



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 3K4C / pdb_00003k4c
Title : Pyranose 2-oxidase H167A/T169G mutant
Authors : Divne, C.; Tan, T.C.
Deposited on : 2009-10-05
Resolution : 1.70 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

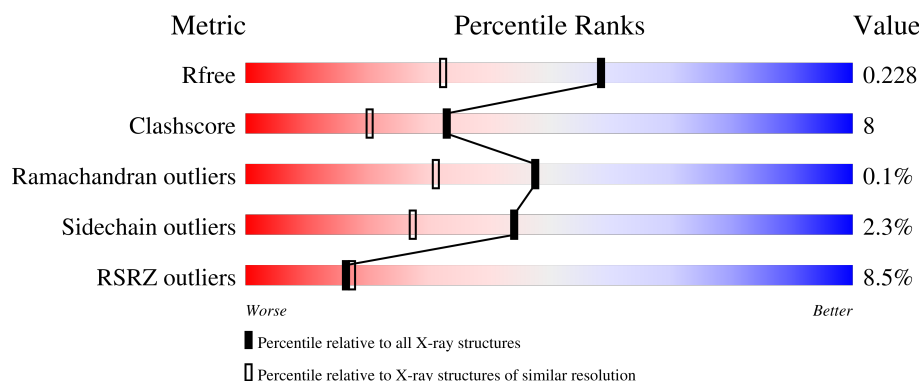
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	623	4% 80% 10% 8%
1	B	623	2% 78% 13% 8%
1	C	623	2% 80% 10% 8%
1	D	623	23% 74% 16% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MES	C	901	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20305 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 Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4534	2863	775	871	25			
1	B	576	Total	C	N	O	S	0	0	0
			4534	2863	775	871	25			
1	C	575	Total	C	N	O	S	0	0	0
			4525	2858	774	869	24			
1	D	574	Total	C	N	O	S	0	0	0
			4518	2854	773	867	24			

There are 8 discrepancies between the modelled and reference sequences:

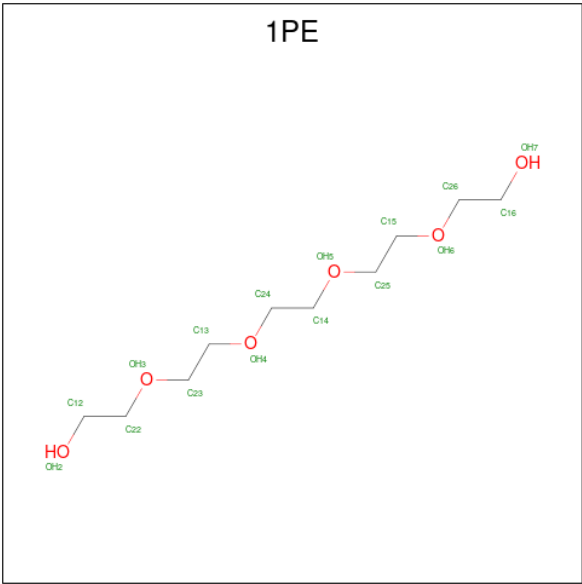
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
A	169	GLY	THR	engineered mutation	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	169	GLY	THR	engineered mutation	UNP Q7ZA32
C	167	ALA	HIS	engineered mutation	UNP Q7ZA32
C	169	GLY	THR	engineered mutation	UNP Q7ZA32
D	167	ALA	HIS	engineered mutation	UNP Q7ZA32
D	169	GLY	THR	engineered mutation	UNP Q7ZA32

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



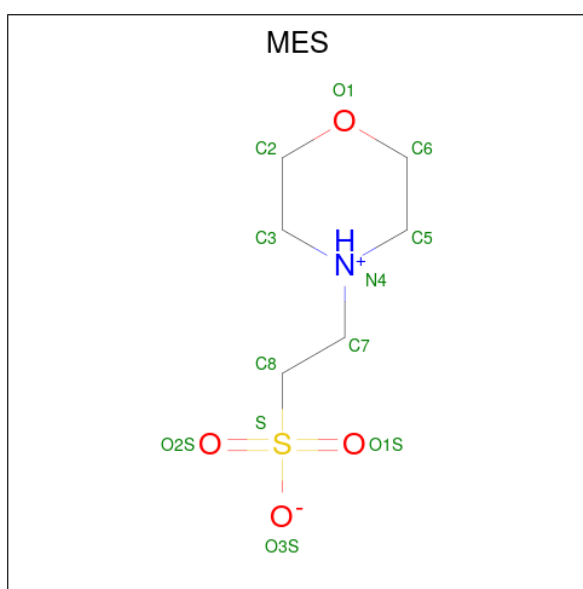
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	9	5		
3	A	1	Total	C	O	0	0
			12	8	4		
3	B	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	498	Total	O	0	0
			498	498		
5	B	554	Total	O	0	0
			554	554		
5	C	504	Total	O	0	0
			504	504		

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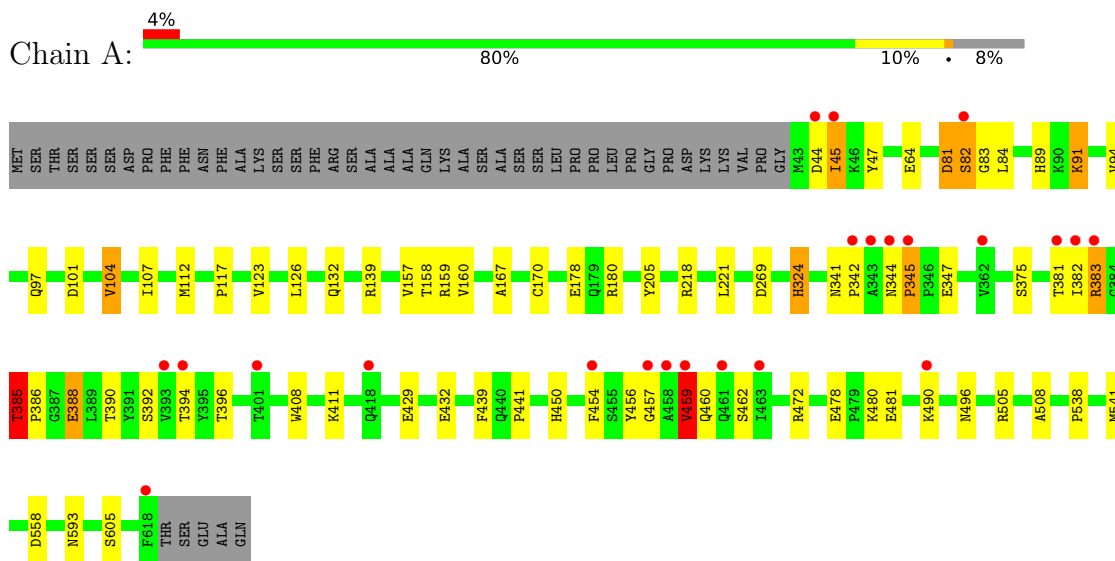
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	344	Total 344	O 344	0	0

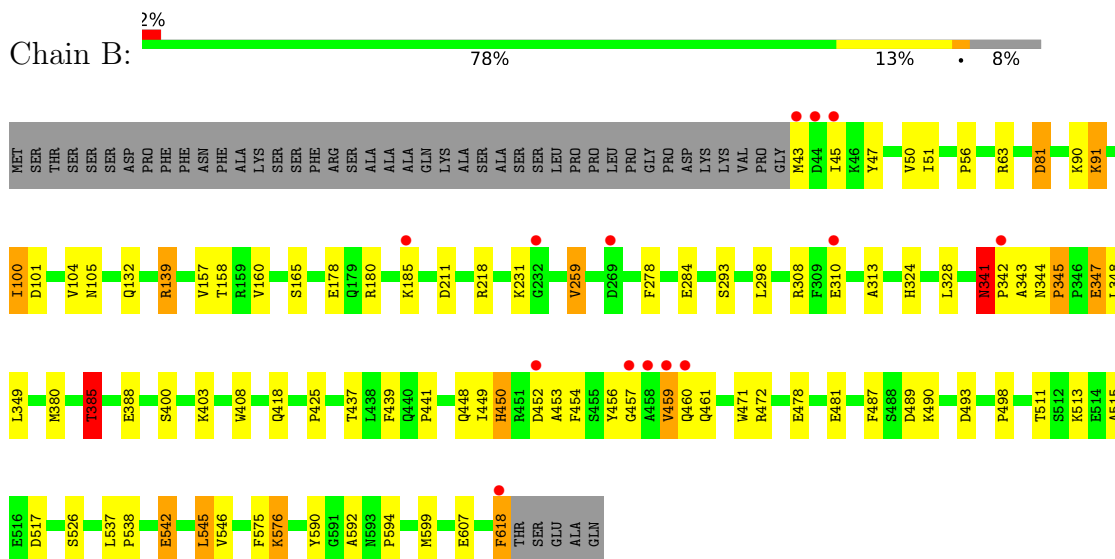
3 Residue-property plots

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.

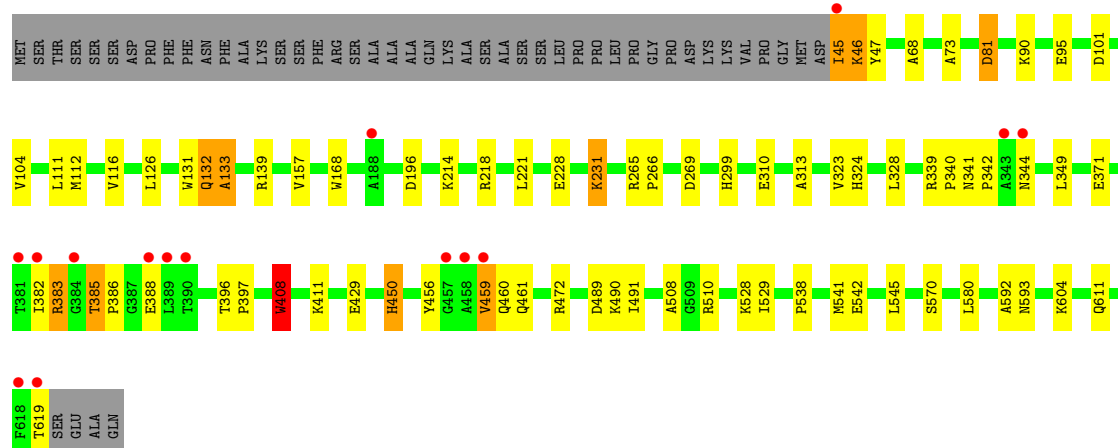
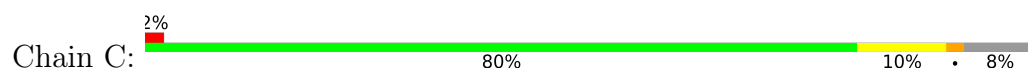
- Molecule 1: Pyranose 2-oxidase



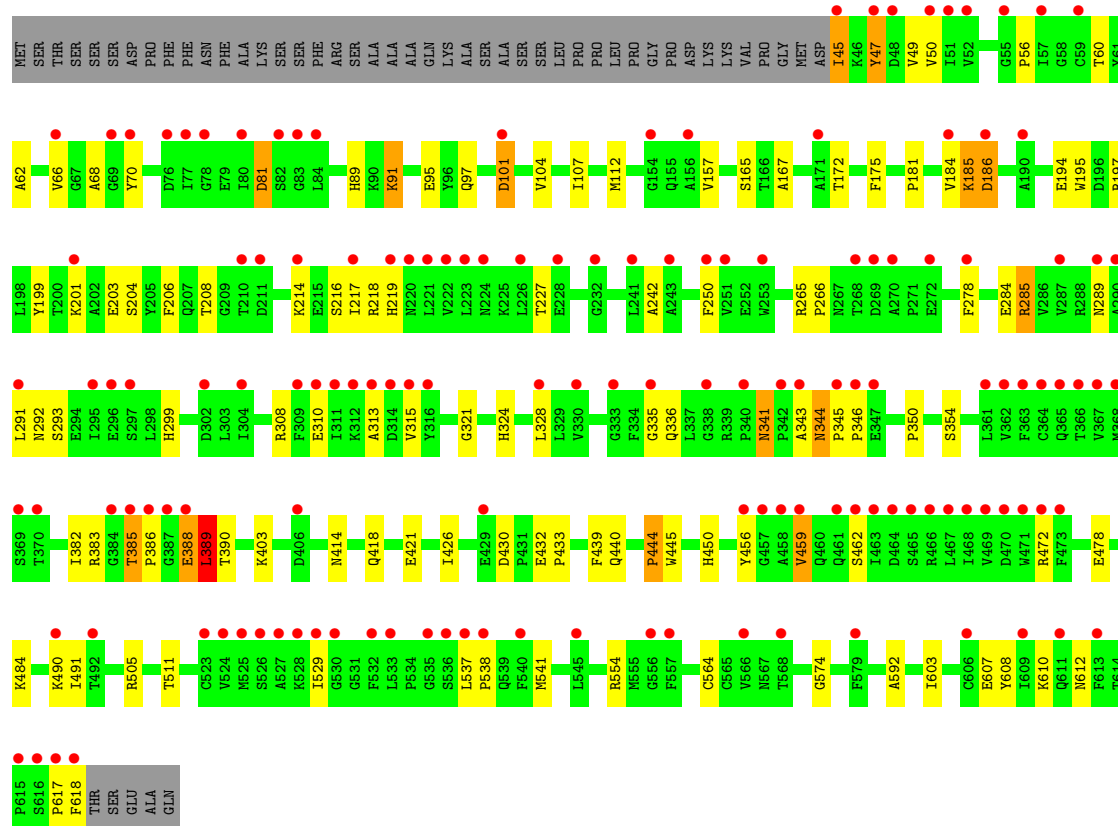
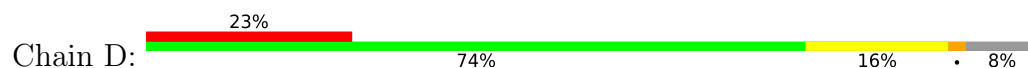
- Molecule 1: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase



• Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.21Å 102.96Å 137.12Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	29.30 – 1.70 29.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.30-1.70) 96.8 (29.30-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.180 , 0.216 0.197 , 0.228	Depositor DCC
R_{free} test set	3027 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l 0.008 for k,h,-l 0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20305	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 1PE, 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	1.49	20/4649 (0.4%)	1.26	18/6320 (0.3%)
1	B	1.45	16/4649 (0.3%)	1.24	13/6320 (0.2%)
1	C	1.31	12/4640 (0.3%)	1.18	13/6309 (0.2%)
1	D	1.20	8/4633 (0.2%)	1.16	12/6299 (0.2%)
All	All	1.37	56/18571 (0.3%)	1.21	56/25248 (0.2%)

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

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

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	SER	N-CA	16.74	1.63	1.46
1	A	112	MET	CA-C	8.50	1.63	1.52
1	B	380	MET	SD-CE	-8.48	1.58	1.79
1	A	82	SER	CB-OG	7.93	1.58	1.42
1	B	298	LEU	C-O	-7.02	1.16	1.24
1	C	592	ALA	CA-CB	-6.58	1.43	1.53
1	A	94	VAL	N-CA	-6.58	1.39	1.46
1	C	133	ALA	CA-C	-6.51	1.44	1.52
1	B	437	THR	C-O	-6.46	1.16	1.24
1	B	546	VAL	CA-CB	6.20	1.63	1.54
1	A	83	GLY	N-CA	6.15	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	GLU	N-CA	-6.11	1.38	1.46
1	A	180	ARG	C-O	-6.06	1.16	1.24
1	A	221	LEU	N-CA	-6.05	1.39	1.46
1	C	132	GLN	CA-C	-5.97	1.45	1.52
1	B	211	ASP	CG-OD1	5.92	1.36	1.25
1	B	592	ALA	CA-CB	-5.92	1.44	1.53
1	A	159	ARG	C-O	-5.91	1.17	1.23
1	A	82	SER	CA-C	5.85	1.60	1.52
1	D	47	TYR	CA-C	5.74	1.59	1.52
1	D	81	ASP	CA-C	5.71	1.57	1.52
1	B	349	LEU	N-CA	5.59	1.50	1.46
1	C	81	ASP	N-CA	5.58	1.53	1.46
1	A	104	VAL	C-O	-5.50	1.17	1.24
1	B	81	ASP	CB-CG	-5.50	1.38	1.52
1	D	70	TYR	C-O	5.50	1.30	1.23
1	C	111	LEU	N-CA	5.49	1.52	1.46
1	C	450	HIS	C-O	-5.46	1.17	1.23
1	D	444	PRO	N-CA	-5.45	1.41	1.47
1	C	221	LEU	N-CA	-5.43	1.40	1.46
1	D	529	ILE	C-O	5.43	1.29	1.23
1	C	371	GLU	CA-C	-5.42	1.46	1.52
1	D	278	PHE	C-O	-5.41	1.19	1.24
1	D	172	THR	CA-C	5.37	1.58	1.52
1	A	117	PRO	N-CA	-5.36	1.40	1.47
1	B	542	GLU	CD-OE1	5.35	1.35	1.25
1	B	51	ILE	CA-CB	5.30	1.61	1.54
1	C	133	ALA	C-O	-5.27	1.17	1.23
1	C	529	ILE	CA-CB	-5.27	1.48	1.54
1	A	508	ALA	N-CA	-5.23	1.38	1.45
1	A	538	PRO	CA-C	5.23	1.58	1.52
1	A	91	LYS	CB-CG	-5.22	1.36	1.52
1	A	123	VAL	CA-CB	5.19	1.59	1.53
1	B	259	VAL	C-O	5.15	1.29	1.24
1	B	450	HIS	CA-C	-5.15	1.46	1.52
1	A	83	GLY	C-O	-5.15	1.17	1.23
1	B	425	PRO	N-CA	-5.12	1.43	1.47
1	C	68	ALA	CA-CB	-5.09	1.45	1.53
1	B	81	ASP	CA-C	5.08	1.59	1.52
1	B	448	GLN	C-O	-5.08	1.18	1.24
1	A	605	SER	N-CA	5.08	1.52	1.46
1	D	321	GLY	N-CA	5.08	1.50	1.45
1	A	170	CYS	CA-CB	-5.07	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	ARG	CG-CD	5.03	1.67	1.52
1	C	510	ARG	C-O	-5.01	1.18	1.24
1	B	481	GLU	CG-CD	5.00	1.64	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASN	CA-C-N	9.50	129.59	119.05
1	A	341	ASN	C-N-CA	9.50	129.59	119.05
1	B	139	ARG	NE-CZ-NH2	-9.45	110.70	119.20
1	A	345	PRO	CA-C-N	-8.40	111.36	119.85
1	A	345	PRO	C-N-CA	-8.40	111.36	119.85
1	B	385	THR	CB-CA-C	8.22	120.52	109.42
1	B	139	ARG	NE-CZ-NH1	7.73	129.23	121.50
1	C	139	ARG	NE-CZ-NH2	-7.69	112.28	119.20
1	A	324	HIS	N-CA-C	7.60	121.81	112.54
1	C	168	TRP	N-CA-C	7.26	119.69	110.33
1	A	82	SER	CA-CB-OG	7.19	125.49	111.10
1	C	344	ASN	CA-C-N	7.07	127.67	120.38
1	C	344	ASN	C-N-CA	7.07	127.67	120.38
1	C	349	LEU	CA-C-N	-6.81	112.78	119.87
1	C	349	LEU	C-N-CA	-6.81	112.78	119.87
1	A	385	THR	CA-C-N	6.68	127.08	119.93
1	A	385	THR	C-N-CA	6.68	127.08	119.93
1	B	81	ASP	CB-CG-OD1	-6.64	103.13	118.40
1	A	385	THR	N-CA-C	6.19	120.32	109.48
1	B	515	ALA	N-CA-C	-6.16	104.64	111.36
1	B	180	ARG	CA-C-N	-6.05	114.04	120.03
1	B	180	ARG	C-N-CA	-6.05	114.04	120.03
1	D	81	ASP	N-CA-C	5.98	120.13	112.12
1	A	396	THR	CB-CA-C	-5.95	103.56	110.17
1	D	426	ILE	N-CA-C	5.82	113.63	108.63
1	A	382	ILE	N-CA-C	5.70	114.94	106.85
1	A	459	VAL	N-CA-C	-5.68	102.25	109.58
1	D	285	ARG	N-CA-C	5.63	117.10	108.42
1	C	408	TRP	N-CA-C	-5.63	105.06	111.14
1	B	91	LYS	CA-CB-CG	5.62	125.35	114.10
1	C	132	GLN	N-CA-C	5.59	117.69	109.24
1	A	112	MET	CB-CA-C	5.56	119.67	110.78
1	C	139	ARG	CG-CD-NE	-5.49	99.92	112.00
1	C	139	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	C	508	ALA	N-CA-C	-5.46	103.69	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	GLN	N-CA-C	-5.45	106.47	113.23
1	B	139	ARG	CD-NE-CZ	5.41	131.98	124.40
1	D	217	ILE	N-CA-C	-5.41	105.45	110.53
1	B	599	MET	N-CA-C	5.39	117.16	111.28
1	A	97	GLN	CA-CB-CG	-5.38	103.35	114.10
1	D	345	PRO	CA-C-N	5.35	125.33	120.03
1	D	345	PRO	C-N-CA	5.35	125.33	120.03
1	C	116	VAL	CB-CA-C	-5.33	104.73	110.85
1	B	341	ASN	O-C-N	5.31	124.95	121.23
1	D	60	THR	N-CA-C	-5.26	105.63	111.36
1	A	81	ASP	CA-C-O	-5.24	114.06	119.51
1	C	323	VAL	N-CA-C	5.22	115.88	110.82
1	D	344	ASN	CA-C-N	-5.20	115.86	119.66
1	D	344	ASN	C-N-CA	-5.20	115.86	119.66
1	D	389	LEU	CB-CG-CD1	-5.20	95.10	110.70
1	B	542	GLU	CB-CG-CD	5.13	121.33	112.60
1	D	321	GLY	CA-C-O	-5.09	118.72	122.23
1	A	81	ASP	CA-C-N	5.08	129.52	121.18
1	A	81	ASP	C-N-CA	5.08	129.52	121.18
1	D	227	THR	N-CA-C	-5.07	105.64	111.07
1	A	139	ARG	NE-CZ-NH1	5.01	126.51	121.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASP	Peptide
1	B	449	ILE	Peptide
1	D	388	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4534	0	4382	50	0
1	B	4534	0	4382	66	0
1	C	4525	0	4376	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4518	0	4369	91	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	29	0	0
2	D	53	0	28	1	0
3	A	26	0	31	0	0
3	B	16	0	22	0	0
3	D	16	0	22	0	0
4	B	12	0	12	3	0
4	C	12	0	12	13	0
5	A	498	0	0	15	0
5	B	554	0	0	10	0
5	C	504	0	0	13	0
5	D	344	0	0	12	0
All	All	20305	0	17727	281	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (281) 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:C:133:ALA:CB	4:C:901:MES:H71	1.40	1.50
1:C:299:HIS:CE1	1:C:310:GLU:HG2	1.60	1.36
1:C:383:ARG:HB2	1:C:383:ARG:NH1	1.45	1.31
1:C:383:ARG:HH11	1:C:383:ARG:CB	1.47	1.25
1:C:133:ALA:CB	4:C:901:MES:C7	2.20	1.18
1:A:45:ILE:H	1:A:45:ILE:HD12	1.01	1.13
1:C:133:ALA:HB2	4:C:901:MES:H71	1.18	1.12
1:C:133:ALA:HB3	4:C:901:MES:H71	1.15	1.11
1:C:101:ASP:O	1:C:104:VAL:HG12	1.50	1.07
1:C:133:ALA:HB2	4:C:901:MES:O1S	1.56	1.04
1:C:133:ALA:HB3	4:C:901:MES:C7	1.86	1.02
1:D:45:ILE:HA	5:D:2497:HOH:O	1.61	0.99
1:A:45:ILE:H	1:A:45:ILE:CD1	1.78	0.94
1:B:576:LYS:HD3	1:B:576:LYS:N	1.79	0.94
1:D:101:ASP:O	1:D:104:VAL:HG12	1.68	0.94
1:A:45:ILE:HD12	1:A:45:ILE:N	1.81	0.94
1:D:343:ALA:O	1:D:344:ASN:ND2	2.00	0.93
1:C:133:ALA:HB2	4:C:901:MES:C7	1.92	0.90
1:C:383:ARG:HB2	1:C:383:ARG:HH11	0.73	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:HIS:CE1	1:C:310:GLU:CG	2.54	0.89
1:C:490:LYS:HD3	1:C:491:ILE:HD13	1.55	0.88
1:B:347:GLU:HG3	1:B:348:LEU:HG	1.55	0.87
1:B:343:ALA:O	1:B:344:ASN:ND2	2.08	0.87
1:C:126:LEU:CD1	1:C:132:GLN:HG3	2.05	0.86
1:B:618:PHE:C	1:B:618:PHE:HD1	1.83	0.86
1:D:343:ALA:C	1:D:344:ASN:HD22	1.84	0.85
1:D:185:LYS:HD3	5:D:2678:HOH:O	1.75	0.85
1:B:101:ASP:O	1:B:104:VAL:HG12	1.77	0.85
1:D:285:ARG:HA	1:D:328:LEU:HD11	1.58	0.85
1:B:618:PHE:C	1:B:618:PHE:CD1	2.55	0.84
1:D:341:ASN:HD21	1:D:343:ALA:HB3	1.43	0.83
1:C:126:LEU:HD12	1:C:132:GLN:HG3	1.62	0.82
1:C:411:LYS:HE3	5:C:2449:HOH:O	1.79	0.81
1:A:101:ASP:OD2	1:A:459:VAL:HG13	1.82	0.80
1:A:84:LEU:HD23	5:B:2054:HOH:O	1.81	0.79
1:A:383:ARG:HB3	1:A:392:SER:HB3	1.65	0.78
1:D:185:LYS:H	1:D:185:LYS:HD2	1.49	0.77
1:B:385:THR:HG23	1:B:388:GLU:OE1	1.85	0.77
1:B:341:ASN:C	1:B:341:ASN:HD22	1.92	0.77
1:D:185:LYS:H	1:D:185:LYS:CD	1.95	0.77
1:D:341:ASN:HD22	1:D:341:ASN:C	1.96	0.74
1:D:341:ASN:HD22	1:D:343:ALA:H	1.36	0.73
1:B:450:HIS:CE1	1:B:472:ARG:HH11	2.07	0.73
1:D:341:ASN:ND2	1:D:343:ALA:H	1.86	0.73
1:D:608:TYR:CZ	1:D:612:ASN:OD1	2.42	0.72
1:A:450:HIS:HD2	5:A:1424:HOH:O	1.72	0.71
1:D:389:LEU:HD12	1:D:389:LEU:C	2.00	0.71
1:A:82:SER:HB2	5:A:1477:HOH:O	1.92	0.70
1:A:505:ARG:HD3	5:A:1785:HOH:O	1.92	0.70
1:D:617:PRO:O	1:D:618:PHE:C	2.35	0.70
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.56	0.69
1:B:450:HIS:HD2	5:B:1237:HOH:O	1.75	0.69
1:D:459:VAL:HG12	1:D:459:VAL:O	1.92	0.69
1:D:505:ARG:NH2	5:D:2273:HOH:O	2.25	0.68
1:D:285:ARG:HA	1:D:328:LEU:CD1	2.24	0.68
1:C:101:ASP:O	1:C:104:VAL:CG1	2.35	0.67
1:C:126:LEU:CD1	1:C:132:GLN:CG	2.72	0.67
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.60	0.66
1:B:450:HIS:HE1	1:B:472:ARG:HH11	1.42	0.66
1:A:344:ASN:HD22	1:A:345:PRO:HD2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ASP:O	1:B:490:LYS:HD2	1.96	0.65
1:D:308:ARG:HG3	1:D:308:ARG:HH11	1.62	0.65
1:C:132:GLN:OE1	4:C:901:MES:H31	1.97	0.64
1:A:132:GLN:HG2	5:A:2468:HOH:O	1.98	0.63
1:B:459:VAL:HG12	1:B:461:GLN:NE2	2.14	0.63
1:B:478:GLU:HG3	1:B:511:THR:OG1	2.00	0.62
1:B:459:VAL:HG22	5:B:2672:HOH:O	1.98	0.62
1:B:459:VAL:CG2	5:B:2672:HOH:O	2.48	0.62
1:D:389:LEU:HD12	1:D:389:LEU:O	1.99	0.61
1:D:450:HIS:HD2	5:D:2499:HOH:O	1.84	0.60
1:C:450:HIS:CE1	1:C:472:ARG:HH11	2.19	0.60
1:D:185:LYS:HD2	1:D:185:LYS:N	2.16	0.60
1:B:81:ASP:OD2	1:B:90:LYS:NZ	2.34	0.60
1:D:45:ILE:CA	5:D:2497:HOH:O	2.34	0.59
1:A:383:ARG:HD2	1:A:390:THR:O	2.02	0.59
1:B:308:ARG:HD2	5:B:2220:HOH:O	2.03	0.59
1:D:444:PRO:HD2	1:D:445:TRP:CZ3	2.38	0.59
1:C:385:THR:OG1	1:C:388:GLU:CD	2.45	0.58
1:B:342:PRO:C	1:B:344:ASN:H	2.11	0.58
1:D:291:LEU:O	1:D:292:ASN:HB2	2.03	0.58
1:D:382:ILE:HD13	5:D:2622:HOH:O	2.03	0.58
1:C:328:LEU:C	1:C:328:LEU:HD23	2.28	0.57
1:A:101:ASP:HB3	1:A:459:VAL:HG22	1.85	0.57
1:D:62:ALA:O	1:D:66:VAL:HG23	2.05	0.57
1:D:459:VAL:O	1:D:459:VAL:CG1	2.52	0.57
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.86	0.57
1:B:63:ARG:HD2	1:B:259:VAL:O	2.04	0.57
1:B:132:GLN:OE1	4:B:901:MES:H31	2.04	0.57
1:A:478:GLU:CD	1:A:480:LYS:HE2	2.30	0.56
1:C:133:ALA:CB	4:C:901:MES:H72	2.28	0.56
1:C:450:HIS:HE1	1:C:472:ARG:HD2	1.70	0.56
1:D:185:LYS:O	1:D:186:ASP:C	2.46	0.56
1:D:414:ASN:O	1:D:418:GLN:HG3	2.06	0.56
1:A:457:GLY:HA2	5:A:2149:HOH:O	2.06	0.56
1:C:126:LEU:HD13	1:C:132:GLN:CG	2.35	0.56
1:D:478:GLU:HG3	1:D:511:THR:OG1	2.06	0.55
1:A:385:THR:O	1:A:388:GLU:HB2	2.06	0.55
1:B:542:GLU:HB2	1:B:545:LEU:HD22	1.88	0.55
1:C:382:ILE:HD13	5:C:2150:HOH:O	2.07	0.55
1:B:293:SER:O	1:B:576:LYS:HE2	2.06	0.55
1:C:131:TRP:O	1:C:132:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HD13	1:B:100:ILE:O	2.07	0.55
1:C:456:TYR:CD2	1:C:541:MET:HE2	2.42	0.55
1:D:308:ARG:HH11	1:D:308:ARG:CG	2.20	0.55
1:A:344:ASN:HD22	1:A:345:PRO:CD	2.20	0.54
1:C:604:LYS:NZ	5:C:1648:HOH:O	2.26	0.54
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.72	0.54
1:B:178:GLU:OE1	1:B:439:PHE:HE1	1.90	0.54
1:C:299:HIS:ND1	1:C:310:GLU:HG2	2.12	0.54
1:C:542:GLU:HB2	1:C:545:LEU:HD22	1.89	0.54
1:A:385:THR:HG22	1:A:386:PRO:HD2	1.89	0.54
1:A:411:LYS:HD3	5:A:2592:HOH:O	2.08	0.54
1:B:100:ILE:CD1	1:B:453:ALA:HB2	2.38	0.54
1:C:450:HIS:HD2	5:C:1651:HOH:O	1.89	0.54
1:C:47:TYR:O	1:C:313:ALA:HA	2.08	0.53
1:C:528:LYS:NZ	5:C:2436:HOH:O	2.40	0.53
1:A:104:VAL:HG13	1:A:454:PHE:O	2.07	0.53
1:C:383:ARG:NH1	1:C:383:ARG:CB	2.30	0.53
1:D:450:HIS:CE1	1:D:472:ARG:HH11	2.25	0.53
1:B:493:ASP:OD2	5:B:1303:HOH:O	2.19	0.53
1:D:341:ASN:C	1:D:341:ASN:ND2	2.67	0.53
1:B:284:GLU:OE1	1:B:308:ARG:NH2	2.42	0.52
1:A:450:HIS:CE1	1:A:472:ARG:HH11	2.27	0.52
1:A:381:THR:HB	1:A:394:THR:OG1	2.09	0.52
1:B:341:ASN:C	1:B:341:ASN:ND2	2.63	0.52
1:D:216:SER:HB3	1:D:219:HIS:HB3	1.91	0.52
1:D:432:GLU:HB2	1:D:433:PRO:HD2	1.92	0.52
1:A:101:ASP:HB3	1:A:459:VAL:CG2	2.40	0.52
1:A:478:GLU:HG2	1:A:480:LYS:HE2	1.92	0.52
1:B:343:ALA:C	1:B:344:ASN:HD22	2.13	0.52
1:C:133:ALA:HB2	4:C:901:MES:C8	2.40	0.52
1:C:385:THR:O	1:C:386:PRO:C	2.50	0.52
1:C:429:GLU:HG2	5:C:2850:HOH:O	2.09	0.52
1:B:100:ILE:HD11	1:B:453:ALA:HB2	1.92	0.52
1:D:335:GLY:O	1:D:346:PRO:HB3	2.10	0.51
1:C:112:MET:HE2	1:D:95:GLU:HG3	1.92	0.51
1:C:95:GLU:HG3	1:D:112:MET:HE2	1.93	0.51
1:A:178:GLU:OE1	1:A:441:PRO:HG3	2.11	0.51
1:B:538:PRO:HG2	1:C:538:PRO:HG2	1.92	0.51
1:C:81:ASP:OD2	1:C:90:LYS:NZ	2.44	0.51
1:D:385:THR:HG22	1:D:386:PRO:HD2	1.92	0.51
1:A:101:ASP:OD2	5:A:2823:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLN:OE1	4:C:901:MES:C3	2.59	0.51
1:D:285:ARG:CA	1:D:328:LEU:HD11	2.38	0.51
1:C:126:LEU:HD13	1:C:132:GLN:HG3	1.92	0.50
1:D:341:ASN:HD21	1:D:343:ALA:CB	2.20	0.50
1:D:50:VAL:HG23	1:D:50:VAL:O	2.11	0.50
1:D:343:ALA:C	1:D:344:ASN:ND2	2.55	0.50
1:D:341:ASN:ND2	1:D:343:ALA:HB3	2.18	0.50
1:D:439:PHE:C	1:D:440:GLN:HG2	2.37	0.49
1:A:456:TYR:CD2	1:A:541:MET:HE2	2.47	0.49
1:A:558:ASP:OD2	5:A:2726:HOH:O	2.19	0.49
1:C:490:LYS:HD3	1:C:491:ILE:CD1	2.37	0.49
1:D:603:ILE:O	1:D:607:GLU:HG3	2.11	0.49
1:D:346:PRO:HG2	1:D:350:PRO:HA	1.94	0.49
1:D:289:ASN:OD1	1:D:292:ASN:N	2.46	0.49
1:C:450:HIS:HE1	1:C:472:ARG:HH11	1.60	0.49
1:D:81:ASP:HB2	5:D:2214:HOH:O	2.13	0.49
1:D:181:PRO:HG2	1:D:195:TRP:HZ2	1.78	0.49
1:A:432:GLU:H	1:A:432:GLU:CD	2.20	0.48
1:C:133:ALA:HB2	4:C:901:MES:S	2.52	0.48
1:C:460:GLN:HB2	5:C:1928:HOH:O	2.13	0.48
1:D:385:THR:O	1:D:388:GLU:HG3	2.13	0.48
1:B:178:GLU:HB2	5:B:1867:HOH:O	2.13	0.48
1:B:459:VAL:HG12	1:B:461:GLN:HE22	1.78	0.48
1:C:81:ASP:OD1	1:C:81:ASP:N	2.47	0.48
1:C:265:ARG:HA	1:C:266:PRO:C	2.38	0.48
1:A:342:PRO:C	1:A:344:ASN:N	2.71	0.48
1:D:308:ARG:CG	1:D:308:ARG:NH1	2.77	0.48
1:B:91:LYS:NZ	1:B:452:ASP:OD1	2.46	0.48
1:C:46:LYS:HG3	1:C:47:TYR:N	2.26	0.48
1:D:194:GLU:OE1	5:D:2796:HOH:O	2.20	0.47
1:A:460:GLN:HB2	5:A:1838:HOH:O	2.14	0.47
1:D:456:TYR:CD2	1:D:541:MET:HE2	2.49	0.47
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.16	0.47
1:B:47:TYR:O	1:B:313:ALA:HA	2.15	0.47
1:A:505:ARG:HD2	5:A:2693:HOH:O	2.14	0.47
1:C:101:ASP:OD2	1:C:459:VAL:HG23	2.15	0.47
1:D:184:VAL:HG13	5:D:2678:HOH:O	2.15	0.47
1:D:199:TYR:O	1:D:203:GLU:HG3	2.14	0.47
1:B:81:ASP:OD1	1:B:81:ASP:C	2.47	0.46
1:B:537:LEU:HB3	1:B:538:PRO:HD2	1.97	0.46
1:A:82:SER:HB3	5:A:2308:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LEU:HD23	1:B:328:LEU:C	2.40	0.46
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.97	0.46
1:D:450:HIS:HE1	1:D:472:ARG:HH11	1.62	0.46
1:B:344:ASN:O	1:B:345:PRO:C	2.58	0.46
1:D:299:HIS:NE2	1:D:310:GLU:CD	2.74	0.46
1:D:385:THR:H	1:D:388:GLU:CD	2.24	0.46
1:A:44:ASP:HB2	1:A:47:TYR:CZ	2.51	0.45
1:D:608:TYR:CD1	1:D:608:TYR:C	2.94	0.45
1:C:231:LYS:HB2	1:C:231:LYS:HE2	1.48	0.45
1:A:408:TRP:CD1	1:A:408:TRP:C	2.95	0.45
1:D:89:HIS:CE1	1:D:91:LYS:HB3	2.50	0.45
1:B:81:ASP:OD1	1:B:81:ASP:N	2.45	0.45
1:C:101:ASP:CG	1:C:459:VAL:HG23	2.40	0.45
1:C:450:HIS:CE1	1:C:472:ARG:HD2	2.51	0.45
1:D:385:THR:OG1	1:D:388:GLU:OE1	2.20	0.45
1:B:104:VAL:HG13	1:B:105:ASN:N	2.32	0.45
1:C:196:ASP:OD1	5:C:2646:HOH:O	2.21	0.45
1:D:47:TYR:O	1:D:313:ALA:HA	2.17	0.45
1:D:218:ARG:HD2	5:D:1256:HOH:O	2.16	0.45
1:A:126:LEU:HD12	1:A:132:GLN:HG3	1.99	0.44
1:B:450:HIS:HE1	1:B:472:ARG:HD2	1.83	0.44
1:C:459:VAL:HG13	1:C:461:GLN:NE2	2.32	0.44
5:C:2186:HOH:O	1:D:462:SER:HB2	2.17	0.44
1:C:570:SER:HB3	1:C:580:LEU:O	2.18	0.44
1:D:56:PRO:HD3	1:D:165:SER:HB3	1.99	0.44
1:D:208:THR:HA	1:D:242:ALA:HA	1.99	0.44
1:A:89:HIS:CE1	1:A:91:LYS:HB2	2.53	0.44
1:C:341:ASN:HA	1:C:342:PRO:HD2	1.90	0.44
1:D:265:ARG:HA	1:D:266:PRO:C	2.43	0.44
1:A:450:HIS:HE1	1:A:472:ARG:HH11	1.64	0.44
1:C:214:LYS:O	5:C:2277:HOH:O	2.21	0.44
1:C:460:GLN:OE1	5:C:1928:HOH:O	2.21	0.44
1:D:107:ILE:HG12	1:D:167:ALA:HB1	1.99	0.44
1:B:607:GLU:HG3	5:B:2890:HOH:O	2.17	0.44
1:D:490:LYS:HG3	1:D:491:ILE:HD13	2.00	0.44
1:A:478:GLU:CG	1:A:480:LYS:HE2	2.48	0.44
1:D:45:ILE:N	5:D:2497:HOH:O	2.50	0.43
4:C:901:MES:H51	4:C:901:MES:H82	1.78	0.43
1:B:456:TYR:O	1:B:457:GLY:C	2.61	0.43
1:C:489:ASP:OD1	1:C:489:ASP:C	2.61	0.43
1:D:68:ALA:HB2	1:D:610:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PRO:C	1:A:344:ASN:H	2.26	0.43
1:B:218:ARG:HD2	5:B:1188:HOH:O	2.18	0.43
1:C:408:TRP:CD1	1:C:408:TRP:C	2.96	0.43
1:A:64:GLU:OE2	1:A:205:TYR:OH	2.29	0.43
1:D:197:ARG:NH2	1:D:607:GLU:OE1	2.47	0.43
1:C:339:ARG:HA	1:C:340:PRO:HD3	1.85	0.43
1:B:43:MET:HE2	1:B:278:PHE:CD1	2.54	0.42
1:B:139:ARG:HD3	4:B:901:MES:O2S	2.19	0.42
1:B:158:THR:HG22	1:B:160:VAL:HG22	2.01	0.42
1:D:421:GLU:H	1:D:421:GLU:CD	2.26	0.42
1:C:228:GLU:HG3	1:C:231:LYS:NZ	2.33	0.42
1:A:505:ARG:NH1	5:A:2693:HOH:O	2.29	0.42
1:D:554:ARG:O	1:D:564:CYS:HB2	2.19	0.42
1:A:462:SER:OG	4:B:901:MES:H61	2.20	0.42
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.42
1:B:487:PHE:HB3	1:B:498:PRO:HB2	2.01	0.42
1:C:218:ARG:HD2	5:C:1133:HOH:O	2.20	0.42
1:B:104:VAL:HG23	1:B:454:PHE:O	2.20	0.42
1:B:513:LYS:NZ	1:B:517:ASP:OD2	2.53	0.42
1:C:45:ILE:HB	1:C:46:LYS:H	1.20	0.42
1:C:396:THR:HA	1:C:397:PRO:HD3	1.90	0.42
1:C:385:THR:N	1:C:388:GLU:OE1	2.47	0.42
1:A:450:HIS:HE1	1:A:472:ARG:HD2	1.85	0.42
1:C:383:ARG:NH1	1:C:383:ARG:CG	2.83	0.42
1:D:201:LYS:HD3	1:D:603:ILE:HG21	2.01	0.42
1:D:299:HIS:CD2	1:D:310:GLU:HG2	2.55	0.42
1:A:218:ARG:HD2	5:A:1396:HOH:O	2.20	0.41
1:A:375:SER:HA	5:A:2923:HOH:O	2.19	0.41
1:B:471:TRP:CH2	1:B:526:SER:HA	2.55	0.41
1:D:175:PHE:CE1	1:D:592:ALA:HB3	2.55	0.41
1:D:293:SER:HA	1:D:574:GLY:O	2.20	0.41
1:B:342:PRO:C	1:B:344:ASN:N	2.75	0.41
1:B:439:PHE:CD1	1:B:439:PHE:C	2.99	0.41
1:B:56:PRO:HD3	1:B:165:SER:HB3	2.03	0.41
1:B:590:TYR:CE2	1:B:594:PRO:HB3	2.55	0.41
1:A:439:PHE:CD1	1:A:439:PHE:C	2.99	0.41
1:B:408:TRP:CD1	1:B:408:TRP:C	2.98	0.41
1:C:611:GLN:HG2	5:C:2779:HOH:O	2.21	0.41
1:B:385:THR:CG2	1:B:388:GLU:OE1	2.62	0.41
1:B:460:GLN:HB2	5:B:2241:HOH:O	2.21	0.41
1:C:81:ASP:CG	1:C:81:ASP:O	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:HH22	1:D:607:GLU:CD	2.29	0.41
1:A:107:ILE:HG12	1:A:167:ALA:HB1	2.02	0.41
5:A:2721:HOH:O	1:B:461:GLN:HB3	2.20	0.41
1:B:185:LYS:H	1:B:185:LYS:HG2	1.68	0.41
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.56	0.41
1:D:336:GLN:NE2	1:D:344:ASN:O	2.53	0.41
1:D:390:THR:HB	5:D:2845:HOH:O	2.20	0.41
1:D:537:LEU:HB3	1:D:538:PRO:HD2	2.02	0.41
1:B:575:PHE:C	1:B:576:LYS:HD3	2.44	0.41
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.20	0.41
1:D:284:GLU:O	1:D:285:ARG:HB3	2.21	0.40
1:D:354:SER:OG	1:D:484:LYS:NZ	2.53	0.40
1:B:576:LYS:N	1:B:576:LYS:CD	2.65	0.40
1:D:49:VAL:HG22	1:D:315:VAL:HB	2.03	0.40
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.56	0.40
2:D:801:FAD:H9	2:D:801:FAD:H1'1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	574/623 (92%)	559 (97%)	15 (3%)	0	100	100
1	B	574/623 (92%)	557 (97%)	16 (3%)	1 (0%)	43	28
1	C	573/623 (92%)	558 (97%)	15 (3%)	0	100	100
1	D	572/623 (92%)	551 (96%)	19 (3%)	2 (0%)	36	22
All	All	2293/2492 (92%)	2225 (97%)	65 (3%)	3 (0%)	48	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	389	LEU
1	D	186	ASP
1	B	345	PRO

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	502/540 (93%)	492 (98%)	10 (2%)	48	32
1	B	502/540 (93%)	488 (97%)	14 (3%)	38	21
1	C	501/540 (93%)	491 (98%)	10 (2%)	48	32
1	D	500/540 (93%)	488 (98%)	12 (2%)	43	26
All	All	2005/2160 (93%)	1959 (98%)	46 (2%)	44	27

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	269	ASP
1	A	347	GLU
1	A	385	THR
1	A	388	GLU
1	A	429	GLU
1	A	459	VAL
1	A	490	LYS
1	A	496	ASN
1	A	593	ASN
1	B	45	ILE
1	B	100	ILE
1	B	231	LYS
1	B	310	GLU
1	B	341	ASN
1	B	347	GLU
1	B	385	THR
1	B	400	SER
1	B	403	LYS

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Mol	Chain	Res	Type
1	B	441	PRO
1	B	459	VAL
1	B	545	LEU
1	B	576	LYS
1	B	618	PHE
1	C	45	ILE
1	C	46	LYS
1	C	231	LYS
1	C	269	ASP
1	C	383	ARG
1	C	385	THR
1	C	408	TRP
1	C	459	VAL
1	C	593	ASN
1	C	619	THR
1	D	45	ILE
1	D	91	LYS
1	D	101	ASP
1	D	185	LYS
1	D	204	SER
1	D	206	PHE
1	D	214	LYS
1	D	341	ASN
1	D	383	ARG
1	D	385	THR
1	D	403	LYS
1	D	459	VAL

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

Mol	Chain	Res	Type
1	A	263	GLN
1	A	276	ASN
1	A	299	HIS
1	A	324	HIS
1	A	341	ASN
1	A	344	ASN
1	A	419	HIS
1	A	450	HIS
1	B	341	ASN
1	B	419	HIS
1	B	450	HIS

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Mol	Chain	Res	Type
1	B	461	GLN
1	B	563	ASN
1	B	611	GLN
1	C	99	ASN
1	C	110	GLN
1	C	263	GLN
1	C	299	HIS
1	C	341	ASN
1	C	344	ASN
1	C	450	HIS
1	C	563	ASN
1	C	611	GLN
1	D	257	ASN
1	D	263	GLN
1	D	276	ASN
1	D	301	HIS
1	D	324	HIS
1	D	341	ASN
1	D	344	ASN
1	D	450	HIS
1	D	539	GLN
1	D	612	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	801	-	58,58,58	1.87	14 (24%)	85,89,89	2.92	34 (40%)
2	FAD	A	801	-	58,58,58	1.44	8 (13%)	85,89,89	1.97	26 (30%)
4	MES	B	901	-	12,12,12	2.46	3 (25%)	15,16,16	4.24	7 (46%)
2	FAD	C	801	-	58,58,58	1.46	13 (22%)	85,89,89	2.18	25 (29%)
3	1PE	A	905	-	11,11,15	0.83	0	10,10,14	0.54	0
4	MES	C	901	-	12,12,12	2.08	1 (8%)	15,16,16	4.11	12 (80%)
3	1PE	D	903	-	15,15,15	0.70	0	14,14,14	0.48	0
3	1PE	A	904	-	13,13,15	0.73	0	12,12,14	0.35	0
3	1PE	B	902	-	15,15,15	0.61	0	14,14,14	0.25	0
2	FAD	B	801	-	58,58,58	1.61	13 (22%)	85,89,89	2.06	24 (28%)

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	801	-	-	3/34/50/50	0/6/6/6
2	FAD	A	801	-	-	2/34/50/50	0/6/6/6
4	MES	B	901	-	-	2/6/14/14	0/1/1/1
2	FAD	C	801	-	-	2/34/50/50	0/6/6/6
3	1PE	A	905	-	-	2/9/9/13	-
4	MES	C	901	-	-	2/6/14/14	0/1/1/1
3	1PE	D	903	-	-	2/13/13/13	-
3	1PE	A	904	-	-	2/11/11/13	-
3	1PE	B	902	-	-	1/13/13/13	-
2	FAD	B	801	-	-	0/34/50/50	0/6/6/6

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	MES	C8-S	-7.85	1.66	1.77
4	C	901	MES	C8-S	-6.66	1.68	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FAD	C6-C5X	5.43	1.48	1.40
2	B	801	FAD	C8A-N9A	-4.48	1.29	1.37
2	D	801	FAD	C8A-N9A	-4.46	1.30	1.37
2	D	801	FAD	PA-O3P	4.14	1.64	1.59
2	B	801	FAD	P-O3P	4.05	1.63	1.59
2	A	801	FAD	C8M-C8	3.92	1.58	1.51
2	D	801	FAD	C10-N1	3.85	1.41	1.33
2	A	801	FAD	C4X-N5	3.59	1.38	1.30
2	D	801	FAD	C5X-N5	-3.59	1.32	1.39
2	A	801	FAD	C9-C9A	3.50	1.45	1.39
2	B	801	FAD	C5A-C4A	-3.26	1.33	1.39
2	D	801	FAD	O2-C2	3.21	1.30	1.24
2	A	801	FAD	C4A-N3A	-3.14	1.28	1.34
2	C	801	FAD	C4'-C3'	3.11	1.58	1.53
2	D	801	FAD	C2-N3	-3.06	1.32	1.39
2	C	801	FAD	C9-C8	2.93	1.43	1.39
2	C	801	FAD	C4-N3	-2.92	1.33	1.38
2	D	801	FAD	O4B-C4B	-2.87	1.38	1.45
2	A	801	FAD	C2A-N1A	-2.82	1.28	1.33
2	A	801	FAD	C8A-N9A	-2.79	1.32	1.37
2	B	801	FAD	PA-O3P	2.78	1.62	1.59
2	D	801	FAD	C2B-C3B	-2.75	1.45	1.53
2	B	801	FAD	C1B-N9A	-2.69	1.38	1.46
2	C	801	FAD	O3B-C3B	-2.59	1.36	1.43
2	B	801	FAD	C8M-C8	2.59	1.55	1.51
2	D	801	FAD	O2B-C2B	-2.58	1.36	1.43
2	D	801	FAD	C5'-C4'	2.58	1.55	1.51
2	C	801	FAD	C4X-N5	2.52	1.36	1.30
2	D	801	FAD	C4X-N5	2.41	1.36	1.30
2	B	801	FAD	C1'-N10	2.41	1.53	1.47
2	B	801	FAD	C4A-N3A	-2.40	1.29	1.34
2	C	801	FAD	O4-C4	2.32	1.28	1.23
2	B	801	FAD	C10-N1	2.32	1.37	1.33
2	C	801	FAD	C2A-N1A	2.32	1.38	1.33
4	B	901	MES	O2S-S	2.32	1.51	1.45
2	B	801	FAD	O3B-C3B	-2.32	1.37	1.43
2	C	801	FAD	O4B-C4B	-2.30	1.39	1.45
2	D	801	FAD	O3B-C3B	-2.25	1.37	1.43
2	C	801	FAD	PA-O2A	-2.25	1.44	1.55
2	B	801	FAD	C2-N3	-2.24	1.34	1.39
2	A	801	FAD	P-O3P	2.23	1.61	1.59
2	C	801	FAD	C5X-N5	-2.20	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C9A-N10	-2.18	1.37	1.41
2	A	801	FAD	C3B-C4B	-2.14	1.47	1.53
4	B	901	MES	O1S-S	2.14	1.51	1.45
2	B	801	FAD	O4B-C4B	-2.10	1.40	1.45
2	C	801	FAD	PA-O3P	-2.09	1.57	1.59
2	C	801	FAD	O5B-C5B	-2.08	1.36	1.44
2	D	801	FAD	C9-C8	2.06	1.42	1.39
2	C	801	FAD	C2B-C3B	-2.02	1.47	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	901	MES	O3S-S-C8	-10.63	85.21	106.00
2	D	801	FAD	C4-N3-C2	-10.29	107.36	125.64
2	D	801	FAD	C4-C4X-N5	9.48	131.30	118.21
4	B	901	MES	O3S-S-C8	-9.12	88.17	106.00
4	B	901	MES	O2S-S-C8	-8.75	93.51	106.73
2	D	801	FAD	C4X-C4-N3	8.25	134.25	113.25
2	D	801	FAD	O4B-C1B-N9A	8.15	123.75	108.09
2	C	801	FAD	C4A-N9A-C8A	7.37	113.48	105.74
4	B	901	MES	C5-N4-C3	7.12	124.18	108.84
4	C	901	MES	C5-N4-C3	6.41	122.64	108.84
2	D	801	FAD	C4A-N9A-C8A	6.33	112.39	105.74
2	D	801	FAD	O4-C4-C4X	-5.76	111.33	126.53
2	C	801	FAD	N9A-C8A-N7A	-5.73	105.81	113.94
2	D	801	FAD	C4-C4X-C10	-5.46	107.58	116.93
2	B	801	FAD	C4-N3-C2	-5.43	116.00	125.64
2	C	801	FAD	C4-C4X-N5	5.25	125.46	118.21
2	B	801	FAD	C4-C4X-N5	4.95	125.04	118.21
4	C	901	MES	O1-C2-C3	-4.88	101.25	111.77
2	C	801	FAD	N3A-C2A-N1A	-4.88	121.20	128.58
2	B	801	FAD	O4-C4-C4X	-4.87	113.69	126.53
2	B	801	FAD	C4X-C4-N3	4.84	125.57	113.25
4	B	901	MES	O3S-S-O2S	4.77	123.32	111.40
2	A	801	FAD	C2A-N1A-C6A	4.49	126.11	118.73
2	A	801	FAD	C4A-C5A-N7A	-4.42	105.52	110.58
2	B	801	FAD	C4A-N9A-C8A	4.38	110.34	105.74
2	C	801	FAD	C2B-C1B-N9A	4.28	123.94	113.30
2	D	801	FAD	O2A-PA-O1A	4.25	132.22	112.44
2	A	801	FAD	C6A-C5A-C4A	4.25	122.97	117.18
2	D	801	FAD	O4B-C4B-C5B	4.17	122.68	109.33
2	B	801	FAD	N3A-C2A-N1A	-4.14	122.31	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	901	MES	O1S-S-C8	-4.14	100.47	106.73
2	C	801	FAD	N3A-C4A-N9A	4.13	134.18	127.17
2	B	801	FAD	C5A-C4A-N3A	-4.10	121.07	126.72
2	C	801	FAD	O2'-C2'-C3'	4.03	118.69	109.25
2	B	801	FAD	N3A-C4A-N9A	4.01	133.99	127.17
2	D	801	FAD	N3-C2-N1	3.90	127.79	119.50
2	D	801	FAD	O2B-C2B-C3B	3.80	124.00	111.82
2	B	801	FAD	C2B-C3B-C4B	3.69	109.74	102.61
2	A	801	FAD	C2B-C1B-N9A	3.69	122.47	113.30
2	A	801	FAD	O4B-C1B-N9A	3.68	115.17	108.09
2	D	801	FAD	N9A-C8A-N7A	-3.68	108.72	113.94
2	B	801	FAD	N9A-C8A-N7A	-3.64	108.77	113.94
2	A	801	FAD	N6A-C6A-N1A	3.63	126.47	118.38
2	A	801	FAD	N9A-C8A-N7A	-3.58	108.85	113.94
2	A	801	FAD	C4-C4X-N5	3.58	123.15	118.21
2	A	801	FAD	N3A-C2A-N1A	-3.56	123.19	128.58
2	C	801	FAD	C1B-N9A-C8A	-3.53	119.26	127.09
2	C	801	FAD	O4B-C1B-N9A	3.51	114.82	108.09
2	A	801	FAD	C7M-C7-C6	-3.45	113.49	119.57
2	D	801	FAD	N3A-C2A-N1A	-3.43	123.39	128.58
4	B	901	MES	O1S-S-C8	-3.42	101.56	106.73
2	A	801	FAD	C4A-N9A-C8A	3.35	109.26	105.74
2	D	801	FAD	O2B-C2B-C1B	3.34	121.59	110.10
2	D	801	FAD	O4-C4-N3	-3.33	113.85	120.11
4	C	901	MES	C7-N4-C5	3.33	120.10	111.24
2	A	801	FAD	C5A-N7A-C8A	3.28	108.61	103.45
2	D	801	FAD	C5B-C4B-C3B	3.25	126.92	115.21
2	A	801	FAD	O4-C4-C4X	-3.17	118.16	126.53
2	C	801	FAD	O2B-C2B-C3B	3.15	121.92	111.82
2	C	801	FAD	C5A-N7A-C8A	3.15	108.40	103.45
2	A	801	FAD	O3B-C3B-C4B	3.13	120.07	111.08
2	C	801	FAD	O2B-C2B-C1B	3.08	120.72	110.10
4	C	901	MES	C2-C3-N4	3.08	114.80	110.12
2	D	801	FAD	N3A-C4A-N9A	3.04	132.33	127.17
2	B	801	FAD	O4B-C1B-C2B	3.01	113.05	106.62
2	B	801	FAD	C4-C4X-C10	-2.98	111.82	116.93
2	B	801	FAD	C2A-N3A-C4A	2.97	119.09	111.83
4	C	901	MES	O3S-S-O1S	2.94	118.76	111.40
2	A	801	FAD	C5A-C6A-N1A	-2.93	110.06	117.51
2	B	801	FAD	O2-C2-N1	-2.91	116.96	121.80
2	C	801	FAD	C5A-C4A-N9A	-2.90	102.65	105.81
2	D	801	FAD	C2B-C1B-N9A	2.88	120.45	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O3P-PA-O1A	-2.88	102.05	110.70
2	D	801	FAD	O5'-P-O1P	-2.88	97.54	108.94
2	B	801	FAD	O2P-P-O3P	-2.84	99.60	107.27
4	C	901	MES	O2S-S-C8	-2.83	102.45	106.73
2	D	801	FAD	C1B-N9A-C8A	-2.82	120.84	127.09
2	A	801	FAD	C5A-C4A-N3A	-2.80	122.87	126.72
2	C	801	FAD	C4X-C4-N3	2.79	120.35	113.25
2	C	801	FAD	C10-C4X-N5	-2.77	119.16	124.81
2	D	801	FAD	O2A-PA-O3P	2.75	114.71	107.27
2	C	801	FAD	O4-C4-C4X	-2.75	119.27	126.53
2	D	801	FAD	O3P-P-O1P	2.71	118.85	110.70
2	C	801	FAD	O4B-C4B-C3B	2.65	110.41	105.15
2	C	801	FAD	C4-N3-C2	-2.62	121.00	125.64
2	C	801	FAD	C5A-C4A-N3A	-2.58	123.17	126.72
2	A	801	FAD	O4'-C4'-C3'	2.57	115.26	109.25
2	D	801	FAD	O5B-PA-O1A	-2.55	98.84	108.94
2	D	801	FAD	C5A-C4A-N9A	-2.54	103.04	105.81
2	D	801	FAD	C7M-C7-C6	-2.51	115.14	119.57
2	C	801	FAD	C2A-N3A-C4A	2.49	117.92	111.83
2	B	801	FAD	O3B-C3B-C4B	2.49	118.22	111.08
4	B	901	MES	C7-N4-C3	2.47	117.83	111.24
2	D	801	FAD	C5X-C6-C7	-2.45	116.28	120.83
4	B	901	MES	C7-N4-C5	2.41	117.67	111.24
2	B	801	FAD	C2B-C1B-N9A	2.40	119.28	113.30
2	A	801	FAD	O2B-C2B-C1B	2.40	118.36	110.10
2	C	801	FAD	O2A-PA-O3P	2.39	113.73	107.27
2	B	801	FAD	O3P-P-O1P	2.38	117.86	110.70
2	B	801	FAD	C6A-C5A-C4A	2.38	120.42	117.18
2	A	801	FAD	C4X-C4-N3	2.38	119.31	113.25
2	D	801	FAD	O2-C2-N3	-2.37	114.03	118.58
4	C	901	MES	O3S-S-O2S	2.37	117.33	111.40
2	B	801	FAD	O2B-C2B-C3B	2.36	119.38	111.82
2	B	801	FAD	N3-C2-N1	2.25	124.29	119.50
2	A	801	FAD	O2B-C2B-C3B	2.23	118.96	111.82
2	D	801	FAD	C10-C4X-N5	-2.22	120.27	124.81
2	D	801	FAD	O2-C2-N1	-2.21	118.13	121.80
2	C	801	FAD	N6A-C6A-N1A	-2.20	113.48	118.38
2	B	801	FAD	O2B-C2B-C1B	2.20	117.67	110.10
2	D	801	FAD	C8M-C8-C9	-2.18	115.73	119.57
2	C	801	FAD	C4X-C10-N10	2.18	119.60	116.48
2	A	801	FAD	C10-N1-C2	2.17	121.55	116.85
2	D	801	FAD	C6A-C5A-C4A	2.16	120.13	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	C5A-C6A-N6A	2.16	128.64	123.29
2	D	801	FAD	C10-N1-C2	2.16	121.52	116.85
4	C	901	MES	C6-O1-C2	-2.10	103.08	109.88
2	D	801	FAD	O3B-C3B-C4B	2.10	117.11	111.08
2	A	801	FAD	O2P-P-O3P	-2.07	101.68	107.27
2	C	801	FAD	O3B-C3B-C4B	2.05	116.97	111.08
2	A	801	FAD	C1B-N9A-C8A	-2.05	122.56	127.09
4	C	901	MES	O2S-S-O1S	2.04	120.45	113.82
2	A	801	FAD	C2B-C3B-C4B	2.04	106.54	102.61
4	C	901	MES	C7-N4-C3	2.03	116.65	111.24
2	A	801	FAD	O2-C2-N1	-2.02	118.44	121.80
2	B	801	FAD	C5A-N7A-C8A	2.02	106.62	103.45
2	A	801	FAD	C9-C8-C7	-2.01	116.74	119.69
2	B	801	FAD	C8M-C8-C9	-2.01	116.03	119.57

There are no chirality outliers.

All (18) torsion outliers are listed below:

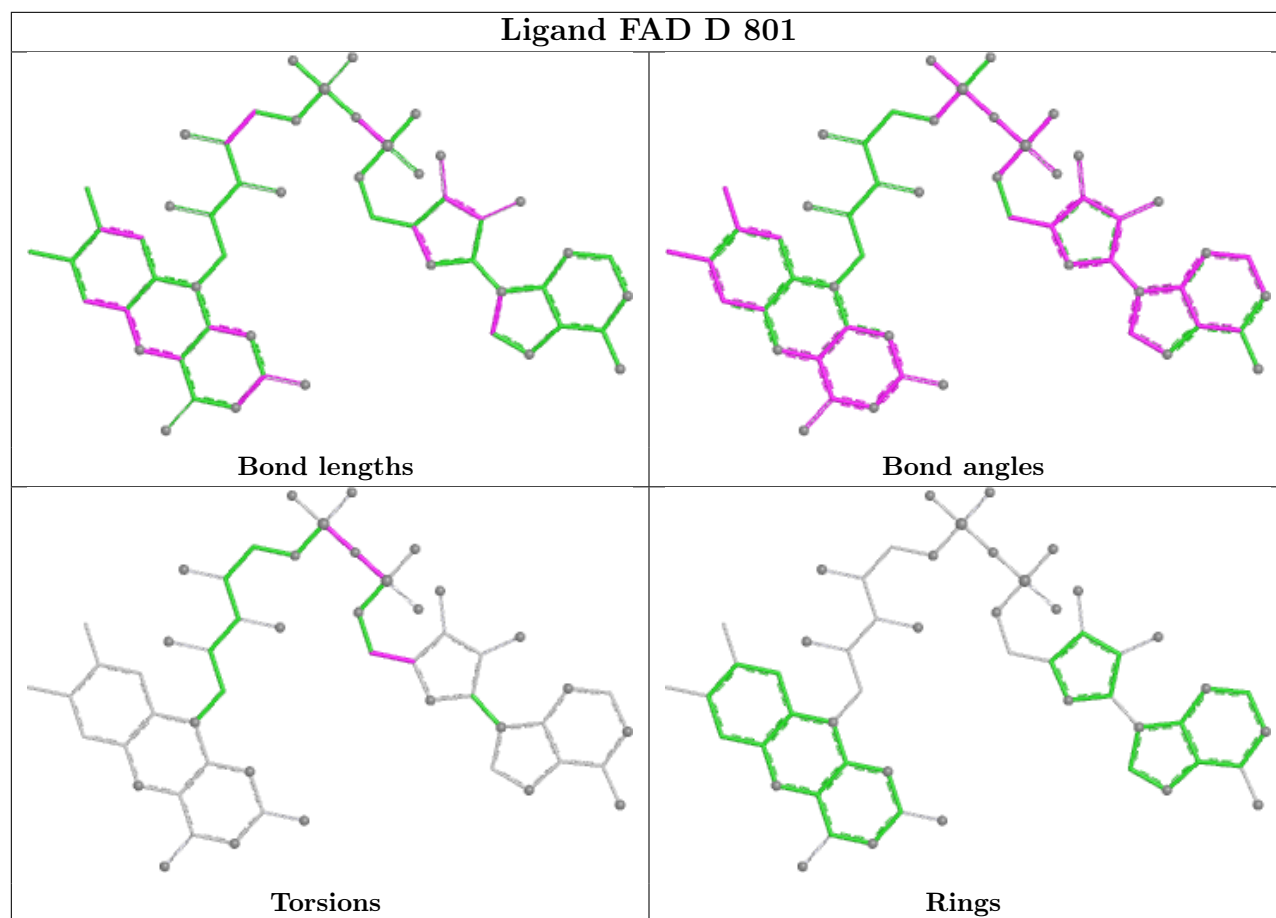
Mol	Chain	Res	Type	Atoms
2	C	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
4	B	901	MES	C8-C7-N4-C5
4	B	901	MES	N4-C7-C8-S
4	C	901	MES	C8-C7-N4-C5
4	C	901	MES	N4-C7-C8-S
2	D	801	FAD	O4B-C4B-C5B-O5B
3	A	905	1PE	OH6-C15-C25-OH5
3	D	903	1PE	OH5-C14-C24-OH4
2	A	801	FAD	PA-O3P-P-O5'
3	D	903	1PE	OH7-C16-C26-OH6
3	A	904	1PE	OH6-C15-C25-OH5
3	A	905	1PE	OH5-C14-C24-OH4
3	B	902	1PE	OH5-C14-C24-OH4
2	A	801	FAD	P-O3P-PA-O2A
2	C	801	FAD	P-O3P-PA-O2A
2	D	801	FAD	P-O3P-PA-O2A
3	A	904	1PE	OH7-C16-C26-OH6

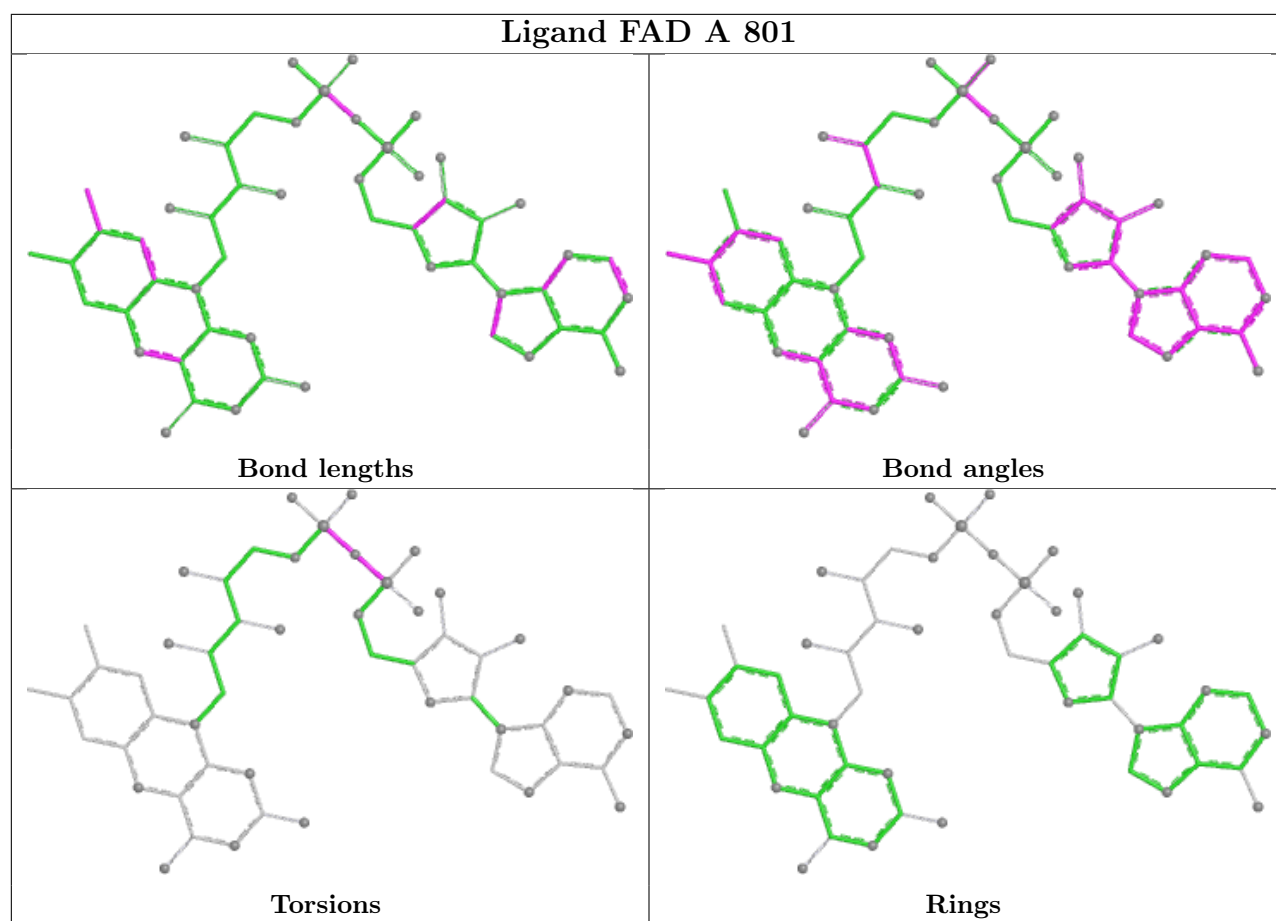
There are no ring outliers.

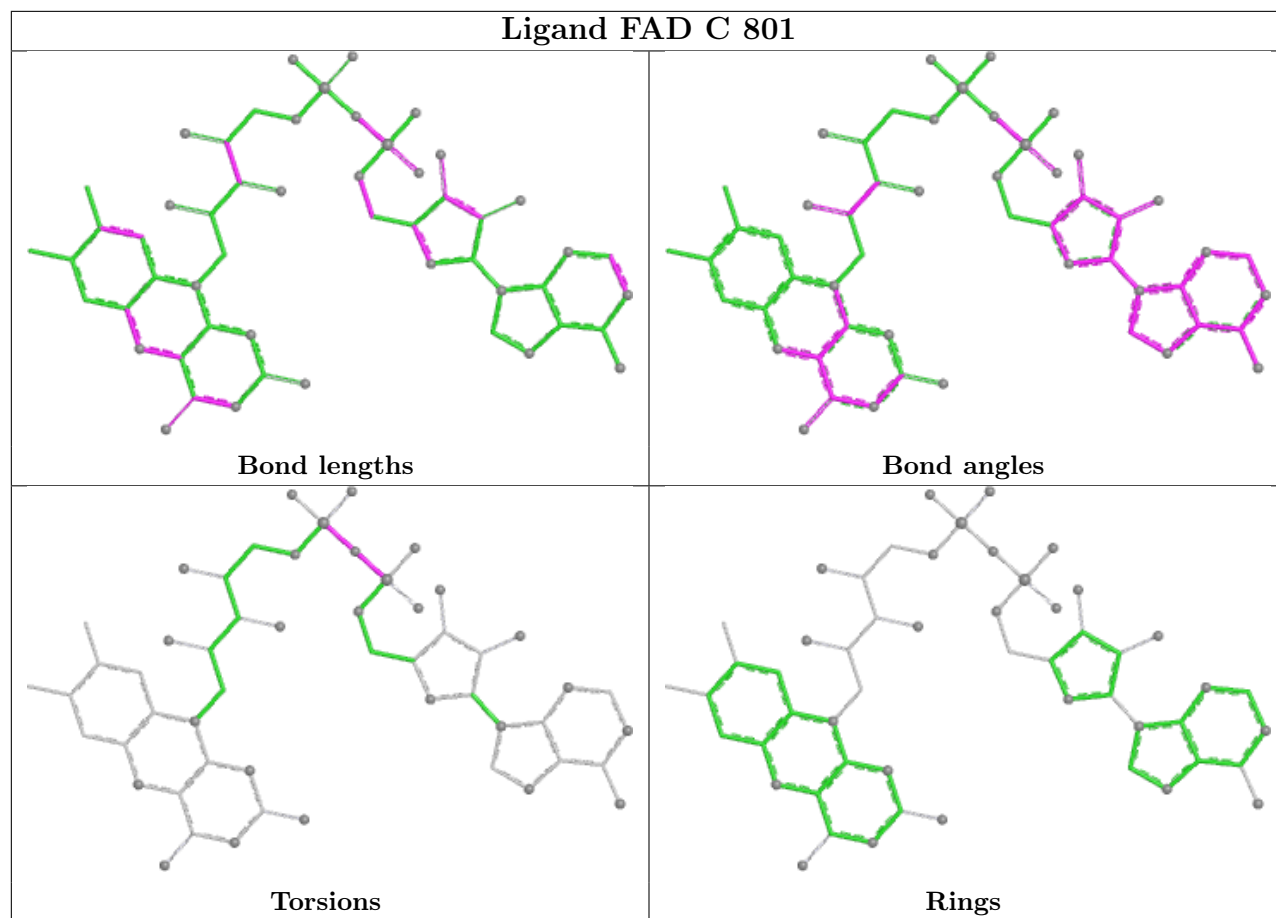
3 monomers are involved in 17 short contacts:

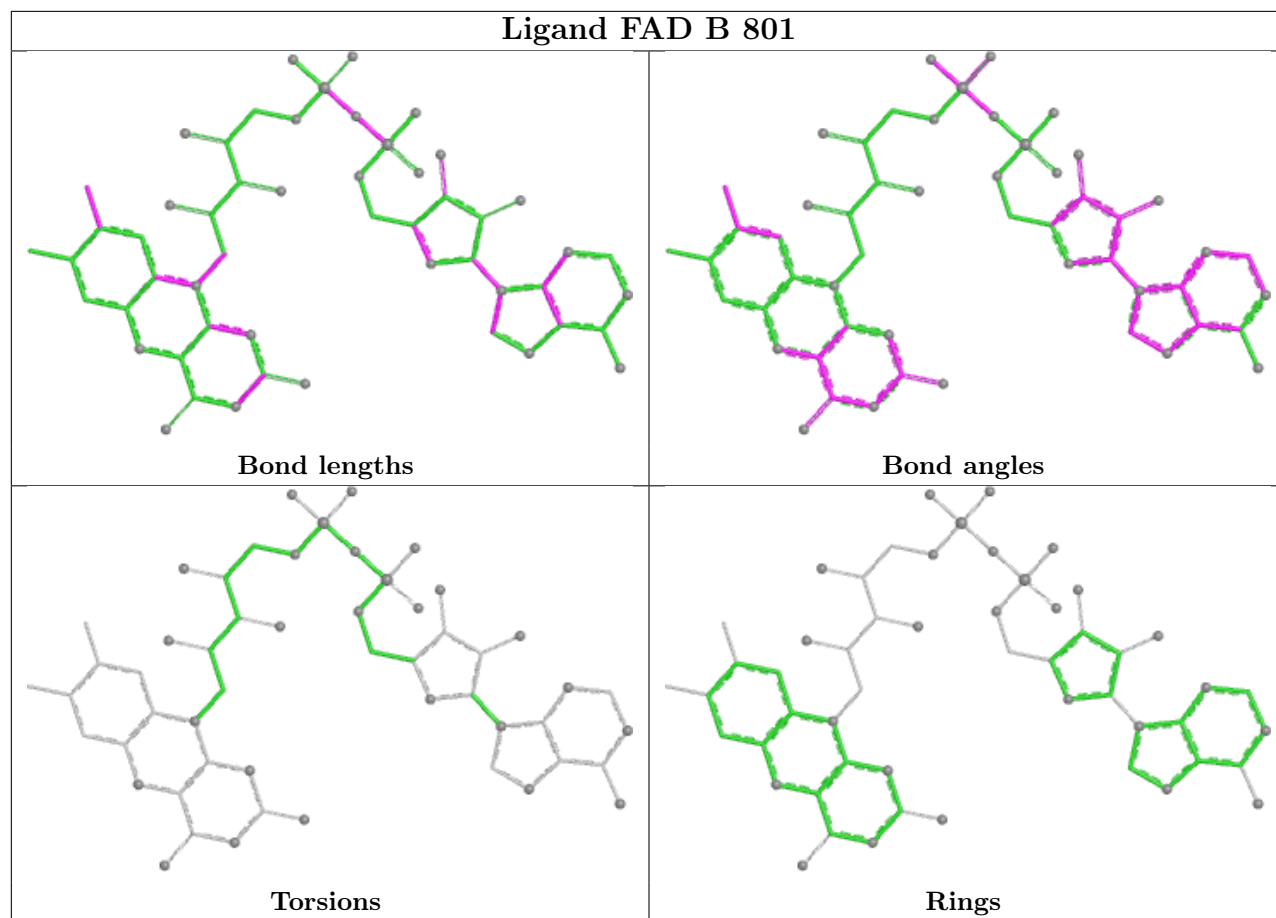
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	FAD	1	0
4	B	901	MES	3	0
4	C	901	MES	13	0

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	576/623 (92%)	-0.00	23 (3%) 42 46	4, 10, 24, 40	0
1	B	576/623 (92%)	-0.14	14 (2%) 59 64	4, 10, 22, 45	0
1	C	575/623 (92%)	0.11	15 (2%) 57 61	6, 13, 28, 39	0
1	D	574/623 (92%)	1.35	143 (24%) 2 1	3, 14, 24, 40	0
All	All	2301/2492 (92%)	0.33	195 (8%) 16 17	3, 12, 25, 45	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	459	VAL	7.3
1	D	290	ALA	6.1
1	C	45	ILE	5.9
1	C	458	ALA	5.7
1	A	459	VAL	5.4
1	D	618	PHE	5.4
1	A	343	ALA	5.2
1	D	367	VAL	5.2
1	D	537	LEU	5.2
1	B	458	ALA	5.1
1	D	385	THR	4.9
1	D	343	ALA	4.9
1	D	617	PRO	4.9
1	D	556	GLY	4.8
1	D	184	VAL	4.7
1	D	469	VAL	4.6
1	D	467	LEU	4.6
1	B	459	VAL	4.4
1	D	221	LEU	4.4
1	D	222	VAL	4.4
1	D	532	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	533	LEU	4.3
1	D	346	PRO	4.3
1	D	471	TRP	4.2
1	D	468	ILE	4.1
1	D	82	SER	4.1
1	D	211	ASP	4.0
1	D	458	ALA	4.0
1	D	312	LYS	4.0
1	D	217	ILE	3.9
1	D	364	CYS	3.9
1	D	368	MET	3.8
1	B	44	ASP	3.8
1	D	226	LEU	3.8
1	D	369	SER	3.8
1	D	366	THR	3.8
1	A	344	ASN	3.7
1	D	465	SER	3.7
1	A	45	ILE	3.7
1	C	343	ALA	3.7
1	B	45	ILE	3.6
1	D	457	GLY	3.6
1	C	389	LEU	3.6
1	D	77	ILE	3.5
1	D	463	ILE	3.5
1	D	309	PHE	3.5
1	D	228	GLU	3.5
1	A	381	THR	3.5
1	D	535	GLY	3.5
1	D	80	ILE	3.4
1	D	462	SER	3.4
1	A	457	GLY	3.4
1	C	619	THR	3.4
1	D	190	ALA	3.4
1	D	47	TYR	3.3
1	C	390	THR	3.3
1	D	291	LEU	3.3
1	D	540	PHE	3.3
1	C	381	THR	3.3
1	D	296	GLU	3.2
1	D	314	ASP	3.2
1	A	82	SER	3.2
1	D	536	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	459	VAL	3.2
1	D	338	GLY	3.1
1	A	394	THR	3.1
1	D	210	THR	3.1
1	C	618	PHE	3.1
1	D	251	VAL	3.0
1	D	304	ILE	3.0
1	A	458	ALA	3.0
1	A	345	PRO	3.0
1	B	457	GLY	3.0
1	D	59	CYS	3.0
1	D	611	GLN	3.0
1	D	616	SER	3.0
1	D	232	GLY	3.0
1	D	83	GLY	2.9
1	D	473	PHE	2.9
1	D	55	GLY	2.9
1	D	490	LYS	2.8
1	D	316	TYR	2.8
1	D	456	TYR	2.8
1	D	84	LEU	2.8
1	D	295	ILE	2.8
1	A	490	LYS	2.8
1	A	44	ASP	2.8
1	D	156	ALA	2.7
1	D	253	TRP	2.7
1	A	362	VAL	2.7
1	D	219	HIS	2.7
1	D	523	CYS	2.7
1	D	606	CYS	2.7
1	D	370	THR	2.7
1	D	527	ALA	2.7
1	D	386	PRO	2.7
1	D	250	PHE	2.7
1	B	232	GLY	2.7
1	A	383	ARG	2.6
1	D	365	GLN	2.6
1	D	526	SER	2.6
1	A	401	THR	2.6
1	D	387	GLY	2.6
1	D	57	ILE	2.6
1	D	529	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	313	ALA	2.6
1	D	492	THR	2.6
1	D	524	VAL	2.6
1	C	344	ASN	2.6
1	D	289	ASN	2.6
1	D	101	ASP	2.5
1	D	538	PRO	2.5
1	D	78	GLY	2.5
1	D	268	THR	2.5
1	D	214	LYS	2.5
1	D	363	PHE	2.5
1	A	342	PRO	2.5
1	D	270	ALA	2.5
1	A	618	PHE	2.5
1	D	223	LEU	2.5
1	D	361	LEU	2.5
1	D	310	GLU	2.5
1	D	272	GLU	2.4
1	D	429	GLU	2.4
1	B	43	MET	2.4
1	D	615	PRO	2.4
1	D	45	ILE	2.4
1	D	287	VAL	2.4
1	D	311	ILE	2.4
1	D	579	PHE	2.4
1	D	362	VAL	2.4
1	D	154	GLY	2.4
1	D	220	ASN	2.4
1	D	545	LEU	2.4
1	C	382	ILE	2.4
1	D	330	VAL	2.4
1	D	171	ALA	2.3
1	D	186	ASP	2.3
1	B	618	PHE	2.3
1	D	557	PHE	2.3
1	D	70	TYR	2.3
1	A	382	ILE	2.3
1	D	52	VAL	2.3
1	D	461	GLN	2.3
1	D	566	VAL	2.3
1	D	464	ASP	2.3
1	D	342	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	328	LEU	2.3
1	A	463	ILE	2.3
1	D	224	ASN	2.3
1	C	388	GLU	2.3
1	D	388	GLU	2.3
1	D	50	VAL	2.3
1	D	335	GLY	2.3
1	D	530	GLY	2.3
1	B	460	GLN	2.3
1	D	297	SER	2.2
1	D	406	ASP	2.2
1	C	457	GLY	2.2
1	D	613	PHE	2.2
1	A	393	VAL	2.2
1	B	310	GLU	2.2
1	D	243	ALA	2.2
1	D	76	ASP	2.2
1	D	269	ASP	2.2
1	D	525	MET	2.2
1	D	69	GLY	2.2
1	D	347	GLU	2.2
1	A	454	PHE	2.2
1	D	278	PHE	2.2
1	D	241	LEU	2.2
1	B	342	PRO	2.2
1	B	452	ASP	2.1
1	D	48	ASP	2.1
1	D	51	ILE	2.1
1	D	466	ARG	2.1
1	D	472	ARG	2.1
1	D	66	VAL	2.1
1	D	470	ASP	2.1
1	D	345	PRO	2.1
1	C	384	GLY	2.1
1	D	528	LYS	2.1
1	B	269	ASP	2.1
1	D	568	THR	2.1
1	D	340	PRO	2.1
1	D	201	LYS	2.1
1	D	609	ILE	2.1
1	A	418	GLN	2.0
1	A	461	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	302	ASP	2.0
1	B	185	LYS	2.0
1	D	333	GLY	2.0
1	D	384	GLY	2.0
1	C	188	ALA	2.0
1	D	315	VAL	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](#)

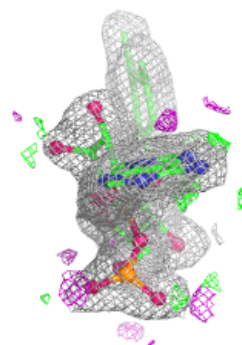
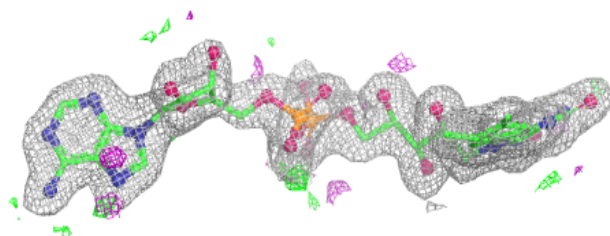
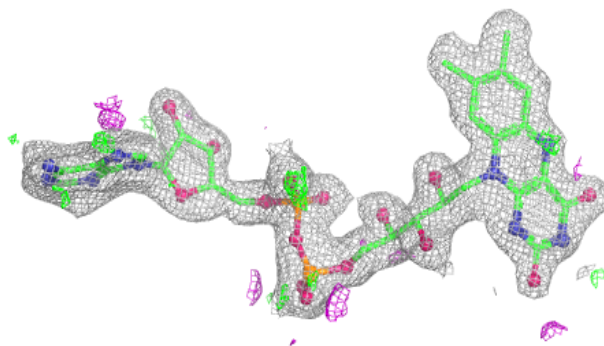
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1PE	A	905	12/16	0.80	0.14	29,31,36,38	0
3	1PE	B	902	16/16	0.86	0.14	35,38,48,55	0
3	1PE	D	903	16/16	0.86	0.14	37,45,51,55	0
3	1PE	A	904	14/16	0.87	0.13	30,35,39,42	0
4	MES	C	901	12/12	0.92	0.09	26,30,32,33	0
4	MES	B	901	12/12	0.95	0.09	24,28,31,31	0
2	FAD	D	801	53/53	0.95	0.08	19,24,29,31	0
2	FAD	C	801	53/53	0.97	0.06	13,17,21,23	0
2	FAD	A	801	53/53	0.98	0.05	8,12,16,19	0
2	FAD	B	801	53/53	0.98	0.05	10,12,15,18	0

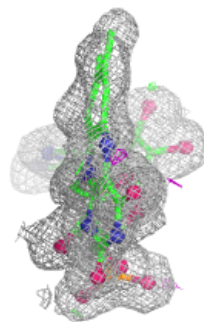
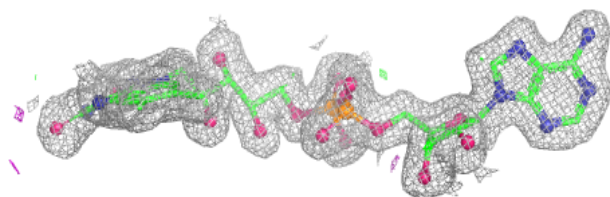
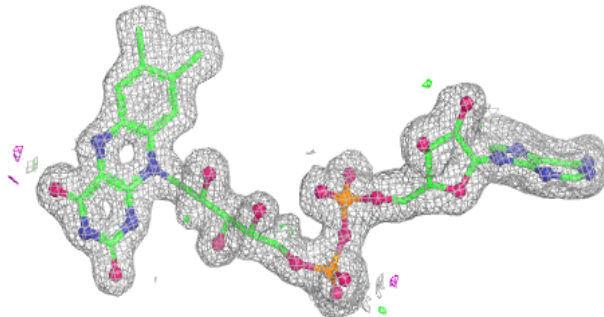
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 801:

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

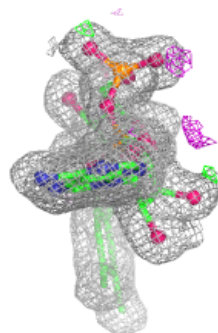
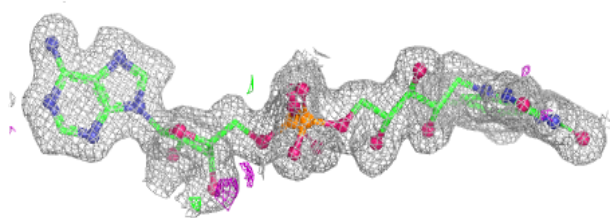
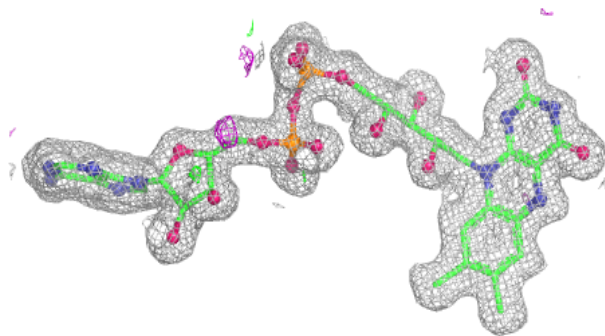
**Electron density around FAD C 801:**

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

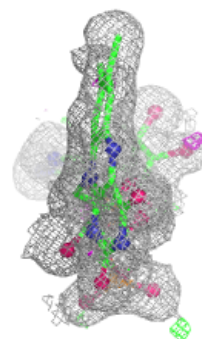
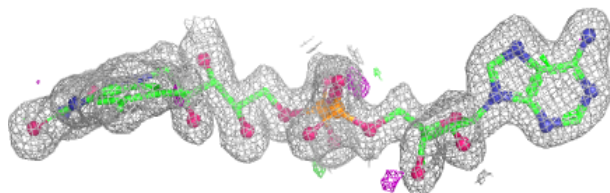
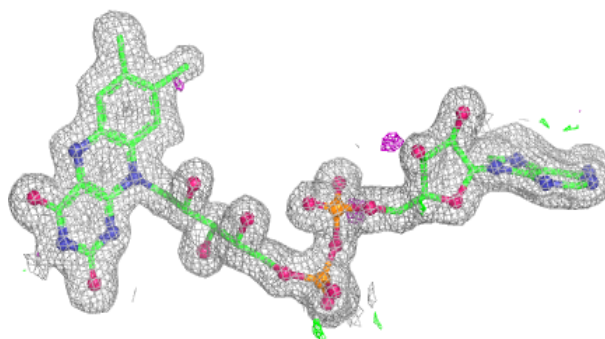


Electron density around FAD A 801:

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

**Electron density around FAD B 801:**

$2mF_o-DF_c$ (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.