



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 1AHZ / pdb_00001ahz
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH 4-(1-HEPTENYL)PHENOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 3.30 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

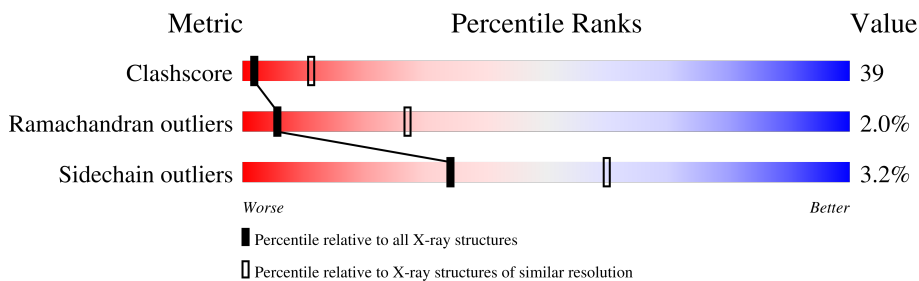
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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	560	
1	B	560	

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
4	EPT	A	602	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8904 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

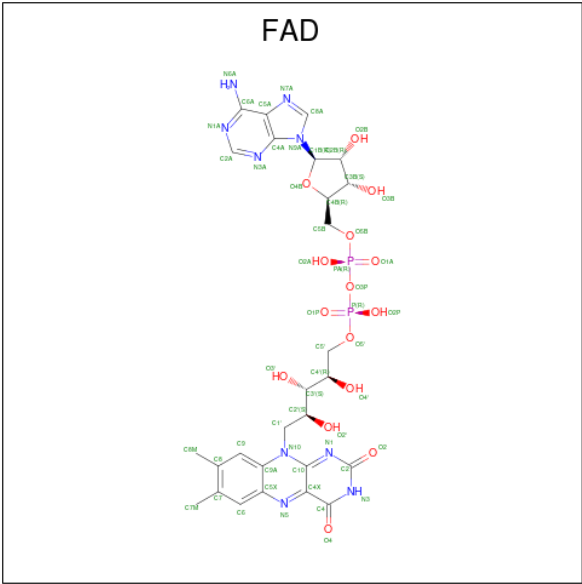
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

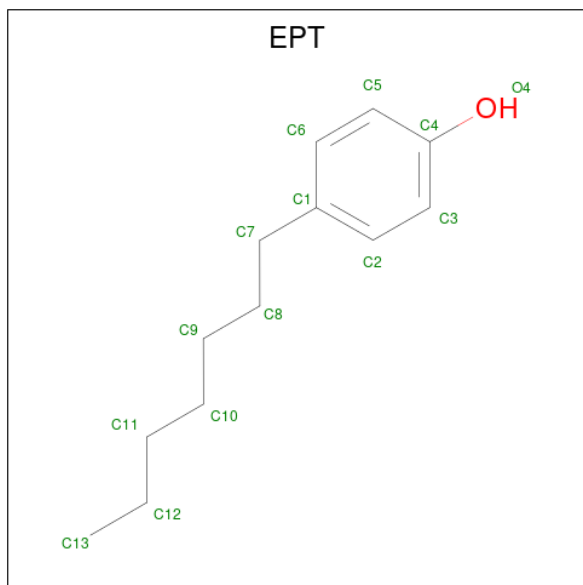
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is HEPTANYL-P-PHENOL (CCD ID: EPT) (formula: $C_{13}H_{20}O$).



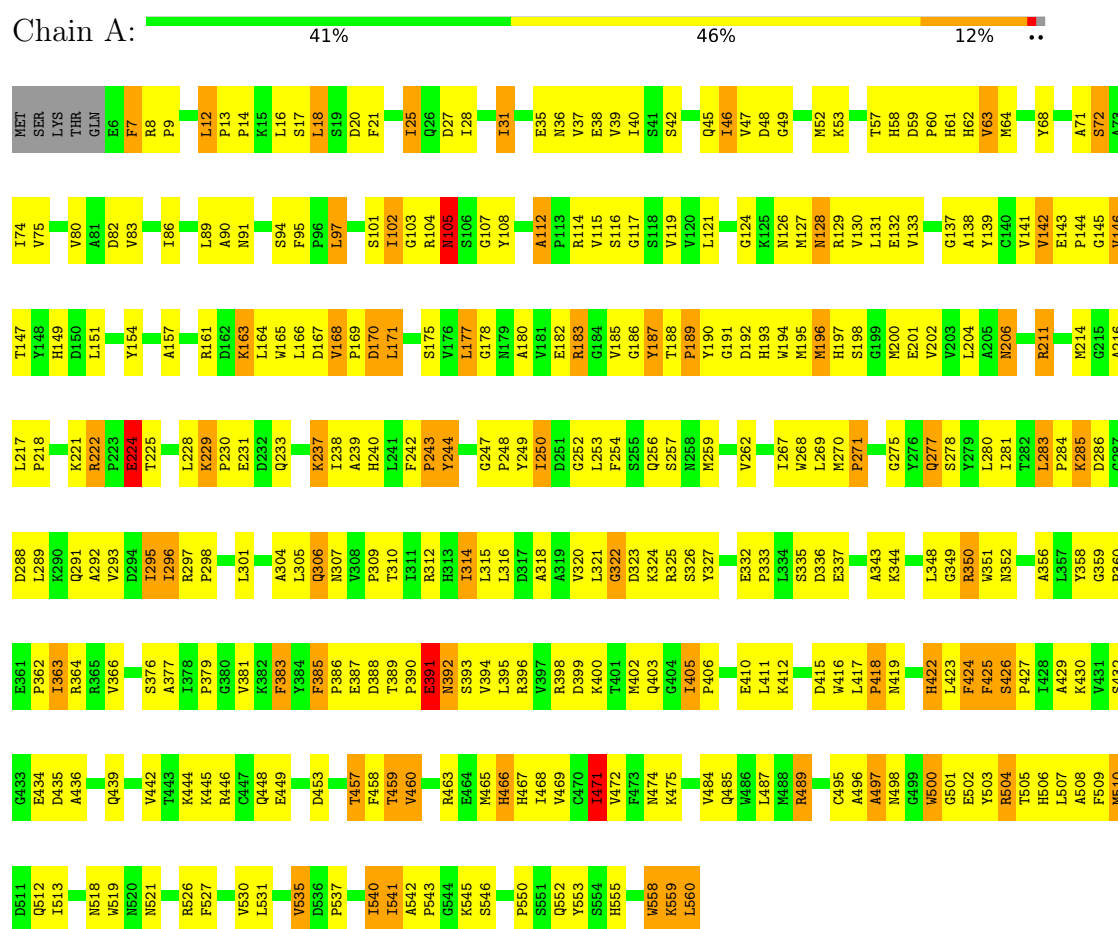
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	13	1		

3 Residue-property plots

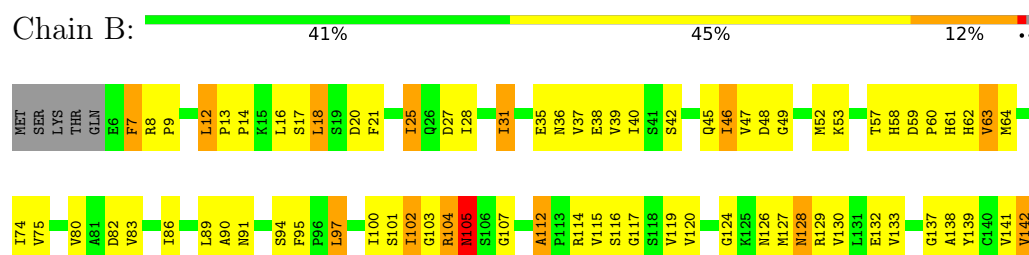
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	140.97 Å 140.97 Å 133.45 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30	Depositor
% Data completeness (in resolution range)	90.7 (30.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.224 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: EPT, FAD, CL

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	0.64	0/4511	1.67	97/6131 (1.6%)
1	B	0.64	0/4511	1.67	95/6131 (1.5%)
All	All	0.64	0/9022	1.67	192/12262 (1.6%)

There are no bond length outliers.

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ARG	N-CA-C	14.24	130.88	110.23
1	A	129	ARG	N-CA-C	14.21	130.83	110.23
1	B	102	ILE	N-CA-C	13.37	123.31	111.81
1	A	102	ILE	N-CA-C	13.33	123.27	111.81
1	A	7	PHE	N-CA-C	11.92	129.80	111.56
1	B	7	PHE	N-CA-C	11.90	129.77	111.56
1	A	187	TYR	N-CA-C	11.34	127.75	112.90
1	B	187	TYR	N-CA-C	11.31	127.72	112.90
1	B	244	TYR	N-CA-C	11.12	124.49	111.71
1	A	244	TYR	N-CA-C	11.08	124.46	111.71
1	B	124	GLY	N-CA-C	10.85	125.75	112.73
1	A	124	GLY	N-CA-C	10.81	125.70	112.73
1	B	558	TRP	N-CA-C	10.78	124.95	111.69
1	A	558	TRP	N-CA-C	10.76	124.92	111.69
1	A	460	VAL	N-CA-C	10.34	123.60	107.98
1	B	460	VAL	N-CA-C	10.32	123.57	107.98
1	A	142	VAL	N-CA-C	9.87	122.53	108.42
1	B	142	VAL	N-CA-C	9.86	122.51	108.42
1	A	410	GLU	N-CA-C	9.85	123.04	111.71
1	B	410	GLU	N-CA-C	9.81	123.00	111.71
1	B	104	ARG	N-CA-C	9.66	124.60	113.01
1	A	104	ARG	N-CA-C	9.65	124.59	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASN	N-CA-C	9.62	123.52	111.69
1	B	36	ASN	N-CA-C	9.60	123.49	111.69
1	A	383	PHE	N-CA-C	9.55	123.78	108.41
1	B	383	PHE	N-CA-C	9.53	123.75	108.41
1	B	250	ILE	N-CA-C	9.10	124.78	112.04
1	A	250	ILE	N-CA-C	9.10	124.78	112.04
1	A	314	ILE	CB-CA-C	-8.84	100.66	111.97
1	B	314	ILE	CB-CA-C	-8.83	100.67	111.97
1	A	457	THR	CB-CA-C	-8.80	94.02	109.86
1	B	457	THR	CB-CA-C	-8.80	94.03	109.86
1	B	306	GLN	N-CA-C	8.39	121.64	111.40
1	A	306	GLN	N-CA-C	8.37	121.61	111.40
1	A	126	ASN	N-CA-C	8.24	122.61	112.23
1	B	126	ASN	N-CA-C	8.24	122.61	112.23
1	B	146	VAL	N-CA-C	8.23	119.70	108.84
1	A	146	VAL	N-CA-C	8.21	119.67	108.84
1	A	425	PHE	N-CA-C	-8.08	96.51	109.76
1	B	425	PHE	N-CA-C	-8.08	96.51	109.76
1	B	385	PHE	N-CA-C	-7.75	100.25	110.40
1	A	385	PHE	N-CA-C	-7.75	100.25	110.40
1	A	72	SER	N-CA-C	-7.73	102.78	112.90
1	B	72	SER	N-CA-C	-7.72	102.78	112.90
1	B	71	ALA	N-CA-C	7.68	120.49	110.43
1	A	63	VAL	N-CA-C	-7.66	101.18	111.44
1	A	71	ALA	N-CA-C	7.64	120.44	110.43
1	B	63	VAL	N-CA-C	-7.64	101.20	111.44
1	A	415	ASP	N-CA-C	7.62	122.22	113.15
1	B	415	ASP	N-CA-C	7.61	122.21	113.15
1	B	535	VAL	N-CA-C	7.61	121.64	111.44
1	A	535	VAL	N-CA-C	7.57	121.59	111.44
1	A	222	ARG	CB-CA-C	7.53	120.47	109.09
1	B	222	ARG	CB-CA-C	7.51	120.43	109.09
1	A	211	ARG	N-CA-CB	7.44	122.37	110.46
1	B	211	ARG	N-CA-CB	7.43	122.35	110.46
1	A	422	HIS	CB-CA-C	7.39	122.77	109.83
1	B	518	ASN	N-CA-C	7.39	126.55	110.80
1	A	518	ASN	N-CA-C	7.37	126.50	110.80
1	B	422	HIS	CB-CA-C	7.37	122.73	109.83
1	A	426	SER	CB-CA-C	-7.24	101.62	110.81
1	B	426	SER	CB-CA-C	-7.22	101.64	110.81
1	B	196	MET	N-CA-C	7.16	123.25	113.37
1	A	196	MET	N-CA-C	7.12	123.19	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	HIS	N-CA-C	6.90	118.45	111.07
1	A	541	ILE	N-CA-C	6.86	118.72	108.23
1	B	47	VAL	N-CA-C	6.85	118.62	109.37
1	A	193	HIS	N-CA-C	6.85	118.40	111.07
1	A	47	VAL	N-CA-C	6.84	118.60	109.37
1	B	541	ILE	N-CA-C	6.84	118.69	108.23
1	B	171	LEU	N-CA-C	-6.80	99.97	110.10
1	A	171	LEU	N-CA-C	-6.79	99.98	110.10
1	B	169	PRO	N-CA-C	-6.63	98.81	112.47
1	A	169	PRO	N-CA-C	-6.63	98.82	112.47
1	A	42	SER	N-CA-C	6.56	119.04	109.07
1	B	42	SER	N-CA-C	6.56	119.04	109.07
1	A	221	LYS	N-CA-C	6.55	119.27	109.25
1	A	237	LYS	N-CA-C	6.52	119.22	111.33
1	B	221	LYS	N-CA-C	6.52	119.23	109.25
1	B	471	ILE	CB-CA-C	-6.51	104.90	111.80
1	A	296	ILE	CB-CA-C	-6.50	103.53	112.24
1	B	237	LYS	N-CA-C	6.49	119.19	111.33
1	B	459	THR	N-CA-C	-6.49	97.69	108.34
1	A	471	ILE	CB-CA-C	-6.48	104.93	111.80
1	A	459	THR	N-CA-C	-6.48	97.71	108.34
1	B	296	ILE	CB-CA-C	-6.45	103.59	112.24
1	A	295	ILE	CB-CA-C	-6.45	102.17	112.16
1	B	295	ILE	CB-CA-C	-6.43	102.19	112.16
1	A	107	GLY	N-CA-C	-6.23	106.64	115.30
1	B	356	ALA	N-CA-C	6.22	117.68	108.60
1	A	356	ALA	N-CA-C	6.20	117.65	108.60
1	B	296	ILE	N-CA-C	6.20	117.75	111.00
1	A	296	ILE	N-CA-C	6.19	117.75	111.00
1	B	130	VAL	N-CA-C	-6.19	97.68	107.15
1	B	107	GLY	N-CA-C	-6.18	106.70	115.30
1	A	130	VAL	N-CA-C	-6.18	97.69	107.15
1	A	363	ILE	N-CA-C	-6.18	104.72	110.53
1	A	103	GLY	N-CA-C	-6.17	106.90	114.92
1	A	424	PHE	N-CA-C	6.16	119.69	109.46
1	B	103	GLY	N-CA-C	-6.16	106.92	114.92
1	B	363	ILE	N-CA-C	-6.15	104.75	110.53
1	B	424	PHE	N-CA-C	6.15	119.67	109.46
1	A	116	SER	N-CA-C	6.13	118.68	110.35
1	B	83	VAL	N-CA-C	-6.11	104.55	110.42
1	A	83	VAL	N-CA-C	-6.11	104.56	110.42
1	B	25	ILE	CB-CA-C	-6.10	103.90	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ILE	CB-CA-C	-6.10	103.91	112.14
1	B	116	SER	N-CA-C	6.09	118.63	110.35
1	B	278	SER	N-CA-C	-6.08	102.68	110.53
1	A	278	SER	N-CA-C	-6.07	102.70	110.53
1	B	521	ASN	N-CA-C	6.00	119.95	111.92
1	B	12	LEU	CA-C-N	5.98	124.02	119.66
1	B	12	LEU	C-N-CA	5.98	124.02	119.66
1	A	521	ASN	N-CA-C	5.96	119.91	111.92
1	B	18	LEU	N-CA-C	-5.91	104.92	111.71
1	A	322	GLY	N-CA-C	5.90	119.70	110.91
1	A	18	LEU	N-CA-C	-5.89	104.94	111.71
1	B	322	GLY	N-CA-C	5.87	119.66	110.91
1	B	14	PRO	CB-CA-C	-5.87	103.30	110.98
1	A	12	LEU	CA-C-N	5.85	123.93	119.66
1	A	12	LEU	C-N-CA	5.85	123.93	119.66
1	A	14	PRO	CB-CA-C	-5.84	103.33	110.98
1	A	542	ALA	N-CA-C	5.81	122.64	109.81
1	B	542	ALA	N-CA-C	5.80	122.62	109.81
1	A	484	VAL	CB-CA-C	-5.79	104.32	112.14
1	B	484	VAL	CB-CA-C	-5.77	104.35	112.14
1	A	224	GLU	N-CA-C	5.73	118.47	111.82
1	B	224	GLU	N-CA-C	5.73	118.47	111.82
1	B	500	TRP	N-CA-C	5.72	118.57	109.24
1	A	500	TRP	N-CA-C	5.71	118.54	109.24
1	A	168	VAL	CB-CA-C	-5.64	101.09	111.36
1	A	506	HIS	N-CA-CB	-5.64	101.88	110.45
1	B	506	HIS	N-CA-CB	-5.63	101.89	110.45
1	B	168	VAL	CB-CA-C	-5.63	101.12	111.36
1	A	510	MET	N-CA-C	-5.60	105.17	111.28
1	B	510	MET	N-CA-C	-5.57	105.21	111.28
1	B	285	LYS	N-CA-C	5.50	118.67	110.52
1	A	285	LYS	N-CA-C	5.50	118.66	110.52
1	A	392	ASN	N-CA-C	-5.45	107.89	114.75
1	A	31	ILE	CB-CA-C	-5.45	104.75	111.94
1	B	392	ASN	N-CA-C	-5.45	107.89	114.75
1	A	137	GLY	N-CA-C	-5.44	107.92	114.66
1	B	31	ILE	CB-CA-C	-5.44	104.76	111.94
1	B	157	ALA	N-CA-C	-5.41	105.29	111.14
1	A	157	ALA	N-CA-C	-5.40	105.31	111.14
1	B	137	GLY	N-CA-C	-5.40	107.97	114.66
1	B	540	ILE	CB-CA-C	-5.40	103.52	112.26
1	A	142	VAL	CB-CA-C	-5.38	101.49	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	VAL	CB-CA-C	-5.37	101.52	111.18
1	A	540	ILE	CB-CA-C	-5.36	103.57	112.26
1	B	405	ILE	CA-C-O	5.34	122.30	119.15
1	A	243	PRO	N-CA-C	5.33	120.54	113.40
1	B	243	PRO	N-CA-C	5.31	120.52	113.40
1	A	405	ILE	CA-C-O	5.30	122.28	119.15
1	B	344	LYS	N-CA-C	-5.30	105.50	111.28
1	B	376	SER	N-CA-C	5.29	117.80	111.71
1	A	376	SER	N-CA-C	5.26	117.76	111.71
1	B	183	ARG	CB-CA-C	-5.25	104.48	111.63
1	A	271	PRO	N-CA-C	-5.25	103.03	111.38
1	B	271	PRO	N-CA-C	-5.24	103.05	111.38
1	B	112	ALA	N-CA-C	5.24	116.29	109.64
1	A	183	ARG	CB-CA-C	-5.23	104.52	111.63
1	A	254	PHE	N-CA-C	5.22	119.65	113.28
1	A	304	ALA	N-CA-C	-5.22	105.50	111.14
1	A	112	ALA	N-CA-C	5.21	116.25	109.64
1	B	254	PHE	N-CA-C	5.21	119.63	113.28
1	A	504	ARG	CB-CA-C	-5.18	101.72	110.43
1	A	344	LYS	N-CA-C	-5.18	105.53	111.07
1	B	147	THR	N-CA-C	-5.18	103.08	110.59
1	B	304	ALA	N-CA-C	-5.17	105.55	111.14
1	B	504	ARG	CB-CA-C	-5.15	101.77	110.43
1	A	12	LEU	O-C-N	5.15	125.00	121.71
1	A	127	MET	N-CA-C	-5.15	97.59	107.57
1	A	350	ARG	N-CA-C	-5.14	106.84	113.01
1	A	147	THR	N-CA-C	-5.13	103.15	110.59
1	B	229	LYS	N-CA-C	-5.13	102.81	110.20
1	A	97	LEU	CA-CB-CG	-5.12	98.36	116.30
1	B	97	LEU	CA-CB-CG	-5.12	98.37	116.30
1	B	350	ARG	N-CA-C	-5.11	106.87	113.01
1	A	229	LYS	N-CA-C	-5.11	102.85	110.20
1	B	180	ALA	N-CA-C	5.10	117.74	111.82
1	B	127	MET	N-CA-C	-5.10	97.68	107.57
1	A	180	ALA	N-CA-C	5.09	117.72	111.82
1	B	12	LEU	O-C-N	5.08	124.96	121.71
1	A	336	ASP	N-CA-C	-5.07	105.75	111.28
1	A	489	ARG	CB-CG-CD	5.06	122.94	111.30
1	B	489	ARG	CB-CG-CD	5.06	122.94	111.30
1	B	466	HIS	N-CA-C	-5.03	100.31	108.41
1	B	336	ASP	N-CA-C	-5.02	105.80	111.28
1	A	466	HIS	N-CA-C	-5.02	100.33	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLY	N-CA-C	5.01	119.80	113.24
1	A	283	LEU	N-CA-C	-5.01	102.36	109.62

There are no chirality outliers.

There are no planarity outliers.

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	4391	0	4330	357	0
1	B	4391	0	4330	352	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	29	9	0
3	B	53	0	29	8	0
4	A	14	0	20	14	0
All	All	8904	0	8738	678	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 39.

All (678) 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)
3:A:600:FAD:H8A	3:A:600:FAD:H51A	1.31	1.10
1:A:510:MET:HE2	1:A:546:SER:H	1.15	1.10
1:A:314:ILE:HD11	1:A:350:ARG:HG3	1.37	1.06
3:B:600:FAD:H51A	3:B:600:FAD:H8A	1.31	1.06
1:B:314:ILE:HD11	1:B:350:ARG:HG3	1.37	1.03
1:B:510:MET:HE2	1:B:546:SER:H	1.15	1.03
1:A:280:LEU:HD12	1:A:281:ILE:H	1.28	0.99
1:B:280:LEU:HD12	1:B:281:ILE:H	1.28	0.98
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.01	0.94
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.01	0.94
1:A:463:ARG:HH12	1:B:138:ALA:HB3	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLY:H	1:B:352:ASN:HD21	1.16	0.92
1:A:138:ALA:HB3	1:B:463:ARG:HH12	1.34	0.91
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.52	0.91
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.52	0.90
1:A:510:MET:HE1	1:A:545:LYS:HD2	1.54	0.90
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.07	0.90
1:B:314:ILE:HD11	1:B:350:ARG:CG	2.02	0.90
1:A:314:ILE:HD11	1:A:350:ARG:CG	2.02	0.89
1:A:349:GLY:H	1:A:352:ASN:HD21	1.16	0.89
1:B:510:MET:HE1	1:B:545:LYS:HD2	1.53	0.89
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.07	0.89
1:A:61:HIS:CD2	1:A:422:HIS:HD1	1.91	0.88
1:B:61:HIS:CD2	1:B:422:HIS:HD1	1.91	0.87
1:A:16:LEU:HD11	1:A:20:ASP:HB2	1.56	0.87
1:A:138:ALA:HB3	1:B:463:ARG:NH1	1.90	0.87
1:B:16:LEU:HD11	1:B:20:ASP:HB2	1.56	0.86
1:B:510:MET:HE2	1:B:546:SER:N	1.90	0.86
1:B:16:LEU:HD11	1:B:20:ASP:CB	2.06	0.86
1:A:510:MET:HE2	1:A:546:SER:N	1.90	0.85
1:A:16:LEU:HD11	1:A:20:ASP:CB	2.06	0.85
1:A:61:HIS:CD2	1:A:422:HIS:H	1.95	0.84
1:B:61:HIS:CD2	1:B:422:HIS:H	1.95	0.84
1:A:463:ARG:NH1	1:B:138:ALA:HB3	1.93	0.83
1:A:248:PRO:HG3	1:B:257:SER:HB3	1.59	0.83
1:B:80:VAL:HB	1:B:231:GLU:HG3	1.61	0.82
1:A:80:VAL:HB	1:A:231:GLU:HG3	1.61	0.82
1:A:163:LYS:HE2	1:A:163:LYS:HA	1.62	0.82
1:B:280:LEU:HD12	1:B:281:ILE:N	1.95	0.82
1:B:206:ASN:H	1:B:206:ASN:HD22	1.29	0.81
1:B:163:LYS:HA	1:B:163:LYS:HE2	1.62	0.81
1:A:206:ASN:HD22	1:A:206:ASN:H	1.29	0.81
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.61	0.80
1:A:457:THR:HG21	4:A:602:EPT:C13	2.12	0.80
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.63	0.80
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.61	0.80
1:A:280:LEU:HD12	1:A:281:ILE:N	1.95	0.79
1:A:349:GLY:N	1:A:352:ASN:HD21	1.80	0.79
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.63	0.79
1:B:314:ILE:HD11	1:B:350:ARG:HA	1.65	0.79
1:A:257:SER:HB3	1:B:248:PRO:HG3	1.65	0.79
1:B:349:GLY:N	1:B:352:ASN:HD21	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ARG:HH21	1:B:316:LEU:HD21	1.49	0.78
1:A:211:ARG:HD3	1:B:519:TRP:CH2	2.19	0.78
1:A:416:TRP:HD1	1:A:417:LEU:HD12	1.49	0.78
1:A:312:ARG:HH21	1:A:316:LEU:HD21	1.49	0.77
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.66	0.77
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.66	0.77
1:A:314:ILE:HD11	1:A:350:ARG:HA	1.65	0.77
1:B:489:ARG:HG2	1:B:512:GLN:OE1	1.85	0.76
1:B:64:MET:HE2	1:B:485:GLN:HE22	1.49	0.76
1:A:161:ARG:O	1:A:161:ARG:HD3	1.86	0.76
1:B:161:ARG:O	1:B:161:ARG:HD3	1.86	0.76
1:A:40:ILE:HA	1:A:45:GLN:OE1	1.86	0.76
1:A:225:THR:O	1:A:228:LEU:HD13	1.86	0.76
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.68	0.76
1:A:510:MET:CE	1:A:546:SER:H	1.97	0.76
1:A:489:ARG:HG2	1:A:512:GLN:OE1	1.85	0.75
1:B:40:ILE:HA	1:B:45:GLN:OE1	1.86	0.75
1:B:225:THR:O	1:B:228:LEU:HD13	1.86	0.75
1:B:416:TRP:HD1	1:B:417:LEU:HD12	1.49	0.75
1:A:292:ALA:O	1:A:296:ILE:HG13	1.87	0.75
1:A:519:TRP:CH2	1:B:211:ARG:HD3	2.22	0.75
1:A:206:ASN:H	1:A:206:ASN:ND2	1.84	0.75
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.22	0.74
1:A:64:MET:HE2	1:A:485:GLN:HE22	1.49	0.74
1:B:314:ILE:CD1	1:B:350:ARG:HA	2.18	0.74
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.22	0.74
1:B:292:ALA:O	1:B:296:ILE:HG13	1.87	0.74
1:A:211:ARG:HD3	1:B:519:TRP:CZ3	2.23	0.74
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.68	0.74
1:A:188:THR:HB	1:A:189:PRO:HD2	1.70	0.73
1:B:526:ARG:O	1:B:530:VAL:HG23	1.89	0.73
1:B:555:HIS:CD2	1:B:559:LYS:HE3	2.24	0.73
1:A:21:PHE:CE1	1:A:25:ILE:HG13	2.24	0.73
1:A:314:ILE:CD1	1:A:350:ARG:HA	2.17	0.73
1:B:419:ASN:O	1:B:474:ASN:HA	1.88	0.73
1:A:419:ASN:O	1:A:474:ASN:HA	1.88	0.73
1:B:320:VAL:O	1:B:412:LYS:HE2	1.89	0.73
1:A:247:GLY:O	1:B:183:ARG:NH2	2.19	0.73
1:B:349:GLY:H	1:B:352:ASN:ND2	1.87	0.73
1:A:362:PRO:O	1:A:366:VAL:HG23	1.89	0.72
1:B:21:PHE:CE1	1:B:25:ILE:HG13	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TRP:CD1	1:B:417:LEU:HD12	2.24	0.72
1:B:171:LEU:HD13	1:B:411:LEU:HD21	1.71	0.72
1:A:320:VAL:O	1:A:412:LYS:HE2	1.89	0.72
1:A:555:HIS:CD2	1:A:559:LYS:HE3	2.24	0.72
1:B:362:PRO:O	1:B:366:VAL:HG23	1.90	0.72
1:A:526:ARG:O	1:A:530:VAL:HG23	1.89	0.72
1:A:171:LEU:HD13	1:A:411:LEU:HD21	1.71	0.71
1:A:416:TRP:CD1	1:A:417:LEU:HD12	2.24	0.71
1:A:64:MET:HE2	1:A:485:GLN:NE2	2.06	0.71
1:B:188:THR:HB	1:B:189:PRO:HD2	1.70	0.71
1:A:359:GLY:O	1:A:364:ARG:HD3	1.90	0.71
1:B:64:MET:HE2	1:B:485:GLN:NE2	2.06	0.71
1:A:349:GLY:H	1:A:352:ASN:ND2	1.87	0.71
1:B:359:GLY:O	1:B:364:ARG:HD3	1.89	0.70
1:B:206:ASN:H	1:B:206:ASN:ND2	1.84	0.70
1:B:510:MET:CE	1:B:546:SER:H	1.97	0.70
1:B:128:ASN:HA	1:B:145:GLY:HA3	1.71	0.70
1:A:128:ASN:HA	1:A:145:GLY:HA3	1.72	0.70
1:A:138:ALA:CB	1:B:463:ARG:HH12	2.05	0.69
1:B:418:PRO:HG2	1:B:474:ASN:HD22	1.57	0.69
1:B:427:PRO:HA	1:B:501:GLY:O	1.93	0.69
1:A:427:PRO:HA	1:A:501:GLY:O	1.93	0.69
1:A:503:TYR:CZ	1:A:504:ARG:HD3	2.28	0.69
1:A:363:ILE:HD12	1:B:363:ILE:HD12	1.76	0.68
1:A:418:PRO:HG2	1:A:474:ASN:HD22	1.57	0.68
1:A:537:PRO:O	1:A:552:GLN:NE2	2.25	0.68
1:B:503:TYR:CZ	1:B:504:ARG:HD3	2.28	0.68
1:B:555:HIS:HD2	1:B:559:LYS:HE3	1.57	0.68
1:B:35:GLU:CD	1:B:35:GLU:H	2.01	0.68
1:A:297:ARG:HH21	1:A:432:SER:HA	1.59	0.68
1:B:537:PRO:O	1:B:552:GLN:NE2	2.25	0.68
1:B:194:TRP:O	1:B:197:HIS:HD2	1.76	0.68
1:A:390:PRO:HB2	1:A:392:ASN:OD1	1.94	0.68
1:A:555:HIS:HD2	1:A:559:LYS:HE3	1.57	0.68
1:A:35:GLU:CD	1:A:35:GLU:H	2.01	0.68
1:B:430:LYS:O	1:B:465:MET:HE2	1.95	0.67
1:B:297:ARG:HH21	1:B:432:SER:HA	1.58	0.67
1:A:194:TRP:O	1:A:197:HIS:HD2	1.76	0.67
1:B:390:PRO:HB2	1:B:392:ASN:OD1	1.94	0.67
1:A:430:LYS:O	1:A:465:MET:HE2	1.95	0.67
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASN:HA	3:B:600:FAD:H5'2	1.77	0.67
1:A:183:ARG:NH2	1:B:247:GLY:O	2.21	0.66
1:B:445:LYS:NZ	1:B:449:GLU:OE2	2.28	0.66
1:A:105:ASN:HA	3:A:600:FAD:H5'2	1.77	0.66
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.25	0.66
1:A:489:ARG:NH2	1:A:508:ALA:O	2.28	0.66
1:A:503:TYR:OH	4:A:602:EPT:O4	2.13	0.66
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.76	0.66
1:A:445:LYS:NZ	1:A:449:GLU:OE2	2.28	0.66
1:A:505:THR:HG21	1:A:513:ILE:CD1	2.25	0.66
1:A:463:ARG:HH12	1:B:138:ALA:CB	2.08	0.65
1:A:519:TRP:CZ3	1:B:211:ARG:HD3	2.32	0.65
1:B:489:ARG:NH2	1:B:508:ALA:O	2.28	0.65
1:A:142:VAL:HG12	1:A:143:GLU:O	1.97	0.65
1:A:275:GLY:HA3	1:A:359:GLY:O	1.96	0.65
1:B:275:GLY:HA3	1:B:359:GLY:O	1.96	0.65
1:A:9:PRO:HG2	1:A:12:LEU:HD21	1.79	0.65
1:A:196:MET:HE3	1:A:268:TRP:HE3	1.62	0.65
1:A:314:ILE:CD1	1:A:350:ARG:HG3	2.21	0.65
1:B:142:VAL:HG12	1:B:143:GLU:O	1.97	0.65
1:A:425:PHE:HB3	1:A:469:VAL:HB	1.78	0.64
1:A:59:ASP:OD2	1:A:62:HIS:HA	1.98	0.64
1:A:108:TYR:OH	4:A:602:EPT:H3	1.97	0.64
1:B:9:PRO:HG2	1:B:12:LEU:HD21	1.78	0.64
1:B:335:SER:HB3	1:B:337:GLU:OE1	1.98	0.64
1:A:271:PRO:HG3	1:B:301:LEU:HB3	1.78	0.64
1:A:335:SER:HB3	1:A:337:GLU:OE1	1.98	0.64
1:B:425:PHE:HB3	1:B:469:VAL:HB	1.78	0.64
1:B:59:ASP:OD2	1:B:62:HIS:HA	1.98	0.64
1:A:12:LEU:HB3	1:A:13:PRO:HD2	1.80	0.64
1:B:177:LEU:HD12	1:B:178:GLY:N	2.13	0.63
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.80	0.63
1:A:363:ILE:HD12	1:B:363:ILE:HG23	1.80	0.63
1:B:12:LEU:HB3	1:B:13:PRO:HD2	1.80	0.63
1:B:552:GLN:OE1	1:B:552:GLN:N	2.28	0.63
1:A:13:PRO:HG3	1:A:117:GLY:O	1.99	0.63
1:B:216:ALA:O	1:B:218:PRO:HD3	1.99	0.63
1:A:91:ASN:ND2	1:A:540:ILE:HG13	2.14	0.63
1:A:312:ARG:HH21	1:A:316:LEU:CD2	2.12	0.63
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.80	0.63
1:B:91:ASN:ND2	1:B:540:ILE:HG13	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HD12	1:A:178:GLY:N	2.14	0.62
1:A:195:MET:HE2	1:B:244:TYR:OH	1.99	0.62
1:A:363:ILE:HG23	1:B:363:ILE:HD12	1.81	0.62
1:A:416:TRP:HD1	1:A:417:LEU:CD1	2.12	0.62
1:A:552:GLN:OE1	1:A:552:GLN:N	2.28	0.62
1:B:425:PHE:HE2	1:B:427:PRO:HG3	1.62	0.62
1:A:216:ALA:O	1:A:218:PRO:HD3	1.98	0.62
1:B:196:MET:HE3	1:B:268:TRP:HE3	1.62	0.62
1:B:312:ARG:HH21	1:B:316:LEU:CD2	2.12	0.62
1:B:419:ASN:H	1:B:474:ASN:ND2	1.98	0.62
1:B:314:ILE:CG1	1:B:350:ARG:HA	2.30	0.62
1:A:419:ASN:H	1:A:474:ASN:ND2	1.98	0.62
1:B:416:TRP:HD1	1:B:417:LEU:CD1	2.12	0.62
1:B:497:ALA:C	1:B:498:ASN:HD22	2.07	0.62
1:A:306:GLN:NE2	1:A:358:TYR:H	1.98	0.62
1:B:13:PRO:HG3	1:B:117:GLY:O	1.99	0.62
1:B:306:GLN:NE2	1:B:358:TYR:H	1.98	0.61
1:B:9:PRO:HG2	1:B:12:LEU:CD2	2.29	0.61
1:B:314:ILE:CD1	1:B:350:ARG:HG3	2.21	0.61
1:B:128:ASN:HD22	1:B:145:GLY:HA3	1.65	0.61
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.29	0.61
1:A:9:PRO:HG2	1:A:12:LEU:CD2	2.29	0.61
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.29	0.61
1:A:314:ILE:CG1	1:A:350:ARG:HA	2.30	0.61
1:A:497:ALA:C	1:A:498:ASN:HD22	2.07	0.61
1:A:425:PHE:HE2	1:A:427:PRO:HG3	1.62	0.61
1:A:244:TYR:OH	1:B:195:MET:HE2	2.01	0.61
1:B:16:LEU:HD12	1:B:17:SER:H	1.67	0.60
1:B:28:ILE:HD13	1:B:89:LEU:HD12	1.83	0.60
1:A:16:LEU:HD12	1:A:17:SER:H	1.67	0.60
1:A:128:ASN:HD22	1:A:145:GLY:HA3	1.65	0.60
1:A:37:VAL:HG12	1:A:38:GLU:N	2.17	0.60
1:A:393:SER:OG	1:A:396:ARG:HG3	2.00	0.60
1:B:417:LEU:HB3	1:B:418:PRO:CD	2.32	0.60
1:A:248:PRO:HG3	1:B:257:SER:CB	2.30	0.60
1:B:21:PHE:CZ	1:B:25:ILE:HG13	2.38	0.59
1:A:28:ILE:HD13	1:A:89:LEU:HD12	1.83	0.59
1:A:310:THR:HG22	1:A:459:THR:HA	1.84	0.59
1:B:393:SER:OG	1:B:396:ARG:HG3	2.01	0.59
1:A:12:LEU:HB3	1:A:13:PRO:CD	2.33	0.59
1:B:471:ILE:HD12	1:B:471:ILE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ILE:N	1:A:471:ILE:HD12	2.18	0.58
1:B:35:GLU:OE1	1:B:35:GLU:N	2.30	0.58
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.32	0.58
1:A:102:ILE:HB	3:A:600:FAD:O2P	2.03	0.58
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.32	0.58
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.18	0.58
1:A:40:ILE:HD11	1:A:57:THR:CG2	2.32	0.58
1:A:429:ALA:HB2	1:A:439:GLN:NE2	2.18	0.58
1:A:495:CYS:HB3	1:A:500:TRP:HB2	1.85	0.58
1:B:7:PHE:O	1:B:18:LEU:HD11	2.04	0.58
1:B:310:THR:HG22	1:B:459:THR:HA	1.84	0.58
1:A:190:TYR:CD2	1:A:196:MET:HE2	2.39	0.58
1:B:37:VAL:HG12	1:B:38:GLU:N	2.17	0.58
1:B:495:CYS:HB3	1:B:500:TRP:HB2	1.85	0.58
1:B:102:ILE:HB	3:B:600:FAD:O2P	2.03	0.58
1:B:429:ALA:HB2	1:B:439:GLN:HE22	1.69	0.58
1:A:188:THR:HB	1:A:189:PRO:CD	2.33	0.58
1:B:312:ARG:NH1	1:B:394:VAL:HG11	2.19	0.58
1:B:190:TYR:CD2	1:B:196:MET:HE2	2.39	0.58
1:A:417:LEU:HB3	1:A:418:PRO:CD	2.32	0.58
1:B:188:THR:HB	1:B:189:PRO:CD	2.33	0.58
1:B:312:ARG:NH2	1:B:316:LEU:HG	2.18	0.58
1:B:343:ALA:HB1	1:B:348:LEU:O	2.04	0.58
1:A:21:PHE:CZ	1:A:25:ILE:HG13	2.38	0.57
1:B:12:LEU:HB3	1:B:13:PRO:CD	2.33	0.57
1:B:256:GLN:NE2	1:B:504:ARG:HG2	2.19	0.57
1:A:312:ARG:NH1	1:A:394:VAL:HG11	2.19	0.57
1:A:61:HIS:HD2	1:A:422:HIS:HD1	1.50	0.57
1:A:256:GLN:NE2	1:A:504:ARG:HG2	2.19	0.57
1:A:312:ARG:NH2	1:A:316:LEU:HG	2.18	0.57
1:A:429:ALA:HB2	1:A:439:GLN:HE22	1.69	0.57
1:B:314:ILE:HG12	1:B:350:ARG:HA	1.86	0.57
1:A:343:ALA:HB1	1:A:348:LEU:O	2.04	0.57
1:A:16:LEU:CD1	1:A:20:ASP:HB2	2.33	0.57
1:B:391:GLU:HA	1:B:396:ARG:HD2	1.87	0.57
1:B:46:ILE:HG22	1:B:46:ILE:O	2.05	0.57
1:B:151:LEU:HG	1:B:166:LEU:HD21	1.87	0.57
1:A:222:ARG:HG3	1:A:225:THR:HG23	1.86	0.57
1:A:35:GLU:OE1	1:A:35:GLU:N	2.30	0.56
1:A:391:GLU:HA	1:A:396:ARG:HD2	1.86	0.56
1:A:7:PHE:O	1:A:18:LEU:HD11	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HG12	1:A:350:ARG:HA	1.86	0.56
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.87	0.56
1:B:40:ILE:HD11	1:B:57:THR:CG2	2.32	0.56
1:B:82:ASP:O	1:B:86:ILE:HG13	2.06	0.56
1:B:417:LEU:CB	1:B:418:PRO:HD2	2.35	0.56
1:A:177:LEU:HD12	1:A:177:LEU:C	2.31	0.56
1:A:214:MET:HB2	1:A:239:ALA:HA	1.87	0.56
1:B:177:LEU:HD12	1:B:177:LEU:C	2.31	0.56
1:B:504:ARG:O	1:B:505:THR:HG23	2.06	0.56
1:A:46:ILE:O	1:A:46:ILE:HG22	2.05	0.56
1:A:82:ASP:O	1:A:86:ILE:HG13	2.06	0.56
1:A:171:LEU:HD11	3:A:600:FAD:HM72	1.88	0.56
1:A:277:GLN:HE21	1:A:277:GLN:HA	1.71	0.56
3:A:600:FAD:H51A	3:A:600:FAD:C8A	2.21	0.56
1:A:225:THR:C	1:A:228:LEU:HD13	2.31	0.55
1:B:202:VAL:HG12	1:B:262:VAL:HA	1.87	0.55
1:B:214:MET:HB2	1:B:239:ALA:HA	1.87	0.55
1:B:277:GLN:HE21	1:B:277:GLN:HA	1.71	0.55
1:B:434:GLU:OE1	1:B:434:GLU:HA	2.05	0.55
1:A:417:LEU:CB	1:A:418:PRO:HD2	2.35	0.55
1:A:151:LEU:HG	1:A:166:LEU:HD21	1.87	0.55
1:B:161:ARG:NH2	1:B:403:GLN:O	2.39	0.55
1:A:434:GLU:HA	1:A:434:GLU:OE1	2.05	0.55
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.87	0.55
1:B:222:ARG:HG3	1:B:225:THR:HG23	1.86	0.55
1:B:446:ARG:HD3	1:B:449:GLU:OE1	2.06	0.55
1:A:112:ALA:O	1:A:507:LEU:HD11	2.07	0.55
1:A:237:LYS:HE2	1:B:498:ASN:O	2.07	0.55
1:A:161:ARG:NH2	1:A:403:GLN:O	2.39	0.55
1:A:202:VAL:HG12	1:A:262:VAL:HA	1.87	0.55
1:A:446:ARG:HD3	1:A:449:GLU:OE1	2.06	0.55
1:A:398:ARG:NH2	4:A:602:EPT:H121	2.21	0.55
1:A:504:ARG:O	1:A:505:THR:HG23	2.06	0.55
1:B:225:THR:C	1:B:228:LEU:HD13	2.31	0.55
1:B:418:PRO:HB2	1:B:474:ASN:ND2	2.23	0.55
1:A:190:TYR:CE1	1:A:270:MET:HB2	2.43	0.54
1:A:281:ILE:HG23	1:A:381:VAL:CG2	2.37	0.54
1:B:171:LEU:HD11	3:B:600:FAD:HM72	1.88	0.54
1:A:418:PRO:HB2	1:A:474:ASN:ND2	2.22	0.54
1:B:16:LEU:CD1	1:B:20:ASP:HB2	2.33	0.54
1:B:112:ALA:O	1:B:507:LEU:HD11	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:HG23	1:B:381:VAL:CG2	2.37	0.54
1:A:337:GLU:OE1	1:A:337:GLU:N	2.29	0.54
1:B:9:PRO:HG3	1:B:21:PHE:CE1	2.42	0.54
1:B:190:TYR:CE1	1:B:270:MET:HB2	2.42	0.54
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.37	0.54
1:A:9:PRO:HG3	1:A:21:PHE:CE1	2.42	0.53
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.37	0.53
1:B:61:HIS:HD2	1:B:422:HIS:HD1	1.50	0.53
1:A:301:LEU:HB3	1:B:271:PRO:HG3	1.89	0.53
1:A:519:TRP:HB2	1:B:218:PRO:HG3	1.90	0.53
1:A:61:HIS:HD2	1:A:422:HIS:H	1.54	0.53
1:A:459:THR:OG1	1:A:466:HIS:HB2	2.09	0.53
1:B:309:PRO:HD2	1:B:460:VAL:HB	1.91	0.53
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.91	0.53
1:A:309:PRO:HD2	1:A:460:VAL:HB	1.91	0.53
1:B:459:THR:OG1	1:B:466:HIS:HB2	2.09	0.52
1:A:385:PHE:CB	1:A:386:PRO:HD2	2.33	0.52
1:B:324:LYS:HB2	1:B:416:TRP:CE2	2.45	0.52
1:A:324:LYS:HB2	1:A:416:TRP:CE2	2.45	0.52
1:B:52:MET:C	1:B:53:LYS:HG3	2.35	0.52
1:B:187:TYR:O	1:B:307:ASN:HB2	2.09	0.52
1:A:187:TYR:O	1:A:307:ASN:HB2	2.09	0.52
1:A:198:SER:O	1:A:240:HIS:HD2	1.92	0.52
1:A:16:LEU:HD12	1:A:17:SER:N	2.25	0.52
1:B:337:GLU:OE1	1:B:337:GLU:N	2.29	0.52
1:B:423:LEU:HB3	1:B:471:ILE:HB	1.92	0.52
1:A:286:ASP:HB2	1:A:350:ARG:CZ	2.40	0.51
1:B:198:SER:O	1:B:240:HIS:HD2	1.92	0.51
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.91	0.51
1:A:257:SER:CB	1:B:248:PRO:HG3	2.38	0.51
1:B:229:LYS:O	1:B:233:GLN:HG3	2.11	0.51
1:A:423:LEU:HB3	1:A:471:ILE:HB	1.92	0.51
1:B:16:LEU:HD11	1:B:20:ASP:HB3	1.92	0.51
1:B:286:ASP:HB2	1:B:350:ARG:CZ	2.40	0.51
3:B:600:FAD:H51A	3:B:600:FAD:C8A	2.21	0.51
1:A:171:LEU:HD22	1:A:411:LEU:HG	1.93	0.51
1:A:238:ILE:O	1:A:238:ILE:HG22	2.11	0.51
1:B:238:ILE:HG22	1:B:238:ILE:O	2.11	0.51
1:A:8:ARG:O	1:A:8:ARG:HG3	2.06	0.51
1:B:163:LYS:HE2	1:B:163:LYS:CA	2.36	0.51
1:B:171:LEU:HD22	1:B:411:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HA	1:A:163:LYS:CE	2.38	0.51
1:A:16:LEU:HD11	1:A:20:ASP:HB3	1.92	0.51
1:A:52:MET:C	1:A:53:LYS:HG3	2.35	0.51
1:A:139:TYR:CD1	1:A:139:TYR:C	2.89	0.51
1:A:457:THR:HG21	4:A:602:EPT:H133	1.91	0.51
1:A:105:ASN:HD22	3:A:600:FAD:H5'2	1.75	0.51
1:A:489:ARG:HH22	1:A:560:LEU:HD22	1.76	0.51
1:A:163:LYS:HE2	1:A:163:LYS:CA	2.36	0.50
1:A:229:LYS:O	1:A:233:GLN:HG3	2.11	0.50
1:B:16:LEU:HD12	1:B:17:SER:N	2.25	0.50
1:B:105:ASN:HD22	3:B:600:FAD:H5'2	1.75	0.50
1:B:318:ALA:O	1:B:322:GLY:N	2.42	0.50
1:A:386:PRO:HG2	1:A:387:GLU:N	2.27	0.50
1:A:386:PRO:HG2	1:A:387:GLU:H	1.76	0.50
1:B:386:PRO:HG2	1:B:387:GLU:N	2.27	0.50
1:A:253:LEU:O	1:A:257:SER:OG	2.29	0.50
1:A:74:ILE:HG22	1:A:75:VAL:N	2.27	0.50
1:B:307:ASN:O	1:B:309:PRO:HD3	2.12	0.50
1:B:386:PRO:HG2	1:B:387:GLU:H	1.76	0.50
1:B:489:ARG:HH22	1:B:560:LEU:HD22	1.76	0.50
1:A:142:VAL:HG13	1:A:146:VAL:CG2	2.41	0.50
1:A:314:ILE:HG13	1:A:350:ARG:O	2.11	0.50
1:B:61:HIS:HD2	1:B:422:HIS:H	1.54	0.50
1:A:444:LYS:O	1:A:448:GLN:HG2	2.11	0.50
1:B:418:PRO:CG	1:B:474:ASN:HD22	2.25	0.50
1:A:231:GLU:OE1	1:A:231:GLU:N	2.36	0.49
1:B:132:GLU:HG2	1:B:133:VAL:N	2.26	0.49
1:B:58:HIS:O	1:B:60:PRO:HD3	2.13	0.49
1:B:139:TYR:CD1	1:B:139:TYR:C	2.89	0.49
1:A:307:ASN:O	1:A:309:PRO:HD3	2.12	0.49
1:A:314:ILE:HD11	1:A:350:ARG:CA	2.40	0.49
1:B:385:PHE:CB	1:B:386:PRO:HD2	2.33	0.49
1:B:444:LYS:O	1:B:448:GLN:HG2	2.11	0.49
1:B:142:VAL:HG13	1:B:146:VAL:CG2	2.41	0.49
1:B:204:LEU:HB3	1:B:206:ASN:HD21	1.77	0.49
1:B:314:ILE:HG13	1:B:350:ARG:O	2.11	0.49
1:A:142:VAL:HG12	1:A:143:GLU:N	2.28	0.49
1:A:457:THR:OG1	4:A:602:EPT:H132	2.13	0.49
1:A:211:ARG:CD	1:B:519:TRP:CH2	2.92	0.49
1:B:426:SER:O	1:B:502:GLU:HA	2.13	0.49
1:B:163:LYS:HA	1:B:163:LYS:CE	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:O	1:B:164:LEU:HD23	2.14	0.48
1:A:418:PRO:CG	1:A:474:ASN:HD22	2.25	0.48
1:B:472:VAL:O	1:B:472:VAL:HG23	2.14	0.48
1:A:142:VAL:CG1	1:A:143:GLU:N	2.76	0.48
1:A:224:GLU:CD	1:A:224:GLU:H	2.22	0.48
1:B:74:ILE:HG22	1:B:75:VAL:N	2.27	0.48
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.46	0.48
1:A:132:GLU:HG2	1:A:133:VAL:N	2.26	0.48
1:B:27:ASP:O	1:B:31:ILE:HG13	2.13	0.48
1:B:168:VAL:HG23	1:B:168:VAL:O	2.14	0.48
1:B:553:TYR:CD1	1:B:553:TYR:N	2.82	0.48
1:A:27:ASP:O	1:A:31:ILE:HG13	2.13	0.48
1:B:267:ILE:HG22	1:B:268:TRP:O	2.14	0.48
1:A:58:HIS:O	1:A:60:PRO:HD3	2.13	0.48
1:B:230:PRO:HA	1:B:233:GLN:HG3	1.95	0.48
1:A:204:LEU:HB3	1:A:206:ASN:HD21	1.77	0.48
1:A:553:TYR:N	1:A:553:TYR:CD1	2.82	0.48
1:B:297:ARG:N	1:B:298:PRO:HD2	2.29	0.48
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.96	0.47
1:A:426:SER:O	1:A:502:GLU:HA	2.13	0.47
1:B:314:ILE:HD11	1:B:350:ARG:CA	2.40	0.47
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.70	0.47
1:A:280:LEU:HB2	1:A:395:LEU:HD22	1.96	0.47
1:A:363:ILE:CD1	1:B:363:ILE:HG23	2.45	0.47
1:A:230:PRO:HA	1:A:233:GLN:HG3	1.95	0.47
1:B:142:VAL:CG1	1:B:143:GLU:N	2.76	0.47
1:B:280:LEU:HB2	1:B:395:LEU:HD22	1.96	0.47
1:A:163:LYS:O	1:A:164:LEU:HD23	2.13	0.47
1:A:297:ARG:N	1:A:298:PRO:HD2	2.29	0.47
1:A:250:ILE:HD12	1:B:527:PHE:CE2	2.50	0.47
1:A:312:ARG:NH2	1:A:316:LEU:CD2	2.78	0.47
1:B:39:VAL:CG1	1:B:40:ILE:N	2.78	0.47
1:B:142:VAL:HG12	1:B:143:GLU:N	2.28	0.47
1:A:168:VAL:HG23	1:A:168:VAL:O	2.14	0.47
1:A:267:ILE:HG22	1:A:268:TRP:O	2.14	0.47
1:A:377:ALA:O	1:A:379:PRO:HD3	2.15	0.47
1:B:97:LEU:HA	1:B:97:LEU:HD23	1.35	0.47
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.96	0.47
1:B:386:PRO:CG	1:B:387:GLU:N	2.78	0.47
1:B:151:LEU:CD2	1:B:166:LEU:HD21	2.45	0.47
1:B:231:GLU:OE1	1:B:231:GLU:N	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LEU:HD22	1:B:351:TRP:CZ2	2.49	0.47
1:A:318:ALA:O	1:A:322:GLY:N	2.42	0.46
1:A:151:LEU:CD2	1:A:166:LEU:HD21	2.45	0.46
1:A:39:VAL:CG1	1:A:40:ILE:N	2.78	0.46
1:A:101:SER:O	1:A:102:ILE:HD13	2.16	0.46
1:A:170:ASP:OD2	4:A:602:EPT:H112	2.15	0.46
1:A:472:VAL:HG23	1:A:472:VAL:O	2.13	0.46
1:B:377:ALA:O	1:B:379:PRO:HD3	2.15	0.46
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.49	0.46
1:A:487:LEU:HD12	1:A:487:LEU:O	2.16	0.46
1:B:105:ASN:HD21	1:B:504:ARG:HH21	1.63	0.46
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.70	0.46
1:B:503:TYR:CZ	1:B:504:ARG:CD	2.97	0.46
1:A:237:LYS:HE3	1:B:500:TRP:NE1	2.30	0.46
1:A:315:LEU:HD22	1:A:416:TRP:CH2	2.51	0.46
1:A:559:LYS:O	1:A:560:LEU:HB2	2.16	0.46
1:B:101:SER:O	1:B:102:ILE:HD13	2.16	0.46
1:A:259:MET:CE	1:A:535:VAL:HG21	2.46	0.46
1:A:386:PRO:CG	1:A:387:GLU:N	2.78	0.46
1:A:399:ASP:O	1:A:403:GLN:HG2	2.16	0.46
1:B:399:ASP:O	1:B:403:GLN:HG2	2.16	0.46
1:B:259:MET:CE	1:B:535:VAL:HG21	2.46	0.46
1:B:321:LEU:HA	1:B:321:LEU:HD23	1.55	0.46
3:B:600:FAD:N1	3:B:600:FAD:O3'	2.39	0.46
1:A:102:ILE:HD13	1:A:102:ILE:HA	1.52	0.45
1:B:312:ARG:NH2	1:B:316:LEU:CD2	2.78	0.45
1:B:487:LEU:C	1:B:487:LEU:HD12	2.41	0.45
1:A:249:TYR:O	1:B:252:GLY:HA3	2.15	0.45
1:B:224:GLU:CD	1:B:224:GLU:H	2.22	0.45
1:B:351:TRP:O	1:B:352:ASN:ND2	2.49	0.45
1:A:190:TYR:CD1	1:A:270:MET:HB2	2.52	0.45
1:A:363:ILE:HD13	1:B:363:ILE:HD13	1.99	0.45
1:B:201:GLU:C	1:B:202:VAL:HG13	2.41	0.45
1:B:256:GLN:HE22	1:B:504:ARG:HG2	1.81	0.45
1:B:315:LEU:HD22	1:B:416:TRP:CH2	2.51	0.45
1:A:351:TRP:O	1:A:352:ASN:ND2	2.49	0.45
1:A:387:GLU:C	1:A:389:THR:H	2.24	0.45
1:A:519:TRP:CA	1:B:218:PRO:HG3	2.45	0.45
3:A:600:FAD:N1	3:A:600:FAD:O3'	2.39	0.45
1:A:166:LEU:HD23	1:A:269:LEU:HD22	1.98	0.45
1:A:386:PRO:CG	1:A:387:GLU:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:HG12	1:B:383:PHE:CD2	2.52	0.45
1:B:166:LEU:HD23	1:B:269:LEU:HD22	1.98	0.45
1:B:190:TYR:CD1	1:B:270:MET:HB2	2.52	0.45
1:B:204:LEU:CB	1:B:206:ASN:HD21	2.30	0.45
1:A:105:ASN:HD21	1:A:504:ARG:HH21	1.62	0.45
1:B:8:ARG:O	1:B:8:ARG:HG3	2.06	0.45
1:B:387:GLU:C	1:B:389:THR:H	2.24	0.45
1:A:324:LYS:HG3	1:A:416:TRP:CZ2	2.51	0.45
1:A:435:ASP:OD1	1:B:237:LYS:NZ	2.49	0.45
1:A:519:TRP:CH2	1:B:211:ARG:CD	2.97	0.45
1:B:324:LYS:HG3	1:B:416:TRP:CZ2	2.51	0.45
1:B:333:PRO:HA	1:B:453:ASP:OD1	2.17	0.45
1:B:386:PRO:CG	1:B:387:GLU:H	2.30	0.45
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.34	0.44
1:A:165:TRP:N	1:A:165:TRP:CD1	2.85	0.44
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.17	0.44
1:A:256:GLN:HE22	1:A:504:ARG:HG2	1.81	0.44
1:A:469:VAL:HG12	1:A:471:ILE:HD12	1.99	0.44
1:A:503:TYR:CZ	1:A:504:ARG:CD	2.97	0.44
1:B:74:ILE:CG2	1:B:75:VAL:N	2.80	0.44
1:B:94:SER:HA	1:B:540:ILE:HD11	1.99	0.44
1:A:8:ARG:HA	1:A:9:PRO:HD3	1.70	0.44
1:A:74:ILE:CG2	1:A:75:VAL:N	2.80	0.44
1:A:281:ILE:HG12	1:A:383:PHE:CD2	2.52	0.44
1:A:333:PRO:HA	1:A:453:ASP:OD1	2.17	0.44
1:B:487:LEU:HD12	1:B:487:LEU:O	2.16	0.44
1:A:291:GLN:O	1:A:295:ILE:HG13	2.17	0.44
1:A:389:THR:HB	1:A:390:PRO:HD2	2.00	0.44
1:A:471:ILE:N	1:A:471:ILE:CD1	2.80	0.44
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.17	0.44
1:A:252:GLY:HA3	1:B:249:TYR:O	2.17	0.44
1:A:363:ILE:HG23	1:B:363:ILE:CD1	2.47	0.44
1:A:465:MET:HE3	1:A:465:MET:HB2	1.86	0.44
1:B:469:VAL:HG12	1:B:471:ILE:HD12	1.99	0.44
1:A:201:GLU:C	1:A:202:VAL:HG13	2.41	0.44
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.55	0.44
1:B:61:HIS:CD2	1:B:422:HIS:N	2.76	0.44
1:A:61:HIS:CD2	1:A:422:HIS:ND1	2.73	0.44
1:A:285:LYS:HG2	1:A:286:ASP:N	2.32	0.44
1:B:559:LYS:O	1:B:560:LEU:HB2	2.16	0.44
1:A:185:VAL:HG12	1:A:186:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:CB	1:A:206:ASN:HD21	2.30	0.44
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.46	0.44
1:A:267:ILE:HD12	1:A:267:ILE:HG23	1.59	0.44
1:A:318:ALA:O	1:A:321:LEU:N	2.50	0.44
1:A:28:ILE:HD13	1:A:89:LEU:CD1	2.48	0.44
1:B:291:GLN:O	1:B:295:ILE:HG13	2.17	0.44
1:A:398:ARG:HH21	4:A:602:EPT:H121	1.82	0.44
1:A:457:THR:HG21	4:A:602:EPT:H132	1.94	0.44
1:B:312:ARG:NH2	1:B:316:LEU:CG	2.81	0.44
1:B:13:PRO:HG2	1:B:95:PHE:CZ	2.53	0.43
1:B:285:LYS:HG2	1:B:286:ASP:N	2.32	0.43
1:B:349:GLY:CA	1:B:352:ASN:HD21	2.30	0.43
1:B:389:THR:HB	1:B:390:PRO:HD2	1.99	0.43
1:A:13:PRO:HG2	1:A:95:PHE:CZ	2.53	0.43
1:A:487:LEU:HD12	1:A:487:LEU:C	2.42	0.43
1:B:204:LEU:HB3	1:B:206:ASN:ND2	2.33	0.43
1:A:363:ILE:CD1	1:B:363:ILE:HD12	2.47	0.43
1:A:527:PHE:CE2	1:B:250:ILE:HD12	2.52	0.43
1:B:200:MET:HE2	1:B:200:MET:HB3	1.76	0.43
1:B:318:ALA:O	1:B:321:LEU:N	2.50	0.43
1:A:405:ILE:HA	1:A:406:PRO:HD2	1.82	0.43
1:A:439:GLN:O	1:A:442:VAL:HG12	2.19	0.43
1:B:9:PRO:CG	1:B:21:PHE:CZ	2.98	0.43
1:B:283:LEU:HD13	1:B:292:ALA:HB2	2.01	0.43
1:A:94:SER:HA	1:A:540:ILE:HD11	1.99	0.43
1:A:200:MET:HE2	1:A:200:MET:HB3	1.76	0.43
1:A:312:ARG:NH2	1:A:316:LEU:CG	2.81	0.43
1:B:39:VAL:HG12	1:B:40:ILE:N	2.32	0.43
1:A:182:GLU:O	1:A:183:ARG:HB2	2.19	0.43
1:B:165:TRP:CD1	1:B:165:TRP:N	2.85	0.43
1:B:389:THR:O	1:B:396:ARG:NH2	2.46	0.43
1:A:204:LEU:HB3	1:A:206:ASN:ND2	2.33	0.43
1:B:242:PHE:HA	1:B:243:PRO:HD3	1.55	0.43
1:B:439:GLN:O	1:B:442:VAL:HG12	2.19	0.43
1:A:280:LEU:CB	1:A:395:LEU:HD22	2.48	0.43
1:B:182:GLU:O	1:B:183:ARG:HB2	2.19	0.43
1:A:37:VAL:CG1	1:A:38:GLU:N	2.82	0.43
1:A:323:ASP:OD1	1:A:324:LYS:N	2.52	0.43
1:A:424:PHE:CD1	4:A:602:EPT:H2	2.54	0.43
1:B:64:MET:CE	1:B:485:GLN:NE2	2.79	0.43
1:B:253:LEU:O	1:B:257:SER:OG	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HG12	1:A:40:ILE:N	2.33	0.43
1:A:349:GLY:CA	1:A:352:ASN:HD21	2.30	0.43
1:B:471:ILE:N	1:B:471:ILE:CD1	2.80	0.43
1:A:170:ASP:OD2	4:A:602:EPT:H101	2.18	0.42
1:B:465:MET:HE3	1:B:465:MET:HB2	1.86	0.42
1:A:281:ILE:CG2	1:A:381:VAL:CG2	2.97	0.42
1:B:171:LEU:HD13	1:B:411:LEU:CD2	2.45	0.42
1:B:185:VAL:HG12	1:B:186:GLY:N	2.33	0.42
1:A:289:LEU:O	1:A:293:VAL:HG23	2.20	0.42
1:A:541:ILE:HD13	1:A:541:ILE:HG21	1.85	0.42
1:B:206:ASN:HD22	1:B:206:ASN:N	2.07	0.42
1:B:323:ASP:OD1	1:B:324:LYS:N	2.52	0.42
1:A:391:GLU:HA	1:A:396:ARG:CD	2.48	0.42
1:B:391:GLU:HA	1:B:396:ARG:CD	2.48	0.42
1:B:445:LYS:HD3	1:B:449:GLU:HG3	2.01	0.42
1:A:61:HIS:CD2	1:A:422:HIS:N	2.76	0.42
1:A:154:TYR:CD1	1:A:154:TYR:C	2.98	0.42
1:A:305:LEU:HA	1:A:305:LEU:HD23	1.75	0.42
1:A:445:LYS:HD3	1:A:449:GLU:HG3	2.02	0.42
1:A:543:PRO:HB3	1:A:550:PRO:HG2	2.02	0.42
1:B:68:TYR:CD1	1:B:68:TYR:C	2.98	0.42
1:B:102:ILE:HD13	1:B:102:ILE:HA	1.52	0.42
1:B:171:LEU:CD1	1:B:411:LEU:CD2	2.98	0.42
1:B:267:ILE:HD12	1:B:267:ILE:HG23	1.59	0.42
1:A:90:ALA:O	1:A:94:SER:N	2.53	0.42
1:A:283:LEU:HD13	1:A:292:ALA:HB2	2.01	0.42
1:A:389:THR:O	1:A:396:ARG:NH2	2.46	0.42
1:B:61:HIS:CD2	1:B:422:HIS:ND1	2.73	0.42
1:B:204:LEU:CB	1:B:206:ASN:ND2	2.83	0.42
1:B:385:PHE:CB	1:B:386:PRO:CD	2.96	0.42
1:A:48:ASP:OD1	1:A:58:HIS:NE2	2.53	0.42
1:A:171:LEU:CD1	1:A:411:LEU:CD2	2.98	0.42
1:A:325:ARG:C	1:A:327:TYR:H	2.28	0.42
1:B:63:VAL:HG11	1:B:423:LEU:HD22	2.02	0.42
1:B:154:TYR:C	1:B:154:TYR:CD1	2.97	0.42
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.48	0.42
1:B:496:ALA:C	1:B:498:ASN:H	2.27	0.42
1:A:436:ALA:HB2	1:A:465:MET:HE1	2.01	0.42
1:A:508:ALA:C	1:A:509:PHE:CG	2.98	0.42
1:A:204:LEU:CB	1:A:206:ASN:ND2	2.83	0.42
1:A:496:ALA:C	1:A:498:ASN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:CG	1:B:166:LEU:HD21	2.50	0.42
1:B:325:ARG:C	1:B:327:TYR:H	2.28	0.42
1:B:418:PRO:HG2	1:B:474:ASN:ND2	2.31	0.42
1:B:28:ILE:HD13	1:B:89:LEU:CD1	2.48	0.41
1:B:201:GLU:OE1	1:B:211:ARG:HD2	2.20	0.41
1:B:297:ARG:HH21	1:B:432:SER:CA	2.31	0.41
1:B:427:PRO:HD2	1:B:467:HIS:O	2.20	0.41
1:B:555:HIS:HB3	1:B:559:LYS:HE3	2.02	0.41
1:A:68:TYR:CD1	1:A:68:TYR:C	2.98	0.41
1:A:131:LEU:O	1:A:132:GLU:HB2	2.21	0.41
1:A:190:TYR:CE2	1:A:196:MET:HE2	2.55	0.41
1:A:363:ILE:CD1	1:B:363:ILE:CD1	2.97	0.41
1:B:37:VAL:CG1	1:B:38:GLU:N	2.82	0.41
1:B:402:MET:HE3	1:B:402:MET:HB2	1.95	0.41
1:B:445:LYS:NZ	1:B:449:GLU:CD	2.79	0.41
1:B:553:TYR:HB3	1:B:558:TRP:CD1	2.56	0.41
1:A:170:ASP:CG	4:A:602:EPT:H101	2.45	0.41
1:A:201:GLU:OE1	1:A:211:ARG:HD2	2.20	0.41
1:A:427:PRO:HD2	1:A:467:HIS:O	2.20	0.41
1:A:527:PHE:CZ	1:A:531:LEU:HD11	2.55	0.41
1:B:8:ARG:HA	1:B:9:PRO:HD3	1.70	0.41
1:B:48:ASP:OD1	1:B:58:HIS:NE2	2.53	0.41
1:B:289:LEU:O	1:B:293:VAL:HG23	2.20	0.41
1:B:405:ILE:HA	1:B:406:PRO:HD2	1.82	0.41
1:A:402:MET:HE3	1:A:402:MET:HB2	1.95	0.41
1:B:281:ILE:CG2	1:B:381:VAL:CG2	2.97	0.41
1:B:527:PHE:CZ	1:B:531:LEU:HD11	2.54	0.41
1:A:314:ILE:HD11	1:A:350:ARG:CB	2.51	0.41
1:A:471:ILE:O	1:A:471:ILE:HG22	2.21	0.41
1:B:21:PHE:CD1	1:B:21:PHE:C	2.99	0.41
1:B:105:ASN:HD21	1:B:504:ARG:NH2	2.19	0.41
1:B:543:PRO:HB3	1:B:550:PRO:HG2	2.02	0.41
1:A:424:PHE:CE1	4:A:602:EPT:H2	2.55	0.41
1:A:427:PRO:HG2	1:A:439:GLN:OE1	2.21	0.41
3:A:600:FAD:N1	3:A:600:FAD:C3'	2.84	0.41
1:B:188:THR:CB	1:B:189:PRO:CD	2.96	0.41
1:B:457:THR:HG22	1:B:458:PHE:O	2.21	0.41
1:B:508:ALA:C	1:B:509:PHE:CG	2.98	0.41
3:B:600:FAD:N1	3:B:600:FAD:C3'	2.84	0.41
1:A:151:LEU:CG	1:A:166:LEU:HD21	2.50	0.41
1:A:171:LEU:HD13	1:A:411:LEU:CD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:HD13	1:A:472:VAL:HG23	2.02	0.41
1:A:553:TYR:HB3	1:A:558:TRP:CD1	2.56	0.41
1:B:90:ALA:O	1:B:94:SER:N	2.53	0.41
1:B:209:LEU:HD23	1:B:209:LEU:HA	1.94	0.41
1:A:63:VAL:HG11	1:A:423:LEU:HD22	2.02	0.41
1:A:250:ILE:HD13	1:A:250:ILE:HG21	1.83	0.41
1:A:321:LEU:HA	1:A:321:LEU:HD23	1.55	0.41
1:A:445:LYS:NZ	1:A:449:GLU:CD	2.78	0.41
1:A:457:THR:HG22	1:A:458:PHE:O	2.21	0.41
3:A:600:FAD:H5'2	3:A:600:FAD:H2'	1.89	0.41
1:B:151:LEU:CD2	1:B:166:LEU:CD2	2.99	0.41
1:B:190:TYR:CE2	1:B:196:MET:HE2	2.56	0.41
1:B:418:PRO:HB2	1:B:474:ASN:HD22	1.86	0.41
1:B:436:ALA:HB2	1:B:465:MET:HE1	2.01	0.41
1:B:541:ILE:HG21	1:B:541:ILE:HD13	1.85	0.41
1:A:128:ASN:HA	1:A:128:ASN:HD22	1.67	0.41
1:A:151:LEU:CD2	1:A:166:LEU:CD2	2.99	0.41
1:A:555:HIS:HB3	1:A:559:LYS:HE3	2.02	0.41
1:B:128:ASN:HD22	1:B:145:GLY:CA	2.31	0.41
1:B:284:PRO:HG2	1:B:288:ASP:OD2	2.21	0.41
1:B:417:LEU:HD13	1:B:472:VAL:HG23	2.02	0.41
1:B:427:PRO:HG2	1:B:439:GLN:OE1	2.21	0.41
1:A:418:PRO:HG2	1:A:474:ASN:ND2	2.31	0.40
1:B:71:ALA:HB2	1:B:120:VAL:HG23	2.04	0.40
1:B:192:ASP:CG	1:B:195:MET:HB2	2.46	0.40
1:B:348:LEU:HA	1:B:348:LEU:HD23	1.83	0.40
1:B:422:HIS:CD2	1:B:424:PHE:CZ	3.09	0.40
1:B:471:ILE:O	1:B:471:ILE:HG22	2.21	0.40
1:A:9:PRO:CG	1:A:21:PHE:CZ	2.98	0.40
1:A:21:PHE:CD1	1:A:21:PHE:C	2.99	0.40
1:A:64:MET:CE	1:A:485:GLN:NE2	2.79	0.40
1:A:72:SER:HB3	1:A:117:GLY:O	2.22	0.40
1:A:121:LEU:HD12	1:A:121:LEU:N	2.36	0.40
1:A:325:ARG:O	1:A:327:TYR:N	2.54	0.40
1:A:141:VAL:C	1:A:142:VAL:HG23	2.46	0.40
1:A:192:ASP:CG	1:A:195:MET:HB2	2.46	0.40
1:A:12:LEU:CB	1:A:13:PRO:CD	2.97	0.40
1:A:217:LEU:HD12	1:B:516:THR:O	2.21	0.40
1:A:284:PRO:HG2	1:A:288:ASP:OD2	2.21	0.40
1:A:468:ILE:HG21	4:A:602:EPT:C2	2.50	0.40
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:HB3	1:B:117:GLY:O	2.22	0.40
1:B:100:ILE:O	1:B:100:ILE:HG13	2.20	0.40
1:B:102:ILE:HG22	1:B:104:ARG:H	1.87	0.40
1:B:297:ARG:CB	1:B:298:PRO:CD	2.98	0.40
1:B:312:ARG:HG2	1:B:457:THR:CG2	2.51	0.40
1:B:325:ARG:O	1:B:327:TYR:N	2.54	0.40
1:A:189:PRO:HD3	1:A:358:TYR:CZ	2.57	0.40
1:A:503:TYR:CD2	1:A:504:ARG:HG3	2.57	0.40
1:B:141:VAL:C	1:B:142:VAL:HG23	2.46	0.40
1:B:189:PRO:HD3	1:B:358:TYR:CZ	2.56	0.40
1:B:238:ILE:HD12	1:B:238:ILE:HG23	1.81	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	553/560 (99%)	503 (91%)	39 (7%)	11 (2%)	6	27
1	B	553/560 (99%)	504 (91%)	38 (7%)	11 (2%)	6	27
All	All	1106/1120 (99%)	1007 (91%)	77 (7%)	22 (2%)	6	27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	388	ASP
1	A	418	PRO
1	A	475	LYS
1	B	46	ILE
1	B	326	SER
1	B	388	ASP

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Mol	Chain	Res	Type
1	B	418	PRO
1	B	475	LYS
1	A	105	ASN
1	A	326	SER
1	A	391	GLU
1	A	497	ALA
1	A	559	LYS
1	B	105	ASN
1	B	391	GLU
1	B	497	ALA
1	B	559	LYS
1	A	49	GLY
1	A	170	ASP
1	B	49	GLY
1	B	170	ASP

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	475/482 (98%)	460 (97%)	15 (3%)	34	60
1	B	475/482 (98%)	460 (97%)	15 (3%)	34	60
All	All	950/964 (98%)	920 (97%)	30 (3%)	34	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	114	ARG
1	A	115	VAL
1	A	128	ASN
1	A	149	HIS
1	A	163	LYS
1	A	177	LEU
1	A	189	PRO

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	224	GLU
1	A	277	GLN
1	A	360	PRO
1	A	391	GLU
1	A	471	ILE
1	A	560	LEU
1	B	105	ASN
1	B	114	ARG
1	B	115	VAL
1	B	128	ASN
1	B	149	HIS
1	B	163	LYS
1	B	177	LEU
1	B	189	PRO
1	B	206	ASN
1	B	224	GLU
1	B	277	GLN
1	B	360	PRO
1	B	391	GLU
1	B	471	ILE
1	B	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	91	ASN
1	A	105	ASN
1	A	128	ASN
1	A	152	HIS
1	A	158	ASN
1	A	197	HIS
1	A	206	ASN
1	A	240	HIS
1	A	277	GLN
1	A	306	GLN
1	A	352	ASN
1	A	485	GLN
1	A	498	ASN
1	A	520	ASN
1	A	528	ASN

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Mol	Chain	Res	Type
1	B	61	HIS
1	B	91	ASN
1	B	105	ASN
1	B	128	ASN
1	B	152	HIS
1	B	158	ASN
1	B	197	HIS
1	B	206	ASN
1	B	240	HIS
1	B	277	GLN
1	B	306	GLN
1	B	352	ASN
1	B	485	GLN
1	B	498	ASN
1	B	520	ASN
1	B	528	ASN
1	B	555	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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
4	EPT	A	602	-	14,14,14	1.29	1 (7%)	16,16,16	1.75	5 (31%)
3	FAD	A	600	1	58,58,58	0.95	5 (8%)	85,89,89	0.77	1 (1%)
3	FAD	B	600	1	58,58,58	0.94	5 (8%)	85,89,89	0.76	1 (1%)

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
4	EPT	A	602	-	-	5/7/7/7	0/1/1/1
3	FAD	A	600	1	-	4/34/50/50	0/6/6/6
3	FAD	B	600	1	-	4/34/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	FAD	P-O3P	3.50	1.63	1.59
3	A	600	FAD	P-O3P	3.37	1.63	1.59
3	A	600	FAD	PA-O3P	3.34	1.63	1.59
3	B	600	FAD	PA-O3P	3.24	1.63	1.59
4	A	602	EPT	C5-C4	-3.16	1.33	1.39
3	A	600	FAD	C9A-N10	-2.35	1.37	1.41
3	B	600	FAD	C5X-N5	-2.34	1.35	1.39
3	A	600	FAD	C5X-N5	-2.32	1.35	1.39
3	B	600	FAD	C9A-N10	-2.31	1.37	1.41
3	A	600	FAD	C4X-N5	2.03	1.35	1.30
3	B	600	FAD	C4X-N5	2.02	1.35	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	EPT	C6-C5-C4	3.72	123.81	119.88
4	A	602	EPT	C9-C8-C7	-3.02	101.14	113.74
4	A	602	EPT	C2-C3-C4	-2.85	116.86	119.88
4	A	602	EPT	C5-C6-C1	-2.84	117.27	121.00
4	A	602	EPT	C3-C2-C1	2.48	124.25	121.00
3	A	600	FAD	C4-N3-C2	-2.42	121.34	125.64
3	B	600	FAD	C4-N3-C2	-2.41	121.37	125.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

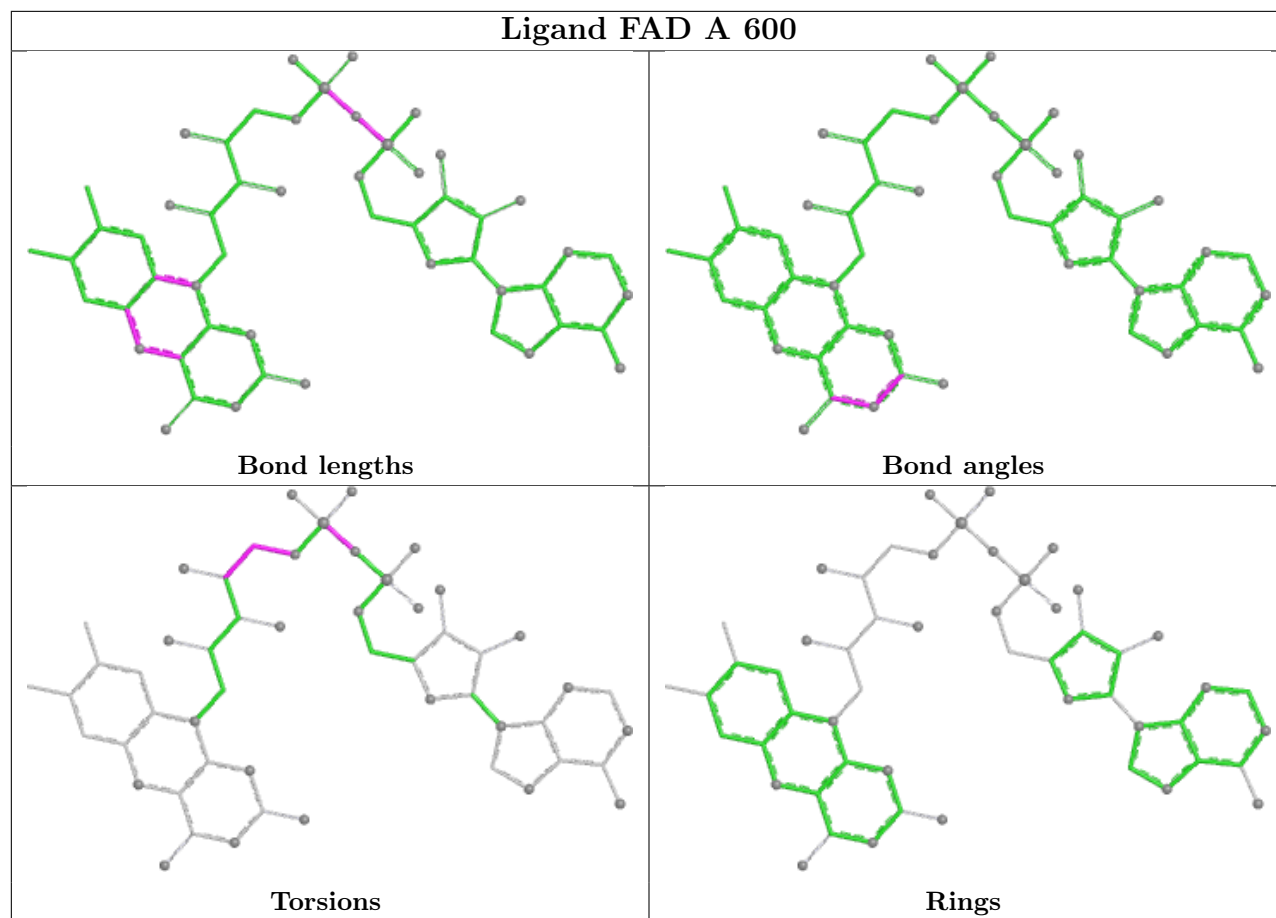
Mol	Chain	Res	Type	Atoms
4	A	602	EPT	C11-C10-C9-C8
3	A	600	FAD	C3'-C4'-C5'-O5'
3	B	600	FAD	C3'-C4'-C5'-O5'
3	A	600	FAD	C4'-C5'-O5'-P
3	B	600	FAD	C4'-C5'-O5'-P
4	A	602	EPT	C10-C11-C12-C13
3	B	600	FAD	O4'-C4'-C5'-O5'
4	A	602	EPT	C6-C1-C7-C8
4	A	602	EPT	C9-C10-C11-C12
3	A	600	FAD	O4'-C4'-C5'-O5'
3	A	600	FAD	PA-O3P-P-O2P
3	B	600	FAD	PA-O3P-P-O2P
4	A	602	EPT	C2-C1-C7-C8

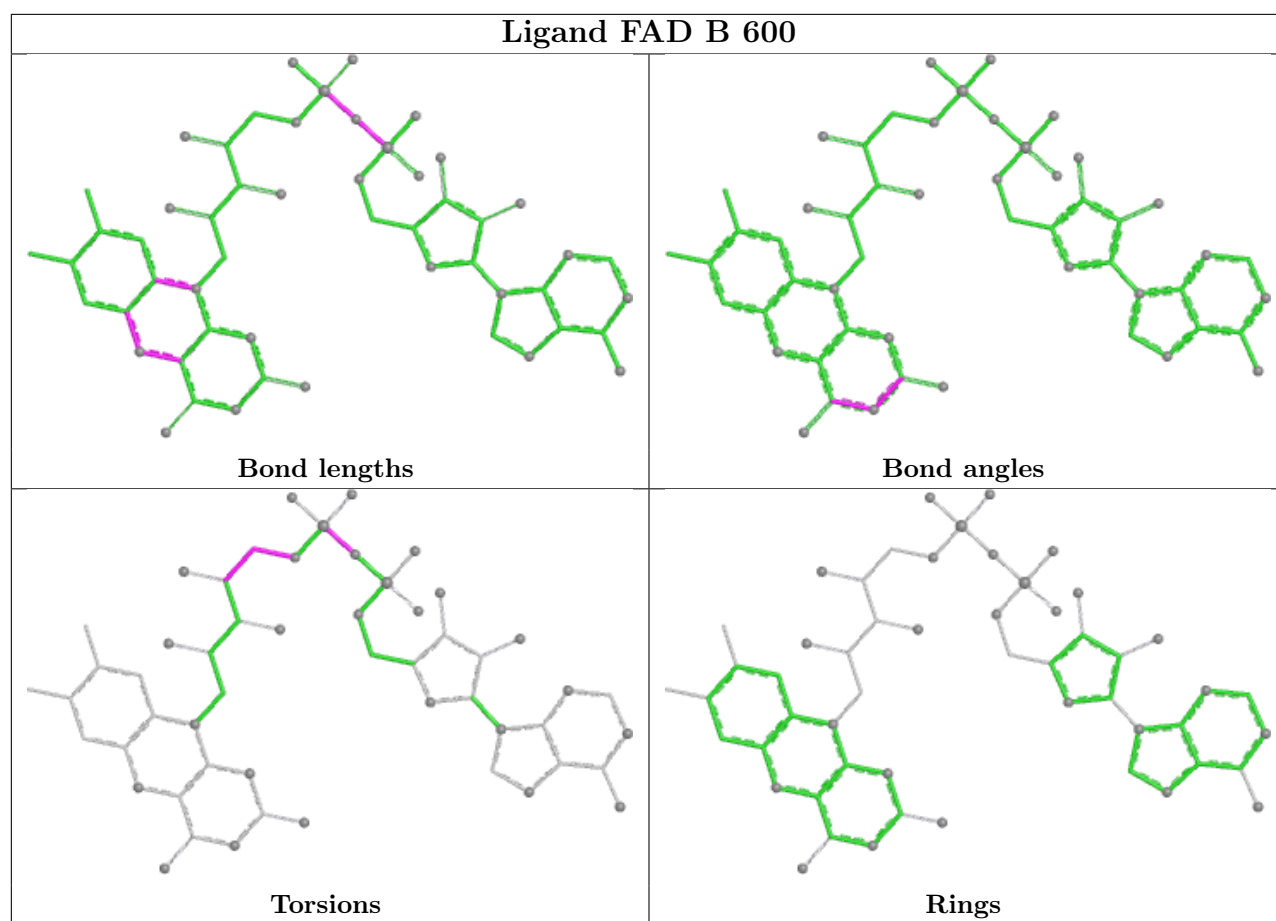
There are no ring outliers.

3 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	EPT	14	0
3	A	600	FAD	9	0
3	B	600	FAD	8	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.