



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:16 PM UTC

PDB ID : 1VAO / pdb_00001vao
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.50 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

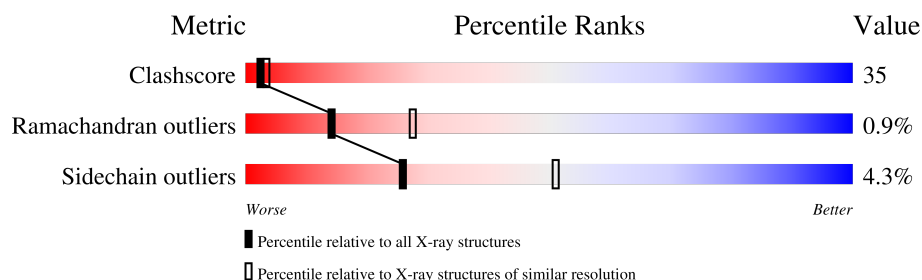
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9134 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			
1	B	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

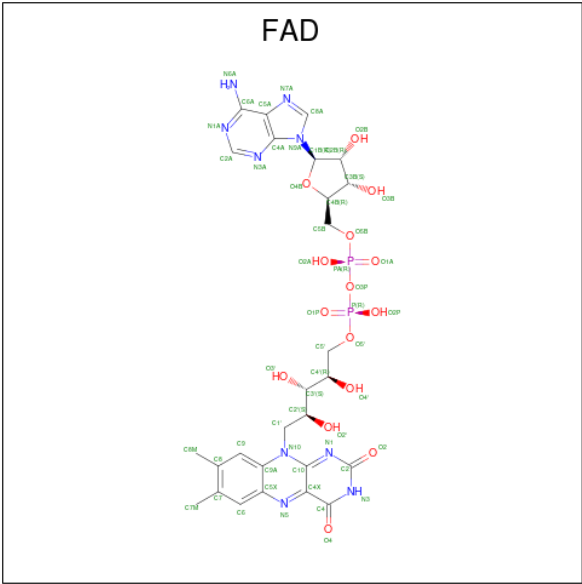


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

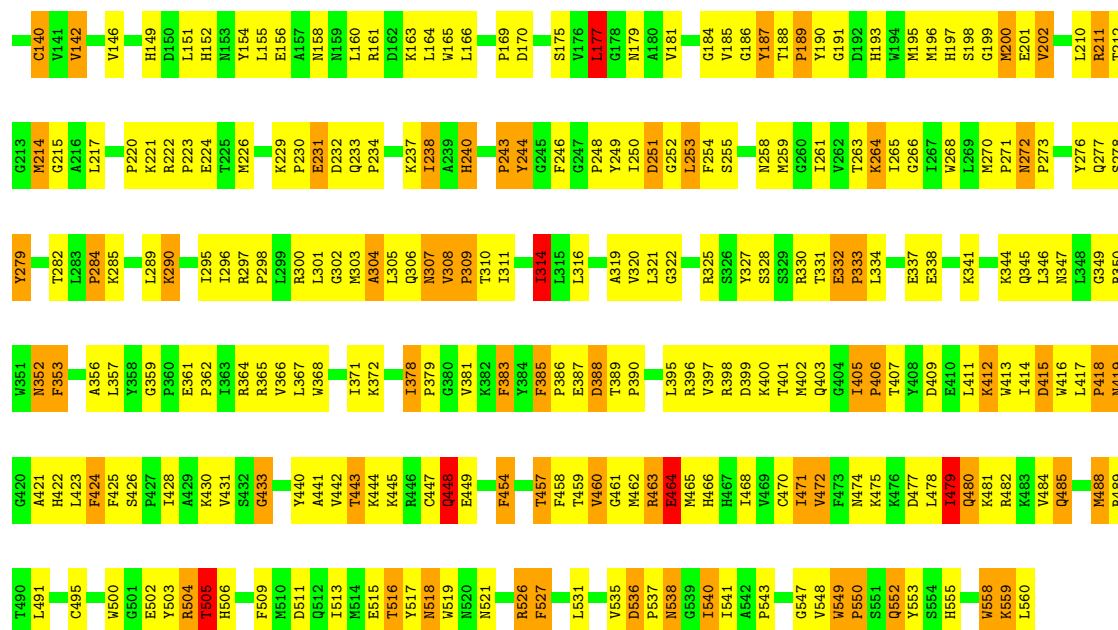
- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	150	Total O 150 150	0	0



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	130.24Å 130.24Å 133.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.9 (30.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.88	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: ACT, CL, 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	0.93	2/4470 (0.0%)	2.18	208/6075 (3.4%)
1	B	0.93	2/4470 (0.0%)	2.18	208/6075 (3.4%)
All	All	0.93	4/8940 (0.0%)	2.18	416/12150 (3.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0
1	B	2	0
All	All	4	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	PHE	CD1-CE1	5.10	1.53	1.38
1	A	7	PHE	CD1-CE1	5.10	1.53	1.38
1	A	296	ILE	CA-CB	-5.09	1.48	1.54
1	B	296	ILE	CA-CB	-5.08	1.48	1.54

All (416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	PHE	N-CA-C	18.91	134.09	111.02
1	A	7	PHE	N-CA-C	18.88	134.06	111.02
1	A	304	ALA	N-CA-C	-15.54	94.42	111.36
1	B	304	ALA	N-CA-C	-15.50	94.47	111.36
1	B	187	TYR	N-CA-C	15.24	132.06	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	TYR	N-CA-C	15.22	132.03	113.16
1	B	129	ARG	N-CA-C	14.68	133.40	110.20
1	A	129	ARG	N-CA-C	14.67	133.38	110.20
1	A	518	ASN	N-CA-C	14.66	129.35	112.93
1	B	518	ASN	N-CA-C	14.65	129.34	112.93
1	B	244	TYR	N-CA-C	13.70	126.22	111.28
1	A	244	TYR	N-CA-C	13.69	126.21	111.28
1	B	62	HIS	N-CA-C	11.61	127.25	109.96
1	A	62	HIS	N-CA-C	11.57	127.20	109.96
1	A	558	TRP	N-CA-C	11.39	128.28	112.45
1	B	558	TRP	N-CA-C	11.36	128.25	112.45
1	B	464	GLU	N-CA-CB	-10.88	94.69	111.56
1	B	505	THR	CB-CA-C	-10.87	89.52	111.91
1	A	464	GLU	N-CA-CB	-10.86	94.73	111.56
1	A	505	THR	CB-CA-C	-10.85	89.55	111.91
1	A	415	ASP	N-CA-C	10.63	125.84	113.19
1	B	415	ASP	N-CA-C	10.61	125.82	113.19
1	A	8	ARG	CB-CA-C	-10.60	98.47	110.98
1	B	8	ARG	CB-CA-C	-10.55	98.53	110.98
1	B	128	ASN	CB-CA-C	-10.51	90.14	110.11
1	A	128	ASN	CB-CA-C	-10.51	90.15	110.11
1	A	25	ILE	CB-CA-C	10.38	125.64	112.04
1	B	25	ILE	CB-CA-C	10.35	125.59	112.04
1	A	112	ALA	CA-C-N	9.97	130.75	119.99
1	A	112	ALA	C-N-CA	9.97	130.75	119.99
1	B	112	ALA	CA-C-N	9.90	130.69	119.99
1	B	112	ALA	C-N-CA	9.90	130.69	119.99
1	A	290	LYS	N-CA-C	9.87	122.95	111.11
1	A	405	ILE	CA-C-N	9.87	129.63	119.76
1	A	405	ILE	C-N-CA	9.87	129.63	119.76
1	B	526	ARG	NE-CZ-NH2	-9.86	110.33	119.20
1	B	290	LYS	N-CA-C	9.85	122.92	111.11
1	A	526	ARG	NE-CZ-NH2	-9.82	110.36	119.20
1	B	405	ILE	CA-C-N	9.81	129.57	119.76
1	B	405	ILE	C-N-CA	9.81	129.57	119.76
1	B	331	THR	N-CA-C	-9.61	99.87	111.69
1	A	331	THR	N-CA-C	-9.61	99.87	111.69
1	B	158	ASN	N-CA-C	-9.59	99.26	112.30
1	A	158	ASN	N-CA-C	-9.53	99.33	112.30
1	A	460	VAL	N-CA-C	9.39	120.70	107.37
1	B	460	VAL	N-CA-C	9.39	120.70	107.37
1	B	308	VAL	N-CA-C	-9.17	98.47	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	VAL	N-CA-C	-9.17	98.48	107.55
1	B	526	ARG	CG-CD-NE	-9.17	91.83	112.00
1	A	526	ARG	CG-CD-NE	-9.16	91.86	112.00
1	A	536	ASP	CA-C-N	9.13	131.25	119.84
1	A	536	ASP	C-N-CA	9.13	131.25	119.84
1	A	457	THR	CB-CA-C	-9.12	93.44	109.86
1	B	457	THR	CB-CA-C	-9.12	93.44	109.86
1	B	536	ASP	CA-C-N	9.10	131.22	119.84
1	B	536	ASP	C-N-CA	9.10	131.22	119.84
1	B	215	GLY	N-CA-C	-9.08	103.17	114.16
1	A	32	VAL	N-CA-C	9.07	125.50	113.07
1	A	215	GLY	N-CA-C	-9.07	103.18	114.16
1	B	32	VAL	N-CA-C	9.06	125.48	113.07
1	A	418	PRO	CA-C-N	-8.89	109.54	123.23
1	A	418	PRO	C-N-CA	-8.89	109.54	123.23
1	B	418	PRO	CA-C-N	-8.89	109.55	123.23
1	B	418	PRO	C-N-CA	-8.89	109.55	123.23
1	A	107	GLY	N-CA-C	-8.82	104.58	115.08
1	B	107	GLY	N-CA-C	-8.80	104.61	115.08
1	B	10	LEU	N-CA-C	-8.78	101.40	112.90
1	A	10	LEU	N-CA-C	-8.75	101.44	112.90
1	B	122	ASP	N-CA-CB	8.75	123.39	110.35
1	A	122	ASP	N-CA-CB	8.75	123.38	110.35
1	A	57	THR	N-CA-C	8.73	121.94	111.82
1	B	57	THR	N-CA-C	8.71	121.92	111.82
1	B	306	GLN	N-CA-C	8.67	124.83	111.56
1	A	306	GLN	N-CA-C	8.63	124.77	111.56
1	A	128	ASN	N-CA-C	8.55	123.55	113.20
1	B	128	ASN	N-CA-C	8.55	123.54	113.20
1	A	232	ASP	N-CA-C	8.53	123.53	113.20
1	A	51	TYR	N-CA-C	-8.53	101.90	111.71
1	B	232	ASP	N-CA-C	8.52	123.51	113.20
1	B	51	TYR	N-CA-C	-8.50	101.94	111.71
1	A	202	VAL	CB-CA-C	-8.48	95.53	110.71
1	B	202	VAL	CB-CA-C	-8.48	95.54	110.71
1	B	448	GLN	CB-CA-C	8.47	124.28	110.90
1	A	426	SER	N-CA-C	8.46	123.32	109.79
1	A	448	GLN	CB-CA-C	8.44	124.24	110.90
1	B	426	SER	N-CA-C	8.43	123.28	109.79
1	A	314	ILE	N-CA-C	8.19	118.97	110.62
1	A	461	GLY	N-CA-C	-8.16	100.12	112.60
1	B	461	GLY	N-CA-C	-8.15	100.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	PRO	CB-CA-C	8.15	121.62	110.95
1	A	289	LEU	N-CA-C	-8.13	101.49	111.33
1	B	220	PRO	CB-CA-C	8.13	121.60	110.95
1	B	314	ILE	N-CA-C	8.13	118.91	110.62
1	B	114	ARG	CB-CG-CD	8.12	129.99	111.30
1	A	114	ARG	CB-CG-CD	8.11	129.96	111.30
1	B	289	LEU	N-CA-C	-8.11	101.52	111.33
1	A	421	ALA	N-CA-C	-8.05	96.36	108.99
1	B	421	ALA	N-CA-C	-8.02	96.41	108.99
1	B	353	PHE	N-CA-C	7.99	121.76	108.73
1	A	353	PHE	N-CA-C	7.99	121.75	108.73
1	B	142	VAL	N-CA-C	7.98	122.15	108.90
1	A	142	VAL	N-CA-C	7.95	122.10	108.90
1	A	231	GLU	N-CA-C	-7.95	101.71	111.33
1	B	231	GLU	N-CA-C	-7.93	101.74	111.33
1	A	419	ASN	N-CA-C	-7.92	89.35	107.48
1	B	321	LEU	N-CA-C	7.90	119.97	111.36
1	A	321	LEU	N-CA-C	7.89	119.97	111.36
1	B	419	ASN	N-CA-C	-7.89	89.40	107.48
1	B	297	ARG	N-CA-C	7.84	127.13	109.81
1	B	549	TRP	N-CA-C	7.83	120.97	109.62
1	A	297	ARG	N-CA-C	7.83	127.11	109.81
1	A	549	TRP	N-CA-C	7.83	120.97	109.62
1	A	468	ILE	CB-CA-C	-7.77	103.82	112.68
1	B	468	ILE	CB-CA-C	-7.76	103.83	112.68
1	A	424	PHE	N-CA-C	7.75	121.37	108.73
1	A	352	ASN	N-CA-C	7.72	121.10	108.52
1	B	352	ASN	N-CA-C	7.71	121.09	108.52
1	B	424	PHE	N-CA-C	7.70	121.27	108.73
1	A	253	LEU	N-CA-C	-7.63	103.72	112.87
1	B	253	LEU	N-CA-C	-7.62	103.73	112.87
1	B	121	LEU	CA-C-N	-7.58	111.26	122.41
1	B	121	LEU	C-N-CA	-7.58	111.26	122.41
1	A	385	PHE	N-CA-C	-7.56	97.26	109.58
1	A	121	LEU	CA-C-N	-7.55	111.31	122.41
1	A	121	LEU	C-N-CA	-7.55	111.31	122.41
1	B	385	PHE	N-CA-C	-7.55	97.28	109.58
1	A	463	ARG	N-CA-CB	-7.52	98.27	111.42
1	B	463	ARG	N-CA-CB	-7.51	98.27	111.42
1	A	29	ILE	N-CA-C	-7.35	103.12	110.62
1	B	29	ILE	N-CA-C	-7.34	103.13	110.62
1	A	395	LEU	N-CA-C	-7.32	103.30	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	LEU	N-CA-C	-7.31	103.31	111.28
1	A	430	LYS	CB-CG-CD	-7.30	94.51	111.30
1	B	430	LYS	CB-CG-CD	-7.29	94.53	111.30
1	A	226	MET	N-CA-C	7.28	120.87	109.96
1	A	468	ILE	N-CA-C	7.26	117.07	106.55
1	B	226	MET	N-CA-C	7.25	120.83	109.96
1	B	468	ILE	N-CA-C	7.25	117.06	106.55
1	A	320	VAL	N-CA-C	-7.21	102.08	111.09
1	B	320	VAL	N-CA-C	-7.17	102.13	111.09
1	B	36	ASN	CB-CA-C	7.11	122.57	110.56
1	B	443	THR	CB-CA-C	-7.10	97.03	110.67
1	A	443	THR	CB-CA-C	-7.10	97.04	110.67
1	A	36	ASN	CB-CA-C	7.08	122.53	110.56
1	B	268	TRP	N-CA-C	7.05	120.46	110.23
1	B	31	ILE	CB-CA-C	-7.04	102.79	111.87
1	B	250	ILE	N-CA-C	7.04	121.78	112.98
1	A	250	ILE	N-CA-C	7.04	121.77	112.98
1	A	268	TRP	N-CA-C	7.03	120.43	110.23
1	B	177	LEU	CB-CA-C	7.03	121.84	110.95
1	A	177	LEU	CB-CA-C	7.02	121.83	110.95
1	A	31	ILE	CB-CA-C	-7.00	102.84	111.87
1	A	211	ARG	CB-CG-CD	7.00	127.40	111.30
1	B	211	ARG	CB-CG-CD	7.00	127.40	111.30
1	B	470	CYS	N-CA-C	6.95	121.03	108.17
1	A	470	CYS	N-CA-C	6.92	120.98	108.17
1	B	200	MET	CG-SD-CE	-6.91	85.70	100.90
1	A	200	MET	CG-SD-CE	-6.90	85.71	100.90
1	A	442	VAL	N-CA-CB	-6.86	102.89	110.51
1	B	442	VAL	N-CA-CB	-6.85	102.90	110.51
1	B	309	PRO	CB-CA-C	-6.82	101.18	110.60
1	A	309	PRO	CB-CA-C	-6.82	101.19	110.60
1	A	120	VAL	N-CA-CB	6.76	118.09	110.72
1	B	75	VAL	N-CA-C	6.75	117.76	107.77
1	B	135	VAL	N-CA-C	6.74	117.53	110.72
1	A	75	VAL	N-CA-C	6.72	117.72	107.77
1	A	24	PHE	N-CA-CB	-6.71	99.94	109.94
1	B	24	PHE	N-CA-CB	-6.71	99.95	109.94
1	A	135	VAL	N-CA-C	6.70	117.49	110.72
1	B	120	VAL	N-CA-CB	6.70	118.02	110.72
1	A	191	GLY	N-CA-C	6.69	120.76	112.73
1	B	191	GLY	N-CA-C	6.68	120.75	112.73
1	A	27	ASP	N-CA-C	-6.67	103.93	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	PHE	CA-C-N	-6.67	112.78	122.19
1	A	93	PHE	C-N-CA	-6.67	112.78	122.19
1	B	93	PHE	CA-C-N	-6.66	112.80	122.19
1	B	93	PHE	C-N-CA	-6.66	112.80	122.19
1	A	272	ASN	N-CA-C	-6.66	101.38	109.57
1	B	27	ASP	N-CA-C	-6.65	103.95	111.07
1	B	264	LYS	CB-CA-C	-6.65	99.26	110.43
1	A	264	LYS	CB-CA-C	-6.64	99.28	110.43
1	B	272	ASN	N-CA-C	-6.63	101.42	109.57
1	A	237	LYS	N-CA-C	6.62	118.50	111.28
1	B	133	VAL	N-CA-C	-6.61	96.14	107.24
1	A	133	VAL	N-CA-C	-6.60	96.15	107.24
1	B	237	LYS	N-CA-C	6.60	118.48	111.28
1	A	11	THR	CB-CA-C	-6.57	98.16	109.65
1	B	11	THR	CB-CA-C	-6.55	98.19	109.65
1	B	479	ILE	CB-CA-C	-6.54	103.31	112.14
1	A	6	GLU	CA-C-N	6.53	129.86	120.79
1	A	6	GLU	C-N-CA	6.53	129.86	120.79
1	A	479	ILE	CB-CA-C	-6.52	103.34	112.14
1	B	6	GLU	CA-C-N	6.51	129.84	120.79
1	B	6	GLU	C-N-CA	6.51	129.84	120.79
1	B	282	THR	CB-CA-C	6.47	120.40	109.80
1	A	221	LYS	N-CA-C	6.46	119.61	110.50
1	B	221	LYS	N-CA-C	6.46	119.61	110.50
1	A	282	THR	CB-CA-C	6.45	120.38	109.80
1	A	106	SER	N-CA-C	-6.42	101.61	110.35
1	B	106	SER	N-CA-C	-6.42	101.61	110.35
1	A	454	PHE	N-CA-C	-6.40	100.09	110.20
1	B	454	PHE	N-CA-C	-6.40	100.09	110.20
1	B	64	MET	N-CA-C	-6.33	99.91	109.79
1	A	64	MET	N-CA-C	-6.33	99.91	109.79
1	A	79	ASN	N-CA-CB	-6.29	100.43	111.49
1	A	548	VAL	CB-CA-C	6.28	120.10	111.31
1	B	79	ASN	N-CA-CB	-6.28	100.44	111.49
1	B	548	VAL	CB-CA-C	6.25	120.06	111.31
1	B	471	ILE	CA-C-N	-6.22	115.08	123.10
1	B	471	ILE	C-N-CA	-6.22	115.08	123.10
1	A	471	ILE	CA-C-N	-6.20	115.11	123.10
1	A	471	ILE	C-N-CA	-6.20	115.11	123.10
1	A	541	ILE	CB-CA-C	-6.20	102.49	110.98
1	A	425	PHE	N-CA-C	-6.17	98.67	108.73
1	B	541	ILE	CB-CA-C	-6.17	102.53	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	MET	N-CA-C	-6.15	105.87	113.19
1	B	425	PHE	N-CA-C	-6.14	98.72	108.73
1	B	214	MET	N-CA-C	-6.13	105.90	113.19
1	B	83	VAL	N-CA-C	-6.11	104.56	110.42
1	A	83	VAL	N-CA-C	-6.10	104.56	110.42
1	A	559	LYS	N-CA-C	6.05	118.14	110.33
1	B	279	TYR	N-CA-C	6.05	117.44	108.60
1	B	559	LYS	N-CA-C	6.03	118.11	110.33
1	B	412	LYS	CA-C-N	-6.03	111.14	120.31
1	B	412	LYS	C-N-CA	-6.03	111.14	120.31
1	A	412	LYS	CA-C-N	-6.03	111.15	120.31
1	A	412	LYS	C-N-CA	-6.03	111.15	120.31
1	A	279	TYR	N-CA-C	6.02	117.39	108.60
1	A	40	ILE	N-CA-C	6.00	115.37	106.85
1	A	170	ASP	N-CA-C	6.00	117.81	111.28
1	B	211	ARG	CB-CA-C	5.99	120.54	109.70
1	A	290	LYS	CA-CB-CG	-5.97	102.16	114.10
1	A	28	ILE	N-CA-C	5.97	116.75	110.72
1	B	28	ILE	N-CA-C	5.97	116.75	110.72
1	A	211	ARG	CB-CA-C	5.97	120.50	109.70
1	B	290	LYS	CA-CB-CG	-5.97	102.17	114.10
1	B	40	ILE	N-CA-C	5.96	115.31	106.85
1	B	378	ILE	CB-CA-C	-5.94	104.23	110.53
1	A	378	ILE	CB-CA-C	-5.93	104.25	110.53
1	B	211	ARG	N-CA-C	-5.92	98.75	108.76
1	B	240	HIS	N-CA-C	5.92	119.26	112.57
1	A	290	LYS	CB-CG-CD	5.92	124.92	111.30
1	A	231	GLU	CA-CB-CG	-5.92	102.27	114.10
1	B	231	GLU	CA-CB-CG	-5.91	102.27	114.10
1	B	425	PHE	CB-CA-C	5.91	119.77	110.19
1	B	290	LYS	CB-CG-CD	5.91	124.89	111.30
1	A	211	ARG	N-CA-C	-5.91	98.78	108.76
1	B	142	VAL	N-CA-CB	-5.90	101.44	112.36
1	A	425	PHE	CB-CA-C	5.89	119.73	110.19
1	A	443	THR	N-CA-C	5.89	118.66	111.82
1	A	240	HIS	N-CA-C	5.89	119.22	112.57
1	B	26	GLN	N-CA-C	5.88	117.77	111.36
1	A	142	VAL	N-CA-CB	-5.87	101.50	112.36
1	A	26	GLN	N-CA-C	5.87	117.75	111.36
1	A	485	GLN	N-CA-C	-5.86	105.03	111.82
1	B	443	THR	N-CA-C	5.86	118.61	111.82
1	B	485	GLN	N-CA-C	-5.85	105.04	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	VAL	CB-CA-C	5.81	119.65	110.81
1	A	406	PRO	N-CA-C	5.81	120.31	111.19
1	B	406	PRO	N-CA-C	5.81	120.31	111.19
1	B	472	VAL	CB-CA-C	5.80	119.63	110.81
1	A	61	HIS	N-CA-C	-5.79	104.38	112.25
1	B	61	HIS	N-CA-C	-5.78	104.39	112.25
1	A	285	LYS	N-CA-C	5.77	119.66	109.96
1	B	285	LYS	N-CA-C	5.76	119.63	109.96
1	B	383	PHE	N-CA-C	5.75	119.63	109.96
1	B	319	ALA	N-CA-C	5.75	118.49	111.82
1	A	383	PHE	N-CA-C	5.75	119.62	109.96
1	B	526	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	319	ALA	N-CA-C	5.73	118.47	111.82
1	A	526	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	70	LEU	N-CA-C	5.73	118.55	108.75
1	B	70	LEU	N-CA-C	5.73	118.54	108.75
1	A	237	LYS	CB-CG-CD	5.72	124.45	111.30
1	B	237	LYS	CB-CG-CD	5.72	124.46	111.30
1	B	177	LEU	N-CA-C	5.71	117.36	111.03
1	A	536	ASP	C-N-CD	-5.70	101.62	125.00
1	B	536	ASP	C-N-CD	-5.70	101.63	125.00
1	B	48	ASP	CA-C-N	-5.69	110.25	121.41
1	B	48	ASP	C-N-CA	-5.69	110.25	121.41
1	A	48	ASP	CA-C-N	-5.68	110.28	121.41
1	A	48	ASP	C-N-CA	-5.68	110.28	121.41
1	A	140	CYS	N-CA-C	-5.68	100.67	109.24
1	B	251	ASP	N-CA-C	5.67	119.01	111.75
1	B	140	CYS	N-CA-C	-5.67	100.68	109.24
1	A	251	ASP	N-CA-C	5.66	119.00	111.75
1	A	193	HIS	N-CA-C	5.66	117.90	111.11
1	B	193	HIS	N-CA-C	5.66	117.90	111.11
1	A	177	LEU	N-CA-C	5.64	117.30	111.03
1	B	527	PHE	N-CA-C	-5.64	105.13	111.28
1	A	527	PHE	N-CA-C	-5.63	105.14	111.28
1	B	87	VAL	CB-CA-C	-5.61	103.47	112.16
1	B	234	PRO	N-CA-C	-5.61	103.37	111.22
1	A	87	VAL	CB-CA-C	-5.60	103.48	112.16
1	A	234	PRO	N-CA-C	-5.59	103.40	111.22
1	A	62	HIS	CA-C-N	5.58	129.48	120.55
1	A	62	HIS	C-N-CA	5.58	129.48	120.55
1	B	488	MET	N-CA-C	5.58	117.83	111.02
1	A	333	PRO	N-CA-C	-5.58	102.37	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	HIS	CA-C-N	5.57	129.47	120.55
1	B	62	HIS	C-N-CA	5.57	129.47	120.55
1	B	333	PRO	N-CA-C	-5.57	102.39	111.68
1	A	526	ARG	CD-NE-CZ	5.56	132.18	124.40
1	A	72	SER	N-CA-C	-5.55	104.73	112.45
1	B	72	SER	N-CA-C	-5.55	104.74	112.45
1	A	488	MET	N-CA-C	5.54	117.78	111.02
1	B	526	ARG	CD-NE-CZ	5.53	132.15	124.40
1	B	264	LYS	CA-C-N	-5.53	114.55	121.96
1	B	264	LYS	C-N-CA	-5.53	114.55	121.96
1	B	189	PRO	N-CA-C	-5.53	107.23	114.03
1	A	189	PRO	N-CA-C	-5.52	107.25	114.03
1	A	264	LYS	CA-C-N	-5.51	114.58	121.96
1	A	264	LYS	C-N-CA	-5.51	114.58	121.96
1	B	547	GLY	CA-C-N	-5.50	115.72	122.93
1	B	547	GLY	C-N-CA	-5.50	115.72	122.93
1	B	495	CYS	N-CA-C	5.47	117.25	111.28
1	A	547	GLY	CA-C-N	-5.47	115.76	122.93
1	A	547	GLY	C-N-CA	-5.47	115.76	122.93
1	A	21	PHE	N-CA-C	-5.47	105.22	111.07
1	B	21	PHE	N-CA-C	-5.46	105.23	111.07
1	B	164	LEU	N-CA-C	5.45	118.33	109.06
1	A	164	LEU	N-CA-C	5.44	118.31	109.06
1	B	165	TRP	N-CA-C	5.44	118.68	109.76
1	B	412	LYS	CA-CB-CG	-5.44	103.23	114.10
1	A	412	LYS	CA-CB-CG	-5.43	103.23	114.10
1	A	165	TRP	N-CA-C	5.43	118.67	109.76
1	A	169	PRO	N-CA-C	-5.42	101.30	112.47
1	A	495	CYS	N-CA-C	5.42	117.18	111.28
1	A	402	MET	N-CA-C	5.42	119.63	113.19
1	B	169	PRO	N-CA-C	-5.41	101.33	112.47
1	B	521	ASN	N-CA-C	5.41	119.04	111.90
1	B	130	VAL	N-CA-C	-5.39	99.84	107.98
1	A	433	GLY	N-CA-C	-5.38	106.27	112.73
1	B	433	GLY	N-CA-C	-5.37	106.28	112.73
1	A	130	VAL	N-CA-C	-5.37	99.87	107.98
1	A	212	THR	N-CA-C	5.37	118.47	110.52
1	A	521	ASN	N-CA-C	5.37	118.99	111.90
1	B	538	ASN	CB-CA-C	-5.36	100.36	110.01
1	A	538	ASN	CB-CA-C	-5.36	100.36	110.01
1	B	212	THR	N-CA-C	5.36	118.45	110.52
1	A	441	ALA	N-CA-C	5.36	116.81	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	MET	N-CA-C	5.35	119.55	113.19
1	B	307	ASN	CA-C-N	-5.34	116.76	122.85
1	B	307	ASN	C-N-CA	-5.34	116.76	122.85
1	B	441	ALA	N-CA-C	5.34	116.79	110.97
1	B	170	ASP	N-CA-C	5.34	117.79	111.33
1	A	307	ASN	CA-C-N	-5.33	116.77	122.85
1	A	307	ASN	C-N-CA	-5.33	116.77	122.85
1	A	249	TYR	CB-CA-C	5.33	120.63	111.68
1	A	271	PRO	CB-CA-C	-5.32	104.01	110.98
1	A	196	MET	N-CA-C	5.32	119.77	113.28
1	B	53	LYS	N-CA-CB	5.31	119.02	111.21
1	B	540	ILE	CB-CA-C	-5.31	98.49	111.02
1	A	332	GLU	N-CA-CB	5.31	119.82	110.37
1	B	196	MET	N-CA-C	5.31	119.75	113.28
1	B	249	TYR	CB-CA-C	5.31	120.59	111.68
1	B	271	PRO	CB-CA-C	-5.31	104.03	110.98
1	A	53	LYS	N-CA-CB	5.30	119.00	111.21
1	B	332	GLU	N-CA-CB	5.30	119.80	110.37
1	A	334	LEU	N-CA-C	-5.29	102.45	110.28
1	A	397	VAL	CB-CA-C	-5.29	105.05	111.87
1	B	243	PRO	CB-CA-C	-5.29	103.90	112.62
1	B	334	LEU	N-CA-C	-5.29	102.45	110.28
1	B	322	GLY	CA-C-N	5.28	128.58	120.82
1	B	322	GLY	C-N-CA	5.28	128.58	120.82
1	A	540	ILE	CB-CA-C	-5.28	98.57	111.02
1	A	243	PRO	CB-CA-C	-5.27	103.92	112.62
1	B	63	VAL	CB-CA-C	-5.27	105.18	112.24
1	B	258	ASN	CB-CA-C	5.27	119.47	110.56
1	A	322	GLY	CA-C-N	5.25	128.54	120.82
1	A	322	GLY	C-N-CA	5.25	128.54	120.82
1	A	63	VAL	CB-CA-C	-5.24	105.22	112.24
1	B	397	VAL	CB-CA-C	-5.24	105.11	111.87
1	B	12	LEU	CA-C-N	5.21	125.74	120.38
1	B	12	LEU	C-N-CA	5.21	125.74	120.38
1	B	314	ILE	CB-CA-C	5.18	119.14	112.14
1	A	284	PRO	N-CA-C	5.18	120.88	113.47
1	B	284	PRO	N-CA-C	5.17	120.87	113.47
1	A	314	ILE	CB-CA-C	5.15	119.09	112.14
1	A	411	LEU	CB-CA-C	-5.14	101.12	110.63
1	B	325	ARG	CB-CA-C	5.14	120.14	110.63
1	A	258	ASN	CB-CA-C	5.14	119.42	110.94
1	B	29	ILE	N-CA-CB	5.14	117.53	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LEU	CA-C-N	5.13	125.67	120.38
1	A	12	LEU	C-N-CA	5.13	125.67	120.38
1	A	29	ILE	N-CA-CB	5.13	117.52	110.54
1	A	550	PRO	N-CA-C	-5.13	103.39	111.34
1	B	464	GLU	CB-CG-CD	5.13	121.32	112.60
1	B	504	ARG	CA-C-O	-5.12	115.75	121.23
1	B	560	LEU	N-CA-C	-5.12	96.65	111.00
1	A	325	ARG	CB-CA-C	5.12	120.11	110.63
1	A	464	GLU	CB-CG-CD	5.12	121.31	112.60
1	B	411	LEU	CB-CA-C	-5.12	101.16	110.63
1	B	259	MET	N-CA-C	5.11	118.62	112.38
1	A	448	GLN	N-CA-CB	5.11	117.48	110.07
1	A	560	LEU	N-CA-C	-5.11	96.70	111.00
1	A	480	GLN	O-C-N	5.10	127.60	122.09
1	B	448	GLN	N-CA-CB	5.09	117.46	110.07
1	B	550	PRO	N-CA-C	-5.09	103.44	111.34
1	A	504	ARG	CA-C-O	-5.09	115.79	121.23
1	B	325	ARG	N-CA-C	5.08	117.56	111.71
1	B	30	ARG	CB-CA-C	5.07	119.21	110.79
1	A	325	ARG	N-CA-C	5.07	117.54	111.71
1	A	74	ILE	CB-CA-C	5.07	117.73	110.84
1	A	187	TYR	N-CA-CB	-5.06	102.70	110.44
1	A	332	GLU	N-CA-C	5.06	120.99	109.81
1	B	366	VAL	CB-CA-C	-5.06	104.32	112.16
1	A	259	MET	N-CA-C	5.05	118.54	112.38
1	B	332	GLU	N-CA-C	5.04	120.96	109.81
1	A	366	VAL	CB-CA-C	-5.04	104.35	112.16
1	B	480	GLN	O-C-N	5.04	127.53	122.09
1	B	74	ILE	CB-CA-C	5.04	117.69	110.84
1	A	30	ARG	CB-CA-C	5.04	119.15	110.79
1	B	187	TYR	N-CA-CB	-5.03	102.75	110.44
1	B	113	PRO	CA-C-O	-5.01	115.47	121.48
1	A	303	MET	N-CA-C	5.01	123.53	113.31

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	PHE	CA
1	A	332	GLU	CA
1	B	7	PHE	CA
1	B	332	GLU	CA

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	4351	0	4288	320	1
1	B	4351	0	4288	302	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	29	5	0
4	B	53	0	29	6	0
5	A	166	0	0	19	0
5	B	150	0	0	11	0
All	All	9134	0	8640	604	1

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 35.

All (604) 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)
4:B:600:FAD:H51A	4:B:600:FAD:H8A	1.22	1.16
4:A:600:FAD:H8A	4:A:600:FAD:H51A	1.23	1.11
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.11	1.07
1:A:211:ARG:HG3	1:B:519:TRP:CZ3	1.99	0.98
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.46	0.97
1:A:91:ASN:HD22	1:A:538:ASN:ND2	1.62	0.97
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.46	0.97
1:B:91:ASN:HD22	1:B:538:ASN:ND2	1.62	0.96
1:B:91:ASN:ND2	1:B:538:ASN:HD22	1.66	0.94
1:A:519:TRP:CZ3	1:B:211:ARG:HG3	2.03	0.93
1:A:91:ASN:ND2	1:A:538:ASN:HD22	1.66	0.91
1:A:448:GLN:HE21	1:A:448:GLN:N	1.70	0.89
1:B:448:GLN:N	1:B:448:GLN:HE21	1.70	0.89
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:THR:HG22	1:A:506:HIS:H	1.37	0.87
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.39	0.87
1:B:505:THR:HG22	1:B:506:HIS:H	1.37	0.86
1:A:91:ASN:HD22	1:A:538:ASN:HD22	0.88	0.85
1:A:445:LYS:HE2	1:A:449:GLU:OE2	1.76	0.85
1:A:341:LYS:O	1:A:344:LYS:HG2	1.77	0.85
4:A:600:FAD:H51A	4:A:600:FAD:C8A	2.06	0.85
1:B:445:LYS:HE2	1:B:449:GLU:OE2	1.76	0.84
1:A:538:ASN:CB	1:A:540:ILE:HD11	2.08	0.84
1:A:78:ARG:HD3	1:A:82:ASP:OD2	1.78	0.84
1:A:550:PRO:HG2	1:A:553:TYR:CD1	2.13	0.84
1:B:538:ASN:CB	1:B:540:ILE:HD11	2.08	0.84
1:B:91:ASN:HD22	1:B:538:ASN:HD22	0.88	0.84
1:B:550:PRO:HG2	1:B:553:TYR:CD1	2.13	0.84
4:B:600:FAD:H51A	4:B:600:FAD:C8A	2.06	0.83
1:B:78:ARG:HD3	1:B:82:ASP:OD2	1.78	0.83
1:B:341:LYS:O	1:B:344:LYS:HG2	1.77	0.83
1:A:349:GLY:H	1:A:352:ASN:HD21	1.27	0.81
1:A:550:PRO:CB	1:A:552:GLN:HE21	1.93	0.80
1:B:349:GLY:H	1:B:352:ASN:HD21	1.27	0.80
1:B:550:PRO:CB	1:B:552:GLN:HE21	1.93	0.80
1:A:538:ASN:HB2	1:A:540:ILE:HD11	1.63	0.79
1:B:416:TRP:C	1:B:417:LEU:HD23	2.08	0.79
1:B:538:ASN:HB2	1:B:540:ILE:HD11	1.63	0.79
1:A:416:TRP:C	1:A:417:LEU:HD23	2.08	0.78
1:A:253:LEU:CD2	1:B:253:LEU:HD21	2.05	0.78
1:A:187:TYR:O	1:A:307:ASN:HB2	1.83	0.77
1:B:187:TYR:O	1:B:307:ASN:HB2	1.83	0.77
1:B:350:ARG:HD2	5:B:694:HOH:O	1.85	0.77
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.67	0.77
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.66	0.77
1:B:21:PHE:O	1:B:25:ILE:HG22	1.86	0.76
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.66	0.76
1:B:516:THR:HG21	5:B:731:HOH:O	1.84	0.76
1:B:304:ALA:HB2	5:B:631:HOH:O	1.86	0.76
1:B:341:LYS:O	1:B:345:GLN:HG3	1.86	0.76
1:B:361:GLU:HB3	1:B:362:PRO:HD3	1.67	0.76
1:A:341:LYS:O	1:A:345:GLN:HG3	1.86	0.76
1:B:482:ARG:HD2	5:B:655:HOH:O	1.86	0.76
1:A:21:PHE:O	1:A:25:ILE:HG22	1.86	0.75
1:B:419:ASN:O	1:B:474:ASN:HA	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:ND2	1:A:82:ASP:H	1.85	0.74
1:A:478:LEU:HD12	1:A:478:LEU:H	1.53	0.74
4:B:600:FAD:H8A	4:B:600:FAD:C5B	2.11	0.74
1:A:515:GLU:HB2	5:A:765:HOH:O	1.87	0.74
1:A:409:ASP:HA	1:A:412:LYS:HE3	1.69	0.74
1:A:419:ASN:O	1:A:474:ASN:HA	1.87	0.74
1:B:79:ASN:ND2	1:B:82:ASP:H	1.85	0.73
1:B:230:PRO:HA	1:B:233:GLN:HG3	1.70	0.73
1:B:409:ASP:HA	1:B:412:LYS:HE3	1.69	0.73
1:B:478:LEU:HD12	1:B:478:LEU:H	1.53	0.72
1:A:91:ASN:ND2	1:A:538:ASN:ND2	2.31	0.72
4:A:600:FAD:H8A	4:A:600:FAD:C5B	2.11	0.72
1:A:516:THR:HG21	5:A:709:HOH:O	1.88	0.72
1:B:114:ARG:NH2	5:B:638:HOH:O	2.23	0.72
1:A:230:PRO:HA	1:A:233:GLN:HG3	1.70	0.72
1:A:253:LEU:HD21	1:B:253:LEU:CD2	2.05	0.72
1:A:314:ILE:HD13	1:A:314:ILE:O	1.91	0.71
1:A:244:TYR:OH	1:B:195:MET:HG2	1.90	0.71
1:B:389:THR:HB	1:B:390:PRO:HD2	1.72	0.71
1:A:37:VAL:HG13	1:A:75:VAL:HG22	1.72	0.70
1:B:314:ILE:HD13	1:B:314:ILE:O	1.91	0.70
1:A:389:THR:HB	1:A:390:PRO:HD2	1.72	0.70
1:B:37:VAL:HG13	1:B:75:VAL:HG22	1.72	0.70
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.74	0.70
1:A:31:ILE:HD13	1:A:85:SER:HB3	1.74	0.70
1:B:463:ARG:HD2	5:B:725:HOH:O	1.92	0.70
1:B:156:GLU:HB2	1:B:161:ARG:NH2	2.07	0.69
1:B:132:GLU:HG2	1:B:133:VAL:N	2.08	0.69
1:A:156:GLU:HB2	1:A:161:ARG:NH2	2.07	0.69
1:B:210:LEU:HD23	1:B:211:ARG:N	2.08	0.69
1:A:210:LEU:HD23	1:A:211:ARG:N	2.08	0.68
1:A:96:PRO:HG3	5:A:746:HOH:O	1.94	0.68
1:A:550:PRO:HG2	1:A:553:TYR:HD1	1.58	0.68
1:A:132:GLU:HG2	1:A:133:VAL:N	2.08	0.67
1:A:538:ASN:HB3	1:A:540:ILE:HD11	1.75	0.67
1:A:162:ASP:HB2	5:A:727:HOH:O	1.95	0.67
1:A:195:MET:HG2	1:B:244:TYR:OH	1.94	0.67
1:B:163:LYS:HG2	5:B:726:HOH:O	1.93	0.67
1:B:513:ILE:O	1:B:516:THR:HB	1.95	0.67
1:B:538:ASN:HB3	1:B:540:ILE:HD11	1.75	0.67
1:A:513:ILE:O	1:A:516:THR:HB	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASN:ND2	1:B:538:ASN:ND2	2.31	0.67
1:B:133:VAL:HG21	1:B:154:TYR:CE2	2.30	0.66
1:A:423:LEU:HD21	1:A:488:MET:HG3	1.78	0.66
1:B:142:VAL:CG2	1:B:146:VAL:HB	2.26	0.66
1:A:133:VAL:HG21	1:A:154:TYR:CE2	2.30	0.66
1:A:142:VAL:CG2	1:A:146:VAL:HB	2.25	0.66
1:B:79:ASN:C	1:B:79:ASN:HD22	2.04	0.66
1:B:550:PRO:HG2	1:B:553:TYR:HD1	1.58	0.66
1:B:156:GLU:HB2	1:B:161:ARG:NE	2.10	0.66
1:B:423:LEU:HD21	1:B:488:MET:HG3	1.78	0.66
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.78	0.66
1:A:222:ARG:HG3	1:A:224:GLU:OE1	1.96	0.65
1:A:156:GLU:HB2	1:A:161:ARG:NE	2.11	0.65
1:A:79:ASN:C	1:A:79:ASN:HD22	2.04	0.65
1:B:349:GLY:N	1:B:352:ASN:HD21	1.94	0.65
1:A:330:ARG:NH1	1:A:338:GLU:OE1	2.30	0.65
1:B:330:ARG:NH1	1:B:338:GLU:OE1	2.30	0.65
1:A:50:SER:OG	1:A:53:LYS:N	2.29	0.65
1:A:379:PRO:HG3	5:A:668:HOH:O	1.97	0.64
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.78	0.64
1:B:222:ARG:HG3	1:B:224:GLU:OE1	1.97	0.64
1:B:505:THR:HG22	1:B:506:HIS:N	2.11	0.64
1:A:99:PRO:HD2	5:A:642:HOH:O	1.97	0.64
1:A:505:THR:HG22	1:A:506:HIS:N	2.11	0.64
1:A:478:LEU:HD12	1:A:478:LEU:N	2.12	0.64
1:B:464:GLU:OE2	1:B:466:HIS:ND1	2.30	0.64
1:A:464:GLU:OE2	1:A:466:HIS:ND1	2.30	0.64
1:A:349:GLY:N	1:A:352:ASN:HD21	1.94	0.64
1:A:543:PRO:HB3	1:A:550:PRO:HG3	1.80	0.64
1:B:224:GLU:CD	1:B:224:GLU:H	2.06	0.63
1:B:550:PRO:HB2	1:B:552:GLN:HG2	1.80	0.63
1:B:65:ASP:OD1	1:B:65:ASP:N	2.31	0.63
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.81	0.63
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.81	0.63
1:B:478:LEU:HD12	1:B:478:LEU:N	2.12	0.63
1:A:224:GLU:CD	1:A:224:GLU:H	2.06	0.63
1:B:50:SER:OG	1:B:53:LYS:N	2.30	0.63
1:A:156:GLU:HB2	1:A:161:ARG:CZ	2.29	0.63
1:A:300:ARG:NH2	1:A:460:VAL:O	2.32	0.63
1:B:156:GLU:HB2	1:B:161:ARG:CZ	2.29	0.62
1:A:550:PRO:HB2	1:A:552:GLN:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ARG:NH2	1:B:460:VAL:O	2.32	0.62
1:B:337:GLU:O	1:B:341:LYS:HG3	1.99	0.62
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.34	0.62
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.34	0.62
1:B:543:PRO:HB3	1:B:550:PRO:HG3	1.80	0.62
1:B:310:THR:HG22	1:B:459:THR:HG22	1.82	0.62
1:A:337:GLU:O	1:A:341:LYS:HG3	2.00	0.62
1:A:211:ARG:HG3	1:B:519:TRP:CE3	2.34	0.61
1:A:310:THR:HG22	1:A:459:THR:HG22	1.82	0.61
1:B:478:LEU:H	1:B:478:LEU:CD1	2.14	0.61
1:A:156:GLU:OE1	1:A:161:ARG:NH2	2.34	0.61
1:A:243:PRO:HD2	1:A:244:TYR:H	1.65	0.61
1:B:156:GLU:OE1	1:B:161:ARG:NH2	2.34	0.61
1:B:243:PRO:HD2	1:B:244:TYR:H	1.65	0.60
1:A:210:LEU:HD23	1:A:210:LEU:C	2.26	0.60
1:B:361:GLU:HB3	1:B:362:PRO:CD	2.31	0.60
1:A:478:LEU:H	1:A:478:LEU:CD1	2.13	0.60
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.83	0.60
1:B:210:LEU:HD23	1:B:210:LEU:C	2.26	0.59
1:A:238:ILE:HG12	5:A:689:HOH:O	2.02	0.59
1:A:316:LEU:HD11	1:A:413:TRP:CD1	2.38	0.59
1:A:505:THR:HG21	1:A:509:PHE:HB2	1.83	0.59
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.37	0.59
1:B:409:ASP:HA	1:B:412:LYS:CE	2.33	0.59
1:A:479:ILE:HD12	1:A:479:ILE:N	2.18	0.59
1:B:316:LEU:HD11	1:B:413:TRP:CD1	2.38	0.59
1:A:361:GLU:HB3	1:A:362:PRO:CD	2.31	0.59
1:A:58:HIS:HA	1:A:112:ALA:HB2	1.85	0.59
1:B:479:ILE:N	1:B:479:ILE:HD12	2.18	0.59
1:A:24:PHE:O	1:A:28:ILE:HG13	2.02	0.58
1:B:22:ASN:HA	1:B:25:ILE:HG22	1.85	0.58
1:A:65:ASP:OD1	1:A:65:ASP:N	2.31	0.58
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.38	0.58
1:B:24:PHE:O	1:B:28:ILE:HG13	2.02	0.58
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.38	0.58
1:A:189:PRO:HA	1:A:307:ASN:HA	1.85	0.58
1:B:152:HIS:CE1	1:B:161:ARG:NH2	2.72	0.58
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.38	0.58
1:A:152:HIS:CE1	1:A:161:ARG:NH2	2.72	0.58
1:B:189:PRO:HA	1:B:307:ASN:HA	1.85	0.58
1:A:409:ASP:HA	1:A:412:LYS:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HD13	1:A:238:ILE:N	2.18	0.57
1:B:238:ILE:N	1:B:238:ILE:HD13	2.18	0.57
1:B:477:ASP:O	1:B:481:LYS:HG3	2.03	0.57
1:A:22:ASN:HA	1:A:25:ILE:HG22	1.86	0.57
1:A:156:GLU:HB2	1:A:161:ARG:HH21	1.68	0.57
1:A:477:ASP:O	1:A:481:LYS:HG3	2.03	0.57
1:A:417:LEU:HD23	1:A:417:LEU:N	2.19	0.57
5:A:724:HOH:O	1:B:519:TRP:HE3	1.86	0.57
1:B:47:VAL:HG13	1:B:66:GLN:HE22	1.70	0.57
1:B:56:HIS:HA	1:B:111:ALA:CB	2.34	0.57
1:B:149:HIS:O	1:B:152:HIS:HB3	2.05	0.57
1:A:56:HIS:HA	1:A:111:ALA:CB	2.34	0.57
1:A:414:ILE:HD11	4:A:600:FAD:HM73	1.87	0.57
1:B:58:HIS:HA	1:B:112:ALA:HB2	1.85	0.57
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.16	0.57
1:A:149:HIS:O	1:A:152:HIS:HB3	2.05	0.56
1:A:361:GLU:O	1:A:365:ARG:HB2	2.05	0.56
1:B:79:ASN:HD21	1:B:82:ASP:H	1.54	0.56
1:A:417:LEU:HB3	1:A:418:PRO:CD	2.35	0.56
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.88	0.56
1:B:417:LEU:HB3	1:B:418:PRO:CD	2.35	0.56
1:A:156:GLU:HB2	1:A:161:ARG:HE	1.70	0.56
1:B:156:GLU:HB2	1:B:161:ARG:HH21	1.68	0.56
1:B:361:GLU:O	1:B:365:ARG:HB2	2.05	0.56
1:B:543:PRO:HB3	1:B:550:PRO:CG	2.36	0.56
1:A:338:GLU:HB3	5:A:670:HOH:O	2.04	0.56
1:A:133:VAL:HG21	1:A:154:TYR:HE2	1.69	0.56
1:A:543:PRO:HB3	1:A:550:PRO:CG	2.36	0.56
1:B:61:HIS:CE1	1:B:422:HIS:HD1	2.24	0.56
1:A:79:ASN:HD21	1:A:82:ASP:H	1.54	0.56
1:A:552:GLN:CD	1:A:552:GLN:H	2.14	0.56
1:A:519:TRP:CH2	1:B:211:ARG:HG3	2.40	0.56
1:B:156:GLU:HB2	1:B:161:ARG:HE	1.70	0.56
1:B:431:VAL:HA	1:B:465:MET:HE2	1.87	0.56
1:B:447:CYS:C	1:B:448:GLN:HE21	2.14	0.55
1:A:431:VAL:HA	1:A:465:MET:HE2	1.87	0.55
1:B:61:HIS:ND1	1:B:422:HIS:ND1	2.51	0.55
1:B:133:VAL:HG21	1:B:154:TYR:HE2	1.69	0.55
1:A:47:VAL:HG13	1:A:66:GLN:HE22	1.70	0.55
1:B:414:ILE:HD11	4:B:600:FAD:HM73	1.87	0.55
1:B:409:ASP:N	1:B:409:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:GLN:CD	1:B:552:GLN:H	2.14	0.55
1:A:238:ILE:O	1:A:238:ILE:HG22	2.07	0.55
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.37	0.55
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.88	0.55
1:B:349:GLY:H	1:B:352:ASN:ND2	2.02	0.55
1:A:200:MET:HB3	1:A:265:ILE:HG13	1.89	0.54
1:A:409:ASP:OD1	1:A:409:ASP:N	2.39	0.54
1:A:447:CYS:C	1:A:448:GLN:HE21	2.14	0.54
1:A:489:ARG:NH2	5:A:630:HOH:O	2.40	0.54
1:B:417:LEU:HD23	1:B:417:LEU:N	2.19	0.54
1:A:36:ASN:HB3	1:A:76:ALA:O	2.08	0.54
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.16	0.54
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.42	0.54
1:A:349:GLY:H	1:A:352:ASN:ND2	2.02	0.54
1:B:151:LEU:HD23	1:B:166:LEU:HD22	1.89	0.54
1:A:24:PHE:CE1	1:A:28:ILE:HD11	2.43	0.54
1:A:388:ASP:OD1	1:A:388:ASP:N	2.37	0.54
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.37	0.54
1:A:300:ARG:HH21	1:A:308:VAL:HA	1.72	0.54
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.43	0.54
1:B:24:PHE:CE1	1:B:28:ILE:HD11	2.43	0.54
1:B:238:ILE:HG22	1:B:238:ILE:O	2.06	0.54
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.08	0.54
1:A:300:ARG:NH2	1:A:308:VAL:HA	2.23	0.54
1:B:300:ARG:HH21	1:B:308:VAL:HA	1.72	0.53
1:B:537:PRO:HD2	1:B:538:ASN:H	1.73	0.53
1:A:11:THR:O	1:A:72:SER:HB3	2.08	0.53
1:A:61:HIS:CE1	1:A:422:HIS:HD1	2.24	0.53
1:A:229:LYS:HD2	1:A:231:GLU:OE2	2.08	0.53
1:B:11:THR:O	1:B:72:SER:HB3	2.08	0.53
1:B:36:ASN:HB3	1:B:76:ALA:O	2.08	0.53
1:A:272:ASN:OD1	1:A:273:PRO:HD2	2.08	0.53
1:B:229:LYS:HD2	1:B:231:GLU:OE2	2.07	0.53
1:B:398:ARG:HA	1:B:401:THR:HB	1.91	0.53
1:B:200:MET:HB3	1:B:265:ILE:HG13	1.89	0.53
1:B:284:PRO:HG2	1:B:379:PRO:O	2.09	0.53
1:A:61:HIS:CE1	1:A:422:HIS:ND1	2.77	0.53
1:A:479:ILE:H	1:A:479:ILE:CD1	2.21	0.53
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.90	0.53
1:B:478:LEU:HD21	5:B:664:HOH:O	2.09	0.53
1:B:422:HIS:CD2	1:B:424:PHE:CZ	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:HIS:CD2	1:A:424:PHE:CZ	2.97	0.53
1:B:479:ILE:H	1:B:479:ILE:CD1	2.21	0.53
1:A:398:ARG:HA	1:A:401:THR:HB	1.91	0.52
1:A:485:GLN:O	1:A:489:ARG:HG3	2.09	0.52
1:A:537:PRO:HD2	1:A:538:ASN:H	1.73	0.52
1:B:300:ARG:NH2	1:B:308:VAL:HA	2.23	0.52
1:A:188:THR:HG21	5:A:691:HOH:O	2.08	0.52
1:A:151:LEU:HD23	1:A:166:LEU:HD22	1.89	0.52
1:A:211:ARG:HG3	1:B:519:TRP:CH2	2.44	0.52
1:A:475:LYS:O	1:A:481:LYS:HD2	2.09	0.52
1:B:61:HIS:CE1	1:B:422:HIS:ND1	2.77	0.52
1:B:485:GLN:O	1:B:489:ARG:HG3	2.09	0.52
1:A:284:PRO:HG2	1:A:379:PRO:O	2.09	0.52
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.91	0.52
1:B:447:CYS:HB2	1:B:448:GLN:HE22	1.75	0.52
1:B:388:ASP:N	1:B:388:ASP:OD1	2.37	0.52
1:A:61:HIS:ND1	1:A:422:HIS:ND1	2.51	0.52
1:B:133:VAL:CG2	1:B:154:TYR:CE2	2.93	0.52
1:B:515:GLU:O	1:B:518:ASN:ND2	2.43	0.52
1:B:475:LYS:O	1:B:481:LYS:HD2	2.09	0.51
1:A:515:GLU:O	1:A:518:ASN:ND2	2.43	0.51
1:A:16:LEU:HD13	1:A:20:ASP:HB2	1.93	0.51
1:A:447:CYS:HB2	1:A:448:GLN:HE22	1.75	0.51
1:B:21:PHE:CE2	1:B:25:ILE:HG21	2.45	0.51
1:A:133:VAL:CG2	1:A:154:TYR:CE2	2.93	0.51
1:B:407:THR:HB	1:B:409:ASP:OD1	2.11	0.51
1:B:414:ILE:HD11	4:B:600:FAD:C7M	2.40	0.51
1:A:407:THR:HB	1:A:409:ASP:OD1	2.11	0.51
1:B:7:PHE:C	1:B:8:ARG:HG3	2.32	0.51
1:B:108:TYR:CZ	1:B:504:ARG:HG2	2.46	0.51
1:A:21:PHE:CE2	1:A:25:ILE:HG21	2.45	0.51
1:A:108:TYR:CZ	1:A:504:ARG:HG2	2.46	0.51
1:B:198:SER:O	1:B:240:HIS:HD2	1.94	0.51
1:A:198:SER:O	1:A:240:HIS:HD2	1.94	0.51
1:A:7:PHE:C	1:A:8:ARG:HG3	2.32	0.50
1:A:443:THR:HA	1:A:491:LEU:HD21	1.92	0.50
1:B:443:THR:HA	1:B:491:LEU:HD21	1.92	0.50
1:B:440:TYR:O	1:B:444:LYS:HB2	2.12	0.50
1:A:414:ILE:HD11	4:A:600:FAD:C7M	2.40	0.50
1:B:447:CYS:HB2	1:B:448:GLN:NE2	2.26	0.50
1:A:350:ARG:HD2	5:A:729:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD13	1:B:20:ASP:HB2	1.93	0.50
1:A:555:HIS:CB	1:A:559:LYS:HE3	2.31	0.50
1:B:6:GLU:CB	1:B:39:VAL:HG21	2.41	0.50
1:B:200:MET:CE	1:B:251:ASP:HB3	2.42	0.50
1:A:6:GLU:CB	1:A:39:VAL:HG21	2.41	0.50
1:A:200:MET:CE	1:A:251:ASP:HB3	2.42	0.50
1:B:479:ILE:HD12	1:B:479:ILE:H	1.76	0.50
1:A:408:TYR:N	5:A:620:HOH:O	2.44	0.50
1:A:447:CYS:HB2	1:A:448:GLN:NE2	2.26	0.50
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.94	0.50
1:A:156:GLU:CD	1:A:161:ARG:NH2	2.70	0.50
1:A:198:SER:HB3	1:A:240:HIS:HA	1.93	0.50
1:A:454:PHE:CD1	1:A:454:PHE:C	2.90	0.50
1:B:230:PRO:HA	1:B:233:GLN:CG	2.42	0.49
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.94	0.49
1:B:198:SER:HB3	1:B:240:HIS:HA	1.93	0.49
1:A:185:VAL:HG12	1:A:186:GLY:N	2.27	0.49
1:A:440:TYR:O	1:A:444:LYS:HB2	2.12	0.49
1:B:555:HIS:CB	1:B:559:LYS:HE3	2.31	0.49
1:B:132:GLU:CG	1:B:133:VAL:N	2.75	0.49
1:B:185:VAL:HG12	1:B:186:GLY:N	2.27	0.49
1:B:108:TYR:HD1	1:B:505:THR:C	2.20	0.49
1:A:201:GLU:HG2	1:A:263:THR:OG1	2.13	0.49
1:B:454:PHE:CD1	1:B:454:PHE:C	2.90	0.49
1:B:156:GLU:CD	1:B:161:ARG:NH2	2.70	0.49
1:B:526:ARG:HA	1:B:526:ARG:HD3	1.58	0.49
1:A:230:PRO:HA	1:A:233:GLN:CG	2.42	0.49
1:A:47:VAL:HG13	1:A:48:ASP:H	1.78	0.48
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.48	0.48
1:A:350:ARG:HD3	1:A:350:ARG:HA	1.75	0.48
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.94	0.48
1:B:457:THR:HG22	1:B:458:PHE:N	2.28	0.48
1:A:132:GLU:CG	1:A:133:VAL:N	2.75	0.48
1:A:457:THR:HG22	1:A:458:PHE:N	2.28	0.48
1:A:479:ILE:N	1:A:479:ILE:CD1	2.77	0.48
1:B:47:VAL:HG13	1:B:48:ASP:H	1.78	0.48
1:B:190:TYR:CE1	1:B:270:MET:HG3	2.48	0.48
1:A:108:TYR:HD1	1:A:505:THR:C	2.20	0.48
1:A:295:ILE:O	1:A:298:PRO:HD2	2.14	0.48
1:A:368:TRP:NE1	1:A:372:LYS:HD2	2.29	0.48
1:A:237:LYS:HD2	1:B:500:TRP:NE1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ILE:HD12	1:A:479:ILE:H	1.76	0.47
1:B:67:ASP:HB2	1:B:70:LEU:HD22	1.97	0.47
1:A:390:PRO:O	1:A:396:ARG:HD2	2.14	0.47
1:A:391:GLU:N	5:A:677:HOH:O	2.26	0.47
1:B:229:LYS:HB3	1:B:231:GLU:OE2	2.14	0.47
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.94	0.47
1:A:463:ARG:HD2	5:B:660:HOH:O	2.14	0.47
1:B:201:GLU:HG2	1:B:263:THR:OG1	2.13	0.47
1:B:295:ILE:O	1:B:298:PRO:HD2	2.14	0.47
1:B:368:TRP:NE1	1:B:372:LYS:HD2	2.29	0.47
1:A:79:ASN:ND2	1:A:79:ASN:C	2.69	0.47
1:A:67:ASP:HB2	1:A:70:LEU:HD22	1.96	0.47
1:A:538:ASN:HB2	1:A:540:ILE:CD1	2.39	0.47
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.49	0.47
1:B:278:SER:HA	1:B:356:ALA:HA	1.96	0.47
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.50	0.47
1:B:433:GLY:N	5:B:622:HOH:O	2.47	0.47
1:A:55:THR:HG21	1:A:58:HIS:CE1	2.49	0.47
1:A:151:LEU:HD23	1:A:166:LEU:CD2	2.44	0.47
1:A:218:PRO:HD2	5:A:685:HOH:O	2.15	0.47
1:A:276:TYR:CE1	1:A:356:ALA:HB1	2.49	0.47
1:A:423:LEU:O	1:A:471:ILE:HB	2.15	0.47
1:B:151:LEU:HD23	1:B:166:LEU:CD2	2.45	0.47
1:B:276:TYR:CE1	1:B:356:ALA:HB1	2.49	0.47
1:B:302:GLY:C	1:B:303:MET:HG3	2.40	0.47
1:B:405:ILE:HA	1:B:406:PRO:HD2	1.56	0.47
1:A:300:ARG:HG3	1:A:462:MET:HA	1.97	0.47
1:B:346:LEU:O	1:B:347:ASN:HB2	2.15	0.47
1:A:114:ARG:NH1	1:A:511:ASP:OD2	2.47	0.47
1:A:316:LEU:HD11	1:A:413:TRP:NE1	2.30	0.47
1:B:390:PRO:O	1:B:396:ARG:HD2	2.14	0.47
1:B:423:LEU:O	1:B:471:ILE:HB	2.15	0.47
1:A:316:LEU:CD1	1:A:413:TRP:CD1	2.98	0.47
1:A:349:GLY:CA	1:A:352:ASN:HD21	2.28	0.47
1:A:536:ASP:N	1:A:537:PRO:HD3	2.16	0.47
1:B:350:ARG:HD3	1:B:350:ARG:HA	1.75	0.47
1:A:47:VAL:CG1	1:A:48:ASP:N	2.78	0.46
1:A:195:MET:CE	1:B:195:MET:HE1	2.45	0.46
1:B:114:ARG:NH1	1:B:511:ASP:OD2	2.47	0.46
1:A:257:SER:HA	5:A:683:HOH:O	2.15	0.46
1:B:252:GLY:C	1:B:254:PHE:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLY:O	1:A:364:ARG:NE	2.48	0.46
1:A:252:GLY:C	1:A:254:PHE:H	2.24	0.46
1:A:252:GLY:C	1:A:254:PHE:N	2.71	0.46
1:A:195:MET:HE1	1:B:195:MET:CE	2.45	0.46
1:A:361:GLU:N	1:A:364:ARG:HH21	2.13	0.46
1:B:10:LEU:HD12	1:B:70:LEU:HD21	1.98	0.46
1:B:527:PHE:CE2	1:B:531:LEU:HD11	2.50	0.46
1:A:93:PHE:N	1:A:93:PHE:CD1	2.83	0.46
1:A:278:SER:HA	1:A:356:ALA:HA	1.96	0.46
1:A:302:GLY:C	1:A:303:MET:HG3	2.40	0.46
1:A:307:ASN:OD1	1:A:307:ASN:N	2.47	0.46
1:B:47:VAL:CG1	1:B:48:ASP:N	2.78	0.46
1:B:316:LEU:CD1	1:B:413:TRP:CD1	2.98	0.46
1:B:277:GLN:O	1:B:357:LEU:N	2.41	0.46
1:B:361:GLU:N	1:B:364:ARG:HH21	2.13	0.46
1:A:412:LYS:H	1:A:412:LYS:HG3	1.37	0.46
1:B:79:ASN:ND2	1:B:79:ASN:C	2.69	0.46
1:A:132:GLU:O	1:A:140:CYS:HA	2.16	0.46
1:A:229:LYS:HB3	1:A:231:GLU:OE2	2.14	0.46
1:A:346:LEU:O	1:A:347:ASN:HB2	2.15	0.46
1:A:491:LEU:HA	1:A:491:LEU:HD23	1.78	0.46
1:B:300:ARG:HG3	1:B:462:MET:HA	1.97	0.46
1:B:416:TRP:HB3	1:B:472:VAL:HG21	1.98	0.46
1:B:540:ILE:HD13	1:B:540:ILE:N	2.31	0.46
1:A:295:ILE:HD12	1:A:378:ILE:HD11	1.97	0.46
1:A:526:ARG:HA	1:A:526:ARG:HD3	1.58	0.46
1:B:359:GLY:O	1:B:364:ARG:NE	2.48	0.46
1:B:540:ILE:HG23	1:B:540:ILE:HD12	1.63	0.46
1:A:22:ASN:HA	1:A:25:ILE:CG2	2.46	0.45
1:A:188:THR:HB	1:A:189:PRO:CD	2.46	0.45
1:B:349:GLY:CA	1:B:352:ASN:HD21	2.28	0.45
1:B:479:ILE:N	1:B:479:ILE:CD1	2.77	0.45
1:A:309:PRO:O	1:A:460:VAL:HG23	2.16	0.45
1:A:383:PHE:CD1	1:A:383:PHE:N	2.85	0.45
1:B:132:GLU:O	1:B:140:CYS:HA	2.16	0.45
1:B:309:PRO:O	1:B:460:VAL:HG23	2.16	0.45
1:B:553:TYR:HD2	1:B:558:TRP:CD1	2.34	0.45
1:B:188:THR:HB	1:B:189:PRO:CD	2.46	0.45
1:B:307:ASN:N	1:B:307:ASN:OD1	2.47	0.45
1:B:538:ASN:HB2	1:B:540:ILE:CD1	2.40	0.45
1:A:332:GLU:CB	1:A:333:PRO:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:HIS:HA	1:B:266:GLY:O	2.16	0.45
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.47	0.45
1:A:278:SER:OG	1:A:399:ASP:OD1	2.31	0.45
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.98	0.45
1:A:67:ASP:OD1	1:A:67:ASP:N	2.49	0.45
1:A:367:LEU:O	1:A:371:ILE:HG13	2.17	0.45
1:B:316:LEU:HD11	1:B:413:TRP:NE1	2.30	0.45
1:A:65:ASP:O	1:A:68:TYR:HB2	2.17	0.45
1:B:252:GLY:C	1:B:254:PHE:H	2.24	0.45
1:B:295:ILE:HD12	1:B:378:ILE:HD11	1.97	0.45
1:B:409:ASP:HA	1:B:412:LYS:NZ	2.31	0.45
1:B:423:LEU:HD21	1:B:488:MET:CG	2.44	0.45
1:B:93:PHE:CD1	1:B:93:PHE:N	2.83	0.45
1:A:197:HIS:HA	1:A:266:GLY:O	2.17	0.45
1:A:409:ASP:HA	1:A:412:LYS:NZ	2.31	0.45
1:B:367:LEU:HD23	1:B:367:LEU:HA	1.66	0.45
1:B:383:PHE:CD1	1:B:383:PHE:N	2.84	0.45
1:A:62:HIS:O	1:A:62:HIS:ND1	2.50	0.45
1:A:132:GLU:HA	5:A:693:HOH:O	2.17	0.45
1:A:361:GLU:N	1:A:362:PRO:HD2	2.32	0.45
1:A:423:LEU:HD21	1:A:488:MET:CG	2.44	0.45
1:B:22:ASN:HA	1:B:25:ILE:CG2	2.46	0.45
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.47	0.45
1:B:361:GLU:N	1:B:362:PRO:HD2	2.32	0.45
1:A:447:CYS:CB	1:A:448:GLN:NE2	2.81	0.44
1:A:505:THR:CG2	1:A:506:HIS:N	2.72	0.44
1:A:553:TYR:HD2	1:A:558:TRP:CD1	2.34	0.44
1:B:151:LEU:CD2	1:B:166:LEU:HD21	2.48	0.44
1:B:155:LEU:HD22	1:B:160:LEU:HB2	1.99	0.44
1:A:426:SER:HA	1:A:427:PRO:HD2	1.63	0.44
1:B:102:ILE:CG1	1:B:175:SER:HB2	2.47	0.44
1:A:10:LEU:HD12	1:A:70:LEU:HD21	1.98	0.44
1:A:277:GLN:O	1:A:357:LEU:N	2.41	0.44
1:B:65:ASP:O	1:B:68:TYR:HB2	2.17	0.44
1:B:367:LEU:O	1:B:371:ILE:HG13	2.17	0.44
1:B:387:GLU:HA	1:B:387:GLU:OE1	2.17	0.44
1:A:519:TRP:CE3	1:B:211:ARG:HG3	2.49	0.44
1:A:540:ILE:N	1:A:540:ILE:HD13	2.31	0.44
1:B:62:HIS:O	1:B:62:HIS:ND1	2.50	0.44
1:B:179:ASN:OD1	1:B:184:GLY:HA3	2.17	0.44
1:A:480:GLN:O	1:A:484:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.53	0.44
1:A:102:ILE:CG1	1:A:175:SER:HB2	2.47	0.44
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.66	0.44
1:A:428:ILE:HD12	1:A:428:ILE:HG23	1.60	0.44
1:A:443:THR:O	1:A:443:THR:HG22	2.18	0.44
1:A:290:LYS:HG3	1:A:433:GLY:HA3	2.00	0.44
1:A:387:GLU:OE1	1:A:387:GLU:HA	2.17	0.44
1:B:108:TYR:CD1	1:B:505:THR:C	2.96	0.44
1:A:151:LEU:CD2	1:A:166:LEU:HD21	2.48	0.44
1:A:179:ASN:OD1	1:A:184:GLY:HA3	2.17	0.44
1:B:344:LYS:HG3	1:B:345:GLN:N	2.33	0.44
1:B:480:GLN:O	1:B:484:VAL:HG23	2.18	0.44
1:A:37:VAL:HG13	1:A:75:VAL:CG2	2.46	0.43
1:B:101:SER:O	1:B:124:GLY:HA3	2.17	0.43
1:A:101:SER:O	1:A:124:GLY:HA3	2.17	0.43
1:A:187:TYR:CD2	1:A:187:TYR:N	2.81	0.43
1:A:241:LEU:HB3	1:B:463:ARG:O	2.17	0.43
1:A:332:GLU:CB	1:A:333:PRO:CD	2.95	0.43
1:B:61:HIS:CE1	1:B:422:HIS:CE1	3.06	0.43
1:A:540:ILE:HD12	1:A:540:ILE:HG23	1.63	0.43
1:B:447:CYS:CB	1:B:448:GLN:NE2	2.80	0.43
1:A:76:ALA:HA	1:A:77:PRO:HD2	1.69	0.43
1:A:155:LEU:HD22	1:A:160:LEU:HB2	1.99	0.43
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.68	0.43
1:B:332:GLU:CB	1:B:333:PRO:CD	2.95	0.43
1:A:108:TYR:CD1	1:A:505:THR:C	2.96	0.43
1:A:361:GLU:N	1:A:362:PRO:CD	2.80	0.43
1:B:201:GLU:OE1	1:B:211:ARG:HD3	2.18	0.43
1:B:535:VAL:C	1:B:537:PRO:HD3	2.43	0.43
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.54	0.43
1:A:12:LEU:HB3	1:A:13:PRO:HD2	2.01	0.43
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.71	0.43
1:A:201:GLU:OE1	1:A:211:ARG:HD3	2.18	0.43
1:A:211:ARG:HD3	1:B:519:TRP:CH2	2.53	0.43
1:A:311:ILE:HG12	1:A:353:PHE:HD1	1.84	0.43
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.54	0.43
1:B:13:PRO:HG3	1:B:95:PHE:CZ	2.53	0.43
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.53	0.43
1:A:13:PRO:HG3	1:A:95:PHE:CZ	2.53	0.43
1:A:244:TYR:HH	1:B:195:MET:HG2	1.84	0.43
1:A:403:GLN:HG3	1:A:405:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:HB2	1:A:223:PRO:HD2	2.01	0.43
1:B:290:LYS:HG3	1:B:433:GLY:HA3	2.00	0.43
1:B:555:HIS:O	1:B:559:LYS:HG3	2.19	0.43
1:A:222:ARG:HA	1:A:223:PRO:HD3	1.76	0.42
1:A:231:GLU:H	1:A:231:GLU:HG3	0.96	0.42
1:A:61:HIS:CE1	1:A:422:HIS:CE1	3.06	0.42
1:A:142:VAL:O	1:A:264:LYS:HA	2.19	0.42
1:A:217:LEU:HD13	1:A:217:LEU:C	2.44	0.42
1:A:344:LYS:HG3	1:A:345:GLN:N	2.33	0.42
1:A:361:GLU:HB2	1:A:364:ARG:NH2	2.34	0.42
1:B:14:PRO:HB2	5:B:749:HOH:O	2.19	0.42
1:B:142:VAL:O	1:B:264:LYS:HA	2.19	0.42
1:A:214:MET:HE1	1:B:517:TYR:OH	2.18	0.42
1:A:385:PHE:CB	1:A:386:PRO:HD2	2.38	0.42
1:B:278:SER:OG	1:B:399:ASP:OD1	2.31	0.42
1:A:188:THR:CB	1:A:189:PRO:CD	2.98	0.42
1:A:304:ALA:HA	1:A:367:LEU:HD22	2.01	0.42
1:B:62:HIS:O	1:B:481:LYS:HE3	2.19	0.42
1:B:156:GLU:CG	1:B:161:ARG:CZ	2.98	0.42
1:B:188:THR:CB	1:B:189:PRO:CD	2.98	0.42
1:B:428:ILE:HG23	1:B:428:ILE:HD12	1.60	0.42
1:A:447:CYS:C	1:A:448:GLN:NE2	2.77	0.42
1:A:478:LEU:N	1:A:478:LEU:CD1	2.79	0.42
1:B:181:VAL:O	1:B:255:SER:HB2	2.20	0.42
1:B:217:LEU:C	1:B:217:LEU:HD13	2.44	0.42
1:B:361:GLU:HB2	1:B:364:ARG:NH2	2.34	0.42
1:B:443:THR:O	1:B:443:THR:HG22	2.18	0.42
1:A:108:TYR:CE1	1:A:504:ARG:HG2	2.54	0.42
1:A:177:LEU:HD22	1:A:265:ILE:HG22	2.01	0.42
1:A:181:VAL:O	1:A:255:SER:HB2	2.20	0.42
1:B:12:LEU:HB3	1:B:13:PRO:HD2	2.01	0.42
1:B:330:ARG:NH1	1:B:338:GLU:CD	2.78	0.42
1:B:361:GLU:N	1:B:362:PRO:CD	2.80	0.42
1:B:413:TRP:C	1:B:415:ASP:N	2.77	0.42
1:B:108:TYR:CE1	1:B:504:ARG:HG2	2.54	0.42
1:A:62:HIS:O	1:A:481:LYS:HE3	2.19	0.42
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.87	0.42
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.93	0.42
1:B:222:ARG:HB2	1:B:223:PRO:HD2	2.01	0.42
1:B:243:PRO:CD	1:B:244:TYR:H	2.32	0.42
1:B:304:ALA:HA	1:B:367:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ILE:HG12	1:B:353:PHE:HD1	1.83	0.42
1:B:491:LEU:HD23	1:B:491:LEU:HA	1.78	0.42
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.71	0.42
1:B:403:GLN:HG3	1:B:405:ILE:HG13	2.00	0.42
1:A:16:LEU:CD1	1:A:21:PHE:N	2.83	0.42
1:A:156:GLU:CG	1:A:161:ARG:CZ	2.98	0.42
1:A:195:MET:CE	1:B:195:MET:CE	2.97	0.42
1:B:177:LEU:HD22	1:B:265:ILE:HG22	2.01	0.42
1:A:330:ARG:NH1	1:A:338:GLU:CD	2.78	0.41
1:B:16:LEU:CD1	1:B:21:PHE:N	2.83	0.41
1:A:12:LEU:HA	1:A:13:PRO:HD3	1.73	0.41
1:A:237:LYS:HD2	1:B:500:TRP:CD1	2.56	0.41
1:A:555:HIS:O	1:A:559:LYS:HG3	2.19	0.41
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.48	0.41
1:B:416:TRP:O	1:B:417:LEU:HD23	2.19	0.41
1:A:217:LEU:CD2	1:B:516:THR:CG2	2.98	0.41
1:A:279:TYR:CD1	1:A:279:TYR:C	2.98	0.41
1:A:416:TRP:O	1:A:417:LEU:HD23	2.19	0.41
1:B:67:ASP:N	1:B:67:ASP:OD1	2.49	0.41
1:B:151:LEU:HG	1:B:166:LEU:HD21	2.03	0.41
1:A:50:SER:C	1:A:52:MET:N	2.78	0.41
1:A:156:GLU:CB	1:A:161:ARG:NE	2.80	0.41
1:A:535:VAL:C	1:A:537:PRO:HD3	2.43	0.41
1:A:553:TYR:HD2	1:A:558:TRP:NE1	2.19	0.41
1:A:413:TRP:C	1:A:415:ASP:N	2.77	0.41
1:B:156:GLU:CB	1:B:161:ARG:NE	2.79	0.41
1:B:536:ASP:N	1:B:537:PRO:HD3	2.16	0.41
1:A:64:MET:HG2	1:A:68:TYR:CD2	2.56	0.41
1:A:151:LEU:HG	1:A:166:LEU:HD21	2.03	0.41
1:A:185:VAL:CG1	1:A:186:GLY:N	2.84	0.41
1:A:213:GLY:HA3	5:A:717:HOH:O	2.20	0.41
1:A:517:TYR:CE1	1:B:246:PHE:CB	3.04	0.41
1:A:537:PRO:HD2	5:A:742:HOH:O	2.19	0.41
1:B:50:SER:O	1:B:54:PRO:N	2.54	0.41
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.89	0.41
1:B:518:ASN:O	1:B:519:TRP:C	2.64	0.41
1:A:311:ILE:O	1:A:457:THR:HG23	2.21	0.41
1:B:12:LEU:HA	1:B:13:PRO:HD3	1.72	0.41
1:B:202:VAL:HA	1:B:261:ILE:O	2.21	0.41
1:B:502:GLU:N	1:B:502:GLU:CD	2.79	0.41
1:A:177:LEU:HB2	1:A:265:ILE:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:TYR:CD1	1:B:279:TYR:C	2.98	0.40
1:A:305:LEU:HA	1:A:305:LEU:HD23	1.89	0.40
1:A:502:GLU:N	1:A:502:GLU:CD	2.79	0.40
1:B:156:GLU:CB	1:B:161:ARG:CZ	2.99	0.40
1:B:6:GLU:CB	1:B:39:VAL:CG2	3.00	0.40
1:B:64:MET:HG2	1:B:68:TYR:CD2	2.56	0.40
1:B:417:LEU:N	1:B:417:LEU:CD2	2.84	0.40
1:B:447:CYS:C	1:B:448:GLN:NE2	2.77	0.40
1:A:47:VAL:HG22	1:A:66:GLN:HE22	1.87	0.40
1:A:151:LEU:CD2	1:A:166:LEU:CD2	2.99	0.40
1:A:272:ASN:HA	1:A:273:PRO:HD3	1.85	0.40
1:A:344:LYS:CG	1:A:345:GLN:N	2.85	0.40
1:B:187:TYR:OH	4:B:600:FAD:O4	2.39	0.40
1:A:243:PRO:CD	1:A:244:TYR:H	2.32	0.40
1:A:517:TYR:OH	1:B:214:MET:HE1	2.21	0.40
1:B:229:LYS:HB3	1:B:231:GLU:CD	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:NH2	1:A:330:ARG:NH2[2_765]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	14	27
1	B	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	14	27
All	All	1092/1120 (98%)	1006 (92%)	76 (7%)	10 (1%)	14	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	48	ASP
1	A	199	GLY
1	A	388	ASP
1	B	199	GLY
1	B	388	ASP
1	A	327	TYR
1	B	327	TYR
1	A	328	SER
1	B	328	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/482 (98%)	450 (96%)	20 (4%)	26	51
1	B	470/482 (98%)	450 (96%)	20 (4%)	26	51
All	All	940/964 (98%)	900 (96%)	40 (4%)	26	51

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	16	LEU
1	A	64	MET
1	A	65	ASP
1	A	79	ASN
1	A	114	ARG
1	A	122	ASP
1	A	177	LEU
1	A	238	ILE
1	A	248	PRO
1	A	301	LEU
1	A	314	ILE
1	A	381	VAL

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Mol	Chain	Res	Type
1	A	448	GLN
1	A	464	GLU
1	A	479	ILE
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	552	GLN
1	B	7	PHE
1	B	16	LEU
1	B	64	MET
1	B	65	ASP
1	B	79	ASN
1	B	114	ARG
1	B	122	ASP
1	B	177	LEU
1	B	238	ILE
1	B	248	PRO
1	B	301	LEU
1	B	314	ILE
1	B	381	VAL
1	B	448	GLN
1	B	464	GLU
1	B	479	ILE
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	79	ASN
1	A	84	GLN
1	A	91	ASN
1	A	152	HIS
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	448	GLN
1	A	480	GLN
1	A	485	GLN

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Mol	Chain	Res	Type
1	A	518	ASN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	56	HIS
1	B	66	GLN
1	B	79	ASN
1	B	84	GLN
1	B	91	ASN
1	B	128	ASN
1	B	152	HIS
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	448	GLN
1	B	480	GLN
1	B	485	GLN
1	B	518	ASN
1	B	520	ASN
1	B	552	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	ACT	B	601	-	3,3,3	1.08	0	3,3,3	0.90	0
4	FAD	A	600	1	58,58,58	1.01	5 (8%)	85,89,89	0.93	4 (4%)
2	ACT	A	601	-	3,3,3	1.06	0	3,3,3	0.90	0
4	FAD	B	600	1	58,58,58	1.01	5 (8%)	85,89,89	0.93	4 (4%)

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	FAD	A	600	1	-	6/34/50/50	0/6/6/6
4	FAD	B	600	1	-	6/34/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	FAD	O5B-C5B	-3.59	1.31	1.44
4	B	600	FAD	O5B-C5B	-3.58	1.31	1.44
4	A	600	FAD	P-O3P	3.11	1.62	1.59
4	B	600	FAD	P-O3P	3.09	1.62	1.59
4	B	600	FAD	PA-O3P	2.79	1.62	1.59
4	A	600	FAD	PA-O3P	2.79	1.62	1.59
4	B	600	FAD	C5X-N5	-2.23	1.35	1.39
4	A	600	FAD	C5X-N5	-2.22	1.35	1.39
4	A	600	FAD	C4X-N5	2.20	1.35	1.30
4	B	600	FAD	C4X-N5	2.19	1.35	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	O4B-C1B-N9A	2.66	113.19	108.09
4	B	600	FAD	O4B-C1B-N9A	2.63	113.14	108.09
4	A	600	FAD	C4'-C3'-C2'	-2.45	109.49	113.57
4	B	600	FAD	C4'-C3'-C2'	-2.43	109.53	113.57
4	B	600	FAD	C4-N3-C2	-2.36	121.46	125.64
4	A	600	FAD	C4-N3-C2	-2.32	121.53	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	FAD	O4B-C4B-C5B	-2.26	102.09	109.33
4	A	600	FAD	O4B-C4B-C5B	-2.25	102.12	109.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

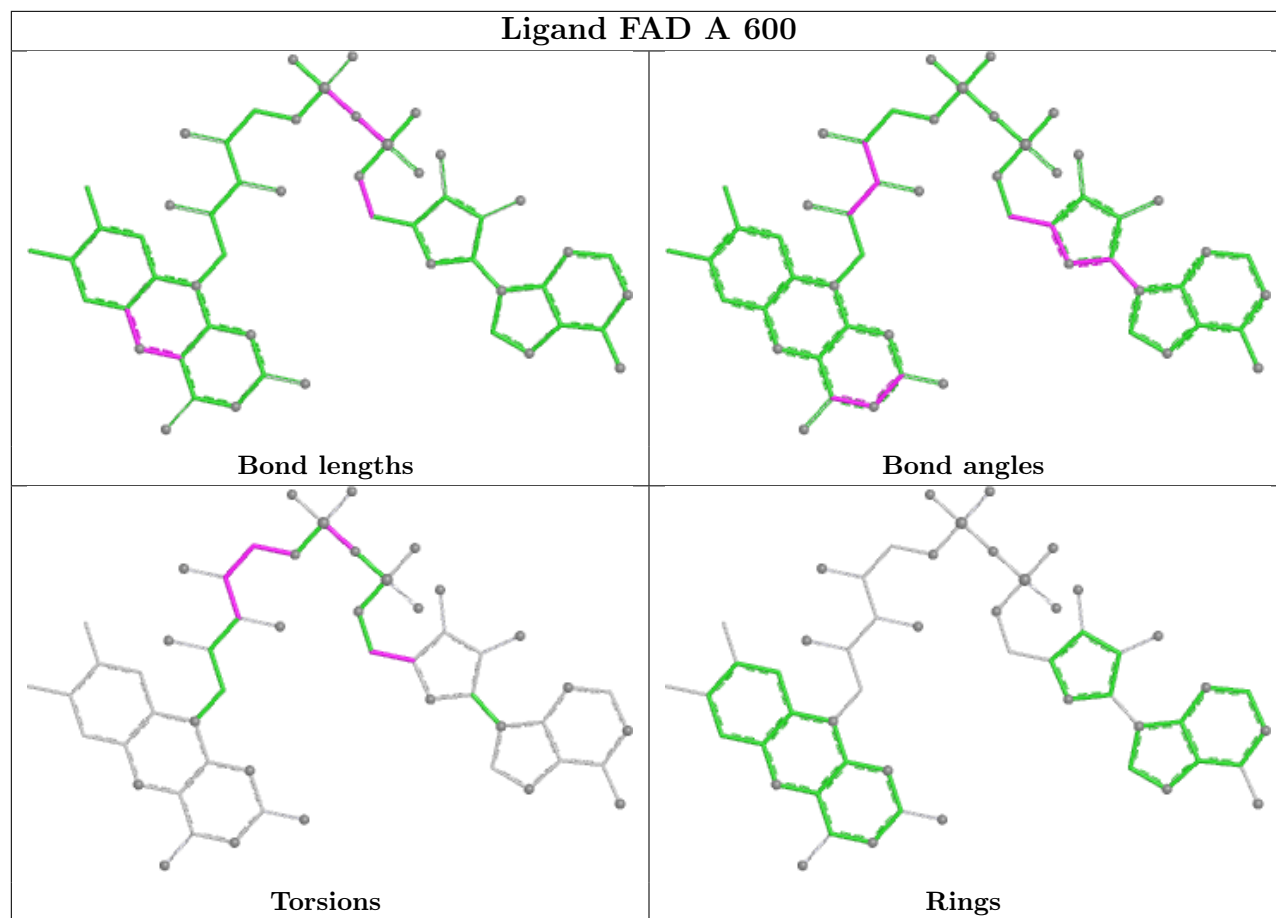
Mol	Chain	Res	Type	Atoms
4	A	600	FAD	C3'-C4'-C5'-O5'
4	A	600	FAD	O4'-C4'-C5'-O5'
4	B	600	FAD	C3'-C4'-C5'-O5'
4	B	600	FAD	O4'-C4'-C5'-O5'
4	A	600	FAD	C4'-C5'-O5'-P
4	B	600	FAD	C4'-C5'-O5'-P
4	A	600	FAD	C2'-C3'-C4'-O4'
4	B	600	FAD	C2'-C3'-C4'-O4'
4	A	600	FAD	PA-O3P-P-O2P
4	B	600	FAD	PA-O3P-P-O2P
4	A	600	FAD	O4B-C4B-C5B-O5B
4	B	600	FAD	O4B-C4B-C5B-O5B

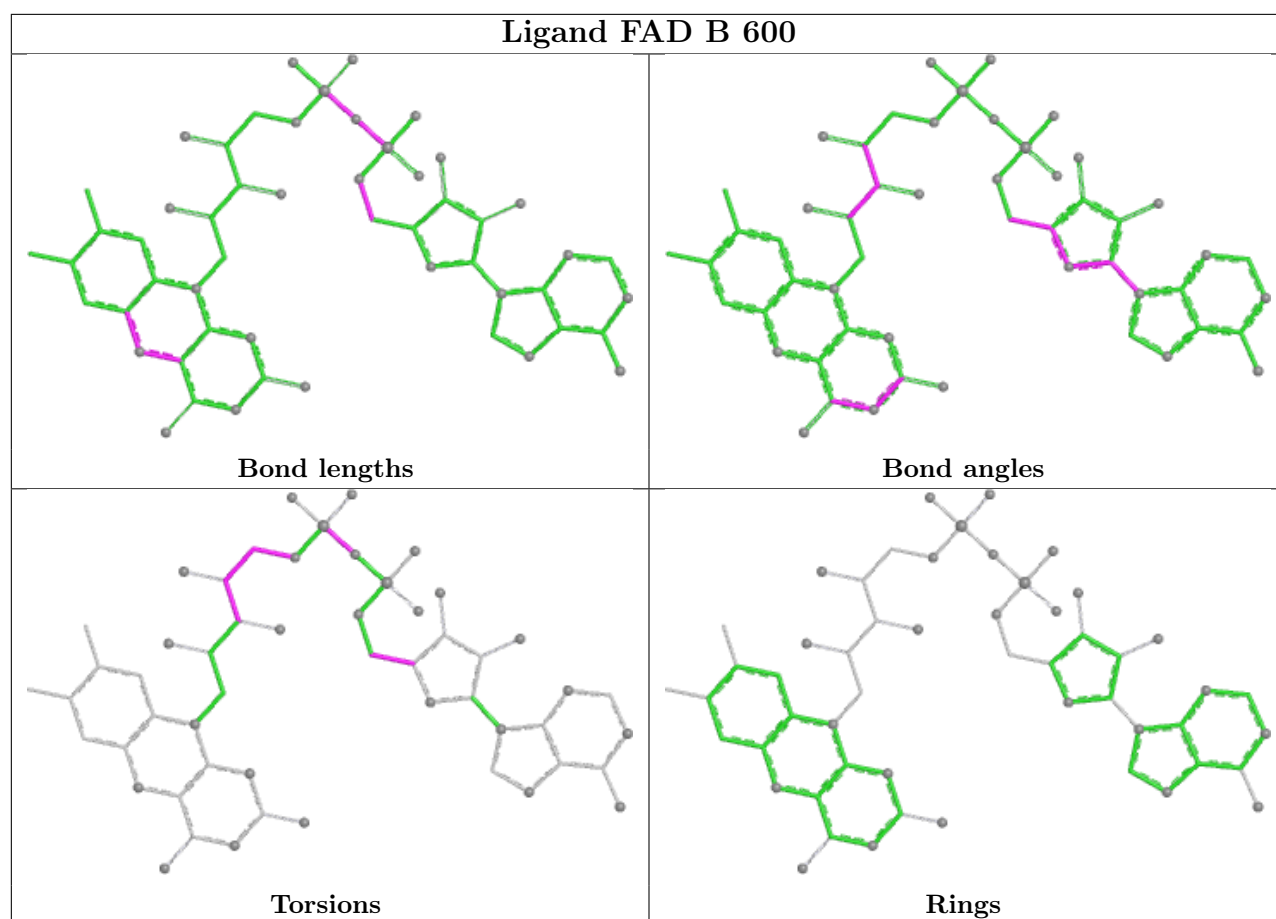
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	FAD	5	0
4	B	600	FAD	6	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.