



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:11 PM UTC

PDB ID : 1FOH / pdb_00001foh
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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

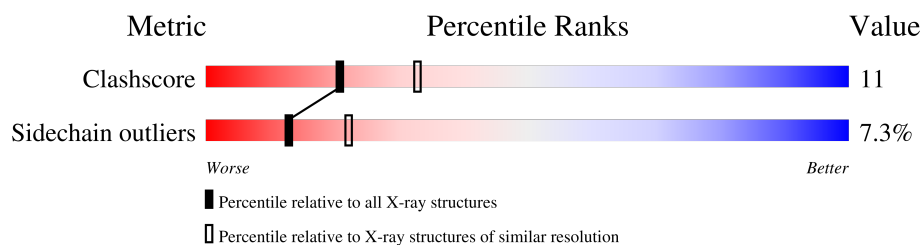
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	664	73% 20% . . .
1	B	664	73% 19% 5% . .
1	C	664	72% 20% 5% . .
1	D	664	73% 20% 5% . .

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:

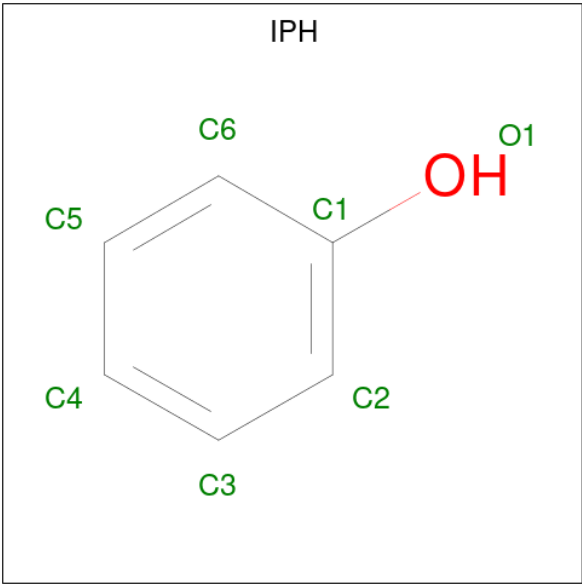
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ARG	PRO	conflict	UNP P15245
B	265	ARG	PRO	conflict	UNP P15245
C	265	ARG	PRO	conflict	UNP P15245
D	265	ARG	PRO	conflict	UNP P15245

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



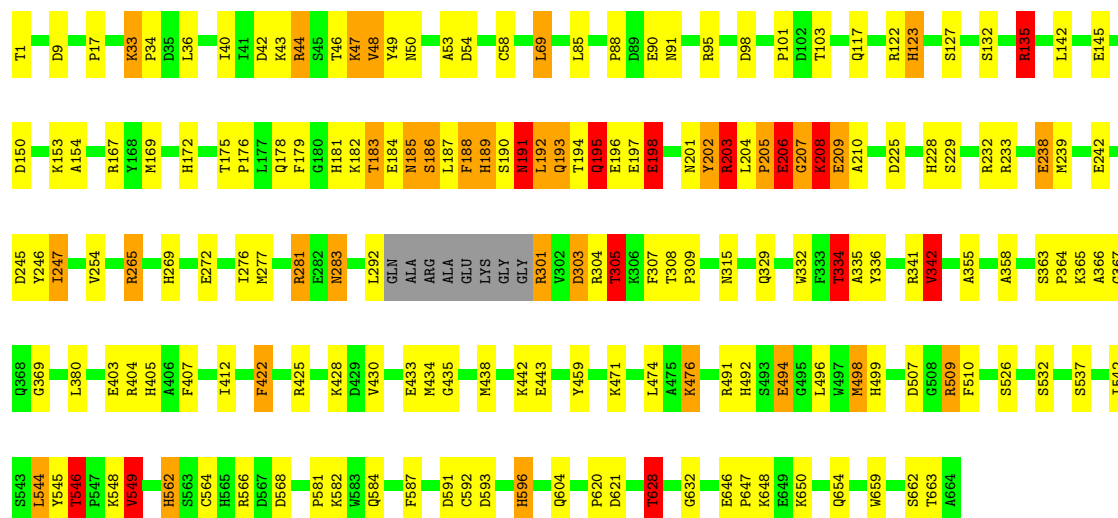
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 6 1	0	0
3	B	1	Total C O 7 6 1	0	0
3	C	1	Total C O 7 6 1	0	0
3	D	1	Total C O 7 6 1	0	0

- Molecule 4 is water.

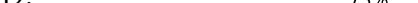
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	341	Total O 341 341	0	0
4	B	296	Total O 296 296	0	0
4	C	302	Total O 302 302	0	0
4	D	250	Total O 250 250	0	0

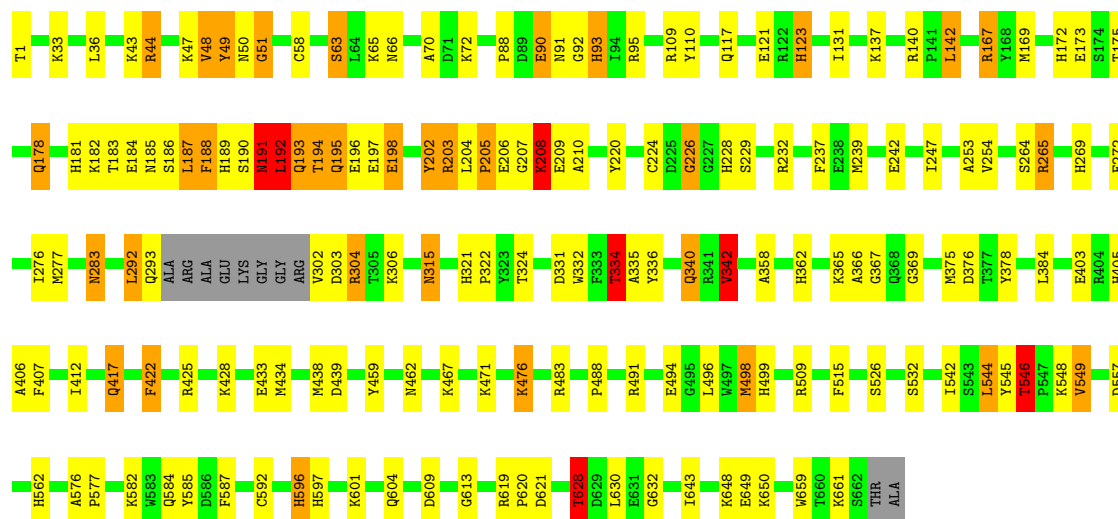
- Molecule 1: PHENOL HYDROXYLASE

Chain C:  72% 20% 5% ..



- Molecule 1: PHENOL HYDROXYLASE

Chain D:  73% 20% 5% ..



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

5.1 Standard geometry

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	0.67	0/5292	1.63	62/7160 (0.9%)
1	B	0.67	0/5304	1.63	85/7177 (1.2%)
1	C	0.72	4/5348 (0.1%)	1.73	97/7235 (1.3%)
1	D	0.71	1/5334 (0.0%)	1.70	99/7216 (1.4%)
All	All	0.69	5/21278 (0.0%)	1.67	343/28788 (1.2%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	562	HIS	CE1-NE2	-10.44	1.22	1.32
1	C	562	HIS	CG-CD2	-6.75	1.28	1.35
1	C	208	LYS	N-CA	-6.65	1.37	1.46
1	C	562	HIS	CG-ND1	-6.15	1.31	1.38
1	D	621	ASP	CA-CB	6.01	1.63	1.53

All (343) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASP	CA-CB-CG	22.85	135.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	562	HIS	ND1-CG-CD2	-20.04	86.06	106.10
1	C	562	HIS	CG-CD2-NE2	18.71	125.91	107.20
1	D	208	LYS	CA-C-O	14.68	137.55	120.66
1	A	620	PRO	CA-C-N	13.99	144.09	120.72
1	A	620	PRO	C-N-CA	13.99	144.09	120.72
1	C	207	GLY	CA-C-N	13.90	148.09	121.54
1	C	207	GLY	C-N-CA	13.90	148.09	121.54
1	D	304	ARG	CD-NE-CZ	13.38	143.13	124.40
1	D	548	LYS	CA-C-N	12.34	144.18	121.97
1	D	548	LYS	C-N-CA	12.34	144.18	121.97
1	D	620	PRO	CA-C-N	12.17	141.05	120.72
1	D	620	PRO	C-N-CA	12.17	141.05	120.72
1	B	548	LYS	CA-C-N	11.96	143.49	121.97
1	B	548	LYS	C-N-CA	11.96	143.49	121.97
1	A	548	LYS	CA-C-N	11.95	143.48	121.97
1	A	548	LYS	C-N-CA	11.95	143.48	121.97
1	C	44	ARG	NE-CZ-NH2	-11.93	108.47	119.20
1	C	620	PRO	CA-C-N	11.50	139.92	120.72
1	C	620	PRO	C-N-CA	11.50	139.92	120.72
1	C	44	ARG	NE-CZ-NH1	11.44	132.94	121.50
1	C	191	ASN	CA-CB-CG	11.32	123.92	112.60
1	C	195	GLN	CA-CB-CG	10.80	135.71	114.10
1	D	172	HIS	CA-CB-CG	-10.06	103.74	113.80
1	B	201	ASN	CA-CB-CG	-10.02	102.58	112.60
1	B	620	PRO	CA-C-N	10.00	140.98	121.18
1	B	620	PRO	C-N-CA	10.00	140.98	121.18
1	C	48	VAL	N-CA-CB	9.95	122.93	110.99
1	D	202	TYR	CA-C-O	9.90	131.10	119.32
1	A	185	ASN	CA-C-O	-9.70	110.48	121.15
1	C	562	HIS	CE1-NE2-CD2	-9.65	99.35	109.00
1	C	123	HIS	CA-CB-CG	-9.56	104.24	113.80
1	D	209	GLU	N-CA-C	-8.95	93.93	108.52
1	D	203	ARG	N-CA-CB	-8.94	95.62	109.48
1	D	210	ALA	N-CA-C	-8.92	97.07	110.28
1	D	188	PHE	CA-C-N	8.90	132.56	120.54
1	D	188	PHE	C-N-CA	8.90	132.56	120.54
1	C	562	HIS	CB-CG-CD2	8.77	142.60	131.20
1	C	562	HIS	CG-ND1-CE1	8.63	123.97	109.30
1	B	123	HIS	CA-CB-CG	-8.35	105.45	113.80
1	A	228	HIS	CA-CB-CG	-8.33	105.47	113.80
1	B	429	ASP	CA-CB-CG	8.27	120.86	112.60
1	C	548	LYS	CA-C-N	8.23	136.78	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	LYS	C-N-CA	8.23	136.78	121.97
1	B	171	ASP	CA-CB-CG	8.16	120.76	112.60
1	C	202	TYR	CA-C-O	8.11	129.16	119.59
1	B	405	HIS	CA-CB-CG	-8.11	105.69	113.80
1	C	172	HIS	CA-CB-CG	-8.06	105.74	113.80
1	B	663	THR	N-CA-CB	7.98	123.97	110.49
1	B	206	GLU	N-CA-C	7.96	122.06	110.28
1	D	203	ARG	NE-CZ-NH2	-7.89	112.10	119.20
1	A	194	THR	CA-C-O	-7.87	112.56	120.82
1	C	203	ARG	NE-CZ-NH2	7.87	126.28	119.20
1	C	407	PHE	CA-CB-CG	-7.86	105.94	113.80
1	B	226	GLY	CA-C-N	7.81	129.97	120.13
1	B	226	GLY	C-N-CA	7.81	129.97	120.13
1	C	509	ARG	NE-CZ-NH2	-7.76	112.22	119.20
1	A	237	PHE	CA-CB-CG	7.76	121.56	113.80
1	A	342	VAL	CB-CA-C	-7.74	97.25	111.18
1	D	192	LEU	N-CA-C	-7.70	104.03	113.50
1	C	210	ALA	N-CA-C	-7.70	99.07	110.23
1	A	557	ASP	CA-CB-CG	7.63	120.23	112.60
1	D	509	ARG	NE-CZ-NH2	-7.59	112.37	119.20
1	C	621	ASP	N-CA-CB	-7.57	97.83	110.39
1	C	205	PRO	CA-C-N	7.55	135.97	121.54
1	C	205	PRO	C-N-CA	7.55	135.97	121.54
1	D	334	THR	N-CA-CB	7.46	124.03	110.76
1	B	91	ASN	CA-CB-CG	7.44	120.04	112.60
1	D	66	ASN	OD1-CG-ND2	-7.43	115.17	122.60
1	B	342	VAL	CB-CA-C	-7.41	97.84	111.18
1	D	557	ASP	CA-CB-CG	7.39	119.99	112.60
1	B	557	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	628	THR	CB-CA-C	-7.36	97.47	114.41
1	C	208	LYS	N-CA-C	7.36	126.47	110.80
1	D	208	LYS	N-CA-C	7.32	121.46	109.24
1	D	167	ARG	CD-NE-CZ	7.24	134.53	124.40
1	C	209	GLU	N-CA-C	-7.22	95.22	107.99
1	A	109	ARG	CD-NE-CZ	7.12	134.37	124.40
1	A	9	ASP	CA-CB-CG	-7.10	105.50	112.60
1	D	315	ASN	OD1-CG-ND2	7.04	129.64	122.60
1	B	206	GLU	CA-CB-CG	-7.03	100.05	114.10
1	D	188	PHE	CA-C-O	7.00	128.11	120.90
1	D	206	GLU	CB-CG-CD	-6.99	100.72	112.60
1	D	405	HIS	CA-CB-CG	-6.97	106.83	113.80
1	B	167	ARG	CD-NE-CZ	6.95	134.13	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	191	ASN	CB-CA-C	6.95	121.83	111.06
1	C	546	THR	N-CA-CB	6.87	120.04	110.01
1	C	537	SER	CA-C-N	6.85	129.76	120.38
1	C	537	SER	C-N-CA	6.85	129.76	120.38
1	C	209	GLU	CA-C-O	-6.84	113.14	120.46
1	B	546	THR	N-CA-CB	6.82	120.40	109.90
1	A	621	ASP	N-CA-CB	-6.81	99.08	110.39
1	C	225	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	123	HIS	CA-CB-CG	-6.78	107.02	113.80
1	C	334	THR	CB-CA-C	-6.77	97.51	113.02
1	A	483	ARG	CD-NE-CZ	6.77	133.88	124.40
1	B	359	CYS	CB-CA-C	-6.75	97.00	109.29
1	C	48	VAL	CB-CA-C	-6.74	101.67	110.84
1	B	407	PHE	CA-CB-CG	-6.73	107.07	113.80
1	C	405	HIS	CA-CB-CG	-6.71	107.09	113.80
1	A	562	HIS	ND1-CG-CD2	-6.71	99.39	106.10
1	B	562	HIS	ND1-CG-CD2	-6.70	99.40	106.10
1	A	206	GLU	N-CA-C	6.68	119.98	109.96
1	B	621	ASP	CA-CB-CG	-6.67	105.93	112.60
1	A	194	THR	O-C-N	6.67	128.94	122.07
1	D	621	ASP	N-CA-CB	-6.67	99.33	110.39
1	B	198	GLU	CB-CA-C	-6.66	99.53	110.85
1	B	562	HIS	CG-CD2-NE2	6.62	113.82	107.20
1	D	66	ASN	CB-CG-ND2	6.62	126.33	116.40
1	D	109	ARG	CD-NE-CZ	6.60	133.64	124.40
1	B	621	ASP	N-CA-CB	-6.60	98.84	110.39
1	D	643	ILE	N-CA-C	6.59	116.83	111.62
1	B	307	PHE	CA-CB-CG	-6.59	107.21	113.80
1	A	172	HIS	CA-CB-CG	-6.58	107.22	113.80
1	B	510	PHE	CA-CB-CG	6.55	120.35	113.80
1	B	173	GLU	CA-CB-CG	6.54	127.17	114.10
1	C	193	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	B	181	HIS	CA-CB-CG	-6.53	107.28	113.80
1	A	197	GLU	N-CA-C	6.52	119.39	111.82
1	A	407	PHE	CA-CB-CG	-6.52	107.28	113.80
1	A	203	ARG	CD-NE-CZ	-6.50	115.29	124.40
1	C	188	PHE	CA-C-N	6.50	129.28	120.38
1	C	188	PHE	C-N-CA	6.50	129.28	120.38
1	D	628	THR	CB-CA-C	-6.50	99.47	114.41
1	D	203	ARG	NH1-CZ-NH2	6.49	127.73	119.30
1	C	9	ASP	CA-CB-CG	-6.43	106.17	112.60
1	A	546	THR	N-CA-CB	6.41	119.78	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	362	HIS	CA-CB-CG	-6.40	107.40	113.80
1	D	44	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	C	188	PHE	CA-CB-CG	6.38	120.19	113.80
1	C	188	PHE	CA-C-O	6.38	127.47	120.90
1	D	597	HIS	O-C-N	6.36	126.39	121.88
1	B	359	CYS	N-CA-CB	-6.35	101.20	110.53
1	D	206	GLU	CA-CB-CG	-6.34	101.41	114.10
1	D	283	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	49	TYR	CA-CB-CG	-6.32	102.52	113.90
1	A	620	PRO	O-C-N	-6.27	114.13	122.22
1	C	265	ARG	N-CA-C	-6.25	101.03	110.28
1	D	178	GLN	CA-C-N	6.25	131.00	122.07
1	D	178	GLN	C-N-CA	6.25	131.00	122.07
1	D	562	HIS	ND1-CG-CD2	-6.21	99.89	106.10
1	D	175	THR	CA-C-O	6.21	123.92	119.32
1	C	178	GLN	CA-C-O	6.20	126.03	119.03
1	B	432	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	499	HIS	CA-CB-CG	-6.17	107.63	113.80
1	C	17	PRO	O-C-N	-6.16	115.53	122.18
1	B	596	HIS	CA-CB-CG	-6.15	107.65	113.80
1	C	628	THR	CB-CA-C	-6.14	98.63	113.19
1	D	596	HIS	CA-CB-CG	-6.12	107.68	113.80
1	A	116	HIS	CA-C-N	6.12	128.76	120.38
1	A	116	HIS	C-N-CA	6.12	128.76	120.38
1	B	205	PRO	N-CA-C	-6.11	101.87	111.34
1	C	91	ASN	CA-CB-CG	-6.09	106.51	112.60
1	C	380	LEU	CA-C-N	6.08	126.86	119.99
1	C	380	LEU	C-N-CA	6.08	126.86	119.99
1	D	549	VAL	N-CA-CB	6.08	121.27	111.23
1	D	621	ASP	CB-CA-C	-6.08	97.61	110.31
1	A	628	THR	CB-CA-C	-6.06	100.46	114.41
1	B	119	ARG	CD-NE-CZ	6.03	132.84	124.40
1	C	203	ARG	N-CA-C	6.01	119.17	110.28
1	A	359	CYS	CB-CA-C	-6.00	99.47	109.55
1	C	246	TYR	N-CA-C	-6.00	100.96	109.96
1	D	206	GLU	N-CA-CB	-6.00	100.35	110.49
1	A	373	SER	O-C-N	-5.99	115.90	122.07
1	B	9	ASP	CA-CB-CG	-5.99	106.61	112.60
1	D	209	GLU	O-C-N	5.99	130.33	123.27
1	C	334	THR	N-CA-CB	5.98	121.41	110.76
1	A	197	GLU	CA-CB-CG	-5.98	102.14	114.10
1	A	334	THR	N-CA-CB	5.98	121.19	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	GLU	N-CA-C	5.97	123.52	110.80
1	B	342	VAL	N-CA-CB	5.97	122.96	111.62
1	A	192	LEU	CA-C-N	5.96	128.59	120.54
1	A	192	LEU	C-N-CA	5.96	128.59	120.54
1	C	192	LEU	N-CA-C	-5.96	105.09	112.90
1	C	207	GLY	CA-C-O	5.95	130.92	120.57
1	D	237	PHE	CA-C-N	5.94	129.55	121.05
1	D	237	PHE	C-N-CA	5.94	129.55	121.05
1	D	209	GLU	N-CA-CB	5.94	119.88	110.55
1	A	309	PRO	CA-C-N	5.92	128.49	120.38
1	A	309	PRO	C-N-CA	5.92	128.49	120.38
1	D	48	VAL	N-CA-CB	5.92	118.14	111.21
1	A	405	HIS	CA-CB-CG	-5.92	107.88	113.80
1	D	621	ASP	CA-CB-CG	-5.92	106.68	112.60
1	B	109	ARG	CD-NE-CZ	5.91	132.67	124.40
1	D	592	CYS	CA-C-N	5.91	130.22	120.94
1	D	592	CYS	C-N-CA	5.91	130.22	120.94
1	C	662	SER	CB-CA-C	5.91	119.53	109.72
1	C	210	ALA	CA-C-O	-5.89	114.71	121.19
1	C	208	LYS	N-CA-CB	-5.88	100.56	110.49
1	D	609	ASP	CA-CB-CG	-5.86	106.74	112.60
1	D	178	GLN	CA-C-O	5.85	125.64	119.03
1	B	88	PRO	CA-C-N	5.85	131.51	121.86
1	B	88	PRO	C-N-CA	5.85	131.51	121.86
1	B	191	ASN	OD1-CG-ND2	5.83	128.43	122.60
1	A	621	ASP	CB-CA-C	-5.83	98.13	110.31
1	D	546	THR	N-CA-CB	5.81	118.85	109.90
1	C	206	GLU	N-CA-CB	-5.81	100.67	110.49
1	D	342	VAL	CB-CA-C	-5.79	100.76	111.18
1	A	191	ASN	CA-C-O	-5.79	114.29	120.42
1	C	566	ARG	CD-NE-CZ	5.78	132.50	124.40
1	D	407	PHE	CA-CB-CG	-5.77	108.03	113.80
1	B	315	ASN	CA-CB-CG	-5.76	106.84	112.60
1	C	562	HIS	CB-CG-ND1	5.76	131.34	122.70
1	C	189	HIS	CA-CB-CG	5.75	119.55	113.80
1	D	188	PHE	O-C-N	-5.74	115.83	122.03
1	A	548	LYS	CA-C-O	5.73	127.49	121.19
1	B	191	ASN	CA-CB-CG	-5.72	106.88	112.60
1	B	283	ASN	CA-CB-CG	5.71	118.31	112.60
1	D	49	TYR	CA-C-O	-5.70	115.53	120.88
1	A	265	ARG	N-CA-C	-5.69	101.85	110.28
1	D	207	GLY	CA-C-N	-5.68	113.52	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	207	GLY	C-N-CA	-5.68	113.52	122.73
1	D	265	ARG	N-CA-C	-5.68	101.87	110.28
1	C	435	GLY	N-CA-C	-5.67	103.63	112.58
1	D	587	PHE	CA-CB-CG	-5.67	108.14	113.80
1	C	254	VAL	N-CA-C	-5.66	102.41	107.56
1	B	462	ASN	CA-CB-CG	5.65	118.25	112.60
1	B	509	ARG	NE-CZ-NH2	-5.65	114.12	119.20
1	A	126	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	111	HIS	CA-C-O	-5.63	114.80	121.16
1	D	483	ARG	CD-NE-CZ	5.63	132.28	124.40
1	C	209	GLU	CA-C-N	-5.62	112.73	120.71
1	C	209	GLU	C-N-CA	-5.62	112.73	120.71
1	C	208	LYS	CB-CA-C	-5.61	99.25	110.42
1	D	226	GLY	CA-C-N	5.61	127.20	120.13
1	D	226	GLY	C-N-CA	5.61	127.20	120.13
1	B	662	SER	CA-C-N	5.61	132.25	121.54
1	B	662	SER	C-N-CA	5.61	132.25	121.54
1	A	309	PRO	O-C-N	-5.60	116.13	122.18
1	D	123	HIS	CA-CB-CG	-5.59	108.21	113.80
1	C	510	PHE	N-CA-C	-5.58	102.26	110.52
1	A	537	SER	CA-C-N	5.56	128.00	120.38
1	A	537	SER	C-N-CA	5.56	128.00	120.38
1	D	51	GLY	CA-C-O	-5.56	116.34	121.63
1	B	116	HIS	CA-C-N	5.55	127.99	120.38
1	B	116	HIS	C-N-CA	5.55	127.99	120.38
1	B	334	THR	N-CA-CB	5.55	123.70	111.87
1	D	376	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	404	ARG	CD-NE-CZ	5.53	132.15	124.40
1	D	192	LEU	CA-C-O	5.53	125.22	119.14
1	D	44	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	D	619	ARG	CA-C-N	5.53	125.36	119.28
1	D	619	ARG	C-N-CA	5.53	125.36	119.28
1	C	69	LEU	N-CA-CB	-5.52	102.53	110.65
1	B	359	CYS	N-CA-C	5.50	120.27	113.50
1	B	621	ASP	CB-CA-C	-5.50	98.96	110.17
1	B	427	ALA	CA-C-N	5.48	128.63	120.31
1	B	427	ALA	C-N-CA	5.48	128.63	120.31
1	B	190	SER	N-CA-C	-5.46	101.89	110.36
1	C	58	CYS	N-CA-C	5.46	117.66	111.11
1	B	466	ASP	N-CA-C	5.46	118.16	107.57
1	C	301	ARG	CD-NE-CZ	5.45	132.03	124.40
1	D	206	GLU	N-CA-C	5.44	122.38	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	VAL	N-CA-CB	5.43	120.19	111.23
1	C	549	VAL	N-CA-CB	5.43	120.19	111.23
1	A	31	ARG	NE-CZ-NH2	5.43	124.08	119.20
1	A	191	ASN	CA-CB-CG	-5.42	107.19	112.60
1	A	54	ASP	CA-CB-CG	5.39	118.00	112.60
1	B	159	ALA	CA-C-N	5.39	129.68	123.15
1	B	159	ALA	C-N-CA	5.39	129.68	123.15
1	D	58	CYS	N-CA-C	5.38	117.57	111.11
1	A	134	THR	CA-C-N	5.35	129.78	120.68
1	A	134	THR	C-N-CA	5.35	129.78	120.68
1	B	161	PRO	CA-C-N	-5.35	116.17	123.12
1	B	161	PRO	C-N-CA	-5.35	116.17	123.12
1	D	188	PHE	N-CA-C	-5.35	105.09	111.03
1	A	201	ASN	CA-CB-CG	-5.34	107.26	112.60
1	A	620	PRO	CA-C-O	5.34	127.67	119.55
1	D	253	ALA	N-CA-CB	-5.34	102.74	111.66
1	B	239	MET	CA-CB-CG	5.34	124.78	114.10
1	B	203	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	B	131	ILE	CB-CA-C	-5.33	105.15	111.97
1	D	205	PRO	CA-C-N	5.33	131.72	121.54
1	D	205	PRO	C-N-CA	5.33	131.72	121.54
1	D	302	VAL	N-CA-CB	-5.33	102.44	111.50
1	D	92	GLY	N-CA-C	-5.30	106.38	115.08
1	D	476	LYS	N-CA-C	5.30	117.97	111.82
1	B	283	ASN	N-CA-C	5.28	118.49	111.30
1	B	46	THR	CA-C-O	5.28	127.64	121.46
1	C	198	GLU	N-CA-CB	5.28	117.66	110.01
1	C	154	ALA	N-CA-C	5.26	117.70	111.33
1	A	281	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	B	52	GLN	CG-CD-NE2	5.25	124.28	116.40
1	C	281	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	B	159	ALA	CA-C-O	5.25	127.97	121.99
1	D	417	GLN	OE1-CD-NE2	5.25	127.85	122.60
1	B	59	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	C	342	VAL	CB-CA-C	-5.24	101.74	111.18
1	C	591	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	140	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	C	305	THR	CA-C-O	5.24	125.97	120.42
1	A	134	THR	CA-CB-OG1	-5.23	101.75	109.60
1	C	596	HIS	CA-CB-CG	-5.23	108.57	113.80
1	B	195	GLN	CB-CG-CD	5.22	121.48	112.60
1	B	55	GLY	O-C-N	-5.22	119.49	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	TYR	CA-CB-CG	-5.21	104.51	113.90
1	D	254	VAL	CA-C-O	5.21	122.04	119.12
1	D	202	TYR	CA-C-N	5.21	128.50	121.05
1	D	202	TYR	C-N-CA	5.21	128.50	121.05
1	A	433	GLU	CA-C-O	-5.19	114.47	120.24
1	D	193	GLN	N-CA-C	-5.19	103.63	110.43
1	A	499	HIS	CA-CB-CG	-5.19	108.61	113.80
1	C	592	CYS	CA-C-N	5.18	129.07	120.94
1	C	592	CYS	C-N-CA	5.18	129.07	120.94
1	A	173	GLU	CA-CB-CG	5.18	124.46	114.10
1	C	548	LYS	CA-C-O	5.17	126.84	121.15
1	A	134	THR	CA-CB-CG2	5.16	119.28	110.50
1	C	568	ASP	CA-CB-CG	-5.15	107.45	112.60
1	D	209	GLU	CA-C-N	-5.15	113.55	120.87
1	D	209	GLU	C-N-CA	-5.15	113.55	120.87
1	B	593	ASP	CA-C-O	-5.15	115.94	121.56
1	B	643	ILE	N-CA-C	5.15	115.99	111.56
1	B	462	ASN	CA-C-O	-5.15	115.59	120.94
1	C	207	GLY	O-C-N	-5.14	116.01	122.70
1	C	186	SER	N-CA-CB	5.13	118.74	111.25
1	C	621	ASP	CA-CB-CG	-5.13	107.47	112.60
1	C	42	ASP	CA-CB-CG	-5.12	107.48	112.60
1	D	237	PHE	N-CA-C	5.12	117.04	108.23
1	C	175	THR	CA-C-O	5.12	123.11	119.32
1	D	315	ASN	CA-CB-CG	-5.12	107.48	112.60
1	B	142	LEU	N-CA-CB	5.12	119.83	111.08
1	C	135	ARG	CD-NE-CZ	5.12	131.56	124.40
1	B	13	VAL	CA-C-O	-5.11	114.89	120.97
1	A	609	ASP	CA-CB-CG	-5.10	107.50	112.60
1	B	349	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	264	SER	CA-C-O	-5.09	115.50	121.46
1	B	315	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	C	283	ASN	CA-CB-CG	5.08	117.68	112.60
1	C	44	ARG	CD-NE-CZ	5.08	131.51	124.40
1	D	283	ASN	O-C-N	-5.08	116.22	122.57
1	A	58	CYS	N-CA-C	5.07	117.20	111.11
1	C	185	ASN	CA-C-N	-5.07	115.61	123.17
1	C	185	ASN	C-N-CA	-5.07	115.61	123.17
1	C	183	THR	N-CA-CB	5.06	117.43	109.69
1	B	197	GLU	N-CA-C	5.05	117.68	111.82
1	C	355	ALA	CA-C-O	-5.04	115.89	121.33
1	D	334	THR	CB-CA-C	-5.03	101.49	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ASP	CA-C-O	5.03	126.15	120.92
1	D	142	LEU	CA-CB-CG	5.03	133.89	116.30
1	A	206	GLU	CA-C-O	5.02	126.58	120.81
1	D	131	ILE	N-CA-CB	5.02	116.42	110.55
1	B	663	THR	CA-CB-OG1	5.02	117.13	109.60
1	D	70	ALA	N-CA-C	5.00	116.54	111.14

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	5038	103	0
1	B	5186	0	5050	90	0
1	C	5230	0	5101	143	0
1	D	5216	0	5084	132	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	6	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	19	0
4	B	296	0	0	17	0
4	C	302	0	0	17	0
4	D	250	0	0	20	0
All	All	22235	0	20415	460	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 11.

All (460) 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:491:ARG:HB2	1:C:498:MET:HE3	1.39	1.05
1:A:491:ARG:HB2	1:A:498:MET:HE3	1.38	1.02
1:D:491:ARG:HB2	1:D:498:MET:HE3	1.40	0.98
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:B:491:ARG:HB2	1:B:498:MET:HE3	1.46	0.94
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:B:438:MET:HE2	4:B:1084:HOH:O	1.71	0.89
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: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: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:A:315:ASN:ND2	4:A:1069:HOH:O	2.16	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:D:425:ARG:HH12	1:D:434:MET:HE2	1.51	0.74
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:D:438:MET:HE2	4:D:969:HOH:O	1.88	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:A:265:ARG:HH21	1:A:277:MET:HE1	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HD3	1:A:498:MET:HE1	1.72	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:C:239:MET:HG2	1:C:341:ARG:HB3	1.73	0.70
1:D:265:ARG:HH21	1:D:277:MET:HE1	1.56	0.70
1:C:204:LEU:HG	1:C:208:LYS:HG3	1.73	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: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:B:496:LEU:HD23	1:B:498:MET:HE2	1.75	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:B:265:ARG:HH21	1:B:277:MET:HE1	1.59	0.66
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
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:194:THR:CG2	1:D:197:GLU:H	2.10	0.65
1:C:44:ARG:NH2	1:C:198:GLU:OE2	2.29	0.65
1:C:190:SER:HA	4:C:888:HOH:O	1.96	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:D:425:ARG:NH1	1:D:434:MET:HE2	2.12	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:HA	1:C:203:ARG:NE	2.12	0.64
1:C:193:GLN:HA	1:C:304:ARG:HH12	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ASN:OD1	1:D:187:LEU:HG	1.98	0.63
1:C:496:LEU:HD23	1:C:498:MET:HE2	1.81	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: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:C:193:GLN:HB3	4:C:1089:HOH:O	2.00	0.62
1:D:186:SER:CB	1:D:332:TRP:HE1	2.13	0.61
1:D:491:ARG:HD3	1:D:498:MET:HE1	1.82	0.61
1:A:277:MET:HE3	1:A:422:PHE:CE2	2.35	0.61
1:D:228:HIS:O	1:D:229:SER:C	2.43	0.61
1:C:265:ARG:HH21	1:C:277:MET:HE1	1.64	0.61
1:A:273:SER:HB3	4:A:1069:HOH:O	2.00	0.61
1:D:467:LYS:NZ	4:D:941:HOH:O	2.31	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
1:C:292:LEU:HD12	1:C:307:PHE:CZ	2.37	0.59
1:C:491:ARG:HD3	1:C:498:MET:HE1	1.84	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:C:169:MET:HE3	1:C:202:TYR:HB3	1.85	0.59
1:C:238:GLU:HG2	1:C:239:MET:N	2.18	0.59
1:B:141:PRO:HD2	1:B:204:LEU:CD2	2.32	0.58
1:B:491:ARG:HD3	1:B:498:MET:HE1	1.85	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:C:628:THR:HG23	4:C:1010:HOH:O	2.02	0.58
1:B:265:ARG:HH21	1:B:277:MET:CE	2.17	0.58
1:A:496:LEU:HD23	1:A:498:MET:HE2	1.84	0.58
1:A:307:PHE:HB3	4:A:1077:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:CE1	4:A:1123:HOH:O	2.57	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:186:SER:CB	1:C:332:TRP:HE1	2.16	0.57
1:C:194:THR:HG23	1:C:197:GLU:H	1.69	0.57
1:C:265:ARG:HH21	1:C:277:MET:CE	2.17	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:A:185:ASN:O	1:A:186:SER:HB3	2.05	0.57
1:B:277:MET:HE3	1:B:422:PHE:CE2	2.40	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:265:ARG:HH21	1:D:277:MET:CE	2.18	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:43:LYS:NZ	1:D:198:GLU:OE1	2.24	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:B:438:MET:HE3	1:B:438:MET:HA	1.87	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
1:B:89:ASP:HB3	1:B:91:ASN:H	1.71	0.55
1:D:192:LEU:HD11	1:D:335:ALA:HB3	1.88	0.55
1:D:198:GLU:O	1:D:202:TYR:HD1	1.89	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: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:C:438:MET:HE2	4:C:1078:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:MET:HE3	1:D:422:PHE:CE2	2.42	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:D:169:MET:HE3	1:D:202:TYR:HB3	1.89	0.54
1:A:202:TYR:O	1:A:203:ARG:HB2	2.05	0.54
1:C:88:PRO:HD3	1:C:269:HIS:O	2.07	0.54
1:C:132:SER:O	1:C:135:ARG:HB2	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:425:ARG:NH1	1:A:434:MET:HE3	2.23	0.54
1:C:194:THR:HG22	1:C:197:GLU:CD	2.33	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:C:193:GLN:HA	1:C:304:ARG:NH1	2.22	0.54
1:D:189:HIS:O	1:D:190:SER:C	2.51	0.54
1:A:122:ARG:HD3	1:A:192:LEU:HD12	1.88	0.54
1:B:228:HIS:O	1:B:229:SER:C	2.51	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:189:HIS:O	1:C:190:SER:C	2.52	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:D:496:LEU:HD23	1:D:498:MET:HE2	1.91	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
1:D:196:GLU:CD	1:D:196:GLU:H	2.18	0.52
1:A:167:ARG:NH2	1:A:173:GLU:OE2	2.32	0.52
1:A:132:SER:O	1:A:133:ASP:C	2.53	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:50:ASN:HA	1:C:188:PHE:HZ	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:49:TYR:OH	1:B:196:GLU:O	2.22	0.51
1:C:363:SER:HB2	1:C:364:PRO:HD2	1.92	0.51
1:D:33:LYS:HG2	1:D:36:LEU:HG	1.92	0.51
1:D:195:GLN:HB3	1:D:228:HIS:CG	2.46	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: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:A:491:ARG:HD3	1:A:498:MET:CE	2.40	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:64:LEU:HD13	1:A:73:ILE:HD12	1.94	0.50
1:A:342:VAL:HG22	1:A:412:ILE:HG12	1.93	0.50
1:A:646:GLU:CD	1:A:650:LYS:HD3	2.35	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: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: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: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:277:MET:HE3	1:C:422:PHE:CE2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:269:HIS:ND1	1:C:438: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:D:194:THR:HG22	1:D:197:GLU:CD	2.38	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: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:D:366:ALA:O	1:D:367:GLY:C	2.57	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:C:491:ARG:NH1	1:C:498:MET:HE1	2.29	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
1:D:220:TYR:CG	1:D:384:LEU:HD11	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:MET:HE3	1:B:422:PHE:HE2	1.80	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
4:B:811:HOH:O	1:D:596:HIS:HE1	1.98	0.47
1:D:50:ASN:HA	1:D:188:PHE:CZ	2.45	0.47
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:HA	1:D:178:GLN:NE2	2.30	0.46
1:D:438:MET:HE3	1:D:438:MET:HA	1.97	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
4:A:811:HOH:O	1:C:596:HIS:HE1	1.99	0.46
1:C:187:LEU:HD23	1:C:334:THR:HA	1.98	0.46
1:C:232:ARG:HD3	1:C:358:ALA:O	2.16	0.46
1:D:425:ARG:NH1	1:D:425:ARG:HB3	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:48:VAL:O	1:D:49:TYR:C	2.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:491:ARG:HD3	1:C:498:MET:CE	2.48	0.44
1:D:576:ALA:HA	1:D:577:PRO:HA	1.75	0.44
1:A:47:LYS:NZ	1:A:196:GLU:OE2	2.51	0.44
1:A:308:THR:HB	1:A:309:PRO:HD2	1.99	0.44
1:A:366:ALA:O	1:A:367:GLY:C	2.61	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:C:169:MET:HE1	1:C:202:TYR:HB3	2.00	0.44
1:A:119:ARG:NH2	1:A:192:LEU:CD2	2.80	0.44
1:A:277:MET:HE3	1:A:422:PHE:HE2	1.79	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:D:375:MET:HE2	1:D:375:MET:HA	1.99	0.44
1:A:403:GLU:HB3	1:A:459:TYR:CE1	2.52	0.43
1:A:491:ARG:HH11	1:A:498:MET:HE1	1.83	0.43
1:A:661:LYS:O	1:A:662:SER:C	2.61	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:C:48:VAL:O	1:C:49:TYR:C	2.62	0.43
1:A:199:ASP:HB3	4:A:804:HOH:O	2.19	0.43
1:B:208:LYS:NZ	1:B:212:GLU:OE2	2.46	0.43
1:B:263:ARG:HG3	1:D:585:TYR:CG	2.54	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:MET:HE1	1:B:365:LYS:O	2.18	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:C:491:ARG:HH11	1:C:498:MET:HE1	1.84	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:HE1	2.34	0.43
1:C:544:LEU:O	1:C:647:PRO:HD2	2.19	0.43
1:C:646:GLU:CD	1:C:650:LYS:HD3	2.44	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:A:247:ILE:HD12	1:A:336:TYR:O	2.17	0.42
1:A:491:ARG:NH1	1:A:498:MET:HE1	2.34	0.42
1:B:116:HIS:HD2	1:B:118:GLY:N	2.15	0.42
1:C:98:ASP:OD2	1:C:442:LYS:NZ	2.51	0.42
1:C:228:HIS:O	1:C:229:SER:C	2.62	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:58:CYS:O	1:B:62:GLU:HG3	2.20	0.42
1:B:515:PHE:O	1:B:613:GLY:HA3	2.19	0.42
1:D:88:PRO:HA	1:D:93:HIS:O	2.19	0.42
1:D:193:GLN:NE2	4:D:888:HOH:O	2.37	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:B:191:ASN:O	1:B:192:LEU:C	2.62	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:A:277:MET:HE1	1:A:365:LYS:O	2.20	0.42
1:A:317:LYS:NZ	4:A:1080:HOH:O	2.53	0.42
1:D:232:ARG:HD3	1:D:358:ALA:O	2.20	0.42
1:A:263:ARG:O	1:C:494:GLU:HB3	2.19	0.42
1:A:351:ARG:HD3	1:A:351:ARG:HA	1.91	0.42
1:A:576:ALA:HA	1:A:577:PRO:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:HD3	1:B:192:LEU:HA	2.02	0.42
1:C:167:ARG:HE	1:C:203:ARG:NH2	2.09	0.41
1:C:366:ALA:O	1:C:367:GLY:C	2.60	0.41
1:D:191:ASN:HD21	2:D:801:FAD:HM82	1.85	0.41
1:D:224:CYS:O	2:D:801:FAD:H52A	2.20	0.41
1:A:252:ASP:O	1:A:330:LEU:HD12	2.20	0.41
1:C:47:LYS:HA	1:C:47:LYS:HD3	1.87	0.41
1:D:33:LYS:HZ2	1:D:36:LEU:CD2	2.33	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:85:LEU:HD13	4:C:943:HOH:O	2.20	0.41
1:C:204:LEU:HB3	1:C:208:LYS:HE3	2.01	0.41
1:D:186:SER:H	1:D:332:TRP:NE1	2.18	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:HG22	1:A:134:THR:O	2.20	0.41
1:C:195:GLN:HB3	1:C:228:HIS:ND1	2.36	0.41
1:D:340:GLN:HB2	1:D:412:ILE:HG13	2.02	0.41
1:D:406:ALA:N	4:D:919:HOH:O	2.31	0.41
1:D:630:LEU:HG	4:D:946:HOH:O	2.21	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:48:VAL:HG21	1:C:176:PRO:HG2	2.03	0.41
1:C:193:GLN:NE2	1:C:201:ASN:ND2	2.69	0.41
1:C:247:ILE:HD11	1:C:307:PHE:CZ	2.56	0.41
1:A:89:ASP:HB3	1:A:91:ASN:H	1.86	0.41
1:A:185:ASN:O	1:A:186:SER:OG	2.37	0.41
1:B:168:TYR:CZ	1:B:208:LYS:HD2	2.56	0.41
1:B:190:SER:OG	1:B:193:GLN:HG3	2.20	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:A:277:MET:HE3	1:A:422:PHE:CZ	2.56	0.40
1:D:90:GLU:HG3	1:D:91:ASN:H	1.85	0.40
1:D:190:SER:CA	4:D:887:HOH:O	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:O	1:D:198:GLU:C	2.65	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: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:72:LYS:HD2	4:D:845:HOH:O	2.21	0.40
1:D:369:GLY:HA3	2:D:801:FAD:O3'	2.22	0.40
1:A:232:ARG:HD3	1:A:358:ALA:O	2.21	0.40
1:B:132:SER:O	1:B:133:ASP:C	2.64	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](#)

There are no protein backbone outliers to report in this entry.

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	563/573 (98%)	526 (93%)	37 (7%)	15	26
1	B	564/573 (98%)	527 (93%)	37 (7%)	15	26
1	C	569/573 (99%)	520 (91%)	49 (9%)	10	16
1	D	568/573 (99%)	525 (92%)	43 (8%)	12	21
All	All	2264/2292 (99%)	2098 (93%)	166 (7%)	13	22

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	95	ARG
1	A	142	LEU
1	A	153	LYS
1	A	173	GLU
1	A	183	THR
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	276	ILE
1	A	283	ASN
1	A	315	ASN
1	A	333	PHE
1	A	334	THR
1	A	342	VAL
1	A	359	CYS
1	A	365	LYS
1	A	422	PHE
1	A	428	LYS
1	A	429	ASP
1	A	430	VAL
1	A	434	MET
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	628	THR
1	A	649	GLU
1	A	655	THR
1	B	89	ASP
1	B	95	ARG
1	B	120	ILE
1	B	134	THR
1	B	142	LEU
1	B	153	LYS

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Mol	Chain	Res	Type
1	B	172	HIS
1	B	174	SER
1	B	192	LEU
1	B	195	GLN
1	B	203	ARG
1	B	213	ILE
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
1	B	347	SER
1	B	365	LYS
1	B	422	PHE
1	B	428	LYS
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	628	THR
1	B	648	LYS
1	B	650	LYS
1	B	655	THR
1	B	662	SER
1	C	1	THR
1	C	33	LYS
1	C	40	ILE
1	C	47	LYS
1	C	90	GLU
1	C	95	ARG
1	C	122	ARG
1	C	135	ARG
1	C	142	LEU
1	C	191	ASN
1	C	195	GLN

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Mol	Chain	Res	Type
1	C	198	GLU
1	C	203	ARG
1	C	206	GLU
1	C	208	LYS
1	C	209	GLU
1	C	238	GLU
1	C	242	GLU
1	C	245	ASP
1	C	247	ILE
1	C	272	GLU
1	C	276	ILE
1	C	283	ASN
1	C	301	ARG
1	C	305	THR
1	C	315	ASN
1	C	329	GLN
1	C	334	THR
1	C	342	VAL
1	C	365	LYS
1	C	422	PHE
1	C	428	LYS
1	C	430	VAL
1	C	433	GLU
1	C	434	MET
1	C	443	GLU
1	C	476	LYS
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	628	THR
1	C	648	LYS
1	C	654	GLN
1	C	663	THR
1	D	1	THR
1	D	47	LYS
1	D	63	SER
1	D	90	GLU

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Mol	Chain	Res	Type
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	191	ASN
1	D	192	LEU
1	D	194	THR
1	D	195	GLN
1	D	198	GLU
1	D	208	LYS
1	D	239	MET
1	D	242	GLU
1	D	247	ILE
1	D	272	GLU
1	D	276	ILE
1	D	283	ASN
1	D	292	LEU
1	D	304	ARG
1	D	315	ASN
1	D	334	THR
1	D	340	GLN
1	D	342	VAL
1	D	365	LYS
1	D	422	PHE
1	D	428	LYS
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	628	THR
1	D	648	LYS
1	D	649	GLU
1	D	650	LYS
1	D	661	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	112	GLN
1	A	116	HIS
1	A	181	HIS
1	A	191	ASN
1	A	195	GLN
1	A	283	ASN
1	A	449	ASN
1	A	499	HIS
1	A	584	GLN
1	A	596	HIS
1	A	597	HIS
1	B	66	ASN
1	B	112	GLN
1	B	116	HIS
1	B	172	HIS
1	B	181	HIS
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	189	HIS
1	C	193	GLN
1	C	195	GLN
1	C	201	ASN
1	C	283	ASN
1	C	315	ASN
1	C	449	ASN
1	C	499	HIS
1	C	562	HIS
1	C	584	GLN
1	C	596	HIS
1	C	604	GLN
1	D	191	ASN
1	D	193	GLN
1	D	243	GLN
1	D	283	ASN
1	D	405	HIS
1	D	449	ASN
1	D	499	HIS
1	D	572	HIS

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Mol	Chain	Res	Type
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 oligosaccharides 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	C	801	-	58,58,58	1.42	8 (13%)	85,89,89	1.52	15 (17%)
3	IPH	D	802	-	7,7,7	1.06	0	8,8,8	0.95	0
2	FAD	B	801	-	58,58,58	1.40	7 (12%)	85,89,89	1.63	23 (27%)
3	IPH	A	802	-	7,7,7	0.59	0	8,8,8	0.61	0
3	IPH	B	802	-	7,7,7	0.78	0	8,8,8	1.15	1 (12%)
3	IPH	C	802	-	7,7,7	0.64	0	8,8,8	0.94	0
2	FAD	D	801	-	58,58,58	1.39	6 (10%)	85,89,89	1.62	20 (23%)
2	FAD	A	801	-	58,58,58	1.47	6 (10%)	85,89,89	1.61	19 (22%)

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	C	801	-	1/1/9/9	5/34/50/50	0/6/6/6
3	IPH	D	802	-	-	-	0/1/1/1
2	FAD	B	801	-	-	2/34/50/50	0/6/6/6
3	IPH	A	802	-	-	-	0/1/1/1
3	IPH	B	802	-	-	-	0/1/1/1
3	IPH	C	802	-	-	-	0/1/1/1
2	FAD	D	801	-	-	5/34/50/50	0/6/6/6
2	FAD	A	801	-	-	4/34/50/50	0/6/6/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C9-C8	-5.18	1.32	1.39
2	B	801	FAD	C9-C8	-5.15	1.32	1.39
2	D	801	FAD	C9-C8	-5.07	1.32	1.39
2	C	801	FAD	C9-C8	-4.89	1.33	1.39
2	A	801	FAD	O2B-C2B	-3.37	1.34	1.43
2	A	801	FAD	C5X-N5	-3.29	1.33	1.39
2	D	801	FAD	O2B-C2B	-3.28	1.34	1.43
2	B	801	FAD	C6-C7	-3.25	1.35	1.39
2	D	801	FAD	C6-C7	-3.13	1.35	1.39
2	C	801	FAD	O2B-C2B	-3.09	1.35	1.43
2	C	801	FAD	C5X-N5	-2.90	1.34	1.39
2	D	801	FAD	C5X-N5	-2.68	1.34	1.39
2	C	801	FAD	C8M-C8	2.64	1.55	1.51
2	B	801	FAD	O2B-C2B	-2.61	1.36	1.43
2	A	801	FAD	C6-C7	-2.53	1.36	1.39
2	B	801	FAD	C1'-N10	2.35	1.53	1.47
2	A	801	FAD	O3B-C3B	2.31	1.48	1.43
2	C	801	FAD	C5'-C4'	2.23	1.54	1.51
2	B	801	FAD	C4X-C4	2.22	1.52	1.44
2	D	801	FAD	C4A-N3A	-2.22	1.30	1.34
2	C	801	FAD	O3B-C3B	2.19	1.48	1.43
2	B	801	FAD	O3B-C3B	2.15	1.48	1.43
2	B	801	FAD	C2A-N3A	-2.09	1.30	1.33
2	C	801	FAD	C4A-N3A	-2.09	1.30	1.34
2	A	801	FAD	C5A-C4A	2.07	1.42	1.39
2	C	801	FAD	C6-C7	-2.04	1.36	1.39
2	D	801	FAD	O2-C2	-2.02	1.20	1.24

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O2B-C2B-C1B	4.97	127.22	110.10
2	C	801	FAD	O2B-C2B-C1B	4.84	126.76	110.10
2	C	801	FAD	O2B-C2B-C3B	4.24	125.41	111.82
2	C	801	FAD	C2B-C1B-N9A	4.03	123.33	113.30
2	B	801	FAD	C7M-C7-C6	3.97	126.57	119.57
2	D	801	FAD	C2B-C1B-N9A	3.88	122.94	113.30
2	D	801	FAD	N3A-C4A-N9A	3.71	133.48	127.17
2	C	801	FAD	N3A-C4A-N9A	3.70	133.47	127.17
2	A	801	FAD	O2B-C2B-C1B	3.69	122.82	110.10
2	B	801	FAD	O2-C2-N1	-3.59	115.84	121.80
2	D	801	FAD	O2-C2-N1	-3.50	115.99	121.80
2	B	801	FAD	N3A-C2A-N1A	-3.43	123.39	128.58
2	A	801	FAD	C2B-C1B-N9A	3.38	121.70	113.30
2	A	801	FAD	O2-C2-N1	-3.33	116.26	121.80
2	D	801	FAD	C4-N3-C2	-3.31	119.76	125.64
2	A	801	FAD	O3B-C3B-C2B	-3.13	101.77	111.82
2	B	801	FAD	C2B-C1B-N9A	3.13	121.07	113.30
2	A	801	FAD	O2'-C2'-C3'	3.12	116.56	109.25
2	A	801	FAD	C10-N1-C2	3.04	123.43	116.85
2	A	801	FAD	C1'-C2'-C3'	3.00	117.80	109.66
2	B	801	FAD	P-O5'-C5'	2.99	138.51	121.35
2	A	801	FAD	O4B-C1B-N9A	2.99	113.83	108.09
2	D	801	FAD	O2B-C2B-C3B	2.96	121.29	111.82
2	B	801	FAD	N3A-C4A-N9A	2.95	132.18	127.17
2	B	801	FAD	O2B-C2B-C1B	2.90	120.09	110.10
2	C	801	FAD	C4A-N9A-C8A	2.77	108.65	105.74
2	A	801	FAD	N3A-C4A-N9A	2.73	131.80	127.17
2	B	801	FAD	O3P-P-O1P	2.72	118.89	110.70
2	D	801	FAD	C4X-C10-N10	2.72	120.37	116.48
2	A	801	FAD	O4B-C1B-C2B	2.72	112.43	106.62
2	C	801	FAD	C5A-C4A-N9A	-2.69	102.88	105.81
2	D	801	FAD	C4A-N9A-C8A	2.69	108.56	105.74
2	B	801	FAD	O4B-C1B-N9A	2.64	113.15	108.09
2	B	801	FAD	O4B-C1B-C2B	2.61	112.20	106.62
2	C	801	FAD	O4B-C1B-C2B	2.61	112.19	106.62
2	B	801	FAD	C5A-C4A-N9A	-2.60	102.98	105.81
2	A	801	FAD	C5A-C4A-N9A	-2.58	103.00	105.81
2	D	801	FAD	C4'-C3'-C2'	-2.56	109.31	113.57
2	C	801	FAD	C10-N1-C2	2.56	122.39	116.85
2	D	801	FAD	O3B-C3B-C2B	-2.53	103.71	111.82
2	B	801	FAD	O2'-C2'-C3'	2.52	115.15	109.25
2	D	801	FAD	C5A-C4A-N3A	-2.51	123.25	126.72
2	A	801	FAD	C8M-C8-C9	-2.51	115.15	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	O2-C2-N1	-2.46	117.71	121.80
2	D	801	FAD	C8M-C8-C9	-2.45	115.26	119.57
2	D	801	FAD	N3A-C2A-N1A	-2.43	124.90	128.58
2	C	801	FAD	C8M-C8-C9	-2.43	115.30	119.57
2	A	801	FAD	O2A-PA-O1A	2.41	123.67	112.44
2	D	801	FAD	C5A-C4A-N9A	-2.36	103.24	105.81
2	B	801	FAD	O2A-PA-O1A	2.32	123.24	112.44
2	A	801	FAD	O2-C2-N3	2.29	122.98	118.58
2	C	801	FAD	C4X-C10-N10	2.29	119.76	116.48
2	B	801	FAD	C4A-N9A-C8A	2.28	108.13	105.74
2	C	801	FAD	C5A-C4A-N3A	-2.25	123.62	126.72
3	B	802	IPH	C4-C3-C2	-2.24	117.47	120.24
2	A	801	FAD	P-O5'-C5'	2.24	134.19	121.35
2	D	801	FAD	O4B-C1B-C2B	2.22	111.37	106.62
2	A	801	FAD	C4A-N9A-C8A	2.20	108.04	105.74
2	A	801	FAD	C2B-C3B-C4B	2.19	106.84	102.61
2	B	801	FAD	C1'-C2'-C3'	2.18	115.56	109.66
2	B	801	FAD	C4X-C10-N10	2.18	119.60	116.48
2	A	801	FAD	C4-N3-C2	-2.18	121.78	125.64
2	B	801	FAD	C10-N1-C2	2.17	121.55	116.85
2	C	801	FAD	C3B-C2B-C1B	2.15	105.53	101.46
2	D	801	FAD	C3B-C2B-C1B	2.14	105.51	101.46
2	C	801	FAD	O4-C4-N3	-2.12	116.14	120.11
2	D	801	FAD	C2A-N3A-C4A	2.10	116.97	111.83
2	B	801	FAD	O3B-C3B-C2B	-2.08	105.16	111.82
2	B	801	FAD	C7M-C7-C8	-2.07	116.52	120.76
2	B	801	FAD	O2B-C2B-C3B	2.07	118.44	111.82
2	B	801	FAD	O2-C2-N3	2.07	122.55	118.58
2	B	801	FAD	C2A-N1A-C6A	2.05	122.10	118.73
2	C	801	FAD	C4-N3-C2	-2.05	122.00	125.64
2	D	801	FAD	C10-N1-C2	2.03	121.23	116.85
2	D	801	FAD	C2B-C3B-C4B	2.03	106.52	102.61
2	A	801	FAD	C7M-C7-C6	2.02	123.14	119.57
2	D	801	FAD	N9A-C8A-N7A	-2.02	111.08	113.94
2	B	801	FAD	C2A-N3A-C4A	2.01	116.74	111.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	801	FAD	C2B

All (16) torsion outliers are listed below:

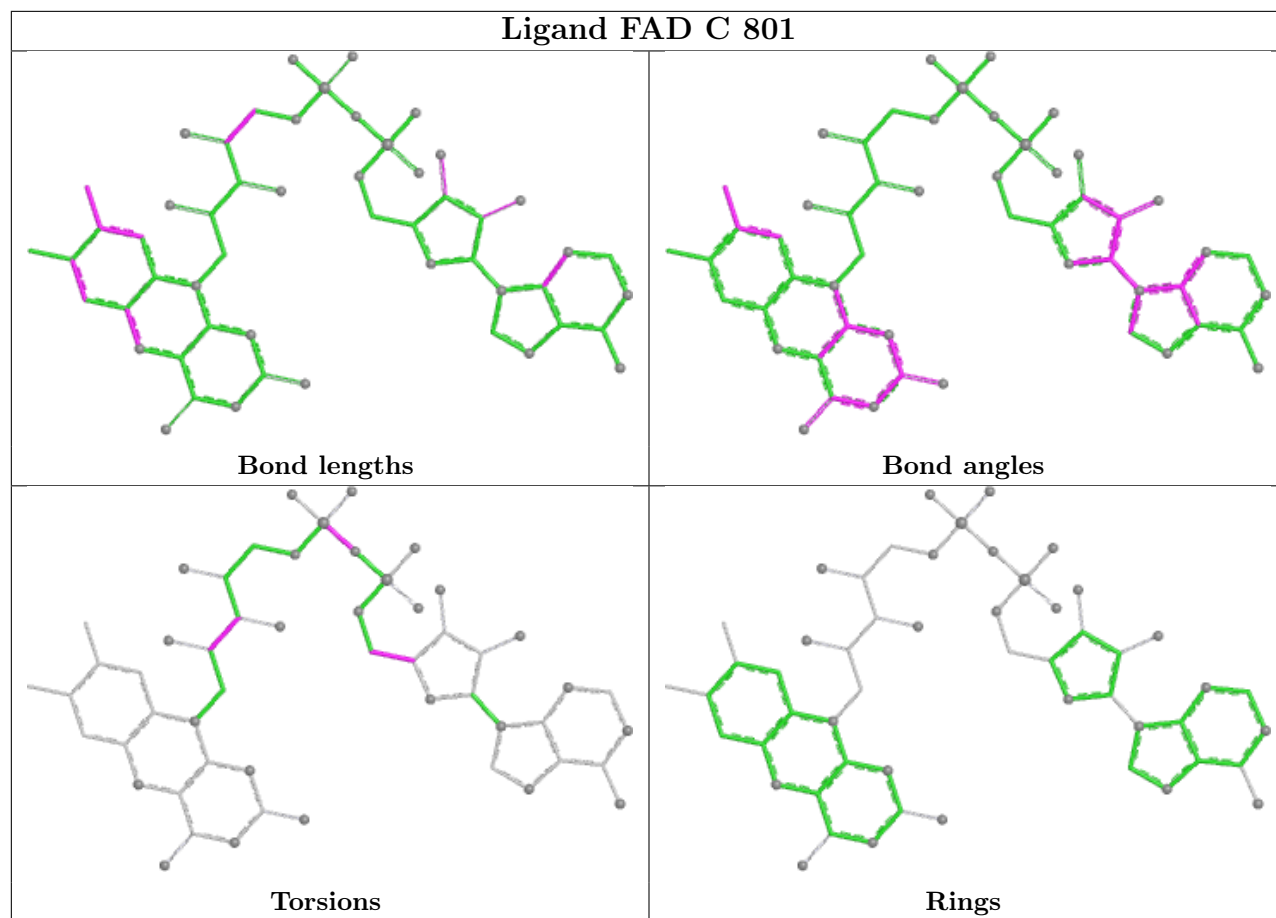
Mol	Chain	Res	Type	Atoms
2	A	801	FAD	N10-C1'-C2'-O2'
2	A	801	FAD	C5'-O5'-P-O1P
2	A	801	FAD	C5'-O5'-P-O3P
2	C	801	FAD	C1'-C2'-C3'-C4'
2	C	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	C1'-C2'-C3'-C4'
2	D	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	O2'-C2'-C3'-C4'
2	A	801	FAD	PA-O3P-P-O5'
2	B	801	FAD	PA-O3P-P-O5'
2	D	801	FAD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

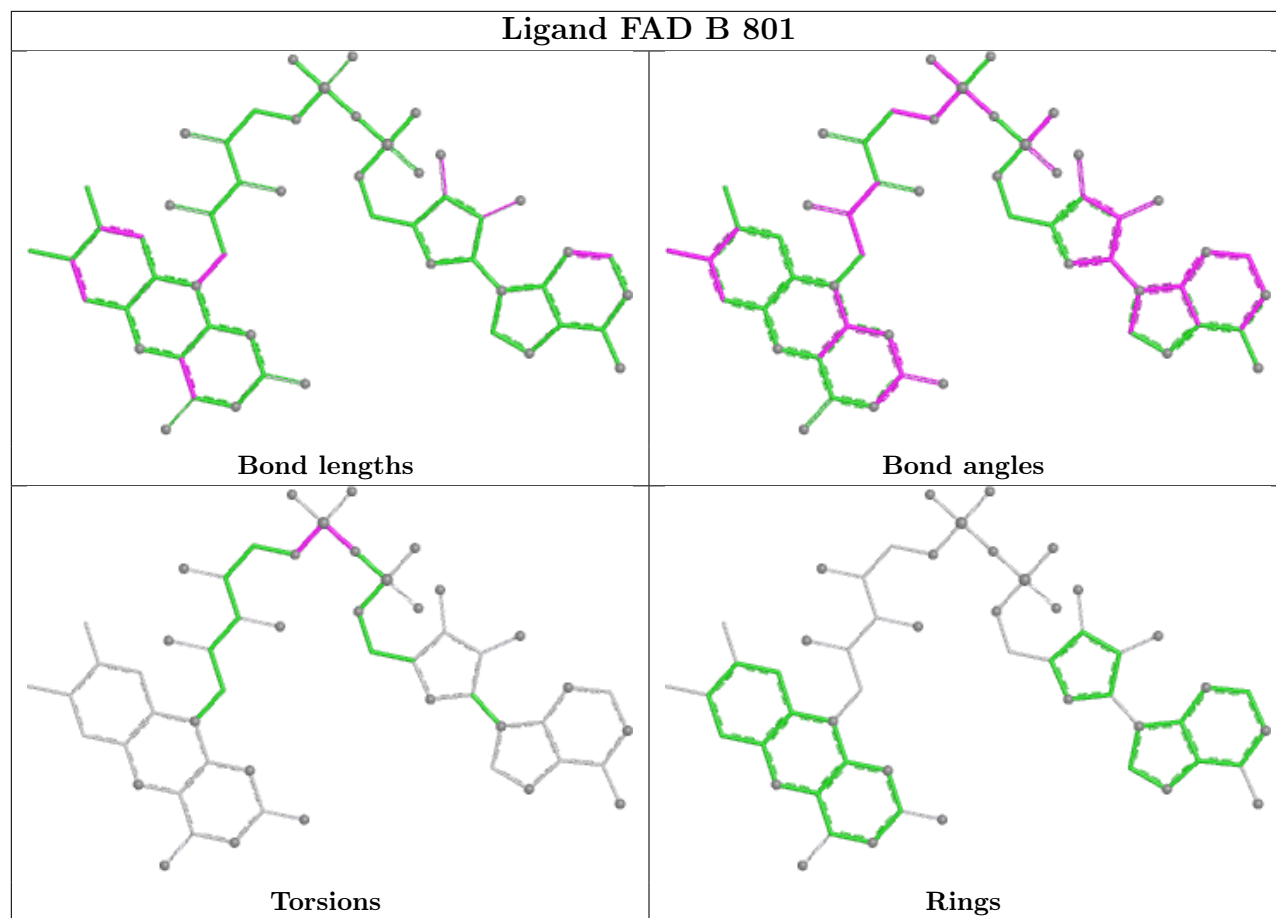
There are no ring outliers.

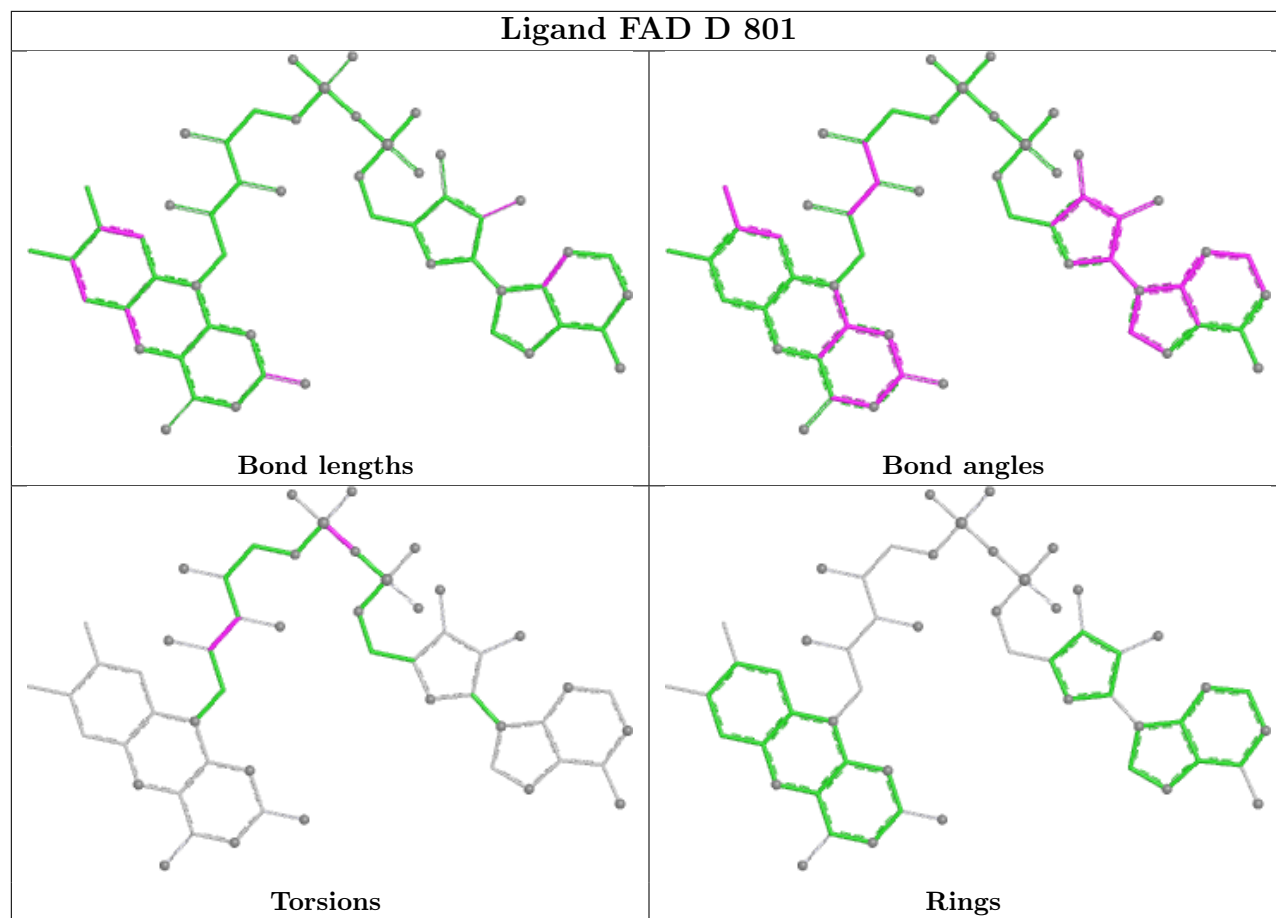
3 monomers are involved in 9 short contacts:

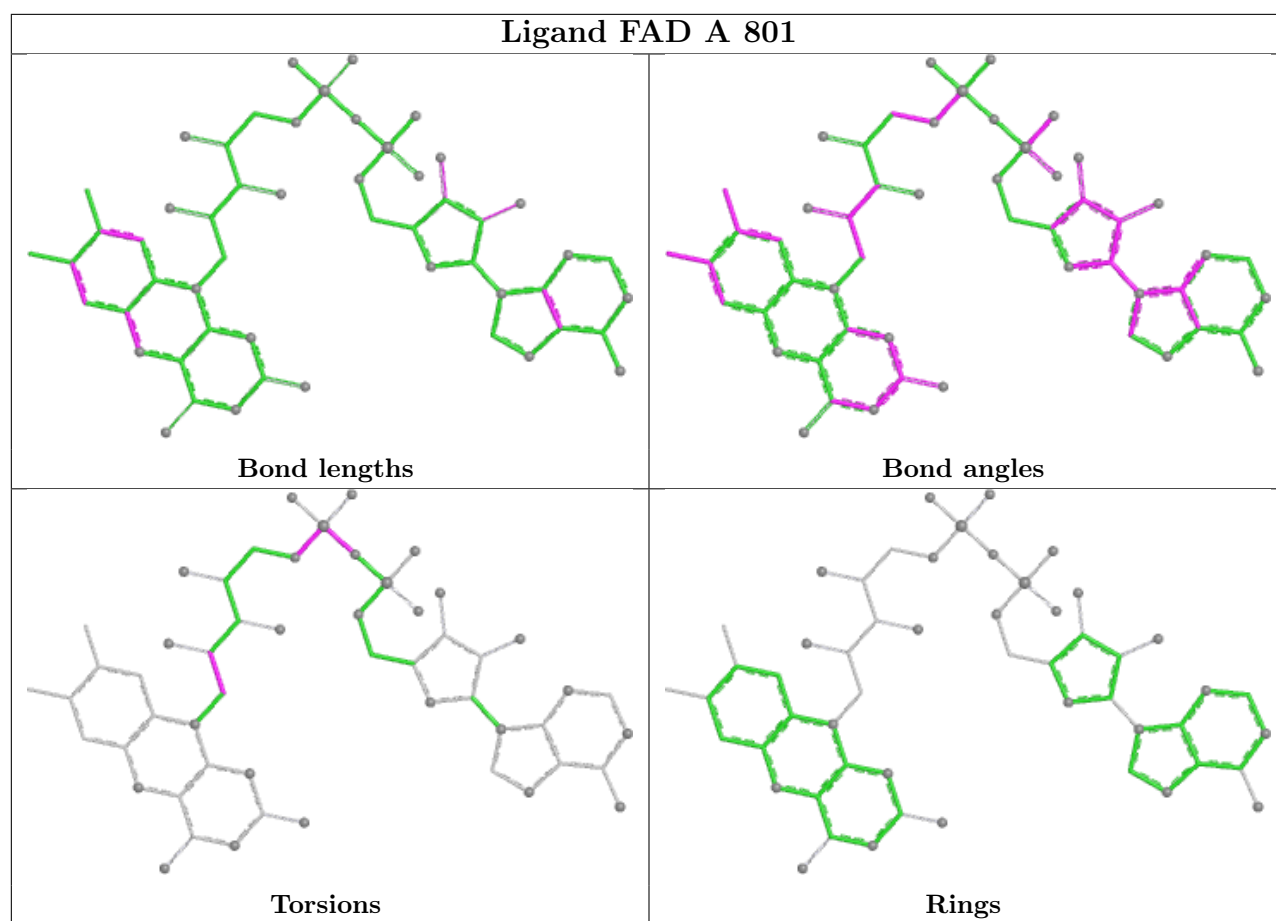
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FAD	2	0
2	D	801	FAD	6	0
2	A	801	FAD	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.