



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2020 – 11:33 pm BST

PDB ID : 1FOH
Title : PHENOL HYDROXYLASE FROM TRICHOSPORON CUTANEUM
Authors : Enroth, C.; Neujahr, H.; Schneider, G.; Lindqvist, Y.
Deposited on : 1998-03-26
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

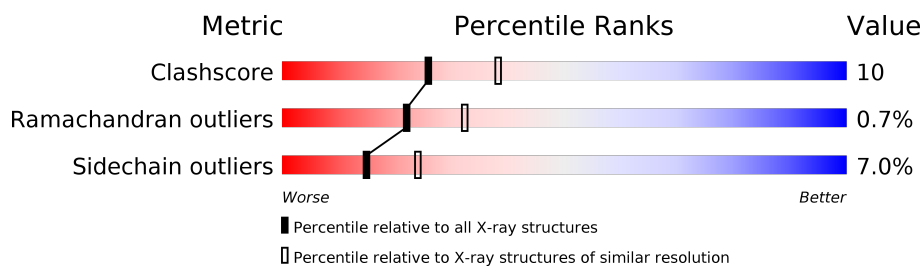
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	664	
1	B	664	
1	C	664	
1	D	664	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	C	801	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22235 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 PHENOL HYDROXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5174	3254	907	989	24			
1	B	651	Total	C	N	O	S	0	0	0
			5186	3261	909	992	24			
1	C	656	Total	C	N	O	S	0	0	0
			5230	3287	920	999	24			
1	D	654	Total	C	N	O	S	0	0	0
			5216	3279	916	997	24			

There are 4 discrepancies between the modelled and reference sequences:

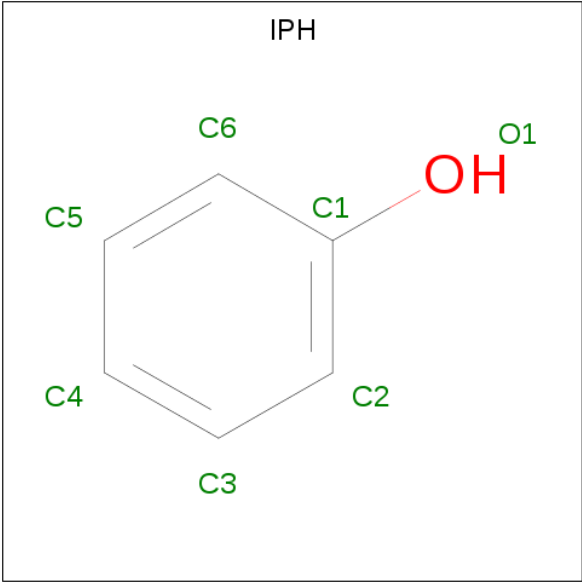
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ARG	PRO	CONFLICT	UNP P15245
B	265	ARG	PRO	CONFLICT	UNP P15245
C	265	ARG	PRO	CONFLICT	UNP P15245
D	265	ARG	PRO	CONFLICT	UNP P15245

- 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		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PHENOL (three-letter code: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 6 1	0	0
3	B	1	Total C O 7 6 1	0	0
3	C	1	Total C O 7 6 1	0	0
3	D	1	Total C O 7 6 1	0	0

- Molecule 4 is water.

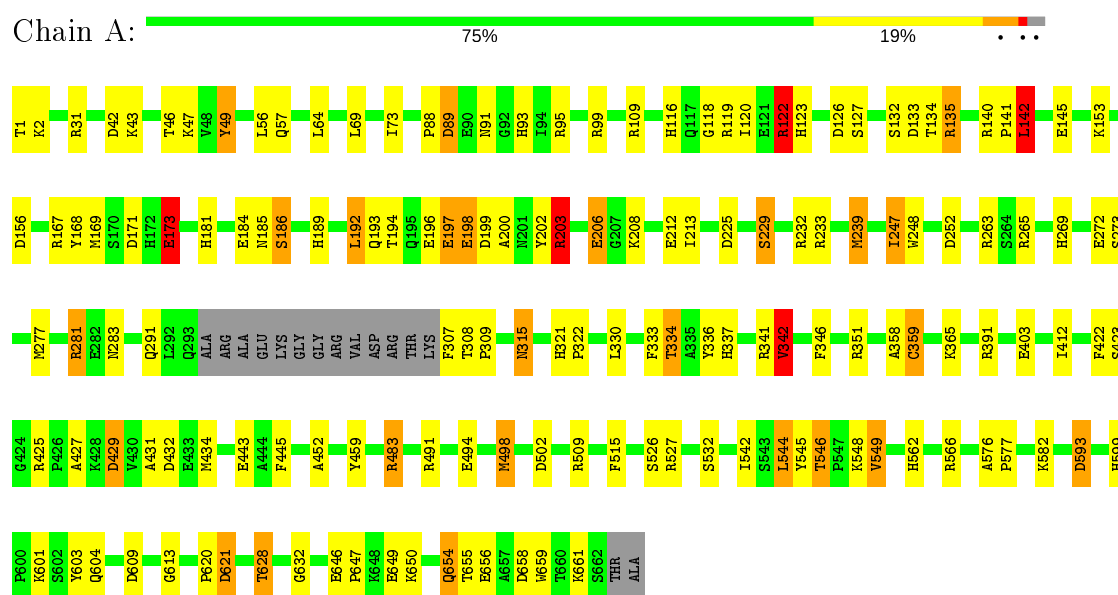
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	341	Total O 341 341	0	0
4	B	296	Total O 296 296	0	0
4	C	302	Total O 302 302	0	0
4	D	250	Total O 250 250	0	0

3 Residue-property plots

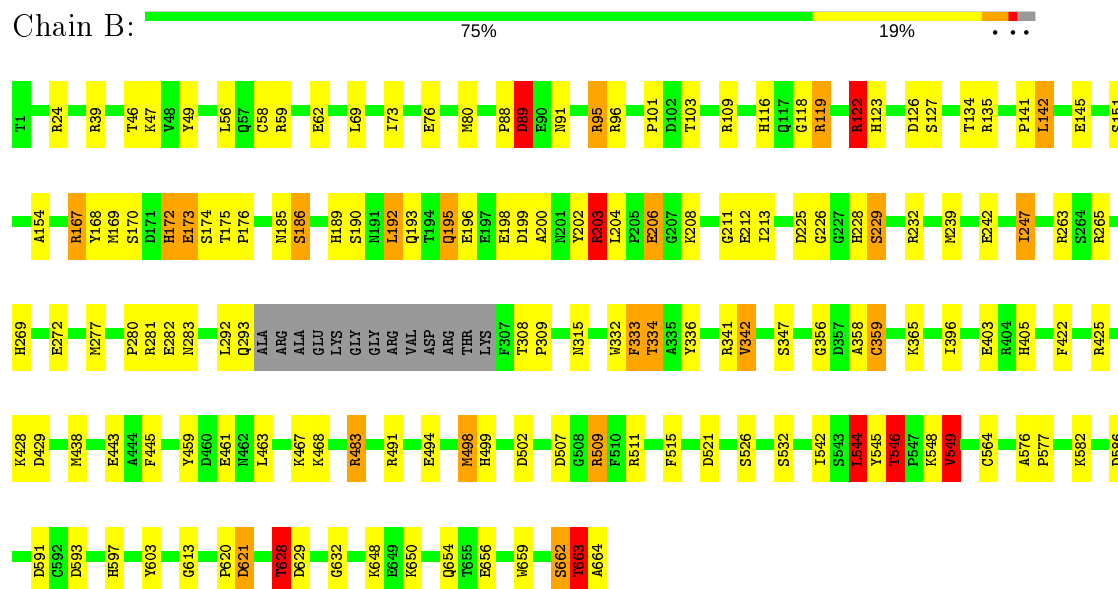
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 was not executed.

• Molecule 1: PHENOL HYDROXYLASE

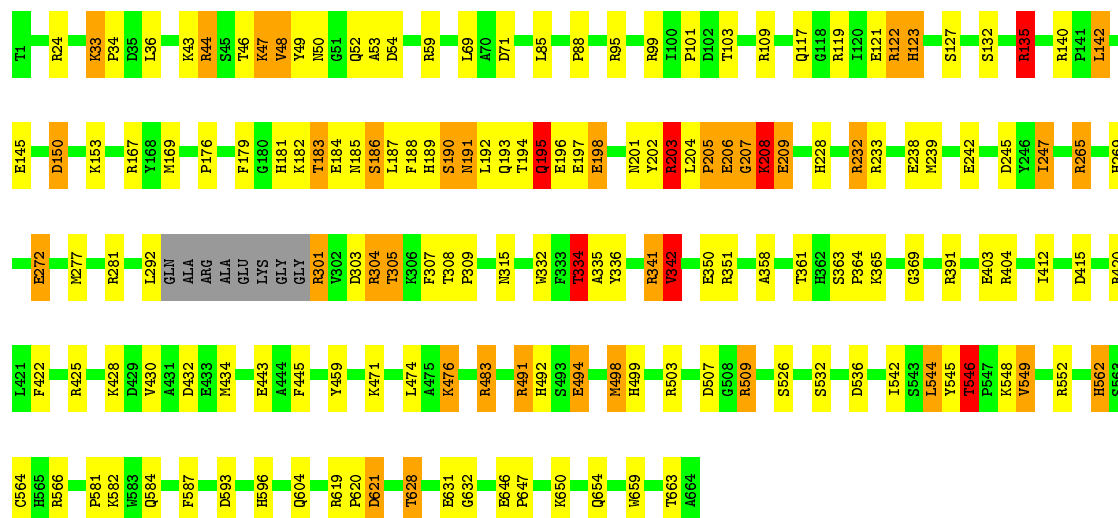


• Molecule 1: PHENOL HYDROXYLASE



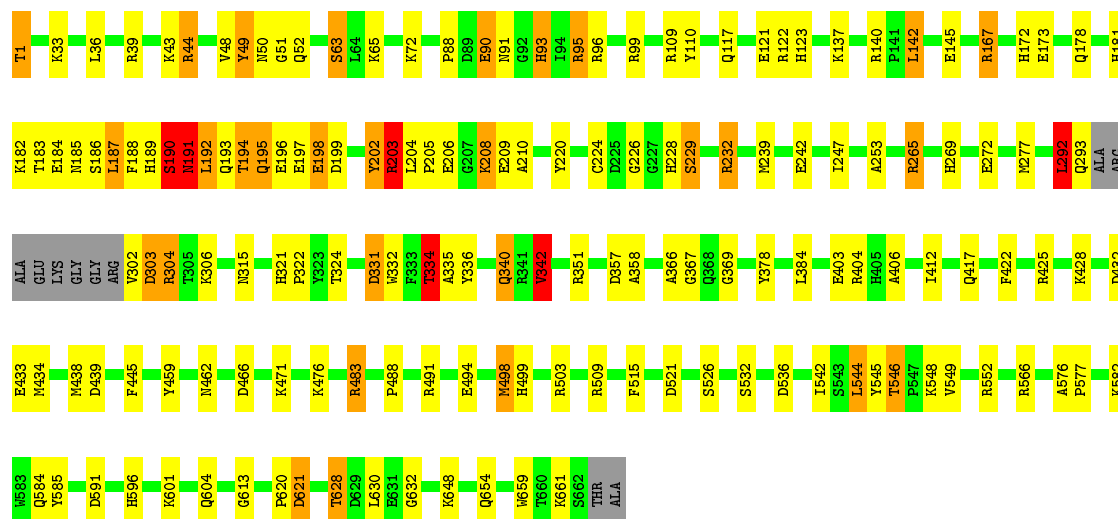
- Molecule 1: PHENOL HYDROXYLASE

Chain C: 74% 18% 5% ..



- Molecule 1: PHENOL HYDROXYLASE

Chain D:  74% 19% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.03Å 150.68Å 114.92Å 90.00° 114.68° 90.00°	Depositor
Resolution (Å)	12.00 – 2.40	Depositor
% Data completeness (in resolution range)	98.0 (12.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22235	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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: IPH, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/5292	1.31	47/7160 (0.7%)
1	B	0.53	0/5304	1.34	58/7177 (0.8%)
1	C	0.55	0/5348	1.44	71/7235 (1.0%)
1	D	0.56	0/5334	1.41	66/7216 (0.9%)
All	All	0.54	0/21278	1.38	242/28788 (0.8%)

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	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	ARG	NE-CZ-NH1	25.27	132.94	120.30
1	C	44	ARG	NE-CZ-NH2	-23.67	108.47	120.30
1	D	203	ARG	NE-CZ-NH2	-16.40	112.10	120.30
1	C	509	ARG	NE-CZ-NH2	-16.17	112.22	120.30
1	D	509	ARG	NE-CZ-NH2	-15.86	112.37	120.30
1	C	562	HIS	ND1-CG-CD2	-14.24	86.06	106.00
1	D	304	ARG	CD-NE-CZ	13.95	143.13	123.60
1	D	44	ARG	NE-CZ-NH2	-13.71	113.45	120.30
1	D	44	ARG	NE-CZ-NH1	13.46	127.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASP	CB-CG-OD1	12.84	129.86	118.30
1	B	509	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	C	135	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	C	203	ARG	NE-CZ-NH2	11.96	126.28	120.30
1	B	203	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	A	566	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	C	562	HIS	CG-ND1-CE1	11.27	123.97	108.20
1	A	122	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	C	207	GLY	C-N-CA	10.55	148.09	121.70
1	D	304	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	C	195	GLN	CA-CB-CG	10.14	135.71	113.40
1	A	233	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	A	171	ASP	CA-CB-CG	10.02	135.45	113.40
1	A	509	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	D	122	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	B	96	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	B	122	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	C	509	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	C	135	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	552	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	D	548	LYS	C-N-CA	8.99	144.18	121.70
1	A	620	PRO	C-N-CA	8.95	144.09	121.70
1	A	156	ASP	CB-CG-OD1	8.82	126.23	118.30
1	C	562	HIS	CG-CD2-NE2	8.80	125.91	109.20
1	B	548	LYS	C-N-CA	8.72	143.49	121.70
1	A	548	LYS	C-N-CA	8.71	143.48	121.70
1	D	203	ARG	N-CA-CB	-8.32	95.62	110.60
1	D	208	LYS	CA-C-O	8.31	137.55	120.10
1	B	122	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	281	ARG	NE-CZ-NH1	-8.11	116.24	120.30
1	B	119	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	B	59	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	D	142	LEU	CA-CB-CG	8.08	133.89	115.30
1	D	39	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	C	142	LEU	CA-CB-CG	8.02	133.75	115.30
1	C	232	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	95	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	B	656	GLU	OE1-CD-OE2	7.96	132.85	123.30
1	C	24	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	D	167	ARG	CD-NE-CZ	7.81	134.53	123.60
1	D	620	PRO	C-N-CA	7.74	141.05	121.70
1	B	620	PRO	C-N-CA	7.71	140.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	CD-NE-CZ	7.69	134.37	123.60
1	D	202	TYR	CB-CG-CD1	-7.68	116.39	121.00
1	C	232	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	24	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	203	ARG	NH1-CZ-NH2	7.57	127.73	119.40
1	A	31	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	A	49	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	B	167	ARG	CD-NE-CZ	7.52	134.13	123.60
1	A	122	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	142	LEU	CA-CB-CG	7.46	132.47	115.30
1	A	342	VAL	CB-CA-C	-7.45	97.25	111.40
1	D	208	LYS	CA-C-N	-7.42	100.87	117.20
1	B	206	GLU	OE1-CD-OE2	7.41	132.19	123.30
1	A	391	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	D	591	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	483	ARG	CD-NE-CZ	7.34	133.88	123.60
1	D	199	ASP	CB-CG-OD1	7.33	124.90	118.30
1	C	621	ASP	CB-CG-OD1	-7.33	111.71	118.30
1	B	341	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	C	620	PRO	C-N-CA	7.29	139.92	121.70
1	D	140	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	D	334	THR	N-CA-CB	7.23	124.03	110.30
1	B	663	THR	N-CA-CB	7.20	123.97	110.30
1	D	109	ARG	CD-NE-CZ	7.17	133.64	123.60
1	C	265	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	342	VAL	CB-CA-C	-7.14	97.84	111.40
1	D	466	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	621	ASP	N-CA-CB	-7.10	97.83	110.60
1	A	126	ASP	CB-CG-OD1	7.07	124.67	118.30
1	B	135	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	334	THR	N-CA-CB	7.05	123.70	110.30
1	A	31	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	D	404	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	B	603	TYR	CB-CG-CD1	6.92	125.15	121.00
1	D	96	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	D	49	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	B	142	LEU	CA-CB-CG	6.87	131.10	115.30
1	D	566	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	225	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	135	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	239	MET	CA-CB-CG	6.75	124.78	113.30
1	C	483	ARG	NE-CZ-NH2	-6.74	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	CYS	CB-CA-C	-6.70	97.00	110.40
1	D	503	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	502	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	119	ARG	CD-NE-CZ	6.60	132.84	123.60
1	A	203	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	206	GLU	OE1-CD-OE2	6.58	131.19	123.30
1	B	621	ASP	N-CA-CB	-6.53	98.84	110.60
1	B	586	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	B	591	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	99	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	B	109	ARG	CD-NE-CZ	6.48	132.67	123.60
1	B	109	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	D	331	ASP	CB-CG-OD1	6.43	124.08	118.30
1	C	391	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	D	109	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	621	ASP	N-CA-CB	-6.40	99.08	110.60
1	D	621	ASP	CB-CA-C	-6.40	97.61	110.40
1	C	350	GLU	OE1-CD-OE2	-6.38	115.64	123.30
1	C	566	ARG	CD-NE-CZ	6.35	132.50	123.60
1	C	351	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	76	GLU	OE1-CD-OE2	-6.34	115.70	123.30
1	D	209	GLU	N-CA-C	-6.32	93.93	111.00
1	A	609	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	D	621	ASP	N-CA-CB	-6.26	99.33	110.60
1	B	173	GLU	CA-CB-CG	6.26	127.17	113.40
1	A	593	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	544	LEU	CA-CB-CG	6.22	129.61	115.30
1	B	96	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	503	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	491	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	D	483	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	197	GLU	OE1-CD-OE2	6.19	130.73	123.30
1	B	521	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	552	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	536	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	359	CYS	CA-CB-SG	6.15	125.07	114.00
1	A	621	ASP	CB-CA-C	-6.13	98.13	110.40
1	C	304	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	404	ARG	CD-NE-CZ	6.11	132.15	123.60
1	B	206	GLU	CA-CB-CG	-6.07	100.05	113.40
1	C	150	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	603	TYR	CB-CG-CD1	6.06	124.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	C	548	LYS	C-N-CA	6.03	136.78	121.70
1	C	301	ARG	CD-NE-CZ	6.02	132.03	123.60
1	D	303	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	466	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	536	ASP	CB-CG-OD1	5.95	123.65	118.30
1	D	483	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	203	ARG	CD-NE-CZ	-5.93	115.29	123.60
1	D	95	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	304	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	502	ASP	CB-CG-OD1	5.85	123.57	118.30
1	C	334	THR	N-CA-CB	5.85	121.41	110.30
1	C	209	GLU	N-CA-C	-5.85	95.22	111.00
1	B	603	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	C	71	ASP	CB-CG-OD1	5.84	123.55	118.30
1	D	265	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	39	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	172	HIS	CA-CB-CG	-5.80	103.74	113.60
1	D	199	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	351	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	A	99	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	C	619	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	334	THR	N-CA-CB	5.73	121.19	110.30
1	C	207	GLY	CA-C-O	5.73	130.92	120.60
1	C	208	LYS	N-CA-C	5.73	126.47	111.00
1	A	49	TYR	CA-CB-CG	-5.73	102.52	113.40
1	B	621	ASP	CB-CA-C	-5.72	98.96	110.40
1	D	191	ASN	CB-CA-C	5.72	121.83	110.40
1	C	205	PRO	C-N-CA	5.71	135.97	121.70
1	C	140	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	D	206	GLU	N-CA-CB	-5.69	100.35	110.60
1	C	135	ARG	CD-NE-CZ	5.69	131.56	123.60
1	C	44	ARG	CD-NE-CZ	5.65	131.51	123.60
1	B	282	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	B	225	ASP	CB-CG-OD1	5.63	123.36	118.30
1	D	342	VAL	CB-CA-C	-5.60	100.76	111.40
1	C	208	LYS	N-CA-CB	-5.58	100.56	110.60
1	C	208	LYS	CB-CA-C	-5.58	99.25	110.40
1	D	302	VAL	CG1-CB-CG2	-5.58	101.98	110.90
1	C	341	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	D	621	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	B	341	ARG	CD-NE-CZ	5.56	131.39	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	206	GLU	N-CA-CB	-5.52	100.67	110.60
1	C	123	HIS	CA-CB-CG	-5.50	104.24	113.60
1	C	186	SER	N-CA-CB	5.49	118.74	110.50
1	A	359	CYS	CB-CA-C	-5.46	99.47	110.40
1	D	145	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	A	621	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	D	206	GLU	CA-CB-CG	-5.45	101.41	113.40
1	B	198	GLU	CB-CA-C	-5.44	99.53	110.40
1	C	203	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
1	A	206	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	C	99	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	562	HIS	CG-ND1-CE1	5.36	115.70	108.20
1	C	109	ARG	CD-NE-CZ	5.36	131.11	123.60
1	A	620	PRO	O-C-N	-5.36	114.13	122.70
1	D	509	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	D	292	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	546	THR	N-CA-CB	5.32	120.40	110.30
1	C	552	ARG	CD-NE-CZ	5.31	131.04	123.60
1	B	203	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	B	24	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	126	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	483	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	253	ALA	N-CA-CB	-5.26	102.74	110.10
1	C	351	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	202	TYR	CA-C-O	5.24	131.10	120.10
1	B	628	THR	CB-CA-C	-5.23	97.47	111.60
1	A	527	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	351	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	D	357	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	359	CYS	N-CA-CB	-5.22	101.20	110.60
1	B	511	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	C	334	THR	CB-CA-C	-5.22	97.51	111.60
1	D	521	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	342	VAL	N-CA-CB	5.21	122.96	111.50
1	C	631	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	A	233	ARG	CD-NE-CZ	5.21	130.89	123.60
1	C	183	THR	CA-CB-CG2	-5.20	105.12	112.40
1	C	48	VAL	N-CA-CB	5.19	122.93	111.50
1	C	420	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	549	VAL	CA-CB-CG2	5.18	118.68	110.90
1	C	301	ARG	NE-CZ-NH2	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	D	49	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	203	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	B	443	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	D	210	ALA	N-CA-C	-5.16	97.07	111.00
1	D	209	GLU	N-CA-CB	5.15	119.88	110.60
1	C	361	THR	N-CA-CB	5.14	120.08	110.30
1	C	546	THR	N-CA-CB	5.13	120.04	110.30
1	D	39	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	48	VAL	CB-CA-C	-5.12	101.67	111.40
1	A	197	GLU	CA-CB-CG	-5.12	102.14	113.40
1	C	415	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	621	ASP	CB-CA-C	-5.09	100.22	110.40
1	B	429	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	342	VAL	CB-CA-C	-5.08	101.74	111.40
1	C	121	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	B	59	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	D	232	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	59	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	173	GLU	CA-CB-CG	5.03	124.46	113.40
1	A	122	ARG	CD-NE-CZ	5.00	130.61	123.60
1	A	140	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	B	621	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	89	ASP	Mainchain
1	C	584	GLN	Mainchain
1	D	488	PRO	Mainchain
1	D	584	GLN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5174	0	5036	96	0
1	B	5186	0	5048	86	0
1	C	5230	0	5099	135	0
1	D	5216	0	5082	124	0
2	A	53	0	30	1	0
2	B	53	0	30	0	0
2	C	53	0	29	2	0
2	D	53	0	29	5	0
3	A	7	0	6	0	0
3	B	7	0	6	0	0
3	C	7	0	6	0	0
3	D	7	0	6	0	0
4	A	341	0	0	18	0
4	B	296	0	0	18	0
4	C	302	0	0	16	0
4	D	250	0	0	20	0
All	All	22235	0	20407	433	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (433) 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:C:167:ARG:NE	1:C:203:ARG:HH21	1.52	1.05
1:C:476:LYS:HE2	4:C:1053:HOH:O	1.62	0.98
1:C:195:GLN:HB2	1:C:228:HIS:HB3	1.47	0.97
1:C:167:ARG:HH21	1:C:203:ARG:HE	1.11	0.91
1:B:628:THR:HG23	4:B:1074:HOH:O	1.70	0.91
1:C:167:ARG:NH2	1:C:203:ARG:HE	1.73	0.86
1:D:208:LYS:HD3	4:D:914:HOH:O	1.74	0.86
1:A:491:ARG:HD3	1:A:498:MET:HE1	1.60	0.84
1:B:265:ARG:HH21	1:B:277:MET:HE2	1.39	0.83
1:D:185:ASN:HB2	1:D:187:LEU:HD21	1.61	0.82
1:B:542:ILE:O	1:B:546:THR:HG23	1.82	0.80
1:D:44:ARG:NH2	1:D:198:GLU:OE2	2.15	0.80
1:C:369:GLY:HA3	2:C:801:FAD:H1'2	1.65	0.79
1:D:369:GLY:HA3	2:D:801:FAD:H1'2	1.64	0.78
1:D:265:ARG:HH21	1:D:277:MET:HE2	1.49	0.78
1:B:119:ARG:HH22	1:B:192:LEU:HD23	1.48	0.78
1:A:542:ILE:O	1:A:546:THR:HG23	1.84	0.77
1:B:491:ARG:HD3	1:B:498:MET:HE1	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ASN:ND2	4:A:1069:HOH:O	2.16	0.77
1:C:491:ARG:HD3	1:C:498:MET:HE3	1.65	0.77
1:D:491:ARG:HD3	1:D:498:MET:HE1	1.67	0.77
1:B:172:HIS:H	1:B:172:HIS:CD2	2.01	0.77
1:C:194:THR:HG23	1:C:196:GLU:HB2	1.67	0.76
1:A:1:THR:HG21	1:A:213:ILE:HD12	1.67	0.75
1:B:192:LEU:HB3	4:B:989:HOH:O	1.86	0.75
1:A:119:ARG:HH22	1:A:192:LEU:HD23	1.52	0.75
1:A:265:ARG:HH21	1:A:277:MET:HE2	1.52	0.73
1:C:542:ILE:O	1:C:546:THR:HG23	1.88	0.73
1:D:205:PRO:HD2	1:D:208:LYS:HD2	1.70	0.73
1:D:204:LEU:HD11	1:D:208:LYS:HB3	1.70	0.73
1:B:628:THR:HG21	1:B:632:GLY:HA3	1.69	0.72
1:C:195:GLN:HE21	1:C:233:ARG:HD3	1.52	0.72
1:D:542:ILE:O	1:D:546:THR:HG23	1.90	0.72
1:B:122:ARG:NH2	1:B:195:GLN:HG3	2.05	0.71
1:C:167:ARG:CZ	1:C:203:ARG:HH21	2.03	0.71
1:A:43:LYS:HG2	2:A:801:FAD:C4A	2.21	0.70
1:C:186:SER:HB2	1:C:332:TRP:HZ2	1.56	0.70
1:D:50:ASN:HA	1:D:188:PHE:HZ	1.56	0.70
1:A:491:ARG:HB2	1:A:498:MET:HE3	1.74	0.70
1:C:239:MET:HG2	1:C:341:ARG:HB3	1.73	0.70
1:C:204:LEU:HG	1:C:208:LYS:HG3	1.73	0.70
1:C:491:ARG:HB2	1:C:498:MET:HE2	1.72	0.70
1:B:265:ARG:NH2	1:B:277:MET:HE2	2.07	0.70
1:A:181:HIS:CE1	1:A:197:GLU:HG3	2.27	0.69
1:D:204:LEU:CD1	1:D:208:LYS:HB3	2.23	0.69
1:C:334:THR:HG21	4:C:888:HOH:O	1.92	0.69
1:D:491:ARG:HB2	1:D:498:MET:HE3	1.74	0.69
1:A:116:HIS:HB3	1:A:281:ARG:NH2	2.07	0.69
1:C:562:HIS:HD2	1:C:564:CYS:H	1.41	0.69
1:A:185:ASN:O	1:A:186:SER:CB	2.42	0.68
1:C:33:LYS:HG2	1:C:36:LEU:HG	1.76	0.67
1:C:604:GLN:HE22	1:D:476:LYS:CB	2.07	0.67
1:C:167:ARG:HE	1:C:203:ARG:HH21	1.42	0.67
1:C:186:SER:HB2	1:C:332:TRP:CZ2	2.30	0.66
1:D:232:ARG:NH2	4:D:1020:HOH:O	2.29	0.66
1:C:476:LYS:HD3	4:D:985:HOH:O	1.96	0.66
1:A:646:GLU:OE2	1:A:650:LYS:HD3	1.96	0.66
1:C:549:VAL:HA	4:C:967:HOH:O	1.96	0.66
1:B:564:CYS:SG	4:B:876:HOH:O	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ARG:NE	1:C:203:ARG:NH2	2.36	0.66
1:B:189:HIS:NE2	4:B:986:HOH:O	2.29	0.65
1:D:433:GLU:HG3	4:D:962:HOH:O	1.95	0.65
1:D:334:THR:HG21	4:D:887:HOH:O	1.95	0.65
1:D:265:ARG:NH2	1:D:277:MET:HE2	2.12	0.65
1:D:194:THR:CG2	1:D:197:GLU:H	2.10	0.65
1:C:190:SER:HA	4:C:888:HOH:O	1.96	0.65
1:C:44:ARG:NH2	1:C:198:GLU:OE2	2.29	0.65
1:D:186:SER:HB2	1:D:332:TRP:CZ2	2.32	0.65
1:A:145:GLU:OE2	1:A:167:ARG:NH1	2.29	0.64
1:A:69:LEU:HD21	1:A:127:SER:HB2	1.79	0.64
1:B:663:THR:HG23	1:D:324:THR:HG22	1.77	0.64
1:A:119:ARG:NH2	1:A:192:LEU:HD23	2.13	0.64
1:A:443:GLU:HB3	4:A:1083:HOH:O	1.98	0.64
1:C:604:GLN:HE22	1:D:476:LYS:HB3	1.62	0.64
1:C:628:THR:HG21	1:C:632:GLY:HA3	1.80	0.64
1:C:203:ARG:NE	1:C:203:ARG:HA	2.12	0.64
1:C:193:GLN:HA	1:C:304:ARG:HH12	1.62	0.64
1:D:185:ASN:OD1	1:D:187:LEU:HG	1.98	0.63
1:A:89:ASP:HB2	1:A:93:HIS:H	1.64	0.63
1:D:190:SER:HA	4:D:887:HOH:O	1.98	0.63
1:D:193:GLN:NE2	1:D:198:GLU:HG2	2.12	0.63
1:B:69:LEU:HD21	1:B:127:SER:HB2	1.79	0.63
1:D:1:THR:N	4:D:1048:HOH:O	2.31	0.62
1:C:206:GLU:CG	1:C:207:GLY:H	2.12	0.62
1:B:116:HIS:HD2	1:B:118:GLY:H	1.47	0.62
1:B:185:ASN:O	1:B:186:SER:CB	2.47	0.62
1:B:116:HIS:HB3	1:B:281:ARG:NH2	2.15	0.62
1:A:265:ARG:HH21	1:A:277:MET:CE	2.13	0.62
1:C:204:LEU:CD2	1:C:208:LYS:HG3	2.30	0.62
1:B:185:ASN:O	1:B:186:SER:HB3	1.99	0.62
1:A:491:ARG:HB2	1:A:498:MET:CE	2.29	0.62
1:C:193:GLN:HB3	4:C:1089:HOH:O	2.00	0.62
1:A:265:ARG:NH2	1:A:277:MET:HE2	2.14	0.61
1:D:186:SER:CB	1:D:332:TRP:HE1	2.13	0.61
1:A:273:SER:HB3	4:A:1069:HOH:O	2.00	0.61
1:C:169:MET:CE	1:C:202:TYR:HB3	2.31	0.60
1:D:303:ASP:HB3	1:D:306:LYS:HE3	1.83	0.60
1:D:191:ASN:HD21	2:D:801:FAD:C8M	2.15	0.60
1:A:46:THR:HG21	1:A:200:ALA:HA	1.83	0.60
1:C:308:THR:HB	1:C:309:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LEU:HD12	1:C:307:PHE:CZ	2.37	0.59
1:C:238:GLU:HG2	1:C:239:MET:N	2.18	0.59
1:C:206:GLU:HG2	1:C:207:GLY:H	1.67	0.59
1:A:56:LEU:HD11	1:A:120:ILE:HD12	1.85	0.59
1:B:247:ILE:HD12	1:B:336:TYR:O	2.02	0.59
1:B:141:PRO:HD2	1:B:204:LEU:CD2	2.32	0.58
1:C:195:GLN:HB2	1:C:228:HIS:CB	2.28	0.58
1:A:194:THR:O	1:A:198:GLU:HG3	2.02	0.58
1:D:491:ARG:NH1	1:D:498:MET:HE2	2.17	0.58
1:D:491:ARG:HB2	1:D:498:MET:CE	2.34	0.58
1:C:628:THR:HG23	4:C:1010:HOH:O	2.02	0.58
1:C:265:ARG:HH21	1:C:277:MET:HE2	1.67	0.58
1:C:265:ARG:HH21	1:C:277:MET:CE	2.17	0.58
1:A:307:PHE:HB3	4:A:1077:HOH:O	2.04	0.57
1:A:123:HIS:CE1	4:A:1123:HOH:O	2.57	0.57
1:A:491:ARG:NH1	1:A:498:MET:HE2	2.19	0.57
1:C:186:SER:N	1:C:332:TRP:NE1	2.52	0.57
1:D:195:GLN:HB3	1:D:228:HIS:HB3	1.85	0.57
1:C:194:THR:HG23	1:C:197:GLU:H	1.69	0.57
1:C:186:SER:CB	1:C:332:TRP:HE1	2.16	0.57
1:C:204:LEU:CG	1:C:208:LYS:HG3	2.33	0.57
1:B:468:LYS:HE3	4:B:1096:HOH:O	2.03	0.57
1:D:342:VAL:HG22	1:D:412:ILE:HG12	1.86	0.57
1:A:123:HIS:HE1	4:A:1123:HOH:O	1.88	0.57
1:A:203:ARG:N	4:A:839:HOH:O	2.38	0.57
1:C:491:ARG:HB2	1:C:498:MET:CE	2.34	0.57
1:A:185:ASN:O	1:A:186:SER:HB3	2.05	0.57
1:D:228:HIS:O	1:D:229:SER:C	2.43	0.56
1:D:88:PRO:HD3	1:D:269:HIS:O	2.06	0.56
1:D:628:THR:HG21	1:D:632:GLY:HA3	1.87	0.56
1:B:123:HIS:CE1	4:B:827:HOH:O	2.57	0.56
1:C:205:PRO:O	1:C:208:LYS:HB2	2.05	0.56
1:C:471:LYS:HG3	4:C:1010:HOH:O	2.05	0.56
1:D:194:THR:HG23	1:D:197:GLU:H	1.70	0.56
1:C:190:SER:HB2	1:C:334:THR:HG22	1.88	0.56
1:D:203:ARG:NE	1:D:204:LEU:O	2.39	0.56
1:B:170:SER:H	1:B:173:GLU:HG2	1.70	0.56
1:C:169:MET:HE1	1:C:202:TYR:HB3	1.88	0.56
1:C:206:GLU:CG	1:C:207:GLY:N	2.68	0.56
1:C:194:THR:CG2	1:C:197:GLU:H	2.18	0.56
1:D:49:TYR:HB2	1:D:184:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASP:HB3	1:B:91:ASN:H	1.71	0.55
1:D:198:GLU:O	1:D:202:TYR:HD1	1.89	0.55
1:D:192:LEU:HD11	1:D:335:ALA:HB3	1.88	0.55
1:C:34:PRO:O	1:C:135:ARG:NH2	2.40	0.55
1:C:145:GLU:OE2	1:C:203:ARG:NH2	2.39	0.55
1:D:192:LEU:HD21	1:D:336:TYR:HA	1.88	0.55
1:B:491:ARG:HB2	1:B:498:MET:CE	2.37	0.55
1:D:194:THR:HG23	1:D:196:GLU:OE1	2.07	0.55
1:D:186:SER:N	1:D:332:TRP:NE1	2.54	0.55
1:D:190:SER:OG	1:D:191:ASN:N	2.39	0.55
1:D:439:ASP:OD2	4:D:966:HOH:O	2.17	0.55
1:D:491:ARG:HD3	1:D:498:MET:CE	2.37	0.55
1:D:417:GLN:OE1	4:D:1009:HOH:O	2.18	0.55
1:D:43:LYS:NZ	1:D:198:GLU:OE1	2.24	0.55
1:B:292:LEU:O	1:B:293:GLN:HB2	2.07	0.55
1:C:604:GLN:HE22	1:D:476:LYS:CG	2.19	0.55
1:C:46:THR:OG1	1:C:47:LYS:HE2	2.06	0.54
1:C:69:LEU:HD21	1:C:127:SER:HB2	1.89	0.54
1:A:202:TYR:O	1:A:203:ARG:HB2	2.05	0.54
1:C:132:SER:O	1:C:135:ARG:HB2	2.07	0.54
1:C:88:PRO:HD3	1:C:269:HIS:O	2.07	0.54
1:C:192:LEU:CD1	1:C:336:TYR:HA	2.38	0.54
1:B:154:ALA:N	4:B:1076:HOH:O	2.40	0.54
1:D:195:GLN:NE2	4:D:1020:HOH:O	2.23	0.54
1:A:192:LEU:HB3	4:A:972:HOH:O	2.06	0.54
1:B:151:SER:HA	4:B:1076:HOH:O	2.07	0.54
1:D:185:ASN:HB2	1:D:187:LEU:CD2	2.33	0.54
1:D:265:ARG:HH21	1:D:277:MET:CE	2.18	0.54
1:C:193:GLN:HA	1:C:304:ARG:NH1	2.22	0.54
1:A:122:ARG:HD3	1:A:192:LEU:HD12	1.88	0.54
1:A:599:HIS:ND1	1:A:601:LYS:HD3	2.22	0.53
1:B:46:THR:HG21	1:B:200:ALA:HA	1.90	0.53
1:C:188:PHE:CG	1:C:189:HIS:N	2.77	0.53
1:C:646:GLU:OE2	1:C:650:LYS:HD3	2.07	0.53
1:C:499:HIS:HD2	4:C:893:HOH:O	1.91	0.53
1:C:204:LEU:HD12	1:C:205:PRO:HD2	1.91	0.53
1:D:186:SER:HB2	1:D:332:TRP:HZ2	1.72	0.53
1:D:188:PHE:CG	1:D:189:HIS:N	2.77	0.53
1:D:190:SER:OG	1:D:192:LEU:HG	2.09	0.53
1:B:203:ARG:N	4:B:840:HOH:O	2.41	0.52
1:B:203:ARG:NH2	1:B:206:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH2	1:A:173:GLU:OE2	2.32	0.52
1:A:88:PRO:HD3	1:A:269:HIS:O	2.10	0.52
1:D:63:SER:HB3	1:D:378:TYR:CZ	2.44	0.52
1:A:544:LEU:HA	1:A:650:LYS:HD2	1.91	0.52
1:C:185:ASN:OD1	1:C:187:LEU:HD12	2.09	0.52
1:C:208:LYS:HG2	1:C:208:LYS:O	2.09	0.52
1:C:50:ASN:HA	1:C:188:PHE:HZ	1.75	0.52
1:D:65:LYS:HD3	1:D:110:TYR:OH	2.10	0.51
1:A:123:HIS:CE1	4:A:827:HOH:O	2.64	0.51
1:A:189:HIS:HD2	1:A:193:GLN:HB3	1.75	0.51
1:B:265:ARG:HH21	1:B:277:MET:CE	2.17	0.51
1:C:363:SER:HB2	1:C:364:PRO:HD2	1.92	0.51
1:D:195:GLN:HB3	1:D:228:HIS:CG	2.46	0.51
1:D:33:LYS:HG2	1:D:36:LEU:HG	1.92	0.51
1:C:135:ARG:CB	1:C:135:ARG:HH11	2.24	0.51
1:A:122:ARG:HD3	1:A:192:LEU:HA	1.93	0.51
1:B:119:ARG:HH22	1:B:192:LEU:CD2	2.21	0.51
1:C:167:ARG:HH21	1:C:203:ARG:NE	1.93	0.51
1:C:265:ARG:NH2	1:C:277:MET:HE2	2.26	0.51
1:D:181:HIS:HB2	1:D:185:ASN:ND2	2.26	0.50
2:C:801:FAD:H8A	4:C:916:HOH:O	2.11	0.50
1:B:232:ARG:HD3	1:B:358:ALA:O	2.12	0.50
1:C:303:ASP:OD1	1:C:305:THR:HB	2.11	0.50
1:C:203:ARG:NE	1:C:204:LEU:H	2.09	0.50
1:A:116:HIS:HD2	1:A:118:GLY:H	1.58	0.50
1:C:582:LYS:HA	1:C:659:TRP:CE2	2.47	0.50
1:A:56:LEU:HD11	1:A:120:ILE:CD1	2.42	0.50
1:A:342:VAL:HG22	1:A:412:ILE:HG12	1.93	0.50
1:A:64:LEU:HD13	1:A:73:ILE:HD12	1.94	0.50
1:D:183:THR:O	1:D:185:ASN:ND2	2.41	0.50
1:A:232:ARG:CZ	1:A:239:MET:HG2	2.41	0.50
1:B:438:MET:HE1	4:B:1084:HOH:O	2.11	0.50
1:C:123:HIS:NE2	4:C:993:HOH:O	2.35	0.50
1:D:167:ARG:CZ	1:D:204:LEU:HB2	2.42	0.50
1:D:403:GLU:HB3	1:D:459:TYR:CE1	2.46	0.50
1:A:47:LYS:HZ2	1:A:196:GLU:CD	2.15	0.49
1:C:195:GLN:HG3	1:C:233:ARG:NE	2.27	0.49
1:C:203:ARG:CZ	1:C:204:LEU:H	2.26	0.49
1:B:491:ARG:HB2	1:B:498:MET:HE3	1.93	0.49
1:C:194:THR:HG22	1:C:197:GLU:CD	2.33	0.49
1:B:438:MET:CE	4:B:1084:HOH:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:LEU:HD23	1:C:545:TYR:CZ	2.48	0.49
1:A:132:SER:O	1:A:135:ARG:HB2	2.12	0.49
1:B:544:LEU:HD23	1:B:545:TYR:CZ	2.48	0.49
1:B:628:THR:HG22	1:B:629:ASP:H	1.77	0.49
1:C:167:ARG:NH2	1:C:203:ARG:NE	2.51	0.49
1:C:403:GLU:HB3	1:C:459:TYR:CE1	2.47	0.49
1:A:628:THR:HG21	1:A:632:GLY:HA3	1.94	0.49
1:B:168:TYR:CD2	1:B:208:LYS:HB3	2.48	0.49
1:B:189:HIS:CE1	4:B:1062:HOH:O	2.64	0.49
1:C:182:LYS:HG3	1:C:183:THR:N	2.27	0.49
1:D:186:SER:HB2	1:D:332:TRP:HE1	1.76	0.49
1:D:189:HIS:O	1:D:190:SER:C	2.51	0.49
1:B:228:HIS:O	1:B:229:SER:C	2.51	0.49
1:C:604:GLN:NE2	1:D:476:LYS:HG2	2.28	0.49
1:A:427:ALA:HB1	1:A:432:ASP:HB3	1.94	0.49
1:C:53:ALA:O	1:C:117:GLN:HB2	2.13	0.49
1:B:403:GLU:HB3	1:B:459:TYR:CE1	2.48	0.49
1:C:49:TYR:O	1:C:188:PHE:HZ	1.96	0.49
1:C:491:ARG:NH1	1:C:498:MET:HE1	2.28	0.49
1:D:186:SER:N	1:D:332:TRP:HE1	2.10	0.49
1:A:337:HIS:HD2	4:A:1073:HOH:O	1.95	0.48
1:C:191:ASN:HB3	4:C:1091:HOH:O	2.13	0.48
1:D:185:ASN:HA	1:D:332:TRP:CD1	2.48	0.48
1:A:582:LYS:HA	1:A:659:TRP:CE2	2.49	0.48
1:B:211:GLY:O	1:B:213:ILE:HD12	2.14	0.48
1:C:604:GLN:HE22	1:D:476:LYS:HG2	1.77	0.48
1:C:189:HIS:O	1:C:190:SER:C	2.52	0.48
1:D:186:SER:HB2	1:D:332:TRP:NE1	2.28	0.48
1:B:141:PRO:HD2	1:B:204:LEU:HD23	1.95	0.48
1:C:198:GLU:O	1:C:202:TYR:HD1	1.96	0.48
1:B:208:LYS:HD3	1:B:212:GLU:OE1	2.14	0.48
1:C:179:PHE:HB2	1:C:181:HIS:CE1	2.49	0.48
1:C:492:HIS:ND1	1:C:562:HIS:HE1	2.11	0.48
1:A:239:MET:HB3	1:A:341:ARG:HD3	1.95	0.48
1:C:49:TYR:O	1:C:188:PHE:CZ	2.67	0.48
1:B:145:GLU:OE2	1:B:167:ARG:NE	2.34	0.47
1:D:196:GLU:CD	1:D:196:GLU:H	2.18	0.47
1:D:544:LEU:HD23	1:D:545:TYR:CZ	2.49	0.47
1:A:193:GLN:HG2	4:A:985:HOH:O	2.13	0.47
1:B:199:ASP:HB3	4:B:804:HOH:O	2.15	0.47
1:D:123:HIS:CE1	4:D:996:HOH:O	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:TYR:CG	1:D:384:LEU:HD11	2.49	0.47
1:A:132:SER:O	1:A:133:ASP:C	2.53	0.47
1:B:663:THR:O	1:B:664:ALA:CB	2.62	0.47
1:B:122:ARG:CZ	1:B:195:GLN:HB3	2.45	0.47
1:C:54:ASP:OD2	1:C:281:ARG:HD3	2.14	0.47
1:C:169:MET:HE3	1:C:202:TYR:HB3	1.97	0.47
1:D:181:HIS:HB2	1:D:185:ASN:HD21	1.80	0.47
1:A:169:MET:HB3	1:A:173:GLU:HG2	1.96	0.47
1:B:47:LYS:NZ	1:B:196:GLU:OE1	2.48	0.47
1:B:582:LYS:HA	1:B:659:TRP:CE2	2.49	0.47
1:C:194:THR:CG2	1:C:196:GLU:HB2	2.41	0.47
1:D:194:THR:HG22	1:D:197:GLU:H	1.77	0.47
1:D:331:ASP:O	1:D:332:TRP:HB2	2.14	0.47
1:B:663:THR:HG23	1:D:324:THR:CG2	2.45	0.47
1:A:604:GLN:HG3	4:A:884:HOH:O	2.14	0.47
1:D:50:ASN:HA	1:D:188:PHE:CZ	2.45	0.47
4:B:811:HOH:O	1:D:596:HIS:HE1	1.98	0.47
1:B:49:TYR:OH	1:B:196:GLU:O	2.22	0.47
1:A:491:ARG:HD3	1:A:498:MET:CE	2.40	0.46
1:C:150:ASP:OD2	1:C:153:LYS:HE3	2.14	0.46
1:D:194:THR:HG22	1:D:197:GLU:HB2	1.97	0.46
1:A:49:TYR:CE2	1:A:181:HIS:HB2	2.51	0.46
1:D:292:LEU:O	1:D:293:GLN:HB2	2.14	0.46
1:D:601:LYS:HD2	1:D:604:GLN:NE2	2.30	0.46
1:B:425:ARG:HB3	1:B:425:ARG:NH1	2.30	0.46
1:C:308:THR:HB	1:C:309:PRO:CD	2.44	0.46
1:D:186:SER:HB2	1:D:332:TRP:CE2	2.49	0.46
1:B:119:ARG:NH2	1:B:192:LEU:HD23	2.23	0.46
1:C:425:ARG:HB3	1:C:425:ARG:NH1	2.31	0.46
1:D:582:LYS:HA	1:D:659:TRP:CE2	2.50	0.46
1:A:229:SER:HB3	1:A:232:ARG:HB3	1.96	0.46
1:C:307:PHE:CE1	1:C:335:ALA:HB2	2.51	0.46
1:D:178:GLN:NE2	1:D:178:GLN:HA	2.30	0.46
1:B:175:THR:HA	1:B:176:PRO:HD3	1.78	0.46
1:C:509:ARG:NH2	4:C:957:HOH:O	2.33	0.46
1:D:601:LYS:HE3	1:D:604:GLN:OE1	2.16	0.46
1:B:88:PRO:HD3	1:B:269:HIS:O	2.15	0.46
1:A:544:LEU:HD23	1:A:545:TYR:CZ	2.51	0.46
1:C:232:ARG:HD3	1:C:358:ALA:O	2.16	0.46
1:C:187:LEU:HD23	1:C:334:THR:HA	1.98	0.46
4:A:811:HOH:O	1:C:596:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:ARG:HB3	1:D:425:ARG:NH1	2.31	0.46
1:B:80:MET:SD	1:B:280:PRO:HD2	2.56	0.45
1:C:201:ASN:ND2	4:C:970:HOH:O	2.45	0.45
1:D:192:LEU:CD2	1:D:336:TYR:HA	2.47	0.45
1:D:499:HIS:HD2	4:D:892:HOH:O	1.99	0.45
1:A:429:ASP:HB2	1:A:431:ALA:H	1.81	0.45
1:B:123:HIS:NE2	4:B:827:HOH:O	2.35	0.45
1:B:499:HIS:HD2	4:B:901:HOH:O	1.98	0.45
1:A:646:GLU:CD	1:A:650:LYS:HD3	2.35	0.45
1:D:471:LYS:HA	4:D:953:HOH:O	2.16	0.45
1:A:168:TYR:CE2	1:A:208:LYS:HG3	2.52	0.45
1:C:204:LEU:HG	1:C:208:LYS:HE3	1.99	0.45
1:B:122:ARG:HG2	1:B:192:LEU:HG	1.99	0.45
1:C:186:SER:N	1:C:332:TRP:HE1	2.15	0.45
1:D:117:GLN:NE2	1:D:121:GLU:OE2	2.46	0.45
1:D:515:PHE:O	1:D:613:GLY:HA3	2.16	0.45
1:A:277:MET:SD	4:A:1092:HOH:O	2.62	0.44
1:B:172:HIS:CD2	1:B:172:HIS:N	2.75	0.44
1:B:101:PRO:HB2	1:B:103:THR:O	2.17	0.44
1:C:195:GLN:CB	1:C:228:HIS:CG	3.00	0.44
1:D:576:ALA:HA	1:D:577:PRO:HA	1.75	0.44
1:A:308:THR:HB	1:A:309:PRO:HD2	1.99	0.44
1:C:194:THR:HG22	1:C:197:GLU:CG	2.47	0.44
1:A:425:ARG:NH1	1:A:425:ARG:HB3	2.32	0.44
1:A:119:ARG:NH2	1:A:192:LEU:CD2	2.80	0.44
1:B:576:ALA:HA	1:B:577:PRO:HA	1.76	0.44
1:C:203:ARG:NH2	1:C:204:LEU:HB2	2.32	0.44
1:D:194:THR:HG22	1:D:197:GLU:CB	2.46	0.44
1:A:123:HIS:CD2	4:A:921:HOH:O	2.70	0.44
1:B:56:LEU:CD1	1:B:73:ILE:HG21	2.48	0.44
1:D:462:ASN:HB2	4:D:889:HOH:O	2.18	0.44
1:C:342:VAL:HG13	1:C:412:ILE:HD13	1.98	0.44
1:C:581:PRO:HG2	1:C:587:PHE:CD2	2.53	0.44
1:D:195:GLN:HB3	1:D:228:HIS:CB	2.47	0.44
1:A:403:GLU:HB3	1:A:459:TYR:CE1	2.52	0.43
1:C:184:GLU:O	1:C:332:TRP:HA	2.18	0.43
1:C:247:ILE:HD11	1:C:307:PHE:CE2	2.53	0.43
1:A:199:ASP:HB3	4:A:804:HOH:O	2.19	0.43
1:B:263:ARG:HG3	1:D:585:TYR:CG	2.54	0.43
1:D:194:THR:HG22	1:D:197:GLU:CD	2.38	0.43
1:D:366:ALA:O	1:D:367:GLY:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:ASP:OD1	1:B:509:ARG:HD3	2.19	0.43
1:A:2:LYS:NZ	1:A:212:GLU:OE1	2.49	0.43
1:A:515:PHE:O	1:A:613:GLY:HA3	2.19	0.43
1:A:321:HIS:HA	1:A:322:PRO:HA	1.69	0.43
1:B:308:THR:HB	1:B:309:PRO:HD2	1.99	0.43
1:D:188:PHE:CD2	1:D:189:HIS:N	2.87	0.43
1:B:332:TRP:CG	1:B:333:PHE:N	2.87	0.43
1:B:491:ARG:NH1	1:B:498:MET:HE2	2.33	0.43
1:C:544:LEU:O	1:C:647:PRO:HD2	2.19	0.43
1:D:198:GLU:O	1:D:202:TYR:CD1	2.69	0.43
1:A:57:GLN:HG3	1:A:452:ALA:O	2.19	0.42
1:A:93:HIS:HA	4:A:1065:HOH:O	2.19	0.42
1:B:202:TYR:O	1:B:203:ARG:CB	2.64	0.42
1:D:50:ASN:OD1	1:D:189:HIS:CD2	2.73	0.42
1:D:438:MET:HE2	4:D:969:HOH:O	2.19	0.42
1:A:247:ILE:HD12	1:A:336:TYR:O	2.17	0.42
1:B:116:HIS:HD2	1:B:118:GLY:N	2.15	0.42
1:D:194:THR:HG22	1:D:197:GLU:CG	2.49	0.42
1:D:434:MET:HG2	1:D:434:MET:O	2.20	0.42
1:C:474:LEU:HD13	4:C:811:HOH:O	2.19	0.42
1:B:515:PHE:O	1:B:613:GLY:HA3	2.19	0.42
1:B:58:CYS:O	1:B:62:GLU:HG3	2.20	0.42
1:D:193:GLN:NE2	4:D:888:HOH:O	2.37	0.42
1:D:88:PRO:HA	1:D:93:HIS:O	2.19	0.42
1:A:184:GLU:HG3	1:A:193:GLN:HG2	2.01	0.42
1:A:291:GLN:NE2	1:A:423:SER:HB3	2.34	0.42
1:C:185:ASN:HA	1:C:332:TRP:CD1	2.55	0.42
1:D:44:ARG:HD2	2:D:801:FAD:O2B	2.20	0.42
1:C:193:GLN:NE2	4:C:889:HOH:O	2.50	0.42
1:C:204:LEU:CG	1:C:208:LYS:HE3	2.50	0.42
1:D:51:GLY:N	1:D:189:HIS:CD2	2.87	0.42
1:A:202:TYR:O	1:A:203:ARG:CB	2.65	0.42
1:D:232:ARG:HD3	1:D:358:ALA:O	2.20	0.42
1:A:351:ARG:HA	1:A:351:ARG:HD3	1.91	0.42
1:A:576:ALA:HA	1:A:577:PRO:HA	1.78	0.42
1:B:122:ARG:HD3	1:B:192:LEU:HA	2.02	0.42
1:C:272:GLU:OE1	1:C:428:LYS:NZ	2.52	0.42
1:A:263:ARG:O	1:C:494:GLU:HB3	2.19	0.42
1:C:167:ARG:HE	1:C:203:ARG:NH2	2.09	0.41
1:D:224:CYS:O	2:D:801:FAD:H52A	2.20	0.41
1:A:247:ILE:HG13	1:A:248:TRP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASP:O	1:A:330:LEU:HD12	2.20	0.41
1:C:47:LYS:HD3	1:C:47:LYS:HA	1.87	0.41
1:D:321:HIS:HA	1:D:322:PRO:HA	1.72	0.41
1:A:654:GLN:HE22	1:A:656:GLU:N	2.17	0.41
1:A:658:ASP:OD2	1:A:661:LYS:HE2	2.20	0.41
1:B:396:ILE:HG22	1:B:463:LEU:HD23	2.02	0.41
1:C:101:PRO:HB2	1:C:103:THR:O	2.20	0.41
1:C:188:PHE:CD2	1:C:189:HIS:N	2.89	0.41
1:C:204:LEU:HB3	1:C:208:LYS:HE3	2.01	0.41
1:C:85:LEU:HD13	4:C:943:HOH:O	2.20	0.41
1:A:142:LEU:HD22	1:A:168:TYR:CD2	2.56	0.41
1:D:195:GLN:NE2	1:D:228:HIS:ND1	2.55	0.41
1:A:134:THR:O	1:A:134:THR:HG22	2.20	0.41
1:C:195:GLN:HB3	1:C:228:HIS:ND1	2.36	0.41
1:D:406:ALA:N	4:D:919:HOH:O	2.31	0.41
1:D:340:GLN:HB2	1:D:412:ILE:HG13	2.02	0.41
1:D:630:LEU:HG	4:D:946:HOH:O	2.21	0.41
1:C:193:GLN:NE2	1:C:201:ASN:ND2	2.69	0.41
1:A:346:PHE:CE1	1:A:359:CYS:HB3	2.56	0.41
1:B:356:GLY:O	1:B:359:CYS:HB2	2.21	0.41
1:B:597:HIS:HB3	4:B:915:HOH:O	2.20	0.41
1:C:247:ILE:HD11	1:C:307:PHE:CZ	2.56	0.41
1:C:48:VAL:HG21	1:C:176:PRO:HG2	2.03	0.41
1:D:48:VAL:O	1:D:49:TYR:C	2.58	0.41
1:A:185:ASN:O	1:A:186:SER:OG	2.37	0.41
1:A:89:ASP:HB3	1:A:91:ASN:H	1.86	0.41
1:B:190:SER:OG	1:B:193:GLN:HG3	2.20	0.41
1:B:168:TYR:CZ	1:B:208:LYS:HD2	2.56	0.41
1:B:226:GLY:O	1:B:358:ALA:HA	2.21	0.41
1:B:405:HIS:CE1	4:B:965:HOH:O	2.73	0.41
1:D:173:GLU:OE2	1:D:205:PRO:HD3	2.21	0.41
1:A:42:ASP:O	1:A:141:PRO:HA	2.21	0.40
1:D:190:SER:CA	4:D:887:HOH:O	2.64	0.40
1:D:90:GLU:HG3	1:D:91:ASN:H	1.85	0.40
1:A:425:ARG:HB3	1:A:425:ARG:HH11	1.85	0.40
1:A:654:GLN:NE2	1:A:656:GLU:H	2.20	0.40
1:B:202:TYR:O	1:B:203:ARG:HB2	2.22	0.40
1:B:169:MET:O	1:B:204:LEU:HD21	2.20	0.40
1:B:461:GLU:HB2	1:B:467:LYS:HG3	2.03	0.40
1:D:369:GLY:HA3	2:D:801:FAD:O3'	2.22	0.40
1:D:72:LYS:HD2	4:D:845:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HD3	1:A:358:ALA:O	2.21	0.40
1:D:226:GLY:O	1:D:358:ALA:HA	2.21	0.40
1:A:546:THR:HG22	4:A:876:HOH:O	2.21	0.40
1:C:43:LYS:NZ	1:C:198:GLU:OE1	2.44	0.40
1:C:507:ASP:OD1	1:C:509:ARG:HD3	2.22	0.40

There are no symmetry-related clashes.

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	645/664 (97%)	612 (95%)	29 (4%)	4 (1%)	25	36
1	B	647/664 (97%)	622 (96%)	19 (3%)	6 (1%)	17	25
1	C	652/664 (98%)	623 (96%)	26 (4%)	3 (0%)	29	41
1	D	650/664 (98%)	627 (96%)	19 (3%)	4 (1%)	25	36
All	All	2594/2656 (98%)	2484 (96%)	93 (4%)	17 (1%)	22	32

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	SER
1	B	186	SER
1	C	190	SER
1	D	190	SER
1	A	229	SER
1	C	52	GLN
1	D	52	GLN
1	A	203	ARG
1	B	203	ARG
1	B	229	SER

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Mol	Chain	Res	Type
1	B	662	SER
1	B	663	THR
1	C	432	ASP
1	D	229	SER
1	D	432	ASP
1	A	549	VAL
1	B	549	VAL

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	563/573 (98%)	525 (93%)	38 (7%)	16	26
1	B	564/573 (98%)	526 (93%)	38 (7%)	16	26
1	C	569/573 (99%)	528 (93%)	41 (7%)	14	23
1	D	568/573 (99%)	526 (93%)	42 (7%)	13	22
All	All	2264/2292 (99%)	2105 (93%)	159 (7%)	15	24

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	95	ARG
1	A	122	ARG
1	A	142	LEU
1	A	153	LYS
1	A	173	GLU
1	A	192	LEU
1	A	198	GLU
1	A	203	ARG
1	A	206	GLU
1	A	239	MET
1	A	247	ILE
1	A	272	GLU
1	A	283	ASN

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Mol	Chain	Res	Type
1	A	315	ASN
1	A	333	PHE
1	A	334	THR
1	A	342	VAL
1	A	365	LYS
1	A	422	PHE
1	A	429	ASP
1	A	434	MET
1	A	445	PHE
1	A	483	ARG
1	A	494	GLU
1	A	498	MET
1	A	526	SER
1	A	532	SER
1	A	544	LEU
1	A	546	THR
1	A	549	VAL
1	A	593	ASP
1	A	621	ASP
1	A	628	THR
1	A	647	PRO
1	A	649	GLU
1	A	654	GLN
1	A	655	THR
1	B	89	ASP
1	B	95	ARG
1	B	122	ARG
1	B	134	THR
1	B	142	LEU
1	B	172	HIS
1	B	174	SER
1	B	192	LEU
1	B	195	GLN
1	B	203	ARG
1	B	242	GLU
1	B	247	ILE
1	B	272	GLU
1	B	283	ASN
1	B	315	ASN
1	B	333	PHE
1	B	334	THR
1	B	342	VAL

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Mol	Chain	Res	Type
1	B	347	SER
1	B	365	LYS
1	B	422	PHE
1	B	428	LYS
1	B	445	PHE
1	B	483	ARG
1	B	494	GLU
1	B	498	MET
1	B	526	SER
1	B	532	SER
1	B	544	LEU
1	B	546	THR
1	B	549	VAL
1	B	593	ASP
1	B	621	ASP
1	B	628	THR
1	B	648	LYS
1	B	650	LYS
1	B	654	GLN
1	B	662	SER
1	C	33	LYS
1	C	47	LYS
1	C	95	ARG
1	C	122	ARG
1	C	135	ARG
1	C	142	LEU
1	C	191	ASN
1	C	195	GLN
1	C	198	GLU
1	C	203	ARG
1	C	208	LYS
1	C	209	GLU
1	C	242	GLU
1	C	245	ASP
1	C	247	ILE
1	C	272	GLU
1	C	301	ARG
1	C	305	THR
1	C	315	ASN
1	C	334	THR
1	C	342	VAL
1	C	365	LYS

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Mol	Chain	Res	Type
1	C	422	PHE
1	C	430	VAL
1	C	434	MET
1	C	443	GLU
1	C	445	PHE
1	C	476	LYS
1	C	483	ARG
1	C	494	GLU
1	C	498	MET
1	C	526	SER
1	C	532	SER
1	C	544	LEU
1	C	546	THR
1	C	549	VAL
1	C	593	ASP
1	C	621	ASP
1	C	628	THR
1	C	654	GLN
1	C	663	THR
1	D	1	THR
1	D	63	SER
1	D	90	GLU
1	D	93	HIS
1	D	95	ARG
1	D	137	LYS
1	D	142	LEU
1	D	182	LYS
1	D	187	LEU
1	D	190	SER
1	D	191	ASN
1	D	192	LEU
1	D	194	THR
1	D	195	GLN
1	D	198	GLU
1	D	203	ARG
1	D	239	MET
1	D	242	GLU
1	D	247	ILE
1	D	272	GLU
1	D	292	LEU
1	D	304	ARG
1	D	315	ASN

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Mol	Chain	Res	Type
1	D	334	THR
1	D	340	GLN
1	D	342	VAL
1	D	422	PHE
1	D	428	LYS
1	D	445	PHE
1	D	483	ARG
1	D	494	GLU
1	D	498	MET
1	D	526	SER
1	D	532	SER
1	D	544	LEU
1	D	546	THR
1	D	549	VAL
1	D	621	ASP
1	D	628	THR
1	D	648	LYS
1	D	654	GLN
1	D	661	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	116	HIS
1	A	191	ASN
1	A	195	GLN
1	A	283	ASN
1	A	449	ASN
1	A	499	HIS
1	A	596	HIS
1	B	116	HIS
1	B	172	HIS
1	B	181	HIS
1	B	195	GLN
1	B	283	ASN
1	B	405	HIS
1	B	449	ASN
1	B	499	HIS
1	B	596	HIS
1	C	93	HIS
1	C	193	GLN

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Mol	Chain	Res	Type
1	C	195	GLN
1	C	201	ASN
1	C	283	ASN
1	C	449	ASN
1	C	499	HIS
1	C	562	HIS
1	C	572	HIS
1	C	596	HIS
1	C	604	GLN
1	D	191	ASN
1	D	193	GLN
1	D	283	ASN
1	D	449	ASN
1	D	499	HIS
1	D	572	HIS
1	D	596	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	801	-	51,58,58	1.98	9 (17%)	60,89,89	2.23	19 (31%)
2	FAD	D	801	-	51,58,58	1.77	8 (15%)	60,89,89	1.82	13 (21%)
2	FAD	A	801	-	51,58,58	1.86	10 (19%)	60,89,89	2.04	16 (26%)
2	FAD	C	801	-	51,58,58	1.87	12 (23%)	60,89,89	1.99	12 (20%)
3	IPH	B	802	-	7,7,7	0.73	0	8,8,8	0.93	0
3	IPH	D	802	-	7,7,7	0.97	0	8,8,8	0.84	0
3	IPH	C	802	-	7,7,7	0.56	0	8,8,8	0.80	0
3	IPH	A	802	-	7,7,7	0.53	0	8,8,8	0.53	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	801	-	-	4/30/50/50	0/6/6/6
2	FAD	D	801	-	-	6/30/50/50	0/6/6/6
2	FAD	A	801	-	-	5/30/50/50	0/6/6/6
2	FAD	C	801	-	1/1/9/9	5/30/50/50	0/6/6/6
3	IPH	B	802	-	-	-	0/1/1/1
3	IPH	D	802	-	-	-	0/1/1/1
3	IPH	C	802	-	-	-	0/1/1/1
3	IPH	A	802	-	-	-	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C4-C4X	6.58	1.52	1.41
2	A	801	FAD	C4-C4X	5.62	1.51	1.41
2	D	801	FAD	C4-C4X	5.59	1.51	1.41
2	C	801	FAD	C4-C4X	5.41	1.50	1.41
2	B	801	FAD	C1'-N10	5.17	1.53	1.48
2	A	801	FAD	C4-N3	5.00	1.41	1.33
2	B	801	FAD	C4-N3	4.63	1.41	1.33
2	D	801	FAD	C4-N3	4.61	1.41	1.33
2	C	801	FAD	C4-N3	4.58	1.41	1.33
2	B	801	FAD	C4X-C10	4.51	1.43	1.38
2	C	801	FAD	C2B-C1B	-4.17	1.47	1.53
2	D	801	FAD	C2B-C1B	-3.98	1.47	1.53
2	D	801	FAD	C4A-N3A	-3.90	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	C4X-C10	3.86	1.42	1.38
2	C	801	FAD	C4A-N3A	-3.73	1.30	1.35
2	A	801	FAD	O2B-C2B	-3.55	1.34	1.43
2	D	801	FAD	O2B-C2B	-3.46	1.34	1.43
2	A	801	FAD	C4X-N5	-3.44	1.28	1.33
2	A	801	FAD	C1'-N10	3.43	1.51	1.48
2	B	801	FAD	C4A-N3A	-3.41	1.30	1.35
2	A	801	FAD	C4X-C10	3.34	1.42	1.38
2	D	801	FAD	C4X-C10	3.26	1.42	1.38
2	C	801	FAD	O2B-C2B	-3.25	1.35	1.43
2	C	801	FAD	C1'-N10	3.20	1.51	1.48
2	A	801	FAD	C2B-C1B	-3.18	1.48	1.53
2	A	801	FAD	C4A-N3A	-3.06	1.31	1.35
2	B	801	FAD	C2B-C1B	-2.99	1.49	1.53
2	C	801	FAD	C4X-N5	-2.82	1.29	1.33
2	B	801	FAD	O2B-C2B	-2.75	1.36	1.43
2	D	801	FAD	C4X-N5	-2.49	1.29	1.33
2	C	801	FAD	C8M-C8	2.46	1.55	1.51
2	A	801	FAD	O3B-C3B	2.42	1.48	1.43
2	C	801	FAD	O3B-C3B	2.30	1.48	1.43
2	B	801	FAD	O3B-C3B	2.25	1.48	1.43
2	B	801	FAD	C4X-N5	-2.23	1.30	1.33
2	C	801	FAD	C5'-C4'	2.16	1.54	1.51
2	D	801	FAD	C1'-N10	2.14	1.50	1.48
2	A	801	FAD	C8A-N7A	-2.03	1.31	1.34
2	C	801	FAD	C6-C5X	-2.01	1.38	1.41

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	C4-N3-C2	8.94	122.69	115.14
2	C	801	FAD	C4-N3-C2	8.13	122.00	115.14
2	A	801	FAD	C4-N3-C2	7.86	121.78	115.14
2	B	801	FAD	C4X-C4-N3	-6.01	115.21	123.43
2	D	801	FAD	C4-N3-C2	5.47	119.76	115.14
2	C	801	FAD	C4X-C4-N3	-5.32	116.15	123.43
2	A	801	FAD	C4X-C4-N3	-5.26	116.24	123.43
2	D	801	FAD	C1'-N10-C9A	4.79	122.07	118.29
2	D	801	FAD	O2B-C2B-C1B	4.43	127.22	110.85
2	D	801	FAD	C4X-C4-N3	-4.43	117.37	123.43
2	B	801	FAD	C1'-N10-C10	4.34	122.30	118.41
2	C	801	FAD	O2B-C2B-C1B	4.31	126.76	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	O2B-C2B-C3B	4.20	125.41	111.82
2	B	801	FAD	C10-C4X-N5	3.80	123.89	121.26
2	A	801	FAD	C4X-N5-C5X	3.77	120.54	116.77
2	A	801	FAD	O4B-C1B-C2B	3.77	112.43	106.93
2	B	801	FAD	O4B-C1B-C2B	3.61	112.20	106.93
2	C	801	FAD	O4B-C1B-C2B	3.60	112.19	106.93
2	B	801	FAD	N3A-C2A-N1A	-3.38	123.39	128.68
2	A	801	FAD	O2B-C2B-C1B	3.24	122.82	110.85
2	A	801	FAD	C1'-N10-C10	3.19	121.26	118.41
2	C	801	FAD	C1'-N10-C9A	3.17	120.78	118.29
2	A	801	FAD	O3B-C3B-C2B	-3.11	101.77	111.82
2	A	801	FAD	O2'-C2'-C3'	3.07	116.56	109.10
2	C	801	FAD	C4-C4X-C10	-3.05	117.93	119.95
2	D	801	FAD	O4B-C1B-C2B	3.04	111.37	106.93
2	C	801	FAD	C3B-C2B-C1B	3.03	105.53	100.98
2	D	801	FAD	C3B-C2B-C1B	3.01	105.51	100.98
2	D	801	FAD	C4-C4X-C10	-2.95	118.00	119.95
2	D	801	FAD	O2B-C2B-C3B	2.93	121.29	111.82
2	B	801	FAD	P-O5'-C5'	2.87	138.51	121.68
2	A	801	FAD	C1'-C2'-C3'	2.87	117.80	109.79
2	B	801	FAD	C9A-N10-C10	-2.78	118.27	121.91
2	D	801	FAD	C9A-N10-C10	-2.68	118.39	121.91
2	B	801	FAD	C7M-C7-C6	2.60	126.57	120.34
2	B	801	FAD	C3B-C2B-C1B	2.52	104.78	100.98
2	D	801	FAD	O3B-C3B-C2B	-2.51	103.71	111.82
2	C	801	FAD	C9A-N10-C10	-2.51	118.62	121.91
2	B	801	FAD	O2B-C2B-C1B	2.50	120.09	110.85
2	B	801	FAD	O2'-C2'-C3'	2.49	115.15	109.10
2	D	801	FAD	N3A-C2A-N1A	-2.42	124.90	128.68
2	B	801	FAD	C4-C4X-C10	-2.39	118.37	119.95
2	D	801	FAD	C10-C4X-N5	2.37	122.90	121.26
2	C	801	FAD	C1'-N10-C10	2.31	120.48	118.41
2	A	801	FAD	O2A-PA-O1A	2.31	123.67	112.24
2	A	801	FAD	C3B-C2B-C1B	2.31	104.45	100.98
2	A	801	FAD	C9A-N10-C10	-2.23	118.99	121.91
2	B	801	FAD	O2A-PA-O1A	2.22	123.24	112.24
2	C	801	FAD	C10-C4X-N5	2.20	122.78	121.26
2	A	801	FAD	C8M-C8-C9	-2.17	115.15	120.34
2	A	801	FAD	C2B-C3B-C4B	2.16	106.84	102.64
2	A	801	FAD	P-O5'-C5'	2.13	134.19	121.68
2	D	801	FAD	C8M-C8-C9	-2.12	115.26	120.34
2	C	801	FAD	C8M-C8-C9	-2.11	115.30	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	C6-C5X-N5	2.10	121.37	119.05
2	B	801	FAD	C1'-C2'-C3'	2.07	115.56	109.79
2	B	801	FAD	O3B-C3B-C2B	-2.06	105.16	111.82
2	B	801	FAD	C7M-C7-C8	-2.06	116.52	120.74
2	B	801	FAD	O2B-C2B-C3B	2.05	118.44	111.82
2	B	801	FAD	C5A-C6A-N6A	2.03	123.43	120.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	801	FAD	C2B

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	FAD	C1'-C2'-C3'-C4'
2	D	801	FAD	PA-O3P-P-O5'
2	A	801	FAD	N10-C1'-C2'-O2'
2	A	801	FAD	C5'-O5'-P-O1P
2	A	801	FAD	C5'-O5'-P-O3P
2	C	801	FAD	C1'-C2'-C3'-C4'
2	C	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	O2'-C2'-C3'-C4'
2	B	801	FAD	PA-O3P-P-O5'
2	A	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	O2'-C2'-C3'-O3'
2	C	801	FAD	O4B-C4B-C5B-O5B
2	B	801	FAD	C5'-O5'-P-O3P
2	C	801	FAD	O2'-C2'-C3'-C4'
2	D	801	FAD	O4B-C4B-C5B-O5B
2	B	801	FAD	C5'-O5'-P-O1P
2	B	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	C1'-C2'-C3'-O3'
2	C	801	FAD	C1'-C2'-C3'-O3'

There are no ring outliers.

3 monomers are involved in 8 short contacts:

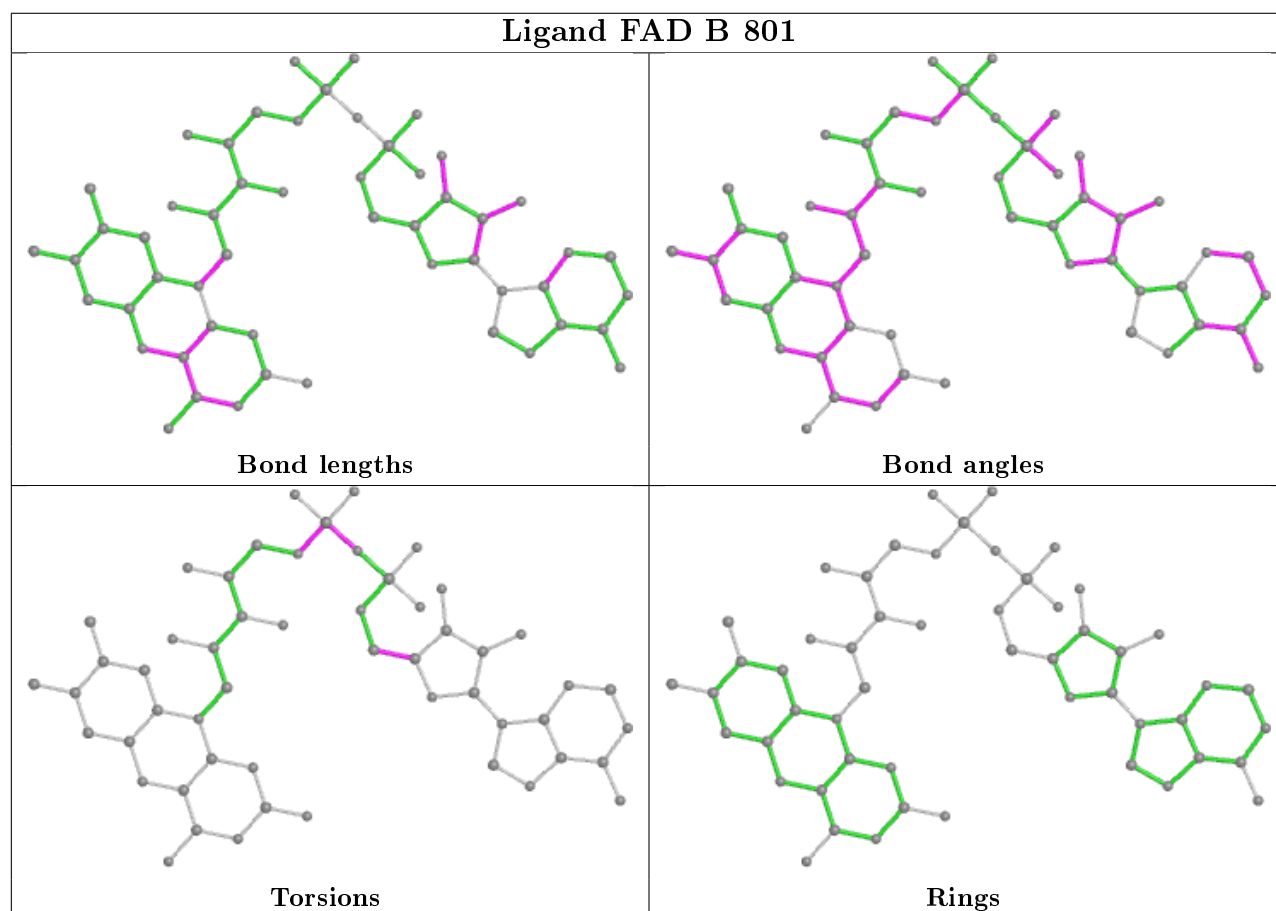
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	FAD	5	0

Continued on next page...

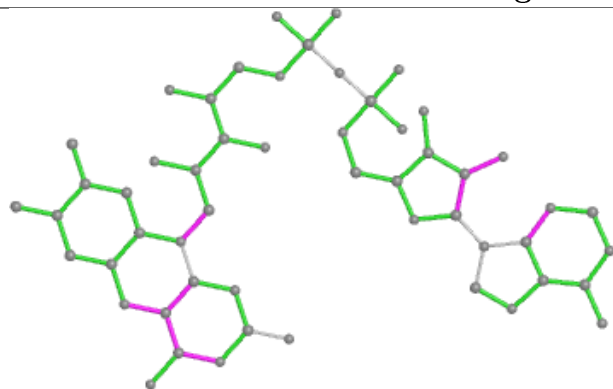
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	1	0
2	C	801	FAD	2	0

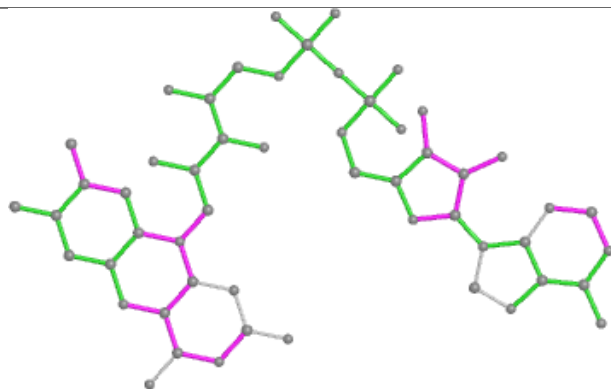
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



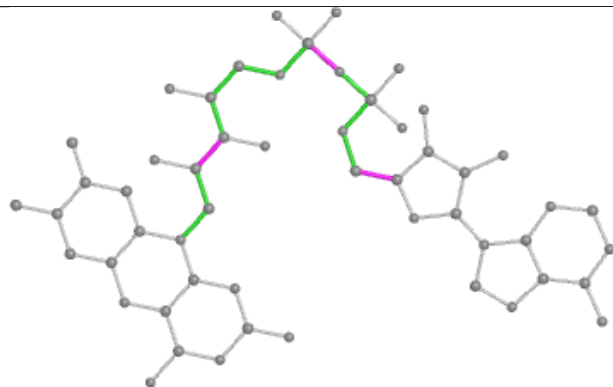
Ligand FAD D 801



Bond lengths



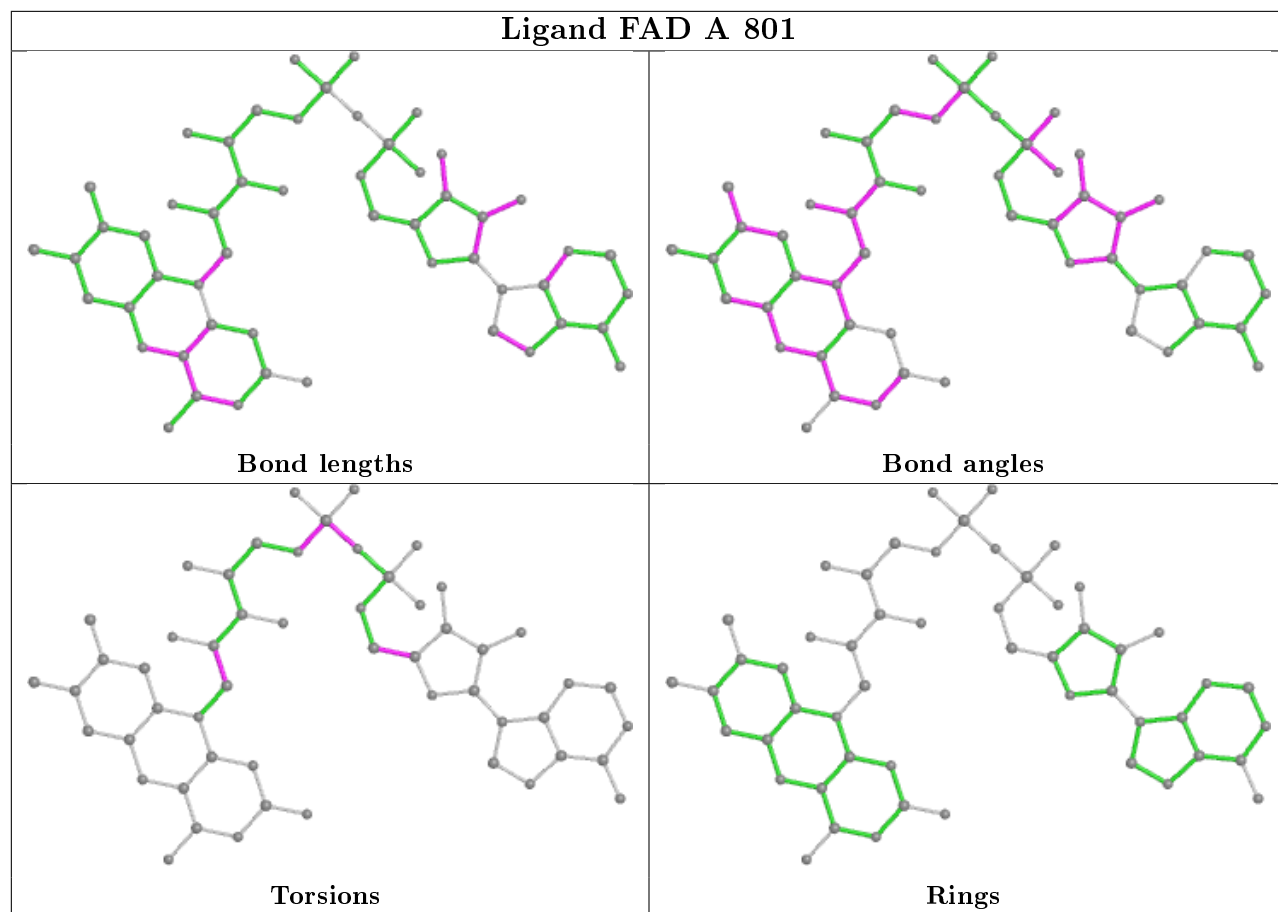
Bond angles

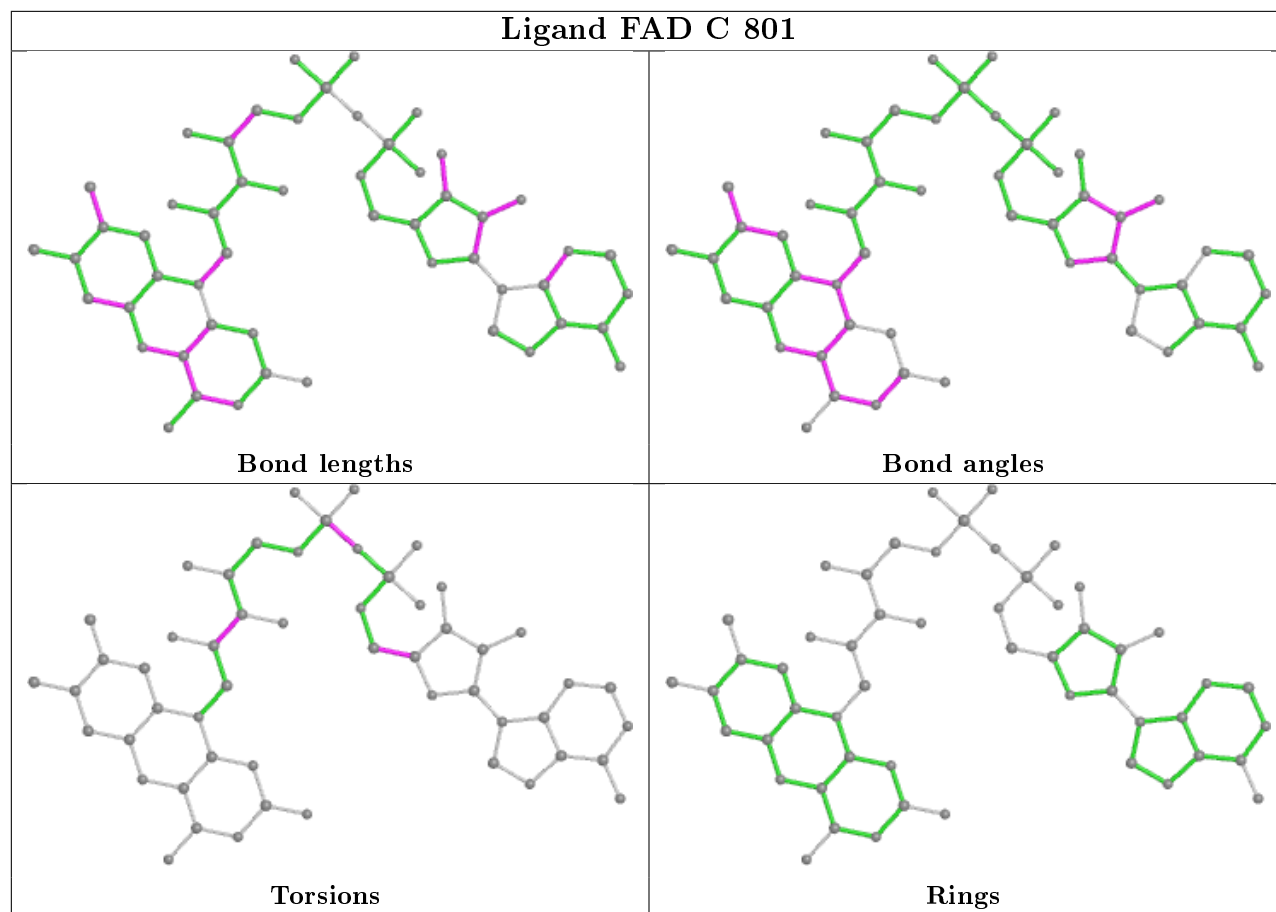


Torsions



Rings





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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.