



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:55 AM UTC

PDB ID : 4BBY / pdb_00004bby
Title : MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE: WILD-TYPE
Authors : Nenci, S.; Piano, V.; Rosati, S.; Aliverti, A.; Pandini, V.; Fraaije, M.W.; Heck, A.J.R.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2012-09-28
Resolution : 1.90 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

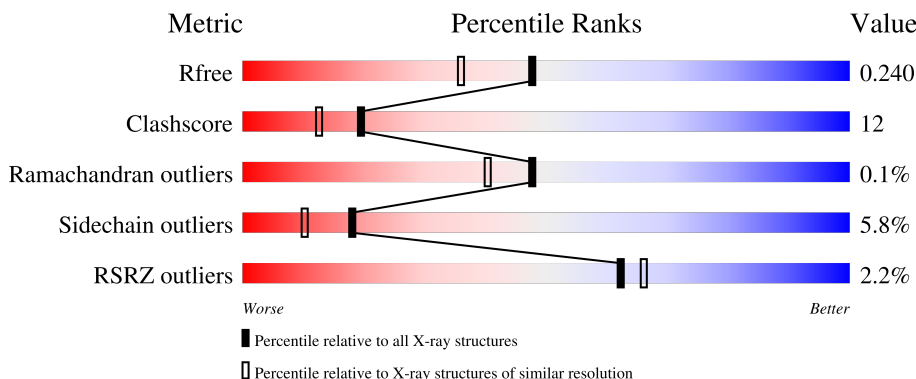
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	658	
1	B	658	
1	C	658	
1	D	658	

2 Entry composition [i](#)

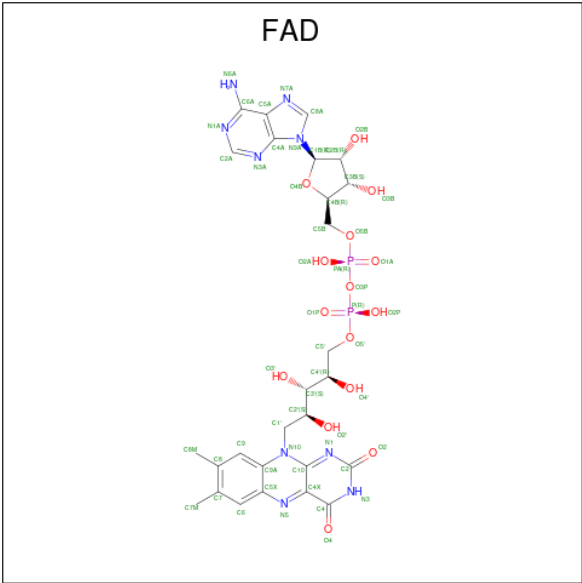
There are 4 unique types of molecules in this entry. The entry contains 18517 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	4	0
			4413	2803	763	821	26			
1	B	543	Total	C	N	O	S	0	0	0
			4301	2732	747	798	24			
1	C	557	Total	C	N	O	S	0	3	0
			4418	2803	766	823	26			
1	D	550	Total	C	N	O	S	0	2	0
			4363	2766	760	812	25			

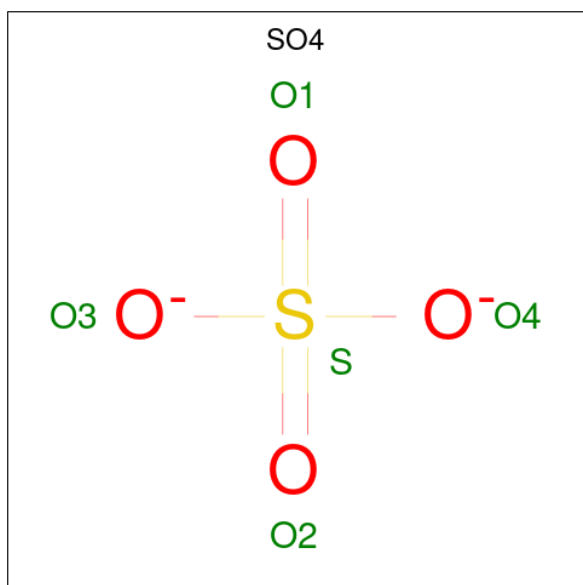
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		
4	B	175	Total	O	0	0
			175	175		
4	C	215	Total	O	0	0
			215	215		

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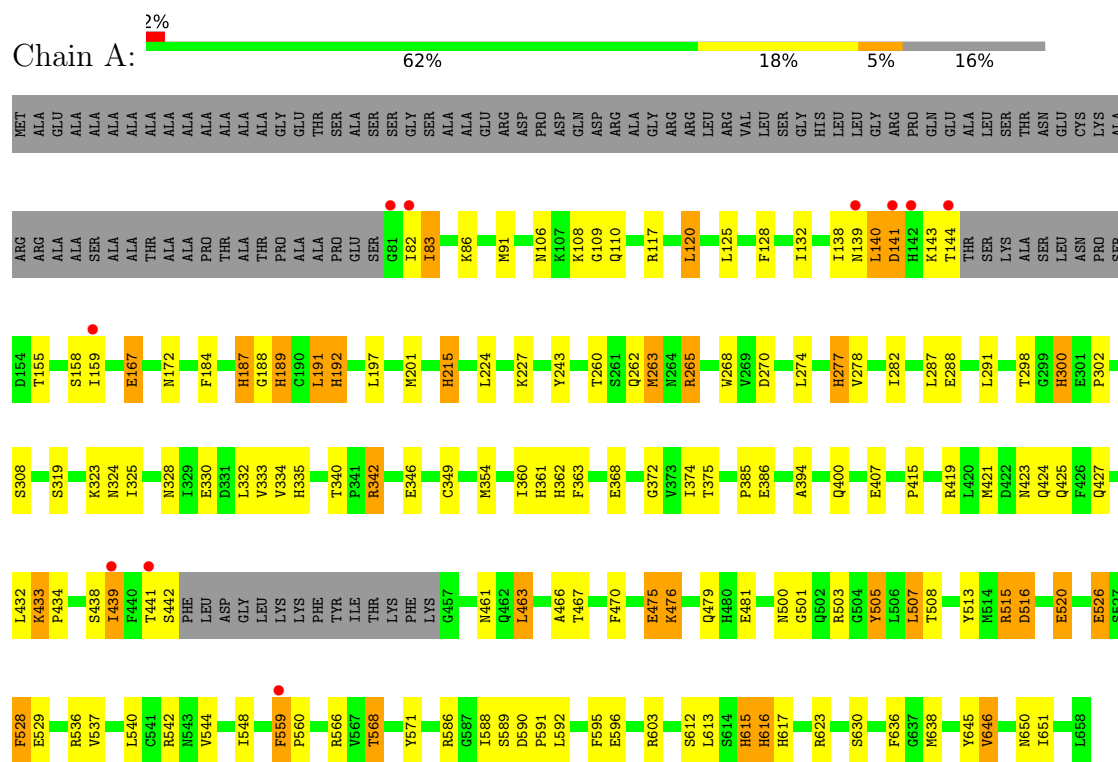
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	173	Total	O	0	0
			173	173		

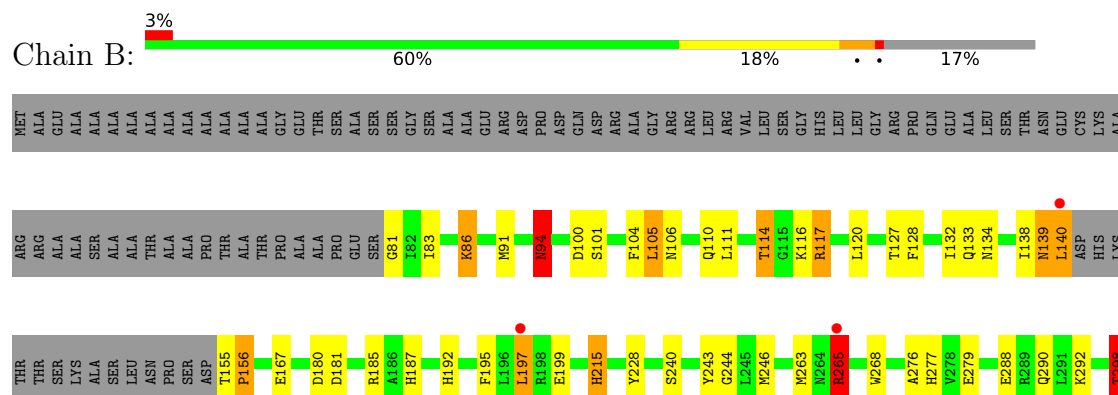
3 Residue-property plots

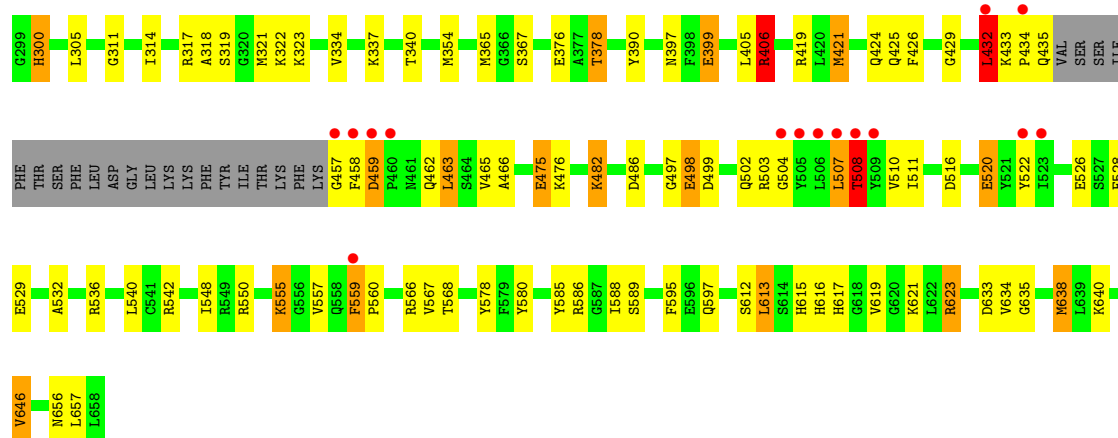
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

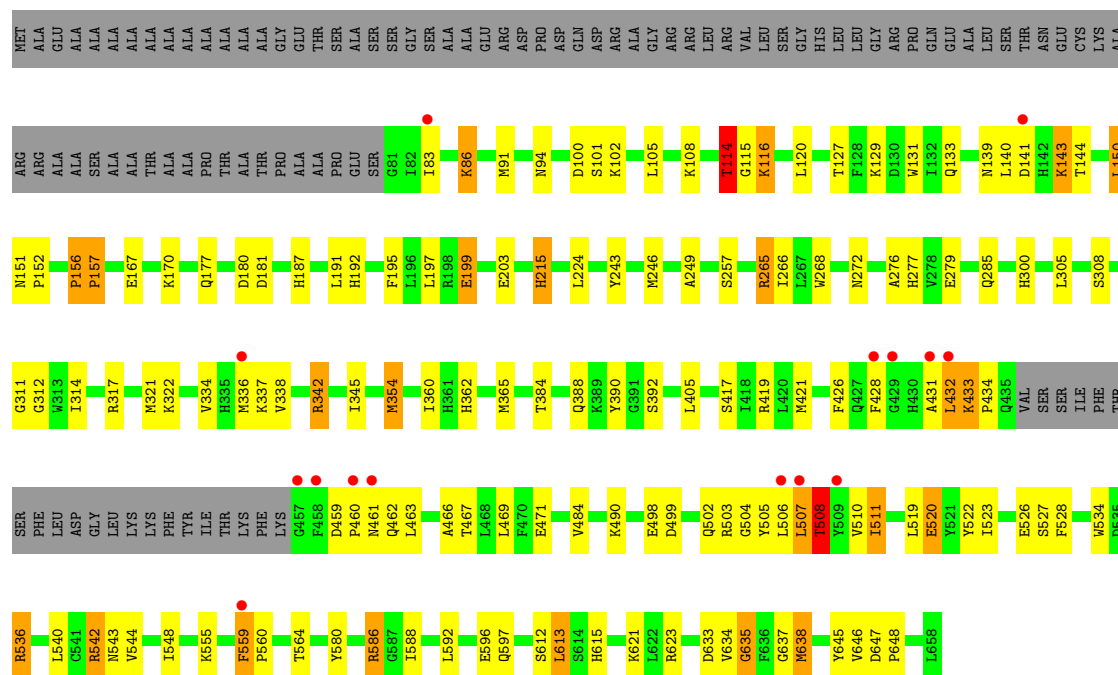


- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

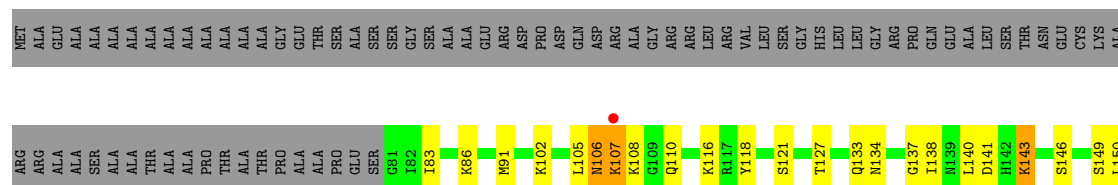


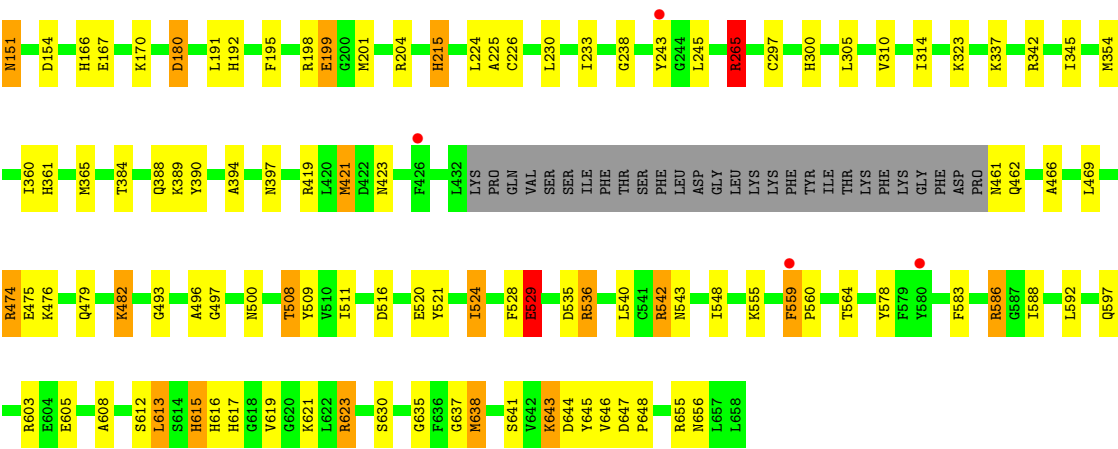


• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.30Å 99.17Å 107.83Å 90.43° 92.18° 94.92°	Depositor
Resolution (Å)	19.98 – 1.90 19.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (19.98-1.90) 92.5 (19.98-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.191 , 0.240 0.192 , 0.240	Depositor DCC
R_{free} test set	2004 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.040 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18517	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, 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	1.66	66/4524 (1.5%)	1.42	41/6114 (0.7%)
1	B	1.48	29/4398 (0.7%)	1.34	29/5944 (0.5%)
1	C	1.49	30/4527 (0.7%)	1.33	36/6119 (0.6%)
1	D	1.47	29/4466 (0.6%)	1.33	29/6036 (0.5%)
All	All	1.53	154/17915 (0.9%)	1.36	135/24213 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	1
1	D	0	1
All	All	1	2

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	ARG	CZ-NH1	-12.34	1.15	1.32
1	A	189	HIS	CE1-NE2	-11.12	1.21	1.32
1	A	189	HIS	CG-ND1	-10.70	1.26	1.38
1	A	362	HIS	CE1-NE2	-10.22	1.22	1.32
1	A	187	HIS	CE1-NE2	-10.11	1.22	1.32
1	A	616	HIS	CE1-NE2	-9.53	1.23	1.32
1	A	615	HIS	CE1-NE2	-9.51	1.23	1.32
1	A	638	MET	SD-CE	-9.27	1.56	1.79
1	D	617	HIS	CG-ND1	-9.15	1.28	1.38
1	C	338	VAL	C-O	8.64	1.33	1.24
1	A	215	HIS	CE1-NE2	-8.60	1.24	1.32
1	A	215	HIS	CG-ND1	-8.54	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	536	ARG	CZ-NH1	-8.37	1.21	1.32
1	A	515	ARG	CZ-NH1	-8.14	1.21	1.32
1	A	528	PHE	CG-CD2	-8.14	1.21	1.38
1	A	650	ASN	CG-ND2	-8.04	1.16	1.33
1	B	187	HIS	CG-ND1	-7.77	1.29	1.38
1	C	177	GLN	CD-NE2	-7.77	1.17	1.33
1	A	515	ARG	CZ-NH2	-7.67	1.23	1.33
1	A	603	ARG	CZ-NH2	-7.67	1.23	1.33
1	C	613	LEU	CA-C	7.58	1.63	1.52
1	A	528	PHE	CG-CD1	-7.48	1.23	1.38
1	A	262	GLN	CD-NE2	-7.47	1.17	1.33
1	A	372	GLY	N-CA	7.30	1.51	1.45
1	A	187	HIS	CG-ND1	-7.24	1.30	1.38
1	D	615	HIS	CG-ND1	-7.21	1.30	1.38
1	D	619	VAL	N-CA	7.20	1.54	1.45
1	A	172	ASN	CG-ND2	-7.16	1.18	1.33
1	D	300	HIS	CE1-NE2	7.09	1.39	1.32
1	D	361	HIS	CG-CD2	7.00	1.43	1.35
1	A	616	HIS	CG-CD2	-6.92	1.28	1.35
1	A	302	PRO	N-CA	-6.81	1.38	1.47
1	D	297	CYS	N-CA	6.74	1.54	1.45
1	B	94	ASN	CG-ND2	-6.67	1.19	1.33
1	B	623	ARG	CZ-NH1	-6.60	1.23	1.32
1	A	400	GLN	CD-OE1	-6.58	1.11	1.23
1	B	300	HIS	ND1-CE1	6.57	1.39	1.32
1	A	302	PRO	CA-C	6.55	1.60	1.52
1	B	94	ASN	CG-OD1	-6.44	1.11	1.23
1	A	363	PHE	CG-CD2	-6.43	1.25	1.38
1	A	167	GLU	CD-OE1	-6.39	1.13	1.25
1	A	184	PHE	CG-CD1	-6.39	1.25	1.38
1	A	636	PHE	CG-CD1	-6.38	1.25	1.38
1	B	318	ALA	C-O	6.36	1.31	1.23
1	B	378	THR	C-O	6.34	1.31	1.24
1	C	215	HIS	CG-ND1	-6.34	1.31	1.38
1	A	300	HIS	CE1-NE2	6.26	1.38	1.32
1	C	177	GLN	CD-OE1	-6.24	1.11	1.23
1	A	278	VAL	N-CA	6.23	1.53	1.46
1	C	647	ASP	N-CA	6.19	1.53	1.46
1	D	361	HIS	ND1-CE1	6.19	1.38	1.32
1	B	567	VAL	N-CA	6.18	1.53	1.46
1	A	83	ILE	CA-C	6.12	1.59	1.52
1	A	363	PHE	CG-CD1	-6.11	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	636	PHE	CG-CD2	-6.08	1.26	1.38
1	A	215	HIS	CG-CD2	-6.08	1.29	1.35
1	C	308	SER	CB-OG	6.08	1.54	1.42
1	C	311	GLY	N-CA	6.08	1.53	1.45
1	A	282	ILE	CA-C	6.07	1.59	1.52
1	A	184	PHE	CG-CD2	-6.06	1.26	1.38
1	C	623	ARG	CD-NE	-6.05	1.37	1.46
1	C	276	ALA	C-O	-6.04	1.16	1.24
1	D	617	HIS	CG-CD2	6.03	1.42	1.35
1	A	400	GLN	CD-NE2	-6.02	1.20	1.33
1	C	638	MET	SD-CE	-6.01	1.64	1.79
1	D	226	CYS	C-O	6.01	1.31	1.24
1	D	300	HIS	ND1-CE1	6.01	1.38	1.32
1	A	172	ASN	CG-OD1	-6.00	1.12	1.23
1	B	367	SER	CA-C	5.95	1.60	1.52
1	D	310	VAL	C-O	5.94	1.31	1.24
1	C	312	GLY	N-CA	5.93	1.53	1.45
1	B	615	HIS	CG-ND1	-5.92	1.31	1.38
1	B	276	ALA	CA-C	5.90	1.59	1.52
1	C	277	HIS	CG-CD2	5.89	1.42	1.35
1	A	362	HIS	CG-ND1	-5.88	1.31	1.38
1	A	361	HIS	ND1-CE1	5.85	1.38	1.32
1	B	586	ARG	N-CA	5.85	1.53	1.46
1	A	526	GLU	CD-OE1	-5.84	1.14	1.25
1	A	407	GLU	C-O	5.84	1.31	1.24
1	D	180	ASP	CG-OD1	-5.84	1.14	1.25
1	B	405	LEU	N-CA	5.80	1.53	1.46
1	B	240	SER	N-CA	5.78	1.53	1.46
1	B	290	GLN	CD-NE2	-5.77	1.21	1.33
1	B	156	PRO	CA-C	5.75	1.55	1.51
1	A	328	ASN	CG-ND2	-5.74	1.21	1.33
1	D	215	HIS	CG-ND1	-5.71	1.31	1.38
1	B	104	PHE	N-CA	5.71	1.53	1.45
1	D	623	ARG	CD-NE	-5.71	1.38	1.46
1	C	362	HIS	ND1-CE1	5.64	1.38	1.32
1	A	270	ASP	N-CA	5.63	1.54	1.46
1	B	532	ALA	C-O	5.57	1.30	1.24
1	A	308	SER	N-CA	5.56	1.52	1.45
1	D	641	SER	CA-C	-5.55	1.45	1.52
1	A	616	HIS	N-CA	5.54	1.52	1.46
1	C	180	ASP	CG-OD1	-5.53	1.14	1.25
1	B	638	MET	SD-CE	-5.53	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	HIS	CG-CD2	5.51	1.42	1.35
1	B	317	ARG	CA-C	5.50	1.60	1.53
1	D	529	GLU	CD-OE2	-5.50	1.15	1.25
1	A	368	GLU	N-CA	5.50	1.54	1.46
1	C	635	GLY	N-CA	5.49	1.52	1.45
1	C	648	PRO	CA-C	5.48	1.60	1.52
1	C	300	HIS	CE1-NE2	5.47	1.38	1.32
1	A	526	GLU	CD-OE2	-5.46	1.15	1.25
1	D	619	VAL	CA-C	5.46	1.58	1.52
1	C	623	ARG	CZ-NH2	-5.43	1.26	1.33
1	D	233	ILE	N-CA	5.43	1.50	1.46
1	B	185	ARG	N-CA	5.42	1.52	1.46
1	C	277	HIS	CE1-NE2	5.42	1.38	1.32
1	D	361	HIS	CG-ND1	-5.38	1.32	1.38
1	C	634	VAL	CA-CB	5.37	1.61	1.54
1	D	233	ILE	CA-CB	5.36	1.59	1.53
1	A	83	ILE	C-N	5.36	1.40	1.33
1	D	300	HIS	CG-CD2	5.34	1.41	1.35
1	A	333	VAL	C-O	5.34	1.29	1.24
1	A	623	ARG	CZ-NH2	-5.34	1.26	1.33
1	C	432	LEU	CA-C	5.32	1.59	1.52
1	A	613	LEU	CA-C	5.32	1.59	1.52
1	C	354[A]	MET	C-O	5.32	1.30	1.23
1	C	354[B]	MET	C-O	5.32	1.30	1.23
1	C	507	LEU	C-O	-5.31	1.18	1.24
1	D	644	ASP	N-CA	5.27	1.52	1.46
1	A	617	HIS	CE1-NE2	5.27	1.37	1.32
1	D	643	LYS	N-CA	5.26	1.52	1.46
1	D	617	HIS	ND1-CE1	5.23	1.37	1.32
1	C	405	LEU	N-CA	5.23	1.52	1.46
1	B	616	HIS	CG-ND1	-5.22	1.32	1.38
1	D	265	ARG	CZ-NH2	-5.22	1.26	1.33
1	D	151	ASN	C-N	5.22	1.40	1.33
1	A	260	THR	N-CA	5.21	1.52	1.46
1	A	386	GLU	N-CA	5.21	1.52	1.46
1	C	157	PRO	CA-C	5.21	1.58	1.52
1	D	616	HIS	CG-ND1	-5.20	1.32	1.38
1	A	300	HIS	CG-CD2	5.19	1.41	1.35
1	B	180	ASP	CG-OD1	-5.19	1.15	1.25
1	B	311	GLY	C-O	5.18	1.30	1.23
1	A	513	TYR	N-CA	5.16	1.52	1.46
1	C	507	LEU	CA-C	-5.12	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	638	MET	SD-CE	-5.12	1.66	1.79
1	B	215	HIS	ND1-CE1	5.11	1.37	1.32
1	D	300	HIS	CG-ND1	-5.10	1.32	1.38
1	B	634	VAL	C-O	5.10	1.30	1.24
1	B	617	HIS	CG-CD2	5.10	1.41	1.35
1	A	277	HIS	ND1-CE1	5.05	1.37	1.32
1	A	324	ASN	CG-ND2	5.05	1.43	1.33
1	A	319	SER	CA-C	-5.03	1.46	1.52
1	A	374	ILE	C-O	5.03	1.29	1.24
1	A	265	ARG	CA-CB	-5.03	1.45	1.53
1	B	406	ARG	CG-CD	-5.02	1.37	1.52
1	C	187	HIS	ND1-CE1	5.02	1.37	1.32
1	A	568	THR	CB-CG2	-5.01	1.36	1.52
1	A	651	ILE	N-CA	5.01	1.52	1.46
1	A	192	HIS	CG-CD2	5.01	1.41	1.35
1	C	615	HIS	ND1-CE1	5.00	1.37	1.32

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	LEU	CD1-CG-CD2	-16.35	74.83	110.80
1	B	265	ARG	NE-CZ-NH2	15.95	133.55	119.20
1	A	542	ARG	NE-CZ-NH2	15.14	132.83	119.20
1	D	265	ARG	NE-CZ-NH2	-13.22	107.31	119.20
1	D	603	ARG	NE-CZ-NH1	12.05	133.56	121.50
1	A	224	LEU	CD1-CG-CD2	-11.52	85.47	110.80
1	A	536	ARG	NE-CZ-NH2	9.92	128.13	119.20
1	D	603	ARG	CD-NE-CZ	9.71	137.99	124.40
1	D	603	ARG	NE-CZ-NH2	-9.23	110.89	119.20
1	D	497	GLY	N-CA-C	9.21	120.70	111.95
1	A	542	ARG	NE-CZ-NH1	-9.00	112.50	121.50
1	D	180	ASP	CB-CA-C	-8.73	97.10	110.90
1	C	623	ARG	NE-CZ-NH1	8.60	130.10	121.50
1	C	623	ARG	NE-CZ-NH2	-8.51	111.54	119.20
1	A	515	ARG	NH1-CZ-NH2	-8.47	108.29	119.30
1	C	536	ARG	CG-CD-NE	-8.32	93.69	112.00
1	C	564	THR	OG1-CB-CG2	-8.22	92.86	109.30
1	B	536	ARG	CG-CD-NE	-8.17	94.02	112.00
1	A	291	LEU	CD1-CG-CD2	-8.10	92.98	110.80
1	A	342	ARG	CA-CB-CG	-7.97	98.15	114.10
1	C	511	ILE	N-CA-C	-7.96	101.30	113.16
1	A	433	LYS	CA-C-N	7.95	127.87	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	LYS	C-N-CA	7.95	127.87	119.05
1	B	334	VAL	CB-CA-C	-7.86	102.31	110.88
1	A	623	ARG	NE-CZ-NH1	7.77	129.27	121.50
1	A	613	LEU	CD1-CG-CD2	-7.68	93.90	110.80
1	A	526	GLU	OE1-CD-OE2	-7.55	104.78	122.90
1	B	334	VAL	CG1-CB-CG2	-7.44	94.42	110.80
1	B	623	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	D	342	ARG	CG-CD-NE	-7.43	95.66	112.00
1	B	265	ARG	NE-CZ-NH1	-7.37	114.13	121.50
1	D	623	ARG	NE-CZ-NH1	7.24	128.74	121.50
1	C	114	THR	N-CA-CB	-7.18	99.53	110.45
1	A	603	ARG	NH1-CZ-NH2	-7.07	110.11	119.30
1	C	342	ARG	CA-CB-CG	-7.02	100.06	114.10
1	B	406	ARG	CG-CD-NE	6.90	127.18	112.00
1	D	536	ARG	CG-CD-NE	-6.86	96.92	112.00
1	D	638	MET	CG-SD-CE	-6.74	86.07	100.90
1	B	298	THR	OG1-CB-CG2	6.73	122.75	109.30
1	D	623	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	B	265	ARG	CD-NE-CZ	-6.66	115.07	124.40
1	D	342	ARG	CB-CG-CD	6.64	126.56	111.30
1	A	528	PHE	CE1-CZ-CE2	-6.61	108.10	120.00
1	C	507	LEU	N-CA-C	-6.57	101.50	111.56
1	A	590	ASP	CA-C-N	6.56	126.80	119.32
1	A	590	ASP	C-N-CA	6.56	126.80	119.32
1	D	265	ARG	CB-CG-CD	-6.56	96.22	111.30
1	A	363	PHE	CE1-CZ-CE2	-6.54	108.23	120.00
1	A	86	LYS	CG-CD-CE	6.53	126.33	111.30
1	B	508	THR	N-CA-C	6.48	119.17	111.71
1	B	432	LEU	N-CA-C	6.44	120.84	112.92
1	A	342	ARG	CB-CG-CD	6.43	126.09	111.30
1	A	385	PRO	CA-C-N	6.37	128.81	120.28
1	A	385	PRO	C-N-CA	6.37	128.81	120.28
1	A	636	PHE	CE1-CZ-CE2	-6.36	108.56	120.00
1	B	429	GLY	N-CA-C	6.31	120.28	112.64
1	B	117	ARG	N-CA-C	6.29	120.16	112.23
1	C	623	ARG	CD-NE-CZ	6.27	133.18	124.40
1	B	195	PHE	N-CA-C	6.25	117.78	110.97
1	D	265	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	A	515	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	B	298	THR	N-CA-CB	-6.18	101.06	110.33
1	B	497	GLY	N-CA-C	6.11	120.37	112.18
1	A	167	GLU	OE1-CD-OE2	-6.08	108.30	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ASN	N-CA-C	6.07	119.97	111.30
1	C	433	LYS	CA-C-N	6.06	126.00	119.76
1	C	433	LYS	C-N-CA	6.06	126.00	119.76
1	A	623	ARG	CD-NE-CZ	6.06	132.88	124.40
1	D	265	ARG	CD-NE-CZ	-6.03	115.95	124.40
1	C	484	VAL	N-CA-C	6.03	116.20	110.42
1	A	537	VAL	N-CA-C	5.99	116.11	110.30
1	A	536	ARG	NH1-CZ-NH2	-5.98	111.53	119.30
1	D	623	ARG	CD-NE-CZ	5.95	132.73	124.40
1	D	630	SER	N-CA-C	5.93	117.42	111.07
1	D	265	ARG	CA-CB-CG	-5.91	102.28	114.10
1	B	536	ARG	CD-NE-CZ	5.91	132.67	124.40
1	A	117	ARG	N-CA-C	5.90	119.66	112.23
1	A	505	TYR	CA-CB-CG	-5.89	103.30	113.90
1	D	180	ASP	N-CA-CB	5.87	118.58	110.07
1	C	265	ARG	CD-NE-CZ	-5.85	116.22	124.40
1	C	638	MET	CG-SD-CE	-5.82	88.09	100.90
1	B	139	ASN	CB-CA-C	5.81	120.02	111.65
1	C	523	ILE	CA-C-N	-5.80	115.62	123.10
1	C	523	ILE	C-N-CA	-5.80	115.62	123.10
1	D	623	ARG	CG-CD-NE	-5.78	99.29	112.00
1	D	655	ARG	N-CA-C	5.77	119.90	112.86
1	B	542	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	D	265	ARG	N-CA-C	5.73	118.96	110.48
1	A	623	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	C	317	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	C	257	SER	N-CA-C	-5.67	99.29	108.41
1	B	265	ARG	NH1-CZ-NH2	-5.63	111.98	119.30
1	A	603	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	C	266	ILE	CB-CA-C	5.61	117.47	111.35
1	C	633	ASP	N-CA-C	5.61	117.84	111.11
1	A	515	ARG	CG-CD-NE	-5.59	99.71	112.00
1	B	319	SER	CA-C-N	-5.58	116.67	122.69
1	B	319	SER	C-N-CA	-5.58	116.67	122.69
1	B	633	ASP	N-CA-C	5.53	117.74	111.11
1	C	536	ARG	CD-NE-CZ	5.53	132.14	124.40
1	C	534	TRP	N-CA-C	5.52	118.01	111.33
1	C	334	VAL	N-CA-C	-5.52	107.44	112.96
1	D	529	GLU	N-CA-CB	-5.50	102.47	111.66
1	D	475	GLU	N-CA-C	5.50	117.73	111.02
1	C	536	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	184	PHE	CE1-CZ-CE2	-5.48	110.14	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	508	THR	N-CA-C	5.46	122.43	110.80
1	D	542	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	325	ILE	CB-CA-C	-5.42	105.32	111.55
1	B	265	ARG	CB-CA-C	-5.41	100.39	109.48
1	C	542	ARG	NE-CZ-NH2	5.41	124.06	119.20
1	C	272	ASN	N-CA-C	5.40	116.97	111.14
1	C	384	THR	CA-C-N	-5.32	114.48	119.85
1	C	384	THR	C-N-CA	-5.32	114.48	119.85
1	A	630	SER	N-CA-C	5.31	117.07	111.28
1	C	623	ARG	CG-CD-NE	-5.31	100.31	112.00
1	B	623	ARG	NH1-CZ-NH2	-5.28	112.44	119.30
1	B	634	VAL	CA-C-N	5.26	125.94	119.99
1	B	634	VAL	C-N-CA	5.26	125.94	119.99
1	A	184	PHE	CD1-CG-CD2	-5.22	110.76	118.60
1	C	265	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	C	342	ARG	CB-CG-CD	5.20	123.25	111.30
1	A	330	GLU	N-CA-C	5.17	117.65	111.71
1	A	334	VAL	CG1-CB-CG2	-5.16	99.45	110.80
1	C	156	PRO	CA-C-N	-5.14	115.27	120.21
1	C	156	PRO	C-N-CA	-5.14	115.27	120.21
1	D	384	THR	CA-C-N	-5.14	114.66	119.85
1	D	384	THR	C-N-CA	-5.14	114.66	119.85
1	B	298	THR	CA-CB-OG1	5.12	117.29	109.60
1	B	117	ARG	CG-CD-NE	-5.07	100.84	112.00
1	C	543	ASN	N-CA-C	5.07	116.81	111.28
1	D	509	TYR	CA-C-N	-5.06	115.64	121.71
1	D	509	TYR	C-N-CA	-5.06	115.64	121.71
1	C	317	ARG	CG-CD-NE	-5.05	100.90	112.00
1	A	363	PHE	CD1-CG-CD2	-5.03	111.05	118.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	298	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	406	ARG	Sidechain
1	D	265	ARG	Sidechain

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	4413	0	4359	100	0
1	B	4301	0	4242	123	7
1	C	4418	0	4365	112	6
1	D	4363	0	4313	95	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
4	A	227	0	0	14	0
4	B	175	0	0	22	0
4	C	215	0	0	15	1
4	D	173	0	0	14	0
All	All	18517	0	17403	408	7

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 12.

All (408) 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:508:THR:HG22	4:D:2095:HOH:O	1.37	1.23
1:A:192:HIS:HB3	1:A:243:TYR:OH	1.43	1.15
1:C:192:HIS:HB3	1:C:243:TYR:OH	1.46	1.14
1:D:192:HIS:HB3	1:D:243:TYR:OH	1.44	1.14
1:A:559:PHE:HE2	1:D:608:ALA:CB	1.58	1.14
1:B:192:HIS:HB3	1:B:243:TYR:OH	1.46	1.13
1:A:419:ARG:HH22	1:A:508:THR:HG21	0.99	1.13
1:B:426:PHE:HE1	4:B:2139:HOH:O	1.29	1.13
1:B:457:GLY:HA3	4:B:2131:HOH:O	1.51	1.10
1:B:503:ARG:HG2	4:B:2140:HOH:O	1.50	1.10
1:C:586:ARG:HG3	1:C:586:ARG:HH11	1.00	1.09
1:C:426:PHE:HB2	4:C:2158:HOH:O	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:SER:HB2	4:D:2036:HOH:O	1.53	1.06
1:B:265:ARG:NH1	1:B:265:ARG:HB3	1.68	1.06
1:B:265:ARG:HB3	1:B:265:ARG:HH11	0.97	1.06
1:C:508:THR:HG22	4:C:2097:HOH:O	1.56	1.05
1:A:349:CYS:SG	1:A:354[B]:MET:HE1	1.97	1.04
1:A:615:HIS:HD2	1:A:616:HIS:HD2	1.03	1.02
1:C:285:GLN:OE1	4:C:2015:HOH:O	1.76	1.02
1:A:559:PHE:HE2	1:D:608:ALA:HB1	1.22	1.01
1:C:419:ARG:HH12	1:C:508:THR:CG2	1.73	1.00
1:A:559:PHE:CE2	1:D:608:ALA:HB1	1.97	1.00
1:B:243:TYR:CD2	4:B:2060:HOH:O	2.14	1.00
1:B:426:PHE:CE1	4:B:2139:HOH:O	2.08	0.98
1:A:419:ARG:NH2	1:A:508:THR:HG21	1.79	0.96
1:A:559:PHE:CE2	1:D:608:ALA:CB	2.48	0.96
1:B:265:ARG:HH11	1:B:265:ARG:CB	1.80	0.94
1:C:586:ARG:HG3	1:C:586:ARG:NH1	1.79	0.94
1:A:394:ALA:HB1	1:A:463:LEU:HD21	1.50	0.93
1:C:421:MET:HE3	4:C:2158:HOH:O	1.68	0.92
1:B:243:TYR:CE2	4:B:2060:HOH:O	2.21	0.91
1:D:586:ARG:HH11	1:D:586:ARG:HG3	1.35	0.91
1:A:476:LYS:HG2	4:A:2177:HOH:O	1.71	0.91
1:C:419:ARG:HH12	1:C:508:THR:HG21	1.35	0.91
1:A:615:HIS:HD2	1:A:616:HIS:CD2	1.90	0.89
1:B:139:ASN:O	1:B:140:LEU:CB	2.16	0.88
1:B:424:GLN:NE2	4:B:2129:HOH:O	2.05	0.87
1:A:419:ARG:HH22	1:A:508:THR:CG2	1.85	0.86
1:A:615:HIS:CD2	1:A:616:HIS:HD2	1.94	0.85
1:B:100:ASP:O	1:B:114:THR:HG23	1.77	0.85
1:A:421[B]:MET:HE1	4:A:2167:HOH:O	1.77	0.85
1:A:423:ASN:HD21	1:A:427:GLN:HE21	1.24	0.83
1:B:139:ASN:O	1:B:140:LEU:HB3	1.79	0.82
1:B:298:THR:HG23	1:B:300:HIS:H	1.44	0.81
1:D:192:HIS:CB	1:D:243:TYR:OH	2.28	0.81
1:B:426:PHE:CD1	1:B:465:VAL:HG21	2.17	0.80
1:C:345:ILE:HD13	1:D:638:MET:HE1	1.64	0.80
1:C:586:ARG:HH11	1:C:586:ARG:CG	1.91	0.79
1:B:127:THR:HG22	1:B:127:THR:O	1.82	0.78
1:B:101:SER:HA	1:B:114:THR:HG22	1.64	0.78
1:A:159:ILE:HA	4:A:2030:HOH:O	1.82	0.77
1:B:555:LYS:NZ	1:B:597:GLN:HE21	1.82	0.77
1:B:246:MET:SD	4:B:2060:HOH:O	2.41	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLY:HA3	1:D:559:PHE:CE2	2.19	0.77
1:C:542:ARG:NH2	4:C:2180:HOH:O	2.16	0.77
1:C:360:ILE:HG12	4:C:2134:HOH:O	1.83	0.77
1:A:192:HIS:CB	1:A:243:TYR:OH	2.30	0.76
1:B:192:HIS:CB	1:B:243:TYR:OH	2.30	0.76
1:A:433:LYS:HB3	1:A:434:PRO:HD2	1.68	0.76
1:A:106[A]:ASN:HB2	1:A:110:GLN:O	1.86	0.76
1:A:349:CYS:SG	1:A:354[B]:MET:CE	2.74	0.76
1:B:457:GLY:C	1:B:458:PHE:HD1	1.94	0.75
1:B:100:ASP:O	1:B:114:THR:CG2	2.33	0.75
1:B:482:LYS:HE3	1:B:486:ASP:OD2	1.86	0.75
1:C:505:TYR:O	1:C:508:THR:OG1	2.01	0.75
1:C:83:ILE:HD12	4:C:2086:HOH:O	1.86	0.74
1:A:559:PHE:HE2	1:D:608:ALA:HB2	1.52	0.74
1:D:496:ALA:O	1:D:500:ASN:ND2	2.21	0.74
1:C:508:THR:HA	1:C:511:ILE:HD13	1.70	0.74
1:D:154:ASP:O	1:D:201:MET:HG2	1.88	0.74
1:C:503:ARG:O	1:C:507:LEU:HB2	1.88	0.73
1:D:648:PRO:O	4:D:2167:HOH:O	2.05	0.73
1:C:388:GLN:NE2	1:C:471:GLU:OE1	2.22	0.73
1:C:83:ILE:HG23	1:C:91:MET:HE1	1.70	0.72
1:D:192:HIS:HB3	1:D:243:TYR:HH	1.53	0.72
1:D:133:GLN:HG2	1:D:138:ILE:O	1.89	0.72
1:D:83:ILE:HG23	1:D:91:MET:HE1	1.72	0.71
1:C:139:ASN:HB2	1:C:141:ASP:OD1	1.91	0.71
1:A:394:ALA:HB1	1:A:463:LEU:CD2	2.21	0.71
1:B:419:ARG:HH22	1:B:508:THR:HG21	1.55	0.71
1:D:215:HIS:CE1	1:D:337:LYS:HD3	2.27	0.70
1:B:550:ARG:HB2	4:B:2153:HOH:O	1.91	0.70
1:B:139:ASN:O	1:B:140:LEU:HB2	1.91	0.70
1:C:192:HIS:CB	1:C:243:TYR:OH	2.32	0.70
1:B:83:ILE:HG23	1:B:91:MET:HE1	1.74	0.70
1:B:640:LYS:HD2	4:B:2169:HOH:O	1.93	0.69
1:A:158:SER:O	4:A:2030:HOH:O	2.10	0.69
1:A:143:LYS:HG3	1:A:144:THR:H	1.56	0.69
1:B:265:ARG:HG2	1:B:279:GLU:OE1	1.92	0.69
1:D:146:SER:CB	4:D:2036:HOH:O	2.24	0.68
1:A:139:ASN:HB3	1:A:141:ASP:OD1	1.93	0.68
1:B:555:LYS:HZ2	1:B:597:GLN:NE2	1.91	0.68
1:C:131:TRP:CZ2	1:C:428:PHE:HD1	2.11	0.68
1:D:192:HIS:CE1	1:D:592:LEU:HD13	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ARG:NH1	1:C:508:THR:HG21	2.08	0.67
1:C:192:HIS:HB3	1:C:243:TYR:HH	1.59	0.67
1:D:419:ARG:HH12	1:D:508:THR:CG2	2.07	0.66
1:A:424:GLN:NE2	4:A:2170:HOH:O	2.15	0.66
1:C:428:PHE:HE2	1:C:507:LEU:HD21	1.61	0.66
1:B:498:GLU:O	1:B:502:GLN:N	2.24	0.66
1:D:474:ARG:HG3	4:D:2136:HOH:O	1.95	0.66
1:B:557:VAL:HG22	1:B:588:ILE:HD11	1.78	0.65
1:D:613:LEU:HD22	1:D:623:ARG:HD3	1.78	0.65
1:B:507:LEU:O	1:B:510:VAL:HG22	1.95	0.65
1:B:555:LYS:NZ	1:B:597:GLN:NE2	2.44	0.65
1:D:360:ILE:HG12	4:D:2122:HOH:O	1.96	0.65
1:A:438:SER:HB3	1:A:441:THR:HG22	1.78	0.65
1:D:555:LYS:NZ	1:D:597:GLN:HE21	1.94	0.65
1:B:399:GLU:CD	1:B:399:GLU:H	2.04	0.65
1:B:613:LEU:HD22	1:B:623:ARG:HD2	1.79	0.65
1:C:421:MET:HE2	1:C:467:THR:HG23	1.78	0.65
1:C:462:GLN:HG2	4:C:2146:HOH:O	1.96	0.65
1:A:189:HIS:HE1	4:A:2043:HOH:O	1.79	0.64
1:D:555:LYS:HZ1	1:D:597:GLN:HE21	1.46	0.64
1:B:425:GLN:HE22	1:B:566:ARG:HD3	1.62	0.64
1:D:586:ARG:HG3	4:D:2153:HOH:O	1.97	0.64
1:A:360:ILE:HG12	4:A:2138:HOH:O	1.96	0.63
1:A:571:TYR:OH	1:A:615:HIS:HE1	1.81	0.63
1:A:442:SER:HB3	1:D:542:ARG:NH1	2.13	0.62
1:C:144:THR:HG22	1:C:520:GLU:HA	1.81	0.62
1:C:265:ARG:NH1	1:C:265:ARG:HG2	2.15	0.62
1:D:578:TYR:CE1	4:D:2152:HOH:O	2.51	0.62
1:C:635:GLY:HA2	1:C:638:MET:HE3	1.82	0.62
1:C:638:MET:HE1	1:D:345:ILE:HD13	1.80	0.62
1:C:586:ARG:NH1	1:C:586:ARG:CG	2.57	0.62
1:B:265:ARG:HD3	4:B:2043:HOH:O	1.98	0.62
1:A:467:THR:HB	1:A:505:TYR:HE1	1.64	0.61
1:B:508:THR:HA	1:B:511:ILE:HD13	1.82	0.61
1:C:129:LYS:O	1:C:133:GLN:HG3	2.01	0.61
1:D:578:TYR:HE1	4:D:2152:HOH:O	1.81	0.61
1:A:83:ILE:HG23	1:A:91:MET:HE1	1.83	0.61
1:B:127:THR:O	1:B:127:THR:CG2	2.47	0.61
1:C:321:MET:HE3	1:C:469:LEU:HD23	1.83	0.61
1:D:635:GLY:HA2	1:D:638:MET:HE3	1.82	0.61
1:A:423:ASN:HD21	1:A:427:GLN:NE2	1.97	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:TYR:C	1:C:507:LEU:H	2.08	0.60
1:D:143:LYS:HG2	1:D:521:TYR:CE1	2.36	0.60
1:A:263:MET:HG2	4:A:2052:HOH:O	2.00	0.60
1:D:540:LEU:C	1:D:540:LEU:HD23	2.27	0.59
1:A:439:ILE:HG13	1:D:535:ASP:HB2	1.84	0.59
1:C:580:TYR:HE1	4:C:2193:HOH:O	1.85	0.59
1:D:192:HIS:ND1	1:D:592:LEU:HD13	2.18	0.59
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.83	0.59
1:C:139:ASN:O	1:C:140:LEU:HB2	2.02	0.59
1:C:421:MET:CE	4:C:2158:HOH:O	2.37	0.59
1:D:529:GLU:OE2	1:D:615:HIS:N	2.33	0.58
1:B:557:VAL:HA	1:B:588:ILE:HD11	1.85	0.58
1:C:321:MET:CE	1:C:469:LEU:HD23	2.34	0.58
1:A:187:HIS:HD2	1:A:188:GLY:O	1.87	0.57
1:A:591:PRO:HD2	4:A:2205:HOH:O	2.04	0.57
1:D:419:ARG:HH12	1:D:508:THR:HG21	1.68	0.57
1:A:432:LEU:HD12	1:A:507:LEU:HD11	1.87	0.56
1:B:215:HIS:CE1	1:B:337:LYS:HD3	2.40	0.56
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.89	0.56
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.85	0.56
1:A:192:HIS:CE1	1:A:592:LEU:HD13	2.39	0.56
1:D:166:HIS:HD2	4:D:2047:HOH:O	1.86	0.56
1:B:277:HIS:HE1	1:B:376:GLU:OE1	1.87	0.56
1:C:508:THR:CB	4:C:2097:HOH:O	2.52	0.56
1:A:415:PRO:HB3	1:A:470:PHE:CE2	2.41	0.56
1:B:434:PRO:HG3	4:B:2130:HOH:O	2.05	0.56
1:D:146:SER:CA	4:D:2036:HOH:O	2.53	0.56
1:B:475:GLU:HB2	4:B:2134:HOH:O	2.06	0.56
1:C:555:LYS:NZ	1:C:597:GLN:HE21	2.02	0.55
1:D:107:LYS:NZ	4:D:2025:HOH:O	2.31	0.55
1:C:345:ILE:HD13	1:D:638:MET:CE	2.36	0.55
1:A:467:THR:HB	1:A:505:TYR:CE1	2.42	0.55
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.88	0.55
1:B:244:GLY:HA2	1:B:656:ASN:HD21	1.70	0.55
1:C:433:LYS:HE2	1:C:503:ARG:NH1	2.21	0.55
1:D:305:LEU:HD12	1:D:305:LEU:C	2.32	0.55
1:B:550:ARG:HD3	4:B:2153:HOH:O	2.06	0.54
1:C:508:THR:CA	1:C:511:ILE:HD13	2.37	0.54
1:C:419:ARG:NH1	1:C:508:THR:CG2	2.58	0.54
1:D:191:LEU:HD13	1:D:191:LEU:C	2.33	0.54
1:C:507:LEU:O	1:C:510:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:GLY:O	1:B:458:PHE:HD1	1.90	0.53
1:D:586:ARG:HH11	1:D:586:ARG:CG	2.16	0.53
1:A:503:ARG:HG3	4:A:2184:HOH:O	2.09	0.53
1:A:612:SER:HB2	1:B:354:MET:HG2	1.90	0.53
1:B:635:GLY:HA2	1:B:638:MET:HE2	1.91	0.53
1:A:120:LEU:CD2	1:A:125:LEU:HD21	2.39	0.53
1:B:106:ASN:HD21	1:B:110:GLN:HG2	1.73	0.53
1:C:156:PRO:HG2	4:C:2058:HOH:O	2.09	0.53
1:B:132:ILE:HG22	1:B:138:ILE:HD11	1.91	0.53
1:C:433:LYS:HE2	1:C:503:ARG:HH12	1.73	0.53
1:A:501:GLY:O	1:A:505:TYR:HD1	1.90	0.53
1:C:203:GLU:OE1	1:C:249:ALA:CB	2.56	0.53
1:C:305:LEU:C	1:C:305:LEU:HD12	2.34	0.53
1:C:508:THR:HA	1:C:511:ILE:CD1	2.38	0.53
1:D:108:LYS:HD3	1:D:110:GLN:NE2	2.24	0.52
1:C:144:THR:CG2	1:C:520:GLU:HA	2.39	0.52
1:A:475:GLU:O	1:A:479:GLN:HG3	2.10	0.52
1:B:243:TYR:HD2	4:B:2060:HOH:O	1.69	0.52
1:C:246:MET:HE2	1:C:621:LYS:HE3	1.92	0.52
1:A:433:LYS:CB	1:A:434:PRO:HD2	2.34	0.52
1:B:298:THR:CG2	1:B:300:HIS:H	2.19	0.52
1:D:105:LEU:HD13	1:D:521:TYR:OH	2.10	0.52
1:B:128:PHE:CD1	1:B:432:LEU:HD11	2.44	0.51
1:B:557:VAL:HG22	1:B:588:ILE:CD1	2.39	0.51
1:D:419:ARG:O	1:D:466:ALA:HA	2.09	0.51
1:D:586:ARG:HG3	1:D:586:ARG:NH1	2.14	0.51
1:C:265:ARG:HD2	1:C:279:GLU:OE1	2.10	0.51
1:A:155:THR:HG22	1:A:201:MET:HE3	1.93	0.51
1:C:505:TYR:C	1:C:507:LEU:N	2.67	0.51
1:B:155:THR:HG22	1:B:156:PRO:O	2.11	0.51
1:D:621:LYS:HG3	1:D:656:ASN:HD22	1.76	0.51
1:C:528:PHE:HZ	1:C:548:ILE:HD11	1.76	0.51
1:B:106:ASN:ND2	1:B:110:GLN:HG2	2.26	0.51
1:B:619:VAL:HB	1:B:657:LEU:HD23	1.92	0.51
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.94	0.50
1:A:143:LYS:HE3	1:A:520:GLU:HB3	1.94	0.50
1:C:215:HIS:CE1	1:C:337:LYS:HD3	2.45	0.50
1:A:265:ARG:NH1	1:A:265:ARG:HG2	2.26	0.50
1:B:265:ARG:HD3	1:B:279:GLU:OE1	2.11	0.50
1:D:397:ASN:HA	1:D:462:GLN:O	2.12	0.50
1:D:643:LYS:NZ	1:D:647:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:TRP:HB2	1:C:431:ALA:HB1	1.95	0.49
1:C:459:ASP:OD1	1:C:460:PRO:HD2	2.13	0.49
1:D:419:ARG:HH22	1:D:508:THR:HG21	1.77	0.49
1:C:195:PHE:CD1	1:C:592:LEU:HD11	2.47	0.49
1:A:566:ARG:HE	1:A:568:THR:HG22	1.77	0.49
1:B:101:SER:CA	1:B:114:THR:HG22	2.37	0.49
1:B:621:LYS:HG3	1:B:656:ASN:HD22	1.77	0.49
1:B:459:ASP:OD1	1:B:459:ASP:C	2.56	0.49
1:D:151:ASN:C	1:D:151:ASN:HD22	2.21	0.49
1:B:292:LYS:HB2	4:B:2073:HOH:O	2.11	0.49
1:A:120:LEU:HD21	1:A:125:LEU:HD21	1.95	0.48
1:B:458:PHE:HB2	1:B:463:LEU:HD12	1.94	0.48
1:C:86:LYS:HE3	1:C:181:ASP:OD1	2.12	0.48
1:C:100:ASP:O	1:C:114:THR:CG2	2.61	0.48
1:D:423:ASN:CG	1:D:461:ASN:O	2.56	0.48
1:A:143:LYS:HG3	1:A:144:THR:N	2.25	0.48
1:C:321:MET:HE2	1:C:322:LYS:HG3	1.95	0.48
1:A:106[B]:ASN:HD21	1:A:110:GLN:HB2	1.78	0.48
1:A:189:HIS:CE1	4:A:2043:HOH:O	2.59	0.48
1:A:612:SER:CB	1:B:354:MET:HG2	2.43	0.48
1:B:419:ARG:O	1:B:466:ALA:HA	2.13	0.48
1:B:397:ASN:HA	1:B:462:GLN:O	2.12	0.48
1:B:457:GLY:CA	4:B:2131:HOH:O	2.32	0.48
1:C:559:PHE:CD1	1:C:560:PRO:HD2	2.49	0.48
1:A:288:GLU:OE1	1:A:298[A]:THR:HG23	2.13	0.48
1:C:157:PRO:HA	4:C:2035:HOH:O	2.14	0.48
1:B:419:ARG:HH12	1:B:508:THR:CG2	2.28	0.47
1:B:94:ASN:HD22	1:B:94:ASN:H	1.63	0.47
1:A:215:HIS:HE1	4:A:2054:HOH:O	1.98	0.47
1:A:526:GLU:CB	1:A:595:PHE:HZ	2.27	0.47
1:C:144:THR:HG21	1:C:519:LEU:O	2.14	0.47
1:C:392:SER:HA	1:C:466:ALA:O	2.14	0.47
1:C:612:SER:HB2	1:D:354[A]:MET:HG2	1.96	0.47
1:D:106:ASN:C	1:D:106:ASN:HD22	2.22	0.47
1:D:323:LYS:HD2	1:D:323:LYS:C	2.40	0.47
1:B:503:ARG:C	4:B:2140:HOH:O	2.58	0.47
1:B:105:LEU:HD13	1:B:111:LEU:HD23	1.97	0.46
1:B:528:PHE:HZ	1:B:548:ILE:HD11	1.80	0.46
1:C:526:GLU:HG3	1:C:527:SER:N	2.30	0.46
1:C:115:GLY:O	1:C:116:LYS:HD2	2.15	0.46
1:D:106:ASN:ND2	1:D:108:LYS:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:HIS:CB	1:C:243:TYR:HH	2.24	0.46
1:D:421:MET:HE2	1:D:421:MET:HB2	1.83	0.46
1:A:419:ARG:NH2	1:A:508:THR:CG2	2.62	0.46
1:B:555:LYS:CE	1:B:597:GLN:HE21	2.28	0.46
1:C:342:ARG:HD2	1:C:645:TYR:CZ	2.50	0.46
1:A:189:HIS:HD2	4:A:2189:HOH:O	1.98	0.46
1:B:419:ARG:HH12	1:B:508:THR:HG21	1.81	0.46
1:B:540:LEU:C	1:B:540:LEU:HD23	2.41	0.46
1:B:265:ARG:HG2	1:B:279:GLU:CD	2.40	0.46
1:D:394:ALA:O	1:D:493:GLY:HA2	2.15	0.46
1:C:505:TYR:O	1:C:508:THR:N	2.48	0.46
1:A:526:GLU:HB2	1:A:595:PHE:HZ	1.80	0.46
1:B:277:HIS:CE1	1:B:376:GLU:OE1	2.69	0.46
1:B:288:GLU:OE1	1:B:298:THR:HB	2.16	0.46
1:C:433:LYS:HD3	1:C:434:PRO:HD2	1.98	0.46
1:D:146:SER:HB3	1:D:198:ARG:HB3	1.98	0.46
1:D:151:ASN:C	1:D:151:ASN:ND2	2.73	0.46
1:C:314:ILE:HG21	1:C:336[B]:MET:SD	2.56	0.46
1:C:555:LYS:HZ2	1:C:597:GLN:NE2	2.14	0.46
1:C:354[A]:MET:HG2	1:D:612:SER:HB2	1.98	0.45
1:A:263:MET:HE2	1:A:263:MET:HB2	1.88	0.45
1:D:586:ARG:NH1	4:D:2153:HOH:O	2.49	0.45
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.52	0.45
1:A:192:HIS:HB3	1:A:243:TYR:HH	1.70	0.45
1:A:287:LEU:HD21	1:A:298[A]:THR:HG21	1.97	0.45
1:B:520:GLU:H	1:B:520:GLU:HG2	1.63	0.45
1:C:555:LYS:NZ	1:C:597:GLN:NE2	2.64	0.45
1:A:340:THR:HB	1:A:646:VAL:HG13	1.98	0.45
1:A:354[A]:MET:HG2	1:B:612:SER:HB2	1.98	0.45
1:A:421[A]:MET:HB2	1:A:425:GLN:HB2	1.99	0.45
1:B:86:LYS:HE3	1:B:181:ASP:OD1	2.16	0.45
1:B:434:PRO:O	1:B:435:GLN:HG2	2.17	0.45
1:C:195:PHE:O	1:C:199:GLU:HB2	2.17	0.45
1:D:192:HIS:CB	1:D:243:TYR:HH	2.22	0.45
1:D:516:ASP:O	1:D:520:GLU:HG2	2.16	0.45
1:D:543:ASN:HB3	1:D:605:GLU:OE2	2.16	0.45
1:B:526:GLU:HB3	1:B:595:PHE:HZ	1.81	0.45
1:C:419:ARG:HH12	1:C:508:THR:HG22	1.71	0.45
1:D:559:PHE:CD1	1:D:560:PRO:HD2	2.52	0.45
1:C:203:GLU:OE1	1:C:249:ALA:HB2	2.16	0.45
1:A:342:ARG:HD2	1:A:645:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:HD22	1:B:94:ASN:N	2.15	0.45
1:B:578:TYR:HE2	1:B:580:TYR:CE1	2.34	0.45
1:A:559:PHE:CD1	1:A:560:PRO:HD2	2.52	0.45
1:A:187:HIS:CE1	1:A:197:LEU:HD11	2.52	0.44
1:B:265:ARG:NH1	1:B:265:ARG:CB	2.53	0.44
1:B:340:THR:HB	1:B:646:VAL:HG13	1.99	0.44
1:B:433:LYS:HA	1:B:434:PRO:HD3	1.75	0.44
1:B:635:GLY:HA2	1:B:638:MET:CE	2.47	0.44
1:C:559:PHE:HD1	1:C:560:PRO:HD2	1.82	0.44
1:A:589:SER:O	1:A:591:PRO:HD3	2.17	0.44
1:A:442:SER:CB	1:D:542:ARG:NH1	2.79	0.44
1:B:244:GLY:HA2	1:B:656:ASN:ND2	2.32	0.44
1:C:321:MET:HE1	1:C:469:LEU:CD2	2.47	0.44
1:C:101:SER:HA	1:C:114:THR:HG22	2.00	0.44
1:C:143:LYS:HE3	1:C:143:LYS:HB3	1.73	0.44
1:C:354[A]:MET:HG2	1:D:612:SER:CB	2.48	0.44
1:B:305:LEU:C	1:B:305:LEU:HD12	2.43	0.44
1:C:419:ARG:O	1:C:466:ALA:HA	2.17	0.44
1:C:426:PHE:C	1:C:428:PHE:N	2.73	0.44
1:C:507:LEU:C	1:C:511:ILE:HD11	2.42	0.44
1:B:81:GLY:HA3	4:B:2001:HOH:O	2.16	0.44
1:B:499:ASP:O	1:B:503:ARG:HB3	2.17	0.44
1:C:116:LYS:HD2	1:C:116:LYS:HA	1.79	0.44
1:C:504:GLY:O	1:C:508:THR:HG23	2.17	0.44
1:A:470:PHE:CZ	1:A:481:GLU:HA	2.53	0.44
1:B:128:PHE:CG	1:B:432:LEU:HD11	2.53	0.44
1:C:522:TYR:CB	1:C:586:ARG:HG2	2.48	0.44
1:D:524:ILE:HD11	1:D:583:PHE:CZ	2.53	0.43
1:B:246:MET:HE2	1:B:621:LYS:HE3	2.00	0.43
1:C:133:GLN:NE2	1:C:139:ASN:O	2.51	0.43
1:C:191:LEU:HD13	1:C:191:LEU:C	2.43	0.43
1:D:106:ASN:ND2	1:D:110:GLN:H	2.17	0.43
1:D:118:TYR:O	1:D:121:SER:HB2	2.18	0.43
1:D:204:ARG:HA	4:D:2063:HOH:O	2.18	0.43
1:A:433:LYS:HB3	1:A:434:PRO:CD	2.45	0.43
1:A:439:ILE:HG13	1:D:535:ASP:CB	2.47	0.43
1:D:482:LYS:HE3	1:D:482:LYS:HB2	1.86	0.43
1:D:419:ARG:NH1	1:D:508:THR:HG21	2.31	0.43
1:D:528:PHE:HZ	1:D:548:ILE:HD11	1.83	0.43
1:D:559:PHE:HD1	1:D:560:PRO:HD2	1.83	0.43
1:A:128:PHE:O	1:A:132:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:HD2	1:A:323:LYS:C	2.44	0.43
1:B:265:ARG:HD3	4:B:2044:HOH:O	2.18	0.43
1:B:559:PHE:CD1	1:B:560:PRO:HD2	2.54	0.43
1:B:421:MET:HG3	1:B:425:GLN:HB3	2.01	0.42
1:C:167:GLU:HA	1:C:170:LYS:HE3	2.01	0.42
1:B:132:ILE:CG2	1:B:138:ILE:HD11	2.48	0.42
1:C:94:ASN:HA	1:C:197:LEU:HD13	2.02	0.42
1:C:417:SER:HB3	1:C:469:LEU:HB3	2.01	0.42
1:D:108:LYS:HD3	1:D:110:GLN:HE22	1.84	0.42
1:A:268:TRP:CE2	1:A:277:HIS:HB2	2.55	0.42
1:D:195:PHE:O	1:D:199:GLU:HB2	2.20	0.42
1:A:167:GLU:OE2	1:A:227:LYS:NZ	2.50	0.42
1:B:277:HIS:HD2	1:B:378:THR:OG1	2.02	0.42
1:B:516:ASP:O	1:B:520:GLU:HG2	2.19	0.42
1:A:419:ARG:O	1:A:466:ALA:HA	2.19	0.42
1:B:292:LYS:HG3	4:B:2076:HOH:O	2.19	0.42
1:B:522:TYR:HD1	1:B:585:TYR:CE1	2.38	0.42
1:C:645:TYR:CZ	1:D:637:GLY:HA3	2.54	0.42
1:A:500:ASN:ND2	1:A:503:ARG:NH1	2.67	0.42
1:A:540:LEU:O	1:A:544:VAL:HG23	2.20	0.42
1:B:458:PHE:CB	1:B:463:LEU:HD12	2.49	0.42
1:D:238:GLY:HA2	1:D:245:LEU:HD11	2.02	0.42
1:C:265:ARG:NH1	1:C:265:ARG:CG	2.72	0.42
1:C:265:ARG:CG	1:C:265:ARG:HH11	2.33	0.42
1:B:321:MET:HE2	1:B:322:LYS:HG3	2.02	0.42
1:B:432:LEU:HD23	1:B:507:LEU:HD21	2.01	0.42
1:B:504:GLY:N	4:B:2140:HOH:O	2.52	0.42
1:C:508:THR:C	1:C:511:ILE:HD13	2.45	0.42
1:C:637:GLY:HA3	1:D:645:TYR:CZ	2.55	0.42
1:A:268:TRP:CZ2	1:A:277:HIS:HB2	2.55	0.41
1:D:225:ALA:HA	1:D:230:LEU:HD12	2.01	0.41
1:D:524:ILE:HD13	1:D:524:ILE:HG21	1.76	0.41
1:D:138:ILE:HD12	1:D:140:LEU:HD23	2.02	0.41
1:A:616:HIS:HE1	4:A:2203:HOH:O	2.02	0.41
1:C:141:ASP:OD1	1:C:141:ASP:N	2.53	0.41
1:C:265:ARG:HD2	4:C:2061:HOH:O	2.19	0.41
1:C:540:LEU:O	1:C:544:VAL:HG23	2.19	0.41
1:A:559:PHE:CE2	1:D:608:ALA:HB2	2.41	0.41
1:B:167:GLU:OE1	1:B:228:TYR:OH	2.29	0.41
1:C:433:LYS:HA	1:C:434:PRO:HD2	1.91	0.41
1:A:300:HIS:HB2	1:A:332:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ASP:O	1:A:520:GLU:HG2	2.21	0.41
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.82	0.41
1:B:390:TYR:CG	1:B:502:GLN:HA	2.56	0.41
2:C:999:FAD:H1'2	2:C:999:FAD:H9	1.86	0.41
1:A:139:ASN:OD1	1:D:536:ARG:NH2	2.54	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.90	0.41
1:A:335:HIS:HE1	1:A:346:GLU:OE2	2.04	0.41
1:A:423:ASN:ND2	1:A:427:GLN:HE21	2.04	0.41
1:A:528:PHE:HZ	1:A:548:ILE:HD11	1.86	0.41
1:B:419:ARG:NH2	1:B:508:THR:HG21	2.28	0.41
1:B:656:ASN:O	1:B:657:LEU:HB2	2.20	0.41
1:D:265:ARG:HH11	1:D:265:ARG:HD3	1.52	0.41
1:D:390:TYR:CE2	1:D:469:LEU:HD13	2.56	0.41
1:A:526:GLU:HB2	1:A:595:PHE:CZ	2.55	0.40
1:B:268:TRP:CE2	1:B:277:HIS:HB2	2.55	0.40
1:B:288:GLU:OE1	1:B:298:THR:HG22	2.20	0.40
1:A:559:PHE:HD1	1:A:560:PRO:HD2	1.86	0.40
1:B:117:ARG:HH11	1:B:117:ARG:HD3	1.67	0.40
1:B:263:MET:HE2	1:B:263:MET:HB2	1.83	0.40
1:B:323:LYS:HD2	1:B:323:LYS:C	2.46	0.40
1:C:390:TYR:CD2	1:C:502:GLN:HG3	2.56	0.40
1:C:508:THR:CA	4:C:2097:HOH:O	2.70	0.40
1:D:167:GLU:HA	1:D:170:LYS:HE3	2.02	0.40
1:B:457:GLY:C	1:B:458:PHE:CD1	2.85	0.40
1:C:342:ARG:HH11	1:C:342:ARG:HD3	1.65	0.40
1:B:133:GLN:OE1	1:B:139:ASN:O	2.40	0.40
1:C:510:VAL:H	1:C:511:ILE:HD12	1.86	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:NE	1:C:151:ASN:OD1[1_556]	1.55	0.65
1:B:265:ARG:NH2	1:C:152:PRO:CD[1_556]	1.67	0.53
1:B:134:ASN:OD1	4:C:2180:HOH:O[1_546]	1.85	0.35
1:B:265:ARG:NH2	1:C:151:ASN:CA[1_556]	1.98	0.22
1:B:265:ARG:NH2	1:C:150:LEU:O[1_556]	2.14	0.06
1:B:265:ARG:NH2	1:C:152:PRO:N[1_556]	2.16	0.04
1:B:139:ASN:ND2	1:C:536:ARG:NH2[1_546]	2.17	0.03

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	553/658 (84%)	542 (98%)	10 (2%)	1 (0%)	43	36
1	B	537/658 (82%)	516 (96%)	21 (4%)	0	100	100
1	C	556/658 (84%)	536 (96%)	18 (3%)	2 (0%)	30	22
1	D	548/658 (83%)	534 (97%)	14 (3%)	0	100	100
All	All	2194/2632 (83%)	2128 (97%)	63 (3%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	506	LEU
1	C	508	THR
1	A	140	LEU

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	480/545 (88%)	458 (95%)	22 (5%)	24	16
1	B	464/545 (85%)	433 (93%)	31 (7%)	15	7
1	C	480/545 (88%)	455 (95%)	25 (5%)	21	13
1	D	473/545 (87%)	442 (93%)	31 (7%)	15	8
All	All	1897/2180 (87%)	1788 (94%)	109 (6%)	18	11

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ILE
1	A	108	LYS
1	A	120	LEU
1	A	138	ILE
1	A	140	LEU
1	A	141	ASP
1	A	191	LEU
1	A	263	MET
1	A	439	ILE
1	A	463	LEU
1	A	475	GLU
1	A	476	LYS
1	A	507	LEU
1	A	515	ARG
1	A	516	ASP
1	A	520	GLU
1	A	529	GLU
1	A	559	PHE
1	A	586	ARG
1	A	588	ILE
1	A	596	GLU
1	A	646	VAL
1	B	86	LYS
1	B	94	ASN
1	B	105	LEU
1	B	114	THR
1	B	116	LYS
1	B	120	LEU
1	B	140	LEU
1	B	197	LEU
1	B	199	GLU
1	B	265	ARG
1	B	298	THR
1	B	399	GLU
1	B	406	ARG
1	B	421	MET
1	B	432	LEU
1	B	459	ASP
1	B	463	LEU
1	B	475	GLU
1	B	476	LYS
1	B	482	LYS
1	B	498	GLU

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Mol	Chain	Res	Type
1	B	507	LEU
1	B	508	THR
1	B	520	GLU
1	B	529	GLU
1	B	555	LYS
1	B	559	PHE
1	B	568	THR
1	B	589	SER
1	B	613	LEU
1	B	646	VAL
1	C	86	LYS
1	C	102	LYS
1	C	105	LEU
1	C	108	LYS
1	C	114	THR
1	C	116	LYS
1	C	120	LEU
1	C	127	THR
1	C	143	LYS
1	C	150	LEU
1	C	199	GLU
1	C	224	LEU
1	C	432	LEU
1	C	461	ASN
1	C	463	LEU
1	C	490	LYS
1	C	498	GLU
1	C	499	ASP
1	C	520	GLU
1	C	559	PHE
1	C	586	ARG
1	C	588	ILE
1	C	596	GLU
1	C	613	LEU
1	C	646	VAL
1	D	86	LYS
1	D	102	LYS
1	D	106	ASN
1	D	107	LYS
1	D	116	LYS
1	D	127	THR
1	D	134	ASN

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Mol	Chain	Res	Type
1	D	141	ASP
1	D	143	LYS
1	D	149	SER
1	D	150	LEU
1	D	180	ASP
1	D	199	GLU
1	D	224	LEU
1	D	388	GLN
1	D	389	LYS
1	D	421	MET
1	D	474	ARG
1	D	476	LYS
1	D	479	GLN
1	D	482	LYS
1	D	508	THR
1	D	511	ILE
1	D	524	ILE
1	D	529	GLU
1	D	559	PHE
1	D	564	THR
1	D	586	ARG
1	D	588	ILE
1	D	613	LEU
1	D	646	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	187	HIS
1	A	189	HIS
1	A	215	HIS
1	A	262	GLN
1	A	272	ASN
1	A	290	GLN
1	A	328	ASN
1	A	335	HIS
1	A	427	GLN
1	A	479	GLN
1	A	500	ASN
1	A	615	HIS
1	A	616	HIS

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Mol	Chain	Res	Type
1	B	94	ASN
1	B	133	GLN
1	B	277	HIS
1	B	335	HIS
1	B	400	GLN
1	B	423	ASN
1	B	425	GLN
1	B	597	GLN
1	B	650	ASN
1	B	656	ASN
1	C	110	GLN
1	C	139	ASN
1	C	151	ASN
1	C	272	ASN
1	C	277	HIS
1	C	285	GLN
1	C	362	HIS
1	C	388	GLN
1	C	400	GLN
1	C	423	ASN
1	C	424	GLN
1	C	427	GLN
1	C	479	GLN
1	C	597	GLN
1	C	650	ASN
1	C	656	ASN
1	D	106	ASN
1	D	110	GLN
1	D	133	GLN
1	D	142	HIS
1	D	151	ASN
1	D	324	ASN
1	D	479	GLN
1	D	597	GLN
1	D	617	HIS
1	D	650	ASN
1	D	656	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	D	999	-	58,58,58	1.45	8 (13%)	85,89,89	1.89	22 (25%)
2	FAD	A	999	-	58,58,58	2.07	19 (32%)	85,89,89	2.16	27 (31%)
3	SO4	A	1659	-	4,4,4	0.70	0	6,6,6	0.60	0
3	SO4	A	1660	-	4,4,4	0.76	0	6,6,6	0.49	0
3	SO4	D	1659	-	4,4,4	0.57	0	6,6,6	0.90	0
2	FAD	B	999	-	58,58,58	2.17	19 (32%)	85,89,89	2.00	26 (30%)
2	FAD	C	999	-	58,58,58	1.95	18 (31%)	85,89,89	1.98	27 (31%)
3	SO4	B	1659	-	4,4,4	0.46	0	6,6,6	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	999	-	-	3/34/50/50	0/6/6/6
2	FAD	B	999	-	-	3/34/50/50	0/6/6/6
2	FAD	C	999	-	-	4/34/50/50	0/6/6/6
2	FAD	A	999	-	-	6/34/50/50	0/6/6/6

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	FAD	C1'-C2'	6.07	1.61	1.52
2	B	999	FAD	C5'-C4'	5.91	1.59	1.51
2	A	999	FAD	C5A-C4A	5.58	1.49	1.39
2	A	999	FAD	C9A-C5X	5.50	1.50	1.41
2	B	999	FAD	C5A-C4A	5.47	1.48	1.39
2	B	999	FAD	C9A-C5X	5.19	1.49	1.41
2	C	999	FAD	C5A-C4A	4.67	1.47	1.39
2	B	999	FAD	C5A-N7A	-4.63	1.30	1.39
2	A	999	FAD	PA-O3P	4.20	1.64	1.59
2	B	999	FAD	C4A-N9A	-4.11	1.29	1.37
2	C	999	FAD	C5X-N5	-4.10	1.31	1.39
2	B	999	FAD	C8-C7	3.74	1.49	1.40
2	D	999	FAD	C4X-N5	3.73	1.38	1.30
2	A	999	FAD	C2A-N1A	3.72	1.40	1.33
2	B	999	FAD	C4X-N5	3.52	1.38	1.30
2	B	999	FAD	C4A-N3A	-3.39	1.28	1.34
2	A	999	FAD	C8-C7	3.38	1.49	1.40
2	A	999	FAD	PA-O2A	-3.34	1.39	1.55
2	A	999	FAD	C8A-N7A	3.32	1.38	1.31
2	C	999	FAD	C4-N3	-3.28	1.32	1.38
2	A	999	FAD	C4X-N5	3.26	1.37	1.30
2	C	999	FAD	C5A-N7A	-3.24	1.33	1.39
2	A	999	FAD	C6-C5X	-3.23	1.35	1.40
2	A	999	FAD	O4B-C1B	3.16	1.49	1.42
2	A	999	FAD	C6A-N6A	3.11	1.42	1.34
2	A	999	FAD	C2A-N3A	3.01	1.39	1.33
2	C	999	FAD	C4X-N5	2.94	1.37	1.30
2	D	999	FAD	C5A-N7A	-2.88	1.33	1.39
2	C	999	FAD	P-O3P	2.87	1.62	1.59
2	B	999	FAD	C1'-C2'	2.85	1.56	1.52
2	D	999	FAD	P-O3P	-2.82	1.56	1.59
2	B	999	FAD	PA-O2A	-2.70	1.42	1.55
2	C	999	FAD	C8M-C8	2.68	1.56	1.51
2	A	999	FAD	C8M-C8	2.65	1.56	1.51
2	C	999	FAD	C2A-N3A	2.64	1.38	1.33
2	B	999	FAD	C2-N3	-2.57	1.33	1.39
2	B	999	FAD	C9A-N10	2.55	1.45	1.41
2	D	999	FAD	C8A-N7A	2.49	1.36	1.31
2	A	999	FAD	O4-C4	2.48	1.28	1.23
2	A	999	FAD	C9-C9A	2.46	1.43	1.39
2	C	999	FAD	O2-C2	2.38	1.29	1.24
2	C	999	FAD	C6-C7	2.37	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	FAD	C8A-N9A	-2.33	1.33	1.37
2	D	999	FAD	C2-N3	-2.32	1.33	1.39
2	D	999	FAD	O4'-C4'	2.29	1.48	1.43
2	D	999	FAD	C8-C7	2.26	1.46	1.40
2	C	999	FAD	C10-N10	-2.25	1.32	1.37
2	B	999	FAD	O2-C2	2.20	1.28	1.24
2	A	999	FAD	P-O3P	2.20	1.61	1.59
2	C	999	FAD	C2-N1	-2.19	1.31	1.36
2	C	999	FAD	C8-C7	2.17	1.46	1.40
2	B	999	FAD	C5X-N5	-2.17	1.35	1.39
2	B	999	FAD	C10-N1	2.15	1.37	1.33
2	B	999	FAD	P-O3P	-2.13	1.57	1.59
2	B	999	FAD	P-O5'	2.12	1.67	1.59
2	C	999	FAD	C9-C8	2.12	1.42	1.39
2	A	999	FAD	C8A-N9A	2.10	1.41	1.37
2	D	999	FAD	C7M-C7	2.09	1.54	1.51
2	C	999	FAD	C2-N3	-2.06	1.34	1.39
2	A	999	FAD	C1B-N9A	2.05	1.52	1.46
2	C	999	FAD	C4'-C3'	2.04	1.57	1.53
2	A	999	FAD	P-O1P	-2.03	1.43	1.50
2	C	999	FAD	C5A-C6A	2.03	1.46	1.41
2	B	999	FAD	PA-O1A	2.02	1.57	1.50

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	N3A-C2A-N1A	-7.43	117.34	128.58
2	B	999	FAD	C4A-C5A-N7A	-5.44	104.37	110.58
2	A	999	FAD	C4-C4X-N5	5.40	125.67	118.21
2	B	999	FAD	C5A-C4A-N3A	-5.34	119.36	126.72
2	D	999	FAD	C5X-C9A-N10	5.18	122.65	117.97
2	A	999	FAD	C5A-C4A-N3A	-5.11	119.68	126.72
2	C	999	FAD	C4-C4X-N5	5.00	125.11	118.21
2	A	999	FAD	C2A-N3A-C4A	4.84	123.65	111.83
2	D	999	FAD	N9A-C8A-N7A	-4.78	107.15	113.94
2	C	999	FAD	C5A-C4A-N3A	-4.70	120.25	126.72
2	C	999	FAD	C4-N3-C2	-4.64	117.41	125.64
2	C	999	FAD	C4X-C4-N3	4.47	124.63	113.25
2	B	999	FAD	O2P-P-O3P	4.44	119.27	107.27
2	B	999	FAD	C5X-C9A-N10	4.41	121.96	117.97
2	C	999	FAD	C10-N1-C2	4.31	126.19	116.85
2	D	999	FAD	C4A-N9A-C8A	4.27	110.22	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	999	FAD	N3A-C4A-N9A	4.21	134.33	127.17
2	D	999	FAD	C5A-C4A-N3A	-4.17	120.97	126.72
2	C	999	FAD	C7M-C7-C6	-4.15	112.26	119.57
2	B	999	FAD	C10-N1-C2	4.06	125.65	116.85
2	A	999	FAD	N3A-C4A-N9A	4.00	133.96	127.17
2	D	999	FAD	C9A-C5X-N5	-3.91	118.30	122.45
2	D	999	FAD	O4-C4-C4X	-3.79	116.54	126.53
2	A	999	FAD	O2-C2-N1	-3.64	115.76	121.80
2	B	999	FAD	C2A-N3A-C4A	3.63	120.69	111.83
2	A	999	FAD	N9A-C8A-N7A	-3.62	108.80	113.94
2	B	999	FAD	C9A-C5X-N5	-3.62	118.62	122.45
2	D	999	FAD	N3A-C4A-N9A	3.59	133.27	127.17
2	B	999	FAD	C4-C4X-N5	3.56	123.12	118.21
2	D	999	FAD	C5A-N7A-C8A	3.49	108.94	103.45
2	A	999	FAD	C5A-N7A-C8A	3.43	108.84	103.45
2	B	999	FAD	N3A-C2A-N1A	-3.28	123.61	128.58
2	A	999	FAD	C8M-C8-C9	3.28	125.36	119.57
2	C	999	FAD	C4X-C10-N1	-3.28	116.54	124.59
2	A	999	FAD	C4A-C5A-N7A	-3.18	106.95	110.58
2	A	999	FAD	C2A-N1A-C6A	3.16	123.93	118.73
2	C	999	FAD	O4-C4-C4X	-3.16	118.18	126.53
2	C	999	FAD	C7M-C7-C8	3.16	127.22	120.76
2	B	999	FAD	C5A-N7A-C8A	3.04	108.23	103.45
2	A	999	FAD	C4X-C4-N3	3.02	120.95	113.25
2	B	999	FAD	N3A-C4A-N9A	3.01	132.29	127.17
2	D	999	FAD	O3P-PA-O1A	-3.01	101.64	110.70
2	C	999	FAD	O4'-C4'-C5'	-3.01	103.34	109.99
2	B	999	FAD	C8M-C8-C9	-3.01	114.28	119.57
2	A	999	FAD	O4-C4-C4X	-3.00	118.61	126.53
2	D	999	FAD	C4B-O4B-C1B	2.97	116.02	109.47
2	B	999	FAD	C4X-C4-N3	2.96	120.80	113.25
2	A	999	FAD	O4'-C4'-C5'	-2.96	103.46	109.99
2	B	999	FAD	O4B-C1B-N9A	-2.91	102.50	108.09
2	A	999	FAD	C7M-C7-C8	-2.88	114.88	120.76
2	B	999	FAD	O2-C2-N3	2.88	124.10	118.58
2	A	999	FAD	C4A-N9A-C8A	2.88	108.76	105.74
2	D	999	FAD	O5'-C5'-C4'	-2.87	101.70	109.36
2	D	999	FAD	O2-C2-N1	-2.81	117.14	121.80
2	C	999	FAD	N3A-C2A-N1A	-2.73	124.45	128.58
2	B	999	FAD	C9A-N10-C10	-2.69	116.64	120.75
2	B	999	FAD	O4B-C1B-C2B	-2.69	100.86	106.62
2	B	999	FAD	O3B-C3B-C4B	-2.69	103.35	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	999	FAD	C4A-N9A-C1B	-2.67	120.38	126.63
2	A	999	FAD	O3P-PA-O1A	-2.65	102.72	110.70
2	C	999	FAD	N6A-C6A-N1A	2.64	124.26	118.38
2	C	999	FAD	C9A-C5X-N5	-2.63	119.66	122.45
2	D	999	FAD	O2A-PA-O1A	2.63	124.69	112.44
2	D	999	FAD	O4-C4-N3	2.56	124.93	120.11
2	B	999	FAD	C6A-C5A-N7A	2.52	136.95	132.09
2	C	999	FAD	O2-C2-N1	-2.51	117.63	121.80
2	C	999	FAD	C2A-N3A-C4A	2.50	117.93	111.83
2	C	999	FAD	C2A-N1A-C6A	2.48	122.80	118.73
2	B	999	FAD	O4-C4-C4X	-2.45	120.06	126.53
2	C	999	FAD	C5A-N7A-C8A	2.44	107.28	103.45
2	B	999	FAD	O2-C2-N1	-2.41	117.79	121.80
2	A	999	FAD	O2A-PA-O3P	2.41	113.78	107.27
2	C	999	FAD	C4A-C5A-N7A	-2.41	107.83	110.58
2	C	999	FAD	C4'-C3'-C2'	2.39	117.55	113.57
2	A	999	FAD	O4B-C1B-N9A	-2.39	103.50	108.09
2	B	999	FAD	C4-C4X-C10	-2.37	112.86	116.93
2	B	999	FAD	C4X-C10-N1	-2.37	118.78	124.59
2	B	999	FAD	C4X-C10-N10	2.31	119.80	116.48
2	A	999	FAD	C6A-C5A-N7A	2.29	136.50	132.09
2	D	999	FAD	C4A-C5A-N7A	-2.27	107.99	110.58
2	D	999	FAD	O4B-C1B-N9A	-2.26	103.75	108.09
2	A	999	FAD	C5'-C4'-C3'	2.26	116.48	112.22
2	D	999	FAD	O2B-C2B-C3B	-2.24	104.63	111.82
2	C	999	FAD	O3P-P-O1P	-2.24	103.98	110.70
2	A	999	FAD	O2-C2-N3	2.22	122.85	118.58
2	D	999	FAD	O4B-C4B-C3B	-2.21	100.77	105.15
2	C	999	FAD	C4X-C10-N10	2.17	119.59	116.48
2	B	999	FAD	C3B-C2B-C1B	2.17	105.56	101.46
2	C	999	FAD	C5X-N5-C4X	2.15	121.57	118.09
2	A	999	FAD	C5X-N5-C4X	2.12	121.51	118.09
2	C	999	FAD	O3'-C3'-C4'	2.11	113.72	108.93
2	D	999	FAD	C2A-N3A-C4A	2.11	116.97	111.83
2	C	999	FAD	C10-C4X-N5	-2.10	120.53	124.81
2	D	999	FAD	C4-C4X-N5	2.07	121.07	118.21
2	A	999	FAD	C10-C4X-N5	-2.07	120.59	124.81
2	C	999	FAD	C4A-N9A-C1B	-2.07	121.80	126.63
2	B	999	FAD	C8M-C8-C7	2.03	124.90	120.76
2	A	999	FAD	C4A-N9A-C1B	-2.02	121.91	126.63
2	D	999	FAD	O3B-C3B-C4B	-2.02	105.29	111.08
2	C	999	FAD	C8M-C8-C7	2.02	124.88	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	C9-C8-C7	-2.01	116.73	119.69
2	A	999	FAD	O5'-C5'-C4'	-2.01	104.00	109.36

There are no chirality outliers.

All (16) torsion outliers are listed below:

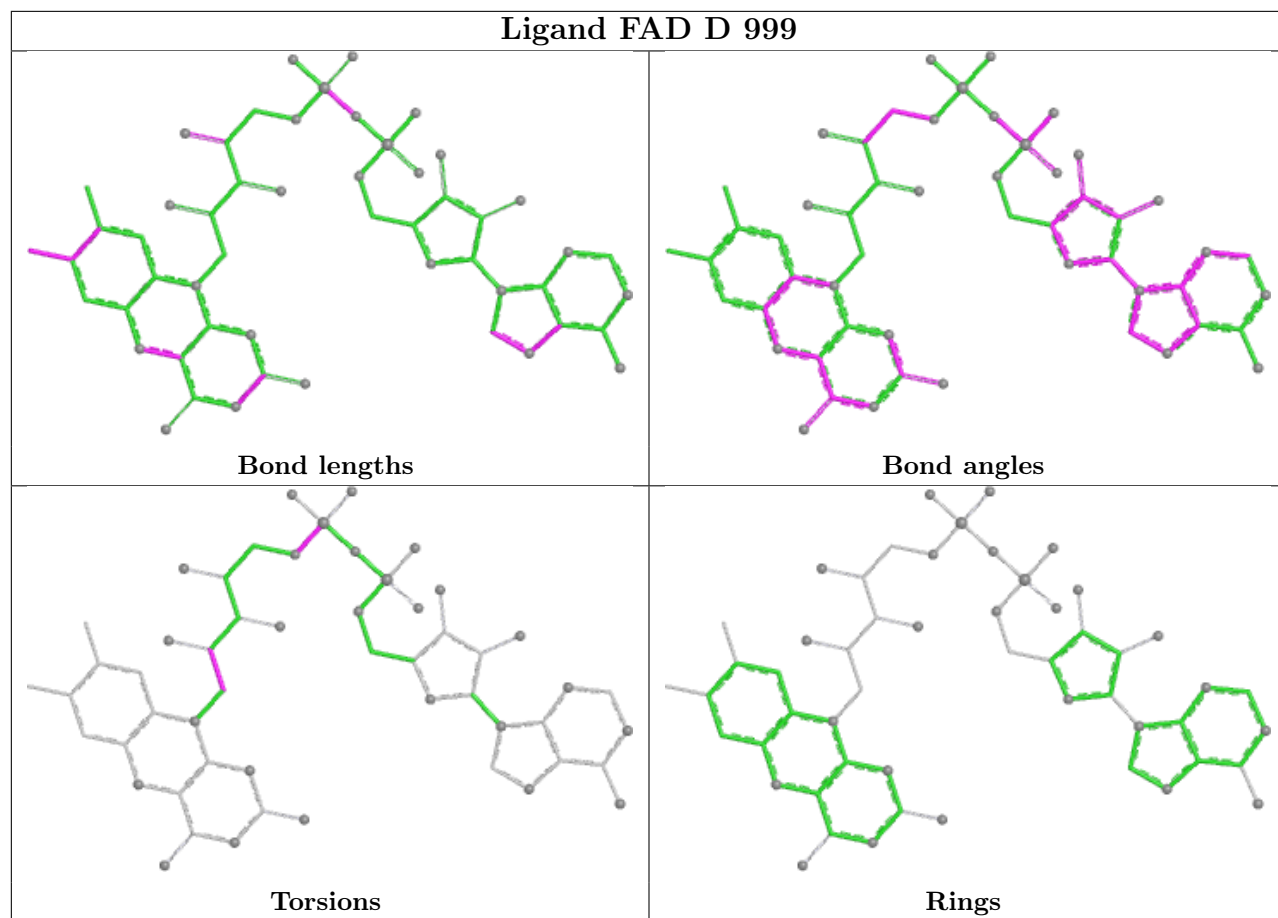
Mol	Chain	Res	Type	Atoms
2	A	999	FAD	N10-C1'-C2'-O2'
2	A	999	FAD	N10-C1'-C2'-C3'
2	B	999	FAD	N10-C1'-C2'-O2'
2	B	999	FAD	N10-C1'-C2'-C3'
2	C	999	FAD	N10-C1'-C2'-O2'
2	C	999	FAD	N10-C1'-C2'-C3'
2	D	999	FAD	N10-C1'-C2'-O2'
2	D	999	FAD	N10-C1'-C2'-C3'
2	A	999	FAD	O4'-C4'-C5'-O5'
2	A	999	FAD	C5'-O5'-P-O1P
2	D	999	FAD	C5'-O5'-P-O1P
2	A	999	FAD	C3'-C4'-C5'-O5'
2	A	999	FAD	PA-O3P-P-O2P
2	B	999	FAD	PA-O3P-P-O1P
2	C	999	FAD	PA-O3P-P-O2P
2	C	999	FAD	PA-O3P-P-O1P

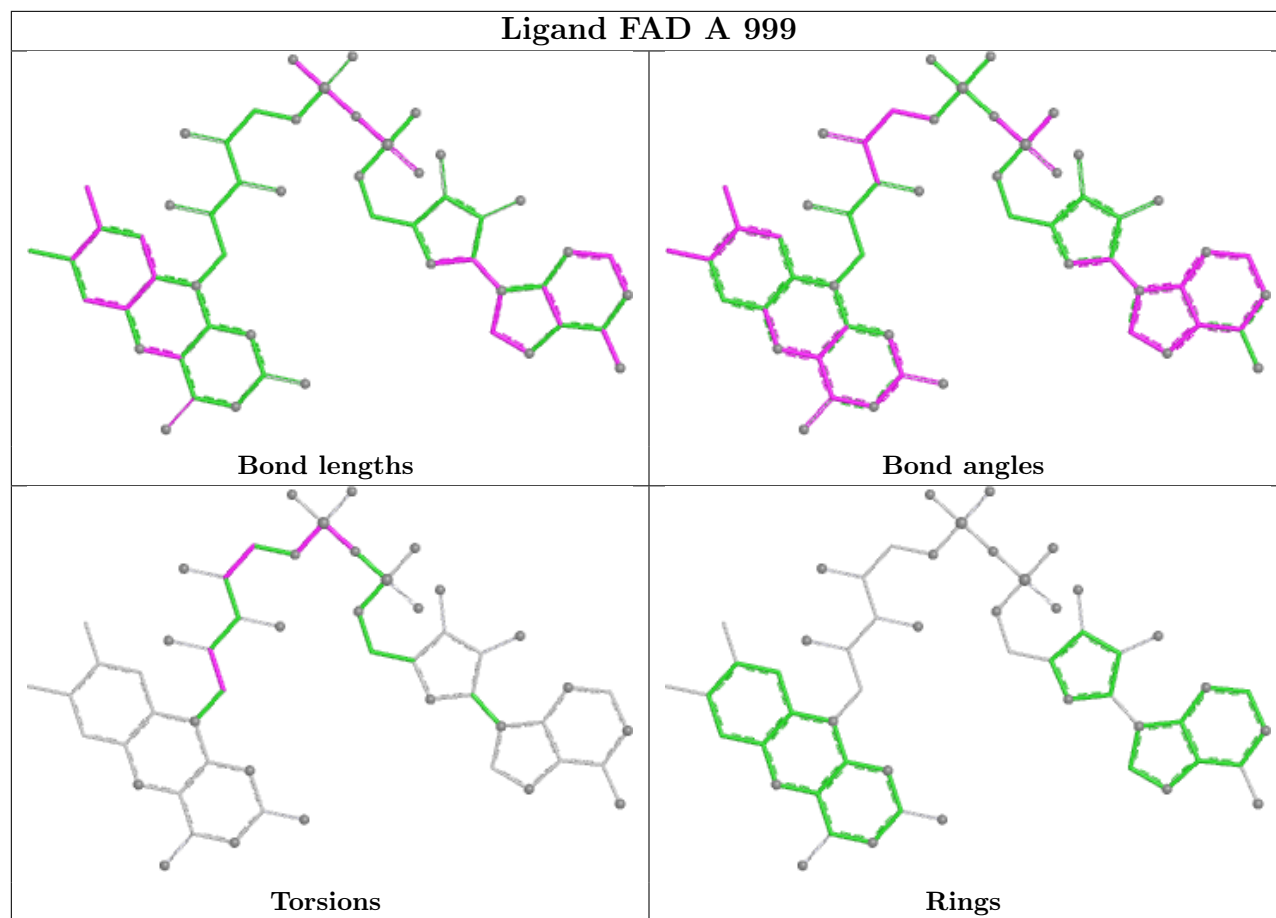
There are no ring outliers.

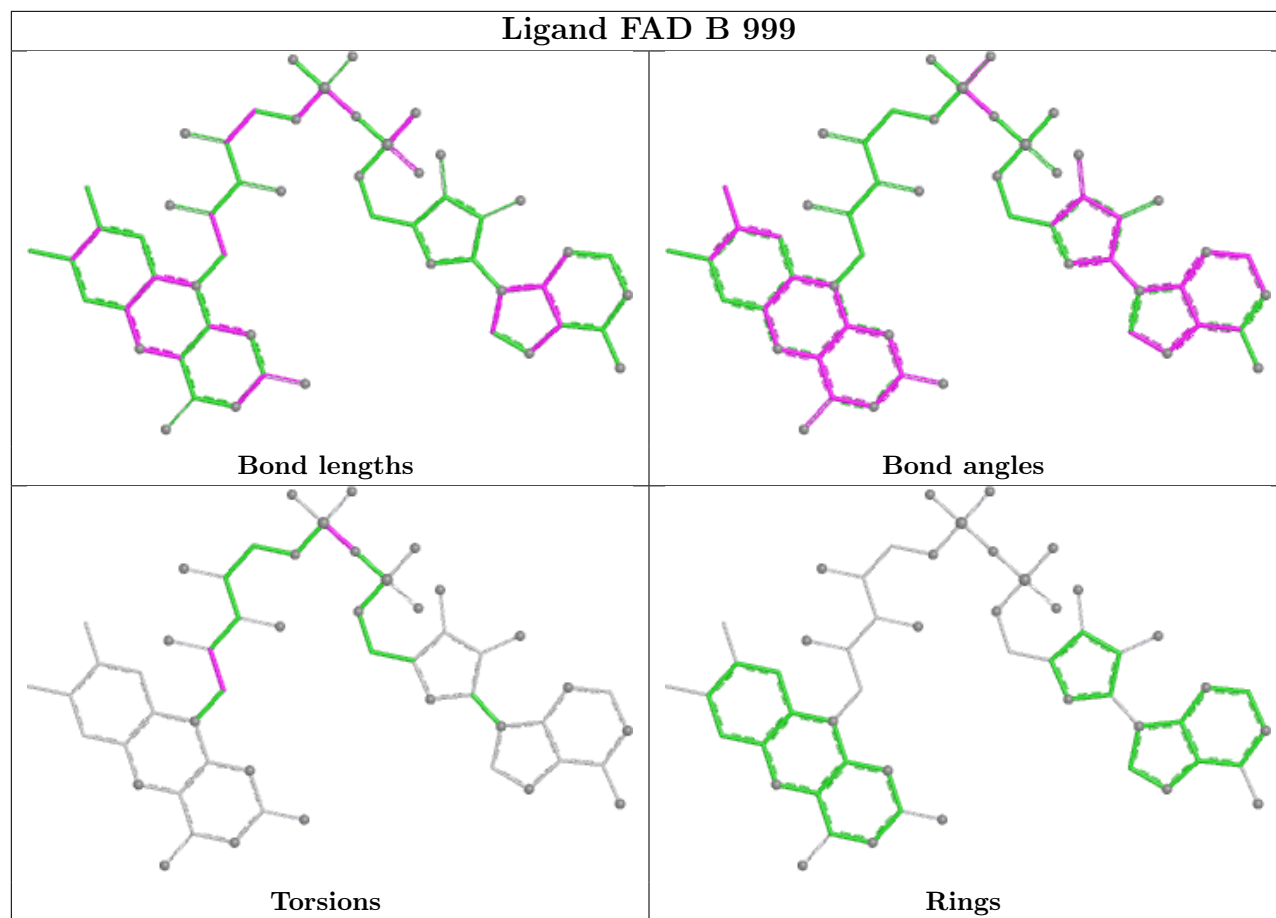
1 monomer is involved in 1 short contact:

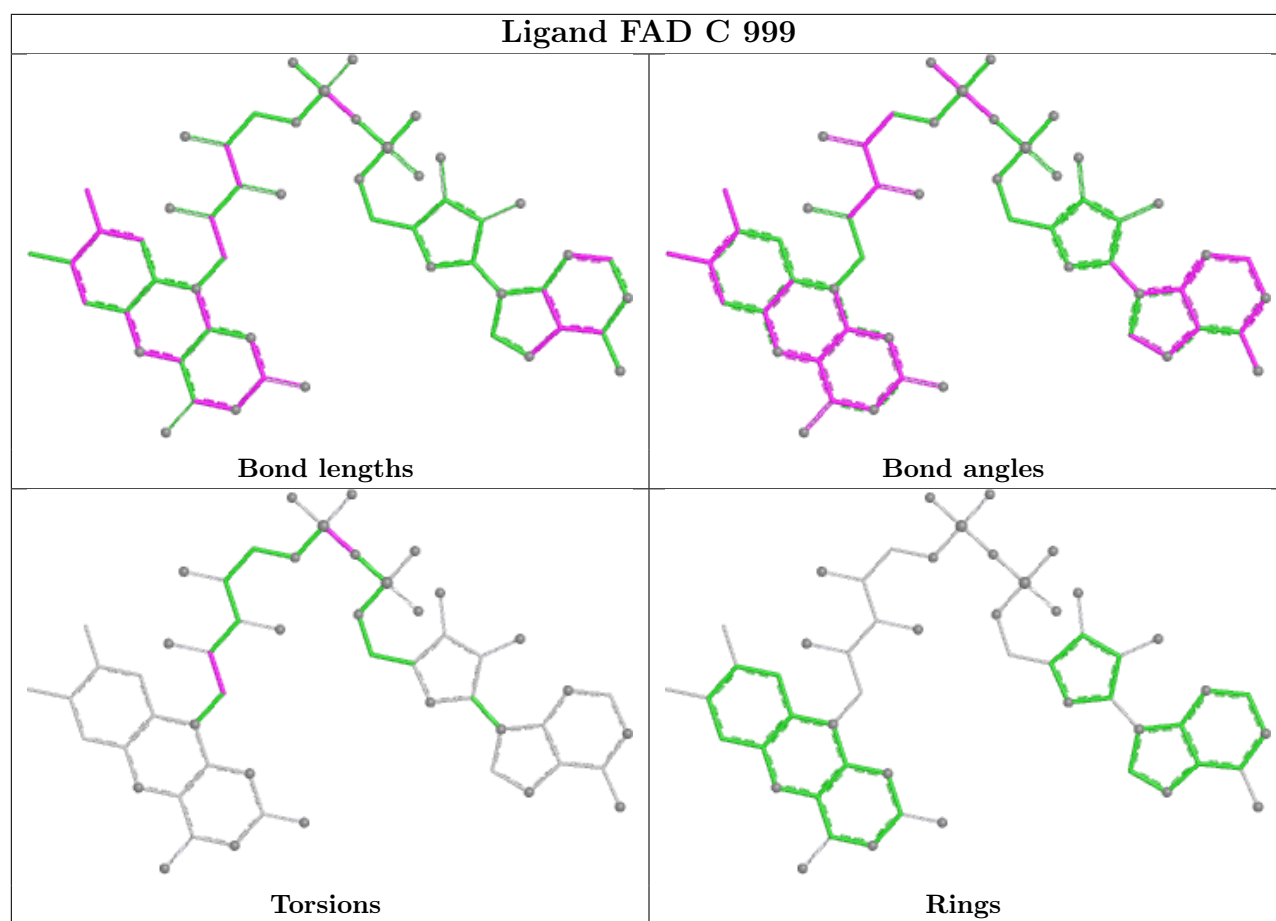
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	999	FAD	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	555/658 (84%)	-0.14	10 (1%) 67 71	9, 26, 55, 88	4 (0%)
1	B	543/658 (82%)	0.05	18 (3%) 49 52	14, 30, 59, 84	0
1	C	557/658 (84%)	-0.08	15 (2%) 56 60	11, 27, 55, 75	3 (0%)
1	D	550/658 (83%)	0.06	5 (0%) 81 83	8, 32, 60, 78	2 (0%)
All	All	2205/2632 (83%)	-0.03	48 (2%) 62 66	8, 29, 58, 88	9 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	PHE	7.4
1	B	559	PHE	6.0
1	B	460	PRO	4.5
1	C	431	ALA	4.3
1	B	458	PHE	4.2
1	D	559	PHE	3.9
1	B	265	ARG	3.5
1	C	457	GLY	3.3
1	A	142	HIS	3.2
1	C	432	LEU	3.1
1	B	457	GLY	3.0
1	C	336[A]	MET	3.0
1	A	141	ASP	2.9
1	B	507	LEU	2.9
1	C	429	GLY	2.8
1	B	434	PRO	2.8
1	B	509	TYR	2.8
1	D	580	TYR	2.8
1	A	144	THR	2.7
1	A	82	ILE	2.6
1	D	426	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	504	GLY	2.6
1	C	460	PRO	2.5
1	C	428	PHE	2.5
1	B	140	LEU	2.5
1	B	432	LEU	2.5
1	B	508	THR	2.5
1	A	81	GLY	2.5
1	A	139	ASN	2.4
1	B	197	LEU	2.4
1	C	458	PHE	2.4
1	C	141	ASP	2.4
1	B	506	LEU	2.3
1	C	507	LEU	2.3
1	A	441	THR	2.3
1	C	509	TYR	2.3
1	C	506	LEU	2.2
1	C	559	PHE	2.2
1	C	461	ASN	2.2
1	C	83	ILE	2.2
1	B	505	TYR	2.1
1	B	523	ILE	2.1
1	A	159	ILE	2.1
1	D	243	TYR	2.1
1	D	107	LYS	2.1
1	A	439	ILE	2.0
1	B	459	ASP	2.0
1	B	522	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 [i](#)

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,

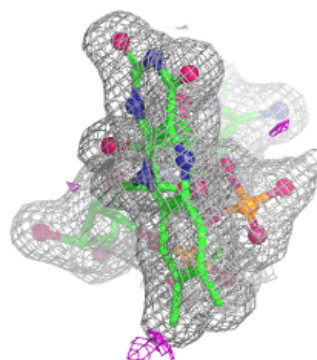
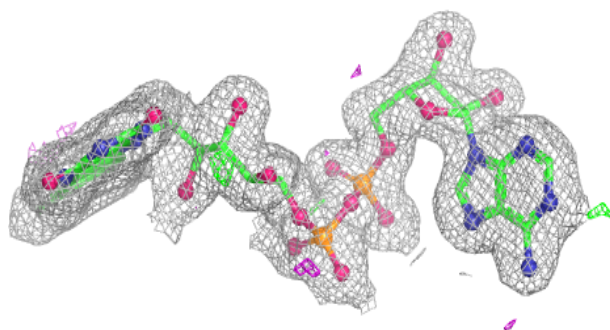
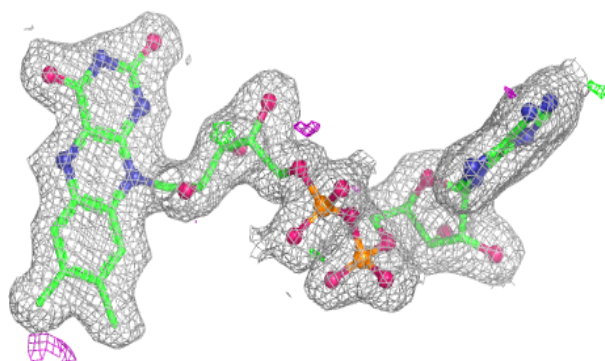
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	1659	5/5	0.90	0.17	41,51,57,66	0
3	SO4	A	1660	5/5	0.92	0.10	47,51,61,62	0
3	SO4	D	1659	5/5	0.92	0.12	39,40,44,58	0
3	SO4	A	1659	5/5	0.93	0.12	34,37,43,59	0
2	FAD	B	999	53/53	0.98	0.04	13,15,19,20	0
2	FAD	D	999	53/53	0.98	0.04	10,13,17,21	0
2	FAD	A	999	53/53	0.98	0.04	10,14,17,18	0
2	FAD	C	999	53/53	0.99	0.04	9,12,16,19	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.

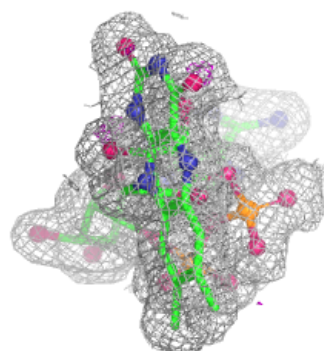
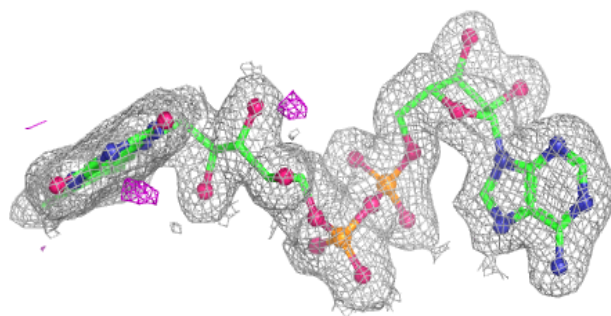
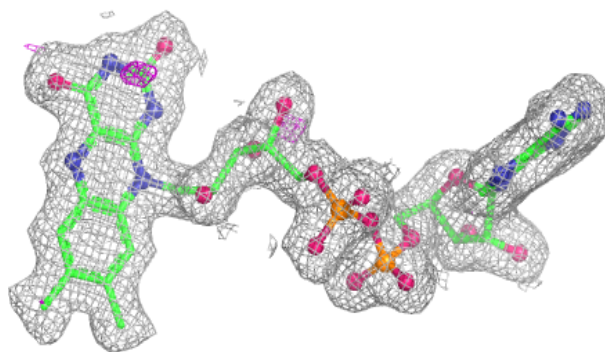
Electron density around FAD B 999:

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

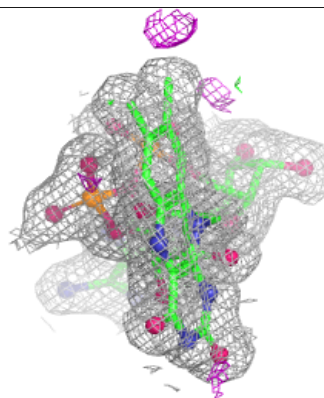
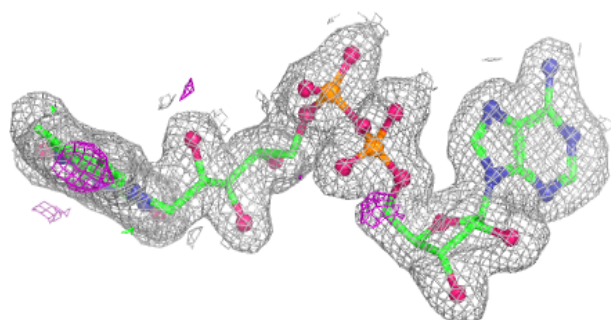
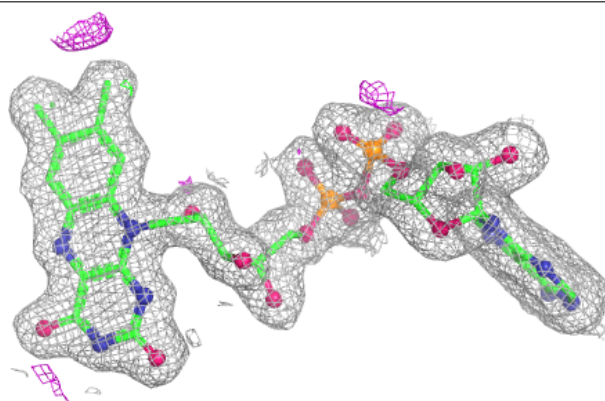


Electron density around FAD D 999:

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

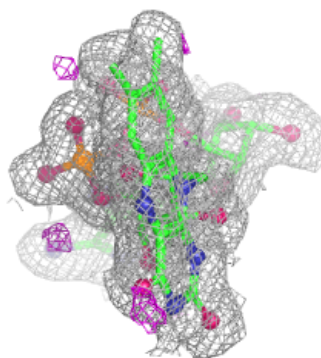
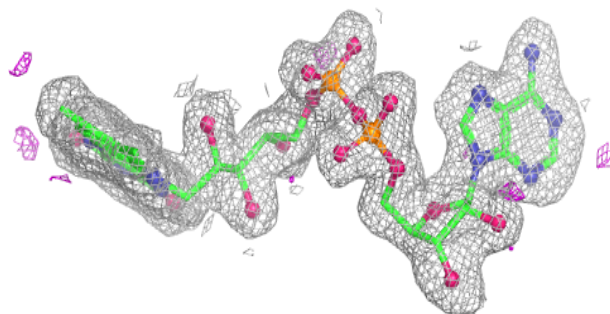
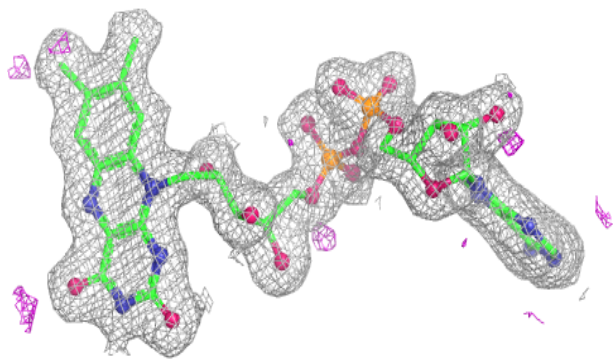
**Electron density around FAD A 999:**

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



Electron density around FAD C 999:

$2mF_o-DF_c$ (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.