



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:34 PM BST

PDB ID : 1F8S
Title : CRYSTAL STRUCTURE OF L-AMINO ACID OXIDASE FROM CALLOSE-LASMA RHODOSTOMA, COMPLEXED WITH THREE MOLECULES OF O-AMINO BENZOATE.
Authors : Pawelek, P.D.; Cheah, J.; Coulombe, R.; Macheroux, P.; Ghisla, S.; Vrielink, A.
Deposited on : 2000-07-04
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

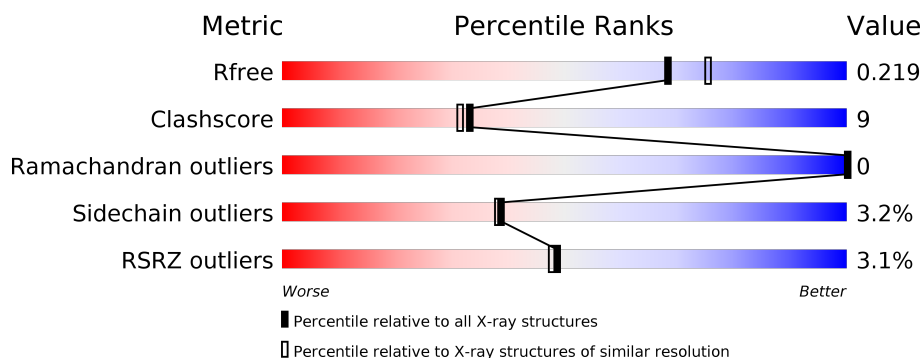
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	498	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>••</div> </div> </div>
1	B	498	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>••</div> </div> </div>
1	C	498	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>••</div> </div> </div>
1	D	498	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>••</div> </div> </div>
1	E	498	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>••</div> </div> </div>
1	F	498	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	498	
1	H	498	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1543	X	-	-	X
3	BE2	G	1544	-	-	X	-
3	BE2	G	1545	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34018 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 L-AMINO ACID OXIDASE.

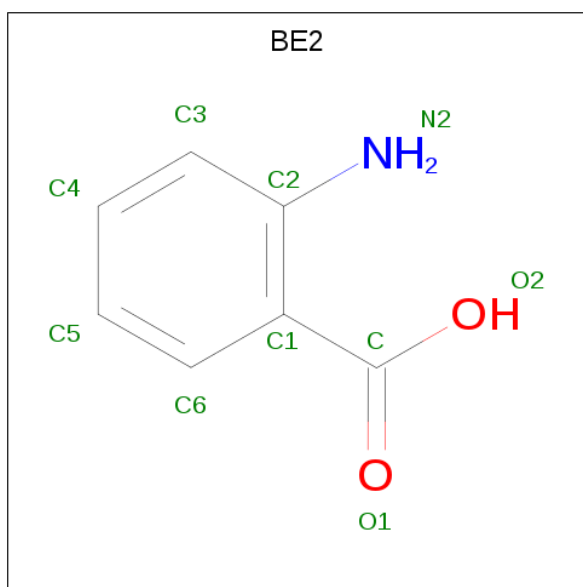
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	B	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	C	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	D	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	E	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	F	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	G	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			
1	H	482	Total	C	N	O	S	0	1	0
			3858	2461	656	729	12			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-AMINOBENZOIC ACID (three-letter code: BE2) (formula: C₇H₇NO₂).



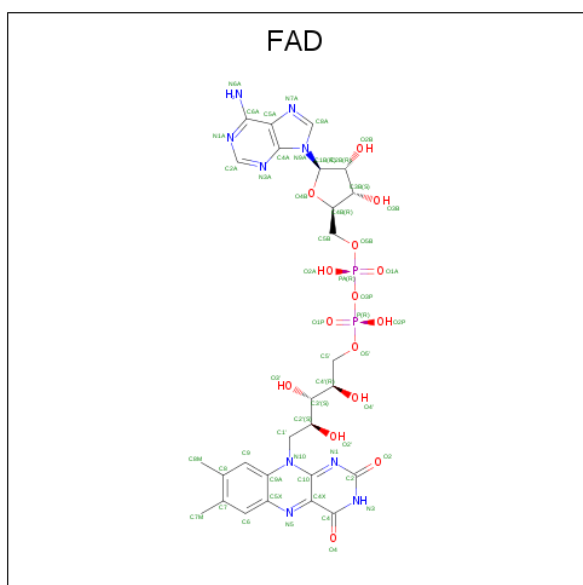
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		
3	E	1	Total	C	N	O	0	0
			10	7	1	2		
3	E	1	Total	C	N	O	0	0
			10	7	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total 10	C 7	N 1	O 2	0	0
3	F	1	Total 10	C 7	N 1	O 2	0	0
3	F	1	Total 10	C 7	N 1	O 2	0	0
3	F	1	Total 10	C 7	N 1	O 2	0	0
3	G	1	Total 10	C 7	N 1	O 2	0	0
3	G	1	Total 10	C 7	N 1	O 2	0	0
3	G	1	Total 10	C 7	N 1	O 2	0	0
3	H	1	Total 10	C 7	N 1	O 2	0	0
3	H	1	Total 10	C 7	N 1	O 2	0	0
3	H	1	Total 10	C 7	N 1	O 2	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

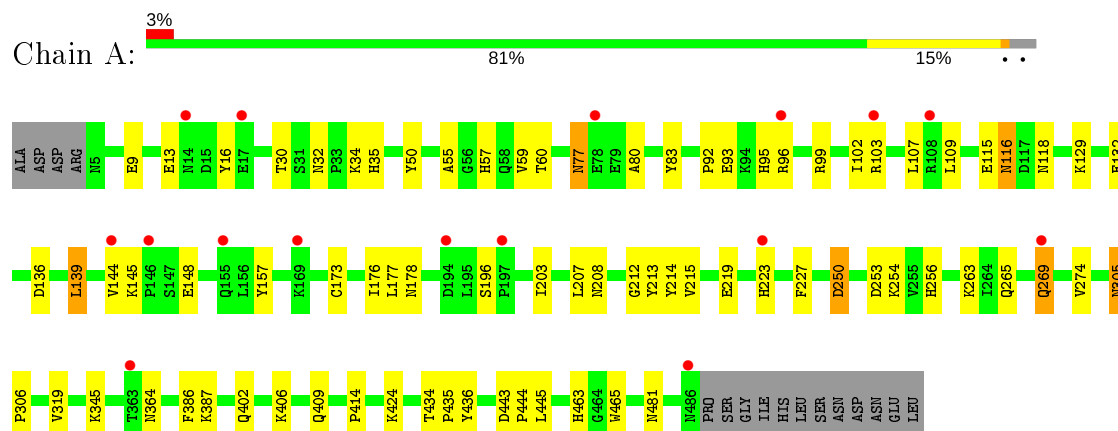
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	292	Total	O	0	0
			292	292		
5	B	305	Total	O	0	0
			305	305		
5	C	350	Total	O	0	0
			350	350		
5	D	341	Total	O	0	0
			341	341		
5	E	281	Total	O	0	0
			281	281		
5	F	292	Total	O	0	0
			292	292		
5	G	285	Total	O	0	0
			285	285		
5	H	232	Total	O	0	0
			232	232		

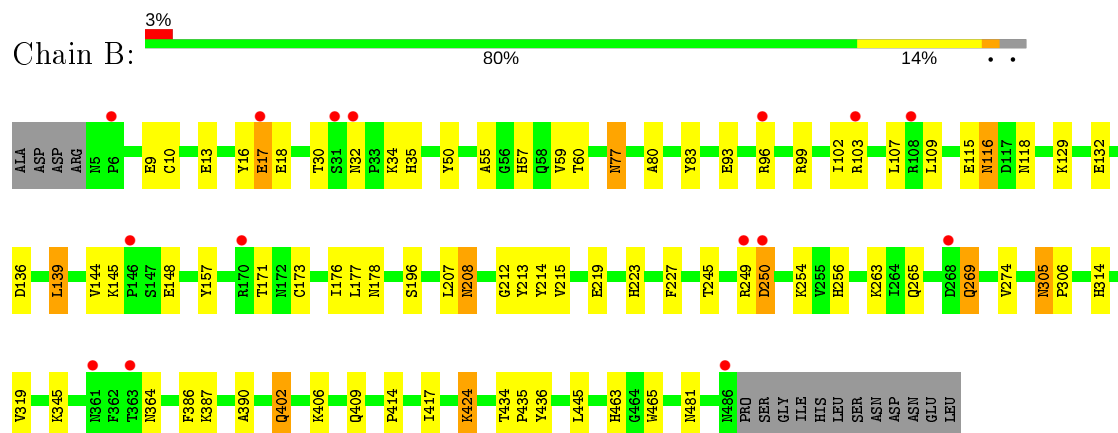
3 Residue-property plots [i](#)

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.

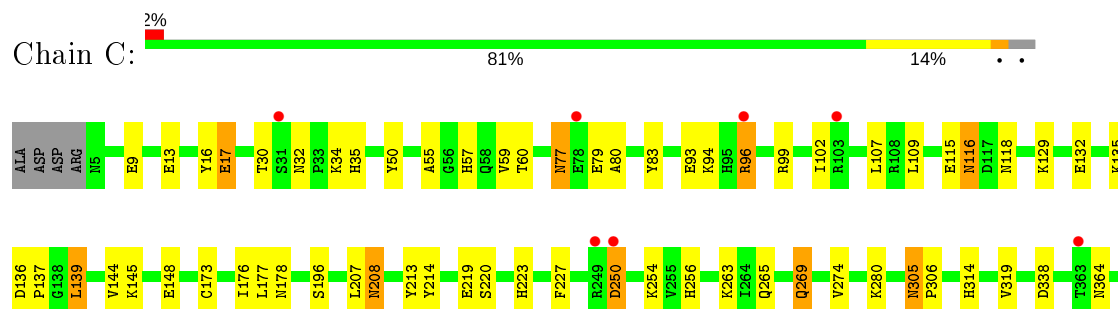
• Molecule 1: L-AMINO ACID OXIDASE



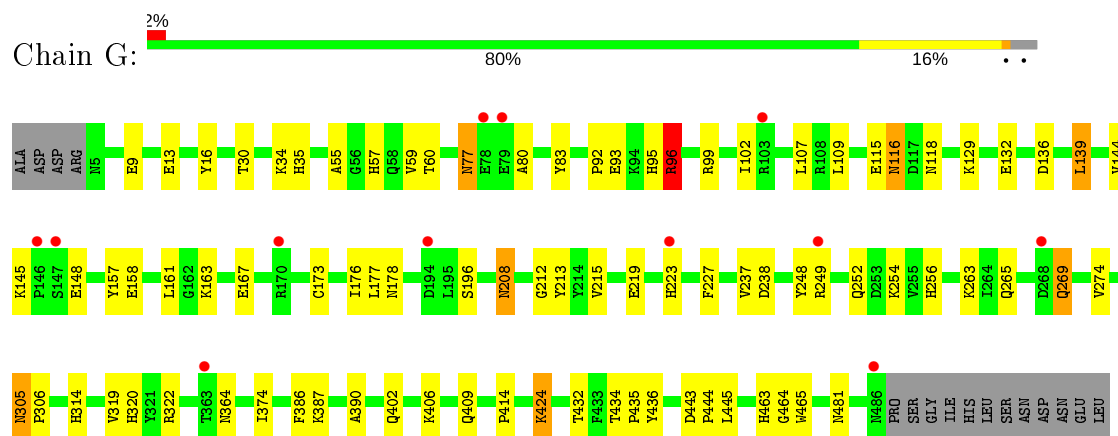
• Molecule 1: L-AMINO ACID OXIDASE



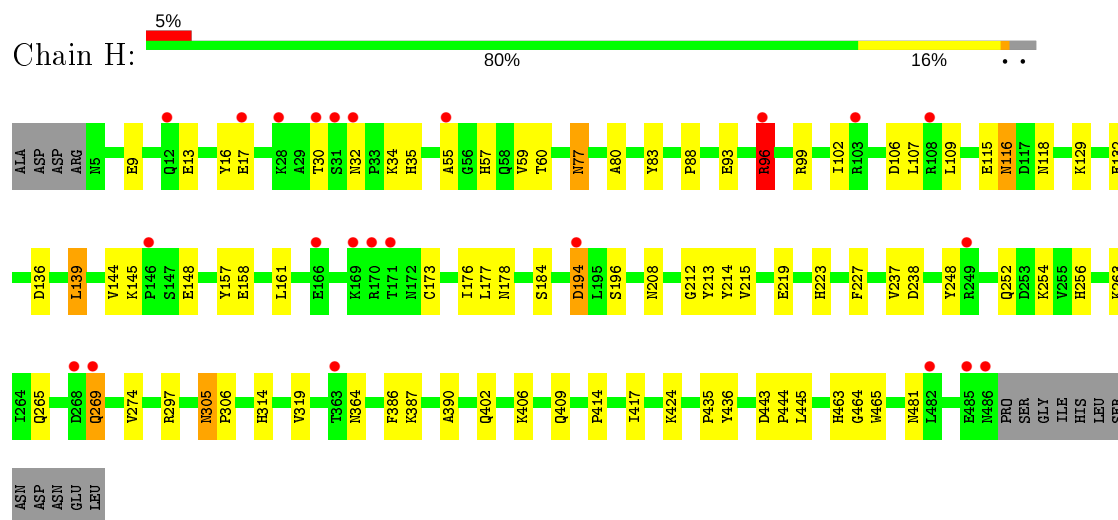
• Molecule 1: L-AMINO ACID OXIDASE



• Molecule 1: L-AMINO ACID OXIDASE



• Molecule 1: L-AMINO ACID OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.55Å 137.18Å 212.63Å 90.00° 105.63° 90.00°	Depositor
Resolution (Å)	500.00 – 2.00 48.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (500.00-2.00) 85.0 (48.80-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.79Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.205 , 0.225 0.199 , 0.219	Depositor DCC
R_{free} test set	33637 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34018	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 57.15 % 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 2.4693e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: BE2, NAG, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/3950	0.64	3/5347 (0.1%)
1	B	0.39	2/3950 (0.1%)	0.62	0/5347
1	C	0.39	2/3950 (0.1%)	0.62	1/5347 (0.0%)
1	D	0.41	0/3950	0.63	1/5347 (0.0%)
1	E	0.37	0/3950	0.64	2/5347 (0.0%)
1	F	0.40	2/3950 (0.1%)	0.62	0/5347
1	G	0.40	0/3950	0.63	3/5347 (0.1%)
1	H	0.38	0/3950	0.63	1/5347 (0.0%)
All	All	0.39	6/31600 (0.0%)	0.63	11/42776 (0.0%)

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	E	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	GLU	CD-OE1	-6.33	1.18	1.25
1	B	17	GLU	CB-CG	-6.19	1.40	1.52
1	C	17	GLU	CG-CD	-5.91	1.43	1.51
1	B	17	GLU	CG-CD	-5.90	1.43	1.51
1	F	17	GLU	CD-OE1	-5.66	1.19	1.25
1	F	17	GLU	CG-CD	-5.35	1.44	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	E	96	ARG	CG-CD-NE	-6.51	98.13	111.80
1	A	96	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	A	103	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	G	96	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	G	249	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	96	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	H	96	ARG	CA-CB-CG	-5.27	101.81	113.40
1	G	249	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	E	96	ARG	CA-CB-CG	-5.12	102.13	113.40
1	D	96	ARG	CB-CG-CD	-5.11	98.31	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	96	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	3858	0	3775	58	1
1	B	3858	0	3775	70	0
1	C	3858	0	3775	67	1
1	D	3858	0	3775	69	2
1	E	3858	0	3775	74	0
1	F	3858	0	3775	68	0
1	G	3858	0	3775	68	0
1	H	3858	0	3775	68	2
2	A	14	0	13	0	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
2	H	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	18	2	0
3	B	30	0	18	4	0
3	C	30	0	18	4	0
3	D	30	0	18	3	0
3	E	30	0	18	2	0
3	F	30	0	18	4	0
3	G	30	0	18	10	0
3	H	30	0	18	2	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	C	53	0	31	0	0
4	D	53	0	31	1	0
4	E	53	0	31	1	0
4	F	53	0	31	0	0
4	G	53	0	31	1	0
4	H	53	0	31	1	0
5	A	292	0	0	4	0
5	B	305	0	0	7	0
5	C	350	0	0	9	0
5	D	341	0	0	4	0
5	E	281	0	0	6	0
5	F	292	0	0	4	0
5	G	285	0	0	8	0
5	H	232	0	0	6	0
All	All	34018	0	30696	536	3

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 9.

All (536) 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:H:96:ARG:CG	1:H:96:ARG:HH11	1.50	1.22
1:E:96:ARG:HG3	1:E:96:ARG:NH1	1.19	1.12
1:E:96:ARG:CG	1:E:96:ARG:HH11	1.58	1.12
1:H:96:ARG:NH1	1:H:96:ARG:HG3	1.31	1.05
1:E:96:ARG:CG	1:E:96:ARG:NH1	2.11	1.02
1:C:17:GLU:OE1	5:C:958:HOH:O	1.78	0.99
1:E:116:ASN:HD22	1:E:118:ASN:H	1.17	0.93
1:A:116:ASN:HD22	1:A:118:ASN:H	1.19	0.90
1:B:17:GLU:OE1	5:B:1363:HOH:O	1.89	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:ASN:HD22	1:F:118:ASN:H	1.18	0.90
1:H:116:ASN:HD22	1:H:118:ASN:H	1.17	0.89
1:B:96:ARG:HH11	1:B:96:ARG:HG3	1.36	0.89
1:G:116:ASN:HD22	1:G:118:ASN:H	1.21	0.87
1:C:116:ASN:HD22	1:C:118:ASN:H	1.22	0.87
1:D:116:ASN:HD22	1:D:118:ASN:H	1.20	0.85
1:B:116:ASN:HD22	1:B:118:ASN:H	1.22	0.82
1:B:34:LYS:H	1:B:57:HIS:HD2	1.28	0.81
1:D:34:LYS:H	1:D:57:HIS:HD2	1.30	0.80
1:G:34:LYS:H	1:G:57:HIS:HD2	1.29	0.80
1:C:34:LYS:H	1:C:57:HIS:HD2	1.29	0.78
1:E:34:LYS:H	1:E:57:HIS:HD2	1.31	0.78
1:D:319:VAL:HG21	1:D:445:LEU:HD11	1.66	0.78
1:D:116:ASN:ND2	1:D:118:ASN:H	1.83	0.77
1:H:219:GLU:OE2	1:H:463:HIS:HD2	1.67	0.77
1:H:116:ASN:ND2	1:H:118:ASN:H	1.84	0.76
1:A:116:ASN:ND2	1:A:118:ASN:H	1.83	0.76
1:B:96:ARG:NH1	1:B:96:ARG:HG3	1.96	0.76
1:H:34:LYS:H	1:H:57:HIS:HD2	1.33	0.76
1:A:319:VAL:HG21	1:A:445:LEU:HD11	1.68	0.76
1:F:34:LYS:H	1:F:57:HIS:HD2	1.31	0.76
1:G:223[A]:HIS:NE2	1:G:227:PHE:CD1	2.54	0.76
1:A:269:GLN:HE21	1:A:269:GLN:HA	1.50	0.76
1:E:116:ASN:ND2	1:E:118:ASN:H	1.85	0.75
1:G:116:ASN:ND2	1:G:118:ASN:H	1.85	0.74
1:F:116:ASN:ND2	1:F:118:ASN:H	1.85	0.74
1:B:269:GLN:HA	1:B:269:GLN:HE21	1.53	0.73
1:E:319:VAL:HG21	1:E:445:LEU:HD11	1.70	0.73
1:C:116:ASN:ND2	1:C:118:ASN:H	1.86	0.73
1:B:116:ASN:ND2	1:B:118:ASN:H	1.86	0.73
1:F:208:ASN:HB3	3:F:1545:BE2:N2	2.03	0.73
1:C:269:GLN:HA	1:C:269:GLN:HE21	1.53	0.72
1:B:219:GLU:OE2	1:B:463:HIS:HD2	1.72	0.72
1:F:219:GLU:OE2	1:F:463:HIS:HD2	1.72	0.72
1:A:34:LYS:H	1:A:57:HIS:HD2	1.35	0.72
1:F:269:GLN:HE21	1:F:269:GLN:HA	1.54	0.72
1:D:269:GLN:HA	1:D:269:GLN:HE21	1.55	0.71
1:H:269:GLN:HE21	1:H:269:GLN:HA	1.55	0.71
1:G:319:VAL:HG21	1:G:445:LEU:HD11	1.72	0.71
1:C:219:GLU:OE2	1:C:463:HIS:HD2	1.73	0.71
1:C:319:VAL:HG21	1:C:445:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:GLN:HA	1:G:269:GLN:HE21	1.57	0.70
1:E:219:GLU:OE2	1:E:463:HIS:HD2	1.73	0.69
1:E:269:GLN:HA	1:E:269:GLN:HE21	1.56	0.69
1:F:223[A]:HIS:CE1	1:F:227:PHE:CD1	2.80	0.69
1:D:219:GLU:OE2	1:D:463:HIS:HD2	1.75	0.69
1:E:145:LYS:HG3	1:E:196:SER:HB3	1.73	0.69
1:G:145:LYS:HG3	1:G:196:SER:HB3	1.74	0.69
1:H:145:LYS:HG3	1:H:196:SER:HB3	1.74	0.68
1:B:34:LYS:H	1:B:57:HIS:CD2	2.10	0.68
1:A:129:LYS:HB2	1:A:132:GLU:HG3	1.76	0.68
1:F:145:LYS:HG3	1:F:196:SER:HB3	1.75	0.68
1:G:223[A]:HIS:CE1	1:G:227:PHE:CD1	2.80	0.68
1:G:219:GLU:OE2	1:G:463:HIS:HD2	1.76	0.68
1:E:96:ARG:HG3	1:E:96:ARG:HH11	0.87	0.67
1:H:319:VAL:HG21	1:H:445:LEU:HD11	1.76	0.67
1:B:319:VAL:HG21	1:B:445:LEU:HD11	1.75	0.67
1:A:145:LYS:HG3	1:A:196:SER:HB3	1.75	0.67
1:C:463:HIS:HE1	5:C:639:HOH:O	1.78	0.67
1:A:219:GLU:OE2	1:A:463:HIS:HD2	1.77	0.67
1:G:34:LYS:H	1:G:57:HIS:CD2	2.13	0.67
1:D:145:LYS:HG3	1:D:196:SER:HB3	1.76	0.66
1:F:34:LYS:H	1:F:57:HIS:CD2	2.13	0.66
1:F:319:VAL:HG21	1:F:445:LEU:HD11	1.78	0.66
1:E:34:LYS:H	1:E:57:HIS:CD2	2.14	0.65
1:H:34:LYS:H	1:H:57:HIS:CD2	2.15	0.64
1:C:145:LYS:HG3	1:C:196:SER:HB3	1.78	0.64
1:E:96:ARG:HH11	1:E:96:ARG:CB	2.09	0.64
1:B:145:LYS:HG3	1:B:196:SER:HB3	1.79	0.64
1:A:34:LYS:H	1:A:57:HIS:CD2	2.16	0.64
1:D:280:LYS:HE2	5:F:1679:HOH:O	1.97	0.63
1:D:96:ARG:N	1:D:96:ARG:HD3	2.13	0.63
1:B:463:HIS:HE1	5:B:1574:HOH:O	1.82	0.63
1:C:34:LYS:H	1:C:57:HIS:CD2	2.13	0.62
1:D:34:LYS:H	1:D:57:HIS:CD2	2.14	0.62
1:G:223[A]:HIS:NE2	1:G:227:PHE:CE1	2.67	0.62
1:B:207:LEU:O	3:B:1545:BE2:N2	2.33	0.62
1:E:129:LYS:HB2	1:E:132:GLU:HG3	1.81	0.62
1:H:463:HIS:HE1	5:H:1549:HOH:O	1.83	0.61
1:F:463:HIS:HE1	5:F:1554:HOH:O	1.84	0.61
1:C:129:LYS:HB2	1:C:132:GLU:HG3	1.83	0.61
1:G:129:LYS:HB2	1:G:132:GLU:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:LEU:O	3:F:1545:BE2:N2	2.35	0.60
1:D:136:ASP:OD2	1:D:139:LEU:HD13	2.01	0.60
1:F:387:LYS:HG2	5:F:1683:HOH:O	2.01	0.60
1:D:57:HIS:HE1	1:D:481:ASN:OD1	1.85	0.60
1:C:57:HIS:HE1	1:C:481:ASN:OD1	1.85	0.60
1:G:136:ASP:OD2	1:G:139:LEU:HD13	2.01	0.60
1:C:96:ARG:HD2	1:C:96:ARG:N	2.17	0.60
1:A:50:TYR:HE1	1:A:250:ASP:OD2	1.85	0.60
1:B:96:ARG:N	1:B:96:ARG:HD2	2.16	0.59
1:E:35:HIS:HE1	1:E:60:THR:OG1	1.85	0.59
1:H:136:ASP:OD2	1:H:139:LEU:HD13	2.02	0.59
1:B:35:HIS:HE1	1:B:60:THR:OG1	1.85	0.59
1:F:129:LYS:HB2	1:F:132:GLU:HG3	1.84	0.59
1:F:59:VAL:HG22	1:F:254:LYS:HD3	1.84	0.59
1:B:136:ASP:OD2	1:B:139:LEU:HD13	2.03	0.59
1:B:129:LYS:HB2	1:B:132:GLU:HG3	1.84	0.59
1:H:305:ASN:HD22	1:H:306:PRO:HA	1.67	0.59
1:C:136:ASP:OD2	1:C:139:LEU:HD13	2.03	0.59
1:G:57:HIS:HE1	1:G:481:ASN:OD1	1.85	0.59
1:F:265:GLN:HG2	1:F:305:ASN:HB3	1.84	0.58
1:C:35:HIS:HE1	1:C:60:THR:OG1	1.86	0.58
1:D:387:LYS:HG2	5:D:1602:HOH:O	2.03	0.58
1:A:136:ASP:OD2	1:A:139:LEU:HD13	2.04	0.58
1:F:116:ASN:HD22	1:F:118:ASN:N	1.97	0.57
1:C:464:GLY:O	3:C:1544:BE2:H3	2.03	0.57
1:H:57:HIS:HE1	1:H:481:ASN:OD1	1.87	0.57
1:G:223[A]:HIS:CE1	1:G:227:PHE:CG	2.93	0.57
1:A:116:ASN:HD22	1:A:118:ASN:N	1.96	0.57
1:A:305:ASN:HD22	1:A:306:PRO:HA	1.70	0.57
1:H:129:LYS:HB2	1:H:132:GLU:HG3	1.87	0.57
1:A:57:HIS:HE1	1:A:481:ASN:OD1	1.88	0.57
1:C:59:VAL:HG22	1:C:254:LYS:HD3	1.86	0.57
1:H:96:ARG:HG3	1:H:96:ARG:HH11	0.58	0.57
1:H:35:HIS:HE1	1:H:60:THR:OG1	1.88	0.56
3:G:1545:BE2:H3	5:G:1481:HOH:O	2.05	0.56
1:B:57:HIS:HE1	1:B:481:ASN:OD1	1.88	0.56
1:H:219:GLU:O	1:H:223[B]:HIS:HD2	1.87	0.56
1:C:305:ASN:HD22	1:C:306:PRO:HA	1.70	0.56
1:F:227:PHE:HE1	1:F:465:TRP:HZ2	1.54	0.56
1:D:305:ASN:HD22	1:D:306:PRO:HA	1.71	0.56
1:D:463:HIS:HE1	5:D:1555:HOH:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:HIS:HE1	1:F:60:THR:OG1	1.87	0.56
1:E:195:LEU:HD23	5:E:1716:HOH:O	2.06	0.55
1:C:50:TYR:HE1	1:C:250:ASP:OD2	1.90	0.55
1:H:269:GLN:HE21	1:H:269:GLN:CA	2.19	0.55
1:H:387:LYS:HG2	5:H:1608:HOH:O	2.06	0.55
1:D:223[A]:HIS:NE2	1:D:227:PHE:CD1	2.74	0.55
1:G:223[A]:HIS:C	1:G:223[A]:HIS:ND1	2.60	0.55
1:B:34:LYS:N	1:B:57:HIS:HD2	2.02	0.55
1:D:77:ASN:ND2	1:D:80:ALA:H	2.05	0.55
1:D:424:LYS:HZ3	1:D:424:LYS:HB2	1.71	0.55
1:F:136:ASP:OD2	1:F:139:LEU:HD13	2.07	0.55
1:E:50:TYR:HE1	1:E:250:ASP:OD2	1.90	0.55
1:F:57:HIS:HE1	1:F:481:ASN:OD1	1.90	0.55
1:C:34:LYS:N	1:C:57:HIS:HD2	2.03	0.55
1:E:93:GLU:HA	1:E:99:ARG:CZ	2.36	0.54
1:F:305:ASN:HD22	1:F:306:PRO:HA	1.72	0.54
1:D:35:HIS:HE1	1:D:60:THR:OG1	1.90	0.54
1:E:223[A]:HIS:NE2	1:E:227:PHE:CD1	2.75	0.54
1:E:269:GLN:HE21	1:E:269:GLN:CA	2.19	0.54
3:G:1544:BE2:H5	3:G:1545:BE2:H5	1.90	0.54
1:F:102:ILE:HG23	1:F:107:LEU:HB2	1.89	0.54
1:H:93:GLU:HA	1:H:99:ARG:CZ	2.38	0.54
1:G:305:ASN:HD22	1:G:306:PRO:HA	1.72	0.54
1:H:59:VAL:HG22	1:H:254:LYS:HD3	1.87	0.54
1:B:59:VAL:HG22	1:B:254:LYS:HD3	1.90	0.54
1:D:126:ILE:HD11	1:D:141:LYS:NZ	2.23	0.54
1:E:305:ASN:HD22	1:E:306:PRO:HA	1.71	0.54
1:E:57:HIS:HE1	1:E:481:ASN:OD1	1.90	0.54
1:G:102:ILE:HG23	1:G:107:LEU:HB2	1.90	0.54
1:G:116:ASN:HD22	1:G:118:ASN:N	2.00	0.54
1:G:463:HIS:HE1	5:G:1362:HOH:O	1.89	0.54
1:A:59:VAL:HG22	1:A:254:LYS:HD3	1.89	0.54
1:D:50:TYR:HE1	1:D:250:ASP:OD2	1.91	0.54
1:C:424:LYS:HB2	1:C:424:LYS:HZ3	1.72	0.54
1:C:77:ASN:ND2	1:C:80:ALA:H	2.05	0.54
1:E:59:VAL:HG22	1:E:254:LYS:HD3	1.88	0.54
1:F:30:THR:HG22	1:F:55:ALA:O	2.07	0.54
1:A:387:LYS:HG2	5:A:1612:HOH:O	2.08	0.53
1:G:59:VAL:HG22	1:G:254:LYS:HD3	1.90	0.53
1:A:35:HIS:HE1	1:A:60:THR:OG1	1.92	0.53
1:E:463:HIS:HE1	5:E:1145:HOH:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:O	3:C:1545:BE2:N2	2.41	0.53
1:E:116:ASN:HD22	1:E:118:ASN:N	1.98	0.53
1:E:265:GLN:HG2	1:E:305:ASN:HB3	1.90	0.53
1:H:116:ASN:HD22	1:H:118:ASN:N	1.97	0.53
1:C:208:ASN:HB3	3:C:1545:BE2:N2	2.23	0.53
1:F:223[A]:HIS:NE2	1:F:227:PHE:CD1	2.76	0.53
1:D:406:LYS:HA	1:D:409:GLN:HE21	1.74	0.53
1:H:223[A]:HIS:NE2	1:H:227:PHE:CD1	2.77	0.53
1:F:269:GLN:HE21	1:F:269:GLN:CA	2.18	0.53
1:F:223[A]:HIS:NE2	1:F:227:PHE:CE1	2.76	0.52
1:B:227:PHE:HE1	1:B:465:TRP:HZ2	1.56	0.52
1:D:59:VAL:HG22	1:D:254:LYS:HD3	1.92	0.52
1:E:464:GLY:O	3:E:1544:BE2:H3	2.09	0.52
1:G:77:ASN:ND2	1:G:80:ALA:H	2.07	0.52
1:B:50:TYR:HE1	1:B:250:ASP:OD2	1.93	0.52
1:B:305:ASN:HD22	1:B:306:PRO:HA	1.73	0.52
1:C:227:PHE:HE1	1:C:465:TRP:HZ2	1.58	0.52
1:D:129:LYS:HB2	1:D:132:GLU:HG3	1.92	0.52
1:G:167:GLU:HG2	5:G:2411:HOH:O	2.08	0.52
1:H:96:ARG:NH1	1:H:96:ARG:CG	2.20	0.52
1:A:212:GLY:O	1:A:215:VAL:HG22	2.10	0.52
1:B:102:ILE:HG23	1:B:107:LEU:HB2	1.92	0.52
1:G:35:HIS:HE1	1:G:60:THR:OG1	1.92	0.52
1:A:34:LYS:N	1:A:57:HIS:HD2	2.07	0.52
1:F:9:GLU:HG2	1:F:173:CYS:SG	2.50	0.52
1:G:465:TRP:CH2	3:G:1544:BE2:N2	2.79	0.51
1:B:223[A]:HIS:NE2	1:B:227:PHE:CD1	2.78	0.51
1:H:297:ARG:HG2	5:H:1571:HOH:O	2.11	0.51
1:G:93:GLU:HA	1:G:99:ARG:CZ	2.40	0.51
1:C:406:LYS:HA	1:C:409:GLN:HE21	1.75	0.51
1:E:50:TYR:CE1	1:E:250:ASP:OD2	2.63	0.51
1:E:30:THR:HG22	1:E:55:ALA:O	2.11	0.51
1:C:220:SER:HA	5:C:2795:HOH:O	2.10	0.51
1:A:77:ASN:ND2	1:A:80:ALA:H	2.09	0.51
1:B:116:ASN:HD22	1:B:118:ASN:N	2.02	0.51
1:B:77:ASN:C	1:B:77:ASN:HD22	2.13	0.51
1:E:223[A]:HIS:CE1	1:E:227:PHE:CD1	2.99	0.51
1:A:463:HIS:HE1	5:A:1557:HOH:O	1.93	0.51
1:C:387:LYS:HG2	5:C:1173:HOH:O	2.11	0.51
1:C:96:ARG:HG3	5:C:2264:HOH:O	2.11	0.51
1:D:9:GLU:HG2	1:D:173:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:LYS:N	1:F:57:HIS:HD2	2.04	0.51
1:H:227:PHE:HE1	1:H:465:TRP:HZ2	1.58	0.51
1:G:227:PHE:HE1	1:G:465:TRP:HZ2	1.59	0.50
1:A:77:ASN:HD22	1:A:77:ASN:C	2.15	0.50
1:D:116:ASN:HD22	1:D:118:ASN:N	2.00	0.50
1:D:93:GLU:HA	1:D:99:ARG:CZ	2.41	0.50
1:F:227:PHE:HE1	1:F:465:TRP:CZ2	2.29	0.50
1:F:386:PHE:CD1	1:F:417:ILE:HD12	2.46	0.50
1:A:80:ALA:O	1:A:364:ASN:ND2	2.44	0.50
1:C:93:GLU:HA	1:C:99:ARG:CZ	2.42	0.50
1:C:116:ASN:HD22	1:C:118:ASN:N	2.01	0.50
1:H:464:GLY:O	3:H:1544:BE2:H3	2.11	0.50
1:F:77:ASN:ND2	1:F:80:ALA:H	2.10	0.50
1:G:322:ARG:NH2	3:G:1545:BE2:H4	2.27	0.50
1:A:30:THR:HG22	1:A:55:ALA:O	2.12	0.50
1:H:263:LYS:HB2	1:H:274:VAL:HB	1.94	0.50
1:H:77:ASN:ND2	1:H:80:ALA:H	2.10	0.50
1:E:136:ASP:OD2	1:E:139:LEU:HD13	2.12	0.50
1:E:9:GLU:HG2	1:E:173:CYS:SG	2.52	0.49
1:G:387:LYS:HG2	5:G:2056:HOH:O	2.12	0.49
1:A:269:GLN:HE21	1:A:269:GLN:CA	2.15	0.49
1:E:34:LYS:N	1:E:57:HIS:HD2	2.04	0.49
1:G:265:GLN:HG2	1:G:305:ASN:HB3	1.94	0.49
1:A:50:TYR:CE1	1:A:250:ASP:OD2	2.65	0.49
1:C:77:ASN:C	1:C:77:ASN:HD22	2.13	0.49
1:D:34:LYS:N	1:D:57:HIS:HD2	2.04	0.49
1:F:223[A]:HIS:CE1	1:F:227:PHE:CG	3.00	0.49
1:F:223[A]:HIS:ND1	1:F:223[A]:HIS:O	2.45	0.49
1:G:9:GLU:HG2	1:G:173:CYS:SG	2.52	0.49
1:A:9:GLU:HG2	1:A:173:CYS:SG	2.52	0.49
1:G:34:LYS:N	1:G:57:HIS:HD2	2.03	0.49
1:G:77:ASN:C	1:G:77:ASN:HD22	2.15	0.49
1:A:93:GLU:HA	1:A:99:ARG:CZ	2.42	0.49
1:B:77:ASN:ND2	1:B:80:ALA:H	2.10	0.49
1:D:157:TYR:CE2	3:D:1546:BE2:H3	2.46	0.49
1:D:269:GLN:CA	1:D:269:GLN:HE21	2.18	0.49
1:E:223[A]:HIS:NE2	1:E:227:PHE:CE1	2.80	0.49
1:B:406:LYS:HA	1:B:409:GLN:HE21	1.78	0.49
1:B:30:THR:HG22	1:B:55:ALA:O	2.12	0.49
1:F:93:GLU:HA	1:F:99:ARG:CZ	2.42	0.49
1:F:406:LYS:HA	1:F:409:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:HE1	1:A:465:TRP:HZ2	1.60	0.49
1:C:79:GLU:HB2	5:E:2565:HOH:O	2.12	0.49
1:D:227:PHE:HE1	1:D:465:TRP:HZ2	1.59	0.49
1:H:34:LYS:N	1:H:57:HIS:HD2	2.06	0.49
1:H:9:GLU:HG2	1:H:173:CYS:SG	2.53	0.49
1:F:263:LYS:HB2	1:F:274:VAL:HB	1.95	0.49
1:B:227:PHE:HE1	1:B:465:TRP:CZ2	2.31	0.49
1:B:93:GLU:HA	1:B:99:ARG:CZ	2.43	0.49
1:D:280:LYS:HG3	1:F:409:GLN:HB3	1.94	0.49
1:G:263:LYS:HB2	1:G:274:VAL:HB	1.95	0.49
1:D:77:ASN:C	1:D:77:ASN:HD22	2.16	0.48
1:E:77:ASN:C	1:E:77:ASN:HD22	2.15	0.48
1:F:212:GLY:O	1:F:215:VAL:HG22	2.13	0.48
1:B:386:PHE:CE2	1:B:414:PRO:HB2	2.48	0.48
1:F:77:ASN:HD22	1:F:77:ASN:C	2.16	0.48
1:D:464:GLY:O	3:D:1544:BE2:H3	2.14	0.48
1:H:77:ASN:HD22	1:H:77:ASN:C	2.15	0.48
1:A:406:LYS:HA	1:A:409:GLN:HE21	1.77	0.48
1:C:80:ALA:O	1:C:364:ASN:ND2	2.47	0.48
1:F:80:ALA:O	1:F:364:ASN:ND2	2.47	0.48
1:A:102:ILE:HG23	1:A:107:LEU:HB2	1.94	0.48
1:A:32:ASN:ND2	1:A:34:LYS:HE2	2.28	0.48
1:A:214:TYR:CD2	1:B:434:THR:HG21	2.49	0.48
1:G:406:LYS:HA	1:G:409:GLN:HE21	1.76	0.48
1:H:80:ALA:O	1:H:364:ASN:ND2	2.47	0.48
1:A:263:LYS:HB2	1:A:274:VAL:HB	1.95	0.48
1:C:94:LYS:O	1:C:96:ARG:HD2	2.14	0.48
1:C:9:GLU:HG2	1:C:173:CYS:SG	2.53	0.48
1:E:102:ILE:HG23	1:E:107:LEU:HB2	1.95	0.48
1:G:435:PRO:O	1:G:436:TYR:HB2	2.14	0.48
1:D:443:ASP:HB2	1:D:444:PRO:HD3	1.96	0.48
1:H:144:VAL:HB	1:H:148:GLU:HB2	1.96	0.48
1:H:32:ASN:ND2	1:H:34:LYS:HE2	2.29	0.48
1:D:80:ALA:O	1:D:364:ASN:ND2	2.47	0.48
1:E:227:PHE:HE1	1:E:465:TRP:HZ2	1.61	0.48
1:F:208:ASN:HB3	3:F:1545:BE2:HN21	1.78	0.48
1:C:263:LYS:HB2	1:C:274:VAL:HB	1.96	0.47
1:D:30:THR:HG22	1:D:55:ALA:O	2.14	0.47
1:F:443:ASP:HB2	1:F:444:PRO:HD3	1.96	0.47
1:H:386:PHE:CE2	1:H:414:PRO:HB2	2.49	0.47
1:D:32:ASN:ND2	1:D:34:LYS:HE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:LYS:HD2	5:G:2411:HOH:O	2.14	0.47
1:G:227:PHE:HE1	1:G:465:TRP:CZ2	2.32	0.47
1:F:50:TYR:CE1	1:F:250:ASP:OD2	2.67	0.47
1:C:227:PHE:HE1	1:C:465:TRP:CZ2	2.32	0.47
1:D:116:ASN:C	1:D:116:ASN:HD22	2.17	0.47
1:C:102:ILE:HG23	1:C:107:LEU:HB2	1.97	0.47
1:F:32:ASN:ND2	1:F:34:LYS:HE2	2.30	0.47
1:H:13:GLU:HB2	1:H:16:TYR:CD1	2.50	0.47
1:H:269:GLN:NE2	1:H:269:GLN:HA	2.28	0.47
1:B:208:ASN:HB3	3:B:1545:BE2:N2	2.30	0.47
1:E:13:GLU:HB2	1:E:16:TYR:CD1	2.50	0.47
1:H:223[A]:HIS:CE1	1:H:227:PHE:CD1	3.03	0.47
1:H:265:GLN:HG2	1:H:305:ASN:HB3	1.97	0.47
1:B:223[A]:HIS:CE1	1:B:227:PHE:CD1	3.02	0.47
1:B:263:LYS:HB2	1:B:274:VAL:HB	1.96	0.47
1:C:269:GLN:HA	1:C:269:GLN:NE2	2.27	0.47
1:C:424:LYS:HG2	5:C:1699:HOH:O	2.15	0.47
1:E:80:ALA:O	1:E:364:ASN:ND2	2.48	0.47
1:G:223[A]:HIS:O	1:G:223[A]:HIS:ND1	2.48	0.47
1:H:102:ILE:HG23	1:H:107:LEU:HB2	1.97	0.47
1:C:269:GLN:CA	1:C:269:GLN:HE21	2.18	0.47
3:G:1544:BE2:C5	3:G:1545:BE2:H5	2.44	0.47
1:E:32:ASN:ND2	1:E:34:LYS:HE2	2.30	0.47
1:F:144:VAL:HB	1:F:148:GLU:HB2	1.97	0.47
1:G:96:ARG:HB3	1:G:96:ARG:HE	1.43	0.47
1:B:269:GLN:NE2	1:B:269:GLN:HA	2.27	0.46
1:C:465:TRP:CH2	3:C:1544:BE2:N2	2.84	0.46
1:D:319:VAL:CG2	1:D:445:LEU:HD11	2.42	0.46
1:B:80:ALA:O	1:B:364:ASN:ND2	2.48	0.46
1:E:212:GLY:O	1:E:215:VAL:HG22	2.16	0.46
1:G:443:ASP:HB2	1:G:444:PRO:HD3	1.98	0.46
1:H:223[A]:HIS:HB3	5:H:1730:HOH:O	2.15	0.46
1:C:32:ASN:ND2	1:C:34:LYS:HE2	2.30	0.46
1:F:223[A]:HIS:ND1	1:F:223[A]:HIS:C	2.67	0.46
1:G:223[B]:HIS:HE1	5:G:1665:HOH:O	1.97	0.46
1:B:116:ASN:C	1:B:116:ASN:HD22	2.19	0.46
1:C:214:TYR:CD2	1:D:434:THR:HG21	2.50	0.46
1:D:102:ILE:HG23	1:D:107:LEU:HB2	1.97	0.46
1:A:227:PHE:HE1	1:A:465:TRP:CZ2	2.34	0.46
1:E:406:LYS:HA	1:E:409:GLN:HE21	1.79	0.46
1:G:144:VAL:HB	1:G:148:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:THR:HG22	1:G:55:ALA:O	2.15	0.46
1:H:406:LYS:HA	1:H:409:GLN:HE21	1.80	0.46
1:B:96:ARG:CG	1:B:96:ARG:NH1	2.64	0.46
1:A:223[A]:HIS:NE2	1:A:227:PHE:CD1	2.84	0.46
1:D:126:ILE:HD11	1:D:141:LYS:HZ2	1.79	0.46
1:E:386:PHE:CD1	1:E:417:ILE:HD12	2.50	0.46
1:H:227:PHE:HE1	1:H:465:TRP:CZ2	2.32	0.46
1:D:227:PHE:HE1	1:D:465:TRP:CZ2	2.34	0.46
1:H:176:ILE:HG13	1:H:177:LEU:N	2.31	0.46
1:E:77:ASN:ND2	1:E:80:ALA:H	2.14	0.46
1:G:464:GLY:O	3:G:1544:BE2:H3	2.16	0.46
1:H:212:GLY:O	1:H:215:VAL:HG22	2.16	0.46
1:E:227:PHE:HE1	1:E:465:TRP:CZ2	2.33	0.46
1:H:256:HIS:CD2	1:H:256:HIS:N	2.84	0.46
1:A:269:GLN:NE2	1:A:269:GLN:HA	2.26	0.45
1:C:402:GLN:HG3	5:C:1814:HOH:O	2.16	0.45
1:D:207:LEU:O	3:D:1545:BE2:N2	2.49	0.45
1:D:79:GLU:HG3	5:D:1789:HOH:O	2.16	0.45
1:C:144:VAL:HB	1:C:148:GLU:HB2	1.98	0.45
1:F:386:PHE:CE2	1:F:414:PRO:HB2	2.51	0.45
1:G:116:ASN:HD22	1:G:116:ASN:C	2.20	0.45
1:G:374:ILE:HD13	3:G:1545:BE2:C5	2.46	0.45
1:E:424:LYS:HB2	1:E:424:LYS:HZ2	1.80	0.45
1:B:387:LYS:HG2	5:B:1202:HOH:O	2.15	0.45
1:D:144:VAL:HB	1:D:148:GLU:HB2	1.98	0.45
1:E:223[A]:HIS:CE1	1:E:227:PHE:CG	3.05	0.45
1:G:208:ASN:HB3	3:G:1545:BE2:C	2.47	0.45
4:G:526:FAD:H8A	5:G:736:HOH:O	2.16	0.45
1:G:80:ALA:O	1:G:364:ASN:ND2	2.50	0.45
1:C:116:ASN:C	1:C:116:ASN:HD22	2.19	0.45
1:F:435:PRO:O	1:F:436:TYR:HB2	2.17	0.45
1:H:223[A]:HIS:CE1	1:H:227:PHE:CG	3.05	0.45
1:A:265:GLN:HG2	1:A:305:ASN:HB3	1.98	0.45
1:F:13:GLU:HB2	1:F:16:TYR:CD1	2.51	0.45
1:A:144:VAL:HB	1:A:148:GLU:HB2	1.99	0.45
1:B:144:VAL:HB	1:B:148:GLU:HB2	1.99	0.45
1:B:9:GLU:HG2	1:B:173:CYS:SG	2.56	0.45
1:F:256:HIS:N	1:F:256:HIS:CD2	2.85	0.45
1:G:386:PHE:CE2	1:G:414:PRO:HB2	2.51	0.45
1:B:265:GLN:HG2	1:B:305:ASN:HB3	1.99	0.45
1:E:214:TYR:CD2	1:F:434:THR:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:ILE:HD13	1:G:109:LEU:HD21	1.99	0.45
1:D:435:PRO:O	1:D:436:TYR:HB2	2.17	0.45
1:E:269:GLN:HA	1:E:269:GLN:NE2	2.30	0.45
1:F:176:ILE:HG13	1:F:177:LEU:N	2.32	0.45
1:H:223[A]:HIS:NE2	1:H:227:PHE:CE1	2.85	0.45
1:A:443:ASP:HB2	1:A:444:PRO:HD3	1.99	0.44
1:D:79:GLU:HB2	5:F:1778:HOH:O	2.17	0.44
1:E:144:VAL:HB	1:E:148:GLU:HB2	2.00	0.44
1:A:116:ASN:ND2	1:A:118:ASN:HB2	2.32	0.44
1:A:319:VAL:CG2	1:A:445:LEU:HD11	2.45	0.44
1:C:30:THR:HG22	1:C:55:ALA:O	2.17	0.44
1:G:269:GLN:CA	1:G:269:GLN:HE21	2.20	0.44
1:H:386:PHE:CD1	1:H:417:ILE:HD12	2.52	0.44
1:B:256:HIS:N	1:B:256:HIS:CD2	2.85	0.44
1:C:434:THR:HG21	1:D:214:TYR:CD2	2.52	0.44
1:F:248:TYR:CZ	1:F:252:GLN:HG3	2.52	0.44
1:H:248:TYR:CZ	1:H:252:GLN:HG3	2.52	0.44
1:G:256:HIS:N	1:G:256:HIS:CD2	2.85	0.44
1:A:13:GLU:HB2	1:A:16:TYR:CD1	2.52	0.44
1:A:83:TYR:CD1	1:A:83:TYR:C	2.91	0.44
1:E:248:TYR:CZ	1:E:252:GLN:HG3	2.52	0.44
1:E:386:PHE:CE2	1:E:414:PRO:HB2	2.53	0.44
1:F:164:VAL:HG23	1:F:188:TYR:OH	2.18	0.44
1:F:83:TYR:C	1:F:83:TYR:CD1	2.90	0.44
1:G:92:PRO:HD2	1:G:95:HIS:ND1	2.33	0.44
1:B:96:ARG:N	1:B:96:ARG:CD	2.73	0.44
1:H:30:THR:HG22	1:H:55:ALA:O	2.17	0.44
1:A:116:ASN:C	1:A:116:ASN:HD22	2.21	0.44
1:C:435:PRO:O	1:C:436:TYR:HB2	2.18	0.44
1:A:116:ASN:HD21	1:A:118:ASN:HB2	1.82	0.44
1:D:263:LYS:HB2	1:D:274:VAL:HB	1.99	0.44
1:E:245:THR:O	1:E:249:ARG:HG2	2.17	0.44
1:F:237:VAL:O	1:F:238:ASP:HB2	2.18	0.44
1:G:176:ILE:HG13	1:G:177:LEU:N	2.32	0.44
1:A:176:ILE:HG13	1:A:177:LEU:N	2.32	0.44
1:A:465:TRP:CH2	3:A:1544:BE2:N2	2.86	0.44
1:E:435:PRO:O	1:E:436:TYR:HB2	2.17	0.44
1:G:424:LYS:HG2	5:G:1557:HOH:O	2.18	0.44
1:B:212:GLY:O	1:B:215:VAL:HG22	2.16	0.43
1:B:269:GLN:CA	1:B:269:GLN:HE21	2.18	0.43
1:E:256:HIS:N	1:E:256:HIS:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:TYR:HE1	1:F:250:ASP:OD2	2.01	0.43
1:H:17:GLU:HB2	5:H:1740:HOH:O	2.16	0.43
1:C:176:ILE:HG13	1:C:177:LEU:N	2.32	0.43
1:C:256:HIS:CD2	1:C:256:HIS:N	2.86	0.43
1:C:280:LYS:HE2	5:E:1883:HOH:O	2.18	0.43
1:E:434:THR:HG21	1:F:214:TYR:CD2	2.53	0.43
1:G:320:HIS:HB3	1:G:432:THR:O	2.18	0.43
1:H:157:TYR:CE2	3:H:1546:BE2:H3	2.53	0.43
1:D:269:GLN:HA	1:D:269:GLN:NE2	2.28	0.43
1:D:424:LYS:HG2	5:D:1634:HOH:O	2.18	0.43
1:C:13:GLU:HB2	1:C:16:TYR:CD1	2.53	0.43
1:C:223[A]:HIS:CE1	1:C:227:PHE:CD1	3.05	0.43
1:E:92:PRO:HD2	1:E:95:HIS:ND1	2.33	0.43
1:H:443:ASP:HB2	1:H:444:PRO:HD3	2.00	0.43
1:B:424:LYS:HZ2	1:B:424:LYS:HB2	1.83	0.43
1:E:184:SER:HB3	5:E:1941:HOH:O	2.17	0.43
1:E:390:ALA:HB1	1:E:414:PRO:HG3	2.01	0.43
1:G:248:TYR:CZ	1:G:252:GLN:HG3	2.53	0.43
1:A:223[B]:HIS:HE1	5:A:1609:HOH:O	2.01	0.43
1:D:212:GLY:O	1:D:215:VAL:HG22	2.19	0.43
1:D:50:TYR:CE1	1:D:250:ASP:OD2	2.70	0.43
1:F:116:ASN:ND2	1:F:118:ASN:HB2	2.33	0.43
1:B:18:GLU:HB2	5:B:2085:HOH:O	2.18	0.43
1:C:102:ILE:HD13	1:C:109:LEU:HD21	2.00	0.43
1:C:443:ASP:HB2	1:C:444:PRO:HD3	1.99	0.43
1:D:223[A]:HIS:NE2	1:D:227:PHE:CE1	2.87	0.43
1:H:219:GLU:O	1:H:223[B]:HIS:CD2	2.70	0.43
1:H:83:TYR:CD1	1:H:83:TYR:C	2.92	0.43
1:B:83:TYR:C	1:B:83:TYR:CD1	2.92	0.43
1:E:120:TRP:CH2	1:E:129:LYS:HE2	2.53	0.43
1:E:263:LYS:HB2	1:E:274:VAL:HB	1.99	0.43
1:A:256:HIS:N	1:A:256:HIS:CD2	2.85	0.42
1:B:10:CYS:SG	1:B:176:ILE:HD11	2.59	0.42
1:D:390:ALA:HB1	1:D:414:PRO:HG3	2.01	0.42
1:G:83:TYR:CD1	1:G:83:TYR:C	2.92	0.42
1:B:245:THR:O	1:B:249:ARG:HG3	2.19	0.42
1:D:13:GLU:HB2	1:D:16:TYR:CD1	2.53	0.42
1:G:212:GLY:O	1:G:215:VAL:HG22	2.19	0.42
1:H:102:ILE:HD13	1:H:109:LEU:HD21	2.01	0.42
1:B:32:ASN:ND2	1:B:34:LYS:HE2	2.34	0.42
1:D:83:TYR:CD1	1:D:83:TYR:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:VAL:HB	1:E:285:VAL:CG1	2.50	0.42
1:A:386:PHE:CE2	1:A:414:PRO:HB2	2.54	0.42
1:C:137:PRO:HG3	5:C:2742:HOH:O	2.18	0.42
1:D:320:HIS:HB3	1:D:432:THR:O	2.20	0.42
1:G:237:VAL:O	1:G:238:ASP:HB2	2.18	0.42
1:H:219:GLU:OE2	1:H:463:HIS:CD2	2.58	0.42
1:C:50:TYR:CE1	1:C:250:ASP:OD2	2.70	0.42
1:E:443:ASP:HB2	1:E:444:PRO:HD3	2.00	0.42
1:G:13:GLU:HB2	1:G:16:TYR:CD1	2.54	0.42
1:A:157:TYR:CE2	3:A:1546:BE2:H3	2.54	0.42
1:B:223[A]:HIS:CE1	1:B:227:PHE:CG	3.07	0.42
1:C:386:PHE:CE2	1:C:414:PRO:HB2	2.54	0.42
1:B:102:ILE:HD13	1:B:109:LEU:HD21	2.01	0.42
1:A:434:THR:HG21	1:B:214:TYR:CD2	2.54	0.42
1:B:390:ALA:HB1	1:B:414:PRO:HG3	2.01	0.42
1:C:135:LYS:HG3	5:C:2949:HOH:O	2.19	0.42
1:D:386:PHE:CE2	1:D:414:PRO:HB2	2.55	0.42
1:E:237:VAL:O	1:E:238:ASP:HB2	2.20	0.42
1:H:435:PRO:O	1:H:436:TYR:HB2	2.19	0.42
1:C:83:TYR:CD1	1:C:83:TYR:C	2.93	0.42
1:D:280:LYS:CG	1:F:409:GLN:HB3	2.50	0.42
1:D:275:TYR:CZ	1:D:283:PRO:HB2	2.55	0.42
1:D:88:PRO:HA	4:D:523:FAD:N5	2.35	0.42
1:F:269:GLN:NE2	1:F:269:GLN:HA	2.28	0.42
1:G:157:TYR:CE2	3:G:1546:BE2:H3	2.55	0.42
1:B:176:ILE:HG13	1:B:177:LEU:N	2.34	0.42
1:B:223[A]:HIS:NE2	1:B:227:PHE:CE1	2.88	0.42
1:B:435:PRO:O	1:B:436:TYR:HB2	2.20	0.42
1:D:256:HIS:N	1:D:256:HIS:CD2	2.86	0.42
1:E:176:ILE:HG13	1:E:177:LEU:N	2.35	0.42
1:E:88:PRO:HA	4:E:524:FAD:C4X	2.50	0.42
1:C:390:ALA:HB1	1:C:414:PRO:HG3	2.01	0.41
1:E:314:HIS:HE1	1:F:210:ASP:OD1	2.02	0.41
1:G:434:THR:HG21	1:H:214:TYR:CD2	2.55	0.41
1:B:345:LYS:HE3	5:B:2288:HOH:O	2.20	0.41
1:E:402:GLN:HG3	5:E:1907:HOH:O	2.21	0.41
1:A:102:ILE:HD13	1:A:109:LEU:HD21	2.03	0.41
1:C:16:TYR:HE2	1:C:96:ARG:HG2	1.86	0.41
1:F:465:TRP:CH2	3:F:1544:BE2:N2	2.89	0.41
1:G:157:TYR:CZ	3:G:1546:BE2:H3	2.56	0.41
1:H:116:ASN:HD22	1:H:116:ASN:C	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:LEU:HA	1:E:92:PRO:HD3	1.96	0.41
1:B:386:PHE:CD1	1:B:417:ILE:HD12	2.55	0.41
1:D:386:PHE:CD1	1:D:417:ILE:HD12	2.55	0.41
1:E:116:ASN:HD22	1:E:116:ASN:C	2.24	0.41
1:F:102:ILE:HD13	1:F:109:LEU:HD21	2.03	0.41
1:B:402:GLN:HG3	5:B:2257:HOH:O	2.20	0.41
1:D:424:LYS:HD3	1:D:425:TYR:CZ	2.54	0.41
1:F:320:HIS:HB3	1:F:432:THR:O	2.21	0.41
1:H:158:GLU:O	1:H:161:LEU:HB2	2.21	0.41
1:B:171:THR:HG22	2:B:1543:NAG:H62	2.03	0.41
1:H:390:ALA:HB1	1:H:414:PRO:HG3	2.03	0.41
1:B:465:TRP:CH2	3:B:1544:BE2:N2	2.89	0.41
1:D:223[A]:HIS:CE1	1:D:227:PHE:CD1	3.09	0.41
1:G:269:GLN:HA	1:G:269:GLN:NE2	2.29	0.41
1:G:390:ALA:HB1	1:G:414:PRO:HG3	2.02	0.41
1:A:435:PRO:O	1:A:436:TYR:HB2	2.21	0.41
1:E:83:TYR:CD1	1:E:83:TYR:C	2.94	0.41
1:H:237:VAL:O	1:H:238:ASP:HB2	2.20	0.41
1:B:13:GLU:HB2	1:B:16:TYR:CD1	2.57	0.40
1:D:92:PRO:HD2	1:D:95:HIS:ND1	2.36	0.40
1:F:390:ALA:HB1	1:F:414:PRO:HG3	2.01	0.40
1:A:203:ILE:HG23	1:A:207:LEU:HD12	2.04	0.40
1:B:157:TYR:CD2	3:B:1546:BE2:H3	2.56	0.40
1:C:96:ARG:N	1:C:96:ARG:CD	2.84	0.40
1:E:207:LEU:O	3:E:1545:BE2:N2	2.53	0.40
1:H:184:SER:HB3	5:H:1718:HOH:O	2.21	0.40
1:A:345:LYS:HE3	5:A:1749:HOH:O	2.20	0.40
1:B:424:LYS:HG2	5:B:967:HOH:O	2.21	0.40
1:C:265:GLN:HG2	1:C:305:ASN:HB3	2.03	0.40
1:E:116:ASN:ND2	1:E:118:ASN:HB2	2.37	0.40
1:F:315:ALA:O	1:F:319:VAL:HG23	2.21	0.40
1:H:88:PRO:HA	4:H:527:FAD:C4X	2.51	0.40
1:A:92:PRO:HD2	1:A:95:HIS:ND1	2.36	0.40
1:G:158:GLU:O	1:G:161:LEU:HB2	2.21	0.40
1:E:441:PHE:C	1:E:444:PRO:HD2	2.41	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:OD1	1:H:106:ASP:OD1[1_655]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ARG:NH1	1:H:194:ASP:OD1[1_656]	2.15	0.05
1:C:338:ASP:OD1	1:D:132:GLU:OE2[2_546]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/498 (97%)	470 (98%)	11 (2%)	0	100	100
1	B	481/498 (97%)	466 (97%)	15 (3%)	0	100	100
1	C	481/498 (97%)	467 (97%)	14 (3%)	0	100	100
1	D	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
1	E	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
1	F	481/498 (97%)	469 (98%)	12 (2%)	0	100	100
1	G	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
1	H	481/498 (97%)	468 (97%)	13 (3%)	0	100	100
All	All	3848/3984 (97%)	3744 (97%)	104 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	414/427 (97%)	402 (97%)	12 (3%)	42	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	414/427 (97%)	400 (97%)	14 (3%)	37	36
1	C	414/427 (97%)	401 (97%)	13 (3%)	40	40
1	D	414/427 (97%)	400 (97%)	14 (3%)	37	36
1	E	414/427 (97%)	401 (97%)	13 (3%)	40	40
1	F	414/427 (97%)	400 (97%)	14 (3%)	37	36
1	G	414/427 (97%)	401 (97%)	13 (3%)	40	40
1	H	414/427 (97%)	400 (97%)	14 (3%)	37	36
All	All	3312/3416 (97%)	3205 (97%)	107 (3%)	39	38

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	115	GLU
1	A	116	ASN
1	A	139	LEU
1	A	178	ASN
1	A	208	ASN
1	A	213	TYR
1	A	250	ASP
1	A	269	GLN
1	A	305	ASN
1	A	402	GLN
1	A	424	LYS
1	B	77	ASN
1	B	103	ARG
1	B	115	GLU
1	B	116	ASN
1	B	139	LEU
1	B	178	ASN
1	B	208	ASN
1	B	213	TYR
1	B	250	ASP
1	B	269	GLN
1	B	305	ASN
1	B	314	HIS
1	B	402	GLN
1	B	424	LYS
1	C	77	ASN
1	C	115	GLU

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Mol	Chain	Res	Type
1	C	116	ASN
1	C	139	LEU
1	C	178	ASN
1	C	208	ASN
1	C	213	TYR
1	C	250	ASP
1	C	269	GLN
1	C	305	ASN
1	C	314	HIS
1	C	402	GLN
1	C	424	LYS
1	D	77	ASN
1	D	103	ARG
1	D	115	GLU
1	D	116	ASN
1	D	139	LEU
1	D	178	ASN
1	D	208	ASN
1	D	213	TYR
1	D	250	ASP
1	D	269	GLN
1	D	305	ASN
1	D	314	HIS
1	D	402	GLN
1	D	424	LYS
1	E	77	ASN
1	E	96	ARG
1	E	115	GLU
1	E	116	ASN
1	E	139	LEU
1	E	178	ASN
1	E	208	ASN
1	E	213	TYR
1	E	269	GLN
1	E	305	ASN
1	E	314	HIS
1	E	402	GLN
1	E	424	LYS
1	F	18	GLU
1	F	77	ASN
1	F	96	ARG
1	F	115	GLU

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Mol	Chain	Res	Type
1	F	116	ASN
1	F	139	LEU
1	F	178	ASN
1	F	208	ASN
1	F	213	TYR
1	F	269	GLN
1	F	305	ASN
1	F	314	HIS
1	F	402	GLN
1	F	424	LYS
1	G	77	ASN
1	G	96	ARG
1	G	115	GLU
1	G	116	ASN
1	G	139	LEU
1	G	178	ASN
1	G	208	ASN
1	G	213	TYR
1	G	269	GLN
1	G	305	ASN
1	G	314	HIS
1	G	402	GLN
1	G	424	LYS
1	H	77	ASN
1	H	96	ARG
1	H	115	GLU
1	H	116	ASN
1	H	139	LEU
1	H	178	ASN
1	H	194	ASP
1	H	208	ASN
1	H	213	TYR
1	H	269	GLN
1	H	305	ASN
1	H	314	HIS
1	H	402	GLN
1	H	424	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS

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Mol	Chain	Res	Type
1	A	57	HIS
1	A	58	GLN
1	A	77	ASN
1	A	116	ASN
1	A	118	ASN
1	A	208	ASN
1	A	256	HIS
1	A	269	GLN
1	A	305	ASN
1	A	314	HIS
1	A	382	GLN
1	A	409	GLN
1	A	439	GLN
1	A	463	HIS
1	B	35	HIS
1	B	57	HIS
1	B	58	GLN
1	B	77	ASN
1	B	116	ASN
1	B	208	ASN
1	B	256	HIS
1	B	269	GLN
1	B	305	ASN
1	B	382	GLN
1	B	409	GLN
1	B	439	GLN
1	B	463	HIS
1	C	35	HIS
1	C	57	HIS
1	C	58	GLN
1	C	77	ASN
1	C	116	ASN
1	C	118	ASN
1	C	208	ASN
1	C	256	HIS
1	C	269	GLN
1	C	305	ASN
1	C	314	HIS
1	C	342	HIS
1	C	382	GLN
1	C	409	GLN
1	C	439	GLN

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Mol	Chain	Res	Type
1	C	463	HIS
1	D	35	HIS
1	D	57	HIS
1	D	58	GLN
1	D	77	ASN
1	D	116	ASN
1	D	208	ASN
1	D	256	HIS
1	D	269	GLN
1	D	305	ASN
1	D	314	HIS
1	D	382	GLN
1	D	409	GLN
1	D	439	GLN
1	D	463	HIS
1	E	35	HIS
1	E	57	HIS
1	E	58	GLN
1	E	77	ASN
1	E	116	ASN
1	E	118	ASN
1	E	125	ASN
1	E	208	ASN
1	E	256	HIS
1	E	269	GLN
1	E	305	ASN
1	E	314	HIS
1	E	382	GLN
1	E	409	GLN
1	E	439	GLN
1	E	463	HIS
1	F	35	HIS
1	F	57	HIS
1	F	58	GLN
1	F	77	ASN
1	F	116	ASN
1	F	208	ASN
1	F	256	HIS
1	F	269	GLN
1	F	305	ASN
1	F	314	HIS
1	F	382	GLN

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Mol	Chain	Res	Type
1	F	409	GLN
1	F	439	GLN
1	F	463	HIS
1	G	35	HIS
1	G	57	HIS
1	G	58	GLN
1	G	77	ASN
1	G	116	ASN
1	G	208	ASN
1	G	256	HIS
1	G	269	GLN
1	G	305	ASN
1	G	314	HIS
1	G	382	GLN
1	G	409	GLN
1	G	463	HIS
1	H	35	HIS
1	H	57	HIS
1	H	58	GLN
1	H	77	ASN
1	H	116	ASN
1	H	208	ASN
1	H	256	HIS
1	H	269	GLN
1	H	305	ASN
1	H	314	HIS
1	H	382	GLN
1	H	409	GLN
1	H	439	GLN
1	H	463	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

40 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$
4	FAD	D	523	-	51,58,58	2.29	14 (27%)	60,89,89	1.71	10 (16%)
2	NAG	E	1543	1	14,14,15	0.57	0	17,19,21	0.74	1 (5%)
3	BE2	C	1544	-	8,10,10	1.47	1 (12%)	9,13,13	0.56	0
4	FAD	B	521	-	51,58,58	2.35	16 (31%)	60,89,89	1.73	10 (16%)
3	BE2	C	1545	-	8,10,10	1.59	2 (25%)	9,13,13	0.71	0
3	BE2	E	1545	-	8,10,10	1.66	2 (25%)	9,13,13	0.62	0
2	NAG	F	1543	1	14,14,15	0.63	0	17,19,21	0.70	0
4	FAD	G	526	-	51,58,58	2.25	15 (29%)	60,89,89	1.78	10 (16%)
3	BE2	A	1546	-	8,10,10	1.75	2 (25%)	9,13,13	0.58	0
3	BE2	A	1545	-	8,10,10	1.58	1 (12%)	9,13,13	0.66	0
2	NAG	C	1543	1	14,14,15	0.55	0	17,19,21	0.62	0
2	NAG	G	1543	1	14,14,15	0.55	0	17,19,21	0.56	0
3	BE2	D	1545	-	8,10,10	1.56	1 (12%)	9,13,13	0.75	0
3	BE2	A	1544	-	8,10,10	1.78	1 (12%)	9,13,13	0.64	0
3	BE2	F	1544	-	8,10,10	1.54	2 (25%)	9,13,13	0.65	0
4	FAD	F	525	-	51,58,58	2.29	16 (31%)	60,89,89	1.81	11 (18%)
2	NAG	D	1543	1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
3	BE2	B	1546	-	8,10,10	1.79	2 (25%)	9,13,13	0.55	0
3	BE2	H	1545	-	8,10,10	1.64	2 (25%)	9,13,13	0.61	0
3	BE2	G	1546	-	8,10,10	1.90	2 (25%)	9,13,13	0.47	0
3	BE2	D	1546	-	8,10,10	1.92	3 (37%)	9,13,13	0.54	0
3	BE2	G	1544	-	8,10,10	1.63	1 (12%)	9,13,13	0.65	0
3	BE2	B	1545	-	8,10,10	1.60	2 (25%)	9,13,13	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	1543	1	14,14,15	0.58	0	17,19,21	0.83	1 (5%)
3	BE2	B	1544	-	8,10,10	1.68	1 (12%)	9,13,13	0.57	0
3	BE2	D	1544	-	8,10,10	1.58	1 (12%)	9,13,13	0.55	0
3	BE2	E	1544	-	8,10,10	1.62	2 (25%)	9,13,13	0.57	0
3	BE2	E	1546	-	8,10,10	1.73	2 (25%)	9,13,13	0.47	0
4	FAD	A	520	-	51,58,58	2.28	14 (27%)	60,89,89	1.75	9 (15%)
3	BE2	G	1545	-	8,10,10	1.71	2 (25%)	9,13,13	0.67	0
3	BE2	C	1546	-	8,10,10	1.76	2 (25%)	9,13,13	0.50	0
4	FAD	H	527	-	51,58,58	2.38	16 (31%)	60,89,89	1.77	9 (15%)
2	NAG	A	1543	1	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
4	FAD	C	522	-	51,58,58	2.29	13 (25%)	60,89,89	1.77	10 (16%)
2	NAG	B	1543	1	14,14,15	0.59	0	17,19,21	0.88	1 (5%)
3	BE2	H	1546	-	8,10,10	1.76	2 (25%)	9,13,13	0.52	0
4	FAD	E	524	-	51,58,58	2.30	16 (31%)	60,89,89	1.83	10 (16%)
3	BE2	F	1545	-	8,10,10	1.80	2 (25%)	9,13,13	0.50	0
3	BE2	F	1546	-	8,10,10	1.65	1 (12%)	9,13,13	0.57	0
3	BE2	H	1544	-	8,10,10	1.67	1 (12%)	9,13,13	0.55	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
4	FAD	D	523	-	-	6/30/50/50	0/6/6/6
2	NAG	E	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	C	1544	-	-	0/0/4/4	0/1/1/1
4	FAD	B	521	-	-	6/30/50/50	0/6/6/6
3	BE2	C	1545	-	-	0/0/4/4	0/1/1/1
3	BE2	E	1545	-	-	0/0/4/4	0/1/1/1
2	NAG	F	1543	1	-	0/6/23/26	0/1/1/1
4	FAD	G	526	-	-	6/30/50/50	0/6/6/6
3	BE2	A	1546	-	-	0/0/4/4	0/1/1/1
3	BE2	A	1545	-	-	0/0/4/4	0/1/1/1
2	NAG	C	1543	1	-	2/6/23/26	0/1/1/1
2	NAG	G	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	D	1545	-	-	0/0/4/4	0/1/1/1
3	BE2	A	1544	-	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BE2	F	1544	-	-	0/0/4/4	0/1/1/1
4	FAD	F	525	-	-	6/30/50/50	0/6/6/6
2	NAG	D	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	B	1546	-	-	0/0/4/4	0/1/1/1
3	BE2	H	1545	-	-	0/0/4/4	0/1/1/1
3	BE2	G	1546	-	-	0/0/4/4	0/1/1/1
3	BE2	D	1546	-	-	0/0/4/4	0/1/1/1
3	BE2	G	1544	-	-	0/0/4/4	0/1/1/1
3	BE2	B	1545	-	-	0/0/4/4	0/1/1/1
2	NAG	H	1543	1	-	0/6/23/26	0/1/1/1
3	BE2	B	1544	-	-	0/0/4/4	0/1/1/1
3	BE2	D	1544	-	-	0/0/4/4	0/1/1/1
3	BE2	E	1544	-	-	0/0/4/4	0/1/1/1
3	BE2	E	1546	-	-	0/0/4/4	0/1/1/1
4	FAD	A	520	-	-	5/30/50/50	0/6/6/6
3	BE2	G	1545	-	-	0/0/4/4	0/1/1/1
3	BE2	C	1546	-	-	0/0/4/4	0/1/1/1
4	FAD	H	527	-	-	6/30/50/50	0/6/6/6
2	NAG	A	1543	1	1/1/5/7	1/6/23/26	0/1/1/1
4	FAD	C	522	-	-	6/30/50/50	0/6/6/6
2	NAG	B	1543	1	-	2/6/23/26	0/1/1/1
3	BE2	H	1546	-	-	0/0/4/4	0/1/1/1
4	FAD	E	524	-	-	5/30/50/50	0/6/6/6
3	BE2	F	1545	-	-	0/0/4/4	0/1/1/1
3	BE2	F	1546	-	-	0/0/4/4	0/1/1/1
3	BE2	H	1544	-	-	0/0/4/4	0/1/1/1

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	525	FAD	C4X-C10	9.21	1.48	1.38
4	H	527	FAD	C4X-C10	9.12	1.47	1.38
4	C	522	FAD	C4X-C10	9.05	1.47	1.38
4	E	524	FAD	C4X-C10	9.03	1.47	1.38
4	D	523	FAD	C4X-C10	8.89	1.47	1.38
4	G	526	FAD	C4X-C10	8.79	1.47	1.38
4	B	521	FAD	C4X-C10	8.75	1.47	1.38
4	A	520	FAD	C4X-C10	8.58	1.47	1.38
4	B	521	FAD	C9A-N10	5.68	1.46	1.38
4	C	522	FAD	C9A-N10	5.45	1.45	1.38
4	H	527	FAD	C9A-N10	5.38	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	525	FAD	C9A-N10	5.19	1.45	1.38
4	A	520	FAD	C9A-N10	5.11	1.45	1.38
4	E	524	FAD	C9A-N10	5.03	1.45	1.38
4	D	523	FAD	C9A-N10	4.87	1.45	1.38
4	G	526	FAD	C9A-N10	4.80	1.45	1.38
4	H	527	FAD	O4B-C1B	4.75	1.47	1.41
4	D	523	FAD	O4B-C1B	4.73	1.47	1.41
4	C	522	FAD	O4B-C1B	4.71	1.47	1.41
4	A	520	FAD	O4B-C1B	4.69	1.47	1.41
4	B	521	FAD	O4B-C1B	4.49	1.47	1.41
4	E	524	FAD	O4B-C1B	4.47	1.47	1.41
4	G	526	FAD	O4B-C1B	4.38	1.47	1.41
4	F	525	FAD	O4B-C1B	4.20	1.46	1.41
4	B	521	FAD	PA-O2A	-4.05	1.36	1.55
4	E	524	FAD	PA-O2A	-3.98	1.36	1.55
4	A	520	FAD	PA-O2A	-3.94	1.36	1.55
4	D	523	FAD	PA-O2A	-3.92	1.36	1.55
4	H	527	FAD	PA-O2A	-3.89	1.37	1.55
4	B	521	FAD	C10-N1	3.78	1.38	1.33
4	G	526	FAD	PA-O2A	-3.78	1.37	1.55
4	C	522	FAD	PA-O2A	-3.76	1.37	1.55
4	D	523	FAD	O5'-C5'	3.68	1.58	1.44
4	F	525	FAD	PA-O2A	-3.66	1.38	1.55
4	G	526	FAD	O5'-C5'	3.66	1.58	1.44
4	H	527	FAD	O5'-C5'	3.63	1.58	1.44
4	A	520	FAD	O5'-C5'	3.63	1.58	1.44
4	C	522	FAD	O5'-C5'	3.63	1.58	1.44
4	B	521	FAD	O5'-C5'	3.62	1.58	1.44
4	A	520	FAD	C10-N1	3.58	1.37	1.33
4	D	523	FAD	P-O2P	-3.57	1.38	1.55
4	E	524	FAD	O5'-C5'	3.55	1.58	1.44
4	H	527	FAD	C4-N3	3.54	1.39	1.33
4	F	525	FAD	O5'-C5'	3.47	1.58	1.44
4	F	525	FAD	C10-N1	3.46	1.37	1.33
4	A	520	FAD	C4-N3	3.44	1.39	1.33
4	H	527	FAD	C4-C4X	3.38	1.47	1.41
4	C	522	FAD	C10-N1	3.36	1.37	1.33
4	E	524	FAD	C10-N1	3.33	1.37	1.33
3	A	1544	BE2	C1-C	-3.32	1.44	1.47
4	E	524	FAD	P-O2P	-3.32	1.39	1.55
4	D	523	FAD	C4-C4X	3.30	1.47	1.41
4	F	525	FAD	P-O2P	-3.26	1.40	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	521	FAD	P-O2P	-3.25	1.40	1.55
4	A	520	FAD	P-O2P	-3.22	1.40	1.55
4	C	522	FAD	P-O2P	-3.21	1.40	1.55
4	H	527	FAD	C10-N1	3.21	1.37	1.33
4	H	527	FAD	P-O2P	-3.20	1.40	1.55
4	G	526	FAD	C4-N3	3.19	1.38	1.33
3	D	1546	BE2	C1-C	-3.11	1.44	1.47
4	G	526	FAD	P-O2P	-3.10	1.40	1.55
3	G	1545	BE2	C1-C	-3.10	1.44	1.47
4	G	526	FAD	C10-N1	3.08	1.37	1.33
4	B	521	FAD	C4-N3	3.02	1.38	1.33
4	B	521	FAD	C2-N3	2.98	1.44	1.38
3	B	1544	BE2	C1-C	-2.97	1.44	1.47
4	F	525	FAD	C4-C4X	2.97	1.46	1.41
3	G	1546	BE2	C1-C	-2.95	1.44	1.47
4	C	522	FAD	C8-C7	2.93	1.48	1.40
4	G	526	FAD	C4-C4X	2.93	1.46	1.41
3	H	1544	BE2	C1-C	-2.92	1.44	1.47
4	E	524	FAD	C4-C4X	2.90	1.46	1.41
4	F	525	FAD	C2-N3	2.86	1.43	1.38
4	D	523	FAD	C4-N3	2.86	1.38	1.33
4	A	520	FAD	C4-C4X	2.86	1.46	1.41
4	F	525	FAD	C4-N3	2.84	1.38	1.33
3	B	1546	BE2	C1-C	-2.84	1.44	1.47
4	D	523	FAD	C10-N1	2.84	1.36	1.33
3	F	1545	BE2	C1-C	-2.84	1.44	1.47
4	H	527	FAD	C8-C7	2.74	1.47	1.40
4	E	524	FAD	C8-C7	2.71	1.47	1.40
4	C	522	FAD	C4-N3	2.70	1.37	1.33
3	F	1545	BE2	C1-C2	2.68	1.47	1.40
4	B	521	FAD	C8-C7	2.67	1.47	1.40
4	H	527	FAD	C2-N3	2.66	1.43	1.38
4	E	524	FAD	C4-N3	2.66	1.37	1.33
4	D	523	FAD	C8-C7	2.66	1.47	1.40
4	C	522	FAD	C2B-C1B	-2.65	1.49	1.53
4	G	526	FAD	C2-N3	2.63	1.43	1.38
4	G	526	FAD	C8-C7	2.62	1.47	1.40
4	C	522	FAD	C4-C4X	2.61	1.45	1.41
3	D	1545	BE2	C1-C2	2.60	1.46	1.40
3	G	1544	BE2	C1-C	-2.58	1.44	1.47
3	D	1544	BE2	C1-C	-2.57	1.45	1.47
4	A	520	FAD	C8-C7	2.56	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	525	FAD	C8-C7	2.55	1.47	1.40
4	H	527	FAD	C2B-C1B	-2.53	1.49	1.53
4	H	527	FAD	C5X-N5	2.51	1.39	1.35
4	B	521	FAD	C4-C4X	2.49	1.45	1.41
3	C	1546	BE2	C1-C	-2.48	1.45	1.47
4	B	521	FAD	C2A-N3A	2.47	1.36	1.32
4	E	524	FAD	C2B-C1B	-2.47	1.50	1.53
4	A	520	FAD	C2A-N3A	2.44	1.36	1.32
4	A	520	FAD	C2-N3	2.41	1.42	1.38
4	E	524	FAD	C2-N3	2.41	1.42	1.38
3	H	1546	BE2	C1-C	-2.40	1.45	1.47
4	H	527	FAD	C4X-N5	2.40	1.36	1.33
3	E	1544	BE2	C1-C	-2.38	1.45	1.47
4	D	523	FAD	C2-N3	2.38	1.42	1.38
4	E	524	FAD	C5X-N5	2.38	1.39	1.35
4	G	526	FAD	C2A-N3A	2.38	1.35	1.32
3	E	1546	BE2	C1-C2	2.37	1.46	1.40
3	C	1544	BE2	C1-C	-2.35	1.45	1.47
4	C	522	FAD	C2-N3	2.35	1.42	1.38
4	B	521	FAD	C2-N1	-2.35	1.33	1.38
4	B	521	FAD	C2B-C1B	-2.34	1.50	1.53
3	E	1545	BE2	C1-C2	2.33	1.46	1.40
4	F	525	FAD	C4A-N3A	2.33	1.38	1.35
3	H	1545	BE2	C1-C	-2.32	1.45	1.47
3	A	1545	BE2	C1-C2	2.29	1.46	1.40
3	D	1546	BE2	C6-C1	2.28	1.43	1.40
3	G	1546	BE2	C6-C1	2.27	1.43	1.40
4	B	521	FAD	C2A-N1A	2.27	1.38	1.33
4	G	526	FAD	C2B-C1B	-2.27	1.50	1.53
4	E	524	FAD	C2A-N3A	2.25	1.35	1.32
3	C	1545	BE2	C1-C	-2.25	1.45	1.47
4	F	525	FAD	C2A-N3A	2.24	1.35	1.32
3	C	1546	BE2	C1-C2	2.21	1.45	1.40
3	H	1545	BE2	C1-C2	2.20	1.45	1.40
4	E	524	FAD	C4A-N3A	2.19	1.38	1.35
4	D	523	FAD	C2B-C1B	-2.19	1.50	1.53
4	A	520	FAD	C5X-N5	2.17	1.38	1.35
3	A	1546	BE2	C6-C1	2.17	1.43	1.40
3	D	1546	BE2	C4-C3	2.17	1.43	1.38
3	E	1544	BE2	C1-C2	2.16	1.45	1.40
4	F	525	FAD	C2B-C1B	-2.16	1.50	1.53
3	F	1544	BE2	C1-C	-2.16	1.45	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1546	BE2	C1-C2	2.15	1.45	1.40
3	H	1546	BE2	C6-C1	2.14	1.43	1.40
3	F	1546	BE2	C1-C	-2.14	1.45	1.47
3	B	1545	BE2	C1-C	-2.14	1.45	1.47
4	H	527	FAD	C2A-N3A	2.13	1.35	1.32
4	B	521	FAD	P-O5'	-2.12	1.50	1.59
4	D	523	FAD	C2A-N3A	2.12	1.35	1.32
3	E	1545	BE2	C1-C	-2.12	1.45	1.47
3	C	1545	BE2	C1-C2	2.12	1.45	1.40
4	F	525	FAD	C2-N1	-2.11	1.34	1.38
3	B	1546	BE2	C1-C2	2.08	1.45	1.40
4	D	523	FAD	C5X-N5	2.07	1.38	1.35
3	G	1545	BE2	C1-C2	2.06	1.45	1.40
4	A	520	FAD	C4A-N3A	2.06	1.38	1.35
3	E	1546	BE2	C6-C1	2.05	1.43	1.40
4	E	524	FAD	C2-N1	-2.04	1.34	1.38
3	B	1545	BE2	C1-C2	2.04	1.45	1.40
4	C	522	FAD	C2A-N3A	2.04	1.35	1.32
4	G	526	FAD	C2-N1	-2.03	1.34	1.38
4	F	525	FAD	P-O5'	-2.02	1.51	1.59
4	H	527	FAD	C4A-N3A	2.02	1.38	1.35
3	F	1544	BE2	C5-C6	2.01	1.43	1.38
4	G	526	FAD	C4A-N3A	2.00	1.38	1.35

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	524	FAD	C4-N3-C2	8.48	122.30	115.14
4	F	525	FAD	C4-N3-C2	8.20	122.07	115.14
4	H	527	FAD	C4-N3-C2	7.94	121.84	115.14
4	C	522	FAD	C4-N3-C2	7.89	121.80	115.14
4	G	526	FAD	C4-N3-C2	7.77	121.70	115.14
4	A	520	FAD	C4-N3-C2	7.68	121.63	115.14
4	B	521	FAD	C4-N3-C2	7.54	121.50	115.14
4	D	523	FAD	C4-N3-C2	7.27	121.28	115.14
4	H	527	FAD	C4X-C4-N3	-4.79	116.88	123.43
4	G	526	FAD	C4X-C4-N3	-4.77	116.91	123.43
4	E	524	FAD	C4X-C4-N3	-4.71	116.99	123.43
4	F	525	FAD	C4X-C4-N3	-4.69	117.01	123.43
4	A	520	FAD	C4X-C4-N3	-4.59	117.16	123.43
4	B	521	FAD	C4X-C4-N3	-4.59	117.16	123.43
4	C	522	FAD	C4X-C4-N3	-4.56	117.20	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	523	FAD	C4X-C4-N3	-4.55	117.20	123.43
4	G	526	FAD	C5'-C4'-C3'	-3.41	105.61	112.20
4	E	524	FAD	C5'-C4'-C3'	-3.40	105.63	112.20
4	C	522	FAD	C5'-C4'-C3'	-3.34	105.76	112.20
4	F	525	FAD	C5'-C4'-C3'	-3.31	105.80	112.20
4	A	520	FAD	O4B-C1B-C2B	-3.28	102.13	106.93
4	H	527	FAD	C5'-C4'-C3'	-3.25	105.92	112.20
4	B	521	FAD	C5'-C4'-C3'	-3.21	106.01	112.20
4	F	525	FAD	O4B-C1B-C2B	-3.17	102.29	106.93
4	G	526	FAD	O4B-C1B-C2B	-3.16	102.30	106.93
4	H	527	FAD	C4-C4X-C10	-3.15	117.86	119.95
4	D	523	FAD	C4-C4X-C10	-3.13	117.88	119.95
4	C	522	FAD	C4-C4X-C10	-3.12	117.89	119.95
4	F	525	FAD	C4-C4X-C10	-3.10	117.90	119.95
4	B	521	FAD	C4-C4X-C10	-3.10	117.90	119.95
4	A	520	FAD	C5'-C4'-C3'	-3.05	106.32	112.20
4	E	524	FAD	C4-C4X-C10	-2.93	118.01	119.95
4	D	523	FAD	C5'-C4'-C3'	-2.92	106.57	112.20
4	A	520	FAD	C4-C4X-C10	-2.92	118.02	119.95
4	H	527	FAD	O4B-C1B-C2B	-2.86	102.74	106.93
4	E	524	FAD	O5B-PA-O1A	-2.84	97.96	109.07
4	H	527	FAD	O5B-PA-O1A	-2.78	98.22	109.07
4	E	524	FAD	O4B-C1B-C2B	-2.77	102.88	106.93
4	F	525	FAD	C5A-C6A-N1A	-2.75	114.13	120.35
4	C	522	FAD	O5B-PA-O1A	-2.72	98.42	109.07
4	G	526	FAD	O5B-PA-O1A	-2.66	98.68	109.07
4	B	521	FAD	O4B-C1B-C2B	-2.62	103.09	106.93
4	A	520	FAD	O5B-PA-O1A	-2.62	98.82	109.07
4	D	523	FAD	O4B-C1B-C2B	-2.62	103.10	106.93
4	F	525	FAD	O5B-PA-O1A	-2.59	98.96	109.07
4	G	526	FAD	C4-C4X-C10	-2.59	118.24	119.95
4	D	523	FAD	O5B-PA-O1A	-2.58	98.99	109.07
4	C	522	FAD	O4B-C1B-C2B	-2.58	103.16	106.93
4	C	522	FAD	C5A-C6A-N6A	2.57	124.25	120.35
4	G	526	FAD	C5A-C6A-N1A	-2.55	114.57	120.35
4	H	527	FAD	C5A-C6A-N1A	-2.54	114.60	120.35
4	D	523	FAD	C2A-N1A-C6A	2.54	123.09	118.75
4	D	523	FAD	C5A-C6A-N1A	-2.52	114.64	120.35
4	B	521	FAD	O5B-PA-O1A	-2.51	99.24	109.07
4	B	521	FAD	C5A-C6A-N1A	-2.50	114.69	120.35
4	A	520	FAD	C5A-C6A-N1A	-2.50	114.69	120.35
4	B	521	FAD	C5A-C6A-N6A	2.49	124.14	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	520	FAD	C5A-C6A-N6A	2.49	124.13	120.35
4	H	527	FAD	C5A-C6A-N6A	2.48	124.12	120.35
4	E	524	FAD	C5A-C6A-N1A	-2.44	114.81	120.35
4	C	522	FAD	C5A-C6A-N1A	-2.44	114.81	120.35
4	G	526	FAD	C5A-C6A-N6A	2.43	124.05	120.35
4	H	527	FAD	C2A-N1A-C6A	2.40	122.86	118.75
4	D	523	FAD	C5A-C6A-N6A	2.37	123.95	120.35
2	D	1543	NAG	C2-N2-C7	-2.35	119.55	122.90
4	E	524	FAD	C2A-N1A-C6A	2.35	122.77	118.75
4	C	522	FAD	C2A-N1A-C6A	2.35	122.77	118.75
4	B	521	FAD	C2A-N1A-C6A	2.32	122.72	118.75
4	C	522	FAD	C5X-C9A-N10	-2.31	116.04	117.72
4	A	520	FAD	C2A-N1A-C6A	2.31	122.70	118.75
4	F	525	FAD	C2A-N1A-C6A	2.30	122.69	118.75
2	H	1543	NAG	C2-N2-C7	-2.28	119.65	122.90
4	E	524	FAD	C5X-C9A-N10	-2.25	116.08	117.72
4	E	524	FAD	C5A-C6A-N6A	2.23	123.74	120.35
4	G	526	FAD	C5X-C9A-N10	-2.22	116.11	117.72
4	G	526	FAD	C2A-N1A-C6A	2.22	122.54	118.75
4	F	525	FAD	C5A-C6A-N6A	2.21	123.71	120.35
2	B	1543	NAG	C2-N2-C7	-2.16	119.82	122.90
4	F	525	FAD	C5X-C9A-N10	-2.12	116.18	117.72
4	D	523	FAD	C5X-C9A-N10	-2.12	116.18	117.72
4	F	525	FAD	C1'-N10-C10	2.07	120.27	118.41
4	B	521	FAD	O5'-P-O1P	-2.07	100.99	109.07
2	E	1543	NAG	C2-N2-C7	-2.07	119.96	122.90
2	A	1543	NAG	O5-C1-C2	-2.06	108.03	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1543	NAG	C1

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	523	FAD	PA-O3P-P-O5'
4	B	521	FAD	PA-O3P-P-O5'
4	G	526	FAD	PA-O3P-P-O5'
4	F	525	FAD	PA-O3P-P-O5'
4	A	520	FAD	PA-O3P-P-O5'
4	H	527	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
4	C	522	FAD	PA-O3P-P-O5'
2	C	1543	NAG	C4-C5-C6-O6
4	D	523	FAD	O3'-C3'-C4'-O4'
2	C	1543	NAG	O5-C5-C6-O6
4	D	523	FAD	O3'-C3'-C4'-C5'
4	G	526	FAD	O3'-C3'-C4'-C5'
4	D	523	FAD	C2'-C3'-C4'-O4'
2	A	1543	NAG	O5-C5-C6-O6
4	F	525	FAD	O3'-C3'-C4'-C5'
4	D	523	FAD	C2'-C3'-C4'-C5'
2	B	1543	NAG	C4-C5-C6-O6
4	G	526	FAD	C2'-C3'-C4'-O4'
4	F	525	FAD	C2'-C3'-C4'-O4'
4	B	521	FAD	O3'-C3'-C4'-C5'
4	G	526	FAD	C2'-C3'-C4'-C5'
4	E	524	FAD	PA-O3P-P-O5'
4	F	525	FAD	C2'-C3'-C4'-C5'
4	B	521	FAD	C2'-C3'-C4'-O4'
4	H	527	FAD	C2'-C3'-C4'-O4'
4	C	522	FAD	C2'-C3'-C4'-O4'
4	A	520	FAD	O3'-C3'-C4'-C5'
4	H	527	FAD	O3'-C3'-C4'-C5'
4	C	522	FAD	O3'-C3'-C4'-C5'
4	G	526	FAD	O3'-C3'-C4'-O4'
4	F	525	FAD	O3'-C3'-C4'-O4'
4	A	520	FAD	C2'-C3'-C4'-O4'
4	B	521	FAD	O3'-C3'-C4'-O4'
4	A	520	FAD	O3'-C3'-C4'-O4'
2	B	1543	NAG	O5-C5-C6-O6
4	E	524	FAD	O3'-C3'-C4'-C5'
4	C	522	FAD	O4B-C4B-C5B-O5B
4	E	524	FAD	C2'-C3'-C4'-O4'
4	H	527	FAD	O3'-C3'-C4'-O4'
4	C	522	FAD	O3'-C3'-C4'-O4'
4	E	524	FAD	O3'-C3'-C4'-O4'
4	B	521	FAD	C2'-C3'-C4'-C5'
4	C	522	FAD	C2'-C3'-C4'-C5'
4	B	521	FAD	O4B-C4B-C5B-O5B
4	G	526	FAD	O4B-C4B-C5B-O5B
4	F	525	FAD	O4B-C4B-C5B-O5B
4	A	520	FAD	O4B-C4B-C5B-O5B
4	H	527	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	E	524	FAD	O4B-C4B-C5B-O5B
4	D	523	FAD	O4B-C4B-C5B-O5B
4	H	527	FAD	C2'-C3'-C4'-C5'

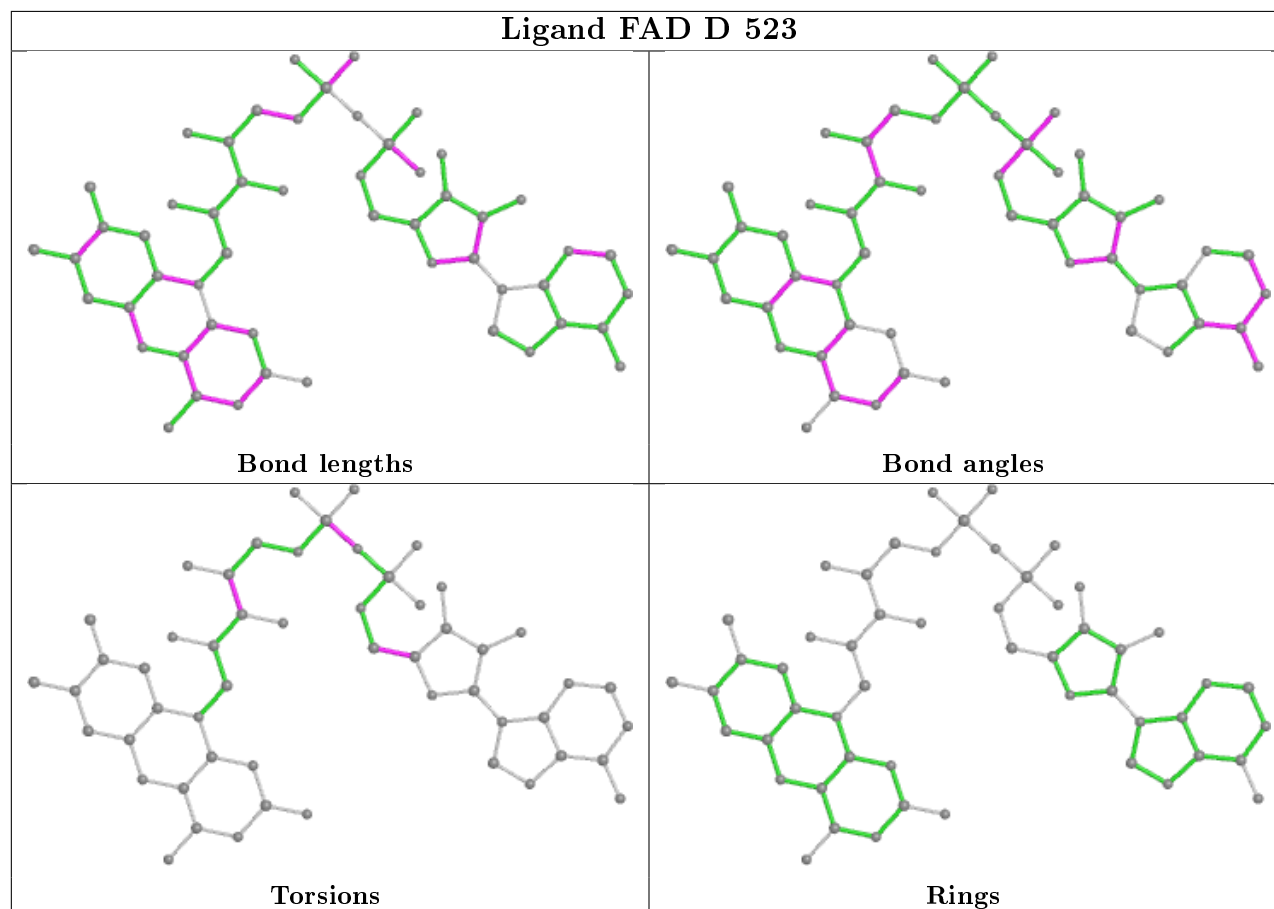
There are no ring outliers.

24 monomers are involved in 36 short contacts:

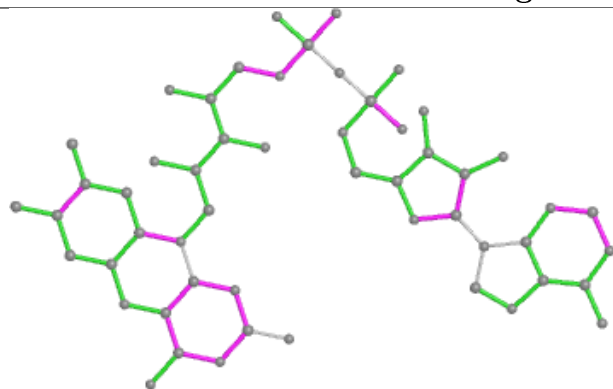
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	523	FAD	1	0
3	C	1544	BE2	2	0
3	C	1545	BE2	2	0
3	E	1545	BE2	1	0
4	G	526	FAD	1	0
3	A	1546	BE2	1	0
3	D	1545	BE2	1	0
3	A	1544	BE2	1	0
3	F	1544	BE2	1	0
3	B	1546	BE2	1	0
3	G	1546	BE2	2	0
3	D	1546	BE2	1	0
3	G	1544	BE2	4	0
3	B	1545	BE2	2	0
3	B	1544	BE2	1	0
3	D	1544	BE2	1	0
3	E	1544	BE2	1	0
3	G	1545	BE2	6	0
4	H	527	FAD	1	0
2	B	1543	NAG	1	0
3	H	1546	BE2	1	0
4	E	524	FAD	1	0
3	F	1545	BE2	3	0
3	H	1544	BE2	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

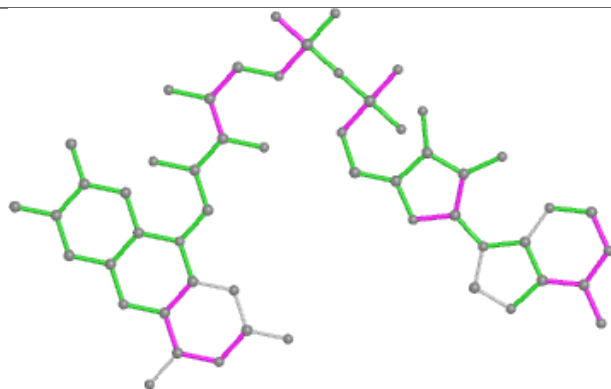
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



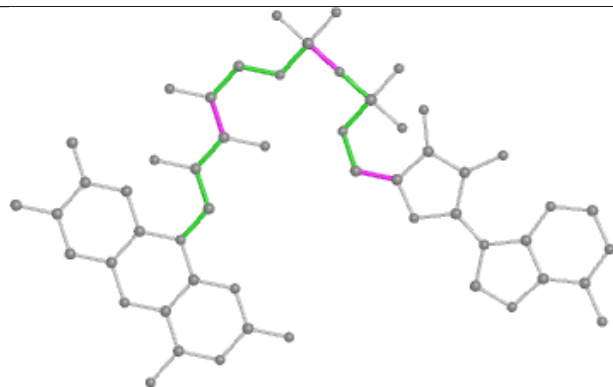
Ligand FAD B 521



Bond lengths



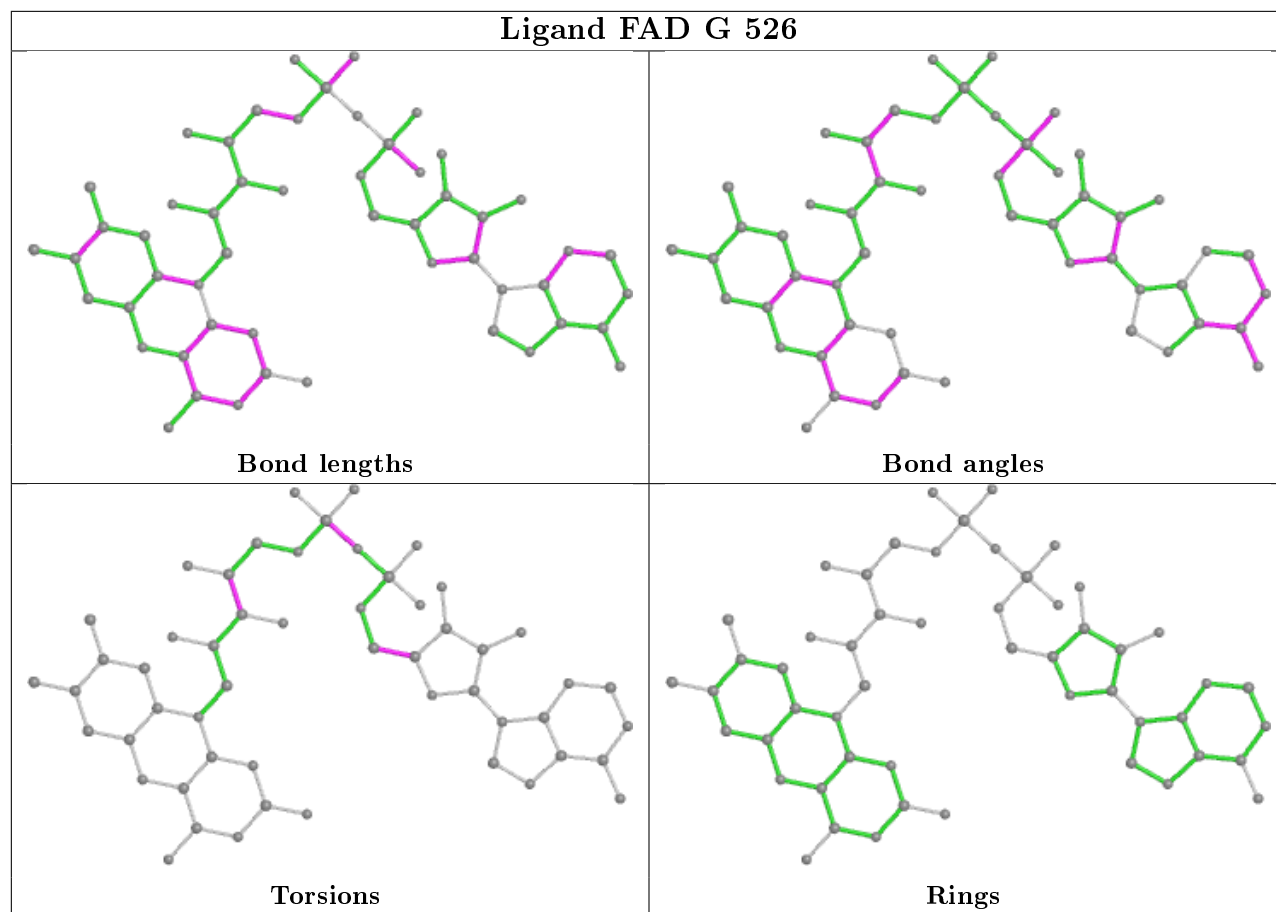
Bond angles



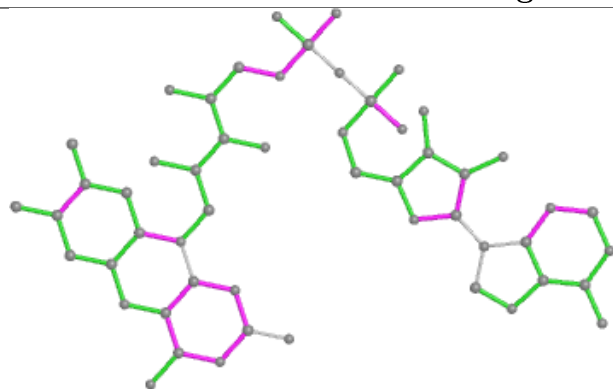
Torsions



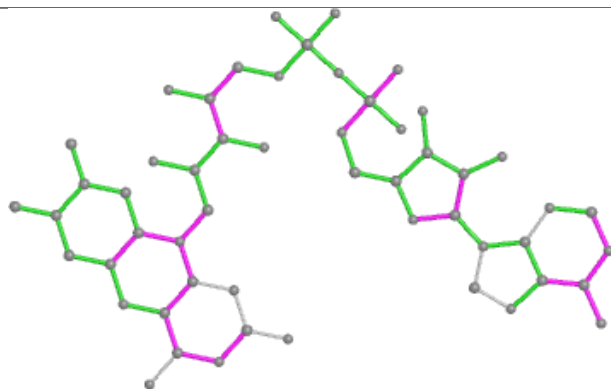
Rings



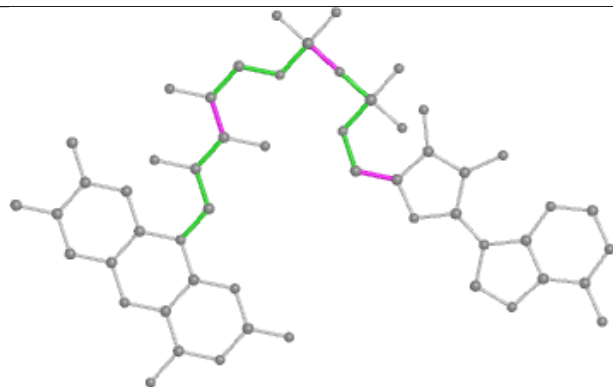
Ligand FAD F 525



Bond lengths



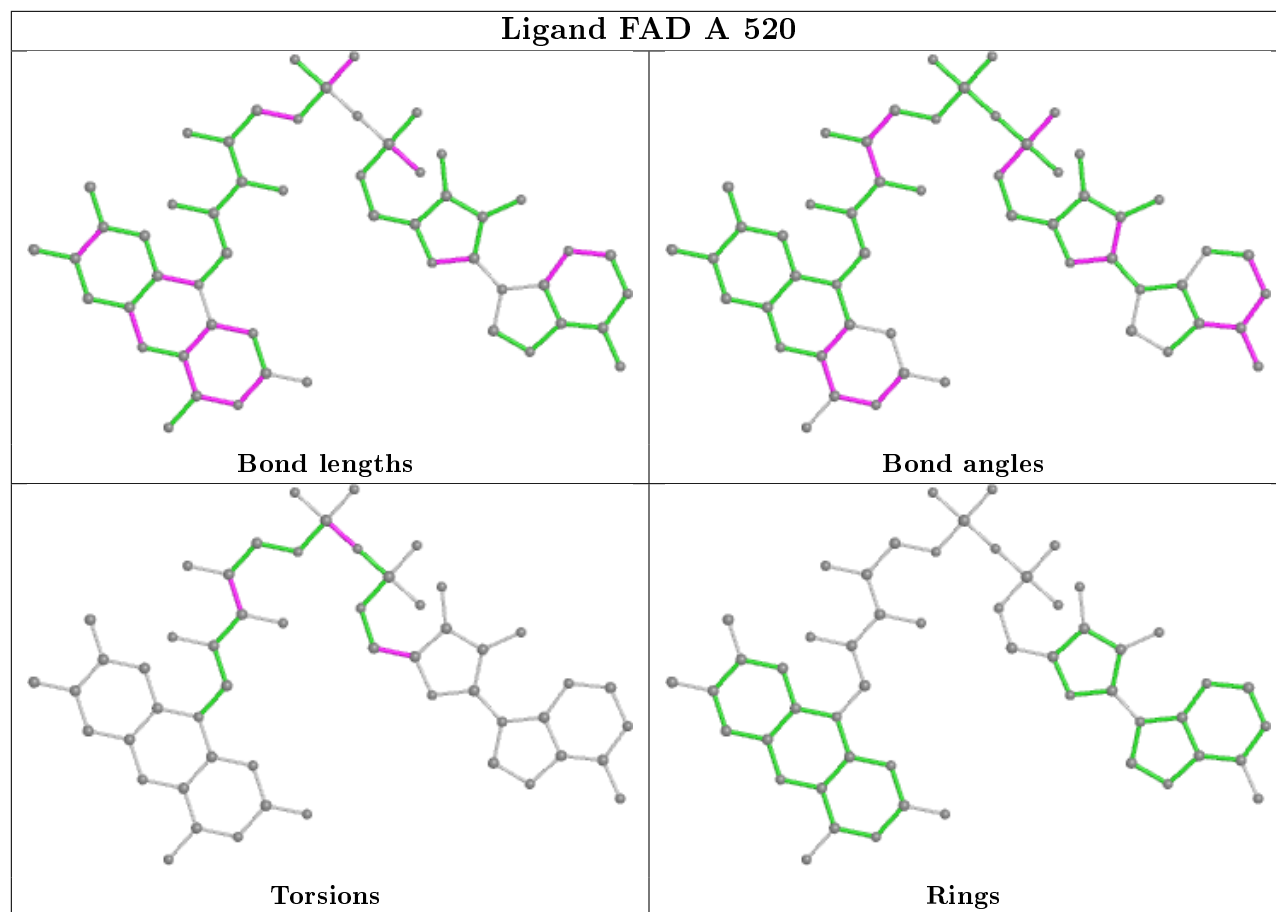
Bond angles

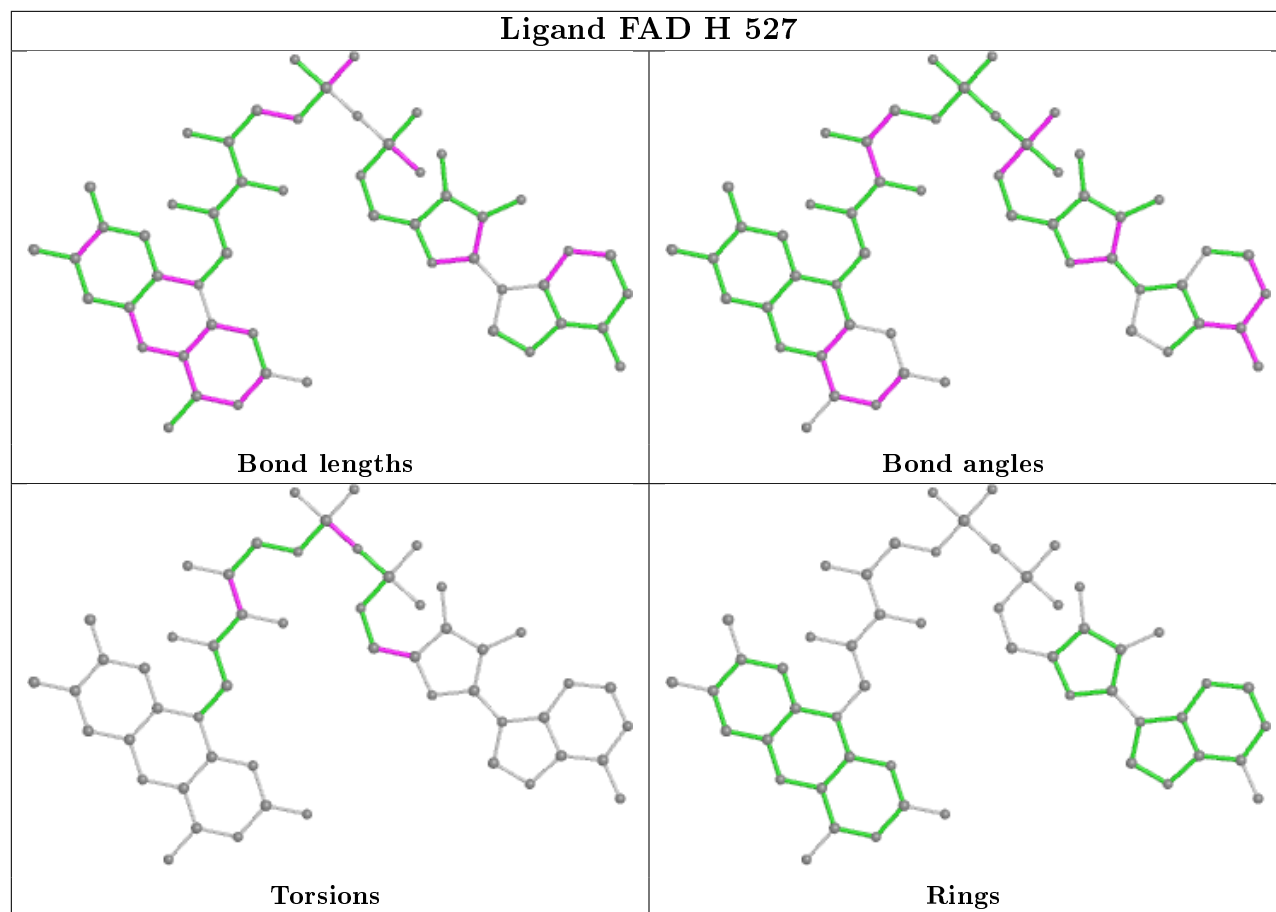


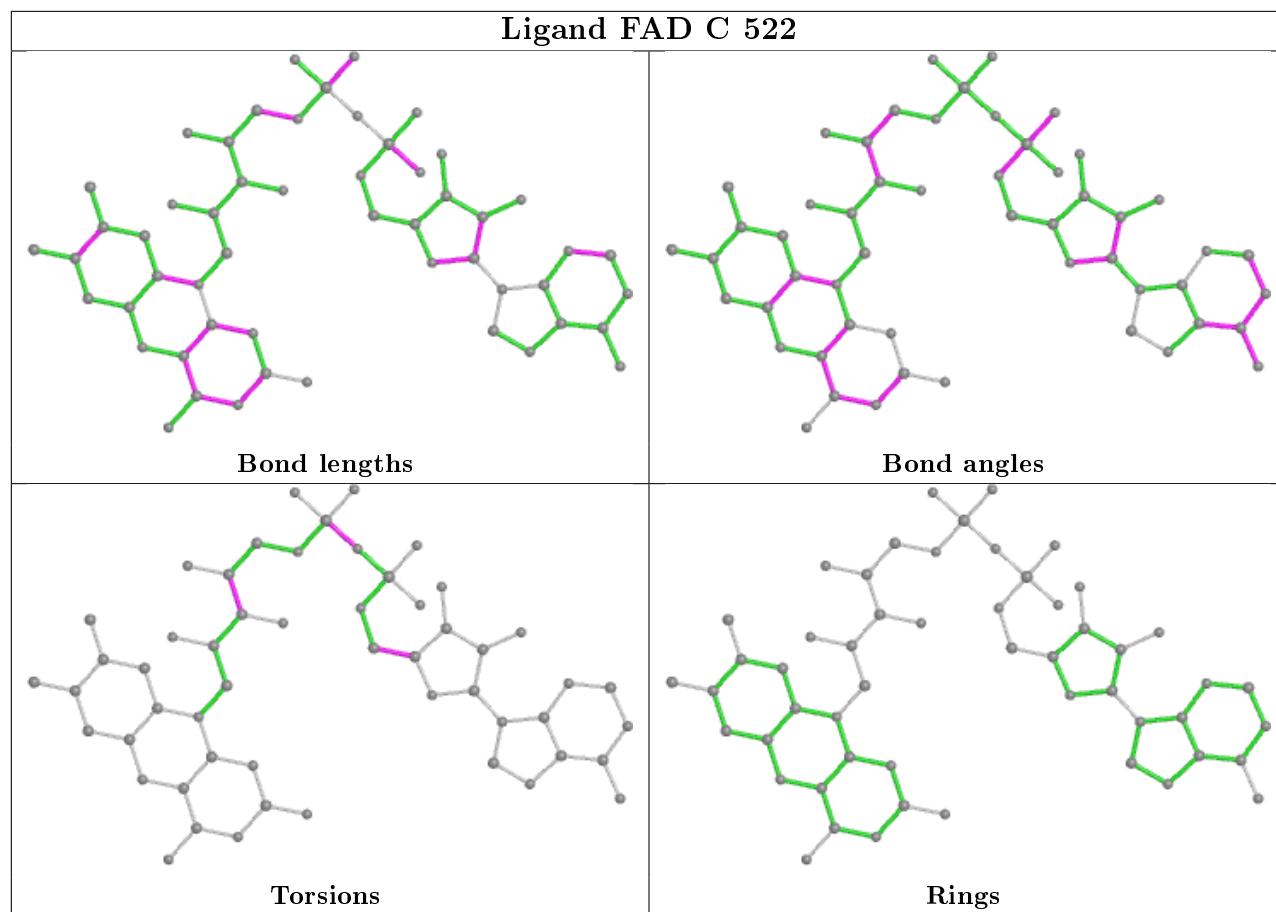
Torsions

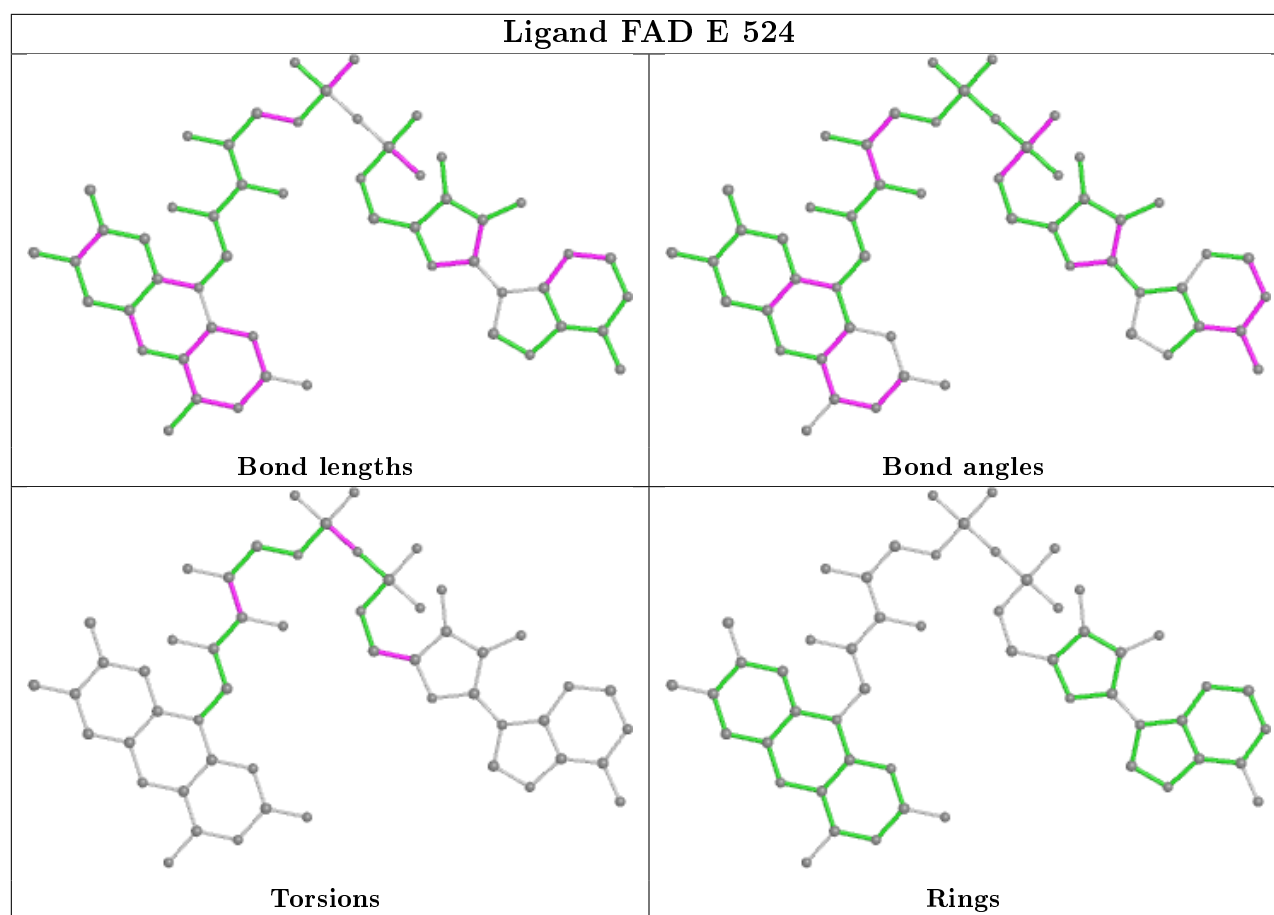


Rings









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	482/498 (96%)	-0.09	16 (3%)	46	45	8, 17, 32, 52	0
1	B	482/498 (96%)	-0.28	15 (3%)	49	48	9, 17, 31, 52	0
1	C	482/498 (96%)	-0.27	9 (1%)	66	65	8, 16, 31, 52	0
1	D	482/498 (96%)	-0.06	10 (2%)	63	62	8, 17, 31, 52	0
1	E	482/498 (96%)	-0.20	18 (3%)	41	41	10, 18, 32, 52	0
1	F	482/498 (96%)	-0.26	17 (3%)	44	43	10, 18, 31, 52	0
1	G	482/498 (96%)	-0.19	12 (2%)	57	56	10, 18, 31, 52	0
1	H	482/498 (96%)	-0.05	23 (4%)	30	29	10, 19, 32, 52	0
All	All	3856/3984 (96%)	-0.17	120 (3%)	49	48	8, 17, 31, 52	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	486	ASN	10.7
1	E	486	ASN	8.3
1	A	363	THR	7.6
1	D	363	THR	7.3
1	G	486	ASN	6.7
1	B	486	ASN	6.6
1	C	486	ASN	5.7
1	F	486	ASN	5.7
1	B	363	THR	5.4
1	C	31	SER	5.2
1	A	486	ASN	5.2
1	D	126	ILE	5.0
1	G	146	PRO	4.7
1	H	194	ASP	4.7
1	G	363	THR	4.5
1	D	486	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	194	ASP	4.4
1	G	194	ASP	4.3
1	C	363	THR	4.1
1	A	78	GLU	3.9
1	H	17	GLU	3.8
1	E	485	GLU	3.8
1	B	268	ASP	3.8
1	A	194	ASP	3.7
1	F	363	THR	3.7
1	C	250	ASP	3.6
1	E	17	GLU	3.6
1	D	194	ASP	3.5
1	H	103	ARG	3.5
1	H	31	SER	3.5
1	E	194	ASP	3.5
1	H	32	ASN	3.5
1	H	108	ARG	3.3
1	A	146	PRO	3.2
1	B	31	SER	3.2
1	A	14	ASN	3.2
1	F	32	ASN	3.1
1	H	12	GLN	3.1
1	F	485	GLU	3.1
1	E	96	ARG	3.0
1	F	269	GLN	3.0
1	H	55	ALA	3.0
1	F	28	LYS	3.0
1	B	96	ARG	2.9
1	H	96	ARG	2.9
1	H	170	ARG	2.9
1	H	482	LEU	2.9
1	G	249	ARG	2.8
1	G	223[A]	HIS	2.8
1	H	268	ASP	2.8
1	D	78	GLU	2.8
1	A	96	ARG	2.8
1	E	31	SER	2.8
1	E	32	ASN	2.7
1	G	147	SER	2.7
1	E	363	THR	2.7
1	H	269	GLN	2.7
1	F	249	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	30	THR	2.7
1	F	268	ASP	2.7
1	B	103	ARG	2.7
1	E	108	ARG	2.6
1	C	249	ARG	2.6
1	F	31	SER	2.6
1	D	250	ASP	2.6
1	H	166	GLU	2.6
1	H	363	THR	2.5
1	B	146	PRO	2.5
1	G	170	ARG	2.5
1	B	250	ASP	2.5
1	H	28	LYS	2.5
1	D	170	ARG	2.4
1	E	269	GLN	2.4
1	F	78	GLU	2.4
1	E	12	GLN	2.4
1	F	103	ARG	2.4
1	G	103	ARG	2.4
1	B	249	ARG	2.4
1	B	361	ASN	2.4
1	C	78	GLU	2.4
1	B	32	ASN	2.3
1	F	146	PRO	2.3
1	G	78	GLU	2.3
1	H	171	THR	2.3
1	E	103	ARG	2.3
1	D	268	ASP	2.3
1	G	268	ASP	2.3
1	A	108	ARG	2.3
1	C	103	ARG	2.3
1	A	197	PRO	2.3
1	A	155	GLN	2.3
1	B	170	ARG	2.3
1	H	485	GLU	2.2
1	A	269	GLN	2.2
1	E	33	PRO	2.2
1	F	223[A]	HIS	2.2
1	A	17	GLU	2.2
1	F	79	GLU	2.2
1	G	79	GLU	2.2
1	E	29	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	484	SER	2.2
1	B	6	PRO	2.1
1	H	146	PRO	2.1
1	C	485	GLU	2.1
1	E	268	ASP	2.1
1	B	108	ARG	2.1
1	H	169	LYS	2.1
1	D	103	ARG	2.1
1	A	144	VAL	2.1
1	A	169	LYS	2.1
1	F	96	ARG	2.1
1	A	223[A]	HIS	2.1
1	A	103	ARG	2.1
1	D	96	ARG	2.0
1	B	17	GLU	2.0
1	E	170	ARG	2.0
1	C	96	ARG	2.0
1	E	171	THR	2.0
1	F	108	ARG	2.0
1	H	249	ARG	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 monosaccharides 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(Å ²)	Q<0.9
3	BE2	E	1545	10/10	0.40	0.40	57,57,57,57	0
3	BE2	G	1545	10/10	0.45	0.56	53,54,54,55	0
3	BE2	H	1545	10/10	0.54	0.34	57,57,57,57	0

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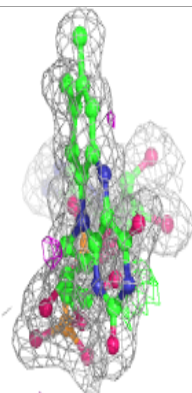
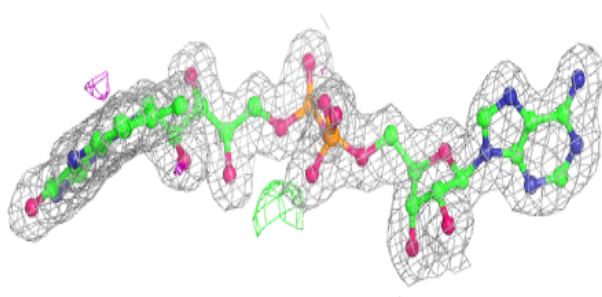
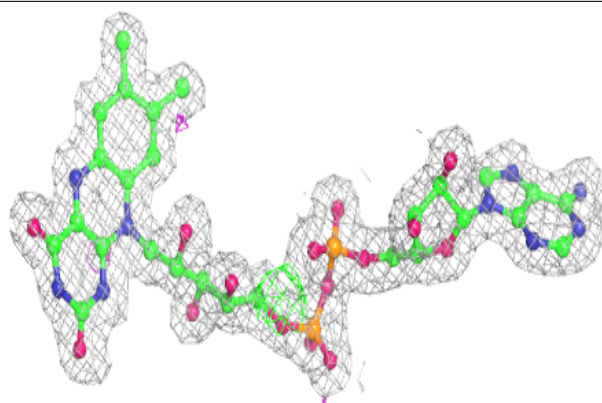
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BE2	A	1545	10/10	0.59	0.33	48,49,49,49	0
2	NAG	A	1543	14/15	0.59	0.41	42,45,48,48	0
3	BE2	H	1544	10/10	0.61	0.29	43,43,44,44	0
3	BE2	E	1544	10/10	0.63	0.30	46,46,46,47	0
3	BE2	B	1545	10/10	0.63	0.28	42,43,43,44	0
3	BE2	D	1546	10/10	0.65	0.24	38,40,40,41	0
3	BE2	A	1546	10/10	0.65	0.23	47,47,48,48	0
3	BE2	D	1545	10/10	0.66	0.31	40,40,41,42	0
3	BE2	C	1545	10/10	0.66	0.25	42,43,43,44	0
3	BE2	F	1546	10/10	0.67	0.18	42,42,42,43	0
3	BE2	C	1544	10/10	0.67	0.20	34,35,35,36	0
3	BE2	F	1545	10/10	0.70	0.40	51,51,52,53	0
3	BE2	E	1546	10/10	0.71	0.23	47,48,48,48	0
3	BE2	G	1546	10/10	0.71	0.18	39,39,40,40	0
3	BE2	H	1546	10/10	0.72	0.23	49,49,50,50	0
3	BE2	C	1546	10/10	0.73	0.18	42,42,43,43	0
3	BE2	F	1544	10/10	0.73	0.23	33,34,35,35	0
3	BE2	G	1544	10/10	0.75	0.25	38,39,39,39	0
2	NAG	H	1543	14/15	0.76	0.26	37,39,40,41	0
2	NAG	D	1543	14/15	0.76	0.18	35,38,40,40	0
2	NAG	F	1543	14/15	0.77	0.17	34,36,37,39	0
3	BE2	B	1544	10/10	0.77	0.22	34,35,35,35	0
3	BE2	D	1544	10/10	0.77	0.23	30,31,32,32	0
2	NAG	G	1543	14/15	0.78	0.16	29,31,32,33	0
2	NAG	E	1543	14/15	0.78	0.27	37,40,43,43	0
2	NAG	C	1543	14/15	0.78	0.18	31,33,37,38	0
2	NAG	B	1543	14/15	0.80	0.16	33,35,37,38	0
3	BE2	A	1544	10/10	0.81	0.25	33,33,34,34	0
3	BE2	B	1546	10/10	0.88	0.19	47,48,48,48	0
4	FAD	H	527	53/53	0.96	0.09	11,14,16,17	0
4	FAD	D	523	53/53	0.97	0.10	6,8,10,11	0
4	FAD	E	524	53/53	0.97	0.08	10,12,14,15	0
4	FAD	F	525	53/53	0.97	0.07	8,10,12,13	0
4	FAD	A	520	53/53	0.97	0.11	7,9,10,10	0
4	FAD	G	526	53/53	0.97	0.08	9,10,11,12	0
4	FAD	B	521	53/53	0.98	0.07	6,8,10,11	0
4	FAD	C	522	53/53	0.98	0.08	4,8,9,10	0

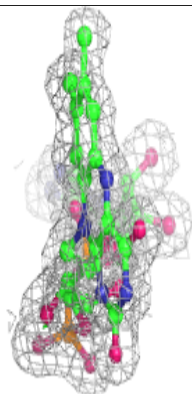
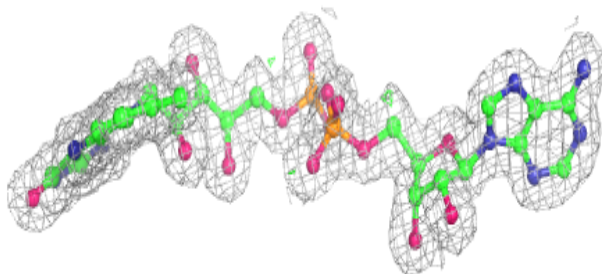
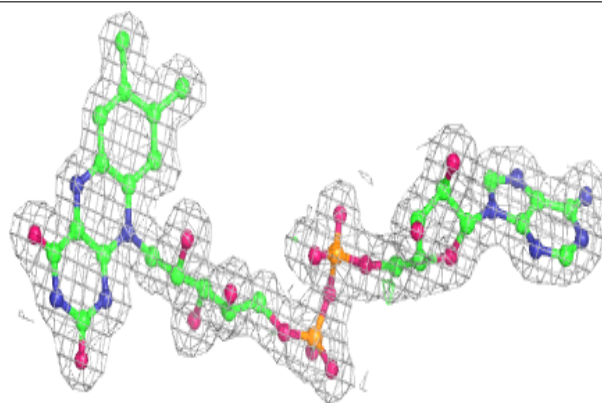
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD H 527:

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

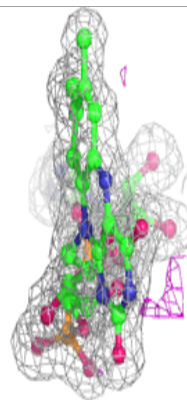
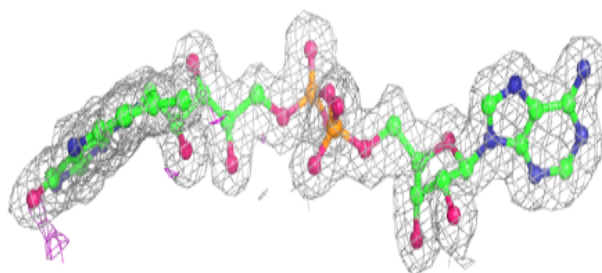
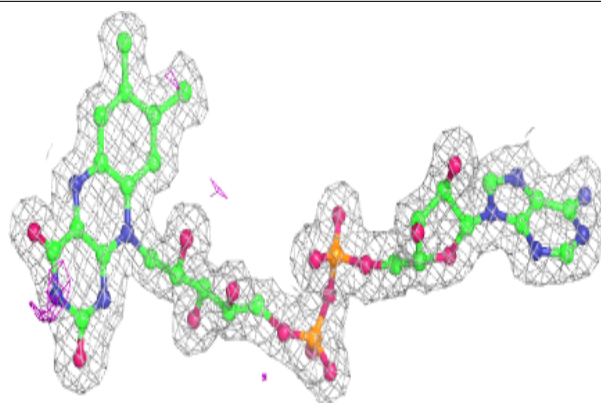
**Electron density around FAD D 523:**

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

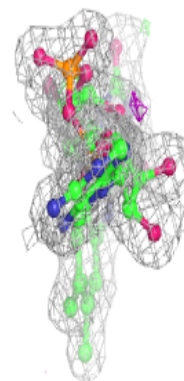
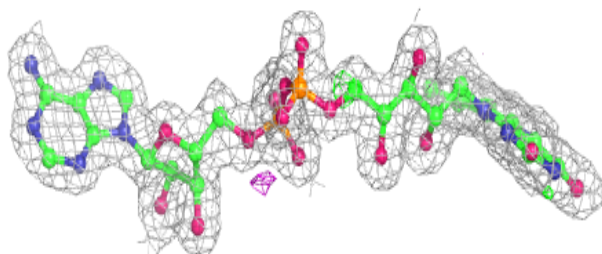
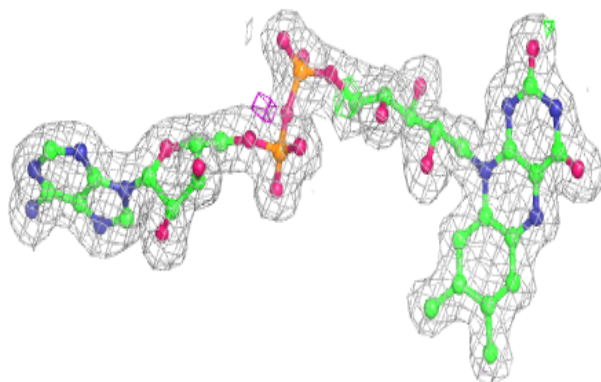


Electron density around FAD E 524:

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

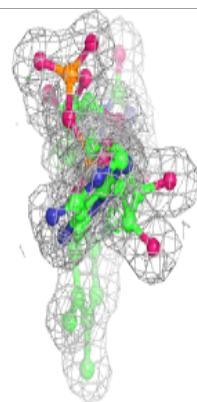
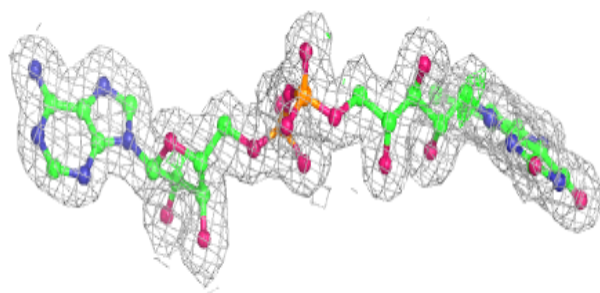
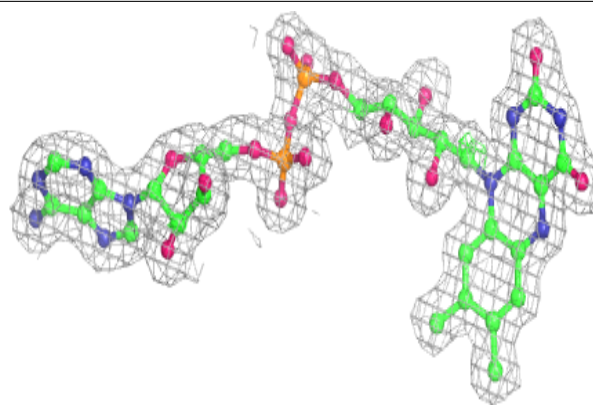
**Electron density around FAD F 525:**

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

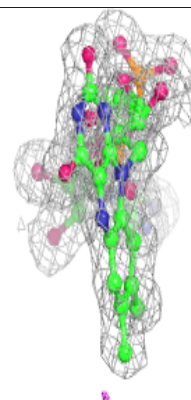
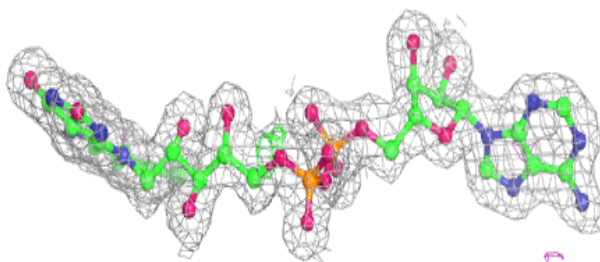
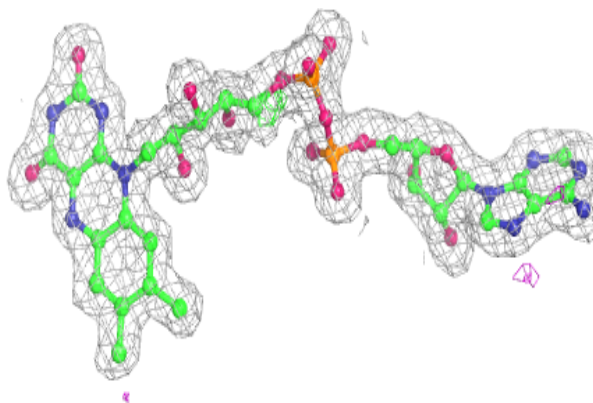


Electron density around FAD A 520:

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

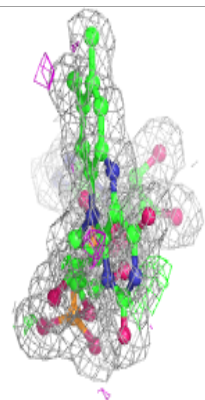
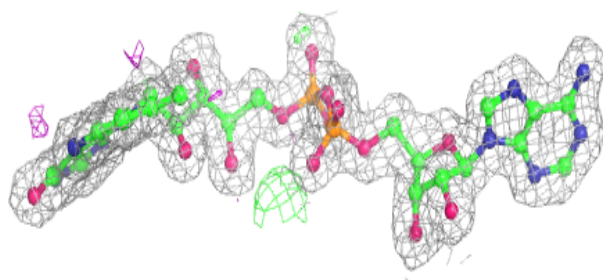
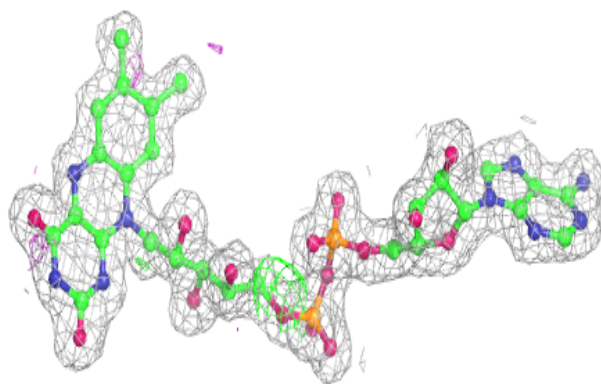
**Electron density around FAD G 526:**

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

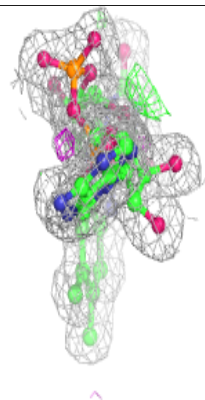
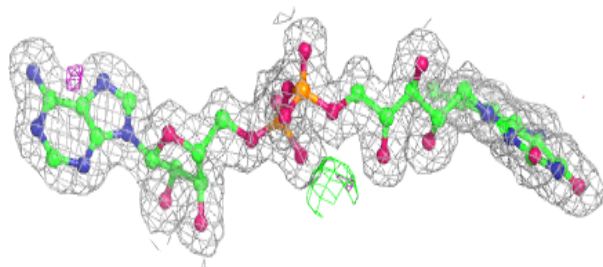
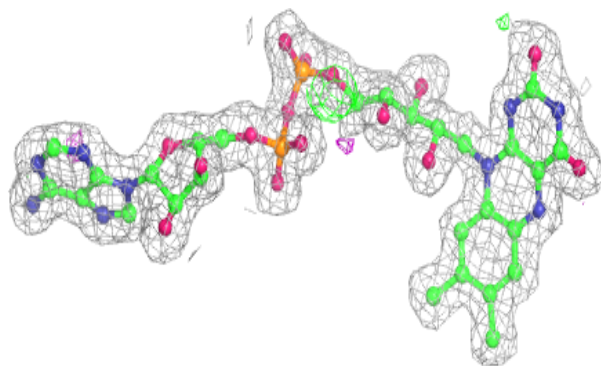


Electron density around FAD B 521:

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

**Electron density around FAD C 522:**

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



6.5 Other polymers

There are no such residues in this entry.