



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:43 PM UTC

PDB ID : 1EJB / pdb_00001ejb
Title : LUMAZINE SYNTHASE FROM SACCHAROMYCES CEREVISIAE
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Deposited on : 2000-03-02
Resolution : 1.85 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

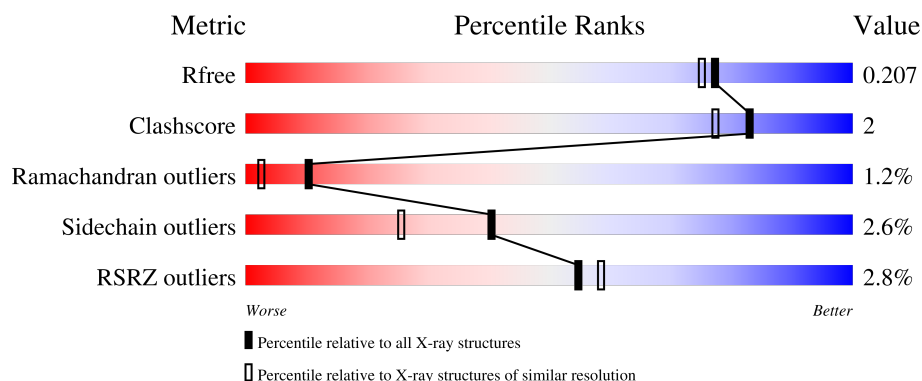
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	168	4% 86% 13% .
1	B	168	2% 86% 10% .
1	C	168	4% 88% 10% ..
1	D	168	2% 89% 10% .
1	E	168	2% 90% 7% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7155 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.

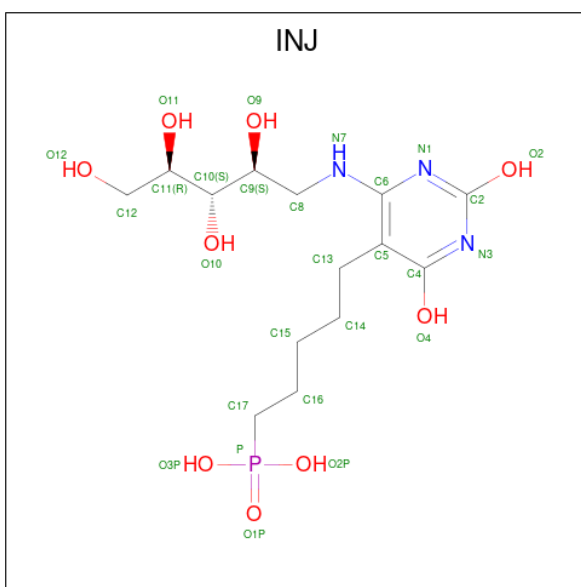
- Molecule 1 is a protein called LUMAZINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	38	0	0
			1294	823	225	238	8			
1	B	168	Total	C	N	O	S	83	0	0
			1294	823	225	238	8			
1	C	168	Total	C	N	O	S	44	0	0
			1294	823	225	238	8			
1	D	168	Total	C	N	O	S	31	0	0
			1294	823	225	238	8			
1	E	168	Total	C	N	O	S	90	0	0
			1294	823	225	238	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	VAL	SEE REMARK 999	UNP P50861
A	50	ASN	LYS	SEE REMARK 999	UNP P50861
B	43	ALA	VAL	SEE REMARK 999	UNP P50861
B	50	ASN	LYS	SEE REMARK 999	UNP P50861
C	43	ALA	VAL	SEE REMARK 999	UNP P50861
C	50	ASN	LYS	SEE REMARK 999	UNP P50861
D	43	ALA	VAL	SEE REMARK 999	UNP P50861
D	50	ASN	LYS	SEE REMARK 999	UNP P50861
E	43	ALA	VAL	SEE REMARK 999	UNP P50861
E	50	ASN	LYS	SEE REMARK 999	UNP P50861

- Molecule 2 is 5-(6-D-RIBITYLAMINO-2,4-DIHYDROXYPYRIMIDIN-5-YL)-1-PENTYL-PHOSPHONIC ACID (CCD ID: INJ) (formula: C₁₄H₂₆N₃O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 14	N 3	O 9	P 1	0	0
2	B	1	Total 27	C 14	N 3	O 9	P 1	0	0
2	C	1	Total 27	C 14	N 3	O 9	P 1	0	0
2	D	1	Total 27	C 14	N 3	O 9	P 1	0	0
2	E	1	Total 27	C 14	N 3	O 9	P 1	0	0

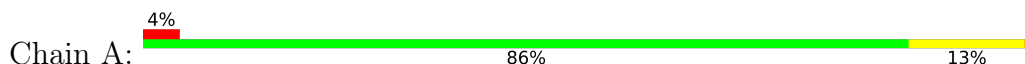
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	B	109	Total O 109 109	0	0
3	C	107	Total O 107 107	0	0
3	D	121	Total O 121 121	0	0
3	E	113	Total O 113 113	0	0

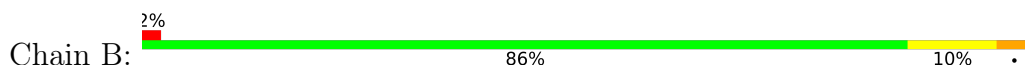
3 Residue-property plots [i](#)

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.

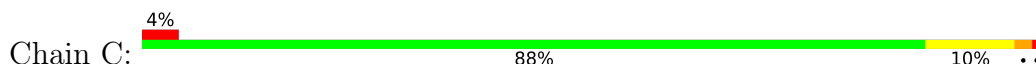
- Molecule 1: LUMAZINE SYNTHASE



- Molecule 1: LUMAZINE SYNTHASE



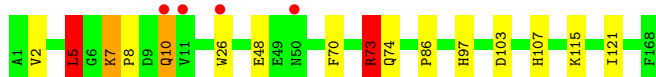
- Molecule 1: LUMAZINE SYNTHASE



- Molecule 1: LUMAZINE SYNTHASE



- Molecule 1: LUMAZINE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.89Å 82.89Å 298.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85 20.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.85) 99.7 (20.00-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.225 0.179 , 0.207	Depositor DCC
R_{free} test set	4549 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7155	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: INJ

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	0.98	6/1319 (0.5%)	1.52	17/1781 (1.0%)
1	B	1.39	10/1319 (0.8%)	1.91	14/1781 (0.8%)
1	C	1.14	8/1319 (0.6%)	1.69	20/1781 (1.1%)
1	D	1.97	15/1319 (1.1%)	1.80	14/1781 (0.8%)
1	E	1.42	7/1319 (0.5%)	1.74	14/1781 (0.8%)
All	All	1.42	46/6595 (0.7%)	1.74	79/8905 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	E	0	1
All	All	0	4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	ARG	CZ-NH2	-35.35	0.87	1.33
1	D	10	GLN	CD-OE1	-31.55	0.63	1.23
1	D	114	GLU	CD-OE1	-30.59	0.67	1.25
1	E	73	ARG	CZ-NH1	28.86	1.73	1.32
1	D	114	GLU	CD-OE2	24.14	1.71	1.25
1	D	10	GLN	CG-CD	22.29	2.07	1.52
1	C	48	GLU	CD-OE2	17.81	1.59	1.25
1	C	50	ASN	CG-OD1	-17.31	0.90	1.23
1	E	48	GLU	CD-OE2	16.55	1.56	1.25
1	D	114	GLU	CG-CD	15.97	1.92	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	48	GLU	CD-OE1	-14.51	0.97	1.25
1	D	73	ARG	CZ-NH1	14.50	1.53	1.32
1	A	1	ALA	C-N	-13.32	1.16	1.33
1	D	10	GLN	CD-NE2	13.26	1.61	1.33
1	E	73	ARG	NE-CZ	-12.67	1.19	1.33
1	D	141	GLU	CD-OE2	12.28	1.48	1.25
1	D	141	GLU	CD-OE1	-12.13	1.02	1.25
1	D	73	ARG	CZ-NH2	-12.02	1.17	1.33
1	B	115	LYS	CG-CD	-11.09	1.19	1.52
1	C	115	LYS	CG-CD	-9.56	1.23	1.52
1	E	73	ARG	CZ-NH2	-9.37	1.21	1.33
1	C	49	GLU	CG-CD	9.03	1.74	1.52
1	D	50	ASN	CG-OD1	-8.81	1.06	1.23
1	E	26	TRP	CD2-CE3	8.48	1.53	1.40
1	B	140	ASP	CA-C	8.44	1.64	1.53
1	A	115	LYS	CG-CD	-8.30	1.27	1.52
1	A	73	ARG	CZ-NH1	8.23	1.44	1.32
1	E	10	GLN	N-CA	-7.40	1.36	1.46
1	A	73	ARG	NE-CZ	-7.30	1.25	1.33
1	C	131	GLU	CD-OE1	7.24	1.39	1.25
1	B	140	ASP	C-O	-7.22	1.14	1.23
1	B	8	PRO	N-CA	-6.80	1.38	1.47
1	B	10	GLN	CB-CG	6.79	1.72	1.52
1	D	73	ARG	CD-NE	-6.53	1.37	1.46
1	C	50	ASN	CB-CG	6.40	1.68	1.52
1	B	8	PRO	CA-C	-6.38	1.43	1.52
1	D	141	GLU	CG-CD	6.32	1.67	1.52
1	D	10	GLN	CA-CB	5.93	1.63	1.53
1	D	36	LYS	CD-CE	5.85	1.70	1.52
1	B	131	GLU	CG-CD	5.78	1.66	1.52
1	A	5	LEU	CB-CG	-5.72	1.42	1.53
1	C	131	GLU	CG-CD	-5.68	1.37	1.52
1	A	1	ALA	CA-CB	-5.33	1.34	1.52
1	B	143	HIS	CB-CG	5.24	1.57	1.50
1	B	8	PRO	C-N	-5.06	1.25	1.33
1	C	5	LEU	CA-CB	-5.00	1.45	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ARG	NE-CZ-NH2	40.18	155.36	119.20
1	D	10	GLN	OE1-CD-NE2	36.94	159.54	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ARG	NH1-CZ-NH2	-30.53	79.61	119.30
1	E	73	ARG	NE-CZ-NH2	23.67	140.50	119.20
1	E	73	ARG	NE-CZ-NH1	-21.84	99.66	121.50
1	D	10	GLN	CG-CD-NE2	-21.13	84.71	116.40
1	E	26	TRP	CD2-CE2-CZ2	-15.03	107.38	122.40
1	D	114	GLU	CG-CD-OE2	-14.82	84.32	118.40
1	B	115	LYS	CB-CG-CD	14.72	145.16	111.30
1	C	1	ALA	CA-C-N	-14.51	101.55	122.45
1	C	1	ALA	C-N-CA	-14.51	101.55	122.45
1	E	73	ARG	CD-NE-CZ	14.29	144.41	124.40
1	C	49	GLU	CG-CD-OE1	-13.05	88.39	118.40
1	C	2	VAL	N-CA-C	12.58	128.70	109.20
1	A	1	ALA	N-CA-CB	11.84	128.15	110.40
1	B	9	ASP	CA-CB-CG	-11.69	100.91	112.60
1	C	2	VAL	CA-C-N	11.38	143.28	121.54
1	C	2	VAL	C-N-CA	11.38	143.28	121.54
1	E	26	TRP	CG-CD2-CE3	-11.28	122.62	133.90
1	C	2	VAL	O-C-N	11.05	134.25	122.76
1	C	7	LYS	CA-CB-CG	10.89	135.88	114.10
1	C	5	LEU	CB-CA-C	10.68	125.86	109.84
1	A	73	ARG	CD-NE-CZ	10.61	139.26	124.40
1	C	115	LYS	CB-CG-CD	10.55	135.57	111.30
1	C	48	GLU	CG-CD-OE2	-10.39	94.50	118.40
1	E	26	TRP	CE2-CD2-CE3	10.29	129.09	118.80
1	D	114	GLU	CB-CG-CD	-10.29	95.11	112.60
1	E	26	TRP	NE1-CE2-CZ2	10.13	145.30	130.10
1	C	50	ASN	OD1-CG-ND2	-10.04	112.56	122.60
1	A	40	GLU	CB-CG-CD	9.68	129.05	112.60
1	E	115	LYS	CD-CE-NZ	9.34	141.78	111.90
1	D	50	ASN	CB-CG-ND2	-9.32	102.42	116.40
1	C	50	ASN	CA-CB-CG	-9.32	103.28	112.60
1	E	73	ARG	NH1-CZ-NH2	-9.01	107.59	119.30
1	D	114	GLU	CG-CD-OE1	8.94	138.96	118.40
1	E	115	LYS	CB-CG-CD	8.59	131.06	111.30
1	C	2	VAL	CA-C-O	8.50	131.87	121.92
1	A	1	ALA	N-CA-C	-8.17	88.13	111.00
1	E	48	GLU	CG-CD-OE1	8.04	136.88	118.40
1	D	50	ASN	OD1-CG-ND2	7.93	130.53	122.60
1	B	143	HIS	CA-CB-CG	-7.83	105.97	113.80
1	A	1	ALA	CB-CA-C	-7.58	99.12	110.50
1	A	130	GLU	CB-CG-CD	7.46	125.29	112.60
1	D	141	GLU	CG-CD-OE2	-7.42	101.34	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ASP	N-CA-C	-7.30	100.69	110.55
1	E	48	GLU	CG-CD-OE2	-7.24	101.76	118.40
1	B	28	ARG	N-CA-C	7.20	119.13	111.28
1	D	10	GLN	CB-CA-C	7.11	123.94	110.51
1	B	8	PRO	O-C-N	6.89	131.94	122.64
1	A	28	ARG	N-CA-C	6.82	118.72	111.28
1	E	26	TRP	CH2-CZ2-CE2	6.81	126.36	117.50
1	D	16	LYS	CB-CG-CD	6.24	125.64	111.30
1	B	70	PHE	CA-CB-CG	6.22	120.02	113.80
1	A	115	LYS	CB-CG-CD	6.15	125.45	111.30
1	C	131	GLU	CB-CG-CD	6.05	122.89	112.60
1	C	70	PHE	CA-CB-CG	5.99	119.79	113.80
1	C	48	GLU	OE1-CD-OE2	5.98	137.26	122.90
1	B	9	ASP	N-CA-C	-5.93	106.09	113.15
1	B	140	ASP	CB-CA-C	-5.91	98.00	109.76
1	A	70	PHE	CA-CB-CG	5.87	119.67	113.80
1	D	115	LYS	CB-CG-CD	5.77	124.57	111.30
1	D	10	GLN	CB-CG-CD	-5.62	103.04	112.60
1	D	114	GLU	OE1-CD-OE2	5.62	136.39	122.90
1	A	2	VAL	CA-CB-CG2	5.60	119.92	110.40
1	E	70	PHE	CA-CB-CG	5.59	119.39	113.80
1	B	9	ASP	CA-C-O	5.58	127.82	119.23
1	A	16	LYS	CA-C-N	-5.58	114.58	122.34
1	A	16	LYS	C-N-CA	-5.58	114.58	122.34
1	A	7	LYS	CG-CD-CE	5.55	124.06	111.30
1	C	50	ASN	CB-CG-OD1	5.51	131.81	120.80
1	A	41	ARG	CD-NE-CZ	5.44	132.01	124.40
1	D	55	GLU	CA-C-O	-5.37	115.33	121.40
1	C	3	LYS	N-CA-C	5.26	122.00	110.80
1	A	5	LEU	CA-C-N	5.24	125.08	120.10
1	A	5	LEU	C-N-CA	5.24	125.08	120.10
1	B	16	LYS	CA-C-N	-5.22	115.09	122.34
1	B	16	LYS	C-N-CA	-5.22	115.09	122.34
1	C	5	LEU	CB-CG-CD2	5.17	126.20	110.70
1	A	41	ARG	NE-CZ-NH1	5.09	126.59	121.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	ASN	Sidechain
1	C	48	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	C	49	GLU	Sidechain
1	E	73	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1294	0	1310	8	0
1	B	1294	0	1310	7	0
1	C	1294	0	1310	7	0
1	D	1294	0	1310	6	0
1	E	1294	0	1310	7	1
2	A	27	0	22	1	0
2	B	27	0	22	1	0
2	C	27	0	22	1	0
2	D	27	0	22	1	0
2	E	27	0	22	0	0
3	A	100	0	0	2	0
3	B	109	0	0	0	0
3	C	107	0	0	2	1
3	D	121	0	0	0	0
3	E	113	0	0	0	0
All	All	7155	0	6660	30	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (30) 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:E:73:ARG:NH1	1:E:73:ARG:NE	2.25	0.82
1:D:114:GLU:CB	1:D:114:GLU:CD	2.54	0.80
1:C:49:GLU:CD	1:C:49:GLU:CB	2.56	0.79
1:E:73:ARG:NH1	1:E:73:ARG:NH2	2.39	0.70
1:E:73:ARG:NH1	1:E:73:ARG:HE	1.96	0.64
1:A:103:ASP:OD2	1:B:107:HIS:HE1	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:O	1:A:77:LEU:HD13	2.05	0.56
1:A:107:HIS:HE1	1:E:103:ASP:OD2	1.89	0.55
1:C:96:MET:HE2	3:C:525:HOH:O	2.07	0.54
1:C:103:ASP:OD2	1:D:107:HIS:HE1	1.91	0.54
1:B:103:ASP:OD2	1:C:107:HIS:HE1	1.91	0.52
1:D:103:ASP:OD2	1:E:107:HIS:HE1	1.91	0.52
1:B:23:HIS:CE1	1:B:56:THR:HG22	2.46	0.50
1:B:86:PRO:HD2	1:B:121:ILE:O	2.14	0.47
1:E:86:PRO:HD2	1:E:121:ILE:O	2.14	0.47
1:A:86:PRO:HD2	1:A:121:ILE:O	2.14	0.47
1:C:86:PRO:HD2	1:C:121:ILE:O	2.15	0.47
1:D:86:PRO:HD2	1:D:121:ILE:O	2.14	0.47
1:B:9:ASP:OD1	1:B:12:TYR:OH	2.28	0.46
1:A:96:MET:HE2	3:A:264:HOH:O	2.15	0.45
1:A:97:HIS:CE1	3:A:247:HOH:O	2.69	0.45
1:E:73:ARG:HH11	1:E:74:GLN:HE21	1.65	0.44
1:D:57:VAL:HB	1:D:58:PRO:HD2	2.00	0.43
1:C:93:GLY:HA3	2:C:400:INJ:H172	2.01	0.43
1:D:61:TYR:HB3	2:D:600:INJ:H101	2.02	0.42
1:A:19:VAL:HG11	1:A:42:MET:SD	2.59	0.42
1:B:93:GLY:HA3	2:B:300:INJ:H172	2.02	0.41
1:B:97:HIS:CE1	3:C:272:HOH:O	2.73	0.41
1:A:93:GLY:HA3	2:A:200:INJ:H172	2.03	0.41
1:C:57:VAL:HB	1:C:58:PRO:HD2	2.01	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:CD1	3:C:461:HOH:O[5_655]	1.86	0.34

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/168 (99%)	160 (96%)	6 (4%)	0	100	100
1	B	166/168 (99%)	157 (95%)	6 (4%)	3 (2%)	6	1
1	C	166/168 (99%)	161 (97%)	3 (2%)	2 (1%)	10	2
1	D	166/168 (99%)	164 (99%)	2 (1%)	0	100	100
1	E	166/168 (99%)	155 (93%)	6 (4%)	5 (3%)	3	0
All	All	830/840 (99%)	797 (96%)	23 (3%)	10 (1%)	10	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	VAL
1	B	5	LEU
1	C	3	LYS
1	E	7	LYS
1	E	8	PRO
1	E	10	GLN
1	C	4	GLY
1	E	5	LEU
1	B	8	PRO
1	E	2	VAL

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	136/136 (100%)	134 (98%)	2 (2%)	57	47
1	B	136/136 (100%)	129 (95%)	7 (5%)	21	7
1	C	136/136 (100%)	133 (98%)	3 (2%)	45	32
1	D	136/136 (100%)	133 (98%)	3 (2%)	45	32
1	E	136/136 (100%)	133 (98%)	3 (2%)	45	32
All	All	680/680 (100%)	662 (97%)	18 (3%)	40	25

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	97	HIS
1	B	3	LYS
1	B	5	LEU
1	B	7	LYS
1	B	10	GLN
1	B	97	HIS
1	B	115	LYS
1	B	140	ASP
1	C	2	VAL
1	C	97	HIS
1	C	115	LYS
1	D	49	GLU
1	D	97	HIS
1	D	115	LYS
1	E	5	LEU
1	E	7	LYS
1	E	97	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	107	HIS
1	B	74	GLN
1	B	107	HIS
1	C	74	GLN
1	C	107	HIS
1	D	107	HIS
1	E	74	GLN
1	E	107	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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	INJ	A	200	-	26,27,27	3.30	10 (38%)	28,37,37	2.59	14 (50%)
2	INJ	D	600	-	26,27,27	3.26	14 (53%)	28,37,37	2.33	10 (35%)
2	INJ	B	300	-	26,27,27	3.43	11 (42%)	28,37,37	2.39	14 (50%)
2	INJ	C	400	-	26,27,27	3.30	10 (38%)	28,37,37	2.23	10 (35%)
2	INJ	E	800	-	26,27,27	3.23	13 (50%)	28,37,37	2.39	10 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	INJ	A	200	-	-	6/24/24/24	0/1/1/1
2	INJ	D	600	-	-	7/24/24/24	0/1/1/1
2	INJ	B	300	-	-	6/24/24/24	0/1/1/1
2	INJ	C	400	-	-	5/24/24/24	0/1/1/1
2	INJ	E	800	-	-	4/24/24/24	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	INJ	C5-C4	9.68	1.50	1.39
2	A	200	INJ	C5-C4	9.34	1.50	1.39
2	E	800	INJ	C5-C4	9.01	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	INJ	C5-C4	8.80	1.49	1.39
2	D	600	INJ	C5-C4	8.68	1.49	1.39
2	B	300	INJ	C11-C10	8.06	1.67	1.53
2	A	200	INJ	C8-C9	7.13	1.61	1.52
2	D	600	INJ	C11-C10	6.83	1.65	1.53
2	E	800	INJ	C11-C10	6.74	1.65	1.53
2	C	400	INJ	C11-C10	6.67	1.65	1.53
2	C	400	INJ	C8-C9	6.65	1.61	1.52
2	A	200	INJ	C11-C10	6.43	1.64	1.53
2	B	300	INJ	C8-C9	6.14	1.60	1.52
2	E	800	INJ	C8-C9	6.00	1.60	1.52
2	D	600	INJ	C8-C9	5.75	1.60	1.52
2	B	300	INJ	P-C17	5.27	1.84	1.78
2	A	200	INJ	C6-N1	4.85	1.43	1.34
2	B	300	INJ	C6-N1	4.58	1.42	1.34
2	C	400	INJ	C13-C5	-4.42	1.41	1.52
2	C	400	INJ	C6-N1	4.42	1.42	1.34
2	E	800	INJ	C6-N1	4.42	1.42	1.34
2	D	600	INJ	C13-C5	-4.27	1.41	1.52
2	A	200	INJ	C8-N7	4.25	1.53	1.45
2	D	600	INJ	C8-N7	4.23	1.53	1.45
2	E	800	INJ	C13-C5	-4.17	1.41	1.52
2	D	600	INJ	C6-N1	4.12	1.41	1.34
2	A	200	INJ	C13-C5	-4.09	1.42	1.52
2	B	300	INJ	C13-C5	-3.92	1.42	1.52
2	E	800	INJ	C8-N7	3.82	1.52	1.45
2	C	400	INJ	C8-N7	3.67	1.52	1.45
2	A	200	INJ	C6-N7	3.66	1.40	1.34
2	C	400	INJ	P-O1P	-3.53	1.43	1.50
2	B	300	INJ	C8-N7	3.35	1.51	1.45
2	E	800	INJ	P-C17	3.30	1.82	1.78
2	D	600	INJ	C6-N7	3.28	1.39	1.34
2	C	400	INJ	C6-N7	3.26	1.39	1.34
2	B	300	INJ	C6-N7	3.14	1.39	1.34
2	E	800	INJ	C6-N7	3.12	1.39	1.34
2	B	300	INJ	C12-C11	3.07	1.59	1.52
2	D	600	INJ	C2-N1	3.03	1.42	1.36
2	D	600	INJ	C12-C11	2.89	1.59	1.52
2	B	300	INJ	C2-N1	2.84	1.42	1.36
2	D	600	INJ	P-O1P	-2.82	1.44	1.50
2	D	600	INJ	C5-C6	2.81	1.47	1.42
2	B	300	INJ	P-O1P	-2.74	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	INJ	C12-C11	2.59	1.58	1.52
2	E	800	INJ	C9-C10	2.55	1.57	1.53
2	D	600	INJ	P-C17	2.41	1.81	1.78
2	C	400	INJ	C2-N1	2.40	1.41	1.36
2	E	800	INJ	P-O1P	-2.37	1.45	1.50
2	E	800	INJ	C2-N1	2.29	1.41	1.36
2	A	200	INJ	P-O1P	-2.28	1.45	1.50
2	D	600	INJ	P-O2P	-2.24	1.49	1.55
2	C	400	INJ	C12-C11	2.18	1.57	1.52
2	D	600	INJ	C9-C10	2.16	1.57	1.53
2	A	200	INJ	C5-C6	2.16	1.46	1.42
2	E	800	INJ	C5-C6	2.16	1.46	1.42
2	A	200	INJ	C2-N1	2.16	1.41	1.36

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	200	INJ	C8-N7-C6	-5.43	113.09	123.18
2	A	200	INJ	C2-N3-C4	5.15	126.15	115.42
2	E	800	INJ	C8-N7-C6	-5.13	113.65	123.18
2	D	600	INJ	C2-N3-C4	4.97	125.78	115.42
2	E	800	INJ	C2-N3-C4	4.96	125.75	115.42
2	D	600	INJ	C8-N7-C6	-4.96	113.97	123.18
2	B	300	INJ	C2-N3-C4	4.82	125.47	115.42
2	A	200	INJ	O11-C11-C10	-4.70	98.25	109.25
2	A	200	INJ	O3P-P-O1P	-4.59	100.50	112.39
2	E	800	INJ	O11-C11-C10	-4.50	98.71	109.25
2	D	600	INJ	O3P-P-O1P	-4.49	100.78	112.39
2	B	300	INJ	O10-C10-C11	-4.43	98.86	108.93
2	C	400	INJ	C2-N3-C4	4.33	124.44	115.42
2	B	300	INJ	O11-C11-C10	-4.31	99.17	109.25
2	C	400	INJ	C8-N7-C6	-4.30	115.19	123.18
2	B	300	INJ	C8-N7-C6	-4.22	115.33	123.18
2	B	300	INJ	O3P-P-O1P	-4.14	101.67	112.39
2	E	800	INJ	O3P-P-O1P	-4.01	102.02	112.39
2	D	600	INJ	O10-C10-C11	-3.99	99.87	108.93
2	C	400	INJ	O11-C11-C10	-3.97	99.97	109.25
2	C	400	INJ	O3P-P-O1P	-3.90	102.30	112.39
2	E	800	INJ	O10-C10-C11	-3.73	100.45	108.93
2	E	800	INJ	P-C17-C16	3.39	119.11	114.94
2	C	400	INJ	O1P-P-C17	3.38	117.82	111.45
2	A	200	INJ	O10-C10-C11	-3.34	101.34	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	INJ	O12-C12-C11	-3.26	104.32	111.16
2	C	400	INJ	O10-C10-C11	-3.18	101.71	108.93
2	A	200	INJ	C12-C11-C10	3.12	118.53	112.17
2	B	300	INJ	C15-C14-C13	-3.11	100.73	113.74
2	C	400	INJ	C15-C14-C13	-3.08	100.86	113.74
2	A	200	INJ	C15-C14-C13	-3.03	101.10	113.74
2	D	600	INJ	O11-C11-C10	-2.97	102.29	109.25
2	B	300	INJ	O12-C12-C11	-2.89	105.09	111.16
2	A	200	INJ	O12-C12-C11	-2.85	105.16	111.16
2	E	800	INJ	C12-C11-C10	2.79	117.86	112.17
2	A	200	INJ	P-C17-C16	2.67	118.23	114.94
2	C	400	INJ	C14-C13-C5	2.63	121.46	113.52
2	E	800	INJ	O3P-P-O2P	2.61	115.39	107.96
2	A	200	INJ	C14-C13-C5	2.61	121.39	113.52
2	B	300	INJ	O3P-P-O2P	2.50	115.08	107.96
2	B	300	INJ	O11-C11-C12	-2.48	103.39	109.03
2	E	800	INJ	C15-C14-C13	-2.47	103.42	113.74
2	D	600	INJ	O10-C10-C9	-2.46	103.33	108.93
2	B	300	INJ	O10-C10-C9	-2.46	103.34	108.93
2	E	800	INJ	C14-C13-C5	2.45	120.93	113.52
2	B	300	INJ	C14-C13-C5	2.38	120.72	113.52
2	D	600	INJ	C15-C14-C13	-2.38	103.79	113.74
2	B	300	INJ	C8-C9-C10	2.38	118.14	110.70
2	B	300	INJ	O2P-P-O1P	2.35	118.46	112.39
2	A	200	INJ	O1P-P-C17	2.31	115.80	111.45
2	C	400	INJ	C8-C9-C10	2.30	117.90	110.70
2	C	400	INJ	C12-C11-C10	2.26	116.78	112.17
2	A	200	INJ	O9-C9-C8	-2.25	105.25	109.67
2	D	600	INJ	C8-C9-C10	2.22	117.64	110.70
2	A	200	INJ	O10-C10-C9	-2.21	103.91	108.93
2	A	200	INJ	O11-C11-C12	-2.16	104.11	109.03
2	D	600	INJ	O3P-P-O2P	2.06	113.83	107.96
2	B	300	INJ	C12-C11-C10	2.01	116.26	112.17

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	600	INJ	C15-C16-C17-P
2	E	800	INJ	C15-C16-C17-P
2	A	200	INJ	C10-C11-C12-O12
2	B	300	INJ	C10-C11-C12-O12

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Mol	Chain	Res	Type	Atoms
2	E	800	INJ	C10-C11-C12-O12
2	C	400	INJ	C5-C6-N7-C8
2	A	200	INJ	C15-C16-C17-P
2	B	300	INJ	C15-C16-C17-P
2	C	400	INJ	C15-C16-C17-P
2	D	600	INJ	C10-C11-C12-O12
2	B	300	INJ	O10-C10-C11-C12
2	C	400	INJ	C10-C11-C12-O12
2	A	200	INJ	N7-C8-C9-O9
2	A	200	INJ	C5-C6-N7-C8
2	B	300	INJ	C13-C14-C15-C16
2	B	300	INJ	C5-C6-N7-C8
2	D	600	INJ	C5-C6-N7-C8
2	D	600	INJ	C5-C13-C14-C15
2	A	200	INJ	O10-C10-C11-C12
2	E	800	INJ	O10-C10-C11-C12
2	A	200	INJ	C13-C14-C15-C16
2	D	600	INJ	N7-C8-C9-O9
2	E	800	INJ	N7-C8-C9-O9
2	B	300	INJ	O10-C10-C9-O9
2	D	600	INJ	O10-C10-C11-C12
2	C	400	INJ	C13-C14-C15-C16
2	D	600	INJ	C16-C17-P-O3P
2	C	400	INJ	C5-C13-C14-C15

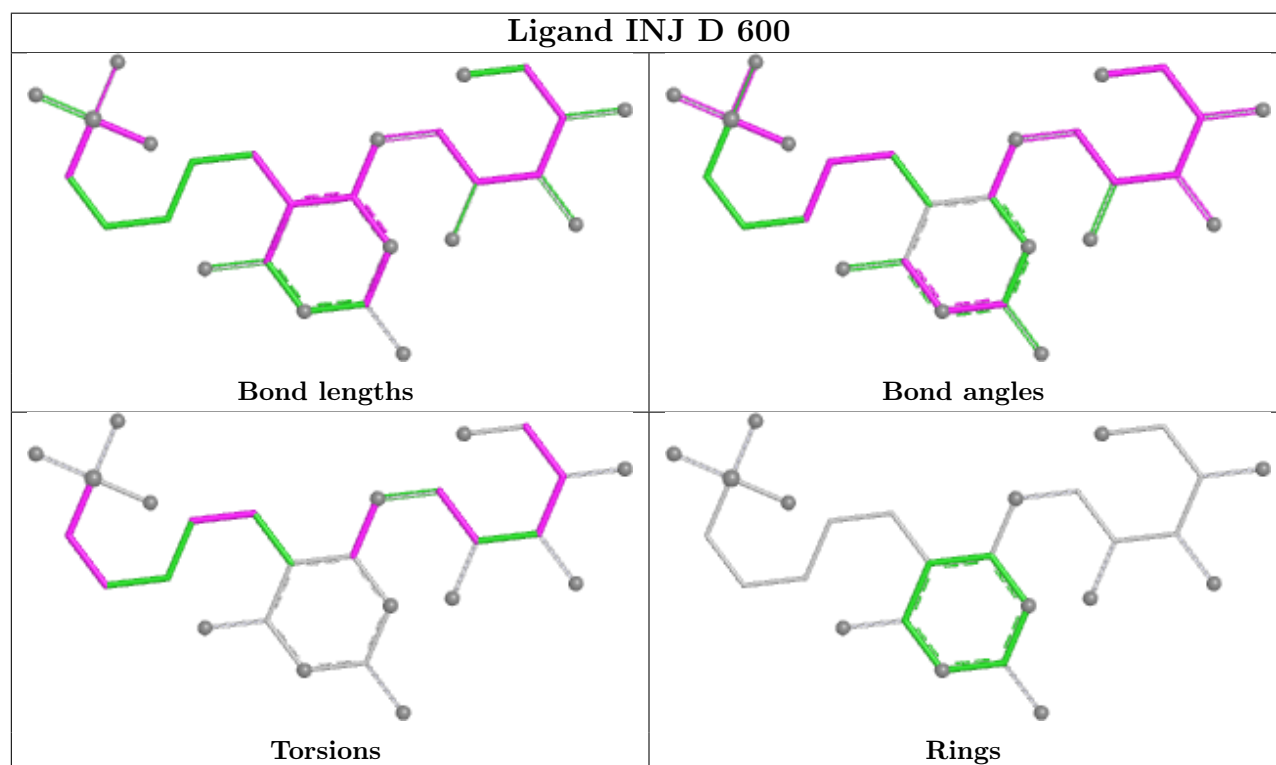
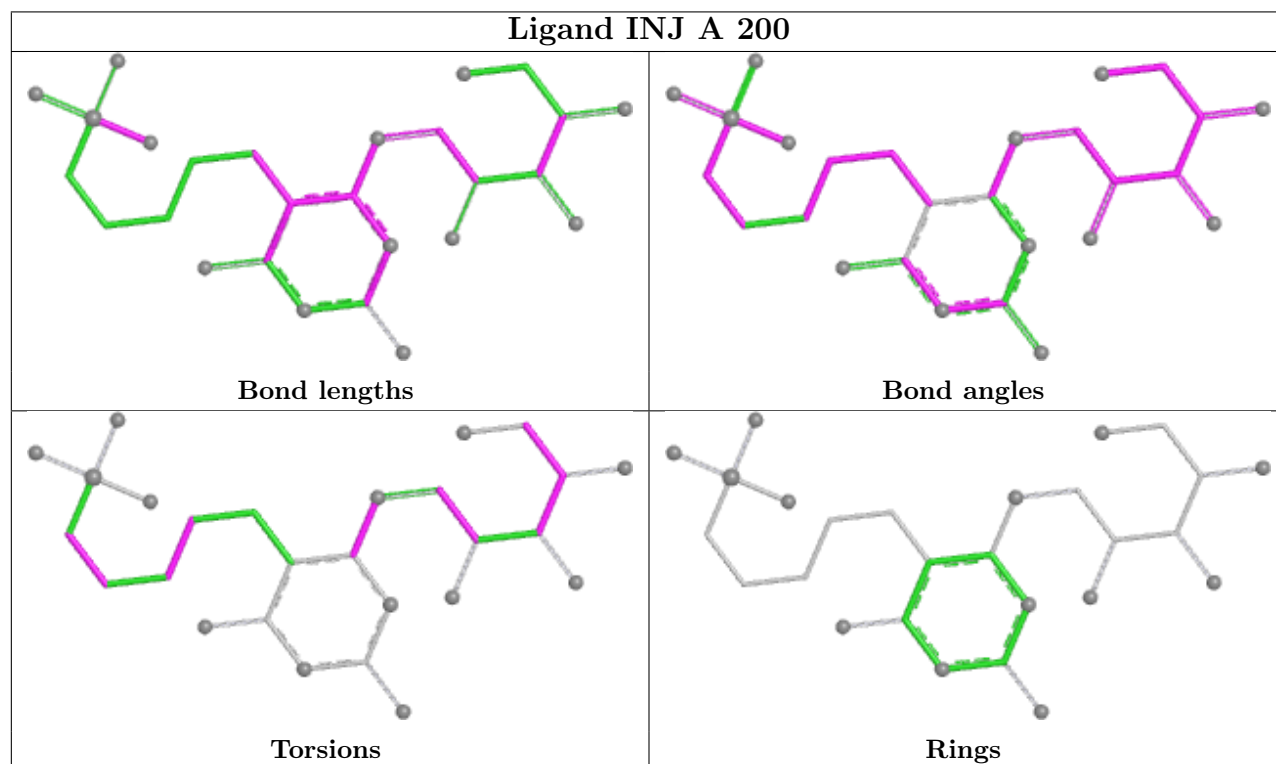
There are no ring outliers.

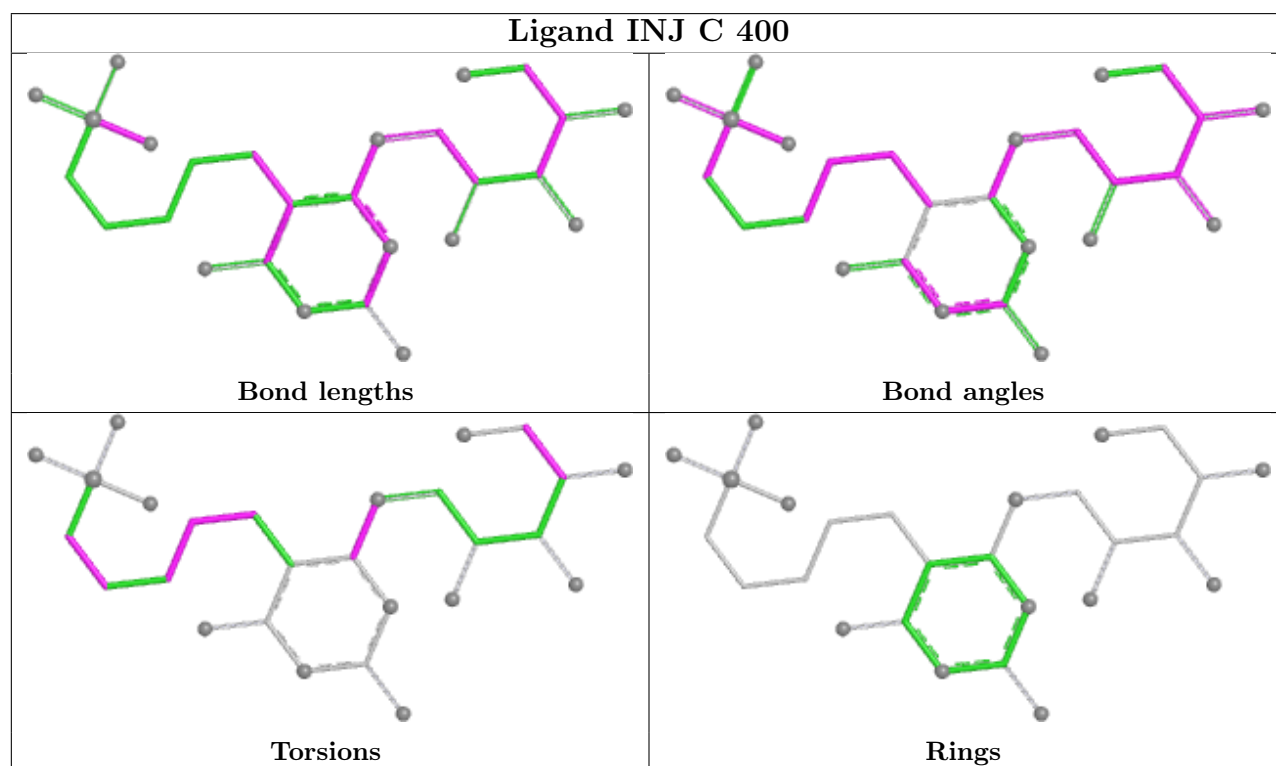
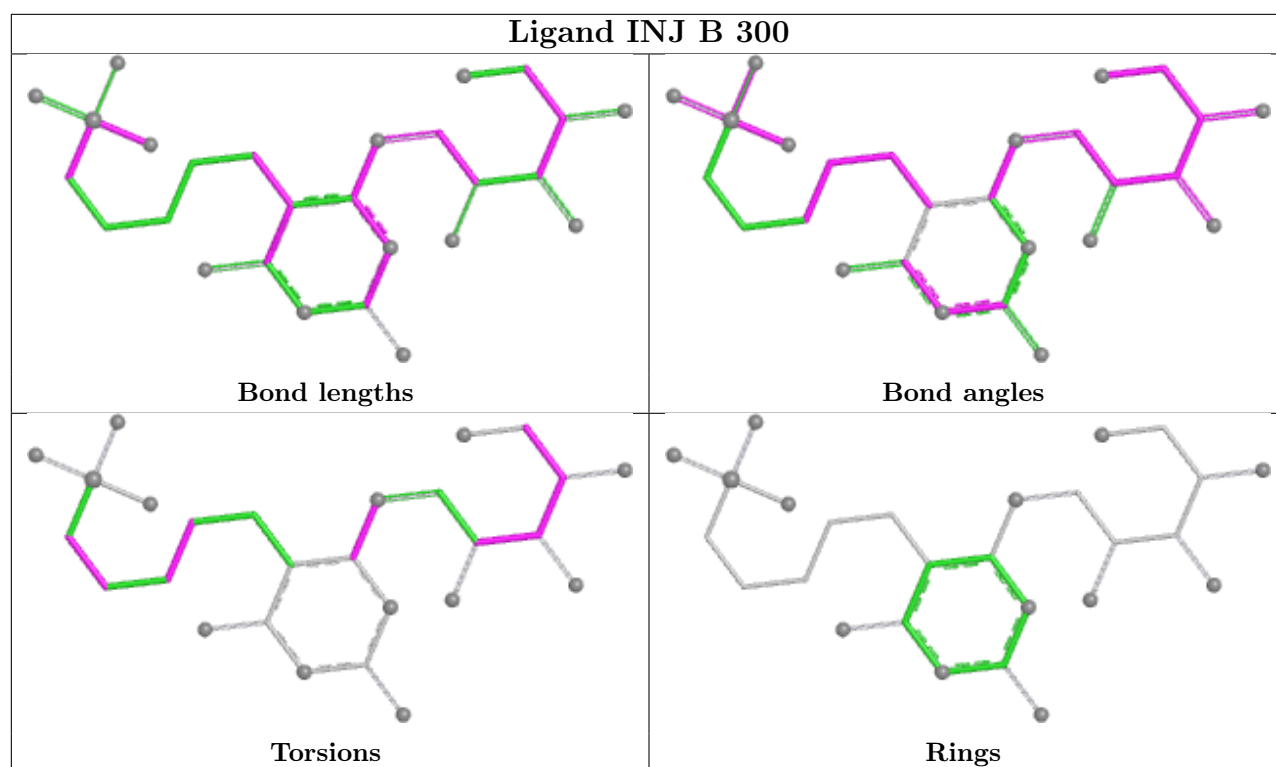
4 monomers are involved in 4 short contacts:

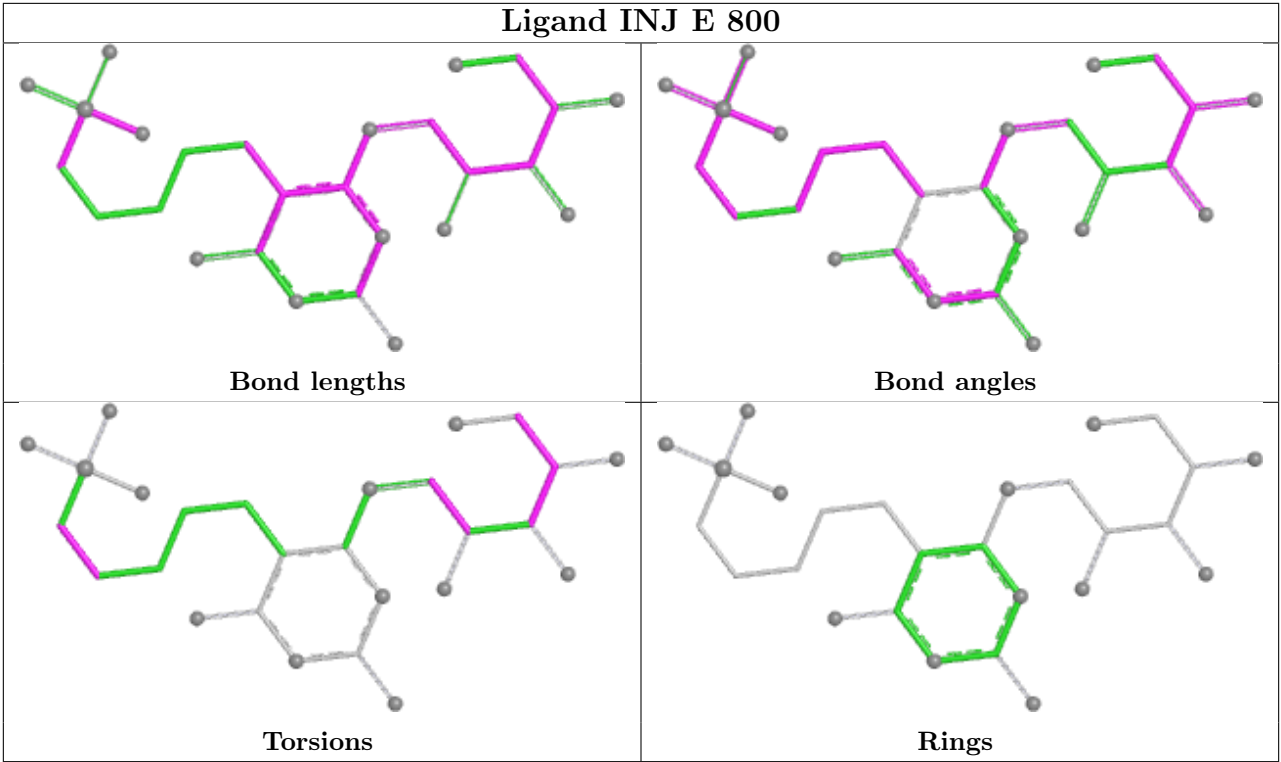
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	INJ	1	0
2	D	600	INJ	1	0
2	B	300	INJ	1	0
2	C	400	INJ	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1:ALA	C	2:VAL	N	1.16

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	168/168 (100%)	-0.13	7 (4%)	40	44	11, 19, 30, 42	14 (8%)
1	B	160/168 (95%)	-0.20	3 (1%)	66	70	10, 19, 30, 41	11 (6%)
1	C	166/168 (98%)	-0.18	6 (3%)	46	50	12, 19, 32, 45	14 (8%)
1	D	168/168 (100%)	-0.24	3 (1%)	67	71	12, 19, 31, 37	14 (8%)
1	E	159/168 (94%)	-0.36	4 (2%)	58	62	9, 18, 26, 31	9 (5%)
All	All	821/840 (97%)	-0.22	23 (2%)	55	58	9, 19, 30, 45	62 (7%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	10.0
1	C	4	GLY	4.8
1	C	3	LYS	4.3
1	C	5	LEU	3.8
1	C	142	ALA	3.8
1	B	9	ASP	3.3
1	B	143	HIS	3.1
1	A	2	VAL	3.0
1	D	49	GLU	2.9
1	C	7	LYS	2.9
1	D	6	GLY	2.8
1	E	11	VAL	2.8
1	A	142	ALA	2.5
1	D	26	TRP	2.5
1	E	10	GLN	2.4
1	A	5	LEU	2.3
1	E	26	TRP	2.2
1	C	6	GLY	2.2
1	A	4	GLY	2.2
1	E	50	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	26	TRP	2.1
1	B	11	VAL	2.1
1	A	12	TYR	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](#)

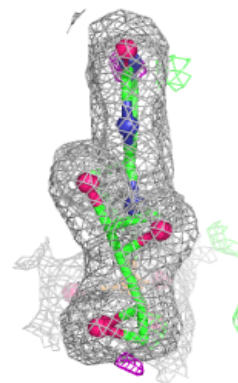
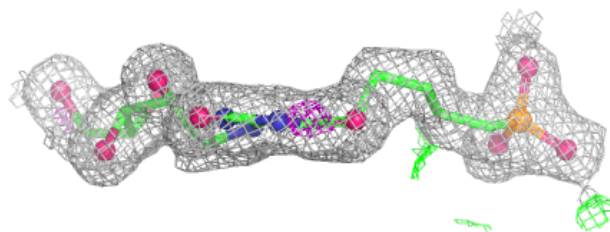
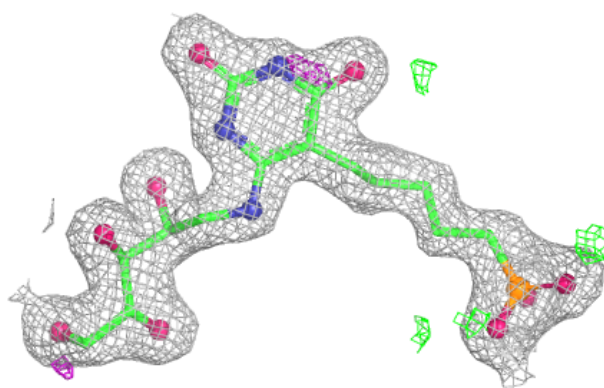
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	INJ	A	200	27/27	0.94	0.07	17,22,28,28	0
2	INJ	C	400	27/27	0.95	0.07	17,22,28,28	0
2	INJ	B	300	27/27	0.96	0.07	17,21,27,28	0
2	INJ	D	600	27/27	0.96	0.06	17,22,28,28	0
2	INJ	E	800	27/27	0.96	0.07	17,21,28,28	0

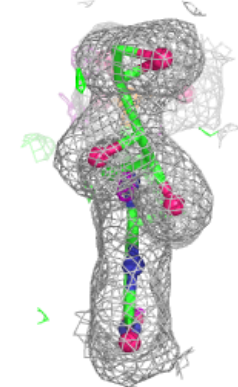
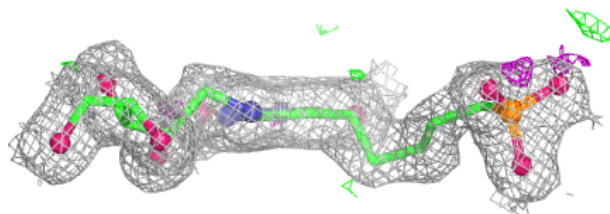
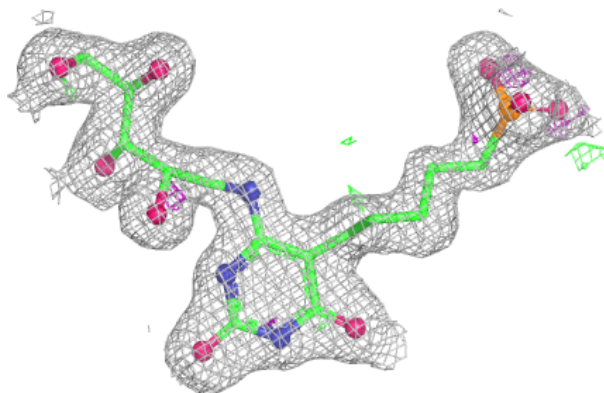
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around INJ A 200:

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

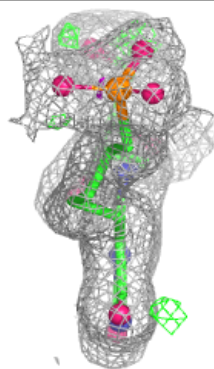
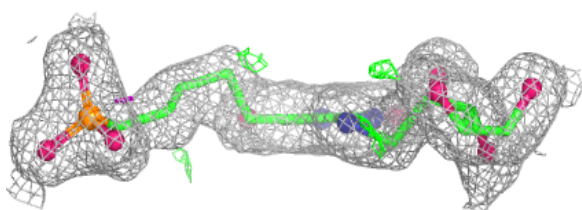
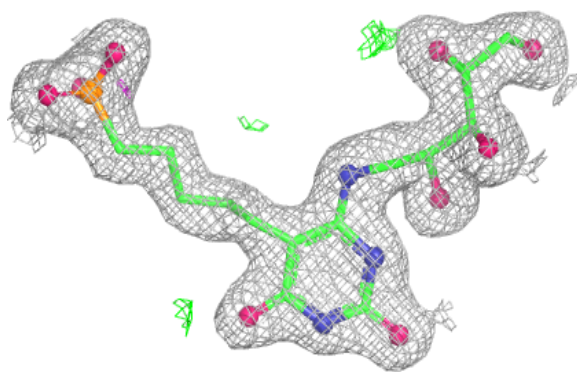
**Electron density around INJ C 400:**

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

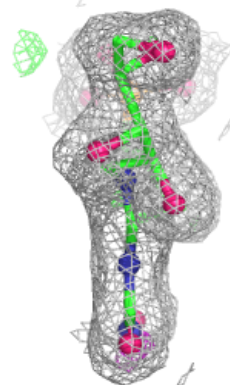
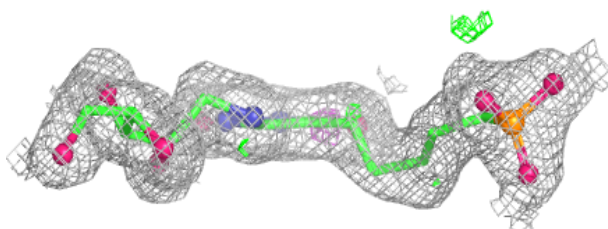
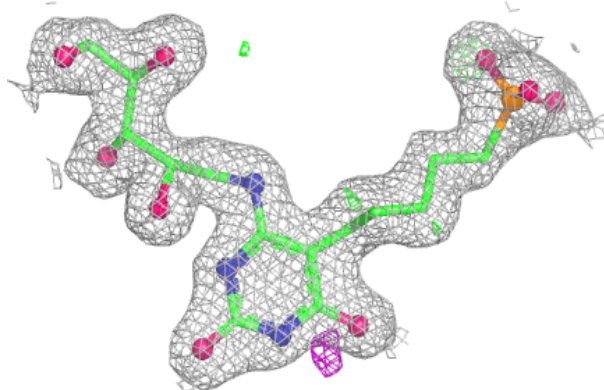


Electron density around INJ B 300:

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

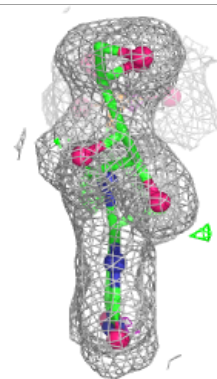
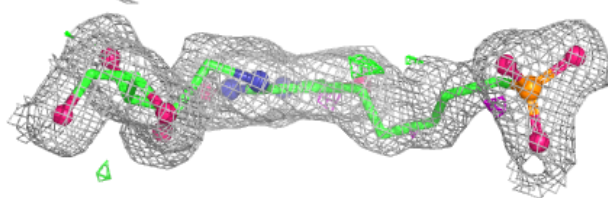
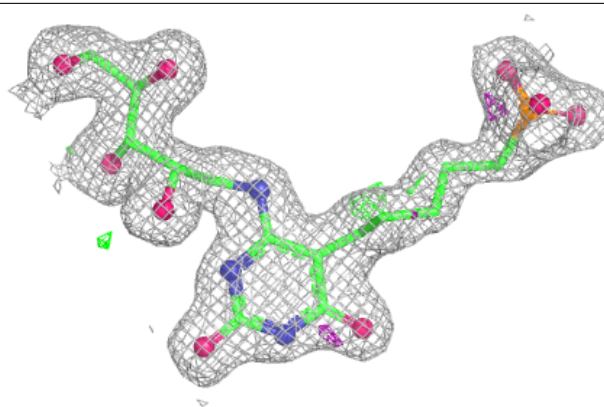
**Electron density around INJ D 600:**

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



Electron density around INJ E 800:

$2mF_o-DF_c$ (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.