



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:46 PM UTC

PDB ID : 5YB8 / pdb_00005yb8
Title : L-Amino acid oxidase/monooxygenase from Pseudomonas sp. AIU 813 - L-arginine complex
Authors : Im, D.; Matsui, D.; Arakawa, T.; Isobe, K.; Asano, Y.; Fushinobu, S.
Deposited on : 2017-09-03
Resolution : 2.30 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

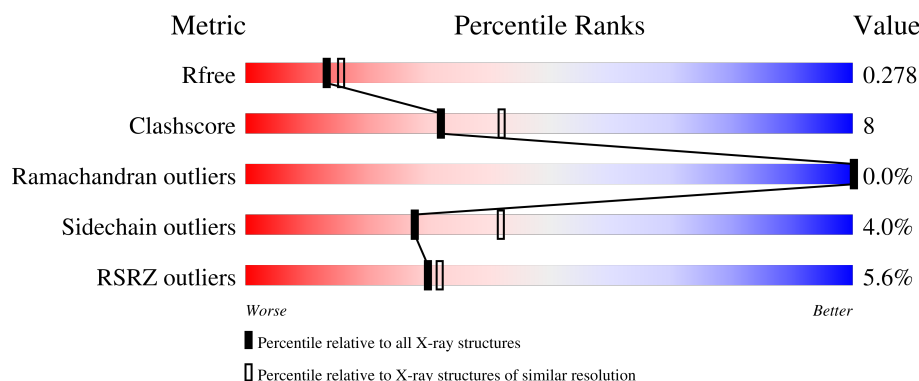
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	580	3% 79% 13% • 5%
1	B	580	3% 78% 16% • 5%
1	C	580	8% 81% 12% • 5%
1	D	580	7% 81% 12% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17837 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-amino acid oxidase/monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			
1	B	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			
1	C	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			
1	D	549	Total	C	N	O	S	0	0	0
			4305	2749	742	791	23			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP W6JQJ6
A	-18	GLY	-	expression tag	UNP W6JQJ6
A	-17	SER	-	expression tag	UNP W6JQJ6
A	-16	SER	-	expression tag	UNP W6JQJ6
A	-15	HIS	-	expression tag	UNP W6JQJ6
A	-14	HIS	-	expression tag	UNP W6JQJ6
A	-13	HIS	-	expression tag	UNP W6JQJ6
A	-12	HIS	-	expression tag	UNP W6JQJ6
A	-11	HIS	-	expression tag	UNP W6JQJ6
A	-10	HIS	-	expression tag	UNP W6JQJ6
A	-9	SER	-	expression tag	UNP W6JQJ6
A	-8	SER	-	expression tag	UNP W6JQJ6
A	-7	GLY	-	expression tag	UNP W6JQJ6
A	-6	LEU	-	expression tag	UNP W6JQJ6
A	-5	VAL	-	expression tag	UNP W6JQJ6
A	-4	PRO	-	expression tag	UNP W6JQJ6
A	-3	ARG	-	expression tag	UNP W6JQJ6
A	-2	GLY	-	expression tag	UNP W6JQJ6
A	-1	SER	-	expression tag	UNP W6JQJ6
A	0	HIS	-	expression tag	UNP W6JQJ6
A	473	PHE	SER	conflict	UNP W6JQJ6

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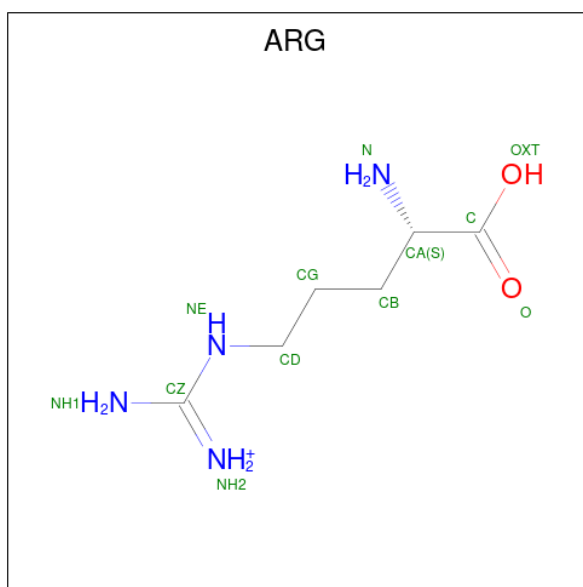
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP W6JQJ6
B	-18	GLY	-	expression tag	UNP W6JQJ6
B	-17	SER	-	expression tag	UNP W6JQJ6
B	-16	SER	-	expression tag	UNP W6JQJ6
B	-15	HIS	-	expression tag	UNP W6JQJ6
B	-14	HIS	-	expression tag	UNP W6JQJ6
B	-13	HIS	-	expression tag	UNP W6JQJ6
B	-12	HIS	-	expression tag	UNP W6JQJ6
B	-11	HIS	-	expression tag	UNP W6JQJ6
B	-10	HIS	-	expression tag	UNP W6JQJ6
B	-9	SER	-	expression tag	UNP W6JQJ6
B	-8	SER	-	expression tag	UNP W6JQJ6
B	-7	GLY	-	expression tag	UNP W6JQJ6
B	-6	LEU	-	expression tag	UNP W6JQJ6
B	-5	VAL	-	expression tag	UNP W6JQJ6
B	-4	PRO	-	expression tag	UNP W6JQJ6
B	-3	ARG	-	expression tag	UNP W6JQJ6
B	-2	GLY	-	expression tag	UNP W6JQJ6
B	-1	SER	-	expression tag	UNP W6JQJ6
B	0	HIS	-	expression tag	UNP W6JQJ6
B	473	PHE	SER	conflict	UNP W6JQJ6
C	-19	MET	-	expression tag	UNP W6JQJ6
C	-18	GLY	-	expression tag	UNP W6JQJ6
C	-17	SER	-	expression tag	UNP W6JQJ6
C	-16	SER	-	expression tag	UNP W6JQJ6
C	-15	HIS	-	expression tag	UNP W6JQJ6
C	-14	HIS	-	expression tag	UNP W6JQJ6
C	-13	HIS	-	expression tag	UNP W6JQJ6
C	-12	HIS	-	expression tag	UNP W6JQJ6
C	-11	HIS	-	expression tag	UNP W6JQJ6
C	-10	HIS	-	expression tag	UNP W6JQJ6
C	-9	SER	-	expression tag	UNP W6JQJ6
C	-8	SER	-	expression tag	UNP W6JQJ6
C	-7	GLY	-	expression tag	UNP W6JQJ6
C	-6	LEU	-	expression tag	UNP W6JQJ6
C	-5	VAL	-	expression tag	UNP W6JQJ6
C	-4	PRO	-	expression tag	UNP W6JQJ6
C	-3	ARG	-	expression tag	UNP W6JQJ6
C	-2	GLY	-	expression tag	UNP W6JQJ6
C	-1	SER	-	expression tag	UNP W6JQJ6
C	0	HIS	-	expression tag	UNP W6JQJ6
C	473	PHE	SER	conflict	UNP W6JQJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP W6JQJ6
D	-18	GLY	-	expression tag	UNP W6JQJ6
D	-17	SER	-	expression tag	UNP W6JQJ6
D	-16	SER	-	expression tag	UNP W6JQJ6
D	-15	HIS	-	expression tag	UNP W6JQJ6
D	-14	HIS	-	expression tag	UNP W6JQJ6
D	-13	HIS	-	expression tag	UNP W6JQJ6
D	-12	HIS	-	expression tag	UNP W6JQJ6
D	-11	HIS	-	expression tag	UNP W6JQJ6
D	-10	HIS	-	expression tag	UNP W6JQJ6
D	-9	SER	-	expression tag	UNP W6JQJ6
D	-8	SER	-	expression tag	UNP W6JQJ6
D	-7	GLY	-	expression tag	UNP W6JQJ6
D	-6	LEU	-	expression tag	UNP W6JQJ6
D	-5	VAL	-	expression tag	UNP W6JQJ6
D	-4	PRO	-	expression tag	UNP W6JQJ6
D	-3	ARG	-	expression tag	UNP W6JQJ6
D	-2	GLY	-	expression tag	UNP W6JQJ6
D	-1	SER	-	expression tag	UNP W6JQJ6
D	0	HIS	-	expression tag	UNP W6JQJ6
D	473	PHE	SER	conflict	UNP W6JQJ6

- Molecule 2 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



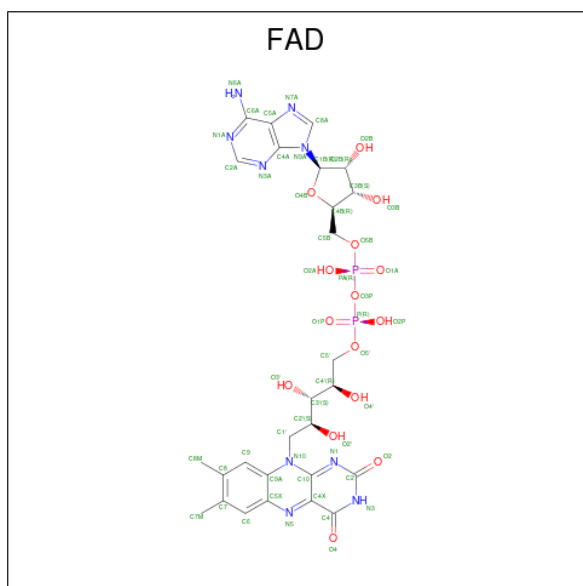
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		
2	C	1	Total	C	N	O	0	0
			12	6	4	2		
2	C	1	Total	C	N	O	0	0
			12	6	4	2		
2	D	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

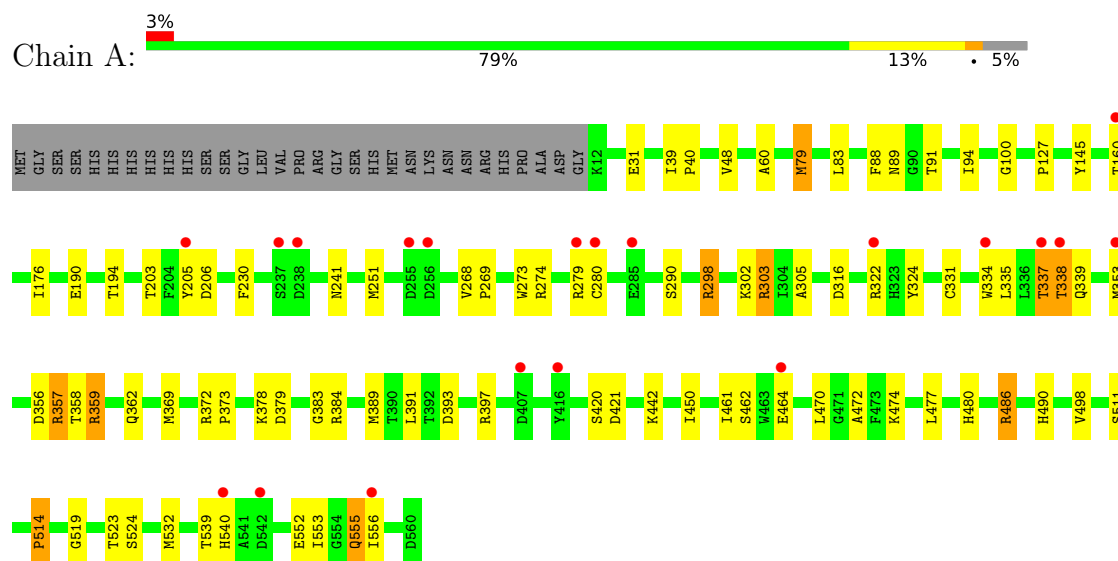
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total 98	O 98	0	0
4	B	108	Total 108	O 108	0	0
4	C	53	Total 53	O 53	0	0
4	D	50	Total 50	O 50	0	0

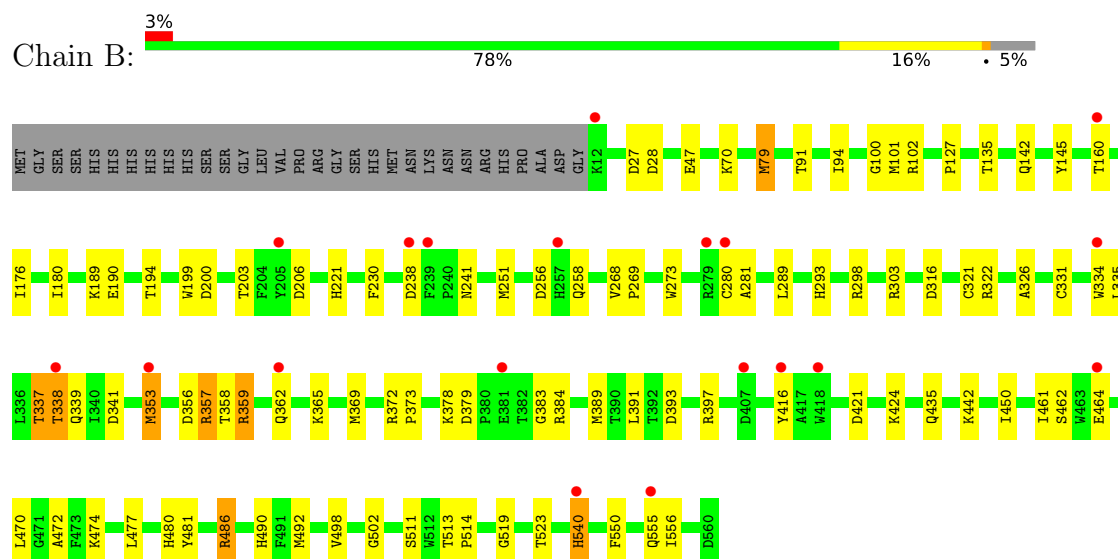
3 Residue-property plots [i](#)

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

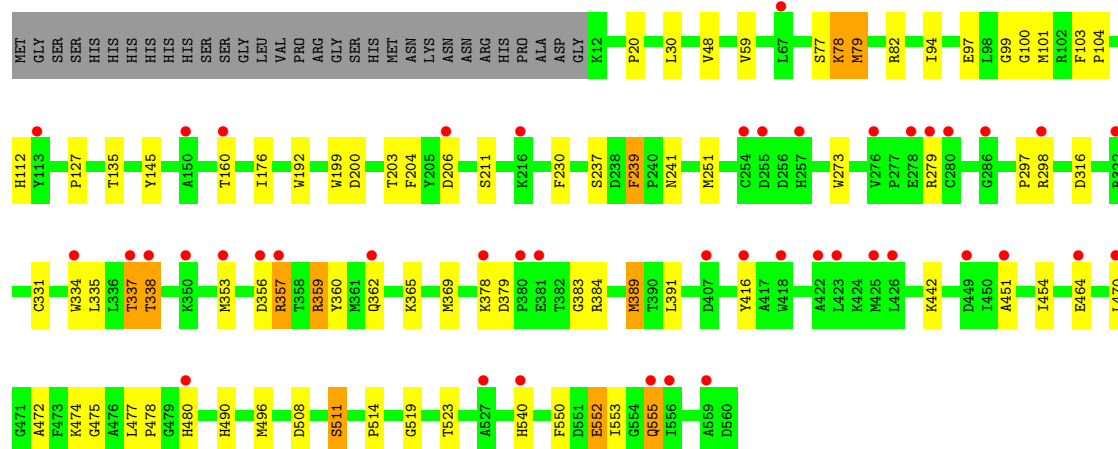
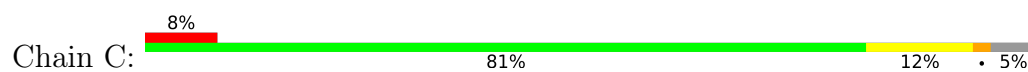
- Molecule 1: L-amino acid oxidase/monooxygenase



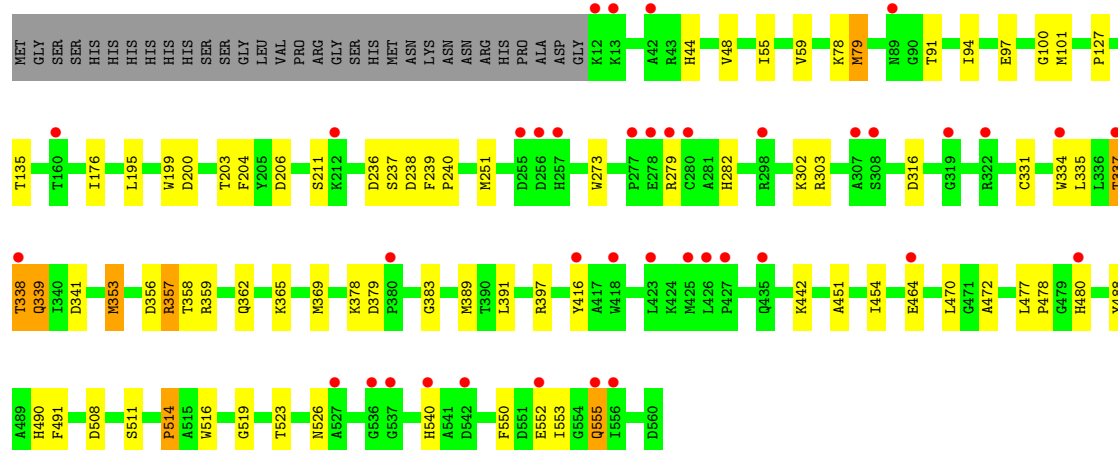
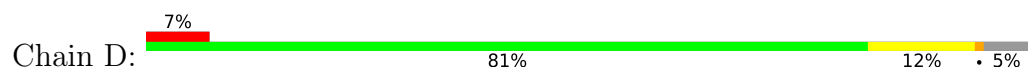
- Molecule 1: L-amino acid oxidase/monooxygenase



- Molecule 1: L-amino acid oxidase/monooxygenase



- Molecule 1: L-amino acid oxidase/monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.20Å 133.00Å 101.50Å 90.00° 112.00° 90.00°	Depositor
Resolution (Å)	94.11 – 2.30 94.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (94.11-2.30) 99.8 (94.11-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.220 , 0.273 0.226 , 0.278	Depositor DCC
R_{free} test set	2009 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.138 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17837	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: 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	1.10	4/4428 (0.1%)	1.08	3/6019 (0.0%)
1	B	1.10	2/4428 (0.0%)	1.10	6/6019 (0.1%)
1	C	0.93	2/4428 (0.0%)	1.00	3/6019 (0.0%)
1	D	0.93	0/4428	1.01	3/6019 (0.0%)
All	All	1.02	8/17712 (0.0%)	1.05	15/24076 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	ARG	C-O	-6.21	1.15	1.24
1	C	239	PHE	C-O	-5.37	1.19	1.24
1	B	293	HIS	N-CA	5.16	1.52	1.46
1	B	281	ALA	N-CA	5.14	1.52	1.46
1	A	324	TYR	N-CA	-5.11	1.39	1.45
1	A	83	LEU	C-O	-5.08	1.18	1.24
1	C	297	PRO	CA-C	-5.05	1.46	1.52
1	A	290	SER	C-O	-5.00	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	513	THR	CA-C-N	-6.14	113.36	119.56
1	B	513	THR	C-N-CA	-6.14	113.36	119.56
1	C	389	MET	N-CA-C	-5.78	101.63	110.30
1	A	514	PRO	N-CA-C	5.65	121.19	113.84
1	D	514	PRO	CA-C-N	-5.64	113.29	122.65
1	D	514	PRO	C-N-CA	-5.64	113.29	122.65
1	C	496	MET	N-CA-C	5.63	116.91	109.93
1	B	353	MET	CG-SD-CE	5.56	113.14	100.90
1	B	289	LEU	N-CA-C	-5.46	104.56	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ILE	N-CA-C	-5.33	105.19	111.00
1	D	195	LEU	N-CA-C	5.32	117.16	111.36
1	C	511	SER	N-CA-C	5.17	117.35	110.53
1	B	180	ILE	N-CA-C	-5.16	105.68	110.53
1	A	486	ARG	N-CA-CB	5.06	117.35	110.01
1	B	450	ILE	N-CA-C	-5.01	105.54	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4305	0	4166	78	0
1	B	4305	0	4164	76	0
1	C	4305	0	4166	71	0
1	D	4305	0	4166	72	0
2	A	36	0	36	1	0
2	B	24	0	24	2	0
2	C	24	0	24	1	0
2	D	12	0	12	2	0
3	A	53	0	31	5	0
3	B	53	0	31	6	0
3	C	53	0	31	6	0
3	D	53	0	31	8	0
4	A	98	0	0	4	0
4	B	108	0	0	10	0
4	C	53	0	0	1	0
4	D	50	0	0	1	0
All	All	17837	0	16882	275	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 (275) 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:B:389:MET:HE1	1:B:391:LEU:HG	1.18	1.15
1:C:389:MET:HE1	1:C:391:LEU:HG	1.23	1.14
1:A:389:MET:HE1	1:A:391:LEU:HG	1.25	1.12
1:D:389:MET:HE1	1:D:391:LEU:HG	1.26	1.11
1:D:203:THR:OG1	1:D:206:ASP:OD2	1.84	0.95
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.29	0.94
1:A:241:ASN:OD1	1:A:359:ARG:NH2	2.07	0.88
1:A:206:ASP:CG	1:D:206:ASP:CG	2.42	0.88
1:C:203:THR:OG1	1:C:206:ASP:OD2	1.91	0.87
1:A:393:ASP:HB2	1:D:353:MET:HE3	1.57	0.85
1:D:127:PRO:HB3	1:D:389:MET:HE2	1.62	0.81
1:B:472:ALA:HB1	3:B:603:FAD:HM82	1.62	0.80
1:B:206:ASP:CG	1:C:206:ASP:CG	2.49	0.80
1:A:464:GLU:OE1	1:A:464:GLU:N	2.14	0.80
1:B:362:GLN:HE22	1:B:464:GLU:HB3	1.46	0.79
1:C:353:MET:HE2	1:C:357:ARG:CZ	2.12	0.79
1:C:127:PRO:HB3	1:C:389:MET:HE2	1.69	0.75
1:D:464:GLU:N	1:D:464:GLU:OE1	2.20	0.74
1:B:464:GLU:N	1:B:464:GLU:OE1	2.20	0.74
1:C:94:ILE:HG21	1:C:369:MET:HE2	1.69	0.74
1:D:238:ASP:OD1	2:D:601:ARG:NH2	2.21	0.73
1:D:472:ALA:HB1	3:D:602:FAD:HM83	1.70	0.73
1:B:127:PRO:HB3	1:B:389:MET:HE2	1.70	0.73
1:A:389:MET:HE1	1:A:391:LEU:CG	2.14	0.73
1:D:358:THR:O	1:D:359:ARG:HD3	1.89	0.73
1:A:127:PRO:HB3	1:A:389:MET:HE2	1.70	0.72
1:C:337:THR:HG21	1:C:356:ASP:OD1	1.90	0.72
1:D:334:TRP:O	1:D:338:THR:HG23	1.90	0.72
1:A:353:MET:CE	1:A:357:ARG:CZ	2.68	0.72
1:C:464:GLU:OE1	1:C:464:GLU:N	2.21	0.71
1:B:389:MET:HE1	1:B:391:LEU:CG	2.10	0.71
1:D:389:MET:C	1:D:389:MET:HE3	2.16	0.71
1:A:477:LEU:HD12	1:A:480:HIS:CE1	2.26	0.71
1:A:362:GLN:HE22	1:A:464:GLU:HB3	1.55	0.70
1:D:337:THR:HG21	1:D:356:ASP:OD1	1.91	0.70
1:A:79:MET:HE1	1:A:273:TRP:CG	2.27	0.70
1:A:303:ARG:HG3	1:A:303:ARG:NH1	1.99	0.69
1:A:334:TRP:O	1:A:338:THR:HG23	1.92	0.69
1:C:353:MET:HE2	1:C:357:ARG:NH1	2.08	0.69
1:B:490:HIS:HD2	4:B:794:HOH:O	1.77	0.68
1:B:189:LYS:HD3	4:B:761:HOH:O	1.94	0.68
1:A:356:ASP:OD2	2:A:603:ARG:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:GLN:HE22	1:D:464:GLU:HB3	1.59	0.68
1:C:353:MET:CE	1:C:357:ARG:CZ	2.72	0.67
1:B:477:LEU:HD12	1:B:480:HIS:CE1	2.29	0.67
1:A:322:ARG:HG2	4:A:777:HOH:O	1.95	0.67
1:A:353:MET:HE2	1:A:357:ARG:CZ	2.25	0.66
1:C:472:ALA:HB1	3:C:603:FAD:HM83	1.77	0.66
1:A:353:MET:HE2	1:A:357:ARG:NH1	2.10	0.66
1:D:358:THR:C	1:D:359:ARG:HD3	2.21	0.66
1:B:142:GLN:HB2	4:B:709:HOH:O	1.94	0.65
1:B:472:ALA:CB	3:B:603:FAD:HM82	2.27	0.65
1:B:91:THR:HG21	1:B:369:MET:HE1	1.80	0.64
1:C:334:TRP:O	1:C:338:THR:HG23	1.97	0.64
1:C:362:GLN:HE22	1:C:464:GLU:HB3	1.62	0.64
1:D:389:MET:HE3	1:D:389:MET:O	1.97	0.64
1:A:472:ALA:O	3:A:604:FAD:HM81	1.98	0.64
1:B:100:GLY:HA2	3:B:603:FAD:C4X	2.27	0.64
1:D:552:GLU:HG2	1:D:553:ILE:HG23	1.79	0.64
1:A:206:ASP:CG	1:D:206:ASP:OD2	2.41	0.64
1:D:94:ILE:HG21	1:D:369:MET:HE2	1.80	0.64
1:B:334:TRP:O	1:B:338:THR:HG23	1.98	0.63
1:A:472:ALA:HB1	3:A:604:FAD:HM83	1.80	0.63
1:B:79:MET:HE1	1:B:273:TRP:CG	2.34	0.62
1:A:490:HIS:HD2	4:A:780:HOH:O	1.81	0.62
1:A:94:ILE:HG21	1:A:369:MET:HE2	1.79	0.62
1:C:389:MET:HE3	1:C:389:MET:C	2.26	0.61
1:B:378:LYS:HE3	1:B:383:GLY:O	2.01	0.61
1:C:477:LEU:HD12	1:C:480:HIS:CE1	2.36	0.61
1:A:353:MET:CE	1:A:357:ARG:NH2	2.63	0.60
1:A:206:ASP:OD1	1:D:206:ASP:OD2	2.19	0.60
1:C:389:MET:HE1	1:C:391:LEU:CG	2.16	0.60
1:A:91:THR:HG21	1:A:369:MET:HE1	1.84	0.60
1:A:206:ASP:OD2	1:D:206:ASP:CG	2.44	0.60
1:D:94:ILE:HG21	1:D:369:MET:CE	2.32	0.59
1:C:362:GLN:OE1	1:C:464:GLU:CD	2.45	0.59
1:A:203:THR:OG1	1:A:206:ASP:OD2	2.14	0.59
1:D:378:LYS:HE3	1:D:383:GLY:O	2.02	0.59
1:D:362:GLN:OE1	1:D:464:GLU:CD	2.44	0.59
1:B:100:GLY:HA2	3:B:603:FAD:N5	2.18	0.58
1:B:362:GLN:NE2	1:B:464:GLU:HB3	2.15	0.58
1:D:472:ALA:O	3:D:602:FAD:HM81	2.03	0.58
1:A:362:GLN:NE2	1:A:464:GLU:HB3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:CYS:SG	4:B:781:HOH:O	2.57	0.58
1:C:331:CYS:HB2	1:C:335:LEU:HD12	1.85	0.58
1:B:472:ALA:CA	3:B:603:FAD:HM82	2.34	0.58
1:C:378:LYS:HE3	1:C:383:GLY:O	2.03	0.58
1:A:206:ASP:OD2	1:D:206:ASP:OD1	2.21	0.58
1:B:206:ASP:OD2	1:C:206:ASP:OD1	2.22	0.57
1:C:362:GLN:NE2	1:C:464:GLU:HB3	2.19	0.57
1:A:206:ASP:CG	1:D:206:ASP:OD1	2.47	0.57
1:D:389:MET:HE1	1:D:391:LEU:CG	2.18	0.57
1:A:100:GLY:HA2	3:A:604:FAD:N5	2.20	0.57
1:B:206:ASP:OD2	1:C:206:ASP:CG	2.47	0.57
1:C:316:ASP:C	1:C:316:ASP:OD1	2.45	0.57
1:C:241:ASN:OD1	1:C:359:ARG:NH1	2.37	0.56
1:A:362:GLN:OE1	1:A:464:GLU:CD	2.48	0.56
1:B:256:ASP:HB2	4:B:724:HOH:O	2.05	0.56
1:C:94:ILE:HG21	1:C:369:MET:CE	2.35	0.56
1:D:362:GLN:NE2	1:D:464:GLU:HB3	2.21	0.56
1:B:206:ASP:CG	1:C:206:ASP:OD2	2.48	0.55
1:C:100:GLY:HA2	3:C:603:FAD:N5	2.22	0.55
1:D:334:TRP:HB2	1:D:470:LEU:HD13	1.88	0.55
1:A:389:MET:C	1:A:389:MET:HE3	2.31	0.55
1:B:362:GLN:OE1	1:B:464:GLU:CD	2.50	0.55
1:A:519:GLY:O	1:A:523:THR:HG23	2.07	0.55
1:B:203:THR:OG1	1:B:206:ASP:OD2	2.12	0.55
1:D:199:TRP:O	1:D:200:ASP:C	2.51	0.54
1:A:206:ASP:OD1	1:D:206:ASP:CG	2.50	0.54
1:D:204:PHE:HB3	1:D:239:PHE:HA	1.89	0.54
1:B:94:ILE:HG21	1:B:369:MET:HE2	1.90	0.54
1:B:145:TYR:CD1	1:B:384:ARG:HD3	2.43	0.54
1:C:176:ILE:HG21	1:C:251:MET:SD	2.48	0.54
1:C:362:GLN:OE1	1:C:464:GLU:OE1	2.25	0.54
1:C:100:GLY:HA2	3:C:603:FAD:C4X	2.38	0.54
1:D:379:ASP:OD1	1:D:379:ASP:C	2.51	0.53
1:D:477:LEU:HD12	1:D:480:HIS:CE1	2.42	0.53
1:C:552:GLU:HG2	1:C:553:ILE:HG23	1.89	0.53
1:B:338:THR:OG1	1:B:339:GLN:N	2.41	0.53
1:A:337:THR:HG21	1:A:356:ASP:OD1	2.09	0.53
1:D:472:ALA:HB1	3:D:602:FAD:C8M	2.39	0.53
1:B:389:MET:HE3	1:B:389:MET:C	2.33	0.53
1:C:334:TRP:HB2	1:C:470:LEU:HD13	1.89	0.53
1:A:206:ASP:OD2	1:D:206:ASP:OD2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:CYS:HB2	1:B:335:LEU:HD12	1.90	0.52
1:D:362:GLN:OE1	1:D:464:GLU:OE1	2.28	0.52
1:D:316:ASP:C	1:D:316:ASP:OD1	2.52	0.52
1:C:508:ASP:OD1	1:C:514:PRO:O	2.28	0.52
1:D:100:GLY:HA2	3:D:602:FAD:C4X	2.40	0.52
1:C:79:MET:HE1	1:C:273:TRP:CG	2.44	0.52
1:B:486:ARG:HD3	4:B:806:HOH:O	2.09	0.51
1:A:353:MET:HE1	1:A:357:ARG:NH2	2.23	0.51
1:B:372:ARG:HB2	1:B:373:PRO:HD2	1.92	0.51
1:D:508:ASP:OD1	1:D:514:PRO:O	2.28	0.51
1:A:338:THR:OG1	1:A:339:GLN:N	2.43	0.51
1:C:359:ARG:HG2	1:C:360:TYR:N	2.26	0.51
1:B:206:ASP:OD1	1:C:206:ASP:OD2	2.28	0.51
1:B:241:ASN:OD1	1:B:359:ARG:NH1	2.43	0.50
1:B:337:THR:HG21	1:B:356:ASP:OD1	2.10	0.50
1:D:100:GLY:HA2	3:D:602:FAD:N5	2.25	0.50
1:A:100:GLY:HA2	3:A:604:FAD:C4X	2.41	0.50
1:B:379:ASP:OD1	1:B:379:ASP:C	2.55	0.50
1:B:303:ARG:HD2	1:B:341:ASP:OD2	2.12	0.50
1:B:206:ASP:CG	1:C:206:ASP:OD1	2.54	0.49
1:A:490:HIS:HE1	4:A:743:HOH:O	1.93	0.49
1:B:472:ALA:HB1	3:B:603:FAD:C8M	2.38	0.49
1:C:472:ALA:HB1	3:C:603:FAD:C8M	2.42	0.49
1:C:334:TRP:HB2	1:C:470:LEU:CD1	2.43	0.49
1:A:378:LYS:HE3	1:A:383:GLY:O	2.12	0.49
1:D:334:TRP:HB2	1:D:470:LEU:CD1	2.41	0.49
1:B:221:HIS:CE1	4:B:793:HOH:O	2.65	0.49
1:D:79:MET:HE1	1:D:273:TRP:CG	2.47	0.49
1:A:334:TRP:HB2	1:A:470:LEU:HD13	1.95	0.49
1:B:461:ILE:HG13	1:B:462:SER:N	2.28	0.49
1:A:268:VAL:HB	1:A:269:PRO:CD	2.42	0.48
1:C:359:ARG:HD3	1:C:475:GLY:O	2.13	0.48
1:C:389:MET:HE3	1:C:389:MET:O	2.13	0.48
1:D:516:TRP:CZ2	2:D:601:ARG:HB3	2.48	0.48
1:A:39:ILE:HG23	1:A:40:PRO:HD2	1.95	0.48
1:D:472:ALA:CB	3:D:602:FAD:HM83	2.41	0.48
1:B:474:LYS:HG2	1:B:514:PRO:HB3	1.95	0.48
1:A:100:GLY:HA2	3:A:604:FAD:C5X	2.43	0.48
1:C:353:MET:CE	1:C:357:ARG:NH1	2.77	0.48
1:C:490:HIS:HE1	4:C:705:HOH:O	1.95	0.48
1:D:303:ARG:HD2	1:D:341:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:CYS:HB2	1:D:335:LEU:HD12	1.94	0.48
1:B:91:THR:HG21	1:B:369:MET:CE	2.44	0.48
1:B:142:GLN:NE2	4:B:709:HOH:O	2.46	0.48
1:C:379:ASP:C	1:C:379:ASP:OD1	2.55	0.48
1:B:334:TRP:CZ2	1:B:358:THR:O	2.67	0.48
1:D:94:ILE:CG2	1:D:369:MET:CE	2.92	0.48
1:A:532:MET:HE1	1:A:539:THR:HG23	1.96	0.47
1:A:91:THR:HG21	1:A:369:MET:CE	2.44	0.47
1:B:519:GLY:O	1:B:523:THR:HG23	2.15	0.47
1:C:100:GLY:HA2	3:C:603:FAD:C5X	2.44	0.47
1:C:77:SER:OG	1:C:78:LYS:N	2.48	0.47
1:C:474:LYS:HG2	1:C:514:PRO:HB3	1.96	0.47
1:D:490:HIS:HD2	4:D:744:HOH:O	1.98	0.46
1:B:397:ARG:NH1	1:B:421:ASP:OD2	2.46	0.46
1:A:176:ILE:HG21	1:A:251:MET:SD	2.55	0.46
1:A:316:ASP:C	1:A:316:ASP:OD1	2.58	0.46
1:B:365:LYS:HG2	1:B:416:TYR:CD1	2.50	0.46
1:C:204:PHE:HB3	1:C:239:PHE:HA	1.97	0.46
1:D:176:ILE:HG21	1:D:251:MET:SD	2.55	0.46
1:A:389:MET:HE3	1:A:389:MET:O	2.16	0.46
1:B:238:ASP:OD2	2:B:601:ARG:NH2	2.48	0.46
2:B:602:ARG:N	1:C:337:THR:HB	2.31	0.46
1:B:190:GLU:O	1:B:194:THR:HG23	2.15	0.46
1:C:94:ILE:CG2	1:C:369:MET:CE	2.93	0.46
1:C:365:LYS:HG2	1:C:416:TYR:CD1	2.51	0.46
1:D:236:ASP:HA	1:D:239:PHE:CD2	2.50	0.46
1:D:365:LYS:HG2	1:D:416:TYR:CD1	2.51	0.46
1:A:145:TYR:CD1	1:A:384:ARG:HD3	2.51	0.45
1:B:206:ASP:OD2	1:C:206:ASP:OD2	2.34	0.45
1:B:102:ARG:HD2	1:B:258:GLN:OE1	2.17	0.45
1:B:334:TRP:HB2	1:B:470:LEU:HD13	1.99	0.45
1:A:464:GLU:N	1:A:464:GLU:CD	2.75	0.45
1:B:206:ASP:OD1	1:C:206:ASP:CG	2.60	0.45
1:C:145:TYR:CD1	1:C:384:ARG:HD3	2.51	0.45
1:D:338:THR:OG1	1:D:339:GLN:N	2.49	0.45
1:B:337:THR:HB	2:C:602:ARG:HB3	1.98	0.44
1:C:97:GLU:HB3	1:C:101:MET:HB3	1.99	0.44
1:A:393:ASP:CB	1:D:353:MET:HE3	2.38	0.44
1:B:101:MET:HE2	1:B:416:TYR:CE2	2.52	0.44
1:C:353:MET:CE	1:C:357:ARG:NH2	2.81	0.44
1:B:160:THR:HB	1:B:230:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ILE:HG22	3:D:602:FAD:O5'	2.18	0.44
1:B:540:HIS:NE2	4:B:702:HOH:O	2.36	0.44
1:D:203:THR:HG22	1:D:478:PRO:HG3	2.00	0.44
1:A:420:SER:HB3	1:D:334:TRP:CZ2	2.52	0.44
1:B:199:TRP:O	1:B:200:ASP:C	2.60	0.44
1:B:393:ASP:HB2	1:C:353:MET:HE1	1.99	0.44
1:A:461:ILE:HG13	1:A:462:SER:N	2.33	0.43
1:D:357:ARG:HE	1:D:357:ARG:HA	1.82	0.43
1:A:160:THR:HB	1:A:230:PHE:CG	2.54	0.43
1:D:488:TYR:HB3	1:D:555:GLN:OE1	2.18	0.43
1:B:389:MET:HE3	1:B:389:MET:O	2.17	0.43
1:A:334:TRP:CZ2	1:A:358:THR:O	2.71	0.43
1:A:474:LYS:HG2	1:A:514:PRO:HB3	2.00	0.43
1:B:540:HIS:CD2	4:B:702:HOH:O	2.72	0.43
1:A:298:ARG:NH1	4:A:703:HOH:O	2.43	0.43
1:C:451:ALA:HA	1:C:454:ILE:HD12	2.01	0.43
1:C:135:THR:HG23	1:C:389:MET:CE	2.48	0.43
1:C:519:GLY:O	1:C:523:THR:HG23	2.18	0.43
1:D:302:LYS:HB3	1:D:302:LYS:HE3	1.81	0.43
1:C:30:LEU:HD13	1:C:112:HIS:CD2	2.54	0.43
1:B:268:VAL:HB	1:B:269:PRO:CD	2.49	0.42
1:A:190:GLU:O	1:A:194:THR:HG23	2.20	0.42
1:D:135:THR:HG23	1:D:389:MET:CE	2.50	0.42
1:B:316:ASP:OD1	1:B:316:ASP:C	2.62	0.42
1:B:424:LYS:HG2	1:C:334:TRP:CE3	2.54	0.42
1:A:88:PHE:O	1:A:89:ASN:C	2.62	0.42
1:A:303:ARG:NE	1:A:305:ALA:HB2	2.33	0.42
1:A:552:GLU:HG2	1:A:553:ILE:HG23	2.01	0.42
1:B:353:MET:CE	1:B:357:ARG:NE	2.75	0.42
1:D:519:GLY:O	1:D:523:THR:HG23	2.20	0.42
1:D:550:PHE:CZ	1:D:555:GLN:NE2	2.87	0.42
1:A:474:LYS:HE2	1:A:514:PRO:HB3	2.02	0.42
1:A:555:GLN:H	1:A:555:GLN:HG3	1.41	0.42
1:A:94:ILE:HG21	1:A:369:MET:CE	2.47	0.42
1:A:379:ASP:OD1	1:A:379:ASP:C	2.61	0.42
1:D:91:THR:HG21	1:D:369:MET:CE	2.50	0.42
1:A:372:ARG:HB2	1:A:373:PRO:HD2	2.02	0.42
1:C:160:THR:HB	1:C:230:PHE:CG	2.55	0.42
1:A:334:TRP:HB2	1:A:470:LEU:CD1	2.50	0.42
1:C:472:ALA:O	3:C:603:FAD:HM81	2.19	0.42
1:A:205:TYR:CD2	1:D:478:PRO:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLY:HA2	3:D:602:FAD:C5X	2.50	0.41
1:C:82:ARG:O	1:C:99:GLY:HA3	2.19	0.41
1:A:203:THR:OG1	1:A:205:TYR:HB2	2.20	0.41
1:B:27:ASP:OD1	1:B:28:ASP:N	2.51	0.41
1:C:103:PHE:HA	1:C:104:PRO:HD2	1.99	0.41
1:D:97:GLU:OE1	1:D:97:GLU:HA	2.20	0.41
1:D:44:HIS:ND1	1:D:282:HIS:HB2	2.35	0.41
1:A:362:GLN:OE1	1:A:464:GLU:OE1	2.38	0.41
1:B:176:ILE:HG21	1:B:251:MET:SD	2.61	0.41
1:B:481:TYR:CD2	1:B:481:TYR:C	2.98	0.41
1:C:203:THR:HG22	1:C:478:PRO:HG3	2.02	0.41
1:A:397:ARG:NH1	1:A:421:ASP:OD2	2.47	0.41
1:A:60:ALA:HB2	1:A:524:SER:OG	2.21	0.41
1:D:239:PHE:N	1:D:240:PRO:CD	2.84	0.41
1:A:331:CYS:HB2	1:A:335:LEU:HD12	2.02	0.41
1:B:135:THR:HG23	1:B:389:MET:CE	2.51	0.41
1:C:199:TRP:O	1:C:200:ASP:C	2.63	0.41
1:C:555:GLN:H	1:C:555:GLN:HG3	1.45	0.41
1:B:326:ALA:HA	1:B:502:GLY:O	2.21	0.40
1:B:353:MET:HE2	1:B:357:ARG:NE	2.06	0.40
1:B:492:MET:HG3	1:B:550:PHE:CD2	2.55	0.40
1:D:101:MET:HE2	1:D:416:TYR:CE2	2.55	0.40
1:C:550:PHE:CZ	1:C:555:GLN:NE2	2.90	0.40
1:A:88:PHE:CD2	1:A:369:MET:HE3	2.57	0.40
1:B:47:GLU:HA	1:B:70:LYS:O	2.20	0.40
1:C:20:PRO:HB2	1:C:192:TRP:CG	2.56	0.40
1:D:451:ALA:HA	1:D:454:ILE:HD12	2.04	0.40
1:D:491:PHE:CE2	1:D:526:ASN:HB3	2.57	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	547/580 (94%)	531 (97%)	16 (3%)	0	100	100
1	B	547/580 (94%)	530 (97%)	17 (3%)	0	100	100
1	C	547/580 (94%)	537 (98%)	10 (2%)	0	100	100
1	D	547/580 (94%)	533 (97%)	13 (2%)	1 (0%)	43	55
All	All	2188/2320 (94%)	2131 (97%)	56 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	397	ARG

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	448/474 (94%)	429 (96%)	19 (4%)	26	40
1	B	448/474 (94%)	432 (96%)	16 (4%)	31	47
1	C	448/474 (94%)	431 (96%)	17 (4%)	29	44
1	D	448/474 (94%)	432 (96%)	16 (4%)	31	47
All	All	1792/1896 (94%)	1724 (96%)	68 (4%)	28	44

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	48	VAL
1	A	79	MET
1	A	279	ARG
1	A	280	CYS
1	A	298	ARG
1	A	302	LYS
1	A	303	ARG
1	A	337	THR
1	A	338	THR

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Mol	Chain	Res	Type
1	A	357	ARG
1	A	359	ARG
1	A	442	LYS
1	A	486	ARG
1	A	498	VAL
1	A	511	SER
1	A	540	HIS
1	A	555	GLN
1	A	556	ILE
1	B	79	MET
1	B	280	CYS
1	B	298	ARG
1	B	322	ARG
1	B	337	THR
1	B	338	THR
1	B	357	ARG
1	B	359	ARG
1	B	435	GLN
1	B	442	LYS
1	B	486	ARG
1	B	498	VAL
1	B	511	SER
1	B	540	HIS
1	B	555	GLN
1	B	556	ILE
1	C	48	VAL
1	C	59	VAL
1	C	78	LYS
1	C	79	MET
1	C	211	SER
1	C	237	SER
1	C	279	ARG
1	C	298	ARG
1	C	337	THR
1	C	338	THR
1	C	357	ARG
1	C	359	ARG
1	C	442	LYS
1	C	511	SER
1	C	540	HIS
1	C	552	GLU
1	C	555	GLN

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Mol	Chain	Res	Type
1	D	48	VAL
1	D	59	VAL
1	D	78	LYS
1	D	79	MET
1	D	211	SER
1	D	237	SER
1	D	279	ARG
1	D	337	THR
1	D	338	THR
1	D	339	GLN
1	D	353	MET
1	D	357	ARG
1	D	442	LYS
1	D	511	SER
1	D	540	HIS
1	D	555	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	157	GLN
1	A	177	GLN
1	A	253	ASN
1	A	267	GLN
1	A	275	HIS
1	A	453	HIS
1	A	480	HIS
1	A	490	HIS
1	B	157	GLN
1	B	267	GLN
1	B	435	GLN
1	B	480	HIS
1	B	485	GLN
1	B	490	HIS
1	C	126	ASN
1	C	142	GLN
1	C	177	GLN
1	C	267	GLN
1	C	468	HIS
1	C	490	HIS
1	D	126	ASN

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Mol	Chain	Res	Type
1	D	142	GLN
1	D	157	GLN
1	D	267	GLN
1	D	428	HIS
1	D	468	HIS
1	D	480	HIS
1	D	490	HIS

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FAD	C	603	-	58,58,58	1.64	13 (22%)	85,89,89	1.97	25 (29%)
2	ARG	A	602	-	10,11,11	0.92	1 (10%)	9,13,13	1.18	1 (11%)
2	ARG	D	601	-	10,11,11	0.68	0	9,13,13	1.09	1 (11%)
2	ARG	C	601	-	10,11,11	0.93	0	9,13,13	1.33	1 (11%)
2	ARG	A	601	-	10,11,11	0.78	0	9,13,13	0.98	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	D	602	-	58,58,58	1.70	11 (18%)	85,89,89	1.91	27 (31%)
2	ARG	A	603	-	10,11,11	0.92	1 (10%)	9,13,13	1.25	1 (11%)
3	FAD	B	603	-	58,58,58	1.71	12 (20%)	85,89,89	2.50	33 (38%)
3	FAD	A	604	-	58,58,58	1.59	11 (18%)	85,89,89	2.28	26 (30%)
2	ARG	C	602	-	10,11,11	0.71	0	9,13,13	1.50	1 (11%)
2	ARG	B	602	-	10,11,11	0.84	1 (10%)	9,13,13	1.12	1 (11%)
2	ARG	B	601	-	10,11,11	0.95	1 (10%)	9,13,13	1.00	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	603	-	-	7/34/50/50	0/6/6/6
2	ARG	A	602	-	-	2/11/11/11	-
2	ARG	D	601	-	-	4/11/11/11	-
2	ARG	C	601	-	-	5/11/11/11	-
2	ARG	A	601	-	-	2/11/11/11	-
3	FAD	D	602	-	-	2/34/50/50	0/6/6/6
2	ARG	A	603	-	-	8/11/11/11	-
3	FAD	B	603	-	-	4/34/50/50	0/6/6/6
3	FAD	A	604	-	-	6/34/50/50	0/6/6/6
2	ARG	C	602	-	-	3/11/11/11	-
2	ARG	B	602	-	-	0/11/11/11	-
2	ARG	B	601	-	-	6/11/11/11	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	FAD	C9A-C5X	6.21	1.51	1.41
3	C	603	FAD	C9A-C5X	5.17	1.49	1.41
3	B	603	FAD	C9A-C5X	5.14	1.49	1.41
3	B	603	FAD	C5A-N7A	-4.65	1.30	1.39
3	C	603	FAD	C5A-C4A	4.54	1.47	1.39
3	D	602	FAD	C5A-C4A	4.34	1.46	1.39
3	A	604	FAD	C1'-C2'	-4.04	1.47	1.52
3	C	603	FAD	C5X-N5	-3.81	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	FAD	P-O3P	3.66	1.63	1.59
3	B	603	FAD	C1'-C2'	-3.51	1.47	1.52
3	B	603	FAD	C8-C7	3.34	1.49	1.40
3	D	602	FAD	C8-C7	3.26	1.48	1.40
3	D	602	FAD	C8A-N7A	3.25	1.37	1.31
3	A	604	FAD	C5A-N7A	-3.22	1.33	1.39
3	A	604	FAD	C5X-N5	-3.20	1.33	1.39
3	D	602	FAD	C1'-C2'	-3.11	1.48	1.52
3	D	602	FAD	PA-O3P	3.10	1.62	1.59
3	A	604	FAD	C4-N3	-3.07	1.33	1.38
3	A	604	FAD	C9A-C5X	3.06	1.46	1.41
3	B	603	FAD	C8A-N9A	-3.06	1.32	1.37
3	C	603	FAD	PA-O3P	3.03	1.62	1.59
3	A	604	FAD	C5A-C4A	2.97	1.44	1.39
3	A	604	FAD	C8-C7	2.93	1.48	1.40
3	D	602	FAD	C5X-N5	-2.77	1.34	1.39
3	C	603	FAD	C6-C5X	-2.71	1.35	1.40
3	A	604	FAD	P-O3P	2.64	1.62	1.59
3	C	603	FAD	C8A-N7A	2.63	1.36	1.31
3	D	602	FAD	C4-N3	-2.62	1.33	1.38
3	C	603	FAD	C8-C7	2.55	1.47	1.40
3	A	604	FAD	C8A-N7A	2.51	1.36	1.31
3	D	602	FAD	C4A-N9A	-2.50	1.32	1.37
3	B	603	FAD	O4'-C4'	2.49	1.48	1.43
3	D	602	FAD	C6-C7	-2.48	1.36	1.39
3	C	603	FAD	C6-C7	-2.44	1.36	1.39
3	B	603	FAD	C5A-C4A	2.39	1.43	1.39
3	B	603	FAD	PA-O3P	2.37	1.62	1.59
3	C	603	FAD	C5A-N7A	-2.33	1.34	1.39
2	A	603	ARG	OXT-C	-2.32	1.23	1.30
3	D	602	FAD	C5A-C6A	2.31	1.47	1.41
2	B	601	ARG	OXT-C	-2.29	1.23	1.30
3	B	603	FAD	C5X-N5	-2.27	1.35	1.39
2	B	602	ARG	OXT-C	-2.26	1.23	1.30
3	C	603	FAD	C4A-N9A	-2.26	1.33	1.37
3	C	603	FAD	C5A-C6A	2.25	1.47	1.41
3	C	603	FAD	C1'-C2'	-2.23	1.49	1.52
3	B	603	FAD	C4-N3	-2.20	1.34	1.38
3	B	603	FAD	O4B-C1B	2.19	1.47	1.42
3	C	603	FAD	C4-N3	-2.12	1.34	1.38
3	A	604	FAD	O4'-C4'	2.11	1.47	1.43
2	A	602	ARG	OXT-C	-2.07	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	FAD	C8A-N9A	-2.07	1.34	1.37

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	FAD	C4B-O4B-C1B	-8.10	91.58	109.47
3	A	604	FAD	C5A-C4A-N3A	-7.27	116.70	126.72
3	B	603	FAD	C5A-C4A-N3A	-6.41	117.88	126.72
3	B	603	FAD	N3A-C4A-N9A	5.73	136.91	127.17
3	A	604	FAD	C4B-O4B-C1B	-5.18	98.03	109.47
3	A	604	FAD	N3A-C4A-N9A	5.11	135.86	127.17
3	B	603	FAD	C5'-C4'-C3'	-5.03	102.73	112.22
3	C	603	FAD	C5A-C4A-N3A	-4.88	120.00	126.72
3	D	602	FAD	C5A-C4A-N3A	-4.69	120.26	126.72
3	B	603	FAD	O4B-C4B-C5B	4.63	124.16	109.33
3	A	604	FAD	C5'-C4'-C3'	-4.61	103.51	112.22
3	A	604	FAD	C2A-N3A-C4A	4.57	122.99	111.83
3	A	604	FAD	O4B-C4B-C5B	4.55	123.92	109.33
3	B	603	FAD	O2A-PA-O3P	-4.52	95.06	107.27
3	B	603	FAD	C5A-N7A-C8A	4.42	110.40	103.45
3	A	604	FAD	O4B-C1B-N9A	4.23	116.22	108.09
3	C	603	FAD	O4-C4-C4X	-4.23	115.38	126.53
3	A	604	FAD	N3A-C2A-N1A	-4.22	122.20	128.58
3	B	603	FAD	O4B-C1B-N9A	4.17	116.10	108.09
3	D	602	FAD	N3A-C2A-N1A	-4.16	122.28	128.58
3	C	603	FAD	O2-C2-N1	-4.16	114.89	121.80
3	A	604	FAD	O2A-PA-O3P	-4.11	96.17	107.27
2	C	602	ARG	OXT-C-O	-4.09	114.79	124.08
3	C	603	FAD	N3A-C4A-N9A	4.00	133.97	127.17
3	D	602	FAD	O2-C2-N1	-3.98	115.19	121.80
3	D	602	FAD	N3A-C4A-N9A	3.91	133.82	127.17
3	D	602	FAD	C4A-N9A-C8A	3.85	109.78	105.74
3	B	603	FAD	N3A-C2A-N1A	-3.85	122.76	128.58
3	B	603	FAD	O2-C2-N1	-3.83	115.43	121.80
3	B	603	FAD	O4-C4-N3	3.82	127.29	120.11
3	C	603	FAD	C6-C5X-C9A	3.81	124.28	119.05
3	B	603	FAD	C5X-C9A-N10	3.81	121.41	117.97
3	B	603	FAD	N9A-C8A-N7A	-3.80	108.55	113.94
3	C	603	FAD	N3A-C2A-N1A	-3.79	122.84	128.58
3	C	603	FAD	O4-C4-N3	3.78	127.23	120.11
3	D	602	FAD	C2A-N3A-C4A	3.77	121.04	111.83
3	B	603	FAD	C2A-N3A-C4A	3.71	120.89	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	FAD	O5B-C5B-C4B	3.69	121.57	108.99
3	A	604	FAD	C4A-C5A-N7A	-3.66	106.39	110.58
3	A	604	FAD	O5B-PA-O1A	3.66	123.46	108.94
3	D	602	FAD	O2A-PA-O1A	3.66	129.45	112.44
2	C	601	ARG	OXT-C-O	-3.65	115.80	124.08
3	D	602	FAD	O4-C4-C4X	-3.65	116.91	126.53
3	C	603	FAD	C4A-N9A-C8A	3.63	109.55	105.74
3	B	603	FAD	C4A-C5A-N7A	-3.53	106.55	110.58
3	C	603	FAD	C2A-N3A-C4A	3.52	120.43	111.83
3	B	603	FAD	O5B-PA-O1A	3.49	122.78	108.94
3	A	604	FAD	O4B-C1B-C2B	-3.48	99.17	106.62
3	B	603	FAD	C4A-N9A-C8A	3.41	109.31	105.74
3	C	603	FAD	C4A-C5A-N7A	-3.39	106.71	110.58
3	A	604	FAD	C5X-C9A-N10	3.33	120.98	117.97
3	B	603	FAD	O4-C4-C4X	-3.27	117.90	126.53
3	D	602	FAD	O4-C4-N3	3.23	126.19	120.11
3	B	603	FAD	O3B-C3B-C4B	-3.22	101.85	111.08
3	D	602	FAD	O4B-C1B-N9A	3.18	114.19	108.09
3	B	603	FAD	C9A-N10-C10	-3.14	115.96	120.75
2	A	603	ARG	OXT-C-O	-3.13	116.98	124.08
3	C	603	FAD	C1'-N10-C9A	3.09	126.63	120.63
3	A	604	FAD	C5A-N7A-C8A	3.05	108.24	103.45
3	D	602	FAD	C6-C5X-C9A	3.04	123.23	119.05
3	C	603	FAD	C4B-O4B-C1B	-3.02	102.80	109.47
3	D	602	FAD	C9A-N10-C10	-3.00	116.18	120.75
3	C	603	FAD	C5X-C9A-N10	2.99	120.67	117.97
3	D	602	FAD	C5X-C9A-N10	2.98	120.66	117.97
3	C	603	FAD	C9A-N10-C10	-2.96	116.23	120.75
3	D	602	FAD	C4B-O4B-C1B	-2.94	102.98	109.47
3	B	603	FAD	O4'-C4'-C3'	2.82	115.84	109.25
3	B	603	FAD	C1'-N10-C9A	2.78	126.04	120.63
2	A	602	ARG	OXT-C-O	-2.76	117.81	124.08
3	C	603	FAD	C2A-N1A-C6A	2.75	123.24	118.73
3	D	602	FAD	C2A-N1A-C6A	2.73	123.21	118.73
2	B	602	ARG	OXT-C-O	-2.71	117.94	124.08
3	C	603	FAD	N9A-C8A-N7A	-2.68	110.13	113.94
2	A	601	ARG	OXT-C-O	-2.67	118.02	124.08
3	B	603	FAD	O4B-C1B-C2B	-2.67	100.91	106.62
3	A	604	FAD	O2'-C2'-C3'	2.65	115.45	109.25
3	C	603	FAD	C5A-N7A-C8A	2.64	107.60	103.45
3	A	604	FAD	O2A-PA-O1A	2.61	124.60	112.44
3	A	604	FAD	O4-C4-N3	2.61	125.02	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	FAD	C1'-N10-C9A	2.60	125.69	120.63
3	C	603	FAD	C9-C8-C7	2.60	123.50	119.69
3	B	603	FAD	O2A-PA-O1A	2.59	124.50	112.44
3	B	603	FAD	N3-C2-N1	2.58	124.99	119.50
3	B	603	FAD	O4'-C4'-C5'	2.56	115.63	109.99
3	B	603	FAD	N6A-C6A-N1A	2.48	123.91	118.38
2	D	601	ARG	OXT-C-O	-2.48	118.46	124.08
3	D	602	FAD	C4A-C5A-N7A	-2.44	107.79	110.58
3	A	604	FAD	O4'-C4'-C5'	2.43	115.35	109.99
3	B	603	FAD	C6-C5X-C9A	2.41	122.36	119.05
3	B	603	FAD	O3'-C3'-C2'	-2.39	103.49	108.93
3	A	604	FAD	O4-C4-C4X	-2.36	120.31	126.53
3	C	603	FAD	O2P-P-O1P	2.35	123.38	112.44
3	D	602	FAD	N3-C2-N1	2.34	124.48	119.50
3	B	603	FAD	C6A-C5A-C4A	2.34	120.38	117.18
3	C	603	FAD	O2A-PA-O1A	2.34	123.31	112.44
3	A	604	FAD	O2P-P-O3P	2.33	113.58	107.27
3	D	602	FAD	N9A-C8A-N7A	-2.28	110.70	113.94
3	D	602	FAD	O4B-C4B-C3B	2.28	109.67	105.15
3	A	604	FAD	N9A-C8A-N7A	-2.27	110.72	113.94
3	C	603	FAD	O2'-C2'-C1'	-2.26	100.92	110.20
3	D	602	FAD	C6A-C5A-N7A	2.25	136.42	132.09
3	A	604	FAD	C9A-C5X-N5	-2.23	120.09	122.45
3	B	603	FAD	C4'-C3'-C2'	-2.23	109.86	113.57
3	D	602	FAD	C4X-C10-N1	-2.21	119.16	124.59
3	D	602	FAD	C4A-N9A-C1B	-2.21	121.45	126.63
3	A	604	FAD	C6-C5X-C9A	2.21	122.08	119.05
3	D	602	FAD	C4X-C10-N10	2.19	119.61	116.48
3	D	602	FAD	O2P-P-O1P	2.13	122.36	112.44
3	D	602	FAD	C9-C8-C7	2.13	122.82	119.69
3	A	604	FAD	C6-C7-C8	-2.11	116.59	119.69
3	D	602	FAD	C4-N3-C2	-2.10	121.91	125.64
3	C	603	FAD	O2'-C2'-C3'	2.10	114.17	109.25
3	C	603	FAD	C2'-C1'-N10	2.09	120.10	110.20
3	C	603	FAD	C4-N3-C2	-2.09	121.94	125.64
3	C	603	FAD	C9A-C5X-N5	-2.07	120.25	122.45
3	A	604	FAD	C9-C8-C7	2.06	122.71	119.69
2	B	601	ARG	OXT-C-O	-2.05	119.43	124.08
3	B	603	FAD	C8M-C8-C9	-2.01	116.03	119.57
3	B	603	FAD	C9-C8-C7	2.00	122.63	119.69

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	ARG	O-C-CA-N
2	A	603	ARG	N-CA-CB-CG
2	A	603	ARG	C-CA-CB-CG
2	B	601	ARG	C-CA-CB-CG
2	C	602	ARG	C-CA-CB-CG
3	A	604	FAD	C5B-O5B-PA-O2A
3	A	604	FAD	C5B-O5B-PA-O3P
3	B	603	FAD	C5B-O5B-PA-O2A
3	B	603	FAD	C5B-O5B-PA-O3P
2	C	602	ARG	NE-CD-CG-CB
2	A	603	ARG	NE-CD-CG-CB
2	D	601	ARG	NE-CD-CG-CB
2	A	603	ARG	CG-CD-NE-CZ
2	C	602	ARG	CG-CD-NE-CZ
2	A	603	ARG	OXT-C-CA-N
2	B	601	ARG	CA-CB-CG-CD
2	B	601	ARG	NE-CD-CG-CB
3	C	603	FAD	O3'-C3'-C4'-C5'
3	C	603	FAD	C2'-C3'-C4'-C5'
3	A	604	FAD	O3'-C3'-C4'-O4'
2	A	602	ARG	NE-CD-CG-CB
3	C	603	FAD	C2'-C3'-C4'-O4'
3	A	604	FAD	N10-C1'-C2'-O2'
3	B	603	FAD	N10-C1'-C2'-O2'
2	B	601	ARG	N-CA-CB-CG
2	C	601	ARG	N-CA-CB-CG
2	D	601	ARG	O-C-CA-CB
3	C	603	FAD	C5'-O5'-P-O1P
3	A	604	FAD	C4B-C5B-O5B-PA
3	C	603	FAD	C2B-C1B-N9A-C8A
2	D	601	ARG	OXT-C-CA-CB
2	A	603	ARG	OXT-C-CA-CB
2	D	601	ARG	CA-CB-CG-CD
2	C	601	ARG	O-C-CA-N
2	A	603	ARG	O-C-CA-CB
2	A	602	ARG	CG-CD-NE-CZ
3	A	604	FAD	O3'-C3'-C4'-C5'
2	B	601	ARG	OXT-C-CA-N
3	C	603	FAD	O3'-C3'-C4'-O4'
3	B	603	FAD	C4B-C5B-O5B-PA
2	C	601	ARG	OXT-C-CA-N
3	C	603	FAD	O4B-C1B-N9A-C8A

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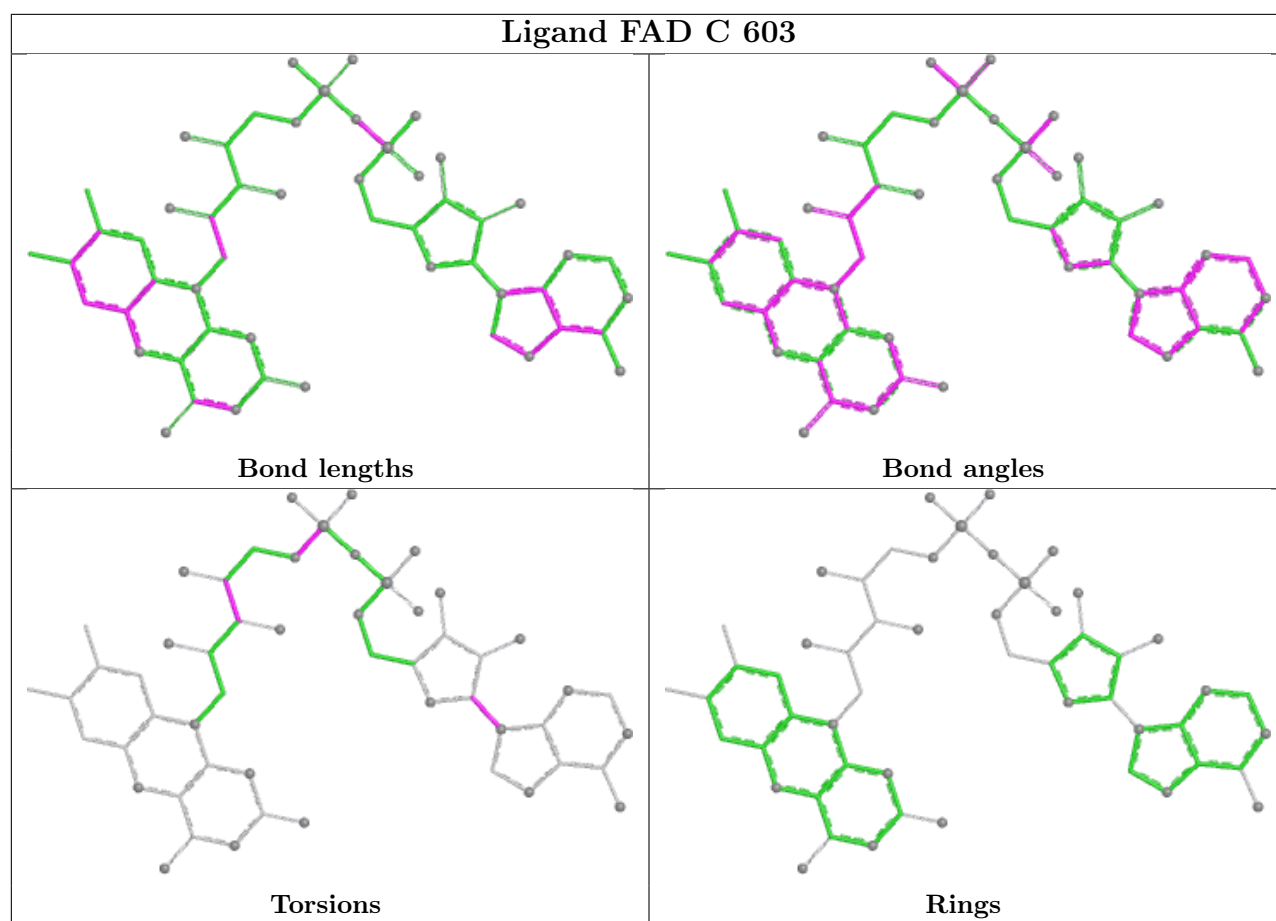
Mol	Chain	Res	Type	Atoms
3	D	602	FAD	C2B-C1B-N9A-C8A
2	C	601	ARG	O-C-CA-CB
3	D	602	FAD	O4B-C4B-C5B-O5B
2	B	601	ARG	CG-CD-NE-CZ
2	C	601	ARG	OXT-C-CA-CB
2	A	601	ARG	OXT-C-CA-N
2	A	601	ARG	O-C-CA-N

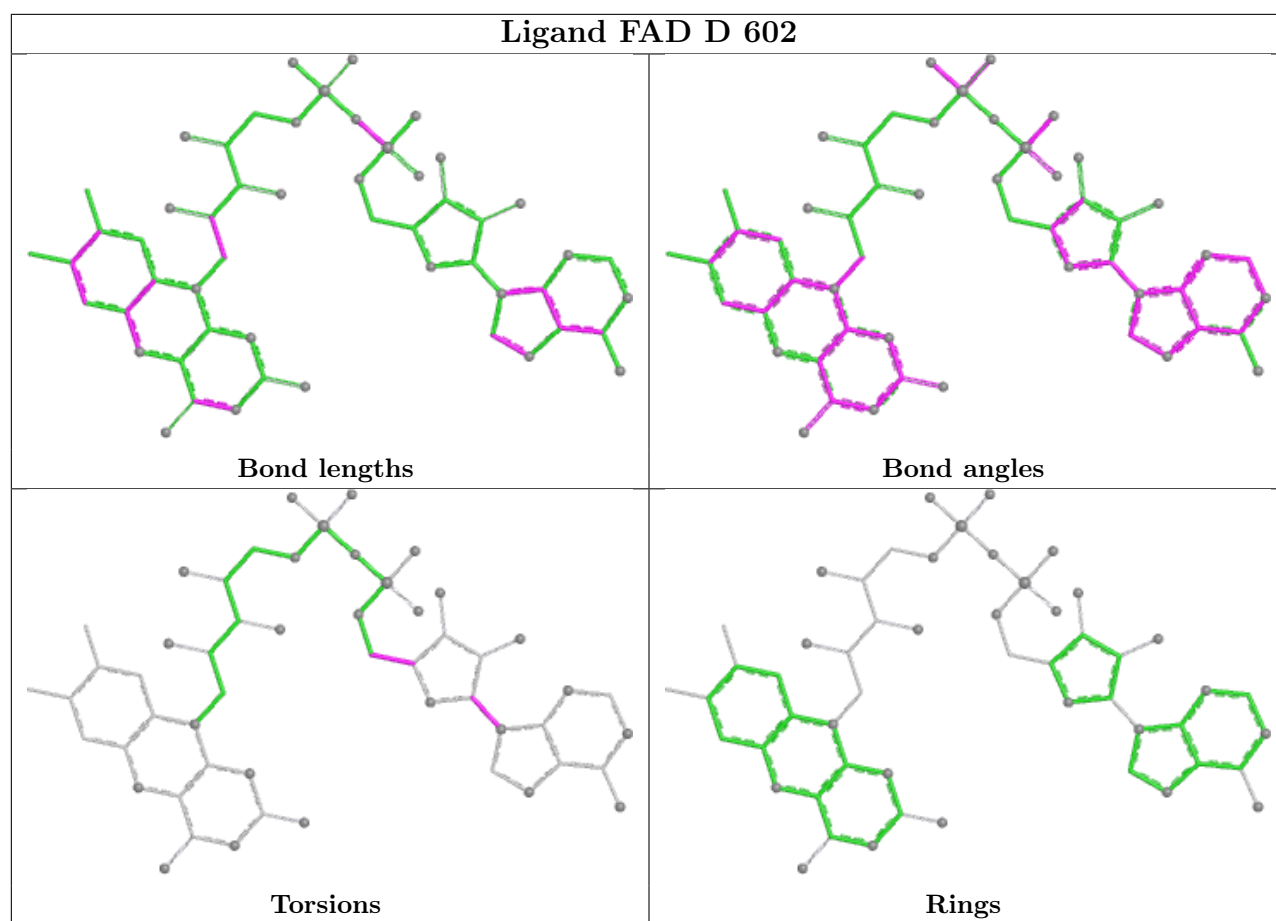
There are no ring outliers.

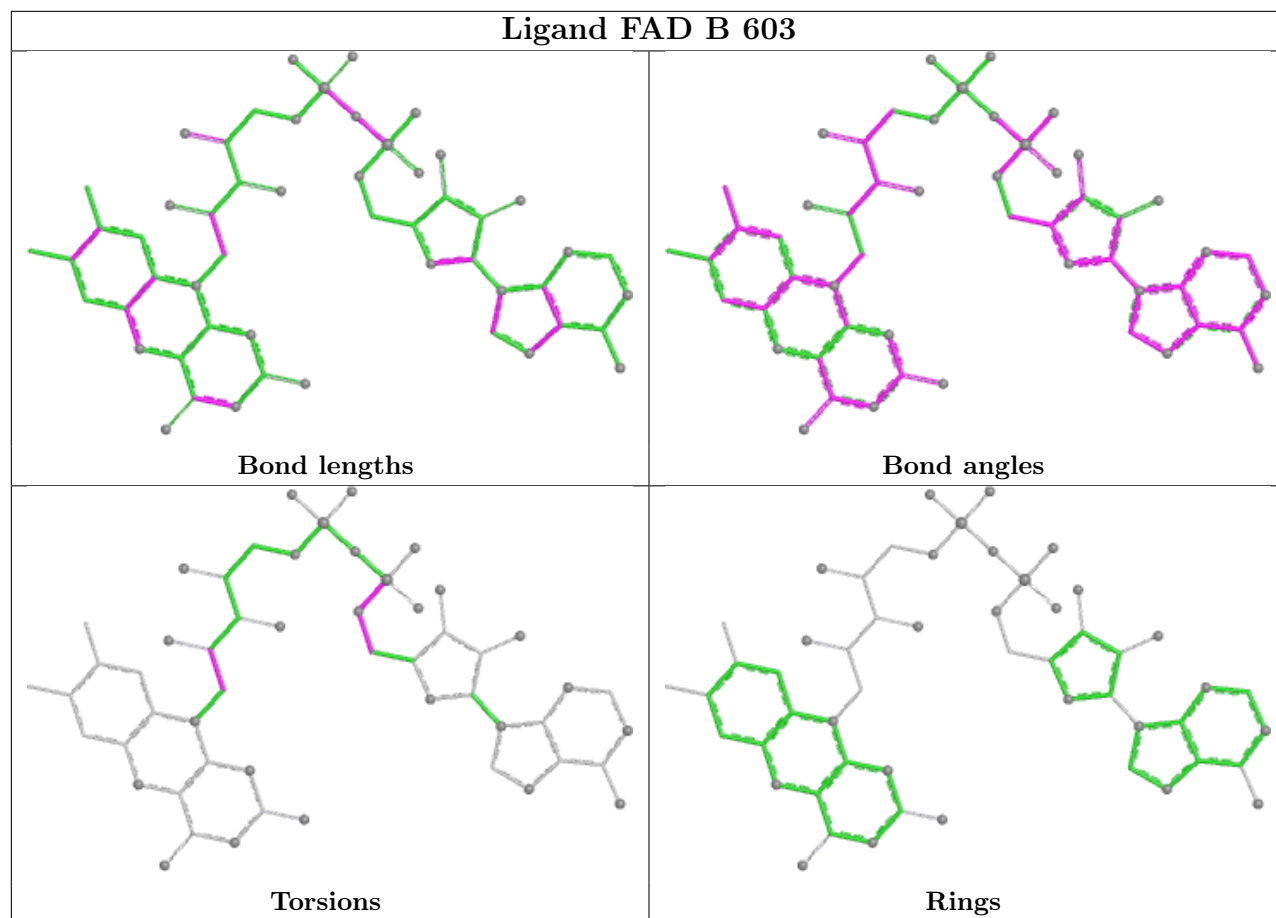
9 monomers are involved in 31 short contacts:

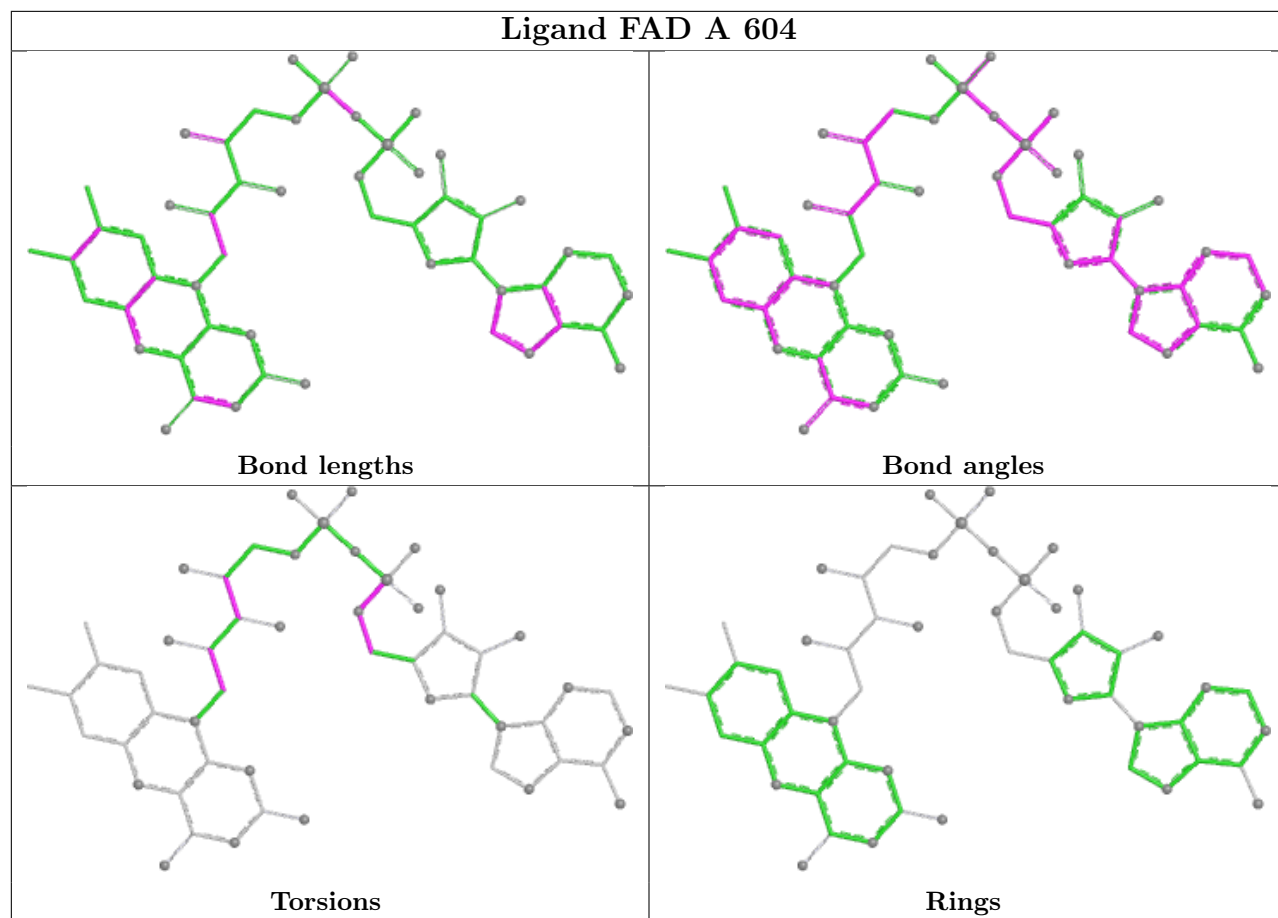
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	FAD	6	0
2	D	601	ARG	2	0
3	D	602	FAD	8	0
2	A	603	ARG	1	0
3	B	603	FAD	6	0
3	A	604	FAD	5	0
2	C	602	ARG	1	0
2	B	602	ARG	1	0
2	B	601	ARG	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	549/580 (94%)	0.35	20 (3%)	46	48	14, 29, 53, 85	0
1	B	549/580 (94%)	0.33	19 (3%)	47	49	15, 29, 51, 83	0
1	C	549/580 (94%)	0.78	44 (8%)	18	20	20, 39, 62, 112	0
1	D	549/580 (94%)	0.79	39 (7%)	22	24	22, 38, 60, 91	0
All	All	2196/2320 (94%)	0.56	122 (5%)	30	32	14, 35, 58, 112	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	HIS	4.6
1	D	338	THR	4.5
1	C	555	GLN	4.4
1	D	160	THR	4.0
1	D	423	LEU	4.0
1	C	279	ARG	3.9
1	A	334	TRP	3.9
1	C	337	THR	3.8
1	B	334	TRP	3.8
1	D	555	GLN	3.7
1	C	257	HIS	3.7
1	C	380	PRO	3.7
1	C	423	LEU	3.6
1	C	160	THR	3.5
1	C	338	THR	3.5
1	A	279	ARG	3.4
1	D	279	ARG	3.4
1	B	338	THR	3.4
1	C	280	CYS	3.4
1	B	353	MET	3.3
1	C	357	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	205	TYR	3.3
1	D	337	THR	3.2
1	D	280	CYS	3.1
1	B	279	ARG	3.1
1	D	257	HIS	3.0
1	A	407	ASP	3.0
1	C	527	ALA	3.0
1	D	556	ILE	3.0
1	A	337	THR	2.9
1	D	89	ASN	2.9
1	C	464	GLU	2.8
1	B	407	ASP	2.8
1	B	205	TYR	2.8
1	C	381	GLU	2.8
1	D	540	HIS	2.7
1	A	542	ASP	2.7
1	D	13	LYS	2.7
1	C	540	HIS	2.7
1	A	338	THR	2.7
1	D	464	GLU	2.7
1	D	380	PRO	2.7
1	D	435	GLN	2.6
1	B	12	LYS	2.6
1	D	319	GLY	2.6
1	B	362	GLN	2.6
1	D	255	ASP	2.6
1	A	160	THR	2.6
1	B	160	THR	2.6
1	D	537	GLY	2.6
1	D	416	TYR	2.6
1	D	256	ASP	2.5
1	D	307	ALA	2.5
1	B	416	TYR	2.5
1	A	280	CYS	2.5
1	C	556	ILE	2.5
1	D	527	ALA	2.5
1	C	278	GLU	2.4
1	D	425	MET	2.4
1	A	540	HIS	2.4
1	C	255	ASP	2.4
1	C	362	GLN	2.4
1	A	464	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	552	GLU	2.4
1	D	12	LYS	2.4
1	D	334	TRP	2.4
1	D	426	LEU	2.4
1	C	416	TYR	2.4
1	C	334	TRP	2.4
1	A	237	SER	2.4
1	A	556	ILE	2.4
1	D	298	ARG	2.4
1	A	256	ASP	2.3
1	C	425	MET	2.3
1	D	322	ARG	2.3
1	C	470	LEU	2.3
1	B	418	TRP	2.3
1	C	418	TRP	2.3
1	D	308	SER	2.3
1	B	555	GLN	2.3
1	D	542	ASP	2.3
1	C	286	GLY	2.3
1	C	298	ARG	2.3
1	C	276	VAL	2.3
1	C	353	MET	2.2
1	A	416	TYR	2.2
1	C	216	LYS	2.2
1	C	113	TYR	2.2
1	D	277	PRO	2.2
1	C	67	LEU	2.2
1	C	407	ASP	2.2
1	A	255	ASP	2.1
1	D	212	LYS	2.1
1	A	353	MET	2.1
1	A	285	GLU	2.1
1	B	238	ASP	2.1
1	C	449	ASP	2.1
1	B	257	HIS	2.1
1	D	427	PRO	2.1
1	D	536	GLY	2.1
1	C	322	ARG	2.1
1	C	150	ALA	2.1
1	C	559	ALA	2.1
1	C	426	LEU	2.1
1	D	278	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	280	CYS	2.1
1	C	350	LYS	2.1
1	C	206	ASP	2.1
1	C	480	HIS	2.1
1	A	322	ARG	2.1
1	D	418	TRP	2.1
1	C	378	LYS	2.0
1	B	464	GLU	2.0
1	C	254	CYS	2.0
1	C	422	ALA	2.0
1	D	42	ALA	2.0
1	D	480	HIS	2.0
1	B	239	PHE	2.0
1	B	381	GLU	2.0
1	C	451	ALA	2.0
1	A	238	ASP	2.0
1	C	356	ASP	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(Å ²)	Q<0.9
2	ARG	A	601	12/12	0.65	0.24	59,70,85,86	0
2	ARG	C	602	12/12	0.67	0.20	68,77,78,80	0
2	ARG	A	603	12/12	0.70	0.17	69,78,82,83	0
2	ARG	B	601	12/12	0.71	0.20	57,61,74,75	0
2	ARG	C	601	12/12	0.73	0.22	58,68,78,80	0
2	ARG	D	601	12/12	0.76	0.20	55,64,78,80	0

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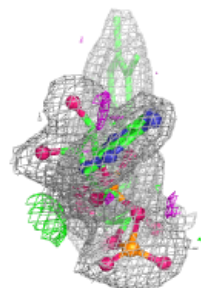
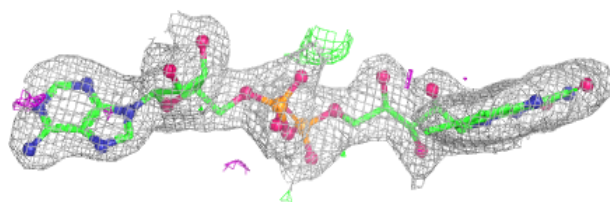
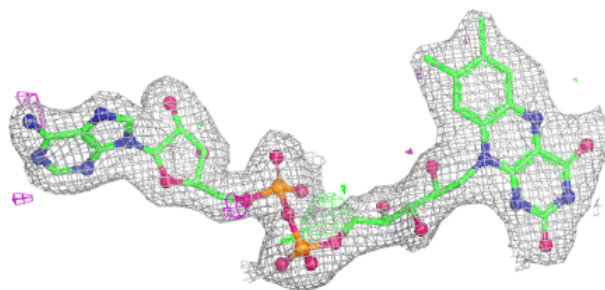
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ARG	B	602	12/12	0.82	0.18	45,55,63,63	0
2	ARG	A	602	12/12	0.83	0.16	40,51,53,55	0
3	FAD	C	603	53/53	0.93	0.09	23,29,32,34	0
3	FAD	B	603	53/53	0.95	0.08	15,21,29,29	0
3	FAD	A	604	53/53	0.95	0.07	17,21,27,31	0
3	FAD	D	602	53/53	0.95	0.08	21,30,37,38	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.

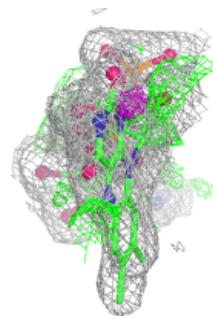
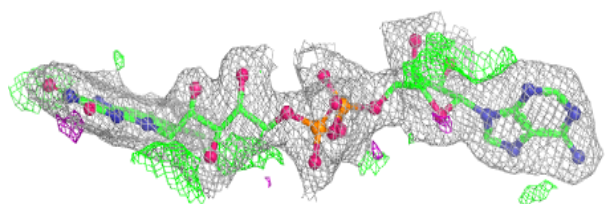
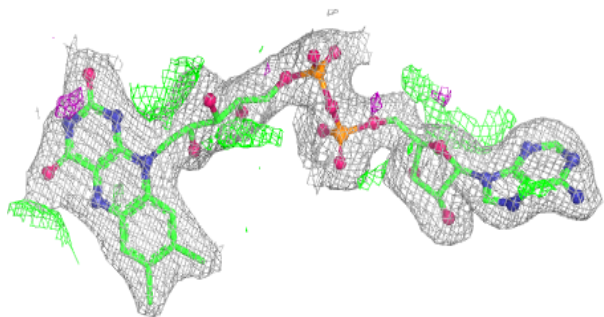
Electron density around FAD C 603:

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

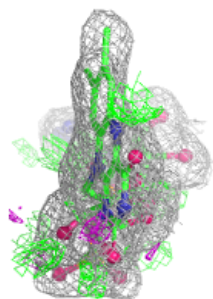
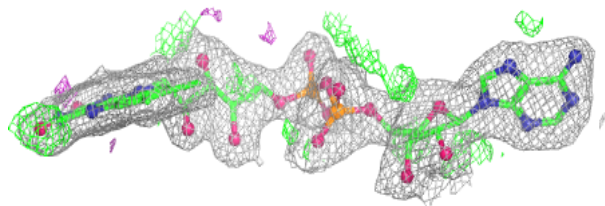
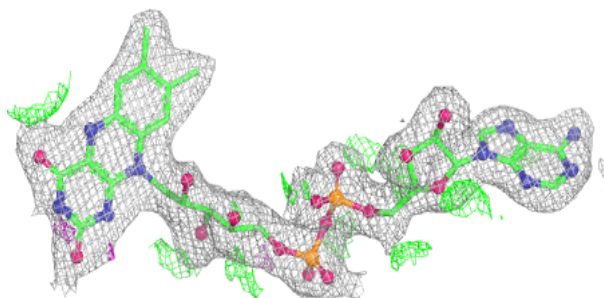


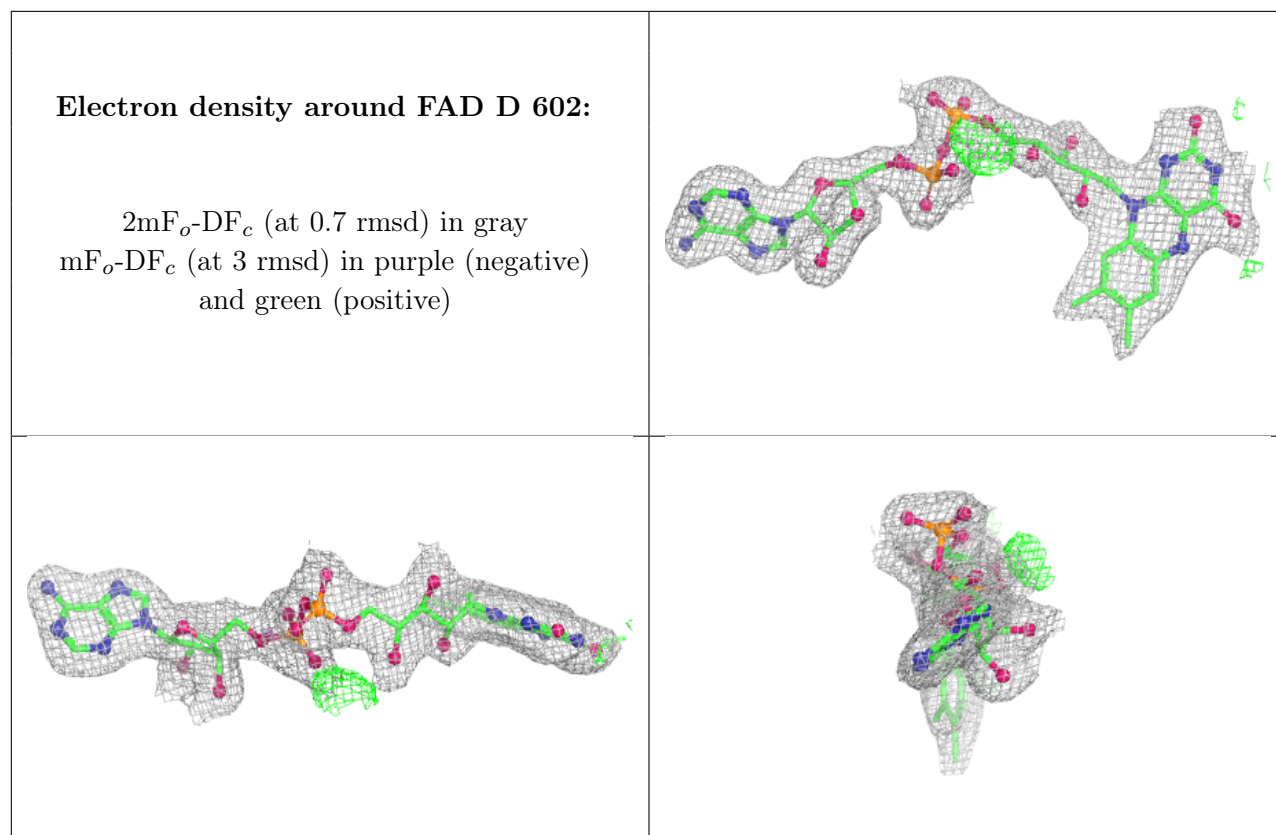
Electron density around FAD B 603:

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

**Electron density around FAD A 604:**

$2mF_o-DF_c$ (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.