



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:12 PM UTC

PDB ID : 3W4K / pdb_00003w4k
Title : Crystal Structure of human DAAO in complex with coumpound 13
Authors : Hondo, T.; Warizaya, M.; Niimi, T.; Namatame, I.; Yamaguchi, T.; Nakanishi, K.; Hamajima, T.; Harada, K.; Sakashita, H.; Matsumoto, Y.; Orita, M.; Watanabe, T.; Takeuchi, M.
Deposited on : 2013-01-09
Resolution : 2.86 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

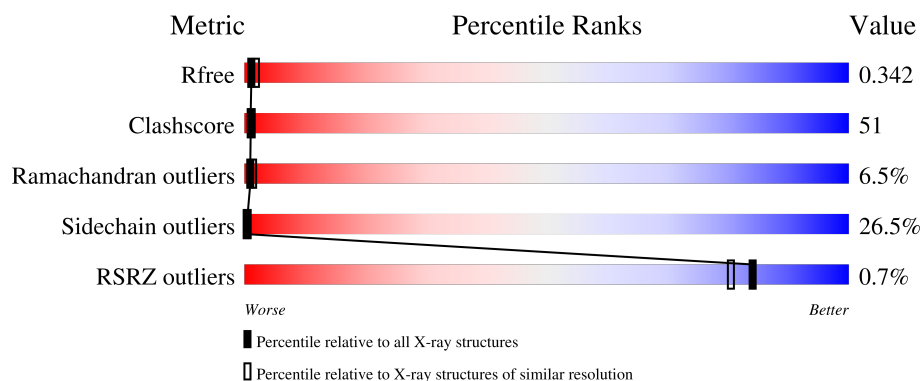
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

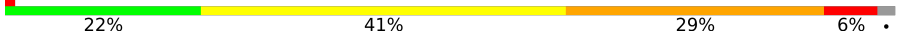
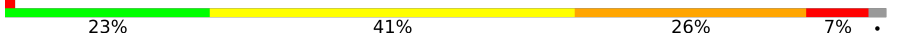
The reported resolution of this entry is 2.86 Å.

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))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	

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
3	3LD	D	402	-	-	X	-

2 Entry composition ⓘ

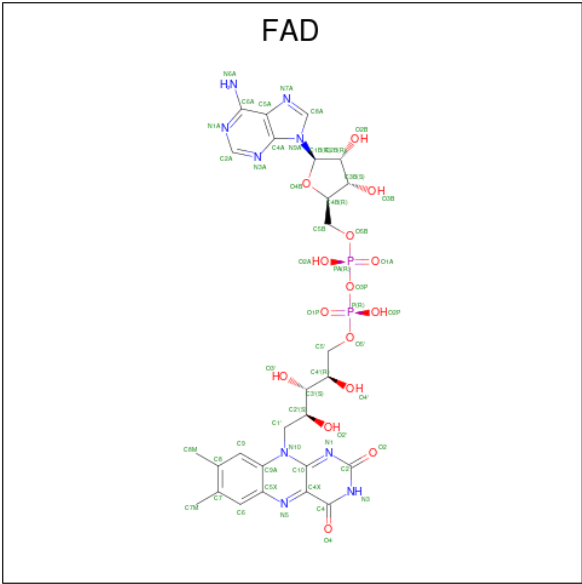
There are 3 unique types of molecules in this entry. The entry contains 11208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	B	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	C	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	D	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			

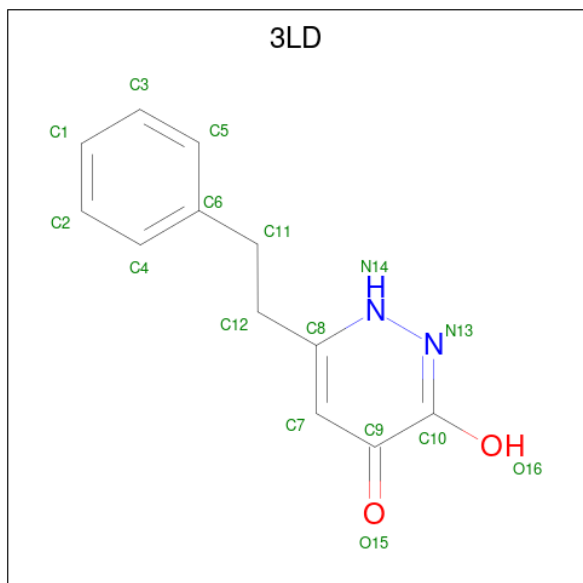
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is 3-hydroxy-6-(2-phenylethyl)pyridazin-4(1H)-one (CCD ID: 3LD) (formula: $C_{12}H_{12}N_2O_2$).

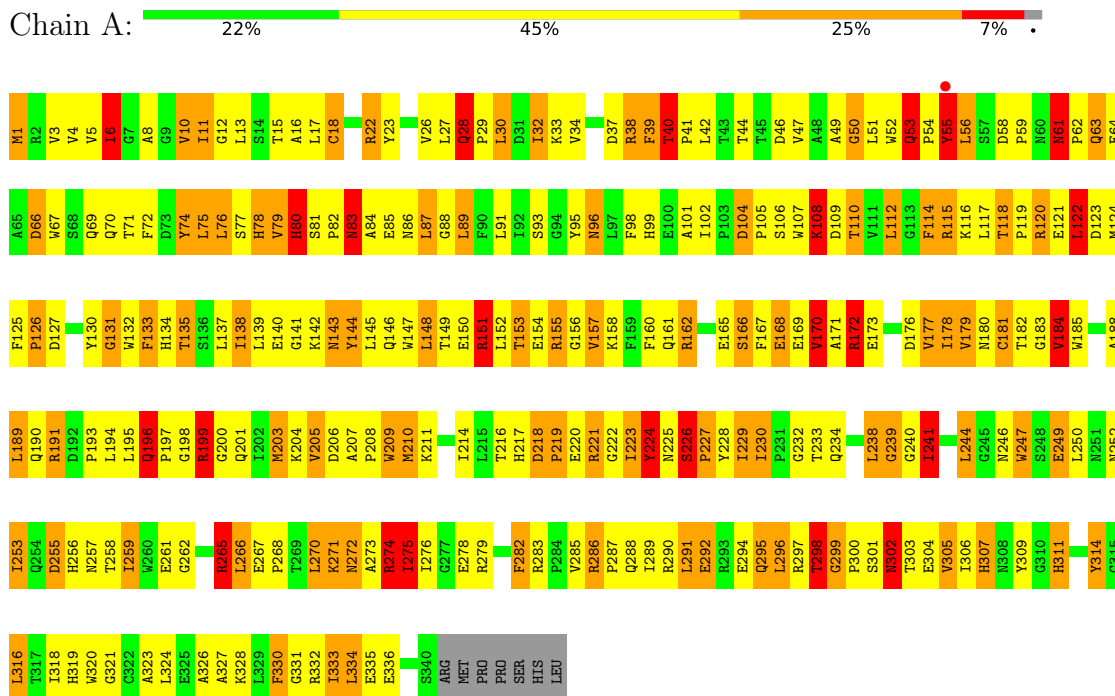


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	12	2	2		
3	B	1	Total	C	N	O	0	0
			16	12	2	2		
3	C	1	Total	C	N	O	0	0
			16	12	2	2		
3	D	1	Total	C	N	O	0	0
			16	12	2	2		

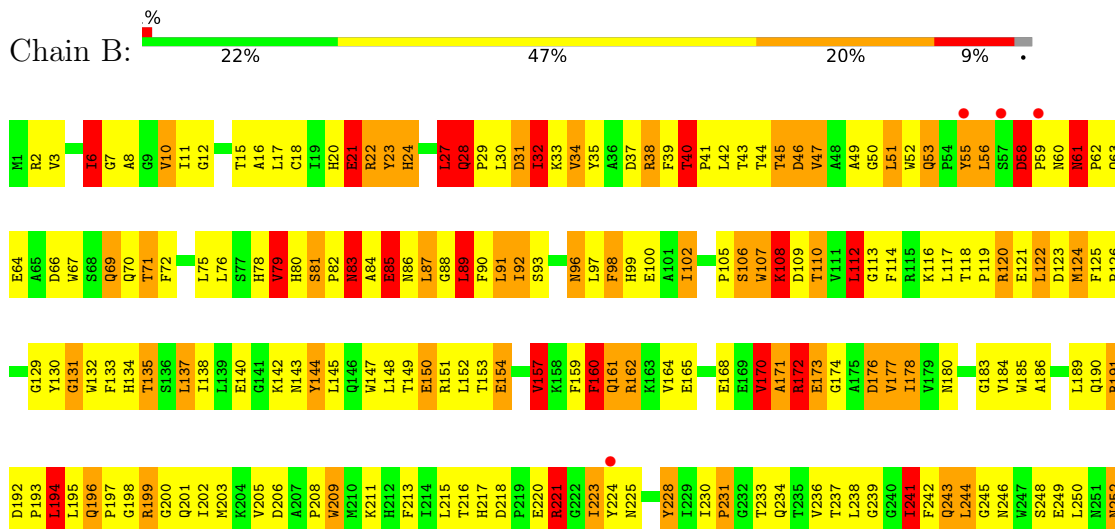
3 Residue-property plots

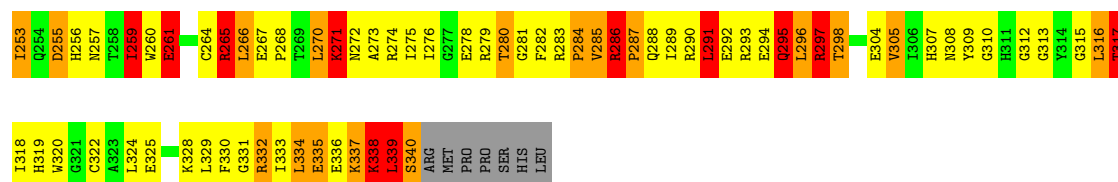
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: D-amino-acid oxidase

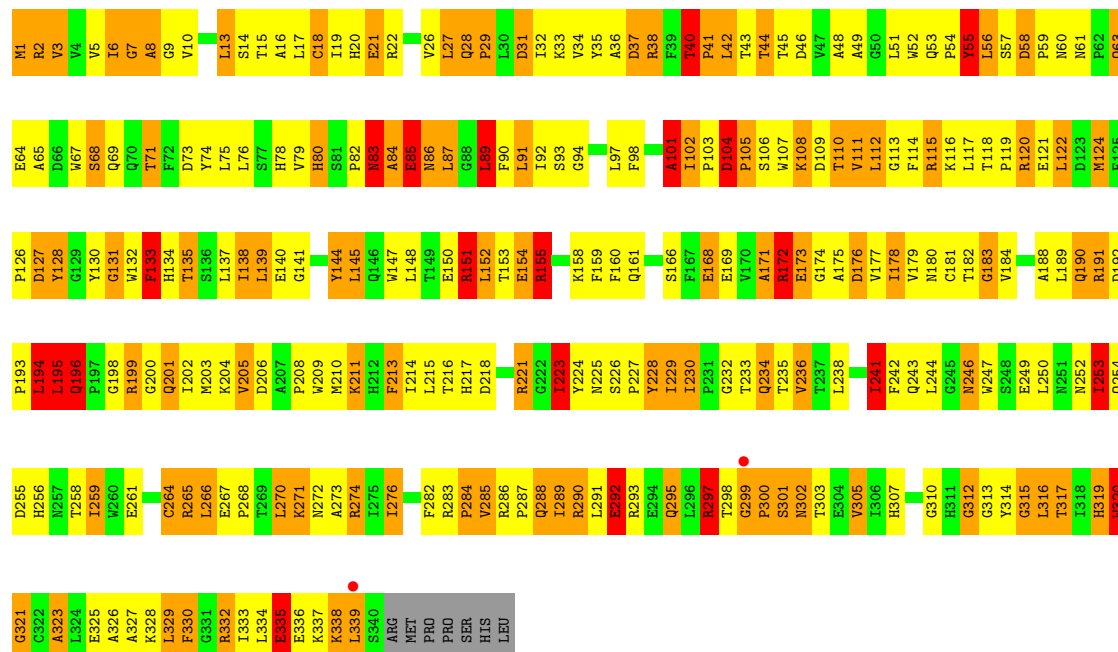
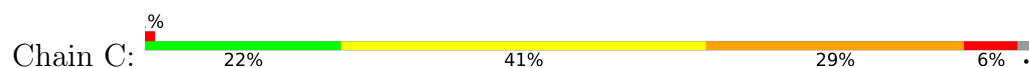


• Molecule 1: D-amino-acid oxidase

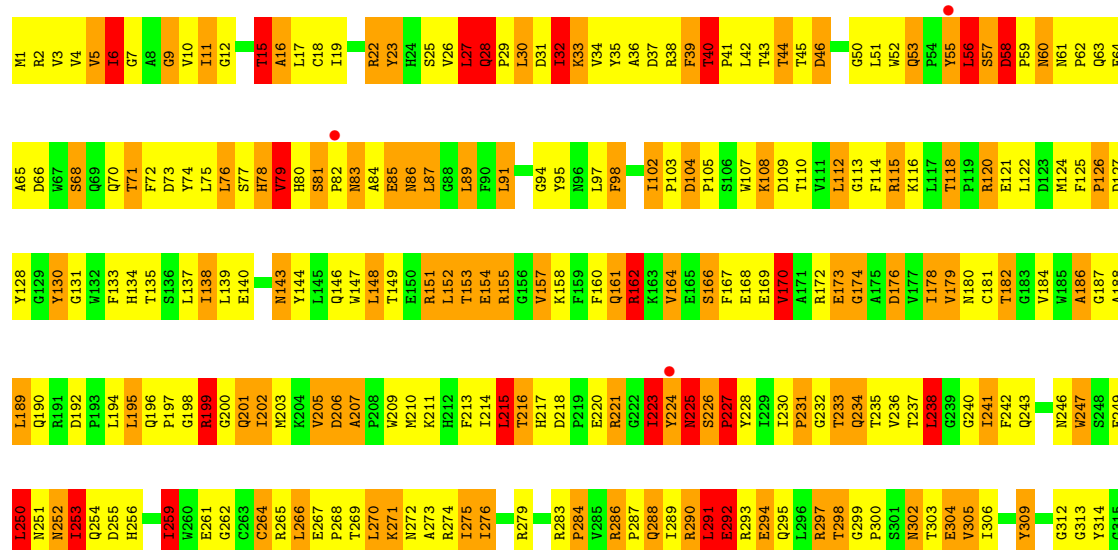
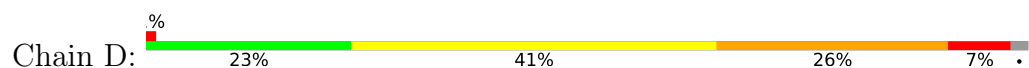




• Molecule 1: D-amino-acid oxidase



• Molecule 1: D-amino-acid oxidase



I316	T317	I318	H319	W320	G321	C322	A323	L324	E325	K328	I333	K337	K338	L339	S340	ARG	MET	PRO	PRO	SER	HIS	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.66Å 182.46Å 50.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.95 – 2.86 38.95 – 2.86	Depositor EDS
% Data completeness (in resolution range)	92.9 (38.95-2.86) 92.9 (38.95-2.86)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.233 , 0.344 0.235 , 0.342	Depositor DCC
R_{free} test set	1566 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11208	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2218e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3LD, 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	1.85	40/2810 (1.4%)	1.88	81/3824 (2.1%)
1	B	1.86	46/2810 (1.6%)	1.95	83/3824 (2.2%)
1	C	1.78	43/2810 (1.5%)	1.91	82/3824 (2.1%)
1	D	1.77	30/2810 (1.1%)	1.87	73/3824 (1.9%)
All	All	1.81	159/11240 (1.4%)	1.90	319/15296 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	6

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	ILE	C-N	28.99	1.69	1.33
1	A	18	CYS	N-CA	-9.25	1.35	1.46
1	B	276	ILE	CA-C	-9.05	1.41	1.52
1	C	289	ILE	CA-CB	-9.00	1.45	1.54
1	B	32	ILE	CA-CB	-8.88	1.43	1.54
1	B	47	VAL	CA-CB	-8.68	1.43	1.54
1	A	138	ILE	CA-CB	-8.62	1.43	1.54
1	D	216	THR	CA-CB	-8.25	1.40	1.53
1	D	250	LEU	N-CA	-7.98	1.36	1.46
1	A	275	ILE	CA-CB	-7.89	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	ILE	CA-CB	7.83	1.63	1.54
1	C	235	THR	N-CA	-7.74	1.36	1.46
1	B	34	VAL	CA-C	-7.54	1.43	1.52
1	B	282	PHE	C-O	-7.45	1.15	1.24
1	C	194	LEU	CA-C	7.42	1.62	1.52
1	B	244	LEU	N-CA	7.42	1.55	1.46
1	A	5	VAL	CA-CB	-7.41	1.45	1.53
1	D	81	SER	CA-C	7.34	1.59	1.52
1	B	76	LEU	CA-C	-7.32	1.42	1.52
1	B	89	LEU	CA-C	-7.25	1.43	1.52
1	A	49	ALA	C-O	-7.17	1.15	1.24
1	B	252	ASN	CA-C	7.14	1.61	1.52
1	D	207	ALA	CA-CB	-7.13	1.42	1.53
1	C	3	VAL	CA-C	7.13	1.61	1.52
1	C	83	ASN	N-CA	7.12	1.55	1.46
1	A	178	ILE	CA-CB	-7.06	1.45	1.54
1	A	230	ILE	CA-CB	-7.05	1.45	1.54
1	B	83	ASN	CA-C	7.03	1.62	1.52
1	D	284	PRO	CA-C	7.01	1.59	1.52
1	A	8	ALA	CA-C	-6.96	1.44	1.52
1	A	11	ILE	CA-CB	-6.90	1.46	1.54
1	B	79	VAL	CA-C	-6.87	1.44	1.52
1	A	99	HIS	CA-C	6.84	1.61	1.52
1	D	252	ASN	N-CA	-6.79	1.38	1.46
1	D	170	VAL	CA-CB	6.75	1.62	1.54
1	B	92	ILE	CA-CB	6.74	1.63	1.54
1	B	102	ILE	CA-CB	6.71	1.62	1.54
1	B	69	GLN	CA-C	-6.71	1.44	1.52
1	B	23	TYR	N-CA	-6.67	1.40	1.46
1	C	276	ILE	CA-C	-6.64	1.45	1.52
1	C	90	PHE	C-O	6.62	1.32	1.23
1	B	339	LEU	CA-C	6.62	1.60	1.52
1	B	255	ASP	CA-C	6.58	1.61	1.52
1	C	89	LEU	C-O	-6.55	1.16	1.24
1	B	289	ILE	CA-CB	-6.55	1.47	1.54
1	B	305	VAL	CA-CB	-6.55	1.46	1.54
1	C	111	VAL	CA-CB	6.50	1.63	1.54
1	C	86	ASN	N-CA	6.47	1.53	1.46
1	C	223	ILE	CA-CB	6.46	1.61	1.54
1	D	4	VAL	N-CA	6.42	1.54	1.46
1	C	330	PHE	CA-C	6.33	1.61	1.52
1	B	11	ILE	CA-C	6.32	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLN	C-O	6.31	1.30	1.24
1	A	80	HIS	CA-C	-6.22	1.45	1.52
1	B	85	GLU	CA-C	6.21	1.61	1.52
1	D	262	GLY	C-O	6.17	1.31	1.23
1	D	78	HIS	CA-C	6.12	1.60	1.52
1	C	276	ILE	C-O	-6.11	1.16	1.24
1	A	326	ALA	CA-CB	-6.11	1.43	1.53
1	D	266	LEU	CA-C	6.11	1.60	1.52
1	C	236	VAL	CA-CB	-6.10	1.46	1.54
1	C	133	PHE	CA-C	-6.09	1.45	1.52
1	A	229	ILE	CA-CB	6.07	1.62	1.54
1	B	31	ASP	CA-C	-6.06	1.45	1.52
1	C	18	CYS	CB-SG	-6.04	1.61	1.81
1	D	237	THR	N-CA	-6.03	1.38	1.46
1	D	157	VAL	CA-CB	-5.97	1.47	1.54
1	A	30	LEU	CA-C	5.97	1.60	1.53
1	A	10	VAL	CA-CB	-5.90	1.46	1.54
1	B	71	THR	CA-CB	5.90	1.62	1.53
1	B	237	THR	CA-C	-5.90	1.45	1.52
1	A	239	GLY	N-CA	5.88	1.51	1.44
1	D	224	TYR	C-N	-5.87	1.25	1.33
1	D	270	LEU	N-CA	-5.86	1.38	1.46
1	B	98	PHE	CA-C	-5.85	1.45	1.52
1	B	21	GLU	CG-CD	5.82	1.66	1.52
1	B	297	ARG	CB-CG	5.82	1.70	1.52
1	C	82	PRO	CA-C	5.82	1.60	1.52
1	B	194	LEU	CA-C	5.81	1.60	1.52
1	D	235	THR	CA-CB	5.81	1.64	1.53
1	A	12	GLY	C-O	5.80	1.30	1.23
1	C	236	VAL	N-CA	-5.77	1.39	1.46
1	B	112	LEU	CA-C	-5.77	1.46	1.52
1	A	196	GLN	N-CA	5.74	1.51	1.45
1	D	16	ALA	CA-CB	-5.73	1.44	1.53
1	A	181	CYS	CA-C	-5.72	1.43	1.52
1	D	4	VAL	CA-CB	5.71	1.60	1.54
1	C	37	ASP	CA-C	-5.70	1.45	1.52
1	A	253	ILE	CA-C	5.69	1.59	1.52
1	B	72	PHE	CA-CB	-5.65	1.44	1.53
1	C	228	TYR	CA-C	5.63	1.59	1.52
1	B	79	VAL	CA-CB	-5.62	1.47	1.54
1	B	275	ILE	CA-C	5.62	1.60	1.52
1	B	96	ASN	CA-C	5.60	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	TYR	CA-C	5.60	1.59	1.52
1	A	265	ARG	C-O	-5.59	1.17	1.24
1	C	196	GLN	N-CA	5.58	1.51	1.45
1	D	5	VAL	CA-CB	-5.58	1.47	1.54
1	C	3	VAL	CA-CB	-5.58	1.47	1.54
1	A	18	CYS	CB-SG	-5.55	1.62	1.81
1	C	303	THR	CA-CB	5.55	1.62	1.53
1	B	275	ILE	CA-CB	5.54	1.61	1.54
1	C	65	ALA	CA-C	-5.54	1.45	1.52
1	A	96	ASN	CA-C	5.52	1.59	1.52
1	A	207	ALA	CA-CB	-5.51	1.46	1.53
1	C	57	SER	CA-C	5.48	1.60	1.52
1	D	98	PHE	CA-C	-5.47	1.45	1.52
1	A	272	ASN	N-CA	-5.47	1.38	1.46
1	C	323	ALA	C-O	5.46	1.30	1.24
1	C	213	PHE	CA-C	5.45	1.59	1.52
1	A	28	GLN	CG-CD	5.45	1.65	1.52
1	A	142	LYS	N-CA	5.44	1.52	1.46
1	A	85	GLU	CA-C	5.41	1.60	1.52
1	B	35	TYR	C-O	5.40	1.30	1.24
1	A	309	TYR	CA-C	-5.40	1.46	1.52
1	D	120	ARG	CA-C	5.39	1.60	1.52
1	B	46	ASP	N-CA	5.39	1.53	1.46
1	D	184	VAL	N-CA	-5.38	1.39	1.46
1	A	286	ARG	CA-C	5.38	1.59	1.52
1	C	56	LEU	N-CA	5.37	1.52	1.46
1	B	165	GLU	C-O	-5.36	1.17	1.24
1	C	300	PRO	CA-C	5.34	1.59	1.52
1	D	265	ARG	C-O	-5.32	1.18	1.24
1	A	282	PHE	C-O	-5.31	1.17	1.24
1	B	55	TYR	N-CA	5.30	1.53	1.46
1	C	320	TRP	CA-C	5.29	1.59	1.52
1	B	157	VAL	CA-CB	-5.28	1.48	1.54
1	B	40	THR	CA-C	-5.25	1.46	1.52
1	C	44	THR	C-O	-5.23	1.18	1.24
1	D	302	ASN	CA-CB	5.22	1.60	1.53
1	C	246	ASN	CB-CG	-5.20	1.39	1.52
1	A	217	HIS	N-CA	5.20	1.52	1.46
1	A	307	HIS	CA-C	-5.20	1.46	1.52
1	C	166	SER	N-CA	5.19	1.52	1.46
1	C	151	ARG	CB-CG	5.18	1.68	1.52
1	A	323	ALA	N-CA	-5.18	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	PHE	C-O	5.16	1.29	1.23
1	C	338	LYS	CA-C	5.16	1.59	1.53
1	B	275	ILE	N-CA	5.15	1.52	1.46
1	D	247	TRP	N-CA	5.14	1.52	1.46
1	C	178	ILE	CA-CB	5.13	1.60	1.54
1	C	55	TYR	CA-C	5.11	1.59	1.52
1	C	284	PRO	C-O	5.11	1.30	1.24
1	D	318	ILE	C-O	-5.10	1.19	1.24
1	A	55	TYR	N-CA	5.09	1.52	1.46
1	A	53	GLN	C-N	5.08	1.40	1.33
1	D	5	VAL	C-O	5.05	1.29	1.24
1	A	50	GLY	C-O	5.04	1.30	1.23
1	B	131	GLY	N-CA	5.04	1.50	1.44
1	C	10	VAL	C-O	-5.04	1.18	1.24
1	B	72	PHE	C-O	5.03	1.29	1.24
1	C	332	ARG	CA-C	5.03	1.59	1.52
1	C	102	ILE	CG1-CD1	5.02	1.71	1.51
1	D	186	ALA	CA-CB	-5.02	1.45	1.53
1	C	229	ILE	CA-C	-5.01	1.46	1.52
1	D	31	ASP	CA-C	-5.01	1.46	1.53
1	A	56	LEU	CA-C	5.00	1.59	1.52
1	A	11	ILE	CG1-CD1	5.00	1.71	1.51
1	C	175	ALA	CA-C	-5.00	1.46	1.52

All (319) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ILE	N-CA-C	-19.83	94.50	111.56
1	C	40	THR	CA-C-N	-18.43	100.95	119.56
1	C	40	THR	C-N-CA	-18.43	100.95	119.56
1	A	28	GLN	CA-C-N	-12.89	103.73	119.84
1	A	28	GLN	C-N-CA	-12.89	103.73	119.84
1	C	102	ILE	CA-C-N	-12.89	107.19	120.98
1	C	102	ILE	C-N-CA	-12.89	107.19	120.98
1	C	276	ILE	CB-CA-C	-12.01	100.36	111.05
1	B	40	THR	CA-C-N	-11.54	108.12	120.47
1	B	40	THR	C-N-CA	-11.54	108.12	120.47
1	C	28	GLN	CA-C-N	-11.48	105.49	119.84
1	C	28	GLN	C-N-CA	-11.48	105.49	119.84
1	D	270	LEU	N-CA-C	-11.08	99.75	113.38
1	D	22	ARG	N-CA-C	10.80	125.84	112.23
1	B	71	THR	N-CA-C	-10.59	98.40	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	THR	N-CA-C	10.00	131.90	109.81
1	A	75	LEU	N-CA-C	-9.86	100.54	111.28
1	D	232	GLY	N-CA-C	-9.67	99.32	112.57
1	D	86	ASN	N-CA-C	9.44	121.51	111.03
1	D	303	THR	N-CA-C	-9.24	94.90	109.50
1	A	218	ASP	CA-C-N	9.18	131.32	119.84
1	A	218	ASP	C-N-CA	9.18	131.32	119.84
1	C	276	ILE	N-CA-CB	9.11	119.11	111.64
1	C	299	GLY	CA-C-N	9.09	131.20	119.84
1	C	299	GLY	C-N-CA	9.09	131.20	119.84
1	B	10	VAL	N-CA-CB	9.07	120.14	110.62
1	D	196	GLN	N-CA-C	9.05	118.74	108.25
1	D	314	TYR	N-CA-C	9.04	125.87	113.21
1	C	57	SER	N-CA-C	8.99	123.79	110.48
1	B	76	LEU	N-CA-C	-8.92	102.53	113.41
1	D	162	ARG	N-CA-C	8.92	122.08	108.52
1	D	58	ASP	CA-C-N	-8.79	110.19	120.13
1	D	58	ASP	C-N-CA	-8.79	110.19	120.13
1	D	265	ARG	N-CA-C	-8.58	101.89	111.07
1	A	276	ILE	N-CA-C	-8.49	105.02	111.90
1	D	40	THR	N-CA-C	8.40	128.37	109.81
1	B	123	ASP	N-CA-C	-8.39	100.78	112.45
1	A	196	GLN	N-CA-C	8.37	117.96	108.25
1	D	266	LEU	N-CA-C	8.34	119.99	111.07
1	D	234	GLN	N-CA-C	-8.30	103.75	114.04
1	B	60	ASN	N-CA-C	-8.26	102.24	111.82
1	A	131	GLY	N-CA-C	8.26	123.10	110.88
1	A	223	ILE	CB-CA-C	-8.25	97.76	111.29
1	C	9	GLY	N-CA-C	-8.24	99.31	112.66
1	A	13	LEU	N-CA-C	-8.22	102.27	111.14
1	B	339	LEU	N-CA-C	-8.16	105.31	114.62
1	A	32	ILE	N-CA-C	8.13	120.32	108.53
1	D	131	GLY	N-CA-C	8.12	122.85	110.18
1	B	40	THR	CB-CA-C	-8.12	94.18	110.17
1	B	177	VAL	N-CA-C	8.11	120.16	108.48
1	C	40	THR	N-CA-C	8.07	127.64	109.81
1	D	94	GLY	N-CA-C	8.05	122.14	110.63
1	D	152	LEU	N-CA-C	7.98	121.96	111.75
1	C	319	HIS	N-CA-C	7.91	124.42	111.37
1	B	338	LYS	N-CA-C	-7.89	101.15	111.02
1	D	199	ARG	NE-CZ-NH1	-7.89	113.61	121.50
1	B	275	ILE	CA-C-N	-7.88	115.12	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ILE	C-N-CA	-7.88	115.12	123.08
1	C	189	LEU	N-CA-C	-7.86	103.00	114.39
1	A	126	PRO	N-CA-C	-7.73	96.54	112.47
1	D	9	GLY	N-CA-C	-7.67	100.12	112.31
1	D	199	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	B	286	ARG	CA-C-N	-7.46	110.82	119.32
1	B	286	ARG	C-N-CA	-7.46	110.82	119.32
1	B	289	ILE	CA-C-N	-7.45	112.24	122.30
1	B	289	ILE	C-N-CA	-7.45	112.24	122.30
1	A	122	LEU	CA-CB-CG	-7.42	90.33	116.30
1	C	338	LYS	N-CA-C	7.38	121.43	111.24
1	B	162	ARG	N-CA-C	7.36	119.93	108.96
1	D	11	ILE	N-CA-C	7.32	117.84	110.23
1	D	226	SER	CA-C-N	-7.31	112.11	119.93
1	D	226	SER	C-N-CA	-7.31	112.11	119.93
1	D	259	ILE	CB-CA-C	-7.31	102.28	112.14
1	B	297	ARG	CB-CA-C	7.25	122.18	110.29
1	B	53	GLN	CA-C-N	7.24	127.67	119.92
1	B	53	GLN	C-N-CA	7.24	127.67	119.92
1	A	157	VAL	CB-CA-C	-7.23	101.07	111.34
1	D	4	VAL	N-CA-C	7.17	118.46	107.99
1	A	83	ASN	CB-CA-C	-7.17	98.61	110.37
1	C	253	ILE	N-CA-C	7.16	118.79	110.62
1	B	280	THR	CB-CA-C	-7.09	96.94	109.71
1	C	44	THR	N-CA-C	-7.08	103.49	111.07
1	A	170	VAL	N-CA-C	-7.06	103.97	110.82
1	C	232	GLY	N-CA-C	-7.04	101.85	112.41
1	A	53	GLN	CA-C-N	6.94	126.86	119.85
1	A	53	GLN	C-N-CA	6.94	126.86	119.85
1	C	335	GLU	N-CA-C	-6.92	103.34	111.03
1	C	153	THR	CB-CA-C	-6.90	100.33	110.96
1	D	201	GLN	N-CA-C	-6.89	98.54	109.23
1	C	320	TRP	N-CA-C	6.87	119.40	111.02
1	D	169	GLU	N-CA-C	-6.87	103.90	112.90
1	B	61	ASN	CB-CA-C	6.83	121.76	110.97
1	B	284	PRO	CB-CA-C	-6.79	106.17	111.87
1	B	265	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	D	272	ASN	N-CA-C	6.76	121.14	113.02
1	C	241	ILE	N-CA-C	6.76	117.62	107.75
1	C	18	CYS	CA-CB-SG	-6.74	98.91	114.40
1	B	170	VAL	N-CA-C	6.70	117.57	111.81
1	A	226	SER	CA-C-N	6.68	128.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	SER	C-N-CA	6.68	128.19	119.84
1	A	247	TRP	N-CA-C	6.67	121.02	113.02
1	C	135	THR	N-CA-C	-6.64	100.66	110.48
1	C	201	GLN	N-CA-C	-6.63	97.79	109.06
1	B	243	GLN	CB-CA-C	-6.63	103.21	111.43
1	C	272	ASN	N-CA-C	6.62	121.21	113.20
1	A	207	ALA	CA-C-N	-6.61	113.00	119.87
1	A	207	ALA	C-N-CA	-6.61	113.00	119.87
1	C	102	ILE	N-CA-C	-6.57	94.69	108.88
1	A	61	ASN	CA-C-N	-6.55	113.40	121.00
1	A	61	ASN	C-N-CA	-6.55	113.40	121.00
1	C	177	VAL	N-CA-C	6.54	117.90	108.48
1	B	149	THR	CA-C-N	-6.51	110.42	120.31
1	B	149	THR	C-N-CA	-6.51	110.42	120.31
1	C	192	ASP	CA-C-N	-6.42	113.32	120.45
1	C	192	ASP	C-N-CA	-6.42	113.32	120.45
1	A	18	CYS	CA-CB-SG	-6.40	99.68	114.40
1	A	232	GLY	N-CA-C	-6.39	102.48	112.58
1	D	305	VAL	N-CA-C	6.39	122.62	109.34
1	D	253	ILE	N-CA-C	6.38	117.13	110.62
1	B	317	THR	N-CA-C	-6.36	104.78	112.54
1	C	104	ASP	CA-C-N	6.34	127.76	119.84
1	C	104	ASP	C-N-CA	6.34	127.76	119.84
1	A	83	ASN	N-CA-C	-6.32	104.63	112.72
1	A	104	ASP	CA-C-N	-6.31	113.45	120.14
1	A	104	ASP	C-N-CA	-6.31	113.45	120.14
1	C	178	ILE	N-CA-C	6.30	116.94	107.80
1	D	6	ILE	CB-CA-C	-6.30	102.36	110.98
1	A	157	VAL	N-CA-C	-6.29	100.66	109.21
1	A	144	TYR	N-CA-C	-6.28	103.71	111.75
1	D	291	LEU	CA-CB-CG	6.28	138.28	116.30
1	B	72	PHE	N-CA-C	6.28	118.64	111.11
1	D	188	ALA	N-CA-C	-6.27	105.48	113.01
1	A	3	VAL	N-CA-C	6.27	117.05	107.77
1	C	235	THR	CA-C-N	-6.26	114.29	122.99
1	C	235	THR	C-N-CA	-6.26	114.29	122.99
1	D	120	ARG	N-CA-C	6.24	118.88	111.33
1	C	145	LEU	N-CA-C	-6.24	104.37	112.23
1	C	56	LEU	CA-C-N	6.23	131.73	121.39
1	C	56	LEU	C-N-CA	6.23	131.73	121.39
1	B	267	GLU	CA-C-N	-6.22	113.35	119.64
1	B	267	GLU	C-N-CA	-6.22	113.35	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	TRP	CA-C-N	-6.22	113.42	122.19
1	A	209	TRP	C-N-CA	-6.22	113.42	122.19
1	B	40	THR	N-CA-C	6.20	123.52	109.81
1	C	288	GLN	N-CA-C	6.20	117.92	108.07
1	A	311	HIS	N-CA-C	-6.18	105.69	113.72
1	A	244	LEU	N-CA-C	6.15	119.52	110.30
1	B	144	TYR	N-CA-C	-6.12	104.61	111.28
1	B	137	LEU	CA-C-N	-6.11	115.61	123.19
1	B	137	LEU	C-N-CA	-6.11	115.61	123.19
1	A	188	ALA	CA-C-N	-6.09	112.66	121.98
1	A	188	ALA	C-N-CA	-6.09	112.66	121.98
1	C	42	LEU	CB-CA-C	-6.08	99.87	111.97
1	D	223	ILE	O-C-N	6.07	130.16	122.57
1	C	234	GLN	CA-C-O	6.07	126.37	119.27
1	C	6	ILE	CB-CA-C	-6.05	102.61	110.84
1	A	6	ILE	N-CA-CB	6.04	117.31	110.72
1	A	118	THR	CB-CA-C	-6.04	98.52	109.45
1	B	208	PRO	N-CA-C	-6.04	106.80	114.35
1	A	314	TYR	N-CA-C	6.02	119.17	109.83
1	A	40	THR	CB-CA-C	-6.02	98.31	110.17
1	A	238	LEU	CA-C-O	-6.00	113.85	120.33
1	B	178	ILE	N-CA-C	5.99	115.36	106.85
1	C	3	VAL	N-CA-C	5.99	116.49	107.80
1	C	303	THR	CB-CA-C	5.98	121.82	110.51
1	C	131	GLY	N-CA-C	5.98	127.36	113.18
1	C	120	ARG	N-CA-C	-5.97	103.94	111.11
1	A	110	THR	N-CA-C	-5.96	104.76	112.68
1	C	46	ASP	N-CA-C	5.96	120.02	112.87
1	A	177	VAL	N-CA-C	-5.93	99.73	108.99
1	A	151	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	B	21	GLU	CB-CA-C	5.91	121.93	110.46
1	A	143	ASN	N-CA-C	5.91	118.22	111.02
1	B	131	GLY	N-CA-C	5.90	121.12	111.27
1	B	339	LEU	CA-CB-CG	5.89	136.93	116.30
1	D	39	PHE	N-CA-C	5.89	118.17	109.69
1	D	238	LEU	CA-C-N	5.89	127.41	122.17
1	D	238	LEU	C-N-CA	5.89	127.41	122.17
1	B	206	ASP	CA-C-N	-5.86	117.12	122.28
1	B	206	ASP	C-N-CA	-5.86	117.12	122.28
1	D	148	LEU	N-CA-C	-5.85	104.82	111.14
1	D	227	PRO	N-CA-C	5.85	120.80	111.26
1	D	181	CYS	CA-CB-SG	-5.85	100.95	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	LYS	CA-C-N	-5.84	113.44	122.49
1	B	271	LYS	C-N-CA	-5.84	113.44	122.49
1	D	224	TYR	N-CA-C	-5.83	103.74	111.02
1	C	89	LEU	CB-CA-C	-5.81	101.47	111.23
1	D	298	THR	N-CA-C	-5.80	98.44	110.80
1	C	199	ARG	NE-CZ-NH1	-5.79	115.71	121.50
1	B	221	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	A	270	LEU	N-CA-C	-5.78	106.20	113.20
1	C	58	ASP	CA-C-N	-5.78	114.65	120.31
1	C	58	ASP	C-N-CA	-5.78	114.65	120.31
1	A	124	MET	N-CA-C	-5.77	106.22	113.20
1	A	274	ARG	N-CA-C	-5.76	99.34	108.73
1	D	58	ASP	N-CA-C	5.74	118.62	110.24
1	A	151	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	B	107	TRP	N-CA-C	5.71	118.28	111.71
1	A	199	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	C	329	LEU	N-CA-C	-5.69	104.28	111.11
1	C	339	LEU	CA-CB-CG	5.69	136.22	116.30
1	A	10	VAL	N-CA-C	-5.69	103.98	111.09
1	D	46	ASP	N-CA-C	5.68	119.31	112.38
1	B	296	LEU	CB-CA-C	-5.68	102.04	110.67
1	B	231	PRO	CA-C-N	-5.66	117.39	122.43
1	B	231	PRO	C-N-CA	-5.66	117.39	122.43
1	B	32	ILE	N-CA-C	5.64	116.61	108.48
1	C	151	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	A	253	ILE	N-CA-C	5.63	121.06	109.34
1	B	8	ALA	N-CA-C	-5.62	106.22	112.57
1	A	316	LEU	N-CA-C	-5.62	105.25	111.71
1	D	36	ALA	N-CA-C	5.62	117.93	109.23
1	B	17	LEU	CA-C-N	-5.58	111.04	120.58
1	B	17	LEU	C-N-CA	-5.58	111.04	120.58
1	D	166	SER	N-CA-C	5.57	116.93	108.07
1	B	294	GLU	N-CA-C	5.56	116.65	107.20
1	C	8	ALA	N-CA-C	-5.56	104.41	113.19
1	A	39	PHE	CB-CA-C	-5.56	99.30	110.30
1	C	101	ALA	N-CA-C	5.56	122.64	110.80
1	A	4	VAL	N-CA-C	5.55	116.10	107.99
1	A	66	ASP	N-CA-C	5.55	118.10	111.71
1	B	34	VAL	N-CA-C	-5.54	100.43	108.36
1	A	169	GLU	N-CA-C	-5.54	104.46	111.11
1	C	7	GLY	N-CA-C	-5.54	100.05	113.18
1	B	308	ASN	CB-CA-C	5.53	119.45	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	ILE	N-CA-C	5.51	116.24	110.62
1	A	255	ASP	N-CA-C	-5.51	105.19	111.14
1	B	69	GLN	N-CA-C	-5.51	105.35	111.36
1	A	199	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	C	230	ILE	N-CA-C	5.50	113.48	107.60
1	C	155	ARG	N-CA-C	5.49	119.23	112.54
1	B	291	LEU	CA-CB-CG	5.48	135.48	116.30
1	B	50	GLY	N-CA-C	-5.48	107.45	115.72
1	B	241	ILE	CB-CA-C	-5.47	104.22	110.73
1	A	74	TYR	N-CA-CB	-5.46	102.15	110.07
1	B	174	GLY	N-CA-C	5.46	126.11	113.18
1	A	148	LEU	N-CA-C	-5.45	104.73	111.33
1	B	253	ILE	CB-CA-C	-5.45	102.36	111.29
1	C	151	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	D	23	TYR	CA-C-N	-5.42	112.38	122.09
1	D	23	TYR	C-N-CA	-5.42	112.38	122.09
1	B	245	GLY	CA-C-N	-5.40	113.94	121.99
1	B	245	GLY	C-N-CA	-5.40	113.94	121.99
1	C	300	PRO	N-CA-C	5.40	123.59	112.47
1	C	80	HIS	N-CA-C	5.39	119.64	112.30
1	D	72	PHE	N-CA-C	5.38	120.19	111.37
1	B	70	GLN	N-CA-C	-5.36	106.58	113.23
1	B	21	GLU	CA-CB-CG	5.34	124.79	114.10
1	A	241	ILE	N-CA-CB	-5.33	105.18	111.90
1	A	204	LYS	N-CA-C	-5.32	101.03	109.59
1	A	30	LEU	N-CA-C	5.32	117.59	109.62
1	B	252	ASN	N-CA-C	5.32	117.40	107.99
1	D	215	LEU	CA-C-N	-5.32	113.06	122.74
1	D	215	LEU	C-N-CA	-5.32	113.06	122.74
1	D	15	THR	N-CA-C	-5.31	105.41	111.14
1	C	42	LEU	N-CA-C	5.29	117.63	110.06
1	C	40	THR	CB-CA-C	-5.29	99.75	110.17
1	C	195	LEU	N-CA-C	5.28	117.34	108.73
1	C	292	GLU	N-CA-C	-5.28	101.45	108.74
1	D	57	SER	N-CA-C	5.28	118.72	110.32
1	A	299	GLY	N-CA-C	5.28	123.11	112.34
1	A	265	ARG	CG-CD-NE	-5.28	100.39	112.00
1	C	128	TYR	CA-CB-CG	-5.28	104.40	113.90
1	C	259	ILE	CB-CA-C	-5.27	105.13	111.88
1	B	160	PHE	N-CA-C	5.27	118.02	108.69
1	B	46	ASP	N-CA-C	5.27	118.49	111.75
1	D	264	CYS	N-CA-C	5.27	116.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	LEU	CA-C-N	-5.27	108.95	121.80
1	D	27	LEU	C-N-CA	-5.27	108.95	121.80
1	D	79	VAL	N-CA-C	5.26	120.29	109.34
1	D	118	THR	CA-C-N	-5.26	113.12	118.85
1	D	118	THR	C-N-CA	-5.26	113.12	118.85
1	B	135	THR	CB-CA-C	-5.25	101.68	110.19
1	C	234	GLN	CA-C-N	-5.25	113.38	122.10
1	C	234	GLN	C-N-CA	-5.25	113.38	122.10
1	D	22	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	D	305	VAL	CA-C-N	-5.22	116.71	123.19
1	D	305	VAL	C-N-CA	-5.22	116.71	123.19
1	D	235	THR	CB-CA-C	5.21	122.93	111.09
1	C	83	ASN	N-CA-C	5.21	121.90	110.80
1	B	334	LEU	N-CA-C	5.20	116.64	111.07
1	C	106	SER	N-CA-C	5.20	119.11	112.87
1	D	32	ILE	N-CA-C	5.19	115.81	107.98
1	C	188	ALA	CA-C-N	-5.18	114.05	121.98
1	C	188	ALA	C-N-CA	-5.18	114.05	121.98
1	D	303	THR	CB-CA-C	5.18	120.20	109.38
1	A	135	THR	N-CA-C	-5.16	101.86	110.17
1	C	178	ILE	CB-CA-C	-5.16	103.42	110.96
1	A	224	TYR	CA-C-N	-5.16	114.42	122.37
1	A	224	TYR	C-N-CA	-5.16	114.42	122.37
1	A	271	LYS	CA-C-N	-5.16	113.00	121.92
1	A	271	LYS	C-N-CA	-5.16	113.00	121.92
1	B	78	HIS	N-CA-C	-5.16	104.69	112.99
1	B	209	TRP	N-CA-C	-5.15	105.74	112.23
1	B	259	ILE	CB-CA-C	-5.15	105.11	111.70
1	A	189	LEU	CA-CB-CG	5.15	134.31	116.30
1	B	275	ILE	O-C-N	-5.13	117.81	122.79
1	C	120	ARG	CA-CB-CG	5.12	124.35	114.10
1	A	239	GLY	N-CA-C	5.12	119.83	111.27
1	A	302	ASN	N-CA-CB	5.12	118.55	110.56
1	D	18	CYS	CA-CB-SG	-5.12	102.61	114.40
1	D	4	VAL	N-CA-CB	5.12	117.20	111.21
1	C	22	ARG	N-CA-C	5.12	119.62	113.17
1	C	139	LEU	CA-C-N	5.12	128.61	121.24
1	C	139	LEU	C-N-CA	5.12	128.61	121.24
1	D	187	GLY	N-CA-C	5.10	120.52	113.99
1	A	178	ILE	CA-C-N	-5.09	116.32	123.10
1	A	178	ILE	C-N-CA	-5.09	116.32	123.10
1	B	45	THR	CA-C-N	5.09	127.81	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	THR	C-N-CA	5.09	127.81	120.38
1	C	144	TYR	N-CA-C	-5.07	105.84	112.23
1	D	333	ILE	CB-CA-C	-5.07	105.55	111.94
1	D	316	LEU	N-CA-C	-5.05	105.87	112.23
1	B	199	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	B	261	GLU	CA-CB-CG	5.04	124.18	114.10
1	D	143	ASN	N-CA-C	5.02	117.48	111.71
1	D	250	LEU	N-CA-C	-5.01	100.10	108.32
1	B	58	ASP	N-CA-C	5.01	116.96	110.40
1	A	330	PHE	CB-CA-C	-5.01	102.48	110.79

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	ASP	Peptide
1	B	58	ASP	Peptide
1	C	301	SER	Peptide
1	C	41	PRO	Peptide
1	C	60	ASN	Peptide
1	D	57	SER	Peptide

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	2733	0	2680	274	0
1	B	2733	0	2680	281	0
1	C	2733	0	2680	323	0
1	D	2733	0	2680	273	0
2	A	53	0	31	4	0
2	B	53	0	31	5	0
2	C	53	0	31	18	0
2	D	53	0	31	6	0
3	A	16	0	11	2	0
3	B	16	0	11	5	0
3	C	16	0	11	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	16	0	11	6	0
All	All	11208	0	10888	1134	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 51.

All (1134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ILE:C	1:D:224:TYR:N	1.69	1.47
1:B:221:ARG:HH21	1:B:221:ARG:CB	1.43	1.31
1:C:264:CYS:SG	1:C:271:LYS:HD3	1.72	1.28
1:C:38:ARG:NH2	2:C:401:FAD:H2B	1.49	1.25
1:B:221:ARG:NH2	1:B:221:ARG:HB2	1.55	1.22
1:C:69:GLN:NE2	1:C:110:THR:HG23	1.60	1.17
1:D:221:ARG:HB2	1:D:221:ARG:HH21	1.08	1.12
1:B:335:GLU:HA	1:B:340:SER:HB3	1.31	1.11
1:C:38:ARG:NH2	2:C:401:FAD:C2B	2.14	1.09
1:C:17:LEU:O	1:C:21:GLU:HG2	1.51	1.09
1:D:264:CYS:SG	1:D:271:LYS:HD2	1.93	1.08
1:C:112:LEU:CD2	1:C:112:LEU:N	2.17	1.07
1:D:221:ARG:HH21	1:D:221:ARG:CB	1.67	1.06
1:A:140:GLU:OE1	1:A:233:THR:HB	1.53	1.06
1:D:264:CYS:SG	1:D:271:LYS:CD	2.44	1.06
1:A:274:ARG:HE	1:A:274:ARG:HA	1.23	1.03
1:D:40:THR:HG22	1:D:41:PRO:HD3	1.40	1.03
1:C:2:ARG:HG3	1:C:176:ASP:OD1	1.58	1.03
1:A:155:ARG:HG2	1:A:155:ARG:HH21	1.25	1.01
1:B:100:GLU:HA	1:B:100:GLU:OE1	1.60	1.01
1:A:221:ARG:HB2	1:A:221:ARG:NH2	1.74	1.01
1:A:178:ILE:HB	1:A:305:VAL:HG22	1.39	1.01
1:D:83:ASN:O	1:D:86:ASN:HB2	1.62	0.99
1:A:168:GLU:O	1:A:172:ARG:HB2	1.62	0.99
1:B:224:TYR:O	1:B:242:PHE:HB2	1.61	0.99
1:A:61:ASN:OD1	1:A:63:GLN:HG3	1.63	0.98
1:A:42:LEU:HD22	1:C:42:LEU:HD22	1.46	0.98
1:B:284:PRO:HG2	1:B:312:GLY:H	1.27	0.98
1:B:241:ILE:HD12	1:B:255:ASP:HB3	1.45	0.98
1:C:2:ARG:HD3	1:C:174:GLY:O	1.64	0.98
1:C:111:VAL:C	1:C:112:LEU:HD22	1.89	0.97
1:A:221:ARG:HB2	1:A:221:ARG:CZ	1.92	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ARG:HH22	2:C:401:FAD:H2B	1.18	0.97
1:C:332:ARG:O	1:C:336:GLU:HG3	1.62	0.97
1:B:55:TYR:HE1	1:B:224:TYR:OH	1.47	0.97
1:D:240:GLY:O	1:D:241:ILE:HD13	1.63	0.97
1:D:28:GLN:HB3	1:D:29:PRO:HD3	1.45	0.96
1:C:38:ARG:HH22	2:C:401:FAD:C2B	1.77	0.95
1:B:290:ARG:HD2	1:B:292:GLU:OE2	1.67	0.94
1:C:252:ASN:HD22	1:C:255:ASP:H	0.95	0.94
1:B:280:THR:HG22	1:B:281:GLY:N	1.79	0.94
1:C:112:LEU:N	1:C:112:LEU:HD23	1.83	0.93
1:B:180:ASN:HD22	1:B:307:HIS:CD2	1.87	0.93
1:B:264:CYS:SG	1:B:271:LYS:HG3	2.09	0.92
1:B:92:ILE:HD11	1:B:231:PRO:HG2	1.48	0.92
1:B:168:GLU:O	1:B:172:ARG:HB2	1.68	0.92
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.03	0.91
1:A:290:ARG:HD2	1:A:292:GLU:OE2	1.71	0.91
1:B:221:ARG:HH21	1:B:221:ARG:HB2	0.75	0.91
1:C:117:LEU:O	1:C:122:LEU:HD11	1.70	0.91
1:A:53:GLN:HE22	1:A:96:ASN:HD21	1.16	0.90
1:C:38:ARG:NH2	2:C:401:FAD:O2B	2.03	0.90
1:D:224:TYR:O	1:D:242:PHE:HB2	1.72	0.89
1:B:335:GLU:CA	1:B:340:SER:HB3	2.02	0.89
1:B:107:TRP:O	1:B:109:ASP:N	2.06	0.89
1:C:228:TYR:OH	3:C:402:3LD:O15	1.88	0.89
1:D:233:THR:CG2	1:D:234:GLN:HG2	2.03	0.89
1:C:69:GLN:NE2	1:C:110:THR:CG2	2.36	0.88
1:D:264:CYS:SG	1:D:271:LYS:HD3	2.12	0.88
1:A:178:ILE:HB	1:A:305:VAL:CG2	2.04	0.88
1:C:264:CYS:HG	1:C:271:LYS:HD3	1.35	0.88
1:D:40:THR:CG2	1:D:41:PRO:HD3	2.03	0.88
1:A:161:GLN:HG3	1:C:249:GLU:O	1.72	0.88
1:C:112:LEU:N	1:C:112:LEU:HD22	1.87	0.87
1:B:205:VAL:HG22	1:B:273:ALA:HB1	1.53	0.87
1:B:199:ARG:HH12	1:B:201:GLN:NE2	1.72	0.87
1:B:199:ARG:NH1	1:B:201:GLN:NE2	2.23	0.87
1:C:1:MET:N	1:C:29:PRO:O	2.07	0.87
1:B:55:TYR:HE1	1:B:224:TYR:CZ	1.92	0.86
1:B:199:ARG:HH12	1:B:201:GLN:HE22	1.22	0.86
1:C:150:GLU:O	1:C:154:GLU:HG2	1.75	0.86
1:C:221:ARG:HB2	1:C:221:ARG:NH2	1.91	0.86
1:A:335:GLU:HG3	1:A:336:GLU:H	1.36	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ILE:HD12	1:C:266:LEU:HD13	1.57	0.86
1:B:221:ARG:CB	1:B:221:ARG:NH2	2.25	0.86
1:A:233:THR:HG23	1:A:234:GLN:N	1.90	0.85
1:C:52:TRP:NE1	1:C:317:THR:HG23	1.91	0.85
1:B:255:ASP:O	1:B:259:ILE:HG13	1.76	0.85
1:B:274:ARG:HH12	1:C:274:ARG:HD2	1.39	0.84
1:A:1:MET:HG2	1:A:27:LEU:HD13	1.59	0.84
1:D:221:ARG:CB	1:D:221:ARG:NH2	2.40	0.84
1:D:43:THR:O	1:D:46:ASP:HB2	1.78	0.84
1:C:242:PHE:HD1	1:C:243:GLN:N	1.75	0.84
1:C:243:GLN:HE22	1:C:246:ASN:HD22	1.26	0.83
1:B:150:GLU:O	1:B:154:GLU:HG2	1.78	0.83
1:C:38:ARG:HH21	2:C:401:FAD:H2B	1.43	0.82
1:A:216:THR:O	1:A:226:SER:HB3	1.80	0.82
1:B:203:MET:HE2	1:B:256:HIS:CE1	2.14	0.81
1:C:151:ARG:HH11	1:C:154:GLU:CD	1.88	0.81
1:C:264:CYS:HB3	1:C:271:LYS:HZ3	1.43	0.81
1:A:101:ALA:HA	1:A:130:TYR:CD2	2.15	0.81
1:A:61:ASN:HD21	1:A:63:GLN:HE21	1.29	0.81
1:D:201:GLN:HE22	1:D:252:ASN:H	1.28	0.80
1:C:69:GLN:CD	1:C:110:THR:HG23	2.06	0.80
1:B:336:GLU:C	1:B:338:LYS:H	1.89	0.80
1:C:79:VAL:HG22	1:C:80:HIS:CD2	2.17	0.80
1:C:1:MET:HE1	1:C:176:ASP:HB2	1.63	0.80
1:C:252:ASN:ND2	1:C:255:ASP:H	1.78	0.80
1:C:79:VAL:HG22	1:C:80:HIS:HD2	1.47	0.80
1:C:111:VAL:C	1:C:112:LEU:CD2	2.54	0.80
1:B:49:ALA:HB1	1:B:230:ILE:HG21	1.64	0.79
1:D:201:GLN:NE2	1:D:252:ASN:H	1.79	0.79
1:B:2:ARG:N	1:B:176:ASP:OD1	2.12	0.79
1:D:240:GLY:C	1:D:241:ILE:HD13	2.07	0.79
1:B:298:THR:HG23	1:B:298:THR:O	1.82	0.79
1:C:79:VAL:HG21	1:C:91:LEU:HD11	1.63	0.79
1:D:81:SER:HB2	1:D:82:PRO:HD2	1.65	0.79
1:B:331:GLY:O	1:B:334:LEU:HB2	1.83	0.78
1:A:27:LEU:HD11	1:A:334:LEU:HD21	1.65	0.78
1:C:283:ARG:NE	3:C:402:3LD:O16	2.13	0.78
1:A:155:ARG:HG2	1:A:155:ARG:NH2	1.88	0.78
1:B:335:GLU:HG2	1:B:336:GLU:N	1.97	0.78
1:B:18:CYS:SG	1:B:324:LEU:HD23	2.23	0.78
1:A:205:VAL:HG22	1:A:273:ALA:HB1	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH1	1:B:193:PRO:HG3	1.99	0.78
1:A:1:MET:HA	1:A:1:MET:CE	2.14	0.78
1:C:54:PRO:HG3	1:C:317:THR:HG21	1.66	0.78
1:A:69:GLN:NE2	1:A:110:THR:HG23	2.00	0.77
1:A:141:GLY:O	1:A:145:LEU:HB2	1.84	0.77
1:C:115:ARG:O	1:C:115:ARG:HG3	1.84	0.77
1:C:55:TYR:CE1	1:C:224:TYR:OH	2.36	0.77
1:A:69:GLN:HE22	1:A:110:THR:HG23	1.50	0.77
1:C:55:TYR:HE1	1:C:224:TYR:HH	1.30	0.77
1:C:117:LEU:HB3	1:C:122:LEU:HD21	1.67	0.77
1:A:233:THR:CG2	1:A:234:GLN:H	1.98	0.76
1:A:1:MET:HE1	1:A:176:ASP:HB3	1.67	0.76
1:D:52:TRP:CD1	1:D:317:THR:HG23	2.21	0.76
1:C:69:GLN:HE22	1:C:110:THR:HG23	1.46	0.76
1:C:295:GLN:CD	1:C:295:GLN:H	1.94	0.76
1:A:1:MET:HA	1:A:1:MET:HE2	1.67	0.76
1:A:108:LYS:HG3	1:A:109:ASP:N	1.99	0.76
1:B:81:SER:HB2	1:B:82:PRO:HD2	1.67	0.76
1:C:286:ARG:HG3	1:C:287:PRO:HD2	1.68	0.76
1:D:5:VAL:HA	1:D:179:VAL:HG23	1.68	0.76
1:B:293:ARG:NH2	1:B:304:GLU:OE2	2.19	0.76
1:C:252:ASN:ND2	1:C:254:GLN:H	1.84	0.76
1:A:223:ILE:O	1:A:223:ILE:HG23	1.85	0.75
1:B:28:GLN:HB3	1:B:29:PRO:HD3	1.68	0.75
1:B:291:LEU:HA	1:B:307:HIS:O	1.87	0.75
1:A:233:THR:CG2	1:A:234:GLN:N	2.49	0.75
1:B:178:ILE:HB	1:B:305:VAL:HG22	1.69	0.75
1:A:53:GLN:HE22	1:A:96:ASN:ND2	1.84	0.74
1:D:50:GLY:HA2	1:D:316:LEU:HD23	1.69	0.74
1:B:55:TYR:HE1	1:B:224:TYR:HH	0.79	0.74
1:B:203:MET:CE	1:B:256:HIS:CE1	2.69	0.74
1:B:224:TYR:O	1:B:242:PHE:CB	2.36	0.74
1:D:1:MET:HG2	1:D:27:LEU:HD11	1.70	0.74
1:C:264:CYS:CB	1:C:271:LYS:HZ3	2.01	0.73
1:B:39:PHE:O	1:B:41:PRO:CD	2.35	0.73
1:A:32:ILE:HB	1:A:157:VAL:HG22	1.71	0.73
1:A:291:LEU:HA	1:A:307:HIS:O	1.89	0.73
1:A:274:ARG:HA	1:A:274:ARG:NE	1.96	0.73
1:D:231:PRO:HA	1:D:236:VAL:HG22	1.71	0.73
1:A:168:GLU:O	1:A:172:ARG:CB	2.35	0.72
1:C:27:LEU:HD11	1:C:334:LEU:CD2	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASN:HB2	1:B:288:GLN:NE2	2.04	0.72
1:C:198:GLY:O	1:C:283:ARG:HG3	1.89	0.72
1:B:202:ILE:HD12	1:B:202:ILE:O	1.89	0.72
1:C:264:CYS:HB3	1:C:271:LYS:NZ	2.05	0.72
1:D:293:ARG:O	1:D:294:GLU:HB2	1.90	0.72
1:A:40:THR:CG2	1:A:41:PRO:HD3	2.20	0.72
1:D:199:ARG:O	1:D:283:ARG:NH2	2.22	0.72
1:B:55:TYR:CE1	1:B:224:TYR:CZ	2.77	0.71
1:C:252:ASN:HD22	1:C:255:ASP:N	1.80	0.71
1:B:55:TYR:CE1	1:B:224:TYR:CE1	2.79	0.71
1:C:55:TYR:HE1	1:C:224:TYR:OH	1.73	0.70
1:D:151:ARG:O	1:D:154:GLU:HG2	1.90	0.70
1:D:23:TYR:O	1:D:30:LEU:HD23	1.91	0.70
1:A:53:GLN:NE2	1:A:96:ASN:HD21	1.89	0.70
1:B:228:TYR:HD1	1:B:230:ILE:HD12	1.54	0.70
1:C:114:PHE:HZ	1:C:132:TRP:CD1	2.09	0.70
1:D:167:PHE:CE1	1:D:189:LEU:HD12	2.27	0.70
1:A:179:VAL:HG13	1:A:306:ILE:HB	1.74	0.70
1:B:200:GLY:O	1:B:280:THR:HG23	1.92	0.70
1:D:76:LEU:HG	1:D:76:LEU:O	1.81	0.70
1:C:5:VAL:HG22	1:C:179:VAL:HB	1.73	0.70
1:D:59:PRO:HG3	1:D:65:ALA:HB2	1.74	0.70
1:C:191:ARG:NH1	1:C:193:PRO:HG3	2.07	0.70
1:D:286:ARG:HH12	1:D:290:ARG:HD3	1.58	0.69
1:A:59:PRO:HG2	1:A:62:PRO:HA	1.75	0.69
1:B:203:MET:CE	1:B:256:HIS:ND1	2.55	0.69
1:B:295:GLN:H	1:B:295:GLN:HE21	1.40	0.69
1:B:180:ASN:ND2	1:B:307:HIS:HD2	1.86	0.69
1:D:3:VAL:HG12	1:D:32:ILE:HG23	1.75	0.69
1:D:233:THR:HG23	1:D:234:GLN:HE21	1.57	0.69
1:D:297:ARG:H	1:D:297:ARG:HD3	1.58	0.69
1:D:221:ARG:HB2	1:D:221:ARG:NH2	1.93	0.69
1:B:40:THR:O	1:B:40:THR:OG1	2.04	0.69
1:C:112:LEU:HB2	1:C:135:THR:HB	1.73	0.69
1:D:233:THR:HG22	1:D:234:GLN:HG2	1.74	0.69
1:B:280:THR:HG22	1:B:281:GLY:H	1.53	0.68
1:A:182:THR:O	2:A:401:FAD:H8A	1.93	0.68
1:B:43:THR:N	1:B:46:ASP:OD1	2.21	0.68
1:B:336:GLU:O	1:B:338:LYS:N	2.26	0.68
1:C:191:ARG:HH11	1:C:193:PRO:HG3	1.57	0.68
1:B:242:PHE:CD1	1:B:242:PHE:C	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ARG:HG3	1:C:287:PRO:CD	2.22	0.68
1:C:83:ASN:O	1:C:86:ASN:HB2	1.93	0.68
1:D:242:PHE:O	1:D:243:GLN:HG3	1.92	0.68
1:A:40:THR:O	1:A:40:THR:OG1	2.06	0.68
1:A:223:ILE:HG13	1:A:224:TYR:N	2.07	0.68
1:A:297:ARG:HG3	1:A:302:ASN:HD22	1.59	0.68
1:B:112:LEU:H	1:B:112:LEU:HD22	1.58	0.68
1:B:309:TYR:CD1	1:B:309:TYR:C	2.72	0.67
1:D:126:PRO:O	1:D:128:TYR:N	2.27	0.67
1:B:168:GLU:OE2	1:B:296:LEU:HD21	1.94	0.67
1:C:52:TRP:CE2	1:C:317:THR:HG23	2.29	0.67
1:D:83:ASN:O	1:D:86:ASN:CB	2.41	0.67
1:D:105:PRO:HD2	1:D:108:LYS:HB3	1.77	0.67
1:B:59:PRO:HG2	1:B:62:PRO:HA	1.76	0.67
1:B:150:GLU:O	1:B:154:GLU:CG	2.43	0.67
1:C:79:VAL:O	1:C:80:HIS:HD2	1.78	0.67
1:B:112:LEU:HD23	1:B:135:THR:O	1.94	0.67
1:C:332:ARG:HA	1:C:335:GLU:CG	2.25	0.67
1:A:38:ARG:HD2	2:A:401:FAD:O2B	1.94	0.66
1:A:335:GLU:HG3	1:A:336:GLU:N	2.07	0.66
1:B:231:PRO:HA	1:B:236:VAL:HG22	1.75	0.66
1:D:179:VAL:HG12	1:D:306:ILE:HB	1.76	0.66
1:C:241:ILE:HD12	1:C:255:ASP:HB3	1.77	0.66
1:D:223:ILE:C	1:D:224:TYR:CA	2.67	0.66
1:A:200:GLY:CA	1:A:283:ARG:HH22	2.07	0.66
1:C:20:HIS:HD2	1:C:32:ILE:HD12	1.61	0.66
1:C:211:LYS:HD3	1:C:211:LYS:N	1.99	0.66
1:D:6:ILE:CD1	1:D:164:VAL:HG11	2.25	0.66
1:B:228:TYR:CD1	1:B:230:ILE:HD12	2.31	0.66
1:A:296:LEU:O	1:A:298:THR:HG22	1.95	0.66
1:C:87:LEU:HD23	1:C:147:TRP:CD2	2.31	0.66
1:C:117:LEU:CB	1:C:122:LEU:HD21	2.25	0.66
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.31	0.65
1:C:194:LEU:HD13	1:C:287:PRO:HG2	1.77	0.65
1:C:242:PHE:CD1	1:C:243:GLN:N	2.63	0.65
1:C:283:ARG:HG2	2:C:401:FAD:HM82	1.79	0.65
1:B:22:ARG:HD2	1:B:23:TYR:CE2	2.31	0.65
1:D:172:ARG:C	1:D:174:GLY:H	2.04	0.65
1:B:325:GLU:OE1	1:B:325:GLU:HA	1.97	0.65
1:C:13:LEU:O	1:C:16:ALA:HB3	1.96	0.65
1:D:250:LEU:HD12	1:D:251:ASN:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:CZ	1:A:221:ARG:CB	2.73	0.65
1:B:22:ARG:HD2	1:B:23:TYR:CZ	2.31	0.65
1:B:184:VAL:HG21	1:B:197:PRO:HB3	1.79	0.65
1:A:61:ASN:ND2	1:A:63:GLN:HE21	1.94	0.65
1:A:67:TRP:O	1:A:71:THR:OG1	2.12	0.65
1:A:257:ASN:O	1:A:261:GLU:OE1	2.14	0.65
1:D:112:LEU:HB2	1:D:135:THR:HB	1.78	0.65
1:C:178:ILE:HB	1:C:305:VAL:HG22	1.79	0.65
2:C:401:FAD:O4	3:C:402:3LD:H9	1.96	0.65
1:B:196:GLN:O	1:B:285:VAL:HG23	1.97	0.65
1:B:274:ARG:NH1	1:C:274:ARG:HD2	2.11	0.65
1:C:223:ILE:HD12	1:C:224:TYR:H	1.61	0.65
1:D:242:PHE:C	1:D:243:GLN:HG3	2.22	0.65
1:C:133:PHE:C	1:C:133:PHE:CD2	2.74	0.64
1:C:320:TRP:O	1:C:321:GLY:C	2.40	0.64
1:D:40:THR:CG2	1:D:41:PRO:CD	2.76	0.64
1:C:150:GLU:HG3	1:C:151:ARG:NH1	2.12	0.64
1:D:201:GLN:HE22	1:D:252:ASN:N	1.94	0.64
1:B:3:VAL:HB	1:B:32:ILE:HG23	1.77	0.64
1:C:243:GLN:HE22	1:C:246:ASN:ND2	1.94	0.64
1:B:284:PRO:HG2	1:B:312:GLY:N	2.09	0.64
1:D:153:THR:C	1:D:155:ARG:H	2.06	0.64
1:D:223:ILE:CA	1:D:224:TYR:N	2.60	0.64
1:A:298:THR:HG21	1:A:303:THR:HG23	1.78	0.64
1:C:71:THR:HG21	1:C:317:THR:O	1.97	0.64
1:B:280:THR:CG2	1:B:281:GLY:N	2.55	0.64
1:C:45:THR:OG1	2:C:401:FAD:O1A	2.16	0.64
1:A:205:VAL:CG2	1:A:273:ALA:HB1	2.28	0.64
1:D:102:ILE:CG1	1:D:103:PRO:CD	2.76	0.64
1:C:114:PHE:CD1	1:C:114:PHE:C	2.76	0.63
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.46	0.63
1:A:332:ARG:O	1:A:333:ILE:C	2.40	0.63
1:B:216:THR:HG23	1:B:266:LEU:HD11	1.80	0.63
1:D:151:ARG:NE	1:D:154:GLU:OE2	2.30	0.63
1:D:202:ILE:HD11	1:D:279:ARG:HB2	1.79	0.63
1:B:112:LEU:HD22	1:B:112:LEU:N	2.14	0.63
1:C:291:LEU:HA	1:C:307:HIS:O	1.99	0.63
1:A:295:GLN:HE21	1:A:295:GLN:N	1.95	0.63
1:B:28:GLN:HB3	1:B:29:PRO:CD	2.28	0.63
1:C:61:ASN:HD21	1:C:63:GLN:HB2	1.63	0.63
1:C:242:PHE:HD1	1:C:242:PHE:C	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:GLU:OE2	1:C:329:LEU:HD21	1.98	0.62
1:A:203:MET:HE3	1:A:259:ILE:CG2	2.29	0.62
1:A:252:ASN:HD22	1:A:255:ASP:H	1.47	0.62
1:B:119:PRO:HA	1:B:122:LEU:HD12	1.80	0.62
1:B:159:PHE:N	1:B:159:PHE:HD2	1.95	0.62
1:B:298:THR:O	1:B:298:THR:CG2	2.47	0.62
1:C:264:CYS:SG	1:C:271:LYS:CD	2.67	0.62
1:A:193:PRO:HD2	1:A:194:LEU:H	1.62	0.62
1:B:38:ARG:NH1	1:B:249:GLU:OE2	2.32	0.62
1:B:221:ARG:HH21	1:B:221:ARG:HB3	1.57	0.62
1:C:221:ARG:HB2	1:C:221:ARG:HH21	1.64	0.62
1:D:140:GLU:OE1	1:D:233:THR:HB	1.99	0.62
1:A:199:ARG:HH12	1:A:201:GLN:NE2	1.96	0.62
1:C:284:PRO:O	1:C:312:GLY:N	2.31	0.62
1:B:24:HIS:H	1:B:24:HIS:CD2	2.17	0.62
1:D:58:ASP:OD2	1:D:59:PRO:HD2	1.99	0.62
1:D:252:ASN:HD21	1:D:254:GLN:HB2	1.65	0.62
1:C:40:THR:HG23	1:C:41:PRO:HD3	1.80	0.62
1:C:74:TYR:CD2	1:C:320:TRP:CD1	2.88	0.62
1:C:160:PHE:N	1:C:160:PHE:CD1	2.66	0.62
1:C:289:ILE:HG22	1:C:290:ARG:N	2.15	0.62
1:D:102:ILE:CG1	1:D:103:PRO:HD2	2.30	0.62
1:B:161:GLN:HG3	1:D:249:GLU:N	2.14	0.62
1:A:42:LEU:HD22	1:C:42:LEU:CD2	2.27	0.61
1:A:286:ARG:HG2	1:A:288:GLN:O	1.99	0.61
1:C:80:HIS:CE1	1:D:267:GLU:OE2	2.53	0.61
1:B:161:GLN:HG3	1:D:249:GLU:H	1.65	0.61
1:C:27:LEU:HD11	1:C:334:LEU:HD22	1.83	0.61
1:B:85:GLU:O	1:B:85:GLU:HG2	2.00	0.61
1:C:332:ARG:HA	1:C:335:GLU:HG2	1.81	0.61
1:A:105:PRO:HB2	1:A:107:TRP:CE2	2.36	0.61
1:B:39:PHE:O	1:B:41:PRO:HD2	2.00	0.61
1:B:186:ALA:HB3	1:B:195:LEU:HD22	1.82	0.61
1:D:59:PRO:HG2	1:D:62:PRO:HA	1.80	0.61
1:C:223:ILE:HD12	1:C:224:TYR:N	2.15	0.61
1:A:40:THR:HG23	1:A:41:PRO:CD	2.31	0.61
1:A:40:THR:HG22	1:A:41:PRO:HD3	1.81	0.61
1:B:41:PRO:HD2	1:B:42:LEU:HG	1.82	0.61
1:B:159:PHE:N	1:B:159:PHE:CD2	2.65	0.61
1:C:284:PRO:HG2	1:C:312:GLY:H	1.65	0.61
1:A:239:GLY:HA2	1:A:259:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ARG:HA	1:C:274:ARG:NE	2.16	0.61
1:B:51:LEU:HD23	3:B:402:3LD:H7	1.82	0.60
1:D:182:THR:HG22	2:D:401:FAD:C8A	2.31	0.60
1:D:318:ILE:O	1:D:319:HIS:C	2.43	0.60
1:B:55:TYR:HE1	1:B:224:TYR:CE1	2.17	0.60
1:B:241:ILE:CD1	1:B:255:ASP:HB3	2.27	0.60
1:C:214:ILE:C	1:C:215:LEU:HD23	2.26	0.60
1:C:221:ARG:HB2	1:C:221:ARG:CZ	2.31	0.60
1:C:289:ILE:CG2	1:C:290:ARG:N	2.64	0.60
1:D:170:VAL:CG1	1:D:178:ILE:HD13	2.31	0.60
1:A:223:ILE:O	1:A:223:ILE:CG2	2.49	0.60
1:C:216:THR:HG1	1:C:226:SER:HG	1.49	0.60
1:C:114:PHE:CZ	1:C:132:TRP:CD1	2.89	0.60
1:A:61:ASN:HB2	1:A:288:GLN:OE1	2.02	0.60
1:A:210:MET:C	1:A:211:LYS:HD3	2.27	0.60
1:C:51:LEU:HD23	3:C:402:3LD:H7	1.83	0.60
1:C:252:ASN:ND2	1:C:254:GLN:N	2.48	0.60
1:D:207:ALA:O	1:D:209:TRP:N	2.34	0.60
1:C:117:LEU:HB3	1:C:122:LEU:CD2	2.30	0.60
1:B:24:HIS:H	1:B:24:HIS:HD2	1.50	0.60
1:B:205:VAL:HG22	1:B:273:ALA:CB	2.31	0.60
1:A:203:MET:HE3	1:A:259:ILE:HG21	1.84	0.60
1:B:63:GLN:O	1:B:64:GLU:C	2.43	0.60
1:C:61:ASN:HD21	1:C:63:GLN:HE21	1.48	0.60
1:D:153:THR:C	1:D:155:ARG:N	2.60	0.60
1:D:241:ILE:HG12	1:D:259:ILE:HD11	1.84	0.60
1:D:293:ARG:O	1:D:294:GLU:CB	2.48	0.60
1:C:61:ASN:ND2	1:C:63:GLN:HB2	2.17	0.60
1:A:51:LEU:HD12	1:A:52:TRP:H	1.66	0.59
1:D:139:LEU:HD11	1:D:144:TYR:CD1	2.37	0.59
1:D:267:GLU:O	1:D:270:LEU:HB2	2.02	0.59
1:A:72:PHE:C	1:A:72:PHE:CD2	2.81	0.59
1:B:32:ILE:HB	1:B:157:VAL:HG13	1.84	0.59
1:B:117:LEU:O	1:B:122:LEU:HD11	2.01	0.59
1:C:112:LEU:HD23	1:C:112:LEU:H	1.67	0.59
1:D:28:GLN:HB3	1:D:29:PRO:CD	2.24	0.59
1:D:71:THR:HG23	1:D:320:TRP:H	1.67	0.59
1:D:223:ILE:HD12	1:D:224:TYR:H	1.68	0.59
1:C:104:ASP:OD1	1:C:104:ASP:N	2.33	0.59
1:D:102:ILE:HG12	1:D:103:PRO:N	2.18	0.59
1:A:272:ASN:O	1:A:273:ALA:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HG21	1:A:266:LEU:HD22	1.84	0.59
1:B:198:GLY:O	1:B:283:ARG:HD2	2.03	0.59
1:C:246:ASN:OD1	1:C:246:ASN:C	2.44	0.59
1:C:43:THR:O	1:C:44:THR:C	2.43	0.59
1:C:87:LEU:HD23	1:C:147:TRP:CE2	2.37	0.59
1:C:289:ILE:HD11	1:C:314:TYR:HE2	1.66	0.59
1:A:146:GLN:O	1:A:149:THR:HB	2.03	0.59
1:B:203:MET:HE2	1:B:256:HIS:ND1	2.17	0.59
1:D:161:GLN:O	1:D:162:ARG:HB3	2.03	0.59
1:C:208:PRO:HG2	1:D:234:GLN:NE2	2.16	0.59
1:D:253:ILE:HD13	1:D:253:ILE:O	2.01	0.59
1:D:172:ARG:O	1:D:174:GLY:N	2.36	0.59
1:A:55:TYR:HE1	1:A:224:TYR:HH	1.46	0.58
1:C:91:LEU:HD23	1:C:137:LEU:HD21	1.85	0.58
1:A:105:PRO:HD3	1:A:132:TRP:CE2	2.38	0.58
1:C:242:PHE:CD1	1:C:242:PHE:C	2.78	0.58
1:A:105:PRO:HD2	1:A:114:PHE:CZ	2.38	0.58
1:B:53:GLN:HE22	1:B:96:ASN:HD21	1.50	0.58
1:D:102:ILE:HG12	1:D:103:PRO:CD	2.33	0.58
1:D:32:ILE:O	1:D:157:VAL:HG13	2.03	0.58
1:D:52:TRP:NE1	1:D:317:THR:HG23	2.19	0.58
1:A:222:GLY:O	1:A:225:ASN:HB3	2.04	0.58
1:A:278:GLU:O	1:A:279:ARG:HG2	2.02	0.58
1:B:92:ILE:CD1	1:B:231:PRO:HG2	2.29	0.58
1:B:114:PHE:CD1	1:B:114:PHE:C	2.82	0.58
1:B:114:PHE:HZ	1:B:132:TRP:CD1	2.21	0.58
1:B:233:THR:HG23	1:B:234:GLN:HG2	1.84	0.58
1:A:203:MET:CE	1:A:259:ILE:HB	2.34	0.58
1:B:286:ARG:O	1:B:287:PRO:C	2.46	0.58
1:C:49:ALA:HB1	1:C:230:ILE:HG21	1.86	0.58
1:A:40:THR:HG23	1:A:41:PRO:HD3	1.86	0.58
1:C:97:LEU:CD2	1:C:117:LEU:CD1	2.82	0.58
1:D:144:TYR:OH	1:D:319:HIS:CE1	2.57	0.57
1:C:102:ILE:HG23	1:C:103:PRO:O	2.04	0.57
1:C:225:ASN:HD22	1:C:242:PHE:H	1.52	0.57
1:A:61:ASN:HD21	1:A:63:GLN:NE2	2.00	0.57
1:B:270:LEU:C	1:B:272:ASN:N	2.61	0.57
1:A:167:PHE:CE1	1:A:189:LEU:HD12	2.40	0.57
1:C:40:THR:HG23	1:C:41:PRO:CD	2.35	0.57
1:D:52:TRP:CE2	1:D:317:THR:HG23	2.40	0.57
1:D:210:MET:HE3	1:D:210:MET:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLY:O	1:B:130:TYR:HB2	2.03	0.57
1:D:224:TYR:O	1:D:242:PHE:CB	2.51	0.57
1:A:1:MET:CE	1:A:1:MET:CA	2.82	0.57
1:A:69:GLN:NE2	1:A:110:THR:CG2	2.67	0.57
1:C:268:PRO:C	1:C:270:LEU:H	2.13	0.57
1:B:171:ALA:O	1:B:172:ARG:C	2.48	0.57
1:D:304:GLU:O	1:D:305:VAL:HG23	2.05	0.57
1:A:27:LEU:HD11	1:A:334:LEU:CD2	2.35	0.57
1:B:328:LYS:O	1:B:329:LEU:C	2.47	0.57
1:C:266:LEU:CD2	1:C:266:LEU:O	2.53	0.57
1:A:1:MET:HE1	1:A:176:ASP:CB	2.33	0.56
1:A:6:ILE:O	1:A:181:CYS:HB2	2.05	0.56
1:A:83:ASN:O	1:A:84:ALA:C	2.48	0.56
1:D:74:TYR:O	1:D:77:SER:OG	2.23	0.56
1:D:207:ALA:HA	1:D:209:TRP:CZ3	2.40	0.56
1:A:1:MET:HG2	1:A:27:LEU:CD1	2.34	0.56
1:A:51:LEU:HD12	1:A:52:TRP:N	2.20	0.56
1:A:83:ASN:O	1:A:86:ASN:N	2.38	0.56
1:B:218:ASP:OD1	1:B:220:GLU:HB2	2.05	0.56
1:D:167:PHE:O	1:D:170:VAL:HG12	2.05	0.56
1:D:228:TYR:OH	3:D:402:3LD:O15	2.21	0.56
1:A:39:PHE:O	1:A:41:PRO:HD2	2.05	0.56
1:A:41:PRO:HD2	1:A:42:LEU:HG	1.88	0.56
1:C:114:PHE:CD1	1:C:115:ARG:N	2.74	0.56
1:D:102:ILE:HG13	1:D:103:PRO:HD2	1.87	0.56
1:D:313:GLY:O	3:D:402:3LD:N13	2.38	0.56
2:B:401:FAD:C5X	3:B:402:3LD:C10	2.83	0.56
1:A:107:TRP:O	1:A:110:THR:N	2.35	0.56
1:C:199:ARG:O	1:C:283:ARG:NH2	2.38	0.56
1:A:233:THR:HG23	1:A:234:GLN:H	1.55	0.56
1:C:119:PRO:HA	1:C:122:LEU:HD12	1.88	0.56
1:C:224:TYR:OH	1:C:313:GLY:HA3	2.06	0.56
1:C:244:LEU:HD21	1:C:285:VAL:HG11	1.86	0.56
1:D:147:TRP:CZ3	1:D:148:LEU:HD23	2.41	0.56
1:D:192:ASP:C	1:D:192:ASP:OD1	2.49	0.56
1:A:67:TRP:HB3	1:A:321:GLY:HA3	1.88	0.56
1:A:39:PHE:O	1:A:41:PRO:CD	2.54	0.56
1:A:200:GLY:CA	1:A:283:ARG:NH2	2.69	0.56
1:A:216:THR:HG23	1:A:266:LEU:HD11	1.87	0.56
2:A:401:FAD:O4	3:A:402:3LD:H9	2.06	0.56
1:B:205:VAL:CG2	1:B:273:ALA:HB1	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LYS:O	1:B:331:GLY:N	2.39	0.56
1:B:336:GLU:C	1:B:338:LYS:N	2.54	0.56
1:C:180:ASN:HD22	1:C:307:HIS:CD2	2.24	0.56
1:A:216:THR:CG2	1:A:266:LEU:HD11	2.36	0.55
1:C:1:MET:CE	1:C:176:ASP:HB2	2.36	0.55
1:C:94:GLY:HA3	1:C:213:PHE:O	2.06	0.55
1:D:37:ASP:N	2:D:401:FAD:N3A	2.51	0.55
1:D:44:THR:O	1:D:45:THR:C	2.47	0.55
1:C:325:GLU:O	1:C:326:ALA:C	2.47	0.55
1:A:221:ARG:NH2	1:A:221:ARG:CB	2.60	0.55
1:B:283:ARG:HG3	2:B:401:FAD:HM82	1.87	0.55
1:C:105:PRO:CD	1:C:105:PRO:O	2.53	0.55
1:C:144:TYR:OH	1:C:319:HIS:CE1	2.60	0.55
1:B:203:MET:HE1	1:B:256:HIS:CE1	2.41	0.55
1:D:121:GLU:O	1:D:124:MET:HG2	2.07	0.55
1:D:293:ARG:HD3	1:D:333:ILE:HD11	1.88	0.55
1:B:6:ILE:HD13	1:B:164:VAL:HG21	1.88	0.55
1:B:27:LEU:O	1:B:28:GLN:O	2.25	0.55
1:D:210:MET:HE3	1:D:210:MET:CA	2.36	0.55
1:D:318:ILE:O	1:D:320:TRP:N	2.40	0.55
1:A:144:TYR:CE2	1:A:148:LEU:HD11	2.41	0.55
1:A:331:GLY:HA2	1:A:334:LEU:HD12	1.89	0.55
1:B:180:ASN:HB3	1:B:307:HIS:HA	1.89	0.55
1:C:3:VAL:N	1:C:31:ASP:O	2.29	0.55
1:C:297:ARG:NH2	1:C:297:ARG:HB2	2.20	0.55
1:D:152:LEU:HG	1:D:157:VAL:HG21	1.89	0.55
1:A:162:ARG:HG3	1:A:162:ARG:O	2.04	0.55
1:B:199:ARG:HB2	1:B:246:ASN:HB3	1.89	0.55
1:C:79:VAL:HG22	1:C:79:VAL:O	2.06	0.55
1:D:221:ARG:NH2	1:D:221:ARG:HB3	2.21	0.55
1:A:268:PRO:HG2	1:B:80:HIS:HB3	1.89	0.54
1:D:255:ASP:O	1:D:259:ILE:HG12	2.07	0.54
1:A:140:GLU:OE1	1:A:233:THR:CB	2.41	0.54
1:A:193:PRO:CD	1:A:194:LEU:H	2.18	0.54
1:A:198:GLY:HA3	1:A:283:ARG:HB2	1.90	0.54
1:D:44:THR:C	1:D:46:ASP:N	2.61	0.54
1:B:252:ASN:HD22	1:B:255:ASP:CG	2.15	0.54
1:C:44:THR:O	1:C:45:THR:C	2.50	0.54
1:C:116:LYS:HD2	1:C:130:TYR:OH	2.06	0.54
1:D:1:MET:CG	1:D:27:LEU:HD11	2.35	0.54
1:C:27:LEU:HD11	1:C:334:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ALA:HB1	1:D:309:TYR:CE2	2.42	0.54
1:D:216:THR:OG1	1:D:226:SER:OG	2.26	0.54
1:B:203:MET:HE3	1:B:278:GLU:OE1	2.07	0.54
1:C:97:LEU:HD23	1:C:117:LEU:HD12	1.89	0.54
1:C:140:GLU:OE1	1:C:233:THR:CG2	2.56	0.54
1:C:210:MET:C	1:C:211:LYS:HD3	2.32	0.54
1:D:286:ARG:HG2	1:D:287:PRO:HD2	1.90	0.54
1:A:252:ASN:ND2	1:A:255:ASP:H	2.04	0.54
1:C:320:TRP:HA	1:C:320:TRP:CE3	2.43	0.54
1:D:52:TRP:CG	1:D:317:THR:HG23	2.43	0.54
1:B:205:VAL:CG2	1:B:273:ALA:CB	2.86	0.54
1:B:284:PRO:HG2	1:B:284:PRO:O	2.08	0.54
1:C:155:ARG:HG2	1:C:155:ARG:HH21	1.73	0.54
1:D:52:TRP:O	1:D:53:GLN:HB2	2.08	0.54
1:D:215:LEU:HD23	1:D:215:LEU:N	2.23	0.54
1:B:81:SER:HB2	1:B:82:PRO:CD	2.36	0.53
1:D:122:LEU:HD22	1:D:130:TYR:HA	1.89	0.53
1:D:197:PRO:HG3	1:D:247:TRP:CE2	2.43	0.53
1:D:233:THR:HG23	1:D:234:GLN:HG2	1.84	0.53
1:A:178:ILE:O	1:A:305:VAL:HA	2.07	0.53
1:A:267:GLU:O	1:A:270:LEU:HB2	2.08	0.53
1:A:297:ARG:CG	1:A:302:ASN:HD22	2.21	0.53
1:B:79:VAL:HG13	1:B:80:HIS:CD2	2.43	0.53
1:B:83:ASN:O	1:B:86:ASN:HB2	2.07	0.53
1:B:22:ARG:HB3	1:B:23:TYR:CD2	2.44	0.53
1:B:255:ASP:C	1:B:259:ILE:HG13	2.34	0.53
1:C:114:PHE:CZ	1:C:132:TRP:CG	2.96	0.53
1:D:199:ARG:HH22	1:D:201:GLN:HE21	1.56	0.53
1:A:115:ARG:NH1	1:B:113:GLY:HA3	2.24	0.53
1:B:61:ASN:OD1	1:B:63:GLN:HG2	2.09	0.53
1:B:309:TYR:HD1	1:B:310:GLY:N	2.05	0.53
1:C:206:ASP:HB2	1:C:276:ILE:HD11	1.91	0.53
1:D:102:ILE:HG13	1:D:103:PRO:CD	2.39	0.53
1:D:286:ARG:O	1:D:287:PRO:C	2.49	0.53
1:A:133:PHE:C	1:A:133:PHE:CD2	2.86	0.53
1:A:239:GLY:HA2	1:A:259:ILE:HD13	1.90	0.53
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.26	0.53
1:B:58:ASP:N	1:B:58:ASP:OD1	2.42	0.53
1:C:113:GLY:HA3	1:D:115:ARG:NH1	2.22	0.53
1:D:2:ARG:N	1:D:176:ASP:OD1	2.41	0.53
1:B:38:ARG:N	2:B:401:FAD:O2B	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASP:O	1:B:69:GLN:HB3	2.09	0.53
1:B:147:TRP:O	1:B:150:GLU:N	2.42	0.53
1:A:1:MET:HE2	1:A:1:MET:CA	2.38	0.53
1:B:47:VAL:O	1:B:47:VAL:HG12	2.09	0.53
1:C:121:GLU:HA	1:C:124:MET:HE2	1.91	0.53
1:D:17:LEU:HB2	1:D:152:LEU:CD1	2.39	0.53
1:B:183:GLY:O	1:B:184:VAL:C	2.52	0.53
1:C:48:ALA:HB1	2:C:401:FAD:C4X	2.39	0.53
1:C:199:ARG:HH12	1:C:201:GLN:NE2	2.07	0.53
1:D:64:GLU:HG2	1:D:289:ILE:HD12	1.90	0.53
1:A:1:MET:HE2	1:A:176:ASP:OD1	2.09	0.52
1:A:17:LEU:O	1:A:18:CYS:C	2.51	0.52
1:D:6:ILE:HD12	1:D:164:VAL:HG11	1.90	0.52
1:A:177:VAL:HG12	1:A:178:ILE:N	2.24	0.52
1:A:194:LEU:HD22	1:A:287:PRO:HG2	1.92	0.52
1:B:316:LEU:O	1:B:319:HIS:HD2	1.91	0.52
1:C:40:THR:O	1:C:40:THR:OG1	2.24	0.52
1:D:9:GLY:HA3	2:D:401:FAD:O1P	2.09	0.52
1:D:30:LEU:C	1:D:30:LEU:HD12	2.35	0.52
1:A:116:LYS:HD2	1:A:130:TYR:OH	2.09	0.52
1:B:39:PHE:C	1:B:41:PRO:CD	2.82	0.52
1:B:56:LEU:HD23	1:B:56:LEU:N	2.25	0.52
1:B:170:VAL:HA	1:B:173:GLU:HG2	1.91	0.52
1:B:290:ARG:HD2	1:B:292:GLU:CD	2.33	0.52
1:C:225:ASN:ND2	1:C:242:PHE:H	2.08	0.52
1:D:152:LEU:HA	1:D:155:ARG:HD2	1.91	0.52
1:A:55:TYR:HE1	1:A:224:TYR:OH	1.92	0.52
1:C:107:TRP:O	1:C:109:ASP:N	2.42	0.52
1:C:286:ARG:NH2	1:C:290:ARG:HB2	2.25	0.52
1:A:69:GLN:HE22	1:A:110:THR:CG2	2.21	0.52
1:B:63:GLN:O	1:B:66:ASP:N	2.43	0.52
1:B:286:ARG:HD3	1:B:288:GLN:O	2.10	0.52
1:B:319:HIS:CG	1:B:320:TRP:N	2.78	0.52
1:C:97:LEU:HD23	1:C:117:LEU:CD1	2.39	0.52
1:D:98:PHE:CD1	1:D:217:HIS:HB2	2.45	0.52
1:D:186:ALA:HB3	1:D:195:LEU:CD2	2.39	0.52
1:A:199:ARG:NH1	1:A:201:GLN:NE2	2.57	0.52
1:B:140:GLU:OE1	1:B:233:THR:HB	2.10	0.52
1:C:56:LEU:HD11	1:C:98:PHE:HE1	1.74	0.52
1:C:139:LEU:HD21	1:C:144:TYR:CG	2.44	0.52
1:C:290:ARG:HD2	1:C:292:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:HG3	1:A:151:ARG:NH2	2.25	0.52
1:B:86:ASN:O	1:B:143:ASN:ND2	2.40	0.52
1:B:100:GLU:OE1	1:B:100:GLU:CA	2.43	0.52
1:B:192:ASP:OD1	1:B:192:ASP:C	2.51	0.52
1:C:114:PHE:HA	1:C:134:HIS:HB3	1.90	0.52
1:C:208:PRO:HG2	1:D:234:GLN:HE22	1.73	0.52
1:D:91:LEU:HD13	1:D:135:THR:HG21	1.92	0.52
1:A:27:LEU:HB3	1:A:30:LEU:HB2	1.91	0.52
1:A:63:GLN:O	1:A:64:GLU:C	2.52	0.52
1:B:96:ASN:O	1:B:131:GLY:HA3	2.10	0.52
1:C:316:LEU:HB2	2:C:401:FAD:O2	2.10	0.52
1:A:66:ASP:O	1:A:70:GLN:HG3	2.10	0.51
1:A:197:PRO:HG2	1:A:247:TRP:CE2	2.44	0.51
1:B:313:GLY:O	3:B:402:3LD:N13	2.43	0.51
1:A:278:GLU:C	1:A:279:ARG:HG2	2.35	0.51
1:B:93:SER:HA	1:B:135:THR:HA	1.92	0.51
1:D:66:ASP:O	1:D:70:GLN:HG3	2.10	0.51
1:D:68:SER:HB3	1:D:317:THR:HG22	1.91	0.51
1:D:213:PHE:O	1:D:214:ILE:HG13	2.10	0.51
1:D:297:ARG:H	1:D:297:ARG:CD	2.18	0.51
1:A:1:MET:CE	1:A:176:ASP:CB	2.88	0.51
1:A:223:ILE:C	1:A:225:ASN:N	2.66	0.51
1:B:112:LEU:CD2	1:B:135:THR:O	2.59	0.51
1:C:150:GLU:HG3	1:C:151:ARG:HH12	1.73	0.51
1:C:171:ALA:O	1:C:172:ARG:C	2.52	0.51
1:D:102:ILE:HG12	1:D:103:PRO:HD2	1.92	0.51
1:B:203:MET:HE1	1:B:256:HIS:ND1	2.26	0.51
1:C:133:PHE:C	1:C:133:PHE:HD2	2.16	0.51
1:C:265:ARG:O	1:C:266:LEU:C	2.52	0.51
1:D:87:LEU:HD12	1:D:147:TRP:CD1	2.46	0.51
1:D:87:LEU:HD13	1:D:87:LEU:H	1.76	0.51
1:D:153:THR:O	1:D:155:ARG:N	2.44	0.51
1:A:28:GLN:HB3	1:A:29:PRO:HD3	1.92	0.51
1:A:221:ARG:O	1:A:225:ASN:HB3	2.10	0.51
1:B:107:TRP:O	1:B:108:LYS:C	2.51	0.51
1:B:228:TYR:OH	3:B:402:3LD:O15	2.23	0.51
1:C:105:PRO:O	1:C:105:PRO:HD2	2.10	0.51
1:A:167:PHE:CE1	1:A:189:LEU:CD1	2.93	0.51
1:B:75:LEU:O	1:B:89:LEU:HD11	2.10	0.51
1:C:283:ARG:CG	2:C:401:FAD:HM82	2.40	0.51
1:D:107:TRP:O	1:D:110:THR:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ARG:HH22	1:D:201:GLN:NE2	2.09	0.51
1:B:81:SER:CB	1:B:82:PRO:HD2	2.37	0.51
1:C:252:ASN:HD21	1:C:254:GLN:H	1.59	0.51
1:C:325:GLU:O	1:C:327:ALA:N	2.44	0.51
1:C:201:GLN:HE22	1:C:252:ASN:H	1.59	0.51
1:B:52:TRP:NE1	1:B:317:THR:HG23	2.25	0.51
1:C:75:LEU:O	1:C:76:LEU:C	2.54	0.51
1:C:113:GLY:O	1:C:114:PHE:C	2.53	0.51
1:C:133:PHE:CD2	1:C:134:HIS:N	2.78	0.51
1:C:205:VAL:HG12	1:C:236:VAL:HB	1.92	0.51
1:C:243:GLN:NE2	1:C:246:ASN:HD22	2.03	0.51
1:A:114:PHE:HA	1:A:134:HIS:HB3	1.93	0.51
1:B:322:CYS:O	1:B:325:GLU:HB3	2.10	0.51
1:C:266:LEU:O	1:C:266:LEU:HD22	2.10	0.51
1:C:297:ARG:HB2	1:C:297:ARG:CZ	2.40	0.51
1:D:122:LEU:CD2	1:D:130:TYR:HA	2.41	0.51
1:A:319:HIS:CG	1:A:320:TRP:N	2.79	0.50
1:B:42:LEU:HD22	1:D:42:LEU:HD22	1.92	0.50
1:B:332:ARG:O	1:B:333:ILE:C	2.52	0.50
1:C:266:LEU:CD2	1:C:266:LEU:C	2.84	0.50
1:D:126:PRO:C	1:D:128:TYR:H	2.19	0.50
1:D:290:ARG:NH2	1:D:292:GLU:OE2	2.45	0.50
1:A:22:ARG:HG2	1:A:23:TYR:CE2	2.47	0.50
1:C:17:LEU:HB2	1:C:152:LEU:CD1	2.42	0.50
1:C:59:PRO:HB2	1:C:61:ASN:H	1.76	0.50
1:C:205:VAL:HG22	1:C:273:ALA:HB1	1.92	0.50
1:A:70:GLN:O	1:A:71:THR:C	2.55	0.50
1:A:107:TRP:O	1:A:109:ASP:N	2.44	0.50
1:B:215:LEU:HD23	1:B:228:TYR:HB2	1.93	0.50
1:B:305:VAL:O	1:B:305:VAL:HG12	2.08	0.50
1:C:71:THR:CG2	1:C:317:THR:O	2.59	0.50
1:C:191:ARG:NH1	1:C:193:PRO:CG	2.75	0.50
1:C:209:TRP:CZ3	1:D:85:GLU:HG3	2.46	0.50
1:D:215:LEU:HD13	3:D:402:3LD:C6	2.41	0.50
1:A:59:PRO:HG2	1:A:61:ASN:O	2.11	0.50
1:A:289:ILE:HG12	1:A:311:HIS:HA	1.94	0.50
1:C:201:GLN:NE2	1:C:252:ASN:H	2.10	0.50
1:D:182:THR:HG22	2:D:401:FAD:N7A	2.26	0.50
1:B:40:THR:HG23	1:B:41:PRO:N	2.25	0.50
1:C:104:ASP:HB3	1:C:105:PRO:CD	2.41	0.50
1:A:294:GLU:C	1:A:295:GLN:HE21	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:THR:O	1:B:46:ASP:OD2	2.30	0.50
1:B:315:GLY:HA3	2:B:401:FAD:O3'	2.11	0.50
1:C:119:PRO:O	1:C:120:ARG:C	2.55	0.50
1:C:316:LEU:HB2	2:C:401:FAD:C2	2.41	0.50
1:D:264:CYS:HG	1:D:271:LYS:HD2	1.71	0.50
1:A:296:LEU:O	1:A:302:ASN:HB3	2.11	0.50
1:C:208:PRO:HB2	1:D:233:THR:O	2.11	0.50
1:B:22:ARG:O	1:B:22:ARG:HD3	2.12	0.49
1:C:200:GLY:CA	1:C:283:ARG:HH22	2.25	0.49
1:C:208:PRO:O	1:C:211:LYS:HE2	2.12	0.49
1:A:330:PHE:O	1:A:333:ILE:HB	2.11	0.49
1:B:114:PHE:CZ	1:B:132:TRP:CD1	3.00	0.49
1:D:5:VAL:HB	1:D:34:VAL:HG22	1.94	0.49
1:A:61:ASN:OD1	1:A:61:ASN:C	2.54	0.49
1:C:139:LEU:HD21	1:C:144:TYR:CD2	2.47	0.49
1:A:54:PRO:O	1:A:55:TYR:O	2.29	0.49
1:A:297:ARG:HG3	1:A:302:ASN:ND2	2.24	0.49
1:B:52:TRP:HA	1:B:317:THR:OG1	2.12	0.49
1:C:190:GLN:O	1:C:191:ARG:C	2.55	0.49
1:C:18:CYS:HB2	1:C:323:ALA:HB1	1.94	0.49
1:A:286:ARG:O	1:A:287:PRO:C	2.55	0.49
1:B:223:ILE:O	1:B:224:TYR:C	2.53	0.49
1:C:284:PRO:HB2	1:C:310:GLY:HA2	1.94	0.49
1:A:15:THR:O	1:A:16:ALA:C	2.54	0.49
1:A:203:MET:HB3	1:A:238:LEU:HB2	1.94	0.49
1:D:198:GLY:O	1:D:283:ARG:HD2	2.13	0.49
1:D:228:TYR:CE1	3:D:402:3LD:H3	2.47	0.49
1:A:115:ARG:NH2	1:A:121:GLU:OE2	2.45	0.49
1:B:168:GLU:CD	1:B:168:GLU:H	2.21	0.49
1:C:79:VAL:C	1:C:80:HIS:HD2	2.20	0.49
1:C:274:ARG:HA	1:C:274:ARG:HE	1.77	0.49
1:D:33:LYS:HG2	1:D:160:PHE:CE1	2.48	0.49
1:D:78:HIS:O	1:D:79:VAL:C	2.56	0.49
1:B:87:LEU:HD11	1:B:147:TRP:CE2	2.47	0.49
1:B:147:TRP:CZ3	1:B:148:LEU:HD23	2.48	0.49
1:D:162:ARG:O	2:D:401:FAD:H2A	2.13	0.49
1:D:223:ILE:C	1:D:224:TYR:C	2.81	0.49
1:A:190:GLN:O	1:A:191:ARG:C	2.55	0.49
1:C:107:TRP:C	1:C:109:ASP:H	2.21	0.49
1:A:79:VAL:HG13	1:A:80:HIS:HB2	1.95	0.48
1:B:108:LYS:HD2	1:B:109:ASP:CG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:OG1	1:B:121:GLU:HG3	2.12	0.48
1:D:28:GLN:CB	1:D:29:PRO:HD3	2.31	0.48
1:C:150:GLU:HG3	1:C:151:ARG:CZ	2.43	0.48
1:A:200:GLY:HA2	1:A:283:ARG:HH22	1.76	0.48
1:B:107:TRP:C	1:B:109:ASP:H	2.21	0.48
1:C:117:LEU:HD22	1:C:121:GLU:CB	2.43	0.48
1:B:52:TRP:CD1	1:B:317:THR:HG23	2.48	0.48
1:B:67:TRP:CH2	1:B:291:LEU:HD23	2.48	0.48
1:B:209:TRP:O	1:B:211:LYS:HG2	2.12	0.48
1:C:325:GLU:C	1:C:327:ALA:N	2.65	0.48
1:D:148:LEU:O	1:D:149:THR:C	2.55	0.48
1:A:1:MET:HA	1:A:1:MET:HE3	1.94	0.48
1:A:112:LEU:HB2	1:A:135:THR:HB	1.95	0.48
1:B:39:PHE:C	1:B:41:PRO:HD3	2.38	0.48
1:B:304:GLU:HB3	1:B:333:ILE:HD13	1.95	0.48
1:D:87:LEU:H	1:D:87:LEU:CD1	2.27	0.48
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.37	0.48
1:B:257:ASN:O	1:B:261:GLU:OE1	2.31	0.48
1:D:44:THR:O	1:D:46:ASP:N	2.47	0.48
1:D:75:LEU:HB3	1:D:89:LEU:HD21	1.94	0.48
1:D:114:PHE:HA	1:D:134:HIS:HB3	1.96	0.48
1:A:196:GLN:O	1:A:285:VAL:HB	2.13	0.48
1:A:272:ASN:O	1:A:273:ALA:O	2.31	0.48
1:C:199:ARG:HG3	1:C:282:PHE:CE1	2.49	0.48
1:C:221:ARG:CZ	1:C:221:ARG:CB	2.92	0.48
1:C:253:ILE:HG22	1:C:254:GLN:NE2	2.28	0.48
1:D:112:LEU:CD2	1:D:112:LEU:N	2.76	0.48
1:A:333:ILE:O	1:A:334:LEU:C	2.54	0.48
1:B:56:LEU:HD11	1:B:217:HIS:CE1	2.49	0.48
1:B:56:LEU:HD11	1:B:217:HIS:ND1	2.28	0.48
1:B:151:ARG:HA	1:B:154:GLU:HG3	1.95	0.48
1:C:114:PHE:CE2	1:C:132:TRP:HB3	2.49	0.48
1:C:283:ARG:HG2	2:C:401:FAD:C8M	2.43	0.48
1:D:79:VAL:HG13	1:D:80:HIS:N	2.29	0.48
1:D:167:PHE:CZ	1:D:189:LEU:HB3	2.49	0.48
1:D:186:ALA:HB3	1:D:195:LEU:HD22	1.94	0.48
1:C:54:PRO:HG3	1:C:317:THR:CG2	2.42	0.48
1:D:95:TYR:CZ	1:D:133:PHE:HE1	2.32	0.48
1:A:1:MET:O	1:A:1:MET:HG3	2.13	0.48
1:A:52:TRP:O	1:A:53:GLN:HB2	2.14	0.48
1:A:30:LEU:HG	1:A:30:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:TYR:C	1:B:309:TYR:HD1	2.22	0.47
1:D:170:VAL:HG11	1:D:178:ILE:HD13	1.94	0.47
1:A:101:ALA:HA	1:A:130:TYR:CE2	2.49	0.47
1:A:114:PHE:C	1:A:114:PHE:CD1	2.92	0.47
1:A:218:ASP:OD1	1:A:218:ASP:C	2.57	0.47
1:A:95:TYR:HD1	1:A:214:ILE:HG12	1.79	0.47
1:B:335:GLU:HG2	1:B:336:GLU:H	1.77	0.47
1:D:172:ARG:C	1:D:174:GLY:N	2.71	0.47
1:A:328:LYS:O	1:A:332:ARG:HG3	2.15	0.47
1:D:200:GLY:HA3	1:D:283:ARG:NH2	2.30	0.47
1:D:286:ARG:NH1	1:D:290:ARG:HD3	2.28	0.47
1:A:160:PHE:CD1	1:A:160:PHE:N	2.82	0.47
1:A:199:ARG:HH12	1:A:201:GLN:HE22	1.62	0.47
1:B:91:LEU:HD23	1:B:137:LEU:CD2	2.43	0.47
1:C:117:LEU:HB2	1:C:131:GLY:O	2.14	0.47
1:D:214:ILE:C	1:D:215:LEU:HD23	2.39	0.47
1:A:114:PHE:HA	1:A:134:HIS:CB	2.45	0.47
1:A:203:MET:HE1	1:A:259:ILE:HB	1.96	0.47
1:B:335:GLU:HA	1:B:340:SER:CB	2.23	0.47
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.46	0.47
1:A:333:ILE:HG22	1:A:334:LEU:N	2.30	0.47
1:B:71:THR:OG1	1:B:318:ILE:O	2.32	0.47
1:B:255:ASP:O	1:B:259:ILE:CG1	2.55	0.47
1:C:208:PRO:HD2	1:C:209:TRP:CZ3	2.50	0.47
1:D:97:LEU:HD11	1:D:125:PHE:CD2	2.49	0.47
1:D:205:VAL:HG13	1:D:273:ALA:HB1	1.95	0.47
1:D:286:ARG:CZ	1:D:290:ARG:HB2	2.45	0.47
1:A:205:VAL:HG23	1:A:275:ILE:HA	1.97	0.47
2:A:401:FAD:O5B	2:A:401:FAD:O1P	2.30	0.47
1:B:87:LEU:CD1	1:B:147:TRP:CE2	2.98	0.47
1:C:178:ILE:CB	1:C:305:VAL:HG22	2.44	0.47
1:C:224:TYR:CZ	1:C:313:GLY:HA3	2.50	0.47
1:D:108:LYS:C	1:D:108:LYS:HD2	2.40	0.47
1:A:42:LEU:CD2	1:C:42:LEU:HD22	2.31	0.47
1:A:197:PRO:HG2	1:A:247:TRP:NE1	2.30	0.47
1:C:79:VAL:HG13	1:C:80:HIS:CD2	2.50	0.47
1:C:266:LEU:O	1:C:266:LEU:HD23	2.15	0.47
1:D:103:PRO:O	1:D:104:ASP:O	2.32	0.47
1:D:107:TRP:O	1:D:109:ASP:N	2.47	0.47
1:C:140:GLU:OE1	1:C:233:THR:HG22	2.14	0.47
1:C:320:TRP:O	1:C:321:GLY:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:NH1	1:D:290:ARG:HB2	2.30	0.47
1:B:243:GLN:HE21	1:B:243:GLN:HB2	1.27	0.46
1:C:265:ARG:O	1:C:267:GLU:N	2.48	0.46
1:D:98:PHE:CE1	1:D:217:HIS:HB2	2.50	0.46
1:A:195:LEU:HB2	1:A:286:ARG:HD2	1.97	0.46
1:C:208:PRO:HD2	1:C:209:TRP:CE3	2.50	0.46
1:D:63:GLN:O	1:D:66:ASP:N	2.44	0.46
1:D:264:CYS:HB3	1:D:271:LYS:NZ	2.30	0.46
1:D:323:ALA:C	1:D:325:GLU:N	2.73	0.46
1:B:59:PRO:HG2	1:B:62:PRO:CA	2.44	0.46
1:B:295:GLN:O	1:B:297:ARG:HD3	2.15	0.46
1:C:180:ASN:HD22	1:C:307:HIS:HD2	1.62	0.46
1:C:327:ALA:O	1:C:330:PHE:HB3	2.15	0.46
1:C:336:GLU:C	1:C:338:LYS:H	2.23	0.46
1:D:199:ARG:NH1	1:D:255:ASP:OD2	2.48	0.46
1:C:120:ARG:HA	1:C:120:ARG:HE	1.81	0.46
1:C:316:LEU:HD13	1:C:316:LEU:HA	1.44	0.46
1:D:60:ASN:C	1:D:60:ASN:OD1	2.58	0.46
1:A:98:PHE:HD2	1:A:131:GLY:HA2	1.79	0.46
1:C:168:GLU:HA	1:C:171:ALA:HB3	1.97	0.46
1:C:69:GLN:HG3	1:C:73:ASP:OD2	2.15	0.46
1:D:10:VAL:HB	1:D:45:THR:HG21	1.98	0.46
1:D:84:ALA:C	1:D:86:ASN:N	2.72	0.46
1:A:118:THR:HB	1:A:119:PRO:HD2	1.98	0.46
1:A:144:TYR:CD2	1:A:148:LEU:HD11	2.51	0.46
1:B:85:GLU:C	1:B:88:GLY:H	2.24	0.46
1:B:241:ILE:HD12	1:B:255:ASP:CB	2.30	0.46
1:B:242:PHE:CD1	1:B:243:GLN:N	2.84	0.46
1:B:270:LEU:C	1:B:272:ASN:H	2.22	0.46
1:C:37:ASP:HB3	1:C:38:ARG:CZ	2.46	0.46
1:C:56:LEU:CD1	1:C:98:PHE:HE1	2.29	0.46
1:C:289:ILE:HD11	1:C:314:TYR:CE2	2.49	0.46
1:D:40:THR:HG23	1:D:41:PRO:CD	2.46	0.46
1:D:201:GLN:HA	1:D:279:ARG:O	2.16	0.46
1:A:311:HIS:O	1:A:314:TYR:CE1	2.69	0.46
1:B:270:LEU:O	1:B:272:ASN:N	2.49	0.46
1:C:93:SER:OG	1:C:135:THR:HA	2.16	0.46
1:C:205:VAL:CG2	1:C:273:ALA:HB1	2.45	0.46
1:D:144:TYR:CE2	1:D:148:LEU:HD11	2.51	0.46
1:D:291:LEU:O	1:D:292:GLU:HB3	2.16	0.46
1:D:323:ALA:C	1:D:325:GLU:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG12	1:A:158:LYS:N	2.31	0.46
1:B:107:TRP:C	1:B:109:ASP:N	2.74	0.46
1:C:202:ILE:HD13	1:C:204:LYS:HE2	1.98	0.46
1:A:123:ASP:C	1:A:125:PHE:H	2.24	0.46
1:A:165:GLU:O	1:A:166:SER:HB3	2.16	0.46
1:B:69:GLN:OE1	1:B:110:THR:HG23	2.16	0.46
1:B:121:GLU:O	1:B:124:MET:HG3	2.16	0.46
1:B:284:PRO:O	1:B:312:GLY:N	2.49	0.46
1:C:68:SER:O	1:C:69:GLN:C	2.56	0.46
1:C:92:ILE:HG21	1:C:138:ILE:HG13	1.98	0.46
1:D:186:ALA:CB	1:D:309:TYR:CD2	2.99	0.46
1:D:267:GLU:HA	1:D:268:PRO:HD3	1.82	0.46
1:A:208:PRO:HD2	1:A:209:TRP:CE3	2.51	0.45
1:A:218:ASP:HA	1:A:219:PRO:HD2	1.49	0.45
1:B:52:TRP:CE2	1:B:317:THR:HG23	2.51	0.45
1:B:213:PHE:HA	1:B:231:PRO:HD2	1.98	0.45
1:C:13:LEU:O	1:C:14:SER:C	2.58	0.45
1:C:74:TYR:CD1	1:C:74:TYR:C	2.89	0.45
1:C:79:VAL:HG21	1:C:91:LEU:HD21	1.97	0.45
1:A:76:LEU:O	1:A:76:LEU:HG	2.15	0.45
1:A:239:GLY:HA2	1:A:259:ILE:HD12	1.97	0.45
1:A:255:ASP:O	1:A:256:HIS:C	2.57	0.45
1:B:64:GLU:O	1:B:67:TRP:N	2.49	0.45
1:B:144:TYR:CE2	1:B:319:HIS:CE1	3.04	0.45
1:D:224:TYR:CE2	1:D:313:GLY:HA3	2.51	0.45
1:D:275:ILE:C	1:D:276:ILE:HD13	2.41	0.45
1:A:328:LYS:HD2	1:A:332:ARG:NH1	2.32	0.45
1:D:126:PRO:C	1:D:128:TYR:N	2.74	0.45
1:D:284:PRO:HD2	1:D:312:GLY:O	2.17	0.45
1:C:20:HIS:ND1	1:C:155:ARG:NH2	2.64	0.45
1:C:55:TYR:CE1	1:C:314:TYR:HD1	2.35	0.45
1:C:205:VAL:HG13	1:C:273:ALA:HB1	1.98	0.45
1:B:92:ILE:HG21	1:B:138:ILE:CD1	2.46	0.45
1:B:97:LEU:HB2	1:B:216:THR:HG22	1.98	0.45
1:C:79:VAL:HG21	1:C:91:LEU:CD1	2.38	0.45
1:A:93:SER:HA	1:A:135:THR:HA	1.99	0.45
1:B:20:HIS:O	1:B:21:GLU:C	2.60	0.45
1:B:147:TRP:NE1	1:B:151:ARG:HH21	2.14	0.45
1:C:68:SER:HB3	1:C:317:THR:HG22	1.99	0.45
1:C:217:HIS:CD2	1:C:217:HIS:N	2.84	0.45
1:C:293:ARG:HD3	1:C:333:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:TYR:O	1:C:317:THR:N	2.50	0.45
1:D:73:ASP:O	1:D:74:TYR:C	2.59	0.45
1:B:96:ASN:O	1:B:131:GLY:CA	2.64	0.45
1:C:6:ILE:HA	1:C:35:TYR:O	2.17	0.45
1:C:71:THR:O	1:C:74:TYR:HB3	2.17	0.45
1:C:268:PRO:C	1:C:270:LEU:N	2.73	0.45
1:D:268:PRO:C	1:D:270:LEU:H	2.25	0.45
1:D:324:LEU:O	1:D:328:LYS:HE2	2.17	0.45
1:A:229:ILE:C	1:A:230:ILE:HG13	2.40	0.45
1:B:43:THR:O	1:B:46:ASP:HB2	2.16	0.45
1:B:293:ARG:NH2	1:B:333:ILE:HG12	2.32	0.45
1:C:205:VAL:HG12	1:C:205:VAL:O	2.16	0.45
1:D:199:ARG:HG3	1:D:246:ASN:HB3	1.97	0.45
1:A:143:ASN:C	1:A:145:LEU:N	2.72	0.45
1:A:249:GLU:N	1:A:282:PHE:HZ	2.15	0.45
1:B:118:THR:HB	1:B:119:PRO:CD	2.46	0.45
1:C:13:LEU:HB2	1:C:148:LEU:HD13	1.99	0.45
1:C:14:SER:O	1:C:15:THR:C	2.59	0.45
1:C:128:TYR:N	1:C:128:TYR:CD1	2.83	0.45
1:C:184:VAL:O	1:C:195:LEU:HD21	2.17	0.45
1:D:223:ILE:HD12	1:D:224:TYR:N	2.31	0.45
1:A:52:TRP:CE2	1:A:72:PHE:HB2	2.52	0.44
1:A:203:MET:O	1:A:238:LEU:N	2.49	0.44
1:C:13:LEU:O	1:C:16:ALA:N	2.50	0.44
1:C:20:HIS:HD2	1:C:32:ILE:CD1	2.29	0.44
1:C:69:GLN:HE22	1:C:110:THR:CG2	2.13	0.44
1:D:61:ASN:HD21	1:D:63:GLN:HB2	1.82	0.44
1:D:138:ILE:HD12	1:D:231:PRO:O	2.17	0.44
1:C:114:PHE:CE2	1:C:132:TRP:CG	3.05	0.44
1:C:205:VAL:HG13	1:C:206:ASP:N	2.32	0.44
1:C:215:LEU:HD23	1:C:215:LEU:N	2.31	0.44
1:D:15:THR:O	1:D:16:ALA:C	2.61	0.44
1:A:50:GLY:O	1:A:138:ILE:HA	2.16	0.44
1:A:196:GLN:NE2	1:A:244:LEU:HD22	2.32	0.44
1:B:83:ASN:HA	1:B:86:ASN:HD22	1.83	0.44
1:B:87:LEU:HD12	1:B:147:TRP:CD2	2.52	0.44
1:C:13:LEU:HD12	1:C:145:LEU:CD1	2.47	0.44
1:C:52:TRP:CD1	1:C:317:THR:HG23	2.50	0.44
1:D:27:LEU:HD12	1:D:30:LEU:HD22	1.99	0.44
1:D:51:LEU:HA	1:D:51:LEU:HD12	1.55	0.44
1:A:193:PRO:CD	1:A:194:LEU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HB	1:B:45:THR:HG21	1.99	0.44
1:B:202:ILE:HD12	1:B:202:ILE:C	2.42	0.44
1:C:34:VAL:C	1:C:35:TYR:HD1	2.25	0.44
1:C:64:GLU:O	1:C:67:TRP:HB2	2.18	0.44
1:D:255:ASP:O	1:D:256:HIS:C	2.60	0.44
1:A:46:ASP:OD2	1:A:145:LEU:HD23	2.18	0.44
1:A:151:ARG:O	1:A:155:ARG:HD2	2.18	0.44
2:C:401:FAD:H1'1	2:C:401:FAD:H9	1.72	0.44
1:D:84:ALA:O	1:D:85:GLU:C	2.59	0.44
1:D:252:ASN:ND2	1:D:254:GLN:HB2	2.32	0.44
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.74	0.44
1:A:168:GLU:O	1:A:172:ARG:N	2.50	0.44
1:A:171:ALA:HB1	1:A:303:THR:HG21	1.98	0.44
1:A:290:ARG:HD2	1:A:292:GLU:CD	2.42	0.44
1:C:8:ALA:O	1:C:13:LEU:HD11	2.18	0.44
1:D:75:LEU:O	1:D:78:HIS:N	2.43	0.44
1:C:202:ILE:C	1:C:202:ILE:HD12	2.43	0.44
1:D:63:GLN:O	1:D:66:ASP:HB2	2.18	0.44
1:A:10:VAL:HG13	1:A:11:ILE:N	2.32	0.44
1:A:28:GLN:HB3	1:A:29:PRO:CD	2.48	0.44
1:A:228:TYR:CD1	1:A:228:TYR:C	2.96	0.44
1:A:229:ILE:CD1	1:A:266:LEU:HD13	2.48	0.44
1:A:233:THR:HG22	1:A:234:GLN:H	1.80	0.44
1:B:265:ARG:HE	1:B:265:ARG:HB2	1.28	0.44
1:D:170:VAL:CG1	1:D:178:ILE:CD1	2.95	0.44
1:D:216:THR:OG1	1:D:227:PRO:O	2.33	0.44
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.67	0.43
1:A:121:GLU:HG3	1:B:112:LEU:HB3	2.00	0.43
1:B:177:VAL:HG22	1:B:304:GLU:HB2	2.00	0.43
1:C:213:PHE:HA	1:C:229:ILE:O	2.18	0.43
1:C:226:SER:HA	1:C:227:PRO:HD2	1.80	0.43
1:D:112:LEU:O	1:D:113:GLY:C	2.61	0.43
1:D:178:ILE:HB	1:D:305:VAL:HG22	2.00	0.43
1:A:11:ILE:HD13	1:A:11:ILE:HA	1.77	0.43
1:A:74:TYR:O	1:A:75:LEU:C	2.58	0.43
1:A:104:ASP:OD1	1:A:116:LYS:CE	2.65	0.43
1:A:274:ARG:HD2	1:D:274:ARG:HH12	1.83	0.43
1:B:7:GLY:O	1:B:12:GLY:HA3	2.17	0.43
1:B:125:PHE:HA	1:B:126:PRO:HD3	1.65	0.43
1:C:79:VAL:O	1:C:80:HIS:CD2	2.64	0.43
1:D:304:GLU:O	1:D:305:VAL:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:O	1:A:53:GLN:CB	2.65	0.43
1:A:138:ILE:CG2	1:A:139:LEU:N	2.77	0.43
1:A:180:ASN:ND2	1:A:307:HIS:HD2	2.14	0.43
1:A:200:GLY:HA3	1:A:283:ARG:NH2	2.32	0.43
1:B:117:LEU:CD2	1:B:133:PHE:HB2	2.48	0.43
1:C:101:ALA:HA	1:C:130:TYR:CD2	2.53	0.43
1:D:10:VAL:HG13	1:D:11:ILE:HG12	1.99	0.43
1:A:84:ALA:O	1:A:88:GLY:N	2.52	0.43
1:A:144:TYR:OH	1:A:319:HIS:HE1	2.01	0.43
1:C:71:THR:HG21	1:C:317:THR:C	2.43	0.43
1:D:207:ALA:C	1:D:209:TRP:H	2.25	0.43
1:D:225:ASN:ND2	1:D:241:ILE:HA	2.34	0.43
1:A:71:THR:HA	1:A:320:TRP:HB3	2.00	0.43
1:B:297:ARG:CZ	1:B:297:ARG:HB2	2.48	0.43
1:C:205:VAL:CG1	1:C:273:ALA:HB1	2.49	0.43
1:C:218:ASP:OD1	1:C:218:ASP:C	2.61	0.43
1:C:233:THR:HG23	1:C:234:GLN:N	2.34	0.43
1:A:246:ASN:OD1	1:A:246:ASN:C	2.61	0.43
1:B:119:PRO:O	1:B:120:ARG:C	2.61	0.43
1:D:140:GLU:CD	1:D:233:THR:HB	2.44	0.43
1:A:153:THR:O	1:A:156:GLY:N	2.46	0.43
1:A:197:PRO:CG	1:A:247:TRP:CE2	3.01	0.43
1:B:198:GLY:H	1:B:285:VAL:CG2	2.32	0.43
1:B:203:MET:HE1	1:B:256:HIS:CG	2.53	0.43
1:B:249:GLU:N	1:D:161:GLN:HG3	2.34	0.43
1:C:213:PHE:C	1:C:214:ILE:HG13	2.41	0.43
1:A:67:TRP:HA	1:A:70:GLN:OE1	2.19	0.43
1:A:229:ILE:HD12	1:A:266:LEU:HD13	2.01	0.43
1:A:265:ARG:HE	1:A:265:ARG:HB2	1.01	0.43
1:B:260:TRP:CD1	1:B:260:TRP:C	2.96	0.43
1:C:41:PRO:HG2	1:C:42:LEU:HG	1.99	0.43
1:A:87:LEU:HD11	1:A:147:TRP:CE2	2.54	0.43
1:B:309:TYR:CD1	1:B:310:GLY:N	2.85	0.43
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.46	0.43
1:C:178:ILE:CG2	1:C:305:VAL:HG22	2.49	0.43
1:D:17:LEU:CA	1:D:152:LEU:HD11	2.49	0.43
1:A:227:PRO:HG3	1:A:262:GLY:HA3	2.00	0.43
1:A:233:THR:HG23	1:A:234:GLN:HG2	2.01	0.43
1:C:155:ARG:HG2	1:C:155:ARG:NH2	2.34	0.43
1:A:143:ASN:O	1:A:144:TYR:C	2.61	0.42
1:B:28:GLN:O	1:B:30:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:O	1:B:81:SER:HB3	2.19	0.42
1:B:83:ASN:O	1:B:84:ALA:C	2.61	0.42
1:B:144:TYR:OH	1:B:319:HIS:HE1	2.01	0.42
1:D:293:ARG:HA	1:D:305:VAL:O	2.19	0.42
1:A:120:ARG:HE	1:A:120:ARG:HA	1.84	0.42
1:A:318:ILE:O	1:A:319:HIS:C	2.60	0.42
1:B:81:SER:CB	1:B:82:PRO:CD	2.97	0.42
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.88	0.42
1:C:139:LEU:HD21	1:C:144:TYR:CD1	2.54	0.42
1:C:225:ASN:OD1	1:C:225:ASN:O	2.36	0.42
1:A:170:VAL:HA	1:A:173:GLU:HG2	2.01	0.42
1:A:228:TYR:CZ	3:A:402:3LD:H3	2.54	0.42
1:C:117:LEU:HD22	1:C:121:GLU:HB3	2.00	0.42
1:A:67:TRP:HD1	1:A:70:GLN:OE1	2.03	0.42
1:A:214:ILE:HG21	1:A:266:LEU:CD2	2.50	0.42
1:D:228:TYR:CE2	1:D:240:GLY:N	2.87	0.42
1:A:178:ILE:N	1:A:304:GLU:O	2.49	0.42
1:B:47:VAL:O	1:B:47:VAL:CG1	2.68	0.42
1:B:147:TRP:HE1	1:B:151:ARG:HH21	1.66	0.42
1:B:183:GLY:C	1:B:185:TRP:N	2.76	0.42
1:B:284:PRO:O	1:B:312:GLY:HA2	2.19	0.42
1:B:325:GLU:OE1	1:B:325:GLU:CA	2.59	0.42
1:C:7:GLY:HA3	1:C:181:CYS:O	2.19	0.42
1:C:150:GLU:O	1:C:154:GLU:CG	2.57	0.42
1:A:104:ASP:OD1	1:A:116:LYS:HE3	2.19	0.42
1:B:335:GLU:CB	1:B:340:SER:HB3	2.47	0.42
1:C:200:GLY:HA3	1:C:283:ARG:NH2	2.34	0.42
1:A:157:VAL:CG1	1:A:158:LYS:N	2.82	0.42
1:A:327:ALA:O	1:A:330:PHE:HB3	2.20	0.42
1:C:105:PRO:O	1:C:105:PRO:CG	2.67	0.42
1:C:127:ASP:N	1:C:127:ASP:OD1	2.52	0.42
1:C:183:GLY:O	1:C:184:VAL:C	2.62	0.42
1:C:314:TYR:O	1:C:315:GLY:C	2.62	0.42
1:D:55:TYR:O	1:D:56:LEU:C	2.62	0.42
1:B:159:PHE:C	1:B:160:PHE:CD1	2.98	0.42
1:B:213:PHE:HA	1:B:231:PRO:CD	2.49	0.42
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.71	0.42
1:D:38:ARG:O	2:D:401:FAD:O3B	2.33	0.42
1:D:95:TYR:O	1:D:215:LEU:N	2.43	0.42
1:D:206:ASP:HB2	1:D:274:ARG:HB3	2.02	0.42
1:A:183:GLY:O	1:A:185:TRP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:H	1:A:241:ILE:HG22	1.84	0.42
1:B:98:PHE:CE1	1:B:217:HIS:HB2	2.55	0.42
1:B:278:GLU:O	1:B:279:ARG:HG2	2.20	0.42
1:C:33:LYS:HE2	1:C:35:TYR:HE1	1.85	0.42
1:D:103:PRO:O	1:D:104:ASP:C	2.62	0.42
1:D:124:MET:HG2	1:D:124:MET:H	1.69	0.42
1:D:203:MET:HB2	1:D:203:MET:HE3	1.76	0.42
1:D:291:LEU:HD21	1:D:322:CYS:HA	2.02	0.42
1:A:18:CYS:SG	1:A:324:LEU:HD23	2.60	0.42
1:A:203:MET:SD	1:A:275:ILE:HD13	2.60	0.42
1:A:218:ASP:OD2	1:A:220:GLU:HB2	2.20	0.42
1:B:105:PRO:O	1:B:106:SER:C	2.62	0.42
1:D:283:ARG:NH1	3:D:402:3LD:O15	2.48	0.42
1:A:40:THR:CG2	1:A:41:PRO:CD	2.90	0.41
1:B:202:ILE:HG22	1:B:239:GLY:HA3	2.02	0.41
1:C:1:MET:CB	1:C:27:LEU:HD22	2.50	0.41
1:C:118:THR:OG1	1:C:121:GLU:HG3	2.20	0.41
1:D:41:PRO:HB2	1:D:42:LEU:HD23	2.01	0.41
1:A:151:ARG:HA	1:A:151:ARG:HE	1.85	0.41
1:B:184:VAL:HG12	1:B:185:TRP:CD2	2.55	0.41
1:C:1:MET:HB2	1:C:27:LEU:HD22	2.02	0.41
1:C:51:LEU:HD12	1:C:51:LEU:HA	1.81	0.41
1:C:316:LEU:CB	2:C:401:FAD:O2	2.68	0.41
1:D:10:VAL:HG13	1:D:11:ILE:H	1.86	0.41
1:D:28:GLN:O	1:D:30:LEU:N	2.53	0.41
1:D:95:TYR:CZ	1:D:133:PHE:CE1	3.08	0.41
1:C:196:GLN:OE1	1:C:244:LEU:HD21	2.20	0.41
1:C:253:ILE:O	1:C:256:HIS:HB3	2.21	0.41
1:D:186:ALA:HB1	1:D:309:TYR:CD2	2.56	0.41
1:B:114:PHE:HA	1:B:134:HIS:HB3	2.02	0.41
1:B:164:VAL:O	1:B:189:LEU:HD21	2.20	0.41
1:C:13:LEU:HD12	1:C:145:LEU:HD12	2.00	0.41
1:C:79:VAL:C	1:C:80:HIS:CD2	2.97	0.41
1:D:44:THR:C	1:D:46:ASP:H	2.28	0.41
1:D:64:GLU:O	1:D:65:ALA:C	2.63	0.41
1:A:37:ASP:OD2	1:A:38:ARG:CZ	2.69	0.41
1:B:105:PRO:HD2	1:B:108:LYS:HB3	2.01	0.41
1:D:286:ARG:HD2	1:D:288:GLN:O	2.21	0.41
1:A:87:LEU:HB3	1:A:89:LEU:HB2	2.03	0.41
1:A:117:LEU:HB2	1:A:122:LEU:HD11	2.02	0.41
1:A:184:VAL:HG12	1:A:185:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:PRO:C	1:B:270:LEU:N	2.78	0.41
1:D:178:ILE:O	1:D:306:ILE:N	2.38	0.41
1:D:201:GLN:NE2	1:D:252:ASN:N	2.57	0.41
1:D:205:VAL:HA	1:D:274:ARG:O	2.21	0.41
1:D:224:TYR:HE1	3:D:402:3LD:C1	2.34	0.41
1:D:283:ARG:HD2	1:D:283:ARG:HH21	1.73	0.41
1:A:107:TRP:C	1:A:109:ASP:N	2.76	0.41
1:A:200:GLY:HA2	1:A:241:ILE:HG22	2.03	0.41
1:A:230:ILE:O	1:A:230:ILE:HG22	2.16	0.41
1:B:108:LYS:HD2	1:B:109:ASP:OD1	2.20	0.41
1:B:330:PHE:O	1:B:331:GLY:C	2.62	0.41
1:D:10:VAL:HG13	1:D:11:ILE:N	2.35	0.41
1:D:27:LEU:CD2	1:D:339:LEU:HD22	2.51	0.41
1:D:51:LEU:CD1	1:D:138:ILE:HG12	2.50	0.41
1:D:253:ILE:CG2	1:D:254:GLN:N	2.82	0.41
1:B:221:ARG:NH2	1:B:221:ARG:HB3	2.24	0.41
1:C:271:LYS:HB2	1:C:271:LYS:HE2	1.87	0.41
1:D:33:LYS:HG2	1:D:160:PHE:HE1	1.86	0.41
1:D:51:LEU:HD13	1:D:138:ILE:HG12	2.03	0.41
1:A:80:HIS:C	1:A:81:SER:O	2.63	0.41
1:A:183:GLY:C	1:A:185:TRP:N	2.78	0.41
1:B:32:ILE:C	1:B:33:LYS:HG3	2.46	0.41
1:B:92:ILE:O	1:B:92:ILE:HG23	2.21	0.41
1:B:199:ARG:NH2	1:B:248:SER:O	2.54	0.41
1:B:242:PHE:HA	1:B:283:ARG:NH2	2.36	0.41
1:B:337:LYS:HB3	1:B:339:LEU:HD22	2.03	0.41
2:B:401:FAD:C4X	3:B:402:3LD:N14	2.84	0.41
1:D:52:TRP:CD2	1:D:317:THR:HG23	2.55	0.41
1:D:114:PHE:CD1	1:D:115:ARG:N	2.88	0.41
1:D:276:ILE:O	1:D:276:ILE:HG22	2.20	0.41
1:B:117:LEU:HD21	1:B:133:PHE:HB2	2.01	0.41
1:B:122:LEU:HD22	1:B:130:TYR:HA	2.01	0.41
1:C:61:ASN:HD21	1:C:63:GLN:CB	2.33	0.41
1:C:87:LEU:HD23	1:C:147:TRP:CG	2.56	0.41
1:C:159:PHE:C	1:C:160:PHE:CD1	2.99	0.41
1:C:253:ILE:HD13	1:C:253:ILE:HA	1.85	0.41
1:D:255:ASP:O	1:D:259:ILE:CG1	2.68	0.41
1:A:39:PHE:CE2	1:C:250:LEU:HD22	2.56	0.40
1:A:78:HIS:O	1:A:80:HIS:N	2.54	0.40
1:A:114:PHE:HB2	1:A:134:HIS:CB	2.51	0.40
1:A:177:VAL:HG21	1:A:330:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:HA	1:C:138:ILE:O	2.21	0.40
1:C:120:ARG:HB3	1:D:112:LEU:HD13	2.02	0.40
1:C:141:GLY:O	1:C:145:LEU:HB2	2.21	0.40
1:C:246:ASN:OD1	1:C:247:TRP:N	2.53	0.40
1:A:333:ILE:O	1:A:335:GLU:N	2.55	0.40
1:B:41:PRO:C	1:B:42:LEU:HD23	2.46	0.40
1:B:270:LEU:O	1:B:271:LYS:C	2.63	0.40
1:C:36:ALA:HA	2:C:401:FAD:C2A	2.52	0.40
1:C:84:ALA:O	1:C:85:GLU:C	2.64	0.40
1:D:166:SER:O	1:D:167:PHE:C	2.64	0.40
1:D:238:LEU:HD11	1:D:270:LEU:HD21	2.03	0.40
1:D:250:LEU:HD12	1:D:250:LEU:C	2.46	0.40
1:D:250:LEU:HD12	1:D:251:ASN:H	1.84	0.40
1:A:183:GLY:C	1:A:185:TRP:H	2.29	0.40
1:B:15:THR:O	1:B:16:ALA:C	2.64	0.40
1:B:144:TYR:O	1:B:148:LEU:HG	2.21	0.40
1:B:223:ILE:HG13	1:B:224:TYR:N	2.35	0.40
1:B:295:GLN:H	1:B:295:GLN:NE2	2.15	0.40
1:C:147:TRP:O	1:C:148:LEU:C	2.64	0.40
1:C:199:ARG:C	1:C:283:ARG:NH2	2.79	0.40
1:D:3:VAL:O	1:D:32:ILE:HG23	2.22	0.40
1:A:145:LEU:HD12	1:A:145:LEU:HA	1.92	0.40
1:B:39:PHE:O	1:B:41:PRO:N	2.54	0.40
1:B:112:LEU:H	1:B:112:LEU:CD2	2.31	0.40
1:B:192:ASP:OD1	1:B:194:LEU:HB2	2.21	0.40
1:D:58:ASP:OD2	1:D:59:PRO:CD	2.67	0.40
1:D:71:THR:HA	1:D:320:TRP:HB3	2.04	0.40
1:D:87:LEU:CD1	1:D:87:LEU:N	2.84	0.40
1:B:200:GLY:HA2	1:B:241:ILE:O	2.22	0.40
1:C:36:ALA:HA	2:C:401:FAD:H2A	2.02	0.40
1:C:79:VAL:CG2	1:C:80:HIS:CD2	2.96	0.40
1:C:104:ASP:HB3	1:C:105:PRO:HD2	2.03	0.40
1:C:209:TRP:CE3	1:D:85:GLU:HG3	2.57	0.40
1:C:266:LEU:C	1:C:266:LEU:HD22	2.46	0.40
1:D:7:GLY:O	1:D:12:GLY:HA3	2.22	0.40
1:D:39:PHE:O	1:D:41:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/347 (97%)	279 (82%)	38 (11%)	21 (6%)	1	2
1	B	338/347 (97%)	257 (76%)	63 (19%)	18 (5%)	1	2
1	C	338/347 (97%)	269 (80%)	44 (13%)	25 (7%)	1	1
1	D	338/347 (97%)	259 (77%)	55 (16%)	24 (7%)	1	1
All	All	1352/1388 (97%)	1064 (79%)	200 (15%)	88 (6%)	1	1

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	TYR
1	A	299	GLY
1	B	28	GLN
1	B	40	THR
1	B	108	LYS
1	B	191	ARG
1	B	223	ILE
1	B	337	LYS
1	C	40	THR
1	C	55	TYR
1	C	83	ASN
1	C	101	ALA
1	C	171	ALA
1	C	299	GLY
1	C	300	PRO
1	D	28	GLN
1	D	40	THR
1	D	56	LEU
1	D	79	VAL
1	D	104	ASP
1	D	118	THR

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Mol	Chain	Res	Type
1	D	127	ASP
1	D	199	ARG
1	A	79	VAL
1	A	108	LYS
1	A	184	VAL
1	A	224	TYR
1	A	333	ILE
1	B	87	LEU
1	B	253	ILE
1	C	21	GLU
1	C	84	ALA
1	C	85	GLU
1	C	108	LYS
1	C	127	ASP
1	C	183	GLY
1	C	297	ARG
1	C	315	GLY
1	C	321	GLY
1	D	154	GLU
1	D	173	GLU
1	D	225	ASN
1	D	294	GLU
1	D	299	GLY
1	D	300	PRO
1	A	191	ARG
1	B	225	ASN
1	B	295	GLN
1	C	104	ASP
1	C	105	PRO
1	D	115	ARG
1	D	126	PRO
1	D	220	GLU
1	D	292	GLU
1	D	298	THR
1	A	126	PRO
1	A	172	ARG
1	A	249	GLU
1	A	298	THR
1	A	300	PRO
1	B	99	HIS
1	B	171	ALA
1	B	190	GLN

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Mol	Chain	Res	Type
1	C	126	PRO
1	C	312	GLY
1	D	83	ASN
1	A	28	GLN
1	A	166	SER
1	B	27	LEU
1	B	81	SER
1	B	124	MET
1	B	194	LEU
1	C	53	GLN
1	C	173	GLU
1	C	302	ASN
1	D	53	GLN
1	D	55	TYR
1	D	174	GLY
1	A	53	GLN
1	A	227	PRO
1	B	172	ARG
1	C	172	ARG
1	A	82	PRO
1	A	240	GLY
1	C	29	PRO
1	A	219	PRO
1	D	223	ILE

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	292/299 (98%)	221 (76%)	71 (24%)	1	0
1	B	292/299 (98%)	223 (76%)	69 (24%)	1	0
1	C	292/299 (98%)	215 (74%)	77 (26%)	0	0
1	D	292/299 (98%)	199 (68%)	93 (32%)	0	0
All	All	1168/1196 (98%)	858 (74%)	310 (26%)	0	0

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ILE
1	A	22	ARG
1	A	26	VAL
1	A	28	GLN
1	A	33	LYS
1	A	34	VAL
1	A	38	ARG
1	A	44	THR
1	A	47	VAL
1	A	56	LEU
1	A	61	ASN
1	A	63	GLN
1	A	76	LEU
1	A	77	SER
1	A	78	HIS
1	A	80	HIS
1	A	83	ASN
1	A	87	LEU
1	A	89	LEU
1	A	91	LEU
1	A	102	ILE
1	A	106	SER
1	A	108	LYS
1	A	112	LEU
1	A	114	PHE
1	A	115	ARG
1	A	120	ARG
1	A	122	LEU
1	A	127	ASP
1	A	133	PHE
1	A	137	LEU
1	A	151	ARG
1	A	152	LEU
1	A	153	THR
1	A	154	GLU
1	A	155	ARG
1	A	162	ARG
1	A	168	GLU
1	A	170	VAL
1	A	172	ARG
1	A	179	VAL

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Mol	Chain	Res	Type
1	A	184	VAL
1	A	196	GLN
1	A	199	ARG
1	A	203	MET
1	A	205	VAL
1	A	206	ASP
1	A	210	MET
1	A	221	ARG
1	A	226	SER
1	A	241	ILE
1	A	250	LEU
1	A	253	ILE
1	A	258	THR
1	A	259	ILE
1	A	265	ARG
1	A	266	LEU
1	A	271	LYS
1	A	274	ARG
1	A	275	ILE
1	A	291	LEU
1	A	292	GLU
1	A	295	GLN
1	A	296	LEU
1	A	298	THR
1	A	301	SER
1	A	302	ASN
1	A	305	VAL
1	A	316	LEU
1	A	334	LEU
1	B	6	ILE
1	B	21	GLU
1	B	22	ARG
1	B	24	HIS
1	B	27	LEU
1	B	28	GLN
1	B	31	ASP
1	B	32	ILE
1	B	34	VAL
1	B	37	ASP
1	B	38	ARG
1	B	44	THR
1	B	51	LEU

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Mol	Chain	Res	Type
1	B	56	LEU
1	B	58	ASP
1	B	61	ASN
1	B	79	VAL
1	B	83	ASN
1	B	85	GLU
1	B	89	LEU
1	B	91	LEU
1	B	102	ILE
1	B	106	SER
1	B	108	LYS
1	B	110	THR
1	B	112	LEU
1	B	116	LYS
1	B	120	ARG
1	B	122	LEU
1	B	142	LYS
1	B	145	LEU
1	B	150	GLU
1	B	152	LEU
1	B	153	THR
1	B	154	GLU
1	B	157	VAL
1	B	160	PHE
1	B	161	GLN
1	B	162	ARG
1	B	170	VAL
1	B	172	ARG
1	B	173	GLU
1	B	176	ASP
1	B	194	LEU
1	B	196	GLN
1	B	221	ARG
1	B	238	LEU
1	B	241	ILE
1	B	250	LEU
1	B	259	ILE
1	B	261	GLU
1	B	265	ARG
1	B	266	LEU
1	B	270	LEU
1	B	271	LYS

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Mol	Chain	Res	Type
1	B	285	VAL
1	B	286	ARG
1	B	287	PRO
1	B	291	LEU
1	B	295	GLN
1	B	297	ARG
1	B	298	THR
1	B	316	LEU
1	B	317	THR
1	B	332	ARG
1	B	335	GLU
1	B	338	LYS
1	B	339	LEU
1	B	340	SER
1	C	1	MET
1	C	2	ARG
1	C	13	LEU
1	C	26	VAL
1	C	27	LEU
1	C	28	GLN
1	C	31	ASP
1	C	38	ARG
1	C	58	ASP
1	C	63	GLN
1	C	68	SER
1	C	71	THR
1	C	78	HIS
1	C	85	GLU
1	C	87	LEU
1	C	89	LEU
1	C	91	LEU
1	C	104	ASP
1	C	108	LYS
1	C	110	THR
1	C	112	LEU
1	C	115	ARG
1	C	122	LEU
1	C	124	MET
1	C	133	PHE
1	C	138	ILE
1	C	151	ARG
1	C	152	LEU

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Mol	Chain	Res	Type
1	C	154	GLU
1	C	155	ARG
1	C	158	LYS
1	C	161	GLN
1	C	168	GLU
1	C	169	GLU
1	C	172	ARG
1	C	173	GLU
1	C	176	ASP
1	C	182	THR
1	C	190	GLN
1	C	191	ARG
1	C	194	LEU
1	C	195	LEU
1	C	196	GLN
1	C	203	MET
1	C	205	VAL
1	C	211	LYS
1	C	221	ARG
1	C	223	ILE
1	C	238	LEU
1	C	241	ILE
1	C	253	ILE
1	C	258	THR
1	C	259	ILE
1	C	261	GLU
1	C	264	CYS
1	C	265	ARG
1	C	266	LEU
1	C	270	LEU
1	C	271	LYS
1	C	274	ARG
1	C	285	VAL
1	C	288	GLN
1	C	290	ARG
1	C	292	GLU
1	C	295	GLN
1	C	297	ARG
1	C	298	THR
1	C	301	SER
1	C	302	ASN
1	C	305	VAL

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Mol	Chain	Res	Type
1	C	316	LEU
1	C	317	THR
1	C	320	TRP
1	C	328	LYS
1	C	335	GLU
1	C	337	LYS
1	C	339	LEU
1	D	6	ILE
1	D	15	THR
1	D	19	ILE
1	D	22	ARG
1	D	25	SER
1	D	26	VAL
1	D	27	LEU
1	D	28	GLN
1	D	30	LEU
1	D	32	ILE
1	D	33	LYS
1	D	35	TYR
1	D	40	THR
1	D	44	THR
1	D	56	LEU
1	D	58	ASP
1	D	60	ASN
1	D	68	SER
1	D	71	THR
1	D	76	LEU
1	D	85	GLU
1	D	87	LEU
1	D	89	LEU
1	D	91	LEU
1	D	102	ILE
1	D	108	LYS
1	D	112	LEU
1	D	116	LYS
1	D	120	ARG
1	D	130	TYR
1	D	137	LEU
1	D	138	ILE
1	D	143	ASN
1	D	146	GLN
1	D	151	ARG

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Mol	Chain	Res	Type
1	D	153	THR
1	D	155	ARG
1	D	158	LYS
1	D	161	GLN
1	D	162	ARG
1	D	164	VAL
1	D	168	GLU
1	D	170	VAL
1	D	173	GLU
1	D	176	ASP
1	D	178	ILE
1	D	179	VAL
1	D	180	ASN
1	D	182	THR
1	D	189	LEU
1	D	190	GLN
1	D	194	LEU
1	D	195	LEU
1	D	199	ARG
1	D	202	ILE
1	D	205	VAL
1	D	206	ASP
1	D	211	LYS
1	D	215	LEU
1	D	218	ASP
1	D	221	ARG
1	D	223	ILE
1	D	225	ASN
1	D	227	PRO
1	D	230	ILE
1	D	231	PRO
1	D	233	THR
1	D	238	LEU
1	D	241	ILE
1	D	250	LEU
1	D	253	ILE
1	D	259	ILE
1	D	261	GLU
1	D	266	LEU
1	D	269	THR
1	D	271	LYS
1	D	275	ILE

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Mol	Chain	Res	Type
1	D	276	ILE
1	D	286	ARG
1	D	288	GLN
1	D	290	ARG
1	D	291	LEU
1	D	292	GLU
1	D	295	GLN
1	D	297	ARG
1	D	302	ASN
1	D	304	GLU
1	D	309	TYR
1	D	316	LEU
1	D	318	ILE
1	D	337	LYS
1	D	338	LYS
1	D	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	63	GLN
1	A	69	GLN
1	A	80	HIS
1	A	161	GLN
1	A	180	ASN
1	A	196	GLN
1	A	201	GLN
1	A	243	GLN
1	A	252	ASN
1	A	295	GLN
1	A	302	ASN
1	A	307	HIS
1	A	319	HIS
1	B	24	HIS
1	B	60	ASN
1	B	78	HIS
1	B	80	HIS
1	B	96	ASN
1	B	201	GLN
1	B	225	ASN
1	B	243	GLN

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Mol	Chain	Res	Type
1	B	252	ASN
1	B	272	ASN
1	B	288	GLN
1	B	295	GLN
1	B	307	HIS
1	B	319	HIS
1	C	61	ASN
1	C	69	GLN
1	C	80	HIS
1	C	134	HIS
1	C	143	ASN
1	C	190	GLN
1	C	201	GLN
1	C	225	ASN
1	C	243	GLN
1	C	252	ASN
1	C	254	GLN
1	C	288	GLN
1	C	307	HIS
1	C	319	HIS
1	D	61	ASN
1	D	63	GLN
1	D	69	GLN
1	D	161	GLN
1	D	201	GLN
1	D	217	HIS
1	D	225	ASN
1	D	234	GLN
1	D	243	GLN
1	D	252	ASN
1	D	295	GLN
1	D	302	ASN
1	D	319	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	3LD	D	402	-	15,17,17	0.75	0	19,22,22	2.74	7 (36%)
2	FAD	C	401	-	58,58,58	1.45	6 (10%)	85,89,89	1.96	33 (38%)
2	FAD	B	401	-	58,58,58	1.56	8 (13%)	85,89,89	1.67	19 (22%)
3	3LD	C	402	-	15,17,17	0.74	0	19,22,22	2.75	7 (36%)
3	3LD	A	402	-	15,17,17	0.74	0	19,22,22	2.74	7 (36%)
2	FAD	D	401	-	58,58,58	1.63	7 (12%)	85,89,89	1.90	24 (28%)
2	FAD	A	401	-	58,58,58	1.43	11 (18%)	85,89,89	1.97	31 (36%)
3	3LD	B	402	-	15,17,17	0.65	0	19,22,22	1.77	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3LD	D	402	-	-	3/5/5/5	0/2/2/2
2	FAD	C	401	-	-	9/34/50/50	0/6/6/6
2	FAD	B	401	-	-	7/34/50/50	0/6/6/6
3	3LD	C	402	-	-	3/5/5/5	0/2/2/2
3	3LD	A	402	-	-	3/5/5/5	0/2/2/2
2	FAD	D	401	-	-	9/34/50/50	0/6/6/6
2	FAD	A	401	-	-	12/34/50/50	0/6/6/6
3	3LD	B	402	-	-	2/5/5/5	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	C1'-C2'	4.82	1.59	1.52
2	D	401	FAD	P-O3P	4.67	1.64	1.59
2	C	401	FAD	C9A-N10	-4.57	1.33	1.41
2	B	401	FAD	C9A-N10	-4.49	1.33	1.41
2	D	401	FAD	C9A-N10	-4.39	1.33	1.41
2	D	401	FAD	C10-N1	4.21	1.41	1.33
2	B	401	FAD	P-O3P	3.95	1.63	1.59
2	A	401	FAD	C9A-N10	-3.79	1.34	1.41
2	D	401	FAD	C5X-N5	-3.74	1.32	1.39
2	C	401	FAD	C5X-N5	-3.74	1.32	1.39
2	C	401	FAD	C4-N3	-3.36	1.32	1.38
2	A	401	FAD	C7M-C7	-3.31	1.44	1.51
2	B	401	FAD	C6-C7	-3.16	1.35	1.39
2	A	401	FAD	C2'-C3'	3.11	1.58	1.53
2	B	401	FAD	C5X-N5	-3.07	1.33	1.39
2	A	401	FAD	C10-N10	-3.01	1.30	1.37
2	B	401	FAD	C5'-C4'	2.98	1.55	1.51
2	D	401	FAD	C4X-C4	2.85	1.55	1.44
2	B	401	FAD	C7M-C7	-2.73	1.45	1.51
2	A	401	FAD	PA-O3P	-2.62	1.56	1.59
2	A	401	FAD	C6-C7	-2.50	1.36	1.39
2	D	401	FAD	O4B-C1B	2.46	1.47	1.42
2	A	401	FAD	C5X-N5	-2.45	1.34	1.39
2	B	401	FAD	C9-C9A	-2.31	1.35	1.39
2	A	401	FAD	O4B-C1B	2.28	1.47	1.42
2	A	401	FAD	C4X-C10	-2.25	1.37	1.44
2	A	401	FAD	C8-C7	-2.14	1.35	1.40
2	C	401	FAD	C6A-N6A	2.08	1.39	1.34
2	C	401	FAD	C10-N10	-2.06	1.32	1.37
2	D	401	FAD	C5'-C4'	2.04	1.54	1.51
2	B	401	FAD	C9A-C5X	-2.02	1.38	1.41
2	A	401	FAD	C10-N1	2.00	1.37	1.33

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	3LD	C7-C8-N14	7.97	126.12	119.54
3	A	402	3LD	C7-C8-N14	7.92	126.08	119.54
3	D	402	3LD	C7-C8-N14	7.84	126.02	119.54
2	B	401	FAD	O3'-C3'-C4'	-4.92	97.75	108.93
2	D	401	FAD	C8M-C8-C7	-4.84	110.88	120.76
2	A	401	FAD	C5X-N5-C4X	-4.80	110.32	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	C1'-N10-C9A	4.75	129.87	120.63
2	C	401	FAD	O3'-C3'-C2'	-4.62	98.42	108.93
3	B	402	3LD	C7-C8-N14	4.50	123.26	119.54
2	A	401	FAD	C2B-C1B-N9A	4.46	124.38	113.30
2	D	401	FAD	O3'-C3'-C4'	-4.46	98.81	108.93
3	D	402	3LD	C10-N13-N14	-4.23	110.61	117.33
3	A	402	3LD	C10-N13-N14	-4.21	110.64	117.33
3	C	402	3LD	C10-N13-N14	-4.19	110.67	117.33
2	C	401	FAD	C5X-C9A-N10	4.15	121.72	117.97
2	C	401	FAD	O3'-C3'-C4'	-4.15	99.50	108.93
2	A	401	FAD	O3B-C3B-C4B	-3.98	99.64	111.08
2	A	401	FAD	C4'-C3'-C2'	3.94	120.13	113.57
2	C	401	FAD	O4'-C4'-C5'	-3.90	101.38	109.99
3	C	402	3LD	C2-C4-C6	-3.89	115.14	120.61
3	D	402	3LD	C2-C4-C6	-3.89	115.14	120.61
3	A	402	3LD	C2-C4-C6	-3.84	115.22	120.61
2	D	401	FAD	C7M-C7-C6	3.75	126.19	119.57
2	C	401	FAD	C5X-N5-C4X	-3.73	112.05	118.09
2	D	401	FAD	O3P-PA-O1A	-3.69	99.60	110.70
2	D	401	FAD	C7M-C7-C8	-3.64	113.32	120.76
2	B	401	FAD	O4'-C4'-C5'	3.62	117.97	109.99
3	D	402	3LD	C12-C8-N14	-3.58	110.53	115.55
2	D	401	FAD	N9A-C8A-N7A	-3.57	108.87	113.94
3	A	402	3LD	C12-C8-N14	-3.55	110.58	115.55
3	C	402	3LD	C12-C8-N14	-3.51	110.63	115.55
2	D	401	FAD	O2P-P-O5'	-3.43	92.02	107.57
2	D	401	FAD	C3B-C2B-C1B	-3.40	95.03	101.46
2	C	401	FAD	N9A-C8A-N7A	-3.40	109.12	113.94
2	D	401	FAD	O2A-PA-O3P	3.36	116.35	107.27
2	A	401	FAD	C8M-C8-C7	-3.35	113.93	120.76
2	C	401	FAD	C7M-C7-C6	-3.33	113.70	119.57
2	D	401	FAD	C4A-N9A-C8A	3.30	109.20	105.74
2	C	401	FAD	C7M-C7-C8	3.30	127.49	120.76
2	B	401	FAD	C4'-C3'-C2'	-3.28	108.11	113.57
2	C	401	FAD	C4-C4X-N5	-3.26	113.71	118.21
2	C	401	FAD	O4B-C1B-N9A	3.21	114.25	108.09
2	B	401	FAD	C4X-C10-N10	3.20	121.06	116.48
3	B	402	3LD	C10-N13-N14	-3.18	112.27	117.33
2	C	401	FAD	C8M-C8-C9	-3.16	114.01	119.57
2	D	401	FAD	C9-C8-C7	3.13	124.29	119.69
2	B	401	FAD	C9-C8-C7	3.13	124.29	119.69
2	B	401	FAD	C2B-C1B-N9A	3.11	121.03	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	C4A-N9A-C8A	3.10	108.99	105.74
2	A	401	FAD	O2'-C2'-C3'	-3.10	101.99	109.25
3	A	402	3LD	C1-C3-C5	-3.09	116.43	120.24
2	A	401	FAD	C4X-C10-N10	3.05	120.85	116.48
3	D	402	3LD	C1-C3-C5	-3.05	116.48	120.24
3	C	402	3LD	C1-C3-C5	-3.04	116.48	120.24
2	D	401	FAD	C9-C9A-N10	-3.04	117.76	121.85
2	A	401	FAD	N9A-C8A-N7A	-3.04	109.62	113.94
2	C	401	FAD	C6A-C5A-N7A	3.01	137.89	132.09
2	D	401	FAD	C8M-C8-C9	2.99	124.83	119.57
2	C	401	FAD	C8M-C8-C7	2.96	126.80	120.76
2	C	401	FAD	C9A-N10-C10	-2.95	116.25	120.75
2	B	401	FAD	O2A-PA-O3P	2.90	115.11	107.27
2	A	401	FAD	C5A-N7A-C8A	2.90	108.00	103.45
2	B	401	FAD	O4B-C1B-C2B	-2.85	100.52	106.62
2	D	401	FAD	C4X-C10-N10	2.83	120.53	116.48
2	B	401	FAD	C1'-N10-C9A	2.80	126.08	120.63
2	A	401	FAD	N3-C2-N1	-2.80	113.56	119.50
2	A	401	FAD	C2B-C3B-C4B	2.76	107.95	102.61
2	B	401	FAD	C3B-C2B-C1B	-2.73	96.29	101.46
2	C	401	FAD	C5A-N7A-C8A	2.73	107.74	103.45
2	A	401	FAD	C1'-C2'-C3'	2.70	116.98	109.66
2	A	401	FAD	C10-N1-C2	2.68	122.66	116.85
2	B	401	FAD	O5B-C5B-C4B	2.68	118.12	108.99
2	A	401	FAD	O3P-P-O1P	-2.65	102.72	110.70
2	B	401	FAD	C10-N1-C2	2.62	122.53	116.85
2	A	401	FAD	PA-O5B-C5B	-2.60	106.44	121.35
3	C	402	3LD	C5-C6-C4	2.60	122.10	118.23
3	A	402	3LD	C5-C6-C4	2.59	122.08	118.23
3	D	402	3LD	C1-C2-C4	2.58	123.42	120.24
2	B	401	FAD	O2P-P-O5'	-2.58	95.87	107.57
3	D	402	3LD	C5-C6-C4	2.57	122.05	118.23
2	A	401	FAD	O4-C4-C4X	-2.57	119.76	126.53
2	A	401	FAD	O2-C2-N3	2.56	123.49	118.58
3	B	402	3LD	C1-C2-C4	-2.54	117.10	120.24
2	C	401	FAD	N6A-C6A-N1A	-2.54	112.72	118.38
3	A	402	3LD	C1-C2-C4	2.53	123.36	120.24
2	A	401	FAD	C9A-N10-C10	-2.53	116.89	120.75
3	C	402	3LD	C1-C2-C4	2.53	123.36	120.24
2	D	401	FAD	C9A-C9-C8	-2.52	114.16	119.22
2	A	401	FAD	N6A-C6A-N1A	-2.51	112.79	118.38
2	D	401	FAD	O5'-P-O1P	2.50	118.83	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	C4X-C10-N10	2.49	120.05	116.48
2	A	401	FAD	C4A-C5A-N7A	-2.48	107.74	110.58
2	D	401	FAD	N3A-C2A-N1A	2.47	132.32	128.58
2	A	401	FAD	O2'-C2'-C1'	-2.44	100.19	110.20
2	A	401	FAD	O2A-PA-O3P	2.43	113.84	107.27
2	D	401	FAD	C6-C5X-N5	-2.41	114.45	118.44
2	A	401	FAD	C7M-C7-C6	2.41	123.81	119.57
2	D	401	FAD	O2P-P-O1P	2.37	123.47	112.44
3	B	402	3LD	C3-C5-C6	-2.36	117.29	120.61
2	A	401	FAD	C5X-C9A-N10	2.35	120.10	117.97
2	C	401	FAD	C9-C9A-N10	-2.33	118.72	121.85
2	A	401	FAD	C9A-C5X-N5	2.33	124.93	122.45
2	A	401	FAD	C5B-C4B-C3B	-2.30	106.94	115.21
2	C	401	FAD	C1'-C2'-C3'	2.28	115.85	109.66
2	C	401	FAD	C4A-N9A-C1B	-2.27	121.31	126.63
2	C	401	FAD	O5B-C5B-C4B	2.26	116.68	108.99
2	C	401	FAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	C	401	FAD	C6A-C5A-C4A	-2.25	114.11	117.18
2	D	401	FAD	C1'-C2'-C3'	2.24	115.73	109.66
2	D	401	FAD	C5X-C6-C7	-2.20	116.74	120.83
2	C	401	FAD	C10-N1-C2	2.20	121.61	116.85
2	C	401	FAD	O5'-P-O1P	2.18	117.58	108.94
2	D	401	FAD	C5A-N7A-C8A	2.17	106.87	103.45
2	C	401	FAD	C4X-C10-N1	-2.17	119.27	124.59
2	C	401	FAD	C5'-C4'-C3'	2.17	116.31	112.22
2	D	401	FAD	C2A-N1A-C6A	-2.15	115.19	118.73
2	A	401	FAD	O4-C4-N3	2.15	124.17	120.11
2	C	401	FAD	C4-C4X-C10	2.15	120.62	116.93
2	A	401	FAD	C6A-C5A-N7A	2.14	136.21	132.09
2	B	401	FAD	O3B-C3B-C4B	-2.13	104.97	111.08
2	C	401	FAD	O2P-P-O3P	-2.13	101.52	107.27
2	C	401	FAD	O2A-PA-O1A	2.12	122.33	112.44
2	B	401	FAD	O2P-P-O1P	2.11	122.27	112.44
2	C	401	FAD	PA-O5B-C5B	-2.11	109.27	121.35
2	A	401	FAD	C8M-C8-C9	2.11	123.29	119.57
2	B	401	FAD	C4-N3-C2	2.11	129.39	125.64
2	A	401	FAD	C9-C8-C7	2.11	122.78	119.69
2	B	401	FAD	C1'-C2'-C3'	2.10	115.35	109.66
2	D	401	FAD	C4X-C10-N1	-2.08	119.48	124.59
2	B	401	FAD	PA-O5B-C5B	-2.08	109.42	121.35
2	B	401	FAD	O2-C2-N3	2.07	122.56	118.58
3	B	402	3LD	C7-C9-C10	2.07	120.53	116.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	O2'-C2'-C1'	2.03	118.55	110.20

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	C5B-O5B-PA-O1A
2	A	401	FAD	C5B-O5B-PA-O2A
2	A	401	FAD	C5B-O5B-PA-O3P
2	A	401	FAD	P-O3P-PA-O5B
2	A	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	C3B-C4B-C5B-O5B
2	A	401	FAD	C5'-O5'-P-O2P
2	A	401	FAD	C5'-O5'-P-O3P
2	B	401	FAD	C5B-O5B-PA-O2A
2	B	401	FAD	C5B-O5B-PA-O3P
2	C	401	FAD	C5B-O5B-PA-O3P
2	C	401	FAD	P-O3P-PA-O5B
2	D	401	FAD	C5B-O5B-PA-O1A
2	D	401	FAD	C5B-O5B-PA-O2A
2	D	401	FAD	C5B-O5B-PA-O3P
2	D	401	FAD	C5'-O5'-P-O3P
3	A	402	3LD	C11-C12-C8-N14
3	C	402	3LD	C11-C12-C8-N14
3	D	402	3LD	C11-C12-C8-N14
2	C	401	FAD	C3B-C4B-C5B-O5B
2	C	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O3'-C3'-C4'-C5'
2	A	401	FAD	O2'-C2'-C3'-O3'
2	B	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	C3B-C4B-C5B-O5B
2	B	401	FAD	O3'-C3'-C4'-O4'
3	A	402	3LD	C11-C12-C8-C7
3	B	402	3LD	C11-C12-C8-C7
3	C	402	3LD	C11-C12-C8-C7
3	D	402	3LD	C11-C12-C8-C7
2	D	401	FAD	P-O3P-PA-O5B
2	C	401	FAD	PA-O3P-P-O1P
2	A	401	FAD	C5'-O5'-P-O1P
2	B	401	FAD	C5B-O5B-PA-O1A

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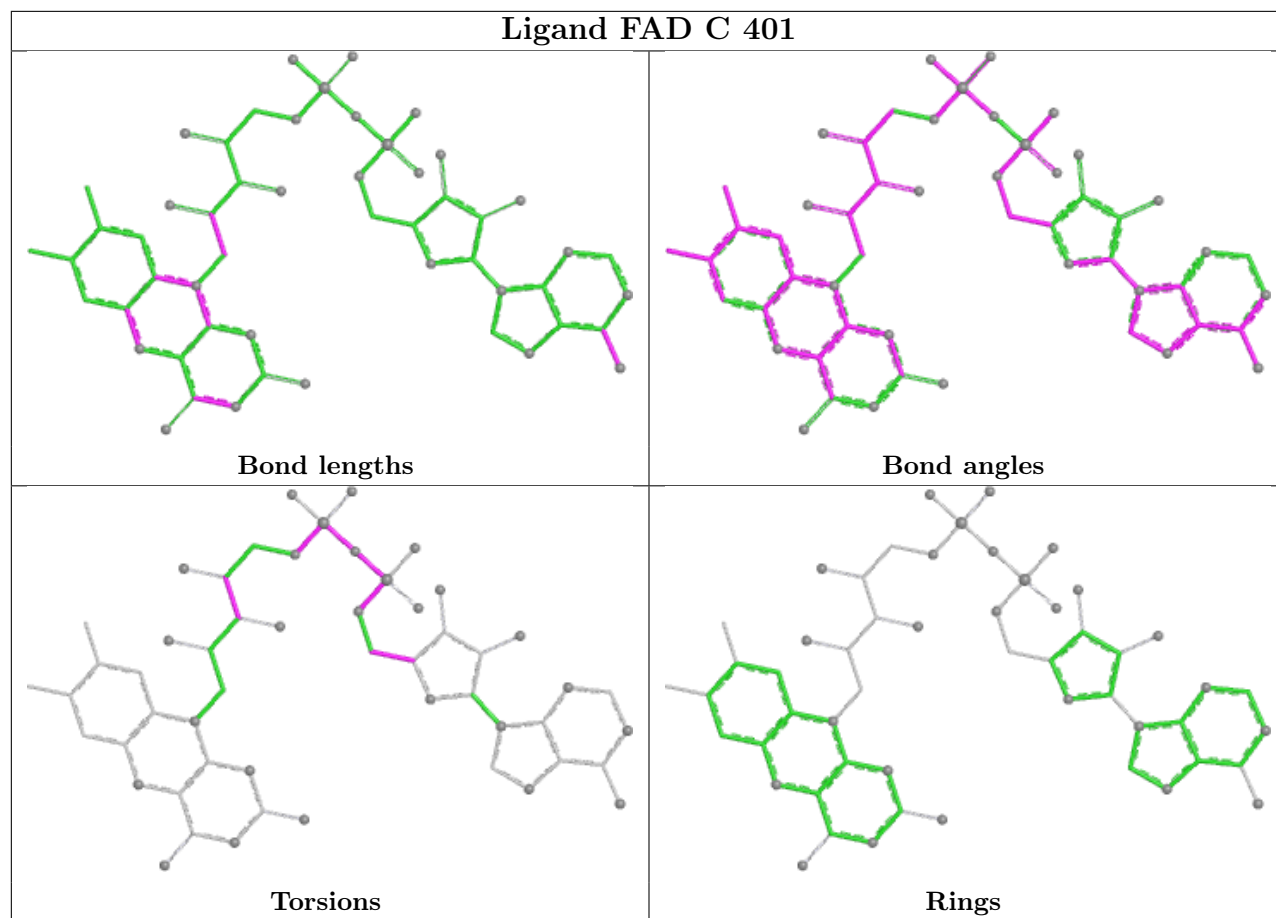
Mol	Chain	Res	Type	Atoms
2	C	401	FAD	C5B-O5B-PA-O1A
2	C	401	FAD	C5'-O5'-P-O3P
3	A	402	3LD	C6-C11-C12-C8
3	C	402	3LD	C6-C11-C12-C8
3	D	402	3LD	C6-C11-C12-C8
2	C	401	FAD	O3'-C3'-C4'-O4'
2	B	401	FAD	C2'-C3'-C4'-O4'
3	B	402	3LD	C11-C12-C8-N14
2	D	401	FAD	C3'-C4'-C5'-O5'
2	D	401	FAD	PA-O3P-P-O1P
2	A	401	FAD	O2'-C2'-C3'-C4'
2	A	401	FAD	PA-O3P-P-O2P

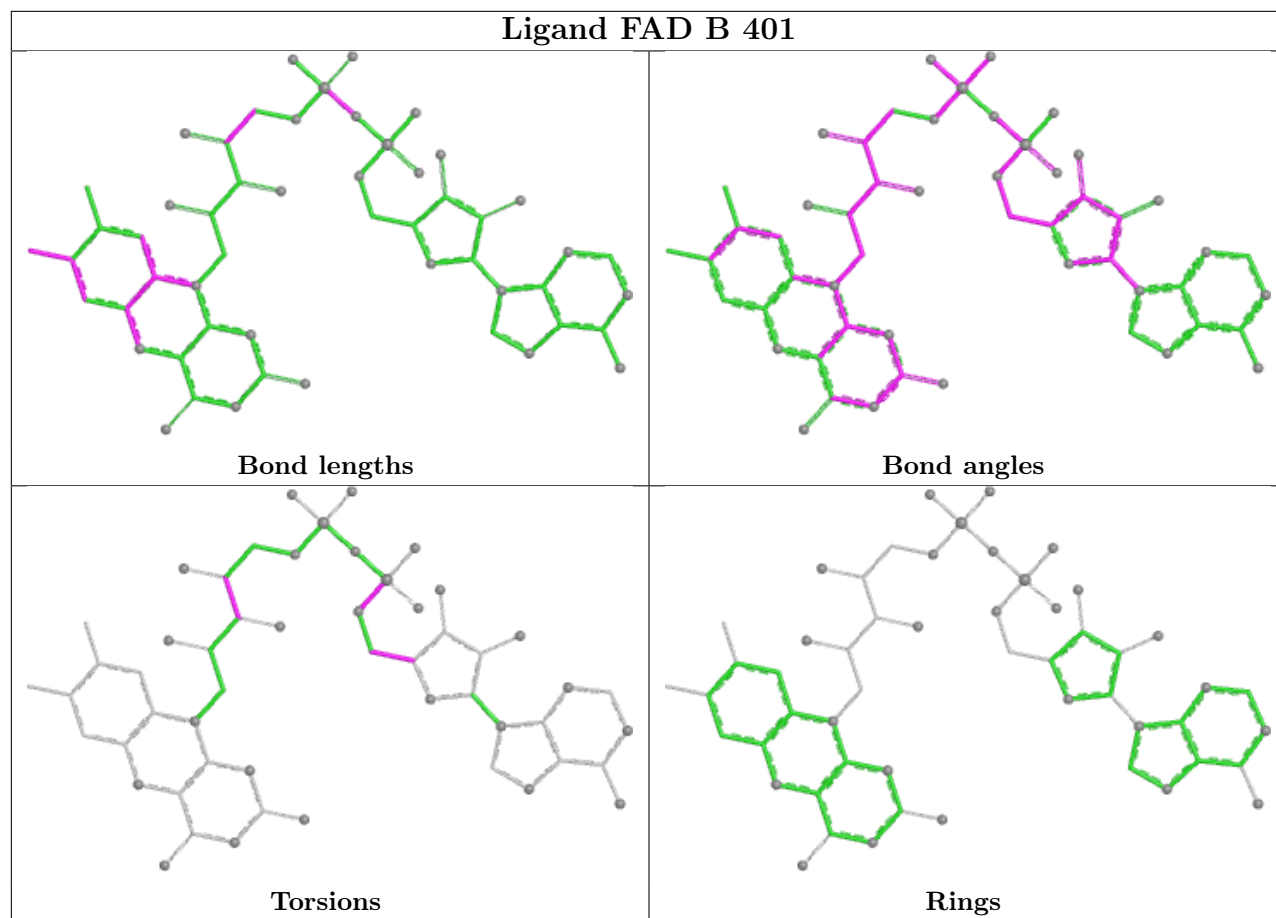
There are no ring outliers.

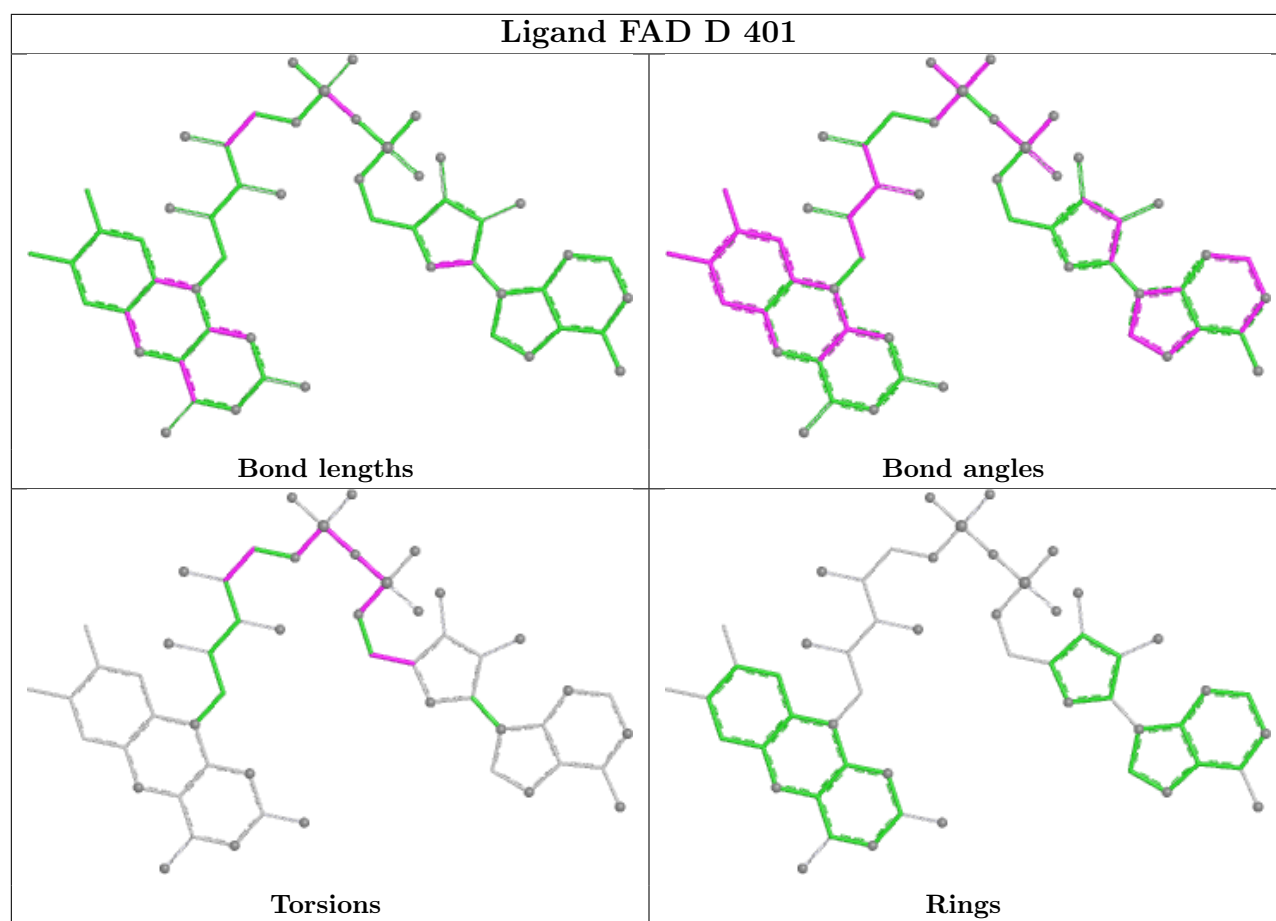
8 monomers are involved in 46 short contacts:

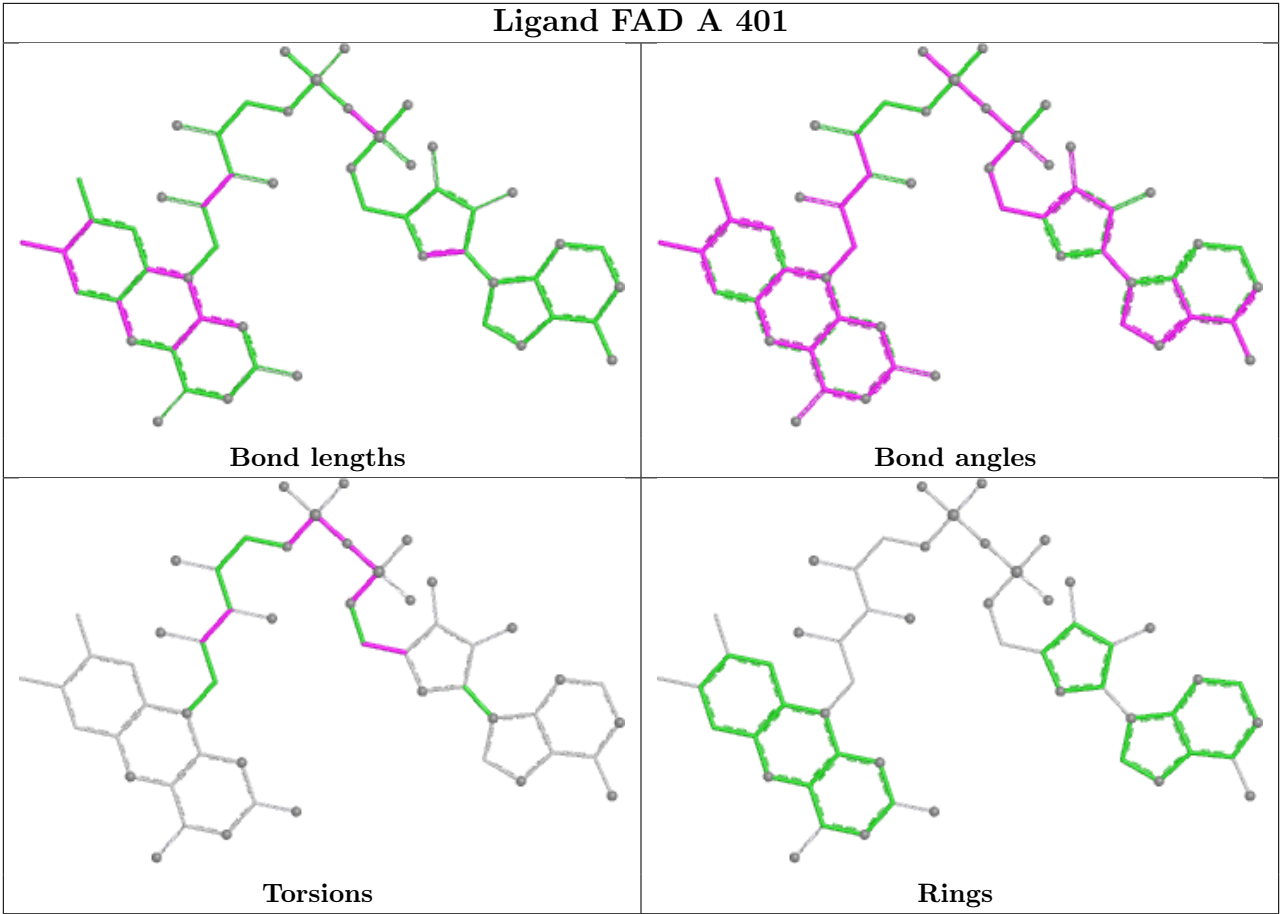
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	3LD	6	0
2	C	401	FAD	18	0
2	B	401	FAD	5	0
3	C	402	3LD	4	0
3	A	402	3LD	2	0
2	D	401	FAD	6	0
2	A	401	FAD	4	0
3	B	402	3LD	5	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	223:ILE	C	224:TYR	N	1.69

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/347 (97%)	-0.28	1 (0%) 90 89	18, 41, 65, 75	0
1	B	340/347 (97%)	-0.25	4 (1%) 76 71	20, 40, 64, 77	0
1	C	340/347 (97%)	-0.03	2 (0%) 85 82	27, 48, 74, 93	0
1	D	340/347 (97%)	-0.08	3 (0%) 81 76	27, 49, 75, 90	0
All	All	1360/1388 (97%)	-0.16	10 (0%) 84 80	18, 44, 69, 93	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	82	PRO	3.0
1	B	224	TYR	2.9
1	A	55	TYR	2.5
1	D	224	TYR	2.4
1	C	339	LEU	2.4
1	C	299	GLY	2.3
1	B	57	SER	2.3
1	B	59	PRO	2.1
1	B	55	TYR	2.0
1	D	55	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

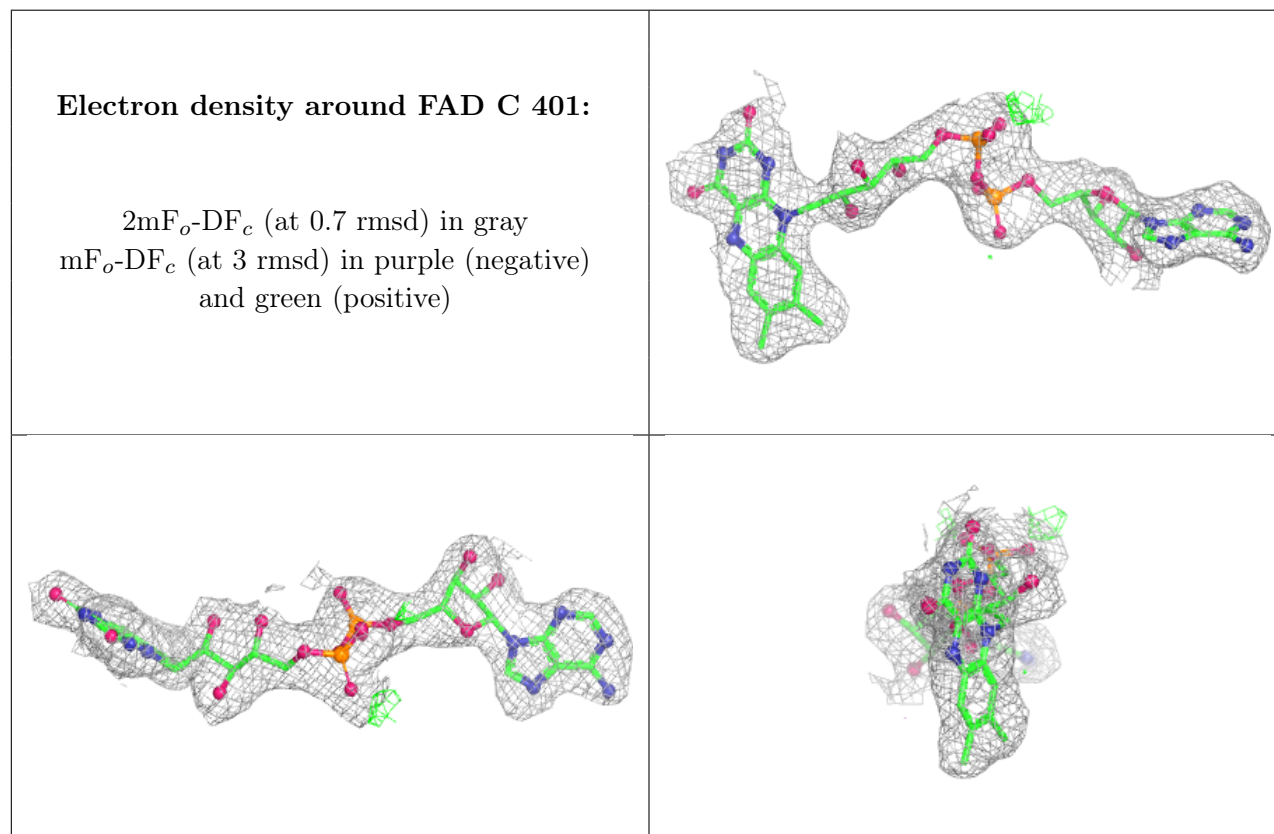
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

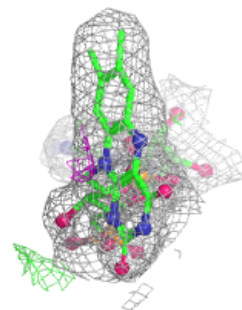
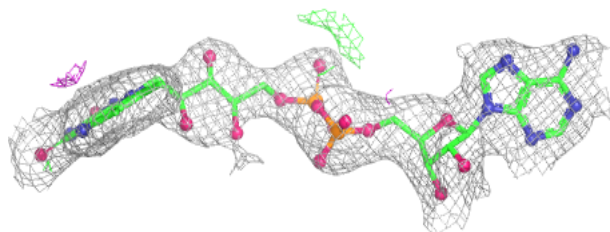
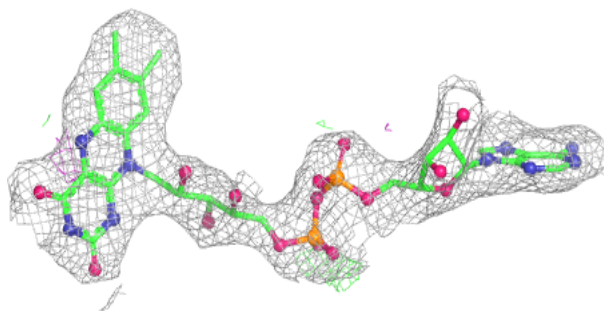
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	3LD	D	402	16/16	0.85	0.11	27,32,47,49	0
3	3LD	C	402	16/16	0.87	0.12	27,32,47,49	0
3	3LD	B	402	16/16	0.87	0.10	32,41,44,44	0
3	3LD	A	402	16/16	0.94	0.08	27,32,47,49	0
2	FAD	C	401	53/53	0.95	0.07	22,30,37,44	0
2	FAD	D	401	53/53	0.95	0.07	20,36,44,47	0
2	FAD	A	401	53/53	0.96	0.07	19,29,38,41	0
2	FAD	B	401	53/53	0.96	0.07	10,30,36,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

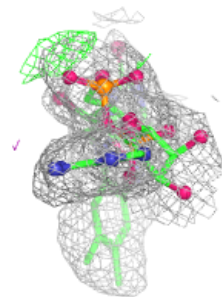
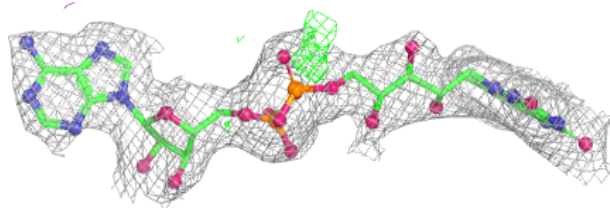
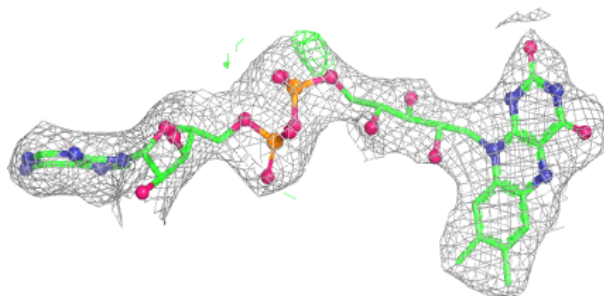


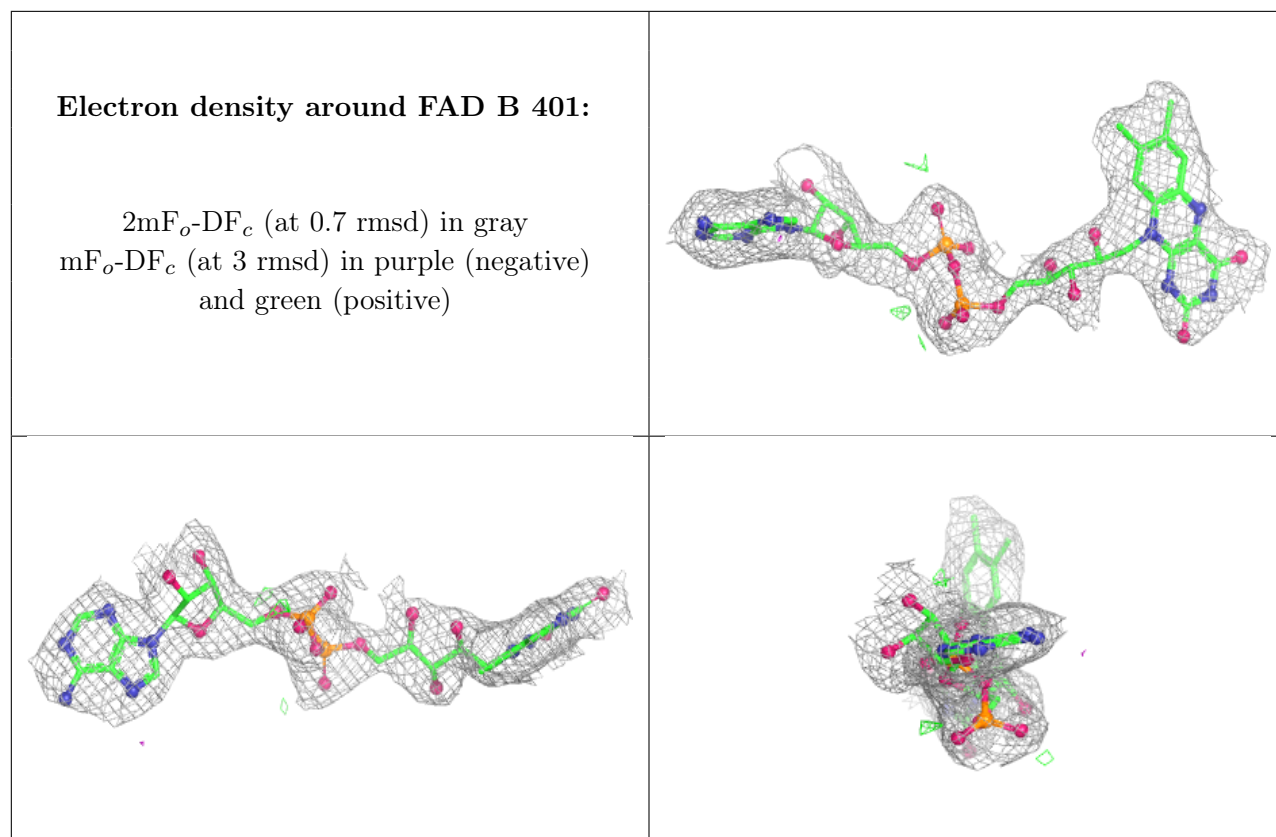
Electron density around FAD D 401:

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

**Electron density around FAD A 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.