



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 10:43 PM JST

PDB ID : 5YB6
Title : L-Amino acid oxidase/monooxygenase from Pseudomonas sp. AIU 813 -
L-lysine complex
Authors : Im, D.; Matsui, D.; Arakawa, T.; Isobe, K.; Asano, Y.; Fushinobu, S.
Deposited on : 2017-09-03
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

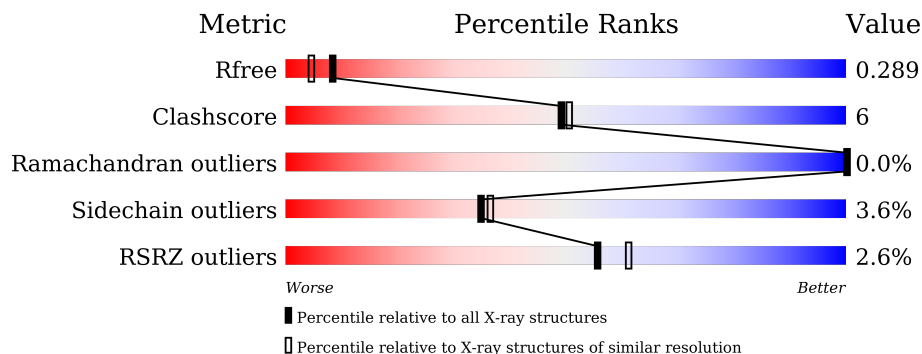
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	580	 2% 83% 12% . .
1	B	580	 2% 83% 12% . .
1	C	580	 3% 84% 11% . .
1	D	580	 3% 83% 11% . .

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 18833 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
			Total	C	N	O	S			
1	A	556	4369	2785	759	802	23	0	1	0
1	B	556	4358	2779	755	801	23	0	0	0
1	C	556	4358	2779	755	801	23	0	0	0
1	D	556	4358	2779	755	801	23	0	0	0

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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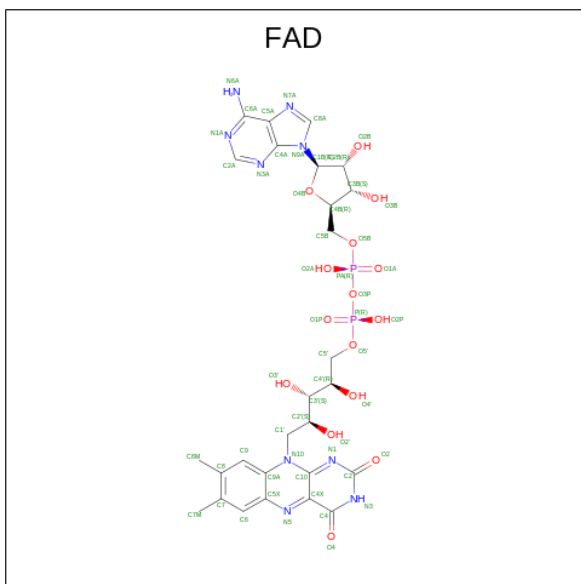
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP W6JQJ6
B	-18	GLY	-	expression tag	UNP W6JQJ6
B	-17	SER	-	expression tag	UNP W6JQJ6
B	-16	SER	-	expression tag	UNP W6JQJ6
B	-15	HIS	-	expression tag	UNP W6JQJ6
B	-14	HIS	-	expression tag	UNP W6JQJ6
B	-13	HIS	-	expression tag	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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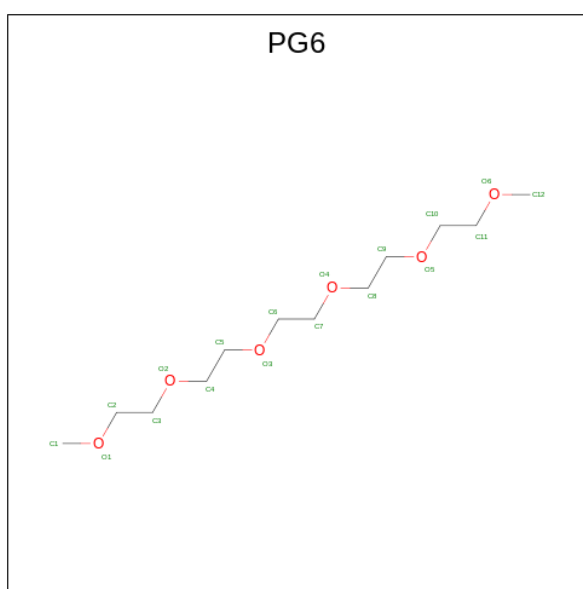
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP W6JQJ6
D	-18	GLY	-	expression tag	UNP W6JQJ6
D	-17	SER	-	expression tag	UNP W6JQJ6
D	-16	SER	-	expression tag	UNP W6JQJ6
D	-15	HIS	-	expression tag	UNP W6JQJ6
D	-14	HIS	-	expression tag	UNP W6JQJ6
D	-13	HIS	-	expression tag	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 FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



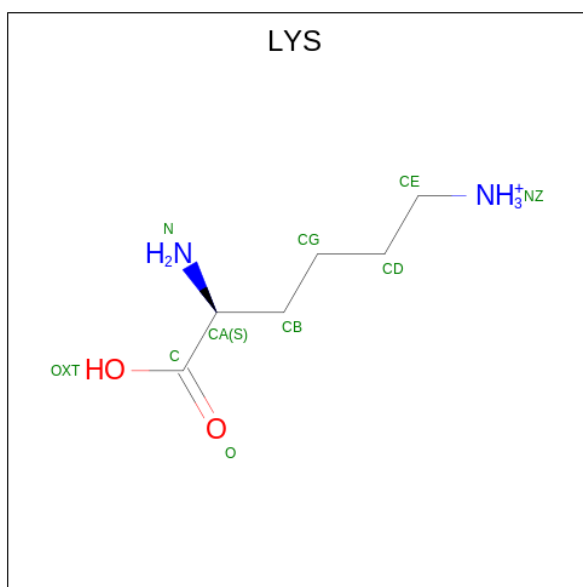
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	18	6	0	0
3	B	1	18	6	0	0
3	C	1	18	6	0	0
3	D	1	18	6	0	0

- Molecule 4 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 10	C 6	N 2	O 2	0	0
4	A	1	Total 10	C 6	N 2	O 2	0	0
4	B	1	Total 10	C 6	N 2	O 2	0	0
4	B	1	Total 10	C 6	N 2	O 2	0	0
4	C	1	Total 10	C 6	N 2	O 2	0	0
4	C	1	Total 10	C 6	N 2	O 2	0	0
4	D	1	Total 10	C 6	N 2	O 2	0	0
4	D	1	Total 10	C 6	N 2	O 2	0	0

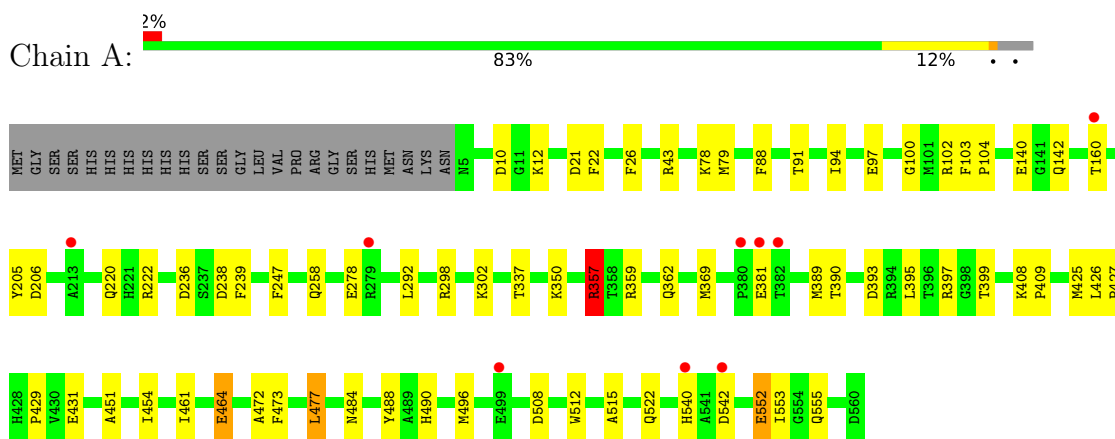
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	272	Total 272	O 272	0	0
5	B	260	Total 260	O 260	0	0
5	C	236	Total 236	O 236	0	0
5	D	258	Total 258	O 258	0	0

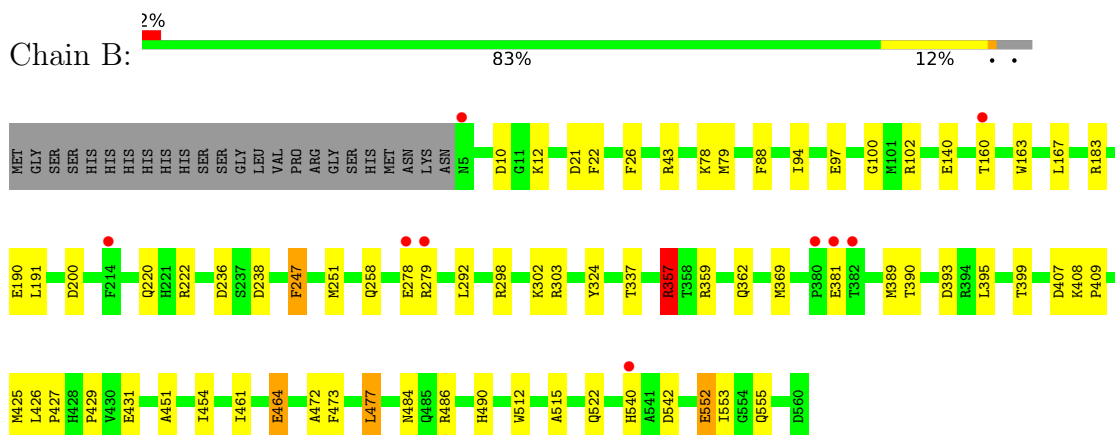
3 Residue-property plots [i](#)

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.

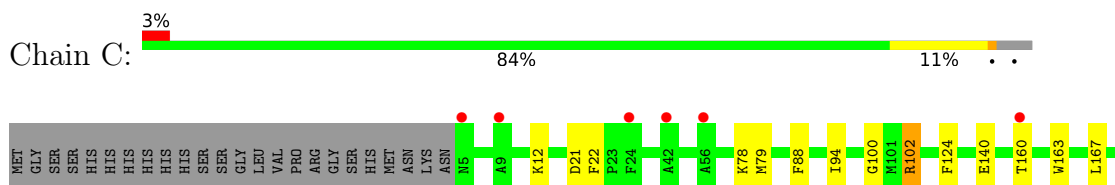
- Molecule 1: L-amino acid oxidase/monooxygenase

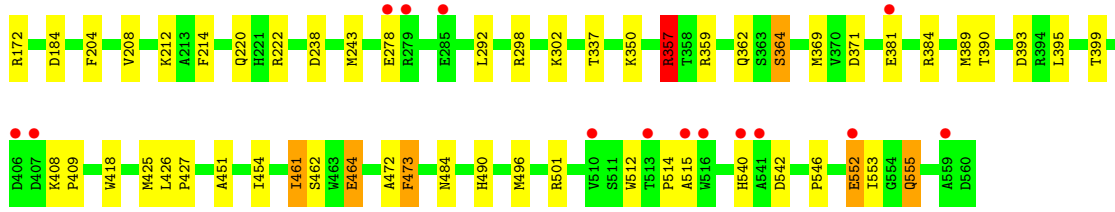


- Molecule 1: L-amino acid oxidase/monooxygenase

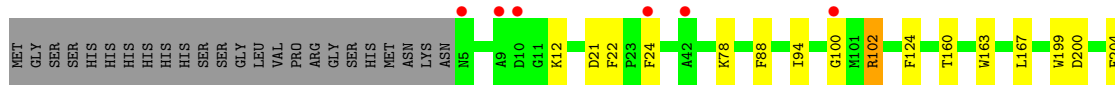
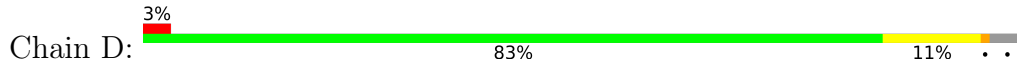


- Molecule 1: L-amino acid oxidase/monooxygenase





• Molecule 1: L-amino acid oxidase/monooxygenase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.07Å 132.29Å 100.96Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.10) 99.4 (38.76-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.234 , 0.283 0.241 , 0.289	Depositor DCC
R_{free} test set	6938 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtrriage
Anisotropy	0.216	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.117 for l,-k,h	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18833	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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, PG6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.90	0/4494	0.95	19/6108 (0.3%)
1	B	0.89	1/4483 (0.0%)	0.96	16/6094 (0.3%)
1	C	0.86	1/4483 (0.0%)	0.95	16/6094 (0.3%)
1	D	0.88	1/4483 (0.0%)	0.95	17/6094 (0.3%)
All	All	0.88	3/17943 (0.0%)	0.95	68/24390 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	364	SER	CB-OG	-6.80	1.33	1.42
1	C	364	SER	CB-OG	-5.81	1.34	1.42
1	B	324	TYR	CE1-CZ	-5.14	1.31	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ARG	NE-CZ-NH2	-12.37	114.11	120.30
1	B	357	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	D	357	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	A	298	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	C	357	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	B	298	ARG	NE-CZ-NH2	-11.11	114.74	120.30
1	A	222	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	B	357	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	A	357	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	A	222	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	298	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	B	222	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	B	298	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	B	236	ASP	CB-CG-OD1	9.57	126.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	D	222	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	D	222	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	C	222	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	B	222	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	D	384	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	D	298	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	C	357	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	D	357	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	298	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	D	298	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	79	MET	CG-SD-CE	-7.76	87.78	100.20
1	C	371	ASP	CB-CG-OD2	-7.75	111.33	118.30
1	A	508	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	236	ASP	CB-CG-OD1	7.71	125.24	118.30
1	D	384	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	C	298	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	79	MET	CG-SD-CE	-7.12	88.81	100.20
1	C	384	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	43	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	C	79	MET	CG-SD-CE	-6.35	90.05	100.20
1	D	496	MET	CG-SD-CE	-6.34	90.05	100.20
1	B	43	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	C	496	MET	CG-SD-CE	-6.17	90.33	100.20
1	C	464	GLU	CB-CA-C	-6.09	98.21	110.40
1	D	206	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	10	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	464	GLU	CB-CA-C	-5.88	98.63	110.40
1	A	247	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	A	464	GLU	CB-CA-C	-5.85	98.70	110.40
1	B	10	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	496	MET	CG-SD-CE	-5.59	91.25	100.20
1	A	298	ARG	CG-CD-NE	-5.55	100.14	111.80
1	D	102	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	464	GLU	CB-CA-C	-5.43	99.54	110.40
1	A	292	LEU	CB-CG-CD2	5.42	120.22	111.00
1	D	403	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	359	ARG	CG-CD-NE	5.35	123.03	111.80
1	C	102	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	501	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	D	359	ARG	CG-CD-NE	5.30	122.94	111.80
1	C	184	ASP	CB-CG-OD1	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	LEU	CB-CG-CD1	5.25	119.93	111.00
1	B	303	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	D	508	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	508	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	486	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	206	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	247	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	B	298	ARG	CG-CD-NE	-5.16	100.96	111.80
1	B	200	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	384	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	357	ARG	CG-CD-NE	-5.07	101.16	111.80
1	D	355	LEU	CB-CG-CD2	5.04	119.57	111.00

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	4369	0	4223	51	0
1	B	4358	0	4211	56	0
1	C	4358	0	4211	47	0
1	D	4358	0	4211	55	0
2	A	53	0	31	3	0
2	B	53	0	31	4	0
2	C	53	0	31	2	0
2	D	53	0	31	2	0
3	A	18	0	26	3	0
3	B	18	0	26	2	0
3	C	18	0	26	2	0
3	D	18	0	26	2	0
4	A	20	0	24	1	0
4	B	20	0	24	3	0
4	C	20	0	24	2	0
4	D	20	0	24	3	0
5	A	272	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	260	0	0	10	0
5	C	236	0	0	4	0
5	D	258	0	0	8	0
All	All	18833	0	17180	205	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 6.

All (205) 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:555:GLN:N	1:A:555:GLN:OE1	1.75	1.20
1:D:555:GLN:OE1	1:D:555:GLN:N	1.75	1.18
1:C:555:GLN:N	1:C:555:GLN:OE1	1.80	1.15
1:B:555:GLN:N	1:B:555:GLN:OE1	1.80	1.14
1:D:220:GLN:HE22	3:D:602:PG6:H92	1.20	1.03
1:D:160:THR:HG22	5:D:950:HOH:O	1.63	0.95
1:B:22:PHE:HB2	1:B:555:GLN:HE22	1.34	0.92
1:B:22:PHE:HB2	1:B:555:GLN:NE2	1.91	0.85
1:A:22:PHE:HB2	1:A:555:GLN:HE22	1.43	0.83
1:D:220:GLN:NE2	3:D:602:PG6:H92	1.92	0.83
1:D:362:GLN:HG3	1:D:464:GLU:HG3	1.60	0.83
1:C:22:PHE:HB2	1:C:555:GLN:HE22	1.44	0.81
1:B:362:GLN:HG3	1:B:464:GLU:CG	2.11	0.80
1:C:362:GLN:HG3	1:C:464:GLU:HG3	1.61	0.80
1:D:22:PHE:HB2	1:D:555:GLN:HE22	1.46	0.80
1:C:94:ILE:HG21	1:C:369:MET:HE2	1.63	0.79
1:A:22:PHE:HB2	1:A:555:GLN:NE2	1.97	0.78
1:A:362:GLN:HG3	1:A:464:GLU:CG	2.13	0.78
1:A:362:GLN:HG3	1:A:464:GLU:HG3	1.65	0.76
1:B:362:GLN:HG3	1:B:464:GLU:HG3	1.66	0.76
1:C:512:TRP:CZ2	1:C:555:GLN:HG2	2.20	0.76
1:C:94:ILE:HG21	1:C:369:MET:CE	2.15	0.76
1:D:275:HIS:HD2	5:D:939:HOH:O	1.69	0.76
1:D:362:GLN:HG3	1:D:464:GLU:CG	2.16	0.76
1:A:512:TRP:CZ2	1:A:555:GLN:HG2	2.22	0.75
1:B:512:TRP:CZ2	1:B:555:GLN:HG2	2.22	0.75
1:B:191:LEU:HG	5:B:843:HOH:O	1.86	0.74
1:B:357:ARG:NH2	1:D:393:ASP:O	2.21	0.74
1:C:362:GLN:HG3	1:C:464:GLU:CG	2.16	0.74
1:D:94:ILE:HG21	1:D:369:MET:HE2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:GLN:H	1:D:555:GLN:CD	1.89	0.74
1:D:512:TRP:CZ2	1:D:555:GLN:HG2	2.22	0.73
1:D:88:PHE:HB2	1:D:369:MET:HE1	1.70	0.73
1:C:22:PHE:HB2	1:C:555:GLN:NE2	2.02	0.73
1:C:88:PHE:HB2	1:C:369:MET:HE1	1.69	0.73
4:B:603:LYS:HE2	5:B:898:HOH:O	1.87	0.72
1:C:512:TRP:HZ2	1:C:555:GLN:HG2	1.54	0.72
1:C:160:THR:HG22	5:C:927:HOH:O	1.88	0.71
1:D:94:ILE:HG21	1:D:369:MET:CE	2.19	0.71
1:D:555:GLN:N	1:D:555:GLN:CD	2.44	0.71
1:D:22:PHE:HB2	1:D:555:GLN:NE2	2.05	0.70
1:D:512:TRP:HZ2	1:D:555:GLN:HG2	1.55	0.69
1:B:337:THR:HG1	4:B:604:LYS:N	1.91	0.69
1:C:555:GLN:N	1:C:555:GLN:CD	2.46	0.68
1:B:395:LEU:HD13	1:B:425:MET:HE1	1.75	0.68
1:A:393:ASP:O	1:C:357:ARG:NH2	2.27	0.67
1:B:512:TRP:HZ2	1:B:555:GLN:HG2	1.60	0.67
1:B:555:GLN:N	1:B:555:GLN:CD	2.48	0.67
1:B:393:ASP:O	1:D:357:ARG:NH2	2.27	0.66
1:B:94:ILE:HG21	1:B:369:MET:HE2	1.77	0.66
1:A:512:TRP:HZ2	1:A:555:GLN:HG2	1.59	0.66
1:A:337:THR:HG1	4:A:604:LYS:N	1.95	0.65
1:A:88:PHE:HB2	1:A:369:MET:HE1	1.79	0.65
1:A:94:ILE:HG21	1:A:369:MET:CE	2.27	0.64
1:D:514:PRO:O	1:D:515:ALA:HB3	1.97	0.64
1:D:337:THR:HG1	4:D:604:LYS:N	1.96	0.63
1:B:94:ILE:HG21	1:B:369:MET:CE	2.29	0.63
1:A:555:GLN:N	1:A:555:GLN:CD	2.49	0.63
1:B:362:GLN:HG3	1:B:464:GLU:HG2	1.80	0.62
1:A:357:ARG:NH2	1:C:393:ASP:O	2.32	0.62
1:D:395:LEU:HD13	1:D:425:MET:CE	2.30	0.62
1:C:395:LEU:HD13	1:C:425:MET:CE	2.30	0.62
1:A:94:ILE:HG21	1:A:369:MET:HE2	1.82	0.61
1:A:395:LEU:HD13	1:A:425:MET:HE1	1.83	0.61
1:C:337:THR:HG1	4:C:604:LYS:N	2.00	0.60
1:C:514:PRO:O	1:C:515:ALA:HB3	2.02	0.60
1:B:359:ARG:NH1	1:B:477:LEU:HD13	2.17	0.59
1:A:21:ASP:HB3	1:A:555:GLN:HG3	1.83	0.59
1:A:359:ARG:NH1	1:A:477:LEU:HD13	2.17	0.59
1:D:222:ARG:NH2	5:D:704:HOH:O	2.36	0.59
1:B:100:GLY:HA2	2:B:601:FAD:C4X	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:LEU:HD13	1:D:425:MET:HE1	1.85	0.58
1:B:160:THR:HG22	5:B:949:HOH:O	2.04	0.56
3:C:602:PG6:H52	5:C:887:HOH:O	2.04	0.56
1:B:102:ARG:HD2	1:B:258:GLN:OE1	2.06	0.56
1:A:362:GLN:HG3	1:A:464:GLU:HG2	1.85	0.56
1:B:21:ASP:HB3	1:B:555:GLN:HG3	1.87	0.56
1:A:102:ARG:HD2	1:A:258:GLN:OE1	2.06	0.56
1:D:472:ALA:HB1	2:D:601:FAD:HM83	1.88	0.56
1:B:140:GLU:OE1	1:D:350:LYS:HD3	2.06	0.55
1:A:160:THR:HG22	5:A:956:HOH:O	2.06	0.54
1:B:88:PHE:HB2	1:B:369:MET:HE1	1.88	0.54
1:B:362:GLN:CG	1:B:464:GLU:HG2	2.38	0.54
1:A:362:GLN:CG	1:A:464:GLU:CG	2.86	0.53
1:C:552:GLU:HG3	1:C:553:ILE:HG23	1.89	0.53
1:A:100:GLY:HA2	2:A:601:FAD:C4X	2.39	0.53
1:A:140:GLU:OE1	1:C:350:LYS:HD3	2.08	0.53
1:D:322:ARG:HD2	5:D:737:HOH:O	2.08	0.53
1:A:472:ALA:HB1	2:A:601:FAD:HM83	1.89	0.53
1:B:395:LEU:HD13	1:B:425:MET:CE	2.39	0.53
1:A:142:GLN:NE2	3:A:602:PG6:H52	2.24	0.53
1:A:395:LEU:HD13	1:A:425:MET:CE	2.38	0.53
1:C:395:LEU:HD13	1:C:425:MET:HE1	1.89	0.53
1:C:490:HIS:HE1	5:C:765:HOH:O	1.92	0.53
1:B:484:ASN:HD21	1:B:512:TRP:HA	1.74	0.53
1:A:362:GLN:CG	1:A:464:GLU:HG2	2.39	0.52
1:D:298:ARG:NH1	5:D:711:HOH:O	2.42	0.52
1:D:94:ILE:CG2	1:D:369:MET:CE	2.88	0.52
1:B:183:ARG:NH1	5:B:707:HOH:O	2.43	0.52
1:B:190:GLU:HB3	5:B:843:HOH:O	2.10	0.52
1:B:425:MET:CE	5:B:883:HOH:O	2.58	0.52
1:C:94:ILE:CG2	1:C:369:MET:CE	2.87	0.51
1:C:362:GLN:CG	1:C:464:GLU:CG	2.87	0.51
1:C:21:ASP:HB3	1:C:555:GLN:HG3	1.93	0.51
1:D:408:LYS:HB3	1:D:409:PRO:HD2	1.93	0.51
1:D:484:ASN:HD21	1:D:512:TRP:HA	1.76	0.51
1:A:552:GLU:HG3	1:A:553:ILE:HG23	1.92	0.51
1:B:552:GLU:HG3	1:B:553:ILE:HG23	1.92	0.50
1:D:512:TRP:CZ2	1:D:555:GLN:CG	2.92	0.50
1:C:512:TRP:CZ2	1:C:555:GLN:CG	2.94	0.50
1:D:418:TRP:CZ2	4:D:603:LYS:HG2	2.47	0.50
1:C:484:ASN:HB3	1:C:512:TRP:CZ3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ASP:HB3	1:D:555:GLN:HG3	1.94	0.50
1:D:100:GLY:HA2	2:D:601:FAD:C4X	2.42	0.50
1:C:408:LYS:HB3	1:C:409:PRO:HD2	1.94	0.49
1:B:220:GLN:HE22	3:B:602:PG6:H42	1.77	0.49
1:B:220:GLN:HE22	3:B:602:PG6:C4	2.26	0.49
1:B:362:GLN:CG	1:B:464:GLU:CG	2.86	0.49
1:B:247:PHE:HA	5:B:915:HOH:O	2.13	0.49
1:D:362:GLN:CG	1:D:464:GLU:CG	2.88	0.49
1:D:514:PRO:O	1:D:515:ALA:CB	2.61	0.48
1:A:26:PHE:CD1	1:A:522:GLN:HG2	2.49	0.48
1:A:484:ASN:HD21	1:A:512:TRP:HA	1.78	0.48
1:C:484:ASN:HD21	1:C:512:TRP:HA	1.77	0.48
1:A:220:GLN:NE2	3:A:602:PG6:H61	2.29	0.48
1:A:512:TRP:CZ2	1:A:555:GLN:CG	2.97	0.48
1:B:472:ALA:HB1	2:B:601:FAD:HM83	1.95	0.47
1:C:451:ALA:HA	1:C:454:ILE:HD12	1.96	0.47
1:D:552:GLU:CG	1:D:553:ILE:HG23	2.44	0.47
1:C:362:GLN:HG3	1:C:464:GLU:HG2	1.95	0.47
1:C:552:GLU:CG	1:C:553:ILE:HG23	2.44	0.47
1:D:362:GLN:HG3	1:D:464:GLU:HG2	1.94	0.47
1:B:425:MET:HE3	5:B:883:HOH:O	2.14	0.47
1:D:552:GLU:HG3	1:D:553:ILE:HG23	1.96	0.47
1:C:390:THR:HB	1:C:399:THR:HB	1.97	0.47
1:B:484:ASN:HB3	1:B:512:TRP:CZ3	2.50	0.47
1:B:100:GLY:HA2	2:B:601:FAD:N5	2.30	0.47
1:C:362:GLN:CG	1:C:464:GLU:HG2	2.45	0.47
1:C:461:ILE:HG13	1:C:462:SER:N	2.30	0.47
1:A:408:LYS:HB3	1:A:409:PRO:HD2	1.97	0.46
1:B:473:PHE:CG	1:B:515:ALA:HB2	2.51	0.46
1:B:512:TRP:CZ2	1:B:555:GLN:CG	2.97	0.45
1:D:362:GLN:CG	1:D:464:GLU:HG2	2.46	0.45
1:B:390:THR:HB	1:B:399:THR:HB	1.98	0.45
1:D:461:ILE:HG13	1:D:462:SER:N	2.31	0.45
1:A:484:ASN:HB3	1:A:512:TRP:CZ3	2.52	0.45
1:B:26:PHE:CD1	1:B:522:GLN:HG2	2.51	0.45
1:B:408:LYS:HB3	1:B:409:PRO:HD2	1.98	0.45
1:B:429:PRO:HB2	1:B:431:GLU:OE1	2.17	0.45
1:A:94:ILE:CG2	1:A:369:MET:CE	2.94	0.45
1:C:418:TRP:CZ2	4:C:603:LYS:HG2	2.51	0.45
1:C:490:HIS:HD2	5:C:890:HOH:O	1.98	0.45
1:B:451:ALA:HA	1:B:454:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TRP:CZ2	1:C:167:LEU:HD11	2.52	0.45
1:A:390:THR:HB	1:A:399:THR:HB	1.97	0.44
1:C:204:PHE:HA	1:C:243:MET:SD	2.58	0.44
1:D:390:THR:HB	1:D:399:THR:HB	1.99	0.44
1:D:204:PHE:HA	1:D:243:MET:SD	2.58	0.44
1:C:100:GLY:HA2	2:C:601:FAD:C4X	2.48	0.44
1:C:472:ALA:HB1	2:C:601:FAD:HM83	1.99	0.44
1:D:199:TRP:O	1:D:200:ASP:C	2.56	0.44
1:A:425:MET:CE	5:A:911:HOH:O	2.66	0.44
1:A:490:HIS:HE1	5:A:743:HOH:O	2.01	0.44
1:A:426:LEU:HB3	1:A:427:PRO:HD3	2.00	0.43
1:A:103:PHE:HA	1:A:104:PRO:HD2	1.93	0.43
1:B:552:GLU:CG	1:B:553:ILE:HG23	2.48	0.43
1:A:473:PHE:CG	1:A:515:ALA:HB2	2.54	0.43
1:A:490:HIS:HD2	5:A:908:HOH:O	2.00	0.43
1:B:251:MET:CE	5:B:915:HOH:O	2.66	0.43
1:D:451:ALA:HA	1:D:454:ILE:HD12	2.01	0.43
1:B:472:ALA:O	2:B:601:FAD:HM81	2.19	0.42
1:A:205:TYR:HB2	1:A:239:PHE:HB3	2.01	0.42
1:B:97:GLU:OE1	1:B:97:GLU:HA	2.19	0.42
1:B:407:ASP:OD1	1:B:408:LYS:HG3	2.20	0.42
1:C:514:PRO:O	1:C:515:ALA:CB	2.65	0.42
1:D:255:ASP:HB2	5:D:803:HOH:O	2.19	0.42
1:A:552:GLU:CG	1:A:553:ILE:HG23	2.49	0.42
1:D:163:TRP:CZ2	1:D:167:LEU:HD11	2.55	0.42
1:B:426:LEU:HB3	1:B:427:PRO:HD3	2.02	0.42
1:A:429:PRO:HB2	1:A:431:GLU:OE1	2.19	0.42
1:B:163:TRP:CZ2	1:B:167:LEU:HD11	2.54	0.42
1:D:275:HIS:CD2	5:D:939:HOH:O	2.56	0.42
1:B:94:ILE:CG2	1:B:369:MET:CE	2.95	0.42
1:B:490:HIS:HE1	5:B:727:HOH:O	2.02	0.42
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.20	0.42
1:B:357:ARG:HD3	1:B:357:ARG:HA	1.81	0.41
1:A:451:ALA:HA	1:A:454:ILE:HD12	2.02	0.41
3:A:602:PG6:H11	5:A:803:HOH:O	2.20	0.41
1:D:490:HIS:HD2	5:D:911:HOH:O	2.02	0.41
1:D:102:ARG:HB3	1:D:124:PHE:CD1	2.55	0.41
1:A:350:LYS:HD3	1:C:140:GLU:OE1	2.20	0.41
1:D:352:TRP:HB3	4:D:604:LYS:HD3	2.03	0.41
1:A:472:ALA:O	2:A:601:FAD:HM81	2.21	0.41
1:B:515:ALA:HB1	4:B:603:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:ASN:HB3	1:D:512:TRP:CZ3	2.54	0.41
1:C:208:VAL:O	1:C:214:PHE:HB2	2.21	0.41
1:C:220:GLN:NE2	3:C:602:PG6:H71	2.36	0.41
1:C:473:PHE:CG	1:C:515:ALA:HB2	2.56	0.41
1:D:208:VAL:O	1:D:214:PHE:HB2	2.21	0.41
1:A:91:THR:HG21	1:A:369:MET:CE	2.51	0.40
1:C:426:LEU:HB3	1:C:427:PRO:HD3	2.03	0.40
1:D:22:PHE:O	1:D:24:PHE:N	2.49	0.40
1:A:488:TYR:CE2	1:A:555:GLN:NE2	2.89	0.40
1:C:102:ARG:HB3	1:C:124:PHE:CD1	2.56	0.40
1:D:357:ARG:HD3	1:D:357:ARG:HA	1.88	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	555/580 (96%)	541 (98%)	13 (2%)	1 (0%)	47	49
1	B	554/580 (96%)	538 (97%)	16 (3%)	0	100	100
1	C	554/580 (96%)	537 (97%)	17 (3%)	0	100	100
1	D	554/580 (96%)	538 (97%)	16 (3%)	0	100	100
All	All	2217/2320 (96%)	2154 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	454/474 (96%)	441 (97%)	13 (3%)	42	46
1	B	453/474 (96%)	438 (97%)	15 (3%)	38	40
1	C	453/474 (96%)	434 (96%)	19 (4%)	30	30
1	D	453/474 (96%)	436 (96%)	17 (4%)	33	34
All	All	1813/1896 (96%)	1749 (96%)	64 (4%)	35	38

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	78	LYS
1	A	238	ASP
1	A	278	GLU
1	A	302	LYS
1	A	357	ARG
1	A	381	GLU
1	A	389	MET
1	A	461	ILE
1	A	477	LEU
1	A	540	HIS
1	A	542	ASP
1	A	552	GLU
1	B	12	LYS
1	B	78	LYS
1	B	238	ASP
1	B	278	GLU
1	B	279	ARG
1	B	292	LEU
1	B	302	LYS
1	B	357	ARG
1	B	381	GLU
1	B	389	MET
1	B	461	ILE

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Mol	Chain	Res	Type
1	B	477	LEU
1	B	540	HIS
1	B	542	ASP
1	B	552	GLU
1	C	12	LYS
1	C	78	LYS
1	C	172	ARG
1	C	212	LYS
1	C	238	ASP
1	C	278	GLU
1	C	292	LEU
1	C	302	LYS
1	C	357	ARG
1	C	364	SER
1	C	381	GLU
1	C	389	MET
1	C	461	ILE
1	C	473	PHE
1	C	540	HIS
1	C	542	ASP
1	C	546	PRO
1	C	552	GLU
1	C	555	GLN
1	D	12	LYS
1	D	78	LYS
1	D	212	LYS
1	D	238	ASP
1	D	278	GLU
1	D	292	LEU
1	D	302	LYS
1	D	357	ARG
1	D	381	GLU
1	D	389	MET
1	D	461	ILE
1	D	473	PHE
1	D	540	HIS
1	D	542	ASP
1	D	546	PRO
1	D	552	GLU
1	D	555	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	220	GLN
1	A	227	GLN
1	A	267	GLN
1	A	275	HIS
1	A	468	HIS
1	A	484	ASN
1	A	490	HIS
1	B	142	GLN
1	B	220	GLN
1	B	267	GLN
1	B	275	HIS
1	B	484	ASN
1	B	490	HIS
1	C	142	GLN
1	C	220	GLN
1	C	267	GLN
1	C	484	ASN
1	C	490	HIS
1	D	142	GLN
1	D	220	GLN
1	D	267	GLN
1	D	275	HIS
1	D	484	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LYS	B	604	-	8,9,9	1.14	1 (12%)	9,10,10	1.06	1 (11%)
4	LYS	C	604	-	8,9,9	0.83	0	9,10,10	1.84	2 (22%)
2	FAD	B	601	-	53,58,58	1.40	7 (13%)	68,89,89	1.72	15 (22%)
4	LYS	B	603	-	8,9,9	1.01	1 (12%)	9,10,10	0.64	0
4	LYS	D	603	-	8,9,9	1.26	1 (12%)	9,10,10	1.74	2 (22%)
3	PG6	B	602	-	17,17,17	0.50	0	16,16,16	0.79	0
4	LYS	C	603	-	8,9,9	1.13	1 (12%)	9,10,10	1.53	1 (11%)
3	PG6	A	602	-	17,17,17	0.52	0	16,16,16	1.05	0
2	FAD	D	601	-	53,58,58	1.45	6 (11%)	68,89,89	1.71	18 (26%)
3	PG6	C	602	-	17,17,17	0.47	0	16,16,16	0.50	0
2	FAD	A	601	-	53,58,58	1.45	9 (16%)	68,89,89	1.62	12 (17%)
3	PG6	D	602	-	17,17,17	0.95	0	16,16,16	1.22	1 (6%)
4	LYS	D	604	-	8,9,9	0.82	0	9,10,10	2.15	2 (22%)
4	LYS	A	604	-	8,9,9	1.01	1 (12%)	9,10,10	1.71	3 (33%)
2	FAD	C	601	-	53,58,58	1.59	9 (16%)	68,89,89	1.70	17 (25%)
4	LYS	A	603	-	8,9,9	1.15	1 (12%)	9,10,10	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LYS	B	604	-	-	1/9/9/9	-
4	LYS	C	604	-	-	0/9/9/9	-
2	FAD	B	601	-	-	6/30/50/50	0/6/6/6
4	LYS	B	603	-	-	1/9/9/9	-
4	LYS	D	603	-	-	0/9/9/9	-
3	PG6	B	602	-	-	7/15/15/15	-
4	LYS	C	603	-	-	0/9/9/9	-
3	PG6	A	602	-	-	5/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	601	-	-	9/30/50/50	0/6/6/6
3	PG6	C	602	-	-	6/15/15/15	-
2	FAD	A	601	-	-	6/30/50/50	0/6/6/6
3	PG6	D	602	-	-	7/15/15/15	-
4	LYS	D	604	-	-	0/9/9/9	-
4	LYS	A	604	-	-	0/9/9/9	-
2	FAD	C	601	-	-	8/30/50/50	0/6/6/6
4	LYS	A	603	-	-	1/9/9/9	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C9A-C5X	5.17	1.49	1.41
2	B	601	FAD	C9A-C5X	5.07	1.49	1.41
2	D	601	FAD	C9A-C5X	4.83	1.49	1.41
2	A	601	FAD	C9A-C5X	4.36	1.48	1.41
2	C	601	FAD	C8-C7	3.60	1.49	1.40
4	D	603	LYS	OXT-C	-3.47	1.19	1.30
2	C	601	FAD	C5X-N5	-3.43	1.32	1.39
2	D	601	FAD	C5X-N5	-3.16	1.33	1.39
2	D	601	FAD	C8-C7	3.14	1.48	1.40
2	C	601	FAD	C5A-C4A	3.04	1.49	1.40
4	C	603	LYS	OXT-C	-2.98	1.20	1.30
2	A	601	FAD	C4A-N3A	2.93	1.39	1.35
2	A	601	FAD	C4-N3	-2.83	1.33	1.38
4	B	604	LYS	OXT-C	-2.81	1.21	1.30
2	C	601	FAD	O4'-C4'	2.68	1.49	1.43
2	B	601	FAD	C8-C7	2.67	1.47	1.40
2	A	601	FAD	C10-N10	2.63	1.43	1.37
2	A	601	FAD	O2-C2	2.59	1.29	1.24
2	B	601	FAD	C10-N10	2.58	1.43	1.37
2	D	601	FAD	C8A-N7A	2.57	1.39	1.34
2	C	601	FAD	O4B-C4B	-2.54	1.39	1.45
2	D	601	FAD	C2B-C1B	-2.53	1.49	1.53
4	B	603	LYS	OXT-C	-2.49	1.22	1.30
2	A	601	FAD	C8-C7	2.41	1.46	1.40
4	A	603	LYS	OXT-C	-2.36	1.22	1.30
2	A	601	FAD	C10-N1	2.34	1.38	1.33
4	A	604	LYS	OXT-C	-2.33	1.22	1.30
2	A	601	FAD	C2A-N1A	2.33	1.38	1.33
2	B	601	FAD	C2A-N3A	2.33	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C5A-C4A	2.32	1.47	1.40
2	B	601	FAD	C4X-C10	2.27	1.50	1.44
2	D	601	FAD	C5A-C4A	2.23	1.46	1.40
2	B	601	FAD	C10-N1	2.14	1.37	1.33
2	C	601	FAD	C8A-N7A	2.09	1.38	1.34
2	C	601	FAD	C4A-N3A	-2.09	1.32	1.35
2	A	601	FAD	C5A-C4A	2.06	1.46	1.40
2	C	601	FAD	C2A-N3A	2.05	1.35	1.32

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C5'-C4'-C3'	-5.33	101.90	112.20
2	B	601	FAD	C5'-C4'-C3'	-4.97	102.60	112.20
2	B	601	FAD	O4-C4-C4X	-4.70	114.13	126.60
2	D	601	FAD	O4-C4-C4X	-4.35	115.07	126.60
4	D	604	LYS	OXT-C-O	-4.34	114.22	124.09
2	A	601	FAD	N3A-C2A-N1A	-4.30	121.96	128.68
2	C	601	FAD	O4-C4-C4X	-4.21	115.42	126.60
2	D	601	FAD	C1B-N9A-C4A	-3.96	119.68	126.64
4	C	603	LYS	OXT-C-O	-3.90	115.23	124.09
4	D	604	LYS	OXT-C-CA	3.89	126.65	113.38
2	B	601	FAD	C4A-C5A-N7A	-3.76	105.48	109.40
4	D	603	LYS	OXT-C-O	-3.70	115.68	124.09
2	B	601	FAD	N3A-C2A-N1A	-3.64	122.99	128.68
2	D	601	FAD	O4-C4-N3	3.59	127.01	120.12
2	A	601	FAD	O4-C4-C4X	-3.58	117.10	126.60
4	C	604	LYS	OXT-C-O	-3.58	115.97	124.09
2	C	601	FAD	C5'-C4'-C3'	-3.54	105.37	112.20
2	D	601	FAD	N3A-C2A-N1A	-3.49	123.22	128.68
2	C	601	FAD	O4-C4-N3	3.44	126.72	120.12
2	B	601	FAD	C4X-C10-N1	-3.41	116.81	124.73
4	D	603	LYS	OXT-C-CA	3.39	124.95	113.38
2	D	601	FAD	O2-C2-N1	-3.35	116.27	121.83
2	C	601	FAD	N3A-C2A-N1A	-3.34	123.46	128.68
4	C	604	LYS	OXT-C-CA	3.30	124.64	113.38
2	A	601	FAD	C4A-C5A-N7A	-3.19	106.07	109.40
2	C	601	FAD	O4'-C4'-C3'	3.17	116.81	109.10
2	C	601	FAD	C4A-C5A-N7A	-3.09	106.18	109.40
2	A	601	FAD	O4'-C4'-C3'	3.09	116.60	109.10
2	B	601	FAD	O4-C4-N3	3.09	126.03	120.12
2	D	601	FAD	C5X-C9A-N10	3.08	121.13	117.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	LYS	OXT-C-O	-3.08	117.11	124.09
2	B	601	FAD	O4'-C4'-C3'	3.06	116.54	109.10
2	C	601	FAD	O4B-C4B-C3B	2.95	110.96	105.11
2	B	601	FAD	O2'-C2'-C3'	2.94	116.24	109.10
4	A	604	LYS	OXT-C-CA	2.93	123.38	113.38
2	A	601	FAD	C4X-C10-N1	-2.92	117.95	124.73
2	A	601	FAD	O5'-C5'-C4'	-2.91	101.60	109.36
2	C	601	FAD	C4X-C10-N1	-2.85	118.12	124.73
2	D	601	FAD	O2'-C2'-C3'	2.78	115.86	109.10
2	C	601	FAD	C6-C5X-C9A	2.76	122.84	118.94
2	C	601	FAD	C1B-N9A-C4A	-2.73	121.85	126.64
2	C	601	FAD	C2A-N1A-C6A	2.68	123.33	118.75
2	A	601	FAD	O4B-C1B-C2B	-2.68	103.02	106.93
2	A	601	FAD	O2'-C2'-C3'	2.65	115.53	109.10
2	D	601	FAD	O4B-C4B-C3B	2.62	110.30	105.11
2	B	601	FAD	O5'-C5'-C4'	-2.57	102.51	109.36
2	B	601	FAD	C4X-C4-N3	2.56	119.70	113.19
2	C	601	FAD	O2A-PA-O1A	2.54	124.80	112.24
2	D	601	FAD	C4X-C10-N1	-2.53	118.86	124.73
2	D	601	FAD	C9A-N10-C10	-2.53	116.83	120.77
2	B	601	FAD	C4-N3-C2	-2.49	121.05	125.64
2	B	601	FAD	O4B-C1B-C2B	-2.48	103.30	106.93
3	D	602	PG6	O5-C9-C8	2.42	121.29	110.39
2	C	601	FAD	O2'-C2'-C3'	2.38	114.89	109.10
2	D	601	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
2	D	601	FAD	C6-C5X-C9A	2.35	122.27	118.94
2	C	601	FAD	C9-C8-C7	2.34	123.02	119.67
2	D	601	FAD	O4'-C4'-C3'	2.33	114.77	109.10
2	A	601	FAD	C4X-C4-N3	2.29	119.02	113.19
2	D	601	FAD	O2A-PA-O1A	2.27	123.48	112.24
2	D	601	FAD	C9-C8-C7	2.27	122.92	119.67
2	D	601	FAD	C2A-N1A-C6A	2.21	122.53	118.75
2	B	601	FAD	O3'-C3'-C4'	-2.20	103.49	108.81
4	A	604	LYS	CB-CA-C	-2.17	105.13	110.30
2	B	601	FAD	C10-N1-C2	2.17	121.24	116.90
2	C	601	FAD	O2-C2-N1	-2.17	118.23	121.83
2	A	601	FAD	C6-C7-C8	-2.16	116.58	119.67
2	D	601	FAD	C4-N3-C2	-2.16	121.66	125.64
2	A	601	FAD	C2A-N1A-C6A	2.11	122.37	118.75
2	D	601	FAD	C5'-C4'-C3'	-2.07	108.21	112.20
4	B	604	LYS	OXT-C-O	-2.06	119.42	124.09
2	B	601	FAD	N10-C10-N1	2.04	124.21	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C5X-C9A-N10	2.04	120.06	117.95
2	C	601	FAD	C4-N3-C2	-2.02	121.92	125.64

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O2A
3	D	602	PG6	C7-C6-O3-C5
2	B	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	C2'-C3'-C4'-O4'
3	D	602	PG6	O1-C2-C3-O2
2	D	601	FAD	C2'-C3'-C4'-C5'
3	C	602	PG6	O5-C10-C11-O6
3	D	602	PG6	O4-C8-C9-O5
3	C	602	PG6	O2-C4-C5-O3
3	A	602	PG6	O3-C6-C7-O4
2	B	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-O4'
3	B	602	PG6	O2-C4-C5-O3
2	A	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	D	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	C2'-C3'-C4'-C5'
4	B	603	LYS	CE-CD-CG-CB
4	B	604	LYS	CE-CD-CG-CB
2	A	601	FAD	O3'-C3'-C4'-O4'
3	A	602	PG6	O4-C8-C9-O5
3	B	602	PG6	O1-C2-C3-O2
2	D	601	FAD	O3'-C3'-C4'-O4'
3	B	602	PG6	C3-C2-O1-C1
3	C	602	PG6	O3-C6-C7-O4
2	C	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	PA-O3P-P-O5'
3	A	602	PG6	C7-C6-O3-C5

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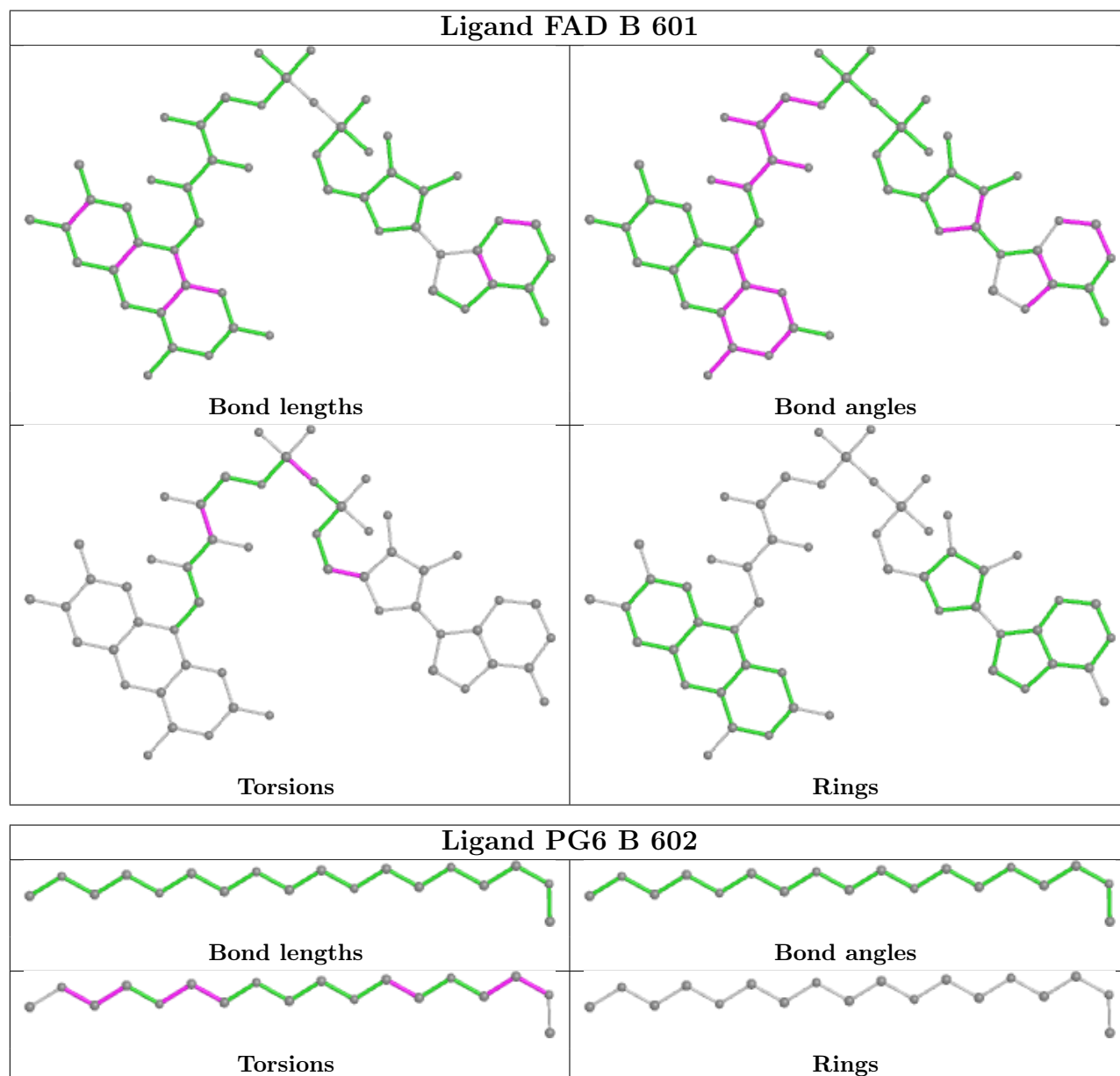
Mol	Chain	Res	Type	Atoms
3	C	602	PG6	C6-C7-O4-C8
2	C	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	O3'-C3'-C4'-C5'
3	C	602	PG6	C7-C6-O3-C5
3	B	602	PG6	O4-C8-C9-O5
3	D	602	PG6	C4-C5-O3-C6
3	A	602	PG6	C5-C4-O2-C3
3	B	602	PG6	C8-C9-O5-C10
2	D	601	FAD	O4B-C4B-C5B-O5B
3	C	602	PG6	C8-C9-O5-C10
2	A	601	FAD	O4B-C4B-C5B-O5B
3	B	602	PG6	C10-C11-O6-C12
3	D	602	PG6	O2-C4-C5-O3
3	B	602	PG6	O5-C10-C11-O6
2	B	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
3	A	602	PG6	C4-C5-O3-C6
2	D	601	FAD	C5B-O5B-PA-O1A
3	D	602	PG6	C6-C7-O4-C8
4	A	603	LYS	CE-CD-CG-CB
3	D	602	PG6	O3-C6-C7-O4

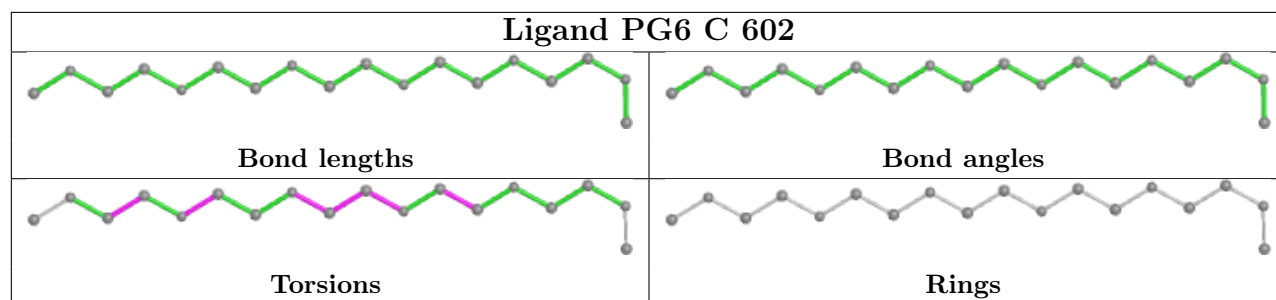
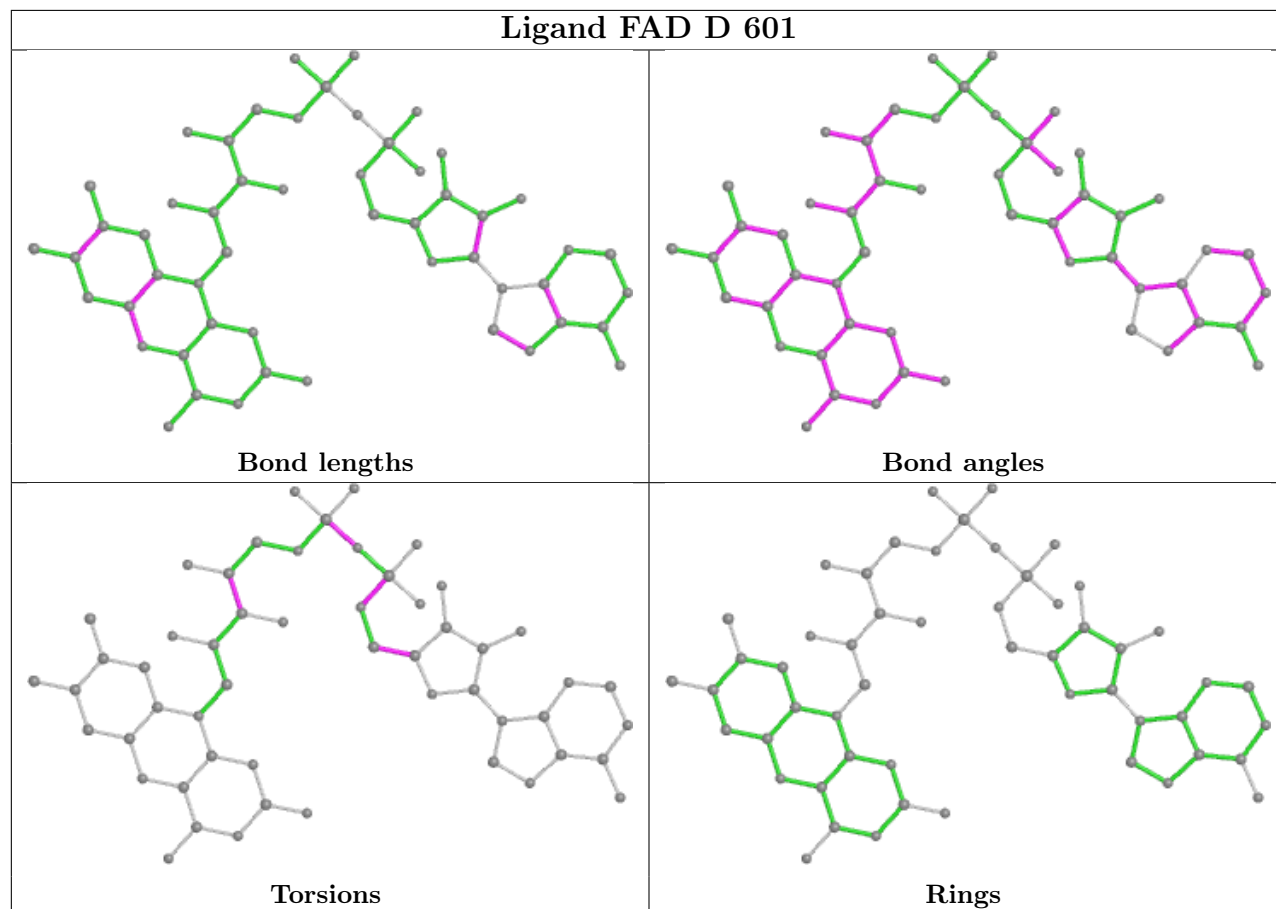
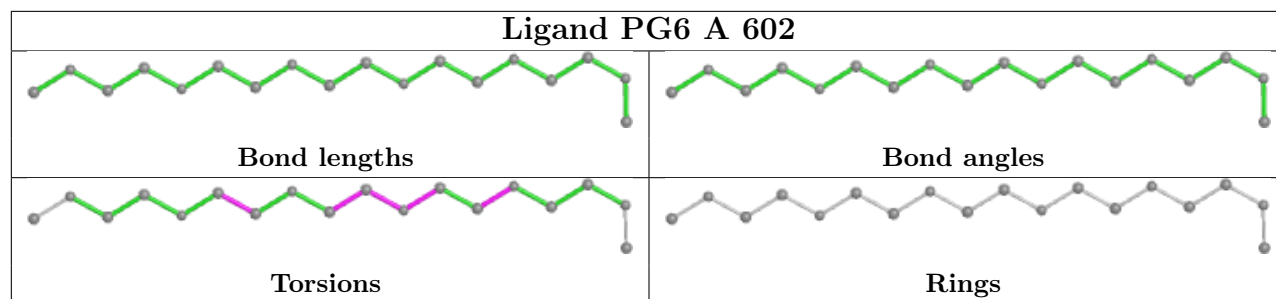
There are no ring outliers.

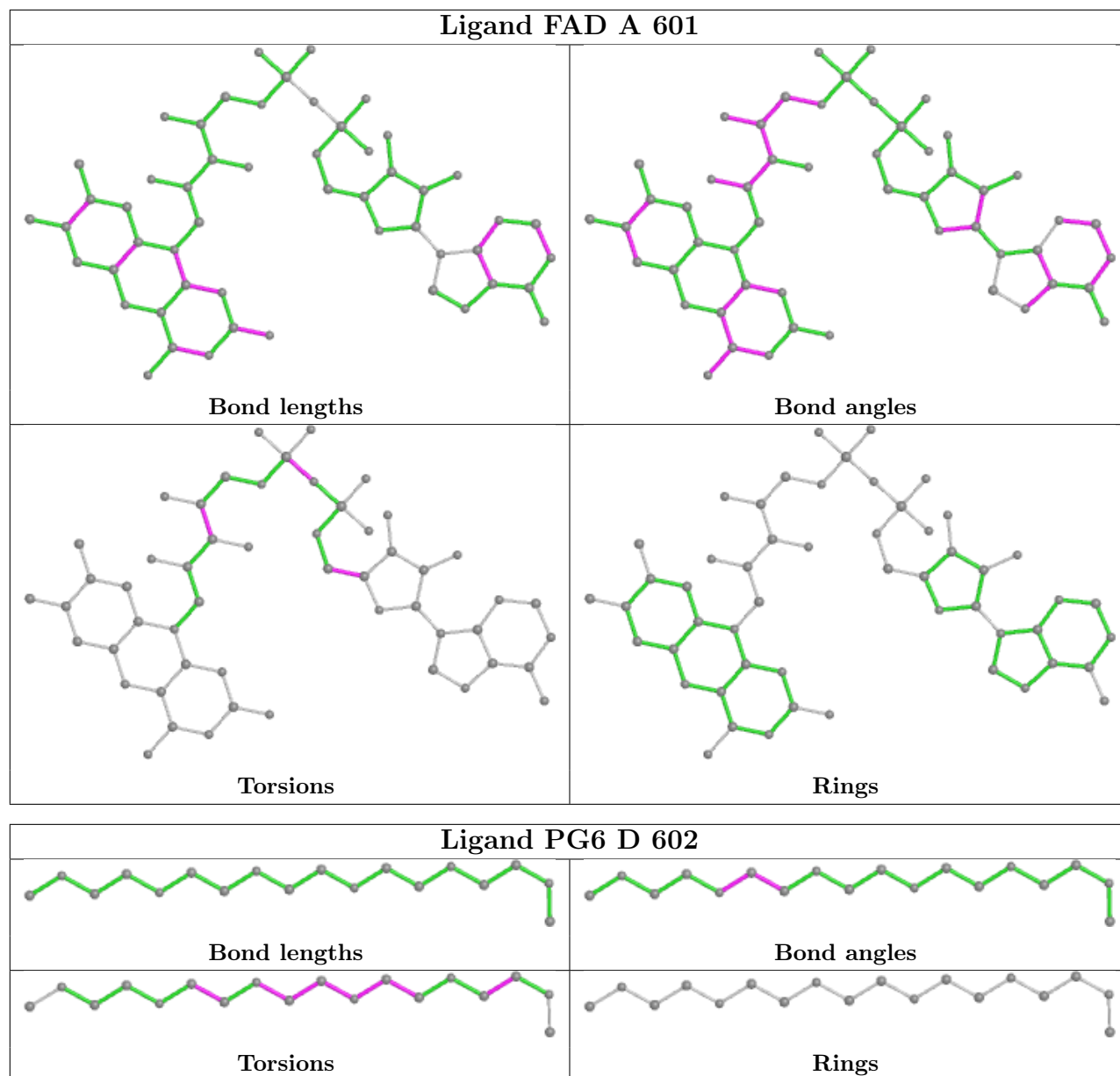
15 monomers are involved in 29 short contacts:

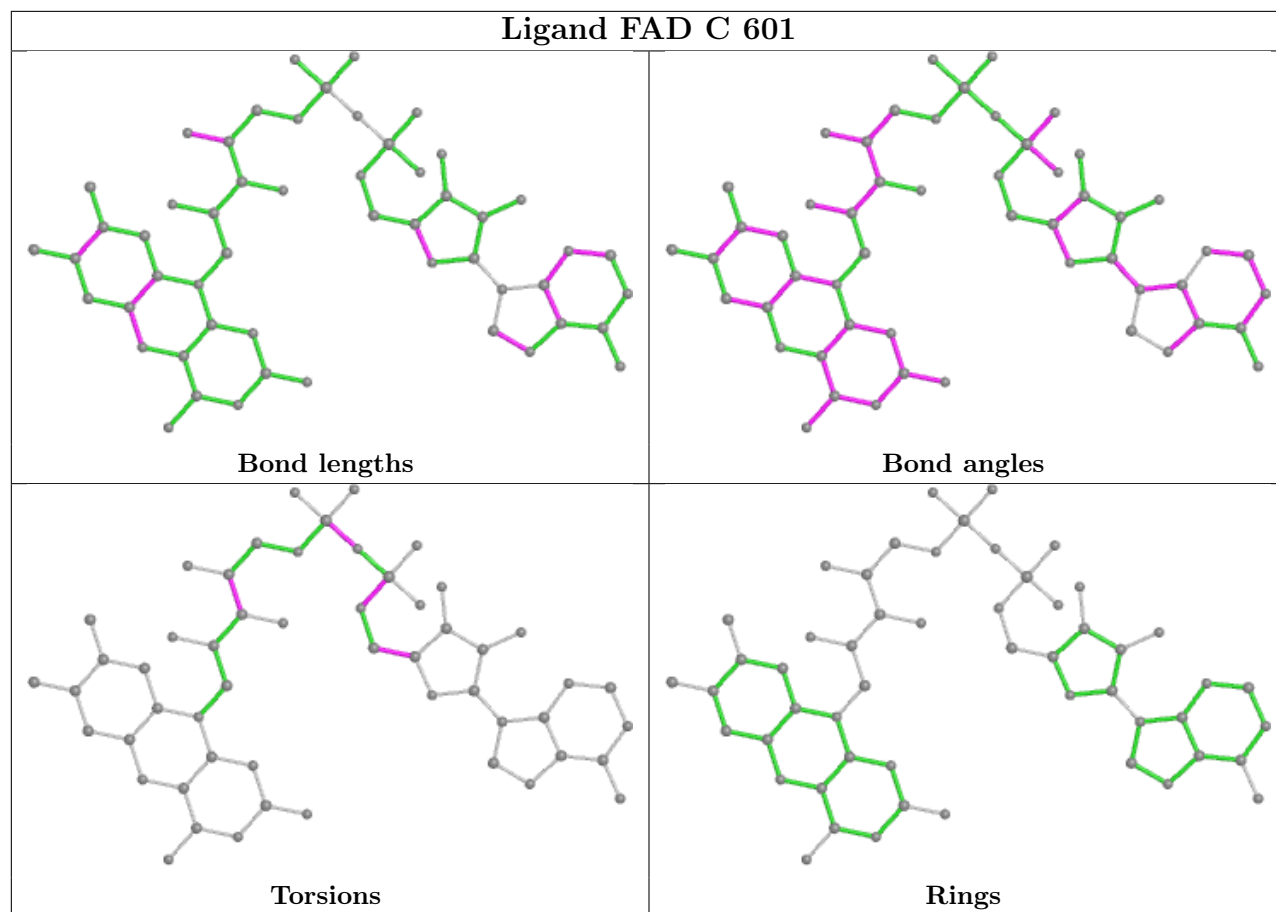
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	LYS	1	0
4	C	604	LYS	1	0
2	B	601	FAD	4	0
4	B	603	LYS	2	0
4	D	603	LYS	1	0
3	B	602	PG6	2	0
4	C	603	LYS	1	0
3	A	602	PG6	3	0
2	D	601	FAD	2	0
3	C	602	PG6	2	0
2	A	601	FAD	3	0
3	D	602	PG6	2	0
4	D	604	LYS	2	0
4	A	604	LYS	1	0
2	C	601	FAD	2	0

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	556/580 (95%)	0.28	9 (1%) 72 75	9, 18, 30, 73	0
1	B	556/580 (95%)	0.31	9 (1%) 72 75	10, 18, 32, 72	0
1	C	556/580 (95%)	0.42	20 (3%) 42 49	11, 18, 31, 59	0
1	D	556/580 (95%)	0.44	19 (3%) 45 51	12, 18, 31, 54	0
All	All	2224/2320 (95%)	0.36	57 (2%) 56 61	9, 18, 31, 73	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	PRO	4.1
1	A	381	GLU	4.0
1	B	279	ARG	4.0
1	B	381	GLU	3.8
1	D	510	VAL	3.6
1	D	407	ASP	3.5
1	B	278	GLU	3.3
1	A	279[A]	ARG	3.3
1	D	5	ASN	3.3
1	D	279	ARG	3.2
1	D	540	HIS	3.0
1	D	515	ALA	2.9
1	B	540	HIS	2.9
1	C	510	VAL	2.9
1	C	515	ALA	2.9
1	C	406	ASP	2.9
1	B	380	PRO	2.8
1	C	279	ARG	2.8
1	C	540	HIS	2.8
1	C	5	ASN	2.8
1	D	406	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	213	ALA	2.7
1	C	381	GLU	2.6
1	D	10	ASP	2.5
1	C	42	ALA	2.5
1	D	42	ALA	2.5
1	C	552	GLU	2.5
1	A	160	THR	2.4
1	B	382	THR	2.4
1	C	513	THR	2.4
1	D	278	GLU	2.4
1	C	24	PHE	2.3
1	C	160	THR	2.3
1	C	407	ASP	2.3
1	D	541	ALA	2.3
1	A	382	THR	2.3
1	D	505	ILE	2.3
1	C	9	ALA	2.2
1	C	56	ALA	2.2
1	C	541	ALA	2.2
1	D	560	ASP	2.2
1	B	160	THR	2.2
1	D	513	THR	2.2
1	D	9	ALA	2.2
1	C	516	TRP	2.1
1	C	559	ALA	2.1
1	A	540	HIS	2.1
1	C	278	GLU	2.1
1	B	214	PHE	2.1
1	B	5	ASN	2.0
1	D	477	LEU	2.0
1	D	24	PHE	2.0
1	D	499	GLU	2.0
1	A	542	ASP	2.0
1	A	499	GLU	2.0
1	C	285	GLU	2.0
1	D	100	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

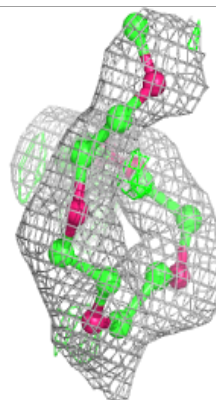
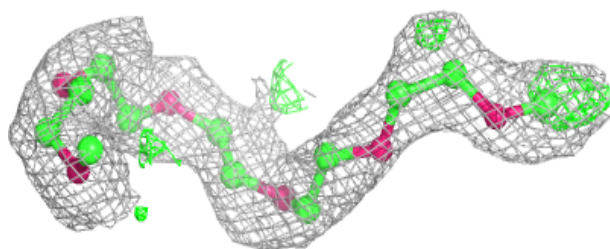
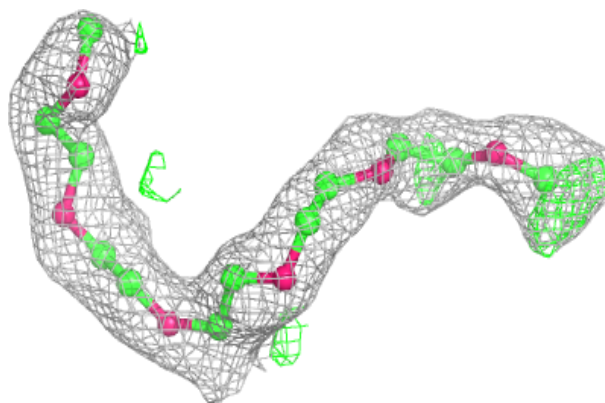
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PG6	D	602	18/18	0.80	0.17	24,28,32,35	0
3	PG6	B	602	18/18	0.82	0.20	24,31,35,40	0
4	LYS	D	603	10/10	0.83	0.27	18,23,25,26	0
4	LYS	C	603	10/10	0.84	0.25	17,22,23,23	0
4	LYS	B	603	10/10	0.87	0.23	21,22,24,25	0
3	PG6	A	602	18/18	0.88	0.17	22,26,30,33	0
4	LYS	B	604	10/10	0.88	0.16	12,15,17,17	0
3	PG6	C	602	18/18	0.89	0.16	26,30,33,33	0
4	LYS	A	604	10/10	0.89	0.15	11,13,15,15	0
4	LYS	A	603	10/10	0.90	0.19	20,21,22,22	0
2	FAD	B	601	53/53	0.92	0.14	12,14,19,21	0
2	FAD	C	601	53/53	0.92	0.15	13,16,21,23	0
2	FAD	A	601	53/53	0.92	0.14	11,14,19,22	0
4	LYS	C	604	10/10	0.93	0.12	8,10,14,16	0
2	FAD	D	601	53/53	0.93	0.14	13,17,21,22	0
4	LYS	D	604	10/10	0.93	0.12	9,11,14,14	0

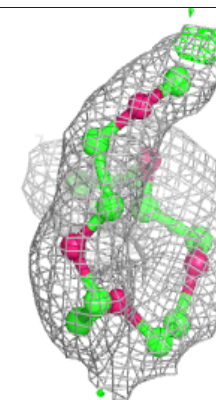
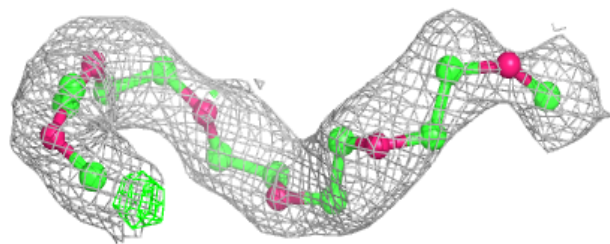
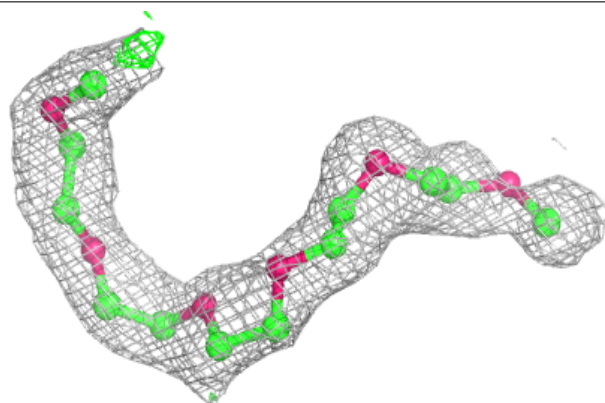
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PG6 D 602:

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

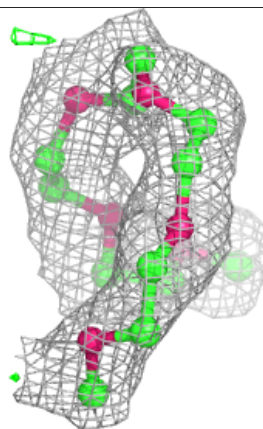
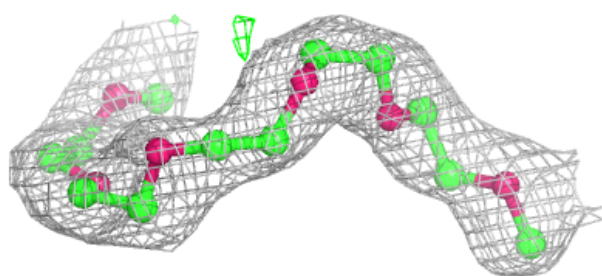
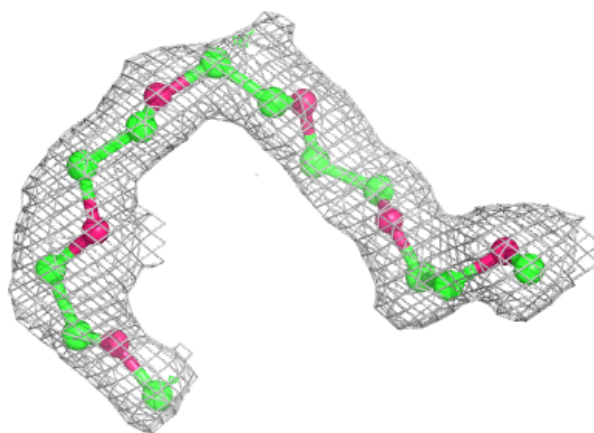
**Electron density around PG6 B 602:**

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

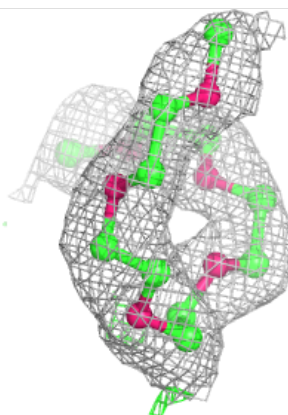
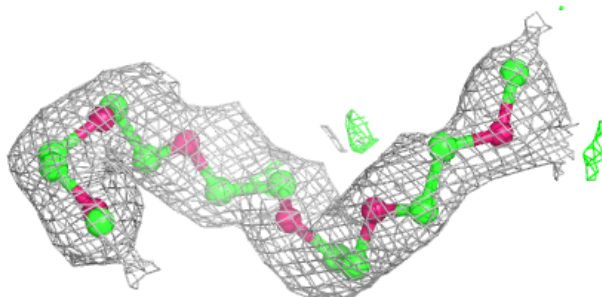
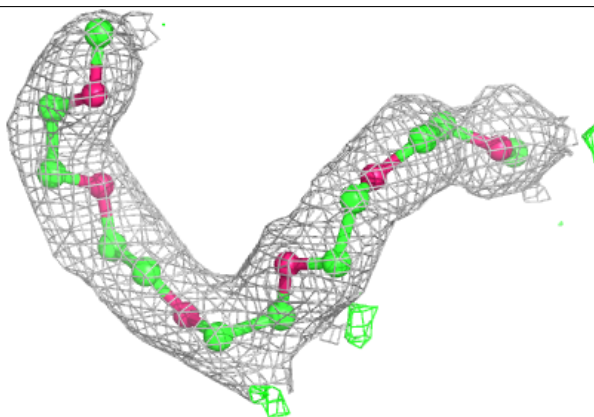


Electron density around PG6 A 602:

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

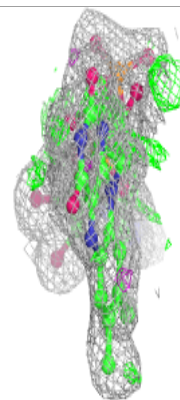
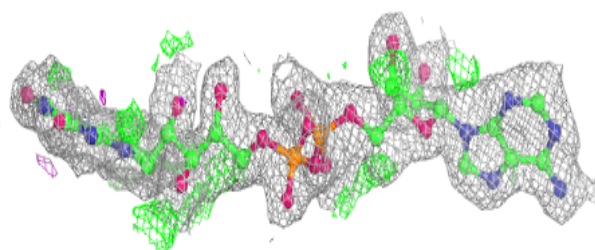
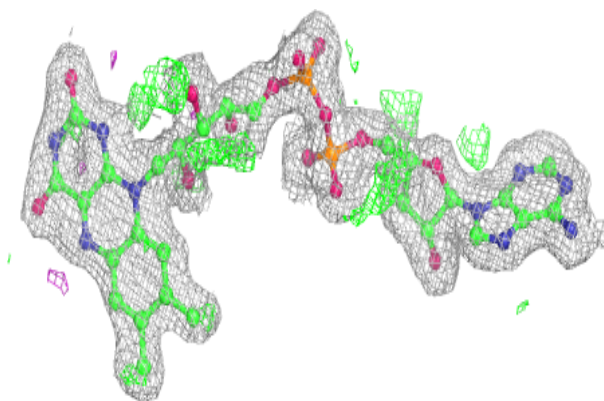
**Electron density around PG6 C 602:**

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

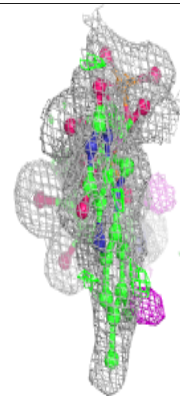
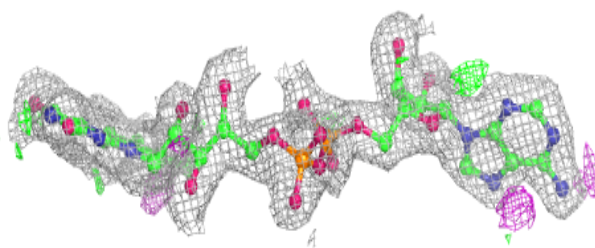
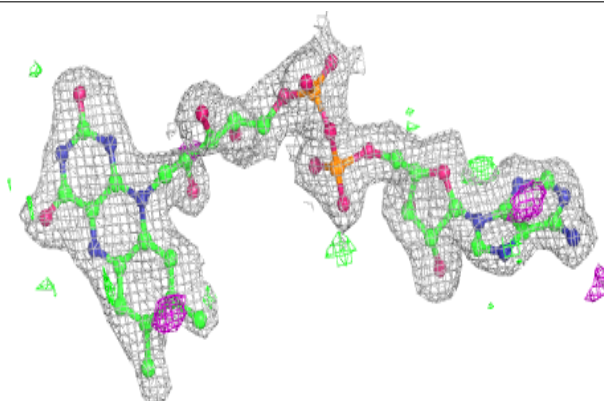


Electron density around FAD B 601:

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

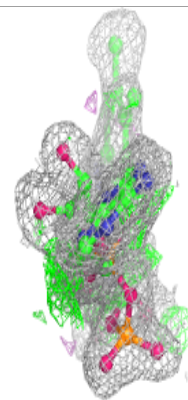
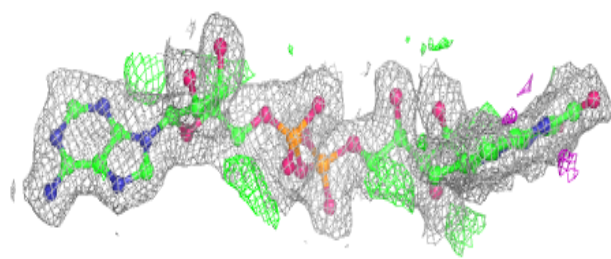
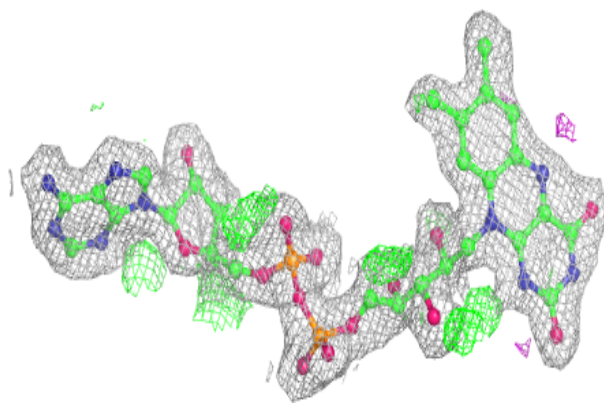
**Electron density around FAD C 601:**

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

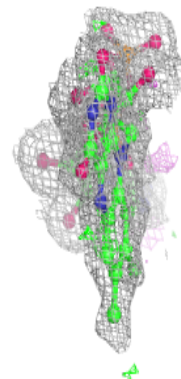
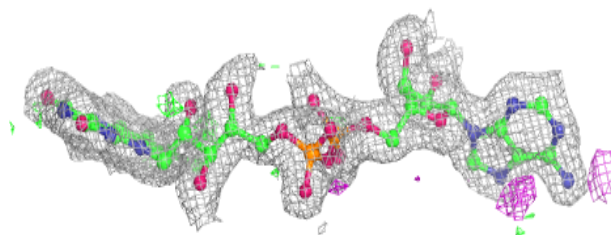
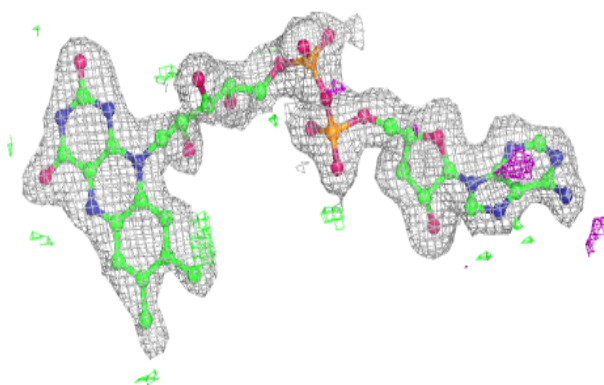


Electron density around FAD A 601:

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

**Electron density around FAD D 601:**

$2mF_o-DF_c$ (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.