



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:10 AM UTC

PDB ID : 3M13 / pdb_00003m13
Title : Crystal Structure of the Lys265Arg PEG-crystallized mutant of monomeric sarcosine oxidase
Authors : Mathews, F.S.; Chen, Z.-W.; Jorns, M.S.
Deposited on : 2010-03-04
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

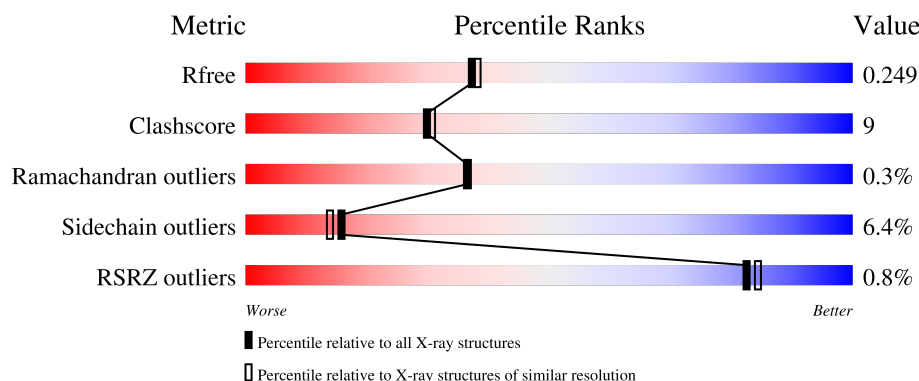
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	389	
1	B	389	
1	C	389	
1	D	389	

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	PO4	D	390	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12635 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.

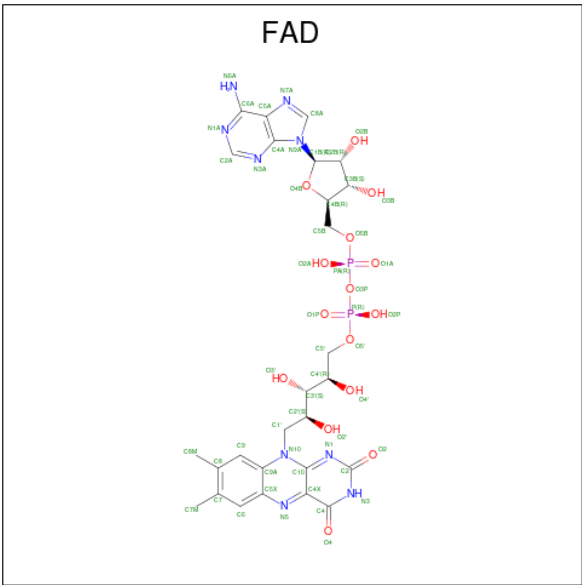
- Molecule 1 is a protein called Monomeric sarcosine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			
1	B	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			
1	C	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			
1	D	381	Total	C	N	O	S	0	0	0
			2978	1897	502	569	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ARG	LYS	engineered mutation	UNP P40859
B	265	ARG	LYS	engineered mutation	UNP P40859
C	265	ARG	LYS	engineered mutation	UNP P40859
D	265	ARG	LYS	engineered mutation	UNP P40859

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

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

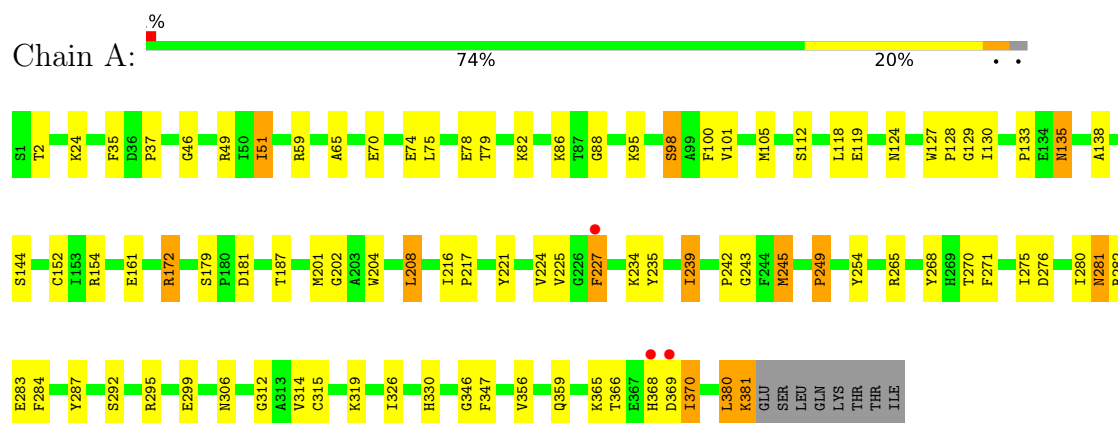
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		
5	B	87	Total	O	0	0
			87	87		
5	C	77	Total	O	0	0
			77	77		
5	D	139	Total	O	0	0
			139	139		

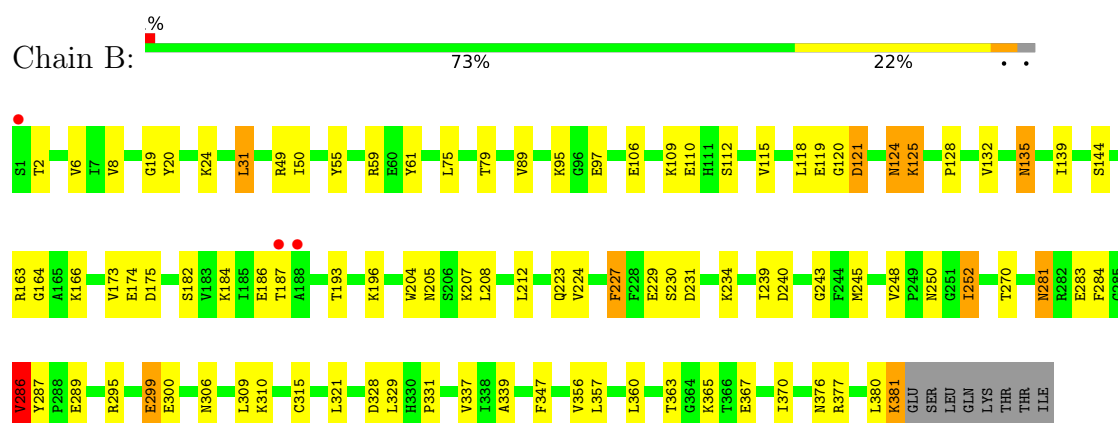
3 Residue-property plots

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.

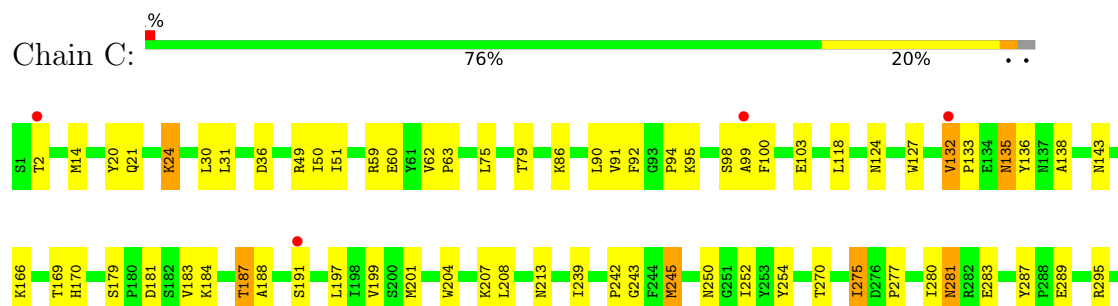
• Molecule 1: Monomeric sarcosine oxidase

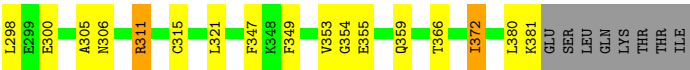


• Molecule 1: Monomeric sarcosine oxidase

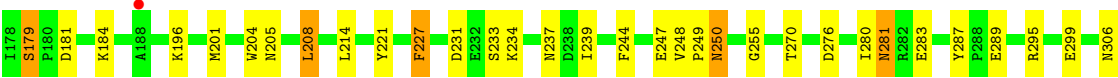
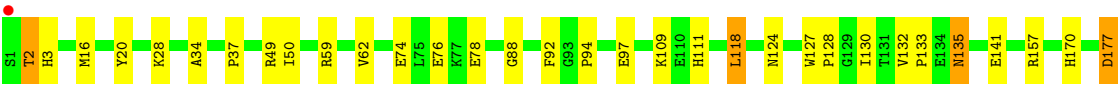
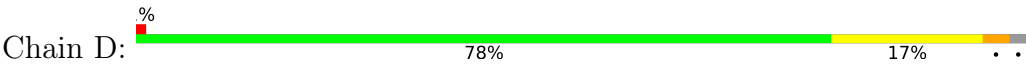


• Molecule 1: Monomeric sarcosine oxidase





● Molecule 1: Monomeric sarcosine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 69.30Å 111.43Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	29.20 – 2.10 29.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.20-2.10) 94.8 (29.20-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.187 , 0.248 0.186 , 0.249	Depositor DCC
R_{free} test set	4212 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12635	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CL, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.52	20/3053 (0.7%)	1.34	19/4135 (0.5%)
1	B	1.15	5/3053 (0.2%)	1.21	12/4135 (0.3%)
1	C	1.16	4/3053 (0.1%)	1.14	7/4135 (0.2%)
1	D	1.38	11/3053 (0.4%)	1.25	10/4135 (0.2%)
All	All	1.31	40/12212 (0.3%)	1.24	48/16540 (0.3%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	PHE	N-CA	7.69	1.56	1.46
1	A	280	ILE	CA-CB	6.62	1.61	1.54
1	A	51	ILE	CA-CB	6.59	1.62	1.54
1	A	370	ILE	N-CA	6.56	1.54	1.46
1	A	369	ASP	C-O	6.50	1.31	1.24
1	D	280	ILE	CA-CB	6.33	1.61	1.54
1	A	138	ALA	CA-C	-6.24	1.45	1.52
1	B	252	ILE	CA-CB	6.14	1.61	1.54
1	D	128	PRO	C-O	6.08	1.31	1.23
1	A	225	VAL	C-O	-6.00	1.17	1.23
1	A	161	GLU	C-O	-5.98	1.17	1.24
1	A	330	HIS	CA-C	5.98	1.59	1.53
1	A	88	GLY	N-CA	5.96	1.52	1.45
1	C	50	ILE	CA-CB	5.94	1.61	1.54
1	D	339	ALA	CA-CB	5.91	1.62	1.53
1	D	237	ASN	CA-C	5.81	1.60	1.52
1	A	187	THR	CA-CB	5.79	1.64	1.53
1	D	340	ALA	CA-CB	5.59	1.64	1.53
1	D	248	VAL	CA-C	5.58	1.58	1.52
1	A	249	PRO	C-O	-5.54	1.16	1.24
1	A	217	PRO	CA-C	5.50	1.59	1.52
1	A	152	CYS	CA-C	-5.49	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	LYS	N-CA	-5.48	1.39	1.46
1	D	92	PHE	CA-C	5.47	1.59	1.52
1	A	65	ALA	CA-CB	5.46	1.61	1.53
1	A	37	PRO	C-O	-5.41	1.20	1.24
1	D	50	ILE	CA-CB	5.38	1.60	1.54
1	B	223	GLN	C-O	5.37	1.30	1.24
1	A	98	SER	CA-C	-5.31	1.47	1.53
1	C	132	VAL	CA-C	5.31	1.58	1.52
1	B	50	ILE	CA-CB	5.30	1.61	1.54
1	D	37	PRO	CA-C	5.28	1.57	1.52
1	A	245	MET	N-CA	-5.28	1.40	1.46
1	D	375	ILE	CA-C	5.25	1.58	1.52
1	A	235	TYR	N-CA	5.24	1.53	1.46
1	B	248	VAL	CA-C	5.14	1.58	1.52
1	C	354	GLY	N-CA	5.13	1.52	1.45
1	D	20	TYR	C-O	5.08	1.29	1.24
1	B	128	PRO	C-O	5.03	1.29	1.23
1	C	51	ILE	CA-CB	5.02	1.61	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ASP	N-CA-C	11.13	122.98	111.07
1	B	286	VAL	CB-CA-C	-10.47	95.93	112.16
1	A	346	GLY	N-CA-C	7.21	123.60	114.66
1	D	2	THR	N-CA-C	7.07	120.39	108.23
1	D	179	SER	CA-C-N	-7.01	112.58	119.87
1	D	179	SER	C-N-CA	-7.01	112.58	119.87
1	B	289	GLU	CB-CA-C	-7.00	99.17	110.79
1	D	276	ASP	N-CA-C	-6.84	100.88	110.31
1	A	243	GLY	N-CA-C	-6.68	103.60	112.82
1	B	243	GLY	N-CA-C	-6.67	103.62	112.82
1	A	370	ILE	N-CA-C	6.61	123.09	109.34
1	A	129	GLY	N-CA-C	-6.55	106.13	113.79
1	A	287	TYR	CA-C-N	-6.05	113.45	119.56
1	A	287	TYR	C-N-CA	-6.05	113.45	119.56
1	D	88	GLY	N-CA-C	-5.85	105.40	112.48
1	A	119	GLU	N-CA-C	5.79	118.08	108.99
1	B	212	LEU	N-CA-C	-5.75	103.62	111.56
1	C	347	PHE	N-CA-CB	5.67	118.45	110.12
1	C	243	GLY	N-CA-C	-5.60	105.09	112.82
1	A	154	ARG	N-CA-CB	-5.53	101.99	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ASP	N-CA-C	-5.51	101.82	110.14
1	A	128	PRO	CA-C-N	-5.45	116.96	123.44
1	A	128	PRO	C-N-CA	-5.45	116.96	123.44
1	B	287	TYR	CA-C-N	-5.40	114.11	119.56
1	B	287	TYR	C-N-CA	-5.40	114.11	119.56
1	D	356	VAL	N-CA-C	5.38	116.01	110.36
1	A	46	GLY	N-CA-C	-5.37	107.80	115.64
1	D	233	SER	N-CA-C	-5.37	106.56	113.01
1	A	326	ILE	CB-CA-C	-5.34	103.19	110.77
1	A	216	ILE	CA-C-N	-5.33	114.07	119.83
1	A	216	ILE	C-N-CA	-5.33	114.07	119.83
1	A	380	LEU	CA-C-N	5.33	131.29	121.70
1	A	380	LEU	C-N-CA	5.33	131.29	121.70
1	D	118	LEU	CA-CB-CG	5.30	134.86	116.30
1	B	175	ASP	N-CA-C	5.22	117.01	109.07
1	C	36	ASP	CA-C-N	5.20	125.73	120.38
1	C	36	ASP	C-N-CA	5.20	125.73	120.38
1	B	182	SER	N-CA-C	5.12	116.07	108.60
1	C	275	ILE	N-CA-C	5.12	115.06	108.82
1	B	61	TYR	N-CA-C	5.10	116.84	111.28
1	A	292	SER	N-CA-C	5.08	116.89	111.36
1	C	14	MET	CA-C-N	5.05	125.70	119.99
1	C	14	MET	C-N-CA	5.05	125.70	119.99
1	D	127	TRP	CA-C-N	-5.04	114.76	119.90
1	D	127	TRP	C-N-CA	-5.04	114.76	119.90
1	B	2	THR	N-CA-C	5.04	116.90	107.99
1	B	119	GLU	N-CA-C	5.01	116.45	108.79
1	B	240	ASP	N-CA-C	5.01	118.97	112.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2978	0	2881	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2978	0	2881	47	0
1	C	2978	0	2881	59	0
1	D	2978	0	2881	46	0
2	A	53	0	31	7	0
2	B	53	0	31	7	0
2	C	53	0	31	6	0
2	D	53	0	31	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	5	0
5	A	194	0	0	3	1
5	B	87	0	0	2	0
5	C	77	0	0	6	0
5	D	139	0	0	2	0
All	All	12635	0	11648	203	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (203) 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:A:315:CYS:SG	2:A:400:FAD:HM82	1.29	1.67
1:B:315:CYS:SG	2:B:400:FAD:HM82	1.40	1.61
1:C:315:CYS:SG	2:C:400:FAD:HM82	1.49	1.52
1:D:315:CYS:SG	2:D:400:FAD:HM81	1.70	1.31
1:A:315:CYS:SG	2:A:400:FAD:C8M	2.21	1.28
1:D:315:CYS:SG	2:D:400:FAD:C8M	2.31	1.18
1:B:315:CYS:SG	2:B:400:FAD:C8M	2.32	1.16
1:C:315:CYS:SG	2:C:400:FAD:C8M	2.42	1.07
1:A:381:LYS:HG3	5:A:530:HOH:O	1.70	0.89
1:B:124:ASN:HD21	1:B:132:VAL:HG22	1.37	0.89
1:C:381:LYS:HG3	5:C:406:HOH:O	1.72	0.88
1:A:95:LYS:HZ2	1:A:95:LYS:HB3	1.40	0.86
1:C:281:ASN:HD22	1:C:283:GLU:H	1.27	0.82
1:B:331:PRO:HB3	1:B:376:ASN:HD21	1.46	0.79
1:A:95:LYS:HB3	1:A:95:LYS:NZ	1.93	0.79
1:D:315:CYS:SG	2:D:400:FAD:HM83	2.24	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:HIS:O	1:D:28:LYS:NZ	2.17	0.76
1:C:100:PHE:CZ	1:C:245:MET:HG2	2.22	0.74
1:B:173:VAL:HG22	1:B:187:THR:HG22	1.71	0.72
1:A:227:PHE:CE1	1:A:265:ARG:NE	2.56	0.72
1:C:281:ASN:ND2	1:C:283:GLU:H	1.86	0.72
1:B:315:CYS:HB3	2:B:400:FAD:HM73	1.72	0.70
1:A:135:ASN:H	1:A:135:ASN:HD22	1.38	0.70
1:A:295:ARG:O	1:A:299:GLU:HG2	1.92	0.70
1:C:94:PRO:HD2	1:C:98:SER:HB2	1.76	0.68
1:A:133:PRO:HB2	1:A:135:ASN:ND2	2.09	0.68
1:C:295:ARG:HD3	1:C:306:ASN:HD21	1.60	0.67
1:C:315:CYS:HB3	2:C:400:FAD:HM73	1.76	0.67
1:B:295:ARG:HH11	1:B:306:ASN:ND2	1.92	0.66
1:C:381:LYS:HB3	5:C:419:HOH:O	1.96	0.65
1:D:295:ARG:HH11	1:D:306:ASN:ND2	1.95	0.64
1:B:124:ASN:ND2	1:B:132:VAL:HG22	2.12	0.63
1:A:172:ARG:NH2	1:A:208:LEU:HD21	2.14	0.63
1:B:245:MET:HE2	1:B:252:ILE:HG21	1.81	0.62
1:C:124:ASN:HD21	1:C:132:VAL:HG22	1.64	0.62
1:C:295:ARG:HH11	1:C:306:ASN:ND2	1.97	0.62
1:A:221:TYR:CE2	1:A:319:LYS:HD2	2.34	0.62
1:D:281:ASN:HD22	1:D:283:GLU:H	1.47	0.62
1:C:281:ASN:HD22	1:C:281:ASN:C	2.08	0.61
1:C:381:LYS:CG	5:C:419:HOH:O	2.48	0.61
1:D:62:VAL:HG21	1:D:111:HIS:CE1	2.35	0.61
1:C:95:LYS:HG3	1:C:135:ASN:O	2.00	0.61
1:D:141:GLU:HG3	4:D:390:PO4:O2	2.02	0.60
1:A:281:ASN:HD22	1:A:283:GLU:H	1.47	0.60
1:B:283:GLU:O	1:B:286:VAL:HG22	2.02	0.60
1:C:95:LYS:HZ2	1:C:95:LYS:HB3	1.65	0.60
1:C:381:LYS:HG2	5:C:419:HOH:O	2.02	0.59
1:D:244:PHE:CZ	1:D:255:GLY:HA3	2.38	0.59
1:A:295:ARG:HH11	1:A:306:ASN:ND2	1.99	0.59
1:B:124:ASN:HD21	1:B:132:VAL:H	1.50	0.59
1:C:95:LYS:HB3	1:C:95:LYS:NZ	2.18	0.58
1:C:179:SER:HB3	1:C:181:ASP:OD1	2.03	0.58
1:A:227:PHE:HE1	1:A:265:ARG:HH21	1.51	0.57
1:D:231:ASP:OD1	1:D:234:LYS:HD2	2.04	0.57
1:A:359:GLN:NE2	1:A:366:THR:OG1	2.38	0.56
1:B:8:VAL:HB	1:B:31:LEU:HD23	1.87	0.56
1:B:328:ASP:OD2	1:B:329:LEU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:MET:HE3	1:C:254:TYR:HB3	1.87	0.56
1:A:227:PHE:CD2	1:A:227:PHE:N	2.73	0.56
1:A:368:HIS:ND1	1:A:368:HIS:N	2.54	0.56
1:B:124:ASN:ND2	1:B:132:VAL:H	2.04	0.56
1:D:133:PRO:HB2	1:D:135:ASN:ND2	2.21	0.55
1:C:381:LYS:CB	5:C:419:HOH:O	2.54	0.55
1:C:245:MET:HE2	1:C:252:ILE:CG2	2.37	0.55
1:A:204:TRP:CE3	2:A:400:FAD:H8A	2.42	0.55
1:B:6:VAL:HG22	1:B:196:LYS:HB2	1.88	0.55
1:B:89:VAL:HG23	1:B:144:SER:HB3	1.88	0.54
1:C:287:TYR:HB3	1:C:289:GLU:OE1	2.08	0.54
1:A:124:ASN:ND2	1:A:130:ILE:O	2.41	0.54
1:A:127:TRP:CD1	1:A:242:PRO:HD3	2.42	0.54
1:B:20:TYR:CZ	1:B:24:LYS:HD3	2.42	0.54
1:A:101:VAL:O	1:A:105:MET:HG3	2.08	0.53
1:A:201:MET:HE1	1:A:208:LEU:HB3	1.90	0.53
1:C:21:GLN:HG3	1:C:355:GLU:HA	1.90	0.53
1:A:281:ASN:HD22	1:A:281:ASN:C	2.17	0.53
1:B:75:LEU:O	1:B:79:THR:HG22	2.09	0.53
1:C:100:PHE:HZ	1:C:245:MET:HG2	1.70	0.53
1:B:250:ASN:ND2	5:B:435:HOH:O	2.26	0.53
1:B:207:LYS:HG3	5:B:427:HOH:O	2.08	0.53
1:B:321:LEU:HD12	1:B:381:LYS:HB2	1.91	0.53
1:D:227:PHE:N	1:D:227:PHE:HD2	2.07	0.53
1:B:347:PHE:HB2	2:B:400:FAD:H2'	1.90	0.52
1:C:207:LYS:HD2	1:C:277:PRO:HG2	1.92	0.51
1:C:49:ARG:HD2	2:C:400:FAD:C4X	2.40	0.51
1:D:94:PRO:HB2	1:D:97:GLU:HB2	1.92	0.51
1:A:74:GLU:O	1:A:78:GLU:HG3	2.10	0.51
1:D:141:GLU:OE2	4:D:390:PO4:O2	2.29	0.51
1:C:92:PHE:C	1:C:92:PHE:CD1	2.89	0.51
1:D:227:PHE:N	1:D:227:PHE:CD2	2.79	0.51
1:D:234:LYS:HE2	5:D:507:HOH:O	2.09	0.51
1:D:311:ARG:HB2	1:D:311:ARG:HH11	1.76	0.51
1:B:295:ARG:HH11	1:B:306:ASN:HD21	1.59	0.50
1:A:234:LYS:HE2	5:A:544:HOH:O	2.11	0.50
1:A:315:CYS:SG	2:A:400:FAD:C8	2.98	0.50
1:C:381:LYS:N	1:C:381:LYS:HD2	2.26	0.50
1:B:363:THR:OG1	1:B:365:LYS:HG2	2.12	0.50
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.76	0.50
1:A:172:ARG:HH22	1:A:204:TRP:CD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:O	1:A:79:THR:HG22	2.12	0.49
1:A:133:PRO:HB2	1:A:135:ASN:HD21	1.77	0.49
1:B:229:GLU:OE1	1:B:310:LYS:HD2	2.12	0.49
1:C:90:LEU:HD11	1:C:138:ALA:HB1	1.95	0.49
1:D:74:GLU:O	1:D:78:GLU:HG3	2.13	0.49
1:B:299:GLU:HG2	1:B:300:GLU:N	2.26	0.49
1:D:250:ASN:O	1:D:250:ASN:OD1	2.30	0.49
1:C:199:VAL:CG1	1:C:201:MET:HE2	2.43	0.49
1:C:91:VAL:HA	1:C:245:MET:O	2.13	0.48
1:C:62:VAL:HB	1:C:63:PRO:HD3	1.95	0.48
1:A:201:MET:O	1:A:202:GLY:C	2.56	0.48
1:C:2:THR:HA	5:C:440:HOH:O	2.13	0.48
1:A:98:SER:OG	1:A:101:VAL:HG23	2.13	0.48
1:C:99:ALA:O	1:C:103:GLU:HB2	2.14	0.47
1:B:19:GLY:HA3	1:B:31:LEU:HD21	1.96	0.47
1:A:275:ILE:HD12	1:A:275:ILE:C	2.38	0.47
1:B:95:LYS:HG3	1:B:135:ASN:O	2.14	0.47
1:D:201:MET:H	1:D:205:ASN:HD21	1.63	0.47
1:A:227:PHE:N	1:A:227:PHE:HD2	2.11	0.47
1:A:245:MET:HE3	1:A:254:TYR:HB3	1.97	0.47
1:C:183:VAL:HG21	1:C:197:LEU:HB2	1.97	0.47
1:A:100:PHE:CZ	1:A:245:MET:HG2	2.50	0.47
1:D:141:GLU:HG2	4:D:390:PO4:O1	2.16	0.46
1:A:239:ILE:HD12	1:A:239:ILE:HA	1.83	0.46
1:B:284:PHE:CE1	1:B:309:LEU:HD21	2.51	0.46
1:A:347:PHE:HB2	2:A:400:FAD:H2'	1.98	0.46
1:C:86:LYS:HD2	1:C:143:ASN:HA	1.97	0.46
1:D:34:ALA:O	1:D:170:HIS:HA	2.15	0.46
1:C:127:TRP:CD1	1:C:242:PRO:HD3	2.50	0.46
1:B:164:GLY:O	1:B:166:LYS:HD3	2.15	0.46
1:B:231:ASP:OD1	1:B:234:LYS:HG3	2.16	0.46
1:A:356:VAL:HG22	1:A:368:HIS:CE1	2.51	0.46
1:A:356:VAL:HG22	1:A:368:HIS:HE1	1.81	0.46
1:C:30:LEU:HA	1:C:166:LYS:O	2.16	0.46
1:C:207:LYS:HB2	1:C:208:LEU:HD22	1.98	0.46
1:C:169:THR:O	1:C:170:HIS:C	2.58	0.46
1:B:95:LYS:HB3	1:B:95:LYS:HE3	1.60	0.45
1:B:356:VAL:HG11	1:B:370:ILE:HG21	1.97	0.45
1:D:124:ASN:ND2	1:D:130:ILE:O	2.50	0.45
1:D:287:TYR:HB3	1:D:289:GLU:OE2	2.15	0.45
1:A:24:LYS:NZ	5:A:415:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:HD3	1:B:163:ARG:HA	1.71	0.45
1:C:359:GLN:HE21	1:C:366:THR:HA	1.82	0.45
1:D:49:ARG:HD2	2:D:400:FAD:C4X	2.46	0.45
1:A:82:LYS:NZ	1:D:76:GLU:OE2	2.39	0.45
1:D:177:ASP:HB2	1:D:184:LYS:HZ2	1.80	0.45
1:A:281:ASN:ND2	1:A:283:GLU:H	2.12	0.45
1:C:321:LEU:HD12	1:C:381:LYS:HB2	1.99	0.44
1:C:49:ARG:HD2	2:C:400:FAD:C10	2.47	0.44
1:C:60:GLU:CD	1:C:372:ILE:HG21	2.42	0.44
1:C:239:ILE:HD12	1:C:239:ILE:HA	1.82	0.44
1:A:268:TYR:CE2	1:A:271:PHE:HB3	2.52	0.44
1:A:49:ARG:HD2	2:A:400:FAD:C4X	2.47	0.44
2:A:400:FAD:H9	2:A:400:FAD:H1'1	1.79	0.44
1:D:347:PHE:HB2	2:D:400:FAD:H2'	1.99	0.44
1:A:224:VAL:HG12	1:A:314:VAL:HG22	2.00	0.44
1:D:221:TYR:OH	5:D:415:HOH:O	2.21	0.44
1:B:284:PHE:HE1	1:B:309:LEU:HD21	1.83	0.43
1:B:315:CYS:CB	2:B:400:FAD:HM73	2.43	0.43
1:D:124:ASN:HD21	1:D:132:VAL:HG22	1.83	0.43
1:B:115:VAL:HG21	1:B:139:ILE:HD11	2.00	0.43
1:A:172:ARG:HH21	1:A:208:LEU:HD21	1.83	0.43
1:C:275:ILE:C	1:C:275:ILE:HD12	2.44	0.43
1:C:311:ARG:HH11	1:C:311:ARG:HB3	1.82	0.43
1:A:172:ARG:NH2	1:A:208:LEU:CD2	2.81	0.43
1:C:20:TYR:CZ	1:C:24:LYS:HD2	2.54	0.43
1:B:204:TRP:CE3	2:B:400:FAD:H8A	2.54	0.43
1:C:298:LEU:HD22	1:C:305:ALA:HB3	2.01	0.43
1:D:133:PRO:HB2	1:D:135:ASN:HD22	1.84	0.43
1:C:349:PHE:O	1:C:353:VAL:HG23	2.19	0.43
1:D:94:PRO:HD3	1:D:247:GLU:O	2.19	0.42
1:D:124:ASN:HD21	1:D:132:VAL:H	1.66	0.42
1:D:295:ARG:O	1:D:299:GLU:HG2	2.18	0.42
1:A:51:ILE:O	1:A:144:SER:HB2	2.19	0.42
1:B:377:ARG:CZ	1:B:380:LEU:HD13	2.50	0.42
1:D:204:TRP:CE3	2:D:400:FAD:H8A	2.54	0.42
1:C:321:LEU:HD23	1:C:321:LEU:HA	1.89	0.42
1:D:201:MET:HE1	1:D:208:LEU:HB3	2.02	0.42
1:B:109:LYS:O	1:B:110:GLU:C	2.63	0.42
1:B:239:ILE:HD12	1:B:239:ILE:HA	1.92	0.42
1:D:214:LEU:HD11	1:D:330:HIS:CD2	2.55	0.42
1:A:70:GLU:OE2	1:A:74:GLU:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:VAL:O	1:B:360:LEU:HG	2.20	0.41
1:D:16:MET:SD	1:D:157:ARG:HB2	2.60	0.41
1:B:49:ARG:HD2	2:B:400:FAD:C10	2.51	0.41
1:B:339:ALA:HB2	1:B:357:LEU:HD21	2.03	0.41
1:C:92:PHE:C	1:C:92:PHE:HD1	2.28	0.41
1:A:284:PHE:CG	1:A:312:GLY:HA3	2.56	0.41
1:C:204:TRP:CE3	2:C:400:FAD:H8A	2.55	0.41
1:D:321:LEU:HD12	1:D:381:LYS:HD3	2.00	0.41
1:C:133:PRO:HG2	1:C:136:TYR:CE1	2.56	0.41
1:D:141:GLU:HG3	4:D:390:PO4:P	2.61	0.41
1:C:75:LEU:O	1:C:79:THR:HG22	2.20	0.41
1:C:281:ASN:ND2	1:C:281:ASN:C	2.78	0.41
1:D:281:ASN:HD22	1:D:281:ASN:C	2.29	0.41
1:D:315:CYS:SG	2:D:400:FAD:C8	3.06	0.41
1:B:121:ASP:O	1:B:125:LYS:HB2	2.21	0.40
1:B:227:PHE:CD2	1:B:227:PHE:N	2.89	0.40
1:B:281:ASN:HD22	1:B:283:GLU:H	1.69	0.40
1:D:380:LEU:HD12	1:D:380:LEU:HA	1.87	0.40
1:D:196:LYS:HD3	1:D:335:ASN:HB2	2.03	0.40
1:C:91:VAL:HG13	1:C:100:PHE:CE2	2.57	0.40
1:C:187:THR:OG1	1:C:188:ALA:N	2.55	0.40
1:D:381:LYS:HD2	1:D:381:LYS:HA	1.75	0.40
1:D:141:GLU:CG	4:D:390:PO4:O2	2.69	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:392:HOH:O	5:A:521:HOH:O[2_656]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/389 (97%)	368 (97%)	10 (3%)	1 (0%)	36	36
1	B	379/389 (97%)	358 (94%)	20 (5%)	1 (0%)	36	36
1	C	379/389 (97%)	362 (96%)	16 (4%)	1 (0%)	36	36
1	D	379/389 (97%)	363 (96%)	15 (4%)	1 (0%)	36	36
All	All	1516/1556 (97%)	1451 (96%)	61 (4%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	250	ASN
1	B	120	GLY
1	A	370	ILE
1	C	280	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/326 (98%)	301 (95%)	17 (5%)	20	19
1	B	318/326 (98%)	291 (92%)	27 (8%)	10	7
1	C	318/326 (98%)	301 (95%)	17 (5%)	20	19
1	D	318/326 (98%)	298 (94%)	20 (6%)	16	14
All	All	1272/1304 (98%)	1191 (94%)	81 (6%)	16	14

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	59	ARG
1	A	112	SER
1	A	118	LEU
1	A	135	ASN
1	A	172	ARG
1	A	179	SER

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Mol	Chain	Res	Type
1	A	181	ASP
1	A	208	LEU
1	A	227	PHE
1	A	239	ILE
1	A	249	PRO
1	A	270	THR
1	A	281	ASN
1	A	365	LYS
1	A	380	LEU
1	A	381	LYS
1	B	31	LEU
1	B	55	TYR
1	B	59	ARG
1	B	97	GLU
1	B	106	GLU
1	B	112	SER
1	B	118	LEU
1	B	121	ASP
1	B	124	ASN
1	B	125	LYS
1	B	135	ASN
1	B	174	GLU
1	B	184	LYS
1	B	186	GLU
1	B	193	THR
1	B	205	ASN
1	B	208	LEU
1	B	224	VAL
1	B	227	PHE
1	B	230	SER
1	B	270	THR
1	B	281	ASN
1	B	286	VAL
1	B	299	GLU
1	B	337	VAL
1	B	367	GLU
1	B	381	LYS
1	C	24	LYS
1	C	31	LEU
1	C	59	ARG
1	C	118	LEU
1	C	135	ASN

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Mol	Chain	Res	Type
1	C	184	LYS
1	C	187	THR
1	C	191	SER
1	C	213	ASN
1	C	245	MET
1	C	250	ASN
1	C	270	THR
1	C	281	ASN
1	C	300	GLU
1	C	311	ARG
1	C	372	ILE
1	C	380	LEU
1	D	2	THR
1	D	59	ARG
1	D	109	LYS
1	D	118	LEU
1	D	135	ASN
1	D	177	ASP
1	D	179	SER
1	D	181	ASP
1	D	208	LEU
1	D	227	PHE
1	D	239	ILE
1	D	249	PRO
1	D	270	THR
1	D	281	ASN
1	D	308	GLU
1	D	311	ARG
1	D	358	SER
1	D	374	SER
1	D	380	LEU
1	D	381	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	41	ASN
1	A	69	GLN
1	A	111	HIS
1	A	124	ASN
1	A	135	ASN

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Mol	Chain	Res	Type
1	A	143	ASN
1	A	189	ASN
1	A	205	ASN
1	A	213	ASN
1	A	281	ASN
1	A	293	ASN
1	A	306	ASN
1	A	359	GLN
1	B	21	GLN
1	B	41	ASN
1	B	124	ASN
1	B	143	ASN
1	B	205	ASN
1	B	213	ASN
1	B	250	ASN
1	B	281	ASN
1	B	293	ASN
1	B	306	ASN
1	B	333	HIS
1	B	359	GLN
1	B	376	ASN
1	C	21	GLN
1	C	41	ASN
1	C	124	ASN
1	C	135	ASN
1	C	189	ASN
1	C	205	ASN
1	C	250	ASN
1	C	281	ASN
1	C	293	ASN
1	C	306	ASN
1	C	359	GLN
1	D	21	GLN
1	D	41	ASN
1	D	124	ASN
1	D	135	ASN
1	D	143	ASN
1	D	170	HIS
1	D	189	ASN
1	D	205	ASN
1	D	213	ASN
1	D	223	GLN

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Mol	Chain	Res	Type
1	D	281	ASN
1	D	306	ASN
1	D	359	GLN
1	D	368	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	C	400	-	58,58,58	1.47	9 (15%)	85,89,89	1.88	22 (25%)
2	FAD	A	400	-	58,58,58	1.71	10 (17%)	85,89,89	1.82	29 (34%)
4	PO4	D	390	-	4,4,4	0.63	0	6,6,6	1.35	0
2	FAD	B	400	-	58,58,58	1.59	10 (17%)	85,89,89	1.62	18 (21%)
4	PO4	B	390	-	4,4,4	1.18	0	6,6,6	0.35	0
2	FAD	D	400	-	58,58,58	1.46	10 (17%)	85,89,89	1.95	20 (23%)

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	B	400	-	-	2/34/50/50	0/6/6/6
2	FAD	D	400	-	-	0/34/50/50	0/6/6/6
2	FAD	C	400	-	-	1/34/50/50	0/6/6/6
2	FAD	A	400	-	-	0/34/50/50	0/6/6/6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	FAD	O4-C4	6.46	1.35	1.23
2	A	400	FAD	O4-C4	6.07	1.35	1.23
2	D	400	FAD	O4-C4	5.74	1.34	1.23
2	C	400	FAD	O4-C4	5.50	1.34	1.23
2	C	400	FAD	PA-O3P	3.80	1.63	1.59
2	A	400	FAD	C4X-N5	3.79	1.38	1.30
2	A	400	FAD	C7M-C7	3.77	1.58	1.51
2	A	400	FAD	PA-O3P	3.45	1.63	1.59
2	D	400	FAD	C8A-N7A	3.33	1.38	1.31
2	D	400	FAD	C4X-N5	3.21	1.37	1.30
2	B	400	FAD	C4X-N5	3.10	1.37	1.30
2	C	400	FAD	C9A-C5X	-3.07	1.36	1.41
2	B	400	FAD	C4A-N3A	3.04	1.40	1.34
2	A	400	FAD	C5A-C6A	3.04	1.49	1.41
2	B	400	FAD	C5'-C4'	3.02	1.55	1.51
2	B	400	FAD	C5A-C6A	3.01	1.49	1.41
2	D	400	FAD	C5A-C6A	2.88	1.49	1.41
2	B	400	FAD	C10-N1	2.85	1.39	1.33
2	A	400	FAD	C4A-N9A	-2.82	1.31	1.37
2	C	400	FAD	C5A-C6A	2.74	1.48	1.41
2	B	400	FAD	C8A-N7A	2.71	1.36	1.31
2	D	400	FAD	C2A-N3A	2.66	1.38	1.33
2	C	400	FAD	C4X-N5	2.58	1.36	1.30
2	B	400	FAD	C4-N3	-2.57	1.34	1.38
2	B	400	FAD	C1'-C2'	-2.54	1.49	1.52
2	D	400	FAD	C8A-N9A	-2.53	1.33	1.37
2	A	400	FAD	C5A-N7A	-2.49	1.34	1.39
2	A	400	FAD	C8A-N9A	-2.48	1.33	1.37
2	D	400	FAD	O2B-C2B	2.48	1.49	1.43
2	C	400	FAD	C5A-N7A	-2.42	1.34	1.39
2	A	400	FAD	C5X-N5	-2.39	1.35	1.39
2	D	400	FAD	C4'-C3'	-2.25	1.49	1.53
2	D	400	FAD	PA-O1A	2.21	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	FAD	C8A-N7A	2.19	1.35	1.31
2	B	400	FAD	P-O3P	2.11	1.61	1.59
2	D	400	FAD	C5X-N5	-2.10	1.35	1.39
2	C	400	FAD	C4X-C10	-2.06	1.38	1.44
2	C	400	FAD	C4A-N9A	-2.04	1.33	1.37
2	C	400	FAD	C2-N3	-2.02	1.34	1.39

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	FAD	C5A-C4A-N3A	-6.38	117.93	126.72
2	C	400	FAD	C5A-C4A-N3A	-5.56	119.06	126.72
2	A	400	FAD	C4-N3-C2	-4.88	116.98	125.64
2	D	400	FAD	N3A-C4A-N9A	4.85	135.42	127.17
2	B	400	FAD	C5A-C4A-N3A	-4.84	120.06	126.72
2	C	400	FAD	N3A-C4A-N9A	4.73	135.21	127.17
2	C	400	FAD	N3A-C2A-N1A	-4.69	121.47	128.58
2	C	400	FAD	C2A-N3A-C4A	4.53	122.89	111.83
2	D	400	FAD	N9A-C8A-N7A	-4.37	107.74	113.94
2	D	400	FAD	C4A-N9A-C8A	4.36	110.32	105.74
2	A	400	FAD	O2-C2-N1	-4.35	114.57	121.80
2	C	400	FAD	O4-C4-C4X	-4.32	115.14	126.53
2	D	400	FAD	O3P-P-O1P	-4.25	97.93	110.70
2	A	400	FAD	C5A-C4A-N3A	-4.24	120.88	126.72
2	D	400	FAD	C2A-N3A-C4A	4.05	121.71	111.83
2	B	400	FAD	N3A-C4A-N9A	3.88	133.76	127.17
2	C	400	FAD	C9A-C5X-N5	-3.81	118.41	122.45
2	D	400	FAD	O4-C4-C4X	-3.77	116.59	126.53
2	D	400	FAD	C5X-C9A-N10	3.66	121.28	117.97
2	B	400	FAD	N3A-C2A-N1A	-3.66	123.05	128.58
2	B	400	FAD	O4-C4-C4X	-3.64	116.91	126.53
2	C	400	FAD	C4-N3-C2	-3.57	119.31	125.64
2	A	400	FAD	N3A-C2A-N1A	-3.54	123.22	128.58
2	A	400	FAD	N9A-C8A-N7A	-3.40	109.12	113.94
2	D	400	FAD	N3A-C2A-N1A	-3.38	123.47	128.58
2	B	400	FAD	C4A-N9A-C8A	3.37	109.28	105.74
2	B	400	FAD	C2A-N3A-C4A	3.27	119.81	111.83
2	C	400	FAD	C8M-C8-C9	-3.26	113.82	119.57
2	D	400	FAD	O2P-P-O3P	3.23	116.02	107.27
2	A	400	FAD	O3P-P-O1P	-3.23	100.99	110.70
2	B	400	FAD	N9A-C8A-N7A	-3.20	109.39	113.94
2	C	400	FAD	C4A-N9A-C8A	3.13	109.02	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	FAD	C9A-C5X-N5	-3.06	119.21	122.45
2	C	400	FAD	N9A-C8A-N7A	-3.02	109.65	113.94
2	B	400	FAD	C4-N3-C2	-3.02	120.28	125.64
2	B	400	FAD	O2-C2-N1	-2.99	116.83	121.80
2	A	400	FAD	C8M-C8-C9	-2.96	114.35	119.57
2	D	400	FAD	C4-N3-C2	-2.93	120.43	125.64
2	A	400	FAD	C2A-N3A-C4A	2.87	118.85	111.83
2	D	400	FAD	C9A-C5X-N5	-2.82	119.46	122.45
2	A	400	FAD	O4-C4-C4X	-2.80	119.15	126.53
2	D	400	FAD	C10-N1-C2	2.77	122.85	116.85
2	A	400	FAD	C9-C8-C7	2.74	123.71	119.69
2	B	400	FAD	C4'-C3'-C2'	-2.73	109.02	113.57
2	A	400	FAD	N3-C2-N1	2.71	125.26	119.50
2	D	400	FAD	C4X-C4-N3	2.66	120.03	113.25
2	C	400	FAD	C5A-C6A-N6A	-2.66	116.71	123.29
2	C	400	FAD	C4X-C4-N3	2.64	119.98	113.25
2	A	400	FAD	C4A-C5A-N7A	-2.64	107.56	110.58
2	D	400	FAD	C5A-N7A-C8A	2.64	107.60	103.45
2	A	400	FAD	C2B-C3B-C4B	2.63	107.69	102.61
2	C	400	FAD	C5X-C9A-N10	2.60	120.32	117.97
2	D	400	FAD	O2A-PA-O5B	2.57	119.22	107.57
2	A	400	FAD	C10-C4X-N5	-2.57	119.57	124.81
2	D	400	FAD	C4A-C5A-N7A	-2.54	107.67	110.58
2	C	400	FAD	O4-C4-N3	2.53	124.88	120.11
2	C	400	FAD	C10-N1-C2	2.53	122.33	116.85
2	A	400	FAD	C9A-C5X-N5	-2.52	119.78	122.45
2	A	400	FAD	O2A-PA-O3P	2.46	113.93	107.27
2	C	400	FAD	N6A-C6A-N1A	2.44	123.82	118.38
2	A	400	FAD	C4A-N9A-C8A	2.44	108.30	105.74
2	A	400	FAD	O5'-C5'-C4'	-2.42	102.91	109.36
2	A	400	FAD	O5B-PA-O1A	-2.39	99.46	108.94
2	A	400	FAD	C4-C4X-N5	2.39	121.50	118.21
2	C	400	FAD	O4B-C1B-C2B	-2.38	101.52	106.62
2	C	400	FAD	C4'-C3'-C2'	-2.37	109.62	113.57
2	C	400	FAD	C4X-C10-N1	-2.36	118.80	124.59
2	A	400	FAD	C1'-C2'-C3'	-2.35	103.29	109.66
2	A	400	FAD	O2'-C2'-C3'	2.34	114.73	109.25
2	B	400	FAD	O4-C4-N3	2.34	124.51	120.11
2	A	400	FAD	C5A-C4A-N9A	2.32	108.34	105.81
2	A	400	FAD	C4X-C4-N3	2.32	119.15	113.25
2	C	400	FAD	C8M-C8-C7	2.29	125.43	120.76
2	D	400	FAD	C4B-O4B-C1B	-2.27	104.45	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	FAD	O3B-C3B-C4B	-2.25	104.61	111.08
2	D	400	FAD	C4X-C10-N1	-2.23	119.13	124.59
2	A	400	FAD	C4X-C10-N10	2.21	119.65	116.48
2	B	400	FAD	C4X-C10-N1	-2.10	119.44	124.59
2	B	400	FAD	C6-C5X-C9A	2.09	121.92	119.05
2	A	400	FAD	C5X-N5-C4X	2.08	121.46	118.09
2	C	400	FAD	C7M-C7-C8	2.07	124.98	120.76
2	C	400	FAD	O2-C2-N1	-2.06	118.38	121.80
2	A	400	FAD	N3A-C4A-N9A	2.06	130.66	127.17
2	A	400	FAD	C5A-N7A-C8A	2.04	106.65	103.45
2	B	400	FAD	C4X-C4-N3	2.03	118.43	113.25
2	A	400	FAD	C6-C7-C8	-2.03	116.71	119.69
2	B	400	FAD	C5X-N5-C4X	2.03	121.36	118.09
2	B	400	FAD	O2A-PA-O1A	2.01	121.78	112.44
2	B	400	FAD	N6A-C6A-N1A	2.01	122.84	118.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	FAD	O4B-C4B-C5B-O5B
2	B	400	FAD	C3B-C4B-C5B-O5B
2	C	400	FAD	O4B-C4B-C5B-O5B

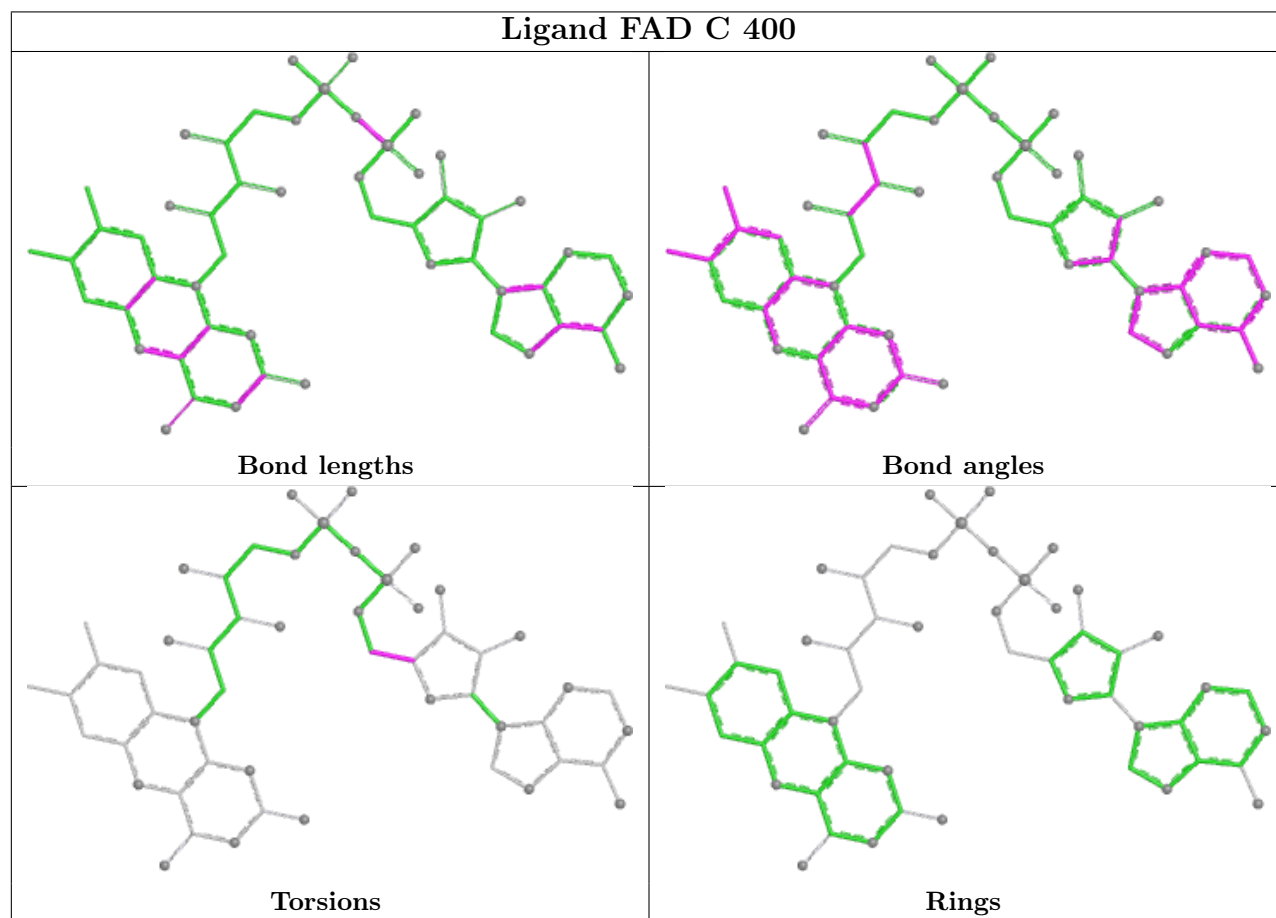
There are no ring outliers.

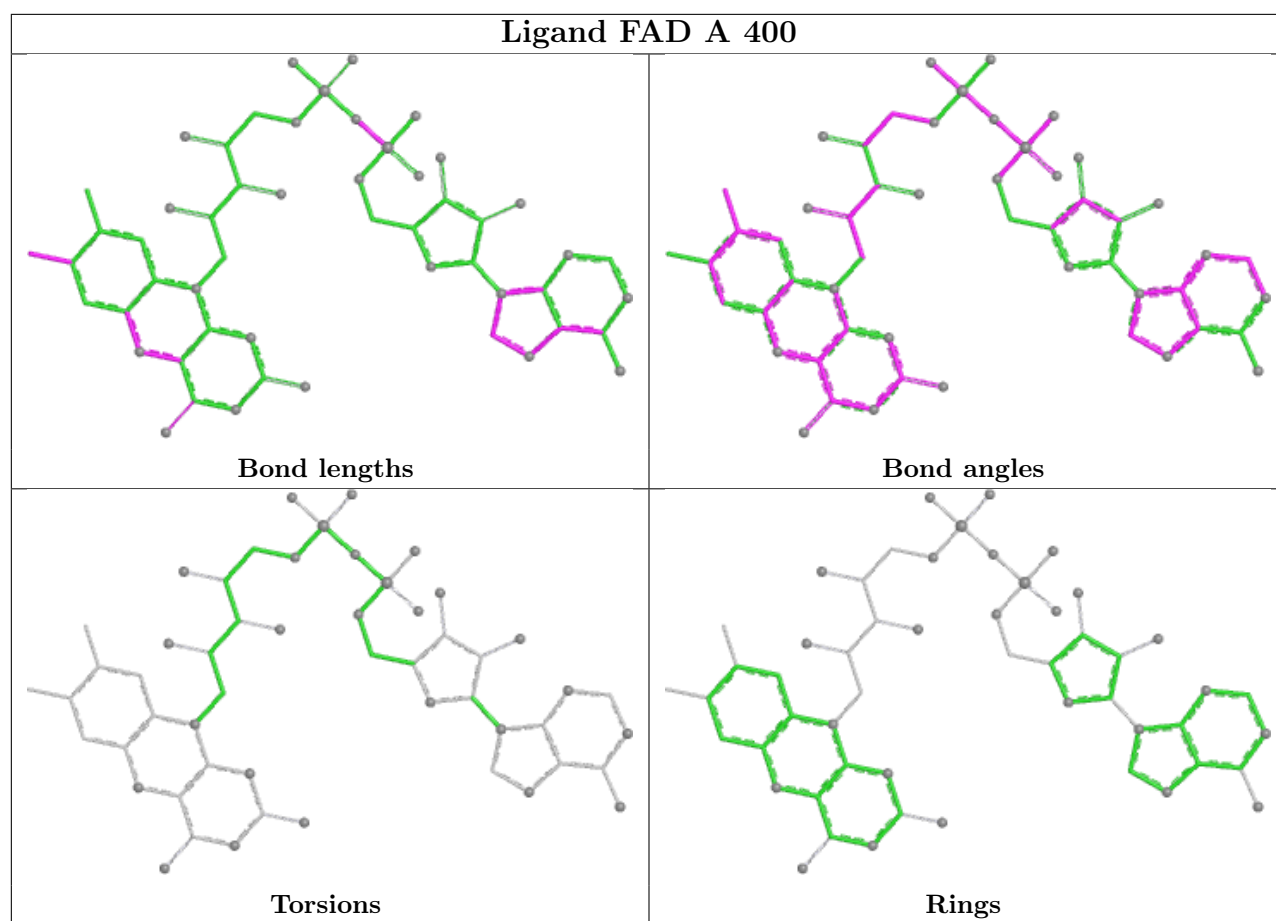
5 monomers are involved in 32 short contacts:

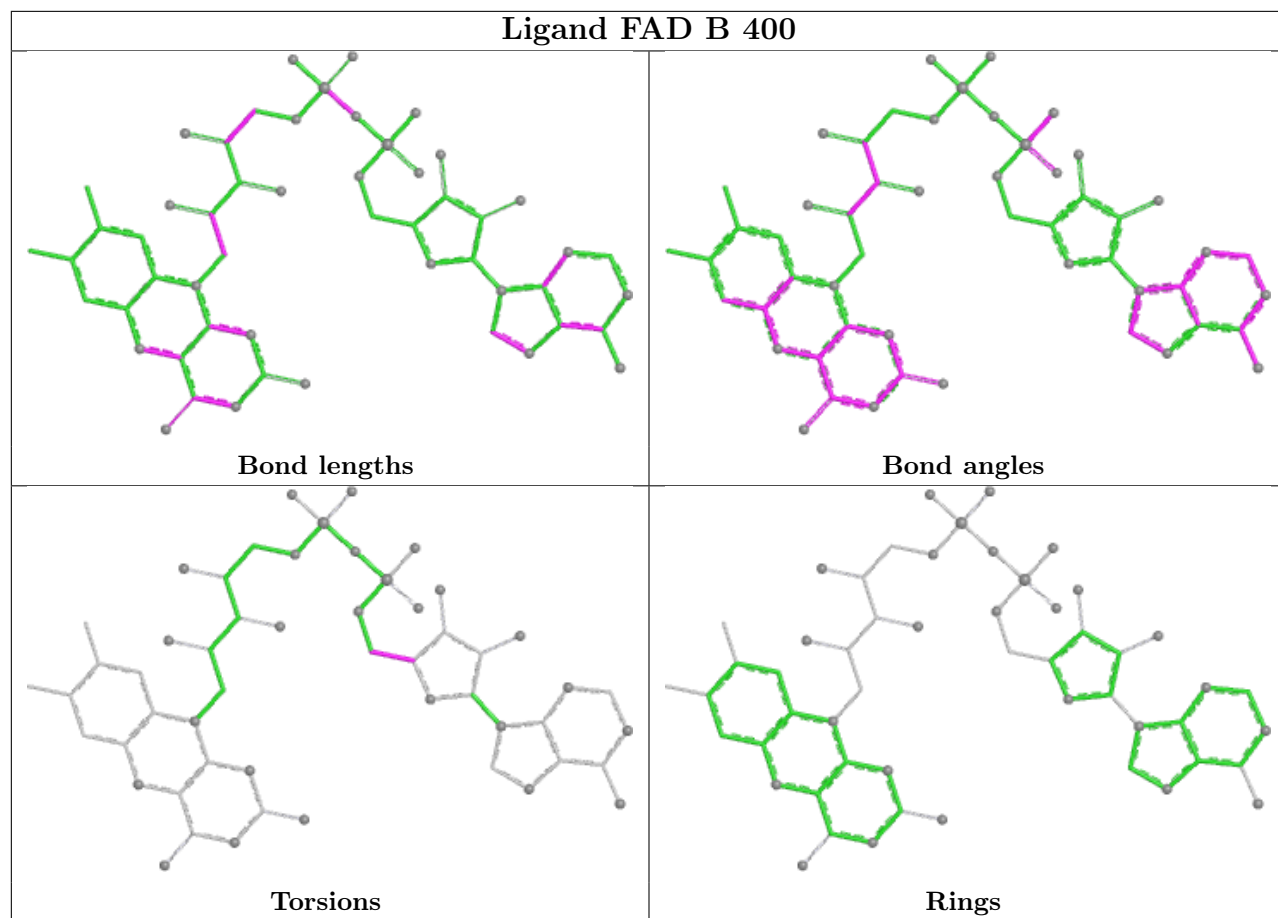
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	FAD	6	0
2	A	400	FAD	7	0
4	D	390	PO4	5	0
2	B	400	FAD	7	0
2	D	400	FAD	7	0

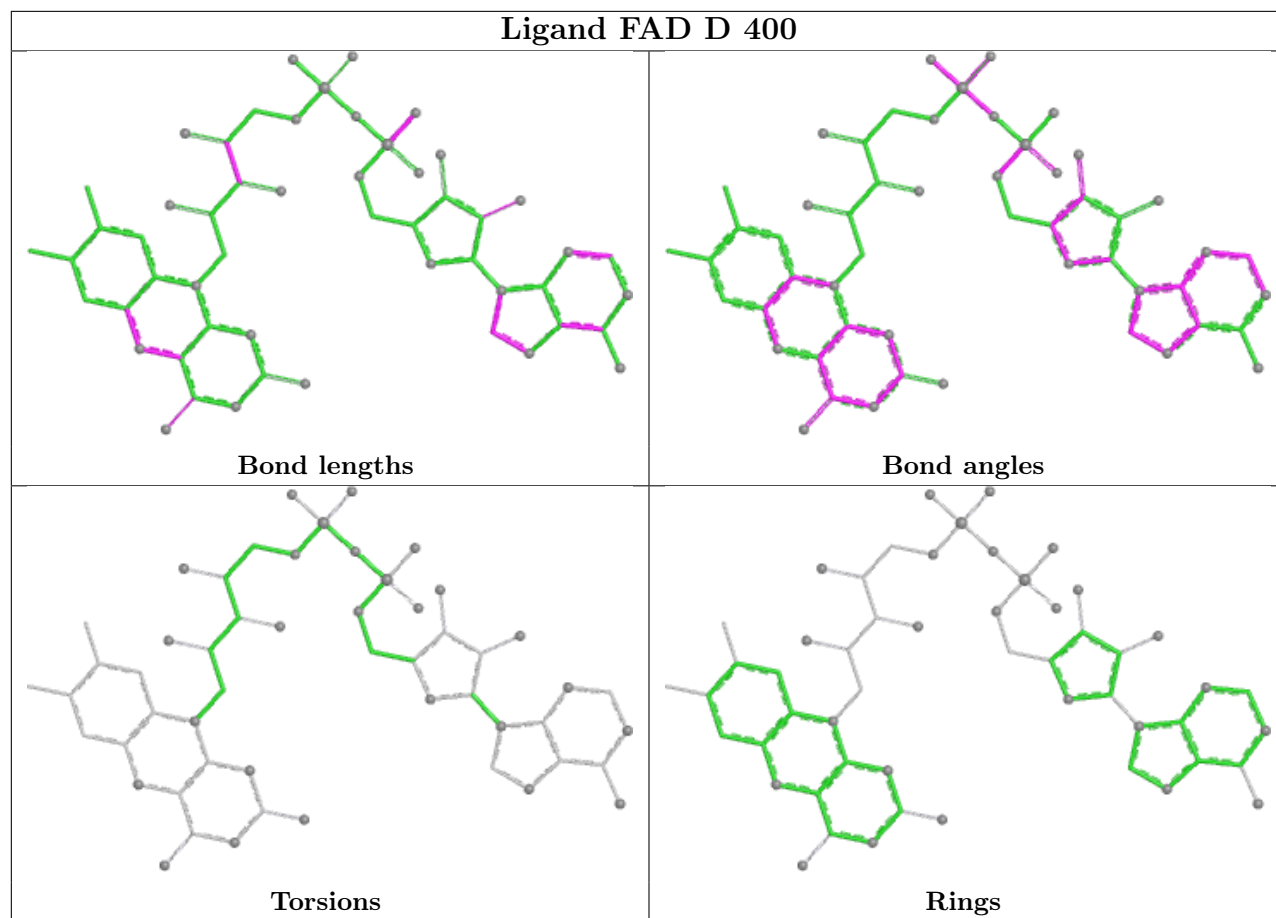
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	381/389 (97%)	-0.42	3 (0%) 82 84	16, 27, 41, 61	0
1	B	381/389 (97%)	0.18	3 (0%) 82 84	26, 41, 65, 81	0
1	C	381/389 (97%)	0.23	4 (1%) 79 81	26, 42, 59, 68	0
1	D	381/389 (97%)	-0.16	2 (0%) 87 88	17, 33, 47, 67	0
All	All	1524/1556 (97%)	-0.04	12 (0%) 82 84	16, 36, 58, 81	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	ALA	3.8
1	D	1	SER	3.7
1	B	187	THR	3.1
1	A	369	ASP	2.9
1	A	227	PHE	2.8
1	C	191	SER	2.7
1	A	368	HIS	2.7
1	B	1	SER	2.6
1	D	188	ALA	2.5
1	C	2	THR	2.3
1	C	99	ALA	2.2
1	C	132	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

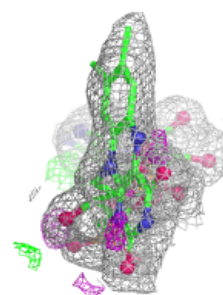
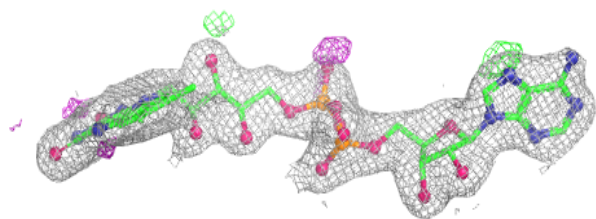
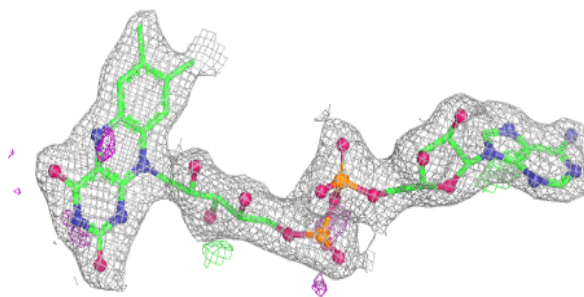
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	B	390	5/5	0.91	0.14	55,62,63,64	0
2	FAD	C	400	53/53	0.94	0.08	23,32,44,46	0
2	FAD	D	400	53/53	0.96	0.06	20,28,36,38	0
4	PO4	D	390	5/5	0.96	0.11	38,44,45,46	0
2	FAD	A	400	53/53	0.97	0.05	13,20,25,27	0
2	FAD	B	400	53/53	0.97	0.06	22,29,37,39	0
3	CL	C	405	1/1	0.98	0.04	31,31,31,31	0
3	CL	A	405	1/1	0.98	0.05	23,23,23,23	0
3	CL	B	405	1/1	0.98	0.04	35,35,35,35	0
3	CL	D	405	1/1	0.99	0.03	26,26,26,26	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.

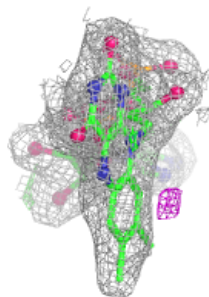
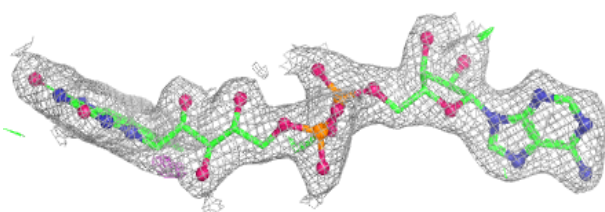
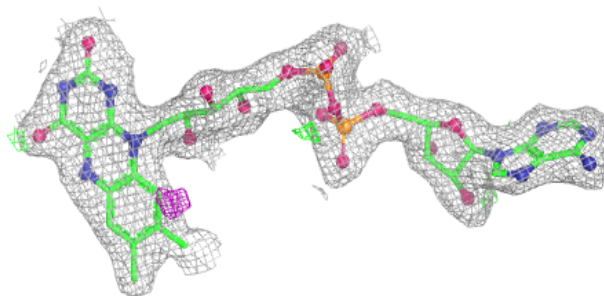
Electron density around FAD C 400:

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

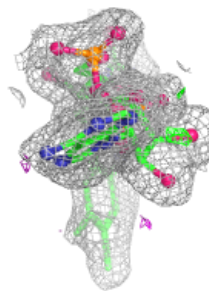
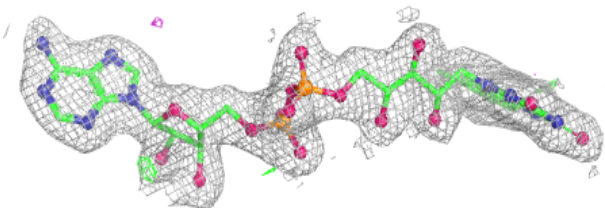
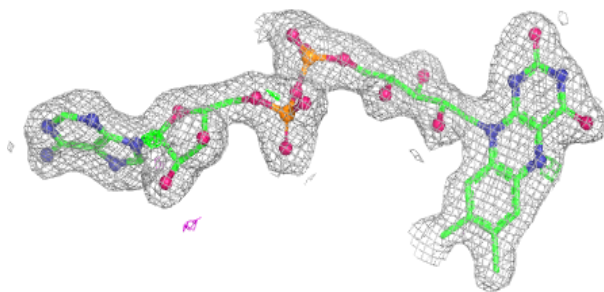


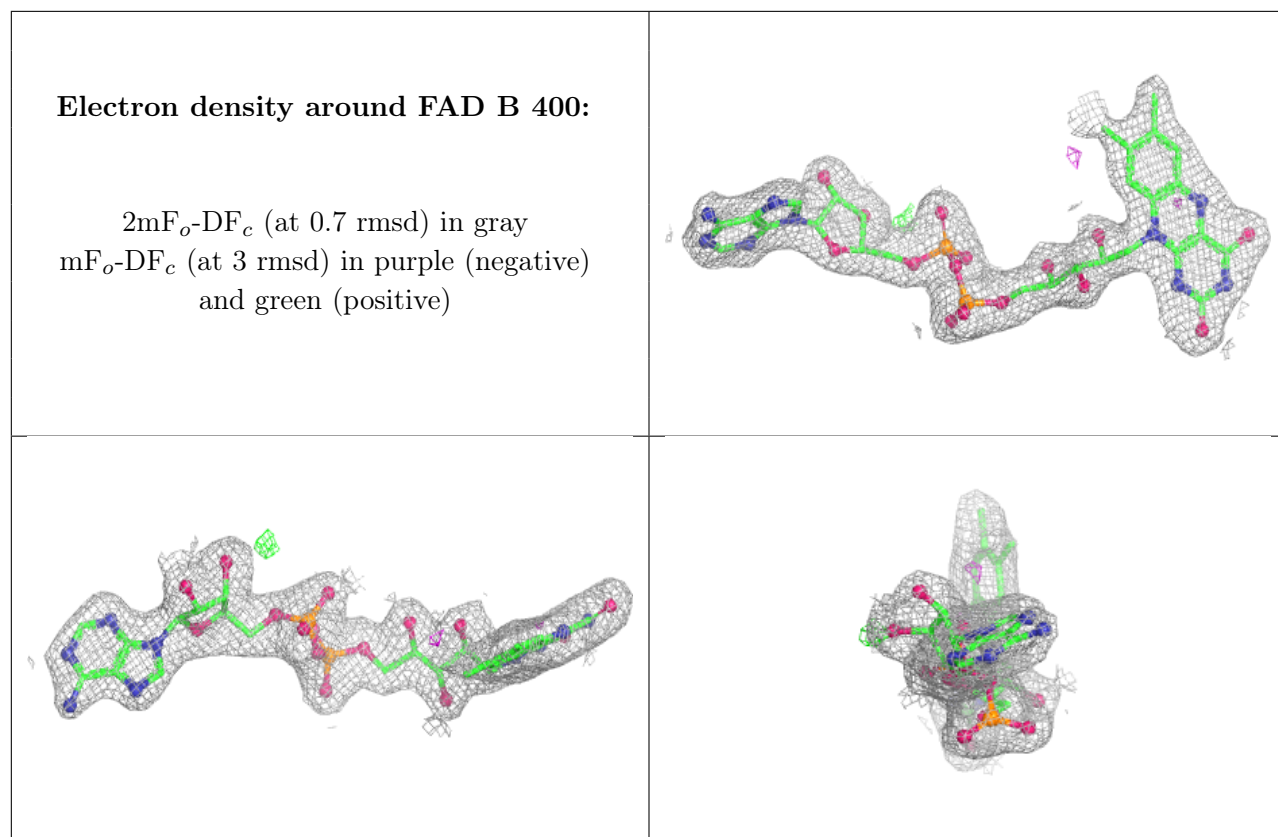
Electron density around FAD D 400:

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

**Electron density around FAD A 400:**

$2mF_o-DF_c$ (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.