	7	PHE	CB-CG	6.87	1.63	1.51
1	A	67	ASP	CA-CB	-6.67	1.39	1.53
1	B	332	GLU	CA-CB	-6.56	1.39	1.53
1	A	8	ARG	CA-CB	-6.38	1.40	1.53
1	A	65	ASP	CA-CB	-6.16	1.40	1.53
1	A	8	ARG	CB-CG	5.66	1.67	1.52
1	B	8	ARG	CB-CG	5.64	1.67	1.52
1	B	341	LYS	CA-CB	-5.36	1.42	1.53
1	A	221	LYS	CG-CD	-5.28	1.34	1.52
1	B	26	GLN	CA-CB	-5.09	1.42	1.53

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CD-NE-CZ	31.00	166.99	123.60
1	A	211	ARG	CD-NE-CZ	30.17	165.84	123.60
1	B	67	ASP	CB-CA-C	20.24	150.88	110.40
1	A	67	ASP	CB-CA-C	20.22	150.85	110.40
1	A	52	MET	CA-CB-CG	-18.37	82.07	113.30
1	B	52	MET	CA-CB-CG	-17.98	82.73	113.30
1	B	303	MET	CB-CA-C	16.72	143.84	110.40
1	B	162	ASP	CB-CG-OD2	-14.49	105.26	118.30
1	A	37	VAL	CA-C-N	13.82	147.61	117.20
1	A	53	LYS	CB-CG-CD	-13.78	75.77	111.60
1	B	53	LYS	CB-CG-CD	-13.78	75.77	111.60
1	B	330	ARG	N-CA-CB	-13.12	86.98	110.60
1	A	303	MET	CB-CA-C	12.89	136.18	110.40
1	B	65	ASP	CB-CA-C	12.66	135.73	110.40
1	B	221	LYS	CB-CG-CD	12.42	143.90	111.60
1	A	330	ARG	N-CA-CB	-12.36	88.36	110.60
1	B	162	ASP	CB-CG-OD1	11.85	128.96	118.30
1	A	297	ARG	NE-CZ-NH1	11.72	126.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CA-CB-CG	11.63	138.98	113.40
1	A	364	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	162	ASP	CB-CG-OD2	-11.42	108.02	118.30
1	A	364	ARG	CD-NE-CZ	11.30	139.42	123.60
1	B	161	ARG	CA-CB-CG	10.72	137.00	113.40
1	B	303	MET	CA-CB-CG	10.69	131.47	113.30
1	A	7	PHE	N-CA-CB	-10.63	91.46	110.60
1	B	53	LYS	N-CA-CB	10.41	129.34	110.60
1	A	53	LYS	N-CA-CB	10.32	129.18	110.60
1	B	66	GLN	N-CA-CB	10.13	128.83	110.60
1	A	211	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	37	VAL	CA-C-O	-10.10	98.89	120.10
1	B	104	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	A	161	ARG	CA-CB-CG	9.76	134.86	113.40
1	B	7	PHE	N-CA-CB	-9.69	93.16	110.60
1	B	297	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	221	LYS	CB-CG-CD	9.62	136.61	111.60
1	B	303	MET	N-CA-CB	-9.17	94.10	110.60
1	B	177	LEU	CA-CB-CG	9.16	136.37	115.30
1	A	161	ARG	CB-CG-CD	9.12	135.32	111.60
1	B	7	PHE	N-CA-C	8.98	135.25	111.00
1	A	177	LEU	CA-CB-CG	8.89	135.76	115.30
1	A	177	LEU	CB-CG-CD1	8.86	126.06	111.00
1	A	162	ASP	CB-CG-OD1	8.85	126.26	118.30
1	A	297	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	303	MET	CA-CB-CG	8.65	128.00	113.30
1	B	161	ARG	CB-CG-CD	8.56	133.87	111.60
1	A	7	PHE	N-CA-C	8.39	133.66	111.00
1	A	211	ARG	CA-CB-CG	8.39	131.86	113.40
1	B	104	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	297	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	A	364	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	364	ARG	CD-NE-CZ	8.20	135.08	123.60
1	B	128	ASN	CB-CA-C	-8.16	94.09	110.40
1	B	412	LYS	CB-CG-CD	-8.08	90.59	111.60
1	A	128	ASN	CB-CA-C	-8.03	94.34	110.40
1	A	344	LYS	CA-CB-CG	-7.99	95.82	113.40
1	B	221	LYS	CG-CD-CE	7.97	135.80	111.90
1	A	446	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	67	ASP	N-CA-CB	-7.69	96.75	110.60
1	A	128	ASN	N-CA-CB	-7.62	96.89	110.60
1	B	312	ARG	NE-CZ-NH2	-7.57	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	364	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	505	THR	N-CA-CB	7.47	124.50	110.30
1	A	211	ARG	CB-CG-CD	7.36	130.74	111.60
1	A	142	VAL	N-CA-CB	-7.29	95.45	111.50
1	B	35	GLU	CB-CG-CD	-7.26	94.59	114.20
1	B	187	TYR	CB-CG-CD1	-7.24	116.65	121.00
1	B	344	LYS	CA-CB-CG	-7.15	97.66	113.40
1	A	200	MET	CA-CB-CG	7.11	125.39	113.30
1	A	221	LYS	CG-CD-CE	7.07	133.09	111.90
1	B	128	ASN	N-CA-CB	-7.04	97.93	110.60
1	B	53	LYS	CB-CA-C	7.01	124.42	110.40
1	A	286	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	344	LYS	CB-CG-CD	-6.93	93.57	111.60
1	A	35	GLU	CB-CG-CD	-6.89	95.58	114.20
1	B	142	VAL	N-CA-CB	-6.88	96.35	111.50
1	A	505	THR	CB-CA-C	-6.88	93.04	111.60
1	A	66	GLN	CB-CA-C	6.87	124.14	110.40
1	B	67	ASP	N-CA-CB	-6.67	98.59	110.60
1	B	560	LEU	CA-C-O	-6.66	106.12	120.10
1	B	504	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	462	MET	CA-CB-CG	-6.62	102.04	113.30
1	B	505	THR	CB-CA-C	-6.61	93.76	111.60
1	B	104	ARG	CD-NE-CZ	6.54	132.75	123.60
1	A	211	ARG	CG-CD-NE	6.51	125.47	111.80
1	B	183	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	457	THR	CB-CA-C	-6.34	94.47	111.60
1	B	177	LEU	CB-CG-CD1	6.29	121.69	111.00
1	B	162	ASP	CA-CB-CG	-6.28	99.58	113.40
1	B	300	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	A	412	LYS	CB-CG-CD	-6.27	95.29	111.60
1	A	30	ARG	N-CA-CB	6.24	121.84	110.60
1	B	482	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	53	LYS	CB-CA-C	6.13	122.66	110.40
1	A	457	THR	CB-CA-C	-6.10	95.13	111.60
1	B	211	ARG	CG-CD-NE	6.09	124.58	111.80
1	A	232	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	306	GLN	CB-CG-CD	5.98	127.16	111.60
1	A	104	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	136	GLU	CA-CB-CG	5.91	126.40	113.40
1	A	190	TYR	CG-CD1-CE1	5.90	126.02	121.30
1	A	419	ASN	CA-CB-CG	-5.90	100.42	113.40
1	A	412	LYS	CA-CB-CG	-5.84	100.54	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	VAL	O-C-N	-5.84	113.36	122.70
1	B	505	THR	N-CA-CB	5.79	121.30	110.30
1	B	244	TYR	CB-CG-CD1	5.77	124.46	121.00
1	A	23	GLU	CA-CB-CG	-5.75	100.74	113.40
1	A	482	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	231	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	A	560	LEU	CA-C-O	-5.72	108.09	120.10
1	A	358	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	306	GLN	CB-CG-CD	5.71	126.44	111.60
1	B	304	ALA	N-CA-CB	5.64	118.00	110.10
1	A	440	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	440	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	B	489	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	B	127	MET	C-N-CA	5.50	135.46	121.70
1	B	482	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	128	ASN	N-CA-C	5.46	125.73	111.00
1	A	217	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	196	MET	CG-SD-CE	5.43	108.89	100.20
1	B	244	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	211	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	255	SER	N-CA-CB	5.37	118.56	110.50
1	B	344	LYS	CB-CG-CD	-5.37	97.64	111.60
1	B	364	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	358	TYR	CB-CG-CD1	5.31	124.19	121.00
1	A	332	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	B	332	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	B	446	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	200	MET	CA-CB-CG	5.17	122.10	113.30
1	A	65	ASP	CB-CA-C	-5.16	100.07	110.40
1	B	231	GLU	CB-CG-CD	5.14	128.09	114.20
1	B	128	ASN	N-CA-C	5.14	124.88	111.00
1	A	104	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	463	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	493	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	162	ASP	CA-CB-CG	-5.07	102.24	113.40
1	A	503	TYR	CB-CG-CD2	5.04	124.03	121.00
1	B	398	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	53	LYS	CA

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

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	73	2
1	B	4348	0	4290	74	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	135	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 8.

All (135) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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:365:ARG:HD2	4:B:2130:HOH:O	2.07	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:387:GLU:CD	1:B:387:GLU:H	2.15	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: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
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:417:LEU:HB3	1:A:418:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.44	0.46
1:A:189:PRO:HG2	1:A:270:MET:CE	2.45	0.46
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.97	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: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:A:79:ASN:HD22	1:A:79:ASN:C	2.23	0.42
1:A:387:GLU:H	1:A:387:GLU:CD	2.22	0.42
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: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:B:365:ARG:O	1:B:369:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:HD22	1:B:79:ASN:C	2.23	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: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 ⓘ

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%)	524 (96%)	21 (4%)	1 (0%)	47	49
1	B	546/560 (98%)	527 (96%)	17 (3%)	2 (0%)	34	32
All	All	1092/1120 (98%)	1051 (96%)	38 (4%)	3 (0%)	41	41

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 ⓘ

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%)	443 (94%)	27 (6%)	20	18
1	B	470/481 (98%)	441 (94%)	29 (6%)	18	15
All	All	940/962 (98%)	884 (94%)	56 (6%)	19	16

All (56) 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	62	HIS
1	A	67	ASP
1	A	79	ASN
1	A	95	PHE
1	A	128	ASN
1	A	142	VAL
1	A	149	HIS
1	A	161	ARG
1	A	177	LEU
1	A	211	ARG
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	503	TYR
1	A	505	THR
1	A	516	THR

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Mol	Chain	Res	Type
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	95	PHE
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	251	ASP
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	462	MET
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	128	ASN
1	A	158	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	439	GLN
1	A	448	GLN
1	A	467	HIS

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Mol	Chain	Res	Type
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	79	ASN
1	B	128	ASN
1	B	158	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	439	GLN
1	B	448	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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
3	FCR	B	601	-	11,11,11	0.74	0	16,16,16	1.61	3 (18%)
2	FAD	B	600	-	53,58,58	1.61	10 (18%)	68,89,89	1.69	16 (23%)
2	FAD	A	600	-	53,58,58	1.51	10 (18%)	68,89,89	1.43	13 (19%)
3	FCR	A	601	-	11,11,11	0.90	0	16,16,16	1.81	5 (31%)

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
3	FCR	B	601	-	-	0/6/6/6	0/1/1/1
2	FAD	B	600	-	-	2/30/50/50	0/6/6/6
2	FAD	A	600	-	-	5/30/50/50	0/6/6/6
3	FCR	A	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	B	600	FAD	PA-O2A	-4.31	1.35	1.55
2	B	600	FAD	C5'-C4'	4.12	1.57	1.51
2	A	600	FAD	PA-O2A	-3.95	1.36	1.55
2	B	600	FAD	O5'-C5'	3.50	1.58	1.44
2	A	600	FAD	O5'-C5'	3.47	1.58	1.44
2	B	600	FAD	P-O2P	-3.36	1.39	1.55
2	A	600	FAD	C5'-C4'	3.13	1.56	1.51
2	B	600	FAD	O4B-C1B	3.08	1.45	1.41
2	A	600	FAD	P-O2P	-2.95	1.41	1.55
2	B	600	FAD	C2B-C1B	-2.93	1.49	1.53
2	B	600	FAD	O2-C2	-2.88	1.18	1.24
2	A	600	FAD	C6-C7	-2.75	1.35	1.39
2	A	600	FAD	O2-C2	-2.59	1.19	1.24
2	A	600	FAD	O4B-C1B	2.54	1.44	1.41
2	B	600	FAD	C1'-C2'	2.41	1.56	1.52
2	B	600	FAD	C6-C7	-2.33	1.36	1.39
2	A	600	FAD	PA-O5B	-2.32	1.49	1.59
2	A	600	FAD	C2B-C1B	-2.19	1.50	1.53
2	B	600	FAD	O4'-C4'	2.02	1.47	1.43
2	A	600	FAD	C5X-N5	-2.01	1.35	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	O4'-C4'-C3'	4.81	120.79	109.10
3	A	601	FCR	F1-C7-C1	3.84	121.37	112.93
3	B	601	FCR	F1-C7-C1	3.75	121.16	112.93
2	B	600	FAD	N6A-C6A-N1A	3.52	125.88	118.57
2	B	600	FAD	C5A-C6A-N1A	-3.41	112.63	120.35
3	A	601	FCR	F2-C7-C1	-3.27	105.75	112.93
2	B	600	FAD	C4-N3-C2	-3.06	119.99	125.64
2	B	600	FAD	O5B-PA-O1A	-3.01	97.30	109.07
2	A	600	FAD	C2A-N1A-C6A	3.01	123.90	118.75
2	A	600	FAD	C4-N3-C2	-2.98	120.14	125.64
2	A	600	FAD	C4X-C10-N1	-2.93	117.92	124.73
2	B	600	FAD	C2A-N1A-C6A	2.92	123.75	118.75
2	B	600	FAD	P-O5'-C5'	2.87	138.49	121.68
2	B	600	FAD	C4A-C5A-N7A	2.79	112.30	109.40
2	B	600	FAD	C4X-C10-N1	-2.71	118.44	124.73
2	A	600	FAD	C10-N1-C2	2.63	122.17	116.90
3	B	601	FCR	F2-C7-C1	-2.63	107.16	112.93
3	B	601	FCR	F3-C7-C1	-2.61	107.19	112.93
2	A	600	FAD	C4A-C5A-N7A	2.60	112.11	109.40
2	A	600	FAD	N3A-C2A-N1A	-2.58	124.64	128.68
2	A	600	FAD	C1'-N10-C9A	-2.53	116.29	120.51
2	A	600	FAD	P-O3P-PA	2.53	141.49	132.83
2	B	600	FAD	C5'-C4'-C3'	-2.52	107.34	112.20
2	B	600	FAD	O2P-P-O1P	2.50	124.58	112.24
2	A	600	FAD	P-O5'-C5'	2.45	136.05	121.68
2	B	600	FAD	O3'-C3'-C2'	-2.37	103.09	108.81
2	A	600	FAD	C5A-C6A-N1A	-2.34	115.04	120.35
2	B	600	FAD	O2P-P-O5'	-2.33	96.93	107.75
3	A	601	FCR	F3-C7-C1	-2.32	107.84	112.93
2	A	600	FAD	C4-C4X-C10	2.29	120.63	116.79
2	B	600	FAD	C10-N1-C2	2.28	121.46	116.90
2	B	600	FAD	O2-C2-N3	-2.18	114.40	118.65
3	A	601	FCR	C5-C4-C3	2.18	123.44	119.77
2	B	600	FAD	C4-C4X-C10	2.14	120.39	116.79
2	A	600	FAD	O4'-C4'-C3'	2.08	114.15	109.10
3	A	601	FCR	C6-C5-C4	-2.07	117.61	119.88
2	A	600	FAD	C4X-C10-N10	2.01	119.42	116.48

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

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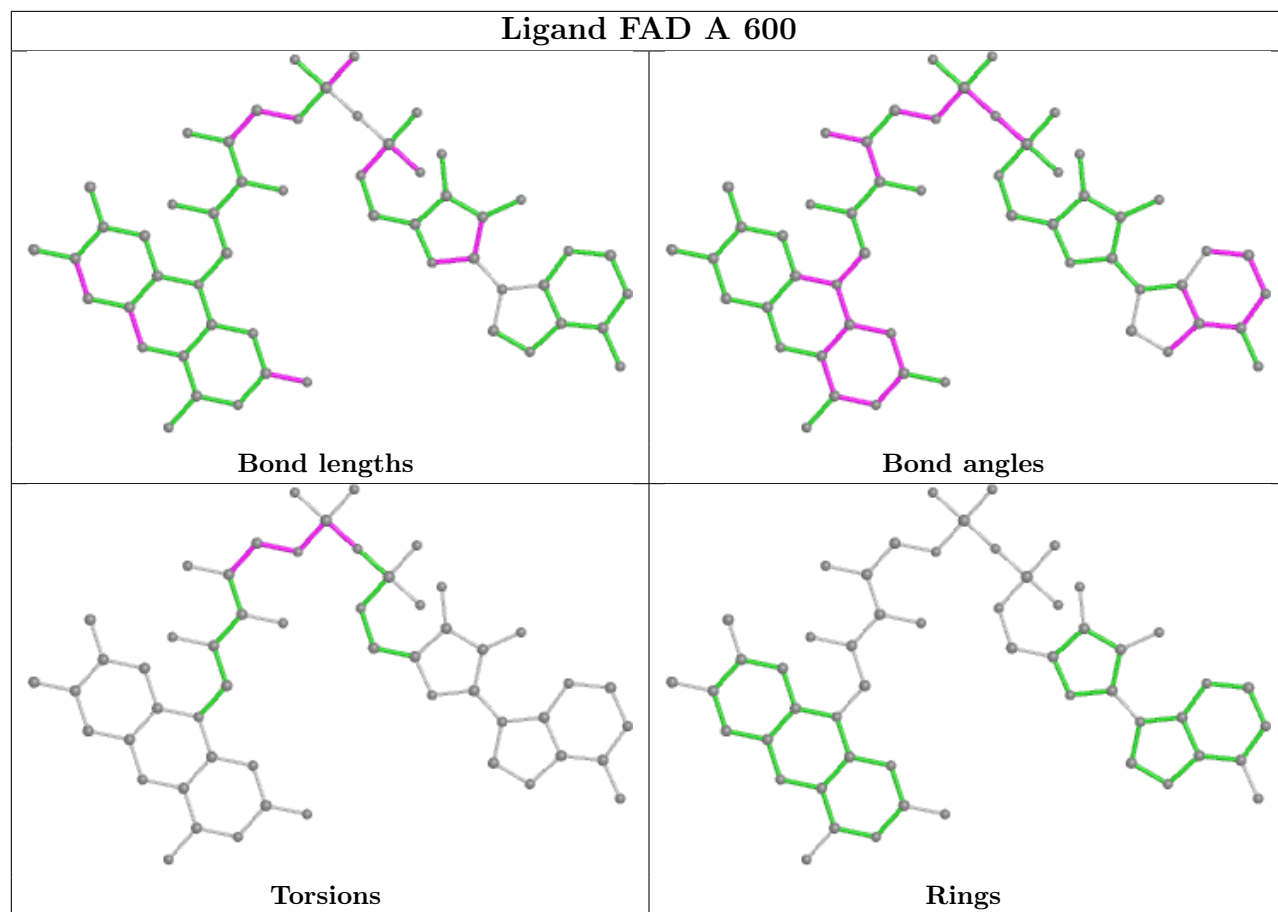| Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	PA-O3P-P-O2P
2	A	600	FAD	PA-O3P-P-O2P
2	A	600	FAD	C3'-C4'-C5'-O5'

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 then 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.

Ligand FAD B 600

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 600

Bond lengths

Bond angles

Torsions

Rings
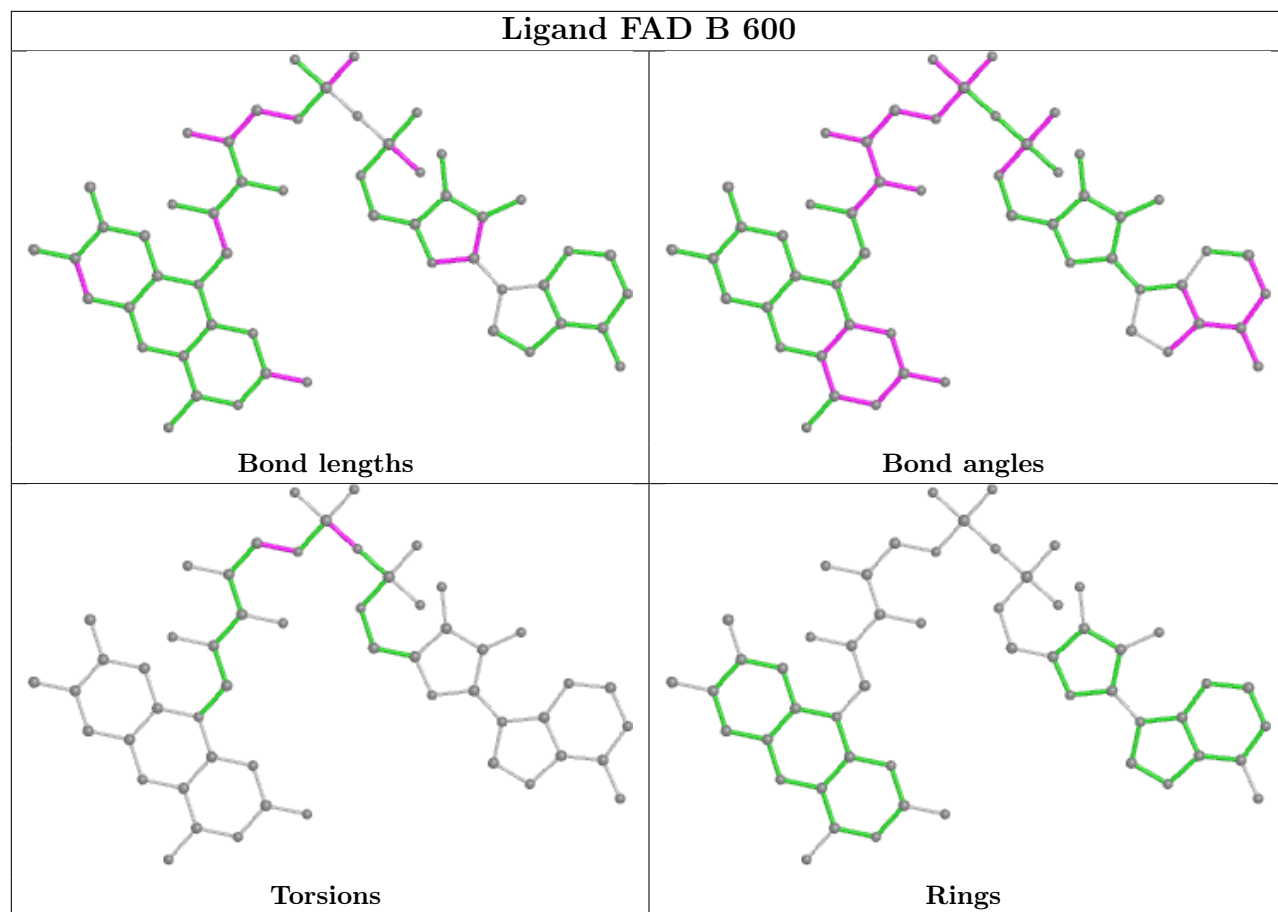
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.16	25 (4%)	33	38	29, 42, 65, 79	24 (4%)
1	B	550/560 (98%)	0.18	39 (7%)	16	20	29, 42, 64, 79	24 (4%)
All	All	1100/1120 (98%)	0.17	64 (5%)	23	28	29, 42, 65, 79	48 (4%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	VAL	6.2
1	A	325	ARG	6.1
1	B	48	ASP	5.6
1	B	50	SER	5.5
1	B	49	GLY	4.5
1	A	330	ARG	4.2
1	A	329	SER	4.2
1	A	61	THR	4.0
1	B	62	HIS	4.0
1	B	329	SER	3.9
1	B	61	THR	3.9
1	A	331	THR	3.8
1	B	66	GLN	3.7
1	B	51	TYR	3.6
1	B	331	THR	3.6
1	B	67	ASP	3.5
1	B	337	GLU	3.5
1	A	7	PHE	3.5
1	B	52	MET	3.3
1	B	391	GLU	3.3
1	A	66	GLN	3.2
1	A	391	GLU	3.2
1	A	302	GLY	3.2
1	A	328	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	62	HIS	3.1
1	B	325	ARG	3.0
1	B	60	PRO	3.0
1	B	415	ASP	3.0
1	B	408	TYR	2.9
1	A	50	SER	2.9
1	B	159	ASN	2.8
1	B	392	ASN	2.8
1	B	365	ARG	2.8
1	B	25	ILE	2.7
1	B	369	GLU	2.7
1	A	285	LYS	2.7
1	A	162	ASP	2.6
1	A	52	MET	2.5
1	B	478	LEU	2.5
1	B	68	TYR	2.5
1	B	303	MET	2.4
1	B	306	GLN	2.4
1	A	395	LEU	2.4
1	A	51	TYR	2.4
1	B	418	PRO	2.3
1	B	19	SER	2.3
1	A	47	VAL	2.3
1	B	274	GLY	2.3
1	B	390	PRO	2.3
1	B	448	GLN	2.3
1	A	30	ARG	2.3
1	B	339	LEU	2.2
1	B	157	ALA	2.2
1	A	41	SER	2.2
1	A	448	GLN	2.1
1	B	409	ASP	2.1
1	A	156	GLU	2.1
1	A	19	SER	2.1
1	B	24	PHE	2.1
1	A	31	ILE	2.1
1	A	49	GLY	2.1
1	B	302	GLY	2.1
1	B	347	ASN	2.1
1	B	77	PRO	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

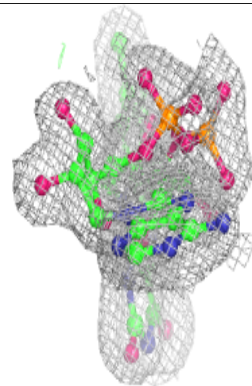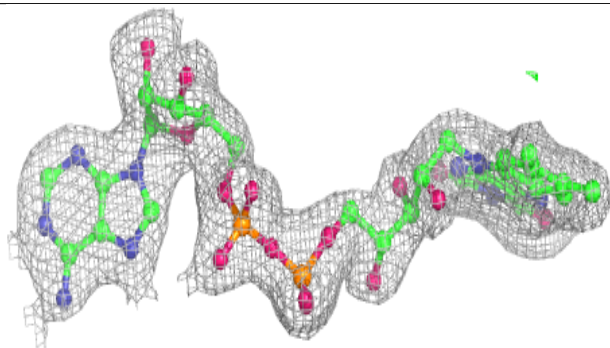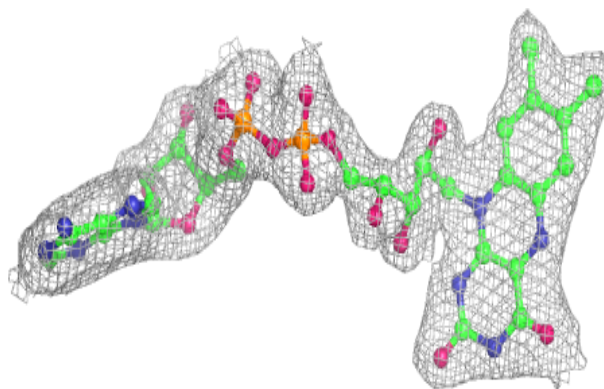| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FCR	B	601	11/11	0.86	0.17	42,44,49,50	0
3	FCR	A	601	11/11	0.88	0.16	42,45,48,49	0
2	FAD	B	600	53/53	0.95	0.10	36,39,43,44	0
2	FAD	A	600	53/53	0.97	0.09	36,39,44,44	0

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.

Electron density around FAD B 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
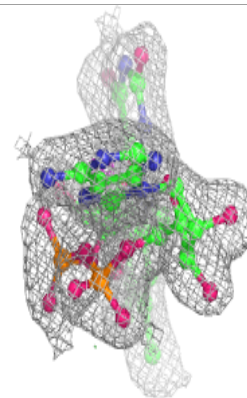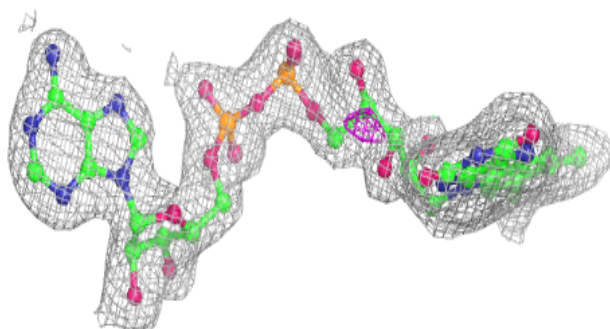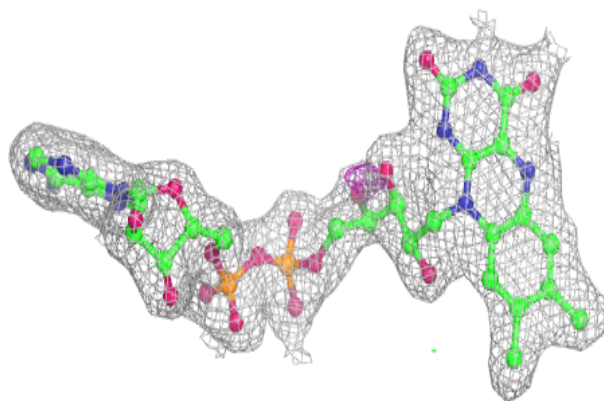
Electron density around FAD A 600:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.